Supplementary Materials

Synthesis of Polysubstituted 1,2-dihydro-3*H*-pyrrolo[1,2-*a*]indol-3-ones through Domino Palladium-Catalyzed Reactions of Indol-2-ylmethyl acetates with 1,3- Dicarbonyl Derivatives

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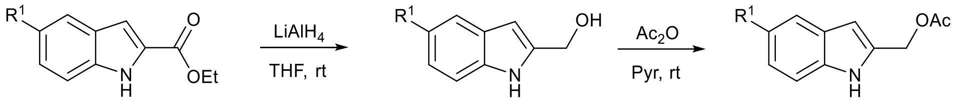
1. SYNTHETIC PROCEDURES

1.1. General procedure for the preparation of (1*H*-indol-2-yl)methyl acetates (1a, 1c, 1d)

(1*H*-indol-2-yl)methyl acetates (**1a, 1c, 1d**) were prepared according to the two-step sequence outlined in Scheme 1 and previously optimized in our laboratory.



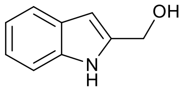
1
R^1 = H, Me, Br

Scheme 1

1.1.a Typical procedure for the preparation of (1*H*-indol-2-yl)methyl acetate (1a)

STEP 1: synthesis of (1H-indol-2-yl)methanol

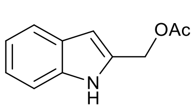
A flame dried three-necked round bottom flask, equipped with a magnetic stirring bar, was charged with ethyl 1*H*-indole-2-carboxylate (1.50 g, 7.93 mmol, 1.0 equiv) dissolved in anhydrous THF (20 mL) under argon. Then, a solution of $LiAlH_4$ in THF (2 M, 4.4 mL, 8.72 mmol, 1.1 equiv) was added dropwise at 0°C and the mixture was stirred for 1 hour. After this time, the mixture was allowed to warm to room temperature and stirred until the disappearance of the starting material, monitoring by TLC (*n*-hexane-EtOAc, 80:20). The reaction was cooled down to 0°C and quenched with an 80 percent aqueous MeOH solution. The mixture was extracted with CH_2Cl_2, washed with a solution of $KHSO_4$ (10% w/w) and with brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product (1*H*-indol-2-yl)methanol) was used in the next step without further purification (1.11 g, 95% yield).



(1*H*-indol-2-yl)methanol: known compound; 95% yield (7.93 mmol scale, 1.11 g); yellow solid; mp: 72-74 °C; lit.[1] mp: 72-73 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3373, 2856, 1617, 1453, 1289, 1004 cm^{-1}; ^1H NMR: (400.13 MHz) (DMSO-d_6): δ 11.0 (s, 1 H), 7.46 (d, J = 7.8 Hz, 1 H), 7.33 (dd, J_1 = 7.8 Hz, J_2 = 0.7 Hz, 1 H), 7.03 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1 H), 6.94 (td, , J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1 H), 6.27 (d, J = 1.2 Hz, 1 H), 5.22 (t, J = 5.6 Hz, 1 H), 4.61 (d, J = 5.6 Hz, 2 H); ^{13}C NMR (100.6 MHz) (DMSO-d_6): δ 140.6 (C), 136.7 (C), 128.3 (C), 121.0 (CH), 120.1 (CH), 119.1 (CH), 111.5 (CH), 98.9 (CH), 57.4 (CH_2); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_{10}NO$: 146.0611; found: 146.0599.

***STEP 2: synthesis of (1H-indol-2-yl)methyl acetate* (1a)**

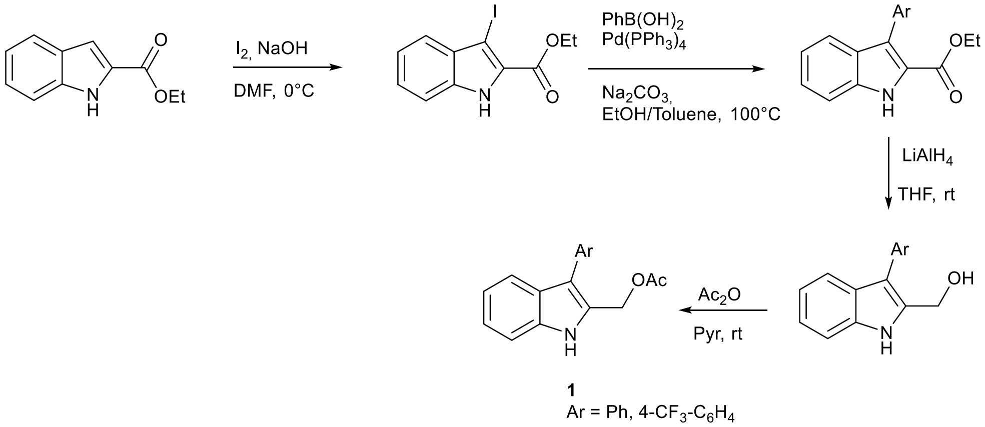
To a stirred solution of (1*H*-indol-2-yl)methanol (1.10 g, 7.47 mmol, 1.0 equiv.) in pyridine (3.0 mL) acetic anhydride (918 µL, 9.72 mmol, 1.3 equiv.) was added at 0°C and the reaction mixture was stirred for 1.5 hours. Then, the reaction was diluted with CH_2Cl_2, washed with a solution of $KHSO_4$ (10% w/w), saturated solution of $NaHCO_3$, and with brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product **1a** was used in the next step without further purification (1.34 g, 95% yield).



(1*H*-indol-2-yl)methyl acetate (1a): known compound; 95% yield (7.47 mmol scale, 1.34 g); yellow solid**;** mp: 104-106 °C; lit.[1] mp: 112 °C; R_f = 0.27 (*n*-hexane-EtOAc, 80:20); IR (neat): 3303, 1726, 1454, 1274, 1045, 805 cm^{-1}; ^{1}H (400.13 MHz) ($CDCl_3$): δ = 8.51 (br s, 1 H), 7.52 (d, *J* = 8.0 Hz, 1 H), 7.27 (d, *J* = 8.0 Hz, 1 H), 7.13 (t, *J* = 7.6 Hz, 1 H), 7.00 (t, J_1 = 7.6 Hz, 1 H), 6.46 (s, 1 H), 5.15 (s, 2 H), 2.03 (s, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ = 172.3 (C), 136.6 (C), 133.0 (C), 127.5 (C), 122.8 (CH), 120.9 (CH), 120.1 (CH), 111.1 (CH), 103.9 (CH), 59.8 (CH_2), 21.0 (CH_3); HRMS: *m/z* [M + H]$^+$ calcd for $C_{11}H_{10}NO_2$: 188.0717; found: 188.0705.

1.2. General procedure for the preparation of (3-aryl-1*H*-indol-2-yl)methyl acetate 1g, 1h

(3-aryl-1*H*-indol-2-yl)methyl acetate **1g**, **1h** were prepared according to the four-steps sequence outlined in Scheme 2.

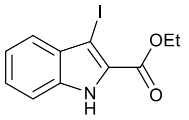


Scheme 2

1.2.a Typical procedure for the preparation of (3-phenyl-1*H*-phenyl-2-yl)methyl acetate (1g)

STEP 1: synthesis of ethyl 3-iodo-1H-indole-2-carboxylate

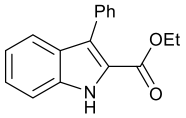
To a solution of ethyl 1*H*-indole-2-carboxylate (1.50 g, 7.92 mmol, 1.0 equiv.) in DMF (9.0 mL) KOH (2.22 g, 39.6 mmol, 5.0 equiv.) was added at 0°C and the resulting mixture was stirred for 10 minutes before a solution of iodine (1.02g, 8.03 mmol,1.05 equiv.) in DMF (10.0 mL) was added dropwise over 5 minutes. After 3h, the mixture was poured into a saturated solution of NH_4Cl and $Na_2S_2O_3$ to precipitate the product. The solid material was filtered off, solubilized in Et_2O, washed with water and dried over Na_2SO_4. After filtration, the mixture was concentrated under reduced pressure to give ethyl 3-iodo-1*H*-indole-2-carboxylate as an off-white powder (2.37 g, 95% yield).



ethyl 3-iodo-1*H*-indole-2-carboxylate: known compound; 85% yield (7.92 mmol scale, 2.37 g); white solid; mp: 133-135 °C; lit.[2] mp: 137-139 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3289, 2896, 1686, 1505, 1255, 859 cm^{-1}; ^{1}H NMR: (400.13 MHz) ($CDCl_3$): δ 9.42 (br s, 1 H), 7.60 (d, *J* = 8.4 Hz, 1 H), 7.43-7.38 (m, 2 H), 7.28-7.24 (m, 1 H), 4.50 (q, *J* = 6.9 Hz, 2 H), 1.50 (t, *J* = 6.9 Hz, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 161.1 (C), 136.3 (C), 131.6 (C), 127.3 (C), 126.7 (CH), 123.6 (CH), 121.8 (CH), 112.2 (CH), 66.2 (C), 61.7 (CH_2), 14.5 (CH_3); HRMS: *m/z* [M + H]$^+$ calcd for $C_{11}H_{10}INO_2Na$: 337.9648; found: 337.9644.

STEP 2*: *synthesis of ethyl 3-phenyl-1H-indole-2-carboxylate

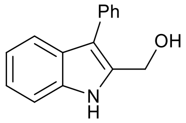
In a three-necked round bottom flask, equipped with a condenser and magnetic stirring bar, [$Pd(PPh_3)_4$] (439.2 mg, 0.38 mmol, 0.05 equiv) was dissolved at room temperature in 25,0 mL of EtOH/Toluene (2:1) under argon; then, ethyl 3-iodo-1*H*-indole-2-carboxylate (2.37 g, 7.52 mmol, 1.0 equiv), phenylboronic acid (2.76 g, 22.6 mmol, 3.0 equiv), and Na_2CO_3 (2.39 g, 22.6 mmol,3.0 equiv) were added and the mixture was refluxed for 16 hours. After this time, the mixture was cooled to room temperature, diluted with CH_2Cl_2 and washed with brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The residue was purified by chromatography on SiO_2 (25-40 µm), eluting with an 80/20 (v/v) *n*-hexane-AcOEt mixture (R_f = 0.22) to obtain the ethyl 3-phenyl-1*H*-indole-2-carboxylate (1.69 g, 85% yield).



ethyl 3-phenyl-1*H*-indole-2-carboxylate: known compound; 85% yield (7.52 mmol scale, 1.69 g); yellow solid; mp: 133-135 °C; lit.[3] mp: 133-135 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3331, 2916, 1675, 1383, 1254 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 9.04 (br s, 1 H), 7.65 (d, *J* = 8.4 Hz, 1 H), 7.58-7.55 (m, 2 H), 7.48-7.44 (m, 3 H), 7.41-7.35 (m, 2 H), 7.18-7.14 (m, 1 H), 4.30 (q, *J* = 7.2 Hz, 2 H), 1.24 (t, *J* = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 162.1 (C), 135.8 (C), 130.8 (C), 128.1 (CH), 127.9 (CH), 127.3 (CH), 125.9, 124.4, 122.9, 121.9, 121.0, 111.8 (CH), 61.0 (CH), 14.2 (CH_2); HRMS: *m/z* [M + Na]$^+$ calcd for $C_{17}H_{15}NO_2Na$: 288.0995; found: 288.0991.

STEP* 3: *synthesis of (3-phenyl-1H-indol-2-yl)methanol

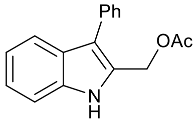
(3-phenyl-1*H*-indol-2-yl)methanol was synthetized according to the typical procedures outlined for (1*H*-indol-2-yl)methanol.



(3-phenyl-1*H*-indol-2-yl)methanol: known compound; 81% yield (6.37 mmol scale, 1.15 g); brown solid; mp: 88-90 °C; lit.[4] mp: R_f = 0.25 (*n*-hexane-EtOAc, 70:30); IR (neat): 3391, 2917, 1730, 1456, 1384, 1231 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 8.56 (br s, 1 H), 7.73 (d, *J* = 8.4 Hz, 1 H), 7.48-7.46 (m, 4 H), 7.37-7.33 (m, 2 H), 7.24 (dt, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H), 7.16 (dt, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H), 4.89 (s, 2 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 135.7 (C), 134.6 (C), 133.7 (C), 129.5 (CH), 128.8 (CH), 127.4 (C), 126.5 (CH), 122.7 (CH), 120.4 (CH), 119.7 (CH), 115.4 (C), 111.2 (CH), 57.2 (CH_2); HRMS: *m/z* [M + H]$^+$ calcd for $C_{15}H_{12}NO$: 222.0924; found: 222.0917.

STEP* 4: *synthesis of (3-phenyl-1H-indol-2-yl)methyl acetate (*1g*)

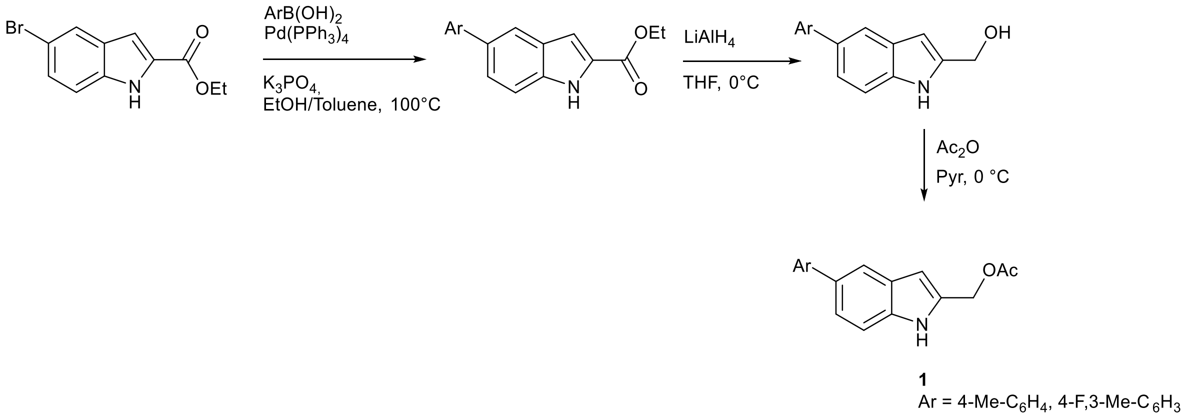
3-phenyl-1*H*-indol-2-yl)methyl acetate **1g** was synthesized according to the typical procedures outlined for **1a**, *step 3*.



(3-phenyl-1*H*-indol-2-yl)methyl acetate (1g): quantitative yield (5.15 mmol scale, 1.37 g); yellow solid; mp: 133-135 °C; R_f = 0.25 (*n*-hexane-EtOAc, 80:20); IR (neat): 3391, 2917, 1730, 1456, 1384, 1231 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 8.71 (br s, 1 H), 7.65 (d, *J* = 8.0 Hz, 1 H), 7.47 (d, *J* = 7.5 Hz, 2 H), 7.41 (t, *J* = 7.5 Hz, 2 H), 7.30 (t, *J* = 8.3 Hz, 2 H), 7.17 (d, *J* = 7.0 Hz, 1 H), 7.06 (t, *J* = 7.5 Hz, 1 H), 5.19 (s, 2 H), 2.06 (s, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 172.8 (C), 135.8 (C), 134.2 (C), 129.8 (CH), 129.4 (C), 128.8 (CH), 126.8 (CH), 126.7 (C) 123.5 (CH), 120.4 (CH), 120.2(CH), 118.8 (C), 111.4(CH), 58.5 (CH_2), 21.2 (CH_3); HRMS: *m/z* [M + H]$^+$ calcd for $C_{17}H_{14}NO_2$: 288.0995; found: 288.0997.

1.3 General procedure for the synthesis of 5-aryl-1*H*-indol-2-yl)methyl acetate (1e, 1f)

The (5-aryl-1*H*-indol-2-yl)methyl acetate (**1e**, **1f**) were synthesized according to the following scheme 3.

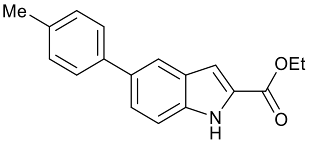


Scheme 3

1.3.a Typical procedure for the preparation of (5-(*p*-tolyl)-1*H*-indol-2-yl)methyl acetate (1e)

STEP 1*: *synthesis of ethyl 5-(p-tolyl)-1H-indole-2-carboxylate

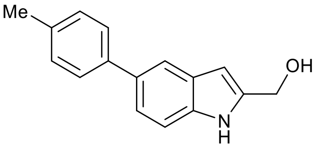
In a three-necked round bottom flask, equipped with a condenser and magnetic stirring bar, [Pd(PPh$_3$)$_4$] (288.75 mg, 0.25 mmol, 0.05 equiv) was dissolved at room temperature in 15,0 mL of EtOH/Toluene (2:1) under argon; then, ethyl 5-bromo-1*H*-indole-2-carboxylate (1.34 g, 5.0 mmol, 1.0 equiv), phenylboronic acid (1.83 g, 15.0 mmol, 3.0 equiv), and K$_3$PO$_4$ (3.18 g, 15.0 mmol,3.0 equiv) were added and the mixture was refluxed for 16 hours. After this time, the mixture was cooled to room temperature, diluted with CH$_2$Cl$_2$ and washed with brine. The organic layer was dried over Na$_2$SO$_4$, filtered, and concentrated under reduced pressure. The residue was purified by chromatography on SiO$_2$ (25-40 µm), eluting with an 80/20 (v/v) *n*-hexane-AcOEt mixture (R$_f$ = 0.23) to obtain the ethyl 3-phenyl-1*H*-indole-2-carboxylate (1.12 g, 80% yield).



ethyl 5-(p-tolyl)-1*H*-indole-2-carboxylate: 80% yield (5.0 mmol scale, 1.12 g), yellow solid; mp: 178-180 °C; R$_f$ = 0.23 (*n*-hexane-EtOAc, 80:20); IR (KBr): 3321.8, 2903.5, 1692.2, 1383.7, 1186.1; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ = 9.32 (bs, 1 H), 7.90 (s, 1 H), 7.63-7.58 (m, 3 H), 7.52 (d, *J* = 8.8 Hz, 1 H), 7.31-7.29 (m, 3 H), 4.50 (q, *J* = 6.8 Hz, 2 H), 2.45 (s, 3 H), 1.49 (d, *J* = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ = 162.3 (C), 139.1 (C), 136.4 (C), 134.3 (C), 129.5 (CH), 128.1 (C), 127.2 (CH), 125.4 (CH), 120.5 (CH), 112.1 (CH), 108.9 (CH), 61.1 (CH$_2$), 21.1 (CH$_3$), 14.4 (CH$_3$). HRMS: *m/z* [M + H]$^+$ calcd for C$_{18}$H$_{18}$NO$_2$: 280.1332; found: 280.1317.

STEP 2*: *(5-(p-tolyl)-1H-indol-2-yl)methanol

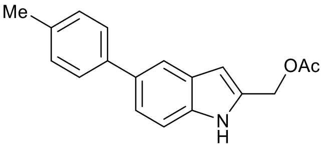
(5-(p-tolyl)-1*H*-indol-2-yl)methanol was synthetized according to the typical procedures outlined for (1*H*-indol-2-yl)methanol, *step 1*.



(5-(p-tolyl)-1*H*-indol-2-yl)methanol: 75% yield (4.0 mmol scale, 713.0 mg); brown solid; mp: 126-128 °C; R$_f$ = 0.25 (*n*-hexane-EtOAc, 75:25); IR (KBr): 3258.1, 2917.8, 1580.4, 1384.6, 1088.6; ^{1}H NMR (400.13 MHz) (DMSO-d$_6$): δ = 11.04 (s, 1 H), 7.71 (t, *J* = 0.6 Hz, 1 H), 7.54 (d, *J* = 8.1 Hz, 2 H), 7.41-7.37 (m, 1 H), 7.34-7.30 (m, 1 H), 7.23 (d, *J* = 8.0 Hz, 2 H), 6.32 (d, *J* = 1.1 Hz, 1 H), 5.26 (t, *J* = 5.5 Hz, 1 H), 4.62 (d, *J* = 5.6 Hz, 2 H), 2.34 (s, 3 H); ^{13}C NMR (100.6 MHz) (DMSO-d$_6$): δ = 141.4, 139.6, 136.2, 135.6 (CH), 131.6, 129.8 (CH), 128.5 (CH), 126.9 (CH), 120.3 (CH),117.9 (CH),111.9 (CH), 99.4 (CH), 57.4 (CH_2), 21.1 (CH_3). HRMS: *m/z* [M + Na]$^+$ calcd for $C_{16}H_{15}NONa$: 260.1046; found: 260.1050.

STEP* 3**: ***synthesis of (5-(p-tolyl)-1H-indol-2-yl)methyl acetate **(1e)**

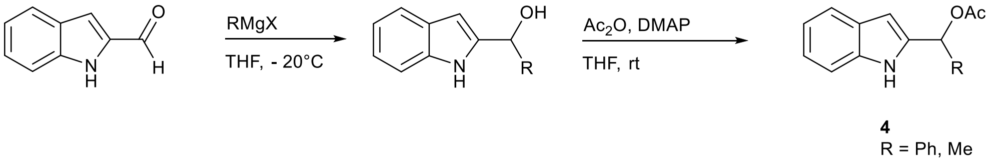
(5-(p-tolyl)-1*H*-indol-2-yl)methyl acetate (**1e**) was synthesized according to the typical procedures outlined for **1a**, *step 3*.



(5-(*p*-tolyl)-1*H*-indol-2-yl)methyl acetate (1e): 98% yield (3.92 mmol scale, 1.10 g); yellow solid; mp: 178-180 °C; IR (KBr): 3398.9, 2918.7, 1727.9, 1384.6, 1235.2; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ = 8.62 (bs, 1 H), 7.79 (s, 1 H), 7.55-7.53 (m, 2 H), 7.45 (dd, J_1 = 8.50 Hz, J_2 = 1.62, 1 H), 7.39 (d, *J* = 8.50 Hz, 1 H), 7.25 (m, 2 H), 6.58 (d, *J* = 1.17 Hz, 1 H), 5.24 (s, 2 H), 2.40 (s, 3 H), 2.11 (s, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ = 172.5 (C), 139.6 (C), 136.1 (C), 136.0 (C), 133.8 (C), 133.7 (C), 129.5 (CH), 128.2 (C), 127.3 (CH), 122.8 (CH), 119.2 (CH), 111.4 (CH), 104.3 (CH), 59.9 (CH_2), 21.2 (CH_3), 21.1 (CH_3); HRMS: *m/z* [M + Na]$^+$ calcd for $C_{18}H_{17}NO_2Na$: 302.1152; found: 302.1153.

1.4. General procedure for the preparation of (1H-indol-2-yl)methyl acetates (**4a, 4b**)

Compounds **4a** and **4b** were prepared according to the two-steps sequence outlined in Scheme 4.

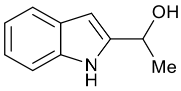


Scheme 4

1.4.a Typical procedure for the preparation of 1-(1*H*-indol-2-yl)ethyl acetate (4b)

STEP 1: synthesis of 1-(1H-indol-2-yl)ethan-1-ol

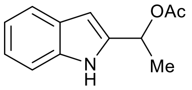
A flame dried three-necked round bottom flask, equipped with a magnetic stirring bar, was charged with 1*H*-indole-2-carbaldehyde (1.00 g, 6.89 mmol, 1.0 equiv) dissolved in anhydrous THF (20 mL) under argon. Then, a solution of MeMgBr in THF (3 M, 9.2 mL, 27.56 mmol, 4.0 equiv) was added dropwise at -78 °C and the mixture was stirred for 1 hour at -20 °C until the disappearance of the starting material, monitoring by TLC (*n*-hexane-EtOAc, 85:15). After this time, the mixture was allowed to warm to room temperature and quenched with a solution of NH_4Cl. Then, the mixture was extracted with CH_2Cl_2, washed with a solution of $KHSO_4$ (10 % w/w), and with brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated under reduced pressure. The resulting crude product 1-(1*H*-indol-2-yl)ethan-1-ol was used in the next step without further purification (1.00 g, 90% yield).



1-(1*H*-indol-2-yl)ethan-1-ol: known compound;[5] 85% yield (6.89 mmol scale, 1.00 g); brown solid; mp: 187-189 C; R_f = 0.23 (*n*-hexane-EtOAc, 85:15); IR (neat): 3384, 2918, 1456, 1384, 1293 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 8.43 (br s, 1 H), 7.58 (d, *J* = 8.0 Hz, 1 H), 7.33 (dd, J_1 = 8.0 Hz, J_2= 0.5 Hz, 1 H), 7.17 (td, J_1 = 7.3 Hz, J_2= 1.1 Hz, 1 H), 7.10 (td, J_1 = 7.3 Hz, J_2= 1.1 Hz, 1 H), 6.35-6.34 (m, 1 H), 5.07 (q, *J* = 6.4 Hz, 1 H), 2.12 (br s, 1 H), 1.63 (d, *J* = 6.4 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ 142.2 (C), 136.0 (C), 128.3 (C), 122.1 (CH), 120.6 (CH), 120.0 (CH), 111.0 (CH), 98.5 (CH), 64.7 (CH), 23.4 (CH$_3$); HRMS: *m/z* [M - H]$^-$ calcd for $C_{10}H_{10}NO$: 160.0768; found: 160.0763.

STEP 2*: *synthesis of 1-(1H-indol-2-yl)ethyl acetate (**4b**)

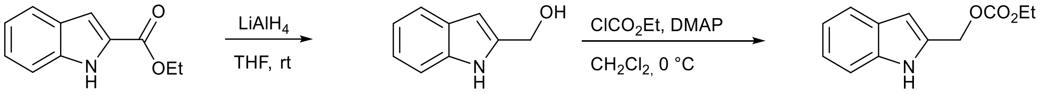
To a stirred solution of 1-(1*H*-indol-2-yl)ethan-1-ol (1.00 g, 6.20 mmol, 1.0 equiv) and DMAP (75.7 mg, 0.62 mmol, 0.1 equiv) in THF (10 mL) acetic anhydride (935 μL, 9.33 mmol, 1.5 equiv) was added at 0 °C and the resulting mixture was allowed to warm to rt. After 1 hour, the reaction was diluted with Et$_2$O, washed with a saturated NaHCO$_3$ solution and with brine. The combined organic layer was dried over Na$_2$SO$_4$, filtered, and concentrated under reduced pressure. The resulting compound **4b** was used in the next step without further purification (2.09 g, 98% yield).



1-(1*H*-indol-2-yl)ethyl acetate (4b): 96% yield (6.20 mmol scale, 1.18 g); brown solid; mp: 209-211 °C; R$_f$ = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3330, 2918,1713, 1455, 1384 cm^{-1}; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ = 8.60 (br s, 1 H), 7.60 (d, *J* = 8.0 Hz, 1 H), 7.35 (dd, J_1 = 8.2 Hz, J_2= 0.7 Hz, 1 H), 7.19 (td, J_1 = 7.2 Hz, J_2= 1.1 Hz, 1 H), 7.10 (td, J_1 = 7.2 Hz, J_2= 1.1 Hz, 1 H), 6.53-6.53 (m, 1 H), 6.07 (q, *J* = 6.4 Hz, 1 H), 2.09 (s, 3 H), 1.74 (d, *J* = 6.4 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ 172.1 (C), 138.0 (C), 136.1 (C), 127.5 (CH), 122.7 (CH), 121.0 (CH), 120.1, 111.2 (CH), 100.7, 66.5 (CH), 21.4 (CH$_3$), 18.7 (CH$_3$); HRMS: *m/z* [M + H]$^+$ calcd for $C_{12}H_{14}NO_2$: 226.0838; found: 226.0838.

1.5. General procedure for the preparation of (1*H*-indol-2-yl)methyl ethyl carbonate (1b)

(1*H*-indol-2-yl)methyl ethyl carbonate **1b** is prepared according to the two-step sequence outlined in Scheme 5 and previously optimized in our laboratory.



1b

Scheme 5

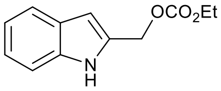
1.5.a Typical procedure for the preparation of (1*H*-indol-2-yl)methyl ethyl carbonate (1b)

STEP 1: synthesis of (1H-indol-2-yl)methanol

(1*H*-indol-2-yl)methanol was synthesized according to the typical procedures outlined for **1a,** *step 1***.**

STEP 2: synthesis of (1H-indol-2-yl)methyl ethyl carbonate **(1b)**

To a stirred solution of 1-(1*H*-indol-2-yl)ethan-1-ol (700.0 mg, 4.76 mmol, 1.0 equiv) and DMAP (581.0 mg mg, 4.76 mmol, 1.0 equiv) in CH$_2$Cl$_2$ (10 mL) ethyl chloroformate (455 μL, 4.76 mmol, 1.0 equiv) was added at 0 °C and the resulting mixture was allowed to warm to rt. After 4 hours, the reaction was diluted with CH$_2$Cl$_2$, washed with a solution of KHSO$_4$ (10% w/w) and with brine. The organic phase was dried over Na$_2$SO$_4$, filtered, and concentrated under reduced pressure. The residue was purified by chromatography on neutral Al$_2$O$_3$ (Brockmann activity I)(60 Å pore size), eluting with a 90/10 (v/v) *n*-hexane/EtOAc mixture (R_f = 0.17) to obtain 490.0 mg (47% yield) of (1*H*-indol-2-yl)methyl ethyl carbonate (**1b**).

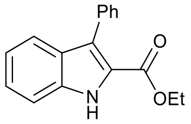


(1*H*-indol-2-yl)methyl ethyl carbonate (1b): 47% yield (4.76 mmol scale, 700.0 mg); yellow oil; R$_f$ = 0.17 (*n*-hexane-EtOAc, 90:10); IR (neat):): 3353, 1778, 1454, 1235, 1032, 815 cm^{-1}; ^{1}H (400.13 MHz) (CDCl$_3$): δ = 8.67 (br s, 1 H), 7.64 (dd, J_1 = 7.97 Hz, J_2= 1.0 Hz, 1 H), 7.39 (dd, J_1 = 8.1 Hz, J_2= 0.9 Hz, 1 H), 7.24 (td, J_1 = 7.51 Hz,

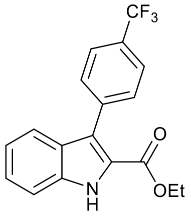
J_2= 1.1 Hz, 1 H), 7.14 (td, J_1 = 7.6 Hz, J_2= 1.0 Hz, 1 H), 6.60 (d, J = 1.54 Hz, 1 H), 5.30 (s, 2 H),), 4.27 (q, J = 7.18 Hz, 2 H), 1.34 (t, J = 7.18 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ = 156.3 (C), 136.7 (C), 132.4 (C), 127.7 (C), 123.0 (CH), 121.2 (CH), 120.2 (CH), 111.3 (CH), 104.5 (CH), 64.7 (CH$_2$), 62.7 (CH$_2$), 14.4 (CH$_3$).

2. CHARACTERIZATION DATA OF STARTING MATERIALS

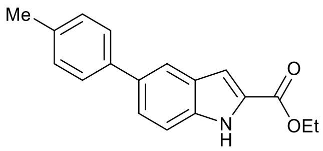
2.1. Characterization data of ethyl 3-and 5-aryl 1*H*-indole-2-carboxylate



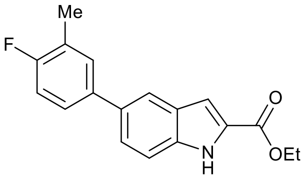
ethyl 3-phenyl-1*H*-indole-2-carboxylate: known compound; 85% yield (7.52 mmol scale, 1.69 g); yellow solid; mp: 133-135 °C; lit.[3] mp: 133-135 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3331, 2916, 1675, 1383, 1254 cm^{-1}; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ = 9.04 (br s, 1 H), 7.65 (d, J = 8.4 Hz, 1 H), 7.58-7.55 (m, 2 H), 7.48-7.44 (m, 3 H), 7.41-7.35 (m, 2 H), 7.18-7.14 (m, 1 H), 4.30 (q, J = 7.2 Hz, 2 H), 1.24 (t, J = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ = 162.1 (C), 135.8 (C), 130.8 (C), 128.1 (CH), 127.9 (CH), 127.3 (CH), 125.9, 124.4, 122.9, 121.9, 121.0, 111.8 (CH), 61.0 (CH), 14.2 (CH$_2$); HRMS: *m/z* [M + Na]$^+$ calcd for $C_{17}H_{15}NO_2Na$: 288.0995; found: 288.0991.



ethyl 3-(4-(trifluoromethyl)phenyl)-1*H*-indole-2-carboxylate: 70% yield (7.52 mmol scale, 1.75 g); brown solid; mp: 133-135 °C; R_f = 0.21 (*n*-hexane-EtOAc, 80:20); IR (neat): 3328, 2933, 1676, 1384, 1255 cm^{-1}; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ 9.21 (br s, 1 H), 7.73-7.68 (m, 4 H), 7.60 (d, J = 8.1 Hz, 1 H), 7.48 (d, J = 8.1 Hz, 1 H), 7.41-7.37 (m, 1 H), 7.21-7.17 (m, 2 H), 4.30 (q, J = 7.2 Hz, 2 H), 1.24 (t, J = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ 161.7 (C), 137.5 (C), 135.7 (C), 131.0 (CH), 129.2 (q, J_{CF} = 31.9 Hz, C), 127.6 (C), 126.1 (CH), 124.6 (q, J_{CF} = 3.7 Hz, CH), 124.4 (q, J_{CF} = 272.3 Hz, C), 123.1 (C), 122.6 (C), 121.33 (CH), 121.28 (CH), 111.9 (CH), 61.2 (CH$_2$), 14.1 (CH$_3$); ^{19}F NMR (376.5 MHz) (CDCl$_3$): δ = -62.4; HRMS: *m/z* [M + Na]$^+$ calcd for $C_{18}H_{14}F_3NO_2Na$: 356.0869; found: 356.0871.

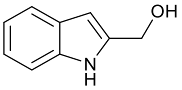


ethyl 5-(p-tolyl)-1*H*-indole-2-carboxylate: 80% yield (5.0 mmol scale, 1.12 g), yellow solid; mp: 178-180 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (KBr): 3321.8, 2903.5, 1692.2, 1383.7, 1186.1; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ = 9.32 (bs, 1 H), 7.90 (s, 1 H), 7.63-7.58 (m, 3 H), 7.52 (d, J = 8.8 Hz, 1 H), 7.31-7.29 (m, 3 H), 4.50 (q, J = 6.8 Hz, 2 H), 2.45 (s, 3 H), 1.49 (d, J = 7.2 Hz, 3 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ = 162.3 (C), 139.1 (C), 136.4 (C), 134.3 (C), 129.5 (CH), 128.1 (C), 127.2 (CH), 125.4 (CH), 120.5 (CH), 112.1 (CH), 108.9 (CH), 61.1 (CH$_2$), 21.1 (CH$_3$), 14.4 (CH$_3$). HRMS: *m/z* [M + H]$^+$ calcd for $C_{18}H_{18}NO_2$: 280.1332; found: 280.1317.

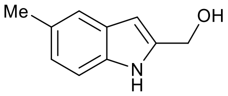


ethyl 5-(4-fluoro-3-methylphenyl)-1*H*-indole-2-carboxylate: 83% yield (5.2 mmol scale, 1.28 g), yellow solid; mp: 98-100 °C; R_f = 0.21 (*n*-hexane-EtOAc, 80:20); IR (KBr): 3366.1, 2918.7, 1712.5, 1472.4, 1384.6, 1265.1; ^{1}H NMR (400.13 MHz) (DMSO-d$_6$): δ = 11.95 (s, 1 H), 7.89 (s, 1 H), 7.59-7.46 (m, 4 H), 7.21-7.17 (m, 2 H), 4.36 (q, *J* = 7.08 Hz, 2 H), 2.31 (d, *J* = 1.4 Hz, 3 H), 1.36 (t, *J* = 7.08 Hz, 3 H); ^{13}C NMR (100.6 MHz) (DMSO-d$_6$): δ = 161.2, 159.9 (d, *J* = 241.5 Hz) (C), 158.8, 137.3 (d, 3.2 Hz), 136.8, 131.8, 129.9 (d, *J* = 5.0 Hz) (CH), 128.0, 127.2, 125.8 (d, *J* = 7.9 Hz) (CH), 124.4 (d, *J* = 17.0 Hz) (C), 124.1 (CH), 119.8 (CH), 115.5 (d, *J* = 22.0 Hz) (CH), 113.0 (CH), 108.0 (CH), 60.5 (CH$_2$), 14.3 (CH$_3$), 14.3 (CH$_3$); ^{1}H-coupled ^{19}F (376.5 MHz) (CDCl$_3$): δ = -121.0 (hept, *J* = 3.0 Hz). HRMS: *m/z* $[M + Na]^+$ calcd for $C_{18}H_{16}FNO_2Na$: 320.1057; found: 320.1051.

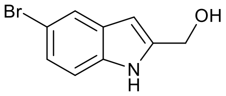
2.2. Characterization data of (1*H*-indol-2-yl)methanols



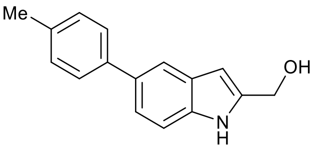
(1*H*-indol-2-yl)methanol: known compound; 95% yield (7.93 mmol scale, 1.11 g); yellow solid; lit. [1] mp: 70-72 °C; mp: 72.5-73.5 °C; R_f = 0.23 (*n*-hexane-EtOAc, 80:20); IR (neat): 3373, 2856, 1617, 1453, 1289, 1004 cm^{-1}; ^{1}H NMR: (400.13 MHz) (DMSO-*d*$_6$): δ 11.0 (s, 1 H), 7.46 (d, *J* = 7.8 Hz, 1 H), 7.33 (dd, J_1 = 7.8 Hz, J_2 = 0.7 Hz, 1 H), 7.03 (td, J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1 H), 6.94 (td, , J_1 = 8.0 Hz, J_2 = 1.2 Hz, 1 H), 6.27 (d, *J* = 1.2 Hz, 1 H), 5.22 (t, *J* = 5.6 Hz, 1 H), 4.61 (d, *J* = 5.6 Hz, 2 H); ^{13}C NMR (100.6 MHz) (DMSO-*d*$_6$): δ 140.6 (C), 136.7 (C), 128.3 (C), 121.0 (CH), 120.1 (CH), 119.1 (CH), 111.5 (CH), 98.9 (CH), 57.4 (CH$_2$); HRMS: *m/z* $[M + H]^+$ calcd for $C_9H_{10}NO$: 146.0611; found: 146.0599.



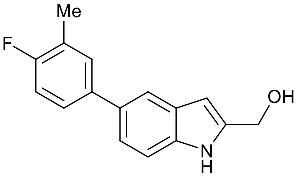
(5-methyl-1*H*-indol-2-yl)methanol: known compound; 98% yield (7.93 mmol scale, 1.25 g); orange solid; lit.[1] mp: 77-79 °C; mp: 77-79 °C; R_f = 0.25 (*n*-hexane-EtOAc, 75:25); IR (neat): 3346, 2932, 1623, 1487, 1197, 1025 cm^{-1}; ^{1}H NMR (400.13 MHz) (CDCl$_3$): δ 8.15 (bs, 1 H), 7.28 (s, 1 H), 7.12 (d, *J* = 8.3 Hz, 1 H), 6.93 (d, *J* = 8.3 Hz, 1 H), 6.23 (br s, 1 H), 4.67 (s, 2 H), 2.36 (s, 3 H), 1.94 (bs, 1 H); ^{13}C NMR (100.6 MHz) (CDCl$_3$): δ 137.6 (C), 134.7 (C), 129.2 (C), 128.4 (C), 123.8 (CH), 120.3 (CH), 110.6 (CH), 100.1 (CH), 58.8 (CH$_2$), 21.4 (CH$_3$); HRMS: *m/z* $[M + H]^+$ calcd for $C_{10}H_{12}NO$: 162.0913; found: 162.0917.



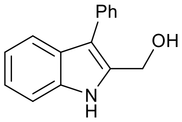
(5-bromo-1*H*-indol-2-yl)methanol: known compound; 98% yield (7.93 mmol scale, 1.76 g); brown solid; lit. [2] mp: 115-117 °C; mp: 113-114 °C; R_f = 0.23 (*n*-hexane-EtOAc, 75:25); IR (neat): 3317, 2892, 1699, 1522, 1383, 1197 cm^{-1}; ^{1}H NMR (400.13 MHz) (DMSO-*d*$_6$): δ 811.3 (br s, 1 H), 7.67 (d, *J* = 1.7 Hz, 1 H), 7.32 (d, *J* = 8.7 Hz, 1 H), 7.17 (dd, J_1 = 8.7 Hz, J_2 = 1.7 Hz, 1 H), 6.30 (s, 1 H), 5.35 (t, *J* = 5.5 Hz, 1 H), 4.65 (d, *J* = 5.5 Hz, 2 H); ^{13}C NMR (100.6 MHz) (DMSO-*d*$_6$): δ 142.0 (C), 134.9 (C), 129.8, (C), 122.9 (CH), 121.8 (CH), 113.0 (CH),111.2 (C), 98.1 (CH), 56.8 (CH$_2$); HRMS: *m/z* $[M + H]^+$ calcd for C_9H_9BrNO: 223.9716; found: 223.9710.



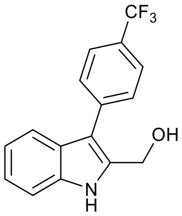
(5-(p-tolyl)-1H-indol-2-yl)methanol: 75% yield (5.8 mmol scale, 1.03 g); brown solid; mp: 126-128 °C; R_f = 0.25 (*n*-hexane-EtOAc, 75:25); IR (KBr): 3258.1, 2917.8, 1580.4, 1384.6, 1088.6; ^{1}H NMR (400.13 MHz) (DMSO-d_6): δ = 11.04 (s, 1 H), 7.71 (t, *J* = 0.6 Hz, 1 H), 7.54 (d, *J* = 8.1 Hz, 2 H), 7.41-7.37 (m, 1 H), 7.34-7.30 (m, 1 H), 7.23 (d, *J* = 8.0 Hz, 2 H), 6.32 (d, *J* = 1.1 Hz, 1 H), 5.26 (t, *J* = 5.5 Hz, 1 H), 4.62 (d, *J* = 5.6 Hz, 2 H), 2.34 (s, 3 H); ^{13}C NMR (100.6 MHz) (DMSO-d_6): δ = 141.4, 139.6, 136.2, 135.6 (CH), 131.6, 129.8 (CH), 128.5 (CH), 126.9 (CH), 120.3 (CH),117.9 (CH),111.9 (CH), 99.4 (CH), 57.4 (CH_2), 21.1 (CH_3). HRMS: *m/z* [M + Na]$^+$ calcd for $C_{16}H_{15}NONa$: 260.1046; found: 260.1050.



(5-(4-fluoro-3-methylphenyl)-1*H*-indol-2-yl)methanol: 73% yield (4.3 mmol scale, 1.04 g); yellow solid; mp: 123-125 °C; R_f = 0.22 (*n*-hexane-EtOAc, 75:25); IR (KBr): 3361.0, 3361.7, 3033.1, 2921.4, ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ = 8.40 (bs, 1 H), 7.72 (s, 1 H), 7.44-7.35 (m, 4 H), 7.05 (t, *J*= 8.77 Hz, 1 H), 6.44 (d, *J*= 1.25 Hz, 1 H), 4.85 (s, 2 H), 2.35 (d, *J* = 1.58 Hz, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ = 161.0 (d, *J* = 241.5 Hz) (C), 138.5 , 138.4 (d, *J* = 3.2 Hz) (C), 135.9 (C), 132.9 (C), 130.5 (d, *J* = 5.0 Hz), 128.8 (C), 126.2 (d, *J* = 8.0 Hz) (CH), 124.9 (d, *J* = 17.5 Hz) (C), 122.0 (CH), 119.1 (CH), 115.19 (d, *J* = 22.0 Hz) (C) , 111.2 (CH), 100.9 (CH), 58.9 (CH_2), 21.2 (CH_3), 14.9 (d, *J* = 3.5 Hz); ^{1}H-coupled ^{19}F (376.5 MHz) ($CDCl_3$): δ = -121.7 (hept, *J* = 3.0 Hz). HRMS: *m/z* [M - H]$^-$ calcd for $C_{16}H_{13}FNO$: 254.0984; found: 254.0982.

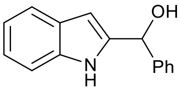


(3-phenyl-1*H*-indol-2-yl)methanol: known compound; 81% yield (6.37 mmol scale, 1.15 g); brown solid; lit. [3] mp: 98-100 °C; mp: 99-100 °C; R_f = 0.25 (*n*-hexane-EtOAc, 70:30); IR (neat): 3391, 2917, 1730, 1456, 1384, 1231 cm^{-1}; ^{1}H NMR: (400.13 MHz) ($CDCl_3$): δ 8.56 (br s, 1 H), 7.73 (d, *J* = 8.4 Hz, 1 H), 7.48-7.46 (m, 4 H), 7.37-7.33 (m, 2 H), 7.24 (dt, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H), 7.16 (dt, J_1 = 8.0 Hz, J_2 = 1.1 Hz, 1 H), 4.89 (s, 2 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 135.7 (C), 134.6 (C), 133.7 (C), 129.5 (CH), 128.8 (CH), 127.4 (C), 126.5 (CH), 122.7 (CH), 120.4 (CH), 119.7 (CH), 115.4 (C), 111.2 (CH), 57.2 (CH_2); HRMS: *m/z* [M + H]$^+$ calcd for $C_{15}H_{13}NO$: 222.0924; found: 222.0917.

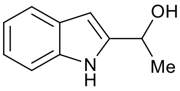


(3-(4-(trifluoromethyl)phenyl)-1*H*-indol-2-yl)methanol: 98% yield (6.37 mmol scale, 1.57 g); yellow solid; mp: 141 – 143 °C; R_f = 0.21 (*n*-hexane-EtOAc, 75:25); IR (neat): 3365, 2917, 1703, 1484, 1385 cm^{-1}; ^{1}H NMR

(400.13 MHz) (DMSO-d_6): δ 11.5 (br s, 1 H), 7.81 (d, *J* = 8.3 Hz, 2 H), 7.76 (d, *J* = 8.3 Hz, 2 H), 7.66 (d, *J* = 7.9 Hz, 1 H), 7.45 (d, *J* = 7.9 Hz, 1 H), 7.15 (dt, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H), 7.07 (dt, J_1 = 7.5 Hz, J_2 = 1.2 Hz, 1 H), 5.47 (t, *J* = 5.42 Hz, 1 H), 4.69 (d, *J* = 5.42 Hz, 2 H), ^{13}C NMR (100.6 MHz) (DMSO-d_6): δ 139.6 (C), 137.2 (C), 135.6 (C), 129.1 (C), 126.1 (CH), 125.9 (q, J_{CF} = 8.3 Hz, C), 125.4 (q, J_{CF} = 3.2 Hz, CH), 124.3 (q, J_{CF} = 232.5 Hz, C), 121.6 (CH), 119.7 (CH), 118.2 (CH), 111.7 (CH), 111.3 (C), 55.2 (CH_2); ^{19}F NMR (376.5 MHz) (DMSO-d_6): δ -60.5; HRMS: *m/z* $[M + H]^+$ calcd for $C_{16}H_{12}F_3NO$: 290.0798; found: 290.0793.



(1*H*-indol-2-yl)(phenyl)methanol: known compound;[4] 90% yield (6.89 mmol scale, 1.38 g); brown solid; mp: 80-82 °C; R_f = 0.24 (*n*-hexane-EtOAc, 80:20); IR (neat): 3391, 2917, 1454, 1384 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 8.45 (br s, 1 H), 7.67 (d, *J* = 8.4 Hz, 1 H), 7.43 (br s, 5 H), 7.29-7.22 (m, 3 H), 6.32 (d, *J* = 1.7 Hz, 1 H), 5.85 (s, 1 H), 3.80 (br s 1 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 141.5 (C), 140.1 (C), 136.2 (C), 128.6 (CH), 128.1 (CH), 127.9 (C), 126.6 (CH), 122.1 (CH), 120.6 (CH), 119.9 (CH), 111.2 (CH), 101.0 (CH), 70.6 (CH HRMS: *m/z* $[M + H]^+$ calcd for $C_{15}H_{13}NO$: 222.0924; found: 222.0920.



1-(1*H*-indol-2-yl)ethan-1-ol: known compound;[5] 85% yield (6.89 mmol scale, 1.00 g); brown solid; mp: 187-189 °C; R_f = 0.23 (*n*-hexane-EtOAc, 85:15); IR (neat): 3384, 2918, 1456, 1384, 1293 cm^{-1}; ^{1}H NMR (400.13 MHz) ($CDCl_3$): δ 8.43 (br s, 1 H), 7.58 (d, *J* = 8.0 Hz, 1 H), 7.33 (dd, J_1 = 8.0 Hz, J_2= 0.5 Hz, 1 H), 7.17 (td, J_1 = 7.3 Hz, J_2= 1.1 Hz, 1 H), 7.10 (td, J_1 = 7.3 Hz, J_2= 1.1 Hz, 1 H), 6.35-6.34 (m, 1 H), 5.07 (q, *J* = 6.4 Hz, 1 H), 2.12 (br s, 1 H), 1.63 (d, *J* = 6.4 Hz, 3 H); ^{13}C NMR (100.6 MHz) ($CDCl_3$): δ 142.2 (C), 136.0 (C), 128.3 (C), 122.1 (CH), 120.6 (CH), 120.0 (CH), 111.0 (CH), 98.5 (CH), 64.7 (CH), 23.4 (CH_3); HRMS: *m/z* $[M + H]^+$ calcd for $C_{10}H_{12}NO$: 160.0768; found: 160.0763.

3. HF CALCULATION ON DIASTEREOISOMERS 5a and 5’a

Stereoisomer trans **5a**

```
+-------------------------------------------------------------------+
  |  Jaguar version 3.5, release  42                                   |
  |                                                                    |
  |  Copyright 1991-1998 Schrodinger, Inc.                             |
  |  All Rights Reserved.                                              |
  |                                                                    |
  |  Use of this program should be acknowledged in publications as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.            |
  +--------------------------------------------------------------------+

  start of program pre
  Job name: WF22711
  Executables used: C:\USERS\GIANCARLO\DOCUMENTS\1.
  Temporary files : LAVORO\C.

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:             3-21g*
  net molecular charge:    0
  multiplicity:            1

  number of basis functions....          210

 Input geometry:
                               angstroms
  atom            x                 y                 z
  H25       1.4305660000     -4.1002650000     -1.7682800000
  C1        1.7700830000     -3.0769040000     -1.8989670000
  C2        2.6834000000     -0.4226530000     -2.2679760000
  C3        1.3067540000     -2.0562360000     -1.0459710000
  C4        2.6617890000     -2.7592810000     -2.9307910000
  C5        3.0982300000     -1.4495770000     -3.1191010000
  C6        1.7955430000     -0.7532560000     -1.2361580000
  C7        0.3695020000     -2.0264770000      0.0382450000
  H27       3.0110100000     -3.5439180000     -3.5976230000
  H28       3.7771430000     -1.2204340000     -3.9375210000
  H30       3.0319160000      0.5969730000     -2.4085260000
  C8        0.3110510000     -0.7248790000      0.4542730000
  H32      -0.2073950000     -2.8584000000      0.4208600000
  C10      -0.3976590000      0.1542770000      1.4065070000
  N2        1.2434290000      0.0050510000     -0.2385740000
  C9        1.3934880000      1.3060500000      0.2091370000
  O1        2.1352170000      2.1153060000     -0.3169060000
  H43      -0.4734580000     -0.3350340000      2.3854890000
  C12      -1.7863570000      0.5666440000      0.9317860000
  C11       0.5494920000      1.4038750000      1.4736160000
  C18       1.4733880000      1.3487920000      2.6887000000
  H48      -0.0079500000      2.3470800000      1.4746980000
  C13      -3.3041190000      1.4274480000     -0.7748770000
  C14      -4.1123880000      1.0546210000      1.4633490000
  C15      -4.3403640000      1.4665450000      0.1522890000
  C16      -2.8455660000      0.6093050000      1.8517350000
  C17      -2.0384750000      0.9812200000     -0.3898970000
  H51      -5.3236280000      1.8190210000     -0.1462460000
  H52      -2.6949690000      0.3062060000      2.8836370000
  H55      -3.4749370000      1.7484370000     -1.7984360000
  H56      -4.9199500000      1.0865410000      2.1868960000
  H59      -1.2571140000      0.9704440000     -1.1443360000
 H60       2.0921750000      0.4437910000      2.6861280000
 H61       0.8954860000      1.3633680000      3.6180520000
 H62       2.1546680000      2.2063210000      2.6947870000

 Molecular weight:    261.12 amu

 Stoichiometry:        C18NH15O
 Molecular Point Group: C1
 Point Group used: C1
 nuclear repulsion energy.......  1452.357863535 hartrees

Non-default options chosen:
  Geometry will be optimized in redundant internal coordinates
  Initial Hessian: from previous calculation

 end of program pre


 start of program onee
 smallest eigenvalue of S:    1.277E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program hfig
 initial wavefunction generated automatically from atomic wavefunctions

 Irreducible     Total no   No of occupied orbitals
 representation  orbitals   Shell_1  Shell_2    ...
 No Symm          210        69
 ------------------------
 Orbital occupation/shell    1.000

 end of program hfig


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     89     91     87     87     84     87
 grid # 2      106    100    100    100    100    100     95     93
 grid # 3      224    186    186    195    184    184    190    182
 grid # 4      223    382    381    401    380    379    374    382

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     82     73     81     98     77
 grid # 2      106    106    105     91    106     88    106     81
 grid # 3      224    224    220    191    224    169    221    165
 grid # 4      224    224    219    377    229    350    400    329

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      112     69     92     82     72     71     88     89
 grid # 2      127     99    106     92     75    101    100    100
 grid # 3      270    209    194    176    143    217    184    185
 grid # 4      473    207    405    352    306    210    380    380
```

```
  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     87     86     73     73     73     73     73
  grid # 2      100     99     98    106    104    106    106    101
  grid # 3      185    183    182    224    216    224    224    217
  grid # 4      380    380    381    224    215    224    224    214

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       72     71     72   2834
  grid # 2       98     99     98   3498
  grid # 3      217    217    220   7056
  grid # 4      223    223    226  10881

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf
 number of electrons..........        138
 number of alpha electrons....         69
 number of beta electrons.....         69
 number of orbitals, total....        210
 number of core orbitals......         69
 number of open shell orbs....          0
 number of occupied orbitals..         69
 number of virtual orbitals...        141
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: HF

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d    total energy     change  change    error

etot   1  N  N  5  M  -812.70807322606           1.1E-01  1.6E-01
etot   2  Y  Y  6  M  -814.63609558920  1.9E+00  1.2E-02  9.5E-02
etot   3  Y  Y  6  M  -814.96677516606  3.3E-01  3.7E-02  6.2E-02
etot   4  N  Y  2  U  -814.18471009137 -7.8E-01  3.4E-02  2.3E-01
etot   5  N  Y  2  U  -814.42871209538  2.4E-01  2.1E-02  1.9E-01
etot   6  Y  Y  6  M  -814.56019712972  1.3E-01  5.1E-03  1.8E-01
etot   7  N  Y  2  U  -814.60294150320  4.3E-02  2.6E-02  1.7E-01
etot   8  Y  Y  6  M  -814.77132966764  1.7E-01  2.4E-02  1.4E-01
etot   9  N  Y  2  U  -814.94917594918  1.8E-01  2.4E-02  9.5E-02
etot  10  Y  Y  6  M  -815.09158938124  1.4E-01  6.6E-03  4.8E-02
etot  11  N  Y  2  U  -815.12806521763  3.6E-02  1.8E-03  1.3E-02
etot  12  Y  Y  6  M  -815.12961784473  1.6E-03  1.2E-04  9.6E-04
etot  13  Y  Y  6  M  -815.12967580265  5.8E-05  4.3E-05  4.1E-04
etot  14  N  Y  2  U  -815.13078749106  1.1E-03  1.5E-05  1.8E-04
etot  15  Y  Y  6  M  -815.13078613640 -1.4E-06  1.0E-05  9.1E-05
etot  16  Y  Y  6  M  -815.13078432059 -1.8E-06  1.4E-06  2.7E-05
etot  17  Y  N  6  M  -815.13078342452 -9.0E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1452.35786353549
   (E)  Total one-electron terms..... -3990.21675173626
   (I)  Total two-electron terms.....  1722.72810477625
   (L)  Electronic energy............ -2267.48864696001  (E+I)
   (N)  Total energy.................  -815.13078342452  (A+L)

SCFE: SCF energy: HF    -815.13078342452 hartrees   iterations:  17


HOMO energy:    -0.28879
LUMO energy:     0.11151

 Orbital energies:
 -20.45677  -15.55469  -11.32558  -11.23562  -11.22365  -11.21575
 -11.21192  -11.20765  -11.19144  -11.18992  -11.18963  -11.18893
 -11.18698  -11.18664  -11.18354  -11.18296  -11.18198  -11.17820
 -11.17761  -11.17541   -1.42360   -1.34244   -1.17799   -1.15691
  -1.11684   -1.08521   -1.03960   -1.02214   -1.01586   -0.99456
  -0.94492   -0.90832   -0.85691   -0.84027   -0.82871   -0.80532
  -0.79385   -0.75915   -0.71616   -0.68597   -0.67827   -0.67105
  -0.65804   -0.64193   -0.63545   -0.62291   -0.60637   -0.60517
  -0.59865   -0.59409   -0.58703   -0.57764   -0.56508   -0.55696
  -0.54334   -0.52608   -0.51383   -0.50745   -0.49721   -0.49452
  -0.49177   -0.48535   -0.45707   -0.42549   -0.39058   -0.34684
  -0.33964   -0.31403   -0.28879    0.11151    0.12858    0.13914
   0.14162    0.20288    0.22529    0.25715    0.26624    0.27025
   0.29633

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
recomputing RwR matrix  20    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     2.710098E-03   9.931418E-03  -1.083884E-03
  2    C1      1.235714E-03   1.840851E-03  -4.397112E-03
  3    C2      1.408141E-03  -2.342416E-03  -1.320422E-03
  4    C3      1.822657E-02  -1.445978E-02  -2.727377E-02
  5    C4     -1.069457E-02  -1.220304E-02   9.670448E-03
  6    C5      1.976768E-03   1.564055E-02   3.180745E-03
  7    C6      2.502822E-02  -4.654627E-03  -1.629752E-02
  8    C7     -2.298166E-02   1.568919E-02   2.159439E-02
  9    H27    -3.962868E-03   8.036541E-03   7.320379E-03
 10    H28    -7.285149E-03  -2.059189E-03   9.150942E-03
 11    H30    -5.228705E-03  -1.143621E-02   5.249053E-03
 12    C8      5.310940E-03  -4.607515E-02  -2.723222E-03
 13    H32     5.612024E-03   1.003896E-02  -5.494555E-03
 14    C10    -8.285301E-03   5.084932E-03   2.083598E-02
 15    N2     -9.058734E-03   2.295617E-02  -9.589230E-03
 16    C9      1.978109E-02   6.704711E-03  -1.785745E-02
 17     O1      -1.183584E-02  -6.856242E-03   1.084779E-02
 18     H43     -7.914041E-04   8.057044E-03  -8.165723E-03
 19     C12     -1.747783E-02   4.303977E-03  -3.829222E-03
 20     C11     -1.112166E-02   1.051317E-02  -5.926035E-04
 21     C18      1.505426E-02   5.905996E-04   1.322731E-02
 22     H48      4.307911E-03  -1.103483E-02  -4.529152E-04
 23     C13      4.888378E-03  -1.733156E-03   3.083228E-03
 24     C14      2.448243E-03   2.215522E-04  -1.371246E-03
 25     C15     -3.837606E-03   3.052164E-04   1.637162E-03
 26     C16     -8.432890E-04   1.767656E-03  -4.749515E-03
 27     C17      4.349286E-04   1.609504E-04   3.479221E-04
 28     H51      9.476532E-03  -3.761478E-03   3.273882E-03
 29     H52      8.450141E-04   1.629853E-03  -9.740699E-03
 30     H55      2.183926E-03  -3.537752E-03   1.011807E-02
 31     H56      7.500918E-03  -7.431302E-04  -5.950180E-03
 32     H59     -4.820475E-03  -2.401999E-03   1.002720E-02
 33     H60     -6.455812E-03   5.156628E-03  -1.263196E-03
 34     H61      2.991080E-03   5.728372E-04  -7.238317E-03
 35     H62     -5.834737E-03  -5.494128E-03  -6.172088E-04
-----------    -------------  -------------  -------------
   total         9.050991E-04   4.096720E-04  -4.434826E-04

 end of program der1b


 start of program geopt   1

 geometry optimization step  1
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.30831E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.44330E-02    1.82052E-02    2.22167E-02
   2.61081E-02    2.83536E-02    2.92815E-02    3.00321E-02    3.13894E-02
   3.27109E-02    3.72510E-02    3.79844E-02    4.41294E-02    4.80993E-02
   7.12060E-02    7.24566E-02    7.29137E-02    7.73630E-02    7.79599E-02
   8.71620E-02    9.52773E-02    1.15259E-01    1.21583E-01    1.27472E-01
   1.33198E-01    1.37133E-01    1.45100E-01    1.45303E-01    1.52229E-01
   1.56516E-01    1.59979E-01    1.61878E-01    1.72414E-01    1.73955E-01
   1.80855E-01    2.04857E-01    2.08572E-01    2.13930E-01    2.17342E-01
   2.25082E-01    2.28259E-01    2.33199E-01    2.34478E-01    2.38673E-01
   2.39778E-01    2.45721E-01    2.56615E-01    2.61083E-01    2.71596E-01
   2.83850E-01    2.90715E-01    2.90805E-01    2.92642E-01    2.95997E-01
   2.99359E-01    3.01632E-01    3.03480E-01    3.04220E-01    3.09861E-01
   3.18892E-01    3.27308E-01    3.28988E-01    3.29382E-01    3.30352E-01
   3.33234E-01    3.34412E-01    3.34841E-01    3.36230E-01    3.36819E-01
   3.39099E-01    3.43853E-01    3.49434E-01    3.50836E-01    3.51003E-01
   3.52695E-01    3.55023E-01    3.58703E-01    3.79455E-01    3.80724E-01
   3.85382E-01    3.88914E-01    4.00754E-01    4.09155E-01    4.18006E-01
   4.27093E-01    4.35040E-01    4.42023E-01    4.50378E-01    4.53940E-01
   4.59273E-01    4.60092E-01    4.83221E-01    5.12605E-01    5.26775E-01
   5.81318E-01    6.62785E-01    7.12908E-01    8.98293E-01    9.98019E-01

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
```

```
    Step size:    0.3001598
    Cos(theta):   0.8403107

    Final level shift:  -6.5067957E-02

   gradient maximum:        2.2292E-02 .  (  4.5000E-04 )
   gradient rms:            7.9695E-03 .  (  3.0000E-04 )
   step size:   0.30011  trust radius:   0.30000
   displacement maximum:    1.1042E-01 .  (  1.8000E-03 )
   displacement rms:        2.6842E-02 .  (  1.2000E-03 )
   predicted energy change:    -1.4167E-02    geom step:   3.0011E-01    full step:
 3.0011E-01
   molecular structure not yet converged...

   center of mass moved by:
      x:    -5.5950E-03     y:     7.6968E-03     z:    -4.4494E-03

   new geometry:
                               angstroms
   atom            x                 y                 z
   H25       1.3000057341     -4.0446715404     -1.8727338343
   C1        1.7026939373     -3.0552926996     -1.9574406747
   C2        2.7925937972     -0.4454117717     -2.1864623609
   C3        1.2756367979     -2.0396021592     -1.1162682346
   C4        2.6510739254     -2.7537778402     -2.9028014140
   C5        3.1850745284     -1.4624565025     -3.0204944936
   C6        1.8389560512     -0.7573766749     -1.2459451927
   C7        0.2746601898     -1.9802721238     -0.0472431354
   H27       2.9921020618     -3.5205509309     -3.5709850587
   H28       3.9180556351     -1.2653155134     -3.7781348023
   H30       3.1967520295      0.5414840374     -2.2539666965
   C8        0.2859364622     -0.7201748586      0.4186213510
   H32      -0.3509002982     -2.7839149072      0.2684123225
   C10      -0.4068794516      0.1748148641      1.4115178091
   N2        1.2283706441      0.0277582731     -0.2839807543
   C9        1.3926480395      1.3238941298      0.1687100607
   O1        2.1502915712      2.1320278797     -0.3146471116
   H43      -0.4840730528     -0.2976550039      2.3806825465
   C12      -1.8056401415      0.5803435977      0.9522133665
   C11       0.5521666204      1.4174770968      1.4500145694
   C18       1.5154311962      1.3618881050      2.6517390944
   H48      -0.0010786736      2.3434826850      1.4616137164
   C13      -3.3245042383      1.3499713474     -0.7328881690
   C14      -4.1026214042      1.0418530975      1.4984843844
   C15      -4.3506035749      1.4042975786      0.1931790739
   C16      -2.8386979422      0.6314940493      1.8731142946
   C17      -2.0623843801      0.9412705690     -0.3591057341
   H51      -5.3299578141      1.7238608156     -0.1036299762
   H52      -2.6610473470      0.3439091297      2.8921391173
   H55      -3.5072558167      1.6255227631     -1.7530350708
   H56      -4.8897581808      1.0755516404      2.2257683902
   H59      -1.2881829644      0.8900692830     -1.0982983159
   H60       2.0921999335      0.4437520187      2.6374524446
   H61       0.9572822454      1.4126318968      3.5786387383
   H62       2.2052787472      2.1965661297      2.6181661050

   nuclear repulsion energy.......  1456.501220668 hartrees
   -------------------------------------------------
  /  end of geometry optimization iteration    1   /
  -------------------------------------------------

   end of program geopt
 start of program onee
 smallest eigenvalue of S:    1.204E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     89     90     87     87     83     85
 grid # 2       106     99     98     99     98     98     90     92
 grid # 3       224    183    182    195    182    182    187    181
 grid # 4       223    379    381    405    379    379    371    378

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     85     73     81     98     77
 grid # 2       106    106    105     91    106     91    107     81
 grid # 3       224    224    220    189    223    175    222    167
 grid # 4       224    224    219    373    229    350    401    331

 number of gridpoints:
    atom         O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1       112     70     91     82     71     70     85     87
 grid # 2       127     98    106     92     77    101     99     99
 grid # 3       271    208    190    176    150    217    181    182
 grid # 4       474    202    399    353    305    206    378    380

 number of gridpoints:
    atom        C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1        89     85     86     73     73     73     73     71
 grid # 2       100     98     98    106    104    106    106    101
 grid # 3       182    181    179    224    215    224    224    216
 grid # 4       379    377    378    224    215    224    224    211

 number of gridpoints:
    atom        H60    H61    H62  total
 grid # 1        71     71     72   2821
 grid # 2        99     99     99   3488
 grid # 3       217    217    220   7034
 grid # 4       218    219    222  10834

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                 RMS     maximum
```

```
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.11300452463           8.2E-04  2.4E-02
etot   2  Y  Y  6  M  -815.13845554450  2.5E-02  3.0E-04  1.0E-02
etot   3  N  Y  2  U  -815.14064468767  2.2E-03  1.3E-04  3.4E-03
etot   4  Y  Y  6  M  -815.14102231127  3.8E-04  5.8E-05  1.5E-03
etot   5  Y  Y  6  M  -815.14107516429  5.3E-05  1.8E-05  3.8E-04
etot   6  Y  Y  6  M  -815.14108493230  9.8E-06  8.9E-06  1.2E-04
etot   7  Y  Y  6  M  -815.14108642610  1.5E-06  2.6E-06  3.0E-05
etot   8  N  N  2  U  -815.14107666406 -9.8E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1456.50122066823
   (E)  Total one-electron terms..... -3998.50139176955
   (I)  Total two-electron terms.....  1726.85909443726
   (L)  Electronic energy............ -2271.64229733229  (E+I)
   (N)  Total energy.................  -815.14107666406  (A+L)

 SCFE: SCF energy: HF    -815.14107666406 hartrees   iterations:   8


 HOMO energy:    -0.29670
 LUMO energy:     0.11667

  Orbital energies:
  -20.45440  -15.55145  -11.32294  -11.23506  -11.22252  -11.21370
  -11.20786  -11.19918  -11.18706  -11.18355  -11.18293  -11.18211
  -11.18043  -11.18027  -11.17843  -11.17777  -11.17714  -11.17579
  -11.17475  -11.17146   -1.42428   -1.33289   -1.18223   -1.16413
   -1.11718   -1.08655   -1.04178   -1.02774   -1.02055   -1.00081
   -0.94644   -0.90533   -0.85641   -0.84329   -0.82973   -0.81198
   -0.79403   -0.76366   -0.72150   -0.68662   -0.67955   -0.66894
   -0.65944   -0.64133   -0.63812   -0.62648   -0.61384   -0.60708
   -0.60310   -0.59819   -0.59138   -0.57931   -0.56391   -0.55409
   -0.54280   -0.53022   -0.51760   -0.51023   -0.49799   -0.49658
   -0.49102   -0.48668   -0.45894   -0.42231   -0.39422   -0.34896
   -0.34152   -0.31515   -0.29670    0.11667    0.13464    0.14410
    0.14610    0.20391    0.22899    0.26095    0.27143    0.27236
    0.30261

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25    -2.575654E-04  -1.377957E-05  -4.102216E-04
  2    C1     -2.921206E-03   1.937730E-04   2.822312E-03
  3    C2      1.858833E-03   1.772500E-03  -3.957725E-04
  4    C3     -2.790645E-03   3.008666E-03   1.631593E-03
  5    C4      6.819097E-03   7.895586E-04  -7.404351E-03
  6    C5      3.991034E-03  -6.501846E-03  -5.765574E-03
  7    C6     -8.295094E-03  -2.212359E-03   7.216076E-03
  8    C7      1.134323E-03   3.532668E-03   1.054047E-03
  9    H27     2.780910E-04   8.549838E-04   3.853479E-05
 10    H28    -1.323298E-04  -9.603221E-04   3.619389E-04
 11    H30    -8.635922E-04   9.383658E-04   9.517932E-04
 12    C8     -1.441258E-03  -6.390285E-03  -2.555182E-03
 13    H32     4.945037E-04   4.862599E-04   5.846434E-04
 14    C10    -1.702306E-03   3.493569E-03  -2.132366E-03
 15    N2     -8.173328E-04   5.735054E-03   1.045233E-03
 16    C9      7.079861E-03  -6.565176E-03   9.773937E-04
 17    O1     -2.761746E-03   1.033521E-03   6.809743E-04
 18    H43     2.463391E-03   1.201338E-03   3.951064E-04
 19    C12     3.528471E-03  -3.033739E-03   4.214148E-03
 20    C11    -3.632064E-03   9.135875E-04  -5.108017E-04
 21    C18     2.612744E-03   8.745695E-04   1.275877E-04
 22    H48    -2.940717E-04  -7.509783E-05  -5.318336E-05
 23    C13    -2.184273E-03   2.031700E-03  -5.345485E-03
 24    C14    -3.952667E-03   1.126668E-04   3.661182E-03
 25    C15    -2.890876E-03   1.817066E-03  -3.261519E-03
 26    C16     2.790241E-03  -1.902126E-03   4.155119E-03
 27    C17     2.128329E-03  -4.447950E-04  -3.503469E-03
 28    H51     3.556837E-04  -2.003766E-04  -9.353409E-05
 29    H52     5.628224E-04   2.813238E-04  -3.052406E-04
 30    H55    -3.578681E-04  -9.991860E-05   3.182582E-04
 31    H56     1.870887E-04  -1.910249E-04   5.330263E-06
 32    H59     7.351639E-04  -2.014384E-04   9.823533E-04
 33    H60    -9.407576E-04  -3.966907E-04   2.070924E-04
 34    H61    -1.014150E-04  -2.044374E-04   2.377736E-05
 35    H62    -3.394196E-04  -1.491331E-05  -4.819000E-04
-----------   -------------  -------------  -------------
   total       3.431898E-04  -3.371549E-04  -7.641063E-04

 end of program der1b


 start of program geopt   2

 geometry optimization step  2
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.26376E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.38656E-02    1.79374E-02    2.24197E-02
   2.60907E-02    2.81363E-02    2.95248E-02    2.99439E-02    3.06786E-02
   3.26181E-02    3.71148E-02    3.85611E-02    4.35651E-02    4.79685E-02
   6.76648E-02    6.97388E-02    7.15610E-02    7.45320E-02    7.53942E-02
   8.25495E-02    9.73693E-02    1.12991E-01    1.17826E-01    1.20233E-01
   1.31245E-01    1.33445E-01    1.37395E-01    1.41868E-01    1.49829E-01
   1.53534E-01    1.57146E-01    1.59863E-01    1.69710E-01    1.71296E-01
   1.77100E-01    2.00128E-01    2.04359E-01    2.10738E-01    2.13691E-01
   2.18355E-01    2.24566E-01    2.29455E-01    2.31275E-01    2.33813E-01
   2.35404E-01    2.41291E-01    2.45137E-01    2.54251E-01    2.59919E-01
```

```
    2.78636E-01    2.81173E-01    2.87824E-01    2.89736E-01    2.96503E-01
    2.99863E-01    3.01550E-01    3.02446E-01    3.03185E-01    3.08887E-01
    3.10192E-01    3.20066E-01    3.26595E-01    3.26861E-01    3.29242E-01
    3.32715E-01    3.33177E-01    3.34949E-01    3.36171E-01    3.39071E-01
    3.41807E-01    3.44186E-01    3.46277E-01    3.48363E-01    3.52291E-01
    3.58215E-01    3.66951E-01    3.74359E-01    3.76156E-01    3.82285E-01
    3.87801E-01    4.03253E-01    4.07438E-01    4.17467E-01    4.28253E-01
    4.35391E-01    4.37442E-01    4.43209E-01    4.51325E-01    4.57444E-01
    4.68068E-01    4.75730E-01    4.88499E-01    5.09972E-01    5.23383E-01
    5.81922E-01    6.54065E-01    6.99931E-01    9.27449E-01    1.01232E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  energy change:           -1.0293E-02 .  (  5.0000E-05 )
  gradient maximum:         9.0587E-03 .  (  4.5000E-04 )
  gradient rms:             2.4046E-03 .  (  3.0000E-04 )
  step size:   0.29345  trust radius:   0.30000
  displacement maximum:     9.9604E-02 .  (  1.8000E-03 )
  displacement rms:         2.6247E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.6638E-03    geom step:   2.9345E-01    full step:
2.9345E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     6.1612E-03     y:    -6.4057E-03     z:    -4.0606E-03

  new geometry:
                              angstroms
  atom           x                 y                 z
  H25       1.1518606918     -4.0098168429     -1.9778502480
  C1        1.6213334988     -3.0412378065     -2.0198094544
  C2        2.8854945661     -0.5061674774     -2.1375642472
  C3        1.2106916162     -2.0237954044     -1.1655115623
  C4        2.6572180524     -2.7892002183     -2.9132967886
  C5        3.2840693794     -1.5321531013     -2.9725294884
  C6        1.8498186945     -0.7716072417     -1.2458480733
  C7        0.1942594179     -1.9359342141     -0.1091129346
  H27       2.9857473521     -3.5649096486     -3.5726003392
  H28       4.0801549607     -1.3620817681     -3.6763623200
  H30       3.3461240517      0.4646787114     -2.1568798680
  C8        0.2618553297     -0.6883215287      0.3821991922
  H32      -0.4681638696     -2.7172745500      0.1901386333
  C10      -0.3975941615      0.2237999717      1.3918814693
  N2        1.2380037561      0.0371308184     -0.3021743921
  C9        1.4521852626      1.3156189960      0.1616775535
  O1        2.2343198160      2.1086661210     -0.3070199295
  H43      -0.4258590119     -0.2337511833      2.3689489433
  C12      -1.8107959507      0.6020767984      0.9735434286
  C11       0.5660949612      1.4604984734      1.4059534484
  C18       1.5050815780      1.4495699586      2.6314972653
  H48       0.0195675120      2.3870243908      1.3648102645
  C13      -3.3661198293      1.4033105312     -0.6804601314
  C14      -4.1304614559      0.9236093394      1.5325150118
  C15      -4.3956846103      1.3521476600      0.2443536745
  C16      -2.8435084195      0.5508352241      1.8928334718
  C17      -2.0838903192      1.0297839732     -0.3191628233
  H51      -5.3894948227      1.6371262915     -0.0361671987
  H52      -2.6501748807      0.2107839874      2.8903083998
  H55      -3.5615758548      1.7281930898     -1.6791037066
  H56      -4.9200189160      0.8719163607      2.2537100009
  H59      -1.2975036389      1.0562731973     -1.0405498146
```

```
 H60       2.0234153991      0.4989957046      2.6957845223
 H61       0.9267575216      1.5940760071      3.5380412645
 H62       2.2363036985      2.2462236996      2.5514206148

 nuclear repulsion energy.......  1451.691619179 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   2   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.267E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     84     85
 grid # 2      106    100     98    100     99     99     90     92
 grid # 3      224    184    184    195    183    183    192    182
 grid # 4      224    382    383    405    377    381    378    378

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     85     73     81     99     77
 grid # 2      106    106    105     91    106     92    109     81
 grid # 3      224    224    220    189    223    175    223    165
 grid # 4      224    224    219    373    229    349    402    325

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      112     69     90     80     71     70     87     87
 grid # 2      123     98    105     91     75    101    100    100
 grid # 3      271    208    190    174    149    217    184    183
 grid # 4      474    202    401    349    305    209    376    379

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1       89     86     86     73     73     73     73     71
 grid # 2      100    100     96    106    104    106    106    101
 grid # 3      182    181    181    224    214    224    224    216
 grid # 4      380    376    374    224    214    224    224    211

 number of gridpoints:
    atom       H60    H61    H62  total
 grid # 1       70     71     71   2818
 grid # 2       99     99     99   3489
 grid # 3      216    218    220   7046
 grid # 4      218    220    221  10834

 end of program grid
```

```
  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.10856900978           7.3E-04  2.3E-02
etot   2  Y  Y  6  M  -815.13699415616  2.8E-02  3.3E-04  9.5E-03
etot   3  N  Y  2  U  -815.14103578522  4.0E-03  1.2E-04  2.9E-03
etot   4  Y  Y  6  M  -815.14134795057  3.1E-04  3.2E-05  7.1E-04
etot   5  Y  Y  6  M  -815.14137251641  2.5E-05  1.6E-05  2.0E-04
etot   6  Y  Y  6  M  -815.14138057381  8.1E-06  5.0E-06  6.2E-05
etot   7  Y  N  6  M  -815.14138192640  1.4E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1451.69161917946
   (E)  Total one-electron terms..... -3988.89311720062
   (I)  Total two-electron terms.....  1722.06011609476
   (L)  Electronic energy............ -2266.83300110586  (E+I)
   (N)  Total energy.................  -815.14138192640  (A+L)

 SCFE: SCF energy: HF    -815.14138192640 hartrees   iterations:   7


 HOMO energy:    -0.29734
 LUMO energy:     0.11639

  Orbital energies:
  -20.45321  -15.55299  -11.32204  -11.23694  -11.22491  -11.21375
  -11.20682  -11.19934  -11.18918  -11.18469  -11.18424  -11.18329
  -11.18180  -11.18146  -11.18132  -11.17931  -11.17887  -11.17874
  -11.17783  -11.17454   -1.42407   -1.33298   -1.18018   -1.16024
   -1.11545   -1.08682   -1.04120   -1.02619   -1.01647   -0.99987
   -0.94624   -0.90518   -0.85586   -0.84416   -0.82958   -0.80997
   -0.79405   -0.76187   -0.72165   -0.68702   -0.67958   -0.66835
   -0.65921   -0.64273   -0.63751   -0.62652   -0.61049   -0.60653
   -0.60301   -0.59843   -0.59123   -0.57758   -0.56225   -0.55362
   -0.54320   -0.53048   -0.51753   -0.50912   -0.49826   -0.49630
   -0.49000   -0.48671   -0.45834   -0.42141   -0.39308   -0.34800
   -0.34190   -0.31344   -0.29734    0.11639    0.13296    0.14186
    0.14452    0.20313    0.22808    0.26208    0.27120    0.27206
    0.30290

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr
 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----    -------------  -------------  -------------
  1    H25     2.098872E-03   3.380861E-03  -1.168343E-03
  2    C1      5.496099E-03  -6.956917E-04  -2.974951E-03
  3    C2     -3.983874E-03   1.177321E-03   4.738758E-03
  4    C3      3.388157E-03   3.089239E-03  -1.574441E-03
  5    C4     -4.182380E-03   4.182366E-03   4.655928E-03
  6    C5     -4.144667E-03  -3.482909E-03   2.243977E-03
  7    C6      1.359420E-03  -1.580591E-03  -7.157283E-03
  8    C7      2.484529E-03   2.864738E-03  -2.743071E-04
  9    H27     1.798075E-04  -1.251287E-03  -7.909477E-04
 10    H28    -2.625419E-03  -1.542959E-03   2.332376E-03
 11    H30    -2.633713E-03  -3.094521E-03   5.034015E-04
 12    C8     -3.169504E-03  -5.212712E-04  -2.036196E-03
 13    H32     8.089568E-04   1.220704E-03   7.917000E-05
 14    C10     7.296106E-04   6.268588E-04  -1.962084E-03
 15    N2      5.964268E-03  -2.540358E-03   1.592548E-03
 16    C9     -2.374178E-03   1.824113E-04  -1.409597E-03
 17    O1      9.993823E-04  -8.270370E-04   9.655266E-04
 18    H43     1.993385E-04  -1.075655E-03   8.894052E-04
 19    C12     2.012208E-04   1.192534E-04   1.749012E-04
 20    C11     2.185718E-03  -9.823637E-04  -7.319136E-04
 21    C18    -2.016583E-03   5.400820E-04   1.711031E-03
 22    H48    -6.955556E-04   1.601647E-03  -5.279066E-04
 23    C13     2.965739E-03  -8.569035E-04   1.179894E-03
 24    C14     3.168776E-04  -3.917690E-04  -4.258883E-04
 25    C15     4.633616E-04  -7.064301E-04   2.447394E-03
 26    C16    -2.482101E-03   4.777271E-05  -2.748550E-04
 27    C17    -2.722128E-03   3.488933E-04   1.071938E-03
 28    H51    -1.516382E-04   1.280466E-04  -1.255269E-04
 29    H52    -1.087607E-04   7.888498E-05   1.344865E-03
 30    H55    -2.157401E-04   7.831934E-04  -2.685911E-03
 31    H56    -6.246669E-04   8.224659E-05   8.782099E-04
 32    H59     1.864034E-03   2.618714E-04  -2.910454E-03
 33    H60     5.295714E-04   7.486976E-04   2.328120E-04
 34    H61     1.255871E-03  -1.451449E-04  -3.410125E-04
 35    H62    -8.772592E-04  -1.152230E-03  -1.981717E-04
-----------    -------------  -------------  -------------
   total       4.826672E-04   6.179652E-04  -5.276526E-04

 end of program der1b


 start of program geopt   3

 geometry optimization step  3
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.25351E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.37059E-02    1.66291E-02    2.21695E-02
```

```
    2.77894E-02    2.83298E-02    3.00506E-02    3.08218E-02    3.09428E-02
    3.39351E-02    3.73791E-02    4.36431E-02    4.52120E-02    5.02468E-02
    6.51205E-02    6.63929E-02    7.16219E-02    7.39902E-02    7.44288E-02
    8.00691E-02    8.70548E-02    1.12362E-01    1.13663E-01    1.15425E-01
    1.21478E-01    1.28463E-01    1.33270E-01    1.39046E-01    1.42773E-01
    1.53576E-01    1.54190E-01    1.60954E-01    1.64182E-01    1.67932E-01
    1.72504E-01    1.88954E-01    1.98079E-01    1.98956E-01    2.05932E-01
    2.11946E-01    2.18216E-01    2.23191E-01    2.24917E-01    2.30268E-01
    2.32960E-01    2.35368E-01    2.42611E-01    2.51571E-01    2.53253E-01
    2.62848E-01    2.70566E-01    2.79141E-01    2.86243E-01    2.89671E-01
    2.97269E-01    2.98703E-01    3.00485E-01    3.07995E-01    3.12061E-01
    3.17593E-01    3.26409E-01    3.29871E-01    3.32476E-01    3.33981E-01
    3.34117E-01    3.36861E-01    3.38562E-01    3.41939E-01    3.45258E-01
    3.47091E-01    3.49729E-01    3.53065E-01    3.56418E-01    3.57719E-01
    3.64812E-01    3.76133E-01    3.77832E-01    3.81172E-01    3.89131E-01
    3.98627E-01    4.15068E-01    4.18376E-01    4.30353E-01    4.39375E-01
    4.41786E-01    4.43884E-01    4.59399E-01    4.67508E-01    4.78749E-01
    4.82375E-01    4.96998E-01    5.06373E-01    5.41864E-01    5.99703E-01
    6.20995E-01    6.77213E-01    7.24138E-01    9.41540E-01    1.05694E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.3000211
   Cos(theta):   0.3699691

   Final level shift:  -3.3930890E-03

  energy change:          -3.0526E-04 .  (  5.0000E-05 )
  gradient maximum:        1.1892E-02 .  (  4.5000E-04 )
  gradient rms:            2.1714E-03 .  (  3.0000E-04 )
  step size:   0.30001  trust radius:   0.30000
  displacement maximum:    1.7324E-01 .  (  1.8000E-03 )
  displacement rms:        2.6834E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.5000E-03    geom step:   3.0001E-01    full step:
3.0001E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1701E-02     y:    -8.4875E-03     z:     5.3236E-03

  new geometry:
                              angstroms
  atom           x                 y                 z
  H25       1.1614190570     -4.0152533188     -1.9128485587
  C1        1.6086208687     -3.0522794650     -1.9818314055
  C2        2.7984426018     -0.5348705802     -2.1771022069
  C3        1.2043923931     -2.0257717304     -1.1339854821
  C4        2.5939478766     -2.8242005058     -2.9131348386
  C5        3.1802412861     -1.5761633223     -3.0100641781
  C6        1.8162588474     -0.7819033370     -1.2494263537
  C7        0.2187483558     -1.9169086228     -0.0521484347
  H27       2.9072186891     -3.6085404749     -3.5673537360
  H28       3.9311282709     -1.4195666234     -3.7399785897
  H30       3.2224166237      0.4345780682     -2.2252236816
  C8        0.2669567905     -0.6672699906      0.3993876946
  H32      -0.4201025246     -2.6898731188      0.2844525025
  C10      -0.3819054453      0.2698931957      1.3980122901
  N2        1.2569609330      0.0390282117     -0.2892173015
  C9        1.5093626556      1.3052147892      0.1764075879
  O1        2.3133717921      2.0816116198     -0.2820004538
```

```
 H43      -0.3916406892     -0.1634111567      2.3860214399
 C12      -1.7964244935      0.6228627455      0.9746968558
 C11       0.5901251536      1.4982564148      1.3929861846
 C18       1.4993549390      1.5232151999      2.6444438604
 H48       0.0507622990      2.4265078689      1.3049029716
 C13      -3.3105468126      1.5463894150     -0.6593153947
 C14      -4.1637618973      0.7431335580      1.4469962012
 C15      -4.3847212370      1.3203164828      0.2039478302
 C16      -2.8716913116      0.3986341852      1.8298430292
 C17      -2.0276768548      1.1945164398     -0.2769447225
 H51      -5.3792592923      1.5836177829     -0.0906898094
 H52      -2.7085231988     -0.0541893670      2.7881336586
 H55      -3.4743324151      1.9857927272     -1.6185445974
 H56      -4.9889142419      0.5537702489      2.1127342653
 H59      -1.1993483024      1.3535275563     -0.9396952544
 H60       1.9945919384      0.5664206563      2.7608144602
 H61       0.9045486745      1.7140557085      3.5308675162
 H62       2.2427731320      2.3021460902      2.5438716690

 nuclear repulsion energy.......  1453.210759158 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   3   /
-------------------------------------------------


 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.167E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     85     87     86     84     86
 grid # 2      106     99     97     98     98     97     91     93
 grid # 3      224    183    182    197    182    183    185    182
 grid # 4      224    376    378    406    375    374    367    376

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     85     73     82    100     75
 grid # 2      106    106    105     91    106     92    108     80
 grid # 3      224    224    220    185    223    172    222    164
 grid # 4      224    222    216    376    227    350    401    332

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      111     69     90     81     71     69     89     88
 grid # 2      123     99    106     91     75    101     99    100
 grid # 3      272    208    195    175    148    217    183    184
 grid # 4      473    202    400    353    305    208    377    380

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
```

```
  grid # 1       89     87     86     73     73     73     73     70
  grid # 2      100    100     97    106    103    106    106    102
  grid # 3      184    182    180    224    215    224    224    216
  grid # 4      378    377    377    224    214    224    224    210

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       70     71     71   2815
  grid # 2       99     99     99   3484
  grid # 3      215    218    220   7036
  grid # 4      217    220    221  10808

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                      RMS    maximum
       e  d  i  u  i                            energy  density    DIIS
       r  t  s  t  d     total energy           change  change     error

etot   1  N  N  2  U  -815.08897379247            9.1E-04  3.7E-02
etot   2  Y  Y  6  M  -815.13304471310  4.4E-02  4.1E-04  1.5E-02
etot   3  N  Y  2  U  -815.13889498757  5.9E-03  1.5E-04  4.9E-03
etot   4  Y  Y  6  M  -815.13944528947  5.5E-04  3.9E-05  1.2E-03
etot   5  Y  Y  6  M  -815.13949633447  5.1E-05  2.0E-05  3.2E-04
etot   6  N  Y  2  U  -815.13952013096  2.4E-05  5.3E-06  6.3E-05
etot   7  Y  Y  6  M  -815.13952466940  4.5E-06  2.2E-06  2.4E-05
etot   8  Y  N  6  M  -815.13952532202  6.5E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1453.21075915848
   (E)  Total one-electron terms..... -3991.88769772517
   (I)  Total two-electron terms.....  1723.53741324468
   (L)  Electronic energy............ -2268.35028448050  (E+I)
   (N)  Total energy.................  -815.13952532202  (A+L)

 SCFE: SCF energy: HF    -815.13952532202 hartrees   iterations:   8


 HOMO energy:    -0.29699
 LUMO energy:     0.11697

  Orbital energies:
  -20.45183  -15.55125  -11.32116  -11.23526  -11.22007  -11.21339
  -11.20644  -11.20145  -11.18720  -11.18662  -11.18656  -11.18592
  -11.18430  -11.18410  -11.17796  -11.17701  -11.17561  -11.17435
  -11.17280  -11.16972   -1.42361   -1.33462   -1.17965   -1.16296
   -1.11681   -1.08978   -1.03943   -1.02605   -1.02232   -0.99931
   -0.94810   -0.90555   -0.85859   -0.84189   -0.83058   -0.81460
   -0.79459   -0.76410   -0.72058   -0.68822   -0.68142   -0.67000
   -0.65944   -0.64364   -0.63883   -0.62952   -0.61294   -0.60633
   -0.60343   -0.60022   -0.59242   -0.57452   -0.56289   -0.55300
   -0.54417   -0.53162   -0.51796   -0.50808   -0.49960   -0.49698
   -0.49014   -0.48760   -0.46005   -0.42007   -0.39285   -0.34847
  -0.34051   -0.31842   -0.29699    0.11697    0.13273    0.14110
   0.14535    0.20646    0.22923    0.26364    0.27133    0.27373
   0.29976

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----    -------------  -------------  -------------
  1    H25     -3.806402E-03  -5.536656E-03   1.423983E-03
  2    C1      -7.595509E-03  -2.805998E-03   6.852796E-03
  3    C2       3.269989E-03  -4.374206E-03  -5.495096E-03
  4    C3      -1.302549E-03  -6.804802E-03   3.353788E-04
  5    C4      -3.482803E-03  -1.274686E-03   2.553103E-03
  6    C5      -7.617634E-04   1.344370E-02   5.614457E-03
  7    C6       6.044798E-03   2.062297E-03  -1.730929E-03
  8    C7      -2.609308E-03  -8.869214E-03  -5.177161E-03
  9    H27      2.187307E-04  -2.077622E-03  -1.030189E-03
 10    H28      7.669363E-03   3.818581E-03  -6.174422E-03
 11    H30      6.067677E-03   6.892154E-03  -2.173920E-03
 12    C8       4.710461E-03   1.145895E-02   7.546522E-03
 13    H32     -4.569118E-03  -4.635587E-03   1.271004E-03
 14    C10      3.032770E-03  -2.481664E-03   9.472803E-04
 15    N2      -1.307554E-03  -2.043169E-04  -2.272438E-03
 16    C9      -8.582600E-03   4.373520E-03  -2.774170E-03
 17    O1       3.396909E-03  -1.139413E-03  -3.619326E-05
 18    H43     -1.821274E-03  -2.496712E-03   8.146571E-04
 19    C12     -5.927197E-03   2.304126E-03   3.638865E-04
 20    C11      4.598454E-03  -2.795029E-03   1.859308E-04
 21    C18     -5.101998E-03  -9.268442E-05   2.163241E-04
 22    H48      1.203985E-04   1.499553E-03  -8.116444E-04
 23    C13     -1.379697E-03  -4.009225E-03   8.690672E-03
 24    C14      1.813768E-03   8.633659E-04  -4.308969E-03
 25    C15      6.202003E-03  -1.624962E-03   1.343779E-03
 26    C16      1.850168E-03   1.397592E-03  -5.846259E-03
 27    C17     -3.224399E-03  -8.897936E-04   5.478460E-03
 28    H51     -6.269819E-04   7.851819E-04  -1.123054E-03
 29    H52      7.635297E-04   4.240073E-04   4.500045E-04
 30    H55     -1.245965E-03   1.191251E-03  -2.529247E-03
 31    H56      3.007047E-03   1.231123E-03  -2.432805E-03
 32    H59     -1.662959E-03   1.369248E-04  -9.669580E-04
 33    H60      1.476641E-03   4.277060E-04  -3.849825E-06
 34    H61      8.023828E-04   3.074340E-04  -2.156559E-04
 35    H62      7.657863E-04  -3.469971E-05   1.554486E-04
-----------    -------------  -------------  -------------
   total        8.028000E-04   4.701943E-04  -8.592716E-04

 end of program der1b
 start of program geopt    4

 geometry optimization step  4
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step    3 **

 Hessian eigenvalues:
  -1.31575E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.25399E-02    1.59841E-02    2.15622E-02
   2.69414E-02    2.81926E-02    2.94072E-02    3.02705E-02    3.13298E-02
   3.31282E-02    3.56779E-02    3.82925E-02    4.63961E-02    5.85155E-02
   6.28471E-02    6.81911E-02    6.92904E-02    7.30826E-02    7.66931E-02
   8.16257E-02    8.52811E-02    1.05202E-01    1.07786E-01    1.14336E-01
   1.21140E-01    1.25371E-01    1.31747E-01    1.34925E-01    1.42338E-01
   1.45462E-01    1.51031E-01    1.59358E-01    1.61852E-01    1.63352E-01
   1.81227E-01    1.83381E-01    1.91528E-01    1.97941E-01    2.00319E-01
   2.08863E-01    2.17701E-01    2.21787E-01    2.24603E-01    2.26075E-01
   2.28541E-01    2.34873E-01    2.39879E-01    2.43922E-01    2.46885E-01
   2.53047E-01    2.62363E-01    2.65660E-01    2.77464E-01    2.80394E-01
   2.89462E-01    2.91191E-01    3.01568E-01    3.05497E-01    3.08922E-01
   3.18556E-01    3.24224E-01    3.25649E-01    3.34348E-01    3.35552E-01
   3.41032E-01    3.42347E-01    3.42809E-01    3.47773E-01    3.48073E-01
   3.49132E-01    3.53173E-01    3.57944E-01    3.63668E-01    3.64657E-01
   3.71424E-01    3.71912E-01    3.83748E-01    3.90436E-01    3.91986E-01
   4.08519E-01    4.18330E-01    4.29417E-01    4.32770E-01    4.43347E-01
   4.43695E-01    4.56224E-01    4.61820E-01    4.80189E-01    4.92057E-01
   4.97869E-01    5.08854E-01    5.73496E-01    5.99870E-01    6.25465E-01
   6.75695E-01    7.33012E-01    8.86780E-01    9.21955E-01    1.03946E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.3003077
  Cos(theta):   0.2681660

  Final level shift:  -4.0869655E-03

 energy change:            1.8566E-03 .  (  5.0000E-05 )
 gradient maximum:         1.1892E-02 .  (  4.5000E-04 )
 gradient rms:             2.1714E-03 .  (  3.0000E-04 )
 step size:   0.30028  trust radius:   0.30000
 displacement maximum:     9.9534E-02 .  (  1.8000E-03 )
 displacement rms:         2.6858E-02 .  (  1.2000E-03 )
 predicted energy change:    -1.1617E-03    geom step:   3.0028E-01    full step:
3.0028E-01
 molecular structure not yet converged...

 center of mass moved by:
    x:     8.3267E-16     y:     1.5005E-16     z:     5.5511E-16

 new geometry:
                               angstroms
 atom            x                 y                  z
 H25       1.2043005006     -4.0177275246     -1.9824602028
 C1        1.6461683306     -3.0412613553     -2.0263296897
 C2        2.8157294014     -0.4844828084     -2.1756613164
 C3        1.2391572476     -2.0321210806     -1.1548460996
 C4        2.6207549813     -2.7668515878     -2.9626563370
 C5        3.1965160839     -1.5041533843     -3.0361944423
 C6        1.8414130481     -0.7752501759     -1.2474890014
 C7        0.2555901030     -1.9603197428     -0.0841142447
 H27       2.9367812303     -3.5378106365     -3.6430836510
 H28       3.9502502530     -1.3184381309     -3.7705770606
 H30       3.2403721099      0.4973471024     -2.2106264468
 C8        0.2901559215     -0.7071386810      0.3940886584
 H32      -0.3894912994     -2.7485350389      0.2361511970
 C10      -0.3811065047      0.1950873568      1.3905290944
 N2        1.2848088368      0.0095097503     -0.2632877246
 C9        1.5115807017      1.2737451115      0.2235131931
 O1        2.3393875286      2.0533846317     -0.2056237943
 H43      -0.4006450301     -0.2786758531      2.3664442759
 C12      -1.7941142920      0.5654501017      0.9725603429
 C11       0.5666942627      1.4394494551      1.4219023295
 C18       1.4220368495      1.4748383266      2.7057167408
 H48       0.0116770276      2.3691264107      1.3155501008
 C13      -3.3557685473      1.3421305392     -0.6951159099
 C14      -4.0760400048      0.9942226112      1.4953952766
 C15      -4.3532183072      1.3696462381      0.2140381847
 C16      -2.7987439255      0.5970491151      1.8737207117
 C17      -2.0865926408      0.9394764816     -0.3186370519
 H51      -5.3362859848      1.6829292210     -0.0793750969
 H52      -2.5862011020      0.3249022895      2.8679202982
 H55      -3.5670310417      1.6335748207     -1.6900741223
 H56      -4.8405281490      1.0189687292      2.1972271293
 H59      -1.3179262930      0.9147403706     -1.0302545291
 H60       1.9819450175      0.5533315242      2.8232761175
 H61       0.7971142817      1.6057123093      3.5820267895
 H62       2.1207731973      2.2942329172      2.6539595437

 nuclear repulsion energy.......  1456.799458232 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration    4   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.190E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      89      87      85      83      85
 grid # 2       106      99      99      98      99      99      88      92
 grid # 3       224     183     183     196     183     183     190     183
 grid # 4       224     380     383     407     380     374     372     377
```

```
  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     85     73     81     99     76
  grid # 2      106    106    105     91    106     91    108     81
  grid # 3      224    224    220    188    223    175    220    164
  grid # 4      224    224    219    372    228    351    399    331

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     70     87     82     72     70     85     85
  grid # 2      127     97     99     92     75    100     96     95
  grid # 3      272    207    192    175    142    217    180    177
  grid # 4      473    200    395    351    308    208    375    373

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       87     85     84     73     73     73     73     71
  grid # 2       97     95     93    106    104    106    106    100
  grid # 3      181    178    177    224    215    223    224    216
  grid # 4      377    371    372    224    214    222    222    212

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2805
  grid # 2       99     99     99   3459
  grid # 3      217    218    220   7018
  grid # 4      217    219    221  10799

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                 RMS    maximum
       e  d  i  u  i                      energy  density    DIIS
       r  t  s  t  d     total energy     change   change    error

etot   1  N  N  2  U  -815.04407421317            1.2E-03  4.3E-02
etot   2  Y  Y  6  M  -815.12312641991  7.9E-02  5.6E-04  1.6E-02
etot   3  N  Y  2  U  -815.13340222471  1.0E-02  2.0E-04  5.1E-03
etot   4  Y  Y  6  M  -815.13433913117  9.4E-04  5.4E-05  1.2E-03
etot   5  Y  Y  6  M  -815.13445674667  1.2E-04  2.7E-05  3.6E-04
etot   6  N  Y  2  U  -815.13449646689  4.0E-05  8.9E-06  1.5E-04
etot   7  Y  Y  6  M  -815.13449765058  1.2E-06  2.5E-06  2.3E-05
etot   8  Y  N  6  M  -815.13449768154  3.1E-08  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1456.79945823214
   (E)  Total one-electron terms..... -3998.96497185383
   (I)  Total two-electron terms.....  1727.03101594015
   (L)  Electronic energy............ -2271.93395591368  (E+I)
   (N)  Total energy.................  -815.13449768154  (A+L)
```

```
SCFE: SCF energy: HF    -815.13449768154 hartrees   iterations:   8


HOMO energy:    -0.29545
LUMO energy:     0.11597

 Orbital energies:
 -20.45267  -15.55305  -11.32297  -11.23537  -11.22122  -11.21329
 -11.20891  -11.19297  -11.18712  -11.17918  -11.17820  -11.17782
 -11.17730  -11.17704  -11.17667  -11.17658  -11.17558  -11.17481
 -11.17461  -11.17194   -1.42054   -1.33686   -1.18932   -1.16645
  -1.11951   -1.09032   -1.04955   -1.02674   -1.02137   -1.00162
  -0.94991   -0.90787   -0.85782   -0.85510   -0.82975   -0.81275
  -0.79688   -0.76315   -0.72917   -0.68720   -0.68069   -0.67304
  -0.65972   -0.64560   -0.64187   -0.62768   -0.61291   -0.60886
  -0.60417   -0.59780   -0.59270   -0.58074   -0.56261   -0.55668
  -0.54407   -0.53172   -0.51797   -0.51161   -0.49986   -0.49822
  -0.49190   -0.48868   -0.45878   -0.42261   -0.39364   -0.35194
  -0.34317   -0.31761   -0.29545    0.11597    0.13523    0.14319
   0.14993    0.20515    0.22854    0.26421    0.27158    0.27366
   0.30332

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -5.446600E-04   7.880534E-04   1.297253E-03
  2    C1     -5.435400E-03  -1.049776E-03   2.999012E-03
  3    C2      4.478573E-03  -2.835526E-03  -6.031144E-03
  4    C3      3.212665E-03  -7.577126E-03  -5.571894E-03
  5    C4     -1.826432E-03  -4.195605E-03   7.457676E-04
  6    C5      2.102396E-03   1.035963E-02   2.255916E-03
  7    C6      9.634430E-03  -4.229946E-04  -2.295816E-03
  8    C7     -9.737597E-03   5.699590E-05   4.582115E-03
  9    H27    -6.248824E-04   2.543975E-03   1.906953E-03
 10    H28     1.605915E-03   1.513637E-03  -1.527714E-03
 11    H30     1.225194E-03  -1.083930E-03  -7.954251E-05
 12    C8      3.371075E-03  -5.926179E-03   2.093759E-03
 13    H32     3.287684E-04   1.124982E-03  -1.461798E-03
 14    C10    -1.169200E-03  -2.882014E-03   4.949229E-03
 15    N2     -5.817599E-03   5.154640E-03  -3.396375E-03
 16    C9      6.715913E-03   8.767624E-03  -5.829239E-03
 17    O1     -7.752344E-03  -7.262822E-03   4.632863E-03
 18    H43    -1.695549E-03   2.055091E-03  -1.453159E-03
 19    C12     1.774907E-02   2.108244E-04  -1.368592E-02
 20    C11    -3.571170E-04   4.062189E-03   1.119940E-03
 21    C18    -2.722761E-04  -5.816456E-05   8.495130E-04
```

```
  22    H48     2.842508E-03  -5.378488E-03   8.125043E-04
  23    C13     2.695179E-02  -3.128174E-03  -1.536489E-02
  24    C14     1.303056E-02  -4.343415E-03   8.254450E-03
  25    C15    -2.218065E-02   3.224380E-03   8.018107E-03
  26    C16    -2.539191E-02   3.994415E-03   1.021359E-02
  27    C17    -5.081644E-03   4.352504E-03  -1.069758E-02
  28    H51    -3.566703E-04  -7.982258E-04   3.141351E-03
  29    H52    -3.004852E-03  -4.070973E-03   1.737877E-02
  30    H55     3.587132E-03   1.806803E-03  -1.207281E-02
  31    H56    -1.913011E-02  -8.545229E-04   2.213306E-02
  32    H59     1.303493E-02  -4.972567E-05  -1.594403E-02
  33    H60    -4.745138E-04  -2.246115E-04  -1.371216E-03
  34    H61    -8.771957E-04   5.493146E-04  -1.386751E-03
  35    H62     2.483237E-03   2.514453E-03   1.692826E-04
 -----------   -------------  -------------  -------------
    total       6.235645E-04   9.372408E-04  -6.164639E-04

  end of program der1b


  start of program geopt   5

  geometry optimization step  5
  [ turning on trust-radius adjustment ]
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  ** restarting optimization from step    3 **

  Hessian eigenvalues:
   -1.32449E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    1.25045E-02    1.73061E-02    2.16834E-02
    2.72948E-02    2.76707E-02    2.96060E-02    3.01889E-02    3.06678E-02
    3.36791E-02    3.64777E-02    4.38813E-02    4.64837E-02    5.68619E-02
    6.65191E-02    7.04141E-02    7.11481E-02    7.37975E-02    7.50855E-02
    8.17991E-02    9.72929E-02    1.11692E-01    1.15875E-01    1.19094E-01
    1.28909E-01    1.34189E-01    1.35981E-01    1.38896E-01    1.44744E-01
    1.53977E-01    1.58229E-01    1.60966E-01    1.64169E-01    1.70004E-01
    1.82336E-01    1.92159E-01    1.95751E-01    1.99271E-01    2.07429E-01
    2.12606E-01    2.15941E-01    2.20481E-01    2.21728E-01    2.29545E-01
    2.31196E-01    2.38891E-01    2.47233E-01    2.49505E-01    2.54425E-01
    2.65228E-01    2.75089E-01    2.81418E-01    2.83117E-01    2.89231E-01
    2.96249E-01    2.97967E-01    3.05576E-01    3.09674E-01    3.13737E-01
    3.16549E-01    3.20642E-01    3.29019E-01    3.30652E-01    3.33851E-01
    3.34377E-01    3.35924E-01    3.36984E-01    3.38274E-01    3.40689E-01
    3.45686E-01    3.49765E-01    3.51771E-01    3.57347E-01    3.62244E-01
    3.65372E-01    3.70015E-01    3.76615E-01    3.86323E-01    3.97235E-01
    4.00359E-01    4.13350E-01    4.20937E-01    4.25994E-01    4.31167E-01
    4.36495E-01    4.48196E-01    4.57905E-01    4.67971E-01    4.77903E-01
    4.93926E-01    5.17783E-01    5.36830E-01    5.62052E-01    6.01832E-01
    6.21762E-01    6.78905E-01    7.07511E-01    9.55830E-01    1.05330E+00

  WARNING: Hessian has wrong number of negative eigenvalues
  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.1500346
   Cos(theta):   0.4789360

   Final level shift:  -1.0201793E-02

  energy change:           6.8842E-03 .  (  5.0000E-05 )
  gradient maximum:        1.1892E-02 .  (  4.5000E-04 )
  gradient rms:            2.1714E-03 .  (  3.0000E-04 )
  step size:   0.15003  trust radius:   0.15000
  displacement maximum:    5.7121E-02 .  (  1.8000E-03 )
  displacement rms:        1.3419E-02 .  (  1.2000E-03 )
  predicted energy change:    -9.8703E-04    geom step:   1.5003E-01    full step:
1.5003E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1102E-16     y:     1.4311E-16     z:    -4.4409E-16

  new geometry:
                               angstroms
  atom            x                  y                  z
  H25       1.1319148883     -3.9952023943     -2.0201534455
  C1        1.6079073375     -3.0322747334     -2.0460887098
  C2        2.8767942829     -0.5008728346     -2.1380186353
  C3        1.2154586647     -2.0198748680     -1.1806074836
  C4        2.6239721541     -2.7736024371     -2.9427220071
  C5        3.2535561867     -1.5219392622     -2.9868950915
  C6        1.8585563093     -0.7735507468     -1.2494420811
  C7        0.2049904068     -1.9321922082     -0.1208563513
  H27       2.9388530842     -3.5439899735     -3.6185506418
  H28       4.0422896680     -1.3540954933     -3.6917786088
  H30       3.3374145292      0.4663934420     -2.1457755513
  C8        0.2749769944     -0.6907197285      0.3773695844
  H32      -0.4658126767     -2.7076886336      0.1732915850
  C10      -0.3858147706      0.2182821505      1.3888253953
  N2        1.2708329236      0.0293390265     -0.2887105241
  C9        1.4984390506      1.2975833189      0.1913462254
  O1        2.3211273174      2.0783670041     -0.2403101446
  H43      -0.4101933121     -0.2512601125      2.3625103070
  C12      -1.8006500292      0.5897401563      0.9735563977
  C11       0.5724399823      1.4566684287      1.4095955328
  C18       1.4637981101      1.4747267378      2.6753465127
  H48       0.0210232667      2.3844395070      1.3273763949
  C13      -3.3599914883      1.3436124963     -0.7031044180
  C14      -4.1094011645      0.9537823114      1.5413821162
  C15      -4.3798588447      1.3368575422      0.2369986575
  C16      -2.8236048606      0.5831930164      1.9069252016
  C17      -2.0811501906      0.9710896558     -0.3374331337
  H51      -5.3716412401      1.6235152351     -0.0471983799
  H52      -2.6214655456      0.2916479169      2.9236197431
  H55      -3.5635633466      1.6319577298     -1.7180613134
  H56      -4.8910870142      0.9444022877      2.2757250750
  H59      -1.2995748955      0.9598940697     -1.0730616392
  H60       1.9996171174      0.5359392808      2.7735200907
  H61       0.8574946359      1.6233019043      3.5623098190
  H62       2.1818653741      2.2786190415      2.6066830579

  nuclear repulsion energy.......  1452.008131448 hartrees
  --------------------------------------------------
 /  end of geometry optimization iteration   5   /
 --------------------------------------------------
 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.220E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     98     98     98     99     90     92
 grid # 3      224    183    183    194    182    182    187    182
 grid # 4      224    380    383    404    379    379    372    378

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     85     73     81    100     77
 grid # 2      106    106    105     91    106     92    108     80
 grid # 3      224    224    220    189    223    175    223    167
 grid # 4      224    224    218    376    229    350    402    331

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      111     69     90     81     71     70     89     87
 grid # 2      127     98    105     91     75    100    100     99
 grid # 3      271    208    191    174    141    217    183    183
 grid # 4      474    201    404    352    308    208    380    380

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1       89     87     86     73     73     73     73     71
 grid # 2      100    100     97    106    104    106    106    100
 grid # 3      183    181    181    224    215    224    224    216
 grid # 4      380    378    376    224    214    224    224    212

 number of gridpoints:
    atom       H60    H61    H62  total
 grid # 1       71     71     71   2824
 grid # 2       99     99     99   3486
 grid # 3      216    218    220   7032
 grid # 4      217    220    221  10850

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
```

```
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.13249458025           5.4E-04  1.3E-02
etot   2  Y  Y  6  M  -815.14037000515  7.9E-03  1.6E-04  5.4E-03
etot   3  N  Y  2  U  -815.14179494739  1.4E-03  6.4E-05  1.9E-03
etot   4  Y  Y  6  M  -815.14193779473  1.4E-04  2.7E-05  7.7E-04
etot   5  Y  Y  6  M  -815.14193886741  1.1E-06  1.0E-05  2.3E-04
etot   6  Y  Y  6  M  -815.14194207983  3.2E-06  4.7E-06  6.5E-05
etot   7  Y  N  6  M  -815.14194132284 -7.6E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1452.00813144791
   (E)  Total one-electron terms..... -3989.53425604140
   (I)  Total two-electron terms.....  1722.38418327065
   (L)  Electronic energy............ -2267.15007277075  (E+I)
   (N)  Total energy.................  -815.14194132284  (A+L)

 SCFE: SCF energy: HF    -815.14194132284 hartrees   iterations:   7


 HOMO energy:    -0.29727
 LUMO energy:     0.11654

  Orbital energies:
  -20.45247  -15.55277  -11.32255  -11.23604  -11.22291  -11.21325
  -11.20784  -11.20010  -11.18842  -11.18572  -11.18522  -11.18427
  -11.18258  -11.18244  -11.17966  -11.17827  -11.17805  -11.17711
  -11.17619  -11.17304   -1.42035   -1.33268   -1.18004   -1.16230
   -1.11570   -1.08827   -1.04029   -1.02650   -1.01978   -0.99961
   -0.94625   -0.90563   -0.85601   -0.84304   -0.82941   -0.81235
   -0.79374   -0.76273   -0.72048   -0.68641   -0.67937   -0.66874
   -0.65881   -0.64143   -0.63752   -0.62643   -0.61237   -0.60559
   -0.60404   -0.59846   -0.59123   -0.57782   -0.56109   -0.55337
   -0.54153   -0.53030   -0.51715   -0.50859   -0.49804   -0.49706
   -0.49052   -0.48653   -0.45833   -0.42146   -0.39424   -0.34883
   -0.34076   -0.31562   -0.29727    0.11654    0.13318    0.14260
    0.14376    0.20396    0.22821    0.26206    0.27075    0.27176
    0.30311

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:   4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x               y               z
 ----  -----   -------------  -------------  -------------
   1    H25     7.747019E-04   1.904519E-03   2.594765E-04
   2    C1     -1.208524E-03  -8.124640E-04   8.118747E-04
  3    C2       1.354522E-03  -3.515997E-04  -1.207683E-03
  4    C3      -5.754820E-04   1.298334E-03   1.713634E-03
  5    C4       2.288511E-03   2.179123E-03  -1.252558E-03
  6    C5      -1.744485E-04  -1.804911E-03  -6.397508E-04
  7    C6      -1.227053E-03  -5.478507E-04   1.747031E-04
  8    C7      -6.840593E-04   4.288574E-04  -4.824150E-04
  9    H27      4.289887E-04   6.674360E-04  -6.510642E-05
 10    H28      1.380576E-04  -3.597287E-04  -5.461356E-04
 11    H30     -3.763603E-04  -1.376703E-03  -1.991947E-04
 12    C8      -2.047190E-05   2.600972E-03   3.093738E-04
 13    H32      5.516610E-04   6.393803E-04  -2.433821E-04
 14    C10      3.965256E-04  -2.348018E-03  -1.487111E-03
 15    N2      -2.167766E-04  -2.238442E-03   9.730863E-04
 16    C9       3.844545E-03   4.398095E-03  -1.067445E-03
 17    O1      -5.680797E-03  -5.926880E-03   2.913074E-03
 18    H43     -2.309548E-06   4.456487E-04   1.810999E-04
 19    C12     -1.030944E-04   9.254577E-04  -2.595683E-03
 20    C11      1.877877E-03   1.845650E-03   1.187967E-03
 21    C18     -2.172053E-03  -3.357024E-04  -1.213236E-03
 22    H48      1.317023E-03  -1.923954E-03   3.201899E-04
 23    C13      4.242615E-05  -2.335291E-04   1.994640E-05
 24    C14     -8.646975E-04   1.247493E-03  -1.858395E-03
 25    C15      4.461087E-04  -9.802746E-04   3.081836E-03
 26    C16     -2.991888E-04   3.397447E-04   7.103576E-04
 27    C17      1.798212E-03  -1.036384E-03   1.436318E-03
 28    H51     -7.577919E-04   5.017058E-05   2.884158E-04
 29    H52     -6.447834E-04   4.260149E-04  -2.830483E-03
 30    H55      4.425220E-04  -4.616190E-04   2.115918E-03
 31    H56     -1.373898E-04   3.560104E-05  -8.699426E-04
 32    H59     -7.445995E-04   5.800883E-05   9.968819E-04
 33    H60     -4.061800E-04   7.724796E-04  -3.832955E-04
 34    H61      3.921711E-05  -1.043718E-04  -1.052892E-03
 35    H62      1.411908E-03   1.184403E-03  -1.346527E-04
-----------   -------------  -------------  -------------
   total        8.567458E-04   6.049555E-04  -6.352097E-04

 end of program der1b


 start of program geopt   6

 geometry optimization step   6
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.75629E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.25210E-02    1.69275E-02    2.22577E-02
   2.76729E-02    2.83528E-02    2.98744E-02    3.05711E-02    3.11340E-02
   3.35441E-02    3.75558E-02    4.42658E-02    4.56072E-02    5.72854E-02
   6.53778E-02    7.05571E-02    7.19937E-02    7.33143E-02    7.56005E-02
   8.05529E-02    9.78298E-02    1.11669E-01    1.13692E-01    1.18946E-01
   1.26842E-01    1.31223E-01    1.37120E-01    1.43005E-01    1.43950E-01
   1.54000E-01    1.57856E-01    1.62747E-01    1.64286E-01    1.76643E-01
```

```
    1.83652E-01    1.92910E-01    1.95417E-01    2.00500E-01    2.08382E-01
    2.08947E-01    2.17425E-01    2.21502E-01    2.25092E-01    2.29146E-01
    2.34610E-01    2.38731E-01    2.43569E-01    2.47642E-01    2.54524E-01
    2.66049E-01    2.73272E-01    2.81773E-01    2.83327E-01    2.89158E-01
    2.97259E-01    2.99377E-01    3.04732E-01    3.10406E-01    3.17168E-01
    3.20911E-01    3.22358E-01    3.29467E-01    3.30684E-01    3.33661E-01
    3.34442E-01    3.35906E-01    3.38650E-01    3.40429E-01    3.45705E-01
    3.47062E-01    3.52498E-01    3.59094E-01    3.59497E-01    3.65692E-01
    3.67622E-01    3.75160E-01    3.81210E-01    3.89566E-01    4.01901E-01
    4.12641E-01    4.20371E-01    4.22796E-01    4.30466E-01    4.38909E-01
    4.42857E-01    4.59071E-01    4.60990E-01    4.77834E-01    4.86711E-01
    5.00035E-01    5.36259E-01    5.40626E-01    5.83078E-01    6.03741E-01
    6.17135E-01    6.74308E-01    7.17611E-01    9.83182E-01    1.07888E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0750400
   Cos(theta):   0.6554389

   Final level shift:  -2.9129815E-02

  energy change:           -5.5940E-04 .  (  5.0000E-05 )
  gradient maximum:         8.7402E-03 .  (  4.5000E-04 )
  gradient rms:             1.4782E-03 .  (  3.0000E-04 )
  step size:   0.07504  trust radius:   0.07500
  displacement maximum:     2.6578E-02 .  (  1.8000E-03 )
  displacement rms:         6.7118E-03 .  (  1.2000E-03 )
  predicted energy change:    -4.8845E-04    geom step:   7.5040E-02    full step:
7.5040E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -4.0348E-03     y:    -1.8733E-03     z:    -3.5063E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       1.1560329223     -3.9972038998     -2.0044562312
  C1        1.6272786794     -3.0369148798     -2.0364735734
  C2        2.8958510944     -0.5173544999     -2.1388127943
  C3        1.2158803634     -2.0217859397     -1.1845242374
  C4        2.6622322427     -2.7865641372     -2.9235101750
  C5        3.2899885671     -1.5407776708     -2.9751501301
  C6        1.8609166934     -0.7795119672     -1.2569835230
  C7        0.1905468410     -1.9282325128     -0.1386831431
  H27       2.9923294849     -3.5608649346     -3.5857702898
  H28       4.0898167324     -1.3796167796     -3.6724541898
  H30       3.3566831296      0.4471980857     -2.1490926784
  C8        0.2655736872     -0.6884272487      0.3632969120
  H32      -0.4825753148     -2.7014887488      0.1527406400
  C10      -0.3903931990      0.2177451769      1.3768801718
  N2        1.2654786297      0.0245953099     -0.3003898058
  C9        1.4923485416      1.2929298421      0.1776985656
  O1        2.3068647038      2.0681855882     -0.2615666360
  H43      -0.4118518307     -0.2479845041      2.3523491537
  C12      -1.8074994974      0.5954454466      0.9713218842
  C11       0.5732111375      1.4560970852      1.3958454979
  C18       1.4663958511      1.4828942571      2.6535863635
  H48       0.0244131452      2.3808417223      1.3146866819
  C13      -3.3712112003      1.3910387723     -0.6650920049
```

```
 C14      -4.1241345771      0.9347014188      1.5573642450
 C15      -4.3948203852      1.3534191201      0.2727318205
 C16      -2.8345998460      0.5593610209      1.9032497415
 C17      -2.0882223209      1.0127543995     -0.3197327670
 H51      -5.3889952411      1.6440309849     -0.0015676919
 H52      -2.6333451649      0.2322706236      2.9043495310
 H55      -3.5756674855      1.7114247886     -1.6657628759
 H56      -4.9072762347      0.8958720068      2.2885914013
 H59      -1.3090154970      1.0298008285     -1.0538280362
 H60       2.0000025899      0.5447709259      2.7538154741
 H61       0.8618012429      1.6365620858      3.5391552487
 H62       2.1902032380      2.2855731881      2.5787426072

 nuclear repulsion energy.......  1451.863060005 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   6   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.220E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     84     85
 grid # 2       106    100     97     98     98     98     90     92
 grid # 3       224    183    183    194    182    182    187    183
 grid # 4       224    378    380    406    379    379    372    377

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     85     73     81    100     76
 grid # 2       106    106    105     91    106     91    108     81
 grid # 3       224    224    220    189    223    176    223    165
 grid # 4       224    224    219    375    229    352    402    326

 number of gridpoints:
    atom         O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1       111     69     91     82     71     70     85     87
 grid # 2       123     98    106     91     78    101    100     99
 grid # 3       271    208    191    175    150    217    183    183
 grid # 4       474    203    398    352    305    209    379    379

 number of gridpoints:
    atom        C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1        88     86     86     73     73     73     73     71
 grid # 2        99     99     98    106    104    106    106    101
 grid # 3       183    182    181    224    214    224    224    216
 grid # 4       379    377    376    224    214    224    224    213

 number of gridpoints:
     atom        H60     H61     H62  total
  grid # 1        71      71      71   2818
  grid # 2        99      99      99   3485
  grid # 3       216     218     220   7042
  grid # 4       217     220     221  10834

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  1  U  -815.13894652292            2.4E-04  7.4E-03
etot   2  Y  Y  4  M  -815.14148871686  2.5E-03  1.0E-04  3.1E-03
etot   3  Y  Y  4  M  -815.14180626252  3.2E-04  3.5E-05  1.0E-03
etot   4  N  Y  1  U  -815.14183282696  2.7E-05  1.3E-05  3.1E-04
etot   5  Y  Y  4  M  -815.14183897215  6.1E-06  5.9E-06  8.9E-05
etot   6  Y  Y  4  M  -815.14183714495 -1.8E-06  2.0E-06  2.9E-05
etot   7  Y  N  4  M  -815.14183878410  1.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1451.86306000473
   (E)  Total one-electron terms..... -3989.21962866864
   (I)  Total two-electron terms.....  1722.21472987980
   (L)  Electronic energy............ -2267.00489878883  (E+I)
   (N)  Total energy.................  -815.14183878410  (A+L)

 SCFE: SCF energy: HF    -815.14183878410 hartrees   iterations:   7


 HOMO energy:    -0.29759
 LUMO energy:     0.11735

  Orbital energies:
  -20.45239  -15.55202  -11.32125  -11.23602  -11.22309  -11.21352
  -11.20676  -11.19963  -11.18787  -11.18502  -11.18435  -11.18373
  -11.18187  -11.18161  -11.17928  -11.17794  -11.17770  -11.17707
  -11.17569  -11.17257   -1.42458   -1.33340   -1.18087   -1.16250
   -1.11623   -1.08803   -1.04122   -1.02673   -1.01859   -1.00091
   -0.94724   -0.90523   -0.85680   -0.84369   -0.83042   -0.81114
   -0.79427   -0.76289   -0.72142   -0.68760   -0.67960   -0.66938
   -0.65920   -0.64205   -0.63831   -0.62741   -0.61136   -0.60668
   -0.60285   -0.59976   -0.59215   -0.57736   -0.56219   -0.55442
   -0.54290   -0.53061   -0.51733   -0.50898   -0.49853   -0.49682
   -0.49057   -0.48686   -0.45902   -0.42126   -0.39338   -0.34851
   -0.34197   -0.31489   -0.29759    0.11735    0.13410    0.14275
    0.14361    0.20495    0.22793    0.26272    0.27164    0.27219
    0.30312

  end of program scf
 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -3.549107E-04  -1.312481E-03  -4.654371E-04
  2    C1      2.948128E-03   3.125256E-05  -2.393555E-03
  3    C2     -2.191822E-03   1.414811E-03   2.699114E-03
  4    C3      9.566401E-05   1.682390E-04  -1.107856E-03
  5    C4     -3.138413E-03  -2.127188E-03   1.662089E-03
  6    C5     -7.521934E-05   5.915997E-04   4.453554E-04
  7    C6      2.166193E-03   1.016054E-03  -1.178001E-03
  8    C7      5.389452E-04  -9.207757E-04   4.121693E-04
  9    H27    -4.009994E-04  -9.243191E-04  -6.372168E-05
 10    H28    -1.113595E-03  -8.504971E-05   9.129198E-04
 11    H30     3.161922E-05   5.313021E-04   2.126557E-04
 12    C8     -4.153228E-04   2.334546E-04  -2.032891E-03
 13    H32     9.796271E-05   5.056365E-05  -2.010776E-04
 14    C10     1.580185E-04   1.271610E-04   7.776333E-04
 15    N2      1.005126E-03  -5.311359E-04   5.106032E-04
 16    C9     -1.633117E-03  -9.966820E-04   1.329665E-04
 17    O1      2.531581E-03   1.943990E-03  -3.737449E-04
 18    H43     2.803865E-04  -3.453601E-04   1.793967E-05
 19    C12    -6.795762E-04  -5.949400E-04   4.767986E-03
 20    C11     3.256853E-04   2.705185E-04  -2.340315E-04
 21    C18     7.037454E-05   2.066673E-04  -1.018867E-04
 22    H48    -3.852887E-04   5.383440E-04  -4.154939E-04
 23    C13    -1.125490E-03   3.415054E-04  -4.621396E-04
 24    C14     1.646764E-03  -1.019525E-03   2.303743E-03
 25    C15     6.057403E-04   9.784646E-04  -4.082322E-03
 26    C16     1.406231E-03  -8.081192E-04   5.681943E-04
 27    C17    -2.291026E-03   1.044472E-03  -1.566749E-03
 28    H51     8.434672E-05   1.534609E-04  -5.228658E-04
 29    H52     4.621364E-04  -1.711185E-04   6.174486E-04
 30    H55    -4.334671E-04   3.206865E-04  -1.050266E-03
 31    H56     4.839442E-04  -5.399322E-05   1.468778E-04
 32    H59     2.006905E-04   1.296257E-04  -1.021161E-03
 33    H60     3.005795E-04  -1.594849E-04   3.052648E-04
 34    H61     6.570786E-05   1.872377E-04   9.834622E-05
 35    H62    -5.966926E-04  -2.459358E-04  -8.745436E-05
-----------   -------------  -------------  -------------
   total       6.708852E-04  -1.669732E-05  -7.693460E-04

 end of program der1b


 start of program geopt   7
 geometry optimization step  7
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -2.87940E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.28498E-02    1.68181E-02    2.22253E-02
   2.76269E-02    2.82155E-02    2.99068E-02    3.05349E-02    3.09858E-02
   3.52391E-02    3.75216E-02    4.39536E-02    4.75793E-02    5.71716E-02
   6.50410E-02    7.14085E-02    7.16572E-02    7.46379E-02    7.60955E-02
   8.34621E-02    9.73583E-02    1.13165E-01    1.13620E-01    1.18176E-01
   1.26811E-01    1.30701E-01    1.36730E-01    1.42882E-01    1.48172E-01
   1.53443E-01    1.58627E-01    1.62482E-01    1.68776E-01    1.74496E-01
   1.82894E-01    1.90762E-01    1.94003E-01    1.99691E-01    2.01869E-01
   2.14197E-01    2.17131E-01    2.21420E-01    2.24942E-01    2.28435E-01
   2.34003E-01    2.37765E-01    2.42714E-01    2.47213E-01    2.53769E-01
   2.64928E-01    2.71708E-01    2.77723E-01    2.81706E-01    2.91395E-01
   2.98189E-01    3.00932E-01    3.07917E-01    3.10045E-01    3.17239E-01
   3.19863E-01    3.26661E-01    3.28139E-01    3.32109E-01    3.33026E-01
   3.34130E-01    3.36906E-01    3.40298E-01    3.40774E-01    3.44926E-01
   3.49462E-01    3.56288E-01    3.59335E-01    3.66036E-01    3.67857E-01
   3.75477E-01    3.80370E-01    3.87294E-01    3.95558E-01    4.05120E-01
   4.09901E-01    4.19847E-01    4.26548E-01    4.33150E-01    4.42557E-01
   4.51023E-01    4.51733E-01    4.73814E-01    4.78411E-01    4.97484E-01
   5.16876E-01    5.33545E-01    5.52741E-01    5.84148E-01    5.93832E-01
   6.06656E-01    6.98813E-01    7.20989E-01    9.78238E-01    1.05514E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0379720
  Cos(theta):   0.7137646

  Final level shift:  -5.5871828E-02

 energy change:           1.0254E-04 .  (  5.0000E-05 )
 gradient maximum:        4.9000E-03 .  (  4.5000E-04 )
 gradient rms:            1.2789E-03 .  (  3.0000E-04 )
 step size:   0.03797  trust radius:   0.03750
 displacement maximum:    1.2543E-02 .  (  1.8000E-03 )
 displacement rms:        3.3963E-03 .  (  1.2000E-03 )
 predicted energy change:    -2.3405E-04    geom step:   3.7972E-02    full step:
3.7972E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     5.0912E-03     y:    -1.3135E-03     z:     2.5471E-03

 new geometry:
                               angstroms
 atom            x                 y                 z
 H25       1.1304575483     -3.9921035851     -2.0223686483
 C1        1.6103546161     -3.0340223526     -2.0479919874
 C2        2.8956938390     -0.5173166812     -2.1328629754
 C3        1.2107530960     -2.0192079694     -1.1878484086
 C4        2.6403057120     -2.7853816590     -2.9355106972
 C5        3.2763198195     -1.5408089242     -2.9777529598
 C6        1.8642016527     -0.7793227516     -1.2524394351
 C7        0.1884690164     -1.9244233447     -0.1395088531
 H27       2.9602461201     -3.5583927620     -3.6047953603
 H28       4.0724961332     -1.3804314230     -3.6765582871
 H30       3.3635227961      0.4449102599     -2.1381457079
 C8        0.2673971942     -0.6849857375      0.3633679125
 H32      -0.4899649017     -2.6948834938      0.1480698793
 C10      -0.3871247045      0.2217244711      1.3780689010
 N2        1.2733971810      0.0250112506     -0.2941141098
 C9        1.5052068394      1.2915174966      0.1870810776
 O1        2.3290656544      2.0634864919     -0.2439244126
 H43      -0.4059057206     -0.2450768510      2.3531839185
 C12      -1.8049107586      0.5967079428      0.9729449283
 C11       0.5764813534      1.4606745919      1.3973271674
 C18       1.4584461100      1.4976634528      2.6623521684
 H48       0.0265433002      2.3842861566      1.3063064802
 C13      -3.3717927552      1.3800084771     -0.6758632669
 C14      -4.1197352771      0.9286289624      1.5519935533
 C15      -4.3934752658      1.3414062776      0.2619192622
 C16      -2.8299413023      0.5589892031      1.9042785285
 C17      -2.0882920786      1.0086508593     -0.3236899923
 H51      -5.3894168668      1.6255825028     -0.0141532133
 H52      -2.6280396446      0.2346686876      2.9061398439
 H55      -3.5778302639      1.6942319322     -1.6787475128
 H56      -4.9034454704      0.8890892561      2.2823975416
 H59      -1.3084314624      1.0236122911     -1.0581471708
 H60       1.9926736480      0.5611298974      2.7758150110
 H61       0.8458662596      1.6582721173      3.5416060184
 H62       2.1803557495      2.3012179601      2.5869501030

 nuclear repulsion energy.......  1451.630424855 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration   7   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.220E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     97     98     98     99     90     92
 grid # 3      224    183    183    194    182    182    187    183
 grid # 4      224    379    382    406    379    379    373    377

 number of gridpoints:
     atom        H27     H28     H30      C8     H32     C10      N2      C9
  grid # 1        73      73      73      85      73      81     100      76
  grid # 2       106     106     105      91     106      92     108      81
  grid # 3       224     224     220     189     223     176     223     165
  grid # 4       224     224     219     374     229     351     401     327

  number of gridpoints:
     atom         O1     H43     C12     C11     C18     H48     C13     C14
  grid # 1       111      69      90      82      72      70      88      87
  grid # 2       123      98     105      91      74     101     100     100
  grid # 3       272     208     191     175     141     217     183     183
  grid # 4       474     201     400     353     306     209     379     379

  number of gridpoints:
     atom        C15     C16     C17     H51     H52     H55     H56     H59
  grid # 1        89      87      86      73      73      73      73      71
  grid # 2       100     100      97     106     104     106     106     101
  grid # 3       183     182     181     224     214     224     224     216
  grid # 4       379     377     376     224     214     224     224     213

  number of gridpoints:
     atom        H60     H61     H62   total
  grid # 1        71      71      71    2824
  grid # 2        99      99      99    3484
  grid # 3       217     218     220    7035
  grid # 4       217     220     221   10838

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                      RMS    maximum
       e  d  i  u  i                            energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14145440966           1.2E-04  2.5E-03
etot   2  Y  Y  4  M  -815.14195316309  5.0E-04  4.2E-05  8.6E-04
etot   3  Y  Y  4  M  -815.14201092146  5.8E-05  1.4E-05  3.0E-04
etot   4  Y  Y  4  M  -815.14201703015  6.1E-06  4.9E-06  8.7E-05
etot   5  Y  N  4  M  -815.14201598780 -1.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1451.63042485522
   (E)  Total one-electron terms..... -3988.76080780577
   (I)  Total two-electron terms.....  1721.98836696276
   (L)  Electronic energy............ -2266.77244084302  (E+I)
   (N)  Total energy.................  -815.14201598780  (A+L)

 SCFE: SCF energy: HF    -815.14201598780 hartrees   iterations:   5


 HOMO energy:    -0.29705
 LUMO energy:     0.11717
 Orbital energies:
 -20.45246  -15.55228  -11.32161  -11.23593  -11.22288  -11.21347
 -11.20686  -11.19990  -11.18803  -11.18516  -11.18468  -11.18390
 -11.18226  -11.18207  -11.17923  -11.17786  -11.17761  -11.17704
 -11.17571  -11.17252   -1.42383   -1.33339   -1.18044   -1.16235
  -1.11604   -1.08798   -1.04101   -1.02669   -1.01949   -1.00018
  -0.94682   -0.90544   -0.85640   -0.84360   -0.83008   -0.81170
  -0.79418   -0.76269   -0.72113   -0.68763   -0.67952   -0.66924
  -0.65909   -0.64197   -0.63817   -0.62708   -0.61186   -0.60637
  -0.60360   -0.59929   -0.59188   -0.57736   -0.56180   -0.55417
  -0.54247   -0.53056   -0.51726   -0.50880   -0.49842   -0.49675
  -0.49058   -0.48676   -0.45896   -0.42142   -0.39357   -0.34852
  -0.34165   -0.31535   -0.29705    0.11717    0.13380    0.14261
   0.14385    0.20469    0.22800    0.26291    0.27131    0.27218
   0.30303

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x             y             z
----  -----   -------------  -------------  -------------
  1    H25     1.359723E-05  -3.466478E-05  -9.627447E-05
  2    C1      6.984586E-05  -8.738348E-05   1.093295E-04
  3    C2     -1.319643E-04  -1.656861E-04  -1.037726E-05
  4    C3      2.655846E-04   1.622017E-05  -4.230537E-04
  5    C4     -5.586107E-04   3.924010E-04   4.933160E-04
  6    C5     -2.069762E-04   1.709694E-04   4.202626E-04
  7    C6     -6.852514E-05  -1.981003E-04  -1.924660E-04
  8    C7     -1.093526E-04  -2.980572E-04  -2.523597E-04
  9    H27     4.660699E-05  -1.978032E-04  -1.606840E-04
 10    H28     4.669475E-05   4.338915E-05  -6.914025E-05
 11    H30    -8.643284E-05  -2.657687E-04  -6.115228E-05
 12    C8     -1.886639E-04   4.370352E-04  -6.357514E-04
 13    H32     2.428191E-04   2.785829E-04  -1.475581E-04
 14    C10     5.081719E-04  -7.293809E-05   2.757845E-04
 15    N2      5.079031E-04  -1.008795E-03   4.313145E-04
 16    C9     -6.598653E-04   1.170071E-04  -3.315036E-04
 17    O1      1.019859E-03   2.695101E-04   1.838224E-04
 18    H43     1.738924E-05  -2.308942E-04   1.984537E-05
 19    C12    -1.990921E-04   2.702134E-04   6.734142E-04
 20    C11     3.195800E-05   4.399625E-05  -2.540453E-04
 21    C18    -3.068506E-04   1.003346E-04   1.684667E-04
 22    H48    -1.744972E-04   3.764032E-04  -5.523677E-04
 23    C13     2.007050E-04  -1.303334E-04   4.827240E-04
 24    C14     2.046691E-04  -2.081235E-04   1.992330E-04
 25    C15     1.416486E-04   5.121125E-05  -1.482842E-04
 26    C16    -1.503977E-04  -1.279791E-04  -5.156088E-04
 27    C17    -6.621979E-04   1.208096E-04   2.363045E-05
 28    H51     2.143096E-04   1.999889E-05  -3.413987E-05
 29    H52     1.716950E-04  -7.173134E-06   6.103983E-04
 30    H55    -3.052410E-05   1.383420E-04  -6.379178E-04
 31    H56     1.587479E-04   5.936810E-05   3.700326E-05
 32    H59     1.189039E-04   1.250673E-04  -4.216355E-04
 33    H60     2.160504E-04   1.988591E-05   1.999422E-04
 34    H61     1.747293E-04   5.555274E-05  -6.674281E-05
 35    H62    -1.577312E-04  -5.750897E-05  -5.049632E-05
-----------   -------------  -------------  -------------
   total       6.802065E-04   1.508895E-05  -7.330719E-04

 end of program der1b


 start of program geopt   8

 geometry optimization step  8
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -2.84991E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.16747E-02    1.66619E-02    2.18108E-02
   2.77488E-02    2.82930E-02    2.99327E-02    3.06019E-02    3.10905E-02
   3.55518E-02    3.76366E-02    4.40449E-02    4.74103E-02    5.73189E-02
   6.47717E-02    7.12975E-02    7.17910E-02    7.47763E-02    7.58519E-02
   8.40352E-02    9.71205E-02    1.12824E-01    1.13260E-01    1.18101E-01
   1.26076E-01    1.30728E-01    1.37144E-01    1.42724E-01    1.48315E-01
   1.54579E-01    1.58912E-01    1.62220E-01    1.72879E-01    1.74848E-01
   1.82750E-01    1.90712E-01    1.92131E-01    1.97594E-01    2.01027E-01
   2.14666E-01    2.16803E-01    2.20894E-01    2.25450E-01    2.28071E-01
   2.34154E-01    2.36386E-01    2.41536E-01    2.46640E-01    2.53741E-01
   2.64441E-01    2.70333E-01    2.76460E-01    2.81568E-01    2.91083E-01
   2.97838E-01    3.01183E-01    3.08951E-01    3.10872E-01    3.16983E-01
   3.19750E-01    3.25911E-01    3.27597E-01    3.30560E-01    3.33441E-01
   3.34321E-01    3.35622E-01    3.40532E-01    3.41131E-01    3.44604E-01
   3.50231E-01    3.58686E-01    3.60702E-01    3.66193E-01    3.68620E-01
   3.75241E-01    3.80533E-01    3.87468E-01    3.99131E-01    4.08245E-01
   4.13679E-01    4.19971E-01    4.27180E-01    4.31716E-01    4.42599E-01
   4.49823E-01    4.54994E-01    4.67029E-01    4.79115E-01    5.01733E-01
   5.10848E-01    5.44815E-01    5.67088E-01    5.87132E-01    6.03253E-01
   6.20295E-01    7.12092E-01    7.26271E-01    9.78631E-01    1.03972E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:     0.0750360
  Cos(theta):    0.6395471

  Final level shift:  -1.7960771E-02
  energy change:          -1.7720E-04 .  (  5.0000E-05 )
  gradient maximum:        1.5447E-03 .  (  4.5000E-04 )
  gradient rms:            3.7106E-04 .  (  3.0000E-04 )
  step size:   0.07504  trust radius:   0.07500
  displacement maximum:    3.2181E-02 .  (  1.8000E-03 )
  displacement rms:        6.7114E-03 .  (  1.2000E-03 )
  predicted energy change:   -1.5010E-04    geom step:   7.5035E-02   full step:
7.5035E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     8.1731E-03     y:    -5.5014E-03     z:     5.1929E-04

  new geometry:
                                angstroms
  atom            x                 y                 z
  H25        1.1063601647     -3.9870092790     -2.0452324985
  C1         1.5963033244     -3.0332824553     -2.0624581680
  C2         2.9082421845     -0.5277214253     -2.1277649857
  C3         1.2020680045     -2.0180591705     -1.2014906554
  C4         2.6341361679     -2.7892575422     -2.9416721274
  C5         3.2835240845     -1.5504740206     -2.9743891415
  C6         1.8692936381     -0.7844522203     -1.2556322063
  C7         0.1736546567     -1.9165634462     -0.1592266790
  H27        2.9510371809     -3.5622435396     -3.6127502977
  H28        4.0861831249     -1.3945294522     -3.6671583099
  H30        3.3852717326      0.4300307804     -2.1256219085
  C8         0.2621841061     -0.6793939169      0.3486986116
  H32       -0.5142822183     -2.6810989061      0.1215825902
  C10       -0.3869336810      0.2276811268      1.3673784363
  N2         1.2819781155      0.0217669200     -0.2971937505
  C9         1.5269808236      1.2838405642      0.1910019694
  O1         2.3775862481      2.0428190466     -0.2191360938
  H43       -0.3991593459     -0.2423683134      2.3413595320
  C12       -1.8079918129      0.6006504425      0.9725428117
  C11        0.5759100158      1.4678044441      1.3840084778
  C18        1.4315997535      1.5286704387      2.6674593726
  H48        0.0252467188      2.3903207426      1.2654037278
  C13       -3.3843308533      1.3896797026     -0.6634034697
  C14       -4.1209093015      0.9151067508      1.5642827306
  C15       -4.4014578254      1.3375403390      0.2787158627
  C16       -2.8281628251      0.5494031016      1.9081752297
  C17       -2.0981735835      1.0220017306     -0.3196356927
  H51       -5.3995339594      1.6193548036      0.0089282867
  H52       -2.6188504895      0.2183021511      2.9066265597
  H55       -3.5967054701      1.7114671876     -1.6630468274
  H56       -4.9008204062      0.8658707472      2.2972748063
  H59       -1.3206074296      1.0473525944     -1.0563633122
  H60        1.9695248998      0.5968848284      2.8095489974
  H61        0.8009004094      1.7017120169      3.5327472740
  H62        2.1485057528      2.3351986463      2.5922022874

  nuclear repulsion energy.......  1450.522675623 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration   8   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.219E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom       H25     C1     C2     C3     C4     C5     C6     C7
  grid # 1       73     89     87     90     87     87     85     85
  grid # 2      106    100     97     98     98     99     90     92
  grid # 3      224    183    182    194    182    182    187    183
  grid # 4      224    379    382    404    379    379    373    377

  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     85     73     81     99     77
  grid # 2      106    106    105     91    106     92    108     81
  grid # 3      224    224    220    189    223    175    223    167
  grid # 4      224    224    218    375    229    351    401    329

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     68     90     82     72     70     87     87
  grid # 2      127     98    105     91     74    100    100    100
  grid # 3      271    208    190    175    146    217    183    183
  grid # 4      474    202    400    354    309    209    379    379

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     86     86     73     73     73     73     71
  grid # 2      100    100     97    106    104    106    106    101
  grid # 3      183    182    181    224    214    224    224    216
  grid # 4      379    378    376    224    214    224    224    213

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2821
  grid # 2       99     99     99   3487
  grid # 3      217    218    220   7038
  grid # 4      217    221    221  10845

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14007792910           1.9E-04  6.4E-03
etot   2  Y  Y  4  M  -815.14181569357  1.7E-03  7.7E-05  1.7E-03
etot   3  Y  Y  4  M  -815.14200816908  1.9E-04  2.4E-05  5.1E-04
etot   4  Y  Y  4  M  -815.14202093310  1.3E-05  7.1E-06  1.6E-04
etot   5  Y  Y  4  M  -815.14202247037  1.5E-06  3.7E-06  8.3E-05
etot   6  N  N  1  U  -815.14203198333  9.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1450.52267562349
   (E)  Total one-electron terms..... -3986.55076182828
   (I)  Total two-electron terms.....  1720.88605422146
   (L)  Electronic energy............ -2265.66470760682  (E+I)
   (N)  Total energy.................  -815.14203198333  (A+L)

 SCFE: SCF energy: HF    -815.14203198333 hartrees   iterations:   6


 HOMO energy:    -0.29709
 LUMO energy:     0.11720

  Orbital energies:
  -20.45243  -15.55265  -11.32224  -11.23613  -11.22272  -11.21357
  -11.20753  -11.19998  -11.18805  -11.18526  -11.18476  -11.18410
  -11.18244  -11.18225  -11.17920  -11.17785  -11.17769  -11.17683
  -11.17566  -11.17254   -1.42182   -1.33298   -1.18052   -1.16241
   -1.11575   -1.08798   -1.04089   -1.02706   -1.01945   -1.00027
   -0.94661   -0.90552   -0.85598   -0.84374   -0.83025   -0.81169
   -0.79411   -0.76262   -0.72117   -0.68749   -0.67918   -0.66917
   -0.65867   -0.64169   -0.63844   -0.62689   -0.61183   -0.60600
   -0.60374   -0.59983   -0.59177   -0.57722   -0.56106   -0.55404
   -0.54197   -0.53052   -0.51699   -0.50859   -0.49867   -0.49685
   -0.49064   -0.48662   -0.45873   -0.42153   -0.39363   -0.34889
   -0.34173   -0.31519   -0.29709    0.11720    0.13386    0.14187
    0.14388    0.20446    0.22741    0.26321    0.27109    0.27232
    0.30232

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x             y             z
 ----  -----   -------------  -------------  -------------
   1    H25     2.151525E-04   3.452281E-04  -6.647457E-05
   2    C1      1.794360E-04  -1.146222E-04  -3.645931E-04
   3    C2     -1.230370E-05   2.254646E-04   4.319000E-05
   4    C3     -3.025544E-04   8.388521E-04   7.246500E-04
   5    C4      2.202499E-04   2.511949E-04  -1.524686E-04
   6    C5     -1.217790E-04  -8.074701E-04  -1.583113E-04
   7    C6     -2.886297E-04  -6.180385E-04   2.798466E-04
  8    C7      5.580646E-04   1.076805E-03  -4.735068E-04
  9    H27     4.775464E-05  -7.114309E-05  -1.231767E-04
 10    H28    -1.673694E-04  -1.654768E-04  -3.054557E-05
 11    H30    -3.120362E-05  -3.266614E-04   9.920676E-05
 12    C8     -5.646786E-05   2.884200E-04  -3.812072E-04
 13    H32     2.397471E-04   3.502991E-04  -2.095105E-04
 14    C10     4.347537E-04  -2.801396E-04  -2.362437E-04
 15    N2      2.554949E-04   1.417855E-04   1.158685E-04
 16    C9      2.598188E-03   1.512231E-03  -3.135181E-04
 17    O1     -3.220044E-03  -3.015410E-03   1.432737E-03
 18    H43     9.812906E-05   6.500958E-05  -1.883177E-05
 19    C12     2.375540E-04   3.491293E-05   6.577273E-04
 20    C11     2.202340E-04   6.383109E-04  -3.733141E-05
 21    C18    -9.345108E-04  -7.344537E-05   1.779801E-04
 22    H48     4.783621E-04  -8.376759E-04  -1.165117E-04
 23    C13    -1.761107E-04   1.671738E-05   1.887860E-04
 24    C14     2.235509E-04   1.711319E-05  -2.486657E-04
 25    C15    -4.913747E-05   6.777839E-05  -8.447060E-05
 26    C16     2.301537E-04  -1.667323E-04  -3.756136E-04
 27    C17    -2.662000E-04   2.726817E-05   2.184171E-04
 28    H51     3.186343E-06   3.044865E-05  -2.503557E-05
 29    H52     7.541528E-06   3.055187E-05   3.880094E-04
 30    H55     2.138375E-05   4.577399E-05  -2.987936E-04
 31    H56    -2.316066E-04   4.774150E-05   2.720347E-04
 32    H59     1.243942E-04   8.148390E-05  -4.135743E-04
 33    H60    -2.821691E-04   6.983565E-04  -2.630499E-04
 34    H61     3.196842E-04  -1.311751E-04  -8.559559E-04
 35    H62     6.262002E-04   3.445098E-04  -3.637170E-05
-----------   -------------  -------------  -------------
   total       1.199130E-03   5.682665E-04  -6.853084E-04

 end of program der1b


 start of program geopt   9

 geometry optimization step  9
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -3.41506E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    4.46929E-03    1.62774E-02    2.14807E-02
   2.77115E-02    2.82544E-02    2.99957E-02    3.07637E-02    3.10674E-02
   3.59918E-02    3.76513E-02    4.39400E-02    4.64681E-02    5.96547E-02
   6.48433E-02    7.12813E-02    7.20029E-02    7.49545E-02    7.84677E-02
   8.38467E-02    9.79209E-02    1.11915E-01    1.13168E-01    1.19062E-01
   1.24938E-01    1.29905E-01    1.36517E-01    1.42226E-01    1.45355E-01
   1.54938E-01    1.58608E-01    1.60936E-01    1.72250E-01    1.77966E-01
   1.83199E-01    1.85586E-01    1.91584E-01    1.97395E-01    2.11259E-01
   2.13553E-01    2.18859E-01    2.19879E-01    2.24296E-01    2.27687E-01
   2.32712E-01    2.35497E-01    2.45301E-01    2.51047E-01    2.55495E-01
   2.66520E-01    2.70597E-01    2.76401E-01    2.88957E-01    2.91921E-01
   3.00259E-01    3.04909E-01    3.08606E-01    3.13711E-01    3.14770E-01
```

```
    3.20737E-01    3.25794E-01    3.27252E-01    3.30359E-01    3.33092E-01
    3.34343E-01    3.38988E-01    3.41894E-01    3.44691E-01    3.50415E-01
    3.55816E-01    3.61838E-01    3.62388E-01    3.71926E-01    3.75622E-01
    3.80629E-01    3.86357E-01    3.91054E-01    4.00131E-01    4.10738E-01
    4.19487E-01    4.24022E-01    4.30906E-01    4.39770E-01    4.44996E-01
    4.48205E-01    4.60922E-01    4.71171E-01    4.82270E-01    5.03382E-01

    5.24339E-01    5.65473E-01    5.67342E-01    5.90272E-01    6.24797E-01
    6.42955E-01    7.30373E-01    7.75522E-01    9.88215E-01    1.33572E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.1502620
   Cos(theta):   0.3321007

   Final level shift:  -1.1513599E-02

  energy change:           -1.5996E-05 *  (  5.0000E-05 )
  gradient maximum:         4.6815E-03 .  (  4.5000E-04 )
  gradient rms:             6.4190E-04 .  (  3.0000E-04 )
  step size:   0.15026  trust radius:   0.15000
  displacement maximum:     6.3053E-02 .  (  1.8000E-03 )
  displacement rms:         1.3439E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.0904E-04    geom step:   1.5026E-01    full step:
1.5026E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.5277E-02     y:    -1.1446E-02     z:     3.3764E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       1.0655987271     -3.9590741881     -2.1204504494
  C1        1.5755939062     -3.0167557911     -2.1110121679
  C2        2.9393133247     -0.5449249047     -2.1106873309
  C3        1.1894524556     -2.0090837086     -1.2376843258
  C4        2.6302323204     -2.7822618974     -2.9711912185
  C5        3.3060380331     -1.5602405230     -2.9708968562
  C6        1.8826004065     -0.7915550796     -1.2589225019
  C7        0.1513970485     -1.9007255209     -0.2070092283
  H27       2.9391190397     -3.5500032684     -3.6516822109
  H28       4.1202339816     -1.4096731420     -3.6472782967
  H30       3.4334597078      0.4024675329     -2.0821562169
  C8        0.2532816522     -0.6741997933      0.3185977997
  H32      -0.5534530323     -2.6547333772      0.0537218948
  C10      -0.3905123529      0.2279109976      1.3468661949
  N2        1.3009984633      0.0126234756     -0.2964436311
  C9        1.5651064129      1.2602487938      0.2133747160
  O1        2.4519315836      1.9986220735     -0.1559371925
  H43      -0.3908321367     -0.2517535221      2.3155866720
  C12      -1.8161238604      0.5998801892      0.9732124515
  C11       0.5701565318      1.4698888187      1.3656002249
  C18       1.3719500898      1.5812503810      2.6797428850
  H48       0.0192196153      2.3841247940      1.1952421435
  C13      -3.4179072666      1.3642289738     -0.6535357753
  C14      -4.1124566332      0.9416513048      1.6022960432
  C15      -4.4151208966      1.3386663450      0.3105771586
  C16      -2.8160355919      0.5751117222      1.9305311524
  C17      -2.1289382608      0.9957159069     -0.3245894278
```

```
 H51      -5.4141710032      1.6219890646      0.0528805200
 H52      -2.5860782016      0.2691957261      2.9339715988
 H55      -3.6477402783      1.6647796775     -1.6582041895
 H56      -4.8759408388      0.9156230927      2.3516536290
 H59      -1.3641499061      1.0003125833     -1.0764934972
 H60       1.9103483599      0.6627437611      2.8770738965
 H61       0.7059822246      1.7765821643      3.5097420421
 H62       2.0830769313      2.3903737169      2.6067287731

 nuclear repulsion energy.......  1449.225446338 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   9   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.206E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      84      85
 grid # 2       106    100      97      98      98      98      90      92
 grid # 3       224    183     182     194     182     182     187     182
 grid # 4       224    379     379     406     379     377     372     376

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      85      73      81     100      76
 grid # 2       106    106     105      91     106      92     108      80
 grid # 3       224    224     220     188     223     175     222     166
 grid # 4       224    224     218     375     228     350     401     333

 number of gridpoints:
    atom         O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1       111     68      90      82      71      70      88      87
 grid # 2       127     99     105      91      75      99     100     100
 grid # 3       272    209     191     175     148     217     183     183
 grid # 4       472    201     404     354     303     208     380     379

 number of gridpoints:
    atom        C15    C16     C17     H51     H52     H55     H56     H59
 grid # 1        88     87      86      73      73      73      73      71
 grid # 2       100    100      97     106     104     106     106     101
 grid # 3       183    182     181     224     215     224     224     216
 grid # 4       378    378     376     224     214     224     224     212

 number of gridpoints:
    atom        H60    H61     H62   total
 grid # 1        71     71      71    2820
 grid # 2        99     99      99    3486
 grid # 3       217    219     220    7041
```

```
  grid # 4      217    221    221  10835

  end of program grid


  start of program rwr
 recomputing RwR matrix   2    grid:  4
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.13382598772           3.9E-04  1.1E-02
etot   2  Y  Y  6  M  -815.14141371182  7.6E-03  1.6E-04  4.2E-03
etot   3  N  Y  2  U  -815.14224728816  8.3E-04  5.5E-05  1.3E-03
etot   4  Y  Y  6  M  -815.14231557346  6.8E-05  1.3E-05  2.6E-04
etot   5  Y  Y  6  M  -815.14232201082  6.4E-06  6.4E-06  9.9E-05
etot   6  Y  Y  6  M  -815.14232373017  1.7E-06  2.1E-06  3.0E-05
etot   7  Y  N  6  M  -815.14232634200  2.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1449.22544633805
   (E)  Total one-electron terms..... -3983.94149407222
   (I)  Total two-electron terms.....  1719.57372139218
   (L)  Electronic energy............ -2264.36777268004  (E+I)
   (N)  Total energy.................  -815.14232634200  (A+L)

 SCFE: SCF energy: HF    -815.14232634200 hartrees   iterations:   7


 HOMO energy:    -0.29729
 LUMO energy:     0.11770

  Orbital energies:
  -20.45214  -15.55248  -11.32187  -11.23584  -11.22213  -11.21341
  -11.20722  -11.20024  -11.18776  -11.18577  -11.18528  -11.18459
  -11.18294  -11.18273  -11.17899  -11.17717  -11.17658  -11.17637
  -11.17516  -11.17223   -1.42167   -1.33346   -1.18049   -1.16285
   -1.11579   -1.08866   -1.04071   -1.02751   -1.02019   -1.00030
   -0.94717   -0.90594   -0.85614   -0.84390   -0.83054   -0.81223
   -0.79454   -0.76276   -0.72100   -0.68840   -0.67936   -0.66959
   -0.65869   -0.64155   -0.63879   -0.62735   -0.61190   -0.60579
   -0.60433   -0.60045   -0.59190   -0.57795   -0.56008   -0.55482
   -0.54132   -0.53093   -0.51713   -0.50845   -0.49885   -0.49708
   -0.49057   -0.48670   -0.45900   -0.42163   -0.39370   -0.34950
   -0.34137   -0.31578   -0.29729    0.11770    0.13378    0.14139
    0.14313    0.20504    0.22732    0.26370    0.27092    0.27271
    0.30241

  end of program scf


  start of program der1a
  end of program der1a
 start of program rwr
recomputing RwR matrix   2    grid:  4
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x             y             z
----  -----   -------------  -------------  -------------
  1    H25    -2.979369E-04  -2.113366E-04   2.735623E-04
  2    C1     -1.142355E-03  -1.498489E-03  -2.944229E-04
  3    C2      4.651867E-04   4.723414E-04  -6.019093E-04
  4    C3     -3.768659E-04   2.235530E-04   1.608663E-03
  5    C4      9.650878E-05  -5.712790E-04  -2.182794E-04
  6    C5     -6.242219E-04   1.252090E-03   1.072153E-03
  7    C6      1.700547E-03  -5.250049E-05  -3.978791E-04
  8    C7     -1.120400E-03  -1.039156E-03  -1.481899E-03
  9    H27     2.143853E-05  -2.154310E-04  -1.368257E-04
 10    H28     1.344776E-03   3.108309E-04  -1.180750E-03
 11    H30     9.444400E-04   2.303329E-04  -1.854111E-04
 12    C8      6.170800E-04   2.122326E-03   1.370800E-03
 13    H32    -7.685106E-04  -4.936087E-04  -1.158703E-05
 14    C10     1.075559E-03  -1.184486E-03  -8.906378E-04
 15    N2     -4.415711E-04   4.248794E-05  -7.961249E-04
 16    C9      2.381696E-03   2.576540E-03  -9.419797E-05
 17    O1     -3.507416E-03  -2.961159E-03   1.063424E-03
 18    H43     1.866055E-04   8.200914E-05   7.001821E-04
 19    C12     4.678822E-04   4.169909E-04  -1.979357E-03
 20    C11     1.177165E-03   3.010082E-04   7.491370E-04
 21    C18    -1.963148E-03   9.918879E-05  -1.247189E-03
 22    H48     4.457004E-04  -5.686639E-04  -1.835047E-04
 23    C13    -4.158363E-04   1.565589E-05   2.287030E-05
 24    C14     2.887893E-04   9.943116E-04  -2.763107E-03
 25    C15     7.080171E-04  -7.092194E-04   2.057841E-03
 26    C16     1.360907E-04   2.650348E-04  -3.435687E-04
 27    C17     1.434782E-03  -6.467176E-04   1.386156E-03
 28    H51    -1.385230E-03   2.155138E-04   1.385573E-04
 29    H52    -4.916570E-04   2.779642E-05  -6.796936E-04
 30    H55     2.437289E-04  -3.031604E-04   1.344353E-03
 31    H56    -1.275697E-03   8.552673E-05   6.017433E-04
 32    H59    -1.821410E-04  -4.691704E-05   3.353121E-04
 33    H60     5.269360E-04  -8.637160E-04  -3.418541E-04
 34    H61    -8.750385E-04   3.197463E-04   7.034138E-04
 35    H62     1.530671E-03   1.425829E-03  -3.440256E-04
-----------   -------------  -------------  -------------
   total       9.255736E-04   1.132743E-04  -7.440575E-04

 end of program der1b


 start of program geopt  10

 geometry optimization step 10
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
```

```
   in five columns format
  reading input hessian of dimension   105
   in five columns format

  Hessian eigenvalues:
   -3.96783E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    2.70395E-03    1.67517E-02    2.17707E-02
    2.82919E-02    2.83973E-02    3.00680E-02    3.07425E-02    3.12100E-02
    3.61534E-02    3.79222E-02    4.45983E-02    4.70562E-02    5.94489E-02
    6.62342E-02    7.13763E-02    7.28004E-02    7.51481E-02    7.87276E-02
    8.30568E-02    1.02777E-01    1.10747E-01    1.13519E-01    1.14939E-01
    1.25147E-01    1.27088E-01    1.35877E-01    1.42955E-01    1.53547E-01
    1.56454E-01    1.58296E-01    1.62818E-01    1.67896E-01    1.70904E-01
    1.78640E-01    1.83921E-01    1.85748E-01    1.97048E-01    2.10071E-01
    2.12860E-01    2.15785E-01    2.19787E-01    2.22406E-01    2.24986E-01
    2.30931E-01    2.32177E-01    2.48101E-01    2.53037E-01    2.53717E-01
    2.66599E-01    2.74147E-01    2.77327E-01    2.90409E-01    2.96632E-01
    2.99225E-01    3.06626E-01    3.10945E-01    3.13813E-01    3.19402E-01
    3.22355E-01    3.23521E-01    3.27977E-01    3.31424E-01    3.34071E-01
    3.37875E-01    3.39703E-01    3.43162E-01    3.49753E-01    3.53760E-01
    3.62134E-01    3.66806E-01    3.69175E-01    3.78263E-01    3.80177E-01
    3.82444E-01    3.90148E-01    3.99086E-01    4.09888E-01    4.14735E-01
    4.20706E-01    4.27214E-01    4.33288E-01    4.39272E-01    4.46790E-01
    4.56737E-01    4.80583E-01    4.82929E-01    4.97147E-01    5.00247E-01
    5.47423E-01    5.69920E-01    5.83972E-01    5.99820E-01    6.36224E-01
    7.23096E-01    7.35473E-01    7.99458E-01    9.84602E-01    1.24031E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.2123793
   Cos(theta):   0.2442891

   Final level shift:  -1.0282018E-02

  energy change:          -2.9436E-04 .  (  5.0000E-05 )
  gradient maximum:        4.7301E-03 .  (  4.5000E-04 )
  gradient rms:            9.9272E-04 .  (  3.0000E-04 )
  step size:   0.21237  trust radius:   0.21213
  displacement maximum:    8.6917E-02 .  (  1.8000E-03 )
  displacement rms:        1.8995E-02 .  (  1.2000E-03 )
  predicted energy change:    -5.1976E-04    geom step:    2.1237E-01    full step:
2.1237E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:      1.9534E-02     y:    -1.3748E-02     z:      5.6645E-03

  new geometry:
                                angstroms
  atom             x                  y                  z
  H25       0.9705592001     -3.9322953709     -2.1809052720
  C1        1.5193343668     -3.0104047554     -2.1470319779
  C2        2.9804516233     -0.5899947654     -2.0829660780
  C3        1.1643435832     -1.9998386246     -1.2603987674
  C4        2.5883808490     -2.8027150827     -2.9914218129
  C5        3.3128023462     -1.6066520545     -2.9576508518
```

```
 C6        1.9044518493    -0.8092275712    -1.2512917825
 C7        0.1172819730    -1.8658653656    -0.2439540285
 H27       2.8713006740    -3.5703711661    -3.6846209842
 H28       4.1388480110    -1.4758982006    -3.6221031905
 H30       3.5120461332     0.3368109731    -2.0306999908
 C8        0.2509685942    -0.6486880926     0.2953723225
 H32      -0.6215400151    -2.5959267813    -0.0059196250
 C10      -0.3800930573     0.2583595288     1.3276411287
 N2        1.3341307517     0.0059264963    -0.2911211180
 C9        1.6204501752     1.2431413714     0.2270788248
 O1        2.5361362848     1.9509468148    -0.1155331072
 H43      -0.3645971218    -0.2195713826     2.2978727893
 C12      -1.8128599331     0.6194235374     0.9729847655
 C11       0.5835792670     1.4996194750     1.3330905430
 C18       1.3230837996     1.6862697103     2.6751167981
 H48       0.0362778236     2.4035976524     1.0943723257
 C13      -3.4348682604     1.4250489710    -0.6138821653
 C14      -4.1290773129     0.8391942857     1.6034944979
 C15      -4.4386764117     1.3039983313     0.3383832529
 C16      -2.8194838909     0.4991490171     1.9176779649
 C17      -2.1328480056     1.0835625856    -0.2987344633
 H51      -5.4482204880     1.5638497791     0.0916213031
 H52      -2.5872512910     0.1359973854     2.9001987532
 H55      -3.6690660293     1.7768516234    -1.5990505258
 H56      -4.8986673323     0.7356020999     2.3429541430
 H59      -1.3627086392     1.1618453238    -1.0422236051
 H60       1.8470888218     0.7750345465     2.9556547998
 H61       0.6189168572     1.9380936879     3.4636968647
 H62       2.0433587928     2.4887530292     2.5806102831

 nuclear repulsion energy.......  1447.232715971 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  10   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.209E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     85     85
 grid # 2       106     99     98     98     98     99     91     92
 grid # 3       224    183    183    194    182    182    186    182
 grid # 4       224    379    380    408    379    377    370    378

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     81    100     75
 grid # 2       106    106    105     91    106     93    109     80
 grid # 3       224    224    220    188    223    175    223    165
```

```
  grid # 4      224    224    218    374    227    347    400    331

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     68     90     82     72     69     88     87
  grid # 2      123     98    105     92     75     99    100    100
  grid # 3      272    209    193    175    141    215    183    183
  grid # 4      473    200    400    351    309    208    379    379

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     87     86     73     73     73     73     70
  grid # 2      100    100     96    106    104    106    106    101
  grid # 3      183    182    180    224    214    224    224    215
  grid # 4      379    378    376    224    214    224    224    214

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2821
  grid # 2       99     99     99   3485
  grid # 3      217    220    220   7032
  grid # 4      219    222    221  10834

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                 RMS    maximum
       e  d  i  u  i                       energy  density   DIIS
       r  t  s  t  d     total energy      change  change    error

etot   1  N  N  2  U  -815.12189927581             5.6E-04  1.7E-02
etot   2  Y  Y  6  M  -815.13976265107  1.8E-02  2.6E-04  7.1E-03
etot   3  N  Y  2  U  -815.14206963265  2.3E-03  9.0E-05  2.3E-03
etot   4  Y  Y  6  M  -815.14226874461  2.0E-04  2.3E-05  5.2E-04
etot   5  Y  Y  6  M  -815.14227748435  8.7E-06  1.3E-05  2.0E-04
etot   6  Y  Y  6  M  -815.14228249213  5.0E-06  4.2E-06  6.2E-05
etot   7  Y  N  6  M  -815.14228511931  2.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1447.23271597093
   (E)  Total one-electron terms..... -3979.95785912359
   (I)  Total two-electron terms.....  1717.58285803335
   (L)  Electronic energy............ -2262.37500109024  (E+I)
   (N)  Total energy.................  -815.14228511931  (A+L)

 SCFE: SCF energy: HF    -815.14228511931 hartrees   iterations:   7


 HOMO energy:    -0.29631
 LUMO energy:     0.11802

  Orbital energies:
  -20.45234  -15.55204  -11.32149  -11.23523  -11.22186  -11.21348
 -11.20764  -11.20055  -11.18758  -11.18626  -11.18578  -11.18531
 -11.18377  -11.18337  -11.17892  -11.17765  -11.17645  -11.17629
 -11.17515  -11.17221   -1.42490   -1.33389   -1.18017   -1.16260
  -1.11522   -1.08849   -1.04063   -1.02695   -1.02075   -0.99972
  -0.94647   -0.90568   -0.85543   -0.84362   -0.83099   -0.81202
  -0.79420   -0.76210   -0.72073   -0.68932   -0.67923   -0.66926
  -0.65839   -0.64131   -0.63978   -0.62700   -0.61224   -0.60604
  -0.60415   -0.60094   -0.59154   -0.57651   -0.55978   -0.55440
  -0.54084   -0.53100   -0.51696   -0.50792   -0.49955   -0.49658
  -0.49090   -0.48634   -0.45944   -0.42162   -0.39349   -0.34914
  -0.34215   -0.31600   -0.29631    0.11802    0.13395    0.14004
   0.14375    0.20572    0.22626    0.26455    0.27057    0.27306
   0.29990

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25     2.144102E-04   1.205084E-03   7.618622E-04
  2    C1     -3.528374E-03  -3.442926E-04   1.850428E-03
  3    C2      1.393434E-03  -1.248786E-03  -2.517157E-03
  4    C3      2.251447E-04  -8.625454E-04   1.473300E-03
  5    C4      2.224675E-03   1.218373E-03  -6.718793E-04
  6    C5     -2.783118E-04   1.334179E-03   8.786158E-04
  7    C6     -2.088593E-04  -4.495554E-04   1.961023E-04
  8    C7     -3.080521E-03  -1.675147E-03  -1.935791E-03
  9    H27     3.735092E-04   7.106930E-04   1.740925E-04
 10    H28     2.066909E-03   1.774400E-04  -1.736806E-03
 11    H30     7.857578E-04  -4.883568E-04  -6.459035E-04
 12    C8      4.173990E-04   1.590100E-03   2.016753E-03
 13    H32    -1.556321E-04   3.729482E-05  -6.487629E-05
 14    C10     1.531558E-03  -8.274530E-04  -4.126476E-04
 15    N2     -1.776214E-03  -2.023195E-03  -5.268804E-04
 16    C9     -2.936967E-03   1.477451E-04   1.582365E-03
 17    O1      3.034302E-03   2.323938E-03  -5.384675E-04
 18    H43     1.686086E-04   1.357831E-04   3.419925E-04
 19    C12    -1.060172E-03  -1.797572E-04   1.898887E-04
 20    C11    -2.303676E-04   5.176430E-04   1.359348E-03
 21    C18    -1.388537E-03  -8.176310E-04   3.793457E-04
 22    H48     1.356169E-03  -1.638542E-03  -1.806817E-04
 23    C13     7.604959E-04  -4.741378E-04   1.031533E-03
 24    C14     1.309029E-03  -1.265251E-05  -7.031787E-04
 25    C15     1.224652E-03  -4.326605E-04   2.761751E-04
 26    C16    -8.800887E-04   6.762355E-04  -9.557361E-04
 27    C17    -5.060357E-04   2.297591E-04   1.922741E-04
 28    H51    -2.099545E-04   1.520753E-04  -1.180830E-04
 29    H52    -1.118498E-04  -2.744263E-05   1.960574E-05
 30    H55    -9.357769E-06   7.741421E-05   2.371021E-04
 31    H56     3.313128E-04   1.772451E-04  -1.495537E-04
 32    H59    -8.432687E-04  -7.881803E-05   2.112795E-04
 33    H60    -1.006530E-03   2.419237E-03  -1.273945E-03
 34    H61     1.317988E-03  -5.168919E-04  -1.988380E-03
 35    H62     4.939274E-04  -2.962030E-04   3.995175E-04
-----------   -------------  -------------  -------------
   total       1.018238E-03   7.361706E-04  -8.483854E-04

 end of program der1b


 start of program geopt  11

 geometry optimization step 11
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -4.78002E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    2.52510E-03    1.68708E-02    1.98993E-02
   2.32295E-02    2.81629E-02    2.97624E-02    3.03768E-02    3.09414E-02
   3.15532E-02    3.73316E-02    3.77454E-02    4.43859E-02    4.47598E-02
   6.09956E-02    6.65899E-02    7.08101E-02    7.16592E-02    7.36847E-02
   8.23790E-02    9.02316E-02    1.06626E-01    1.12174E-01    1.15315E-01
   1.23087E-01    1.29414E-01    1.34017E-01    1.40555E-01    1.45694E-01
   1.49292E-01    1.51200E-01    1.56004E-01    1.63404E-01    1.72225E-01
   1.76187E-01    1.80774E-01    1.81700E-01    1.86372E-01    1.96361E-01
   1.98752E-01    2.09752E-01    2.13691E-01    2.16561E-01    2.21328E-01
   2.27396E-01    2.29089E-01    2.39348E-01    2.47251E-01    2.49668E-01
   2.52253E-01    2.62048E-01    2.63433E-01    2.81784E-01    2.83875E-01
   2.97440E-01    2.99402E-01    3.04905E-01    3.12713E-01    3.14779E-01
   3.21797E-01    3.24537E-01    3.29579E-01    3.30925E-01    3.34830E-01
   3.40009E-01    3.40502E-01    3.45284E-01    3.48624E-01    3.59369E-01
   3.61214E-01    3.66596E-01    3.72744E-01    3.81138E-01    3.83647E-01
   3.87472E-01    3.95542E-01    4.01276E-01    4.05138E-01    4.20077E-01
   4.22811E-01    4.29389E-01    4.39644E-01    4.48683E-01    4.56045E-01
   4.67856E-01    4.75835E-01    4.87364E-01    4.99252E-01    5.14924E-01
   5.28923E-01    5.64094E-01    6.01734E-01    6.10715E-01    6.64414E-01
   7.16860E-01    7.49634E-01    8.22700E-01    1.03181E+00    1.36247E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.1061566
  Cos(theta):   0.6185673

  Final level shift:  -4.8991655E-02

 energy change:           4.1223E-05 *   (  5.0000E-05 )
 gradient maximum:        4.1685E-03 .   (  4.5000E-04 )
 gradient rms:            1.1798E-03 .   (  3.0000E-04 )
 step size:   0.10615  trust radius:   0.10607
 displacement maximum:    3.2417E-02 .   (  1.8000E-03 )
 displacement rms:        9.4947E-03 .   (  1.2000E-03 )
```

```
  predicted energy change:    -7.0909E-04    geom step:   1.0615E-01    full step:
1.0615E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.3318E-04     y:     5.7594E-04     z:    -2.1807E-03

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.9350673315     -3.9078266325     -2.2289740236
  C1        1.5075047820     -3.0009932433     -2.1756346448
  C2        3.0431614539     -0.6147978193     -2.0482258413
  C3        1.1534365049     -1.9897145691     -1.2912350378
  C4        2.6186480562     -2.8080883728     -2.9820528530
  C5        3.3812324117     -1.6303086254     -2.9160819741
  C6        1.9256209142     -0.8159857738     -1.2537495466
  C7        0.0782973067     -1.8458130674     -0.3050905515
  H27       2.9097064251     -3.5750567377     -3.6723519341
  H28       4.2437337784     -1.5166721395     -3.5524914701
  H30       3.6093958229      0.2929708214     -1.9698567655
  C8        0.2385099650     -0.6399430346      0.2619826996
  H32      -0.6866910667     -2.5608615839     -0.0988539199
  C10      -0.3851602041      0.2548807499      1.3067223253
  N2        1.3332303805      0.0056989668     -0.3082330222
  C9        1.6186897862      1.2421136552      0.2191078059
  O1        2.5439224526      1.9414991874     -0.1072820720
  H43      -0.3711477533     -0.2375494630      2.2711625243
  C12      -1.8211573223      0.6261525687      0.9699790563
  C11       0.5806935310      1.4956436814      1.3182504534
  C18       1.3136022095      1.6992460227      2.6521043954
  H48       0.0345551363      2.3928290930      1.0770261748
  C13      -3.4822296144      1.4183264428     -0.5809148285
  C14      -4.1209395142      0.8500914341      1.6453800915
  C15      -4.4625660491      1.3039199268      0.3884341571
  C16      -2.8062954378      0.5122777669      1.9323456340
  C17      -2.1728128901      1.0815009458     -0.2925357908
  H51      -5.4793015792      1.5589844742      0.1608877483
  H52      -2.5558908890      0.1484767944      2.9116831787
  H55      -3.7405056601      1.7600994146     -1.5627577951
  H56      -4.8724572018      0.7484118356      2.4027006234
  H59      -1.4282772932      1.1498844369     -1.0563893348
  H60       1.8383647638      0.7969638036      2.9370290356
  H61       0.6059576189      1.9543219941      3.4285869141
  H62       2.0397646853      2.5022772647      2.5580291374

  nuclear repulsion energy.......  1445.954963252 hartrees
  --------------------------------------------------
 /  end of geometry optimization iteration  11   /
 --------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.240E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe
  start of program grid

  number of gridpoints:
     atom        H25     C1      C2      C3      C4      C5      C6      C7
  grid # 1        73     89      88      90      87      87      85      85
  grid # 2       106    100      98      98      98      99      91      92
  grid # 3       224    183     183     195     182     182     188     183
  grid # 4       224    380     383     404     379     379     374     379

  number of gridpoints:
     atom        H27    H28     H30      C8     H32     C10      N2      C9
  grid # 1        73     73      73      86      73      81     100      76
  grid # 2       106    106     105      91     106      92     109      81
  grid # 3       224    224     220     190     223     175     223     164
  grid # 4       224    224     219     372     228     351     401     327

  number of gridpoints:
     atom         O1    H43     C12     C11     C18     H48     C13     C14
  grid # 1       111     68      90      81      71      69      87      87
  grid # 2       123     98     105      93      76     100     100      98
  grid # 3       272    209     191     171     150     216     183     183
  grid # 4       474    202     400     352     305     205     380     378

  number of gridpoints:
     atom        C15    C16     C17     H51     H52     H55     H56     H59
  grid # 1        89     87      85      73      73      73      73      71
  grid # 2       100     99      98     106     104     106     106     101
  grid # 3       182    180     181     224     214     224     224     215
  grid # 4       380    377     375     224     214     224     224     215

  number of gridpoints:
     atom        H60    H61     H62   total
  grid # 1        71     71      71    2820
  grid # 2        99     99      99    3488
  grid # 3       217    220     220    7039
  grid # 4       218    222     221   10838

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                     RMS    maximum
       e  d  i  u  i                        energy   density    DIIS
       r  t  s  t  d    total energy        change    change     error

etot   1  N  N  1  U  -815.13511620078             3.7E-04  1.3E-02
etot   2  Y  Y  4  M  -815.14109616859  6.0E-03  1.5E-04  5.2E-03
etot   3  N  Y  1  U  -815.14179411455  7.0E-04  5.3E-05  1.6E-03
etot   4  Y  Y  4  M  -815.14186107932  6.7E-05  1.8E-05  5.1E-04
etot   5  Y  Y  4  M  -815.14186679143  5.7E-06  6.8E-06  1.4E-04
etot   6  Y  Y  4  M  -815.14186734030  5.5E-07  2.9E-06  4.0E-05
etot   7  Y  N  4  M  -815.14186819667  8.6E-07  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
  (A)  Nuclear repulsion............  1445.95496325192
  (E)  Total one-electron terms..... -3977.40453177892
  (I)  Total two-electron terms.....  1716.30770033034
  (L)  Electronic energy............ -2261.09683144859  (E+I)
  (N)  Total energy.................  -815.14186819667  (A+L)

SCFE: SCF energy: HF    -815.14186819667 hartrees   iterations:   7


HOMO energy:    -0.29645
LUMO energy:     0.11861

 Orbital energies:
 -20.45269  -15.55215  -11.32105  -11.23561  -11.22340  -11.21383
 -11.20610  -11.19987  -11.18789  -11.18543  -11.18486  -11.18437
 -11.18282  -11.18249  -11.17985  -11.17781  -11.17669  -11.17662
 -11.17592  -11.17356   -1.42634   -1.33322   -1.18119   -1.16177
  -1.11549   -1.08733   -1.04232   -1.02717   -1.01880   -1.00061
  -0.94647   -0.90555   -0.85508   -0.84446   -0.83080   -0.80972
  -0.79418   -0.76178   -0.72123   -0.69085   -0.67860   -0.66845
  -0.65854   -0.64086   -0.63999   -0.62645   -0.61150   -0.60693
  -0.60357   -0.60049   -0.59215   -0.57746   -0.55942   -0.55527
  -0.54130   -0.53112   -0.51642   -0.50838   -0.49938   -0.49609
  -0.49121   -0.48635   -0.45907   -0.42211   -0.39314   -0.34910
  -0.34351   -0.31390   -0.29645    0.11861    0.13467    0.13957
   0.14364    0.20522    0.22560    0.26444    0.27093    0.27290
   0.30060

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25      1.287006E-03   1.169534E-03  -4.934181E-04
  2    C1       4.982090E-03   2.097602E-03  -2.375867E-03
  3    C2      -2.498465E-03   7.570800E-04   2.917767E-03
  4    C3       1.024460E-03   7.778499E-04  -3.948986E-04
  5    C4      -2.958431E-04   7.023582E-04   9.626116E-04
  6    C5       3.222860E-06  -3.884697E-03  -2.449964E-03
  7    C6      -1.295333E-03   1.314017E-03  -1.352881E-03
  8    C7       1.043197E-03   2.515804E-03   2.950928E-04
  9    H27     -1.444873E-04   3.919244E-05   2.156971E-04
 10    H28     -4.036505E-03  -1.412069E-03   2.471712E-03
 11    H30     -2.381193E-03  -1.560881E-03   2.902841E-05
 12    C8      -3.743770E-03  -1.834222E-03  -2.699784E-03
 13    H32      1.330956E-03   7.780944E-04   2.312532E-04
 14    C10      7.308707E-04   7.940108E-04  -7.274642E-04
 15    N2      2.636299E-03  -2.325157E-03   1.849266E-03
 16    C9     -2.391351E-03  -4.793206E-03   1.662832E-03
 17    O1      5.711572E-03   4.753976E-03  -1.638427E-03
 18    H43     1.278466E-03   7.906435E-04  -2.935122E-04
 19    C12     1.137079E-03  -1.605896E-03   1.068971E-03
 20    C11    -1.195006E-03  -2.033543E-04  -1.272718E-03
 21    C18     2.282753E-03   1.593426E-03   2.648320E-04
 22    H48    -1.177564E-03   1.785104E-03  -1.769165E-03
 23    C13     2.740815E-03   3.200306E-04  -2.388940E-03
 24    C14    -2.911957E-04  -1.192819E-03   3.248866E-03
 25    C15    -2.306720E-03   4.751624E-04   3.228107E-04
 26    C16    -2.707736E-03  -5.302930E-04   3.490894E-03
 27    C17    -1.274693E-03   4.353794E-04  -1.815591E-03
 28    H51     7.707843E-04  -9.740377E-05   3.492333E-04
 29    H52    -3.493259E-04   6.169750E-04  -7.296322E-04
 30    H55     5.096521E-04   2.799782E-04  -5.684600E-04
 31    H56     3.389988E-05   1.111685E-04   3.299452E-04
 32    H59     1.987920E-03   4.147087E-04  -1.884503E-03
 33    H60     7.088841E-04  -1.229240E-03   9.248530E-04
 34    H61    -3.960131E-04   3.790184E-04   1.723255E-03
 35    H62    -2.372659E-03  -1.876090E-03  -2.797159E-04
-----------   -------------  -------------  -------------
   total       1.342069E-03   3.557834E-04  -7.760215E-04

 end of program der1b


 start of program geopt  12

 geometry optimization step 12
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   11 **

 Hessian eigenvalues:
  -1.20277E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    2.30049E-03    6.46729E-03    2.13182E-02
   2.19821E-02    2.81735E-02    3.02288E-02    3.07258E-02    3.08945E-02
   3.16739E-02    3.70653E-02    3.83479E-02    4.46544E-02    4.92337E-02
   5.68994E-02    6.45936E-02    6.72933E-02    7.26298E-02    7.33660E-02
   7.99358E-02    8.22371E-02    9.09971E-02    1.04407E-01    1.11888E-01
   1.12558E-01    1.22101E-01    1.31926E-01    1.40071E-01    1.42155E-01
   1.46233E-01    1.50373E-01    1.53689E-01    1.55621E-01    1.60397E-01
   1.73847E-01    1.79098E-01    1.81871E-01    1.84617E-01    1.88481E-01
   1.97911E-01    2.00665E-01    2.08140E-01    2.12802E-01    2.16731E-01
   2.18923E-01    2.31322E-01    2.32532E-01    2.44599E-01    2.49001E-01
   2.56293E-01    2.60377E-01    2.62299E-01    2.66239E-01    2.79760E-01
   2.83643E-01    2.91588E-01    2.98586E-01    3.05677E-01    3.11708E-01
   3.15283E-01    3.20066E-01    3.25015E-01    3.31259E-01    3.33186E-01
   3.34189E-01    3.36228E-01    3.38734E-01    3.47969E-01    3.58054E-01
   3.62440E-01    3.68459E-01    3.75294E-01    3.77863E-01    3.89220E-01
   3.92363E-01    4.01662E-01    4.06751E-01    4.12260E-01    4.22308E-01
   4.26232E-01    4.36783E-01    4.54613E-01    4.60872E-01    4.66859E-01
   4.71745E-01    4.91055E-01    5.03734E-01    5.08794E-01    5.14482E-01
   5.24585E-01    5.63490E-01    5.82795E-01    6.17863E-01    6.80942E-01
   7.11914E-01    7.35067E-01    8.22024E-01    1.06549E+00    1.33348E+00
  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0539062
   Cos(theta):   0.5974702

   Final level shift:  -1.7661307E-01

  energy change:           4.1692E-04 .  (  5.0000E-05 )
  gradient maximum:        4.1685E-03 .  (  4.5000E-04 )
  gradient rms:            1.1798E-03 .  (  3.0000E-04 )
  step size:   0.05391  trust radius:   0.05303
  displacement maximum:    1.8827E-02 .  (  1.8000E-03 )
  displacement rms:        4.8215E-03 .  (  1.2000E-03 )
  predicted energy change:    -4.6902E-04    geom step:   5.3906E-02    full step:
5.3906E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.6653E-16     y:     6.7654E-17     z:    -5.5511E-17

  new geometry:
                               angstroms
  atom            x                 y                  z
  H25       0.9771529403     -3.9291962865     -2.1761041238
  C1        1.5252186106     -3.0098785058     -2.1410383377
  C2        2.9911669335     -0.5964973151     -2.0841128923
  C3        1.1578846408     -1.9969396451     -1.2705582265
  C4        2.6106606158     -2.8038946234     -2.9737313692
  C5        3.3385000696     -1.6140921013     -2.9447638486
  C6        1.8997578672     -0.8098905310     -1.2637516546
  C7        0.1019824108     -1.8579171945     -0.2641846338
  H27       2.9081267727     -3.5752894123     -3.6583312498
  H28       4.1788698916     -1.4903279841     -3.5978736927
  H30       3.5223938864      0.3294601910     -2.0318062568
  C8        0.2411792534     -0.6424488685      0.2802221285
  H32      -0.6363960026     -2.5859567622     -0.0225341537
  C10      -0.3849203517      0.2625189530      1.3138637665
  N2        1.3239710006      0.0087522134     -0.3093139257
  C9        1.6167867343      1.2441715951      0.2117297241
  O1        2.5570892964      1.9387197261     -0.1088568271
  H43      -0.3691621114     -0.2229466121      2.2807762570
  C12      -1.8191168699      0.6219572683      0.9671953027
  C11       0.5797115978      1.5016733976      1.3176650440
  C18       1.3157981603      1.6765428729      2.6613535177
  H48       0.0400160640      2.4123995049      1.0746856579
  C13      -3.4504836170      1.4345815485     -0.5962620203
  C14      -4.1275203727      0.8364306687      1.6170220404
  C15      -4.4447803250      1.3083086739      0.3625082863
  C16      -2.8173791607      0.4956972754      1.9181657639
  C17      -2.1482637861      1.0918644094     -0.2964082841
  H51      -5.4562583777      1.5722799864      0.1253494707
  H52      -2.5757572976      0.1350236371      2.9016902668
  H55      -3.6954677824      1.7937398601     -1.5765453393
  H56      -4.8900296317      0.7342465417      2.3613469313
  H59      -1.3851637463      1.1769950215     -1.0441231342
  H60       1.8436440783      0.7675305911      2.9331544845
  H61       0.6175967480      1.9124617954      3.4569807131
  H62       2.0270258039      2.4835471399      2.5749027876
```

```
 nuclear repulsion energy.......  1447.577731398 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  12   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.202E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     84     85
 grid # 2      106    100     97     98     98     99     91     92
 grid # 3      224    182    182    194    182    182    187    183
 grid # 4      224    380    379    404    379    378    370    377

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     86     73     81    100     76
 grid # 2      106    106    105     91    106     92    109     80
 grid # 3      224    224    220    188    223    175    223    165
 grid # 4      224    224    218    374    227    349    402    332

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      111     68     90     82     72     69     87     87
 grid # 2      127     98    106     94     74    100    100     98
 grid # 3      272    209    193    176    141    216    183    183
 grid # 4      473    199    398    352    307    208    379    379

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1       87     87     86     73     73     73     73     70
 grid # 2       99    100     96    106    104    106    106    101
 grid # 3      183    182    180    224    214    224    224    215
 grid # 4      379    377    376    224    214    224    224    214

 number of gridpoints:
    atom       H60    H61    H62  total
 grid # 1       71     71     71   2818
 grid # 2       99     99     99   3488
 grid # 3      216    220    220   7033
 grid # 4      218    222    221  10829

 end of program grid


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr
```

```
  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                    energy  density    DIIS
       r  t  s  t  d     total energy    change  change     error

etot   1  N  N  1  U  -815.13716243958           3.2E-04  1.2E-02
etot   2  Y  Y  4  M  -815.14139067976  4.2E-03  1.3E-04  4.8E-03
etot   3  Y  Y  4  M  -815.14190974434  5.2E-04  4.5E-05  1.5E-03
etot   4  N  Y  1  U  -815.14195024401  4.0E-05  2.1E-05  4.8E-04
etot   5  Y  Y  4  M  -815.14195632242  6.1E-06  7.9E-06  1.3E-04
etot   6  Y  Y  4  M  -815.14195799197  1.7E-06  3.1E-06  3.6E-05
etot   7  Y  N  4  M  -815.14195691538 -1.1E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1447.57773139812
   (E)  Total one-electron terms..... -3980.63883502023
   (I)  Total two-electron terms.....  1717.91914670673
   (L)  Electronic energy............ -2262.71968831350  (E+I)
   (N)  Total energy.................  -815.14195691538  (A+L)

 SCFE: SCF energy: HF    -815.14195691538 hartrees   iterations:   7


 HOMO energy:    -0.29717
 LUMO energy:     0.11831

  Orbital energies:
  -20.45214  -15.55250  -11.32196  -11.23551  -11.22193  -11.21339
  -11.20825  -11.20005  -11.18702  -11.18585  -11.18477  -11.18466
  -11.18309  -11.18243  -11.17862  -11.17646  -11.17630  -11.17615
  -11.17470  -11.17215   -1.42153   -1.33362   -1.18169   -1.16360
   -1.11601   -1.08886   -1.04150   -1.02802   -1.01954   -1.00139
   -0.94726   -0.90605   -0.85597   -0.84433   -0.83146   -0.81126
   -0.79450   -0.76258   -0.72153   -0.68895   -0.67880   -0.66958
   -0.65809   -0.64095   -0.64042   -0.62717   -0.61156   -0.60612
   -0.60405   -0.60170   -0.59195   -0.57721   -0.56002   -0.55478
   -0.54061   -0.53085   -0.51648   -0.50835   -0.49998   -0.49717
   -0.49116   -0.48640   -0.45908   -0.42181   -0.39348   -0.34975
   -0.34297   -0.31500   -0.29717    0.11831    0.13476    0.13950
    0.14386    0.20576    0.22596    0.26446    0.27089    0.27319
    0.29902

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b
 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -8.793163E-05  -7.284415E-04   1.534319E-04
  2    C1      1.747961E-03  -6.803971E-04  -3.966347E-03
  3    C2     -2.067343E-03   2.433051E-03   1.947151E-03
  4    C3     -7.890831E-04   6.051085E-04   2.509989E-03
  5    C4     -4.938475E-04  -4.985741E-03  -1.362581E-03
  6    C5      5.793989E-04   7.104740E-04  -1.054380E-04
  7    C6      3.145290E-03   2.044709E-03  -4.853383E-04
  8    C7     -1.488022E-03  -5.328551E-04   3.300460E-04
  9    H27    -8.386920E-04   3.191751E-04   9.685245E-04
 10    H28    -2.225737E-04  -2.864975E-04  -2.532800E-04
 11    H30     7.809458E-04   3.425289E-04   2.908721E-04
 12    C8     -2.603187E-04  -8.865512E-05  -1.987860E-03
 13    H32    -6.127370E-04  -6.092375E-04  -3.584395E-04
 14    C10     5.651113E-04  -1.163365E-03  -9.741275E-04
 15    N2     -2.312682E-05   1.306153E-03  -3.344962E-04
 16    C9      6.164547E-03   1.128648E-03   3.196440E-03
 17    O1     -4.991206E-03  -1.836981E-03   3.221816E-04
 18    H43     7.817195E-04   1.050869E-03   4.930786E-04
 19    C12     7.356808E-05  -9.513266E-04   2.679000E-03
 20    C11    -1.630663E-03   2.377751E-03   6.442379E-04
 21    C18    -1.100031E-03  -4.006181E-04  -1.728066E-04
 22    H48     1.191621E-03  -3.495483E-03   1.274216E-03
 23    C13    -7.352532E-04   6.926293E-04  -1.914636E-03
 24    C14     1.291275E-03  -4.520763E-04   2.542060E-03
 25    C15    -2.196224E-03   1.043310E-03  -3.250652E-03
 26    C16     7.451240E-04   4.279297E-05   2.409415E-03
 27    C17     4.349237E-04   6.441672E-04  -1.093577E-03
 28    H51     1.867769E-04   4.062917E-05  -1.077784E-04
 29    H52    -4.147278E-04   1.698793E-05  -1.604662E-03
 30    H55     2.565444E-04  -2.954245E-06   3.699215E-04
 31    H56    -5.434186E-04  -3.047336E-04   9.616781E-04
 32    H59     2.335698E-05  -1.040448E-04  -6.909369E-04
 33    H60     1.544427E-04   1.067695E-03  -1.552558E-03
 34    H61    -7.385815E-04   2.757002E-04  -1.684118E-03
 35    H62     2.602469E-03   1.146247E-03   5.298051E-04
-----------   -------------  -------------  -------------
   total       1.491294E-03   6.652188E-04  -2.775832E-04

 end of program der1b


 start of program geopt  13

 geometry optimization step 13
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   11 **

 Hessian eigenvalues:
  -2.90898E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.61667E-03    1.88858E-02    2.02850E-02
   2.79562E-02    2.85503E-02    3.00689E-02    3.05410E-02    3.09044E-02
```

```
     3.42799E-02     3.72812E-02     4.16096E-02     4.56745E-02     5.68035E-02
     5.91995E-02     6.97156E-02     7.16291E-02     7.40225E-02     7.49961E-02
     8.20739E-02     8.89180E-02     1.03662E-01     1.06898E-01     1.11938E-01
     1.12878E-01     1.23845E-01     1.35239E-01     1.40650E-01     1.44275E-01
     1.47228E-01     1.51483E-01     1.52608E-01     1.55654E-01     1.64763E-01
     1.73532E-01     1.76736E-01     1.80022E-01     1.85830E-01     1.96711E-01
     2.00657E-01     2.06538E-01     2.12790E-01     2.15422E-01     2.20288E-01
     2.21296E-01     2.30514E-01     2.32196E-01     2.47940E-01     2.49890E-01
     2.55421E-01     2.58159E-01     2.67247E-01     2.75476E-01     2.85021E-01
     2.90170E-01     3.00392E-01     3.06122E-01     3.09510E-01     3.16790E-01
     3.18881E-01     3.22160E-01     3.24405E-01     3.28727E-01     3.33404E-01
     3.34528E-01     3.38383E-01     3.46252E-01     3.50535E-01     3.55123E-01
     3.59079E-01     3.63714E-01     3.68358E-01     3.74953E-01     3.84356E-01
     3.87029E-01     3.96984E-01     4.03835E-01     4.10045E-01     4.19408E-01
     4.22810E-01     4.31781E-01     4.46500E-01     4.56560E-01     4.59526E-01
     4.66990E-01     4.78307E-01     4.86584E-01     5.01405E-01     5.15234E-01
     5.35939E-01     5.45233E-01     5.86235E-01     6.24710E-01     6.67357E-01
     6.87698E-01     7.32078E-01     7.83296E-01     1.05679E+00     1.26916E+00

   WARNING: Hessian has wrong number of negative eigenvalues


   Level shifts adjusted to satisfy step-size constraints
    Step size:    0.0265681
    Cos(theta):   0.8678432

    Final level shift:  -1.9439479E-01

   energy change:            3.2820E-04 .  (  5.0000E-05 )
   gradient maximum:         4.1685E-03 .  (  4.5000E-04 )
   gradient rms:             1.1798E-03 .  (  3.0000E-04 )
   step size:   0.02657  trust radius:   0.02652
   displacement maximum:     6.8365E-03 .  (  1.8000E-03 )
   displacement rms:         2.3763E-03 .  (  1.2000E-03 )
   predicted energy change:    -2.2067E-04    geom step:   2.6568E-02    full step:
 2.6568E-02
   molecular structure not yet converged...

   center of mass moved by:
      x:    -1.6653E-16     y:     6.7654E-17     z:    -5.5511E-17

   new geometry:
                               angstroms
   atom           x                 y                 z
   H25       0.9710761692     -3.9286413642     -2.1828451837
   C1        1.5210628282     -3.0085086925     -2.1487172297
   C2        2.9891060011     -0.5928392197     -2.0809386577
   C3        1.1605174873     -1.9975481736     -1.2659005475
   C4        2.5995847207     -2.8039496956     -2.9867406663
   C5        3.3274194457     -1.6103340597     -2.9514545732
   C6        1.9044304502     -0.8083880317     -1.2544071872
   C7        0.1055663203     -1.8636015171     -0.2563000348
   H27       2.8874490623     -3.5721748397     -3.6761909147
   H28       4.1601039206     -1.4825610291     -3.6112498125
   H30       3.5241459795      0.3321462181     -2.0273647060
   C8        0.2444275768     -0.6476496065      0.2883165349
   H32      -0.6354004276     -2.5936217966     -0.0228418196
   C10      -0.3830287784      0.2576910899      1.3234829307
   N2        1.3296985246      0.0065527973     -0.2961160580
   C9        1.6190886794      1.2430987080      0.2263345077
   O1        2.5425730769      1.9496310973     -0.1077971456
   H43      -0.3662424600     -0.2210625444      2.2933013467
 C12      -1.8167080643      0.6206555444      0.9733676575
 C11       0.5811843550      1.4983172005      1.3298749907
 C18       1.3236511200      1.6854695713      2.6674527418
 H48       0.0355598932      2.4006846895      1.0914397457
 C13      -3.4435010259      1.4260073169     -0.6079216112
 C14      -4.1283552859      0.8417968781      1.6117041540
 C15      -4.4428476458      1.3060953669      0.3476532957
 C16      -2.8193215751      0.5012118945      1.9213524917
 C17      -2.1416529372      1.0841747355     -0.2974143576
 H51      -5.4530667511      1.5665501699      0.1044683608
 H52      -2.5843705111      0.1375866592      2.9031055975
 H55      -3.6816104404      1.7776198332     -1.5918554636
 H56      -4.8944365154      0.7394763208      2.3542858101
 H59      -1.3762357040      1.1606002751     -1.0444961466
 H60       1.8481366833      0.7770713691      2.9426397013
 H61       0.6217691853      1.9341274667      3.4555084934
 H62       2.0440604976      2.4879423273      2.5745757944

 nuclear repulsion energy.......  1446.844283190 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  13   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.217E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     85     85
 grid # 2       106     99     97     98     98     99     91     92
 grid # 3       224    183    183    194    182    182    187    182
 grid # 4       224    379    380    407    379    379    374    377

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     81    100     76
 grid # 2       106    106    105     91    106     93    109     80
 grid # 3       224    224    220    188    223    175    223    165
 grid # 4       224    224    218    374    228    348    400    334

 number of gridpoints:
    atom         O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1       111     68     90     82     71     69     88     87
 grid # 2       127     98    105     94     76     99    100    100
 grid # 3       272    209    193    175    148    215    183    183
 grid # 4       473    201    400    352    306    208    379    379

 number of gridpoints:
    atom        C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1        89     87     86     73     73     73     73     70
```

```
  grid # 2      100    100     96    106    104    106    106    101
  grid # 3      183    182    181    224    214    224    224    215
  grid # 4      379    378    376    224    214    224    224    214

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2821
  grid # 2       99     99     99   3491
  grid # 3      217    220    220   7041
  grid # 4      218    222    221  10841

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change   change    error

etot   1  N  N  1  U  -815.14149424438              1.4E-04  3.6E-03
etot   2  Y  Y  4  M  -815.14216459325  6.7E-04  4.9E-05  1.0E-03
etot   3  Y  Y  4  M  -815.14223278719  6.8E-05  1.6E-05  3.5E-04
etot   4  Y  Y  4  M  -815.14223995311  7.2E-06  6.3E-06  1.5E-04
etot   5  Y  Y  4  M  -815.14224081391  8.6E-07  2.2E-06  5.3E-05
etot   6  N  N  1  U  -815.14224334138  2.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1446.84428318973
   (E)  Total one-electron terms..... -3979.18371144226
   (I)  Total two-electron terms.....  1717.19718491114
   (L)  Electronic energy............ -2261.98652653112  (E+I)
   (N)  Total energy.................  -815.14224334138  (A+L)

 SCFE: SCF energy: HF    -815.14224334138 hartrees   iterations:   6


 HOMO energy:    -0.29654
 LUMO energy:     0.11796

  Orbital energies:
  -20.45227  -15.55257  -11.32177  -11.23587  -11.22238  -11.21360
  -11.20718  -11.20055  -11.18774  -11.18603  -11.18552  -11.18503
  -11.18357  -11.18321  -11.17902  -11.17694  -11.17678  -11.17653
  -11.17533  -11.17234   -1.42293   -1.33329   -1.18043   -1.16234
   -1.11547   -1.08820   -1.04094   -1.02744   -1.02007   -1.00000
   -0.94674   -0.90584   -0.85546   -0.84376   -0.83109   -0.81144
   -0.79426   -0.76214   -0.72100   -0.68955   -0.67902   -0.66925
   -0.65827   -0.64122   -0.63977   -0.62705   -0.61176   -0.60580
   -0.60410   -0.60113   -0.59179   -0.57676   -0.55927   -0.55465
   -0.54109   -0.53107   -0.51674   -0.50801   -0.49952   -0.49650
   -0.49091   -0.48653   -0.45909   -0.42171   -0.39337   -0.34949
   -0.34226   -0.31539   -0.29654    0.11796    0.13398    0.13979
    0.14373    0.20530    0.22619    0.26461    0.27082    0.27323
    0.30011

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     1.179817E-04   4.866811E-04   2.915231E-04
   2    C1     -1.235021E-03   2.241895E-05   1.895621E-04
   3    C2     -2.771048E-04  -5.719622E-04  -5.936928E-04
   4    C3      7.221481E-04  -4.451166E-04   5.015560E-04
   5    C4      3.836452E-04   6.637549E-04   5.597747E-04
   6    C5     -5.791712E-04   1.000569E-03   7.709635E-04
   7    C6      5.878341E-04  -7.244541E-04  -5.787658E-04
   8    C7     -1.070790E-03   1.383827E-04  -1.274090E-03
   9    H27     1.491187E-04   2.314319E-06  -8.848191E-06
  10    H28     9.134500E-04   2.867911E-06  -7.500650E-04
  11    H30     3.900779E-04  -4.435394E-04  -2.741252E-04
  12    C8      1.257371E-04   6.584917E-04   5.335397E-04
  13    H32     1.245686E-04   4.140946E-04  -7.694066E-05
  14    C10     1.188972E-03  -4.449516E-04  -1.066796E-04
  15    N2     -2.217309E-04  -6.400183E-04  -2.994458E-04
  16    C9      3.091174E-04   1.062786E-03   1.765236E-04
  17    O1     -7.617849E-04  -9.212584E-04   3.047989E-04
  18    H43     2.658259E-04  -7.234424E-05   3.234769E-04
  19    C12    -5.893941E-04  -1.855076E-04  -2.801349E-04
  20    C11     6.093686E-04   2.864218E-04   3.107997E-04
  21    C18    -1.398873E-03   2.433899E-04   1.013341E-04
  22    H48     3.812528E-04  -2.835115E-04  -4.969214E-04
  23    C13     3.758253E-04  -2.281232E-04   6.800739E-04
  24    C14     1.902920E-04   2.699950E-04  -8.370655E-04
  25    C15     4.579277E-04  -3.961056E-04   7.617007E-04
  26    C16    -2.208390E-04   3.710826E-04  -3.723683E-04
  27    C17     2.152106E-04  -7.800421E-05   5.608093E-04
  28    H51    -2.809388E-04   1.376977E-04  -2.026562E-05
  29    H52    -4.240987E-05   2.612596E-05  -7.924644E-06
  30    H55     1.239186E-05   1.188466E-04  -3.692739E-05
  31    H56    -5.321630E-05   1.356248E-04   2.327213E-05
  32    H59    -9.669621E-05  -1.373468E-05  -1.292145E-04
  33    H60     9.105557E-05   3.205210E-04  -2.740002E-04
  34    H61     3.787267E-04  -7.804601E-05  -3.885609E-04
  35    H62     2.244349E-04  -1.041814E-04  -3.586584E-05
 -----------   -------------  -------------  -------------
    total       1.386993E-03   7.312069E-04  -7.521941E-04

  end of program der1b
```

```
start of program geopt  14

geometry optimization step 14
reading input hessian of dimension   105
 in five columns format
reading input hessian of dimension   105
 in five columns format

Hessian eigenvalues:
 -2.97418E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    2.63127E-03    1.83963E-02    1.90283E-02
  2.43600E-02    2.82220E-02    2.96024E-02    3.06129E-02    3.09529E-02
  3.17052E-02    3.73316E-02    4.43038E-02    4.53679E-02    4.82289E-02
  5.93986E-02    6.50534E-02    7.10790E-02    7.19334E-02    7.51098E-02
  8.05618E-02    9.29380E-02    1.04526E-01    1.05953E-01    1.12179E-01
  1.15527E-01    1.23756E-01    1.27717E-01    1.38944E-01    1.42585E-01
  1.49171E-01    1.52284E-01    1.54516E-01    1.55982E-01    1.63659E-01
  1.71930E-01    1.76443E-01    1.81932E-01    1.85501E-01    1.95030E-01
  2.02172E-01    2.05498E-01    2.09726E-01    2.15266E-01    2.18817E-01
  2.22371E-01    2.28154E-01    2.31477E-01    2.45502E-01    2.48159E-01
  2.54514E-01    2.62812E-01    2.64579E-01    2.82061E-01    2.86060E-01
  2.88147E-01    2.98442E-01    2.99841E-01    3.09865E-01    3.13554E-01
  3.16553E-01    3.20555E-01    3.27186E-01    3.28041E-01    3.33675E-01
  3.34939E-01    3.35987E-01    3.39925E-01    3.48837E-01    3.55004E-01
  3.56475E-01    3.64348E-01    3.67695E-01    3.72464E-01    3.74847E-01
  3.83739E-01    3.89854E-01    4.03506E-01    4.05744E-01    4.15961E-01
  4.23465E-01    4.29602E-01    4.40586E-01    4.53439E-01    4.55371E-01
  4.61758E-01    4.76220E-01    4.87989E-01    4.96019E-01    5.06823E-01
  5.23366E-01    5.59003E-01    5.79574E-01    6.20808E-01    6.75828E-01
  7.16385E-01    7.37925E-01    7.84620E-01    1.08451E+00    1.27755E+00

WARNING: Hessian has wrong number of negative eigenvalues


Level shifts adjusted to satisfy step-size constraints
 Step size:    0.0375488
 Cos(theta):   0.6951004

 Final level shift:  -6.9066508E-02

energy change:           4.1778E-05 *  (  5.0000E-05 )
gradient maximum:        1.6601E-03 .  (  4.5000E-04 )
gradient rms:            4.7825E-04 .  (  3.0000E-04 )
step size:   0.03755  trust radius:   0.03750
displacement maximum:    1.6080E-02 .  (  1.8000E-03 )
displacement rms:        3.3585E-03 .  (  1.2000E-03 )
predicted energy change:    -1.1847E-04    geom step:   3.7549E-02    full step:
3.7549E-02
molecular structure not yet converged...

center of mass moved by:
   x:     2.5025E-03     y:    -1.8247E-03     z:    -2.1789E-04

new geometry:
                              angstroms
atom            x                 y                 z
H25       0.9589695046     -3.9191206159     -2.1987768391
C1        1.5157997707     -3.0044661203     -2.1589845316
```

```
 C2        3.0026280297     -0.6010594024     -2.0735006242
 C3        1.1572307715     -1.9937575446     -1.2766036420
 C4        2.6038166599     -2.8052935157     -2.9864837734
 C5        3.3410342525     -1.6180797162     -2.9426214909
 C6        1.9100404655     -0.8108990893     -1.2568789389
 C7        0.0951531335     -1.8551669208     -0.2753875450
 H27       2.8926170419     -3.5737084202     -3.6754352570
 H28       4.1821227047     -1.4968870892     -3.5953345921
 H30       3.5469285212      0.3177749450     -2.0129824400
 C8        0.2418523574     -0.6438554310      0.2775506822
 H32      -0.6538219067     -2.5791501559     -0.0499838853
 C10      -0.3827996017      0.2582442755      1.3165353347
 N2        1.3332495877      0.0054208854     -0.3001184665
 C9        1.6250205200      1.2394457985      0.2271555077
 O1        2.5531538121      1.9404545161     -0.0990626140
 H43      -0.3633874063     -0.2244610111      2.2849663110
 C12      -1.8185589893      0.6215505971      0.9730325540
 C11       0.5812780371      1.4991091728      1.3231102103
 C18       1.3109740696      1.6976587815      2.6645913754
 H48       0.0365150297      2.3990433036      1.0743742548
 C13      -3.4544199043      1.4267342198     -0.5971209918
 C14      -4.1270750118      0.8404861564      1.6238270400
 C15      -4.4487705207      1.3053238789      0.3629989675
 C16      -2.8162842291      0.5007445739      1.9257385486
 C17      -2.1506708167      1.0857308231     -0.2947614348
 H51      -5.4605700154      1.5656266210      0.1251807352
 H52      -2.5764215386      0.1365405753      2.9060857829
 H55      -3.6982624878      1.7795610711     -1.5794644457
 H56      -4.8888042664      0.7375789349      2.3706843183
 H59      -1.3905551905      1.1628790517     -1.0471752601
 H60       1.8342053389      0.7921456412      2.9513475791
 H61       0.6025599111      1.9522647918      3.4445545631
 H62       2.0327365134      2.4990092717      2.5712906042

 nuclear repulsion energy.......  1446.685357034 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  14   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.212E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      98      91      92
 grid # 3       224    183     182     194     182     182     187     182
 grid # 4       224    379     381     406     379     379     372     377

 number of gridpoints:
      atom        H27     H28     H30      C8     H32     C10      N2      C9
   grid # 1        73      73      73      86      73      81     100      76
   grid # 2       106     106     105      91     106      92     109      81
   grid # 3       224     224     220     188     223     175     223     165
   grid # 4       224     224     219     374     228     351     401     330

   number of gridpoints:
      atom         O1     H43     C12     C11     C18     H48     C13     C14
   grid # 1       111      68      90      82      71      70      88      87
   grid # 2       123      98     105      94      75      99     100     100
   grid # 3       272     209     193     174     141     215     183     183
   grid # 4       474     200     400     352     308     208     379     379

   number of gridpoints:
      atom        C15     C16     C17     H51     H52     H55     H56     H59
   grid # 1        89      87      86      73      73      73      73      70
   grid # 2       100     100      97     106     104     106     106     101
   grid # 3       183     182     181     224     214     224     224     215
   grid # 4       379     377     376     224     214     224     224     214

   number of gridpoints:
      atom        H60     H61     H62   total
   grid # 1        71      71      71    2822
   grid # 2        99      99      99    3487
   grid # 3       217     220     220    7032
   grid # 4       218     223     221   10842

   end of program grid


   start of program rwr
  recomputing RwR matrix  15    grid:  4
   end of program rwr


   start of program scf

       i  u  d  i  g
       t  p  i  c  r                                       RMS    maximum
       e  d  i  u  i                         energy  density   DIIS
       r  t  s  t  d     total energy        change  change     error

 etot   1  N  N  1  U  -815.14170113503            1.1E-04  3.7E-03
 etot   2  Y  Y  4  M  -815.14224578714  5.4E-04  4.5E-05  1.5E-03
 etot   3  Y  Y  4  M  -815.14230797425  6.2E-05  1.5E-05  4.6E-04
 etot   4  Y  Y  4  M  -815.14231339573  5.4E-06  4.3E-06  1.2E-04
 etot   5  Y  N  4  M  -815.14231612826  2.7E-06  0.0E+00  0.0E+00


  Energy components, in hartrees:
    (A)  Nuclear repulsion............  1446.68535703399
    (E)  Total one-electron terms..... -3978.86466946382
    (I)  Total two-electron terms.....  1717.03699630157
    (L)  Electronic energy............ -2261.82767316225  (E+I)
    (N)  Total energy.................  -815.14231612826  (A+L)

  SCFE: SCF energy: HF    -815.14231612826 hartrees   iterations:   5


  HOMO energy:    -0.29655
  LUMO energy:     0.11832
 Orbital energies:
 -20.45247  -15.55212  -11.32139  -11.23560  -11.22224  -11.21357
 -11.20688  -11.20049  -11.18749  -11.18592  -11.18538  -11.18494
 -11.18348  -11.18310  -11.17880  -11.17665  -11.17658  -11.17632
 -11.17530  -11.17224   -1.42408   -1.33327   -1.18063   -1.16263
  -1.11556   -1.08814   -1.04111   -1.02752   -1.02010   -1.00026
  -0.94681   -0.90573   -0.85548   -0.84377   -0.83111   -0.81124
  -0.79423   -0.76224   -0.72103   -0.68996   -0.67889   -0.66920
  -0.65834   -0.64106   -0.63997   -0.62707   -0.61184   -0.60619
  -0.60400   -0.60119   -0.59194   -0.57680   -0.55937   -0.55488
  -0.54100   -0.53115   -0.51670   -0.50806   -0.49959   -0.49653
  -0.49106   -0.48641   -0.45927   -0.42176   -0.39340   -0.34950
  -0.34248   -0.31528   -0.29655    0.11832    0.13423    0.13987
   0.14373    0.20559    0.22613    0.26464    0.27090    0.27320
   0.30015

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -8.025048E-05  -1.795033E-04   4.146906E-05
  2    C1     -1.409234E-04   3.505474E-04  -1.822963E-04
  3    C2      3.149233E-04   9.171207E-05  -2.950762E-04
  4    C3     -7.823079E-05  -3.377136E-04   4.745332E-04
  5    C4      2.346343E-04  -2.271952E-04   3.509597E-05
  6    C5      1.918872E-04   2.140402E-04  -3.111634E-04
  7    C6     -2.692367E-04   1.623176E-04   3.721926E-04
  8    C7     -4.910106E-04   2.691617E-04  -7.824689E-04
  9    H27     4.208542E-05  -6.633096E-05   3.193454E-05
 10    H28    -6.543623E-06  -9.775006E-06  -3.595065E-05
 11    H30     1.177477E-04  -9.060800E-05  -1.351522E-04
 12    C8     -4.770779E-04   5.362225E-04  -2.265859E-04
 13    H32     1.263171E-04   1.448655E-04  -4.217583E-05
 14    C10     7.571020E-04  -3.820697E-04  -2.697170E-04
 15    N2     -2.619029E-05  -7.668667E-04   2.703872E-04
 16    C9     -9.793730E-04  -7.803880E-04   8.537382E-04
 17    O1      1.629758E-03   1.111533E-03  -4.626050E-04
 18    H43     4.365384E-04   1.957163E-04  -3.310185E-06
 19    C12     9.077640E-05  -5.568121E-04   3.856700E-04
 20    C11    -2.785692E-04   1.674835E-04   1.968460E-04
 21    C18    -6.521093E-04   9.195429E-05   1.361220E-04
 22    H48     1.762756E-04  -1.495686E-04  -5.976015E-04
 23    C13     1.412589E-04   8.196726E-05  -9.370457E-05
 24    C14     1.403468E-04   8.737614E-05  -1.275262E-05
 25    C15     9.059954E-05  -5.327267E-05   6.143330E-05
 26    C16    -2.433591E-04   2.510468E-04   8.712440E-05
 27    C17     1.591009E-04   2.679170E-05  -1.843492E-05
 28    H51    -8.903734E-05   8.069521E-05   9.095047E-06
 29    H52     2.091611E-05   1.818073E-05  -1.471576E-05
 30    H55     7.355751E-05   3.488312E-05   7.478818E-05
 31    H56    -5.746227E-05   5.823815E-05   1.023537E-04
 32    H59     5.975291E-06   6.814520E-06  -3.284648E-05
 33    H60     5.230320E-05   2.616353E-04  -1.651178E-04
 34    H61     3.268409E-04  -2.977286E-05  -3.066233E-04
 35    H62     1.107722E-04  -4.860867E-05   1.566509E-05
-----------   -------------  -------------  -------------
   total       1.370343E-03   5.646977E-04  -8.398501E-04

 end of program der1b


 start of program geopt  15

 geometry optimization step 15
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.16865E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    2.24865E-03    6.17521E-03    2.03372E-02
   2.28466E-02    2.82016E-02    2.95058E-02    3.04158E-02    3.08239E-02
   3.14464E-02    3.73674E-02    4.44871E-02    4.49529E-02    4.81535E-02
   6.01426E-02    6.42246E-02    7.09405E-02    7.16561E-02    7.39448E-02
   8.35376E-02    9.14068E-02    9.60798E-02    1.04420E-01    1.12159E-01
   1.13063E-01    1.21838E-01    1.36531E-01    1.38116E-01    1.41806E-01
   1.43189E-01    1.51188E-01    1.54812E-01    1.56221E-01    1.62468E-01
   1.73250E-01    1.80272E-01    1.83818E-01    1.85391E-01    1.90626E-01
   2.00924E-01    2.03598E-01    2.12704E-01    2.15711E-01    2.19584E-01
   2.25173E-01    2.32776E-01    2.40499E-01    2.46385E-01    2.50839E-01
   2.53010E-01    2.61928E-01    2.63572E-01    2.72997E-01    2.89038E-01
   2.92838E-01    2.97757E-01    3.03365E-01    3.10116E-01    3.10285E-01
   3.15249E-01    3.22864E-01    3.25237E-01    3.29462E-01    3.34166E-01
   3.35666E-01    3.37742E-01    3.42882E-01    3.48691E-01    3.53683E-01
   3.59917E-01    3.64845E-01    3.78690E-01    3.83184E-01    3.86408E-01
   3.94975E-01    4.03419E-01    4.05910E-01    4.16094E-01    4.23411E-01
   4.30353E-01    4.35163E-01    4.53803E-01    4.58307E-01    4.61693E-01
   4.66577E-01    4.87167E-01    4.97582E-01    5.03693E-01    5.22749E-01
   5.31423E-01    5.81086E-01    5.94415E-01    6.48742E-01    6.88192E-01
   7.05064E-01    7.29895E-01    8.48785E-01    1.06634E+00    1.42378E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0537587
  Cos(theta):   0.7523557

  Final level shift:  -4.2249227E-02

 energy change:           -7.2787E-05 .  (  5.0000E-05 )
 gradient maximum:         1.9722E-03 .  (  4.5000E-04 )
 gradient rms:             3.0998E-04 .  (  3.0000E-04 )
 step size:   0.05376  trust radius:   0.05303
 displacement maximum:     2.3073E-02 .  (  1.8000E-03 )
```

```
  displacement rms:        4.8083E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.3114E-04    geom step:   5.3758E-02    full step:
5.3758E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.0467E-03     y:    -3.6590E-03     z:     1.1536E-03

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.9464246191     -3.9104500176     -2.2213508009
  C1        1.5111468239     -3.0004541363     -2.1739024670
  C2        3.0190054840     -0.6107595698     -2.0665858253
  C3        1.1532106891     -1.9904717079     -1.2896703181
  C4        2.6090102518     -2.8079848559     -2.9917960682
  C5        3.3558419245     -1.6270903345     -2.9377466029
  C6        1.9169593416     -0.8141927235     -1.2584020109
  C7        0.0833013311     -1.8470465407     -0.2980641099
  H27       2.8972678578     -3.5763464050     -3.6809112157
  H28       4.2027774827     -1.5098868331     -3.5841704762
  H30       3.5717810467      0.3025681022     -1.9987604082
  C8        0.2369179753     -0.6397560314      0.2630442074
  H32      -0.6739179651     -2.5656947773     -0.0822946124
  C10      -0.3846281323      0.2586676522      1.3058823131
  N2        1.3386005592      0.0021416272     -0.3025163871
  C9        1.6369649032      1.2318648702      0.2329939987
  O1        2.5795114971      1.9241326233     -0.0781883160
  H43      -0.3601341219     -0.2269978617      2.2729930481
  C12      -1.8223203601      0.6230584314      0.9719009211
  C11       0.5798060189      1.4999002708      1.3141009327
  C18       1.2906894515      1.7175712928      2.6618451733
  H48       0.0362741124      2.3956535638      1.0474814929
  C13      -3.4697283652      1.4294168195     -0.5850213941
  C14      -4.1277001005      0.8420339496      1.6396501862
  C15      -4.4581094092      1.3072590736      0.3815722581
  C16      -2.8145254152      0.5020863477      1.9313711553
  C17      -2.1632864258      1.0882648449     -0.2926419091
  H51      -5.4719338530      1.5673933922      0.1508194639
  H52      -2.5685683397      0.1360351276      2.9095281178
  H55      -3.7201156665      1.7829178294     -1.5653303263
  H56      -4.8844683413      0.7379516967      2.3918860043
  H59      -1.4092127132      1.1658628911     -1.0507898874
  H60       1.8123781797      0.8172020443      2.9675454150
  H61       0.5710810235      1.9816298086      3.4282224194
  H62       2.0137114338      2.5187121183      2.5682871097

  nuclear repulsion energy.......  1445.663368389 hartrees
  --------------------------------------------------
 /  end of geometry optimization iteration  15   /
 --------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.217E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom         H25     C1      C2      C3      C4      C5      C6      C7
  grid # 1         73     89      87      90      87      87      85      85
  grid # 2        106    100      97      98      98      98      91      92
  grid # 3        224    183     182     194     182     182     187     183
  grid # 4        224    379     381     404     379     379     374     378

  number of gridpoints:
     atom         H27    H28     H30      C8     H32     C10      N2      C9
  grid # 1         73     73      73      86      73      82     100      76
  grid # 2        106    106     105      91     106      92     109      81
  grid # 3        224    224     220     188     223     175     223     165
  grid # 4        224    224     219     374     228     351     402     332

  number of gridpoints:
     atom          O1    H43     C12     C11     C18     H48     C13     C14
  grid # 1        111     68      90      81      71      70      87      87
  grid # 2        127     98     105      93      76      99     100     100
  grid # 3        272    209     193     172     149     215     183     183
  grid # 4        473    200     401     352     306     208     379     379

  number of gridpoints:
     atom         C15    C16     C17     H51     H52     H55     H56     H59
  grid # 1         89     87      86      73      73      73      73      70
  grid # 2        100     99      97     106     104     106     106     101
  grid # 3        183    182     181     224     214     224     224     215
  grid # 4        379    377     376     224     214     224     224     214

  number of gridpoints:
     atom         H60    H61     H62   total
  grid # 1         71     71      71    2821
  grid # 2         99     99      99    3490
  grid # 3        217    220     220    7039
  grid # 4        218    223     221   10844

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                       RMS    maximum
       e  d  i  u  i                             energy  density   DIIS
       r  t  s  t  d      total energy           change  change    error

etot   1  N  N  1  U  -815.14120200169                   1.5E-04  4.2E-03
etot   2  Y  Y  4  M  -815.14219652930   9.9E-04  5.9E-05  1.7E-03
etot   3  Y  Y  4  M  -815.14230765529   1.1E-04  1.9E-05  5.1E-04
etot   4  Y  Y  4  M  -815.14231403103   6.4E-06  5.0E-06  1.3E-04
etot   5  Y  N  4  M  -815.14231592662   1.9E-06  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
  (A)  Nuclear repulsion............  1445.66336838851
  (E)  Total one-electron terms..... -3976.82146986510
  (I)  Total two-electron terms.....  1716.01578554997
  (L)  Electronic energy............ -2260.80568431513  (E+I)
  (N)  Total energy.................  -815.14231592662  (A+L)

SCFE: SCF energy: HF    -815.14231592662 hartrees   iterations:   5


HOMO energy:    -0.29653
LUMO energy:     0.11818

 Orbital energies:
 -20.45245  -15.55237  -11.32175  -11.23581  -11.22244  -11.21384
 -11.20715  -11.20079  -11.18759  -11.18611  -11.18553  -11.18512
 -11.18371  -11.18329  -11.17902  -11.17683  -11.17679  -11.17622
 -11.17549  -11.17244   -1.42270   -1.33306   -1.18060   -1.16237
  -1.11552   -1.08804   -1.04112   -1.02755   -1.01983   -1.00032
  -0.94689   -0.90581   -0.85521   -0.84383   -0.83134   -0.81092
  -0.79421   -0.76206   -0.72101   -0.69020   -0.67883   -0.66918
  -0.65820   -0.64096   -0.63998   -0.62698   -0.61152   -0.60586
  -0.60378   -0.60134   -0.59200   -0.57680   -0.55877   -0.55515
  -0.54085   -0.53113   -0.51657   -0.50795   -0.49968   -0.49638
  -0.49112   -0.48640   -0.45906   -0.42197   -0.39328   -0.34953
  -0.34270   -0.31511   -0.29653    0.11818    0.13419    0.13935
   0.14334    0.20532    0.22581    0.26463    0.27091    0.27324
   0.29988

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.570739E-04   8.424059E-05  -7.381299E-05
  2    C1      3.186481E-04   2.333582E-04  -4.029628E-04
  3    C2     -4.969000E-04  -1.767584E-04   2.013582E-04
  4    C3      5.982224E-04  -2.945436E-04  -4.549820E-04
  5    C4     -6.454716E-04  -1.267695E-04   6.634476E-04
  6    C5     -1.455411E-04   3.567310E-04   7.264008E-05
  7    C6      3.202791E-04  -2.516367E-04  -2.954228E-04
  8    C7     -3.911236E-04   6.651443E-04  -3.578150E-04
  9    H27    -4.182916E-05  -1.428398E-04   1.918705E-05
 10    H28    -1.778199E-04  -4.945258E-05   2.082284E-04
 11    H30    -4.020726E-05  -5.756403E-05   2.784976E-05
 12    C8     -5.462853E-04  -4.611201E-04  -9.405994E-04
 13    H32     2.674490E-04   2.811162E-04  -6.183473E-05
 14    C10     7.834954E-04   3.322594E-05   4.515573E-04
 15    N2      7.767932E-04   3.637155E-04   3.509830E-04
 16    C9      1.694126E-03   2.552446E-04  -8.182069E-05
 17    O1     -1.554054E-03  -1.060326E-03   4.584320E-04
 18    H43     4.465841E-04   1.287624E-04  -6.478301E-05
 19    C12    -5.266706E-04  -5.829531E-04   9.650472E-04
 20    C11    -1.024872E-04   7.583695E-04  -2.155732E-04
 21    C18    -2.878586E-04   1.661926E-04   3.783266E-04
 22    H48     2.116432E-04  -1.094423E-04  -6.231249E-04
 23    C13     1.454765E-04   6.164526E-05  -6.507602E-05
 24    C14     3.927815E-04  -1.460863E-04   2.194062E-04
 25    C15     1.443101E-04   1.834018E-04  -4.120524E-04
 26    C16     1.106905E-04   7.025176E-05   1.362942E-04
 27    C17    -4.213989E-04   1.387119E-04  -1.546211E-04
 28    H51     1.690670E-04   5.178363E-05  -2.218872E-05
 29    H52     1.136166E-04   6.716084E-05  -4.154337E-06
 30    H55     3.284630E-06   6.966898E-05  -2.961049E-05
 31    H56     1.932974E-04   9.192205E-05  -4.268338E-05
 32    H59     1.447218E-04   2.944065E-05  -1.282085E-04
 33    H60    -1.445779E-04   2.787547E-04  -1.360400E-04
 34    H61     4.126012E-04  -7.978368E-05  -1.786583E-04
 35    H62    -3.748518E-04  -3.139767E-04  -1.249488E-04
-----------   -------------  -------------  -------------
   total       1.507085E-03   5.155893E-04  -7.182163E-04

 end of program der1b


 start of program geopt  16

 geometry optimization step 16
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -4.38427E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.63852E-03    4.69712E-03    2.10648E-02
   2.15102E-02    2.80567E-02    2.90900E-02    3.05050E-02    3.06261E-02
   3.17325E-02    3.72670E-02    3.84317E-02    4.43567E-02    4.77655E-02
   6.14351E-02    6.76064E-02    7.07438E-02    7.26910E-02    7.47792E-02
   8.39751E-02    8.81213E-02    9.68901E-02    1.04232E-01    1.10696E-01
   1.12257E-01    1.29101E-01    1.32116E-01    1.37281E-01    1.42455E-01
   1.44673E-01    1.49828E-01    1.53236E-01    1.56664E-01    1.65392E-01
   1.66210E-01    1.76449E-01    1.81084E-01    1.86503E-01    1.87763E-01
   1.99946E-01    2.05382E-01    2.12337E-01    2.14853E-01    2.17211E-01
   2.24082E-01    2.30289E-01    2.31641E-01    2.38003E-01    2.46956E-01
   2.57112E-01    2.61366E-01    2.66748E-01    2.72468E-01    2.79900E-01
   2.92132E-01    2.98016E-01    3.01860E-01    3.09506E-01    3.13687E-01
   3.17064E-01    3.21902E-01    3.25311E-01    3.28604E-01    3.33082E-01
   3.36230E-01    3.37463E-01    3.46266E-01    3.51421E-01    3.56689E-01
   3.58814E-01    3.64430E-01    3.73422E-01    3.80993E-01    3.89561E-01
   3.98501E-01    4.03973E-01    4.13525E-01    4.19958E-01    4.23882E-01
   4.33310E-01    4.47536E-01    4.50427E-01    4.57800E-01    4.67255E-01
   4.79486E-01    5.00022E-01    5.06475E-01    5.12319E-01    5.30358E-01
   5.69119E-01    5.93412E-01    6.20045E-01    6.54845E-01    7.21719E-01
   7.35608E-01    7.54020E-01    8.18619E-01    1.05199E+00    1.49250E+00
  WARNING: Hessian has wrong number of negative eigenvalues
  WARNING: positive P-RFO shift not converged: using initial-guess shift


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0750251
   Cos(theta):   0.1128800

   Final level shift:  -4.4082528E-01

  energy change:           2.0163E-07 !  (  5.0000E-05 )
  gradient maximum:        1.9857E-03 .  (  4.5000E-04 )
  gradient rms:            3.7383E-04 .  (  3.0000E-04 )
  step size:   0.07503  trust radius:   0.07500
  displacement maximum:    2.6324E-02 .  (  1.8000E-03 )
  displacement rms:        6.7104E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.2583E-03    geom step:   7.5025E-02    full step:
7.5025E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.3259E-04     y:     1.1815E-03     z:     2.6723E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25        0.9289584197     -3.8896118279     -2.2181338061
  C1         1.4943447819     -2.9902717573     -2.1748002361
  C2         3.0045499141     -0.5995714175     -2.0710983457
  C3         1.1472377419     -1.9771282779     -1.2951797558
  C4         2.5826381262     -2.7945961631     -2.9887733519
  C5         3.3276208327     -1.6183629817     -2.9350836699
  C6         1.9143345342     -0.8039334713     -1.2708367124
  C7         0.0771172003     -1.8400623931     -0.3003845095
  H27        2.8692958711     -3.5637687145     -3.6795090569
  H28        4.1743458393     -1.5217667366     -3.5876596717
  H30        3.5633387732      0.3033850213     -2.0106191293
  C8         0.2390027606     -0.6375437226      0.2669857332
  H32       -0.6810454354     -2.5563613245     -0.0859189390
  C10       -0.3759700394      0.2532772353      1.3145221304
  N2         1.3435970121      0.0022548278     -0.3010169525
  C9         1.6450143655      1.2303194551      0.2409885441
  O1         2.5918995738      1.9174012940     -0.0696289198
  H43       -0.3532115848     -0.2408631992      2.2839204722
  C12       -1.8176115657      0.6223659547      0.9807619046
  C11        0.5915033106      1.4962278274      1.3260768549
  C18        1.3016969717      1.7291171271      2.6669559709
  H48        0.0511760374      2.3954376522      1.0680212327
  C13       -3.4456611495      1.4045945394     -0.5928361865
  C14       -4.1355539217      0.8348959727      1.6261336407
  C15       -4.4492366591      1.2880056812      0.3649499759
  C16       -2.8264498641      0.5025933721      1.9297183894
  C17       -2.1439142415      1.0734909458     -0.2884747832
  H51       -5.4628207751      1.5443898162      0.1173058585
  H52       -2.5996009206      0.1318979101      2.9058886539
  H55       -3.6845259432      1.7532818558     -1.5819183038
  H56       -4.9022207663      0.7363122460      2.3730346815
  H59       -1.3880959164      1.1359441821     -1.0548769048
  H60        1.8347948787      0.8336866210      2.9750604510
  H61        0.5829306047      1.9951590797      3.4326146022
  H62        2.0246703066      2.5331126107      2.5652961958
```

```
 nuclear repulsion energy.......  1447.431432624 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  16   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.178E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     89     90     87     87     84     85
 grid # 2      106     99     99     98     98     98     91     92
 grid # 3      224    183    182    194    182    182    185    183
 grid # 4      224    376    379    404    379    379    368    376

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     86     73     81     99     76
 grid # 2      106    106    105     91    106     92    109     81
 grid # 3      224    224    220    186    223    175    223    164
 grid # 4      224    224    219    378    228    352    401    328

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      111     69     90     81     72     68     86     87
 grid # 2      127     98    106     94     74    100     98     99
 grid # 3      272    208    193    173    139    216    183    183
 grid # 4      473    201    401    358    308    205    380    380

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1       87     86     85     73     73     73     73     71
 grid # 2       99     99     97    106    104    106    106    101
 grid # 3      183    181    181    224    215    224    224    215
 grid # 4      378    374    378    224    215    224    224    212

 number of gridpoints:
    atom       H60    H61    H62  total
 grid # 1       71     71     71   2816
 grid # 2       99     99     99   3488
 grid # 3      218    220    220   7026
 grid # 4      218    223    221  10836

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
recomputing RwR matrix  20    grid:  4
```

```
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  1  U  -815.14026970350            2.2E-04  2.9E-03
etot   2  Y  Y  4  M  -815.14119249524  9.2E-04  5.7E-05  7.8E-04
etot   3  Y  Y  4  M  -815.14126661934  7.4E-05  2.1E-05  2.3E-04
etot   4  Y  Y  4  M  -815.14127482102  8.2E-06  9.1E-06  1.3E-04
etot   5  Y  Y  4  M  -815.14127612194  1.3E-06  3.1E-06  5.7E-05
etot   6  N  N  1  U  -815.14127287773 -3.2E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1447.43143262418
   (E)  Total one-electron terms..... -3980.36089320291
   (I)  Total two-electron terms.....  1717.78818770099
   (L)  Electronic energy............ -2262.57270550192  (E+I)
   (N)  Total energy.................  -815.14127287773  (A+L)

 SCFE: SCF energy: HF    -815.14127287773 hartrees   iterations:   6


 HOMO energy:    -0.29650
 LUMO energy:     0.11867

  Orbital energies:
  -20.45196  -15.55155  -11.32147  -11.23535  -11.22123  -11.21472
  -11.20698  -11.20128  -11.18660  -11.18579  -11.18507  -11.18488
  -11.18335  -11.18316  -11.17631  -11.17618  -11.17596  -11.17444
  -11.17368  -11.17011   -1.42208   -1.33185   -1.18123   -1.16494
   -1.11605   -1.08846   -1.04153   -1.02836   -1.02267   -1.00128
   -0.94695   -0.90513   -0.85536   -0.84233   -0.83187   -0.81211
   -0.79365   -0.76337   -0.72062   -0.69043   -0.67805   -0.66939
   -0.65829   -0.64023   -0.63968   -0.62757   -0.61493   -0.60623
   -0.60339   -0.60161   -0.59274   -0.57595   -0.55838   -0.55486
   -0.54064   -0.53097   -0.51587   -0.50779   -0.49971   -0.49631
   -0.49237   -0.48623   -0.45925   -0.42166   -0.39443   -0.35032
   -0.34233   -0.31621   -0.29650    0.11867    0.13518    0.14067
    0.14374    0.20599    0.22547    0.26409    0.27116    0.27333
    0.29998

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
 recomputing RwR matrix  20    grid:  4
  end of program rwr


  start of program der1b
 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -3.182148E-03  -5.791438E-03  -3.936352E-04
  2    C1     -2.321122E-03   5.052126E-03   3.465752E-03
  3    C2      4.985214E-03  -6.294323E-04  -4.848171E-03
  4    C3     -3.677428E-03  -3.088240E-03   3.616024E-04
  5    C4      4.019578E-03  -4.644853E-03  -5.577130E-03
  6    C5      7.804161E-03  -2.687728E-03  -8.144120E-03
  7    C6     -1.176219E-02  -3.702051E-04   1.317444E-02
  8    C7      2.484805E-03   2.257305E-03  -9.894787E-04
  9    H27     3.935654E-04   7.974040E-04   2.343719E-04
 10    H28    -6.752203E-04   1.681033E-03   1.141628E-03
 11    H30     1.944835E-03   3.987048E-03   8.797874E-04
 12    C8      1.566433E-03  -6.168732E-04  -2.276586E-03
 13    H32    -1.949085E-04  -5.757300E-04  -2.101582E-04
 14    C10    -1.542310E-03   9.756121E-04   6.581975E-03
 15    N2     -1.891823E-03   4.503349E-03   2.165183E-03
 16    C9      2.833826E-03  -1.791783E-03  -1.270455E-03
 17    O1     -2.257764E-03  -4.319169E-04   9.756649E-04
 18    H43     7.666361E-04   2.155396E-03  -3.362620E-03
 19    C12     5.204391E-04  -3.314306E-03   4.799107E-03
 20    C11    -1.429599E-03   1.611784E-03  -1.297786E-03
 21    C18     3.812273E-03  -1.900054E-03   1.936037E-03
 22    H48    -1.073620E-03  -3.762429E-04  -2.596776E-03
 23    C13    -6.806639E-03   3.036759E-03  -2.746038E-03
 24    C14    -1.247197E-03  -1.561032E-04   2.630014E-03
 25    C15    -9.456881E-04   2.937336E-03  -7.667763E-03
 26    C16     6.114122E-03  -9.035865E-04  -1.798210E-03
 27    C17     1.803647E-03   7.835260E-05  -5.156296E-03
 28    H51     2.126230E-03  -2.731267E-04   1.046543E-04
 29    H52     2.296745E-03  -4.690640E-04   3.202855E-03
 30    H55    -2.388165E-04  -1.162494E-03   2.589928E-03
 31    H56     1.920944E-03  -2.049787E-04  -1.432720E-03
 32    H59    -2.090497E-03   3.601520E-04   4.299304E-03
 33    H60    -1.326809E-03   1.365154E-03   4.705905E-04
 34    H61     5.680783E-04  -2.392318E-04   2.841900E-04
 35    H62    -2.137550E-03  -1.323336E-03  -1.465678E-04
-----------   -------------  -------------  -------------
   total       1.160206E-03  -1.519152E-04  -6.174285E-04

 end of program der1b


 start of program geopt  17

 geometry optimization step 17
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   16 **

 Hessian eigenvalues:
  -3.30224E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.69512E-03    7.38869E-03    1.97963E-02
```

```
    2.40255E-02    2.81534E-02    3.00017E-02    3.03010E-02    3.09412E-02
    3.18626E-02    3.70739E-02    4.39602E-02    4.61787E-02    5.03111E-02
    5.72984E-02    6.73999E-02    6.76515E-02    7.22182E-02    7.46345E-02
    7.87597E-02    9.39556E-02    9.89467E-02    1.05040E-01    1.10374E-01
    1.12866E-01    1.26272E-01    1.36114E-01    1.42279E-01    1.43484E-01
    1.47533E-01    1.52281E-01    1.54339E-01    1.56734E-01    1.67010E-01
    1.72112E-01    1.78776E-01    1.82328E-01    1.89342E-01    1.96299E-01
    2.01827E-01    2.04582E-01    2.12865E-01    2.17204E-01    2.18543E-01
    2.29677E-01    2.31469E-01    2.38792E-01    2.46765E-01    2.52012E-01
    2.54654E-01    2.64887E-01    2.70369E-01    2.78040E-01    2.87295E-01
    2.96207E-01    3.00488E-01    3.01852E-01    3.13176E-01    3.17083E-01
    3.21490E-01    3.25063E-01    3.28631E-01    3.29760E-01    3.32995E-01
    3.36410E-01    3.42601E-01    3.47231E-01    3.50606E-01    3.55206E-01
    3.64522E-01    3.71023E-01    3.79779E-01    3.85053E-01    3.86924E-01
    3.98321E-01    4.05671E-01    4.12733E-01    4.15693E-01    4.29985E-01
    4.32342E-01    4.42654E-01    4.55952E-01    4.64769E-01    4.74982E-01
    4.84493E-01    4.93326E-01    5.00073E-01    5.24181E-01    5.32266E-01
    5.56195E-01    5.89351E-01    6.13701E-01    6.59622E-01    7.18861E-01
    7.35175E-01    7.53097E-01    7.89095E-01    1.02095E+00    1.45214E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0384194
   Cos(theta):   0.6369791

   Final level shift:  -5.8782893E-02

  energy change:           1.0430E-03 .  (  5.0000E-05 )
  gradient maximum:        1.9857E-03 .  (  4.5000E-04 )
  gradient rms:            3.7383E-04 .  (  3.0000E-04 )
  step size:   0.03842  trust radius:   0.03750
  displacement maximum:    1.6279E-02 .  (  1.8000E-03 )
  displacement rms:        3.4363E-03 .  (  1.2000E-03 )
  predicted energy change:    -9.4525E-05    geom step:   3.8419E-02    full step:
3.8419E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.5511E-16     y:     6.7654E-17     z:     0.0000E+00

  new geometry:
                               angstroms
  atom           x                 y                  z
  H25       0.9366700265     -3.9028853138     -2.2395394086
  C1        1.5069057822     -2.9971821045     -2.1849638552
  C2        3.0294826243     -0.6183687952     -2.0598321763
  C3        1.1504306666     -1.9883581843     -1.2992595500
  C4        2.6112661450     -2.8091220300     -2.9950763652
  C5        3.3653553283     -1.6338300482     -2.9322984229
  C6        1.9214507868     -0.8175023480     -1.2593138203
  C7        0.0764887917     -1.8417493392     -0.3125367242
  H27       2.8989966587     -3.5772712427     -3.6848053574
  H28       4.2177901721     -1.5208170856     -3.5724712024
  H30       3.5879590716      0.2908371635     -1.9848815326
  C8        0.2356070138     -0.6383446340      0.2547140938
  H32      -0.6859415929     -2.5561157505     -0.1020242072
  C10      -0.3827821520      0.2582575353      1.3010474292
  N2        1.3442416754     -0.0011500289     -0.3029545504
  C9        1.6459387900      1.2249699857      0.2371143694
  O1        2.5928586189      1.9128395940     -0.0666879556
```

```
 H43      -0.3525184792     -0.2296284341      2.2672883663
 C12      -1.8221273467      0.6214821012      0.9736893717
 C11       0.5809594090      1.4999506116      1.3084109837
 C18       1.2789642592      1.7298375173      2.6602677778
 H48       0.0391150596      2.3934799853      1.0290076738
 C13      -3.4747845612      1.4274314607     -0.5784381618
 C14      -4.1249974144      0.8404140569      1.6492311931
 C15      -4.4596546821      1.3054403340      0.3919218549
 C16      -2.8108571434      0.5005304742      1.9369405011
 C17      -2.1675703461      1.0862517119     -0.2901958985
 H51      -5.4743817027      1.5654776057      0.1646351151
 H52      -2.5613805407      0.1354054548      2.9147477621
 H55      -3.7287868297      1.7809287152     -1.5580405409
 H56      -4.8791327135      0.7371264847      2.4041554071
 H59      -1.4157089849      1.1633393770     -1.0506936544
 H60       1.7993760625      0.8335883575      2.9776351844
 H61       0.5538583128      1.9989026916      3.4183483372
 H62       2.0009221680      2.5310268886      2.5658389805

 nuclear repulsion energy.......  1445.508147999 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  17   /
--------------------------------------------------


 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.214E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      85      85
 grid # 2       106     100      97      98      98      98      91      92
 grid # 3       224     183     182     194     182     182     187     183
 grid # 4       224     379     381     406     379     379     372     378

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      82     100      76
 grid # 2       106     106     105      91     106      92     109      80
 grid # 3       224     224     220     188     223     175     223     164
 grid # 4       224     224     219     374     228     351     402     332

 number of gridpoints:
    atom         O1     H43     C12     C11     C18     H48     C13     C14
 grid # 1       111      69      90      81      71      70      88      87
 grid # 2       127      98     105      93      78      99     100     100
 grid # 3       272     209     194     171     150     215     183     183
 grid # 4       473     200     400     352     306     208     379     379

 number of gridpoints:
    atom        C15     C16     C17     H51     H52     H55     H56     H59
```

```
  grid # 1       89     87     86     73     73     73     73     70
  grid # 2      100    100     97    106    104    106    106    101
  grid # 3      183    182    181    224    214    224    224    215
  grid # 4      379    377    376    224    214    224    224    212

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2823
  grid # 2       99     99     99   3492
  grid # 3      217    220    220   7039
  grid # 4      218    222    221  10840

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                          energy  density   DIIS
       r  t  s  t  d     total energy         change  change    error

etot   1  N  N  2  U  -815.14120544926          2.3E-04  3.7E-03
etot   2  Y  Y  6  M  -815.14229963769  1.1E-03  6.8E-05  1.3E-03
etot   3  Y  Y  6  M  -815.14240063709  1.0E-04  2.4E-05  4.4E-04
etot   4  Y  Y  6  M  -815.14240333278  2.7E-06  1.1E-05  2.0E-04
etot   5  Y  Y  6  M  -815.14240719045  3.9E-06  3.5E-06  6.9E-05
etot   6  N  N  2  U  -815.14262970700  2.2E-04  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1445.50814799889
   (E)  Total one-electron terms..... -3976.50431503215
   (I)  Total two-electron terms.....  1715.85353732626
   (L)  Electronic energy............ -2260.65077770589  (E+I)
   (N)  Total energy.................  -815.14262970700  (A+L)

 SCFE: SCF energy: HF    -815.14262970700 hartrees   iterations:   6


 HOMO energy:    -0.29660
 LUMO energy:     0.11827

  Orbital energies:
  -20.45241  -15.55235  -11.32149  -11.23574  -11.22249  -11.21378
  -11.20699  -11.20081  -11.18761  -11.18627  -11.18565  -11.18524
  -11.18376  -11.18345  -11.17895  -11.17681  -11.17673  -11.17583
  -11.17543  -11.17236   -1.42333   -1.33325   -1.18061   -1.16251
   -1.11557   -1.08822   -1.04112   -1.02763   -1.02001   -1.00039
   -0.94700   -0.90592   -0.85530   -0.84384   -0.83145   -0.81100
   -0.79421   -0.76208   -0.72102   -0.69044   -0.67884   -0.66920
   -0.65830   -0.64099   -0.64008   -0.62707   -0.61164   -0.60601
   -0.60393   -0.60148   -0.59206   -0.57692   -0.55876   -0.55525
   -0.54073   -0.53131   -0.51658   -0.50792   -0.49980   -0.49646
   -0.49121   -0.48642   -0.45918   -0.42193   -0.39339   -0.34963
   -0.34267   -0.31518   -0.29660    0.11827    0.13410    0.13925
    0.14317    0.20544    0.22574    0.26458    0.27088    0.27330
   0.29963

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
   1    H25     6.085692E-06  -1.870643E-04  -6.898939E-05
   2    C1      4.497896E-04   3.693031E-05  -6.479080E-04
   3    C2     -3.008053E-04  -9.938999E-05   9.608955E-05
   4    C3      2.290085E-04  -6.235991E-04  -4.483329E-04
   5    C4     -7.277382E-04  -4.840529E-04   4.870225E-04
   6    C5      3.830313E-04   4.777196E-04  -2.406587E-04
   7    C6      8.063741E-04   3.080345E-04  -1.094578E-04
   8    C7     -5.588610E-04   4.097632E-04  -1.487481E-04
   9    H27    -7.626640E-05  -8.842524E-05   5.492422E-05
  10    H28    -2.966574E-04   2.174867E-05   2.725932E-04
  11    H30    -2.628459E-05  -2.380873E-05   1.481522E-05
  12    C8     -4.066106E-04  -1.098953E-05  -6.154393E-04
  13    H32     1.157067E-04   1.180615E-04  -1.226810E-04
  14    C10     6.138316E-04  -1.386863E-04   4.346157E-04
  15    N2      3.039157E-04  -2.206831E-04   3.022041E-04
  16    C9      5.577019E-04   1.789495E-04   1.913350E-04
  17    O1     -2.871064E-04  -2.200467E-04   1.093937E-04
  18    H43     2.896994E-04   2.366219E-04  -2.728419E-04
  19    C12    -4.171111E-04  -5.881082E-04   9.312531E-04
  20    C11    -4.267134E-04   6.398246E-04  -9.444764E-05
  21    C18    -1.249866E-04   2.313846E-04  -1.354948E-04
  22    H48     2.838656E-04  -4.349902E-04  -5.523851E-04
  23    C13    -2.362666E-05   7.797889E-05  -4.267742E-06
  24    C14     3.430857E-04  -9.157796E-06   3.993001E-05
  25    C15     1.115285E-04   1.055584E-04  -2.743753E-04
  26    C16     1.304467E-04   2.060837E-04  -2.861160E-05
  27    C17    -3.363183E-04   7.343606E-05   7.102319E-05
  28    H51     2.406432E-04   3.318046E-05   8.640545E-06
  29    H52     9.783412E-05   7.271221E-05  -1.484886E-04
  30    H55     5.889580E-05  -1.140713E-05   1.158138E-04
  31    H56     1.569552E-04   6.378854E-05  -6.130711E-05
  32    H59     1.055457E-04   2.731150E-05  -1.010497E-04
  33    H60     1.038272E-04  -1.246032E-04  -3.867003E-05
  34    H61    -1.662217E-04   8.213011E-05   1.647212E-04
  35    H62    -3.450816E-05  -2.187049E-05  -1.262760E-04
-----------   -------------  -------------  -------------
   total        1.177956E-03   1.143351E-04  -9.460558E-04

 end of program der1b
 start of program geopt  18

 geometry optimization step 18
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -3.30199E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    1.69451E-03    7.38841E-03    1.97961E-02
   2.40257E-02    2.81534E-02    3.00017E-02    3.03009E-02    3.09412E-02
   3.18626E-02    3.70739E-02    4.39602E-02    4.61783E-02    5.03112E-02
   5.72984E-02    6.73999E-02    6.76516E-02    7.22182E-02    7.46345E-02
   7.87596E-02    9.39550E-02    9.89470E-02    1.05041E-01    1.10374E-01
   1.12866E-01    1.26272E-01    1.36114E-01    1.42279E-01    1.43484E-01
   1.47531E-01    1.52280E-01    1.54339E-01    1.56733E-01    1.67009E-01
   1.72113E-01    1.78777E-01    1.82328E-01    1.89341E-01    1.96299E-01
   2.01827E-01    2.04582E-01    2.12865E-01    2.17204E-01    2.18543E-01
   2.29677E-01    2.31469E-01    2.38791E-01    2.46765E-01    2.52012E-01
   2.54654E-01    2.64886E-01    2.70369E-01    2.78039E-01    2.87293E-01
   2.96206E-01    3.00488E-01    3.01852E-01    3.13175E-01    3.17083E-01
   3.21490E-01    3.25063E-01    3.28631E-01    3.29758E-01    3.32995E-01
   3.36409E-01    3.42600E-01    3.47231E-01    3.50606E-01    3.55206E-01
   3.64522E-01    3.71023E-01    3.79779E-01    3.85053E-01    3.86923E-01
   3.98320E-01    4.05670E-01    4.12734E-01    4.15693E-01    4.29985E-01
   4.32342E-01    4.42654E-01    4.55951E-01    4.64768E-01    4.74982E-01
   4.84493E-01    4.93325E-01    5.00072E-01    5.24180E-01    5.32266E-01
   5.56194E-01    5.89350E-01    6.13695E-01    6.59623E-01    7.18861E-01
   7.35167E-01    7.53095E-01    7.89091E-01    1.02095E+00    1.45214E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0750317
  Cos(theta):   0.6314568

  Final level shift:  -4.3557486E-02

 energy change:          -3.1378E-04 .  (  5.0000E-05 )
 gradient maximum:        1.1946E-03 .  (  4.5000E-04 )
 gradient rms:            3.0204E-04 .  (  3.0000E-04 )
 step size:   0.07503  trust radius:   0.07500
 displacement maximum:    2.4933E-02 .  (  1.8000E-03 )
 displacement rms:        6.7110E-03 .  (  1.2000E-03 )
 predicted energy change:    -2.0261E-04    geom step:   7.5032E-02    full step:
7.5032E-02
 molecular structure not yet converged...

 center of mass moved by:
    x:     8.3122E-03     y:    -6.7724E-03     z:     2.2632E-03

 new geometry:
                              angstroms
 atom            x                 y                 z
 H25       0.9509812428     -3.9122830054     -2.2518427039
 C1        1.5218481426     -3.0044329004     -2.1948050359
 C2        3.0476768605     -0.6260318891     -2.0537237868
 C3        1.1662190151     -1.9988511911     -1.3059426769
 C4        2.6231306466     -2.8127057375     -2.9997011658
 C5        3.3765948096     -1.6337231631     -2.9322049642
 C6        1.9411808324     -0.8292695008     -1.2526564701
 C7        0.0795537749     -1.8455278126     -0.3361182295
 H27       2.9123590680     -3.5758108679     -3.6935544192
 H28       4.2211956957     -1.5084378066     -3.5756498440
 H30       3.6093967045      0.2794460956     -1.9783296869
 C8        0.2347237855     -0.6433130655      0.2377984531
 H32      -0.6919701087     -2.5552966949     -0.1459483408
 C10      -0.3913884882      0.2470690004      1.2836901829
 N2        1.3490357641     -0.0112633259     -0.3060157452
 C9        1.6455918475      1.2189176093      0.2386763323
 O1        2.6066737330      1.8974831438     -0.0461581347
 H43      -0.3676198389     -0.2448480866      2.2452738844
 C12      -1.8303705291      0.6189500249      0.9634802027
 C11       0.5675903235      1.4933489759      1.2960669082
 C18       1.2381113786      1.7466876346      2.6551690571
 H48       0.0209546187      2.3748701014      0.9916051162
 C13      -3.4968309171      1.4434139296     -0.5615551419
 C14      -4.1144339896      0.8654650391      1.6743360392
 C15      -4.4652996310      1.3328820081      0.4224094422
 C16      -2.8034809368      0.5108228470      1.9404694615
 C17      -2.1907295212      1.0877996300     -0.2944947812
 H51      -5.4798255663      1.6045590611      0.2128771549
 H52      -2.5405817363      0.1443590370      2.9143181177
 H55      -3.7604936743      1.7981964911     -1.5370523238
 H56      -4.8576082491      0.7682975661      2.4427560734
 H59      -1.4512211253      1.1654238522     -1.0707686956
 H60       1.7613145438      0.8599251247      2.9975344820
 H61       0.4931838744      2.0201254508      3.3941462487
 H62       1.9545992533      2.5543799056      2.5649786060

 nuclear repulsion energy.......  1444.793128394 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  18   /
 ------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.207E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      84      85
 grid # 2       106      99      98      98      98      99      91      92
 grid # 3       224     183     182     195     182     182     187     182
 grid # 4       224     379     381     402     379     377     374     377

 number of gridpoints:
      atom        H27    H28    H30     C8    H32    C10     N2     C9
   grid # 1        73     73     73     86     73     81     99     77
   grid # 2       106    106    105     91    106     92    109     81
   grid # 3       224    224    220    190    223    175    223    165
   grid # 4       224    224    219    372    229    351    402    330

   number of gridpoints:
      atom         O1    H43    C12    C11    C18    H48    C13    C14
   grid # 1       111     68     90     81     71     69     86     87
   grid # 2       127     98    105     93     78     99     99     99
   grid # 3       272    209    193    171    149    216    183    183
   grid # 4       474    200    400    353    307    208    379    379

   number of gridpoints:
      atom        C15    C16    C17    H51    H52    H55    H56    H59
   grid # 1        89     85     85     73     73     73     73     70
   grid # 2       100     99     98    106    104    106    106    101
   grid # 3       183    182    181    224    214    224    224    216
   grid # 4       379    378    378    224    214    224    224    214

   number of gridpoints:
      atom        H60    H61    H62  total
   grid # 1        71     71     71   2814
   grid # 2        99     99     99   3492
   grid # 3       217    220    220   7042
   grid # 4       218    222    221  10840

   end of program grid


   start of program rwr
  recomputing RwR matrix  14    grid:  4
  recomputing RwR matrix  15    grid:  4
   end of program rwr


   start of program scf

        i  u  d  i  g
        t  p  i  c  r                                    RMS    maximum
        e  d  i  u  i                          energy  density   DIIS
        r  t  s  t  d     total energy        change  change    error

etot    1  N  N  1  U  -815.14043509785           2.1E-04  4.3E-03
etot    2  Y  Y  4  M  -815.14213811498  1.7E-03  8.0E-05  1.1E-03
etot    3  Y  Y  4  M  -815.14231624065  1.8E-04  2.8E-05  3.5E-04
etot    4  Y  Y  4  M  -815.14233004633  1.4E-05  1.1E-05  1.8E-04
etot    5  Y  Y  4  M  -815.14233439363  4.3E-06  4.2E-06  6.0E-05
etot    6  N  N  1  U  -815.14234091476  6.5E-06  0.0E+00  0.0E+00


  Energy components, in hartrees:
    (A)  Nuclear repulsion............  1444.79312839407
    (E)  Total one-electron terms..... -3975.06978645940
    (I)  Total two-electron terms.....  1715.13431715058
    (L)  Electronic energy........... -2259.93546930882  (E+I)
    (N)  Total energy.................  -815.14234091476  (A+L)

  SCFE: SCF energy: HF    -815.14234091476 hartrees   iterations:   6


  HOMO energy:    -0.29618
```

```
LUMO energy:     0.11872

 Orbital energies:
 -20.45306  -15.55236  -11.32226  -11.23522  -11.22226  -11.21364
 -11.20723  -11.20068  -11.18694  -11.18573  -11.18533  -11.18483
 -11.18398  -11.18314  -11.17846  -11.17621  -11.17614  -11.17584
 -11.17459  -11.17186   -1.42269   -1.33304   -1.18159   -1.16298
  -1.11610   -1.08726   -1.04156   -1.02859   -1.02046   -1.00066
  -0.94687   -0.90625   -0.85469   -0.84401   -0.83178   -0.81095
  -0.79459   -0.76228   -0.72127   -0.69118   -0.67878   -0.66931
  -0.65802   -0.64066   -0.64034   -0.62665   -0.61176   -0.60624
  -0.60416   -0.60173   -0.59175   -0.57760   -0.55842   -0.55580
  -0.54063   -0.53153   -0.51687   -0.50826   -0.49966   -0.49679
  -0.49101   -0.48629   -0.45950   -0.42254   -0.39310   -0.35050
  -0.34283   -0.31507   -0.29618    0.11872    0.13415    0.13946
   0.14352    0.20539    0.22565    0.26443    0.27131    0.27359
   0.29899

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     6.429836E-04   1.435730E-03  -1.663890E-04
  2    C1     -2.208926E-03  -2.243559E-03   1.324801E-03
  3    C2     -8.988649E-04   2.781811E-04   1.396494E-03
  4    C3     -4.144242E-04   2.861408E-03   1.265476E-03
  5    C4      3.237553E-03   1.537947E-03  -2.006512E-03
  6    C5     -4.954327E-04  -2.223491E-03  -7.544223E-04
  7    C6     -2.640582E-03   2.691410E-04  -8.081468E-04
  8    C7     -1.417013E-03  -1.301908E-04   5.456034E-04
  9    H27     1.117215E-04  -3.039393E-04  -3.442256E-04
 10    H28     1.631160E-03  -9.132043E-04  -1.165032E-03
 11    H30     1.230044E-04   1.133578E-03   3.495599E-04
 12    C8     -2.306530E-03  -2.755663E-03  -2.467396E-03
 13    H32     1.608802E-05  -1.284916E-04   6.884732E-04
 14    C10     5.424433E-04   1.636204E-03  -1.655539E-03
 15    N2      3.614240E-03   3.362112E-03   1.385707E-03
 16    C9      4.902873E-03  -3.357420E-03   6.457833E-04
 17    O1     -3.287106E-03  -7.217628E-04   3.544385E-04
 18    H43     1.339537E-03  -3.117824E-04   1.444795E-03
 19    C12     1.585453E-03  -8.319603E-04  -6.841584E-04
 20    C11    -9.709603E-04   5.381427E-04  -2.004648E-03
 21    C18    -3.120061E-05   6.712524E-04   1.031769E-03
 22    H48     6.076200E-05   6.240473E-04   3.244456E-04
 23    C13     3.292338E-05   1.587924E-04  -1.303306E-03
 24    C14    -3.509863E-03  -1.132091E-04   1.100372E-03
```

```
25    C15    -1.313179E-03   9.458745E-05   1.293462E-03
26    C16     9.737429E-04  -6.883449E-04   1.917243E-03
27    C17     3.364401E-03   2.281349E-04  -1.625091E-03
28    H51    -4.635873E-04   1.383733E-04  -1.360200E-04
29    H52    -2.227883E-04   4.287965E-05  -1.031691E-04
30    H55    -3.002464E-04   4.059049E-04  -4.943533E-04
31    H56     6.060196E-04   4.676608E-04  -8.768542E-04
32    H59    -7.156723E-04  -8.402087E-04   1.788917E-03
33    H60    -4.512960E-04   4.633384E-04  -5.182050E-04
34    H61     7.150803E-04  -1.740271E-04  -1.722258E-04
35    H62    -3.986130E-04  -4.801328E-04  -1.448087E-04
-----------    -------------  -------------  -------------
   total       1.453700E-03   1.300279E-04  -5.731622E-04

end of program der1b


start of program geopt  19

geometry optimization step 19
reading input hessian of dimension   105
 in five columns format
reading input hessian of dimension   105
 in five columns format
** restarting optimization from step   18 **

Hessian eigenvalues:
 -1.30845E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
  0.00000E+00    0.00000E+00    2.21695E-03    1.36849E-02    2.02633E-02
  2.58333E-02    2.84407E-02    2.89538E-02    3.03762E-02    3.08352E-02
  3.25410E-02    3.71636E-02    4.04608E-02    4.29866E-02    4.90003E-02
  5.81243E-02    6.78499E-02    7.01367E-02    7.40998E-02    7.58770E-02
  8.00100E-02    8.72603E-02    9.41555E-02    9.73942E-02    1.10007E-01
  1.12446E-01    1.23337E-01    1.29097E-01    1.31601E-01    1.41646E-01
  1.42927E-01    1.47076E-01    1.51928E-01    1.54618E-01    1.59488E-01
  1.66977E-01    1.72837E-01    1.82558E-01    1.85950E-01    1.87486E-01
  2.00251E-01    2.03410E-01    2.06170E-01    2.12368E-01    2.16128E-01
  2.24858E-01    2.28361E-01    2.32104E-01    2.36787E-01    2.43216E-01
  2.54617E-01    2.58277E-01    2.62368E-01    2.73016E-01    2.80065E-01
  2.86797E-01    2.92323E-01    2.98446E-01    3.05339E-01    3.06468E-01
  3.15892E-01    3.18652E-01    3.24888E-01    3.28838E-01    3.32482E-01
  3.32817E-01    3.37323E-01    3.43656E-01    3.47254E-01    3.49432E-01
  3.59230E-01    3.61371E-01    3.69050E-01    3.81727E-01    3.88977E-01
  3.94855E-01    4.05146E-01    4.15088E-01    4.21612E-01    4.29215E-01
  4.37337E-01    4.44896E-01    4.59894E-01    4.71203E-01    4.74842E-01
  4.81419E-01    4.95319E-01    5.11990E-01    5.22530E-01    5.25088E-01
  5.54815E-01    6.03678E-01    6.36444E-01    6.50302E-01    6.73623E-01
  7.44522E-01    7.82475E-01    8.08085E-01    1.04237E+00    1.51499E+00

WARNING: Hessian has wrong number of negative eigenvalues


Level shifts adjusted to satisfy step-size constraints
 Step size:     0.0383807
 Cos(theta):    0.7554660

 Final level shift:  -5.7857995E-02
```

```
  energy change:           2.8879E-04 .  (  5.0000E-05 )
  gradient maximum:        1.1946E-03 .  (  4.5000E-04 )
  gradient rms:            3.0204E-04 .  (  3.0000E-04 )
  step size:   0.03838  trust radius:   0.03750
  displacement maximum:    1.6447E-02 .  (  1.8000E-03 )
  displacement rms:        3.4329E-03 .  (  1.2000E-03 )
  predicted energy change:    -9.1572E-05    geom step:   3.8381E-02    full step:
3.8381E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.5511E-17     y:     9.5410E-17     z:    -2.2204E-16

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.9329130509     -3.8988216180     -2.2589732411
  C1        1.5076668300     -2.9963260232     -2.1973827346
  C2        3.0428959490     -0.6260062736     -2.0526201429
  C3        1.1506635087     -1.9892951307     -1.3102729740
  C4        2.6186487320     -2.8105839380     -2.9985688985
  C5        3.3792902263     -1.6392127291     -2.9266569099
  C6        1.9286673533     -0.8223029601     -1.2601292850
  C7        0.0702852508     -1.8400113213     -0.3293961024
  H27       2.9074469027     -3.5773181534     -3.6889870997
  H28       4.2358710506     -1.5274850285     -3.5606184956
  H30       3.6055732429      0.2798809836     -1.9704121209
  C8        0.2332907240     -0.6400923385      0.2444351652
  H32      -0.6969120313     -2.5513461128     -0.1267134932
  C10      -0.3835080153      0.2544597862      1.2943028765
  N2        1.3485171764     -0.0063849753     -0.3048677688
  C9        1.6525212646      1.2171866854      0.2402027915
  O1        2.6060368544      1.9003665286     -0.0531682342
  H43      -0.3500795197     -0.2357623382      2.2587131529
  C12      -1.8239863603      0.6191200564      0.9745175790
  C11       0.5792270602      1.4971598715      1.3013451375
  C18       1.2645053378      1.7417232806      2.6569862899
  H48       0.0379234021      2.3863011755      1.0095526585
  C13      -3.4828302720      1.4265201631     -0.5693681037
  C14      -4.1202331512      0.8458692086      1.6632571773
  C15      -4.4612890164      1.3094108849      0.4071143145
  C16      -2.8063418802      0.5027694446      1.9437709791
  C17      -2.1758204121      1.0821075917     -0.2881947313
  H51      -5.4761442091      1.5721810556      0.1857619887
  H52      -2.5514108879      0.1392154968      2.9204305396
  H55      -3.7416758472      1.7788473572     -1.5476185790
  H56      -4.8695937146      0.7465598931      2.4227062260
  H59      -1.4283076990      1.1558294818     -1.0527216078
  H60       1.7820128154      0.8489038739      2.9891039423
  H61       0.5312158744      2.0196411386      3.4049930784
  H62       1.9869733984      2.5420879604      2.5604575430

  nuclear repulsion energy.......  1445.105114809 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  19   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.215E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom       H25     C1     C2     C3     C4     C5     C6     C7
  grid # 1       73     89     87     90     87     87     85     85
  grid # 2      106    100     97     98     98     99     91     92
  grid # 3      224    183    182    194    182    182    187    183
  grid # 4      224    379    381    404    379    379    374    377

  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     86     73     82    100     76
  grid # 2      106    106    105     91    106     92    109     81
  grid # 3      224    224    220    188    223    175    223    164
  grid # 4      224    224    219    374    228    350    402    332

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     68     90     81     71     70     88     87
  grid # 2      127     98    105     93     76    100    100    100
  grid # 3      272    209    193    171    148    215    183    183
  grid # 4      473    200    400    351    306    208    379    379

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     87     86     73     73     73     73     70
  grid # 2      100    100     96    106    104    106    106    101
  grid # 3      183    182    181    224    214    224    224    215
  grid # 4      379    377    376    224    214    224    224    212

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     71     71   2822
  grid # 2       99     99     99   3492
  grid # 3      217    220    220   7036
  grid # 4      218    222    221  10837

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14158405516           1.5E-04  3.1E-03
etot   2  Y  Y  4  M  -815.14238354153  8.0E-04  5.6E-05  7.1E-04
etot   3  Y  Y  4  M  -815.14246649663  8.3E-05  2.0E-05  2.4E-04
etot   4  Y  Y  4  M  -815.14247311310  6.6E-06  8.2E-06  1.4E-04
etot   5  Y  Y  4  M  -815.14247378525  6.7E-07  3.0E-06  4.1E-05
etot   6  N  N  1  U  -815.14246928853 -4.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1445.10511480906
   (E)  Total one-electron terms..... -3975.70049000285
   (I)  Total two-electron terms.....  1715.45290590526
   (L)  Electronic energy............ -2260.24758409758  (E+I)
   (N)  Total energy.................  -815.14246928853  (A+L)

 SCFE: SCF energy: HF    -815.14246928853 hartrees   iterations:   6


 HOMO energy:    -0.29674
 LUMO energy:     0.11843

  Orbital energies:
  -20.45244  -15.55234  -11.32146  -11.23585  -11.22257  -11.21374
  -11.20681  -11.20065  -11.18771  -11.18604  -11.18548  -11.18500
  -11.18359  -11.18329  -11.17893  -11.17685  -11.17673  -11.17570
  -11.17538  -11.17235   -1.42331   -1.33297   -1.18079   -1.16249
   -1.11552   -1.08803   -1.04113   -1.02798   -1.01992   -1.00047
   -0.94694   -0.90588   -0.85507   -0.84396   -0.83155   -0.81097
   -0.79423   -0.76203   -0.72120   -0.69071   -0.67873   -0.66914
   -0.65822   -0.64093   -0.64020   -0.62706   -0.61163   -0.60601
   -0.60399   -0.60172   -0.59205   -0.57715   -0.55834   -0.55520
   -0.54047   -0.53141   -0.51661   -0.50790   -0.49983   -0.49641
   -0.49113   -0.48637   -0.45917   -0.42198   -0.39337   -0.34987
   -0.34265   -0.31499   -0.29674    0.11843    0.13423    0.13932
    0.14326    0.20538    0.22582    0.26476    0.27110    0.27359
    0.29970

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   4    grid:  4
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x             y             z
 ----  -----   -------------  -------------  -------------
   1    H25     9.039735E-05  -1.295770E-04  -1.559117E-04
   2    C1      4.567170E-04   4.018140E-07  -5.736836E-04
   3    C2     -3.478091E-04   2.212115E-04   3.420346E-04
   4    C3      1.907708E-04   5.369560E-04   2.508664E-04
   5    C4     -2.735343E-04  -1.929635E-04   2.647466E-04
   6    C5     -3.779371E-04  -1.622912E-04  -3.399880E-05
  7    C6     -2.869867E-04  -3.007315E-04   5.398571E-05
  8    C7      1.143653E-04   4.055755E-04  -4.577916E-04
  9    H27    -4.300463E-05  -2.749719E-04  -1.170146E-04
 10    H28     6.153270E-06  -1.023517E-04   2.255534E-05
 11    H30     8.667344E-06   6.766074E-05   4.754569E-05
 12    C8     -3.091938E-04   1.424151E-04  -1.072543E-03
 13    H32     3.861177E-05   9.287580E-05  -5.620798E-05
 14    C10     7.120931E-04  -1.514412E-05   1.187047E-04
 15    N2      6.680637E-04  -3.304244E-04   4.168498E-04
 16    C9      5.718285E-04  -2.344571E-04   4.712025E-04
 17    O1      4.094204E-05  -7.405950E-05  -1.080648E-06
 18    H43     4.794769E-04   6.526275E-05   1.351280E-04
 19    C12     4.439654E-05  -6.290584E-04   3.096449E-04
 20    C11    -1.666060E-04   4.271503E-04  -4.026804E-05
 21    C18    -6.295140E-04   1.141440E-04   1.250653E-04
 22    H48     2.321387E-05   3.671619E-05  -6.558310E-04
 23    C13    -2.384790E-04   1.319345E-04  -6.347761E-05
 24    C14    -2.275233E-04   1.516956E-04  -1.500602E-04
 25    C15    -1.914697E-04   5.271049E-05   7.273050E-05
 26    C16     4.506627E-04   8.191575E-05   2.496570E-04
 27    C17     4.143977E-04  -4.220802E-05   2.179080E-04
 28    H51    -1.205446E-04   1.103765E-04  -6.372009E-06
 29    H52     8.517684E-05  -1.265550E-05   7.113625E-05
 30    H55    -3.199210E-05   1.083707E-04  -2.065778E-04
 31    H56    -1.889050E-04   5.012139E-05   1.893690E-04
 32    H59     3.002526E-04   1.678680E-05  -3.068919E-04
 33    H60     1.609915E-05   5.240561E-05  -9.398131E-06
 34    H61     2.719173E-04  -1.503996E-04  -6.990390E-05
 35    H62     2.574238E-05  -1.688952E-05  -1.464338E-04
-----------   -------------  -------------  -------------
   total       1.576447E-03   1.985042E-04  -7.643164E-04

 end of program der1b


 start of program geopt  20

 geometry optimization step 20
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -4.92083E-03    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    2.42462E-03    1.42212E-02    2.05065E-02
   2.75060E-02    2.88712E-02    2.97149E-02    3.05542E-02    3.10775E-02
   3.29447E-02    3.72550E-02    4.36451E-02    4.50321E-02    5.59923E-02
   5.93210E-02    6.58776E-02    6.99218E-02    7.31347E-02    7.45796E-02
   8.35382E-02    8.60020E-02    9.67931E-02    1.04036E-01    1.12326E-01
   1.17956E-01    1.24473E-01    1.33610E-01    1.36388E-01    1.41732E-01
   1.46108E-01    1.47473E-01    1.53339E-01    1.60439E-01    1.61587E-01
   1.70684E-01    1.79255E-01    1.81557E-01    1.86775E-01    1.89154E-01
   2.03633E-01    2.06457E-01    2.09357E-01    2.14971E-01    2.19705E-01
   2.25589E-01    2.29827E-01    2.32431E-01    2.44514E-01    2.49985E-01
   2.55128E-01    2.59997E-01    2.69728E-01    2.82167E-01    2.86218E-01
   2.89182E-01    2.95988E-01    3.00273E-01    3.10229E-01    3.15228E-01
   3.19193E-01    3.25968E-01    3.28971E-01    3.31777E-01    3.34440E-01
```

```
    3.38177E-01    3.40219E-01    3.45327E-01    3.47980E-01    3.56467E-01
    3.56821E-01    3.61188E-01    3.74760E-01    3.84077E-01    3.95884E-01
    4.02686E-01    4.10628E-01    4.17813E-01    4.26488E-01    4.30241E-01
    4.40275E-01    4.46385E-01    4.60207E-01    4.71054E-01    4.78409E-01
    4.81772E-01    4.97888E-01    5.02505E-01    5.11350E-01    5.38838E-01
    5.71440E-01    5.96299E-01    6.05686E-01    6.34469E-01    6.68546E-01
    7.44107E-01    7.51127E-01    7.89392E-01    1.03660E+00    1.51803E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0754282
   Cos(theta):   0.7409694

   Final level shift:  -3.0725091E-02

  energy change:            1.6042E-04 .  (  5.0000E-05 )
  gradient maximum:         1.1336E-03 .  (  4.5000E-04 )
  gradient rms:             3.2456E-04 .  (  3.0000E-04 )
  step size:   0.07543  trust radius:   0.07500
  displacement maximum:     3.1467E-02 .  (  1.8000E-03 )
  displacement rms:         6.7465E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.8881E-04    geom step:   7.5428E-02    full step:
7.5428E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     7.0022E-03     y:    -4.9549E-03     z:     2.2705E-03

  new geometry:
                              angstroms
  atom           x                 y                 z
  H25       0.9163260706     -3.8838836842     -2.2947234504
  C1        1.5007287505     -2.9885383106     -2.2200095222
  C2        3.0621174720     -0.6395784961     -2.0404975802
  C3        1.1463478138     -1.9837633377     -1.3284364642
  C4        2.6221779423     -2.8120522794     -3.0077612276
  C5        3.3952723093     -1.6506569701     -2.9189986191
  C6        1.9374613006     -0.8275970768     -1.2604636320
  C7        0.0578761712     -1.8274166436     -0.3590573705
  H27       2.9089005670     -3.5779685406     -3.7001999511
  H28       4.2603074982     -1.5446553344     -3.5425075331
  H30       3.6352740365      0.2583491999     -1.9452632618
  C8        0.2287224023     -0.6340852469      0.2251566998
  H32      -0.7205237317     -2.5299739857     -0.1696195420
  C10      -0.3852453869      0.2561668835      1.2803546711
  N2        1.3576027880     -0.0107812066     -0.3062578495
  C9        1.6690323848      1.2060554354      0.2499805715
  O1        2.6387705334      1.8773049478     -0.0225470680
  H43      -0.3437725996     -0.2388851991      2.2421933137
  C12      -1.8280426393      0.6203127447      0.9728426964
  C11       0.5774073282      1.4990303541      1.2888323386
  C18       1.2344244990      1.7667809124      2.6519884415
  H48       0.0397373353      2.3817623510      0.9710616474
  C13      -3.5034396977      1.4254943335     -0.5564643489
  C14      -4.1184978552      0.8509576962      1.6845255725
  C15      -4.4724652683      1.3114767261      0.4302343013
  C16      -2.8010793039      0.5073874296      1.9525139487
  C17      -2.1926258549      1.0807482137     -0.2876489158
  H51      -5.4894987959      1.5743855212      0.2184461130
  H52      -2.5360744255      0.1465924758      2.9281516738
```

```
 H55      -3.7721677469      1.7752220608     -1.5336746256
 H56      -4.8602474829      0.7540108048      2.4524449761
 H59      -1.4526102575      1.1524880592     -1.0606733050
 H60       1.7502649740      0.8851098726      3.0057148947
 H61       0.4880653452      2.0480340249      3.3798341874
 H62       1.9537971132      2.5691308853      2.5594563641

 nuclear repulsion energy.......  1444.238800790 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  20   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.212E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom         H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1         73     89     87     90     87     87     85     85
 grid # 2        106    100     97     98     98     99     91     92
 grid # 3        224    183    182    194    182    182    188    183
 grid # 4        224    379    381    406    379    379    374    377

 number of gridpoints:
    atom         H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1         73     73     73     86     73     82     99     75
 grid # 2        106    106    105     91    106     93    109     80
 grid # 3        224    224    220    188    223    175    223    164
 grid # 4        224    224    219    373    228    349    402    334

 number of gridpoints:
    atom          O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1        111     69     90     81     71     69     88     87
 grid # 2        127     98    105     93     74     99    100    100
 grid # 3        272    208    193    172    142    216    183    183
 grid # 4        473    201    400    352    305    208    380    379

 number of gridpoints:
    atom         C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1         89     87     85     73     73     73     73     70
 grid # 2        100    100     97    106    104    106    106    101
 grid # 3        183    182    181    224    214    224    224    215
 grid # 4        379    378    376    224    214    224    224    212

 number of gridpoints:
    atom         H60    H61    H62  total
 grid # 1         71     71     71   2819
 grid # 2         99     99     99   3490
 grid # 3        217    220    220   7032
 grid # 4        218    222    221  10842
```

```
  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                 RMS    maximum
       e  d  i  u  i                       energy  density   DIIS
       r  t  s  t  d     total energy     change   change    error

etot   1  N  N  1  U  -815.14049630175           1.9E-04  5.9E-03
etot   2  Y  Y  4  M  -815.14234406790  1.8E-03  8.2E-05  2.4E-03
etot   3  Y  Y  4  M  -815.14255162518  2.1E-04  2.7E-05  7.3E-04
etot   4  N  Y  1  U  -815.14257118464  2.0E-05  7.5E-06  1.6E-04
etot   5  Y  Y  4  M  -815.14257065930 -5.3E-07  4.5E-06  6.0E-05
etot   6  Y  N  4  M  -815.14257165259  9.9E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1444.23880078977
   (E)  Total one-electron terms..... -3973.96210494348
   (I)  Total two-electron terms.....  1714.58073250112
   (L)  Electronic energy............ -2259.38137244236  (E+I)
   (N)  Total energy.................  -815.14257165259  (A+L)

 SCFE: SCF energy: HF    -815.14257165259 hartrees   iterations:   6


 HOMO energy:    -0.29669
 LUMO energy:     0.11846

  Orbital energies:
  -20.45245  -15.55239  -11.32159  -11.23572  -11.22248  -11.21385
  -11.20684  -11.20095  -11.18759  -11.18647  -11.18589  -11.18547
  -11.18404  -11.18370  -11.17892  -11.17678  -11.17666  -11.17539
  -11.17446  -11.17231   -1.42247   -1.33314   -1.18064   -1.16252
   -1.11569   -1.08819   -1.04125   -1.02772   -1.02030   -1.00044
   -0.94727   -0.90623   -0.85510   -0.84400   -0.83164   -0.81106
   -0.79418   -0.76199   -0.72102   -0.69123   -0.67877   -0.66913
   -0.65823   -0.64084   -0.64026   -0.62712   -0.61158   -0.60584
   -0.60412   -0.60165   -0.59213   -0.57743   -0.55805   -0.55560
   -0.54037   -0.53161   -0.51660   -0.50777   -0.49994   -0.49651
   -0.49121   -0.48637   -0.45919   -0.42218   -0.39333   -0.34977
   -0.34279   -0.31521   -0.29669    0.11846    0.13399    0.13901
    0.14282    0.20542    0.22584    0.26467    0.27125    0.27391
    0.29946

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -5.590149E-05  -3.870109E-05  -4.335196E-05
  2    C1     -9.580971E-05  -2.803892E-04  -1.169699E-04
  3    C2     -2.597715E-04  -1.276678E-04   1.489579E-04
  4    C3      2.398921E-04  -3.856143E-05  -2.763762E-04
  5    C4     -3.842977E-04  -1.045407E-04   2.506730E-04
  6    C5      1.045618E-04   5.579275E-04   2.046451E-04
  7    C6      8.646678E-04   1.218533E-04  -6.563139E-04
  8    C7     -7.072315E-04  -1.903583E-04  -3.846562E-04
  9    H27    -7.288527E-05  -1.357228E-04  -4.586758E-05
 10    H28    -3.479510E-05  -5.710454E-05   4.001539E-05
 11    H30     7.552734E-05   1.104444E-04   1.423703E-05
 12    C8     -6.393986E-04   2.723840E-04  -5.898228E-04
 13    H32    -1.631785E-05  -4.003301E-05  -2.710056E-05
 14    C10     1.018555E-03  -1.299700E-04   1.122802E-04
 15    N2      8.652664E-04   3.661115E-05   5.000355E-04
 16    C9      2.401113E-03   7.281648E-04  -1.113410E-04
 17    O1     -1.981303E-03  -1.324548E-03   5.443576E-04
 18    H43     3.450412E-04   7.613875E-05   1.523468E-04
 19    C12    -4.781526E-04  -3.970645E-04   2.881204E-04
 20    C11    -1.744470E-04   5.130172E-04  -6.834861E-04
 21    C18     2.039834E-05   6.370190E-04  -1.542724E-03
 22    H48     6.160058E-05   9.992152E-05  -5.899728E-04
 23    C13     3.644883E-04  -5.934096E-05  -5.048361E-05
 24    C14     2.939735E-04   1.387311E-05  -1.167209E-04
 25    C15     3.250199E-04  -7.557025E-05   2.812143E-04
 26    C16    -1.220484E-04   2.512147E-04   1.636867E-04
 27    C17    -1.602012E-04   1.127346E-04  -1.197069E-05
 28    H51     1.493578E-05   5.714623E-05   2.703222E-05
 29    H52    -7.571553E-05   9.560980E-05  -3.377796E-04
 30    H55     1.217777E-04  -1.814425E-05   2.389206E-04
 31    H56     9.604136E-05   9.189443E-05  -1.005150E-04
 32    H59    -9.976177E-05  -4.646901E-05   1.213953E-04
 33    H60     1.001511E-03  -1.894392E-03   6.263527E-04
 34    H61    -1.687354E-03   7.800341E-04   1.825364E-03
 35    H62     3.974147E-04   5.722640E-04  -3.568094E-04
-----------   -------------  -------------  -------------
   total       1.566394E-03   1.696754E-04  -5.026273E-04

 end of program der1b


 start of program geopt  21

 geometry optimization step 21
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -3.14757E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
```

```
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    1.14827E-03    1.22180E-02    2.07238E-02
    2.21114E-02    2.83976E-02    3.03852E-02    3.06736E-02    3.11876E-02
    3.14045E-02    3.60114E-02    3.77495E-02    4.47000E-02    5.54533E-02
    5.71840E-02    6.68602E-02    6.72899E-02    7.35070E-02    7.45084E-02
    8.12096E-02    8.74327E-02    9.46968E-02    1.06797E-01    1.09777E-01
    1.12819E-01    1.24281E-01    1.30571E-01    1.41436E-01    1.43111E-01
    1.45896E-01    1.48389E-01    1.51472E-01    1.57095E-01    1.65049E-01
    1.72361E-01    1.77388E-01    1.81810E-01    1.88122E-01    1.94169E-01
    1.99512E-01    2.06415E-01    2.11374E-01    2.12893E-01    2.16652E-01
    2.27496E-01    2.31795E-01    2.33926E-01    2.45808E-01    2.49952E-01
    2.54159E-01    2.59991E-01    2.62132E-01    2.67731E-01    2.85040E-01
    2.90925E-01    2.92250E-01    3.01023E-01    3.03930E-01    3.11295E-01
    3.19461E-01    3.21509E-01    3.25957E-01    3.31560E-01    3.32022E-01
    3.35449E-01    3.41717E-01    3.43569E-01    3.45540E-01    3.57984E-01
    3.61961E-01    3.68036E-01    3.79848E-01    3.86923E-01    3.93588E-01
    4.04733E-01    4.08780E-01    4.12637E-01    4.29958E-01    4.33652E-01
    4.40668E-01    4.46746E-01    4.58509E-01    4.72606E-01    4.73764E-01
    4.85686E-01    4.91019E-01    5.14278E-01    5.16673E-01    5.38872E-01
    5.61877E-01    5.90160E-01    6.31005E-01    6.33462E-01    6.68420E-01
    7.11911E-01    7.44248E-01    8.08616E-01    1.05071E+00    1.54996E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.1063933
   Cos(theta):   0.5224784

   Final level shift:  -3.8591377E-02

  energy change:           -1.0236E-04 .   (  5.0000E-05 )
  gradient maximum:         2.6602E-03 .   (  4.5000E-04 )
  gradient rms:             5.0184E-04 .   (  3.0000E-04 )
  step size:   0.10639  trust radius:   0.10607
  displacement maximum:     4.4366E-02 .   (  1.8000E-03 )
  displacement rms:         9.5160E-03 .   (  1.2000E-03 )
  predicted energy change:    -3.7437E-04    geom step:   1.0639E-01    full step:
1.0639E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:     9.0810E-03     y:    -8.5668E-03     z:     6.1758E-03

  new geometry:
                              angstroms
  atom            x                y                 z
  H25       0.8868853718     -3.8538237866     -2.3549578724
  C1        1.4837868608     -2.9697672869     -2.2572258918
  C2        3.0789702156     -0.6443771088     -2.0254273541
  C3        1.1384600915     -1.9751093575     -1.3534929969
  C4        2.6129498816     -2.7886538464     -3.0349414433
  C5        3.4028395048     -1.6415500459     -2.9199515447
  C6        1.9466974999     -0.8319491307     -1.2598711135
  C7        0.0446199884     -1.8217242164     -0.3898154184
  H27       2.8945050041     -3.5432626532     -3.7427867054
  H28       4.2750036412     -1.5365387705     -3.5356366533
  H30       3.6622456715      0.2460141691     -1.9064161827
  C8        0.2244423872     -0.6362641434      0.2098149381
```

```
 H32      -0.7423573544     -2.5200741666     -0.2170304743
 C10      -0.3877191282      0.2499584354      1.2724133332
 N2        1.3717397968     -0.0229453572     -0.2979024555
 C9        1.6890543629      1.1822088200      0.2749779532
 O1        2.6691608102      1.8403948475      0.0322190325
 H43      -0.3512001752     -0.2610736613      2.2267800208
 C12      -1.8301342769      0.6216054084      0.9722868041
 C11       0.5774407869      1.4899701601      1.2826881111
 C18       1.1976851341      1.7984641052      2.6527543905
 H48       0.0477268513      2.3627184166      0.9361657115
 C13      -3.5194142239      1.3855959827     -0.5600494649
 C14      -4.1028128638      0.8916492284      1.7052961487
 C15      -4.4709654450      1.3135140126      0.4425205626
 C16      -2.7874784654      0.5457157165      1.9674507545
 C17      -2.2109775538      1.0415933628     -0.2963966927
 H51      -5.4865790643      1.5775692639      0.2346220224
 H52      -2.5125272855      0.2160862461      2.9561884931
 H55      -3.8003644330      1.7018916555     -1.5478831289
 H56      -4.8307746568      0.8318289291      2.4851291557
 H59      -1.4859175062      1.0736251330     -1.0803134418
 H60       1.6942660010      0.9252011410      3.0571730167
 H61       0.4286905478      2.1159346012      3.3489500907
 H62       1.9281853299      2.5912055660      2.5472124318

 nuclear repulsion energy.......  1444.706032409 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  21   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.210E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom         H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1         73     89      87      90      87      87      85      85
 grid # 2        106    100      97      98      98      98      91      92
 grid # 3        224    182     181     194     182     182     187     182
 grid # 4        224    379     381     404     379     379     374     378

 number of gridpoints:
    atom         H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1         73     73      73      86      73      81      99      75
 grid # 2        106    106     105      91     106      93     109      80
 grid # 3        224    224     220     187     223     175     223     164
 grid # 4        224    224     219     374     229     346     400     330

 number of gridpoints:
    atom          O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1        111     68      90      81      72      69      87      87
 grid # 2        123     97     105      94      75      98     100      99
```

```
  grid # 3      272    210    193    171    141    216    183    183
  grid # 4      473    201    400    353    309    208    380    377

  number of gridpoints:
     atom        C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       87     87     85     73     73     73     73     70
  grid # 2      100     99     96    106    103    106    106    102
  grid # 3      183    181    180    224    215    224    224    215
  grid # 4      378    376    375    224    214    224    224    212

  number of gridpoints:
     atom        H60    H61    H62  total
  grid # 1       71     72     71   2816
  grid # 2       99     99     99   3482
  grid # 3      217    221    220   7027
  grid # 4      218    222    221  10833

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                   RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy       change  change    error

etot   1  N  N  2  U  -815.13657410208           3.2E-04  9.3E-03
etot   2  Y  Y  6  M  -815.14208125466  5.5E-03  1.4E-04  3.9E-03
etot   3  N  Y  2  U  -815.14265337798  5.7E-04  4.9E-05  1.2E-03
etot   4  Y  Y  6  M  -815.14270901645  5.6E-05  1.4E-05  3.1E-04
etot   5  Y  Y  6  M  -815.14271742217  8.4E-06  7.0E-06  1.2E-04
etot   6  Y  Y  6  M  -815.14271796120  5.4E-07  2.7E-06  4.3E-05
etot   7  Y  N  6  M  -815.14271783004 -1.3E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1444.70603240922
   (E)  Total one-electron terms..... -3974.87914107188
   (I)  Total two-electron terms.....  1715.03039083262
   (L)  Electronic energy............ -2259.84875023927  (E+I)
   (N)  Total energy.................  -815.14271783004  (A+L)

 SCFE: SCF energy: HF    -815.14271783004 hartrees   iterations:   7


 HOMO energy:    -0.29706
 LUMO energy:     0.11893

  Orbital energies:
  -20.45246  -15.55195  -11.32074  -11.23607  -11.22226  -11.21381
  -11.20554  -11.20033  -11.18754  -11.18629  -11.18498  -11.18474
  -11.18288  -11.18268  -11.17897  -11.17708  -11.17650  -11.17529
  -11.17456  -11.17233   -1.42594   -1.33366   -1.18164   -1.16333
   -1.11590   -1.08863   -1.04175   -1.02873   -1.02032   -1.00078
   -0.94714   -0.90637   -0.85490   -0.84450   -0.83177   -0.81100
   -0.79446   -0.76214   -0.72133   -0.69248   -0.67867   -0.66899
  -0.65850   -0.64116   -0.64060   -0.62735   -0.61202   -0.60660
  -0.60427   -0.60220   -0.59227   -0.57865   -0.55723   -0.55580
  -0.53911   -0.53181   -0.51652   -0.50811   -0.49996   -0.49661
  -0.49154   -0.48607   -0.45965   -0.42241   -0.39405   -0.35047
  -0.34287   -0.31487   -0.29706    0.11893    0.13462    0.13955
   0.14270    0.20583    0.22599    0.26443    0.27123    0.27424
   0.29998

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -3.663028E-05  -4.741978E-04  -2.663808E-06
  2    C1      1.768989E-03   1.189622E-03  -1.943889E-03
  3    C2      5.134526E-04   2.093609E-03   7.119634E-04
  4    C3      3.709753E-05  -3.975426E-04   1.050316E-03
  5    C4     -2.159458E-04  -2.337768E-03  -8.433983E-04
  6    C5      1.300080E-03  -4.217482E-04  -1.146168E-03
  7    C6     -1.637070E-04  -2.997039E-04   5.815640E-04
  8    C7     -3.269365E-04   1.671040E-03  -7.650070E-04
  9    H27    -2.682197E-04  -1.393285E-05   3.352124E-04
 10    H28    -8.821173E-04  -3.417881E-04   3.534498E-04
 11    H30    -2.756155E-04  -1.012351E-03  -3.042168E-04
 12    C8     -3.662004E-04   1.999609E-04   4.930198E-04
 13    H32     1.705535E-04   6.631806E-04  -1.114962E-04
 14    C10     1.104105E-03  -1.601743E-03  -1.406674E-03
 15    N2     -2.398230E-03  -2.024751E-03   6.361978E-05
 16    C9     -3.679754E-03  -2.338797E-03   1.548841E-03
 17    O1      5.788842E-03   3.498514E-03  -1.773722E-03
 18    H43     1.312289E-03   1.491637E-03   4.477060E-04
 19    C12     1.627440E-03  -2.106577E-03  -1.205476E-04
 20    C11    -4.805831E-04  -1.320863E-03   2.226307E-03
 21    C18    -1.280678E-03   9.406960E-04   1.220578E-03
 22    H48    -1.295742E-03   1.915519E-03  -2.123247E-03
 23    C13    -7.375047E-04   1.246492E-03  -3.371602E-03
 24    C14    -3.482536E-04   9.602880E-04  -4.804191E-04
 25    C15    -1.552890E-03  -1.058338E-04   1.001914E-03
 26    C16     4.891969E-04  -1.570713E-04   4.471378E-03
 27    C17     1.638560E-03  -9.913141E-04   7.867225E-04
 28    H51    -1.535195E-03   3.173970E-04   3.227441E-04
 29    H52    -6.644208E-04   8.294817E-04  -3.524280E-03
 30    H55     6.110513E-04  -4.765425E-04   1.975115E-03
 31    H56    -2.029590E-03  -3.676835E-04   1.693869E-03
 32    H59     2.310703E-03   4.517719E-04  -2.035586E-03
 33    H60     3.659181E-04  -7.000803E-04  -3.797985E-05
 34    H61     1.162188E-03  -7.353260E-05  -2.462660E-04
 35    H62    -3.812451E-04  -2.221828E-04   3.111071E-04
 -----------   -------------  -------------  -------------
    total       1.281007E-03  -3.167965E-04  -6.417356E-04

  end of program der1b


  start of program geopt  22

  geometry optimization step 22
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format

  Hessian eigenvalues:
   -2.42667E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    5.00000E-04    9.09872E-03    1.68957E-02
    2.07508E-02    2.81801E-02    3.03422E-02    3.07550E-02    3.12153E-02
    3.17552E-02    3.68292E-02    3.81138E-02    4.50996E-02    4.64393E-02
    5.78097E-02    6.26703E-02    6.85846E-02    7.15560E-02    7.31183E-02
    7.76495E-02    8.65580E-02    9.89387E-02    9.91277E-02    1.04731E-01
    1.13246E-01    1.21523E-01    1.26560E-01    1.38741E-01    1.43114E-01
    1.44343E-01    1.44978E-01    1.49351E-01    1.54851E-01    1.58970E-01
    1.60949E-01    1.66894E-01    1.73009E-01    1.82222E-01    1.86723E-01
    1.87702E-01    2.00069E-01    2.06350E-01    2.12569E-01    2.16172E-01
    2.23879E-01    2.28912E-01    2.31548E-01    2.43107E-01    2.46820E-01
    2.50927E-01    2.61339E-01    2.64429E-01    2.72875E-01    2.82267E-01
    2.91075E-01    2.93603E-01    2.96301E-01    3.04250E-01    3.08131E-01
    3.19085E-01    3.19940E-01    3.26975E-01    3.29080E-01    3.33960E-01
    3.35376E-01    3.39029E-01    3.43514E-01    3.53400E-01    3.56274E-01
    3.62607E-01    3.76510E-01    3.83476E-01    3.89809E-01    3.96256E-01
    4.09023E-01    4.12220E-01    4.20393E-01    4.22298E-01    4.38301E-01
    4.40025E-01    4.50030E-01    4.66634E-01    4.71353E-01    4.80036E-01
    4.84496E-01    5.00048E-01    5.09121E-01    5.34311E-01    5.42539E-01
    5.76385E-01    6.13798E-01    6.36938E-01    6.39193E-01    6.46659E-01
    7.01880E-01    7.49040E-01    8.85182E-01    1.03105E+00    1.40722E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0539963
   Cos(theta):   0.6862566

   Final level shift:  -7.0368007E-02

  energy change:          -1.4618E-04 .  (  5.0000E-05 )
  gradient maximum:        6.9454E-03 .  (  4.5000E-04 )
  gradient rms:            1.3878E-03 .  (  3.0000E-04 )
  step size:   0.05400  trust radius:   0.05303
  displacement maximum:    1.7436E-02 .  (  1.8000E-03 )
  displacement rms:        4.8296E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.9020E-04    geom step:   5.3996E-02    full step:
5.3996E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.5419E-03     y:    -1.6432E-03     z:    -1.6400E-03
 new geometry:
                              angstroms
 atom             x                  y                  z
 H25       0.8884538578     -3.8546497541     -2.3642824164
 C1        1.4877437387     -2.9705683923     -2.2648093682
 C2        3.0896507854     -0.6506169450     -2.0244049569
 C3        1.1382225120     -1.9736595798     -1.3617245322
 C4        2.6222283120     -2.7991996328     -3.0363580650
 C5        3.4160785682     -1.6529841346     -2.9168688092
 C6        1.9503258271     -0.8321650674     -1.2637104236
 C7        0.0398042963     -1.8148177912     -0.4027903654
 H27       2.9021888182     -3.5586304493     -3.7391179231
 H28       4.2908900859     -1.5527127596     -3.5269412233
 H30       3.6760350861      0.2377259210     -1.9048715984
 C8        0.2215346279     -0.6320109922      0.1999037170
 H32      -0.7513599989     -2.5091251661     -0.2323600125
 C10      -0.3881809090      0.2511095606      1.2644681776
 N2        1.3735118735     -0.0225580417     -0.3020162357
 C9        1.6953969332      1.1810673550      0.2741793912
 O1        2.6838611879      1.8357220869      0.0331759728
 H43      -0.3379422117     -0.2517350785      2.2223966386
 C12      -1.8339793987      0.6181641607      0.9736595073
 C11       0.5743457409      1.4947590106      1.2759840099
 C18       1.1826140372      1.8076754101      2.6546355948
 H48       0.0423660212      2.3672369893      0.9158193967
 C13      -3.5282443906      1.3953573285     -0.5477565081
 C14      -4.1100626432      0.8877245024      1.7195059183
 C15      -4.4810535311      1.3173737679      0.4593099000
 C16      -2.7909675515      0.5397664110      1.9732356902
 C17      -2.2158336557      1.0470279021     -0.2926541025
 H51      -5.4987251921      1.5843431929      0.2571539827
 H52      -2.5114201154      0.2063544041      2.9533174017
 H55      -3.8110587708      1.7200037405     -1.5301723099
 H56      -4.8382452667      0.8205590546      2.5018736076
 H59      -1.4881395469      1.0897489686     -1.0794431268
 H60       1.6771465982      0.9289129315      3.0674156735
 H61       0.4073950200      2.1311251598      3.3484187455
 H62       1.9144730860      2.5997411565      2.5507483064

 nuclear repulsion energy.......  1442.806977358 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  22   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.221E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
```

```
  grid # 1        73     89     87     90     87     87     85     85
  grid # 2       106    100     97     98     98     99     90     92
  grid # 3       224    183    184    194    182    182    188    183
  grid # 4       224    379    383    404    379    379    375    378

  number of gridpoints:
     atom        H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1        73     73     73     86     73     82     99     75
  grid # 2       106    106    105     91    106     93    109     80
  grid # 3       224    224    220    187    223    175    224    164
  grid # 4       224    224    219    374    229    348    400    333

  number of gridpoints:
     atom         O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1       111     69     90     81     71     69     88     87
  grid # 2       127     96    105     93     75     99    100    100
  grid # 3       272    210    194    171    149    216    183    183
  grid # 4       474    201    401    352    308    207    380    379

  number of gridpoints:
     atom        C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1        88     87     85     73     73     73     73     70
  grid # 2       100    100     96    106    103    106    106    102
  grid # 3       183    182    181    224    215    224    224    215
  grid # 4       379    378    377    224    214    224    224    211

  number of gridpoints:
     atom        H60    H61    H62  total
  grid # 1        71     72     71   2819
  grid # 2        99     99     99   3487
  grid # 3       217    221    220   7045
  grid # 4       222    225    221  10853

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14218412194          1.2E-04  1.8E-03
etot   2  Y  Y  4  M  -815.14261906998  4.3E-04  4.1E-05  7.0E-04
etot   3  Y  Y  4  M  -815.14266175783  4.3E-05  1.4E-05  2.5E-04
etot   4  Y  Y  4  M  -815.14266711775  5.4E-06  6.3E-06  9.5E-05
etot   5  Y  Y  4  M  -815.14266759708  4.8E-07  1.9E-06  2.7E-05
etot   6  N  N  1  U  -815.14266679234 -8.0E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1442.80697735765
   (E)  Total one-electron terms..... -3971.10637949937
   (I)  Total two-electron terms.....  1713.15673534938
   (L)  Electronic energy............ -2257.94964414999  (E+I)
   (N)  Total energy.................  -815.14266679234  (A+L)
```

```
SCFE: SCF energy: HF    -815.14266679234 hartrees   iterations:   6


HOMO energy:    -0.29699
LUMO energy:     0.11836

 Orbital energies:
 -20.45253  -15.55245  -11.32162  -11.23614  -11.22293  -11.21402
 -11.20731  -11.20103  -11.18814  -11.18655  -11.18594  -11.18565
 -11.18404  -11.18384  -11.17941  -11.17737  -11.17726  -11.17641
 -11.17589  -11.17271   -1.42289   -1.33288   -1.18039   -1.16214
  -1.11495   -1.08826   -1.04056   -1.02790   -1.01971   -1.00030
  -0.94659   -0.90584   -0.85396   -0.84411   -0.83184   -0.81092
  -0.79391   -0.76140   -0.72093   -0.69139   -0.67860   -0.66883
  -0.65803   -0.64074   -0.64016   -0.62685   -0.61145   -0.60559
  -0.60377   -0.60203   -0.59180   -0.57765   -0.55683   -0.55514
  -0.53849   -0.53132   -0.51659   -0.50757   -0.50003   -0.49615
  -0.49129   -0.48589   -0.45906   -0.42231   -0.39362   -0.34987
  -0.34268   -0.31500   -0.29699    0.11836    0.13412    0.13872
   0.14201    0.20504    0.22553    0.26446    0.27103    0.27380
   0.29957

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     3.192333E-04   5.326342E-04   1.806305E-04
  2    C1     -1.223526E-04   5.697246E-04  -4.494685E-04
  3    C2     -4.547650E-04  -1.413896E-04  -1.481679E-04
  4    C3      1.408441E-03   2.342490E-04  -9.902121E-05
  5    C4     -2.730675E-04   3.437948E-04   8.181828E-04
  6    C5     -1.136605E-03   1.659947E-04   8.484056E-04
  7    C6      4.782418E-04  -1.631313E-03  -1.322041E-04
  8    C7     -3.147908E-04   4.820229E-04  -1.324488E-03
  9    H27     1.492729E-04   1.752891E-04   8.616813E-05
 10    H28     1.345701E-04   3.547692E-06  -1.472583E-04
 11    H30    -3.223086E-04  -1.102190E-03  -1.533227E-04
 12    C8      5.326385E-04   3.700578E-04   3.846201E-04
 13    H32     3.015810E-04   5.346964E-04  -2.850694E-04
 14    C10     9.861856E-04  -2.389510E-04   2.637073E-04
 15    N2     -1.193228E-03  -7.268826E-04  -7.515909E-05
 16    C9      9.922477E-04   1.211180E-03   4.237352E-04
 17    O1     -9.457376E-04  -6.529947E-04   4.502855E-04
 18    H43     4.518899E-04   2.314445E-04   3.095807E-05
 19    C12    -1.207821E-05  -9.158280E-04   4.552698E-04
 20    C11    -7.892053E-04   7.972653E-04   9.197864E-04
 21    C18    -1.578750E-03  -1.104875E-03   2.292974E-03
 22    H48     8.825922E-04  -8.658837E-04  -3.960822E-04
 23    C13    -3.392289E-04   1.218595E-04   7.891205E-05
 24    C14     1.224961E-03   3.408026E-04  -9.626915E-04
 25    C15     7.787939E-04  -5.118233E-05  -6.734334E-04
 26    C16     2.217550E-04   7.968759E-04  -6.557962E-04
 27    C17    -4.129834E-04   4.066402E-05   2.075776E-04
 28    H51    -2.091311E-04   6.187455E-05   4.319105E-05
 29    H52     1.707936E-04  -4.145325E-04   3.597738E-04
 30    H55     6.950949E-05  -6.297227E-05   6.339366E-04
 31    H56    -4.453699E-04  -9.292177E-05   5.135813E-04
 32    H59    -2.942846E-04   4.357988E-05   1.734875E-04
 33    H60    -1.647601E-03   3.205569E-03  -1.800439E-03
 34    H61     3.089146E-03  -1.329657E-03  -2.749993E-03
 35    H62    -2.369505E-04  -6.183610E-04   6.287088E-04
-----------   -------------  -------------  -------------
   total       1.463415E-03   3.131936E-04  -2.587033E-04

 end of program der1b


 start of program geopt  23

 geometry optimization step 23
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -3.83606E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.90629E-04    5.38054E-03    2.15963E-02
   2.48849E-02    2.81962E-02    3.06522E-02    3.09594E-02    3.11644E-02
   3.20400E-02    3.73883E-02    3.85046E-02    4.44754E-02    4.90746E-02
   5.80580E-02    6.59110E-02    6.87646E-02    7.35102E-02    7.51973E-02
   7.93701E-02    8.70959E-02    9.49946E-02    1.01766E-01    1.13106E-01
   1.21173E-01    1.24897E-01    1.34824E-01    1.37962E-01    1.41576E-01
   1.43074E-01    1.47719E-01    1.49593E-01    1.55546E-01    1.62882E-01
   1.71373E-01    1.75551E-01    1.79623E-01    1.81773E-01    1.87302E-01
   1.93500E-01    2.02365E-01    2.09047E-01    2.13942E-01    2.16037E-01
   2.20427E-01    2.29755E-01    2.36331E-01    2.41740E-01    2.48141E-01
   2.55973E-01    2.59793E-01    2.61140E-01    2.71653E-01    2.81628E-01
   2.89383E-01    2.94682E-01    2.97165E-01    3.05934E-01    3.09721E-01
   3.17542E-01    3.19086E-01    3.25104E-01    3.26599E-01    3.35271E-01
   3.38210E-01    3.43633E-01    3.50775E-01    3.53050E-01    3.57023E-01
   3.67772E-01    3.72420E-01    3.78827E-01    3.92021E-01    3.98098E-01
   4.01745E-01    4.09171E-01    4.14721E-01    4.30055E-01    4.39270E-01
   4.52731E-01    4.53933E-01    4.57689E-01    4.72318E-01    4.77204E-01
   4.89326E-01    4.96022E-01    5.14614E-01    5.51225E-01    5.69792E-01
   5.70496E-01    5.85849E-01    6.28370E-01    6.43699E-01    6.67694E-01
   7.34277E-01    7.50423E-01    8.70012E-01    1.11027E+00    1.42349E+00

 WARNING: Hessian has wrong number of negative eigenvalues


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0271616
  Cos(theta):   0.8629647
```

```
   Final level shift:  -2.2188195E-01

  energy change:           5.1038E-05 .  (  5.0000E-05 )
  gradient maximum:        4.2912E-03 .  (  4.5000E-04 )
  gradient rms:            7.9961E-04 .  (  3.0000E-04 )
  step size:   0.02716  trust radius:   0.02652
  displacement maximum:    1.1158E-02 .  (  1.8000E-03 )
  displacement rms:        2.4294E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.8662E-04    geom step:   2.7162E-02    full step:
2.7162E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.0275E-03     y:    -3.2369E-04     z:     1.0144E-04

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.8855316275     -3.8501435885     -2.3697838860
  C1        1.4881065953     -2.9690946966     -2.2680407168
  C2        3.0977118448     -0.6575709608     -2.0183515248
  C3        1.1405572337     -1.9723653909     -1.3652727053
  C4        2.6256583400     -2.8020469368     -3.0338827965
  C5        3.4235151369     -1.6598287127     -2.9095108156
  C6        1.9548788502     -0.8351491275     -1.2627895953
  C7        0.0396523966     -1.8093992311     -0.4119793029
  H27       2.9058129802     -3.5614021566     -3.7368400291
  H28       4.3017609904     -1.5623717163     -3.5154666903
  H30       3.6885116848      0.2263702812     -1.8959784481
  C8        0.2223236485     -0.6296174442      0.1949275267
  H32      -0.7563587481     -2.4987097194     -0.2469347629
  C10      -0.3881456189      0.2513134764      1.2593184134
  N2        1.3745783567     -0.0221441650     -0.3046974115
  C9        1.6940135878      1.1820679276      0.2726050247
  O1        2.6818691326      1.8350823541      0.0356531122
  H43      -0.3373783363     -0.2517836993      2.2166695333
  C12      -1.8340083048      0.6171898812      0.9703214234
  C11       0.5715665356      1.4958844750      1.2710744448
  C18       1.1743249208      1.8099673398      2.6484123960
  H48       0.0409955095      2.3654168104      0.9047710840
  C13      -3.5353164762      1.4004933995     -0.5397977607
  C14      -4.1084417269      0.8854500552      1.7259436883
  C15      -4.4845805943      1.3190196505      0.4702810819
  C16      -2.7878859383      0.5367591123      1.9726712837
  C17      -2.2211070324      1.0507633158     -0.2921606858
  H51      -5.5041410900      1.5867223309      0.2742793914
  H52      -2.5045735140      0.2019692575      2.9508041880
  H55      -3.8218281047      1.7286609883     -1.5188262312
  H56      -4.8348297148      0.8146355874      2.5119259870
  H59      -1.4955665056      1.0996635369     -1.0823560577
  H60       1.6673565144      0.9362593560      3.0587483135
  H61       0.4011968279      2.1274593522      3.3380208731
  H62       1.9042615917      2.6025395255      2.5492825245

  nuclear repulsion energy.......  1443.237806597 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  23   /
 ------------------------------------------------

  end of program geopt
 start of program onee
 smallest eigenvalue of S:    1.211E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      99      91      92
 grid # 3       224    183     182     194     182     182     188     183
 grid # 4       224    379     383     404     379     379     372     378

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      82      99      75
 grid # 2       106    106     105      91     106      93     109      80
 grid # 3       224    224     220     187     223     175     224     164
 grid # 4       224    224     219     374     228     349     402     332

 number of gridpoints:
    atom         O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1       111     69      90      81      71      69      87      87
 grid # 2       123     96     106      93      75      99     100     100
 grid # 3       272    210     193     172     141     216     183     183
 grid # 4       473    201     398     355     308     209     379     379

 number of gridpoints:
    atom        C15    C16     C17     H51     H52     H55     H56     H59
 grid # 1        88     87      85      73      73      73      73      70
 grid # 2        99    100      98     106     103     106     106     102
 grid # 3       183    182     181     224     215     224     224     215
 grid # 4       379    378     377     224     214     224     224     211

 number of gridpoints:
    atom        H60    H61     H62  total
 grid # 1        71     72      71   2818
 grid # 2        99     99      99   3486
 grid # 3       217    221     220   7035
 grid # 4       218    222     221  10844

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                         energy  density   DIIS
      r  t  s  t  d     total energy    change  change    error
```

```
etot   1  N  N  1  U  -815.14257620959           7.4E-05  1.8E-03
etot   2  Y  Y  4  M  -815.14276636194  1.9E-04  2.5E-05  7.5E-04
etot   3  Y  Y  4  M  -815.14278623418  2.0E-05  8.8E-06  2.5E-04
etot   4  Y  Y  4  M  -815.14278832808  2.1E-06  4.1E-06  1.1E-04
etot   5  Y  N  4  M  -815.14278906639  7.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1443.23780659711
   (E)  Total one-electron terms..... -3971.95568885951
   (I)  Total two-electron terms.....  1713.57509319601
   (L)  Electronic energy............ -2258.38059566350  (E+I)
   (N)  Total energy.................  -815.14278906639  (A+L)

 SCFE: SCF energy: HF    -815.14278906639 hartrees   iterations:   5


 HOMO energy:    -0.29688
 LUMO energy:     0.11877

  Orbital energies:
  -20.45257  -15.55196  -11.32121  -11.23553  -11.22262  -11.21375
  -11.20669  -11.20095  -11.18761  -11.18645  -11.18591  -11.18560
  -11.18420  -11.18381  -11.17910  -11.17698  -11.17660  -11.17559
  -11.17467  -11.17247   -1.42426   -1.33326   -1.18069   -1.16267
   -1.11563   -1.08827   -1.04109   -1.02766   -1.02036   -1.00058
   -0.94716   -0.90610   -0.85451   -0.84413   -0.83186   -0.81102
   -0.79394   -0.76171   -0.72092   -0.69200   -0.67876   -0.66908
   -0.65824   -0.64069   -0.64036   -0.62704   -0.61174   -0.60612
   -0.60410   -0.60177   -0.59205   -0.57801   -0.55744   -0.55580
   -0.53901   -0.53181   -0.51669   -0.50777   -0.50004   -0.49657
   -0.49138   -0.48608   -0.45947   -0.42233   -0.39354   -0.34968
   -0.34291   -0.31525   -0.29688    0.11877    0.13432    0.13893
    0.14210    0.20560    0.22583    0.26446    0.27122    0.27408
    0.29959

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     1.350579E-04   2.741675E-04   7.481409E-05
   2    C1     -2.378481E-04  -7.230226E-05  -2.589889E-04
   3    C2     -2.692388E-04   2.138113E-05   5.783063E-05
   4    C3      3.292319E-04   2.579849E-04   2.760825E-04
   5    C4      1.925447E-04  -2.048571E-04  -1.810400E-05
   6    C5     -3.515494E-04   1.359277E-04   2.036013E-04
   7    C6      5.673017E-04   3.376347E-04   1.704376E-04
   8    C7     -1.584157E-03  -6.406681E-04  -6.802053E-04
  9    H27     8.172896E-05   1.874937E-04   1.738475E-04
 10    H28    -4.685708E-07  -5.859149E-05  -8.111187E-05
 11    H30    -1.534611E-04  -3.929726E-04  -5.928572E-05
 12    C8      4.726562E-05   1.884753E-04  -5.777532E-04
 13    H32     1.783034E-04   5.688829E-06  -1.593956E-04
 14    C10     4.772527E-04  -3.491906E-05  -1.205943E-04
 15    N2     -7.778618E-06  -7.766610E-04   2.982370E-04
 16    C9     -4.525494E-04  -9.669624E-04   8.596498E-04
 17    O1      2.078895E-03   1.593225E-03  -3.019907E-04
 18    H43     5.307163E-04   7.226982E-05   2.328912E-04
 19    C12    -6.460192E-04  -7.626877E-04   1.227142E-03
 20    C11    -1.034918E-03   2.620373E-04  -3.374878E-04
 21    C18    -5.103751E-04   1.442696E-04  -2.156988E-05
 22    H48     2.586969E-04  -2.025763E-04  -2.432985E-04
 23    C13     2.769440E-04  -1.664652E-04   2.723611E-04
 24    C14     9.926921E-04  -2.929296E-04   1.020283E-03
 25    C15     9.387157E-05   3.360789E-04  -1.648624E-03
 26    C16    -2.517079E-04   8.057617E-04  -4.182559E-04
 27    C17    -3.022872E-04   5.188546E-04  -8.798559E-04
 28    H51     4.620089E-04  -4.629588E-05  -9.545173E-05
 29    H52     2.149477E-04  -5.994828E-04   6.041814E-04
 30    H55    -8.991934E-05   2.086922E-04  -1.133807E-04
 31    H56     5.355338E-04   2.615741E-05  -2.722817E-04
 32    H59    -1.014874E-03  -1.847225E-04   7.840525E-04
 33    H60     3.184770E-04  -3.911398E-05  -2.646256E-04
 34    H61     6.715510E-05   1.317919E-04  -2.359414E-04
 35    H62     3.810810E-04   2.070301E-04   3.496000E-04
-----------   -------------  -------------  -------------
   total       1.312555E-03   2.727143E-04  -1.831912E-04

 end of program der1b


 start of program geopt  24

 geometry optimization step 24
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -7.29006E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.73260E-04    1.34656E-02    2.14066E-02
   2.21309E-02    2.83999E-02    2.99087E-02    3.08451E-02    3.10436E-02
   3.19254E-02    3.50439E-02    3.74082E-02    4.48327E-02    4.66508E-02
   5.67245E-02    6.65260E-02    6.76234E-02    7.28251E-02    7.55252E-02
   7.63163E-02    8.91777E-02    9.74103E-02    1.06375E-01    1.13290E-01
   1.19272E-01    1.20977E-01    1.31824E-01    1.35690E-01    1.42984E-01
   1.43389E-01    1.46309E-01    1.54007E-01    1.61558E-01    1.62648E-01
   1.66493E-01    1.72578E-01    1.76020E-01    1.83375E-01    1.85976E-01
   1.91468E-01    1.97171E-01    2.07283E-01    2.11965E-01    2.16621E-01
   2.23719E-01    2.29699E-01    2.32056E-01    2.34680E-01    2.42720E-01
   2.48272E-01    2.56464E-01    2.60525E-01    2.72567E-01    2.75181E-01
   2.89315E-01    2.94360E-01    2.98094E-01    3.03244E-01    3.08641E-01
   3.10024E-01    3.21458E-01    3.25847E-01    3.29838E-01    3.30575E-01
   3.36093E-01    3.40151E-01    3.46141E-01    3.53085E-01    3.56451E-01
   3.74074E-01    3.75596E-01    3.77891E-01    3.87332E-01    3.96742E-01
```

```
    3.97290E-01    4.13952E-01    4.21425E-01    4.23358E-01    4.39971E-01
    4.42365E-01    4.52813E-01    4.58712E-01    4.73893E-01    4.79189E-01
    4.89555E-01    5.02894E-01    5.14075E-01    5.15455E-01    5.36270E-01
    5.55222E-01    5.82251E-01    6.34084E-01    6.43248E-01    6.54151E-01
    7.21341E-01    7.57830E-01    8.72071E-01    1.07051E+00    1.50566E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0136983
   Cos(theta):   0.8599705

   Final level shift:  -2.6579083E-01

  energy change:           -1.2227E-04 .  (  5.0000E-05 )
  gradient maximum:         2.5854E-03 .  (  4.5000E-04 )
  gradient rms:             5.2685E-04 .  (  3.0000E-04 )
  step size:   0.01370  trust radius:   0.01326
  displacement maximum:     3.6148E-03 .  (  1.8000E-03 )
  displacement rms:         1.2252E-03 .  (  1.2000E-03 )
  predicted energy change:    -5.9631E-05    geom step:   1.3698E-02    full step:
1.3698E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.0252E-03     y:    -3.7445E-04     z:     8.9330E-04

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.8798105701     -3.8456848703     -2.3745928221
  C1        1.4842980031     -2.9667989361     -2.2711962489
  C2        3.0978997808     -0.6596144279     -2.0154376243
  C3        1.1387186146     -1.9711480835     -1.3668715961
  C4        2.6228462289     -2.8003229729     -3.0353626945
  C5        3.4219611474     -1.6601712201     -2.9080421729
  C6        1.9553039662     -0.8362309983     -1.2613393908
  C7        0.0359254693     -1.8082864616     -0.4151269583
  H27       2.9030811328     -3.5578770209     -3.7395872719
  H28       4.3004713859     -1.5630614050     -3.5138890617
  H30       3.6898574857      0.2221105267     -1.8909535806
  C8        0.2213796612     -0.6292950566      0.1933866751
  H32      -0.7619197199     -2.4961091825     -0.2542076494
  C10      -0.3879433315      0.2519247227      1.2589484983
  N2        1.3758383896     -0.0230353950     -0.3034358790
  C9        1.6977858741      1.1807132984      0.2750575054
  O1        2.6886526753      1.8328764008      0.0414295002
  H43      -0.3371281304     -0.2522642068      2.2160621435
  C12      -1.8336014412      0.6187476622      0.9702691677
  C11       0.5722919734      1.4963267533      1.2705504360
  C18       1.1733731119      1.8142624982      2.6480597436
  H48       0.0424115319      2.3654730354      0.9026358643
  C13      -3.5369789730      1.3975992477     -0.5415977461
  C14      -4.1060777398      0.8851158846      1.7256532102
  C15      -4.4843836801      1.3165070472      0.4686146705
  C16      -2.7858980327      0.5379584484      1.9731340493
  C17      -2.2230748542      1.0499741729     -0.2927803494
  H51      -5.5042452477      1.5820251527      0.2728598875
  H52      -2.5020012131      0.2002541030      2.9515511280
  H55      -3.8249100282      1.7238932335     -1.5209099076
  H56      -4.8314696315      0.8141606778      2.5122962102
```

```
 H59      -1.4999675272      1.0954471468     -1.0830604421
 H60       1.6656850525      0.9421322637      3.0611637166
 H61       0.3990610104      2.1345246802      3.3340330547
 H62       1.9039810724      2.6068689543      2.5491819153

 nuclear repulsion energy.......  1443.233524766 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  24   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.208E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      98      91      92
 grid # 3       224    183     182     194     182     182     187     183
 grid # 4       224    379     380     406     379     379     372     377

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      82      99      75
 grid # 2       106    106     105      91     106      93     109      80
 grid # 3       224    224     220     187     223     175     224     164
 grid # 4       224    224     219     374     229     349     402     333

 number of gridpoints:
    atom         O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1       111     69      90      81      71      69      88      87
 grid # 2       127     96     105      93      76      99     100     100
 grid # 3       272    210     193     173     148     216     183     183
 grid # 4       474    201     400     356     306     208     379     379

 number of gridpoints:
    atom        C15    C16     C17     H51     H52     H55     H56     H59
 grid # 1        89     87      85      73      73      73      73      70
 grid # 2       100    100      96     106     103     106     106     102
 grid # 3       183    182     181     224     214     224     224     215
 grid # 4       379    378     377     224     214     224     224     211

 number of gridpoints:
    atom        H60    H61     H62   total
 grid # 1        71     72      71    2820
 grid # 2        99     99      99    3488
 grid # 3       217    221     220    7041
 grid # 4       218    222     221   10845

 end of program grid
 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                              RMS    maximum
      e  d  i  u  i                    energy  density   DIIS
      r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14278245545           5.8E-05  9.8E-04
etot   2  Y  Y  4  M  -815.14283771100  5.5E-05  1.6E-05  4.0E-04
etot   3  Y  Y  4  M  -815.14284471084  7.0E-06  5.9E-06  1.4E-04
etot   4  Y  Y  4  M  -815.14284509616  3.9E-07  2.7E-06  5.8E-05
etot   5  Y  N  4  M  -815.14284578473  6.9E-07  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1443.23352476568
  (E)  Total one-electron terms..... -3971.94629468740
  (I)  Total two-electron terms.....  1713.56992413699
  (L)  Electronic energy............ -2258.37637055041  (E+I)
  (N)  Total energy.................  -815.14284578473  (A+L)

SCFE: SCF energy: HF    -815.14284578473 hartrees   iterations:   5


HOMO energy:    -0.29693
LUMO energy:     0.11878

 Orbital energies:
 -20.45275  -15.55220  -11.32157  -11.23579  -11.22243  -11.21387
 -11.20678  -11.20090  -11.18748  -11.18645  -11.18589  -11.18544
 -11.18399  -11.18374  -11.17893  -11.17678  -11.17662  -11.17535
 -11.17452  -11.17229   -1.42338   -1.33315   -1.18080   -1.16287
  -1.11560   -1.08835   -1.04115   -1.02786   -1.02047   -1.00061
  -0.94721   -0.90617   -0.85450   -0.84423   -0.83184   -0.81111
  -0.79397   -0.76191   -0.72098   -0.69205   -0.67868   -0.66907
  -0.65827   -0.64062   -0.64041   -0.62715   -0.61192   -0.60609
  -0.60424   -0.60183   -0.59212   -0.57807   -0.55716   -0.55571
  -0.53898   -0.53190   -0.51664   -0.50772   -0.49999   -0.49661
  -0.49149   -0.48609   -0.45947   -0.42239   -0.39367   -0.34986
  -0.34286   -0.31533   -0.29693    0.11878    0.13421    0.13897
   0.14223    0.20547    0.22576    0.26446    0.27131    0.27417
   0.29955

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr
 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -4.693129E-05  -8.955542E-05  -3.947449E-05
  2    C1     -3.400762E-05  -1.115335E-04  -2.973969E-04
  3    C2      2.873871E-05   5.530545E-05  -8.613525E-05
  4    C3     -2.896385E-04  -3.505482E-04   2.538094E-04
  5    C4      1.343388E-05  -3.899574E-04  -8.270230E-05
  6    C5      5.542569E-04   3.568880E-05  -5.237625E-04
  7    C6      2.191685E-04   5.807666E-04   4.014931E-04
  8    C7     -8.780115E-04   2.671671E-04  -7.346376E-04
  9    H27     4.797173E-05  -1.153414E-04  -1.696471E-05
 10    H28    -2.318651E-05  -5.102009E-05   9.860963E-06
 11    H30     2.791345E-04   2.282415E-04  -1.913709E-05
 12    C8     -2.506698E-04   4.859804E-04  -2.613423E-05
 13    H32     5.615176E-05  -3.484797E-06   3.726353E-05
 14    C10     6.312939E-04  -6.380115E-05  -4.457213E-04
 15    N2      3.107649E-04  -5.898393E-04   4.845005E-04
 16    C9      3.817864E-04  -1.815168E-04   5.098035E-04
 17    O1      1.546469E-06  -1.238997E-04   5.519581E-06
 18    H43     5.281791E-04   2.455802E-04   7.357829E-05
 19    C12    -4.430054E-04  -8.794639E-04   6.425886E-04
 20    C11    -3.528337E-04   3.858928E-04  -2.068393E-04
 21    C18    -4.086160E-04   4.829425E-04  -3.522413E-04
 22    H48     2.638336E-04  -2.130394E-04  -4.614152E-04
 23    C13     3.231652E-04  -2.843605E-05   1.413580E-04
 24    C14     7.585485E-05   2.002462E-06   5.584545E-04
 25    C15    -1.510532E-04   4.869886E-05  -5.007211E-05
 26    C16    -2.632720E-04   3.620964E-04   3.487420E-04
 27    C17     1.113749E-04   5.330038E-05  -1.284709E-04
 28    H51     2.097836E-04   4.897233E-06   2.629053E-05
 29    H52    -8.817246E-05  -3.232563E-05  -2.360050E-04
 30    H55     7.280615E-05   1.230035E-04  -1.132583E-04
 31    H56     2.771566E-04   4.430355E-05  -2.838972E-04
 32    H59     5.369438E-06   3.164462E-05  -7.975462E-05
 33    H60     3.761009E-04  -3.527690E-04  -4.450671E-05
 34    H61    -2.077395E-04   1.030444E-04   2.206652E-04
 35    H62     1.277019E-04  -3.674696E-05   1.110622E-04
-----------   -------------  -------------  -------------
   total       1.458436E-03  -7.272195E-05  -4.035372E-04

 end of program der1b


 start of program geopt  25

 geometry optimization step 25
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.82117E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
```

```
    0.00000E+00     0.00000E+00     6.52529E-04     7.41854E-03     1.84635E-02
    2.19593E-02     2.82810E-02     3.07952E-02     3.09397E-02     3.13815E-02
    3.21759E-02     3.70318E-02     3.78907E-02     4.45499E-02     4.74001E-02
    5.61643E-02     6.64131E-02     6.84285E-02     7.27107E-02     7.31956E-02
    7.78541E-02     8.31257E-02     8.79940E-02     9.75192E-02     1.01009E-01
    1.13267E-01     1.17254E-01     1.22465E-01     1.32600E-01     1.40934E-01
    1.42020E-01     1.44747E-01     1.51866E-01     1.52455E-01     1.59745E-01
    1.60524E-01     1.71134E-01     1.75642E-01     1.80878E-01     1.86995E-01
    1.88272E-01     1.96159E-01     2.03891E-01     2.08329E-01     2.14125E-01
    2.16325E-01     2.27330E-01     2.31544E-01     2.38915E-01     2.45552E-01
    2.47445E-01     2.56277E-01     2.60870E-01     2.74961E-01     2.82870E-01
    2.88104E-01     2.93600E-01     2.99808E-01     3.07669E-01     3.10155E-01
    3.19136E-01     3.21845E-01     3.22660E-01     3.30318E-01     3.34142E-01
    3.37382E-01     3.40888E-01     3.46579E-01     3.55369E-01     3.56657E-01
    3.59455E-01     3.69444E-01     3.75835E-01     3.83156E-01     3.98477E-01
    4.02884E-01     4.06663E-01     4.15187E-01     4.27910E-01     4.39754E-01
    4.42362E-01     4.57093E-01     4.60532E-01     4.73932E-01     4.79567E-01
    4.86413E-01     4.92669E-01     5.02571E-01     5.18220E-01     5.31835E-01
    5.81737E-01     6.22814E-01     6.33183E-01     6.43254E-01     6.75129E-01
    7.26921E-01     7.62644E-01     9.14152E-01     1.05385E+00     1.41236E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0193202
   Cos(theta):   0.7050332

   Final level shift:  -2.2503852E-01

  energy change:           -5.6718E-05 .   (  5.0000E-05 )
  gradient maximum:         1.2011E-03 .   (  4.5000E-04 )
  gradient rms:             2.9935E-04 *   (  3.0000E-04 )
  step size:   0.01932  trust radius:   0.01875
  displacement maximum:    6.2298E-03 .   (  1.8000E-03 )
  displacement rms:         1.7280E-03 .   (  1.2000E-03 )
  predicted energy change:    -6.4795E-05    geom step:   1.9320E-02    full step:
1.9320E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.5181E-04     y:    -1.0610E-03     z:     9.4421E-04

  new geometry:
                                 angstroms
  atom            x                  y                  z
  H25       0.8841756139      -3.8451128079      -2.3795592096
  C1        1.4879296826      -2.9659977738      -2.2737930892
  C2        3.1018943504      -0.6607036755      -2.0161313320
  C3        1.1383171520      -1.9707973192      -1.3698328867
  C4        2.6288812749      -2.8004560371      -3.0367062030
  C5        3.4280688933      -1.6612984794      -2.9088313835
  C6        1.9558508169      -0.8357197208      -1.2621017370
  C7        0.0334225028      -1.8087360242      -0.4200989883
  H27       2.9110068367      -3.5580169192      -3.7398497200
  H28       4.3069377004      -1.5634243110      -3.5126057552
  H30       3.6929270099       0.2217927325      -1.8912047758
  C8        0.2182109361      -0.6299838437       0.1903019831
  H32      -0.7627238467      -2.4986365935      -0.2602937808
  C10      -0.3906345666       0.2502214520       1.2562746241
  N2        1.3743100093      -0.0244700072      -0.3042321663
  C9        1.6973457886       1.1787296992       0.2764979684
```

```
 O1        2.6930158166      1.8300973548      0.0477779367
 H43      -0.3366406432     -0.2525658007      2.2134897509
 C12      -1.8369157955      0.6169948823      0.9717284713
 C11       0.5693903446      1.4948253541      1.2675289180
 C18       1.1702129061      1.8169705749      2.6429154796
 H48       0.0409065050      2.3612546844      0.8953812070
 C13      -3.5371197893      1.3998631594     -0.5385323588
 C14      -4.1071567664      0.8883718615      1.7315410780
 C15      -4.4842797939      1.3208469259      0.4739431928
 C16      -2.7888980317      0.5385859423      1.9769770096
 C17      -2.2252636861      1.0492280099     -0.2918724447
 H51      -5.5030379021      1.5890390546      0.2794734473
 H52      -2.5048169564      0.2020161883      2.9554687691
 H55      -3.8242474859      1.7272717684     -1.5181301127
 H56      -4.8323517595      0.8194668824      2.5190044769
 H59      -1.5019823261      1.0952077314     -1.0838825327
 H60       1.6629127227      0.9470384239      3.0571680126
 H61       0.3954939955      2.1371955723      3.3273443000
 H62       1.9005568797      2.6095472398      2.5438498268

 nuclear repulsion energy.......  1442.875343304 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  25   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.214E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1       73     89      87      90      87      87      85      85
 grid # 2      106    100      97      98      98      99      91      92
 grid # 3      224    183     184     194     182     182     188     182
 grid # 4      224    379     380     404     379     379     374     377

 number of gridpoints:
    atom       H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1       73     73      73      86      73      82      99      75
 grid # 2      106    106     105      91     106      93     109      80
 grid # 3      224    224     220     187     223     175     224     164
 grid # 4      224    224     219     374     229     349     402     332

 number of gridpoints:
    atom        O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1      111     69      90      81      72      69      88      87
 grid # 2      127     96     105      93      74      99     100     100
 grid # 3      272    210     193     173     147     216     183     183
 grid # 4      474    201     399     355     306     209     379     380

 number of gridpoints:
    atom       C15     C16     C17     H51     H52     H55     H56     H59
 grid # 1       89      86      85      73      73      73      73      70
 grid # 2      100     100      97     106     103     106     106     102
 grid # 3      183     182     181     224     215     224     224     215
 grid # 4      379     378     376     224     214     224     224     211

 number of gridpoints:
    atom       H60     H61     H62  total
 grid # 1       71      72      71   2820
 grid # 2       99      99      99   3488
 grid # 3      217     221     220   7043
 grid # 4      218     222     221  10843

 end of program grid


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                     RMS    maximum
      e  d  i  u  i                          energy  density   DIIS
      r  t  s  t  d     total energy        change   change    error

etot   1  N  N  1  U  -815.14272301303           7.7E-05  8.7E-04
etot   2  Y  Y  4  M  -815.14279348689  7.0E-05  1.9E-05  2.8E-04
etot   3  Y  Y  4  M  -815.14279737496  3.9E-06  6.0E-06  1.6E-04
etot   4  Y  Y  4  M  -815.14279768359  3.1E-07  2.8E-06  5.7E-05
etot   5  Y  N  4  M  -815.14279837106  6.9E-07  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1442.87534330388
  (E)  Total one-electron terms..... -3971.22858528973
  (I)  Total two-electron terms.....  1713.21044361479
  (L)  Electronic energy............ -2258.01814167494  (E+I)
  (N)  Total energy.................  -815.14279837106  (A+L)

SCFE: SCF energy: HF    -815.14279837106 hartrees   iterations:   5


HOMO energy:    -0.29703
LUMO energy:     0.11849

 Orbital energies:
 -20.45259  -15.55264  -11.32178  -11.23616  -11.22281  -11.21398
 -11.20657  -11.20126  -11.18771  -11.18661  -11.18601  -11.18556
 -11.18418  -11.18395  -11.17912  -11.17711  -11.17699  -11.17539
 -11.17409  -11.17237   -1.42170   -1.33292   -1.18081   -1.16257
  -1.11578   -1.08823   -1.04094   -1.02850   -1.02015   -1.00058
  -0.94734   -0.90640   -0.85448   -0.84392   -0.83228   -0.81089
  -0.79413   -0.76180   -0.72106   -0.69213   -0.67872   -0.66921
  -0.65811   -0.64057   -0.64032   -0.62718   -0.61155   -0.60567
  -0.60413   -0.60234   -0.59209   -0.57807   -0.55705   -0.55555
  -0.53908   -0.53184   -0.51665   -0.50774   -0.50004   -0.49649
  -0.49140   -0.48628   -0.45921   -0.42246   -0.39350   -0.35040
  -0.34258   -0.31509   -0.29703    0.11849    0.13403    0.13866
```

```
    0.14192     0.20519     0.22573     0.26433     0.27142     0.27439
    0.29939

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25    -9.714313E-05  -1.161049E-04   2.170986E-05
   2    C1      2.675129E-04   2.377839E-05  -6.904508E-04
   3    C2     -1.639912E-03   2.578062E-04   1.020052E-03
   4    C3      9.890870E-04   5.463815E-05  -2.482887E-04
   5    C4     -9.214562E-04  -5.603544E-04   6.284403E-04
   6    C5     -6.136311E-04   9.668785E-04   9.461156E-04
   7    C6      1.094747E-03  -8.535263E-04  -9.540568E-04
   8    C7     -2.252493E-04   6.766657E-04  -7.108219E-04
   9    H27    -1.679923E-04  -3.709626E-04  -6.913642E-05
  10    H28     4.647765E-04  -4.077575E-05  -3.232213E-04
  11    H30     3.236270E-04   6.519178E-05   5.141983E-05
  12    C8      6.495391E-05  -3.593817E-04  -8.308884E-04
  13    H32    -1.263261E-04   1.102556E-04   3.004845E-05
  14    C10     8.164836E-04   1.993241E-04   4.602473E-04
  15    N2      1.354779E-03   8.481349E-04   3.685790E-04
  16    C9      3.401833E-03   1.013205E-03  -6.343755E-04
  17    O1     -3.778897E-03  -2.692785E-03   5.867877E-04
  18    H43     4.721782E-04  -1.401710E-04   3.513388E-04
  19    C12    -6.575662E-04  -6.672790E-04   6.086884E-04
  20    C11     5.382694E-04   4.074872E-04  -5.385166E-04
  21    C18    -9.002836E-04   7.500707E-04  -6.117966E-05
  22    H48    -3.457176E-04   7.078513E-04  -6.176515E-04
  23    C13    -1.670271E-03   2.527050E-04   4.705650E-04
  24    C14    -9.115917E-04   5.133206E-04  -4.939391E-04
  25    C15     4.113568E-04   1.356194E-05  -5.384865E-04
  26    C16     2.001140E-03   9.825150E-05  -3.029240E-04
  27    C17     1.441721E-03  -1.994314E-04   2.383057E-04
  28    H51    -2.335675E-04   1.366882E-04  -1.752295E-04
  29    H52     2.055371E-04  -2.132495E-04  -1.630348E-04
  30    H55    -1.914988E-04   8.238032E-05   2.619522E-04
  31    H56     3.930219E-04   1.034902E-04  -5.575606E-04
  32    H59    -5.849048E-04  -2.118714E-04   8.644616E-04
  33    H60     6.803009E-04  -1.042593E-03   3.898281E-04
  34    H61    -4.529563E-04   3.080447E-04   7.126579E-04
  35    H62     8.688231E-05   8.014975E-05  -1.534116E-04
 -----------   -------------  -------------  -------------
    total       1.489243E-03   2.013943E-04  -5.197603E-05

  end of program der1b
  start of program geopt  26

  geometry optimization step 26
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  ** restarting optimization from step   25 **

  Hessian eigenvalues:
   -9.50741E-02    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    5.00000E-04    5.54763E-03    1.83969E-02
    2.19097E-02    2.81661E-02    3.01001E-02    3.08749E-02    3.09439E-02
    3.18809E-02    3.72485E-02    3.96545E-02    4.47471E-02    4.91724E-02
    5.67172E-02    6.73853E-02    7.02131E-02    7.26847E-02    7.48824E-02
    8.11748E-02    8.45493E-02    9.98910E-02    1.00596E-01    1.13237E-01
    1.16024E-01    1.21635E-01    1.26979E-01    1.34212E-01    1.42662E-01
    1.43925E-01    1.44749E-01    1.49759E-01    1.54288E-01    1.59350E-01
    1.64841E-01    1.68966E-01    1.77131E-01    1.78959E-01    1.86760E-01
    1.94322E-01    1.96588E-01    2.07546E-01    2.12306E-01    2.13982E-01
    2.21543E-01    2.28459E-01    2.32084E-01    2.42437E-01    2.46850E-01
    2.51215E-01    2.57651E-01    2.59895E-01    2.71479E-01    2.76551E-01
    2.88772E-01    2.96009E-01    2.99385E-01    3.07320E-01    3.10338E-01
    3.15981E-01    3.19213E-01    3.23842E-01    3.26952E-01    3.32122E-01
    3.35880E-01    3.39794E-01    3.45924E-01    3.50062E-01    3.58316E-01
    3.69125E-01    3.73231E-01    3.76178E-01    3.86041E-01    3.94643E-01
    4.06418E-01    4.14289E-01    4.16602E-01    4.25483E-01    4.39494E-01
    4.45643E-01    4.55445E-01    4.62867E-01    4.70296E-01    4.79539E-01
    4.81378E-01    4.94331E-01    5.15395E-01    5.24289E-01    5.52069E-01
    5.69824E-01    6.31151E-01    6.41566E-01    6.47624E-01    6.52209E-01
    7.20171E-01    7.62977E-01    9.20144E-01    1.03799E+00    1.35537E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0104182
   Cos(theta):   0.9189322

   Final level shift:  -2.5678303E-01

  energy change:            4.7414E-05 *  (  5.0000E-05 )
  gradient maximum:         1.2011E-03 .  (  4.5000E-04 )
  gradient rms:             2.9935E-04 *  (  3.0000E-04 )
  step size:   0.01042  trust radius:   0.01000
  displacement maximum:     4.0372E-03 .  (  1.8000E-03 )
  displacement rms:         9.3183E-04 *  (  1.2000E-03 )
  predicted energy change:   -2.9961E-05   geom step:   1.0418E-02   full step:
1.0418E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.6613E-16     y:    -6.5919E-17     z:     2.7756E-16

  new geometry:
                                angstroms
  atom            x                 y                 z
```

```
 H25       0.8789559773     -3.8448035041     -2.3785695524
 C1        1.4845402129     -2.9667843613     -2.2737414561
 C2        3.1015611087     -0.6616819373     -2.0140721951
 C3        1.1385505149     -1.9710570901     -1.3692330626
 C4        2.6250348108     -2.8016479682     -3.0359195317
 C5        3.4258817706     -1.6624518958     -2.9068638050
 C6        1.9570529398     -0.8370211427     -1.2615576646
 C7        0.0340358951     -1.8073664343     -0.4191473871
 H27       2.9055717035     -3.5594210859     -3.7398161267
 H28       4.3056581807     -1.5663217199     -3.5113271478
 H30       3.6951361945      0.2191299559     -1.8883931835
 C8        0.2207035204     -0.6290878578      0.1910075371
 H32      -0.7648811198     -2.4943088238     -0.2597946796
 C10      -0.3880097043      0.2515891425      1.2572161684
 N2        1.3767999468     -0.0241733923     -0.3037758620
 C9        1.6991720839      1.1791983536      0.2755077326
 O1        2.6910257258      1.8302847377      0.0432380324
 H43      -0.3352748305     -0.2524390288      2.2144591729
 C12      -1.8343456345      0.6182214846      0.9707889668
 C11       0.5718600355      1.4963833273      1.2685270130
 C18       1.1698971841      1.8172255287      2.6466242273
 H48       0.0424146855      2.3646608579      0.8976562610
 C13      -3.5387503721      1.3988758086     -0.5385262694
 C14      -4.1057152833      0.8847904597      1.7289478989
 C15      -4.4851360209      1.3172896112      0.4725456681
 C16      -2.7856278199      0.5370707343      1.9747303731
 C17      -2.2248466408      1.0505491455     -0.2915303374
 H51      -5.5050165250      1.5833340850      0.2779998336
 H52      -2.5009659309      0.1983567685      2.9523074216
 H55      -3.8275877423      1.7263264329     -1.5172342690
 H56      -4.8302724323      0.8134237470      2.5158180717
 H59      -1.5027396487      1.0967697650     -1.0825101342
 H60       1.6625117464      0.9459471518      3.0618646646
 H61       0.3937646550      2.1378749174      3.3306733290
 H62       1.9000754278      2.6102599579      2.5485962602

 nuclear repulsion energy.......  1443.022478286 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  26   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.212E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
   atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1       73     89      87      90      87      87      85      85
 grid # 2      106    100      97      98      98      98      91      92
 grid # 3      224    183     182     194     182     182     188     183
 grid # 4      224    379     381     406     379     379     372     377
```

```
  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     86     73     82     99     75
  grid # 2      106    106    105     91    106     93    109     80
  grid # 3      224    224    220    187    223    175    224    164
  grid # 4      224    224    219    374    228    349    402    333

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     69     90     81     71     69     88     87
  grid # 2      127     96    105     93     76     99    100    100
  grid # 3      272    210    193    173    149    216    183    183
  grid # 4      474    201    401    356    306    208    378    379

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     87     85     73     73     73     73     70
  grid # 2      100    100     97    106    103    106    106    102
  grid # 3      183    182    181    224    214    224    224    215
  grid # 4      379    378    376    224    214    224    224    211

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     72     71   2820
  grid # 2       99     99     99   3489
  grid # 3      217    221    220   7043
  grid # 4      218    222    221  10844

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14277440044           5.9E-05  7.3E-04
etot   2  Y  Y  4  M  -815.14282147841  4.7E-05  1.4E-05  2.0E-04
etot   3  Y  Y  4  M  -815.14282701493  5.5E-06  4.8E-06  1.5E-04
etot   4  Y  N  4  M  -815.14282784723  8.3E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1443.02247828638
   (E)  Total one-electron terms..... -3971.52479359741
   (I)  Total two-electron terms.....  1713.35948746380
   (L)  Electronic energy............ -2258.16530613362  (E+I)
   (N)  Total energy.................  -815.14282784723  (A+L)

 SCFE: SCF energy: HF    -815.14282784723 hartrees   iterations:   4


 HOMO energy:    -0.29691
 LUMO energy:     0.11872
 Orbital energies:
 -20.45248  -15.55229  -11.32163  -11.23590  -11.22256  -11.21395
 -11.20688  -11.20095  -11.18761  -11.18646  -11.18587  -11.18543
 -11.18398  -11.18373  -11.17902  -11.17688  -11.17677  -11.17554
 -11.17458  -11.17242   -1.42334   -1.33307   -1.18079   -1.16272
  -1.11557   -1.08822   -1.04109   -1.02796   -1.02035   -1.00056
  -0.94716   -0.90615   -0.85442   -0.84424   -0.83190   -0.81100
  -0.79398   -0.76180   -0.72104   -0.69207   -0.67863   -0.66905
  -0.65822   -0.64064   -0.64040   -0.62709   -0.61183   -0.60601
  -0.60419   -0.60194   -0.59210   -0.57802   -0.55711   -0.55565
  -0.53896   -0.53191   -0.51666   -0.50770   -0.50003   -0.49655
  -0.49146   -0.48614   -0.45940   -0.42233   -0.39359   -0.34993
  -0.34286   -0.31522   -0.29691    0.11872    0.13418    0.13892
   0.14218    0.20535    0.22573    0.26447    0.27131    0.27418
   0.29949

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -1.418465E-05  -6.482077E-05  -5.232393E-05
  2    C1      1.327387E-04   3.328931E-04  -1.056546E-04
  3    C2     -1.401040E-04  -4.385918E-05  -6.262136E-06
  4    C3      7.510581E-05   9.402452E-06   1.557679E-04
  5    C4     -1.590224E-06  -1.831958E-04   6.936016E-05
  6    C5      6.660999E-06  -2.693865E-06  -1.393898E-04
  7    C6     -9.389368E-05  -1.244106E-04   1.897775E-04
  8    C7     -2.842837E-04   6.403235E-04  -8.413399E-04
  9    H27     1.594529E-05  -1.141470E-04  -3.921277E-06
 10    H28    -1.375583E-04  -5.477686E-05   1.010127E-04
 11    H30     9.594328E-05   8.504632E-05   2.642337E-06
 12    C8     -2.302025E-04   1.812065E-04  -3.203690E-04
 13    H32     6.592407E-05  -5.690603E-06   1.620745E-05
 14    C10     5.428340E-04   3.018413E-05  -2.278840E-04
 15    N2      4.442705E-04  -4.401613E-04   5.080769E-04
 16    C9      1.755508E-04  -2.307928E-04   4.006757E-04
 17    O1      1.444185E-04  -9.723184E-05   1.117759E-04
 18    H43     4.632526E-04   2.062685E-04  -1.821814E-05
 19    C12    -2.710081E-04  -8.828715E-04   6.430544E-04
 20    C11    -2.944421E-04   4.693575E-04  -2.986546E-04
 21    C18    -4.324201E-04   3.224197E-04  -1.784564E-04
 22    H48     2.720362E-04  -2.633121E-04  -4.377055E-04
 23    C13     1.560807E-04   2.792447E-05   3.589385E-05
 24    C14     4.737722E-05   7.692290E-05   2.491746E-04
 25    C15    -1.016630E-04   5.268981E-05  -9.203413E-06
 26    C16    -6.581472E-05   3.079911E-04   1.877716E-04
 27    C17     9.447180E-05   2.508150E-05  -4.247505E-06
 28    H51     1.551168E-04   3.173427E-05   2.501224E-05
 29    H52    -9.209584E-06  -6.297352E-05  -7.042321E-05
 30    H55     6.878818E-05   1.042174E-04  -9.382444E-05
 31    H56     1.054882E-04   4.624873E-05  -5.906166E-05
 32    H59     9.067291E-05  -5.345254E-06  -1.285165E-04
 33    H60     2.558064E-04  -2.052772E-04  -6.340874E-05
 34    H61    -1.039576E-04   2.810835E-05   1.495370E-04
 35    H62     1.376270E-04   3.405769E-06   2.476452E-05
-----------   -------------  -------------  -------------
   total       1.365777E-03   1.998658E-04  -1.883601E-04

 end of program der1b


 start of program geopt  27

 geometry optimization step 27
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.39181E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.00000E-04    2.99096E-03    2.18068E-02
   2.39126E-02    2.81591E-02    2.96236E-02    3.04541E-02    3.10836E-02
   3.21481E-02    3.61879E-02    3.73578E-02    4.46589E-02    5.13883E-02
   5.72032E-02    6.26431E-02    6.95108E-02    7.39887E-02    7.60631E-02
   7.95039E-02    8.45084E-02    9.30603E-02    9.81680E-02    1.10657E-01
   1.13777E-01    1.18526E-01    1.29260E-01    1.33796E-01    1.41860E-01
   1.42993E-01    1.46245E-01    1.51672E-01    1.53968E-01    1.61594E-01
   1.65382E-01    1.70163E-01    1.73067E-01    1.79252E-01    1.91223E-01
   1.92164E-01    1.97509E-01    2.05485E-01    2.10793E-01    2.18453E-01
   2.19181E-01    2.25576E-01    2.31226E-01    2.37216E-01    2.42520E-01
   2.48981E-01    2.54285E-01    2.57649E-01    2.82986E-01    2.86286E-01
   2.89048E-01    2.95252E-01    3.04138E-01    3.07846E-01    3.14220E-01
   3.18553E-01    3.21649E-01    3.24063E-01    3.26203E-01    3.29975E-01
   3.36616E-01    3.38065E-01    3.40959E-01    3.53495E-01    3.56261E-01
   3.76683E-01    3.77953E-01    3.87916E-01    3.93922E-01    3.98506E-01
   4.04501E-01    4.12562E-01    4.26384E-01    4.33447E-01    4.37663E-01
   4.54439E-01    4.67650E-01    4.74725E-01    4.79839E-01    4.81886E-01
   4.88727E-01    4.99888E-01    5.11870E-01    5.29038E-01    5.63373E-01
   5.75005E-01    6.14696E-01    6.41734E-01    6.50422E-01    7.10122E-01
   7.37612E-01    8.37001E-01    1.03856E+00    1.06750E+00    1.36852E+00

 WARNING: Hessian has wrong number of negative eigenvalues
 WARNING: positive P-RFO shift not converged: using initial-guess shift


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0143152
  Cos(theta):   0.9172034

  Final level shift:  -1.9447812E-01

 energy change:           1.7937E-05 *  (  5.0000E-05 )
 gradient maximum:        1.0830E-03 .  (  4.5000E-04 )
 gradient rms:            2.5022E-04 *  (  3.0000E-04 )
```

```
  step size:   0.01432  trust radius:   0.01414
  displacement maximum:    5.6914E-03 .  (  1.8000E-03 )
  displacement rms:        1.2804E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.8297E-05    geom step:   1.4315E-02    full step:
1.4315E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.2197E-03     y:    -1.2543E-03     z:     6.9472E-04

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.8762564274     -3.8415745856     -2.3859327936
  C1        1.4838846979     -2.9650153357     -2.2780619256
  C2        3.1050351571     -0.6643072970     -2.0114989424
  C3        1.1387135994     -1.9702469354     -1.3720246931
  C4        2.6252574527     -2.8014802971     -3.0383973185
  C5        3.4280825851     -1.6642224812     -2.9059637101
  C6        1.9593216140     -0.8381565407     -1.2605667864
  C7        0.0332171439     -1.8054800894     -0.4238157335
  H27       2.9051726401     -3.5586555444     -3.7432782072
  H28       4.3078745690     -1.5681621116     -3.5089258714
  H30       3.7002932907      0.2150917095     -1.8834996258
  C8        0.2202436032     -0.6283196631      0.1884203827
  H32      -0.7672263185     -2.4911312967     -0.2673408582
  C10      -0.3887314537      0.2515691239      1.2546920167
  N2        1.3782775854     -0.0255289961     -0.3032191851
  C9        1.7009888511      1.1771873167      0.2770513891
  O1        2.6944444086      1.8259675903      0.0476440436
  H43      -0.3344995209     -0.2522628667      2.2116207087
  C12      -1.8355029822      0.6176775311      0.9708220197
  C11       0.5709290907      1.4967144391      1.2656390692
  C18       1.1634893633      1.8224484538      2.6446358403
  H48       0.0424842602      2.3630957358      0.8899026329
  C13      -3.5407725084      1.3990495656     -0.5359094328
  C14      -4.1046964127      0.8860847939      1.7327679746
  C15      -4.4854528573      1.3184037640      0.4766826871
  C16      -2.7851138035      0.5376662373      1.9764238462
  C17      -2.2273714564      1.0498810658     -0.2910784896
  H51      -5.5051078217      1.5850594632      0.2838256040
  H52      -2.4988968958      0.1992718666      2.9532963178
  H55      -3.8306354075      1.7265491466     -1.5141837773
  H56      -4.8281395566      0.8153325982      2.5203989867
  H59      -1.5063848853      1.0965293136     -1.0834900422
  H60       1.6549235449      0.9523982607      3.0647492041
  H61       0.3839738535      2.1453922798      3.3245628006
  H62       1.8941132809      2.6154013711      2.5476806675

  nuclear repulsion energy.......  1443.043531714 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  27   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.210E-03
  number of canonical orbitals.....          210
  end of program onee
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H25     C1      C2      C3      C4      C5      C6      C7
  grid # 1        73     89      87      90      87      87      85      85
  grid # 2       106    100      97      98      98      99      91      92
  grid # 3       224    183     182     194     182     182     187     183
  grid # 4       224    379     381     404     379     379     372     377

  number of gridpoints:
     atom        H27    H28     H30      C8     H32     C10      N2      C9
  grid # 1        73     73      73      86      73      82      99      75
  grid # 2       106    106     105      91     106      93     109      80
  grid # 3       224    224     220     187     223     175     224     164
  grid # 4       224    224     219     374     228     349     402     332

  number of gridpoints:
     atom         O1    H43     C12     C11     C18     H48     C13     C14
  grid # 1       111     69      90      81      71      69      87      87
  grid # 2       123     96     105      93      77      99     100     100
  grid # 3       272    210     193     172     149     216     183     183
  grid # 4       474    201     401     356     305     208     378     379

  number of gridpoints:
     atom        C15    C16     C17     H51     H52     H55     H56     H59
  grid # 1        89     86      85      73      73      73      73      70
  grid # 2       100    100      97     106     103     106     106     102
  grid # 3       183    182     181     224     214     224     224     215
  grid # 4       379    378     376     224     214     224     224     211

  number of gridpoints:
     atom        H60    H61     H62   total
  grid # 1        71     72      71    2818
  grid # 2        99     99      99    3487
  grid # 3       217    221     220    7041
  grid # 4       218    222     221   10840

  end of program grid


  start of program rwr
 recomputing RwR matrix  14    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                RMS    maximum
       e  d  i  u  i                     energy  density    DIIS
       r  t  s  t  d     total energy    change   change    error

etot   1  N  N  1  U  -815.14280969734            5.0E-05  1.1E-03
etot   2  Y  Y  4  M  -815.14286250291  5.3E-05  1.5E-05  4.4E-04
etot   3  Y  Y  4  M  -815.14286718030  4.7E-06  4.8E-06  1.4E-04
etot   4  Y  N  4  M  -815.14286771519  5.3E-07  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
  (A)  Nuclear repulsion...........  1443.04353171359
  (E)  Total one-electron terms..... -3971.56379385594
  (I)  Total two-electron terms.....  1713.37739442716
  (L)  Electronic energy........... -2258.18639942878  (E+I)
  (N)  Total energy................  -815.14286771519  (A+L)

SCFE: SCF energy: HF    -815.14286771519 hartrees   iterations:   4


HOMO energy:    -0.29681
LUMO energy:     0.11875

 Orbital energies:
 -20.45283  -15.55212  -11.32141  -11.23575  -11.22258  -11.21388
 -11.20670  -11.20098  -11.18758  -11.18633  -11.18575  -11.18532
 -11.18395  -11.18369  -11.17899  -11.17683  -11.17675  -11.17532
 -11.17467  -11.17226   -1.42374   -1.33323   -1.18093   -1.16280
  -1.11563   -1.08819   -1.04107   -1.02822   -1.02044   -1.00052
  -0.94717   -0.90620   -0.85437   -0.84424   -0.83208   -0.81102
  -0.79410   -0.76178   -0.72115   -0.69224   -0.67872   -0.66913
  -0.65823   -0.64065   -0.64052   -0.62712   -0.61182   -0.60608
  -0.60422   -0.60214   -0.59208   -0.57805   -0.55713   -0.55568
  -0.53895   -0.53200   -0.51674   -0.50774   -0.50008   -0.49656
  -0.49142   -0.48617   -0.45949   -0.42241   -0.39355   -0.35012
  -0.34280   -0.31528   -0.29681    0.11875    0.13418    0.13900
   0.14221    0.20544    0.22584    0.26450    0.27139    0.27432
   0.29945

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x               y               z
----  -----   -------------  -------------  -------------
  1    H25     5.536507E-05   1.009587E-04   4.972662E-05
  2    C1     -3.989019E-04   1.408619E-05   8.000543E-05
  3    C2     -8.102358E-05  -1.450321E-05  -3.267739E-05
  4    C3      1.959152E-04   5.665780E-05   2.097242E-04
  5    C4      2.199285E-04  -6.881441E-05  -5.965728E-06
  6    C5     -2.928512E-04   2.773931E-04   2.625893E-04
  7    C6     -1.928033E-04  -2.375571E-04  -3.312746E-05
  8    C7     -7.587958E-04   4.044530E-04  -7.515646E-04
  9    H27    -7.134534E-06  -6.586448E-05   5.135270E-06
 10    H28     4.172658E-04  -5.370583E-05  -2.632260E-04
 11    H30     1.103792E-04   2.589041E-05  -6.516174E-05
 12    C8     -2.038889E-04  -3.229695E-04  -6.789807E-04
 13    H32    -1.715685E-05  -5.543916E-05   6.339978E-05
 14    C10     6.392731E-04   2.578378E-04   1.829044E-05
 15    N2      7.850015E-04  -3.018746E-04   4.299509E-04
 16    C9     -1.186536E-04  -5.850359E-04   5.707698E-04
 17    O1      7.240532E-04   4.453162E-04  -7.495729E-05
 18    H43     5.043722E-04   4.955469E-05   2.184360E-04
 19    C12    -1.543278E-04  -7.383911E-04   3.943102E-04
 20    C11    -2.828955E-04   4.492621E-04  -1.583964E-04
 21    C18    -5.125772E-04   2.802292E-04   1.993410E-04
 22    H48     1.274753E-04  -3.383880E-05  -5.078225E-04
 23    C13    -3.093525E-04   1.344736E-04  -5.315293E-05
 24    C14    -3.212942E-04   1.830832E-04  -5.325624E-05
 25    C15    -1.527675E-04   3.328053E-05   5.454941E-05
 26    C16     5.292555E-04   1.733152E-04   1.149952E-04
 27    C17     6.903139E-04   3.794942E-05  -6.614406E-05
 28    H51    -1.114371E-04   8.602323E-05  -4.892655E-05
 29    H52     6.232425E-05  -1.578207E-04   1.605981E-04
 30    H55    -2.171484E-05   1.352268E-04  -1.419888E-04
 31    H56    -1.759742E-05   4.010799E-05   6.055829E-05
 32    H59    -1.453458E-05  -1.025774E-04   1.123527E-04
 33    H60     9.483755E-05  -2.301336E-06  -1.147813E-04
 34    H61     1.902297E-04  -1.218181E-04  -3.025538E-05
 35    H62     2.885088E-05  -6.721982E-05  -6.047267E-05
-----------   -------------  -------------  -------------
   total       1.405133E-03   2.553679E-04  -1.361251E-04

 end of program der1b


 start of program geopt  28

 geometry optimization step 28
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -1.11929E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.00000E-04    2.75903E-03    2.09042E-02
   2.28789E-02    2.82011E-02    2.97817E-02    3.08737E-02    3.11769E-02
   3.17706E-02    3.55129E-02    3.74101E-02    4.44379E-02    5.09892E-02
   5.67234E-02    6.35169E-02    7.01962E-02    7.20938E-02    7.48144E-02
   7.67875E-02    8.62471E-02    9.51092E-02    9.78841E-02    1.09466E-01
   1.13788E-01    1.16667E-01    1.23785E-01    1.35217E-01    1.41516E-01
   1.44886E-01    1.48730E-01    1.52072E-01    1.56368E-01    1.62262E-01
   1.69466E-01    1.70883E-01    1.74381E-01    1.79946E-01    1.91980E-01
   1.98687E-01    2.02083E-01    2.05670E-01    2.11286E-01    2.17633E-01
   2.21922E-01    2.29240E-01    2.31979E-01    2.39414E-01    2.45351E-01
   2.49951E-01    2.53072E-01    2.60662E-01    2.76096E-01    2.84800E-01
   2.88286E-01    2.99944E-01    3.08328E-01    3.12046E-01    3.14401E-01
   3.16406E-01    3.19509E-01    3.26727E-01    3.27263E-01    3.32579E-01
   3.36729E-01    3.43072E-01    3.47957E-01    3.54450E-01    3.59656E-01
   3.74618E-01    3.79420E-01    3.82385E-01    3.84015E-01    3.94369E-01
   4.07458E-01    4.17401E-01    4.21048E-01    4.33157E-01    4.41591E-01
   4.54382E-01    4.61946E-01    4.63908E-01    4.78974E-01    4.83786E-01
   4.88898E-01    5.02225E-01    5.11453E-01    5.25525E-01    5.59083E-01
   5.80431E-01    6.08632E-01    6.42404E-01    6.56377E-01    6.86415E-01
```

```
    7.49177E-01    7.81609E-01    9.47080E-01    1.04454E+00    1.32233E+00

  WARNING: Hessian has wrong number of negative eigenvalues


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0201984
   Cos(theta):   0.8445332

   Final level shift:  -1.8279453E-01

  energy change:          -3.9868E-05 *  (  5.0000E-05 )
  gradient maximum:        9.6437E-04 .  (  4.5000E-04 )
  gradient rms:            2.8312E-04 *  (  3.0000E-04 )
  step size:   0.02020  trust radius:   0.02000
  displacement maximum:    5.9365E-03 .  (  1.8000E-03 )
  displacement rms:        1.8066E-03 .  (  1.2000E-03 )
  predicted energy change:    -6.4293E-05    geom step:   2.0198E-02    full step:
2.0198E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.3454E-04     y:     1.1136E-03     z:    -8.2184E-04

  new geometry:
                                angstroms
  atom            x                  y                  z
  H25       0.8738413172     -3.8395126865     -2.3880074182
  C1        1.4823771565     -2.9641670753     -2.2796172648
  C2        3.1088378346     -0.6660601406     -2.0104479052
  C3        1.1356667011     -1.9675515396     -1.3760684112
  C4        2.6285798581     -2.8048139871     -3.0358437892
  C5        3.4341194971     -1.6685466187     -2.9024254258
  C6        1.9591508693     -0.8372601631     -1.2633235157
  C7        0.0273899614     -1.8012125337     -0.4306555570
  H27       2.9085673743     -3.5651042014     -3.7376095766
  H28       4.3188929829     -1.5778038716     -3.5025266163
  H30       3.7070515623      0.2123122648     -1.8815227743
  C8        0.2185345792     -0.6259554664      0.1835737015
  H32      -0.7746513383     -2.4853957181     -0.2739752425
  C10      -0.3871491064      0.2533881144      1.2529689920
  N2        1.3798834071     -0.0244556996     -0.3051342287
  C9        1.7042648905      1.1768656725      0.2772162695
  O1        2.6986868413      1.8264491196      0.0478237842
  H43      -0.3273172182     -0.2511607111      2.2101487875
  C12      -1.8353728682      0.6185797333      0.9719679566
  C11       0.5721540253      1.4982942043      1.2639027723
  C18       1.1621426501      1.8220061121      2.6445611869
  H48       0.0440741557      2.3652947313      0.8867454990
  C13      -3.5459865584      1.3986414206     -0.5320189121
  C14      -4.1065410637      0.8836802522      1.7361256168
  C15      -4.4902421326      1.3164571579      0.4811583359
  C16      -2.7843196607      0.5363666339      1.9782751816
  C17      -2.2295392076      1.0507074659     -0.2889076812
  H51      -5.5110104152      1.5821772495      0.2887421749
  H52      -2.4977012363      0.1964471475      2.9542401645
  H55      -3.8378129506      1.7267997116     -1.5100299323
  H56      -4.8286153981      0.8119901212      2.5238830547
  H59      -1.5098119344      1.0959965074     -1.0812569317
  H60       1.6540373854      0.9507197956      3.0633027555
  H61       0.3817231106      2.1423687530      3.3252673160
  H62       1.8920483112      2.6150609687      2.5483179491
```

```
 nuclear repulsion energy.......  1442.523823494 hartrees
 ------------------------------------------------
/  end of geometry optimization iteration  28   /
------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.216E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     97     98     98     98     91     92
 grid # 3      224    183    182    194    182    182    188    183
 grid # 4      224    379    383    405    379    379    374    377

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     86     73     82     99     75
 grid # 2      106    106    105     91    106     93    109     80
 grid # 3      224    224    220    187    223    175    224    164
 grid # 4      224    224    219    374    228    349    401    333

 number of gridpoints:
    atom        O1    H43    C12    C11    C18    H48    C13    C14
 grid # 1      111     69     90     81     71     69     87     87
 grid # 2      127     96    105     93     74     99    100    100
 grid # 3      272    208    193    173    139    216    183    183
 grid # 4      475    201    401    355    307    208    379    379

 number of gridpoints:
    atom       C15    C16    C17    H51    H52    H55    H56    H59
 grid # 1       89     87     85     73     73     73     73     70
 grid # 2      100    100     98    106    103    106    106    102
 grid # 3      183    182    181    224    215    224    224    215
 grid # 4      379    377    377    224    214    224    224    211

 number of gridpoints:
    atom       H60    H61    H62  total
 grid # 1       71     72     71   2819
 grid # 2       99     99     99   3488
 grid # 3      217    221    220   7032
 grid # 4      218    222    221  10848

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr
```

```
  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14274984067           6.4E-05  1.0E-03
etot   2  Y  Y  4  M  -815.14283441889  8.5E-05  1.8E-05  4.2E-04
etot   3  Y  Y  4  M  -815.14284245552  8.0E-06  6.5E-06  1.4E-04
etot   4  Y  Y  4  M  -815.14284407133  1.6E-06  2.7E-06  5.3E-05
etot   5  Y  N  4  M  -815.14284261108 -1.5E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1442.52382349407
   (E)  Total one-electron terms..... -3970.52966655893
   (I)  Total two-electron terms.....  1712.86300045379
   (L)  Electronic energy............ -2257.66666610514  (E+I)
   (N)  Total energy.................  -815.14284261108  (A+L)

 SCFE: SCF energy: HF    -815.14284261108 hartrees   iterations:   5


 HOMO energy:    -0.29702
 LUMO energy:     0.11861

  Orbital energies:
  -20.45262  -15.55241  -11.32170  -11.23604  -11.22288  -11.21406
  -11.20695  -11.20109  -11.18787  -11.18659  -11.18596  -11.18568
  -11.18411  -11.18386  -11.17915  -11.17719  -11.17712  -11.17590
  -11.17473  -11.17259   -1.42286   -1.33291   -1.18056   -1.16242
   -1.11546   -1.08827   -1.04107   -1.02754   -1.02014   -1.00051
   -0.94703   -0.90614   -0.85426   -0.84437   -0.83176   -0.81089
   -0.79379   -0.76161   -0.72104   -0.69202   -0.67856   -0.66884
   -0.65830   -0.64078   -0.64022   -0.62699   -0.61171   -0.60583
   -0.60415   -0.60175   -0.59213   -0.57793   -0.55705   -0.55554
   -0.53875   -0.53181   -0.51661   -0.50750   -0.50016   -0.49652
   -0.49148   -0.48605   -0.45922   -0.42234   -0.39367   -0.34957
   -0.34307   -0.31510   -0.29702    0.11861    0.13408    0.13863
    0.14196    0.20513    0.22566    0.26447    0.27116    0.27407
    0.29947

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y               z
```

```
----  -----   -------------  -------------  -------------
  1    H25    -1.184316E-04  -1.592729E-04  -6.207227E-05
  2    C1      6.603408E-04   5.109037E-04  -3.586909E-04
  3    C2      1.836873E-05  -3.486972E-04  -2.528074E-04
  4    C3      4.651232E-04  -2.189672E-04  -4.516129E-04
  5    C4     -4.783517E-04   2.720486E-04   5.741075E-04
  6    C5     -2.144340E-05  -1.653835E-04  -1.246811E-04
  7    C6      6.492401E-04  -2.977891E-04  -6.408855E-05
  8    C7      2.229574E-04   7.431298E-04  -7.248244E-04
  9    H27     1.011378E-04   1.359528E-04   6.263466E-05
 10    H28    -8.771328E-04   9.012589E-05   6.432466E-04
 11    H30    -4.474036E-04  -4.891673E-04   4.620147E-05
 12    C8      3.466963E-05   8.406533E-04   1.667482E-04
 13    H32     1.615509E-04   1.102869E-04  -1.501911E-04
 14    C10     2.994149E-04  -1.605620E-04  -1.368404E-04
 15    N2     -1.420113E-04  -7.164698E-04   5.964335E-04
 16    C9      8.066099E-04   8.625824E-04  -1.938297E-04
 17    O1     -9.259055E-04  -9.600683E-04   5.324046E-04
 18    H43     8.753082E-06   1.846301E-04  -3.953546E-04
 19    C12    -2.294939E-04  -9.103137E-04   1.036095E-03
 20    C11    -3.911700E-04   3.265715E-04  -2.919776E-04
 21    C18    -4.823798E-04  -1.080611E-04   1.531590E-04
 22    H48     5.118240E-04  -4.815420E-04  -3.313102E-04
 23    C13     1.206448E-03  -7.693322E-05  -2.100000E-04
 24    C14     1.422260E-03  -1.292129E-04  -5.856680E-05
 25    C15     4.021125E-04   4.047898E-05  -2.578471E-04
 26    C16    -1.075714E-03   5.742479E-04  -2.930558E-04
 27    C17    -1.715940E-03   3.516449E-04   5.184368E-05
 28    H51     4.343475E-04  -6.445100E-05   1.438144E-04
 29    H52     1.284785E-04  -1.217573E-04   3.360721E-04
 30    H55     2.266887E-04  -4.089598E-05   1.130808E-04
 31    H56    -2.774198E-04  -1.140167E-04   6.206160E-04
 32    H59     2.396625E-04   1.839869E-04  -5.630890E-04
 33    H60    -6.507287E-05   4.075232E-04  -2.464762E-04
 34    H61     3.791023E-04  -9.356802E-05  -2.942180E-04
 35    H62     2.867157E-04   2.127984E-04   2.377116E-04
-----------   -------------  -------------  -------------
   total       1.417936E-03   1.904361E-04  -1.473653E-04

 end of program der1b


 start of program geopt  29

 geometry optimization step 29
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format


 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0106751
  Cos(theta):   0.8554045

  Final level shift:  -2.7216740E-01

 energy change:            2.5104E-05 *  (  5.0000E-05 )
 gradient maximum:         1.7322E-03 .  (  4.5000E-04 )
 gradient rms:             4.8087E-04 .  (  3.0000E-04 )
```

```
  step size:   0.01068  trust radius:   0.01000
  displacement maximum:    4.0301E-03 .  (  1.8000E-03 )
  displacement rms:        9.5481E-04 *  (  1.2000E-03 )
  predicted energy change:    -4.0055E-05    geom step:   1.0675E-02    full step:
1.0675E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     9.2653E-04     y:    -1.1014E-03     z:     4.8047E-04

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.8714616765     -3.8371703048     -2.3931862273
  C1        1.4816463038     -2.9630130629     -2.2826838675
  C2        3.1108976339     -0.6686089516     -2.0079198001
  C3        1.1358189846     -1.9672251043     -1.3781920609
  C4        2.6286631322     -2.8043737289     -3.0367402139
  C5        3.4353817057     -1.6699268661     -2.9006072484
  C6        1.9606838737     -0.8386905673     -1.2625490034
  C7        0.0266097208     -1.7995359902     -0.4346070977
  H27       2.9088989458     -3.5636476154     -3.7393795939
  H28       4.3203169671     -1.5790091921     -3.4990706864
  H30       3.7097618371      0.2083399928     -1.8768179783
  C8        0.2182110698     -0.6251488743      0.1813578786
  H32      -0.7772704671     -2.4821143483     -0.2807147299
  C10      -0.3879903923      0.2534985997      1.2508009254
  N2        1.3808251559     -0.0253376652     -0.3051509855
  C9        1.7055734885      1.1755202646      0.2780041585
  O1        2.7015370565      1.8228563153      0.0519317012
  H43      -0.3286941490     -0.2518415752      2.2072820479
  C12      -1.8361982453      0.6183528287      0.9713706252
  C11       0.5715163076      1.4984115630      1.2616079124
  C18       1.1579206042      1.8266218797      2.6425722615
  H48       0.0445129775      2.3642041329      0.8810452084
  C13      -3.5474338046      1.3999855731     -0.5301897088
  C14      -4.1052276979      0.8832618136      1.7388816448
  C15      -4.4900447597      1.3170192972      0.4844131583
  C16      -2.7835869189      0.5356785008      1.9790876016
  C17      -2.2317996551      1.0516630014     -0.2889307692
  H51      -5.5108598823      1.5829510400      0.2940409276
  H52      -2.4953044615      0.1952294453      2.9547490320
  H55      -3.8403501659      1.7288402187     -1.5074784391
  H56      -4.8265802917      0.8107965791      2.5280060870
  H59      -1.5129680148      1.0982880211     -1.0825908458
  H60       1.6487180523      0.9572934676      3.0654372550
  H61       0.3758873306      2.1492246442      3.3196636203
  H62       1.8882590647      2.6196083983      2.5465086102

  nuclear repulsion energy.......  1442.636300728 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  29   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.212E-03
  number of canonical orbitals.....          210
  end of program onee
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom       H25     C1     C2     C3     C4     C5     C6     C7
  grid # 1       73     89     87     90     87     87     85     85
  grid # 2      106    100     97     98     98     98     91     92
  grid # 3      224    183    182    194    182    182    188    183
  grid # 4      224    379    382    406    379    379    372    377

  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     86     73     82     99     75
  grid # 2      106    106    105     91    106     93    109     80
  grid # 3      224    224    220    187    223    175    224    164
  grid # 4      224    224    219    374    228    348    402    333

  number of gridpoints:
     atom        O1    H43    C12    C11    C18    H48    C13    C14
  grid # 1      111     69     90     81     72     69     87     87
  grid # 2      127     96    105     93     74     99    100    100
  grid # 3      272    209    194    173    145    216    183    183
  grid # 4      475    201    401    355    309    208    379    379

  number of gridpoints:
     atom       C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1       89     87     85     73     73     73     73     70
  grid # 2      100    100     97    106    103    106    106    102
  grid # 3      183    182    181    224    215    224    224    215
  grid # 4      379    377    377    224    214    224    224    211

  number of gridpoints:
     atom       H60    H61    H62  total
  grid # 1       71     72     71   2820
  grid # 2       99     99     99   3487
  grid # 3      217    221    220   7040
  grid # 4      218    222    221  10848

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14284111676           3.4E-05  8.5E-04
etot   2  Y  Y  4  M  -815.14287877129  3.8E-05  1.2E-05  3.5E-04
etot   3  Y  Y  4  M  -815.14288187736  3.1E-06  4.0E-06  1.1E-04
etot   4  Y  N  4  M  -815.14288061777 -1.3E-06  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
  (A)  Nuclear repulsion............  1442.63630072842
  (E)  Total one-electron terms..... -3970.75208371619
  (I)  Total two-electron terms.....  1712.97290237000
  (L)  Electronic energy............ -2257.77918134618  (E+I)
  (N)  Total energy.................  -815.14288061777  (A+L)

SCFE: SCF energy: HF    -815.14288061777 hartrees   iterations:   4


HOMO energy:    -0.29694
LUMO energy:     0.11870

 Orbital energies:
 -20.45259  -15.55233  -11.32165  -11.23596  -11.22264  -11.21401
 -11.20689  -11.20108  -11.18766  -11.18656  -11.18596  -11.18554
 -11.18407  -11.18387  -11.17905  -11.17695  -11.17687  -11.17556
 -11.17457  -11.17242   -1.42323   -1.33306   -1.18071   -1.16265
  -1.11556   -1.08827   -1.04107   -1.02784   -1.02031   -1.00053
  -0.94710   -0.90620   -0.85430   -0.84429   -0.83192   -0.81096
  -0.79389   -0.76170   -0.72106   -0.69220   -0.67860   -0.66893
  -0.65829   -0.64070   -0.64037   -0.62704   -0.61177   -0.60595
  -0.60419   -0.60194   -0.59211   -0.57798   -0.55707   -0.55559
  -0.53877   -0.53194   -0.51665   -0.50757   -0.50015   -0.49657
  -0.49149   -0.48609   -0.45935   -0.42236   -0.39365   -0.34984
  -0.34296   -0.31519   -0.29694    0.11870    0.13406    0.13877
   0.14204    0.20529    0.22573    0.26444    0.27128    0.27421
   0.29934

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -2.421480E-05  -4.082669E-05  -3.620988E-05
  2    C1      2.402631E-04   1.787689E-04  -1.728427E-04
  3    C2      1.006648E-04  -1.078201E-04  -1.354065E-04
  4    C3      1.592936E-04  -1.115510E-04  -1.913749E-04
  5    C4     -2.571083E-04  -2.972422E-05   1.958248E-04
  6    C5      6.087421E-05  -8.848977E-05  -1.338892E-04
  7    C6      3.606655E-04  -8.129384E-05   2.482216E-05
  8    C7     -1.991047E-04   6.087127E-04  -5.614202E-04
  9    H27     5.760924E-05   5.239777E-05   3.654153E-05
 10    H28    -3.947184E-04   5.026680E-05   2.952371E-04
 11    H30    -1.465291E-04  -1.483397E-04   1.195051E-05
 12    C8     -1.993866E-04   4.300910E-04  -1.367757E-04
 13    H32     1.544724E-04   5.411054E-05  -7.706662E-05
 14    C10     4.945095E-04  -1.120474E-04  -2.162887E-04
```

```
  15    N2      1.343601E-04  -6.583381E-04   6.025248E-04
  16    C9      3.329858E-04   1.645385E-04   1.403213E-04
  17    O1     -1.977608E-04  -3.336795E-04   2.463235E-04
  18    H43     2.200435E-04   1.766815E-04  -1.720630E-04
  19    C12    -1.579770E-04  -7.311479E-04   7.578276E-04
  20    C11    -3.627884E-04   3.893172E-04  -1.870219E-04
  21    C18    -3.316296E-04   1.165485E-04   6.195855E-05
  22    H48     3.201243E-04  -3.144429E-04  -4.074456E-04
  23    C13     4.634872E-04  -4.169900E-06  -7.251404E-05
  24    C14     5.702396E-04   2.203143E-07  -1.116968E-05
  25    C15     1.811637E-04   2.291774E-05  -2.485849E-05
  26    C16    -3.753569E-04   3.606406E-04  -7.678446E-05
  27    C17    -6.342739E-04   1.612402E-04   7.773192E-05
  28    H51     2.483131E-04  -8.896122E-06   5.101693E-05
  29    H52     6.295316E-05  -5.875142E-05   9.177141E-05
  30    H55     1.412103E-04   1.079184E-05   3.711564E-05
  31    H56    -5.328302E-05  -2.352958E-05   2.194740E-04
  32    H59     1.284464E-04   7.371313E-05  -2.509467E-04
  33    H60     4.680046E-05   1.144589E-04  -1.428912E-04
  34    H61     1.590259E-04  -4.181104E-05  -7.457538E-05
  35    H62     1.389224E-04   9.546446E-05   9.553130E-05
 -----------   -------------  -------------  -------------
   total        1.442297E-03   1.660215E-04  -1.355719E-04

  end of program der1b


  start of program geopt  30

  geometry optimization step 30
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0208413
   Cos(theta):   0.8610597

   Final level shift:  -1.1089669E-01

  energy change:           -3.8007E-05 *  (  5.0000E-05 )
  gradient maximum:         1.0579E-03 .  (  4.5000E-04 )
  gradient rms:             2.7191E-04 *  (  3.0000E-04 )
  step size:   0.02084  trust radius:   0.02000
  displacement maximum:     8.6634E-03 .  (  1.8000E-03 )
  displacement rms:         1.8641E-03 .  (  1.2000E-03 )
  predicted energy change:    -5.1362E-05    geom step:   2.0841E-02    full step:
2.0841E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.8817E-03     y:    -1.6619E-03     z:     8.4341E-04

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.8660293121     -3.8322109784     -2.4033618609
  C1        1.4792681908     -2.9606225236     -2.2890314817
 C2        3.1163905785     -0.6730504482     -2.0035643214
 C3        1.1348217750     -1.9656745849     -1.3832320359
 C4        2.6288913454     -2.8044463212     -3.0390043350
 C5        3.4392747636     -1.6732800225     -2.8977096130
 C6        1.9637110545     -0.8406340578     -1.2619605383
 C7        0.0233596734     -1.7957896032     -0.4430075303
 H27       2.9089169741     -3.5628677398     -3.7425606436
 H28       4.3257342993     -1.5835771916     -3.4931747274
 H30       3.7176917979      0.2013689848     -1.8686028095
 C8        0.2170274356     -0.6235256282      0.1762580213
 H32      -0.7832562220     -2.4758528470     -0.2936561026
 C10      -0.3886683239      0.2540363189      1.2465517034
 N2        1.3833875895     -0.0271840044     -0.3049611261
 C9        1.7093162504      1.1723192929      0.2805523031
 O1        2.7085184261      1.8163507869      0.0601453951
 H43      -0.3280123757     -0.2523623725      2.2022133222
 C12      -1.8372051301      0.6186113720      0.9706005684
 C11       0.5707440011      1.4990423434      1.2575355174
 C18       1.1493303296      1.8349082881      2.6398062724
 H48       0.0453512225      2.3625159249      0.8698272068
 C13      -3.5518342801      1.4010301977     -0.5260582684
 C14      -4.1036780099      0.8831730168      1.7444080717
 C15      -4.4915500441      1.3174490268      0.4911040755
 C16      -2.7818366483      0.5355536250      1.9808715156
 C17      -2.2360742661      1.0526203626     -0.2884345835
 H51      -5.5126913193      1.5833217328      0.3036205576
 H52      -2.4908165009      0.1942678277      2.9556207238
 H55      -3.8472145109      1.7303428332     -1.5023638403
 H56      -4.8230399737      0.8100559847      2.5355387877
 H59      -1.5194434119      1.0998821720     -1.0842023891
 H60       1.6386151524      0.9685632086      3.0696160566
 H61       0.3634195290      2.1602121619      3.3106357224
 H62       1.8794631657      2.6282354487      2.5443108095

 nuclear repulsion energy.......  1442.555067466 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  30   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.211E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     97     98     98     98     91     92
 grid # 3      224    183    182    194    182    182    188    183
 grid # 4      224    379    381    404    379    379    372    377

 number of gridpoints:
      atom        H27     H28     H30      C8     H32     C10      N2      C9
   grid # 1        73      73      73      86      73      82      99      75
   grid # 2       106     106     105      91     106      93     109      80
   grid # 3       224     224     220     187     223     175     224     164
   grid # 4       224     224     219     374     228     348     401     333

   number of gridpoints:
      atom         O1     H43     C12     C11     C18     H48     C13     C14
   grid # 1       111      69      90      81      71      69      88      87
   grid # 2       127      96     105      93      76      99     100     100
   grid # 3       272     209     194     173     149     216     183     183
   grid # 4       475     201     401     356     306     209     378     379

   number of gridpoints:
      atom        C15     C16     C17     H51     H52     H55     H56     H59
   grid # 1        89      87      85      73      73      73      73      70
   grid # 2       100     100      97     106     103     106     106     102
   grid # 3       183     182     181     224     214     224     224     215
   grid # 4       379     377     377     224     214     224     224     211

   number of gridpoints:
      atom        H60     H61     H62   total
   grid # 1        71      72      71    2820
   grid # 2        99      99      99    3489
   grid # 3       217     221     220    7043
   grid # 4       218     222     221   10842

   end of program grid


   start of program rwr
  recomputing RwR matrix  15    grid:  4
   end of program rwr


   start of program scf

        i  u  d  i  g
        t  p  i  c  r                                   RMS    maximum
        e  d  i  u  i                          energy  density   DIIS
        r  t  s  t  d     total energy         change  change    error

 etot   1  N  N  1  U  -815.14274629560            5.5E-05  1.8E-03
 etot   2  Y  Y  4  M  -815.14289288404  1.5E-04  2.3E-05  7.4E-04
 etot   3  Y  Y  4  M  -815.14290806696  1.5E-05  7.9E-06  2.2E-04
 etot   4  Y  Y  4  M  -815.14290973653  1.7E-06  1.9E-06  4.8E-05
 etot   5  Y  N  4  M  -815.14290998481  2.5E-07  0.0E+00  0.0E+00


  Energy components, in hartrees:
    (A)  Nuclear repulsion............  1442.55506746588
    (E)  Total one-electron terms..... -3970.58648362099
    (I)  Total two-electron terms.....  1712.88850617031
    (L)  Electronic energy............ -2257.69797745068  (E+I)
    (N)  Total energy................  -815.14290998481  (A+L)

  SCFE: SCF energy: HF    -815.14290998481 hartrees   iterations:   5


  HOMO energy:    -0.29691
  LUMO energy:     0.11875
 Orbital energies:
 -20.45267  -15.55227  -11.32163  -11.23589  -11.22260  -11.21396
 -11.20686  -11.20109  -11.18757  -11.18655  -11.18592  -11.18556
 -11.18410  -11.18384  -11.17897  -11.17686  -11.17680  -11.17551
 -11.17441  -11.17237   -1.42333   -1.33311   -1.18084   -1.16276
  -1.11562   -1.08828   -1.04109   -1.02804   -1.02040   -1.00056
  -0.94715   -0.90626   -0.85429   -0.84429   -0.83206   -0.81099
  -0.79392   -0.76174   -0.72110   -0.69239   -0.67863   -0.66898
  -0.65830   -0.64066   -0.64047   -0.62706   -0.61184   -0.60601
  -0.60425   -0.60209   -0.59212   -0.57802   -0.55704   -0.55555
  -0.53872   -0.53207   -0.51668   -0.50759   -0.50020   -0.49659
  -0.49152   -0.48614   -0.45940   -0.42241   -0.39367   -0.35000
  -0.34294   -0.31521   -0.29691    0.11875    0.13405    0.13878
   0.14204    0.20533    0.22578    0.26444    0.27137    0.27436
   0.29922

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label        x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -2.051522E-05  -6.764223E-06  -3.942405E-05
  2    C1      8.775645E-05   1.004751E-04  -6.534047E-05
  3    C2      5.630100E-05  -8.456519E-05  -9.716387E-05
  4    C3      1.298569E-04   1.538558E-05  -2.835017E-05
  5    C4      1.607664E-05   5.486790E-06   2.375553E-05
  6    C5     -1.759749E-05  -9.659544E-05  -5.966782E-05
  7    C6      3.671409E-05  -1.366190E-04   7.461461E-05
  8    C7     -2.762498E-04   5.424871E-04  -6.160270E-04
  9    H27     2.506194E-05   5.186647E-06  -6.452225E-06
 10    H28    -7.535678E-05  -1.235977E-05   5.082610E-05
 11    H30     7.969046E-06  -3.802506E-05  -6.605250E-06
 12    C8     -2.494289E-04   3.054807E-04  -2.275347E-04
 13    H32     1.006061E-05  -2.143657E-05  -1.547601E-05
 14    C10     5.872659E-04  -4.210294E-05  -1.582728E-04
 15    N2      2.952738E-04  -5.320834E-04   6.129639E-04
 16    C9      2.625630E-04   4.852846E-05   2.123701E-04
 17    O1     -3.511851E-05  -2.357916E-04   1.929524E-04
 18    H43     3.147886E-04   1.203774E-04  -2.302228E-05
 19    C12    -1.589432E-04  -6.689990E-04   7.112721E-04
 20    C11    -3.057941E-04   3.741394E-04  -1.582928E-04
 21    C18    -3.242370E-04   2.396581E-04  -8.552424E-05
 22    H48     2.494714E-04  -2.236363E-04  -4.572753E-04
 23    C13     1.380184E-04   4.455916E-05  -4.129527E-05
 24    C14     2.065927E-04   3.283868E-05   3.713833E-05
 25    C15     6.889160E-05   6.032397E-05  -3.136971E-05
 26    C16    -7.196840E-05   2.252362E-04   4.499926E-05
 27    C17    -1.682442E-04   7.719094E-05   3.913180E-05
 28    H51     7.373208E-05   4.262176E-05   1.944865E-05
 29    H52     3.116120E-05  -2.280932E-06  -1.842582E-05
 30    H55     8.315011E-05   3.651504E-05   7.906755E-06
 31    H56    -3.013610E-06   1.639404E-05   9.528406E-05
 32    H59     1.354807E-04   3.444385E-05  -1.443632E-04
 33    H60     1.478419E-04  -8.371876E-05  -5.164987E-05
 34    H61    -4.803084E-06   3.065945E-06   5.758170E-05
 35    H62     1.125341E-04   5.181814E-05   3.511478E-06
-----------   -------------  -------------  -------------
   total       1.365292E-03   1.972349E-04  -1.477760E-04

 end of program der1b


 start of program geopt  31

 geometry optimization step 31
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format

 Hessian eigenvalues:
  -4.09040E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.00000E-04    6.97072E-03    1.66592E-02
   2.16079E-02    2.82322E-02    3.02614E-02    3.06977E-02    3.12066E-02
   3.21365E-02    3.36547E-02    3.72705E-02    4.07111E-02    4.47474E-02
   5.16853E-02    5.65834E-02    6.68761E-02    7.12834E-02    7.33470E-02
   7.58093E-02    7.71930E-02    8.56713E-02    9.11005E-02    1.01371E-01
   1.13235E-01    1.16291E-01    1.21295E-01    1.32943E-01    1.33676E-01
   1.42629E-01    1.46347E-01    1.49760E-01    1.52712E-01    1.56163E-01
   1.62941E-01    1.64114E-01    1.69326E-01    1.74201E-01    1.82953E-01
   1.88379E-01    1.89802E-01    2.01725E-01    2.09826E-01    2.12135E-01
   2.13588E-01    2.24552E-01    2.26246E-01    2.32065E-01    2.37818E-01
   2.47277E-01    2.49106E-01    2.56914E-01    2.66335E-01    2.77074E-01
   2.77858E-01    2.86309E-01    2.94166E-01    3.04742E-01    3.06553E-01
   3.13862E-01    3.18451E-01    3.20654E-01    3.25150E-01    3.27106E-01
   3.32470E-01    3.38341E-01    3.43951E-01    3.48563E-01    3.53882E-01
   3.70415E-01    3.73193E-01    3.78149E-01    3.82664E-01    3.96370E-01
   3.98240E-01    4.08370E-01    4.20351E-01    4.32522E-01    4.47834E-01
   4.52904E-01    4.63354E-01    4.69873E-01    4.77078E-01    4.83062E-01
   4.97901E-01    5.18795E-01    5.26182E-01    5.39431E-01    5.65357E-01
   5.79910E-01    6.05408E-01    6.32019E-01    6.74188E-01    7.34899E-01
   7.45555E-01    7.83401E-01    8.57813E-01    1.02740E+00    1.16586E+00

 WARNING: Hessian has wrong number of negative eigenvalues
 WARNING: positive P-RFO shift not converged: using initial-guess shift

 WARNING: failed to converge rfo shift adjustments

 Level shifts adjusted to satisfy step-size constraints
  Step size:    0.0497028
  Cos(theta):   0.0572212

  Final level shift:  -4.0927321E+00

 energy change:           -2.9367E-05 *  (  5.0000E-05 )
 gradient maximum:         1.0424E-03 .  (  4.5000E-04 )
 gradient rms:             2.3207E-04 *  (  3.0000E-04 )
```

```
  step size:   0.04970  trust radius:   0.02828
  displacement maximum:    2.8505E-02 .  (  1.8000E-03 )
  displacement rms:        4.4455E-03 .  (  1.2000E-03 )
  predicted energy change:    -5.0590E-03    geom step:   4.9703E-02    full step:
4.9703E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.9325E-03     y:     2.8549E-04     z:    -2.3576E-03

  new geometry:
                               angstroms
  atom            x                  y                  z
  H25       0.8740169175     -3.8378248023     -2.4136404539
  C1        1.4867393214     -2.9648214187     -2.2911652812
  C2        3.1252915746     -0.6814921308     -1.9934262157
  C3        1.1379664970     -1.9689807987     -1.3850419577
  C4        2.6377945227     -2.8136871507     -3.0352183088
  C5        3.4501911580     -1.6841290950     -2.8876560937
  C6        1.9667787143     -0.8472021954     -1.2583795091
  C7        0.0301138242     -1.7909182160     -0.4514795252
  H27       2.9168168215     -3.5771014069     -3.7385003557
  H28       4.3387028967     -1.5943607912     -3.4762671934
  H30       3.7283732542      0.1926596683     -1.8551532056
  C8        0.2226755754     -0.6208717051      0.1701213513
  H32      -0.7802598636     -2.4664343679     -0.3023257614
  C10      -0.3926871148      0.2522802634      1.2361566355
  N2        1.3890860130     -0.0274951104     -0.3067510499
  C9        1.7093709884      1.1754358472      0.2769321220
  O1        2.7210152248      1.8251600132      0.0469382911
  H43      -0.3432595507     -0.2625783072      2.1873065235
  C12      -1.8405135028      0.6171013363      0.9603386575
  C11       0.5660353974      1.4982635749      1.2497517134
  C18       1.1341602984      1.8333629254      2.6388617473
  H48       0.0372234724      2.3602661804      0.8553752609
  C13      -3.5753485672      1.4152933478     -0.5149079791
  C14      -4.1013867560      0.8824365175      1.7584273208
  C15      -4.5030495084      1.3255087089      0.5122263045
  C16      -2.7749519171      0.5311391910      1.9795295361
  C17      -2.2549892444      1.0618434335     -0.2932654993
  H51      -5.5247851144      1.5954624062      0.3354471288
  H52      -2.4711244404      0.1914515758      2.9535529241
  H55      -3.8828800132      1.7520495135     -1.4895707014
  H56      -4.8102792253      0.8036273705      2.5587888276
  H59      -1.5465394980      1.1233237190     -1.1037268742
  H60       1.6213079174      0.9661125677      3.0788139638
  H61       0.3413783781      2.1580466891      3.3073112283
  H62       1.8681222500      2.6245679418      2.5485914213

  nuclear repulsion energy.......  1441.081895109 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  31   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.202E-03
  number of canonical orbitals.....          210
  end of program onee
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom        H25     C1      C2      C3      C4      C5      C6      C7
  grid # 1        73     89      87      90      87      87      85      85
  grid # 2       106     99      99      98      98      99      91      92
  grid # 3       224    183     183     195     182     182     186     182
  grid # 4       224    379     383     404     379     377     372     377

  number of gridpoints:
     atom        H27    H28     H30      C8     H32     C10      N2      C9
  grid # 1        73     73      73      86      73      81      99      75
  grid # 2       106    106     105      91     106      92     109      80
  grid # 3       224    224     220     187     223     175     223     164
  grid # 4       224    224     219     372     227     350     401     338

  number of gridpoints:
     atom         O1    H43     C12     C11     C18     H48     C13     C14
  grid # 1       111     68      90      81      71      69      88      87
  grid # 2       127     96     105      94      75     100     100      98
  grid # 3       272    210     193     171     142     217     184     183
  grid # 4       475    201     400     351     307     206     380     378

  number of gridpoints:
     atom        C15    C16     C17     H51     H52     H55     H56     H59
  grid # 1        87     87      85      73      73      73      73      71
  grid # 2       100    100      98     106     103     106     106     102
  grid # 3       183    182     182     224     214     224     224     216
  grid # 4       379    378     378     224     214     224     224     213

  number of gridpoints:
     atom        H60    H61     H62  total
  grid # 1        71     72      72   2818
  grid # 2        99     99      99   3490
  grid # 3       217    221     220   7036
  grid # 4       220    221     221  10844

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                   RMS    maximum
       e  d  i  u  i                       energy   density    DIIS
       r  t  s  t  d     total energy      change    change     error

etot   1  N  N  1  U  -815.14130215200             1.7E-04  3.3E-03
etot   2  Y  Y  4  M  -815.14205935245  7.6E-04  6.3E-05  9.9E-04
etot   3  Y  Y  4  M  -815.14212422012  6.5E-05  2.5E-05  9.4E-04
etot   4  Y  Y  4  M  -815.14213866210  1.4E-05  1.1E-05  2.1E-04
etot   5  Y  Y  4  M  -815.14213925520  5.9E-07  3.9E-06  1.3E-04
etot    6  N  N  1  U  -815.14214611940  6.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1441.08189510906
   (E)  Total one-electron terms..... -3967.65054297617
   (I)  Total two-electron terms.....  1711.42650174770
   (L)  Electronic energy........... -2256.22404122847  (E+I)
   (N)  Total energy................  -815.14214611940  (A+L)

 SCFE: SCF energy: HF    -815.14214611940 hartrees   iterations:   6


 HOMO energy:    -0.29641
 LUMO energy:     0.11758

  Orbital energies:
  -20.45204  -15.55336  -11.32349  -11.23517  -11.22239  -11.21448
  -11.20909  -11.20205  -11.18757  -11.18739  -11.18692  -11.18683
  -11.18606  -11.18456  -11.17918  -11.17703  -11.17613  -11.17608
  -11.17543  -11.17271   -1.41424   -1.33260   -1.18071   -1.16293
   -1.11591   -1.08904   -1.04131   -1.02721   -1.02067   -1.00037
   -0.94719   -0.90738   -0.85414   -0.84432   -0.83196   -0.81144
   -0.79393   -0.76173   -0.72037   -0.69163   -0.67866   -0.66874
   -0.65818   -0.64017   -0.63975   -0.62627   -0.61134   -0.60403
   -0.60377   -0.60120   -0.59141   -0.57801   -0.55728   -0.55504
   -0.53839   -0.53088   -0.51624   -0.50748   -0.49994   -0.49683
   -0.49157   -0.48605   -0.45804   -0.42336   -0.39341   -0.34985
   -0.34349   -0.31591   -0.29641    0.11758    0.13303    0.13733
    0.14140    0.20467    0.22478    0.26346    0.27113    0.27384
    0.29798

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     1.002550E-04   1.319520E-03   8.160926E-04
   2    C1     -2.864101E-03  -1.459598E-03   8.926958E-04
   3    C2      2.484690E-04  -1.945250E-03  -1.671730E-03
   4    C3      2.139377E-03  -1.245815E-04  -1.365837E-03
   5    C4      1.640963E-03  -2.331649E-04  -1.092182E-03
   6    C5     -7.582049E-04   1.858203E-03   1.699483E-03
   7    C6      5.386234E-03   2.338160E-03  -2.596505E-03
   8    C7     -5.013260E-03  -2.306836E-03   1.373438E-03
   9    H27    -1.567901E-04   2.030549E-03   1.397841E-03
  10    H28     1.245795E-03  -5.166798E-05  -9.132537E-04
  11    H30    -5.880327E-04  -8.368117E-04  -6.734541E-05
  12    C8     -3.058885E-03  -3.499521E-04  -7.855526E-04
 13    H32    -1.447583E-04  -2.242942E-04  -6.757707E-05
 14    C10     1.379611E-03  -9.063864E-05  -2.324004E-03
 15    N2      1.834741E-04   1.072775E-03   2.234669E-03
 16    C9      2.030512E-02   9.367724E-03  -6.312617E-03
 17    O1     -2.124309E-02  -1.254340E-02   6.020019E-03
 18    H43     1.555165E-03   1.130415E-03   7.595824E-04
 19    C12    -1.878739E-03   7.098464E-04  -1.044459E-03
 20    C11    -4.686581E-04   2.190783E-03   1.218545E-03
 21    C18    -1.171353E-04  -4.412562E-04   1.641496E-03
 22    H48     1.528766E-03  -1.442571E-03   9.086033E-04
 23    C13     2.370680E-03  -4.506079E-04  -1.542463E-03
 24    C14     2.108015E-03  -7.148117E-04   7.396690E-04
 25    C15     2.246239E-04  -1.726797E-04   2.729960E-04
 26    C16    -2.424755E-03   9.721200E-04   6.478413E-04
 27    C17     1.723116E-03   7.906501E-04  -2.664252E-03
 28    H51    -2.236133E-04  -9.918889E-05   4.656033E-04
 29    H52    -8.942324E-04   1.100310E-04  -1.708197E-03
 30    H55     1.275518E-03  -8.300922E-04   2.930355E-03
 31    H56    -6.827451E-05   3.090640E-04  -2.419881E-04
 32    H59    -2.278817E-03  -9.870716E-04   3.732971E-03
 33    H60    -1.176210E-03   1.507236E-03  -1.979119E-03
 34    H61     1.610472E-03  -2.044818E-04  -1.856401E-03
 35    H62    -5.290356E-04   1.172643E-04   2.720101E-04
-----------   -------------  -------------  -------------
   total       1.139062E-03   3.153796E-04  -2.095699E-04

 end of program der1b


 start of program geopt  32

 geometry optimization step 32
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   31 **

 Hessian eigenvalues:
  -2.45157E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    5.00000E-04    3.22831E-03    1.95788E-02
   2.23668E-02    2.83085E-02    2.95499E-02    3.07469E-02    3.13562E-02
   3.16719E-02    3.40783E-02    3.77272E-02    4.36008E-02    4.70212E-02
   5.47491E-02    6.61232E-02    7.04255E-02    7.25842E-02    7.56677E-02
   8.09144E-02    8.16887E-02    8.95661E-02    9.92070E-02    1.13675E-01
   1.14500E-01    1.18667E-01    1.27853E-01    1.37032E-01    1.38394E-01
   1.44829E-01    1.49042E-01    1.52171E-01    1.56173E-01    1.61934E-01
   1.68598E-01    1.71579E-01    1.80575E-01    1.84090E-01    1.88577E-01
   1.96030E-01    2.00666E-01    2.05755E-01    2.11917E-01    2.18536E-01
   2.23275E-01    2.30153E-01    2.31542E-01    2.41041E-01    2.46930E-01
   2.55975E-01    2.61981E-01    2.68057E-01    2.83560E-01    2.85748E-01
   2.92153E-01    2.96894E-01    2.99922E-01    3.07469E-01    3.11050E-01
   3.16926E-01    3.23327E-01    3.25165E-01    3.32366E-01    3.36353E-01
   3.41413E-01    3.45293E-01    3.53768E-01    3.64474E-01    3.66180E-01
   3.76690E-01    3.82687E-01    3.88511E-01    3.97050E-01    4.00622E-01
   4.07182E-01    4.12870E-01    4.26660E-01    4.39355E-01    4.47745E-01
```

```
    4.60030E-01    4.62146E-01    4.84170E-01    4.84612E-01    4.90203E-01
    4.93846E-01    5.07126E-01    5.28186E-01    5.31382E-01    5.63448E-01
    5.69052E-01    6.12130E-01    6.20044E-01    6.53981E-01    6.58503E-01
    7.34149E-01    8.40260E-01    8.91243E-01    9.34513E-01    1.13266E+00

  WARNING: Hessian has wrong number of negative eigenvalues
  WARNING: positive P-RFO shift not converged: using initial-guess shift

  WARNING: failed to converge rfo shift adjustments

  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0161090
   Cos(theta):   0.1972358

   Final level shift:  -2.4732431E+00

  energy change:            7.6387E-04 .  (  5.0000E-05 )
  gradient maximum:         1.0424E-03 .  (  4.5000E-04 )
  gradient rms:             2.3207E-04 *  (  3.0000E-04 )
  step size:   0.01611  trust radius:   0.01414
  displacement maximum:     4.4509E-03 .  (  1.8000E-03 )
  displacement rms:         1.4408E-03 .  (  1.2000E-03 )
  predicted energy change:    -3.2502E-04    geom step:   1.6109E-02    full step:
1.6109E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.2204E-16     y:    -4.5103E-17     z:     3.8858E-16

  new geometry:
                              angstroms
  atom           x                  y                  z
  H25       0.8555223374     -3.8227640767     -2.4046995325
  C1        1.4725685271     -2.9544279981     -2.2896713992
  C2        3.1202875626     -0.6757241476     -2.0024873742
  C3        1.1332235179     -1.9607952935     -1.3810974147
  C4        2.6224126199     -2.8020411585     -3.0411027188
  C5        3.4382852005     -1.6753333151     -2.8987461469
  C6        1.9660662125     -0.8393061929     -1.2583918229
  C7        0.0218053265     -1.7888470066     -0.4408301930
  H27       2.8982826369     -3.5593124566     -3.7466707448
  H28       4.3248659475     -1.5876874187     -3.4956320456
  H30       3.7271094566      0.1942464605     -1.8668588812
  C8        0.2169123338     -0.6190509970      0.1796382645
  H32      -0.7882154689     -2.4648253014     -0.2948299553
  C10      -0.3879864380      0.2574462734      1.2504026541
  N2        1.3842689514     -0.0256150694     -0.3008840424
  C9        1.7114301812      1.1726199293      0.2856002846
  O1        2.7130074559      1.8121796824      0.0670110467
  H43      -0.3289837254     -0.2493767490      2.2052259629
  C12      -1.8369200494      0.6211416416      0.9724405545
  C11       0.5723487481      1.5022238953      1.2619571889
  C18       1.1564316110      1.8364768966      2.6423611265
  H48       0.0475583017      2.3672795294      0.8751648452
  C13      -3.5541281224      1.3923142268     -0.5317836627
  C14      -4.1043090262      0.8806431958      1.7413970867
  C15      -4.4942542516      1.3094356575      0.4846050046
  C16      -2.7816777193      0.5377903865      1.9813487049
  C17      -2.2375733499      1.0495400981     -0.2900489993
  H51      -5.5160652179      1.5709524919      0.2935228498
  H52      -2.4898962014      0.1975518210      2.9552491218
  H55      -3.8497155602      1.7165752072     -1.5110717918
```

```
 H56      -4.8229340791      0.8075350102      2.5333922480
 H59      -1.5224367068      1.0933357857     -1.0898237618
 H60       1.6510487084      0.9684527349      3.0656676220
 H61       0.3734592988      2.1561075790      3.3190664533
 H62       1.8821427585      2.6340413444      2.5449099165

 nuclear repulsion energy.......  1442.448526258 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  32   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.212E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      99      91      92
 grid # 3       224    183     183     194     182     182     187     182
 grid # 4       224    379     381     406     379     379     372     376

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      82      99      75
 grid # 2       106    106     105      91     106      93     109      80
 grid # 3       224    224     220     187     223     175     224     164
 grid # 4       224    224     219     374     227     350     402     332

 number of gridpoints:
    atom         O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1       111     69      90      81      72      69      88      87
 grid # 2       123     96     105      93      75      99     100     100
 grid # 3       272    210     193     174     142     216     183     183
 grid # 4       475    201     400     358     307     208     379     379

 number of gridpoints:
    atom        C15    C16     C17     H51     H52     H55     H56     H59
 grid # 1        89     86      84      73      73      73      73      70
 grid # 2       100    100      97     106     103     106     106     102
 grid # 3       183    182     181     224     214     224     224     215
 grid # 4       380    378     377     224     214     224     224     212

 number of gridpoints:
    atom        H60    H61     H62   total
 grid # 1        71     72      71    2819
 grid # 2        99     99      99    3485
 grid # 3       217    221     220    7036
 grid # 4       218    222     221   10849

 end of program grid
 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

       i  u  d  i  g
       t  p  i  c  r                                     RMS    maximum
       e  d  i  u  i                         energy  density   DIIS
       r  t  s  t  d     total energy        change  change     error

etot   1  N  N  1  U  -815.14171771491             1.9E-04  3.7E-03
etot   2  Y  Y  4  M  -815.14276388742  1.0E-03  7.1E-05  1.0E-03
etot   3  Y  Y  4  M  -815.14285022807  8.6E-05  2.7E-05  9.8E-04
etot   4  Y  Y  4  M  -815.14286860293  1.8E-05  1.2E-05  1.9E-04
etot   5  Y  Y  4  M  -815.14287259667  4.0E-06  3.9E-06  1.3E-04
etot   6  N  N  1  U  -815.14286488410 -7.7E-06  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1442.44852625766
  (E)  Total one-electron terms..... -3970.37931040962
  (I)  Total two-electron terms.....  1712.78791926786
  (L)  Electronic energy............ -2257.59139114176  (E+I)
  (N)  Total energy.................  -815.14286488410  (A+L)

SCFE: SCF energy: HF    -815.14286488410 hartrees   iterations:   6


HOMO energy:    -0.29710
LUMO energy:     0.11904

 Orbital energies:
 -20.45252  -15.55208  -11.32128  -11.23553  -11.22291  -11.21402
 -11.20698  -11.20126  -11.18741  -11.18656  -11.18612  -11.18569
 -11.18443  -11.18414  -11.17891  -11.17716  -11.17637  -11.17563
 -11.17455  -11.17235   -1.42371   -1.33307   -1.18054   -1.16259
  -1.11547   -1.08827   -1.04095   -1.02788   -1.02014   -1.00070
  -0.94726   -0.90589   -0.85419   -0.84408   -0.83183   -0.81070
  -0.79407   -0.76168   -0.72088   -0.69242   -0.67869   -0.66900
  -0.65816   -0.64050   -0.64035   -0.62704   -0.61174   -0.60603
  -0.60430   -0.60175   -0.59204   -0.57835   -0.55700   -0.55540
  -0.53859   -0.53200   -0.51671   -0.50762   -0.49996   -0.49656
  -0.49140   -0.48617   -0.45947   -0.42220   -0.39346   -0.35006
  -0.34275   -0.31511   -0.29710    0.11904    0.13372    0.13888
   0.14199    0.20555    0.22583    0.26438    0.27141    0.27429
   0.29935

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  14    grid:  4
recomputing RwR matrix  15    grid:  4
```

```
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -1.514248E-04  -2.792285E-04  -1.722642E-04
  2    C1      8.114116E-04  -1.792538E-04  -5.124113E-04
  3    C2     -1.160958E-03  -1.963073E-05   1.176708E-03
  4    C3      7.736421E-06   3.513821E-05  -6.788201E-05
  5    C4     -6.192335E-04  -4.547057E-05   4.047724E-04
  6    C5      3.142228E-06   1.805409E-04  -9.969590E-06
  7    C6      2.668670E-04   2.799277E-04  -3.137022E-04
  8    C7     -7.989876E-04  -7.239971E-04  -1.416046E-03
  9    H27    -3.818984E-06  -4.106222E-04  -2.312948E-04
 10    H28    -5.215306E-04  -1.062947E-04   4.067767E-04
 11    H30    -7.198350E-05   3.738749E-04   1.208990E-04
 12    C8      4.983585E-04   4.886852E-04  -3.967248E-04
 13    H32    -1.501858E-04  -4.929260E-04   6.146184E-05
 14    C10     2.590415E-04   7.768088E-04  -6.937216E-04
 15    N2      1.540179E-03  -4.335730E-05   5.675750E-04
 16    C9     -4.104963E-04  -2.386356E-04   1.098947E-04
 17    O1      9.583879E-04   8.626685E-04   2.098299E-04
 18    H43     4.349224E-04  -7.872842E-05   4.003883E-04
 19    C12    -2.233672E-04  -2.629756E-04  -1.426450E-03
 20    C11    -1.088463E-04   6.489676E-04  -5.115777E-04
 21    C18    -2.801965E-04  -4.864829E-04   1.220832E-04
 22    H48     4.947611E-04  -6.672318E-04  -3.842102E-04
 23    C13     3.370921E-04   1.537764E-04  -1.951038E-04
 24    C14    -6.420815E-04   4.742911E-04  -8.389821E-04
 25    C15     4.585901E-04  -3.678629E-04   1.650732E-03
 26    C16    -6.957720E-04   5.334133E-04  -8.414238E-04
 27    C17     1.225255E-03  -3.667744E-04  -4.652565E-04
 28    H51     1.637162E-04  -6.781788E-05   4.554837E-04
 29    H52    -7.514129E-05   1.208019E-05   7.341165E-04
 30    H55     4.039963E-04  -2.859952E-04   8.685491E-04
 31    H56    -1.875877E-04   6.387621E-05  -1.793423E-04
 32    H59    -3.289693E-04   4.734322E-05   1.287930E-03
 33    H60    -5.163989E-05   8.198256E-04  -1.509034E-04
 34    H61    -1.368821E-04   4.083854E-06   1.069850E-04
 35    H62     1.461243E-04  -3.926560E-04   1.329876E-04
-----------   -------------  -------------  -------------
   total       1.390479E-03   2.393599E-04   9.907883E-06

 end of program der1b


 start of program geopt  33

 geometry optimization step 33
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   31 **

 Hessian eigenvalues:
  -4.20567E-01    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
   0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
```

```
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00    0.00000E+00
    0.00000E+00    0.00000E+00    5.00000E-04    5.15896E-03    1.73714E-02
    2.28745E-02    2.76232E-02    2.83389E-02    3.07971E-02    3.08982E-02
    3.18489E-02    3.27276E-02    3.59196E-02    3.78231E-02    4.60852E-02
    5.33994E-02    6.32670E-02    6.66121E-02    6.95851E-02    7.28332E-02
    7.42753E-02    7.97754E-02    8.86076E-02    9.60765E-02    1.00697E-01
    1.07976E-01    1.13382E-01    1.16870E-01    1.27308E-01    1.38031E-01
    1.42098E-01    1.42660E-01    1.44943E-01    1.46981E-01    1.58029E-01
    1.62386E-01    1.65945E-01    1.69399E-01    1.77760E-01    1.80256E-01
    1.86680E-01    1.90911E-01    1.94302E-01    2.06298E-01    2.07793E-01
    2.14462E-01    2.20216E-01    2.25195E-01    2.33898E-01    2.39049E-01
    2.46267E-01    2.50449E-01    2.57600E-01    2.59049E-01    2.63970E-01
    2.82291E-01    2.91642E-01    2.96811E-01    3.06300E-01    3.08209E-01
    3.15114E-01    3.16749E-01    3.24052E-01    3.28516E-01    3.31977E-01
    3.36192E-01    3.43298E-01    3.53676E-01    3.56500E-01    3.63230E-01
    3.65184E-01    3.72679E-01    3.79282E-01    3.84745E-01    3.93350E-01
    4.01011E-01    4.05923E-01    4.23173E-01    4.28703E-01    4.35692E-01
    4.52559E-01    4.65625E-01    4.76872E-01    4.83390E-01    4.88003E-01
    4.92977E-01    5.06521E-01    5.11549E-01    5.30269E-01    5.50764E-01
    5.64480E-01    5.75561E-01    6.32766E-01    6.53812E-01    7.14040E-01
    7.29725E-01    7.59680E-01    9.07053E-01    9.29412E-01    1.09319E+00

  WARNING: Hessian has wrong number of negative eigenvalues
  WARNING: positive P-RFO shift not converged: using initial-guess shift

  WARNING: failed to converge rfo shift adjustments

  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0278280
   Cos(theta):   0.2148434

   Final level shift:  -4.2123425E-01

  energy change:           4.5101E-05 *  (  5.0000E-05 )
  gradient maximum:        1.0424E-03 .  (  4.5000E-04 )
  gradient rms:            2.3207E-04 *  (  3.0000E-04 )
  step size:   0.02783  trust radius:   0.01000
  displacement maximum:    8.8118E-03 .  (  1.8000E-03 )
  displacement rms:        2.4890E-03 .  (  1.2000E-03 )
  predicted energy change:   -1.7086E-04   geom step:   2.7828E-02   full step:
2.7828E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.6653E-16     y:    -4.5103E-17     z:     0.0000E+00

  new geometry:
                              angstroms
  atom           x                 y                 z
  H25       0.8685141544     -3.8289165667     -2.4082184296
  C1        1.4809823266     -2.9581767422     -2.2924207914
  C2        3.1192113762     -0.6756177653     -2.0038771824
  C3        1.1370150088     -1.9651369511     -1.3816091342
  C4        2.6284119557     -2.8046223217     -3.0444076913
  C5        3.4391519401     -1.6757007337     -2.9021888813
  C6        1.9672643619     -0.8413135534     -1.2579213881
  C7        0.0262997405     -1.7938832886     -0.4410117914
  H27       2.9048170441     -3.5620912049     -3.7493204350
  H28       4.3223618519     -1.5854951586     -3.5002364953
  H30       3.7211482302      0.1968374252     -1.8685799831
```

```
 C8        0.2177881805     -0.6256393928      0.1804848490
 H32      -0.7820123733     -2.4710766049     -0.2933962565
 C10      -0.3904611920      0.2494673674      1.2510860510
 N2        1.3863128396     -0.0309336857     -0.2973480449
 C9        1.7095028677      1.1678195126      0.2894081603
 O1        2.7054807145      1.8188323576      0.0595335305
 H43      -0.3305450747     -0.2573200830      2.2057166365
 C12      -1.8396196512      0.6145273814      0.9742277035
 C11       0.5683929977      1.4950838651      1.2615841520
 C18       1.1510021274      1.8421590327      2.6387556470
 H48       0.0405729108      2.3537857949      0.8722554159
 C13      -3.5513233044      1.4009596405     -0.5223571491
 C14      -4.1068709799      0.8837794861      1.7412053592
 C15      -4.4929365700      1.3189516911      0.4900901079
 C16      -2.7852998058      0.5337019456      1.9797484974
 C17      -2.2364580917      1.0496924037     -0.2826553976
 H51      -5.5120271351      1.5872303012      0.2976270400
 H52      -2.4944232852      0.1923500374      2.9493822232
 H55      -3.8436496568      1.7320303192     -1.4980294532
 H56      -4.8249489452      0.8107709707      2.5290120956
 H59      -1.5191883775      1.0971121099     -1.0781093210
 H60       1.6423876520      0.9795105613      3.0727747470
 H61       0.3641939947      2.1703429899      3.3074896957
 H62       1.8828939054      2.6337615645      2.5356362497

 nuclear repulsion energy.......  1442.544030789 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  33   /
 --------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.210E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106     99      97      98      98      98      91      92
 grid # 3       224    183     184     194     182     182     188     182
 grid # 4       224    379     380     408     379     379     374     376

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      82      99      75
 grid # 2       106    106     105      91     106      93     109      80
 grid # 3       224    224     220     186     223     175     224     164
 grid # 4       224    224     219     376     227     349     402     333

 number of gridpoints:
    atom         O1    H43     C12     C11     C18     H48     C13     C14
 grid # 1       111     69      90      81      71      69      87      87
```

```
  grid # 2       127     96    105     93     76     99    100     98
  grid # 3       272    209    192    173    149    216    183    183
  grid # 4       475    201    400    356    305    208    378    376

  number of gridpoints:
     atom        C15    C16    C17    H51    H52    H55    H56    H59
  grid # 1        87     85     84     73     73     73     73     70
  grid # 2       100    100     97    106    103    106    106    102
  grid # 3       183    182    181    224    214    224    224    215
  grid # 4       379    375    376    224    214    224    224    211

  number of gridpoints:
     atom        H60    H61    H62  total
  grid # 1        71     72     72   2815
  grid # 2        99     99     99   3486
  grid # 3       217    221    220   7041
  grid # 4       218    222    221  10840

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                        energy  density   DIIS
       r  t  s  t  d     total energy      change   change    error

etot   1  N  N  1  U  -815.14240442792            1.1E-04  2.7E-03
etot   2  Y  Y  4  M  -815.14272628312  3.2E-04  3.5E-05  7.7E-04
etot   3  Y  Y  4  M  -815.14276073817  3.4E-05  1.3E-05  3.3E-04
etot   4  Y  Y  4  M  -815.14276320490  2.5E-06  5.8E-06  1.1E-04
etot   5  Y  Y  4  M  -815.14276314733 -5.8E-08  1.9E-06  4.6E-05
etot   6  N  N  1  U  -815.14276354093  3.9E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1442.54403078922
   (E)  Total one-electron terms..... -3970.55663474941
   (I)  Total two-electron terms.....  1712.86984041926
   (L)  Electronic energy............ -2257.68679433015  (E+I)
   (N)  Total energy.................  -815.14276354093  (A+L)

 SCFE: SCF energy: HF    -815.14276354093 hartrees   iterations:   6


 HOMO energy:    -0.29713
 LUMO energy:     0.11856

  Orbital energies:
  -20.45199  -15.55227  -11.32129  -11.23550  -11.22299  -11.21425
  -11.20666  -11.20059  -11.18782  -11.18586  -11.18539  -11.18505
  -11.18372  -11.18340  -11.17901  -11.17720  -11.17648  -11.17562
  -11.17437  -11.17225   -1.42129   -1.33272   -1.18156   -1.16292
   -1.11596   -1.08863   -1.04182   -1.02807   -1.02070   -1.00093
   -0.94785   -0.90616   -0.85439   -0.84528   -0.83217   -0.81120
   -0.79434   -0.76176   -0.72191   -0.69271   -0.67895   -0.66934
  -0.65826   -0.64100   -0.64058   -0.62726   -0.61187   -0.60527
  -0.60436   -0.60198   -0.59246   -0.57857   -0.55732   -0.55503
  -0.53927   -0.53198   -0.51693   -0.50792   -0.50031   -0.49652
  -0.49146   -0.48656   -0.45909   -0.42231   -0.39340   -0.34978
  -0.34385   -0.31564   -0.29713    0.11856    0.13429    0.13864
   0.14208    0.20535    0.22578    0.26491    0.27156    0.27464
   0.29987

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -7.730016E-04  -5.124978E-04   5.473418E-05
  2    C1     -1.289582E-03   3.647156E-04   1.437368E-03
  3    C2     -8.429366E-04  -1.370869E-03  -8.462852E-05
  4    C3      1.109121E-03  -4.210770E-04  -1.221547E-03
  5    C4     -4.605337E-04   6.100920E-04   6.622196E-04
  6    C5     -4.414109E-04   2.061370E-03   1.488608E-03
  7    C6      2.760964E-04  -8.615921E-04  -4.590633E-04
  8    C7     -1.801301E-03  -2.607574E-03  -1.808522E-03
  9    H27     1.427103E-04  -3.375529E-04  -3.323421E-04
 10    H28     8.137571E-04   2.982234E-04  -2.407148E-04
 11    H30     6.518773E-04   6.959804E-04  -8.460174E-05
 12    C8      9.057729E-04   1.545103E-03   3.170024E-04
 13    H32    -4.209968E-04  -6.950629E-04  -1.287361E-04
 14    C10     8.703350E-04   3.754785E-04  -4.043090E-05
 15    N2      1.324029E-03   3.389700E-04   6.881740E-04
 16    C9      3.094736E-03   3.548460E-03  -4.037896E-03
 17    O1     -3.372225E-03  -3.026781E-03   2.245705E-03
 18    H43     4.152405E-04  -1.564509E-04   5.364890E-04
 19    C12     1.758741E-03  -6.609335E-04  -9.649744E-05
 20    C11     1.145875E-03  -5.236223E-05   3.904124E-04
 21    C18    -1.117114E-03  -2.237456E-04   7.026597E-04
 22    H48     2.694897E-05   1.022595E-03  -1.385353E-03
 23    C13     1.761017E-03   1.319712E-04  -1.553878E-03
 24    C14     2.031517E-03  -6.521927E-04   8.042769E-04
 25    C15    -4.539852E-04   3.293806E-04  -4.863020E-04
 26    C16    -2.014838E-03   7.710041E-04  -8.060916E-04
 27    C17    -3.748306E-04   8.415705E-04  -2.559436E-03
 28    H51    -3.424461E-04   2.881254E-05   4.276512E-04
 29    H52     2.690992E-04  -1.035979E-03   3.514058E-03
 30    H55     8.535088E-05   1.806752E-04  -7.219892E-04
 31    H56    -1.614602E-03  -1.735350E-04   2.113054E-03
 32    H59     2.415843E-05   3.919954E-05  -1.083514E-04
 33    H60     2.422856E-05  -3.616377E-04   2.920942E-04
 34    H61     6.290094E-04   2.287964E-04   3.907289E-04
 35    H62    -6.653468E-04   8.093501E-07  -1.171101E-04
-----------   -------------  -------------  -------------
```

```
   total       1.374472E-03   2.633645E-04  -2.082536E-04

 end of program der1b


 start of program geopt  34

 geometry optimization step 34
** stopping now - optimization seems to be stuck **


 ********************************************************
 **           Geometry optimization complete           **
 ********************************************************

 center of mass moved by:
    x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00

 final geometry:
                              angstroms
 atom            x                 y                 z
 H25       0.8685141544     -3.8289165667     -2.4082184296
 C1        1.4809823266     -2.9581767422     -2.2924207914
 C2        3.1192113762     -0.6756177653     -2.0038771824
 C3        1.1370150088     -1.9651369511     -1.3816091342
 C4        2.6284119557     -2.8046223217     -3.0444076913
 C5        3.4391519401     -1.6757007337     -2.9021888813
 C6        1.9672643619     -0.8413135534     -1.2579213881
 C7        0.0262997405     -1.7938832886     -0.4410117914
 H27       2.9048170441     -3.5620912049     -3.7493204350
 H28       4.3223618519     -1.5854951586     -3.5002364953
 H30       3.7211482302      0.1968374252     -1.8685799831
 C8        0.2177881805     -0.6256393928      0.1804848490
 H32      -0.7820123733     -2.4710766049     -0.2933962565
 C10      -0.3904611920      0.2494673674      1.2510860510
 N2        1.3863128396     -0.0309336857     -0.2973480449
 C9        1.7095028677      1.1678195126      0.2894081603
 O1        2.7054807145      1.8188323576      0.0595335305
 H43      -0.3305450747     -0.2573200830      2.2057166365
 C12      -1.8396196512      0.6145273814      0.9742277035
 C11       0.5683929977      1.4950838651      1.2615841520
 C18       1.1510021274      1.8421590327      2.6387556470
 H48       0.0405729108      2.3537857949      0.8722554159
 C13      -3.5513233044      1.4009596405     -0.5223571491
 C14      -4.1068709799      0.8837794861      1.7412053592
 C15      -4.4929365700      1.3189516911      0.4900901079
 C16      -2.7852998058      0.5337019456      1.9797484974
 C17      -2.2364580917      1.0496924037     -0.2826553976
 H51      -5.5120271351      1.5872303012      0.2976270400
 H52      -2.4944232852      0.1923500374      2.9493822232
 H55      -3.8436496568      1.7320303192     -1.4980294532
 H56      -4.8249489452      0.8107709707      2.5290120956
 H59      -1.5191883775      1.0971121099     -1.0781093210
 H60       1.6423876520      0.9795105613      3.0727747470
 H61       0.3641939947      2.1703429899      3.3074896957
 H62       1.8828939054      2.6337615645      2.5356362497

 nuclear repulsion energy.......  1442.544030789 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  34   /
--------------------------------------------------
```

```
 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:    2188.203   user+sys:    2188.203
```

Stereoisomer cis **5’a**

```
+--------------------------------------------------------------------+
  |  Jaguar version 3.5, release  42                                   |
  |                                                                    |
  |  Copyright 1991-1998 Schrodinger, Inc.                             |
  |  All Rights Reserved.                                              |
  |                                                                    |
  |  Use of this program should be acknowledged in publications as:    |
  |  Jaguar 3.5, Schrodinger, Inc., Portland, Oregon, 1998.            |
  +--------------------------------------------------------------------+

  start of program pre
  Job name: WF29705
  Executables used: C:\USERS\GIANCARLO\DOCUMENTS\1.
  Temporary files : LAVORO\C.

  Input file comments:
    Molecule001
    This file created by Spartan

  basis set:              3-21g*
  net molecular charge:     0
  multiplicity:             1

  number of basis functions....           210

 Input geometry:
                                angstroms
  atom            x                 y                 z
  H25       0.6886900000      2.3544670000     -3.9937660000
  C1        1.3750520000      2.2734170000     -3.1390250000
  C2        3.1750530000      2.0861580000     -0.9285270000
  C3        1.1383800000      1.3403620000     -2.1349640000
  C4        2.4920260000      3.0976570000     -3.0405700000
  C5        3.3742850000      3.0037670000     -1.9550370000
  C6        2.0557450000      1.2524780000     -1.0164380000
  C7        0.0957650000      0.3425340000     -1.9264760000
  H27       2.6898920000      3.8389280000     -3.8289430000
  H28       4.2474270000      3.6727650000     -1.9132950000
  H30       3.8681870000      2.0136070000     -0.0784040000
  C8        0.3831890000     -0.2976200000     -0.7409320000
  H32      -0.7409340000      0.1600350000     -2.5950360000
  C10      -0.1361960000     -1.4227000000      0.1031630000
  N2        1.5769130000      0.2513240000     -0.1637720000
  C9        1.9474810000     -0.4225660000      1.0095210000
  O1        2.9471210000     -0.1768780000      1.6869020000
  H43      -0.0649790000     -2.3743750000     -0.4983350000
  C12      -1.5497210000     -1.2402180000      0.5399010000
  C11       0.8902860000     -1.5130810000      1.2775300000
  C19       0.2982570000     -1.3342840000      2.6500090000
  C13      -3.7119580000     -2.2138530000      1.0439530000
  C14      -3.3957740000      0.1717130000      1.2257040000
  C15      -4.2202500000     -0.9479390000      1.3340210000
  C16      -2.0666360000      0.0279860000      0.8307490000
  C17      -2.3841030000     -2.3609000000      0.6471610000
  H49      -4.3596040000     -3.0991830000      1.1256260000
  H50      -3.7933710000      1.1725120000      1.4504100000
  H51      -5.2688150000     -0.8329270000      1.6450770000
  H52      -1.4200870000      0.9147090000      0.7388970000
  H53      -1.9911600000     -3.3622750000      0.4156240000
  H1        1.1120370000     -1.3363630000      3.4165330000
  H2       -0.4122190000     -2.1680220000      2.8690440000
 H3       -0.2595340000     -0.3685300000      2.7224590000
 H4        1.4195540000     -2.5027080000      1.2212370000

 Molecular weight:    261.12 amu

 Stoichiometry:        C18NH15O
 Molecular Point Group: C1
 Point Group used: C1
 nuclear repulsion energy.......  1440.472808068 hartrees

Non-default options chosen:
  Geometry will be optimized in redundant internal coordinates
  Initial Hessian: from previous calculation

 end of program pre


 start of program onee
 smallest eigenvalue of S:    1.347E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program hfig
 initial wavefunction generated automatically from atomic wavefunctions

 Irreducible     Total no   No of occupied orbitals
 representation  orbitals   Shell_1  Shell_2    ...
 No Symm          210         69
 ------------------------
 Orbital occupation/shell    1.000

 end of program hfig


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      89      91      87      86      85      85
 grid # 2       106    100     100      96     100     100      93      92
 grid # 3       224    184     185     196     183     184     196     185
 grid # 4       227    380     384     411     380     380     383     384

 number of gridpoints:
    atom        H27     H28     H30     C8      H32     C10     N2      C9
 grid # 1        73     73      73      87      73      81      99      82
 grid # 2       106    106     106      90     105      88     108      82
 grid # 3       224    224     220     189     223     171     225     169
 grid # 4       228    228     223     380     230     350     410     339

 number of gridpoints:
    atom        O1      H43     C12     C11     C19     C13     C14     C15
 grid # 1       111     71      90      82      73      89      89      89
 grid # 2       127    100     106      93      77      99      99     100
 grid # 3       274    211     192     175     148     184     184     185
 grid # 4       478    207     401     352     322     379     378     379
```

```
  number of gridpoints:
     atom       C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1       86     88     73     73     73     69     71     72
  grid # 2       98     99    106    106    106    102    104     99
  grid # 3      181    183    224    224    224    212    216    220
  grid # 4      379    378    228    227    228    214    219    225

  number of gridpoints:
     atom        H2     H3     H4  total
  grid # 1       71     70     71   2837
  grid # 2       99     96    100   3494
  grid # 3      218    214    218   7069
  grid # 4      219    216    213  10959

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf
 number of electrons..........        138
 number of alpha electrons....         69
 number of beta electrons.....         69
 number of orbitals, total....        210
 number of core orbitals......         69
 number of open shell orbs....          0
 number of occupied orbitals..         69
 number of virtual orbitals...        141
 number of hamiltonians.......          1
 number of shells.............          1
 SCF type: HF

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                      energy  density    DIIS
       r  t  s  t  d     total energy     change   change     error

etot   1  N  N  5  M  -812.78268348650            3.8E-02  1.4E-01
etot   2  Y  Y  6  M  -814.79138137081  2.0E+00  6.2E-03  1.1E-01
etot   3  Y  Y  6  M  -815.04716877384  2.6E-01  1.0E-02  5.3E-02
etot   4  N  Y  2  U  -814.82979416740 -2.2E-01  1.4E-02  1.4E-01
etot   5  N  Y  2  U  -814.92391575147  9.4E-02  2.1E-02  1.1E-01
etot   6  Y  Y  6  M  -815.05560708398  1.3E-01  8.3E-03  6.7E-02
etot   7  N  Y  2  U  -815.10629835254  5.1E-02  3.4E-03  3.1E-02
etot   8  Y  Y  6  M  -815.11687634204  1.1E-02  1.4E-03  8.8E-03
etot   9  N  Y  2  U  -815.11876800244  1.9E-03  1.5E-04  2.5E-03
etot  10  Y  Y  6  M  -815.11892424704  1.6E-04  1.2E-04  1.4E-03
etot  11  Y  Y  6  M  -815.11899599696  7.2E-05  5.4E-05  3.9E-04
etot  12  Y  Y  6  M  -815.11902866522  3.3E-05  7.2E-06  8.3E-05
etot  13  Y  Y  6  M  -815.11902706488 -1.6E-06  3.1E-06  3.5E-05
etot  14  N  N  2  U  -815.11889544947 -1.3E-04  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1440.47280806809
   (E)  Total one-electron terms..... -3966.66504906832
   (I)  Total two-electron terms.....  1711.07334555075
   (L)  Electronic energy............ -2255.59170351756  (E+I)
   (N)  Total energy.................  -815.11889544947  (A+L)
```

```
SCFE: SCF energy: HF    -815.11889544947 hartrees   iterations:  14


HOMO energy:    -0.29298
LUMO energy:     0.11127

 Orbital energies:
 -20.45306  -15.55949  -11.32866  -11.24422  -11.23573  -11.21699
 -11.21406  -11.20362  -11.19611  -11.19433  -11.19377  -11.19309
 -11.19166  -11.19114  -11.18700  -11.18641  -11.18586  -11.18257
 -11.17972  -11.17707   -1.40470   -1.31339   -1.17846   -1.15442
  -1.11573   -1.07956   -1.03706   -1.02388   -1.01487   -0.99554
  -0.94221   -0.90070   -0.84708   -0.83850   -0.82642   -0.80022
  -0.77997   -0.75564   -0.71186   -0.68097   -0.67852   -0.66623
  -0.65399   -0.63994   -0.63075   -0.61940   -0.60945   -0.60171
  -0.59658   -0.59512   -0.58645   -0.57797   -0.55614   -0.54311
  -0.52339   -0.51844   -0.51208   -0.50894   -0.49547   -0.49384
  -0.48760   -0.48203   -0.45234   -0.42182   -0.39553   -0.34941
  -0.34169   -0.31254   -0.29298    0.11127    0.12947    0.13244
   0.13351    0.20008    0.20866    0.25301    0.26027    0.26847
   0.29523

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.222434E-02  -1.130955E-03   1.475894E-02
  2    C1     -3.862275E-03   2.737511E-03  -7.805375E-03
  3    C2      2.504355E-05  -5.982400E-03   8.093392E-03
  4    C3      1.824739E-02  -2.839439E-03   2.442479E-02
  5    C4      5.932779E-04   7.123474E-03  -9.049019E-03
  6    C5      9.754677E-03   6.434136E-03   1.629568E-03
  7    C6     -2.075858E-03   9.178370E-03  -1.195066E-02
  8    C7      2.814102E-03  -1.688764E-02   2.728656E-02
  9    H27    -3.601753E-03  -1.344203E-02   1.429580E-02
 10    H28    -1.618132E-02  -1.246861E-02  -6.839243E-04
 11    H30    -1.422930E-02  -2.330306E-05  -1.529101E-02
 12    C8      1.113915E-02   2.840004E-02  -2.792182E-02
 13    H32     1.100067E-02   5.734086E-04   1.135553E-02
 14    C10     1.100992E-02  -2.716938E-02  -2.172544E-02
 15    N2     -2.642436E-02  -1.787194E-02  -1.339288E-02
 16    C9      3.756980E-02   1.780946E-02   9.691310E-03
 17    O1     -3.642113E-02  -6.246066E-03  -2.360412E-02
 18    H43    -2.726170E-03   2.319800E-02   1.412277E-02
 19    C12    -2.503282E-02   5.942381E-04   6.987730E-04
 20    C11     2.291762E-02  -1.625845E-02  -1.382487E-02
 21    C19    -1.122013E-02   3.781163E-03   3.485740E-02
```

```
  22    C13    -6.222051E-03  -7.340124E-03   1.835546E-03
  23    C14    -2.100249E-03   8.017839E-03   2.423074E-03
  24    C15    -9.018741E-03   9.260244E-05   2.603245E-03
  25    C16     2.484457E-03   5.593248E-03  -1.759100E-04
  26    C17     1.658169E-03  -2.011237E-03  -3.138985E-04
  27    H49     1.147389E-02   1.599304E-02  -1.585371E-03
  28    H50     7.181397E-03  -1.816341E-02  -4.054648E-03
  29    H51     1.885804E-02  -2.067966E-03  -5.807676E-03
  30    H52    -1.279500E-02  -1.700501E-02   6.616159E-04
  31    H53    -6.624328E-03   1.771002E-02   3.386624E-03
  32    H1     -1.668550E-02  -1.218845E-04  -1.565712E-02
  33    H2      1.418806E-02   1.879594E-02  -1.788669E-03
  34    H3      1.210608E-02  -2.195092E-02   7.916222E-04
  35    H4     -1.004245E-02   2.361926E-02   2.461792E-03
 -----------   -------------  -------------  -------------
    total      -1.734733E-05   6.709873E-04   7.459507E-04

  end of program der1b


  start of program geopt   1

  geometry optimization step  1
  reading input hessian of dimension   105
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:     0.3002118
   Cos(theta):    0.8389975

   Final level shift:  -5.2179595E-02

  gradient maximum:         4.3794E-02 .  (  4.5000E-04 )
  gradient rms:             1.2223E-02 .  (  3.0000E-04 )
  step size:   0.30021  trust radius:   0.30000
  displacement maximum:     8.3134E-02 .  (  1.8000E-03 )
  displacement rms:         2.6852E-02 .  (  1.2000E-03 )
  predicted energy change:    -1.9562E-02    geom step:   3.0021E-01    full step:
3.0021E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.5964E-02     y:     3.1437E-03     z:    -1.5951E-02

  new geometry:
                               angstroms
  atom            x                 y                 z
  H25       0.7398635828      2.3367211526     -3.9707796120
  C1        1.3970254542      2.2609998714     -3.1233397783
  C2        3.1709742893      2.0580296859     -0.8990496105
  C3        1.1577112601      1.3275223397     -2.1201753592
  C4        2.5073978646      3.0810069952     -3.0137823157
  C5        3.3866487924      2.9800275972     -1.9156684517
  C6        2.0540438730      1.2437912485     -1.0200550701
  C7        0.1099068234      0.3246151920     -1.9226775600
  H27       2.7082674462      3.8072463629     -3.7805661819
  H28       4.2315797784      3.6402143553     -1.8577954237
  H30       3.8181514571      1.9754010688     -0.0481640993
  C8        0.3794964387     -0.2997446904     -0.7654776965
  H32      -0.7048999624      0.1355785631     -2.5857085597
  C10      -0.1452156126     -1.4251614525      0.0944573269
 N2         1.5559400303      0.2349014172     -0.2012571471
 C9         1.9480381272     -0.3850638524      0.9820617363
 O1         2.9233635939     -0.1035785071      1.6405677795
 H43       -0.0856436979     -2.3554720229     -0.4606881258
 C12       -1.5805958252     -1.2454924987      0.5312993868
 C11        0.9066836483     -1.4865678440      1.2716609096
 C19        0.3834741654     -1.3140966297      2.6981957081
 C13       -3.7271863089     -2.2203706947      1.0329615607
 C14       -3.4137964209      0.1638916814      1.2324837756
 C15       -4.2343853551     -0.9542946417      1.3357872613
 C16       -2.1001085773      0.0178182649      0.8299138102
 C17       -2.4091543907     -2.3591848007      0.6315497115
 H49       -4.3642165665     -3.0852147864      1.1000203386
 H50       -3.7944386113      1.1411778907      1.4659213387
 H51       -5.2578097521     -0.8427607631      1.6441330522
 H52       -1.4701816191      0.8867454110      0.7444147448
 H53       -2.0285817643     -3.3352537171      0.3855835579
 H1         1.2237931433     -1.3765631446      3.3738415393
 H2        -0.3342642682     -2.0942130342      2.9351286210
 H3        -0.0993880779     -0.3663307952      2.8439572923
 H4         1.4431813633     -2.4245539315      1.2066820334

 nuclear repulsion energy.......  1445.086679319 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   1   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.280E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      89      91      87      87      84      85
 grid # 2       106     100     100      99      99      99      91      92
 grid # 3       224     183     183     194     183     185     192     182
 grid # 4       224     382     385     403     379     382     377     379

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      83      99      80
 grid # 2       106     106     105      91     105      91     108      81
 grid # 3       224     224     220     183     223     173     224     168
 grid # 4       224     224     219     379     228     352     407     333

 number of gridpoints:
    atom         O1     H43     C12     C11     C19     C13     C14     C15
 grid # 1       111      69      90      81      72      88      89      89
 grid # 2       127      98     105      92      74      99     100     100
 grid # 3       274     211     192     173     145     182     182     184
 grid # 4       475     206     398     356     302     380     379     379
```

```
  number of gridpoints:
     atom        C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1        85     86     73     73     73     70     71     71
  grid # 2        97     99    106    106    106    101    103     96
  grid # 3       181    183    224    224    224    214    216    220
  grid # 4       380    378    224    223    224    211    215    219

  number of gridpoints:
     atom         H2     H3     H4  total
  grid # 1        71     71     69   2827
  grid # 2        97     98     99   3482
  grid # 3       219    217    218   7048
  grid # 4       216    213    211  10866

  end of program grid


  start of program rwr
 recomputing RwR matrix   4    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                   RMS    maximum
       e  d  i  u  i                        energy  density    DIIS
       r  t  s  t  d     total energy       change   change     error

etot   1  N  N  2  U  -815.12760518104             7.2E-04  7.2E-03
etot   2  Y  Y  6  M  -815.13767931827  1.0E-02  1.8E-04  1.9E-03
etot   3  N  Y  2  U  -815.13789955582  2.2E-04  6.7E-05  1.3E-03
etot   4  Y  Y  6  M  -815.13792619566  2.7E-05  2.7E-05  3.2E-04
etot   5  Y  Y  6  M  -815.13793533269  9.1E-06  8.7E-06  2.0E-04
etot   6  Y  Y  6  M  -815.13793357215 -1.8E-06  4.2E-06  5.6E-05
etot   7  Y  N  6  M  -815.13793352362 -4.9E-08  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1445.08667931854
   (E)  Total one-electron terms..... -3975.79206470248
   (I)  Total two-electron terms.....  1715.56745186032
   (L)  Electronic energy............ -2260.22461284216  (E+I)
   (N)  Total energy.................  -815.13793352362  (A+L)

 SCFE: SCF energy: HF    -815.13793352362 hartrees   iterations:   7


 HOMO energy:    -0.29608
 LUMO energy:     0.11778

  Orbital energies:
  -20.45377  -15.55301  -11.32351  -11.23699  -11.22760  -11.21457
  -11.20825  -11.20185  -11.19003  -11.18887  -11.18820  -11.18703
  -11.18648  -11.18508  -11.18079  -11.18069  -11.17912  -11.17796
  -11.17499  -11.16610   -1.42036   -1.32425   -1.17772   -1.15711
   -1.11197   -1.08473   -1.03791   -1.02795   -1.01739   -0.99887
   -0.94752   -0.90173   -0.85264   -0.84182   -0.82960   -0.80805
   -0.78803   -0.75931   -0.71787   -0.68415   -0.68106   -0.66905
   -0.65571   -0.64293   -0.63677   -0.62308   -0.61471   -0.60606
  -0.60307   -0.60158   -0.58967   -0.58280   -0.55726   -0.54617
  -0.53219   -0.52452   -0.51600   -0.51183   -0.49844   -0.49445
  -0.49062   -0.48446   -0.45674   -0.42034   -0.39463   -0.35087
  -0.34044   -0.31317   -0.29608    0.11778    0.13179    0.13696
   0.13912    0.20433    0.21826    0.26296    0.27011    0.27843
   0.30321

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.082376E-03   2.860015E-04   2.281768E-03
  2    C1      3.222330E-03  -1.585870E-04   1.836401E-03
  3    C2     -5.136555E-03   2.238841E-03  -6.126828E-03
  4    C3      7.972063E-03   1.605087E-03   6.142764E-03
  5    C4      4.783526E-03  -1.837015E-03   6.120872E-03
  6    C5     -6.951960E-03  -1.869077E-03  -1.501968E-03
  7    C6     -7.877590E-03  -2.013762E-03  -6.614666E-03
  8    C7      2.324878E-03   2.668237E-04   3.840875E-03
  9    H27    -1.030510E-04  -1.556590E-03   2.187182E-03
 10    H28    -1.073646E-03  -1.573911E-03  -5.068402E-04
 11    H30    -1.072145E-03  -8.072346E-04  -1.908643E-03
 12    C8      8.461190E-03   3.537095E-03  -7.681314E-04
 13    H32     3.677220E-04   2.713555E-04   1.631253E-03
 14    C10     4.261853E-03  -1.606562E-03   2.587965E-04
 15    N2     -5.150917E-03  -7.681990E-03   4.407027E-03
 16    C9      2.803416E-04   4.767250E-03  -7.996029E-03
 17    O1     -5.488620E-03   1.176252E-03  -3.363509E-03
 18    H43     1.243694E-03   2.002689E-03  -4.705330E-04
 19    C12    -7.955533E-03   6.713513E-03   9.211370E-04
 20    C11     5.644125E-03   5.336180E-03  -4.764648E-03
 21    C19    -2.746204E-03  -8.127269E-03   2.220314E-03
 22    C13    -6.017972E-03   9.420573E-03   2.397737E-03
 23    C14    -2.752859E-03  -5.818407E-03   9.412731E-04
 24    C15     3.007362E-03  -5.755522E-03  -1.330078E-03
 25    C16     6.142501E-03  -3.906929E-03  -2.808611E-04
 26    C17     8.481408E-04   3.385474E-03   1.125427E-04
 27    H49     2.016984E-03   2.797799E-03   1.455498E-04
 28    H50     3.152453E-05  -2.233240E-03  -7.607697E-04
 29    H51     2.102534E-03  -7.884871E-04  -7.388283E-04
 30    H52    -1.875499E-03  -3.625785E-03  -8.817577E-04
 31    H53    -2.978004E-04   2.186788E-03   6.440159E-04
 32    H1      8.646609E-04  -6.290993E-04   2.061954E-03
 33    H2      2.892355E-03   1.728978E-03   5.846091E-04
 34    H3     -2.498431E-03   5.215111E-03  -1.569047E-03
 35    H4     -4.071073E-04  -1.202637E-03   9.652473E-04
-----------   -------------  -------------  -------------
```

```
    total       1.442718E-04   1.743710E-03   1.181800E-04

  end of program der1b


  start of program geopt   2

  geometry optimization step  2
  reading input hessian of dimension   105
   in five columns format


  energy change:          -1.9038E-02 .  (  5.0000E-05 )
  gradient maximum:        1.5112E-02 .  (  4.5000E-04 )
  gradient rms:            3.9810E-03 .  (  3.0000E-04 )
  step size:   0.19393  trust radius:   0.30000
  displacement maximum:    5.2508E-02 .  (  1.8000E-03 )
  displacement rms:        1.7345E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.4874E-03    geom step:   1.9393E-01    full step:
1.9393E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -9.1451E-03     y:     5.7245E-03     z:    -8.6685E-03

  new geometry:
                               angstroms
  atom            x                  y                  z
  H25       0.7967260056      2.3299018677     -3.9857803870
  C1        1.4350552114      2.2470470588     -3.1302158988
  C2        3.1283906435      2.0568506211     -0.8781592526
  C3        1.1717758371      1.3080134690     -2.1402986284
  C4        2.5382161341      3.0723658784     -2.9890298644
  C5        3.3739719773      2.9820723567     -1.8719761634
  C6        2.0290344166      1.2313051884     -1.0324418956
  C7        0.1192569272      0.2994461727     -1.9529932793
  H27       2.7578960807      3.7969745514     -3.7433059465
  H28       4.2187418778      3.6343781462     -1.7889011473
  H30       3.7568061523      1.9584819367     -0.0173633228
  C8        0.3931011506     -0.3356880661     -0.8047252733
  H32      -0.6981143562      0.1139484770     -2.6132475788
  C10      -0.1345300353     -1.4498695090      0.0731199874
  N2        1.5406187330      0.2121584957     -0.2301351582
  C9        1.9197607438     -0.3472592728      0.9693225814
  O1        2.8601281695     -0.0062431820      1.6459629914
  H43      -0.0723505993     -2.3801380751     -0.4689640688
  C12      -1.5763049703     -1.2459444137      0.5110623919
  C11       0.9218202784     -1.4793124559      1.2572126749
  C19       0.3866400189     -1.3294505456      2.6907977333
  C13      -3.7299280302     -2.2037612738      1.0635112955
  C14      -3.3840615928      0.1532990657      1.2654439928
  C15      -4.2171030909     -0.9517970593      1.3890197856
  C16      -2.0768445187      0.0095389688      0.8244966889
  C17      -2.4184919437     -2.3452322200      0.6280627563
  H49      -4.3611343315     -3.0661896878      1.1428437857
  H50      -3.7524013898      1.1296861103      1.5075599138
  H51      -5.2246937354     -0.8347534890      1.7251651001
  H52      -1.4526613471      0.8730615904      0.7163835312
  H53      -2.0526004711     -3.3214508488      0.3762451729
  H1        1.2181467842     -1.3334586393      3.3860816770
  H2       -0.2748264783     -2.1404264500      2.9293103096
  H3       -0.1519777723     -0.3950452424      2.7982047617
```

```
 H4        1.4769903361     -2.4067640012      1.2037165899

 nuclear repulsion energy.......  1449.525488251 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration   2   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.224E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     85     85
 grid # 2       106    100     97     98     98     99     91     92
 grid # 3       224    183    183    195    182    183    187    182
 grid # 4       224    379    381    406    377    380    372    378

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     82     99     76
 grid # 2       106    106    105     91    105     93    109     80
 grid # 3       224    224    220    187    223    175    225    164
 grid # 4       224    224    219    373    228    350    402    332

 number of gridpoints:
    atom         O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1       111     69     90     81     71     87     87     89
 grid # 2       123     97    106     93     75     99     99     99
 grid # 3       272    210    195    175    142    182    183    183
 grid # 4       473    204    401    358    305    378    378    376

 number of gridpoints:
    atom        C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1        86     84     73     73     73     70     72     71
 grid # 2        98     98    106    106    106    101    103     99
 grid # 3       182    182    224    223    224    213    216    219
 grid # 4       378    377    224    223    224    211    215    220

 number of gridpoints:
    atom         H2     H3     H4  total
 grid # 1        71     71     70   2817
 grid # 2        99     97    100   3480
 grid # 3       219    216    218   7039
 grid # 4       218    212    212  10836

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
```

```
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.13064395291           5.6E-04  1.0E-02
etot   2  Y  Y  6  M  -815.13890364201  8.3E-03  1.8E-04  3.1E-03
etot   3  N  Y  2  U  -815.13975268411  8.5E-04  7.2E-05  1.2E-03
etot   4  Y  Y  6  M  -815.13974997335 -2.7E-06  3.0E-05  6.4E-04
etot   5  Y  Y  6  M  -815.13979028527  4.0E-05  9.3E-06  2.4E-04
etot   6  Y  Y  6  M  -815.13979256254  2.3E-06  5.3E-06  1.2E-04
etot   7  Y  Y  6  M  -815.13979576879  3.2E-06  1.6E-06  2.8E-05
etot   8  N  N  2  U  -815.13987365587  7.8E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1449.52548825116
   (E)  Total one-electron terms..... -3984.60110961014
   (I)  Total two-electron terms.....  1719.93574770311
   (L)  Electronic energy............ -2264.66536190703  (E+I)
   (N)  Total energy.................  -815.13987365587  (A+L)

 SCFE: SCF energy: HF    -815.13987365587 hartrees   iterations:   8


 HOMO energy:    -0.29764
 LUMO energy:     0.11945

  Orbital energies:
  -20.45232  -15.55246  -11.32119  -11.23673  -11.22347  -11.21587
  -11.20772  -11.20117  -11.18840  -11.18708  -11.18654  -11.18598
  -11.18444  -11.18389  -11.17965  -11.17791  -11.17741  -11.17573
  -11.17271  -11.16601   -1.42321   -1.33209   -1.17920   -1.16156
   -1.11234   -1.08768   -1.03870   -1.02659   -1.01869   -1.00183
   -0.94965   -0.90312   -0.85408   -0.84343   -0.83130   -0.81075
   -0.79120   -0.76136   -0.72035   -0.68609   -0.68135   -0.66945
   -0.65684   -0.64394   -0.63875   -0.62522   -0.61304   -0.60757
   -0.60360   -0.60066   -0.59238   -0.58503   -0.55509   -0.54833
   -0.53333   -0.52475   -0.51722   -0.51154   -0.49910   -0.49503
   -0.49029   -0.48462   -0.45819   -0.42114   -0.39345   -0.34863
   -0.34346   -0.31528   -0.29764    0.11945    0.13368    0.13676
    0.14074    0.20588    0.22009    0.26462    0.27184    0.28131
    0.30470

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b
 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -2.623631E-04   1.700799E-04  -9.124781E-04
  2    C1      2.432552E-03   1.211666E-03   1.198601E-03
  3    C2      4.715643E-04  -1.986015E-03   1.585579E-03
  4    C3     -2.309690E-03   1.324897E-03   1.417885E-03
  5    C4     -2.901685E-03  -2.200260E-03   1.309211E-03
  6    C5     -2.227007E-03  -2.432971E-03  -4.164661E-04
  7    C6      1.152702E-03  -8.780845E-04  -1.388603E-03
  8    C7      2.507957E-03  -3.639032E-04  -1.920657E-03
  9    H27    -7.319205E-05   1.405911E-03  -1.903195E-03
 10    H28     3.709943E-04   5.340245E-04  -2.523943E-05
 11    H30    -8.085029E-04  -1.240634E-04   1.837915E-04
 12    C8     -9.385822E-04   1.294605E-03   1.523497E-03
 13    H32     8.071532E-04   1.553965E-04   7.331486E-04
 14    C10     7.039373E-04   4.384921E-03   2.559956E-03
 15    N2      1.616081E-03   1.728965E-03   2.708001E-03
 16    C9     -1.452199E-03  -3.213018E-03  -3.834215E-03
 17    O1      2.642902E-04   2.610004E-03   3.916516E-04
 18    H43     2.483463E-04  -2.741756E-03  -9.976686E-04
 19    C12    -1.760753E-03  -2.663642E-03   6.550794E-04
 20    C11     9.484241E-04   5.584168E-04   1.445251E-03
 21    C19     6.898760E-04   6.450851E-03  -2.802946E-03
 22    C13     3.774411E-03   2.060100E-04  -1.101554E-03
 23    C14     7.584081E-04  -7.842765E-04  -6.667253E-04
 24    C15     5.840972E-03   2.406323E-03  -1.670542E-03
 25    C16    -4.367034E-03   1.831214E-04   1.745718E-03
 26    C17    -9.944412E-04   1.458779E-04   7.299726E-04
 27    H49     1.822174E-04  -2.359941E-04  -3.828083E-05
 28    H50    -3.804916E-04   4.367151E-04   9.030745E-05
 29    H51    -1.948547E-03   6.697194E-04   7.302620E-04
 30    H52     1.577978E-05   3.903787E-04  -1.480019E-05
 31    H53     3.570102E-04  -5.758122E-04  -1.327843E-04
 32    H1      2.534299E-04   3.851687E-04  -2.025601E-03
 33    H2     -4.427410E-03  -3.812410E-03   2.056013E-03
 34    H3      1.660708E-04  -2.589512E-03   1.227096E-03
 35    H4      1.130577E-03  -6.645597E-04  -1.252721E-03
-----------   -------------  -------------  -------------
   total      -1.591435E-04   1.386774E-03   1.186543E-03

 end of program der1b


 start of program geopt   3

 geometry optimization step  3
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format


 energy change:          -1.9401E-03 .   (  5.0000E-05 )
 gradient maximum:        6.1173E-03 .   (  4.5000E-04 )
 gradient rms:            1.7467E-03 .   (  3.0000E-04 )
 step size:    0.17236  trust radius:    0.30000
 displacement maximum:    6.7777E-02 .   (  1.8000E-03 )
 displacement rms:        1.5416E-02 .   (  1.2000E-03 )
```

```
  predicted energy change:    -5.8629E-04    geom step:   1.7236E-01    full step:
1.7236E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -8.0592E-03     y:     1.4053E-02     z:     6.2813E-03

  new geometry:
                              angstroms
  atom             x                  y                  z
  H25       0.8072865483      2.2760293482     -4.0143546838
  C1        1.4325178336      2.2130871857     -3.1459662973
  C2        3.0976253171      2.0667490363     -0.8651597197
  C3        1.1712748712      1.2791840973     -2.1512836582
  C4        2.5153655009      3.0583921385     -2.9938746906
  C5        3.3377384538      2.9858852701     -1.8643249838
  C6        2.0119854774      1.2279304907     -1.0311111308
  C7        0.1465784669      0.2438782778     -1.9771518293
  H27       2.7315919265      3.7820441542     -3.7521825163
  H28       4.1726912194      3.6515563018     -1.7754703926
  H30       3.7097514806      1.9852447292      0.0091292579
  C8        0.4010099143     -0.3570219534     -0.8084213467
  H32      -0.6501742014      0.0275017732     -2.6496760436
  C10      -0.1229729538     -1.4639393444      0.0786221673
  N2        1.5189677339      0.2254555354     -0.2157299573
  C9        1.9020989706     -0.3217707669      0.9829327639
  O1        2.8151205517      0.0629398142      1.6772920803
  H43      -0.0678278284     -2.4005658225     -0.4590942179
  C12      -1.5631049639     -1.2451359645      0.5189991882
  C11       0.9418899756     -1.4894534200      1.2530039693
  C19       0.4011021736     -1.4041869419      2.6862463752
  C13      -3.7226329608     -2.1688535666      1.0469508290
  C14      -3.3466156121      0.1851923676      1.2619589087
  C15      -4.1902105651     -0.9090297665      1.3697187430
  C16      -2.0442039099      0.0183278048      0.8369931969
  C17      -2.4164110075     -2.3337937945      0.6249984247
  H49      -4.3682653523     -3.0199658461      1.1178566307
  H50      -3.7060294944      1.1666422173      1.5007293633
  H51      -5.2008383429     -0.7766856075      1.6958622372
  H52      -1.4071642828      0.8716104968      0.7311012260
  H53      -2.0627003799     -3.3147832946      0.3713148177
  H1        1.2439048961     -1.3948340451      3.3666321408
  H2       -0.2266020434     -2.2519354554      2.9147482339
  H3       -0.1771930683     -0.5044698803      2.8328919287
  H4        1.5287631081     -2.3957569091      1.1654660655

  nuclear repulsion energy.......  1452.259395357 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration   3   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.213E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe
```

```
   start of program grid

   number of gridpoints:
      atom        H25     C1     C2     C3     C4     C5     C6     C7
   grid # 1        73     89     87     90     87     87     85     85
   grid # 2       106    100     97     98     98     99     91     92
   grid # 3       224    183    183    194    182    182    187    183
   grid # 4       224    379    383    404    379    379    372    376

   number of gridpoints:
      atom        H27    H28    H30     C8    H32    C10     N2     C9
   grid # 1        73     73     73     86     73     82    100     76
   grid # 2       106    106    105     91    105     93    109     80
   grid # 3       224    224    220    187    223    175    224    164
   grid # 4       224    224    219    372    227    352    402    334

   number of gridpoints:
      atom         O1    H43    C12    C11    C19    C13    C14    C15
   grid # 1       111     69     92     81     71     87     87     88
   grid # 2       127     97    106     93     78     99     99    100
   grid # 3       272    210    192    175    149    182    182    183
   grid # 4       474    203    396    359    307    377    379    377

   number of gridpoints:
      atom        C16    C17    H49    H50    H51    H52    H53     H1
   grid # 1        84     84     73     73     73     71     72     71
   grid # 2        97     98    106    106    106    101    103     99
   grid # 3       181    182    224    223    224    214    216    219
   grid # 4       375    378    224    223    224    212    215    220

   number of gridpoints:
      atom         H2     H3     H4  total
   grid # 1        71     71     69   2817
   grid # 2        98     97    100   3486
   grid # 3       219    215    218   7039
   grid # 4       218    214    211  10836

   end of program grid


   start of program rwr
  recomputing RwR matrix  15    grid:  4
   end of program rwr


   start of program scf

        i  u  d  i  g
        t  p  i  c  r                                 RMS    maximum
        e  d  i  u  i                       energy  density   DIIS
        r  t  s  t  d     total energy      change  change    error

 etot   1  N  N  2  U  -815.13359031216             3.8E-04  9.0E-03
 etot   2  Y  Y  6  M  -815.13965737775  6.1E-03  1.5E-04  3.4E-03
 etot   3  N  Y  2  U  -815.14024597539  5.9E-04  5.0E-05  1.0E-03
 etot   4  Y  Y  6  M  -815.14026120740  1.5E-05  1.9E-05  4.1E-04
 etot   5  Y  Y  6  M  -815.14028900003  2.8E-05  8.3E-06  1.4E-04
 etot   6  Y  Y  6  M  -815.14029029074  1.3E-06  3.5E-06  6.8E-05
 etot   7  Y  N  6  M  -815.14029185985  1.6E-06  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
  (A)  Nuclear repulsion............  1452.25939535683
  (E)  Total one-electron terms..... -3990.06157287361
  (I)  Total two-electron terms.....  1722.66188565694
  (L)  Electronic energy............ -2267.39968721667  (E+I)
  (N)  Total energy.................  -815.14029185985  (A+L)

SCFE: SCF energy: HF    -815.14029185985 hartrees   iterations:   7


HOMO energy:    -0.29751
LUMO energy:     0.11942

 Orbital energies:
 -20.45210  -15.55235  -11.32113  -11.23569  -11.22260  -11.21520
 -11.20773  -11.20061  -11.18781  -11.18611  -11.18531  -11.18480
 -11.18354  -11.18295  -11.17940  -11.17699  -11.17692  -11.17559
 -11.17260  -11.16545   -1.42254   -1.33385   -1.18059   -1.16278
  -1.11297   -1.08898   -1.03871   -1.02898   -1.01946   -1.00185
  -0.94904   -0.90414   -0.85404   -0.84396   -0.83155   -0.81171
  -0.79190   -0.76122   -0.72113   -0.68612   -0.68111   -0.66955
  -0.65664   -0.64425   -0.63886   -0.62544   -0.61349   -0.60747
  -0.60429   -0.60263   -0.59182   -0.58432   -0.55535   -0.54830
  -0.53251   -0.52410   -0.51766   -0.51191   -0.49913   -0.49462
  -0.49002   -0.48521   -0.45820   -0.42147   -0.39394   -0.35031
  -0.34292   -0.31547   -0.29751    0.11942    0.13357    0.13855
   0.14128    0.20607    0.22031    0.26454    0.27197    0.28119
   0.30560

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.010580E-04   1.942380E-05  -3.552070E-05
  2    C1      5.074994E-04   4.964675E-04  -1.266648E-04
  3    C2     -6.766024E-04  -9.589108E-04   4.736512E-04
  4    C3     -1.953185E-04  -6.409867E-04  -8.061010E-04
  5    C4     -9.044525E-04  -1.230562E-03   1.115862E-03
  6    C5      8.100580E-04   1.482815E-04  -8.885323E-04
  7    C6     -1.376086E-04   2.105949E-03   1.479087E-03
  8    C7      1.557922E-04   1.843155E-03  -6.733394E-04
  9    H27     2.462770E-04   8.110729E-04  -6.671167E-04
 10    H28    -2.242361E-04   4.001475E-04  -2.982147E-04
 11    H30    -6.346412E-04   1.426222E-04  -2.171208E-04
 12    C8     -1.289446E-03  -1.883674E-03   2.165353E-03
 13    H32    -2.924584E-04  -6.572313E-05  -5.545253E-04
 14    C10     9.545611E-04   1.787046E-03  -3.436936E-04
```

```
  15    N2      3.326501E-03  -4.700836E-04  -1.308199E-03
  16    C9     -1.133265E-03   2.086582E-04   2.772878E-03
  17    O1     -1.033850E-03  -1.216126E-04  -1.558166E-03
  18    H43    -4.363843E-04  -8.567623E-04   4.806195E-05
  19    C12     2.341601E-03  -1.197351E-03   6.101532E-04
  20    C11    -2.071413E-03  -2.757577E-04   2.607449E-04
  21    C19     2.364914E-03   1.127246E-03   2.555360E-04
  22    C13    -1.171573E-03   2.179477E-04   6.241987E-04
  23    C14    -2.023048E-03   6.421807E-05   4.696616E-04
  24    C15    -6.651299E-04   8.090348E-04   4.455158E-04
  25    C16     1.390028E-03  -3.219050E-04  -1.600996E-03
  26    C17     2.658039E-03  -1.094508E-05  -8.144298E-04
  27    H49    -9.230256E-04  -4.685583E-04   2.637308E-04
  28    H50    -5.172524E-05  -3.106668E-04   1.206580E-04
  29    H51    -1.168443E-03   6.195567E-05   2.968585E-04
  30    H52     1.203254E-03   5.984256E-04   1.510966E-04
  31    H53     2.525677E-04   9.793345E-05   2.755141E-05
  32    H1     -5.641611E-04   6.756994E-04   3.445955E-04
  33    H2     -1.004026E-03  -1.611655E-03  -1.380153E-04
  34    H3     -3.083528E-04   5.235400E-04   2.332260E-04
  35    H4      5.023782E-04  -4.648487E-04  -7.979136E-04
 -----------   -------------  -------------  -------------
    total      -9.463140E-05   1.248822E-03   1.329869E-03

  end of program der1b


  start of program geopt   4

  geometry optimization step  4
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:          -4.1820E-04 .  (  5.0000E-05 )
  gradient maximum:        3.4808E-03 .  (  4.5000E-04 )
  gradient rms:            8.6489E-04 .  (  3.0000E-04 )
  step size:   0.12936  trust radius:   0.30000
  displacement maximum:    5.2835E-02 .  (  1.8000E-03 )
  displacement rms:        1.1571E-02 .  (  1.2000E-03 )
  predicted energy change:    -2.1245E-04    geom step:   1.2936E-01    full step:
1.2936E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.9215E-05     y:     9.9106E-04     z:     7.1413E-04

  new geometry:
                               angstroms
  atom            x                 y                  z
  H25       0.7971728644      2.2788644224     -4.0061444076
  C1        1.4208187167      2.2167246925     -3.1373359925
  C2        3.0833185063      2.0685756628     -0.8556339552
  C3        1.1686646005      1.2715228110     -2.1504975179
  C4        2.4920270548      3.0725243510     -2.9770316540
  C5        3.3153295384      2.9976324606     -1.8492382985
  C6        2.0084442984      1.2201275787     -1.0299260254
  C7        0.1542915881      0.2261191337     -1.9856358417
 H27       2.7002286996      3.8084924687     -3.7288020235
 H28       4.1386185412      3.6768717965     -1.7547889150
 H30       3.6891010041      1.9903230738      0.0204351535
 C8        0.4134985652     -0.3841207353     -0.8212229852
 H32      -0.6404945515      0.0089886275     -2.6598308865
 C10      -0.1149989585     -1.4807588295      0.0720047200
 N2        1.5331951653      0.1973221852     -0.2311141871
 C9        1.8876571739     -0.3219473858      0.9907675648
 O1        2.7804022497      0.0887181541      1.7013369128
 H43      -0.0723242168     -2.4260811476     -0.4551827176
 C12      -1.5485503169     -1.2473907255      0.5149149371
 C11       0.9445626114     -1.5049765934      1.2471248647
 C19       0.3976244387     -1.4436765611      2.6773594604
 C13      -3.7096764648     -2.1450107608      1.0846319371
 C14      -3.3265823197      0.2141151856      1.2134605377
 C15      -4.1734859629     -0.8729496446      1.3626069905
 C16      -2.0254074096      0.0279171718      0.7899165733
 C17      -2.4040174809     -2.3291908113      0.6634824294
 H49      -4.3599908435     -2.9908229876      1.1896650309
 H50      -3.6811279041      1.2041585751      1.4211081108
 H51      -5.1852252049     -0.7264529610      1.6865655428
 H52      -1.3822667972      0.8757593893      0.6563392551
 H53      -2.0536835868     -3.3196722055      0.4443587969
 H1        1.2359945838     -1.4272358678      3.3621063119
 H2       -0.2193508808     -2.3096898193      2.8890726002
 H3       -0.1979147328     -0.5584397401      2.8376325835
 H4        1.5488227375     -2.3992270283      1.1439156061

 nuclear repulsion energy.......  1453.856370874 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   4   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.209E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106     99      97      98      98      98      91      92
 grid # 3       224    183     183     194     182     182     187     183
 grid # 4       224    379     380     405     379     379     373     377

 number of gridpoints:
    atom        H27     H28     H30     C8      H32     C10     N2      C9
 grid # 1        73     73      73      86      73      82      99      75
 grid # 2       106    106     105      91     105      93     109      80
 grid # 3       224    224     220     186     223     175     223     163
 grid # 4       224    224     218     372     227     350     402     333
```

```
  number of gridpoints:
     atom        O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1      111     69     92     81     71     87     88     89
  grid # 2      127     97    106     93     75    100     99    100
  grid # 3      272    210    193    175    143    182    182    183
  grid # 4      475    205    396    359    303    379    379    379

  number of gridpoints:
     atom       C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1       85     84     73     73     73     70     72     71
  grid # 2       97     99    106    106    106    101    103     99
  grid # 3      181    182    224    223    224    213    216    220
  grid # 4      376    378    224    223    224    212    215    221

  number of gridpoints:
     atom        H2     H3     H4  total
  grid # 1       71     71     69   2817
  grid # 2       98     98    100   3484
  grid # 3      219    216    218   7032
  grid # 4      218    214    211  10837

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                    energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.13572766272           3.0E-04  6.9E-03
etot   2  Y  Y  6  M  -815.13999463142  4.3E-03  1.2E-04  2.9E-03
etot   3  Y  Y  6  M  -815.14048790420  4.9E-04  4.3E-05  8.5E-04
etot   4  N  Y  2  U  -815.14047681929 -1.1E-05  1.4E-05  3.0E-04
etot   5  Y  Y  6  M  -815.14048249198  5.7E-06  7.0E-06  1.1E-04
etot   6  Y  Y  6  M  -815.14048109639 -1.4E-06  2.2E-06  3.4E-05
etot   7  Y  N  6  M  -815.14048184542  7.5E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1453.85637087401
   (E)  Total one-electron terms..... -3993.25555717667
   (I)  Total two-electron terms.....  1724.25870445724
   (L)  Electronic energy............ -2268.99685271943  (E+I)
   (N)  Total energy.................  -815.14048184542  (A+L)

 SCFE: SCF energy: HF    -815.14048184542 hartrees   iterations:   7


 HOMO energy:    -0.29716
 LUMO energy:     0.11902

  Orbital energies:
  -20.45239  -15.55245  -11.32148  -11.23577  -11.22237  -11.21496
  -11.20797  -11.20029  -11.18768  -11.18638  -11.18575  -11.18493
  -11.18384  -11.18306  -11.17915  -11.17713  -11.17667  -11.17560
 -11.17253  -11.16566   -1.42098   -1.33377   -1.18091   -1.16293
  -1.11387   -1.08882   -1.03893   -1.02849   -1.01996   -1.00159
  -0.94916   -0.90456   -0.85399   -0.84385   -0.83164   -0.81176
  -0.79153   -0.76122   -0.72095   -0.68663   -0.68120   -0.66910
  -0.65735   -0.64364   -0.63922   -0.62535   -0.61371   -0.60779
  -0.60381   -0.60209   -0.59208   -0.58389   -0.55452   -0.54889
  -0.53184   -0.52403   -0.51719   -0.51233   -0.49905   -0.49506
  -0.49039   -0.48508   -0.45820   -0.42181   -0.39395   -0.35002
  -0.34291   -0.31579   -0.29716    0.11902    0.13350    0.13788
   0.14164    0.20580    0.21992    0.26417    0.27197    0.28143
   0.30648

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x               y               z
----  -----   -------------  -------------  -------------
  1    H25    -3.441725E-04   7.867304E-05  -3.358111E-04
  2    C1     -6.810300E-04  -5.433485E-04   1.988254E-05
  3    C2     -5.462027E-04   9.048680E-04  -1.405041E-03
  4    C3     -1.002052E-04  -2.925457E-04  -1.393725E-03
  5    C4      3.969773E-04   8.946297E-05  -2.457347E-04
  6    C5      4.027622E-04   8.079543E-04   7.270992E-04
  7    C6      4.855956E-04  -2.987928E-04  -2.763502E-04
  8    C7     -4.753323E-06   3.356626E-04   9.055734E-05
  9    H27    -5.506455E-05  -4.331423E-04   4.008450E-04
 10    H28     9.773562E-05  -3.552234E-06   8.238032E-05
 11    H30     8.050837E-04  -1.583338E-05   9.943578E-04
 12    C8      1.389044E-04  -7.010970E-04  -5.437636E-04
 13    H32    -7.016485E-04   1.637367E-04  -5.328706E-04
 14    C10     8.052453E-04  -1.594617E-03  -1.239903E-03
 15    N2      3.460582E-04   1.825580E-03   3.900681E-03
 16    C9      4.763710E-03   1.578913E-03   2.313807E-03
 17    O1     -5.275677E-03  -1.788269E-03  -4.008281E-03
 18    H43     1.186111E-04   4.519452E-04   2.360278E-04
 19    C12    -1.531970E-04   1.668178E-04   3.803062E-04
 20    C11    -1.022065E-03   1.379460E-03   3.217867E-04
 21    C19     4.700400E-04  -2.962397E-03   1.251723E-03
 22    C13    -8.478524E-04  -5.329280E-04   3.923850E-04
 23    C14    -1.361897E-03  -2.017479E-04   5.067244E-04
 24    C15    -1.580103E-03   9.467885E-04   6.432528E-04
 25    C16     1.760169E-03   8.792614E-04  -6.371640E-04
 26    C17     1.180897E-03   1.521576E-04  -4.193959E-04
 27    H49     5.370760E-05   1.595859E-04   4.485439E-05
 28    H50    -1.057536E-04  -1.501169E-04   1.332931E-05
 29    H51     4.912426E-04  -7.199618E-05  -1.492869E-04
 30    H52    -3.160148E-04  -7.582056E-04   1.237614E-04
 31    H53     1.520809E-04   4.341062E-05  -5.119927E-05
 32    H1     -3.497523E-04   7.508782E-05   6.801302E-04
```

```
  33    H2      1.173676E-03   1.166402E-03   4.775717E-05
  34    H3     -5.276980E-04   1.060908E-03  -6.574441E-04
  35    H4     -5.167100E-05  -2.984202E-04   4.328851E-05
 -----------   -------------  -------------  -------------
    total      -3.822621E-04   1.619666E-03   1.318966E-03

  end of program der1b


  start of program geopt   5

  geometry optimization step  5
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:          -1.8999E-04 .  (  5.0000E-05 )
  gradient maximum:        6.8972E-03 .  (  4.5000E-04 )
  gradient rms:            8.8976E-04 .  (  3.0000E-04 )
  step size:   0.19647  trust radius:   0.30000
  displacement maximum:    7.3864E-02 .  (  1.8000E-03 )
  displacement rms:        1.7573E-02 .  (  1.2000E-03 )
  predicted energy change:   -2.6389E-04   geom step:   1.9647E-01   full step:
1.9647E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1720E-02     y:     1.7754E-02     z:     4.7623E-03

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.8725858787      2.1919439159     -4.0734749107
  C1        1.4647532381      2.1636710497     -3.1799266399
  C2        3.0426007357      2.1088784674     -0.8290102703
  C3        1.1891914498      1.2452586589     -2.1745715680
  C4        2.5201854214      3.0356716476     -3.0042315667
  C5        3.3044980681      3.0070775224     -1.8439280798
  C6        1.9860040607      1.2422188678     -1.0196000372
  C7        0.1801972233      0.1933284036     -2.0176631286
  H27       2.7480087537      3.7501643608     -3.7698669984
  H28       4.1133200966      3.7006202214     -1.7404504022
  H30       3.6115424321      2.0678830004      0.0744652805
  C8        0.4112311018     -0.3864105783     -0.8308500409
  H32      -0.5892372452     -0.0511779959     -2.7155036103
  C10      -0.1117151010     -1.4869252063      0.0585790388
  N2        1.4935762550      0.2390943274     -0.2085050305
  C9        1.8547419124     -0.2890747350      1.0031248101
  O1        2.7319757970      0.1417439421      1.7193974832
  H43      -0.0800662711     -2.4311060060     -0.4665759979
  C12      -1.5401625422     -1.2486968993      0.5151984956
  C11       0.9497608799     -1.5129098739      1.2298566628
  C19       0.4142759840     -1.5251009984      2.6731899269
  C13      -3.7123736281     -2.1267587595      1.0875858607
  C14      -3.3026572564      0.2213554566      1.2480069716
  C15      -4.1631350637     -0.8548554438      1.3885634451
  C16      -2.0031589337      0.0265320807      0.8100245891
  C17      -2.4077565825     -2.3195551440      0.6521327053
  H49      -4.3729125082     -2.9646222335      1.1829344145
  H50      -3.6417221596      1.2096904784      1.4766719521
 H51      -5.1707996342     -0.7021666679      1.7216189233
 H52      -1.3483785649      0.8654629146      0.6918379720
 H53      -2.0713671004     -3.3084487731      0.4135313486
 H1        1.2552496893     -1.4547308094      3.3524015936
 H2       -0.1307021715     -2.4487293336      2.8721056280
 H3       -0.2552508221     -0.6904497293      2.8577062567
 H4        1.5894393050     -2.3805896512      1.0834423287

 nuclear repulsion energy.......  1453.823275600 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   5   /
-------------------------------------------------


 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.216E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106     99     97     98     98     98     89     92
 grid # 3      224    183    183    194    182    182    188    183
 grid # 4      224    379    380    404    379    379    375    379

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     86     73     82     99     75
 grid # 2      106    106    105     91    105     93    109     80
 grid # 3      224    224    220    186    223    175    225    163
 grid # 4      224    224    218    376    229    353    401    336

 number of gridpoints:
    atom        O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1      111     69     92     80     71     87     87     89
 grid # 2      127     97    106     92     75    100     99    100
 grid # 3      272    211    192    175    142    182    183    182
 grid # 4      476    206    397    360    310    378    375    379

 number of gridpoints:
    atom       C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1       86     85     73     73     73     71     72     71
 grid # 2       97     99    106    106    106    101    103     99
 grid # 3      182    182    224    223    224    213    216    220
 grid # 4      376    376    224    223    224    211    215    221

 number of gridpoints:
    atom        H2     H3     H4  total
 grid # 1       72     71     69   2819
 grid # 2       99     97    100   3481
 grid # 3      219    215    218   7034
 grid # 4      223    213    210  10857
 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                RMS    maximum
      e  d  i  u  i                      energy  density   DIIS
      r  t  s  t  d    total energy      change  change    error

etot   1  N  N  2  U  -815.12907646171            4.6E-04  1.5E-02
etot   2  Y  Y  6  M  -815.13899341516  9.9E-03  1.9E-04  6.1E-03
etot   3  N  Y  2  U  -815.14025250021  1.3E-03  6.6E-05  1.8E-03
etot   4  Y  Y  6  M  -815.14034107144  8.9E-05  1.8E-05  4.8E-04
etot   5  Y  Y  6  M  -815.14036054883  1.9E-05  1.0E-05  1.9E-04
etot   6  Y  Y  6  M  -815.14036035375 -2.0E-07  3.5E-06  8.8E-05
etot   7  Y  N  6  M  -815.14036254175  2.2E-06  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1453.82327560033
  (E)  Total one-electron terms..... -3993.20732217510
  (I)  Total two-electron terms.....  1724.24368403302
  (L)  Electronic energy............ -2268.96363814208  (E+I)
  (N)  Total energy.................  -815.14036254175  (A+L)

SCFE: SCF energy: HF    -815.14036254175 hartrees   iterations:   7


HOMO energy:    -0.29741
LUMO energy:     0.11824

 Orbital energies:
 -20.45193  -15.55227  -11.32106  -11.23618  -11.22268  -11.21488
 -11.20950  -11.19967  -11.18801  -11.18618  -11.18573  -11.18471
 -11.18353  -11.18276  -11.17940  -11.17823  -11.17676  -11.17595
 -11.17265  -11.16784   -1.42174   -1.33337   -1.18045   -1.16245
  -1.11321   -1.08903   -1.03888   -1.02665   -1.01897   -1.00185
  -0.94869   -0.90441   -0.85363   -0.84461   -0.83092   -0.81164
  -0.79132   -0.76094   -0.72109   -0.68591   -0.68087   -0.66883
  -0.65739   -0.64301   -0.63949   -0.62490   -0.61396   -0.60693
  -0.60393   -0.60072   -0.59259   -0.58384   -0.55339   -0.54875
  -0.53104   -0.52410   -0.51633   -0.51262   -0.49901   -0.49501
  -0.49027   -0.48534   -0.45765   -0.42128   -0.39447   -0.34854
  -0.34328   -0.31535   -0.29741    0.11824    0.13359    0.13861
   0.14202    0.20553    0.21993    0.26506    0.27206    0.28096
   0.30644

 end of program scf


 start of program der1a
 end of program der1a
 start of program rwr
recomputing RwR matrix   2    grid:  4
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.610549E-04   1.387182E-04   3.655966E-04
  2    C1     -5.199381E-04  -5.772333E-04  -2.071234E-04
  3    C2      6.420465E-05   1.550665E-03  -1.926293E-03
  4    C3     -8.341138E-04   1.176940E-03  -1.377802E-04
  5    C4      2.158482E-03   7.688971E-04   5.396956E-04
  6    C5     -2.302115E-03   2.219589E-04  -4.008076E-04
  7    C6     -1.381531E-03   5.222113E-05  -1.093454E-03
  8    C7      1.697058E-04  -9.989974E-04  -5.115276E-05
  9    H27     2.042715E-04   7.908634E-05   4.549655E-05
 10    H28     7.177791E-04   3.661620E-04  -8.436291E-06
 11    H30     7.004748E-04  -3.017645E-04   4.950372E-04
 12    C8      6.345711E-04   9.351139E-04  -4.571445E-04
 13    H32     1.091509E-03   1.100508E-04   6.060228E-04
 14    C10    -1.165806E-03  -8.402070E-04   1.480283E-03
 15    N2     -1.760636E-03  -2.803578E-03  -2.284888E-03
 16    C9      2.975561E-03   1.370084E-03   4.080293E-03
 17    O1     -3.790249E-03  -2.331461E-03  -1.241195E-03
 18    H43     8.327076E-04  -4.980762E-04  -8.819169E-04
 19    C12    -1.446996E-03   1.892659E-03  -2.393923E-04
 20    C11     1.635663E-03   1.525338E-03   2.879748E-03
 21    C19    -3.224491E-03  -3.017507E-03  -7.708463E-04
 22    C13     1.780345E-03  -5.958838E-04  -1.011483E-03
 23    C14     2.780770E-03  -3.019732E-04  -5.842073E-04
 24    C15     5.920118E-04  -6.724473E-04  -2.441611E-04
 25    C16    -1.913232E-03   8.562396E-04   1.906450E-03
 26    C17    -3.385241E-03  -7.572077E-05   1.201576E-03
 27    H49     1.628584E-04  -8.520542E-04   1.000642E-05
 28    H50    -3.882901E-04   1.734599E-03   4.116707E-05
 29    H51     5.221705E-04  -4.701179E-05  -7.074078E-05
 30    H52    -3.811876E-05   8.341995E-04  -2.942853E-04
 31    H53     1.828695E-04  -1.436121E-03  -6.569234E-05
 32    H1     -5.242451E-04  -2.195692E-04  -1.475811E-04
 33    H2      3.020365E-03   5.070497E-03  -7.907824E-04
 34    H3      2.791594E-03  -2.796167E-03  -1.630458E-03
 35    H4     -1.362443E-03   1.427401E-03   1.176364E-03
-----------   -------------  -------------  -------------
   total      -8.584754E-04   1.745059E-03   2.879145E-04

 end of program der1b


 start of program geopt   6

 geometry optimization step   6
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
```

```
   in five columns format


  energy change:           1.1930E-04 .  (  5.0000E-05 )
  gradient maximum:        5.8653E-03 .  (  4.5000E-04 )
  gradient rms:            1.3405E-03 .  (  3.0000E-04 )
  step size:   0.07098  trust radius:   0.30000
  displacement maximum:    3.7656E-02 .  (  1.8000E-03 )
  displacement rms:        6.3484E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.5944E-04    geom step:   7.0978E-02    full step:
7.0978E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.4069E-03     y:     1.0945E-03     z:     8.7299E-04

  new geometry:
                              angstroms
  atom             x                  y                  z
  H25       0.8758801078      2.1810458813     -4.0820611168
  C1        1.4635784596      2.1564222691     -3.1845790885
  C2        3.0268805721      2.1164429140     -0.8278258370
  C3        1.1886774012      1.2359059393     -2.1815497531
  C4        2.5112722535      3.0379813915     -3.0023625258
  C5        3.2855453132      3.0184401507     -1.8377482687
  C6        1.9783491101      1.2396186807     -1.0222222330
  C7        0.1926080158      0.1714608660     -2.0290907633
  H27       2.7396605924      3.7533880742     -3.7675426970
  H28       4.0926999356      3.7163185613     -1.7299614418
  H30       3.5964598534      2.0758280604      0.0779377238
  C8        0.4181531302     -0.4008272740     -0.8365471394
  H32      -0.5697214295     -0.0819384196     -2.7313763810
  C10      -0.1060508443     -1.4970424321      0.0585286919
  N2        1.4902062594      0.2347076117     -0.2094677845
  C9        1.8477129459     -0.2845063594      1.0080176946
  O1        2.7128768506      0.1576228506      1.7321840757
  H43      -0.0715355561     -2.4449167088     -0.4647775325
  C12      -1.5343205576     -1.2491689979      0.5142958678
  C11       0.9535668004     -1.5147854130      1.2325984000
  C19       0.4129787609     -1.5373199431      2.6708491312
  C13      -3.7092800186     -2.1154096201      1.0816391871
  C14      -3.2835451798      0.2302566369      1.2554120597
  C15      -4.1496887156     -0.8413224598      1.3893100143
  C16      -1.9862278694      0.0288298775      0.8173554369
  C17      -2.4077915440     -2.3158767158      0.6455873276
  H49      -4.3749200255     -2.9506193107      1.1742918493
  H50      -3.6184940671      1.2215849771      1.4862343425
  H51      -5.1567285219     -0.6832698430      1.7233334500
  H52      -1.3253373824      0.8634058794      0.6993402199
  H53      -2.0767620214     -3.3075959833      0.4031999203
  H1        1.2425144604     -1.4987425721      3.3569941373
  H2       -0.1538337162     -2.4357160437      2.8580820614
  H3       -0.2262147529     -0.6908840898      2.8560682307
  H4        1.5971520379     -2.3813047062      1.0879008745

  nuclear repulsion energy.......  1454.627415472 hartrees
  --------------------------------------------------
 /  end of geometry optimization iteration   6   /
 --------------------------------------------------

  end of program geopt
 start of program onee
 smallest eigenvalue of S:    1.212E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      98      90      92
 grid # 3       224    183     182     194     182     182     187     183
 grid # 4       224    380     381     404     379     379     375     379

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      82     100      75
 grid # 2       106    106     105      91     105      93     109      80
 grid # 3       224    224     220     186     223     175     224     163
 grid # 4       224    224     218     374     229     353     401     335

 number of gridpoints:
    atom         O1    H43     C12     C11     C19     C13     C14     C15
 grid # 1       111     69      90      80      71      87      87      89
 grid # 2       127     98     106      92      74     100      99     100
 grid # 3       272    210     192     175     139     182     183     182
 grid # 4       476    205     397     359     307     379     379     379

 number of gridpoints:
    atom        C16    C17     H49     H50     H51     H52     H53      H1
 grid # 1        86     85      73      73      73      71      72      71
 grid # 2        97     99     106     106     106     101     103      99
 grid # 3       181    182     224     223     224     213     216     220
 grid # 4       376    378     224     223     224     211     215     221

 number of gridpoints:
    atom         H2     H3      H4   total
 grid # 1        72     71      69    2818
 grid # 2        99     98     100    3484
 grid # 3       219    215     218    7026
 grid # 4       218    214     214   10858

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                         energy  density    DIIS
      r  t  s  t  d     total energy        change  change     error
```

```
etot   1  N  N  2  U  -815.13959330036           1.6E-04  3.1E-03
etot   2  Y  Y  6  M  -815.14056922901  9.8E-04  5.7E-05  1.2E-03
etot   3  Y  Y  6  M  -815.14066740204  9.8E-05  1.8E-05  4.0E-04
etot   4  Y  Y  6  M  -815.14067546782  8.1E-06  7.5E-06  1.5E-04
etot   5  Y  Y  6  M  -815.14067519538 -2.7E-07  2.2E-06  4.0E-05
etot   6  N  N  2  U  -815.14065358156 -2.2E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1454.62741547179
   (E)  Total one-electron terms..... -3994.80829153250
   (I)  Total two-electron terms.....  1725.04022247915
   (L)  Electronic energy............ -2269.76806905335  (E+I)
   (N)  Total energy.................  -815.14065358156  (A+L)

 SCFE: SCF energy: HF    -815.14065358156 hartrees   iterations:   6


 HOMO energy:    -0.29733
 LUMO energy:     0.11829

  Orbital energies:
  -20.45222  -15.55244  -11.32126  -11.23626  -11.22260  -11.21524
  -11.20913  -11.19984  -11.18800  -11.18615  -11.18569  -11.18482
  -11.18344  -11.18292  -11.17952  -11.17813  -11.17669  -11.17564
  -11.17258  -11.16453   -1.42167   -1.33358   -1.18064   -1.16272
   -1.11345   -1.08883   -1.03878   -1.02713   -1.01954   -1.00186
   -0.94932   -0.90490   -0.85391   -0.84455   -0.83088   -0.81151
   -0.79133   -0.76090   -0.72121   -0.68602   -0.68094   -0.66868
   -0.65731   -0.64317   -0.63929   -0.62512   -0.61357   -0.60726
   -0.60421   -0.60108   -0.59221   -0.58399   -0.55365   -0.54912
   -0.53281   -0.52469   -0.51664   -0.51241   -0.49895   -0.49498
   -0.49004   -0.48551   -0.45774   -0.42159   -0.39431   -0.34901
   -0.34311   -0.31540   -0.29733    0.11829    0.13335    0.13906
    0.14200    0.20568    0.22007    0.26468    0.27174    0.28093
    0.30705

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label          x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     6.242294E-04  -2.393983E-06   7.371625E-04
   2    C1     -1.262006E-04   5.122522E-05  -4.342059E-04
   3    C2      5.197442E-04  -1.597181E-04   1.352066E-03
   4    C3     -2.746153E-04  -2.310974E-04   6.312942E-04
   5    C4      2.179673E-04   8.164083E-04  -9.618337E-04
   6    C5      4.647529E-04   8.556599E-04  -5.924191E-04
```

```
    7     C6      -9.372527E-05   1.458043E-03  -1.162963E-04
    8     C7      -5.344341E-04  -9.139478E-04   1.286034E-03
    9     H27     -1.429755E-04  -1.426416E-04   1.610712E-04
   10     H28     -6.251118E-04  -3.575221E-04  -1.323583E-04
   11     H30     -5.018717E-04   4.804563E-05  -6.634466E-04
   12     C8       2.337373E-04   8.588311E-04  -1.550361E-03
   13     H32      9.607872E-04   1.698987E-05   6.460219E-04
   14     C10     -8.759897E-04  -1.096061E-03   3.574011E-04
   15     N2      -4.704903E-04  -1.557480E-03  -2.563149E-03
   16     C9       2.920720E-03   1.310811E-03   4.743945E-03
   17     O1      -3.702990E-03  -2.482970E-03  -2.012557E-03
   18     H43      1.488482E-05   7.973514E-04   5.317373E-04
   19     C12      3.652128E-05   1.136742E-03  -4.182061E-04
   20     C11      1.978979E-03  -1.562089E-03   1.381472E-03
   21     C19      3.326708E-04   5.608830E-04  -4.015796E-03
   22     C13      3.986355E-04  -1.070369E-03  -3.516975E-04
   23     C14      2.070954E-03   1.233866E-03  -4.510410E-04
   24     C15     -1.060880E-03  -1.097222E-03   2.195759E-04
   25     C16     -8.909418E-04   1.691476E-04   6.490318E-04
   26     C17     -1.984796E-03  -6.758543E-04   7.177752E-04
   27     H49      2.160970E-04  -9.038756E-05  -2.687023E-05
   28     H50      1.332503E-04   3.107469E-04  -3.869171E-05
   29     H51      7.917418E-04  -1.557635E-04  -1.963101E-04
   30     H52     -1.398933E-04   6.125469E-04  -1.309709E-05
   31     H53     -2.128029E-04  -7.064469E-05   1.123810E-04
   32     H1       3.603672E-03   4.149605E-04   1.933533E-03
   33     H2      -1.278009E-03  -2.337257E-03  -3.774310E-04
   34     H3      -1.697816E-03   2.112647E-03   3.237520E-04
   35     H4      -1.256837E-03   2.405223E-03   6.290650E-04
  -----------   -------------  -------------  -------------
     total      -3.510350E-04   1.166708E-03   1.497551E-03

   end of program der1b


   start of program geopt   7

   geometry optimization step   7
   reading input hessian of dimension   105
    in five columns format
   reading input hessian of dimension   105
    in five columns format


   energy change:          -2.9104E-04 .  (  5.0000E-05 )
   gradient maximum:        4.8069E-03 .  (  4.5000E-04 )
   gradient rms:            1.0251E-03 .  (  3.0000E-04 )
   step size:   0.08272  trust radius:   0.30000
   displacement maximum:    3.8986E-02 .  (  1.8000E-03 )
   displacement rms:        7.3991E-03 .  (  1.2000E-03 )
   predicted energy change:    -2.0957E-04    geom step:   8.2724E-02    full step:
 8.2724E-02
   molecular structure not yet converged...

   center of mass moved by:
      x:     2.5992E-03     y:    -6.3545E-03     z:     2.0569E-04

   new geometry:
                              angstroms
   atom            x                 y                 z
   H25       0.8505922988      2.2045278124     -4.0596232903
   C1        1.4456713616      2.1720468451     -3.1692545485
 C2        3.0326678558      2.1097826594     -0.8332301322
 C3        1.1813116718      1.2419376220     -2.1720321579
 C4        2.4936600680      3.0540457729     -2.9921443841
 C5        3.2776955272      3.0237431690     -1.8358581421
 C6        1.9831456539      1.2334743269     -1.0229987478
 C7        0.1920576094      0.1720808827     -2.0191820324
 H27       2.7132354621      3.7763066809     -3.7533743955
 H28       4.0858831213      3.7198325681     -1.7308827271
 H30       3.6138636728      2.0576359560      0.0631132606
 C8        0.4231391334     -0.4058995255     -0.8330230241
 H32      -0.5719313106     -0.0771491419     -2.7168893168
 C10      -0.1070541692     -1.4988912359      0.0639918355
 N2        1.5037879080      0.2179112408     -0.2150310643
 C9        1.8550033854     -0.3005237716      1.0072489402
 O1        2.7241628377      0.1221583596      1.7284848187
 H43      -0.0724105437     -2.4468814361     -0.4582906571
 C12      -1.5366580174     -1.2441407660      0.5148502332
 C11       0.9529845820     -1.5170989829      1.2374832290
 C19       0.4137363982     -1.5284776727      2.6698391078
 C13      -3.7076521185     -2.1100780488      1.0832006226
 C14      -3.2825023344      0.2417265750      1.2316805517
 C15      -4.1460953769     -0.8317704564      1.3737885662
 C16      -1.9873092034      0.0375211650      0.8027524244
 C17      -2.4084146497     -2.3129592690      0.6565258956
 H49      -4.3718857372     -2.9447967915      1.1835490643
 H50      -3.6214714440      1.2361109258      1.4463314356
 H51      -5.1534356366     -0.6701267553      1.7015902218
 H52      -1.3283902654      0.8722717935      0.6734811327
 H53      -2.0740299602     -3.3070464157      0.4270952388
 H1        1.2503570059     -1.4511001810      3.3580479495
 H2       -0.1301763773     -2.4420300623      2.8693736420
 H3       -0.2517743657     -0.6932639236      2.8356091524
 H4        1.5864179988     -2.3851728718      1.1020158271

 nuclear repulsion energy.......  1455.488475538 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   7   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.206E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     97     98     98     98     91     92
 grid # 3      224    183    182    194    182    182    187    182
 grid # 4      224    379    379    406    379    379    371    377

 number of gridpoints:
     atom        H27     H28     H30      C8     H32     C10      N2      C9
  grid # 1        73      73      73      86      73      82      99      75
  grid # 2       106     106     105      91     105      93     109      80
  grid # 3       224     224     220     186     223     175     225     163
  grid # 4       224     224     219     372     228     353     402     329

  number of gridpoints:
     atom         O1     H43     C12     C11     C19     C13     C14     C15
  grid # 1       111      69      92      81      71      87      87      88
  grid # 2       123      98     106      93      75     100      99     100
  grid # 3       272     211     192     174     142     181     182     183
  grid # 4       475     204     396     359     309     379     379     379

  number of gridpoints:
     atom        C16     C17     H49     H50     H51     H52     H53      H1
  grid # 1        86      84      73      73      73      71      72      71
  grid # 2        96      99     106     106     106     101     103      99
  grid # 3       181     181     224     223     224     214     216     220
  grid # 4       377     378     224     223     224     211     215     221

  number of gridpoints:
     atom         H2      H3      H4   total
  grid # 1        72      71      69    2818
  grid # 2        98      97     100    3480
  grid # 3       219     215     218    7028
  grid # 4       219     212     210   10839

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

      i  u  d  i  g
      t  p  i  c  r                                      RMS    maximum
      e  d  i  u  i                            energy  density   DIIS
      r  t  s  t  d     total energy           change  change    error

etot   1  N  N  2  U  -815.13916126058            1.9E-04  3.5E-03
etot   2  Y  Y  6  M  -815.14055849858  1.4E-03  7.1E-05  1.4E-03
etot   3  Y  Y  6  M  -815.14070071593  1.4E-04  2.3E-05  4.4E-04
etot   4  Y  Y  6  M  -815.14071839733  1.8E-05  1.0E-05  1.8E-04
etot   5  Y  Y  6  M  -815.14071512292 -3.3E-06  4.0E-06  7.8E-05
etot   6  N  N  2  U  -815.14066653255 -4.9E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1455.48847553819
   (E)  Total one-electron terms..... -3996.51292383122
   (I)  Total two-electron terms.....  1725.88378176047
   (L)  Electronic energy............ -2270.62914207075  (E+I)
   (N)  Total energy.................  -815.14066653255  (A+L)

 SCFE: SCF energy: HF    -815.14066653255 hartrees   iterations:   6


 HOMO energy:    -0.29712
```

```
LUMO energy:     0.11910

 Orbital energies:
 -20.45264  -15.55208  -11.32073  -11.23544  -11.22249  -11.21474
 -11.20692  -11.19984  -11.18760  -11.18575  -11.18520  -11.18449
 -11.18315  -11.18256  -11.17923  -11.17675  -11.17667  -11.17547
 -11.17250  -11.16528   -1.42537   -1.33454   -1.18117   -1.16325
  -1.11405   -1.08873   -1.03859   -1.02891   -1.02008   -1.00157
  -0.94903   -0.90452   -0.85369   -0.84411   -0.83133   -0.81158
  -0.79193   -0.76103   -0.72164   -0.68697   -0.68179   -0.66881
  -0.65733   -0.64411   -0.63942   -0.62539   -0.61377   -0.60831
  -0.60455   -0.60260   -0.59186   -0.58371   -0.55400   -0.54953
  -0.53268   -0.52422   -0.51695   -0.51280   -0.49904   -0.49493
  -0.48968   -0.48516   -0.45857   -0.42194   -0.39418   -0.35025
  -0.34246   -0.31590   -0.29712    0.11910    0.13360    0.13909
   0.14243    0.20625    0.22042    0.26472    0.27176    0.28209
   0.30746

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -2.362318E-04  -2.132386E-04  -2.806466E-04
  2    C1     -1.226583E-04   6.176358E-05  -4.625988E-04
  3    C2      1.319865E-04  -3.610784E-04   1.173014E-03
  4    C3      4.983991E-04  -1.047995E-03  -2.433032E-04
  5    C4     -7.689024E-04   2.394108E-04  -6.268629E-04
  6    C5      1.551621E-03   5.973486E-04  -4.575321E-05
  7    C6      5.129845E-04   4.994763E-04   1.034409E-03
  8    C7     -2.081709E-03   8.115142E-04  -1.208331E-03
  9    H27    -1.903779E-04  -1.686588E-04   1.747336E-04
 10    H28    -2.463294E-04   4.148760E-06   1.937111E-04
 11    H30     1.773401E-04   4.691650E-04   1.520724E-04
 12    C8      1.901328E-04  -1.037259E-03  -6.542565E-04
 13    H32    -9.659943E-04  -3.494470E-04  -6.609230E-04
 14    C10    -3.246636E-04  -6.655255E-04  -4.124526E-04
 15    N2      7.472318E-04   1.582363E-03   5.346544E-04
 16    C9     -1.398342E-03  -1.744832E-03  -1.945884E-03
 17    O1      3.130797E-03   2.997075E-03   3.172939E-03
 18    H43    -3.853396E-04   4.363201E-04   4.964129E-04
 19    C12     1.750490E-03  -8.030674E-04  -6.562082E-04
 20    C11    -1.301618E-03  -6.448383E-04  -7.233143E-04
 21    C19     1.015582E-03   1.969058E-03   1.882940E-03
 22    C13    -1.658435E-03   1.578417E-04   8.769960E-04
 23    C14    -1.956631E-03   1.005860E-03   6.390548E-04
 24    C15    -2.571830E-03   1.569391E-04   7.471176E-04
 25    C16     2.187562E-03  -5.123739E-04  -1.182526E-03
```

```
  26    C17     2.391953E-03  -2.246457E-04  -8.740877E-04
  27    H49    -4.031671E-04  -4.805240E-05   1.134502E-04
  28    H50     3.667200E-05  -4.104785E-04   1.826655E-04
  29    H51    -1.358038E-04  -1.743317E-06   7.698322E-05
  30    H52     1.126712E-04   1.476414E-04   9.892803E-05
  31    H53    -3.314863E-05   3.327849E-04   3.045347E-05
  32    H1     -1.884112E-03  -4.456033E-04  -1.405665E-03
  33    H2      4.131727E-05  -1.523113E-04   2.862021E-04
  34    H3      1.822935E-04  -3.634442E-04   8.143398E-04
  35    H4      1.181780E-03  -8.754076E-04  -4.985469E-04
 -----------   -------------  -------------  -------------
    total      -8.244798E-04   1.398710E-03   7.997182E-04

  end of program der1b


  start of program geopt   8

  geometry optimization step  8
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:           -1.2951E-05 *  (  5.0000E-05 )
  gradient maximum:         5.1668E-03 .  (  4.5000E-04 )
  gradient rms:             1.0215E-03 .  (  3.0000E-04 )
  step size:   0.22897  trust radius:   0.30000
  displacement maximum:     9.3501E-02 .  (  1.8000E-03 )
  displacement rms:         2.0480E-02 .  (  1.2000E-03 )
  predicted energy change:    -3.3182E-04    geom step:   2.2897E-01    full step:
2.2897E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.4102E-02     y:     1.5813E-02     z:     3.8822E-03

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.9071867646      2.1019281546     -4.1180847885
  C1        1.4681925676      2.1093005143     -3.2047209945
  C2        2.9677440872      2.1497885388     -0.8007496107
  C3        1.2000215554      1.1869375532     -2.1999852224
  C4        2.4741425867      3.0359422954     -3.0013326134
  C5        3.2165828604      3.0555978341     -1.8108267913
  C6        1.9578305888      1.2331167688     -1.0206174051
  C7        0.2395856723      0.0827610727     -2.0660086857
  H27       2.6932173460      3.7518777665     -3.7641986354
  H28       3.9907811377      3.7840016745     -1.6838352421
  H30       3.5124673976      2.1349949824      0.1194662453
  C8        0.4506042369     -0.4623071633     -0.8631077281
  H32      -0.4919333774     -0.2060733984     -2.7851918696
  C10      -0.0889804845     -1.5365949291      0.0554663440
  N2        1.4866559914      0.2108749646     -0.2185659597
  C9        1.8118980138     -0.2567260162      1.0349557281
  O1        2.6188173285      0.2407146403      1.7984113410
  H43      -0.0692233008     -2.4931127314     -0.4394347340
  C12      -1.5162518513     -1.2459479061      0.5042901392
 C11       0.9751621867     -1.5314828452      1.2288084415
 C19       0.4387470415     -1.6285861162      2.6669849118
 C13      -3.7135069037     -2.0529457707      1.0669287797
 C14      -3.2099441388      0.2819792404      1.2571134672
 C15      -4.1082087682     -0.7671132162      1.3852978872
 C16      -1.9252803112      0.0442417635      0.8163805187
 C17      -2.4230137789     -2.2879141950      0.6301925504
 H49      -4.4019836081     -2.8660892274      1.1533353126
 H50      -3.5140532514      1.2807494266      1.4931292113
 H51      -5.1048610983     -0.5784016333      1.7228735702
 H52      -1.2444287045      0.8595506966      0.6967621544
 H53      -2.1236926819     -3.2864804061      0.3802968513
 H1        1.2793417824     -1.5469747574      3.3471422402
 H2       -0.0611089163     -2.5799380301      2.8263667835
 H3       -0.2643804927     -0.8294043816      2.8807517166
 H4        1.6612462396     -2.3554408593      1.0580410281

 nuclear repulsion energy.......  1456.043748144 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration   8   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.228E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      84      85
 grid # 2       106     100      97      98      99      99      90      92
 grid # 3       224     183     184     195     182     182     187     182
 grid # 4       224     379     380     408     377     379     373     378

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      82      99      76
 grid # 2       106     106     105      92     106      93     109      80
 grid # 3       224     224     220     187     223     175     224     164
 grid # 4       224     224     217     373     229     353     400     335

 number of gridpoints:
    atom         O1     H43     C12     C11     C19     C13     C14     C15
 grid # 1       111      69      92      81      71      87      86      88
 grid # 2       127      98     106      93      76     100      98     100
 grid # 3       272     210     192     174     150     181     182     182
 grid # 4       476     205     397     359     307     375     378     376

 number of gridpoints:
    atom        C16     C17     H49     H50     H51     H52     H53      H1
 grid # 1        86      84      73      73      73      71      72      71
 grid # 2        96      98     106     106     106     100     103      99
```

```
  grid # 3      181    182    224    223    224    215    216    220
  grid # 4      374    378    224    223    224    211    215    221

  number of gridpoints:
     atom         H2     H3     H4  total
  grid # 1        72     71     69   2817
  grid # 2        99     97    100   3486
  grid # 3       219    215    218   7040
  grid # 4       219    212    211  10838

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                 RMS    maximum
       e  d  i  u  i                       energy  density   DIIS
       r  t  s  t  d     total energy      change   change    error

etot   1  N  N  2  U  -815.11828010280             6.2E-04  1.8E-02
etot   2  Y  Y  6  M  -815.13771483113  1.9E-02  2.6E-04  7.4E-03
etot   3  N  Y  2  U  -815.14019194804  2.5E-03  8.7E-05  2.3E-03
etot   4  Y  Y  6  M  -815.14034964728  1.6E-04  2.2E-05  5.6E-04
etot   5  Y  Y  6  M  -815.14037543149  2.6E-05  1.3E-05  2.1E-04
etot   6  Y  Y  6  M  -815.14037485600 -5.8E-07  4.3E-06  7.8E-05
etot   7  Y  N  6  M  -815.14037782599  3.0E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1456.04374814385
   (E)  Total one-electron terms..... -3997.66001909393
   (I)  Total two-electron terms.....  1726.47589312410
   (L)  Electronic energy........... -2271.18412596984  (E+I)
   (N)  Total energy.................  -815.14037782599  (A+L)

 SCFE: SCF energy: HF    -815.14037782599 hartrees   iterations:   7


 HOMO energy:    -0.29796
 LUMO energy:     0.11802

  Orbital energies:
  -20.45387  -15.55279  -11.32287  -11.23593  -11.22266  -11.21536
  -11.20904  -11.20011  -11.18829  -11.18547  -11.18473  -11.18413
  -11.18287  -11.18216  -11.17983  -11.17787  -11.17711  -11.17635
  -11.17298  -11.16655   -1.41838   -1.33342   -1.18046   -1.16208
   -1.11243   -1.08876   -1.03772   -1.02894   -1.01841   -1.00180
   -0.94819   -0.90470   -0.85195   -0.84400   -0.83121   -0.81207
   -0.79180   -0.76026   -0.72219   -0.68606   -0.68086   -0.66788
   -0.65636   -0.64267   -0.64010   -0.62475   -0.61327   -0.60713
   -0.60433   -0.60264   -0.59228   -0.58293   -0.55121   -0.54925
   -0.53181   -0.52421   -0.51694   -0.51239   -0.49920   -0.49460
   -0.48878   -0.48497   -0.45796   -0.42201   -0.39435   -0.35013
   -0.34226   -0.31506   -0.29796    0.11802    0.13231    0.14018
    0.14269    0.20385    0.22135    0.26578    0.27234    0.28138
   0.30586

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.841171E-04   9.685182E-05  -3.961196E-05
  2    C1      8.758269E-04   4.764937E-04   9.461125E-04
  3    C2     -1.555725E-03  -3.722300E-05  -1.735444E-03
  4    C3      6.713278E-04   5.351658E-04  -1.776705E-03
  5    C4      1.678627E-04  -2.234414E-03   4.000651E-03
  6    C5     -1.708607E-03  -4.255747E-04  -2.626105E-03
  7    C6     -1.310706E-03  -1.488211E-03  -9.069032E-04
  8    C7      7.193123E-04   3.188106E-03  -2.312803E-03
  9    H27     5.993744E-04   1.533616E-03  -1.346753E-03
 10    H28     3.377900E-04   8.279419E-04  -4.638826E-04
 11    H30    -1.123245E-04   2.545567E-04   1.712792E-04
 12    C8     -2.875061E-04  -3.545378E-03   3.912930E-03
 13    H32     3.391624E-05   3.090086E-04   7.884368E-05
 14    C10     7.436448E-04   3.714275E-03   1.235824E-03
 15    N2      3.938310E-03   3.604811E-03   6.490407E-03
 16    C9      4.545228E-03   2.371708E-03   5.075382E-03
 17    O1     -1.001724E-02  -5.506987E-03  -1.056373E-02
 18    H43    -3.554645E-05  -2.929869E-03  -1.205119E-03
 19    C12     2.742592E-03  -1.448209E-03   4.510851E-04
 20    C11    -3.117888E-03   8.051949E-04   4.111657E-03
 21    C19    -1.088031E-04   6.881283E-04  -1.290269E-03
 22    C13    -5.126589E-04   2.652491E-03   6.583254E-04
 23    C14    -2.645677E-03  -1.433389E-03   4.921983E-04
 24    C15    -3.484725E-05   9.276068E-04   6.696387E-05
 25    C16     1.384955E-03  -1.650478E-03  -1.314249E-03
 26    C17     3.454314E-03   3.789442E-04  -1.186983E-03
 27    H49    -1.611915E-03  -1.452210E-03   3.436331E-04
 28    H50    -5.201623E-04   8.740562E-04   3.739374E-04
 29    H51    -1.970359E-03   2.383120E-04   6.551981E-04
 30    H52     1.622118E-03   1.451065E-03   1.479797E-04
 31    H53     5.552732E-04  -8.158356E-04  -7.188324E-05
 32    H1     -1.640405E-03  -2.747552E-04   1.731209E-04
 33    H2      1.348510E-03   2.708392E-03  -1.223504E-04
 34    H3      2.740504E-03  -3.013180E-03  -1.148156E-03
 35    H4     -2.612877E-04  -6.829678E-05  -2.063461E-04
-----------   -------------  -------------  -------------
   total      -7.866891E-04   1.312713E-03   1.068237E-03

 end of program der1b
```

```
  start of program geopt   9

  geometry optimization step  9
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:           2.8871E-04 .  (  5.0000E-05 )
  gradient maximum:        1.5564E-02 .  (  4.5000E-04 )
  gradient rms:            2.0457E-03 .  (  3.0000E-04 )
  step size:   0.17911  trust radius:   0.30000
  displacement maximum:    7.6122E-02 .  (  1.8000E-03 )
  displacement rms:        1.6020E-02 .  (  1.2000E-03 )
  predicted energy change:    -6.9150E-04    geom step:   1.7911E-01    full step:
1.7911E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.1515E-02     y:     1.3339E-02     z:     6.4557E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.9854086380      2.0207486693     -4.1692767745
  C1        1.5151720192      2.0609155825     -3.2371774704
  C2        2.9236455825      2.1887108181     -0.7858762307
  C3        1.2231581786      1.1636294646     -2.2167251284
  C4        2.4981481077      3.0035528328     -3.0276774059
  C5        3.2002134183      3.0644852326     -1.8188159854
  C6        1.9365560815      1.2524364386     -1.0101221723
  C7        0.2659330805      0.0609801861     -2.0851292275
  H27       2.7339598606      3.7050942661     -3.8054733646
  H28       3.9566863749      3.8120581167     -1.6898498501
  H30       3.4308488302      2.2169615239      0.1547584782
  C8        0.4550894242     -0.4658475709     -0.8636725472
  H32      -0.4442594203     -0.2485766469     -2.8193024991
  C10      -0.0810926187     -1.5423609805      0.0480174892
  N2        1.4531709198      0.2481760739     -0.1937840340
  C9        1.7738660515     -0.2366468779      1.0499993693
  O1        2.5512325248      0.2820494795      1.8200814932
  H43      -0.0707903298     -2.5044992626     -0.4490730120
  C12      -1.4984835199     -1.2514213482      0.5043416953
  C11       0.9786200470     -1.5398631325      1.2176761040
  C19       0.4559551003     -1.6915920556      2.6502581684
  C13      -3.7135694043     -2.0303464070      1.0657639041
  C14      -3.1873948871      0.2854252716      1.2853809202
  C15      -4.1015690701     -0.7481161438      1.4037065514
  C16      -1.8981584486      0.0364994064      0.8340384995
  C17      -2.4185840825     -2.2781975495      0.6172021624
  H49      -4.4150545570     -2.8373401549      1.1436899333
  H50      -3.4754318005      1.2833070075      1.5436111130
  H51      -5.0994948026     -0.5541903682      1.7490896749
  H52      -1.2019502153      0.8451372957      0.7349102883
  H53      -2.1332280312     -3.2772937631      0.3525224729
  H1        1.2897563415     -1.6269682922      3.3285480303
  H2       -0.0265174297     -2.6532600573      2.7838484535
  H3       -0.2546075259     -0.9227759725      2.9012273069
  H4        1.6954156508     -2.3351017121      1.0100509046
```

```
 nuclear repulsion energy.......  1457.325387747 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration   9   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.219E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     84     85
 grid # 2       106     99     98     98     98     98     89     92
 grid # 3       224    183    183    194    182    182    189    183
 grid # 4       224    379    381    403    379    380    375    379

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     81     99     75
 grid # 2       106    106    105     92    106     93    109     81
 grid # 3       224    224    220    189    223    175    222    163
 grid # 4       224    224    219    378    229    349    400    329

 number of gridpoints:
    atom         O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1       111     69     90     80     71     87     86     89
 grid # 2       127     98    105     92     75     99     99    100
 grid # 3       272    212    192    176    148    182    183    181
 grid # 4       476    206    399    361    307    378    378    379

 number of gridpoints:
    atom        C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1        86     86     73     73     73     71     72     71
 grid # 2        98     98    106    106    106    100    103     99
 grid # 3       182    181    224    223    224    215    216    220
 grid # 4       378    376    224    223    224    211    215    221

 number of gridpoints:
    atom         H2     H3     H4  total
 grid # 1        72     71     70   2816
 grid # 2        99     97    100   3483
 grid # 3       219    215    219   7044
 grid # 4       220    212    215  10855

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
```

```
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                    RMS    maximum
       e  d  i  u  i                         energy  density    DIIS
       r  t  s  t  d     total energy        change  change     error

etot   1  N  N  2  U  -815.13170234446            4.3E-04  1.4E-02
etot   2  Y  Y  6  M  -815.13972400376  8.0E-03  1.7E-04  5.6E-03
etot   3  N  Y  2  U  -815.14055391488  8.3E-04  6.2E-05  1.7E-03
etot   4  Y  Y  6  M  -815.14065382104  1.0E-04  2.2E-05  5.1E-04
etot   5  Y  Y  6  M  -815.14066553823  1.2E-05  9.7E-06  1.9E-04
etot   6  Y  Y  6  M  -815.14066682514  1.3E-06  5.1E-06  1.0E-04
etot   7  Y  Y  6  M  -815.14066931502  2.5E-06  2.0E-06  5.2E-05
etot   8  N  N  2  U  -815.14065149339 -1.8E-05  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1457.32538774698
   (E)  Total one-electron terms..... -4000.21518124494
   (I)  Total two-electron terms.....  1727.74914200456
   (L)  Electronic energy............ -2272.46603924038  (E+I)
   (N)  Total energy.................  -815.14065149339  (A+L)

 SCFE: SCF energy: HF    -815.14065149339 hartrees   iterations:   8


 HOMO energy:    -0.29678
 LUMO energy:     0.11710

  Orbital energies:
  -20.45302  -15.55217  -11.32145  -11.23636  -11.22307  -11.21522
  -11.20959  -11.19913  -11.18830  -11.18608  -11.18561  -11.18463
  -11.18318  -11.18266  -11.17922  -11.17874  -11.17703  -11.17612
  -11.17250  -11.16454   -1.42256   -1.33294   -1.18041   -1.16223
   -1.11418   -1.08807   -1.03941   -1.02476   -1.02022   -1.00141
   -0.94910   -0.90554   -0.85298   -0.84473   -0.83010   -0.81131
   -0.79097   -0.76025   -0.72170   -0.68612   -0.68109   -0.66795
   -0.65755   -0.64255   -0.64017   -0.62482   -0.61415   -0.60737
   -0.60409   -0.59866   -0.59320   -0.58333   -0.55203   -0.55032
   -0.53258   -0.52488   -0.51641   -0.51316   -0.49846   -0.49492
   -0.48986   -0.48557   -0.45809   -0.42187   -0.39454   -0.34716
   -0.34355   -0.31570   -0.29678    0.11710    0.13247    0.14071
    0.14346    0.20489    0.22121    0.26515    0.27149    0.28017
    0.30596

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr
 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----  -------------  -------------  -------------
  1    H25     2.085293E-04  -1.046698E-05   7.370282E-04
  2    C1     -3.011216E-03  -2.369182E-03  -4.153569E-04
  3    C2      8.820340E-04   2.707386E-03  -2.934834E-03
  4    C3     -5.640292E-04   2.073818E-03   4.076406E-04
  5    C4      3.319910E-03   2.099172E-03  -1.759108E-04
  6    C5     -1.082347E-03   6.303644E-04   1.609525E-03
  7    C6     -1.755569E-03  -7.349231E-04  -1.330661E-03
  8    C7      2.102999E-03  -2.641627E-03   2.888564E-03
  9    H27    -7.476275E-05  -9.221204E-04   1.134848E-03
 10    H28     3.225140E-04  -1.070248E-04   1.316972E-04
 11    H30     5.809125E-04  -7.097146E-05   1.317981E-04
 12    C8     -1.402956E-03   3.076145E-03  -3.032829E-03
 13    H32     1.266553E-03   6.751857E-05   8.243169E-04
 14    C10     4.795093E-04  -2.336623E-03  -5.043974E-04
 15    N2     -2.121528E-03  -4.785538E-03  -3.802862E-03
 16    C9      2.080575E-03   4.491790E-03   3.688794E-03
 17    O1     -2.288802E-03  -3.556847E-03  -1.184714E-03
 18    H43     8.674013E-04   1.161676E-03   1.489318E-04
 19    C12    -2.602619E-03   2.614437E-03   1.011454E-03
 20    C11     1.663462E-03   2.314590E-04   8.355147E-04
 21    C19    -4.665851E-04  -4.903428E-03  -2.631098E-03
 22    C13     2.992048E-03  -2.832475E-03  -1.995211E-03
 23    C14     5.820262E-03   5.008609E-04  -1.460642E-03
 24    C15     1.034263E-03  -9.168821E-04  -3.721609E-04
 25    C16    -4.339708E-03   2.932509E-03   3.081072E-03
 26    C17    -5.979479E-03  -9.943937E-04   2.031374E-03
 27    H49     7.859148E-04  -6.150844E-04  -2.153347E-04
 28    H50     2.050302E-04   1.461473E-03  -2.331327E-04
 29    H51     1.605449E-03  -3.396873E-04  -5.372033E-04
 30    H52    -7.557658E-04   6.483084E-04   4.919089E-05
 31    H53    -3.254942E-04  -9.582932E-04   1.928005E-04
 32    H1      3.237668E-03   6.769430E-04   3.026972E-03
 33    H2      3.835886E-04   6.817858E-04  -5.918747E-04
 34    H3     -1.339432E-03   2.559805E-03  -9.076618E-04
 35    H4     -2.454481E-03   1.601868E-03   1.484388E-03
-----------  -------------  -------------  -------------
   total      -7.261503E-04   1.121753E-03   1.090027E-03

 end of program der1b


 start of program geopt  10

 geometry optimization step 10
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format


 energy change:           -2.7367E-04 .  (   5.0000E-05 )
 gradient maximum:         6.9580E-03 .  (   4.5000E-04 )
 gradient rms:             1.7238E-03 .  (   3.0000E-04 )
 step size:   0.09722  trust radius:   0.30000
```

```
  displacement maximum:     5.0420E-02 .  (  1.8000E-03 )
  displacement rms:         8.6955E-03 .  (  1.2000E-03 )
  predicted energy change:    -4.5108E-04    geom step:   9.7219E-02    full step:
9.7219E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     5.6825E-03     y:    -8.5801E-03     z:    -3.0798E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.9418882259      2.0515174508     -4.1466436424
  C1        1.4838762869      2.0796167120     -3.2211756076
  C2        2.9306495962      2.1794791167     -0.7919017598
  C3        1.2080719958      1.1704109103     -2.2092650003
  C4        2.4733901891      3.0218945442     -3.0105940904
  C5        3.1906945249      3.0717670148     -1.8098959557
  C6        1.9395994139      1.2426854728     -1.0140914895
  C7        0.2607966831      0.0588160449     -2.0779561407
  H27       2.6994624482      3.7309026429     -3.7820749470
  H28       3.9523510333      3.8151413536     -1.6804581957
  H30       3.4561532547      2.1910501104      0.1409968892
  C8        0.4536078125     -0.4699521114     -0.8607095141
  H32      -0.4537492025     -0.2476595311     -2.8078788528
  C10      -0.0821932964     -1.5441637339      0.0556003134
  N2        1.4669159451      0.2289660725     -0.2017015945
  C9        1.7921377034     -0.2531600382      1.0415338362
  O1        2.5935326481      0.2403972651      1.7975048846
  H43      -0.0688336765     -2.5054053154     -0.4406717331
  C12      -1.5018544401     -1.2470122599      0.5121435280
  C11       0.9769453070     -1.5406864087      1.2267697412
  C19       0.4538851355     -1.6691831844      2.6609047208
  C13      -3.7136705863     -2.0280898465      1.0550098428
  C14      -3.1858657818      0.2969250424      1.2700616100
  C15      -4.0984391591     -0.7399564252      1.3815848334
  C16      -1.8982505198      0.0460682360      0.8349234456
  C17      -2.4201493500     -2.2782854918      0.6231584555
  H49      -4.4151233188     -2.8350927160      1.1309668726
  H50      -3.4784491631      1.2985893245      1.5156798931
  H51      -5.0984542341     -0.5430996142      1.7136443264
  H52      -1.2020485365      0.8542114455      0.7337192645
  H53      -2.1310966828     -3.2797164465      0.3671755442
  H1        1.2840363883     -1.5766571704      3.3490161580
  H2       -0.0229116356     -2.6288907786      2.8118081594
  H3       -0.2644384576     -0.8949889931      2.8813322842
  H4        1.6749373834     -2.3517552245      1.0352935905

  nuclear repulsion energy.......  1457.637666912 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  10   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.217E-03
  number of canonical orbitals.....          210
  end of program onee
  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom       H25     C1     C2     C3     C4     C5     C6     C7
  grid # 1       73     89     87     90     87     87     85     85
  grid # 2      106    100     97     98     98     99     90     92
  grid # 3      224    183    183    194    182    182    187    183
  grid # 4      224    380    382    404    379    379    374    379

  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     86     73     82     99     76
  grid # 2      106    106    105     92    106     93    109     81
  grid # 3      224    224    220    189    223    175    223    163
  grid # 4      224    224    219    375    229    353    400    330

  number of gridpoints:
     atom        O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1      111     69     90     80     71     87     87     89
  grid # 2      123     98    105     91     75    100     99    100
  grid # 3      272    210    192    176    143    182    182    182
  grid # 4      476    206    399    361    302    379    379    379

  number of gridpoints:
     atom       C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1       86     85     73     73     73     71     72     71
  grid # 2       97     99    106    106    106    100    103     99
  grid # 3      181    182    224    223    224    215    216    220
  grid # 4      376    378    224    223    224    211    215    221

  number of gridpoints:
     atom        H2     H3     H4  total
  grid # 1       72     71     69   2818
  grid # 2       99     97    100   3481
  grid # 3      219    214    218   7034
  grid # 4      220    212    210  10850

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:   4
 recomputing RwR matrix  15    grid:   4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  2  U  -815.13860408996           2.2E-04  6.3E-03
etot   2  Y  Y  6  M  -815.14073347678  2.1E-03  8.7E-05  1.9E-03
etot   3  Y  Y  6  M  -815.14097323414  2.4E-04  2.8E-05  5.7E-04
etot   4  N  Y  2  U  -815.14102486623  5.2E-05  1.1E-05  2.1E-04
etot   5  Y  Y  6  M  -815.14102676651  1.9E-06  5.3E-06  8.8E-05
etot   6  Y  Y  6  M  -815.14102794136  1.2E-06  2.4E-06  4.5E-05
etot   7  Y  N  6  M  -815.14102835379  4.1E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1457.63766691214
   (E)  Total one-electron terms..... -4000.83596030380
   (I)  Total two-electron terms.....  1728.05726503786
   (L)  Electronic energy............ -2272.77869526594  (E+I)
   (N)  Total energy................  -815.14102835379  (A+L)

 SCFE: SCF energy: HF    -815.14102835379 hartrees   iterations:   7


 HOMO energy:    -0.29744
 LUMO energy:     0.11794

  Orbital energies:
  -20.45300  -15.55204  -11.32095  -11.23595  -11.22305  -11.21495
  -11.20810  -11.19967  -11.18806  -11.18579  -11.18533  -11.18450
  -11.18310  -11.18258  -11.17962  -11.17795  -11.17707  -11.17596
  -11.17281  -11.16473   -1.42469   -1.33378   -1.18047   -1.16243
   -1.11375   -1.08839   -1.03823   -1.02723   -1.01940   -1.00163
   -0.94881   -0.90496   -0.85283   -0.84414   -0.83043   -0.81118
   -0.79143   -0.76057   -0.72189   -0.68636   -0.68140   -0.66795
   -0.65699   -0.64316   -0.63998   -0.62501   -0.61358   -0.60757
   -0.60468   -0.60106   -0.59224   -0.58324   -0.55198   -0.55015
   -0.53300   -0.52479   -0.51613   -0.51326   -0.49879   -0.49498
   -0.48952   -0.48504   -0.45816   -0.42168   -0.39458   -0.34911
   -0.34234   -0.31510   -0.29744    0.11794    0.13250    0.14091
    0.14322    0.20545    0.22129    0.26515    0.27160    0.28123
    0.30682

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     4.942888E-04   1.085106E-04   6.777792E-04
   2    C1      9.149954E-04   1.277964E-03  -2.580834E-04
   3    C2     -2.906137E-04  -8.953488E-04   1.449004E-03
   4    C3      2.533503E-04  -8.174955E-04   8.078189E-04
   5    C4      1.766098E-05   2.977986E-04  -8.117422E-04
   6    C5     -6.666134E-04   4.286042E-04  -1.459685E-03
   7    C6      5.392638E-04   1.064791E-03   8.723250E-05
   8    C7     -6.969799E-04  -1.844274E-04   8.410534E-04
   9    H27    -2.599920E-05  -1.732855E-05   6.052677E-05
  10    H28    -4.743331E-04  -2.440486E-04  -2.516310E-04
  11     H30    -3.885976E-04  -1.352475E-04  -7.203910E-04
  12     C8      6.123525E-04   8.751091E-05  -8.510351E-04
  13     H32     4.879794E-04   1.101571E-04   4.192584E-04
  14     C10    -6.657436E-04  -5.432465E-04   6.618698E-04
  15     N2     -1.922156E-03  -3.427584E-04  -2.088374E-03
  16     C9     -8.779267E-05  -1.542378E-03  -6.724825E-06
  17     O1      1.117678E-03   1.168967E-03   2.504592E-03
  18     H43    -4.327281E-05   3.193259E-04   1.730451E-04
  19     C12     2.087354E-04   9.716727E-04  -4.801166E-04
  20     C11     8.670897E-04  -3.848822E-04   2.433786E-04
  21     C19    -2.665666E-05   1.518712E-04  -7.441307E-04
  22     C13    -3.313531E-04   4.117694E-04   2.866083E-04
  23     C14     6.551073E-04   3.571361E-04  -6.505991E-05
  24     C15    -7.789026E-04  -1.287632E-03   2.367100E-05
  25     C16     2.194202E-04  -6.839796E-04   1.211889E-05
  26     C17    -6.493763E-04   2.819037E-04   2.493719E-04
  27     H49     9.533104E-06   4.872716E-05   5.550205E-05
  28     H50     5.287651E-05  -1.799942E-04  -5.608688E-05
  29     H51     1.888451E-04  -1.464445E-04  -4.886211E-05
  30     H52    -4.857083E-05   2.017186E-04  -2.441456E-05
  31     H53    -6.347714E-05   1.187900E-04   1.012850E-04
  32     H1      6.177986E-04  -1.876919E-05  -2.036923E-04
  33     H2     -1.126628E-04  -2.663228E-04  -7.761274E-05
  34     H3     -6.426653E-04   6.956461E-04   2.875296E-04
  35     H4     -1.318604E-04   7.347958E-04   2.818405E-04
 -----------    -------------  -------------  -------------
    total       -7.906521E-04   1.147357E-03   1.075844E-03

  end of program der1b


  start of program geopt  11

  geometry optimization step 11
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:           -3.7686E-04 .  (  5.0000E-05 )
  gradient maximum:         2.7460E-03 .  (  4.5000E-04 )
  gradient rms:             6.1862E-04 .  (  3.0000E-04 )
  step size:   0.08078  trust radius:   0.30000
  displacement maximum:     2.8158E-02 .  (  1.8000E-03 )
  displacement rms:         7.2256E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.0545E-04    geom step:   8.0785E-02    full step:
8.0785E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -6.8974E-03     y:     7.0898E-03     z:     4.1518E-03

  new geometry:
                                angstroms
  atom             x                  y                  z
  H25       0.9629736427       2.0249301356      -4.1597022725
  C1        1.4968230847       2.0634681169      -3.2319814596
  C2        2.9188034942       2.1870473069      -0.7944456956
  C3        1.2155879527       1.1596148710      -2.2151111946
```

```
C4        2.4791839753      3.0107124310     -3.0263112467
C5        3.1832208564      3.0714275653     -1.8205833318
C6        1.9339996954      1.2459012461     -1.0143161363
C7        0.2741683171      0.0425223778     -2.0833985113
H27       2.7099585473      3.7130528261     -3.8015670991
H28       3.9422400855      3.8168627145     -1.6926976514
H30       3.4391381238      2.2071293568      0.1389854473
C8        0.4602164023     -0.4794423144     -0.8642766582
H32      -0.4294365104     -0.2731370820     -2.8175380067
C10      -0.0774572409     -1.5507314957      0.0561399846
N2        1.4554337917      0.2362726364     -0.1982753841
C9        1.7741907288     -0.2349055448      1.0556476221
O1        2.5505418953      0.2795771220      1.8304145178
H43      -0.0646931662     -2.5139965607     -0.4351656178
C12      -1.4970949276     -1.2469673053      0.5101645892
C11       0.9825712212     -1.5391353097      1.2266161506
C19       0.4628760429     -1.6980172521      2.6570665755
C13      -3.7168299237     -2.0189440429      1.0383916732
C14      -3.1681138243      0.2969219112      1.2896378545
C15      -4.0903353507     -0.7339865605      1.3848293157
C16      -1.8826669461      0.0432497921      0.8519964275
C17      -2.4254351567     -2.2715799002      0.6041644451
H49      -4.4242406308     -2.8210396432      1.1006317292
H50      -3.4531070538      1.2965519619      1.5503397114
H51      -5.0880073657     -0.5334184007      1.7198883219
H52      -1.1811362851      0.8468729921      0.7633331367
H53      -2.1442585100     -3.2711424673      0.3326970116
H1        1.2936000951     -1.5957346638      3.3453700006
H2        0.0100601913     -2.6715701697      2.7936925370
H3       -0.2747206209     -0.9427698513      2.8876363148
H4        1.6970968675     -2.3322251261      1.0246405805

nuclear repulsion energy.......  1457.777338860 hartrees
-------------------------------------------------
/  end of geometry optimization iteration  11   /
-------------------------------------------------

end of program geopt


start of program onee
smallest eigenvalue of S:    1.210E-03
number of canonical orbitals.....          210
end of program onee


start of program probe
end of program probe


start of program grid

number of gridpoints:
   atom       H25     C1      C2      C3      C4      C5      C6      C7
grid # 1       73     89      87      90      87      87      84      85
grid # 2      106     99      97      98      98      98      90      92
grid # 3      224    183     182     194     182     182     187     182
grid # 4      224    379     381     407     379     379     371     376

number of gridpoints:
   atom       H27    H28     H30      C8     H32     C10      N2      C9
grid # 1       73     73      73      86      73      82      99      76
```

```
   grid # 2       106     106     105      92     106      93     109      81
   grid # 3       224     224     220     187     223     175     223     164
   grid # 4       224     224     219     376     229     351     399     330

   number of gridpoints:
      atom         O1     H43     C12     C11     C19     C13     C14     C15
   grid # 1       111      69      91      80      72      87      86      89
   grid # 2       127      98     106      91      74     100      99     100
   grid # 3       272     211     192     175     139     182     182     182
   grid # 4       476     205     397     361     308     378     378     378

   number of gridpoints:
      atom        C16     C17     H49     H50     H51     H52     H53      H1
   grid # 1        86      85      73      73      73      71      72      71
   grid # 2        97      99     106     106     106     100     103      99
   grid # 3       181     182     224     223     224     216     216     220
   grid # 4       375     378     224     223     224     211     215     220

   number of gridpoints:
      atom         H2      H3      H4   total
   grid # 1        72      71      69    2818
   grid # 2        99      97     100    3483
   grid # 3       219     214     218    7028
   grid # 4       220     212     209   10840

   end of program grid


   start of program rwr
  recomputing RwR matrix   4    grid:  4
  recomputing RwR matrix  15    grid:  4
   end of program rwr


   start of program scf

       i  u  d  i  g
       t  p  i  c  r                                      RMS     maximum
       e  d  i  u  i                            energy  density    DIIS
       r  t  s  t  d     total energy           change  change     error

 etot   1  N  N  1  U  -815.13839756236          2.3E-04  5.9E-03
 etot   2  Y  Y  4  M  -815.14054954178  2.2E-03  8.9E-05  1.6E-03
 etot   3  Y  Y  4  M  -815.14080117381  2.5E-04  2.8E-05  4.9E-04
 etot   4  N  Y  1  U  -815.14081383399  1.3E-05  1.1E-05  1.6E-04
 etot   5  Y  Y  4  M  -815.14081703386  3.2E-06  6.3E-06  8.0E-05
 etot   6  Y  Y  4  M  -815.14081761458  5.8E-07  1.9E-06  2.4E-05
 etot   7  Y  N  4  M  -815.14081777425  1.6E-07  0.0E+00  0.0E+00


  Energy components, in hartrees:
    (A)  Nuclear repulsion............  1457.77733886019
    (E)  Total one-electron terms..... -4001.11822458234
    (I)  Total two-electron terms.....  1728.20006794790
    (L)  Electronic energy............ -2272.91815663444  (E+I)
    (N)  Total energy.................  -815.14081777425  (A+L)

  SCFE: SCF energy: HF    -815.14081777425 hartrees   iterations:   7


  HOMO energy:    -0.29726
  LUMO energy:     0.11769
 Orbital energies:
 -20.45391  -15.55228  -11.32202  -11.23575  -11.22283  -11.21528
 -11.20819  -11.19965  -11.18785  -11.18558  -11.18503  -11.18431
 -11.18289  -11.18231  -11.17919  -11.17743  -11.17694  -11.17580
 -11.17237  -11.16473   -1.42189   -1.33343   -1.18069   -1.16266
  -1.11397   -1.08819   -1.03822   -1.02746   -1.02004   -1.00150
  -0.94903   -0.90491   -0.85235   -0.84401   -0.83075   -0.81146
  -0.79158   -0.76046   -0.72225   -0.68651   -0.68130   -0.66786
  -0.65715   -0.64287   -0.64004   -0.62512   -0.61383   -0.60776
  -0.60450   -0.60104   -0.59230   -0.58284   -0.55146   -0.55041
  -0.53286   -0.52484   -0.51636   -0.51316   -0.49877   -0.49483
  -0.48935   -0.48520   -0.45834   -0.42201   -0.39435   -0.34914
  -0.34245   -0.31590   -0.29726    0.11769    0.13221    0.14140
   0.14365    0.20489    0.22182    0.26541    0.27182    0.28097
   0.30595

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -3.556138E-04  -1.671816E-04  -5.890125E-04
  2    C1     -1.067576E-03  -9.830863E-04  -8.034071E-04
  3    C2      3.721726E-04   7.363976E-04  -4.481067E-04
  4    C3     -3.055205E-04  -2.574975E-05  -3.277892E-04
  5    C4      1.539307E-04   8.779456E-05   6.377039E-04
  6    C5      1.086584E-03   4.459042E-04   8.062370E-04
  7    C6     -1.237775E-03  -1.714081E-04   5.931581E-04
  8    C7      5.024405E-05   2.264508E-04  -9.155206E-04
  9    H27    -6.945315E-05   1.990438E-04  -2.805352E-04
 10    H28    -2.892582E-05   7.879841E-05   1.602097E-04
 11    H30     2.418721E-04   3.888469E-04   6.806829E-04
 12    C8     -5.051504E-04   4.138593E-04   9.297371E-04
 13    H32    -3.827551E-04  -3.356723E-04  -5.421653E-04
 14    C10     1.407968E-04   4.608890E-04   1.851972E-04
 15    N2      3.213095E-03  -3.578236E-04   2.291375E-03
 16    C9      1.639834E-03   1.917560E-03   2.106272E-03
 17    O1     -3.510309E-03  -2.144232E-03  -3.823264E-03
 18    H43    -5.224398E-05   7.419927E-05   1.358377E-04
 19    C12     4.752834E-04  -5.561932E-04  -1.256769E-04
 20    C11     3.705402E-04   1.284676E-04   2.425146E-04
 21    C19     1.737153E-04   7.501079E-04   3.410695E-04
 22    C13    -1.861337E-04   3.981059E-04   1.181416E-04
 23    C14    -3.539349E-04   2.618534E-04   1.229171E-04
 24    C15    -3.066416E-04  -3.001389E-05   1.255333E-04
 25    C16    -1.571717E-04  -4.721544E-04  -5.523683E-05
 26    C17     7.182871E-04  -3.056450E-04  -2.525316E-04
```

```
  27    H49    -2.955119E-04  -3.212097E-04   9.707874E-05
  28    H50    -1.595242E-05   1.152517E-04   3.007410E-05
  29    H51    -2.033661E-04  -1.144511E-05   6.566678E-05
  30    H52     4.755975E-04   8.268037E-04   1.385464E-05
  31    H53    -5.628792E-06   5.449310E-05   1.492274E-04
  32    H1     -5.603850E-04   1.022143E-05  -4.177039E-04
  33    H2     -2.206289E-04  -1.257292E-04   1.933007E-04
  34    H3      3.674765E-04  -2.482146E-04   2.566545E-04
  35    H4      3.428726E-05   9.817103E-05  -4.610339E-05
 -----------   -------------  -------------  -------------
    total      -3.069620E-04   1.417461E-03   1.655389E-03

  end of program der1b


  start of program geopt  12

  geometry optimization step 12
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:            2.1058E-04 .  (  5.0000E-05 )
  gradient maximum:         5.6759E-03 .  (  4.5000E-04 )
  gradient rms:             7.2282E-04 .  (  3.0000E-04 )
  step size:   0.07000  trust radius:   0.30000
  displacement maximum:     2.5590E-02 .  (  1.8000E-03 )
  displacement rms:         6.2611E-03 .  (  1.2000E-03 )
  predicted energy change:    -7.3227E-05    geom step:   7.0002E-02    full step:
7.0002E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.4685E-03     y:     2.9347E-03     z:     1.4732E-03

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.9821859575      1.9923598495     -4.1778990947
  C1        1.5030394553      2.0446669770     -3.2417865055
  C2        2.8923662701      2.2034485510     -0.7807142184
  C3        1.2219670356      1.1435894625     -2.2213406065
  C4        2.4681877280      3.0081282054     -3.0261785915
  C5        3.1568983960      3.0859182847     -1.8091916309
  C6        1.9244374053      1.2466328825     -1.0103469327
  C7        0.2926245258      0.0154403256     -2.0958539111
  H27       2.6975524867      3.7098355374     -3.8030351869
  H28       3.9018567693      3.8435146553     -1.6746184631
  H30       3.3992694742      2.2363579346      0.1608185955
  C8        0.4712073982     -0.4952455578     -0.8695693791
  H32      -0.3989489633     -0.3141620758     -2.8376071615
  C10      -0.0717526626     -1.5603266492      0.0548476442
  N2        1.4568067554      0.2298762439     -0.1974967505
  C9        1.7614842816     -0.2312991505      1.0613884012
  O1        2.5186257520      0.2967116100      1.8426993627
  H43      -0.0666008951     -2.5250116980     -0.4313401850
  C12      -1.4891630422     -1.2447229002      0.5074914611
  C11       0.9892252258     -1.5472100848      1.2231315216
 C19       0.4720174129    -1.7301978200      2.6531626736
 C13      -3.7160213882    -1.9966744251      1.0402375260
 C14      -3.1474135032     0.3144644362      1.2864651844
 C15      -4.0789662280    -0.7086431057      1.3846026748
 C16      -1.8640989832     0.0493127162      0.8476796951
 C17      -2.4263285289    -2.2609425065      0.6050369521
 H49      -4.4295457522    -2.7935406864      1.1050945589
 H50      -3.4229312395     1.3171076964      1.5454932697
 H51      -5.0742950373    -0.4994009844      1.7202061520
 H52      -1.1563824224     0.8486956287      0.7566549316
 H53      -2.1543691772    -3.2637708946      0.3368997639
 H1        1.3046702834    -1.6378242009      3.3360170260
 H2        0.0235902088    -2.7081548594      2.7777669466
 H3       -0.2667523852    -0.9824544967      2.9015065478
 H4        1.7149496436    -2.3274611753      1.0094065084

 nuclear repulsion energy.......  1458.402573227 hartrees
 --------------------------------------------------
/  end of geometry optimization iteration  12   /
--------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.222E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     84     85
 grid # 2       106     99     98     98     98     99     90     92
 grid # 3       224    183    183    194    182    182    187    183
 grid # 4       224    379    381    407    379    379    373    377

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     81     99     76
 grid # 2       106    106    105     92    106     93    109     81
 grid # 3       224    224    220    187    223    175    223    163
 grid # 4       224    224    219    375    229    349    399    328

 number of gridpoints:
    atom         O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1       111     69     90     80     71     87     86     89
 grid # 2       127     97    106     92     76    100     99    100
 grid # 3       273    211    192    174    149    182    182    182
 grid # 4       475    205    397    360    305    378    378    378

 number of gridpoints:
    atom        C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1        86     85     73     73     73     71     72     71
 grid # 2        97     98    106    106    106    100    103     99
 grid # 3       181    182    224    223    224    216    216    220
 grid # 4      376    377    224    223    224    211    215    220

 number of gridpoints:
    atom        H2     H3     H4  total
 grid # 1       72     71     69   2815
 grid # 2       99     97    100   3486
 grid # 3      220    214    219   7041
 grid # 4      221    212    211  10836

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                  RMS    maximum
      e  d  i  u  i                        energy  density   DIIS
      r  t  s  t  d     total energy      change  change    error

etot   1  N  N  1  U  -815.13885786835            2.5E-04  6.4E-03
etot   2  Y  Y  4  M  -815.14053535960  1.7E-03  7.9E-05  2.6E-03
etot   3  Y  Y  4  M  -815.14072622945  1.9E-04  2.8E-05  8.0E-04
etot   4  Y  Y  4  M  -815.14074207598  1.6E-05  9.1E-06  2.3E-04
etot   5  Y  Y  4  M  -815.14074236696  2.9E-07  3.8E-06  8.2E-05
etot   6  N  N  1  U  -815.14076067622  1.8E-05  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1458.40257322696
  (E)  Total one-electron terms..... -4002.37422815778
  (I)  Total two-electron terms.....  1728.83089425460
  (L)  Electronic energy............ -2273.54333390318  (E+I)
  (N)  Total energy.................  -815.14076067622  (A+L)

SCFE: SCF energy: HF    -815.14076067622 hartrees   iterations:   6


HOMO energy:    -0.29710
LUMO energy:     0.11745

 Orbital energies:
 -20.45388  -15.55216  -11.32163  -11.23573  -11.22316  -11.21486
 -11.20818  -11.19953  -11.18827  -11.18551  -11.18498  -11.18425
 -11.18280  -11.18230  -11.17963  -11.17785  -11.17730  -11.17621
 -11.17284  -11.16459   -1.42345   -1.33355   -1.18040   -1.16222
  -1.11377   -1.08806   -1.03815   -1.02700   -1.01979   -1.00121
  -0.94858   -0.90530   -0.85216   -0.84386   -0.83051   -0.81128
  -0.79150   -0.76019   -0.72228   -0.68650   -0.68136   -0.66764
  -0.65681   -0.64283   -0.64030   -0.62478   -0.61385   -0.60778
  -0.60456   -0.60051   -0.59246   -0.58257   -0.55121   -0.55038
  -0.53303   -0.52495   -0.51638   -0.51338   -0.49859   -0.49473
  -0.48899   -0.48512   -0.45831   -0.42206   -0.39446   -0.34878
  -0.34237   -0.31554   -0.29710    0.11745    0.13222    0.14155
   0.14389    0.20471    0.22209    0.26551    0.27169    0.28106
   0.30573
 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x             y             z
----  -----   -------------  -------------  -------------
  1    H25     2.011708E-04  -9.306334E-05   5.148739E-04
  2    C1     -7.662316E-04  -8.980852E-04   4.662703E-04
  3    C2      1.045704E-04   8.500277E-04  -1.372132E-03
  4    C3      2.280399E-04   3.204608E-04  -1.476427E-06
  5    C4      9.776529E-04   3.303159E-05   1.606021E-03
  6    C5     -7.044640E-04  -1.356714E-04  -5.135340E-04
  7    C6     -3.620839E-04  -7.633864E-04  -9.405624E-04
  8    C7      1.879348E-04   2.010893E-04   1.533414E-05
  9    H27     1.782558E-04   1.282640E-04   1.765797E-04
 10    H28     1.937737E-04   4.216643E-04  -5.229801E-05
 11    H30    -2.251337E-05   2.909429E-04  -1.073933E-04
 12    C8     -3.600201E-04  -5.507328E-04  -1.798444E-04
 13    H32     2.867983E-04   2.146759E-04   5.131084E-04
 14    C10     3.582999E-04   4.188446E-04  -2.351722E-04
 15    N2     -1.004548E-03   9.819884E-04  -4.583167E-04
 16    C9      9.789034E-04   4.677299E-04   1.554489E-03
 17    O1     -8.844065E-04  -7.917812E-04  -7.823750E-04
 18    H43     1.302638E-04  -6.604575E-04  -1.752657E-04
 19    C12     2.023390E-04  -2.958080E-04   5.564862E-04
 20    C11    -1.386757E-03  -1.233017E-04   1.025217E-03
 21    C19    -5.959108E-05  -1.839814E-04  -1.227900E-03
 22    C13     3.636125E-04  -1.376352E-04  -1.247337E-04
 23    C14    -8.869557E-05  -6.530894E-05  -6.511584E-05
 24    C15     4.452336E-04   4.484264E-04  -3.155066E-05
 25    C16    -4.049063E-04   1.996871E-04   1.694209E-06
 26    C17     2.593563E-04  -1.132965E-04  -6.214955E-05
 27    H49    -1.333866E-04  -1.516496E-04   5.779107E-05
 28    H50    -9.094372E-05   1.400613E-04   5.331753E-05
 29    H51    -4.106356E-04   9.524111E-05   1.524459E-04
 30    H52    -1.325195E-05   9.525865E-05   1.308699E-04
 31    H53     7.914668E-05  -2.860516E-05   4.829597E-05
 32    H1      8.175413E-04   3.767627E-04   1.272542E-03
 33    H2     -2.752270E-06   1.924453E-04  -2.788320E-04
 34    H3      1.919286E-04   2.011393E-04  -2.280176E-04
 35    H4     -2.276243E-04   9.117969E-05   1.698567E-04
-----------   -------------  -------------  -------------
   total      -7.379901E-04   1.176157E-03   1.478523E-03

 end of program der1b


 start of program geopt  13
```

```
  geometry optimization step 13
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:           5.7098E-05 .  (  5.0000E-05 )
  gradient maximum:        1.9403E-03 .  (  4.5000E-04 )
  gradient rms:            4.5887E-04 .  (  3.0000E-04 )
  step size:   0.04376  trust radius:   0.30000
  displacement maximum:    1.7327E-02 .  (  1.8000E-03 )
  displacement rms:        3.9137E-03 .  (  1.2000E-03 )
  predicted energy change:   -4.5801E-05    geom step:   4.3756E-02    full step:
4.3756E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     2.6044E-03     y:    -2.8800E-03     z:    -1.1773E-03

  new geometry:
                              angstroms
  atom            x                  y                 z
  H25       0.9780137671      1.9972409320     -4.1729589406
  C1        1.5017589175      2.0468983917     -3.2390598519
  C2        2.8998708018      2.2026166209     -0.7866079705
  C3        1.2202434228      1.1472178500     -2.2196228911
  C4        2.4715869948      3.0085184618     -3.0241385143
  C5        3.1648365198      3.0856832457     -1.8123446644
  C6        1.9273499873      1.2472474115     -1.0119555355
  C7        0.2861137841      0.0241293414     -2.0919453225
  H27       2.7007075406      3.7109374553     -3.8007255351
  H28       3.9117812714      3.8428434161     -1.6794511195
  H30       3.4090230781      2.2362581351      0.1539079416
  C8        0.4651768265     -0.4874373999     -0.8662860852
  H32      -0.4095546862     -0.3013610703     -2.8308318831
  C10      -0.0744347190     -1.5558079667      0.0552647761
  N2        1.4550719615      0.2345388269     -0.1962378888
  C9        1.7695971217     -0.2368093368      1.0574429753
  O1        2.5405953551      0.2789510974      1.8316647996
  H43      -0.0663073744     -2.5205847594     -0.4338972902
  C12      -1.4919142463     -1.2459648632      0.5101186582
  C11       0.9848333813     -1.5447975692      1.2246150379
  C19       0.4674494037     -1.7124615381      2.6543001917
  C13      -3.7180496883     -2.0031963882      1.0359730743
  C14      -3.1557115945      0.3085471435      1.2931977752
  C15      -4.0849305687     -0.7165955743      1.3856259342
  C16      -1.8708239297      0.0466691987      0.8548466907
  C17      -2.4267221154     -2.2643049429      0.6011951018
  H49      -4.4313191486     -2.8014247941      1.0963552755
  H50      -3.4332789454      1.3095273193      1.5572011024
  H51      -5.0821779079     -0.5109735130      1.7210895662
  H52      -1.1634201656      0.8474776261      0.7696375576
  H53      -2.1524972367     -3.2652956545      0.3284245856
  H1        1.2984049997     -1.6174258405      3.3410443805
  H2        0.0129758679     -2.6863278215      2.7847446894
  H3       -0.2666527946     -0.9591924484      2.8942250372
  H4        1.7035592531     -2.3329825027      1.0166220630

  nuclear repulsion energy.......  1458.127010856 hartrees
```

```
 --------------------------------------------------
/  end of geometry optimization iteration  13   /
 --------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.217E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      85      85
 grid # 2       106    100      97      98      98      98      90      92
 grid # 3       224    183     183     194     182     182     187     183
 grid # 4       224    379     381     404     379     379     374     377

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      81      99      76
 grid # 2       106    106     105      92     106      93     109      81
 grid # 3       224    224     220     188     223     175     223     163
 grid # 4       224    224     219     377     229     351     401     330

 number of gridpoints:
    atom         O1    H43     C12     C11     C19     C13     C14     C15
 grid # 1       111     69      90      80      71      87      87      89
 grid # 2       123     98     105      91      78     100      99     100
 grid # 3       272    211     193     175     149     182     182     182
 grid # 4       475    205     399     361     306     379     379     379

 number of gridpoints:
    atom        C16    C17     H49     H50     H51     H52     H53      H1
 grid # 1        86     86      73      73      73      71      72      71
 grid # 2        97     99     106     106     106     100     103      99
 grid # 3       181    182     224     223     224     216     216     220
 grid # 4       376    377     224     223     224     211     215     221

 number of gridpoints:
    atom         H2     H3      H4   total
 grid # 1        72     71      69    2818
 grid # 2        99     97     100    3483
 grid # 3       219    214     218    7041
 grid # 4       220    212     211   10849

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr
```

```
  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14032657107           1.6E-04  3.0E-03
etot   2  Y  Y  4  M  -815.14077652460  4.5E-04  4.0E-05  8.2E-04
etot   3  Y  Y  4  M  -815.14082066760  4.4E-05  1.4E-05  2.9E-04
etot   4  Y  Y  4  M  -815.14082476245  4.1E-06  6.1E-06  1.4E-04
etot   5  Y  Y  4  M  -815.14082690422  2.1E-06  1.9E-06  5.5E-05
etot   6  N  N  1  U  -815.14082034438 -6.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.12701085585
   (E)  Total one-electron terms..... -4001.82078209807
   (I)  Total two-electron terms.....  1728.55295089784
   (L)  Electronic energy............ -2273.26783120023  (E+I)
   (N)  Total energy.................  -815.14082034438  (A+L)

 SCFE: SCF energy: HF    -815.14082034438 hartrees   iterations:   6


 HOMO energy:    -0.29737
 LUMO energy:     0.11774

  Orbital energies:
  -20.45366  -15.55209  -11.32154  -11.23586  -11.22323  -11.21501
  -11.20800  -11.19969  -11.18802  -11.18570  -11.18522  -11.18446
  -11.18302  -11.18260  -11.17945  -11.17769  -11.17720  -11.17593
  -11.17264  -11.16443   -1.42395   -1.33340   -1.18037   -1.16225
   -1.11401   -1.08811   -1.03823   -1.02676   -1.01953   -1.00157
   -0.94891   -0.90504   -0.85241   -0.84390   -0.83033   -0.81097
   -0.79132   -0.76047   -0.72206   -0.68643   -0.68147   -0.66771
   -0.65698   -0.64295   -0.64007   -0.62499   -0.61377   -0.60758
   -0.60467   -0.60046   -0.59247   -0.58296   -0.55162   -0.55047
   -0.53313   -0.52485   -0.51616   -0.51338   -0.49862   -0.49487
   -0.48930   -0.48508   -0.45834   -0.42185   -0.39453   -0.34872
   -0.34241   -0.31523   -0.29737    0.11774    0.13210    0.14154
    0.14366    0.20516    0.22180    0.26528    0.27164    0.28090
    0.30591

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

```
atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.026659E-04   7.940149E-05   1.259725E-05
  2    C1      7.385166E-04   1.041774E-03   3.640578E-04
  3    C2     -4.277132E-04  -7.121912E-04   1.072111E-03
  4    C3      1.823096E-04   6.080676E-05   1.454382E-04
  5    C4     -3.486319E-04  -3.976083E-05  -1.220409E-03
  6    C5     -5.429509E-04  -4.812900E-05  -4.274587E-04
  7    C6      3.672095E-04   5.257589E-04  -3.842109E-05
  8    C7      2.893655E-06   1.343825E-04   3.563527E-04
  9    H27    -1.093378E-04  -9.313943E-05  -3.686873E-05
 10    H28    -2.670753E-04  -1.689756E-04  -7.354570E-05
 11    H30    -1.011360E-04  -1.262256E-04  -1.134469E-04
 12    C8      2.466115E-04  -1.841046E-04  -2.789220E-06
 13    H32     1.183894E-04  -1.492649E-07   7.505712E-05
 14    C10    -1.088954E-04  -3.050312E-04   3.274031E-05
 15    N2     -2.361920E-04  -2.591109E-04  -1.990486E-04
 16    C9     -2.497903E-04   2.943137E-04  -9.796197E-05
 17    O1      1.494034E-04   2.322840E-04   5.475614E-04
 18    H43     2.600056E-05   3.197115E-04   1.694046E-04
 19    C12    -4.228763E-04   6.821343E-04   9.625218E-05
 20    C11     5.009918E-04   9.438437E-05  -1.252887E-04
 21    C19     1.971033E-04  -5.222753E-04  -9.278954E-06
 22    C13     6.038922E-05  -2.142518E-05  -4.345160E-05
 23    C14     8.153282E-04  -1.398940E-04  -2.323116E-04
 24    C15     2.480760E-05  -5.737902E-04  -8.793533E-05
 25    C16    -2.556205E-04   8.766221E-05   2.826419E-04
 26    C17    -7.535824E-04   1.782726E-04   3.604845E-04
 27    H49     2.093788E-04   9.060593E-05   2.126575E-05
 28    H50     1.481243E-05   3.272972E-05  -7.716648E-05
 29    H51     3.048751E-04  -1.315100E-04  -1.100336E-04
 30    H52    -2.503398E-04  -4.975195E-05   1.524432E-05
 31    H53    -3.700165E-05  -2.203874E-05   1.048956E-04
 32    H1      3.894079E-04   5.726540E-05   2.053742E-04
 33    H2     -1.556112E-04  -6.858125E-05   1.288347E-04
 34    H3     -5.878188E-04   7.010178E-04   1.067378E-04
 35    H4     -1.286037E-04   1.323384E-04   2.160125E-04
-----------   -------------  -------------  -------------
   total      -5.320828E-04   1.278759E-03   1.417648E-03

 end of program der1b


 start of program geopt  14

 geometry optimization step 14

the energy is increasing and lowest energy was more than two iters back
.

 [ turning on trust-radius adjustment ]
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   11 **


 energy change:           -5.9668E-05 .  (  5.0000E-05 )
 gradient maximum:         2.7460E-03 .  (  4.5000E-04 )
```

```
  gradient rms:             6.1862E-04 .  (  3.0000E-04 )
  step size:   0.10441  trust radius:   0.15000
  displacement maximum:     4.0660E-02 .  (  1.8000E-03 )
  displacement rms:         9.3389E-03 .  (  1.2000E-03 )
  predicted energy change:    -8.6925E-05    geom step:   1.0441E-01    full step:
1.0441E-01
  molecular structure not yet converged...

  center of mass moved by:
     x:    -1.6653E-16     y:    -5.2736E-16     z:    -5.5511E-16

  new geometry:
                              angstroms
  atom            x                y                 z
  H25       0.9715887888      2.0064928669     -4.1681976290
  C1        1.4966283010      2.0538213252     -3.2349789190
  C2        2.8972095262      2.2030389824     -0.7829284628
  C3        1.2155229947      1.1516447003     -2.2169710276
  C4        2.4666121697      3.0144107691     -3.0197543180
  C5        3.1614273275      3.0877726973     -1.8078830205
  C6        1.9235507522      1.2498604204     -1.0096146466
  C7        0.2815940008      0.0276098562     -2.0899943305
  H27       2.6952795850      3.7180502409     -3.7949084686
  H28       3.9096047975      3.8435217998     -1.6745107867
  H30       3.4072076158      2.2331024230      0.1567619932
  C8        0.4613947828     -0.4853898844     -0.8655314237
  H32      -0.4145138032     -0.2966773894     -2.8288468681
  C10      -0.0788354461     -1.5532330514      0.0569438632
  N2        1.4500755708      0.2367776120     -0.1955507463
  C9        1.7646362376     -0.2320410488      1.0590265144
  O1        2.5330447844      0.2882322622      1.8355653230
  H43      -0.0710249041     -2.5179716080     -0.4312574566
  C12      -1.4966273085     -1.2423886106      0.5109448423
  C11       0.9816192815     -1.5410214900      1.2259898323
  C19       0.4636878689     -1.7097856316      2.6557765545
  C13      -3.7215514039     -1.9993794701      1.0434403894
  C14      -3.1598728119      0.3133601179      1.2901797719
  C15      -4.0884173080     -0.7118738702      1.3882350616
  C16      -1.8755160919      0.0507904949      0.8510288399
  C17      -2.4309824101     -2.2608717223      0.6077351319
  H49      -4.4338672003     -2.7975024969      1.1079199859
  H50      -3.4380169530      1.3150348310      1.5501650088
  H51      -5.0849480843     -0.5051905932      1.7241501582
  H52      -1.1688920771      0.8509646167      0.7608462131
  H53      -2.1563158873     -3.2625827431      0.3382229938
  H1        1.2945824471     -1.6085448627      3.3420044008
  H2        0.0160083860     -2.6869158952      2.7875796078
  H3       -0.2761293950     -0.9608532730      2.8941412473
  H4        1.7016389697     -2.3275795861      1.0180796769

  nuclear repulsion energy.......  1458.206394548 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  14   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.218E-03
  number of canonical orbitals.....          210
  end of program onee
 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1      C2      C3      C4      C5      C6      C7
 grid # 1        73     89      87      90      87      87      84      85
 grid # 2       106    100      97      98      98      99      90      92
 grid # 3       224    183     182     194     182     182     187     182
 grid # 4       224    379     380     406     379     379     374     378

 number of gridpoints:
    atom        H27    H28     H30      C8     H32     C10      N2      C9
 grid # 1        73     73      73      86      73      81      99      76
 grid # 2       106    106     105      92     106      93     109      81
 grid # 3       224    224     220     187     223     175     223     163
 grid # 4       224    224     219     375     229     350     400     330

 number of gridpoints:
    atom         O1    H43     C12     C11     C19     C13     C14     C15
 grid # 1       111     69      90      80      71      87      87      89
 grid # 2       127     97     106      91      76     100      99     100
 grid # 3       272    211     192     176     150     182     182     182
 grid # 4       475    206     397     361     305     378     379     378

 number of gridpoints:
    atom        C16    C17     H49     H50     H51     H52     H53      H1
 grid # 1        86     85      73      73      73      71      72      71
 grid # 2        97     99     106     106     106     100     103      99
 grid # 3       181    182     224     223     224     216     216     220
 grid # 4       376    377     224     223     224     211     215     221

 number of gridpoints:
    atom         H2     H3      H4  total
 grid # 1        72     71      69   2816
 grid # 2        99     97     100   3486
 grid # 3       219    214     219   7040
 grid # 4       221    212     210  10843

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                 RMS    maximum
      e  d  i  u  i                      energy  density    DIIS
      r  t  s  t  d     total energy     change  change     error

etot   1  N  N  2  U  -815.14095613282            6.6E-05  9.5E-04
etot   2  Y  Y  6  M  -815.14103547368  7.9E-05  1.7E-05  3.7E-04
etot   3  Y  Y  6  M  -815.14105073503  1.5E-05  6.2E-06  1.2E-04
etot   4  Y  Y  6  M  -815.14104947192 -1.3E-06  3.0E-06  5.5E-05
etot   5  Y  N  6  M  -815.14105019647  7.2E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.20639454760
   (E)  Total one-electron terms..... -4001.97464933021
   (I)  Total two-electron terms.....  1728.62720458614
   (L)  Electronic energy............ -2273.34744474407  (E+I)
   (N)  Total energy.................  -815.14105019647  (A+L)

 SCFE: SCF energy: HF    -815.14105019647 hartrees   iterations:   5


 HOMO energy:    -0.29744
 LUMO energy:     0.11757

  Orbital energies:
  -20.45373  -15.55228  -11.32176  -11.23588  -11.22318  -11.21516
  -11.20812  -11.19965  -11.18813  -11.18568  -11.18517  -11.18442
  -11.18298  -11.18248  -11.17950  -11.17774  -11.17720  -11.17604
  -11.17270  -11.16458   -1.42295   -1.33360   -1.18048   -1.16233
   -1.11399   -1.08825   -1.03831   -1.02691   -1.01965   -1.00163
   -0.94892   -0.90517   -0.85240   -0.84402   -0.83048   -0.81127
   -0.79148   -0.76041   -0.72218   -0.68648   -0.68142   -0.66774
   -0.65701   -0.64287   -0.64020   -0.62501   -0.61385   -0.60760
   -0.60468   -0.60055   -0.59255   -0.58292   -0.55151   -0.55046
   -0.53300   -0.52486   -0.51627   -0.51336   -0.49869   -0.49484
   -0.48924   -0.48524   -0.45834   -0.42199   -0.39453   -0.34878
   -0.34251   -0.31538   -0.29744    0.11757    0.13202    0.14138
    0.14361    0.20482    0.22191    0.26530    0.27164    0.28085
    0.30584

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----   -------------  -------------  -------------
   1    H25     7.642063E-05   2.228009E-05  -5.784614E-05
   2    C1      1.990428E-04   4.592703E-04   3.392988E-04
   3    C2     -4.355800E-04  -2.759023E-04   2.627708E-04
   4    C3      3.616522E-04   3.096878E-04  -5.668802E-05
   5    C4      6.743136E-05  -2.178968E-04  -2.124141E-04
   6    C5     -4.485339E-04   3.675195E-05  -4.929463E-04
   7    C6     -3.983617E-04   1.033620E-04  -3.776749E-04
   8    C7      3.606249E-05   5.311642E-04  -3.250841E-04
   9    H27    -3.453411E-05   7.310908E-05  -1.515938E-04
  10    H28    -2.288304E-04  -9.263876E-05  -6.446956E-05
  11    H30     3.214381E-05   4.893072E-05   1.421391E-04
  12    C8     -1.837265E-04  -4.297444E-04   3.247033E-04
  13    H32     7.099220E-05  -4.485450E-05   1.251749E-05
  14    C10     1.931686E-04   3.975476E-05  -9.584003E-05
  15    N2      1.112921E-03   2.295018E-05   8.860574E-04
  16    C9      7.074941E-04   1.485733E-03   1.572049E-03
  17    O1     -1.768044E-03  -1.325477E-03  -1.848039E-03
  18    H43     8.249322E-05   1.864236E-05   4.033652E-05
  19    C12    -1.968266E-04   2.018880E-04   2.938186E-04
  20    C11    -1.705260E-04   1.772935E-04   4.573836E-04
  21    C19     3.486310E-04  -5.211619E-04  -7.112175E-05
  22    C13     2.400181E-04   4.842769E-05  -1.513940E-04
  23    C14     5.937683E-04  -9.760248E-05  -2.094124E-04
  24    C15     9.990594E-05  -2.137299E-04  -1.623275E-05
  25    C16    -5.251307E-04   1.050158E-04   2.914697E-04
  26    C17    -3.153649E-04  -7.684957E-05   1.633692E-04
  27    H49    -1.176554E-05  -1.758050E-04   3.844575E-05
  28    H50     1.228499E-05   1.699379E-04  -1.854845E-05
  29    H51     8.262888E-05  -8.675548E-05  -2.379603E-05
  30    H52    -3.661522E-05   3.368161E-04   8.394570E-05
  31    H53    -3.525729E-05  -8.316147E-05   1.209114E-04
  32    H1      1.542859E-04   8.677659E-05   2.735419E-04
  33    H2     -1.146601E-04   1.219578E-04   6.468406E-05
  34    H3     -2.078806E-04   4.660569E-04   2.260729E-06
  35    H4     -1.083501E-04  -1.211125E-04   1.125285E-04
 -----------   -------------  -------------  -------------
    total      -7.486429E-04   1.103115E-03   1.309130E-03

  end of program der1b


  start of program geopt  15

  geometry optimization step 15
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:          -2.1843E-05 *  (  5.0000E-05 )
  gradient maximum:        2.9280E-03 .  (  4.5000E-04 )
  gradient rms:            3.9444E-04 .  (  3.0000E-04 )
  step size:   0.03577  trust radius:   0.15000
  displacement maximum:    1.0946E-02 .  (  1.8000E-03 )
  displacement rms:        3.1992E-03 .  (  1.2000E-03 )
  predicted energy change:    -2.4323E-05    geom step:   3.5768E-02    full step:
3.5768E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.3877E-03     y:    -2.6169E-04     z:    -1.1880E-04

  new geometry:
                              angstroms
  atom           x                 y                 z
  H25       0.9628770552      2.0193285669     -4.1638889067
  C1        1.4935408546      2.0623282836     -3.2334932157
  C2        2.9084026940      2.1969390307     -0.7900338448
  C3        1.2123962294      1.1610553684     -2.2142601873
 C4         2.4729218265      3.0129449231     -3.0261256242
 C5         3.1731896506      3.0796062625     -1.8177301723
 C6         1.9278151831      1.2510106110     -1.0110563088
 C7         0.2723376428      0.0434054291     -2.0831797484
 H27        2.7035328033      3.7141323690     -3.8032171072
 H28        3.9285309058      3.8281887399     -1.6886578631
 H30        3.4262187959      2.2222081320      0.1459155375
 C8         0.4582127908     -0.4767817257     -0.8617184970
 H32       -0.4295514713     -0.2755250135     -2.8189013667
 C10       -0.0804255394     -1.5470660706      0.0587490318
 N2         1.4549983983      0.2385676904     -0.1950029308
 C9         1.7678083254     -0.2316129189      1.0596452197
 O1         2.5417082210      0.2812914585      1.8329451566
 H43       -0.0687009551     -2.5103983857     -0.4324051712
 C12       -1.4994123676     -1.2420340897      0.5128222978
 C11        0.9780612527     -1.5367210779      1.2295799135
 C19        0.4584760543     -1.6981362334      2.6602424141
 C13       -3.7210956272     -2.0112965750      1.0370260412
 C14       -3.1691895230      0.3031592205      1.2955681002
 C15       -4.0933246835     -0.7266847030      1.3870054683
 C16       -1.8836559926      0.0484861183      0.8580798504
 C17       -2.4292538227     -2.2653746048      0.6032469423
 H49       -4.4298683505     -2.8132013080      1.0969139577
 H50       -3.4520037927      1.3027746385      1.5592426993
 H51       -5.0910323376     -0.5260510861      1.7220405431
 H52       -1.1808884116      0.8527344319      0.7730126864
 H53       -2.1499072007     -3.2650752120      0.3305864403
 H1         1.2901676011     -1.6092180497      3.3466612018
 H2        -0.0046746319     -2.6670391758      2.7931406310
 H3        -0.2696325560     -0.9367322987      2.8974733967
 H4         1.6931232446     -2.3296832421      1.0257831728

 nuclear repulsion energy.......  1457.800540722 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  15   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.215E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     84     85
 grid # 2       106     99     97     98     98     98     90     92
 grid # 3       224    183    182    194    182    182    187    183
 grid # 4       224    379    382    406    379    379    372    378

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     82     99     76
```

```
  grid # 2       106    106    105     92    106     93    109     81
  grid # 3       224    224    220    188    223    175    223    163
  grid # 4       224    224    219    377    229    351    400    331

  number of gridpoints:
     atom         O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1       111     69     90     80     71     87     86     89
  grid # 2       123     98    106     90     75    100     99    100
  grid # 3       272    211    192    175    142    182    182    182
  grid # 4       476    205    397    361    309    378    379    378

  number of gridpoints:
     atom        C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1        86     85     73     73     73     71     72     71
  grid # 2        97     99    106    106    106    100    103     99
  grid # 3       181    182    224    223    224    216    216    220
  grid # 4       376    377    224    223    224    211    215    221

  number of gridpoints:
     atom         H2     H3     H4  total
  grid # 1        72     71     69   2816
  grid # 2        99     97    100   3479
  grid # 3       219    214    218   7032
  grid # 4       220    212    210  10850

  end of program grid


  start of program rwr
 recomputing RwR matrix   2    grid:  4
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14041016071           1.4E-04  3.0E-03
etot   2  Y  Y  4  M  -815.14085786302  4.5E-04  4.1E-05  1.2E-03
etot   3  Y  Y  4  M  -815.14090804473  5.0E-05  1.4E-05  3.7E-04
etot   4  Y  Y  4  M  -815.14091171062  3.7E-06  5.5E-06  1.2E-04
etot   5  Y  Y  4  M  -815.14091325030  1.5E-06  2.1E-06  4.1E-05
etot   6  N  N  1  U  -815.14090435872 -8.9E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1457.80054072206
   (E)  Total one-electron terms..... -4001.16714833897
   (I)  Total two-electron terms.....  1728.22570325819
   (L)  Electronic energy............ -2272.94144508078  (E+I)
   (N)  Total energy.................  -815.14090435872  (A+L)

 SCFE: SCF energy: HF    -815.14090435872 hartrees   iterations:   6


 HOMO energy:    -0.29705
 LUMO energy:     0.11774
 Orbital energies:
 -20.45374  -15.55209  -11.32164  -11.23584  -11.22308  -11.21498
 -11.20807  -11.19966  -11.18800  -11.18558  -11.18509  -11.18437
 -11.18290  -11.18249  -11.17932  -11.17760  -11.17711  -11.17586
 -11.17256  -11.16456   -1.42389   -1.33330   -1.18049   -1.16245
  -1.11390   -1.08794   -1.03813   -1.02722   -1.01994   -1.00124
  -0.94886   -0.90497   -0.85234   -0.84386   -0.83058   -0.81113
  -0.79143   -0.76042   -0.72213   -0.68649   -0.68142   -0.66780
  -0.65703   -0.64303   -0.64002   -0.62498   -0.61373   -0.60780
  -0.60451   -0.60085   -0.59226   -0.58286   -0.55150   -0.55045
  -0.53310   -0.52493   -0.51633   -0.51330   -0.49869   -0.49487
  -0.48936   -0.48503   -0.45840   -0.42192   -0.39440   -0.34901
  -0.34232   -0.31571   -0.29705    0.11774    0.13225    0.14149
   0.14375    0.20517    0.22168    0.26533    0.27166    0.28102
   0.30599

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   2    grid:  4
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x             y             z
----  -----   -------------  -------------  -------------
  1    H25    -6.436108E-05  -1.190955E-04   6.848711E-05
  2    C1     -9.552618E-04  -7.122507E-04  -9.032131E-04
  3    C2      5.385183E-04   5.841831E-04  -1.271506E-04
  4    C3     -2.594356E-04  -1.934042E-04   3.587599E-04
  5    C4      4.563910E-04   6.140661E-04   2.899082E-04
  6    C5      2.174784E-04  -2.104989E-05   4.781555E-04
  7    C6     -1.947910E-04  -4.885665E-05   1.538015E-04
  8    C7     -2.740086E-05  -5.570203E-04   1.850285E-05
  9    H27    -1.218011E-05   3.858357E-06   7.199887E-05
 10    H28     9.360981E-05   2.334213E-04   7.058816E-05
 11    H30    -1.226692E-04   2.266955E-04  -7.441474E-05
 12    C8     -8.478174E-05   5.354356E-04   2.663392E-05
 13    H32     2.846009E-06  -4.375968E-05   4.567013E-05
 14    C10    -1.335133E-04   1.464726E-04   2.164126E-04
 15    N2     -1.706169E-04  -2.774102E-05  -2.559249E-04
 16    C9      2.031810E-04  -3.612411E-04  -2.496135E-04
 17    O1     -1.688275E-04   2.466108E-04   2.615854E-04
 18    H43    -9.358747E-05   4.085757E-05   1.249766E-04
 19    C12     1.510792E-04   7.532251E-06  -1.071990E-04
 20    C11     2.475192E-04  -1.300633E-04   2.487299E-05
 21    C19    -1.064998E-04   5.635889E-04  -4.615977E-04
 22    C13    -2.772288E-04   1.300808E-04   1.988728E-04
 23    C14    -1.195257E-04   1.142410E-04   4.288076E-05
 24    C15    -9.268623E-05  -2.790353E-04  -4.680051E-06
 25    C16     1.558280E-04  -3.700738E-04  -7.645453E-05
```

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  26    C17     1.714749E-04   3.179176E-05   4.482059E-05
  27    H49    -2.724407E-05   4.312251E-05   5.724637E-05
  28    H50    -6.332008E-05  -5.325421E-06  -2.415754E-06
  29    H51    -1.679837E-04   1.935835E-05   4.655891E-05
  30    H52     9.739645E-05   1.497840E-04  -2.923301E-05
  31    H53     4.553215E-05   7.647045E-05   6.076668E-05
  32    H1      3.795902E-04   1.413362E-04   3.122034E-04
  33    H2     -2.545972E-04  -3.364018E-04   2.978531E-05
  34    H3     -6.628000E-05   1.120113E-04   1.456635E-04
  35    H4     -1.355503E-04   4.770405E-04   1.340745E-04
 -----------   -------------  -------------  -------------
    total      -8.378977E-04   1.292641E-03   9.913298E-04

  end of program der1b


  start of program geopt  16

  geometry optimization step 16
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:            1.4584E-04 .  (  5.0000E-05 )
  gradient maximum:         1.3500E-03 .  (  4.5000E-04 )
  gradient rms:             2.4088E-04 *  (  3.0000E-04 )
  step size:   0.04650  trust radius:   0.07500
  displacement maximum:     1.7065E-02 .  (  1.8000E-03 )
  displacement rms:         4.1592E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.3638E-05    geom step:   4.6501E-02    full step:
4.6501E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -3.2655E-03     y:     2.5025E-03     z:     1.2806E-03

  new geometry:
                                angstroms
  atom            x                 y                 z
  H25       0.9809504977      1.9933633407     -4.1773919824
  C1        1.5015608236      2.0467844734     -3.2418443144
  C2        2.8915159352      2.2088818154     -0.7842208154
  C3        1.2180173127      1.1496249911     -2.2196942299
  C4        2.4709195136      3.0080766602     -3.0285881900
  C5        3.1588218880      3.0881696194     -1.8135825205
  C6        1.9209656114      1.2528515514     -1.0099662465
  C7        0.2856870098      0.0249000417     -2.0919890851
  H27       2.7032649371      3.7073316316     -3.8070056423
  H28       3.9056076874      3.8450800813     -1.6806767799
  H30       3.3989878477      2.2451195857      0.1571008386
  C8        0.4625420086     -0.4849782956     -0.8649112239
  H32      -0.4064527433     -0.3039244030     -2.8327662809
  C10      -0.0777143108     -1.5523720273      0.0576985200
  N2        1.4488571985      0.2405964825     -0.1932018788
  C9        1.7579802025     -0.2263947030      1.0638170614
  O1        2.5209988575      0.2942832667      1.8424136825
  H43      -0.0700832373     -2.5173417783     -0.4304175571
  C12      -1.4949180759     -1.2413892368      0.5129493676
 C11       0.9811773400     -1.5398482564      1.2270907973
 C19       0.4659579500     -1.7178383191      2.6568353895
 C13      -3.7222254631     -1.9981252113      1.0329216537
 C14      -3.1549314258      0.3109585359      1.3030473642
 C15      -4.0861862206     -0.7131167138      1.3891999051
 C16      -1.8709214494      0.0498545045      0.8645245825
 C17      -2.4314927785     -2.2586745468      0.5982152992
 H49      -4.4365138582     -2.7954896888      1.0884376683
 H50      -3.4309460803      1.3110397472      1.5719954712
 H51      -5.0828851243     -0.5073983284      1.7251130478
 H52      -1.1627481673      0.8502299116      0.7839994527
 H53      -2.1587629174     -3.2587445123      0.3207055370
 H1        1.2980171047     -1.6270403360      3.3432357362
 H2        0.0115670538     -2.6923926226      2.7817438135
 H3       -0.2684937664     -0.9654949508      2.9022079174
 H4        1.7040615676     -2.3234022778      1.0152955883

 nuclear repulsion energy.......  1458.164269921 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  16   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.218E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      84      85
 grid # 2       106     100      97      98      98      98      90      92
 grid # 3       224     183     182     194     182     182     187     183
 grid # 4       224     379     383     406     379     379     373     378

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      81      99      76
 grid # 2       106     106     105      92     106      93     109      81
 grid # 3       224     224     220     188     223     175     223     163
 grid # 4       224     224     219     377     229     351     401     328

 number of gridpoints:
    atom         O1     H43     C12     C11     C19     C13     C14     C15
 grid # 1       111      69      90      80      71      87      86      89
 grid # 2       123      98     105      91      75     100      99     100
 grid # 3       272     211     192     175     143     182     182     182
 grid # 4       475     205     398     361     302     378     379     378

 number of gridpoints:
    atom        C16     C17     H49     H50     H51     H52     H53      H1
 grid # 1        86      85      73      73      73      71      72      71
 grid # 2        97      99     106     106     106     100     103      99
```

```
  grid # 3      181    182    224    223    224    216    216    220
  grid # 4      376    377    224    223    224    211    215    221

  number of gridpoints:
     atom        H2     H3     H4  total
  grid # 1       72     71     69   2815
  grid # 2       99     97    100   3480
  grid # 3      219    214    219   7034
  grid # 4      220    212    210  10843

  end of program grid


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.13986953342           2.3E-04  4.7E-03
etot   2  Y  Y  4  M  -815.14072515920  8.6E-04  5.9E-05  1.9E-03
etot   3  Y  Y  4  M  -815.14082701500  1.0E-04  2.0E-05  5.8E-04
etot   4  Y  Y  4  M  -815.14083598704  9.0E-06  4.7E-06  1.1E-04
etot   5  Y  N  4  M  -815.14083440092 -1.6E-06  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.16426992119
   (E)  Total one-electron terms..... -4001.89442968404
   (I)  Total two-electron terms.....  1728.58932536193
   (L)  Electronic energy............ -2273.30510432211  (E+I)
   (N)  Total energy.................  -815.14083440092  (A+L)

 SCFE: SCF energy: HF    -815.14083440092 hartrees   iterations:   5


 HOMO energy:    -0.29718
 LUMO energy:     0.11762

  Orbital energies:
  -20.45370  -15.55225  -11.32170  -11.23594  -11.22328  -11.21502
  -11.20808  -11.19960  -11.18803  -11.18554  -11.18505  -11.18429
  -11.18286  -11.18244  -11.17945  -11.17767  -11.17729  -11.17597
  -11.17265  -11.16454   -1.42404   -1.33338   -1.18051   -1.16232
   -1.11399   -1.08794   -1.03814   -1.02704   -1.01975   -1.00135
   -0.94882   -0.90503   -0.85225   -0.84387   -0.83046   -0.81098
   -0.79139   -0.76042   -0.72223   -0.68647   -0.68145   -0.66769
   -0.65693   -0.64298   -0.64014   -0.62496   -0.61380   -0.60771
   -0.60460   -0.60062   -0.59238   -0.58275   -0.55145   -0.55046
   -0.53312   -0.52496   -0.51629   -0.51340   -0.49866   -0.49493
   -0.48932   -0.48500   -0.45833   -0.42193   -0.39443   -0.34887
   -0.34234   -0.31548   -0.29718    0.11762    0.13218    0.14173
    0.14375    0.20506    0.22177    0.26537    0.27161    0.28088
    0.30576

  end of program scf
 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.197154E-05  -3.880915E-06   1.229694E-04
  2    C1      2.984185E-04   4.405875E-05   4.568057E-04
  3    C2      1.595001E-05   8.264179E-05   9.744505E-05
  4    C3     -1.959970E-04  -1.769603E-04  -9.598780E-06
  5    C4     -1.869471E-04  -3.814459E-05  -1.383476E-04
  6    C5     -6.366497E-05   1.084360E-04  -2.396776E-05
  7    C6      1.042933E-04   1.069312E-04   8.012181E-05
  8    C7      4.713100E-04  -1.117033E-04   1.123877E-03
  9    H27    -5.305310E-05  -3.678573E-05   5.243826E-05
 10    H28    -7.178770E-05   3.900799E-05  -5.230254E-05
 11    H30    -1.215360E-04   4.206664E-05  -1.432929E-04
 12    C8      5.393340E-05   2.967724E-04  -5.197674E-04
 13    H32     7.980840E-05   4.358165E-05   1.381620E-04
 14    C10    -1.029962E-04  -1.452853E-04   1.431289E-04
 15    N2     -5.316417E-04  -1.233132E-04  -2.141295E-04
 16    C9     -8.354953E-08  -1.962254E-04  -2.192286E-04
 17    O1      1.518070E-04   3.110927E-04   4.136169E-04
 18    H43     3.056671E-05   1.269001E-04   1.276372E-04
 19    C12    -2.194066E-05   2.231110E-04  -1.390691E-05
 20    C11     2.798599E-04  -4.182236E-06   6.130963E-05
 21    C19    -1.670035E-05   2.200723E-04  -2.037433E-04
 22    C13    -5.759361E-05  -4.186729E-05   7.847741E-05
 23    C14     9.782830E-06   7.701788E-05   4.211381E-05
 24    C15    -1.405726E-04  -1.131644E-04   3.090309E-05
 25    C16     1.086979E-05  -3.001966E-06  -4.073413E-05
 26    C17    -1.597667E-04  -3.806436E-05   9.914423E-05
 27    H49     4.698751E-05   1.635266E-05   5.677084E-05
 28    H50    -6.116839E-05   2.871414E-05  -3.141397E-05
 29    H51     5.079675E-05  -2.489822E-05  -2.660579E-05
 30    H52    -4.261081E-05  -5.051763E-05  -1.129702E-05
 31    H53     4.514738E-05  -1.740629E-05   6.404544E-05
 32    H1      1.641576E-04   4.680346E-05   1.000537E-04
 33    H2     -9.250118E-05  -1.377518E-04   9.033128E-05
 34    H3     -1.964247E-04   2.572398E-04   1.096879E-04
 35    H4     -6.153486E-05   3.005876E-04   1.449111E-04
-----------   -------------  -------------  -------------
   total      -3.528606E-04   1.108235E-03   1.985614E-03

 end of program der1b


 start of program geopt  17

 geometry optimization step 17
 reading input hessian of dimension   105
```

```
    in five columns format
  reading input hessian of dimension   105
    in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0751531
   Cos(theta):   0.1398944

   Final level shift:  -9.9750025E-04

  energy change:           6.9958E-05 .  (  5.0000E-05 )
  gradient maximum:        1.1687E-03 .  (  4.5000E-04 )
  gradient rms:            1.9272E-04 *  (  3.0000E-04 )
  step size:   0.07515  trust radius:   0.07500
  displacement maximum:    2.8963E-02 .  (  1.8000E-03 )
  displacement rms:        6.7219E-03 .  (  1.2000E-03 )
  predicted energy change:    -1.4143E-05    geom step:   7.5153E-02    full step:
7.5153E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     6.5403E-03     y:    -5.5485E-03     z:    -1.3898E-03

  new geometry:
                              angstroms
  atom           x                  y                 z
  H25       0.9523043544      2.0228844652     -4.1578761179
  C1        1.4882412669      2.0651082600     -3.2308003563
  C2        2.9171873624      2.1964471422     -0.7955204938
  C3        1.2113743989      1.1636526768     -2.2108299389
  C4        2.4692560474      3.0161864616     -3.0274055224
  C5        3.1761045804      3.0809891666     -1.8229365206
  C6        1.9338937434      1.2505648816     -1.0115573822
  C7        0.2687725184      0.0487746506     -2.0763253576
  H27       2.6955995100      3.7184775796     -3.8047714502
  H28       3.9323554031      3.8294981639     -1.6965985259
  H30       3.4412635550      2.2216222956      0.1365995127
  C8        0.4577771765     -0.4715581071     -0.8565310416
  H32      -0.4374290286     -0.2676874363     -2.8085482367
  C10      -0.0822124159     -1.5426073678      0.0627312163
  N2        1.4623187192      0.2370446324     -0.1946817732
  C9        1.7789750641     -0.2387776618      1.0575874800
  O1        2.5579191190      0.2664833247      1.8298383584
  H43      -0.0689153689     -2.5045272812     -0.4314433251
  C12      -1.5027841764     -1.2409589637      0.5135244266
  C11       0.9777674755     -1.5352407914      1.2322599107
  C19       0.4551635531     -1.6806102949      2.6615929317
  C13      -3.7263843810     -2.0156193855      1.0277806658
  C14      -3.1774463774      0.2970466493      1.2998435515
  C15      -4.1013044448     -0.7343880633      1.3836439773
  C16      -1.8901359996      0.0464515357      0.8646329904
  C17      -2.4326361583     -2.2654154957      0.5963478763
  H49      -4.4339265189     -2.8190866444      1.0810592084
  H50      -3.4620841359      1.2953736400      1.5673938833
  H51      -5.1000801483     -0.5365813545      1.7173350416
  H52      -1.1894722085      0.8537524980      0.7841806965
  H53      -2.1517059326     -3.2634470667      0.3192560660
  H1        1.2910925935     -1.6164362241      3.3456089994
  H2       -0.0341695894     -2.6355055403      2.7952512699
  H3       -0.2502945170     -0.9001490950      2.9010905744
  H4        1.6846639744     -2.3358167404      1.0363003378
```

```
 nuclear repulsion energy.......  1457.320589003 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  17   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.216E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1       73     89     87     90     87     87     85     85
 grid # 2      106    100     97     98     98     98     90     92
 grid # 3      224    183    182    194    182    182    187    182
 grid # 4      224    379    381    406    379    379    372    376

 number of gridpoints:
    atom       H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1       73     73     73     86     73     81     99     76
 grid # 2      106    106    105     92    106     93    109     81
 grid # 3      224    224    220    188    223    175    223    163
 grid # 4      224    224    219    375    229    350    400    329

 number of gridpoints:
    atom        O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1      111     69     91     80     71     87     86     89
 grid # 2      123     98    106     90     78    100     99    100
 grid # 3      272    210    192    175    150    182    182    182
 grid # 4      476    205    397    361    305    378    379    378

 number of gridpoints:
    atom       C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1       86     85     73     73     73     71     72     71
 grid # 2       98     98    106    106    106    100    103     99
 grid # 3      181    182    224    223    224    216    216    220
 grid # 4      376    377    224    223    224    211    215    220

 number of gridpoints:
    atom        H2     H3     H4  total
 grid # 1       72     71     69   2817
 grid # 2       99     97    100   3483
 grid # 3      219    215    218   7039
 grid # 4      220    212    210  10837

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr
```

```
  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                   RMS    maximum
       e  d  i  u  i                        energy  density    DIIS
       r  t  s  t  d     total energy       change   change     error

etot   1  N  N  1  U  -815.13865806584             2.6E-04  6.4E-03
etot   2  Y  Y  4  M  -815.14059660199  1.9E-03  8.6E-05  2.6E-03
etot   3  Y  Y  4  M  -815.14081510825  2.2E-04  2.8E-05  7.7E-04
etot   4  N  Y  1  U  -815.14081752837  2.4E-06  8.8E-06  2.0E-04
etot   5  Y  Y  4  M  -815.14082012224  2.6E-06  5.8E-06  7.6E-05
etot   6  Y  Y  4  M  -815.14081890741 -1.2E-06  1.4E-06  1.8E-05
etot   7  Y  N  4  M  -815.14081864226 -2.7E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1457.32058900316
   (E)  Total one-electron terms..... -4000.20645587416
   (I)  Total two-electron terms.....  1727.74504822875
   (L)  Electronic energy............ -2272.46140764542  (E+I)
   (N)  Total energy.................  -815.14081864226  (A+L)

 SCFE: SCF energy: HF    -815.14081864226 hartrees   iterations:   7


 HOMO energy:    -0.29712
 LUMO energy:     0.11806

  Orbital energies:
  -20.45371  -15.55210  -11.32146  -11.23558  -11.22333  -11.21487
  -11.20760  -11.19972  -11.18793  -11.18565  -11.18509  -11.18446
  -11.18298  -11.18258  -11.17936  -11.17737  -11.17723  -11.17591
  -11.17264  -11.16418   -1.42414   -1.33316   -1.18043   -1.16236
   -1.11400   -1.08796   -1.03832   -1.02714   -1.01993   -1.00138
   -0.94893   -0.90487   -0.85243   -0.84374   -0.83058   -0.81091
   -0.79141   -0.76054   -0.72203   -0.68667   -0.68149   -0.66791
   -0.65693   -0.64321   -0.63985   -0.62509   -0.61383   -0.60778
   -0.60453   -0.60071   -0.59242   -0.58301   -0.55180   -0.55049
   -0.53307   -0.52479   -0.51659   -0.51330   -0.49865   -0.49479
   -0.48922   -0.48516   -0.45853   -0.42185   -0.39435   -0.34891
   -0.34253   -0.31559   -0.29712    0.11806    0.13236    0.14130
    0.14347    0.20540    0.22151    0.26530    0.27158    0.28109
    0.30593

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total
```

```
atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -9.714509E-05  -3.257278E-05  -1.121528E-04
  2    C1     -5.265814E-05  -2.693681E-05   1.131277E-04
  3    C2     -1.952882E-04  -1.443699E-04  -1.273786E-04
  4    C3     -1.316005E-04  -1.217149E-04   2.407945E-05
  5    C4     -2.992417E-04  -2.174768E-04   5.100155E-06
  6    C5      2.184925E-04  -5.758959E-05   3.679022E-04
  7    C6      1.913134E-04   7.440717E-05   2.585191E-04
  8    C7      3.738927E-04   2.401980E-04   1.769582E-04
  9    H27    -3.651172E-05  -3.443829E-05   5.519440E-05
 10    H28    -5.209564E-05   8.625356E-05   3.790467E-05
 11    H30    -7.893815E-05   6.391138E-05   1.915184E-04
 12    C8     -9.496197E-05  -1.952724E-04   2.783432E-04
 13    H32    -1.638826E-04  -6.141544E-07  -1.086887E-04
 14    C10     5.812520E-04   2.101190E-04  -5.842982E-04
 15    N2      6.798214E-05   2.388671E-04   2.010705E-04
 16    C9     -9.466315E-04   4.679452E-06  -7.650692E-04
 17    O1      8.266055E-04   7.731313E-04   4.903099E-04
 18    H43    -1.184080E-04   2.799531E-05   2.039415E-04
 19    C12    -7.060573E-06  -5.426534E-04   3.914983E-04
 20    C11    -5.394716E-04   2.453575E-04  -4.424123E-04
 21    C19     6.348664E-04  -1.302009E-05   4.374722E-04
 22    C13     1.414945E-04  -5.315286E-04  -3.384947E-05
 23    C14    -3.197303E-04   1.713609E-04   8.139079E-05
 24    C15     1.692794E-04   7.068616E-04   1.260571E-04
 25    C16    -3.596334E-05   6.468250E-04  -1.687591E-04
 26    C17     3.884811E-04  -1.305372E-04  -5.514099E-05
 27    H49     5.970259E-06   2.710949E-05   5.098301E-05
 28    H50    -3.394615E-05  -1.874641E-04  -2.031334E-05
 29    H51    -1.106429E-04   4.755142E-05   1.155310E-05
 30    H52     3.537694E-06  -2.338354E-04   8.117635E-05
 31    H53     6.897872E-05   5.498239E-05   5.403514E-05
 32    H1      2.216998E-04   3.777372E-04   5.846765E-04
 33    H2     -5.599748E-04  -8.675184E-04   9.457231E-05
 34    H3     -4.848391E-04   6.374137E-04   1.803960E-04
 35    H4      1.634506E-04  -1.760632E-04  -2.178885E-04
-----------   -------------  -------------  -------------
   total      -3.016952E-04   1.121156E-03   1.861829E-03

 end of program der1b


 start of program geopt  18

 geometry optimization step 18
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
 ** restarting optimization from step   17 **


 energy change:            1.5759E-05 *  (  5.0000E-05 )
 gradient maximum:         1.1687E-03 .  (  4.5000E-04 )
 gradient rms:             1.9272E-04 *  (  3.0000E-04 )
 step size:    0.02271  trust radius:    0.03750
 displacement maximum:     8.7344E-03 .  (  1.8000E-03 )
 displacement rms:         2.0313E-03 .  (  1.2000E-03 )
```

```
  predicted energy change:    -6.8780E-06    geom step:   2.2710E-02    full step:
2.2710E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.1102E-16     y:    -3.6082E-16     z:    -1.9429E-16

  new geometry:
                              angstroms
  atom             x                 y                 z
  H25       0.9691123401      2.0026052249     -4.1682374285
  C1        1.4959039365      2.0520277423     -3.2360989400
  C2        2.9008081761      2.2038027082     -0.7874684015
  C3        1.2162795977      1.1524833078     -2.2154569619
  C4        2.4680917158      3.0108306486     -3.0264011266
  C5        3.1637220597      3.0858023170     -1.8156263311
  C6        1.9264330285      1.2504843245     -1.0096435851
  C7        0.2817883561      0.0304766669     -2.0855509728
  H27       2.6966918383      3.7119562671     -3.8041645925
  H28       3.9129563436      3.8407758309     -1.6854507989
  H30       3.4139669784      2.2363381494      0.1505218551
  C8        0.4631899543     -0.4834104631     -0.8618808724
  H32      -0.4154905750     -0.2937410206     -2.8232490637
  C10      -0.0772984410     -1.5517571311      0.0593485400
  N2        1.4548027425      0.2373941836     -0.1932554808
  C9        1.7660730069     -0.2317557082      1.0622776853
  O1        2.5335999013      0.2852691803      1.8391901330
  H43      -0.0688662411     -2.5158397838     -0.4304096692
  C12      -1.4954578168     -1.2424988550      0.5129606892
  C11       0.9824188093     -1.5407415500      1.2283701049
  C19       0.4646744849     -1.7108803820      2.6578471986
  C13      -3.7216987793     -2.0025538841      1.0337037536
  C14      -3.1600576730      0.3090200073      1.2949625992
  C15      -4.0890157520     -0.7170141458      1.3842969181
  C16      -1.8749294132      0.0490639810      0.8589459755
  C17      -2.4299685751     -2.2617535171      0.6013162198
  H49      -4.4342283300     -2.8012858302      1.0915651582
  H50      -3.4388838231      1.3096730404      1.5589866507
  H51      -5.0866240691     -0.5121877952      1.7179744726
  H52      -1.1685220787      0.8507890933      0.7753405810
  H53      -2.1546207922     -3.2622027141      0.3276576760
  H1        1.2977642999     -1.6267729688      3.3438826657
  H2        0.0013374820     -2.6812715426      2.7843894868
  H3       -0.2630988223     -0.9515104119      2.9017504428
  H4        1.7013290169     -2.3284347886      1.0198974999

  nuclear repulsion energy.......  1458.041289416 hartrees
  -------------------------------------------------
 /  end of geometry optimization iteration  18   /
 -------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.216E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe
  start of program grid

  number of gridpoints:
     atom        H25     C1      C2      C3      C4      C5      C6      C7
  grid # 1        73     89      87      90      87      87      84      85
  grid # 2       106    100      97      98      98      98      90      92
  grid # 3       224    183     182     194     182     182     187     182
  grid # 4       224    379     381     404     379     379     373     377

  number of gridpoints:
     atom        H27    H28     H30      C8     H32     C10      N2      C9
  grid # 1        73     73      73      86      73      81      99      76
  grid # 2       106    106     105      92     106      93     109      81
  grid # 3       224    224     220     188     223     175     223     163
  grid # 4       224    224     219     377     229     351     401     330

  number of gridpoints:
     atom         O1    H43     C12     C11     C19     C13     C14     C15
  grid # 1       111     69      90      80      71      87      86      89
  grid # 2       123     98     106      91      75     100      99     100
  grid # 3       272    211     192     175     148     182     182     182
  grid # 4       475    205     397     361     306     378     379     378

  number of gridpoints:
     atom        C16    C17     H49     H50     H51     H52     H53      H1
  grid # 1        86     85      73      73      73      71      72      71
  grid # 2        97     99     106     106     106     100     103      99
  grid # 3       181    182     224     223     224     216     216     220
  grid # 4       376    377     224     223     224     211     215     221

  number of gridpoints:
     atom         H2     H3      H4   total
  grid # 1        72     71      69    2815
  grid # 2        99     97     100    3481
  grid # 3       219    214     218    7037
  grid # 4       220    212     211   10844

  end of program grid


  start of program rwr
 recomputing RwR matrix   4    grid:  4
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                       RMS    maximum
       e  d  i  u  i                            energy  density    DIIS
       r  t  s  t  d     total energy           change   change     error

etot   1  N  N  1  U  -815.13977302674                  1.7E-04  4.2E-03
etot   2  Y  Y  4  M  -815.14074943281  9.8E-04  6.0E-05  1.7E-03
etot   3  Y  Y  4  M  -815.14085562208  1.1E-04  2.0E-05  5.1E-04
etot   4  Y  Y  4  M  -815.14086453518  8.9E-06  6.1E-06  1.4E-04
etot   5  Y  Y  4  M  -815.14086402956 -5.1E-07  2.8E-06  5.7E-05
etot   6  N  N  1  U  -815.14086918459  5.2E-06  0.0E+00  0.0E+00
```

```
Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.04128941568
   (E)  Total one-electron terms..... -4001.64966974635
   (I)  Total two-electron terms.....  1728.46751114608
   (L)  Electronic energy............ -2273.18215860027  (E+I)
   (N)  Total energy.................  -815.14086918459  (A+L)

SCFE: SCF energy: HF    -815.14086918459 hartrees   iterations:   6


HOMO energy:    -0.29724
LUMO energy:     0.11777

 Orbital energies:
 -20.45378  -15.55207  -11.32152  -11.23561  -11.22326  -11.21490
 -11.20788  -11.19960  -11.18792  -11.18560  -11.18509  -11.18435
 -11.18293  -11.18246  -11.17942  -11.17743  -11.17728  -11.17596
 -11.17266  -11.16451   -1.42384   -1.33333   -1.18047   -1.16239
  -1.11397   -1.08812   -1.03817   -1.02707   -1.01977   -1.00144
  -0.94885   -0.90500   -0.85232   -0.84384   -0.83049   -0.81100
  -0.79140   -0.76046   -0.72215   -0.68653   -0.68143   -0.66777
  -0.65702   -0.64298   -0.64006   -0.62498   -0.61382   -0.60773
  -0.60459   -0.60066   -0.59243   -0.58277   -0.55153   -0.55050
  -0.53303   -0.52491   -0.51633   -0.51338   -0.49865   -0.49485
  -0.48923   -0.48503   -0.45839   -0.42185   -0.39452   -0.34889
  -0.34239   -0.31553   -0.29724    0.11777    0.13217    0.14154
   0.14376    0.20521    0.22183    0.26534    0.27160    0.28100
   0.30576

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   4    grid:  4
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -4.693834E-06  -8.536052E-06  -9.477689E-06
  2    C1      5.312281E-05   2.333710E-04  -2.483551E-04
  3    C2     -1.833768E-04  -6.200875E-05   1.213958E-04
  4    C3      2.360595E-05   1.543685E-04  -1.769862E-04
  5    C4     -1.190726E-04  -3.329791E-05  -1.044302E-04
  6    C5      1.324267E-04   2.879325E-04  -3.543594E-05
  7    C6      1.939427E-04   9.500827E-05   4.294962E-04
  8    C7     -5.427043E-04  -1.815920E-04  -7.488224E-04
  9    H27    -3.809239E-05  -2.832740E-05   4.267616E-05
 10    H28    -8.183383E-05   9.564089E-06   3.065118E-05
 11    H30    -8.362424E-06   5.785376E-05   1.054813E-04
```

```
  12    C8      9.885833E-05  -3.409003E-05   3.741176E-04
  13    H32    -2.808300E-05  -4.455581E-05  -3.076627E-06
  14    C10     1.443162E-04   3.807262E-05  -2.955898E-05
  15    N2     -5.342666E-05   2.652246E-06   8.271801E-05
  16    C9     -6.922791E-05   8.144113E-05   9.138950E-05
  17    O1      1.041462E-04   1.331836E-04   2.390290E-04
  18    H43     6.315669E-05   6.748431E-05   1.211675E-04
  19    C12    -9.873606E-06   4.843629E-06   6.704167E-05
  20    C11    -4.701879E-05   3.425245E-05   5.484379E-05
  21    C19     7.101177E-05  -9.360090E-05   6.413146E-05
  22    C13     1.140034E-06  -8.721278E-05   4.191634E-05
  23    C14    -6.656143E-05   4.531795E-07   1.070701E-05
  24    C15    -7.789365E-05   9.935069E-05   3.943782E-05
  25    C16     7.039105E-05   1.858857E-04   5.823771E-05
  26    C17     1.499683E-05   5.168636E-05   4.994690E-05
  27    H49     4.346869E-05   6.611577E-06   4.935697E-05
  28    H50    -5.249022E-05  -2.031589E-05  -5.083300E-06
  29    H51     4.523268E-05  -2.634252E-05  -1.244838E-05
  30    H52    -1.127282E-04  -5.029799E-05   2.311132E-05
  31    H53     3.027417E-05   1.288317E-06   7.768338E-05
  32    H1      7.148042E-05   1.292712E-04   1.911439E-04
  33    H2     -1.856161E-05   3.442169E-05   7.260594E-05
  34    H3     -1.450266E-04   2.548167E-04   6.706089E-05
  35    H4     -4.577715E-05   1.177452E-04   1.090271E-04
 -----------   -------------  -------------  -------------
    total      -5.432339E-04   1.411381E-03   1.240700E-03

  end of program der1b


  start of program geopt  19

  geometry optimization step 19
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  energy change:          -3.4784E-05 *  (  5.0000E-05 )
  gradient maximum:        7.9740E-04 .  (  4.5000E-04 )
  gradient rms:            1.4807E-04 *  (  3.0000E-04 )
  step size:   0.02057  trust radius:   0.03750
  displacement maximum:    8.1281E-03 .  (  1.8000E-03 )
  displacement rms:        1.8398E-03 .  (  1.2000E-03 )
  predicted energy change:    -5.0538E-06    geom step:   2.0569E-02    full step:
2.0569E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:    -2.1783E-03     y:     1.9267E-03     z:    -5.4660E-05

  new geometry:
                              angstroms
  atom            x                 y                 z
  H25       0.9818550776      1.9972801411     -4.1755921599
  C1        1.5035662044      2.0487348174     -3.2405840752
  C2        2.8954433299      2.2063464126     -0.7842616669
  C3        1.2193303606      1.1504055055     -2.2195473053
  C4        2.4740838515      3.0082393961     -3.0275099185
 C5        3.1636657740      3.0863436732     -1.8132345501
 C6        1.9231995801      1.2520087950     -1.0094927038
 C7        0.2859811523      0.0259566200     -2.0924979019
 H27       2.7066263905      3.7077415529     -3.8054893319
 H28       3.9121041894      3.8414115578     -1.6808896174
 H30       3.4040148155      2.2402602466      0.1563966254
 C8        0.4630033868     -0.4845998200     -0.8657563713
 H32      -0.4068094184     -0.3014848451     -2.8333605909
 C10      -0.0774172777     -1.5523228495      0.0562450893
 N2        1.4496847525      0.2397859861     -0.1935734784
 C9        1.7589712801     -0.2276254023      1.0633228445
 O1        2.5225814148      0.2927658607      1.8424425761
 H43      -0.0693641985     -2.5169798697     -0.4320253828
 C12      -1.4948376199     -1.2421815161      0.5116663259
 C11       0.9811669604     -1.5404250426      1.2260893492
 C19       0.4651956910     -1.7186846674      2.6558241784
 C13      -3.7192219353     -2.0018648841      1.0393947534
 C14      -3.1566177948      0.3094136028      1.2992014420
 C15      -4.0852370599     -0.7162358910      1.3914427975
 C16      -1.8729160009      0.0494596538      0.8588267705
 C17      -2.4290286435     -2.2611193444      0.6026220874
 H49      -4.4315175099     -2.8004336815      1.0998504652
 H50      -3.4344224628      1.3096826723      1.5649294039
 H51      -5.0814784885     -0.5115310569      1.7287971910
 H52      -1.1663593547      0.8504059457      0.7739018933
 H53      -2.1544833771     -3.2615647434      0.3283553469
 H1        1.2971650295     -1.6271720341      3.3427392660
 H2        0.0114235914     -2.6942232448      2.7803626009
 H3       -0.2704675963     -0.9663762880      2.9005583831
 H4        1.7036434509     -2.3239227438      1.0141499674

 nuclear repulsion energy.......  1458.077810503 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  19   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.218E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      84      85
 grid # 2       106      99      97      98      98      99      90      92
 grid # 3       224     183     182     194     182     182     187     183
 grid # 4       224     379     381     404     379     379     374     378

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      81      99      76
 grid # 2       106     106     105      92     106      93     109      81
```

```
  grid # 3      224    224    220    188    223    175    223    163
  grid # 4      224    224    219    377    229    351    401    328

  number of gridpoints:
     atom         O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1      111     69     90     80     71     87     86     89
  grid # 2      127     98    105     90     75    100     99    100
  grid # 3      272    211    192    175    143    182    182    182
  grid # 4      475    205    398    361    302    378    378    378

  number of gridpoints:
     atom        C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1       86     85     73     73     73     71     72     71
  grid # 2       97     99    106    106    106    100    103     99
  grid # 3      181    182    224    223    224    216    216    220
  grid # 4      376    377    224    223    224    211    215    221

  number of gridpoints:
     atom         H2     H3     H4  total
  grid # 1       72     71     69   2815
  grid # 2       99     97    100   3483
  grid # 3      219    214    219   7034
  grid # 4      220    212    211  10840

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                       RMS    maximum
       e  d  i  u  i                          energy  density    DIIS
       r  t  s  t  d     total energy    change  change     error

etot   1  N  N  1  U  -815.14068106164            7.4E-05  1.7E-03
etot   2  Y  Y  4  M  -815.14082673905  1.5E-04  2.5E-05  6.9E-04
etot   3  Y  Y  4  M  -815.14084364367  1.7E-05  8.2E-06  2.0E-04
etot   4  Y  Y  4  M  -815.14084582692  2.2E-06  2.8E-06  6.5E-05
etot   5  Y  N  4  M  -815.14084528445 -5.4E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion...........  1458.07781050310
   (E)  Total one-electron terms..... -4001.72287518358
   (I)  Total two-electron terms.....  1728.50421939603
   (L)  Electronic energy............ -2273.21865578755  (E+I)
   (N)  Total energy.................  -815.14084528445  (A+L)

 SCFE: SCF energy: HF    -815.14084528445 hartrees   iterations:   5


 HOMO energy:    -0.29718
 LUMO energy:     0.11756

  Orbital energies:
  -20.45386  -15.55223  -11.32170  -11.23591  -11.22330  -11.21493
 -11.20802  -11.19952  -11.18816  -11.18551  -11.18503  -11.18428
 -11.18284  -11.18237  -11.17945  -11.17779  -11.17730  -11.17602
 -11.17266  -11.16476   -1.42368   -1.33331   -1.18050   -1.16228
  -1.11397   -1.08792   -1.03814   -1.02705   -1.01972   -1.00135
  -0.94878   -0.90504   -0.85219   -0.84392   -0.83048   -0.81108
  -0.79139   -0.76036   -0.72224   -0.68647   -0.68145   -0.66768
  -0.65700   -0.64293   -0.64012   -0.62492   -0.61381   -0.60765
  -0.60457   -0.60065   -0.59240   -0.58273   -0.55138   -0.55037
  -0.53302   -0.52497   -0.51627   -0.51337   -0.49866   -0.49484
  -0.48929   -0.48501   -0.45832   -0.42196   -0.39445   -0.34887
  -0.34235   -0.31550   -0.29718    0.11756    0.13213    0.14165
   0.14386    0.20493    0.22186    0.26539    0.27161    0.28089
   0.30571

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label        x              y              z
----  -----  -------------  -------------  -------------
  1    H25     2.424568E-05  -3.115446E-05   7.463959E-05
  2    C1     -1.555598E-04  -3.829115E-04   3.065764E-04
  3    C2      1.294631E-04   1.999968E-04  -5.868255E-06
  4    C3      1.624728E-04   8.827454E-05   3.035139E-04
  5    C4      1.652816E-04   1.988854E-04   9.723509E-05
  6    C5     -3.737918E-04  -3.152560E-04   5.301535E-05
  7    C6     -3.332694E-04   3.176134E-05  -5.941027E-04
  8    C7      1.859352E-04   1.574059E-04   4.077391E-04
  9    H27    -4.683888E-05   1.755935E-05  -6.516968E-06
 10    H28     8.422774E-06   1.454940E-04   3.008530E-05
 11    H30    -7.952955E-05   1.303564E-04  -2.745551E-05
 12    C8      3.701530E-05   5.490657E-05  -1.536830E-04
 13    H32     1.105457E-04   7.260766E-07   1.788229E-04
 14    C10    -2.146618E-04  -4.734726E-05   2.206708E-04
 15    N2     -6.621686E-05   1.170240E-04  -1.106757E-04
 16    C9      2.970400E-04   2.100465E-04   3.229260E-04
 17    O1     -4.180399E-04  -1.464746E-04  -1.941379E-04
 18    H43     2.826537E-05  -1.560312E-06   3.341359E-05
 19    C12     1.095271E-04   1.680786E-04  -5.617205E-05
 20    C11     1.843508E-04   4.756667E-05   2.076465E-04
 21    C19    -2.162867E-04   2.089874E-04  -1.151779E-04
 22    C13    -2.201426E-05   3.751327E-05   3.511998E-05
 23    C14     1.338730E-04   9.182780E-05  -3.520179E-05
 24    C15    -1.109228E-04  -2.412548E-04   4.269815E-06
 25    C16    -3.150924E-05  -1.047533E-04   1.303484E-04
 26    C17    -1.469854E-04  -6.085954E-05   1.215089E-04
 27    H49    -2.744107E-05  -7.441840E-05   3.749067E-05
 28    H50    -6.029451E-05   1.530210E-04  -4.934888E-06
 29    H51    -6.258494E-05   3.056009E-06   1.130083E-05
```

```
   30    H52      9.100027E-06   1.994005E-04  -1.231526E-05
   31    H53      2.069299E-05  -4.328999E-05   6.340328E-05
   32    H1      -4.565300E-05   3.175692E-05  -3.037080E-05
   33    H2       5.821561E-05   2.757288E-04   7.592706E-05
   34    H3       1.349333E-04  -9.437877E-05   3.255550E-05
   35    H4       4.843881E-05   1.113567E-04   1.452244E-04
 -----------   -------------  -------------  -------------
     total      -5.637807E-04   1.137072E-03   1.546821E-03

   end of program der1b


   start of program geopt  20

   geometry optimization step 20
   reading input hessian of dimension   105
    in five columns format
   reading input hessian of dimension   105
    in five columns format
   reading input hessian of dimension   105
    in five columns format


   energy change:           2.3900E-05 *  (  5.0000E-05 )
   gradient maximum:        6.4249E-04 .  (  4.5000E-04 )
   gradient rms:            1.4253E-04 *  (  3.0000E-04 )
   step size:   0.00819  trust radius:   0.01875
   displacement maximum:    4.8630E-03 .  (  1.8000E-03 )
   displacement rms:        7.3297E-04 *  (  1.2000E-03 )
   predicted energy change:    -3.0160E-06    geom step:   8.1948E-03    full step:
 8.1948E-03
   molecular structure not yet converged...

   center of mass moved by:
      x:     5.4452E-04     y:    -5.5842E-04     z:     2.3272E-04

   new geometry:
                              angstroms
   atom           x                 y                 z
   H25       0.9780486660      1.9961213859     -4.1739967801
   C1        1.5008336761      2.0480116596     -3.2396574468
   C2        2.8954368886      2.2065876594     -0.7851978873
   C3        1.2183324032      1.1498756138     -2.2183868326
   C4        2.4708341224      3.0084897295     -3.0277426499
   C5        3.1614359311      3.0869342845     -1.8142090384
   C6        1.9235589862      1.2514883525     -1.0096161345
   C7        0.2852020013      0.0257653097     -2.0902565089
   H27       2.7017607315      3.7082905097     -3.8059179428
   H28       3.9092329942      3.8429759519     -1.6823444360
   H30       3.4049726926      2.2413275299      0.1548902333
   C8        0.4638310224     -0.4853600022     -0.8643297795
   H32      -0.4086725090     -0.3014624790     -2.8299116928
   C10      -0.0765879561     -1.5529835400      0.0578494034
   N2        1.4512867532      0.2389371751     -0.1931910842
   C9        1.7610046795     -0.2284615371      1.0636910123
   O1        2.5247323699      0.2914246810      1.8425639254
   H43      -0.0685591520     -2.5176747174     -0.4305278007
   C12      -1.4941710230     -1.2422634388      0.5125447714
   C11       0.9826110193     -1.5408239610      1.2271839336
   C19       0.4660866737     -1.7173425538      2.6565273184
   C13      -3.7207076005     -2.0003850902      1.0347895574
   C14      -3.1559086270      0.3101198811      1.2990287889
 C15      -4.0860222215     -0.7148367995      1.3878242176
 C16      -1.8715278555      0.0493450768      0.8611129013
 C17      -2.4298128304     -2.2604277464      0.6003731687
 H49      -4.4340360687     -2.7983749290      1.0924054967
 H50      -3.4332310023      1.3105940230      1.5651689592
 H51      -5.0828510353     -0.5093524391      1.7231330963
 H52      -1.1643148489      0.8501601142      0.7781489175
 H53      -2.1559524324     -3.2608420377      0.3250133694
 H1        1.2987075117     -1.6308470329      3.3429331878
 H2        0.0075520288     -2.6903664105      2.7806146151
 H3       -0.2654108223     -0.9618400553      2.9023581637
 H4        1.7047472495     -2.3249671724      1.0161251348

 nuclear repulsion energy.......  1458.113445894 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  20   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.217E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1       73      89      87      90      87      87      84      85
 grid # 2      106     100      97      98      98      98      90      92
 grid # 3      224     183     182     194     182     182     187     183
 grid # 4      224     379     381     404     379     379     373     378

 number of gridpoints:
    atom       H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1       73      73      73      86      73      81      99      76
 grid # 2      106     106     105      92     106      93     109      81
 grid # 3      224     224     220     188     223     175     223     163
 grid # 4      224     224     219     377     229     351     401     328

 number of gridpoints:
    atom        O1     H43     C12     C11     C19     C13     C14     C15
 grid # 1      111      69      90      80      72      87      86      89
 grid # 2      123      98     105      91      74     100      99     100
 grid # 3      273     211     192     175     145     182     182     182
 grid # 4      475     205     397     361     308     378     379     378

 number of gridpoints:
    atom       C16     C17     H49     H50     H51     H52     H53      H1
 grid # 1       86      85      73      73      73      71      72      71
 grid # 2       97      99     106     106     106     100     103      99
 grid # 3      181     182     224     223     224     216     216     220
 grid # 4      376     377     224     223     224     211     215     221

 number of gridpoints:
    atom        H2     H3     H4  total
 grid # 1       72     71     69   2816
 grid # 2       99     97    100   3479
 grid # 3      219    214    219   7037
 grid # 4      220    212    211  10845

 end of program grid


 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

        i  u  d  i  g
        t  p  i  c  r                                RMS    maximum
        e  d  i  u  i                      energy  density   DIIS
        r  t  s  t  d     total energy     change   change    error

etot    1  N  N  1  U  -815.14079876061            3.3E-05  5.6E-04
etot    2  Y  Y  4  M  -815.14082533615  2.7E-05  1.1E-05  2.0E-04
etot    3  Y  Y  4  M  -815.14082991026  4.6E-06  3.3E-06  6.3E-05
etot    4  Y  N  4  M  -815.14082868622 -1.2E-06  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1458.11344589424
  (E)  Total one-electron terms..... -4001.79392558639
  (I)  Total two-electron terms.....  1728.53965100593
  (L)  Electronic energy............ -2273.25427458046  (E+I)
  (N)  Total energy.................  -815.14082868622  (A+L)

SCFE: SCF energy: HF    -815.14082868622 hartrees   iterations:   4


HOMO energy:    -0.29720
LUMO energy:     0.11766

 Orbital energies:
 -20.45379  -15.55221  -11.32168  -11.23582  -11.22328  -11.21496
 -11.20797  -11.19962  -11.18798  -11.18557  -11.18507  -11.18434
 -11.18288  -11.18244  -11.17943  -11.17759  -11.17730  -11.17598
 -11.17268  -11.16458   -1.42383   -1.33334   -1.18046   -1.16232
  -1.11398   -1.08797   -1.03813   -1.02704   -1.01975   -1.00137
  -0.94880   -0.90503   -0.85223   -0.84385   -0.83046   -0.81103
  -0.79138   -0.76040   -0.72220   -0.68649   -0.68144   -0.66771
  -0.65698   -0.64295   -0.64011   -0.62495   -0.61380   -0.60771
  -0.60458   -0.60064   -0.59240   -0.58275   -0.55144   -0.55045
  -0.53306   -0.52495   -0.51630   -0.51338   -0.49866   -0.49485
  -0.48926   -0.48503   -0.45838   -0.42191   -0.39445   -0.34887
  -0.34235   -0.31550   -0.29720    0.11766    0.13210    0.14164
   0.14383    0.20505    0.22188    0.26536    0.27161    0.28091
   0.30573

 end of program scf


 start of program der1a
 end of program der1a
 start of program rwr
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label          x              y              z
----  -----   -------------  -------------  -------------
  1    H25     1.812915E-05  -2.766039E-05   4.707356E-05
  2    C1     -7.089778E-06  -4.019904E-05   1.440926E-04
  3    C2     -2.028233E-05   7.654699E-05   5.486318E-05
  4    C3     -9.562110E-05  -1.607636E-04   2.144656E-04
  5    C4      4.643877E-06   5.431443E-05   1.466458E-05
  6    C5     -1.363600E-04  -6.356268E-05   2.737090E-05
  7    C6     -1.230375E-04   5.185798E-05  -1.439237E-04
  8    C7      6.094317E-04   1.554960E-04   8.675479E-04
  9    H27    -2.745385E-05   8.271607E-06  -3.242029E-06
 10    H28    -7.012470E-05   5.055046E-05   2.228500E-06
 11    H30    -8.514611E-05   8.517052E-05  -1.482511E-05
 12    C8     -6.515310E-05   1.666852E-04  -2.074684E-04
 13    H32     4.148572E-05  -1.315540E-05   4.361482E-05
 14    C10     1.737517E-05   3.339913E-05   1.193228E-04
 15    N2     -7.626788E-05  -1.431270E-05   5.975845E-06
 16    C9     -9.664519E-06  -1.177071E-05   5.064286E-06
 17    O1     -5.795894E-05   1.134155E-04   8.725729E-05
 18    H43     1.094856E-05   4.191556E-05   8.590097E-05
 19    C12     1.416655E-05   7.095468E-05   4.725708E-05
 20    C11     8.681527E-05   2.265826E-05   7.092116E-05
 21    C19    -3.444562E-05   1.034229E-04  -2.629556E-05
 22    C13     1.489727E-05   2.785608E-05   4.505978E-05
 23    C14     9.330672E-06   2.787970E-06  -7.790729E-06
 24    C15    -2.640668E-05  -5.795500E-05   1.433778E-05
 25    C16    -2.944042E-05  -4.977597E-05   2.773794E-06
 26    C17    -2.032582E-05   3.694601E-05   6.817067E-05
 27    H49     1.634454E-05  -1.427022E-05   6.198647E-05
 28    H50    -4.695122E-05   1.953656E-05  -1.195998E-05
 29    H51    -2.321015E-05  -1.212242E-05   1.480052E-05
 30    H52    -2.386207E-05   6.257389E-05   4.411822E-06
 31    H53     2.731504E-05   1.882658E-05   8.348701E-05
 32    H1      5.931836E-05   1.039116E-04   1.247230E-04
 33    H2     -2.688154E-05   5.765152E-05   7.511585E-05
 34    H3     -4.127689E-05   9.617275E-05   4.711949E-05
 35    H4     -3.957826E-05   1.299747E-04   1.216823E-04
-----------   -------------  -------------  -------------
   total      -1.563366E-04   1.125349E-03   2.085784E-03

 end of program der1b


 start of program geopt  21

 geometry optimization step 21
 reading input hessian of dimension   105
  in five columns format
 reading input hessian of dimension   105
  in five columns format
  energy change:           1.6598E-05 *  (  5.0000E-05 )
  gradient maximum:        7.9456E-04 .  (  4.5000E-04 )
  gradient rms:            1.3298E-04 *  (  3.0000E-04 )
  step size:   0.01505  trust radius:   0.01875
  displacement maximum:    5.5946E-03 .  (  1.8000E-03 )
  displacement rms:        1.3457E-03 .  (  1.2000E-03 )
  predicted energy change:   -3.6834E-06   geom step:   1.5045E-02   full step:
1.5045E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     1.6490E-03     y:    -1.4211E-03     z:     3.7132E-04

  new geometry:
                                  angstroms
  atom            x                 y                 z
  H25       0.9679252140      1.9995865025     -4.1685695377
  C1        1.4942765518      2.0504903076     -3.2362485236
  C2        2.8983907431      2.2054239111     -0.7872535192
  C3        1.2159798640      1.1512715132     -2.2151129252
  C4        2.4651427962      3.0110198391     -3.0266126689
  C5        3.1597442600      3.0874706532     -1.8155219675
  C6        1.9257540708      1.2502367326     -1.0095001459
  C7        0.2833941252      0.0283325203     -2.0850736485
  H27       2.6930790201      3.7121552437     -3.8046278870
  H28       3.9077584865      3.8439593980     -1.6850912561
  H30       3.4114228299      2.2394925776      0.1508885164
  C8        0.4648374494     -0.4853881381     -0.8615831873
  H32      -0.4132907043     -0.2969342577     -2.8227460590
  C10      -0.0760738086     -1.5532452003      0.0596746863
  N2        1.4557458587      0.2362897095     -0.1928646593
  C9        1.7659006672     -0.2323681061      1.0635163228
  O1        2.5310278902      0.2856205735      1.8421794536
  H43      -0.0682821675     -2.5175957578     -0.4301255372
  C12      -1.4939641773     -1.2421258641      0.5130251511
  C11       0.9835472390     -1.5423213040      1.2284536950
  C19       0.4652749284     -1.7136764323      2.6569296068
  C13      -3.7215659559     -1.9997650225      1.0323073128
  C14      -3.1574946064      0.3112650565      1.2933851244
  C15      -4.0877041931     -0.7138524773      1.3823460222
  C16      -1.8722501509      0.0499204747      0.8586583833
  C17      -2.4298154666     -2.2603253997      0.6009079149
  H49      -4.4349206374     -2.7979443154      1.0899417612
  H50      -3.4356423453      1.3125462746      1.5566535494
  H51      -5.0854179979     -0.5078120278      1.7153970222
  H52      -1.1654893432      0.8514857610      0.7747401729
  H53      -2.1554169838     -3.2612607540      0.3275720461
  H1        1.2977799451     -1.6331087809      3.3435872640
  H2       -0.0008132081     -2.6820625162      2.7816154724
  H3       -0.2598332994     -0.9530804288      2.9015742349
  H4        1.7028937814     -2.3295423747      1.0196947165

  nuclear repulsion energy.......  1458.177165184 hartrees
  ------------------------------------------------
 /  end of geometry optimization iteration  21   /
 ------------------------------------------------

  end of program geopt


  start of program onee
  smallest eigenvalue of S:    1.215E-03
  number of canonical orbitals.....          210
  end of program onee


  start of program probe
  end of program probe


  start of program grid

  number of gridpoints:
     atom       H25     C1     C2     C3     C4     C5     C6     C7
  grid # 1       73     89     87     90     87     87     84     85
  grid # 2      106    100     97     98     98     98     90     92
  grid # 3      224    183    182    194    182    182    187    182
  grid # 4      224    379    381    404    379    379    372    377

  number of gridpoints:
     atom       H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1       73     73     73     86     73     81     99     76
  grid # 2      106    106    105     92    106     93    109     81
  grid # 3      224    224    220    188    223    175    223    163
  grid # 4      224    224    219    376    229    351    401    330

  number of gridpoints:
     atom        O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1      111     69     90     80     71     87     86     89
  grid # 2      123     98    106     91     75    100     99    100
  grid # 3      272    211    192    175    148    182    182    182
  grid # 4      475    205    397    361    305    378    379    378

  number of gridpoints:
     atom       C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1       86     85     73     73     73     71     72     71
  grid # 2       97     99    106    106    106    100    103     99
  grid # 3      181    182    224    223    224    216    216    220
  grid # 4      376    377    224    223    224    211    215    221

  number of gridpoints:
     atom        H2     H3     H4  total
  grid # 1       72     71     69   2815
  grid # 2       99     97    100   3481
  grid # 3      219    214    218   7037
  grid # 4      220    212    210  10840

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change     error

etot   1  N  N  1  U  -815.14059337867           1.2E-04  1.1E-03
etot   2  Y  Y  4  M  -815.14067358434  8.0E-05  2.0E-05  4.6E-04
etot   3  Y  Y  4  M  -815.14068202080  8.4E-06  6.5E-06  1.4E-04
etot   4  Y  Y  4  M  -815.14068193861 -8.2E-08  2.5E-06  5.3E-05
etot   5  Y  N  4  M  -815.14068209397  1.6E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.17716518382
   (E)  Total one-electron terms..... -4001.92051216917
   (I)  Total two-electron terms.....  1728.60266489138
   (L)  Electronic energy............ -2273.31784727779  (E+I)
   (N)  Total energy.................  -815.14068209397  (A+L)

 SCFE: SCF energy: HF    -815.14068209397 hartrees   iterations:   5


 HOMO energy:    -0.29723
 LUMO energy:     0.11778

  Orbital energies:
  -20.45374  -15.55207  -11.32160  -11.23553  -11.22329  -11.21489
  -11.20784  -11.19966  -11.18787  -11.18560  -11.18508  -11.18436
  -11.18291  -11.18249  -11.17952  -11.17733  -11.17726  -11.17598
  -11.17273  -11.16424   -1.42377   -1.33332   -1.18049   -1.16244
   -1.11406   -1.08817   -1.03817   -1.02706   -1.01983   -1.00146
   -0.94890   -0.90500   -0.85233   -0.84378   -0.83048   -0.81095
   -0.79137   -0.76053   -0.72213   -0.68661   -0.68143   -0.66779
   -0.65700   -0.64297   -0.64003   -0.62496   -0.61385   -0.60781
   -0.60456   -0.60061   -0.59238   -0.58276   -0.55152   -0.55057
   -0.53312   -0.52493   -0.51635   -0.51339   -0.49864   -0.49490
   -0.48927   -0.48505   -0.45843   -0.42186   -0.39454   -0.34888
   -0.34238   -0.31557   -0.29723    0.11778    0.13214    0.14153
    0.14375    0.20523    0.22185    0.26531    0.27148    0.28098
    0.30584

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   2    grid:  4
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program der1b

  forces (hartrees/bohr) : total

 atom  label         x              y              z
 ----  -----  -------------  -------------  -------------
   1    H25   -1.688655E-05  -3.056567E-05   2.385646E-05
   2    C1     2.728351E-05   4.646382E-04  -7.192114E-04
   3    C2    -2.862088E-04  -2.719874E-04   3.115467E-04
   4    C3     4.025810E-05  -1.918451E-04   1.167544E-04
   5    C4    -1.725060E-04   1.172023E-04  -2.969702E-04
   6    C5     3.337644E-04   3.630490E-04   2.358131E-05
   7    C6     2.814975E-04   1.778009E-04   5.464056E-04
   8    C7     -6.548318E-04  -1.840545E-04  -9.188242E-04
   9    H27    -4.251039E-05  -6.149480E-05   8.445876E-05
  10    H28    -1.935085E-04  -9.944477E-05  -3.923875E-06
  11    H30    -6.527282E-05   3.756360E-05   3.436658E-05
  12    C8      1.937927E-04  -3.853050E-05   4.219804E-04
  13    H32    -8.605334E-05  -3.943488E-05  -6.889428E-05
  14    C10     1.904174E-04  -5.676588E-05  -1.926976E-04
  15    N2     -3.474712E-05   1.073859E-04   2.631866E-04
  16    C9     -5.181040E-05   1.277560E-04   2.467982E-05
  17    O1      6.474832E-05   1.231457E-04   7.541010E-05
  18    H43     1.577187E-05   2.128632E-04   2.412473E-04
  19    C12    -1.161600E-04  -1.030079E-04   1.079076E-04
  20    C11     7.837876E-05  -2.130151E-05  -1.350451E-04
  21    C19     3.564182E-04   7.389850E-05   7.399370E-05
  22    C13    -3.355686E-05  -1.840837E-04   6.815161E-05
  23    C14    -2.178328E-04   6.743230E-05   9.229953E-05
  24    C15    -1.482935E-04   2.667255E-04   1.073959E-04
  25    C16     1.102813E-04   2.397501E-04  -7.959590E-05
  26    C17     1.678882E-04  -5.860225E-05   2.172210E-05
  27    H49     9.213284E-05   8.155424E-05   3.775842E-05
  28    H50    -7.519537E-06  -1.798684E-04  -2.700181E-05
  29    H51     1.334257E-04  -3.846099E-05  -4.969179E-05
  30    H52    -1.182300E-04  -1.847872E-04   5.913585E-05
  31    H53     2.220681E-05   9.523529E-05   9.062399E-05
  32    H1      2.798840E-04   1.477425E-04   3.147974E-04
  33    H2     -2.455495E-04  -5.281776E-04   1.275178E-04
  34    H3     -5.414461E-04   6.419939E-04   2.253192E-04
  35    H4     -2.576777E-05   1.435856E-04   6.100669E-05
 -----------   -------------  -------------  -------------
    total      -6.705421E-04   1.216910E-03   1.063248E-03

  end of program der1b


  start of program geopt  22

  geometry optimization step 22
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  ** restarting optimization from step   21 **


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0102289
   Cos(theta):   0.5598262

   Final level shift:  -5.9526998E-03

  energy change:           1.4659E-04 .   (  5.0000E-05 )
  gradient maximum:        7.9456E-04 .   (  4.5000E-04 )
  gradient rms:            1.3298E-04 *   (  3.0000E-04 )
  step size:   0.01023  trust radius:   0.01000
  displacement maximum:    3.3561E-03 .   (  1.8000E-03 )
  displacement rms:        9.1490E-04 *   (  1.2000E-03 )
  predicted energy change:    -4.5683E-06    geom step:   1.0229E-02    full step:
1.0229E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:     8.3267E-16     y:    -4.4409E-16     z:     5.5511E-16
 new geometry:
                               angstroms
 atom            x                 y                 z
 H25       0.9709847000      1.9943485287     -4.1702911763
 C1        1.4955429179      2.0474583568     -3.2372709516
 C2        2.8944584332      2.2070271846     -0.7851336403
 C3        1.2172159044      1.1487689012     -2.2151846540
 C4        2.4643492880      3.0097885580     -3.0269421330
 C5        3.1565045258      3.0880810218     -1.8143274237
 C6        1.9241597738      1.2503147321     -1.0082075334
 C7        0.2864921918      0.0244288368     -2.0858247638
 H27       2.6927521707      3.7103915109     -3.8051190979
 H28       3.9028733044      3.8456762382     -1.6833679431
 H30       3.4054655484      2.2430341092      0.1537362611
 C8        0.4666969459     -0.4881726006     -0.8617627226
 H32      -0.4081392094     -0.3027293423     -2.8246613907
 C10      -0.0744225441     -1.5554604158      0.0597754981
 N2        1.4548772379      0.2360244433     -0.1916074142
 C9        1.7633413886     -0.2314040062      1.0656646899
 O1        2.5246327483      0.2890291917      1.8462537553
 H43      -0.0679627438     -2.5199365567     -0.4289164235
 C12      -1.4918157714     -1.2421805538      0.5131810205
 C11       0.9852015538     -1.5440963638      1.2283136609
 C19       0.4679451148     -1.7205307979      2.6566095103
 C13      -3.7208328491     -1.9965700163      1.0326275100
 C14      -3.1531418624      0.3138132765      1.2929775902
 C15      -4.0851356711     -0.7099227360      1.3822437210
 C16      -1.8682194981      0.0505542932      0.8583296956
 C17      -2.4293794803     -2.2589395621      0.6013105733
 H49      -4.4353094756     -2.7936882130      1.0903842101
 H50      -3.4296548934      1.3154526647      1.5561141644
 H51      -5.0823730018     -0.5022856234      1.7151360487
 H52      -1.1604980431      0.8511003070      0.7743822621
 H53      -2.1565972746     -3.2602712989      0.3280820399
 H1        1.3006947122     -1.6350803828      3.3433936446
 H2        0.0082933769     -2.6935539593      2.7795177551
 H3       -0.2635313006     -0.9646922263      2.9023560384
 H4        1.7069743397     -2.3279404523      1.0172218649

 nuclear repulsion energy.......  1458.343626022 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  22   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.215E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom       H25     C1     C2     C3     C4     C5     C6     C7
```

```
  grid # 1        73     89     87     90     87     87     84     85
  grid # 2       106    100     97     98     98     98     90     92
  grid # 3       224    183    182    194    182    182    187    182
  grid # 4       224    379    381    406    379    379    372    377

  number of gridpoints:
     atom        H27    H28    H30     C8    H32    C10     N2     C9
  grid # 1        73     73     73     86     73     81     99     76
  grid # 2       106    106    105     92    106     93    109     81
  grid # 3       224    224    220    187    223    175    223    163
  grid # 4       224    224    219    376    229    351    401    329

  number of gridpoints:
     atom         O1    H43    C12    C11    C19    C13    C14    C15
  grid # 1       111     69     90     80     71     87     86     89
  grid # 2       123     98    106     91     74    100     99    100
  grid # 3       273    211    192    175    147    182    182    182
  grid # 4       475    205    397    361    305    378    379    378

  number of gridpoints:
     atom        C16    C17    H49    H50    H51    H52    H53     H1
  grid # 1        86     85     73     73     73     71     72     71
  grid # 2        97     99    106    106    106    100    103     99
  grid # 3       181    182    224    223    224    216    216    220
  grid # 4       376    377    224    223    224    211    215    221

  number of gridpoints:
     atom         H2     H3     H4  total
  grid # 1        72     71     69   2815
  grid # 2        99     97    100   3480
  grid # 3       219    214    219   7037
  grid # 4       220    212    210  10841

  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                               RMS    maximum
       e  d  i  u  i                     energy  density   DIIS
       r  t  s  t  d     total energy    change  change    error

etot   1  N  N  1  U  -815.14057271703           1.4E-04  1.2E-03
etot   2  Y  Y  4  M  -815.14063223326  6.0E-05  1.9E-05  3.6E-04
etot   3  Y  Y  4  M  -815.14063782775  5.6E-06  4.7E-06  1.2E-04
etot   4  Y  N  4  M  -815.14063795184  1.2E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.34362602168
   (E)  Total one-electron terms..... -4002.25448851981
   (I)  Total two-electron terms.....  1728.77022454629
   (L)  Electronic energy............ -2273.48426397352  (E+I)
   (N)  Total energy.................  -815.14063795184  (A+L)
```

```
SCFE: SCF energy: HF    -815.14063795184 hartrees   iterations:   4


HOMO energy:    -0.29717
LUMO energy:     0.11774

 Orbital energies:
 -20.45387  -15.55198  -11.32154  -11.23542  -11.22320  -11.21476
 -11.20776  -11.19961  -11.18787  -11.18559  -11.18508  -11.18434
 -11.18292  -11.18241  -11.17959  -11.17728  -11.17723  -11.17604
 -11.17282  -11.16467   -1.42388   -1.33333   -1.18045   -1.16243
  -1.11406   -1.08817   -1.03813   -1.02701   -1.01986   -1.00139
  -0.94881   -0.90498   -0.85225   -0.84374   -0.83047   -0.81096
  -0.79137   -0.76055   -0.72216   -0.68665   -0.68146   -0.66778
  -0.65701   -0.64293   -0.64011   -0.62491   -0.61394   -0.60785
  -0.60455   -0.60055   -0.59237   -0.58268   -0.55144   -0.55055
  -0.53298   -0.52493   -0.51629   -0.51344   -0.49860   -0.49492
  -0.48924   -0.48503   -0.45843   -0.42188   -0.39456   -0.34883
  -0.34232   -0.31564   -0.29717    0.11774    0.13221    0.14158
   0.14375    0.20520    0.22195    0.26540    0.27152    0.28101
   0.30574

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   2    grid:  4
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
  1    H25    -9.297692E-05  -3.446842E-05  -5.908082E-05
  2    C1      2.702430E-05   2.480234E-04  -3.416288E-04
  3    C2     -9.349053E-05   6.856195E-05  -6.144869E-05
  4    C3     -5.693217E-05  -6.350050E-06  -1.418257E-04
  5    C4     -1.008624E-04  -6.023304E-05   1.764901E-05
  6    C5      1.950921E-04   3.533048E-04   2.564745E-05
  7    C6      1.586238E-04  -8.430720E-05   4.819420E-04
  8    C7     -6.938552E-04  -3.016917E-04  -1.058903E-03
  9    H27    -1.457972E-05   5.759269E-06   4.970174E-05
 10    H28    -2.211050E-05   4.479908E-05   3.583940E-05
 11    H30     7.052739E-05   7.045849E-05   1.916845E-04
 12    C8      2.228411E-04  -1.357705E-05   4.539425E-04
 13    H32    -8.288187E-05  -2.306154E-05  -2.675018E-05
 14    C10     9.099274E-05   1.103408E-04  -2.336217E-05
 15    N2     -1.780922E-04   1.153398E-04   1.854953E-04
 16    C9     -1.231872E-04   9.996482E-05  -2.400056E-05
 17    O1      1.707156E-04   1.781259E-04   4.294235E-05
 18    H43     6.413036E-05  -1.474315E-05   8.573206E-05
 19    C12    -2.363941E-04  -2.025369E-04   9.961007E-05
 20    C11    -2.646624E-04   3.370099E-04  -9.236004E-06
```

```
  21    C19    -1.174006E-04  -1.038197E-04   3.895163E-04
  22    C13     2.244443E-05  -2.232245E-05   5.462872E-05
  23    C14    -2.957471E-04  -1.022502E-04   1.173352E-04
  24    C15     1.541933E-04   2.743651E-04   2.365406E-05
  25    C16    -1.043650E-04   1.415756E-04  -6.815826E-05
  26    C17     1.931746E-04   5.222045E-05   1.943141E-05
  27    H49     8.680522E-05   6.550208E-05   3.904493E-05
  28    H50    -4.129499E-05  -9.465647E-05  -2.377689E-05
  29    H51     1.520830E-05  -4.759156E-06  -9.392908E-06
  30    H52    -2.390591E-05  -1.561630E-04   5.482847E-05
  31    H53     5.600193E-05   4.654257E-05   9.253156E-05
  32    H1     -1.738186E-04   7.678866E-05   9.304826E-05
  33    H2      9.819621E-05   2.668080E-04   1.455594E-04
  34    H3      1.127351E-04   2.336613E-05   3.919433E-05
  35    H4      1.378237E-04  -9.885976E-05   2.808879E-05
 -----------   -------------  -------------  -------------
    total      -8.400274E-04   1.255057E-03   9.194834E-04

  end of program der1b


  start of program geopt  23

  geometry optimization step 23
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format
  ** restarting optimization from step   21 **


  energy change:           1.9073E-04 .  (  5.0000E-05 )
  gradient maximum:        7.9456E-04 .  (  4.5000E-04 )
  gradient rms:            1.3298E-04 *  (  3.0000E-04 )
  step size:   0.00372  trust radius:   0.01000
  displacement maximum:    1.4271E-03 *  (  1.8000E-03 )
  displacement rms:        3.3276E-04 *  (  1.2000E-03 )
  predicted energy change:    -1.6098E-06   geom step:   3.7203E-03    full step:
3.7203E-03
  molecular structure not yet converged...

  center of mass moved by:
     x:     3.8858E-16     y:     2.2204E-16     z:    -8.6042E-16

  new geometry:
                                angstroms
  atom            x                 y                  z
  H25       0.9754393767      1.9958564099     -4.1725371865
  C1        1.4990699123      2.0481032803     -3.2387684431
  C2        2.8955865720      2.2066404840     -0.7852119429
  C3        1.2179949956      1.1497452096     -2.2171381244
  C4        2.4689201749      3.0090698007     -3.0274372279
  C5        3.1602721434      3.0871938981     -1.8142756191
  C6        1.9239842497      1.2511797348     -1.0090717751
  C7        0.2854931333      0.0257955134     -2.0884951956
  H27       2.6990749606      3.7091545068     -3.8055686008
  H28       3.9078434094      3.8435406024     -1.6827913148
  H30       3.4058552836      2.2416677548      0.1543558526
  C8        0.4646111178     -0.4858040558     -0.8632447616
  H32      -0.4088011315     -0.3012451447     -2.8278434821
 C10      -0.0760560570     -1.5534698845      0.0585203290
 N2        1.4525328990      0.2381394570     -0.1925308940
 C9        1.7624421879     -0.2298730157      1.0640742257
 O1        2.5261162178      0.2895035555      1.8431533636
 H43      -0.0684737206     -2.5179214967     -0.4302772946
 C12      -1.4936808527     -1.2422277286      0.5127468833
 C11       0.9834858838     -1.5419116781      1.2274608227
 C19       0.4666546459     -1.7178687096      2.6565332906
 C13      -3.7206857675     -1.9996158305      1.0345089244
 C14      -3.1557567858      0.3110567182      1.2965759499
 C15      -4.0860885764     -0.7137444887      1.3859921067
 C16      -1.8711579933      0.0497058265      0.8596953110
 C17      -2.4295665540     -2.2601825846      0.6011223030
 H49      -4.4341091400     -2.7975085665      1.0924947825
 H50      -3.4331262700      1.3119097835      1.5613342718
 H51      -5.0830901073     -0.5077775904      1.7204991837
 H52      -1.1639993566      0.8506010826      0.7760521085
 H53      -2.1557240016     -3.2608751090      0.3268254886
 H1        1.2995203266     -1.6329405755      3.3429249037
 H2        0.0065898160     -2.6902801017      2.7802798389
 H3       -0.2638061714     -0.9613827946      2.9025393654
 H4        1.7050776197     -2.3263972464      1.0164967537

 nuclear repulsion energy.......  1458.165316215 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  23   /
-------------------------------------------------

 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.217E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25      C1      C2      C3      C4      C5      C6      C7
 grid # 1        73      89      87      90      87      87      84      85
 grid # 2       106     100      97      98      98      98      90      92
 grid # 3       224     183     182     194     182     182     187     182
 grid # 4       224     379     381     406     379     379     373     377

 number of gridpoints:
    atom        H27     H28     H30      C8     H32     C10      N2      C9
 grid # 1        73      73      73      86      73      81      99      76
 grid # 2       106     106     105      92     106      93     109      81
 grid # 3       224     224     220     188     223     175     223     163
 grid # 4       224     224     219     377     229     351     401     330

 number of gridpoints:
    atom         O1     H43     C12     C11     C19     C13     C14     C15
 grid # 1       111      69      90      80      71      87      86      89
 grid # 2       123      98     106      91      75     100      99     100
 grid # 3       273     211     192     175     147     182     182     182
 grid # 4      475    205    397    361    303    378    379    378

 number of gridpoints:
    atom         C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1         86     85     73     73     73     71     72     71
 grid # 2         97     99    106    106    106    100    103     99
 grid # 3        181    182    224    223    224    216    216    220
 grid # 4        376    377    224    223    224    211    215    221

 number of gridpoints:
    atom          H2     H3     H4  total
 grid # 1         72     71     69   2815
 grid # 2         99     97    100   3481
 grid # 3        219    214    219   7038
 grid # 4        220    212    211  10843

 end of program grid


 start of program rwr
recomputing RwR matrix   8    grid:  4
recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program scf

      i  u  d  i  g
      t  p  i  c  r                                    RMS    maximum
      e  d  i  u  i                          energy  density   DIIS
      r  t  s  t  d     total energy         change  change    error

etot   1  N  N  1  U  -815.14077889952           1.8E-04  1.2E-03
etot   2  Y  Y  4  M  -815.14081762226  3.9E-05  1.7E-05  1.5E-04
etot   3  Y  Y  4  M  -815.14081861901  1.0E-06  3.8E-06  5.5E-05
etot   4  Y  N  4  M  -815.14081809752 -5.2E-07  0.0E+00  0.0E+00


Energy components, in hartrees:
  (A)  Nuclear repulsion............  1458.16531621535
  (E)  Total one-electron terms..... -4001.89615490508
  (I)  Total two-electron terms.....  1728.59002059222
  (L)  Electronic energy............ -2273.30613431286  (E+I)
  (N)  Total energy.................  -815.14081809752  (A+L)

SCFE: SCF energy: HF    -815.14081809752 hartrees   iterations:   4


HOMO energy:    -0.29721
LUMO energy:     0.11768

 Orbital energies:
 -20.45373  -15.55215  -11.32166  -11.23576  -11.22332  -11.21494
 -11.20796  -11.19964  -11.18810  -11.18554  -11.18503  -11.18430
 -11.18284  -11.18247  -11.17945  -11.17757  -11.17732  -11.17594
 -11.17261  -11.16459   -1.42387   -1.33339   -1.18048   -1.16236
  -1.11400   -1.08809   -1.03815   -1.02703   -1.01979   -1.00139
  -0.94882   -0.90504   -0.85227   -0.84384   -0.83047   -0.81102
  -0.79140   -0.76046   -0.72219   -0.68656   -0.68146   -0.66777
  -0.65699   -0.64297   -0.64010   -0.62493   -0.61388   -0.60775
  -0.60461   -0.60061   -0.59242   -0.58275   -0.55146   -0.55050
  -0.53305   -0.52495   -0.51631   -0.51340   -0.49864   -0.49488
  -0.48925   -0.48504   -0.45840   -0.42189   -0.39453   -0.34885
  -0.34235   -0.31555   -0.29721    0.11768    0.13212    0.14160
   0.14383    0.20512    0.22187    0.26535    0.27159    0.28092
   0.30570

 end of program scf


 start of program der1a
 end of program der1a


 start of program rwr
recomputing RwR matrix   8    grid:   4
recomputing RwR matrix  15    grid:   4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x              y              z
----  -----   -------------  -------------  -------------
   1    H25   -2.835388E-06  -2.819158E-06  -4.902329E-07
   2    C1     1.040395E-04  -2.433384E-05   3.127439E-04
   3    C2    -8.033582E-05   2.414625E-05  -1.126008E-05
   4    C3     1.002489E-04   1.980184E-04  -5.688413E-05
   5    C4    -1.468930E-04  -1.386828E-04   2.566270E-05
   6    C5    -4.060293E-05   9.364192E-05  -1.565305E-06
   7    C6    -4.937338E-06   3.561842E-05   7.198085E-05
   8    C7    -2.247212E-04  -6.073031E-05  -3.117498E-04
   9    H27   -3.133986E-05   3.575414E-05  -8.099211E-06
  10    H28   -6.468266E-05   7.010483E-05   7.867262E-06
  11    H30   -3.370461E-05   7.805225E-05   5.496078E-05
  12    C8     6.764739E-05  -3.143127E-05   1.825368E-04
  13    H32    8.253951E-06  -1.502475E-05   3.535706E-05
  14    C10    4.005453E-05   2.962190E-05   4.063639E-05
  15    N2    -4.648961E-05   6.425144E-05   7.010081E-06
  16    C9    -9.139593E-05  -7.904895E-06  -3.165349E-05
  17    O1     7.451213E-05   2.168090E-04   1.990827E-04
  18    H43    2.721443E-05   7.701451E-06   8.568685E-05
  19    C12   -3.522405E-05   1.028688E-05   1.048420E-04
  20    C11   -8.690775E-05   8.500984E-05   1.023015E-04
  21    C19   -2.848396E-05   2.657463E-05   9.628403E-05
  22    C13    2.408297E-05  -2.138977E-05   3.597858E-05
  23    C14   -3.159769E-05  -2.940765E-06   2.798203E-06
  24    C15    1.020427E-05   3.868718E-05   3.242492E-06
  25    C16   -1.107397E-05   7.164699E-05   3.714214E-05
  26    C17    2.454009E-05   2.740372E-05   6.781483E-05
  27    H49    1.555452E-05  -9.131242E-06   4.457840E-05
  28    H50   -5.263221E-05   3.066533E-06  -1.417887E-05
  29    H51   -3.446707E-05  -2.603146E-06  -3.186609E-06
  30    H52   -6.139078E-05  -1.108176E-05   3.143102E-05
  31    H53    3.062427E-05  -3.748239E-06   8.360005E-05
  32    H1     5.724637E-06   1.214301E-04   1.349199E-04
  33    H2    -7.023272E-06   8.461312E-05   8.590751E-05
  34    H3    -1.280987E-05   9.890039E-05   4.868153E-05
  35    H4     5.345632E-06   6.172204E-05   9.464836E-05
-----------   -------------  -------------  -------------
   total      -5.915017E-04   1.151239E-03   1.558628E-03
  end of program der1b


  start of program geopt  24

  geometry optimization step 24
  reading input hessian of dimension   105
   in five columns format
  reading input hessian of dimension   105
   in five columns format


  Level shifts adjusted to satisfy step-size constraints
   Step size:    0.0101083
   Cos(theta):   0.2841773

   Final level shift:  -2.7110409E-03

  energy change:           1.0589E-05 *  (  5.0000E-05 )
  gradient maximum:        3.0562E-04 *  (  4.5000E-04 )
  gradient rms:            6.5247E-05 *  (  3.0000E-04 )
  step size:   0.01011  trust radius:   0.01000
  displacement maximum:    3.9909E-03 .  (  1.8000E-03 )
  displacement rms:        9.0411E-04 *  (  1.2000E-03 )
  predicted energy change:   -1.1862E-06   geom step:   1.0108E-02   full step:
1.0108E-02
  molecular structure not yet converged...

  center of mass moved by:
     x:   -5.5493E-04     y:    2.0702E-04     z:     1.7874E-04

  new geometry:
                              angstroms
  atom            x                  y                  z
  H25       0.9766539762      1.9935215693     -4.1731207013
  C1        1.4989411433      2.0466001137     -3.2386265740
  C2        2.8921639234      2.2078907946     -0.7840752370
  C3        1.2183098758      1.1475386639     -2.2178317329
  C4        2.4664628156      3.0094685773     -3.0264607303
  C5        3.1563744008      3.0891002060     -1.8128108169
  C6        1.9226429236      1.2504886507     -1.0089283485
  C7        0.2875732485      0.0215021191     -2.0906347417
  H27       2.6958765398      3.7103067773     -3.8043311438
  H28       3.9020557818      3.8472617214     -1.6805837341
  H30       3.4010893793      2.2440421376      0.1561088029
  C8        0.4661463414     -0.4890998209     -0.8644654096
  H32      -0.4052396066     -0.3068563486     -2.8308017097
  C10      -0.0749003226     -1.5555369124      0.0585569919
  N2        1.4524279464      0.2365025989     -0.1930562643
  C9        1.7603183817     -0.2294338346      1.0650410267
  O1        2.5212077596      0.2927189970      1.8454459318
  H43      -0.0684257450     -2.5208869936     -0.4288319332
  C12      -1.4919766276     -1.2422585441      0.5130584387
  C11       0.9842665898     -1.5431047873      1.2274804060
  C19       0.4684082036     -1.7223945943      2.6562604396
  C13      -3.7203308437     -1.9958955062      1.0345510214
  C14      -3.1520685342      0.3142215507      1.2947845848
  C15      -4.0840512628     -0.7091095688      1.3844264952
  C16      -1.8675920028      0.0505629947      0.8589311550
  C17      -2.4292917471     -2.2588449670      0.6021289594
  H49      -4.4351249856     -2.7926492403      1.0928861391
  H50      -3.4281134758      1.3157288753      1.5585673954
```

```
 H51      -5.0811370596     -0.5012737439      1.7179385773
 H52      -1.1590893275      0.8503554591      0.7752083360
 H53      -2.1567653513     -3.2602438341      0.3289517437
 H1        1.3009494112     -1.6365619841      3.3429010813
 H2        0.0106765116     -2.6959230479      2.7784688928
 H3       -0.2633972733     -0.9681846735      2.9036210871
 H4        1.7076795392     -2.3255506320      1.0149252583

 nuclear repulsion energy.......  1458.306385664 hartrees
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/  end of geometry optimization iteration  24   /
-------------------------------------------------


 end of program geopt


 start of program onee
 smallest eigenvalue of S:    1.216E-03
 number of canonical orbitals.....          210
 end of program onee


 start of program probe
 end of program probe


 start of program grid

 number of gridpoints:
    atom        H25     C1     C2     C3     C4     C5     C6     C7
 grid # 1        73     89     87     90     87     87     84     85
 grid # 2       106    100     97     98     98     98     90     92
 grid # 3       224    183    182    194    182    182    187    183
 grid # 4       224    379    381    406    379    379    373    378

 number of gridpoints:
    atom        H27    H28    H30     C8    H32    C10     N2     C9
 grid # 1        73     73     73     86     73     81     99     76
 grid # 2       106    106    105     92    106     93    109     81
 grid # 3       224    224    220    188    223    175    223    163
 grid # 4       224    224    219    377    229    351    401    328

 number of gridpoints:
    atom         O1    H43    C12    C11    C19    C13    C14    C15
 grid # 1       111     69     90     80     71     87     86     89
 grid # 2       127     98    106     91     74    100     99    100
 grid # 3       273    211    192    175    149    182    182    182
 grid # 4       475    205    397    361    304    378    379    378

 number of gridpoints:
    atom        C16    C17    H49    H50    H51    H52    H53     H1
 grid # 1        86     85     73     73     73     71     72     71
 grid # 2        97     99    106    106    106    100    103     99
 grid # 3       181    182    224    223    224    216    216    220
 grid # 4       376    377    224    223    224    211    215    221

 number of gridpoints:
    atom         H2     H3     H4  total
 grid # 1        72     71     69   2815
 grid # 2        99     97    100   3484
 grid # 3       219    214    219   7041
 grid # 4       220    212    211  10843
```

```
  end of program grid


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
  end of program rwr


  start of program scf

       i  u  d  i  g
       t  p  i  c  r                                  RMS    maximum
       e  d  i  u  i                     energy  density    DIIS
       r  t  s  t  d     total energy    change   change    error

etot   1  N  N  1  U  -815.14075946834           1.4E-04  1.2E-03
etot   2  Y  Y  4  M  -815.14080035572  4.1E-05  1.7E-05  2.7E-04
etot   3  Y  Y  4  M  -815.14080267659  2.3E-06  4.2E-06  8.8E-05
etot   4  Y  N  4  M  -815.14080332844  6.5E-07  0.0E+00  0.0E+00


 Energy components, in hartrees:
   (A)  Nuclear repulsion............  1458.30638566351
   (E)  Total one-electron terms..... -4002.18191050153
   (I)  Total two-electron terms.....  1728.73472150958
   (L)  Electronic energy............ -2273.44718899195  (E+I)
   (N)  Total energy.................  -815.14080332844  (A+L)

 SCFE: SCF energy: HF    -815.14080332844 hartrees   iterations:   4


 HOMO energy:    -0.29718
 LUMO energy:     0.11766

  Orbital energies:
  -20.45408  -15.55201  -11.32157  -11.23571  -11.22323  -11.21484
  -11.20782  -11.19953  -11.18798  -11.18558  -11.18509  -11.18432
  -11.18290  -11.18238  -11.17939  -11.17765  -11.17729  -11.17601
  -11.17267  -11.16452   -1.42374   -1.33327   -1.18045   -1.16235
   -1.11404   -1.08794   -1.03812   -1.02700   -1.01979   -1.00135
   -0.94882   -0.90505   -0.85222   -0.84380   -0.83043   -0.81100
   -0.79133   -0.76041   -0.72219   -0.68652   -0.68144   -0.66768
   -0.65698   -0.64292   -0.64012   -0.62491   -0.61381   -0.60775
   -0.60456   -0.60056   -0.59240   -0.58269   -0.55139   -0.55049
   -0.53309   -0.52501   -0.51627   -0.51344   -0.49861   -0.49486
   -0.48924   -0.48498   -0.45836   -0.42194   -0.39446   -0.34883
   -0.34233   -0.31552   -0.29718    0.11766    0.13220    0.14167
    0.14378    0.20501    0.22191    0.26536    0.27156    0.28089
    0.30572

  end of program scf


  start of program der1a
  end of program der1a


  start of program rwr
 recomputing RwR matrix   8    grid:  4
 recomputing RwR matrix  15    grid:  4
 end of program rwr


 start of program der1b

 forces (hartrees/bohr) : total

atom  label         x               y               z
----  -----   -------------   -------------   -------------
  1    H25    -2.174256E-05   -2.010735E-05    2.420233E-05
  2    C1     -2.784272E-05   -1.054690E-05   -7.113078E-05
  3    C2     -7.060032E-05    7.905332E-05   -8.275811E-06
  4    C3      5.946665E-06   -4.789096E-06    5.474077E-06
  5    C4     -3.732817E-05    6.827876E-05   -8.270808E-05
  6    C5     -1.779339E-05    7.021575E-05    1.359203E-04
  7    C6      5.547163E-05   -3.015761E-05   -6.643653E-06
  8    C7      5.893936E-05    4.455628E-05    2.244565E-04
  9    H27    -6.648433E-05   -8.801143E-05    6.113848E-05
 10    H28    -8.479674E-05   -2.361985E-05    3.163262E-05
 11    H30    -1.734745E-05    6.300727E-05    7.830478E-05
 12    C8      1.690917E-05    3.371846E-05   -7.239758E-05
 13    H32     1.077967E-05    1.818886E-06    7.584221E-05
 14    C10    -5.525958E-05   -1.672886E-04    3.993986E-05
 15    N2     -2.211731E-04    1.580615E-04    2.293587E-04
 16    C9      2.784162E-04    3.048050E-04    2.073943E-04
 17    O1     -2.578751E-04   -5.917226E-05   -3.545012E-04
 18    H43     4.731811E-05    1.335886E-04    1.238564E-04
 19    C12    -6.108574E-05    2.773814E-05    1.659213E-06
 20    C11     1.202707E-04    7.768341E-05   -7.001198E-05
 21    C19     6.427689E-05   -2.926116E-05    7.536898E-05
 22    C13     6.417692E-06   -6.316425E-05    3.602753E-05
 23    C14    -7.686390E-05   -1.470637E-05    5.727246E-05
 24    C15    -5.817094E-05    6.750750E-05    5.096151E-05
 25    C16    -1.002148E-04    5.487732E-05   -2.871763E-05
 26    C17    -2.653686E-05    4.756824E-05    5.031013E-05
 27    H49     8.655136E-05    4.087091E-05    4.432713E-05
 28    H50    -2.919648E-05   -2.713686E-05   -1.629858E-05
 29    H51     8.598651E-05   -2.996359E-05   -1.817425E-05
 30    H52    -6.435736E-05   -6.654054E-05    2.016367E-05
 31    H53     2.490063E-05    4.157492E-05    7.352076E-05
 32    H1      6.064471E-05    1.110858E-04    7.882446E-05
 33    H2     -5.897999E-05   -1.389542E-05    1.112756E-04
 34    H3     -2.222331E-04    2.909106E-04    8.961558E-05
 35    H4      4.030149E-06    6.583437E-05    1.228312E-04
-----------   -------------   -------------   -------------
   total      -6.490233E-04    1.134394E-03    1.320819E-03

 end of program der1b


 start of program geopt  25

 geometry optimization step 25
** stopping now - optimization seems to be stuck **


 *********************************************************
 **             Geometry optimization complete          **
 *********************************************************

 center of mass moved by:
    x:     0.0000E+00     y:     0.0000E+00     z:     0.0000E+00
 final geometry:
                              angstroms
 atom          x                  y                  z
 H25       0.9766539762       1.9935215693      -4.1731207013
 C1        1.4989411433       2.0466001137      -3.2386265740
 C2        2.8921639234       2.2078907946      -0.7840752370
 C3        1.2183098758       1.1475386639      -2.2178317329
 C4        2.4664628156       3.0094685773      -3.0264607303
 C5        3.1563744008       3.0891002060      -1.8128108169
 C6        1.9226429236       1.2504886507      -1.0089283485
 C7        0.2875732485       0.0215021191      -2.0906347417
 H27       2.6958765398       3.7103067773      -3.8043311438
 H28       3.9020557818       3.8472617214      -1.6805837341
 H30       3.4010893793       2.2440421376       0.1561088029
 C8        0.4661463414      -0.4890998209      -0.8644654096
 H32      -0.4052396066      -0.3068563486      -2.8308017097
 C10      -0.0749003226      -1.5555369124       0.0585569919
 N2        1.4524279464       0.2365025989      -0.1930562643
 C9        1.7603183817      -0.2294338346       1.0650410267
 O1        2.5212077596       0.2927189970       1.8454459318
 H43      -0.0684257450      -2.5208869936      -0.4288319332
 C12      -1.4919766276      -1.2422585441       0.5130584387
 C11       0.9842665898      -1.5431047873       1.2274804060
 C19       0.4684082036      -1.7223945943       2.6562604396
 C13      -3.7203308437      -1.9958955062       1.0345510214
 C14      -3.1520685342       0.3142215507       1.2947845848
 C15      -4.0840512628      -0.7091095688       1.3844264952
 C16      -1.8675920028       0.0505629947       0.8589311550
 C17      -2.4292917471      -2.2588449670       0.6021289594
 H49      -4.4351249856      -2.7926492403       1.0928861391
 H50      -3.4281134758       1.3157288753       1.5585673954
 H51      -5.0811370596      -0.5012737439       1.7179385773
 H52      -1.1590893275       0.8503554591       0.7752083360
 H53      -2.1567653513      -3.2602438341       0.3289517437
 H1        1.3009494112      -1.6365619841       3.3429010813
 H2        0.0106765116      -2.6959230479       2.7784688928
 H3       -0.2633972733      -0.9681846735       2.9036210871
 H4        1.7076795392      -2.3255506320       1.0149252583

 nuclear repulsion energy.......  1458.306385664 hartrees
 -------------------------------------------------
/  end of geometry optimization iteration  25   /
-------------------------------------------------

 end of program geopt


 start of program post
 Writing a SPARTAN archive file
 end of program post

Total cpu seconds     user:    1404.719   user+sys:    1404.719
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4. REFERENCES

[1] A. Arcadi, A. Calcaterra, M. Chiarini, G. Fabrizi, A. Fochetti, A. Goggiamani, A. Iazzetti, F. Marrone, V. Marsicano, A. Serraiocco, *Synthesis* 2021**, 54**, 741-753.

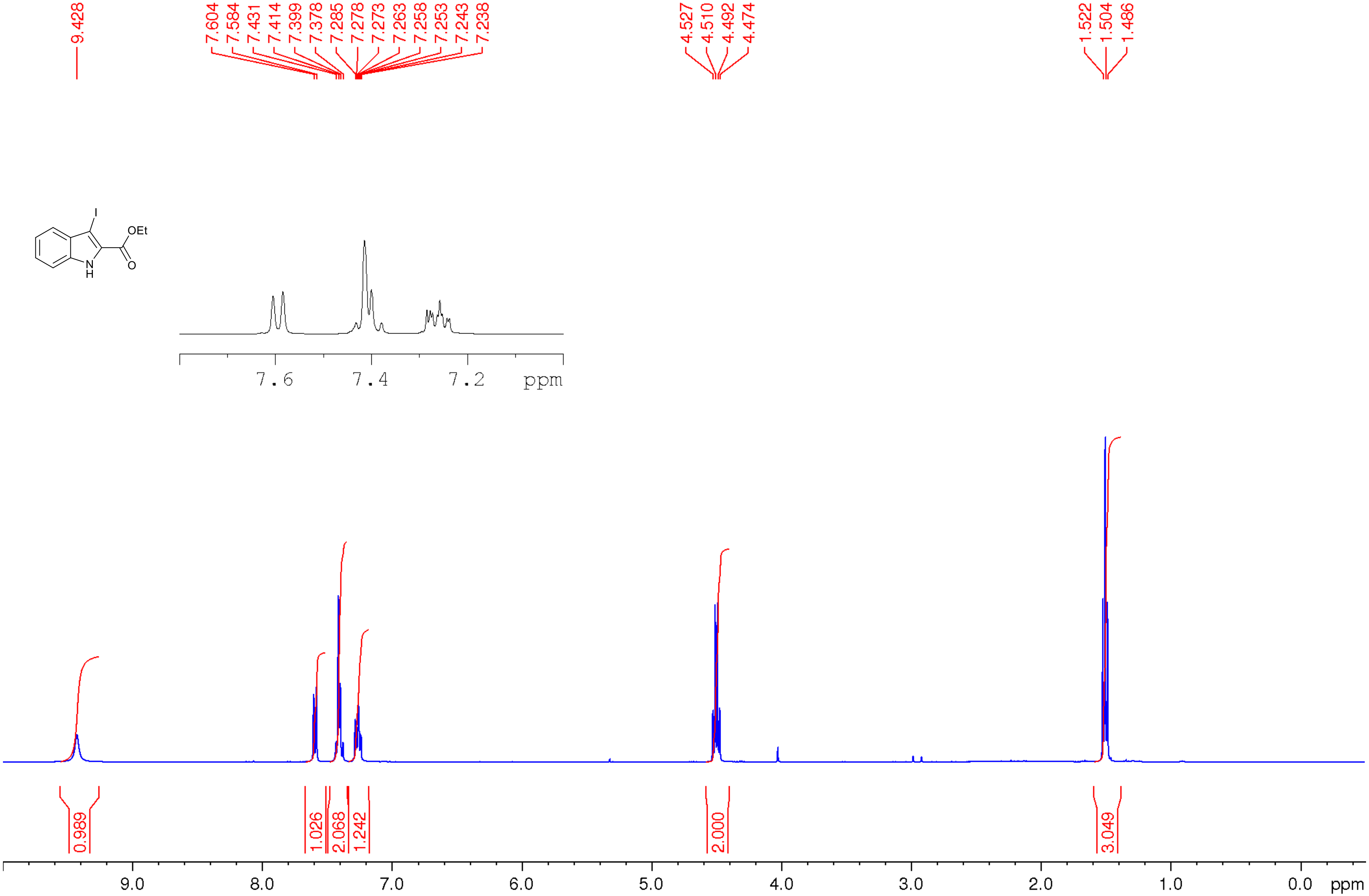
[2] S. Hammoud, E. Anselmi, K. Cherry, J.-C. Kizirian, J. Thibonnet, *Eur. J. Org. Chem.* 2018**, 45**, 6314-6327.

[3] Y. Goriya, C. V. Ramana, *Chem. Comm.* 2014**, 50**, 7790-7792.

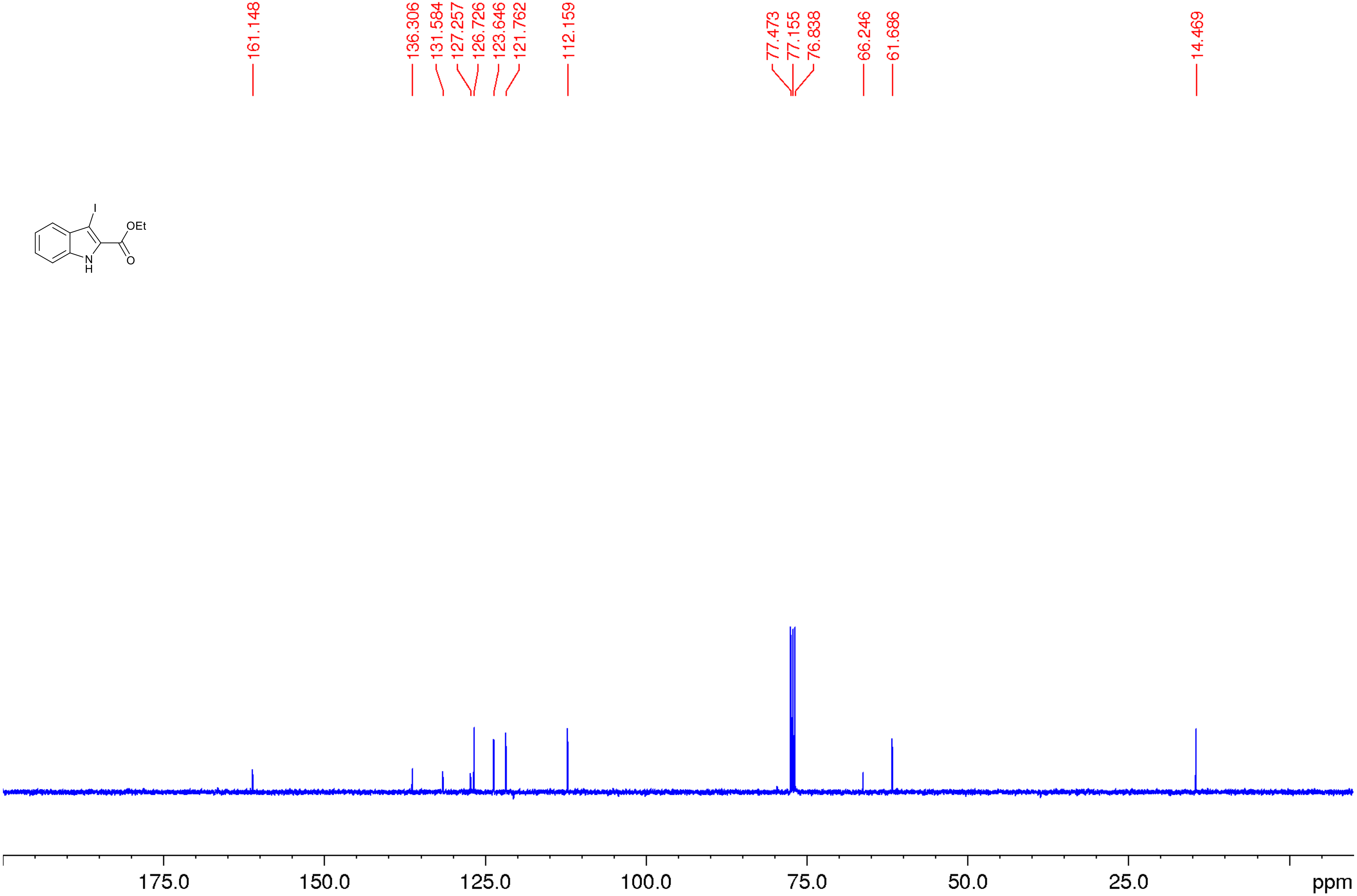
[4] V. Collot, M. Schmitt, P. Marwah, J.-J. Bourguignon, *Heterocycles*, 1999, **51**, 2823-2847.

[5] R. Akunuri, V. Veerareddy, G. Kaul, A. Akhir, T. Unnissa, R. Parupalli, Y. V. Madhavi, S. Chopra, S. Nanduri, *Bioorg. Chem.* 2021**, 116**, 105288.

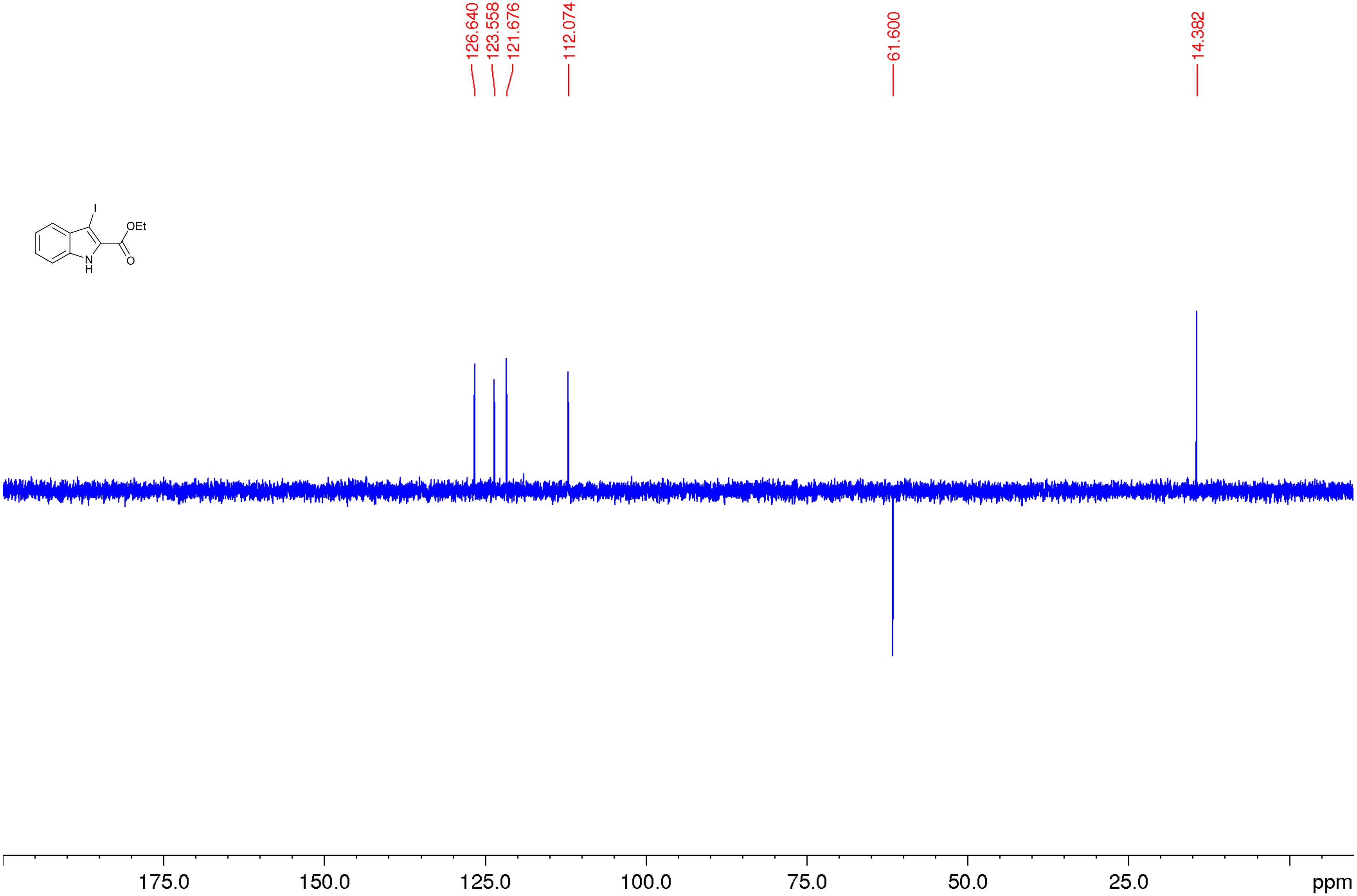
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



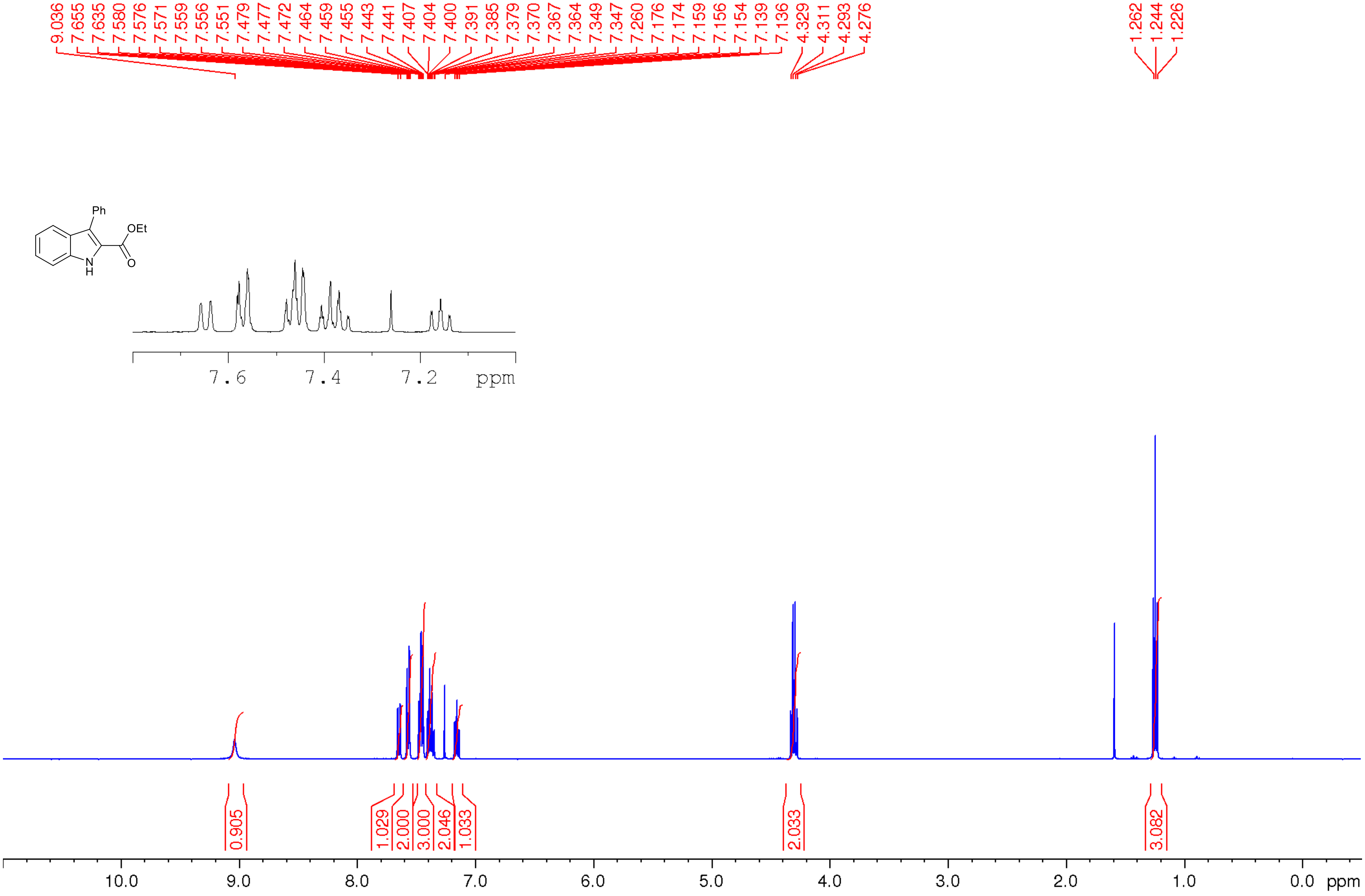
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



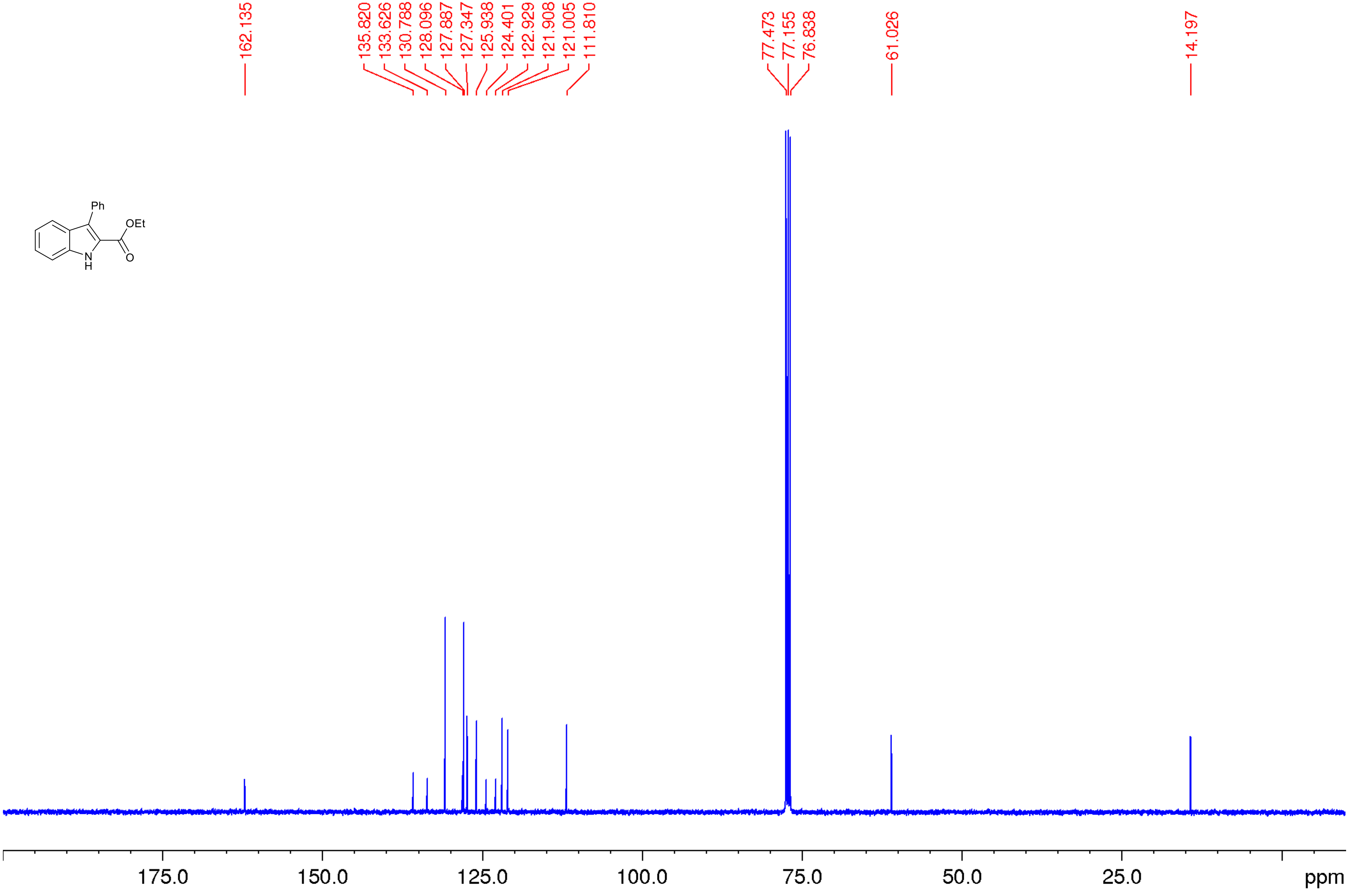
DEPT 135 NMR-spectrum ($CDCl_3$)



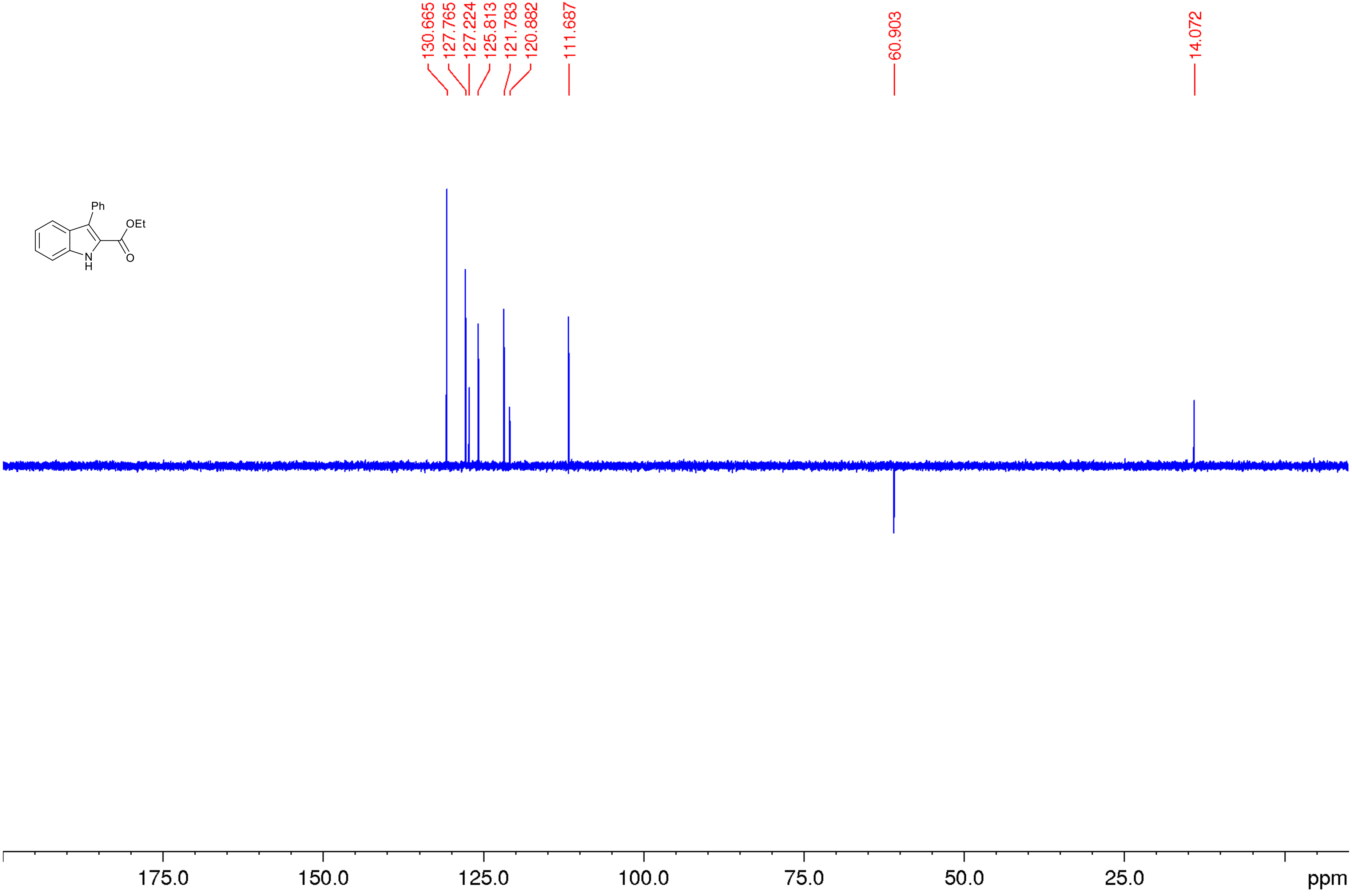
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



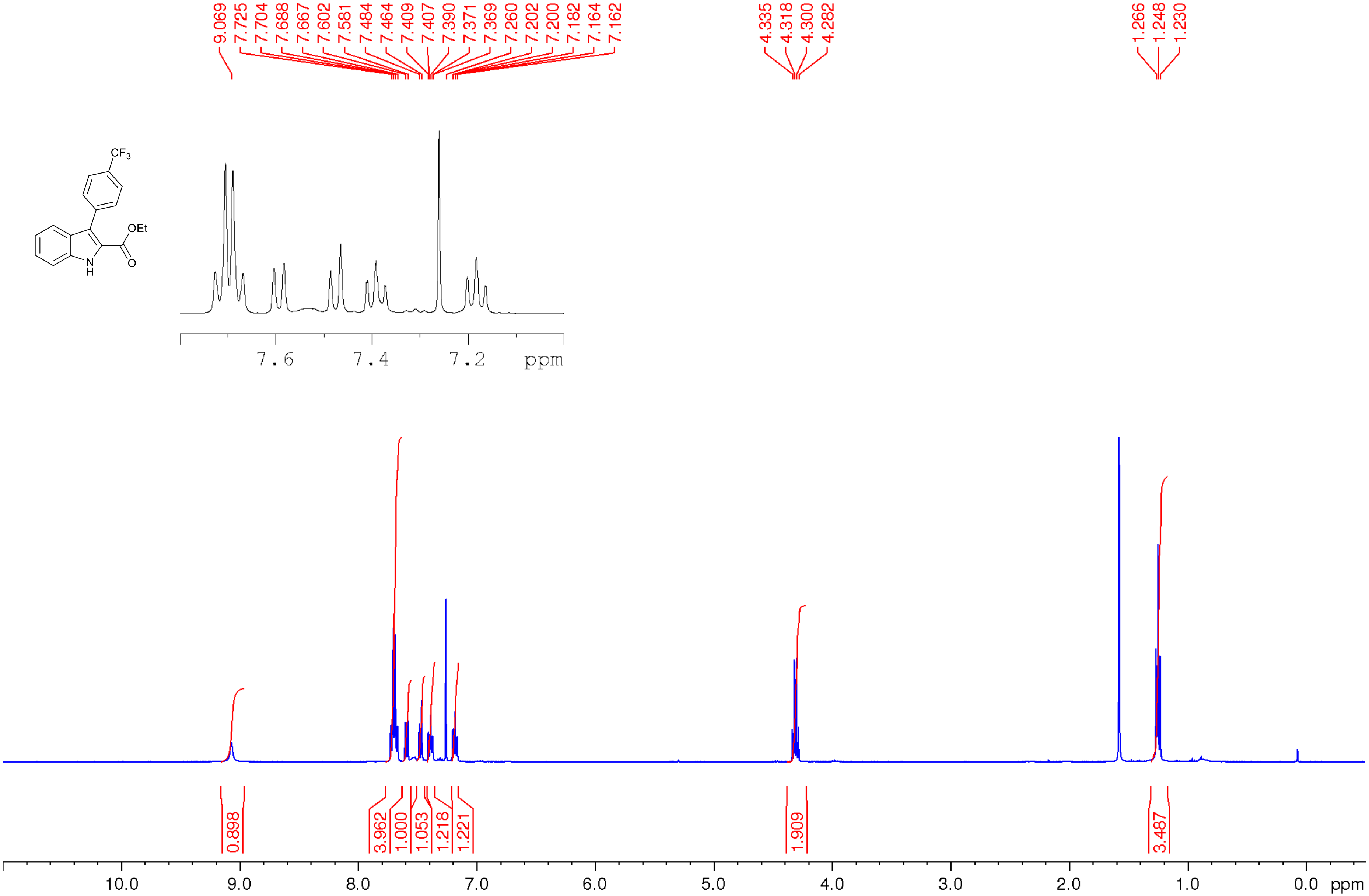
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



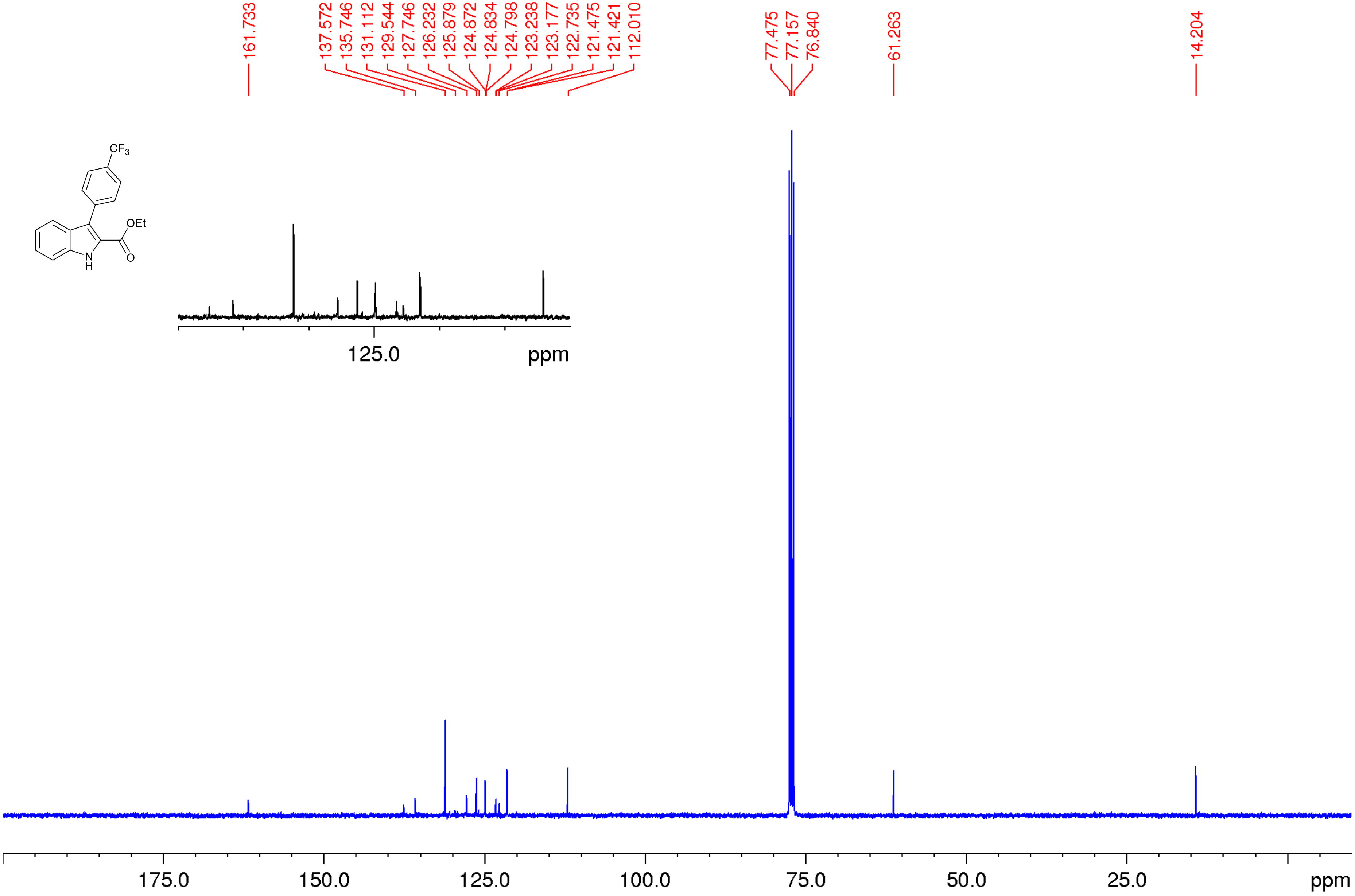
DEPT 135 NMR-spectrum ($CDCl_3$)



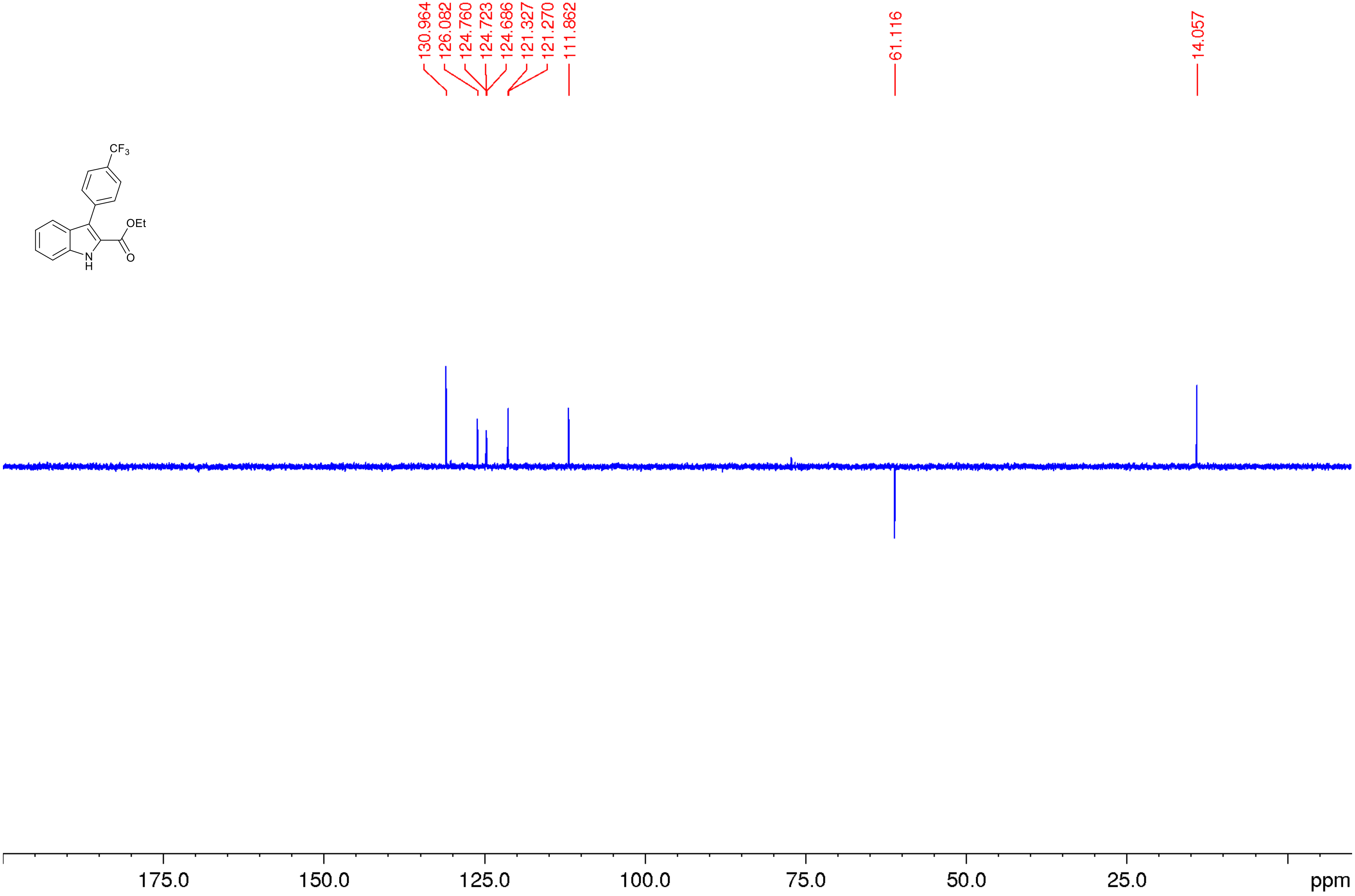
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



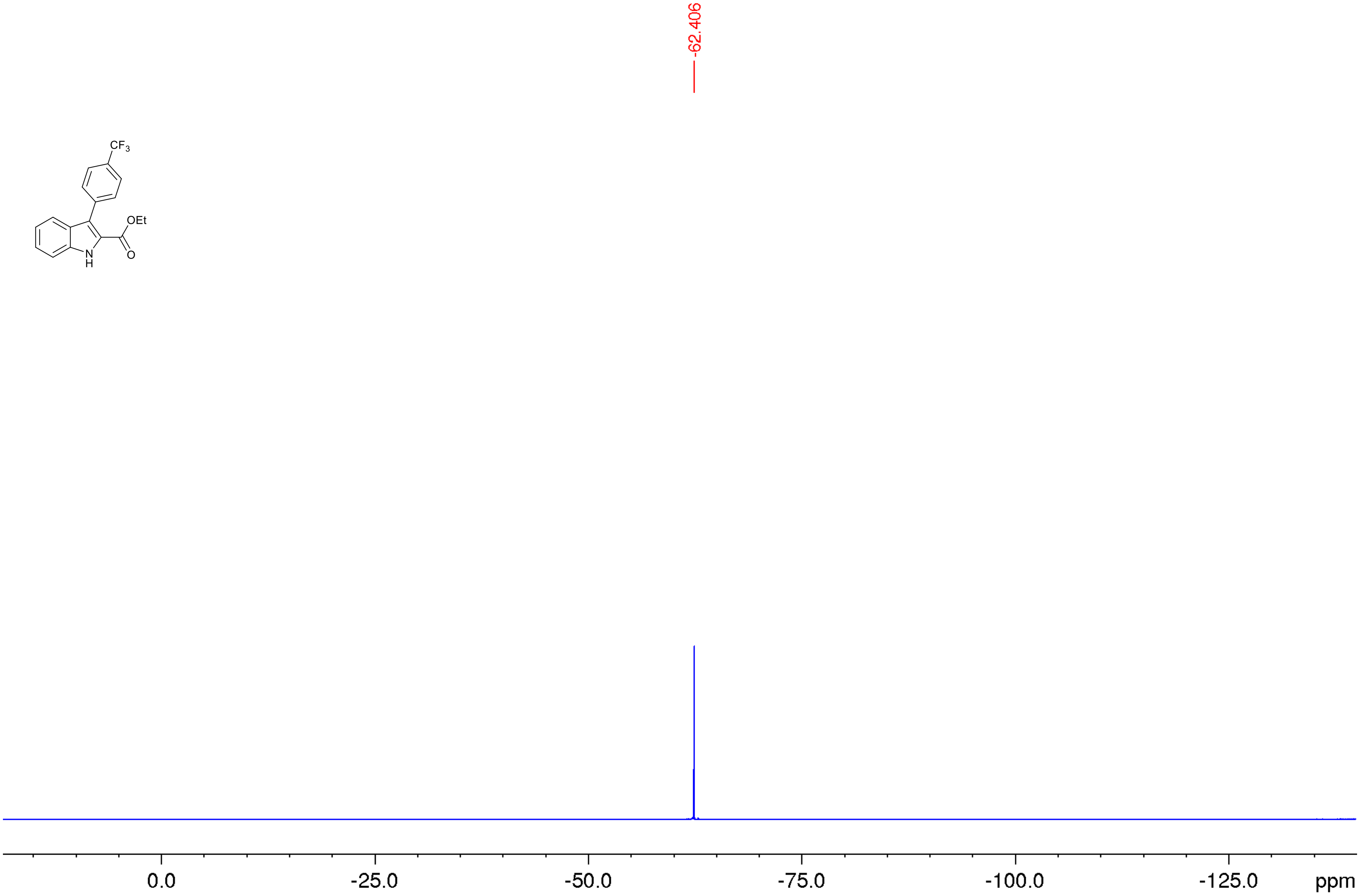
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



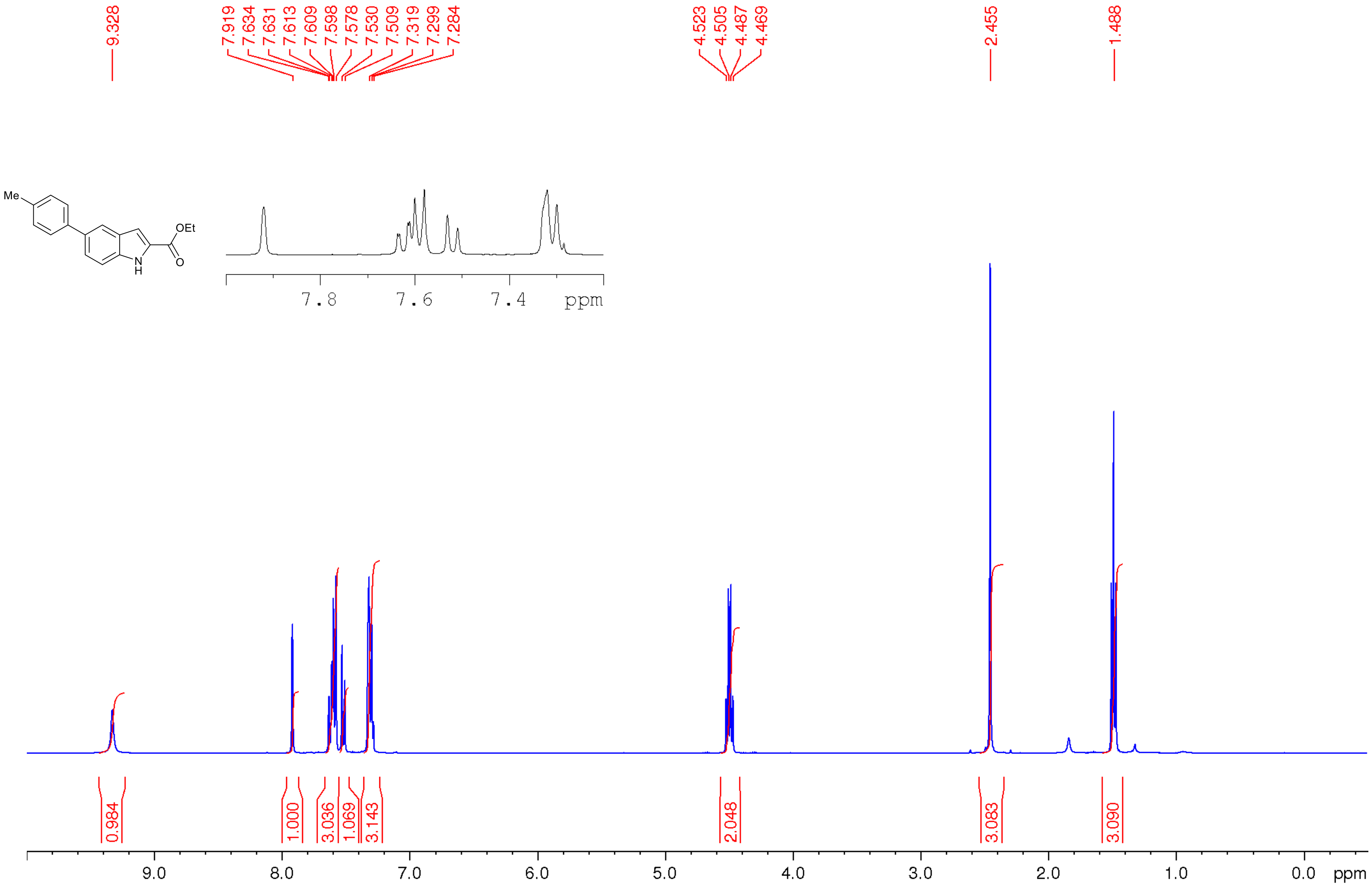
DEPT 135 NMR-spectrum ($CDCl_3$)



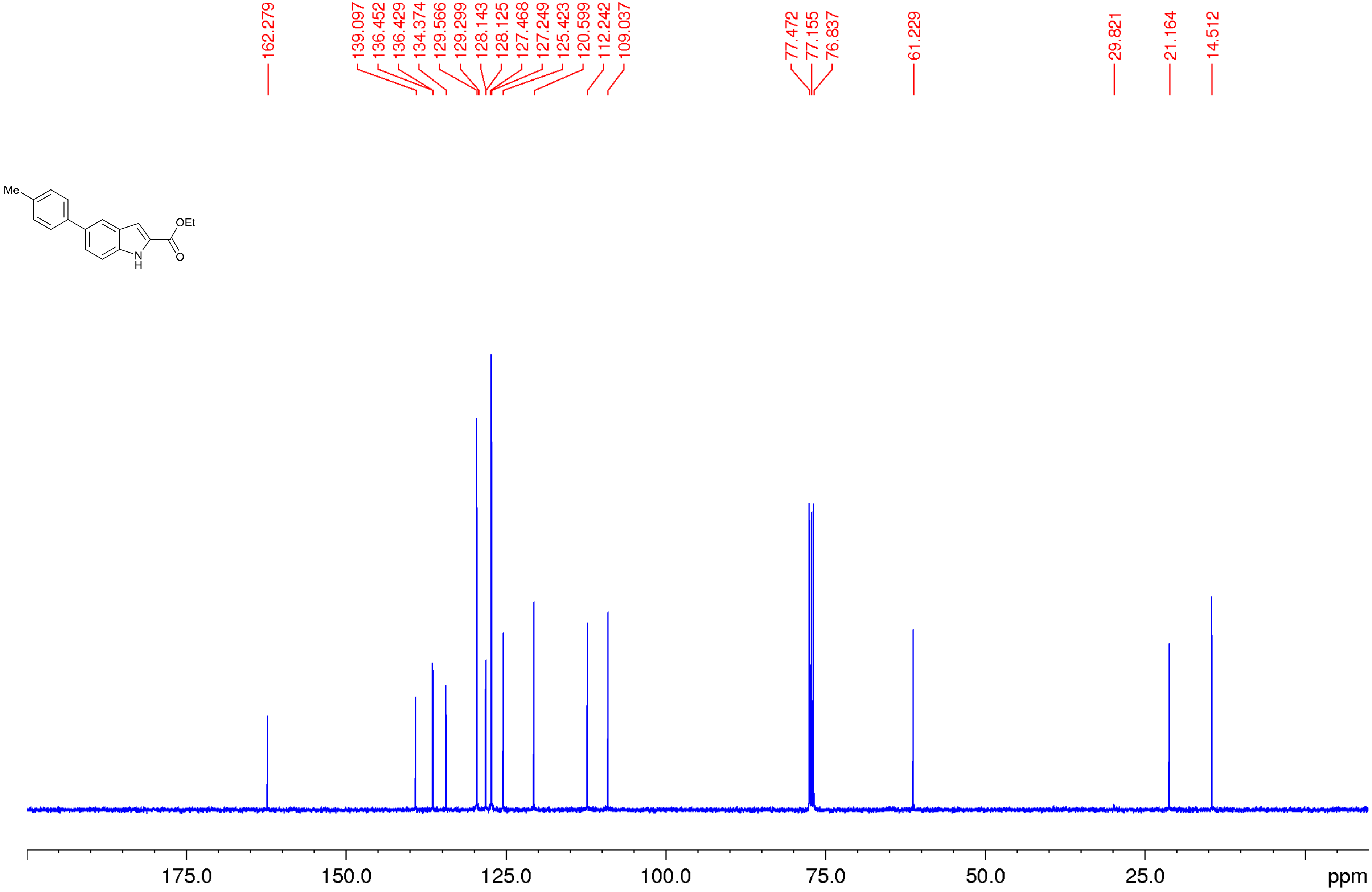
^{19}F NMR-spectrum (376.5 MHz, $CDCl_3$)



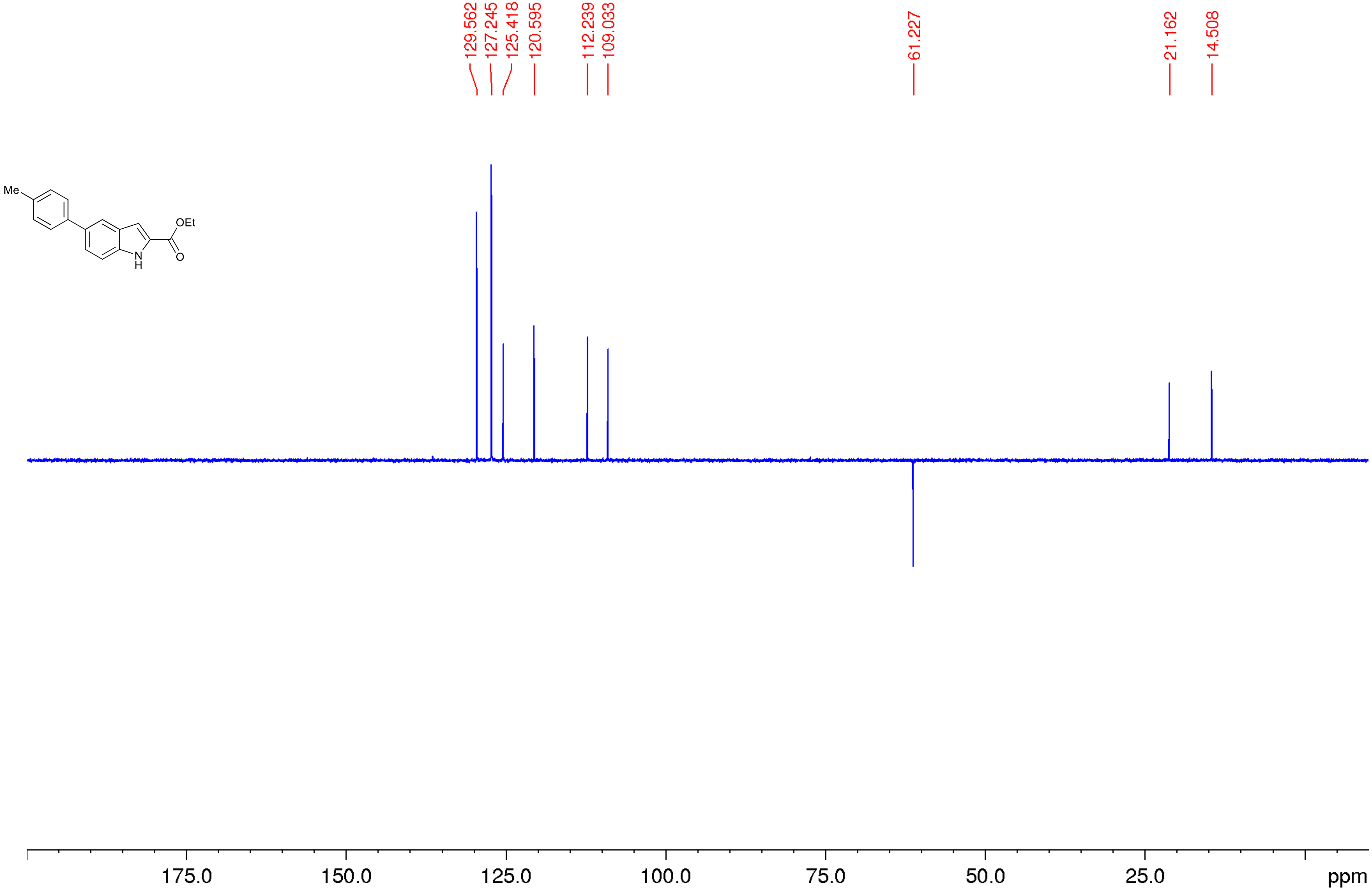
^1H NMR-spectrum (400 MHz, $CDCl_3$)



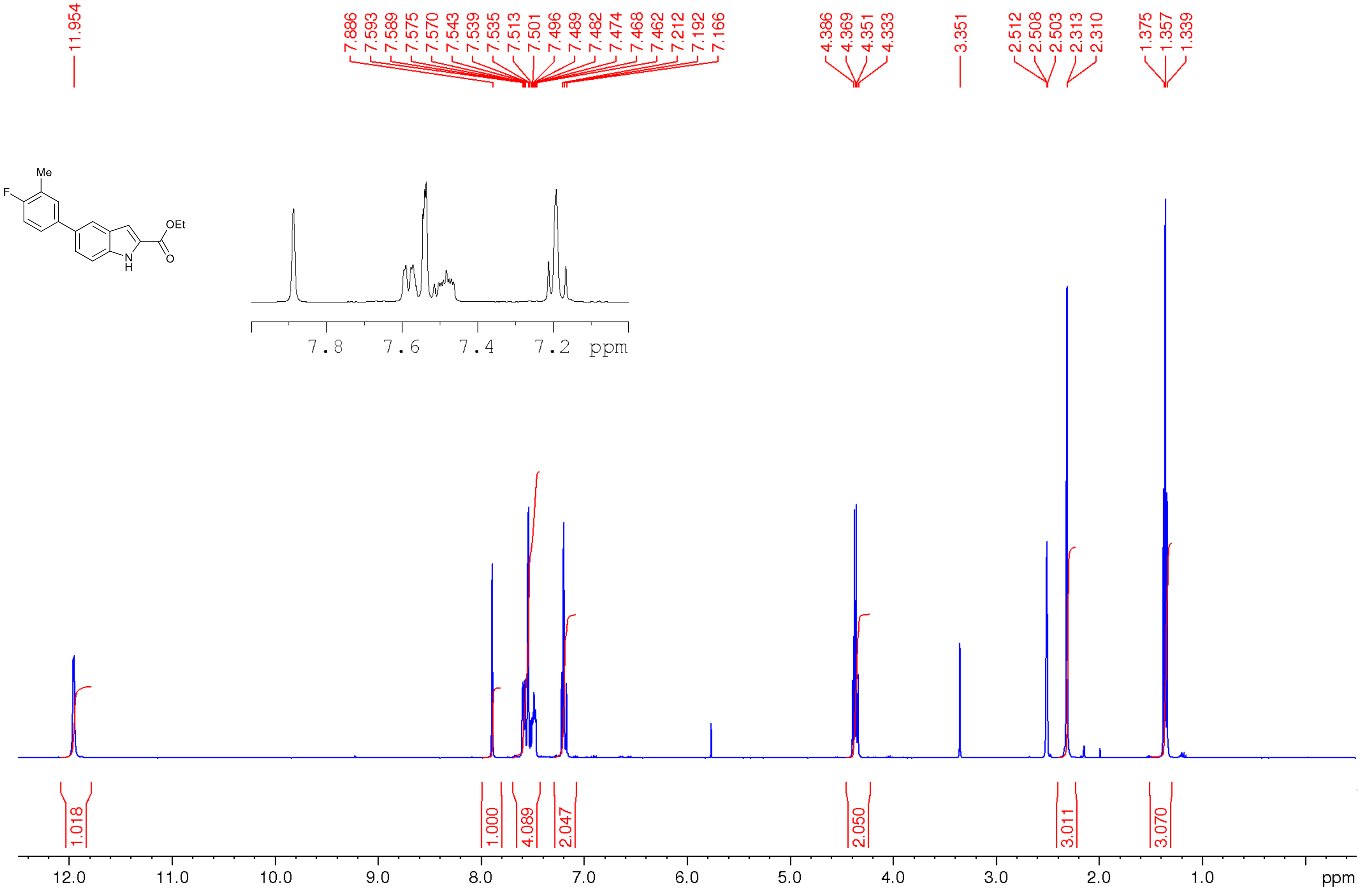
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



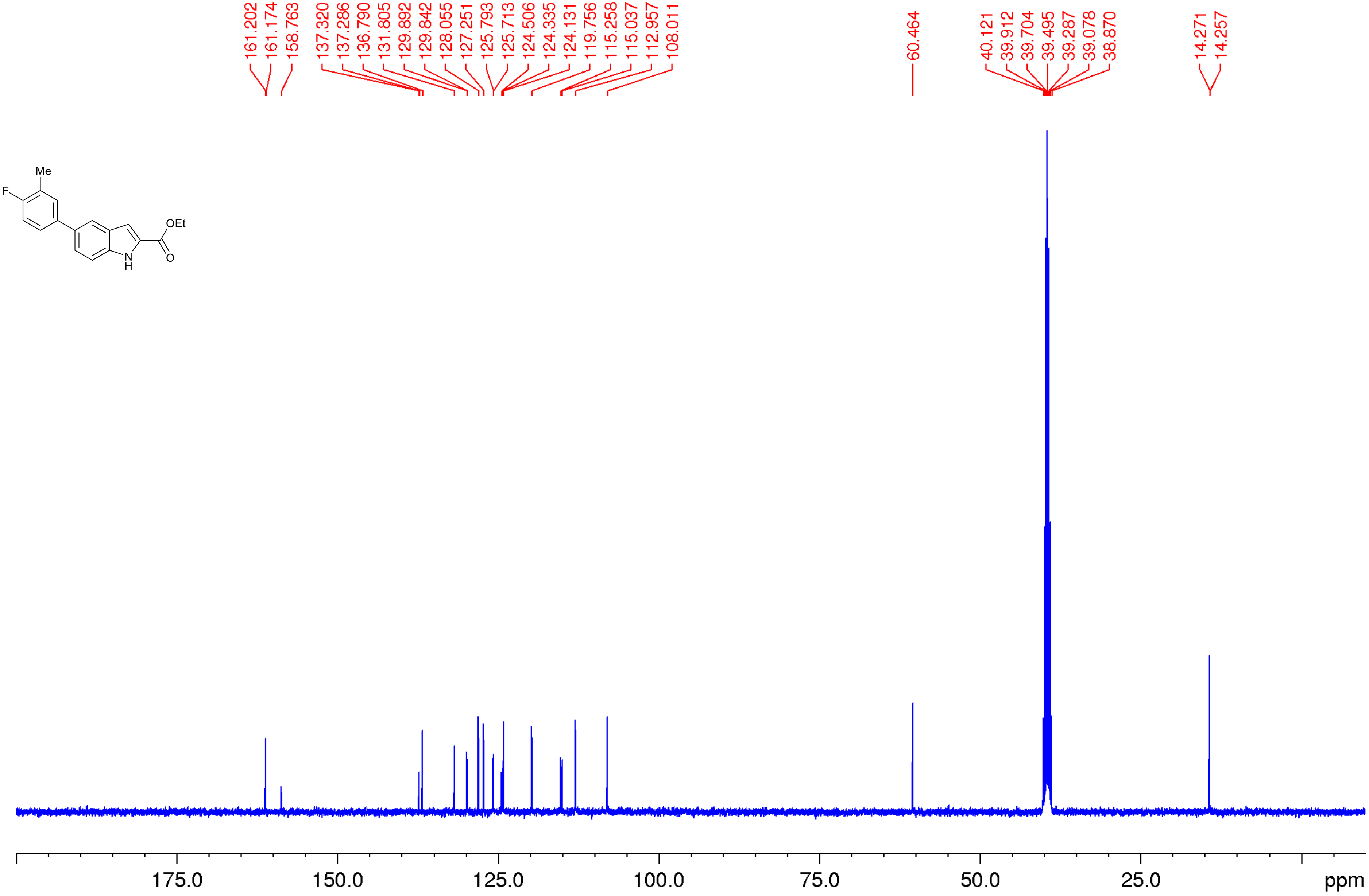
DEPT 135 NMR-spectrum ($CDCl_3$)



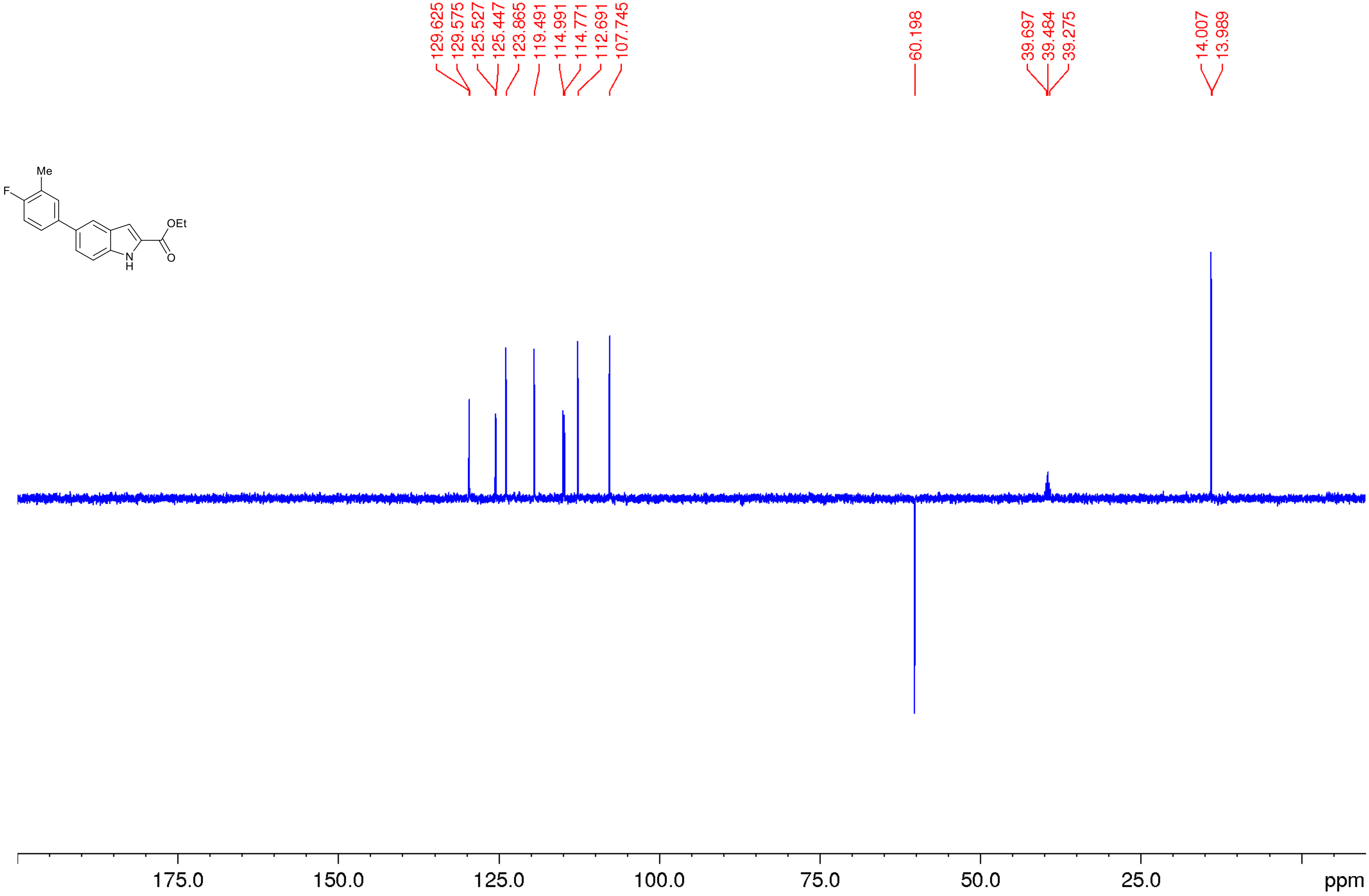
^{1}H NMR-spectrum (400 MHz, DMSO-d_6)



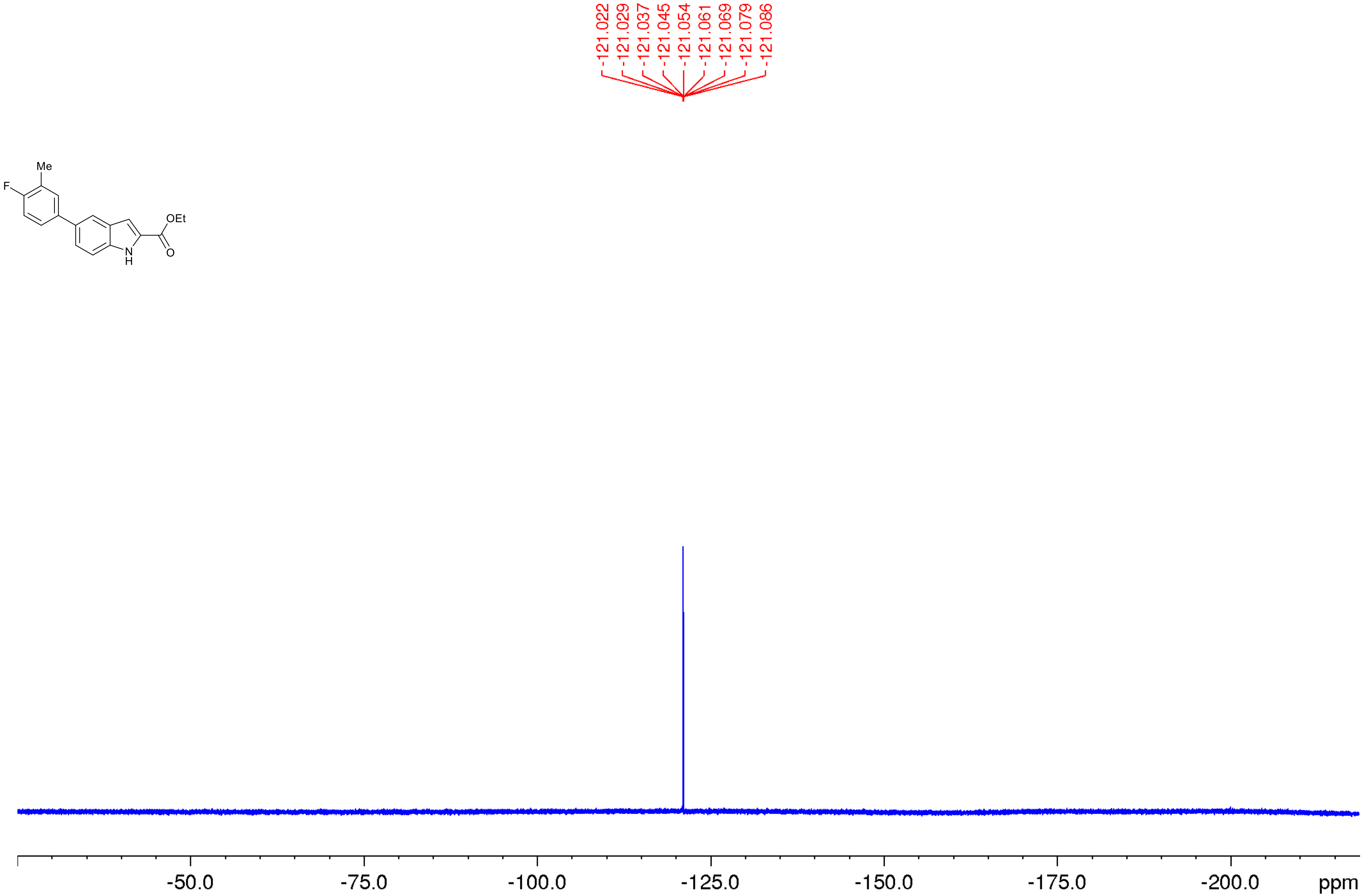
^{13}C NMR-spectrum (100 MHz, DMSO-d_6)



DEPT 135 NMR-spectrum (DMSO-d_6)



^{19}F NMR-spectrum (376.5, DMSO-d_6)



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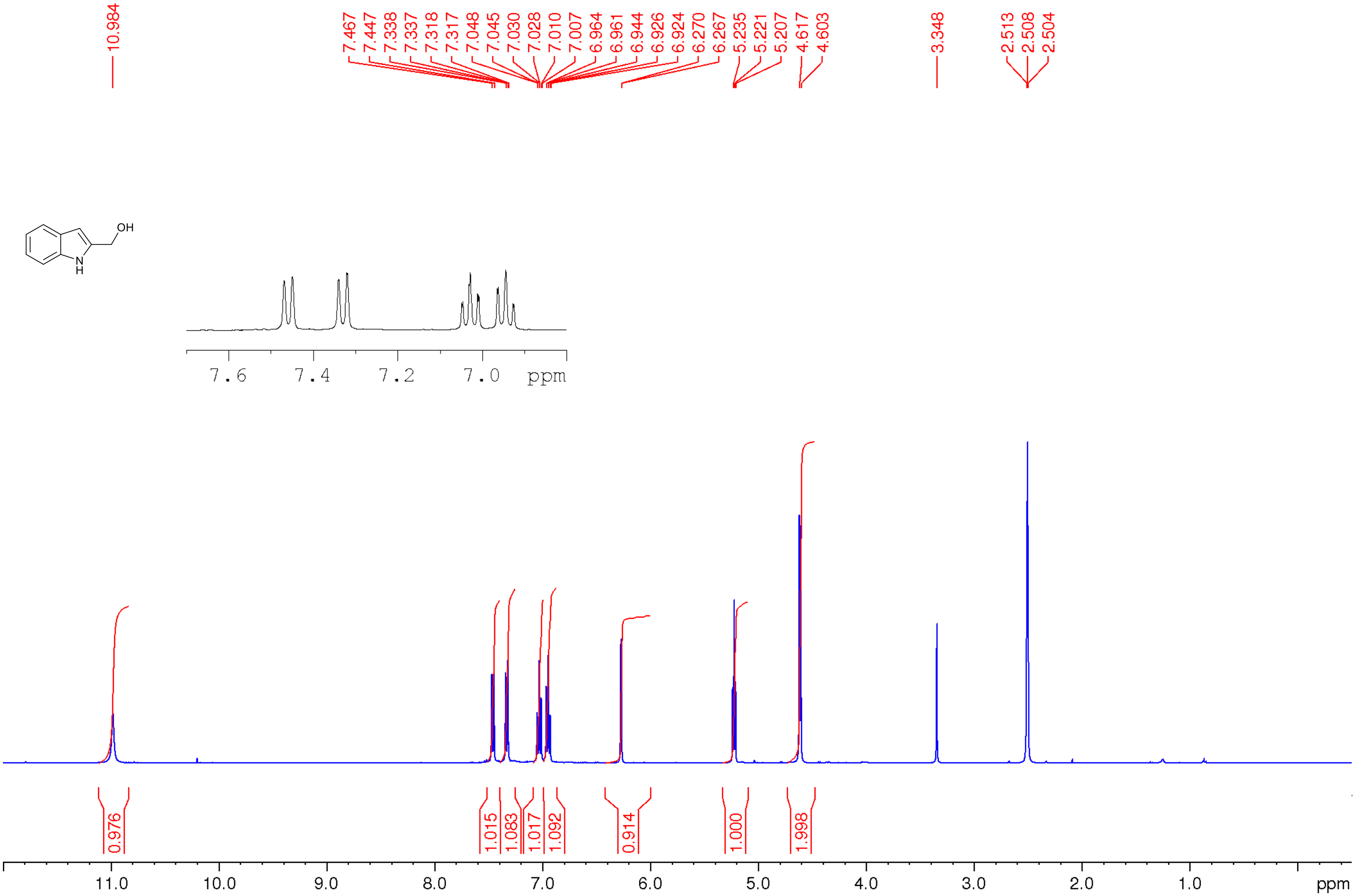
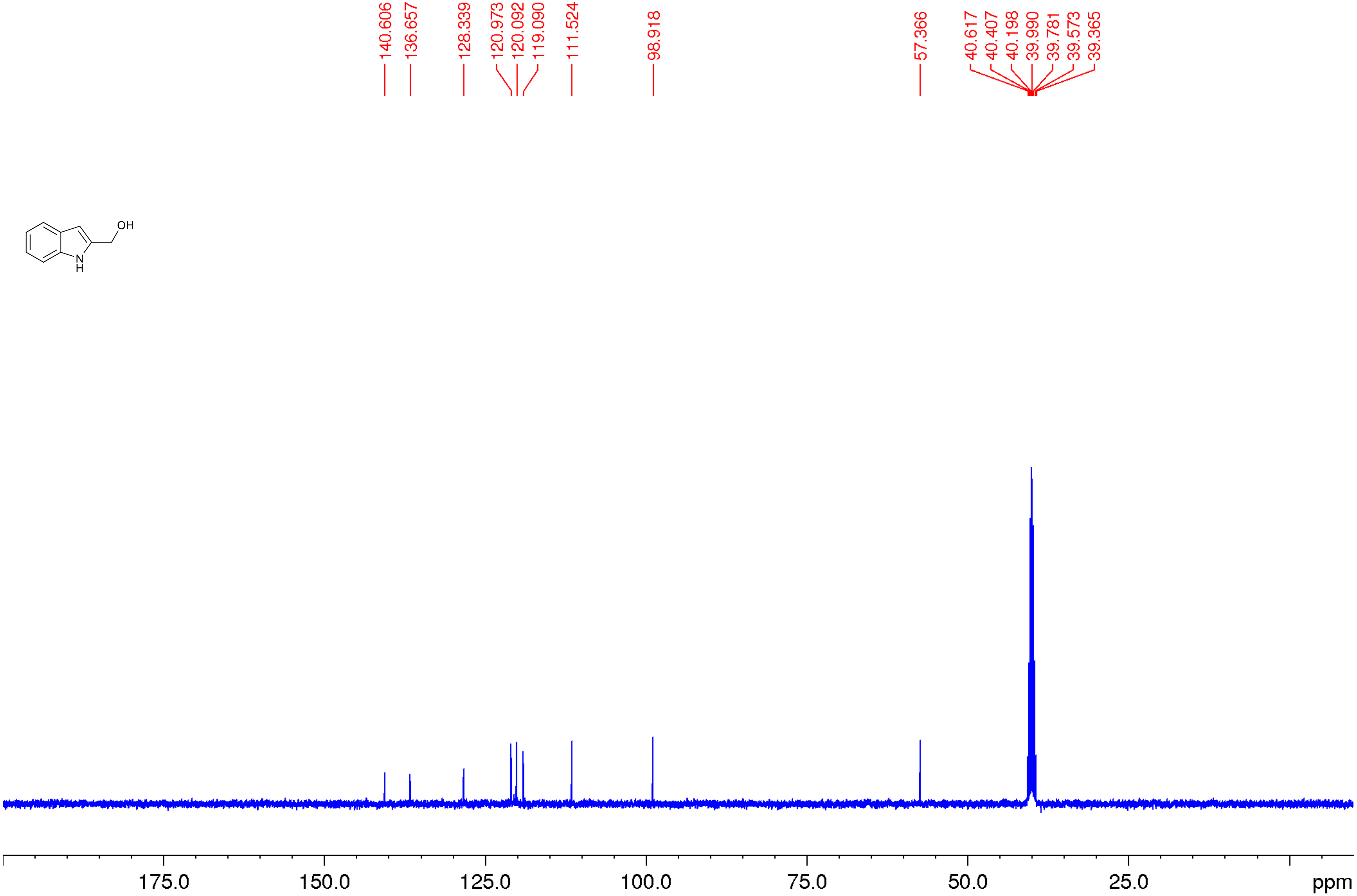
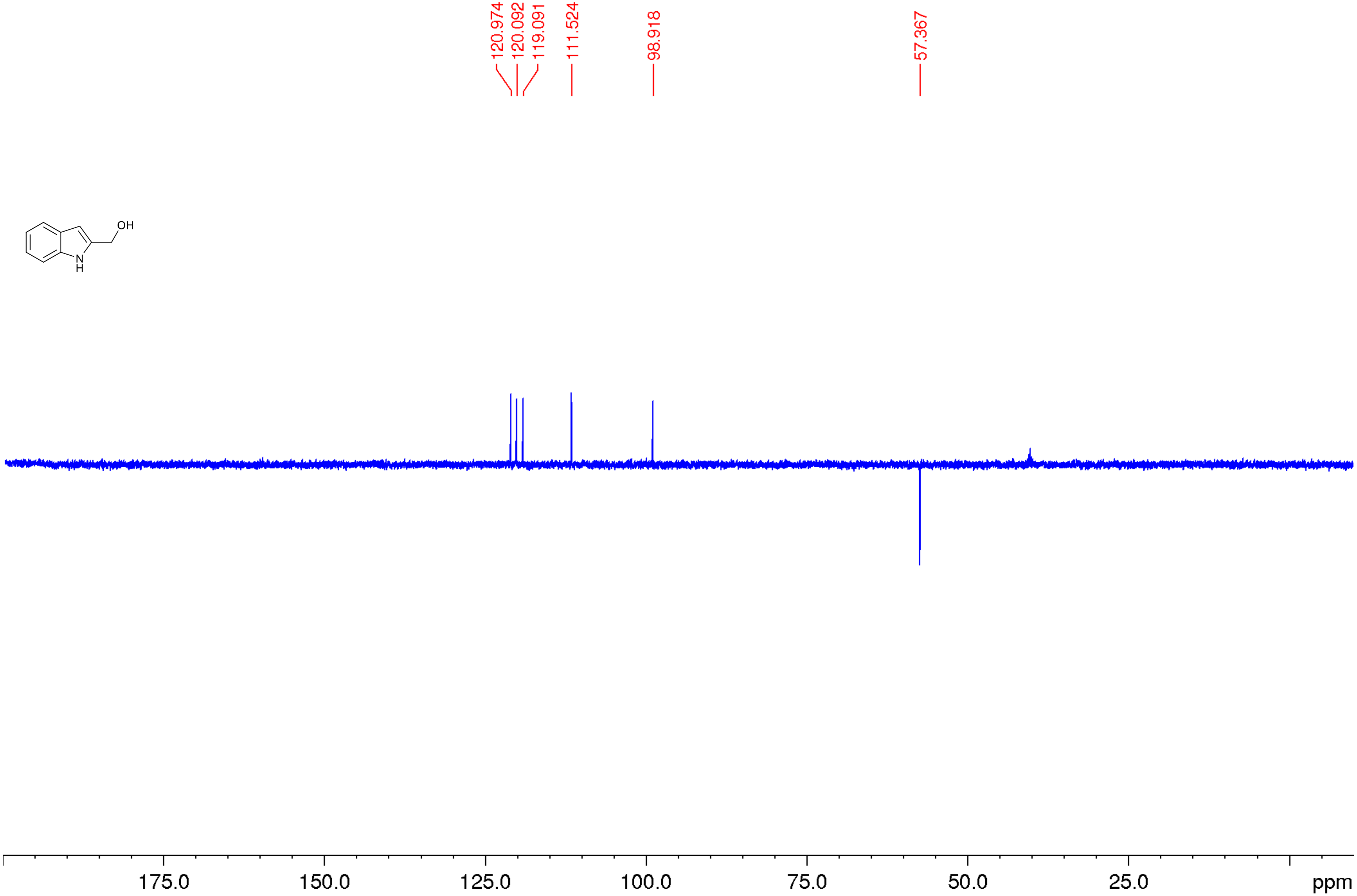


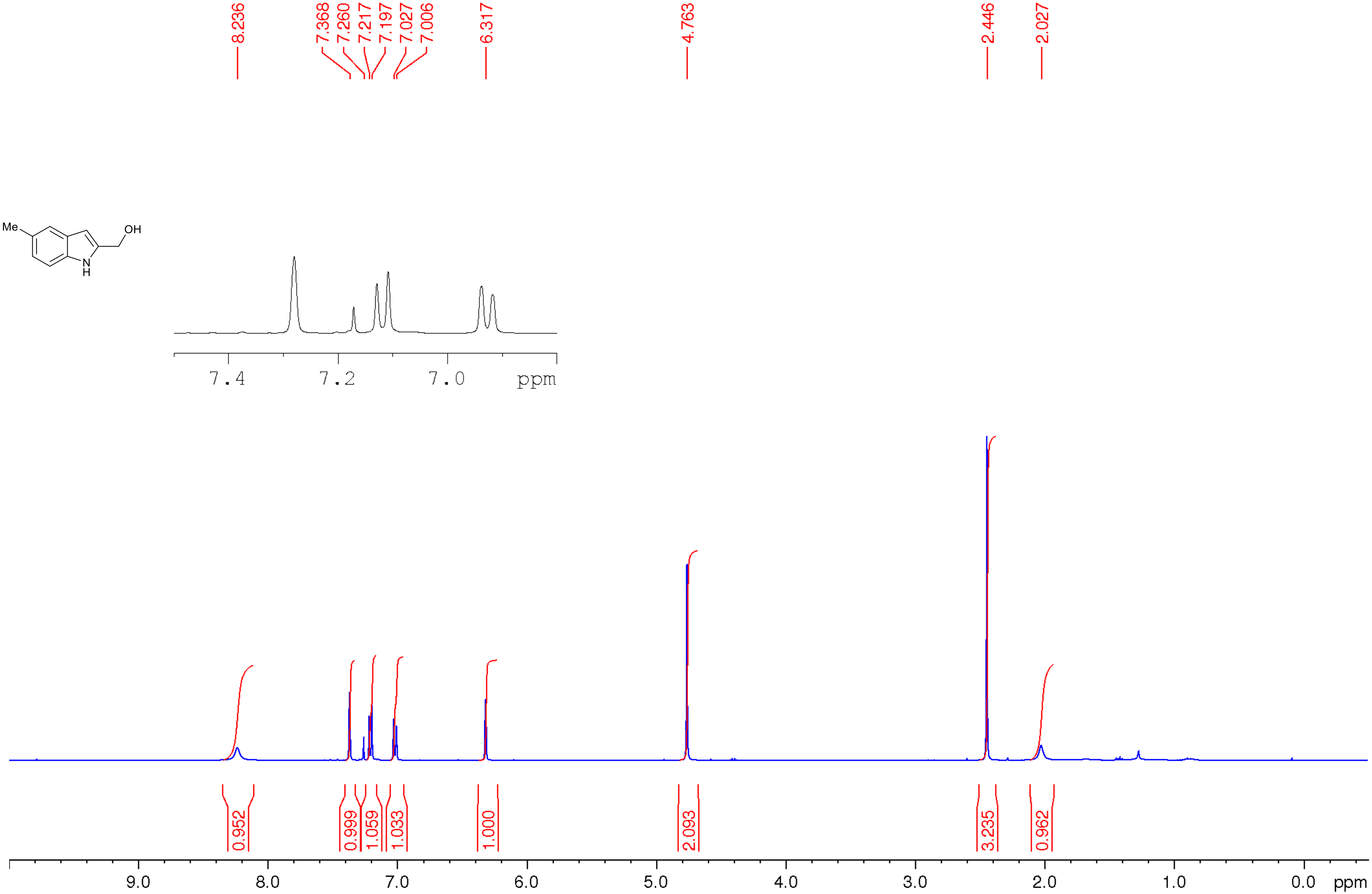
^{13}C NMR-spectrum (100 MHz, DMSO-d_6)



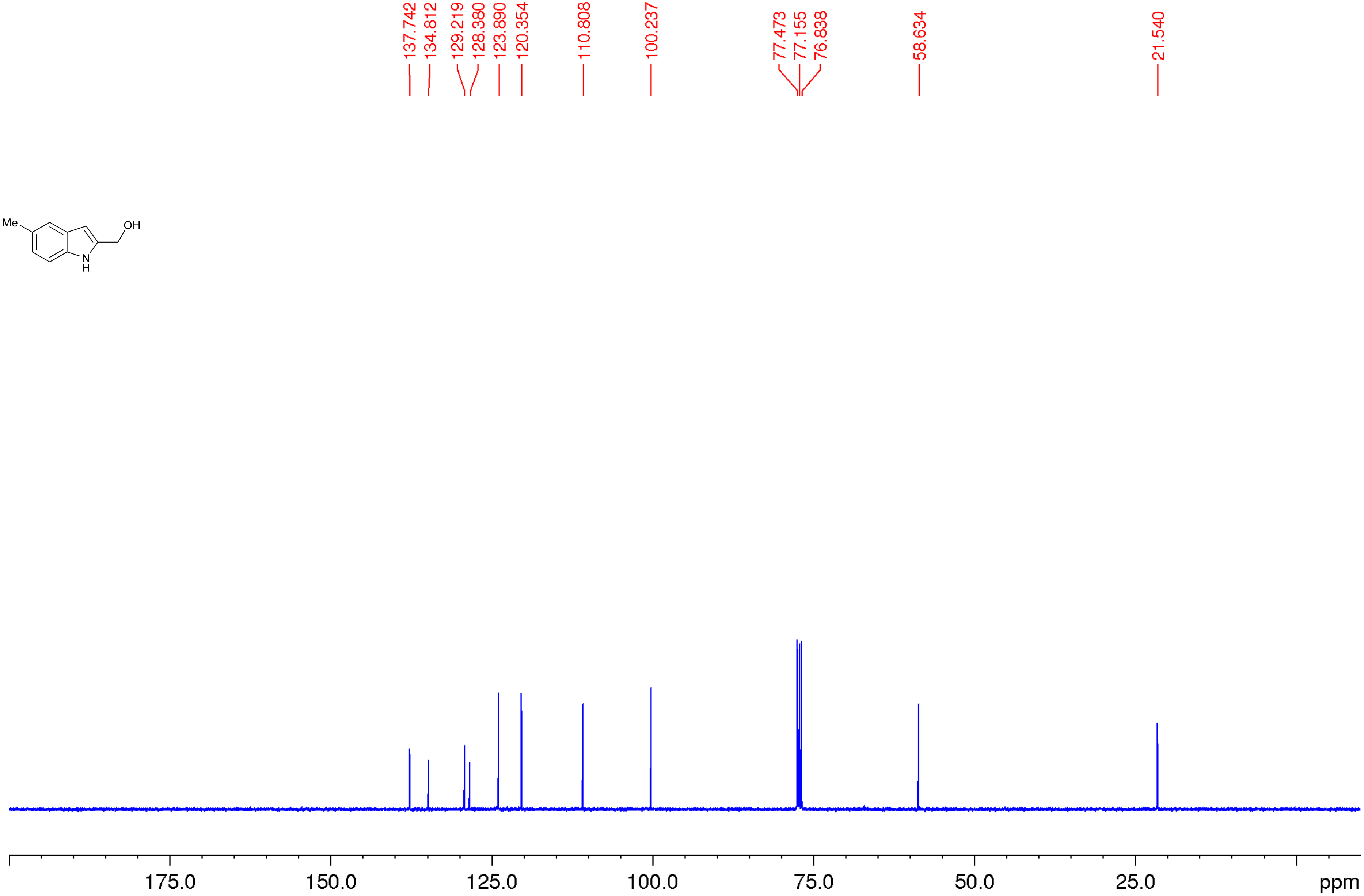
DEPT 135 NMR-spectrum (DMSO-d_6)



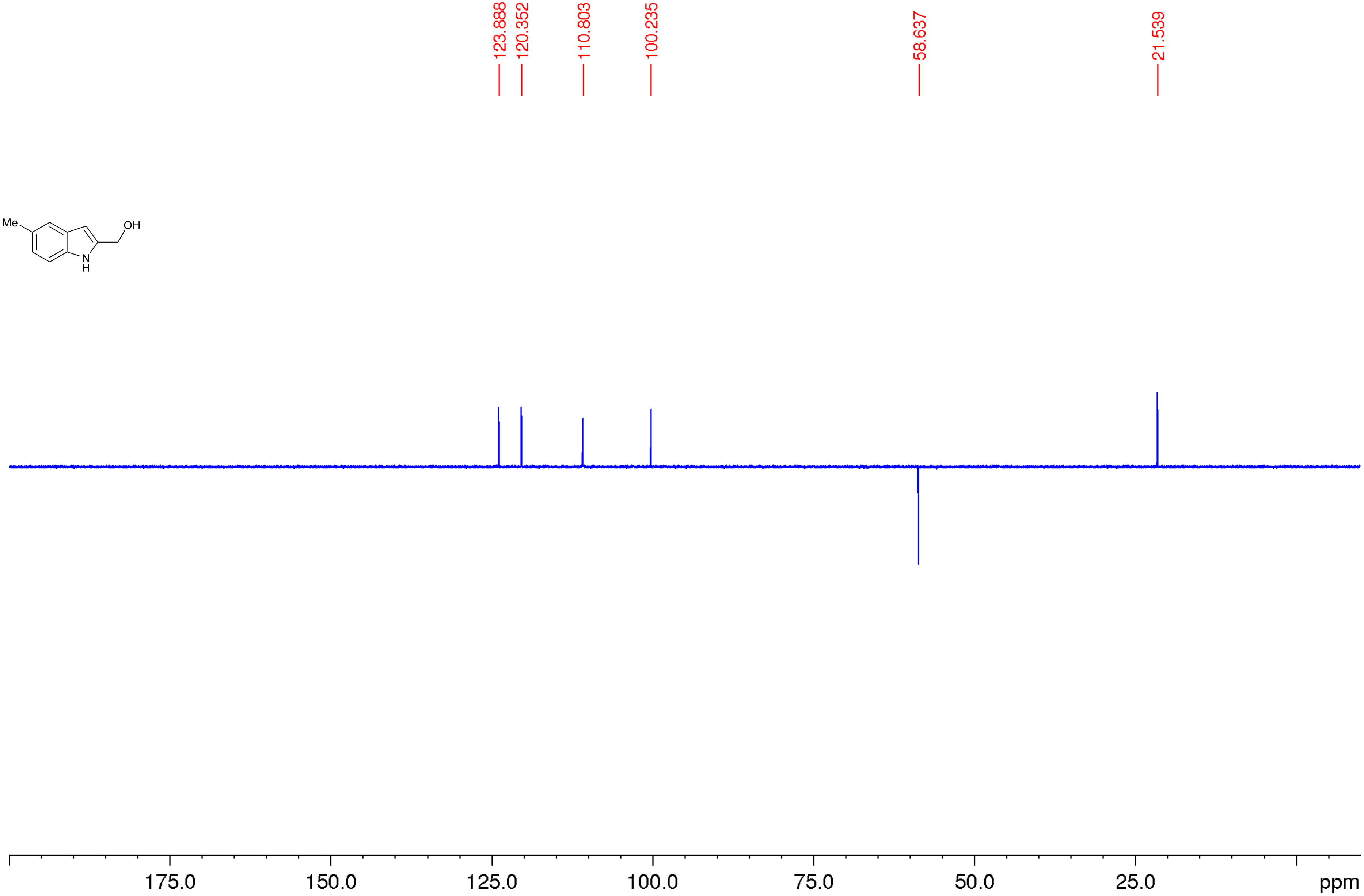
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



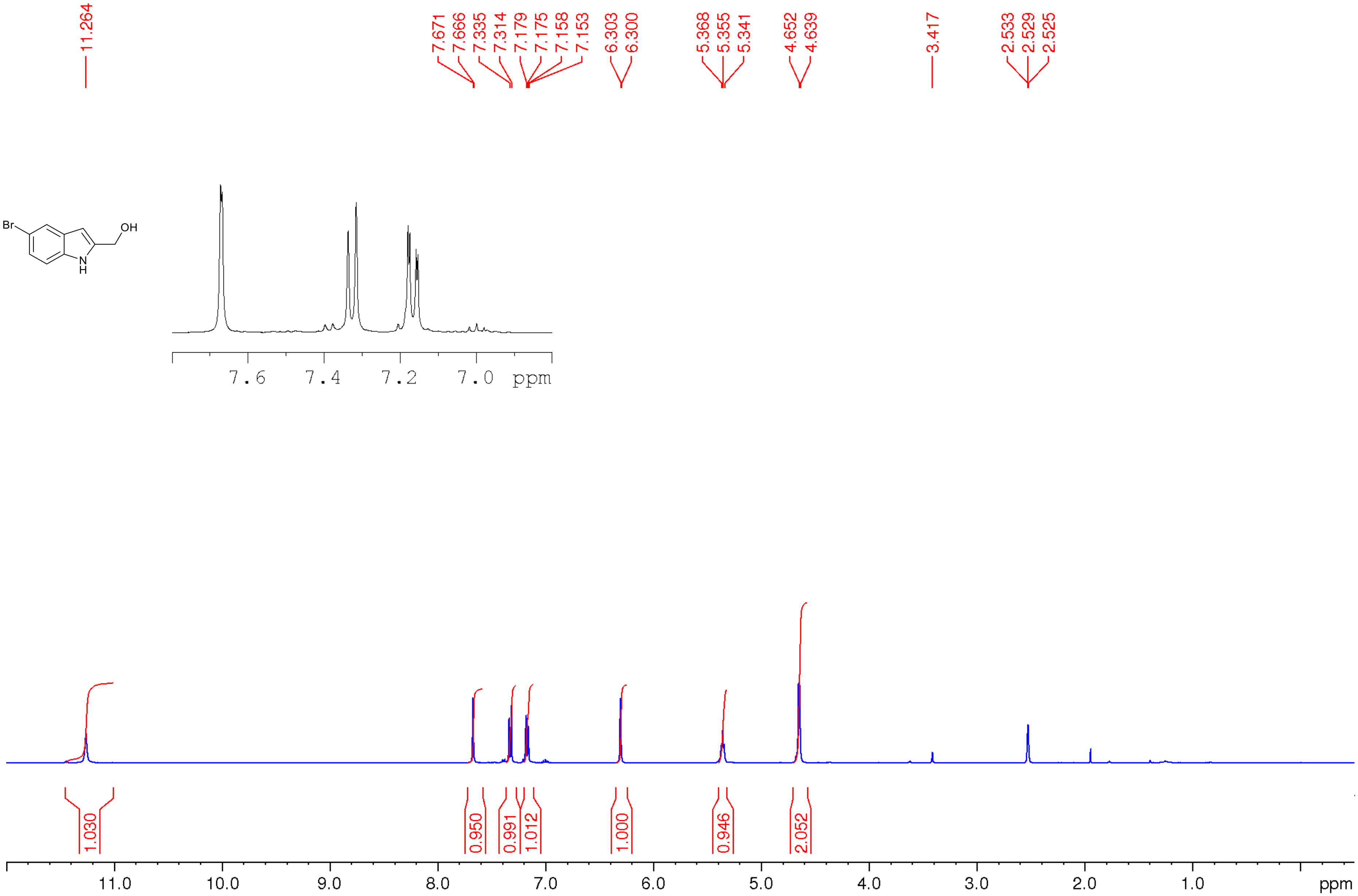
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



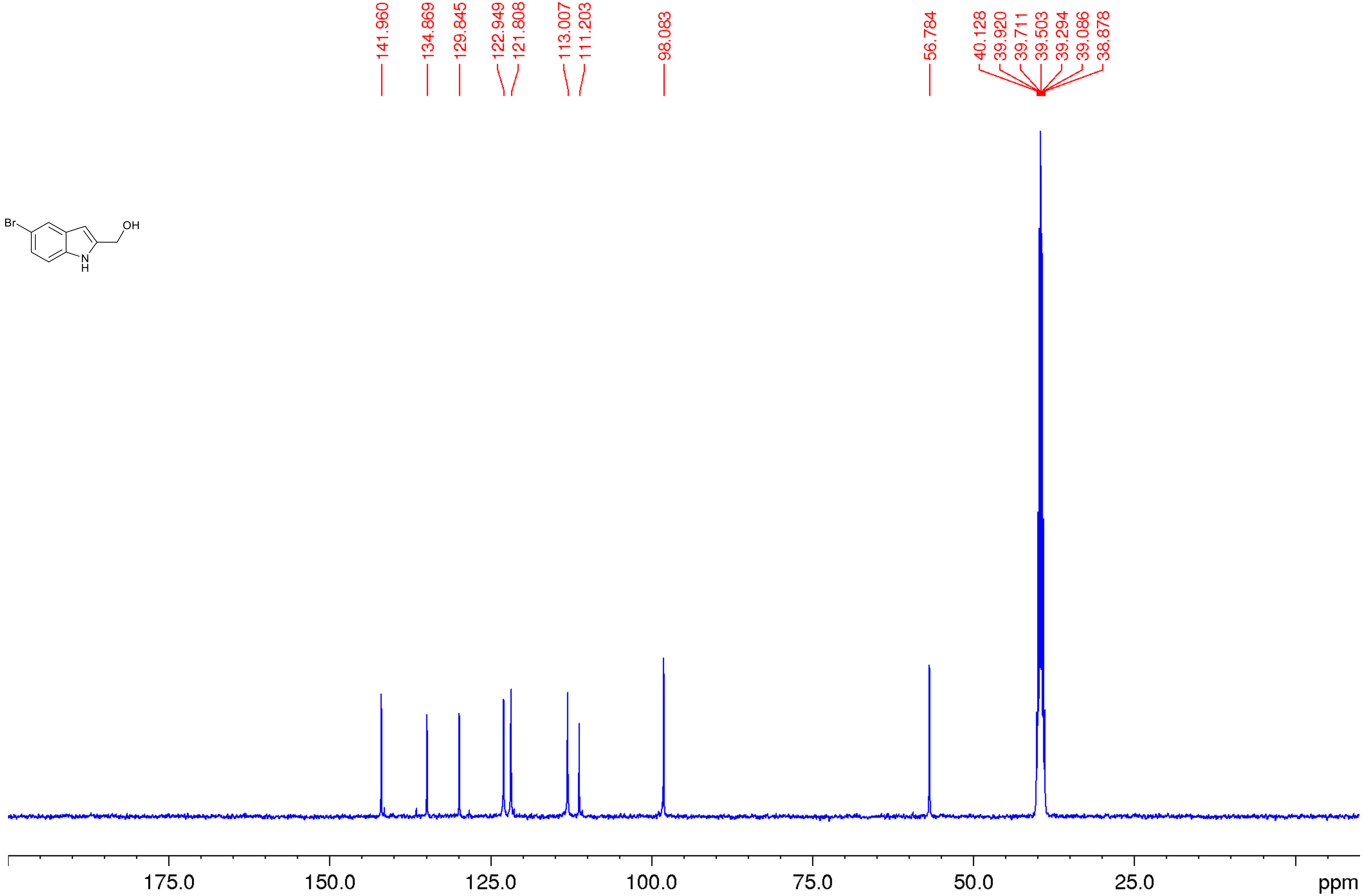
DEPT 135 NMR-spectrum ($CDCl_3$)



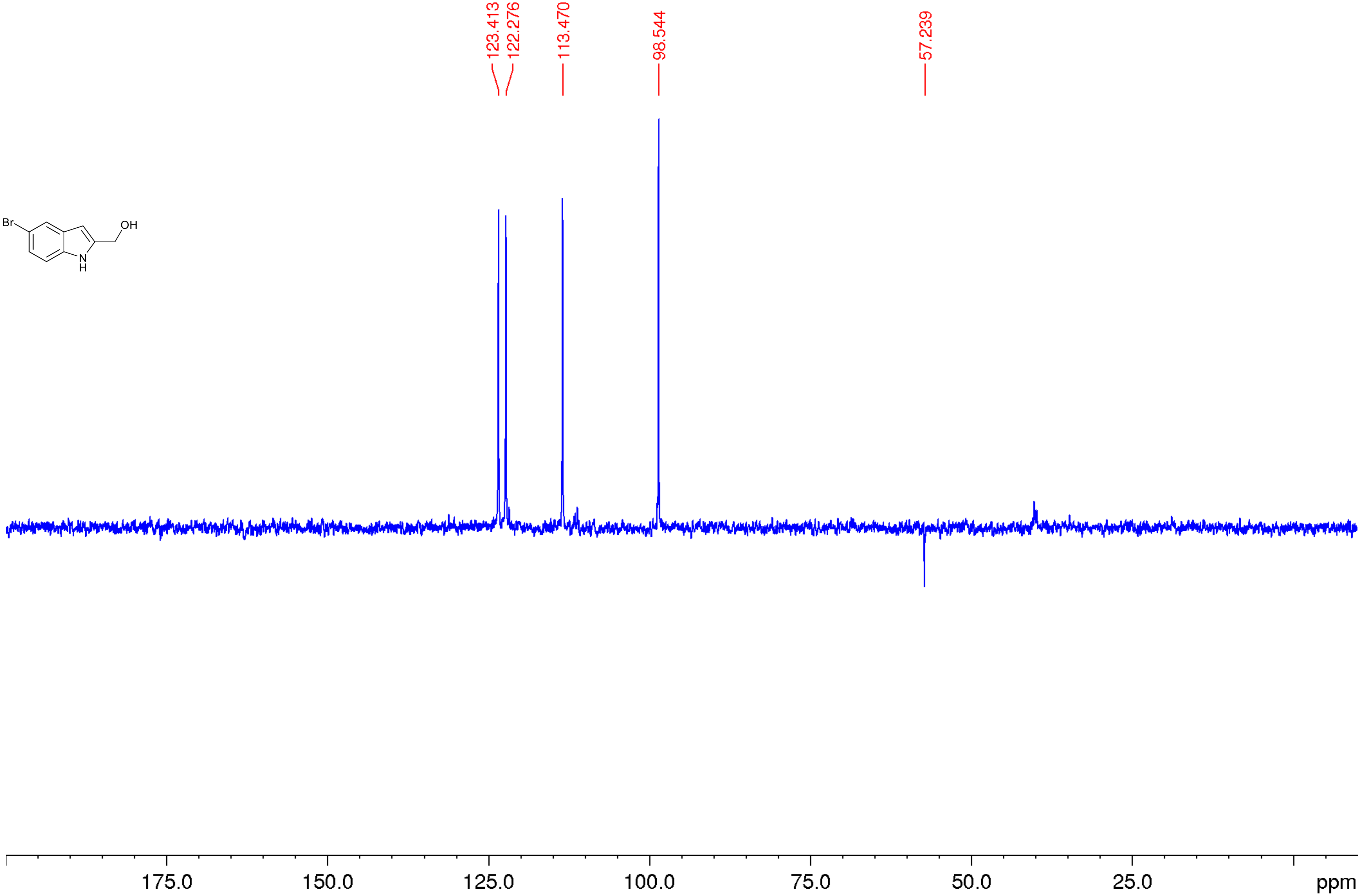
^{1}H NMR-spectrum (400 MHz, DMSO-d_6)



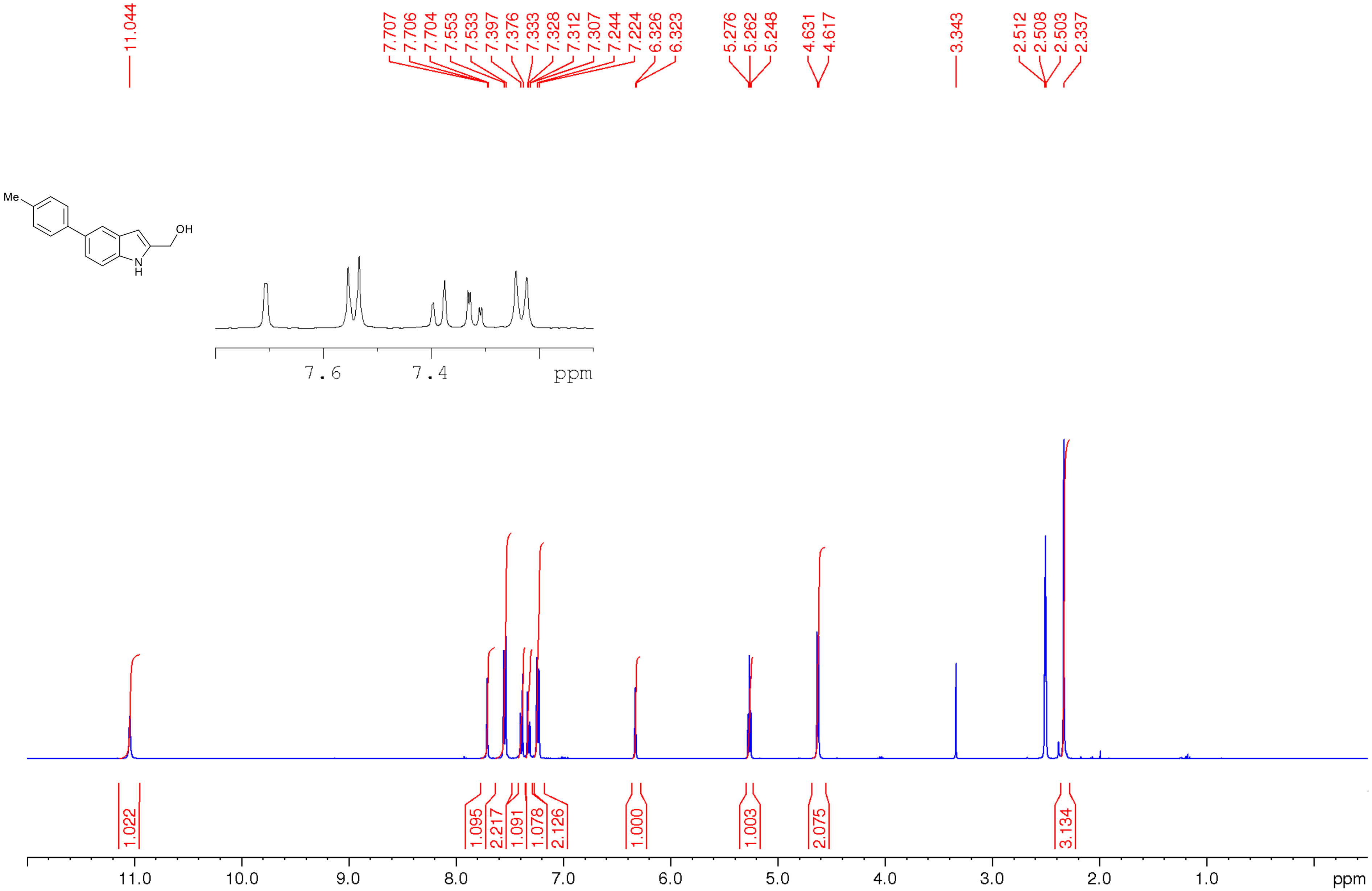
^{13}C NMR-spectrum (100 MHz, DMSO-d_6)



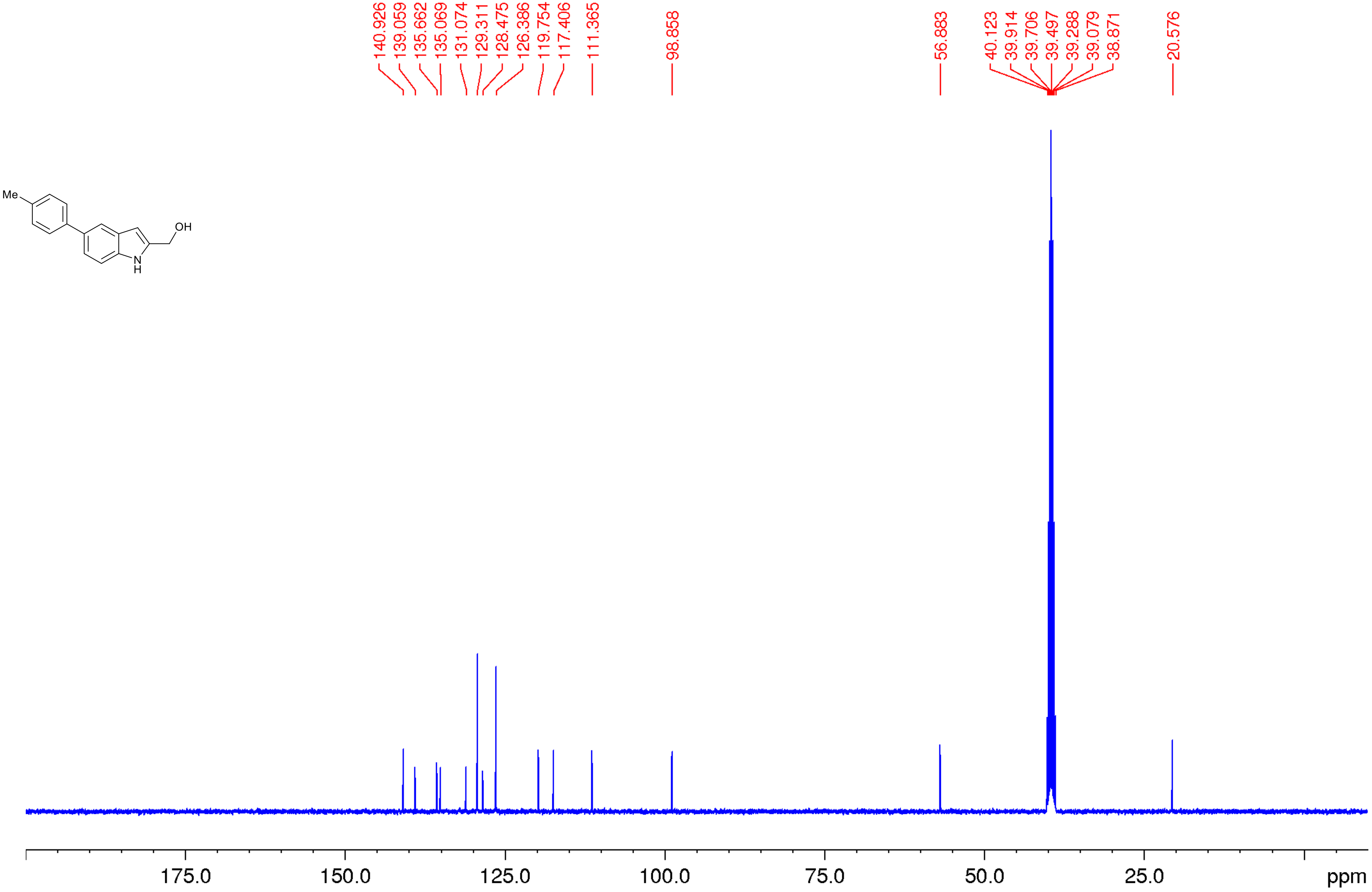
DEPT 135 NMR-spectrum (DMSO-d_6)



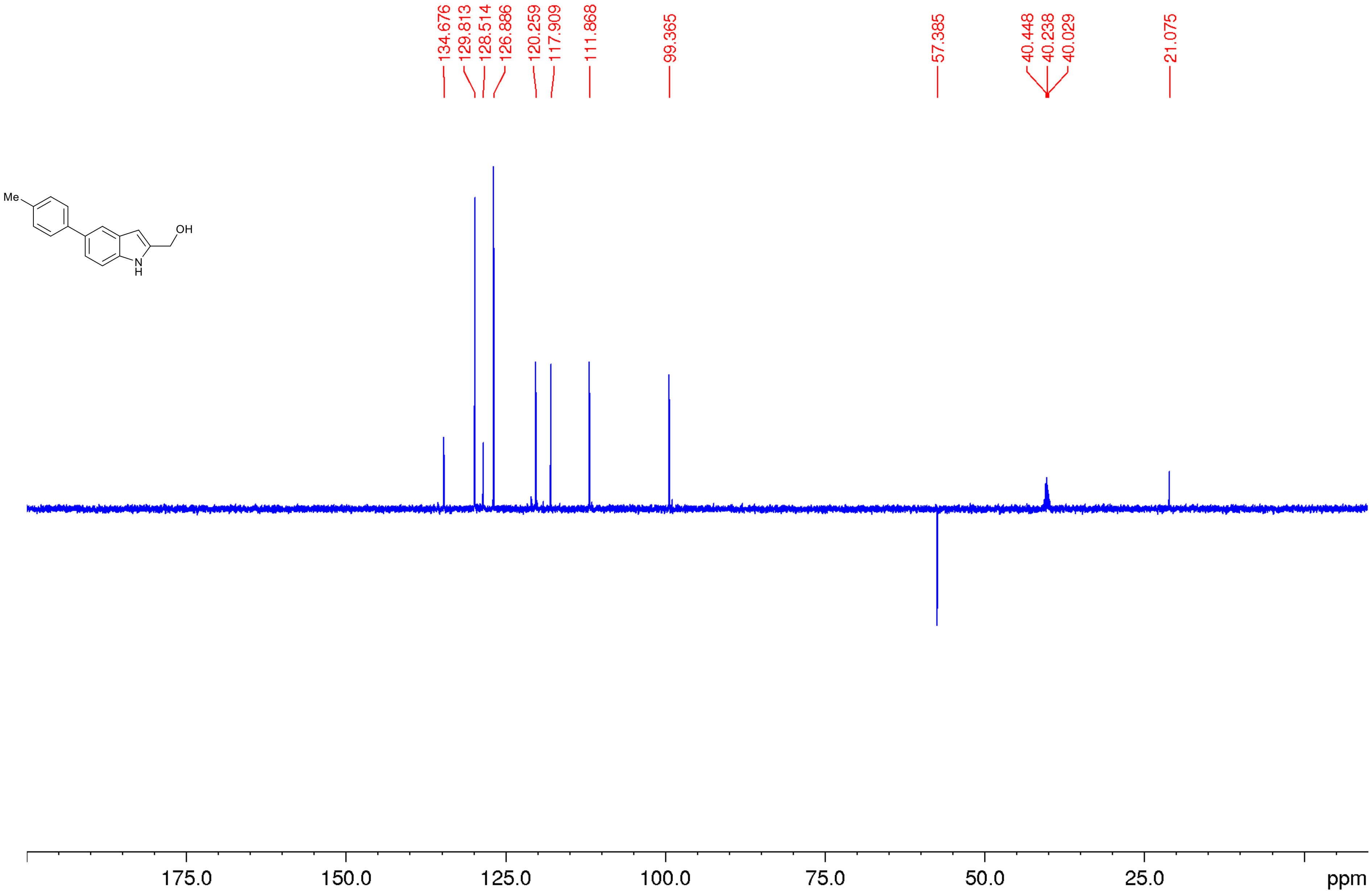
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



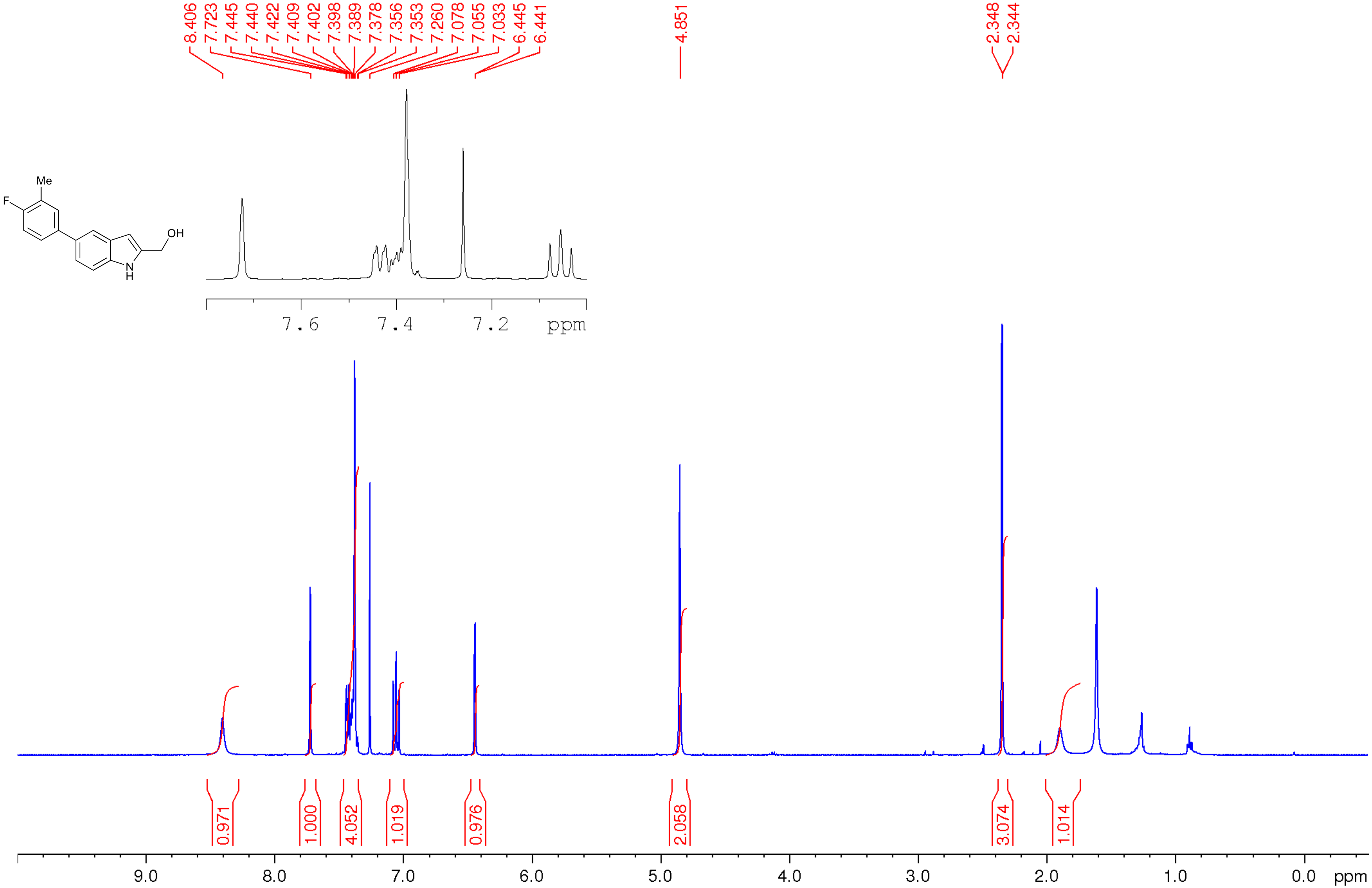
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



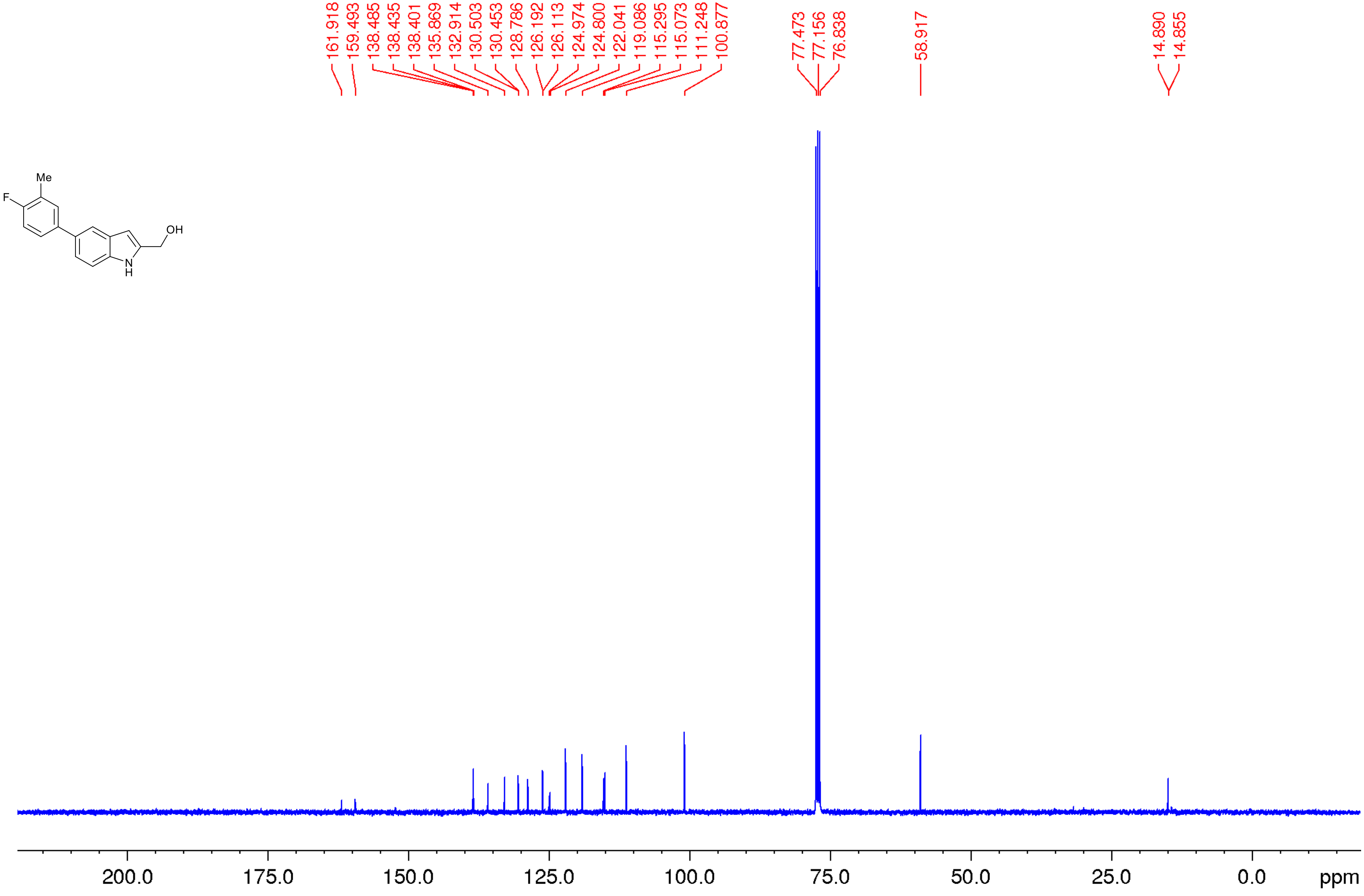
DEPT 135 NMR-spectrum (DMSO-d_6)



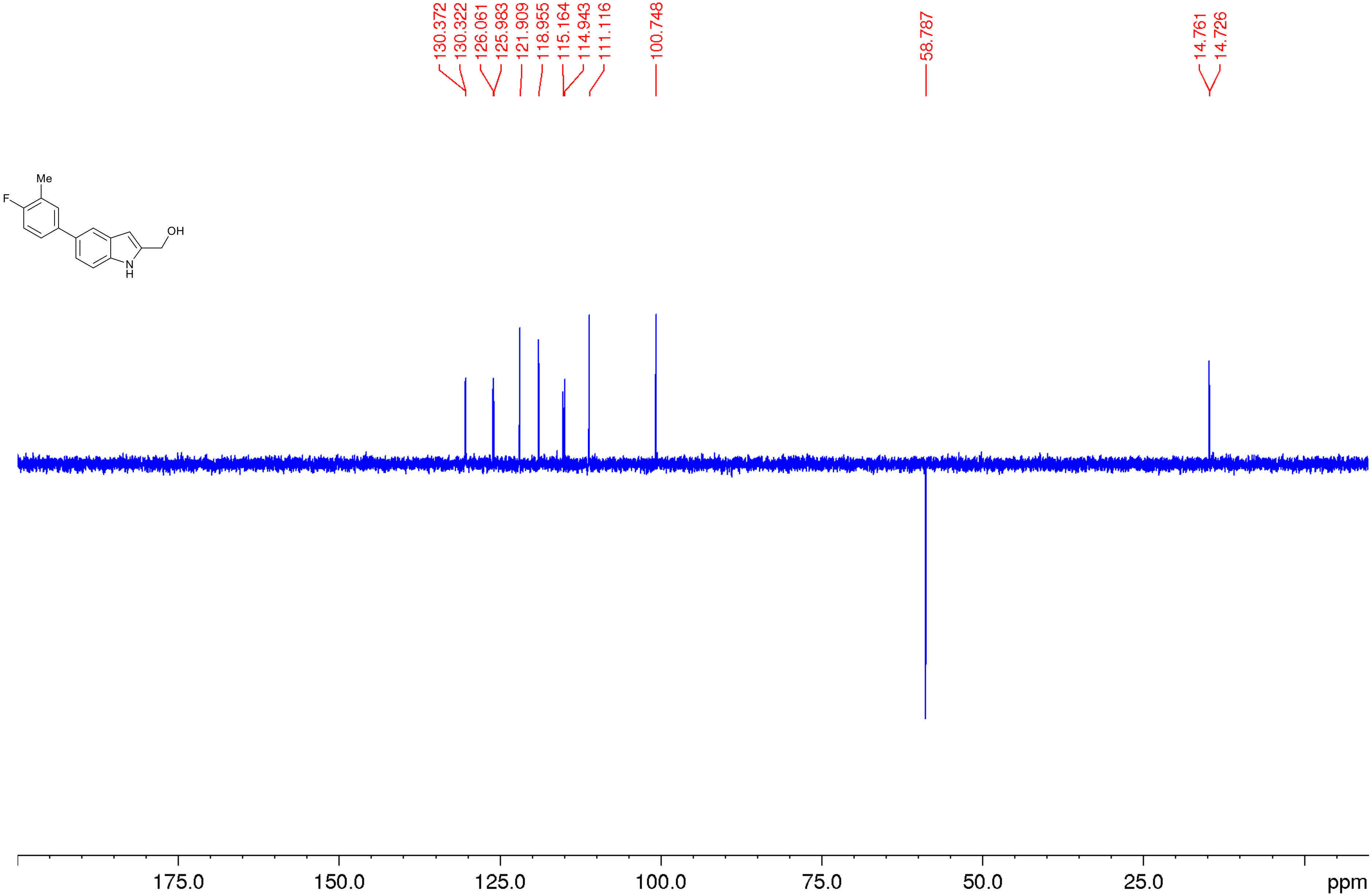
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



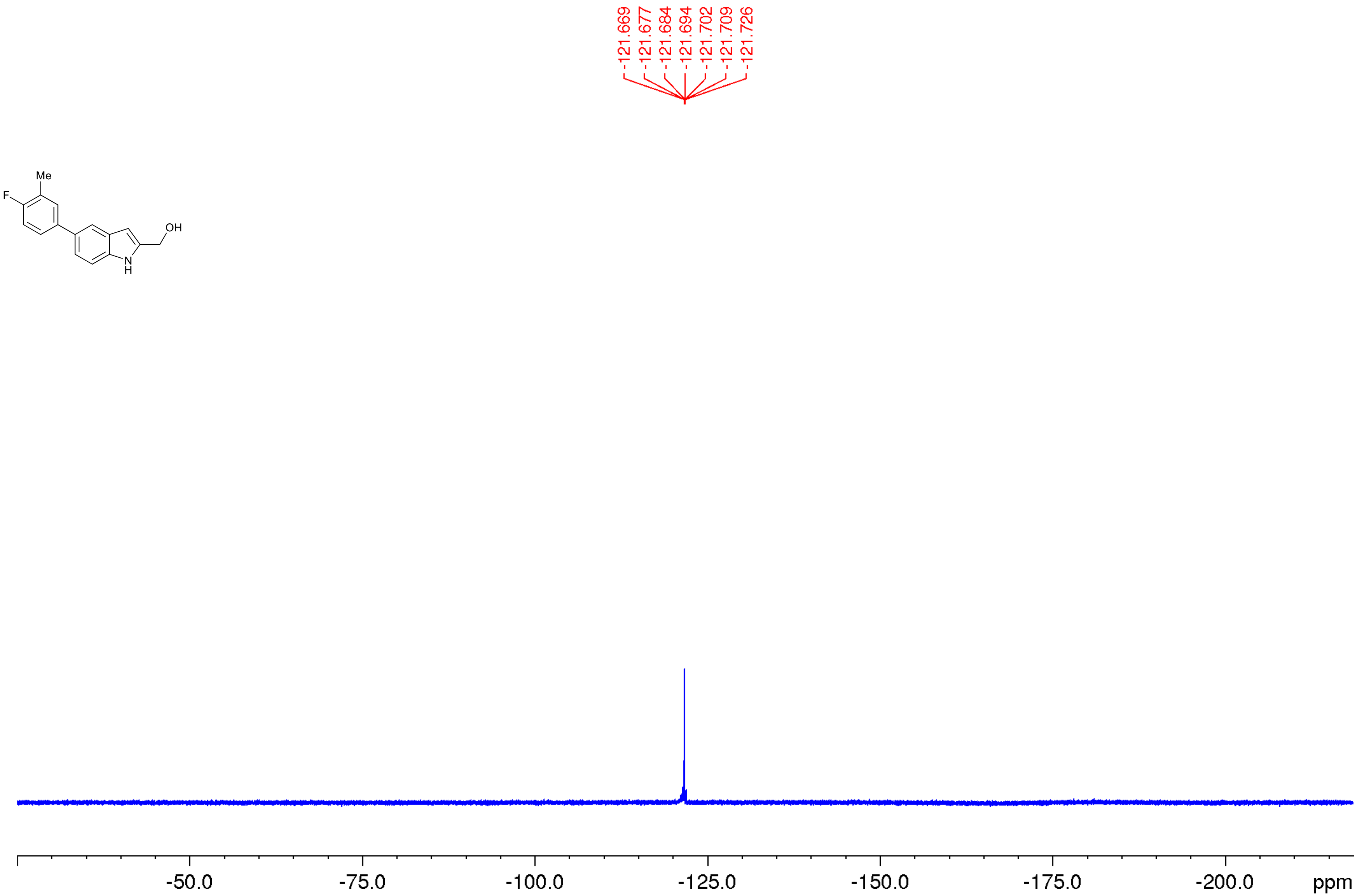
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



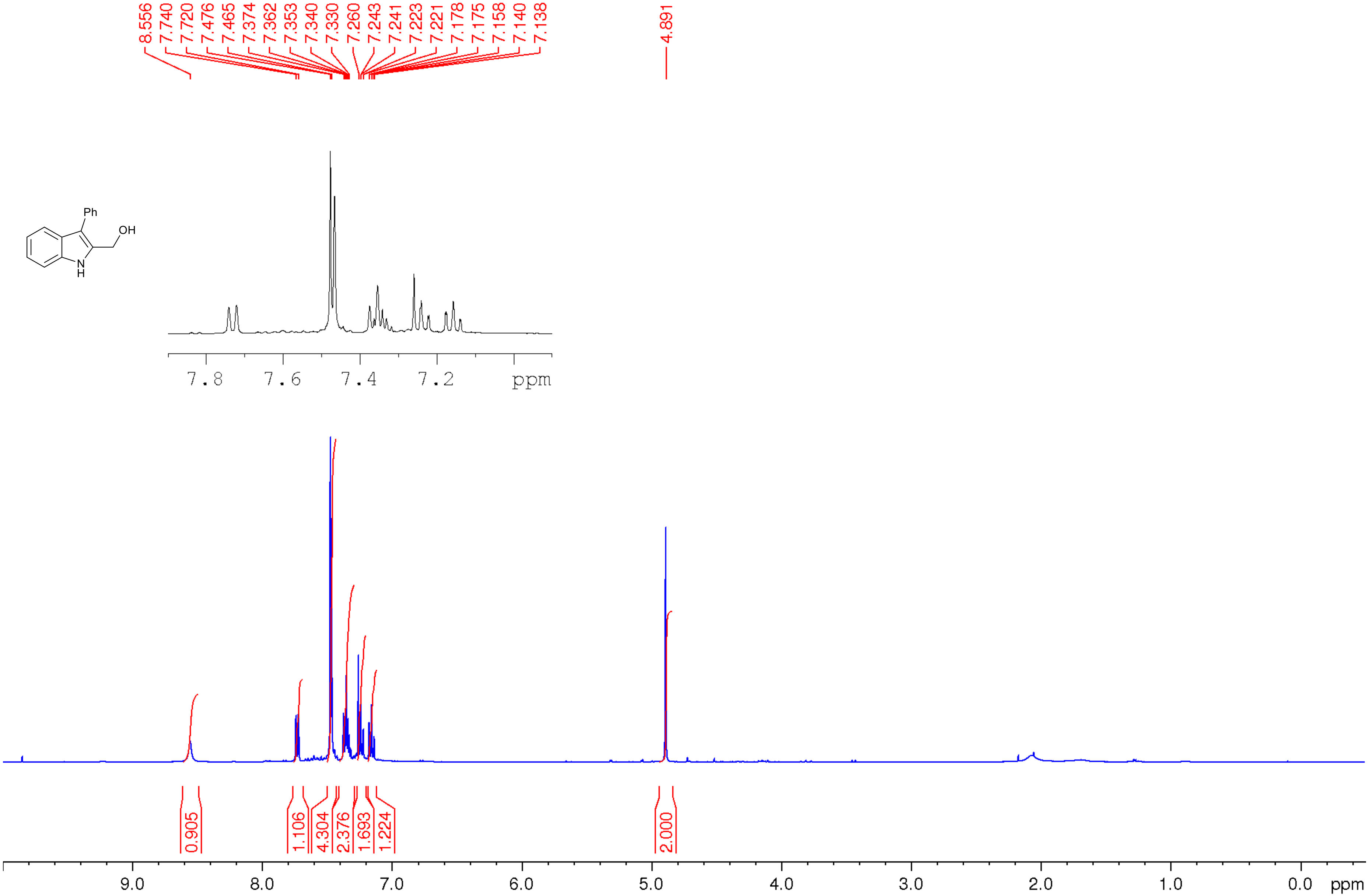
DEPT 135 NMR-spectrum ($CDCl_3$)



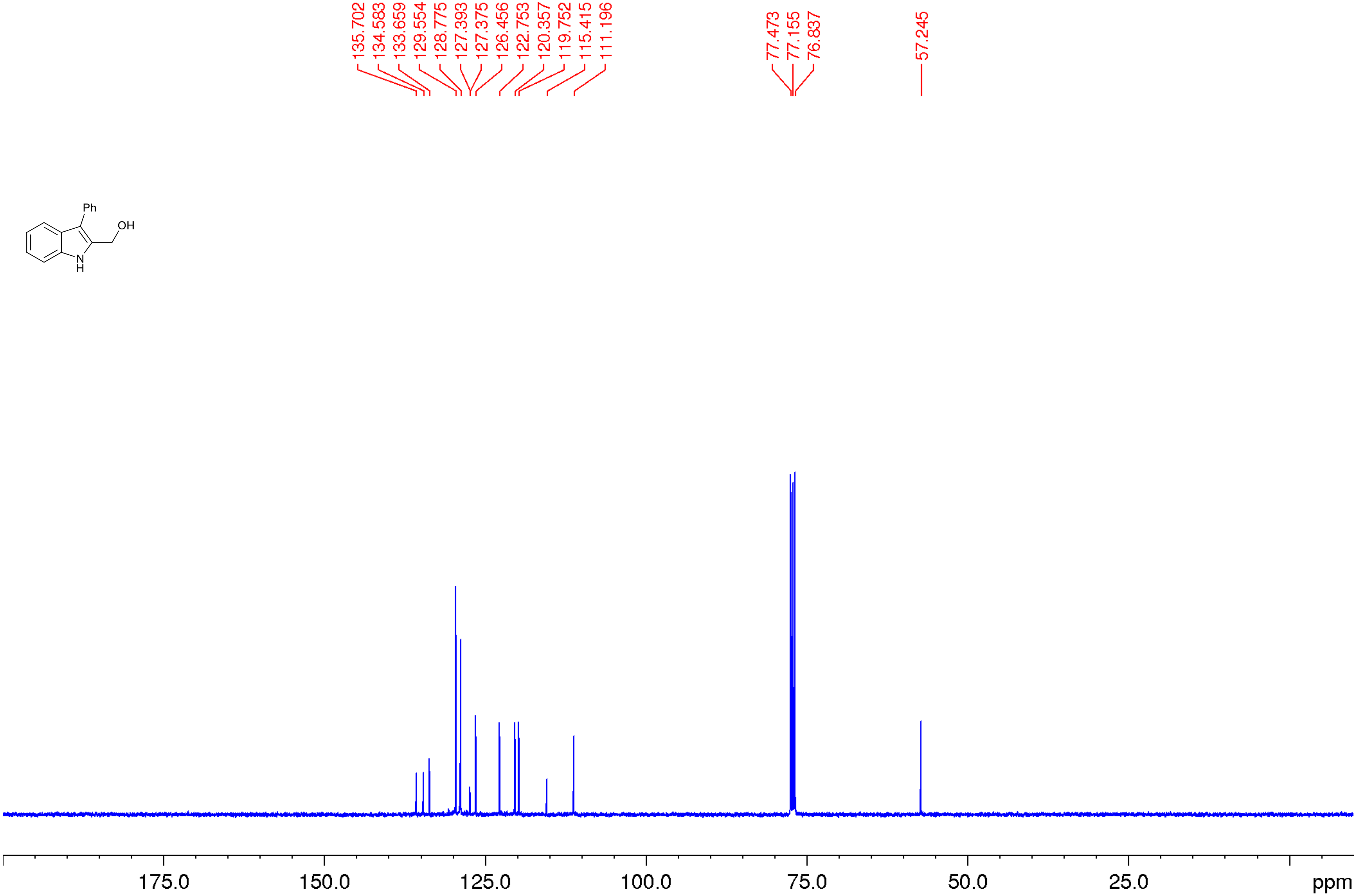
^{19}F NMR-spectrum (376.5, DMSO-d_6)



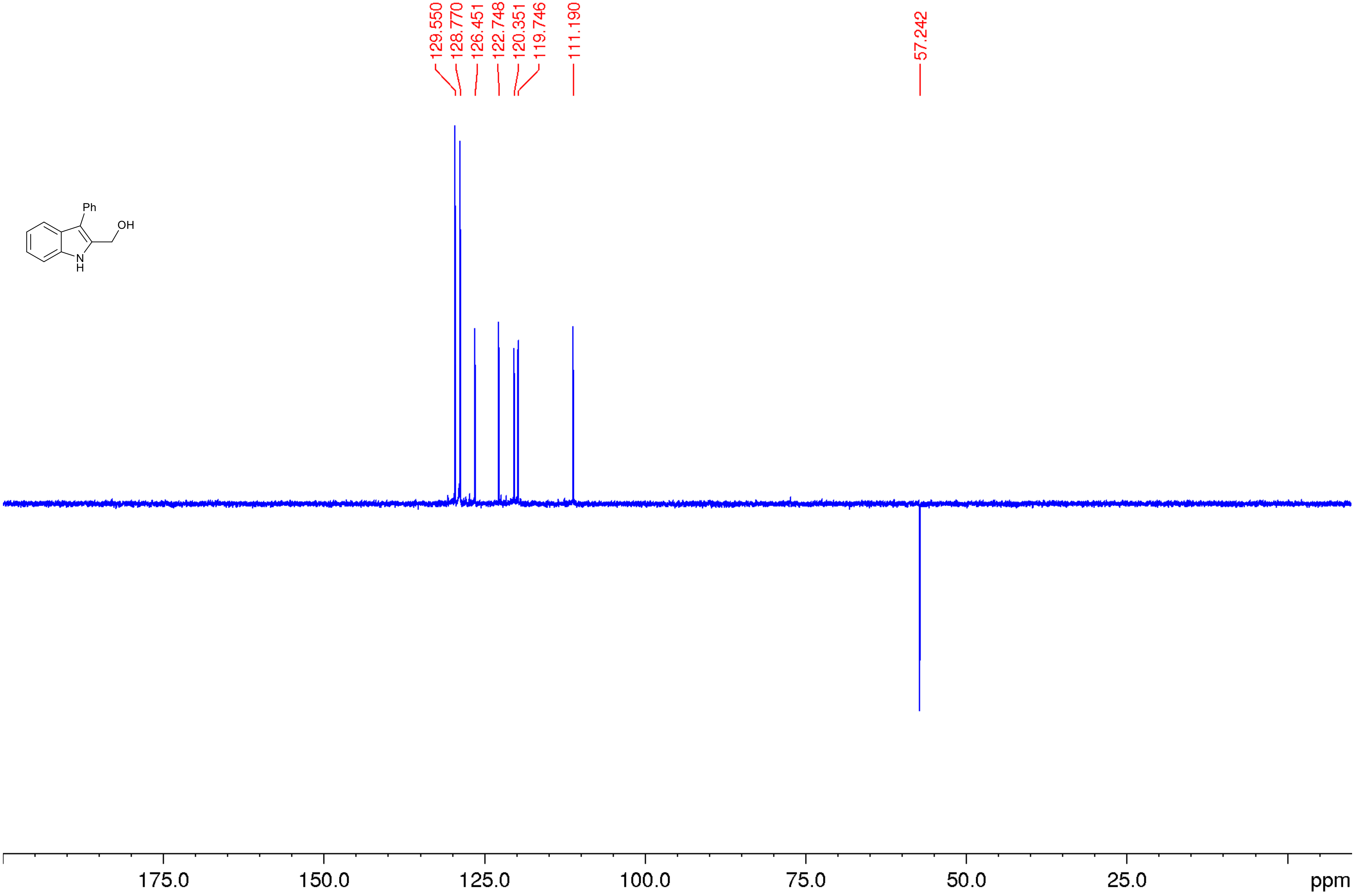
^1H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)



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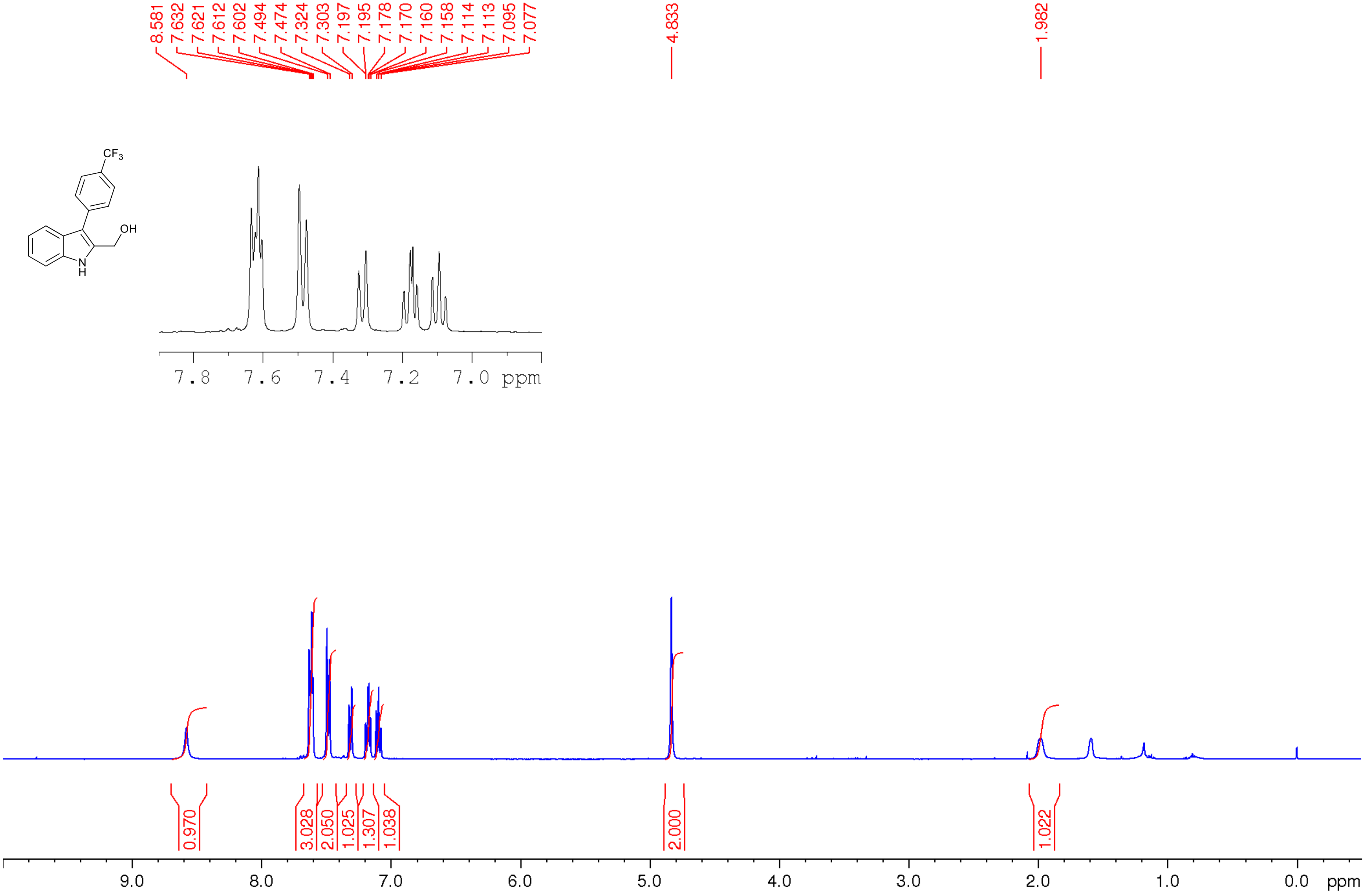

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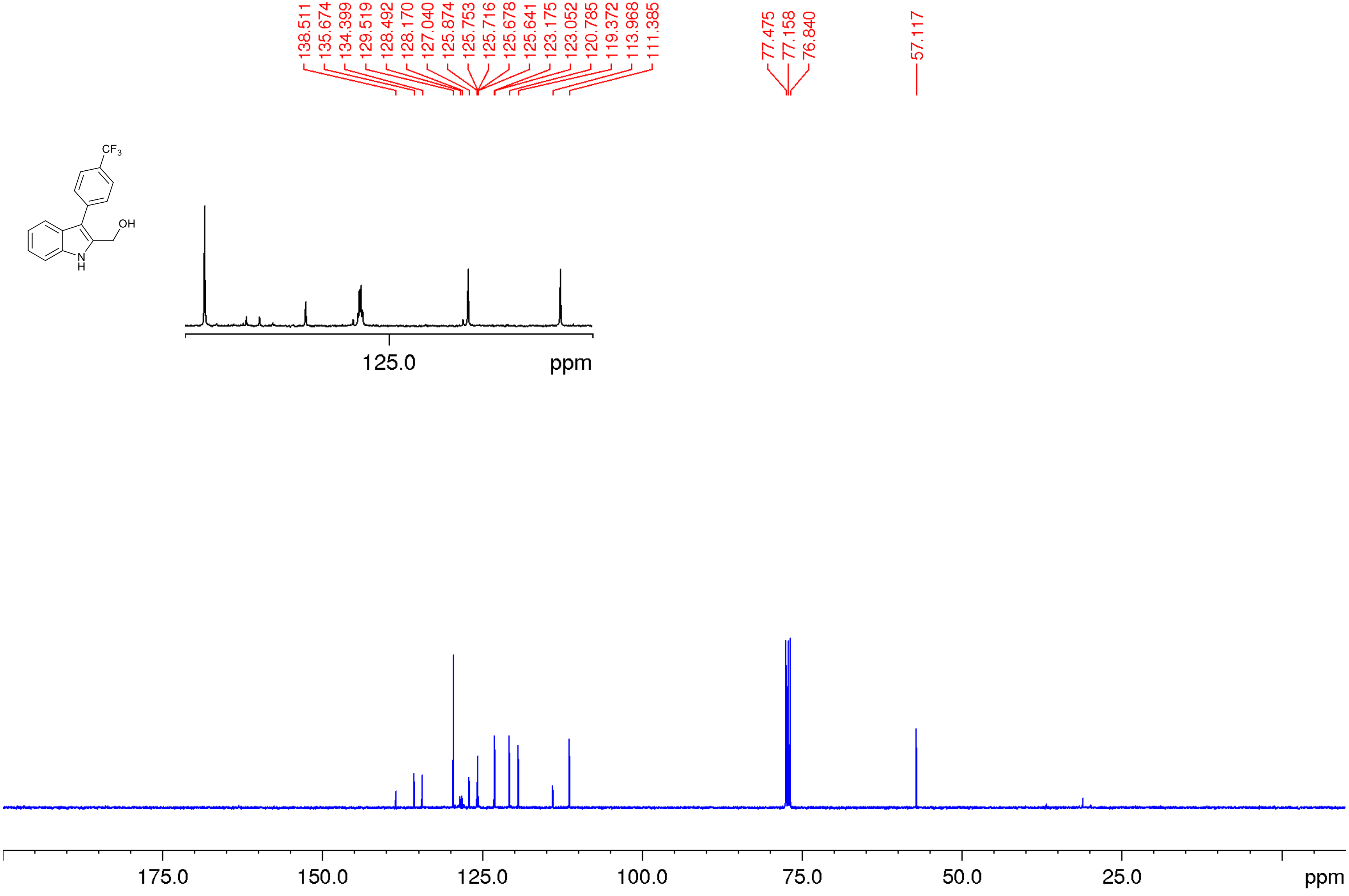
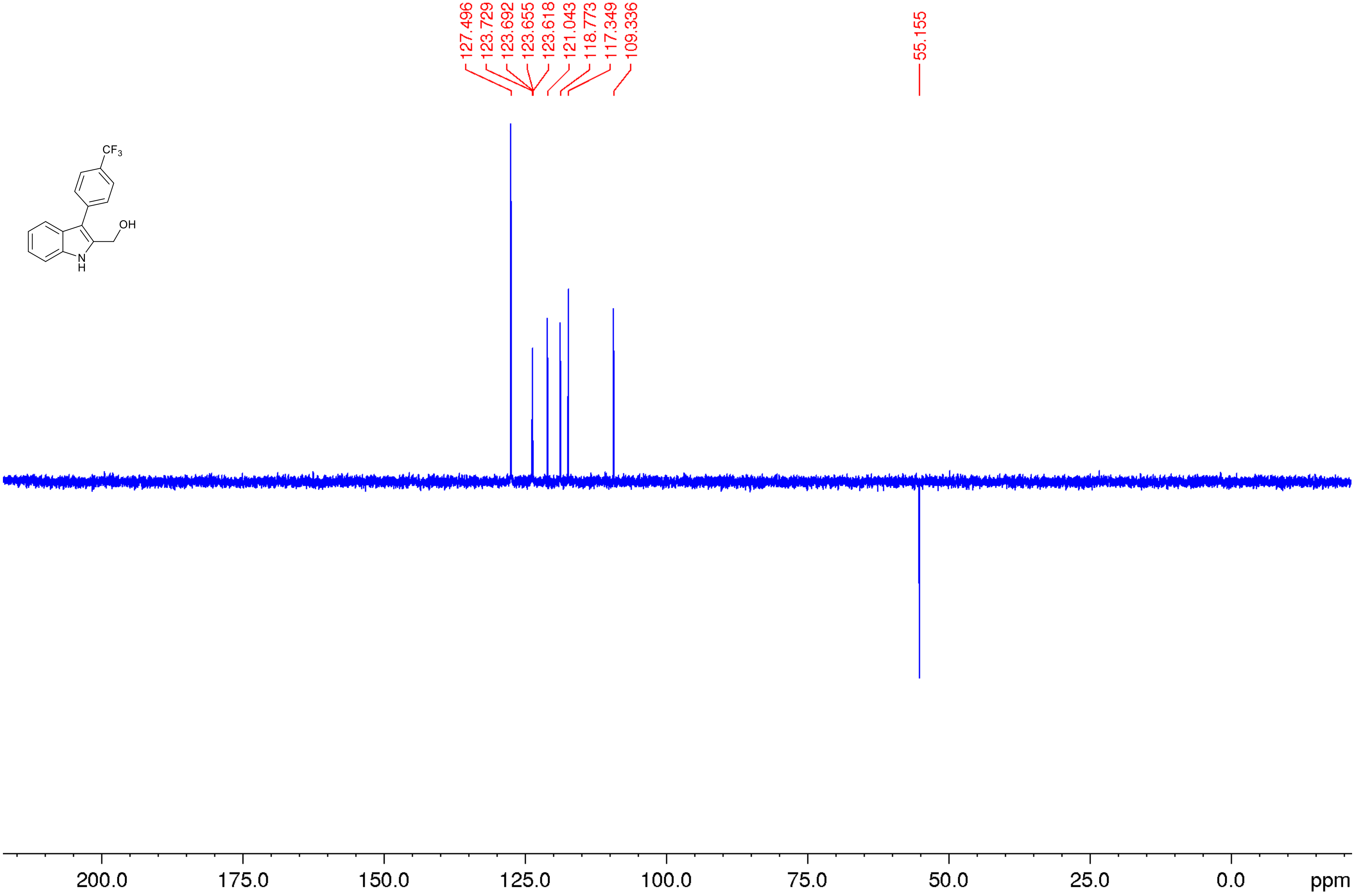
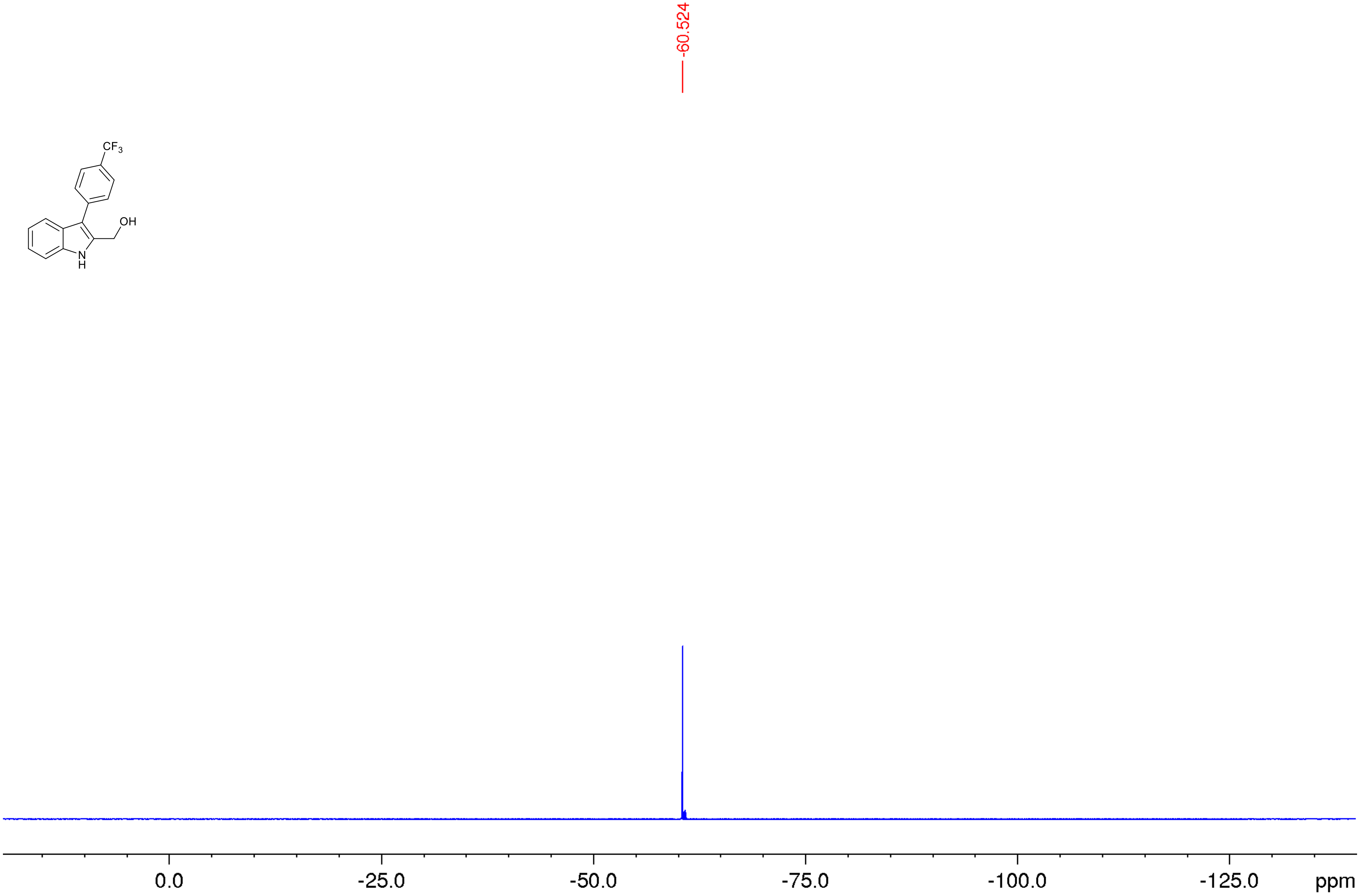


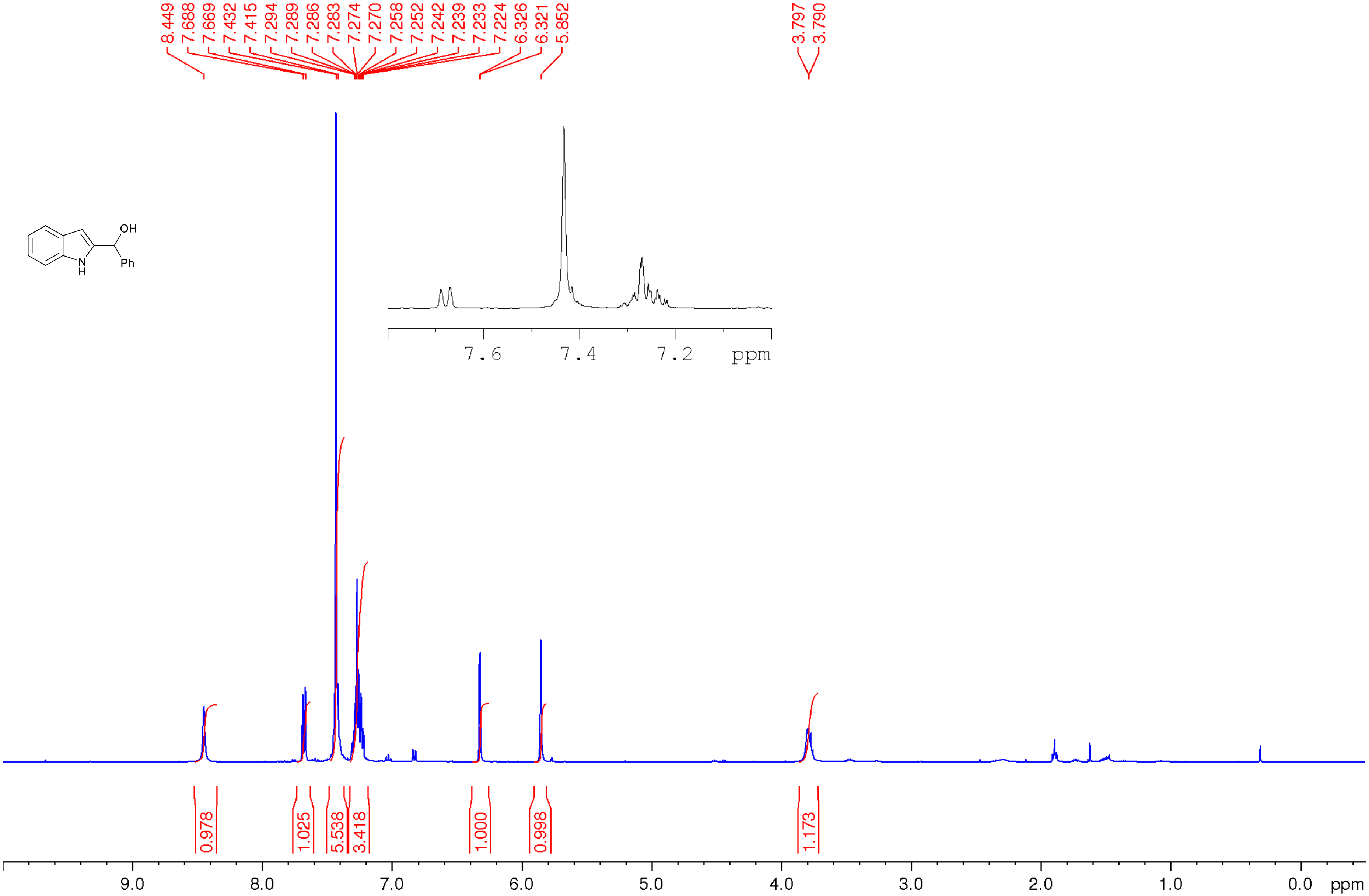
DEPT 135 NMR-spectrum ($CDCl_3$)



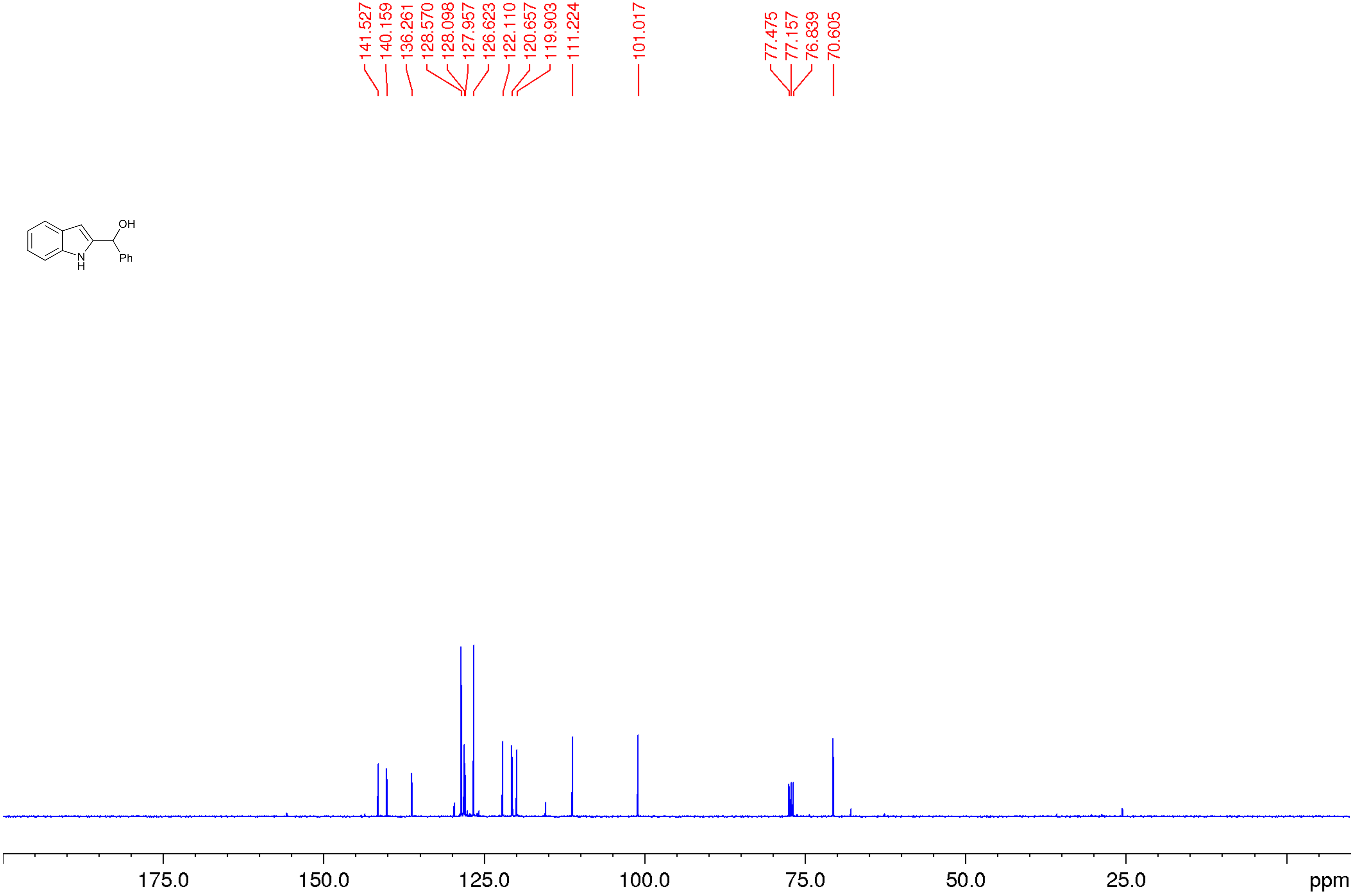
^{19}F NMR-spectrum (376.5, DMSO-d_6)



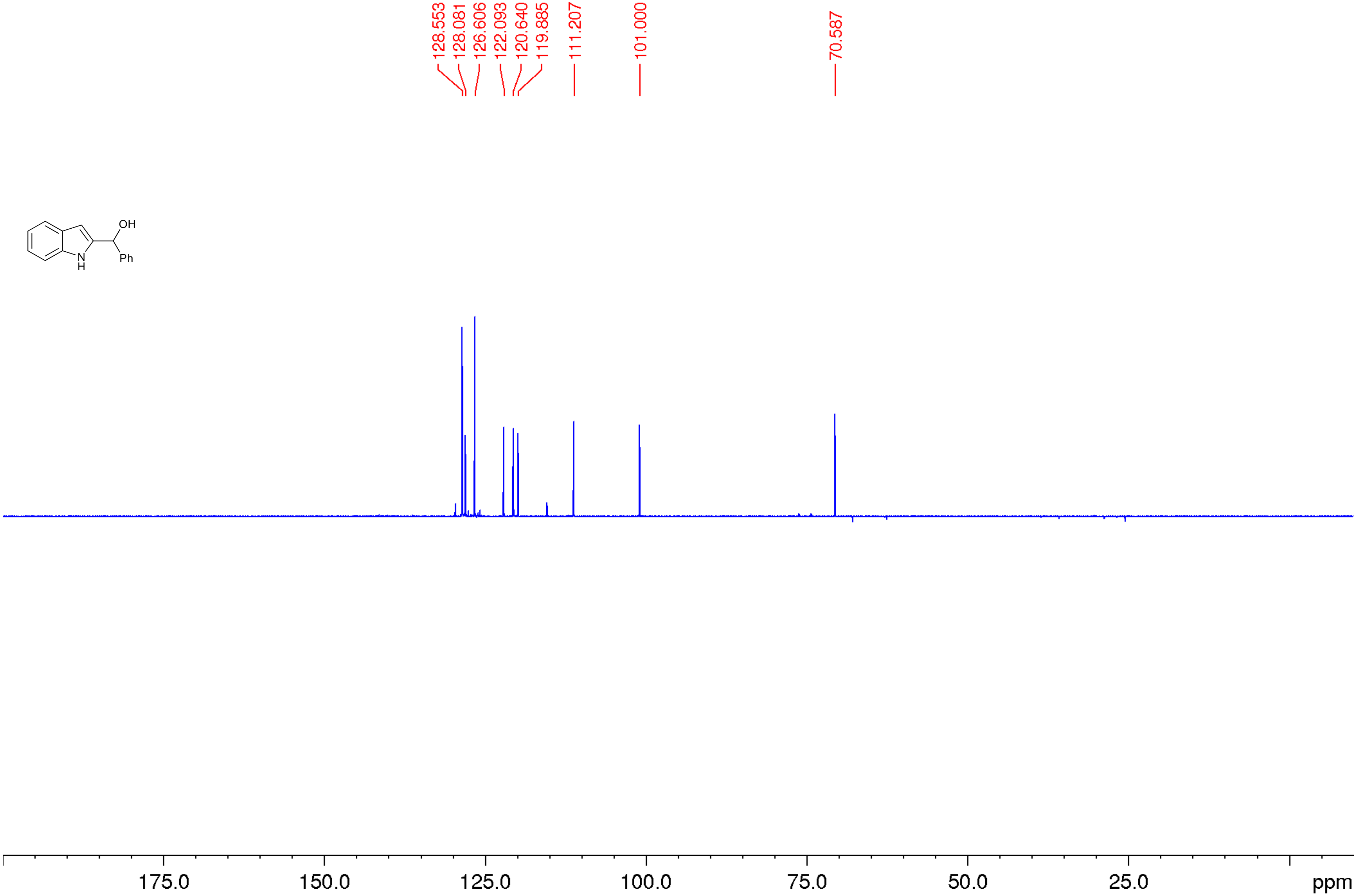
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)



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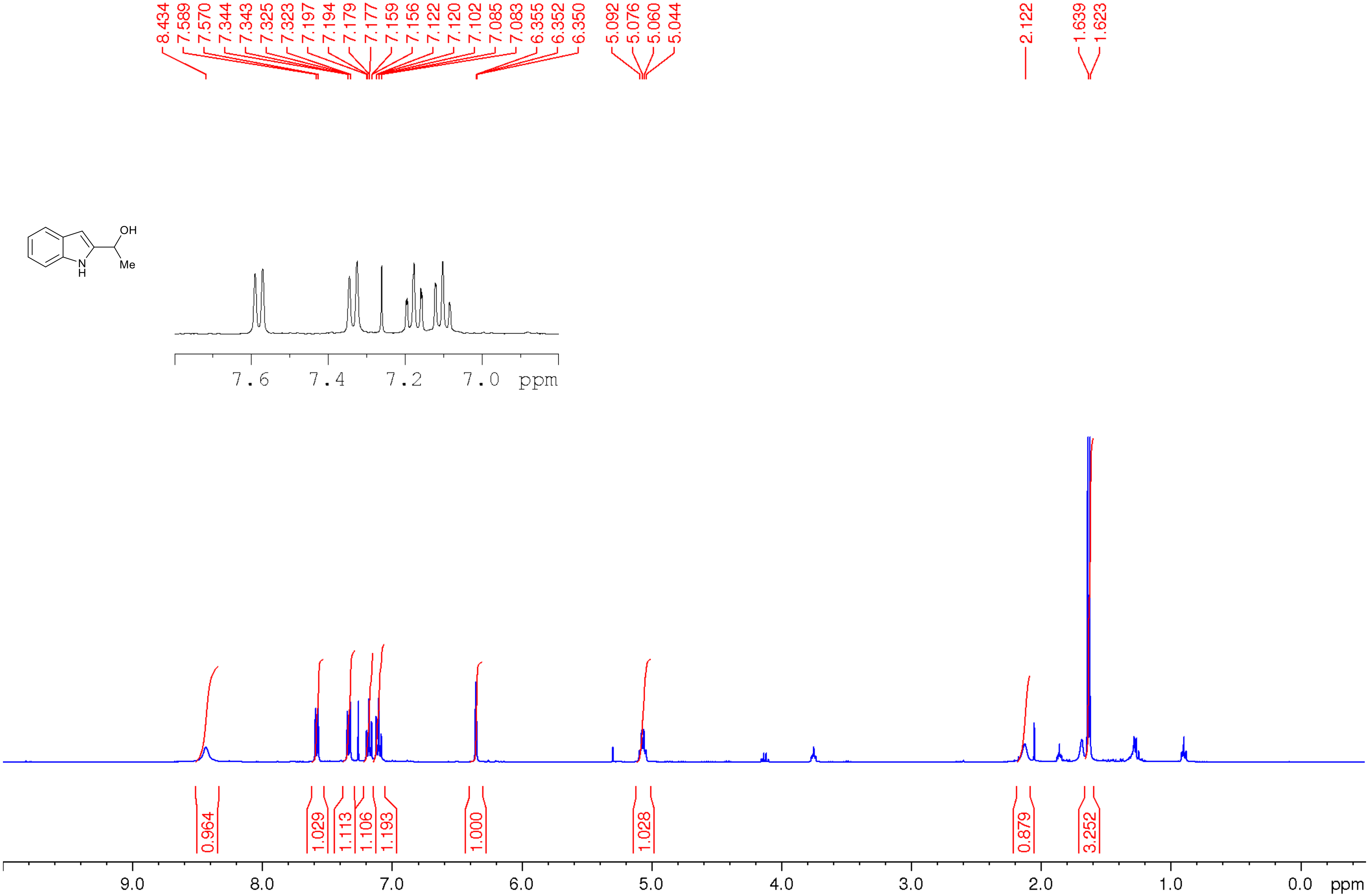

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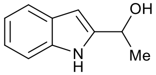

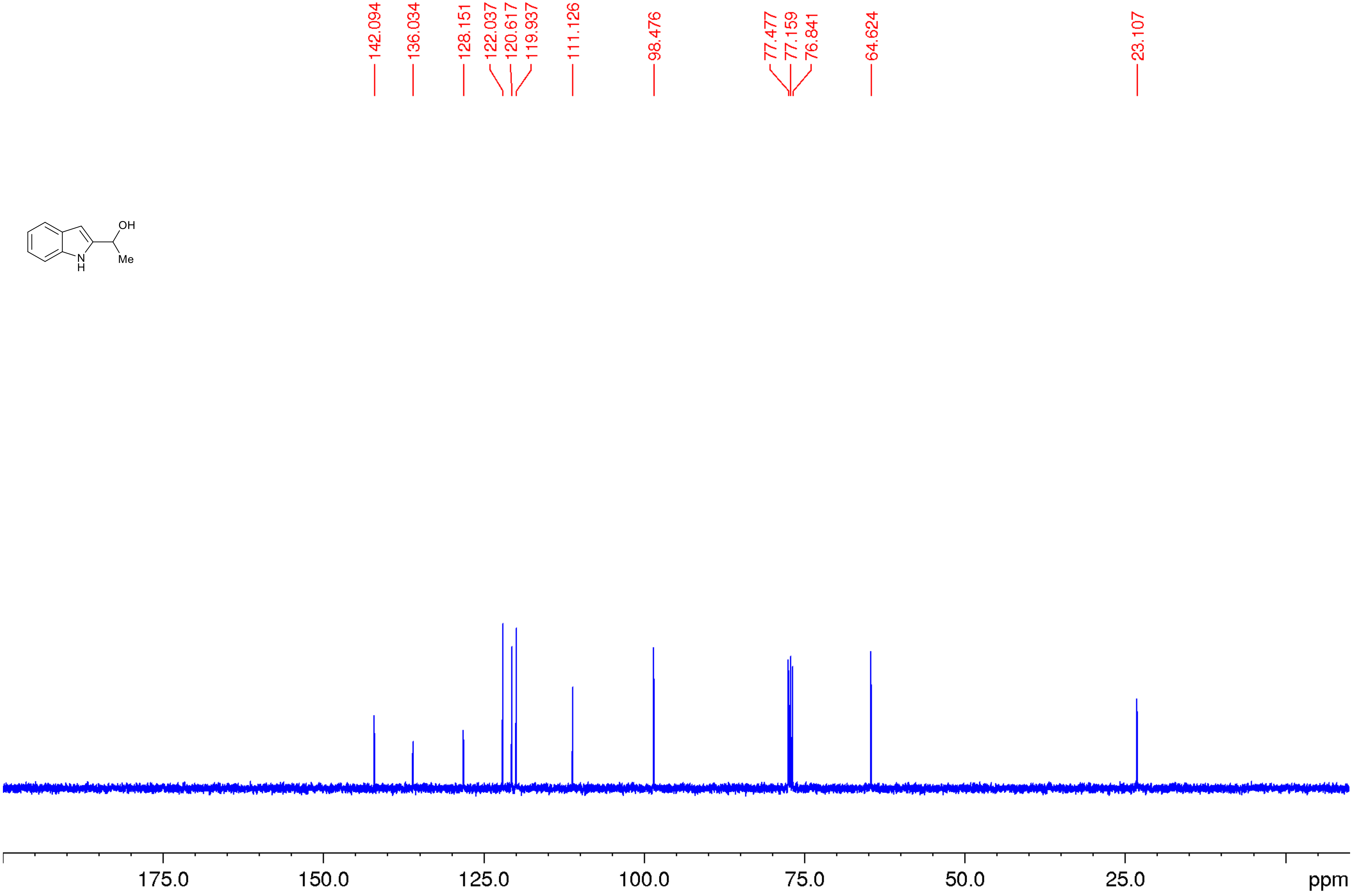

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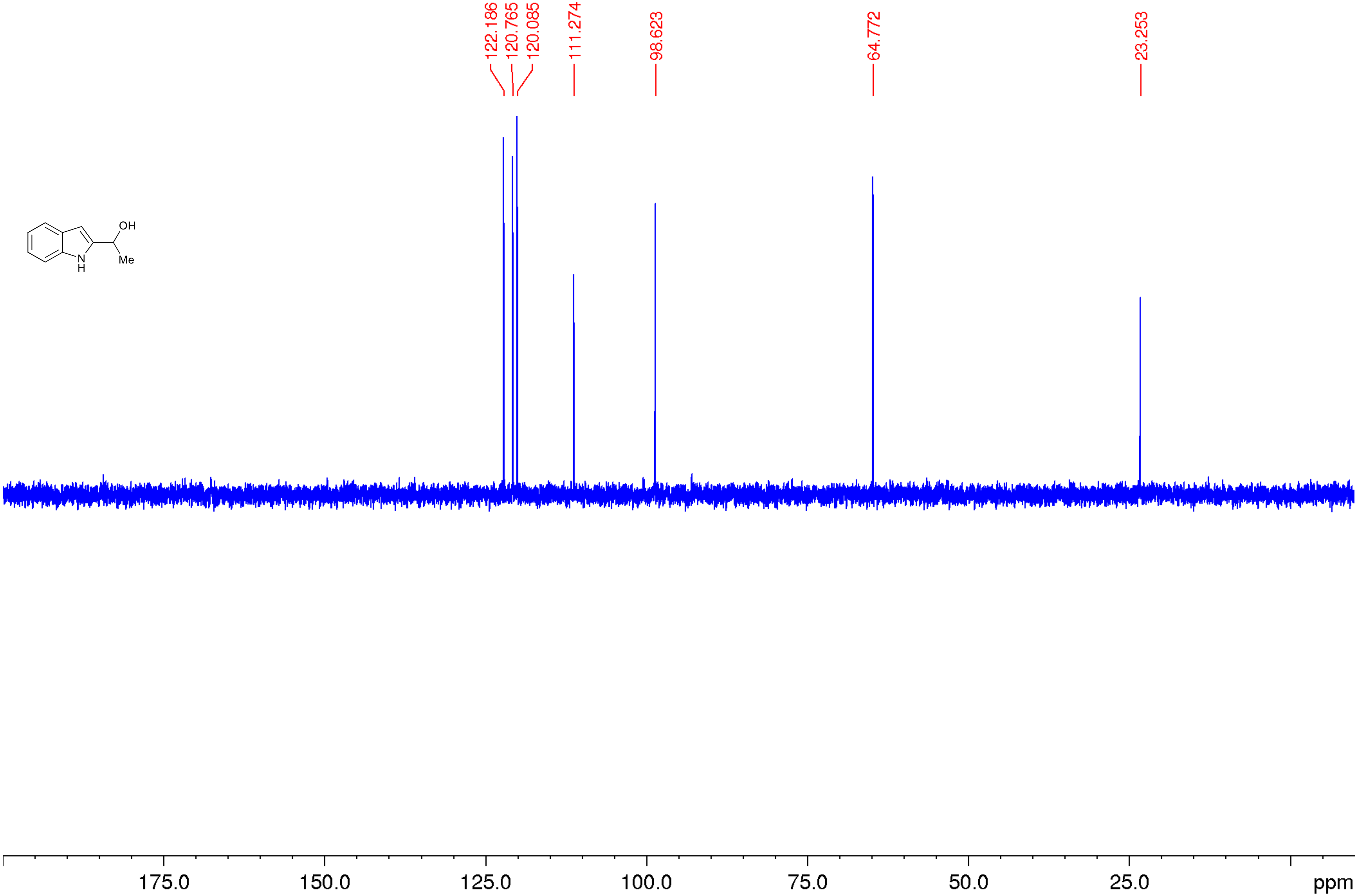

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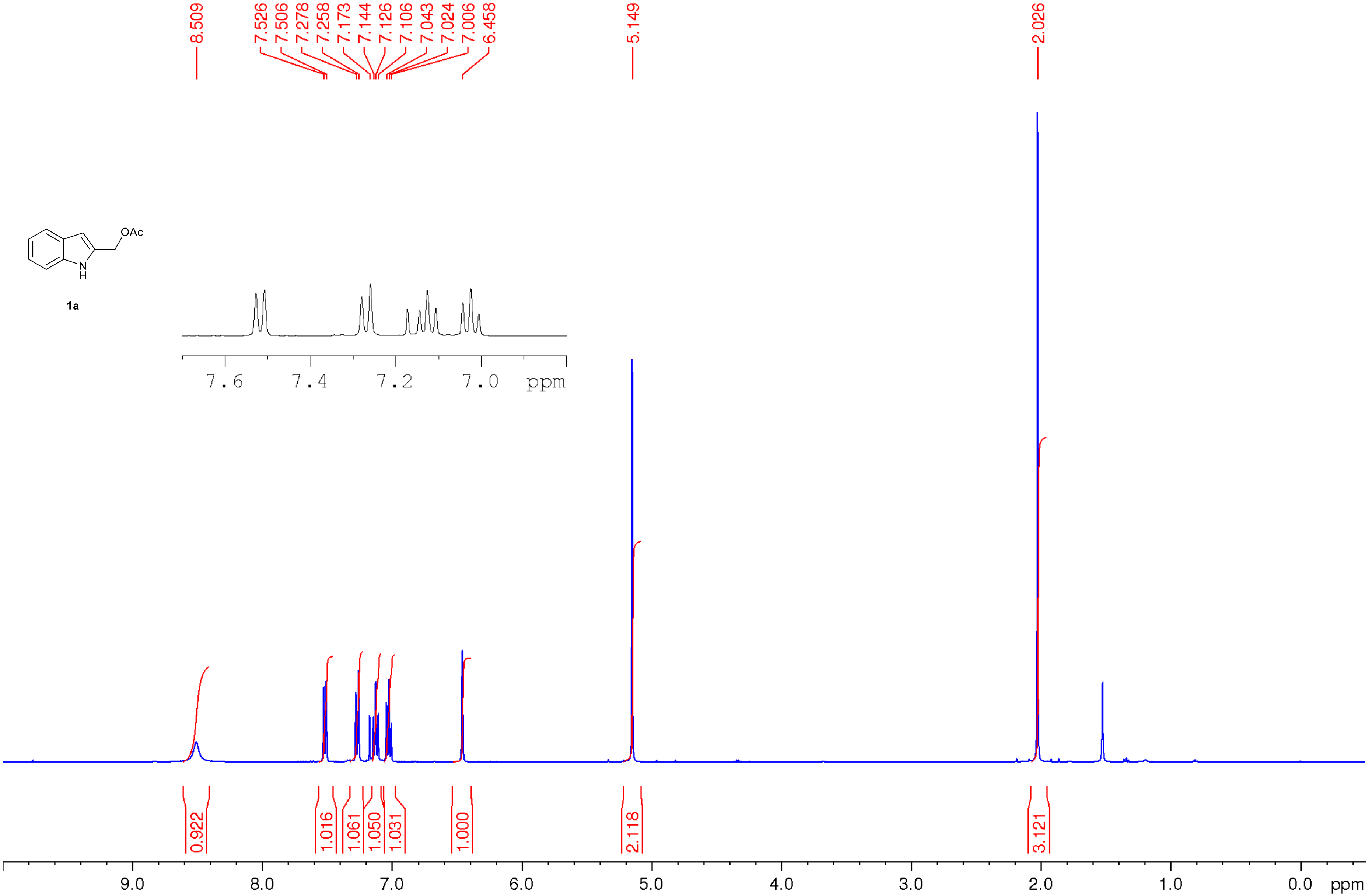
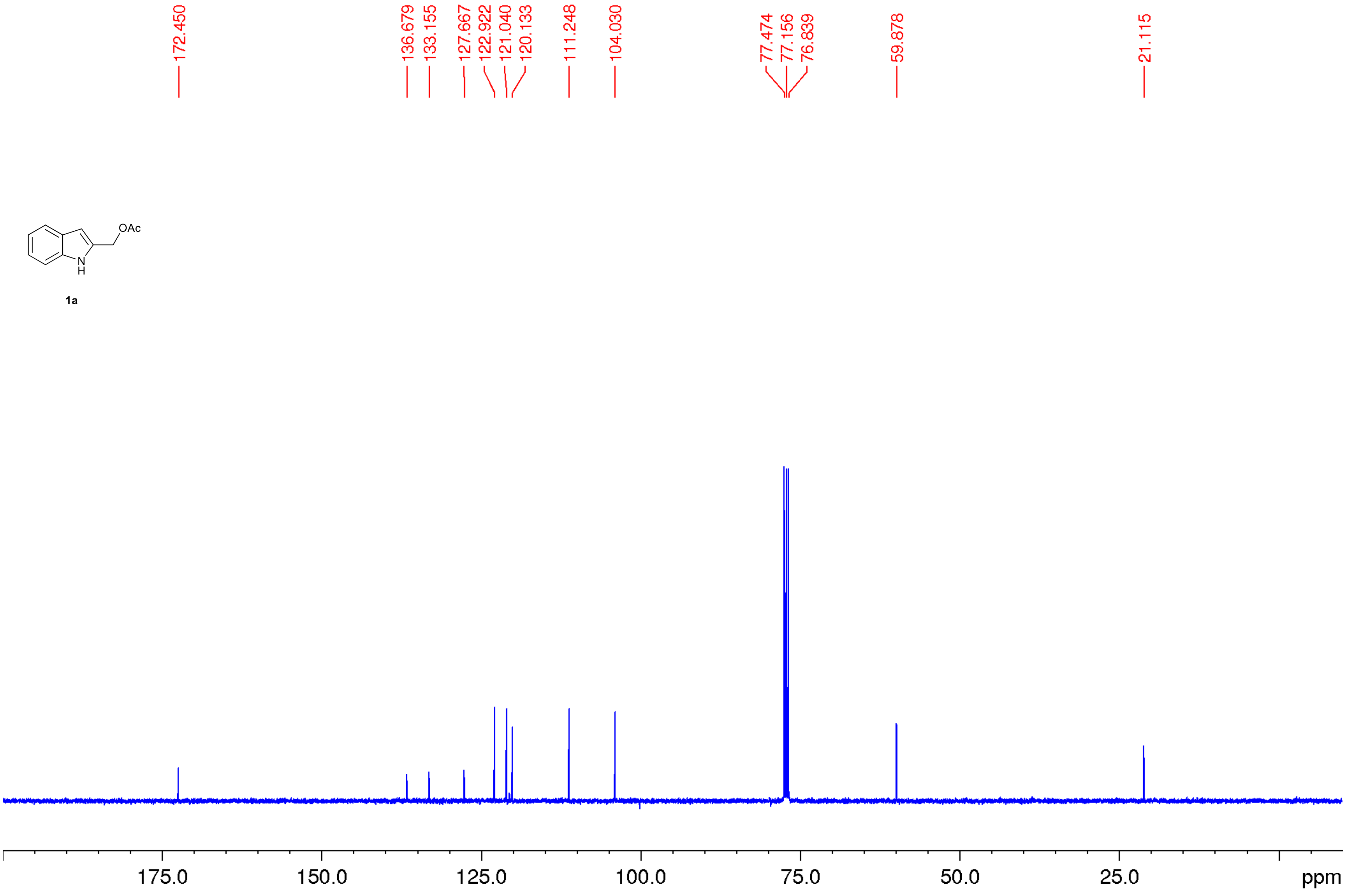


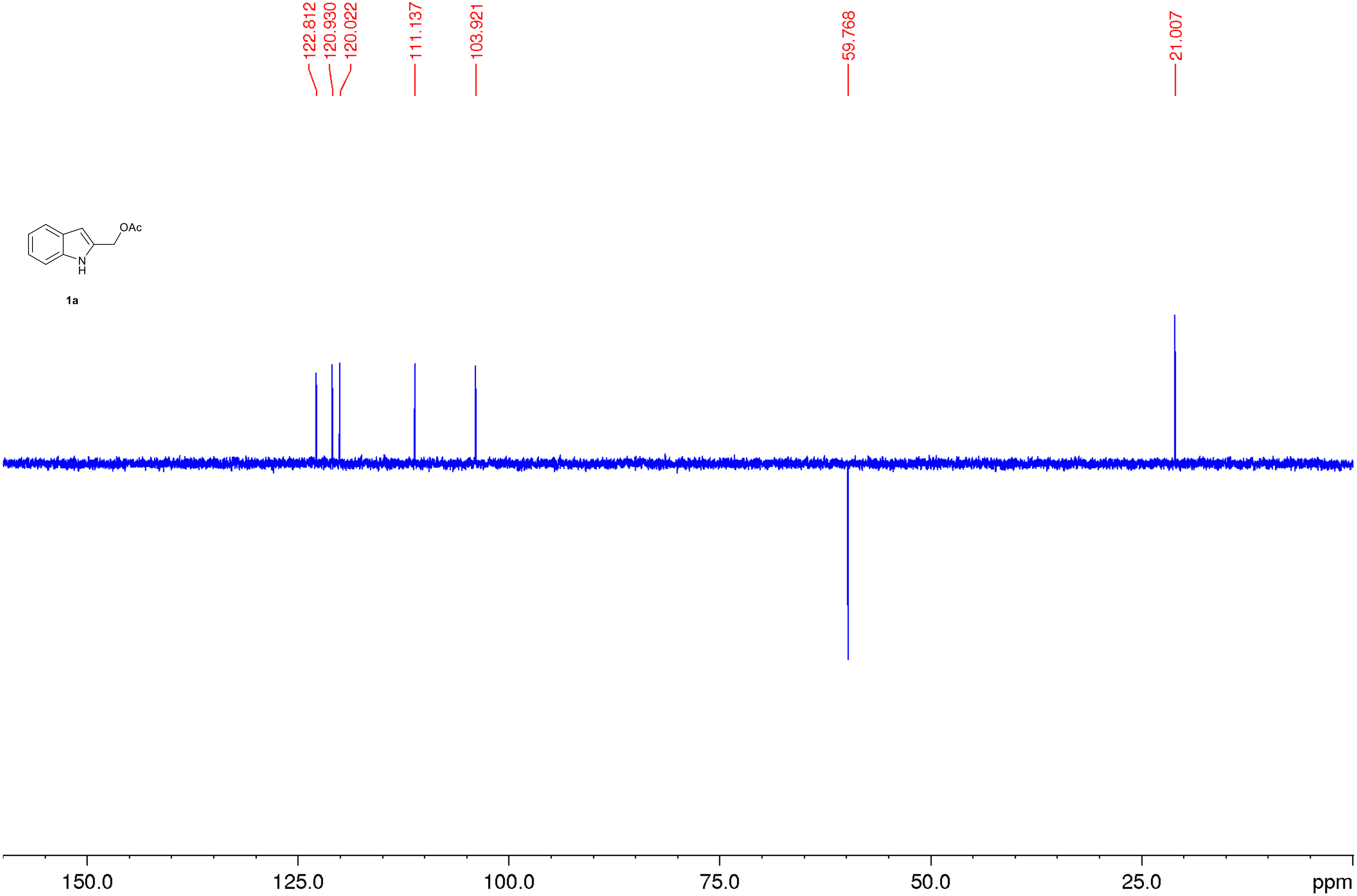
1a

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

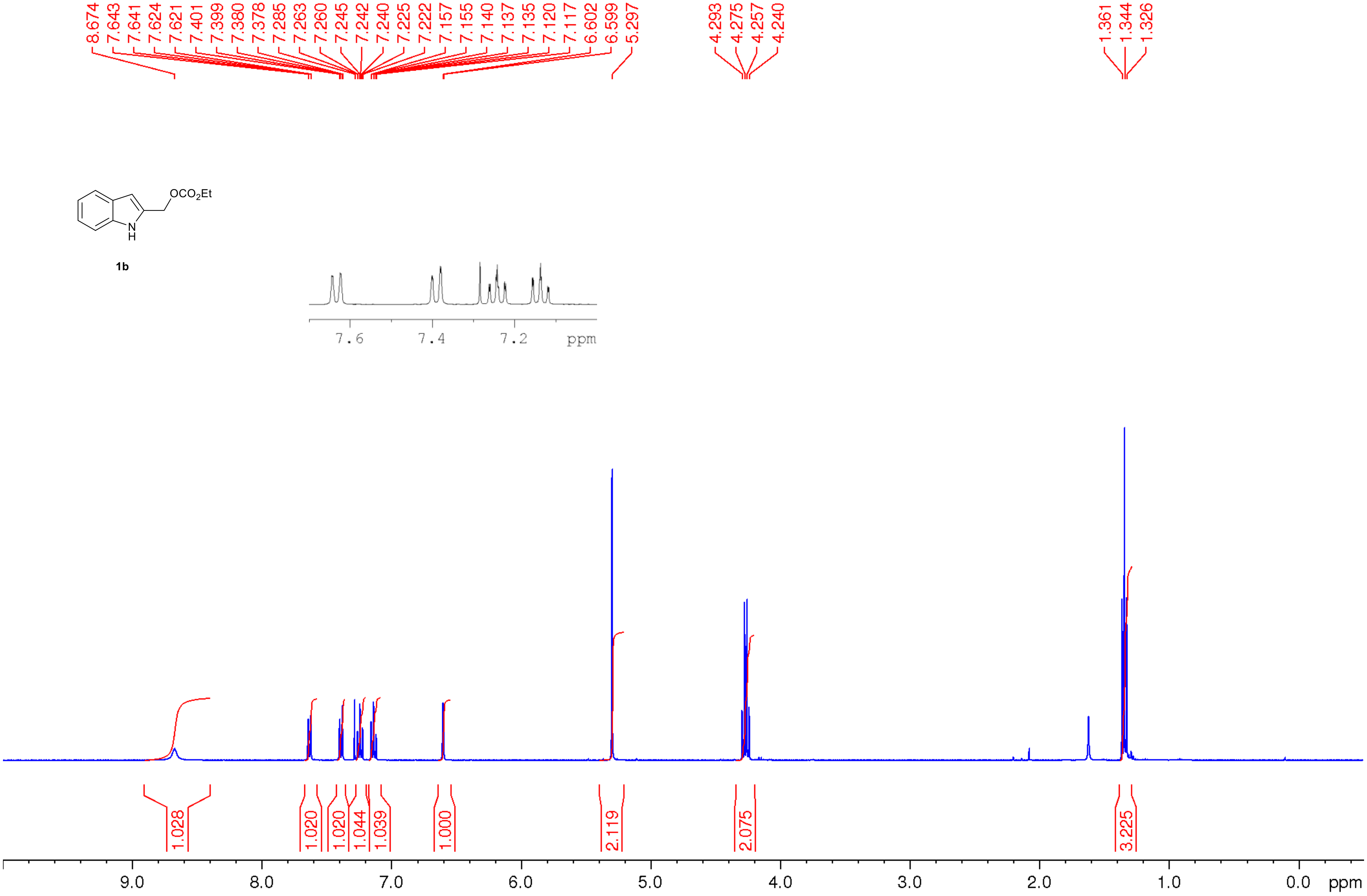


DEPT 135 NMR-spectrum ($CDCl_3$)

1a

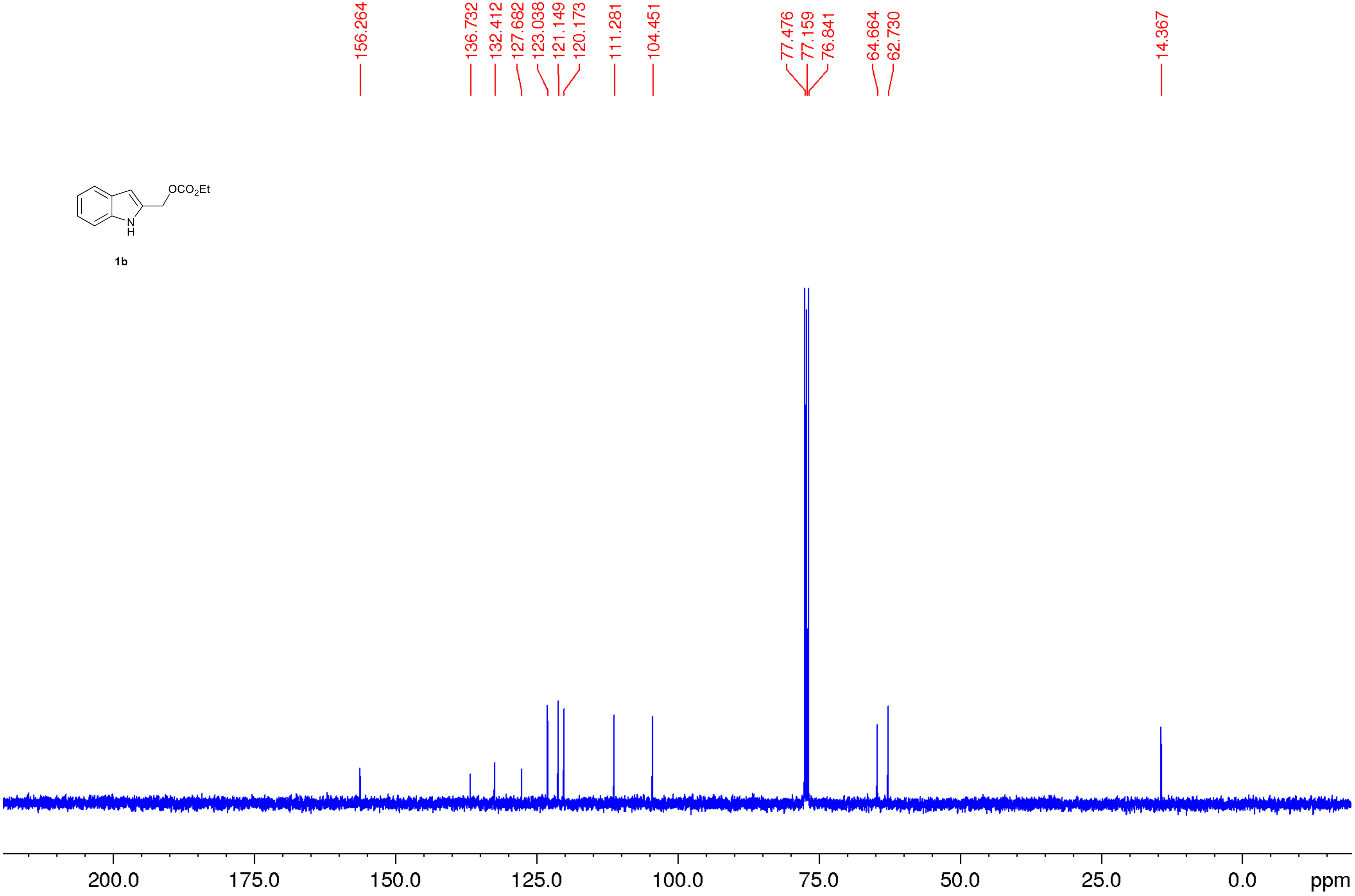


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



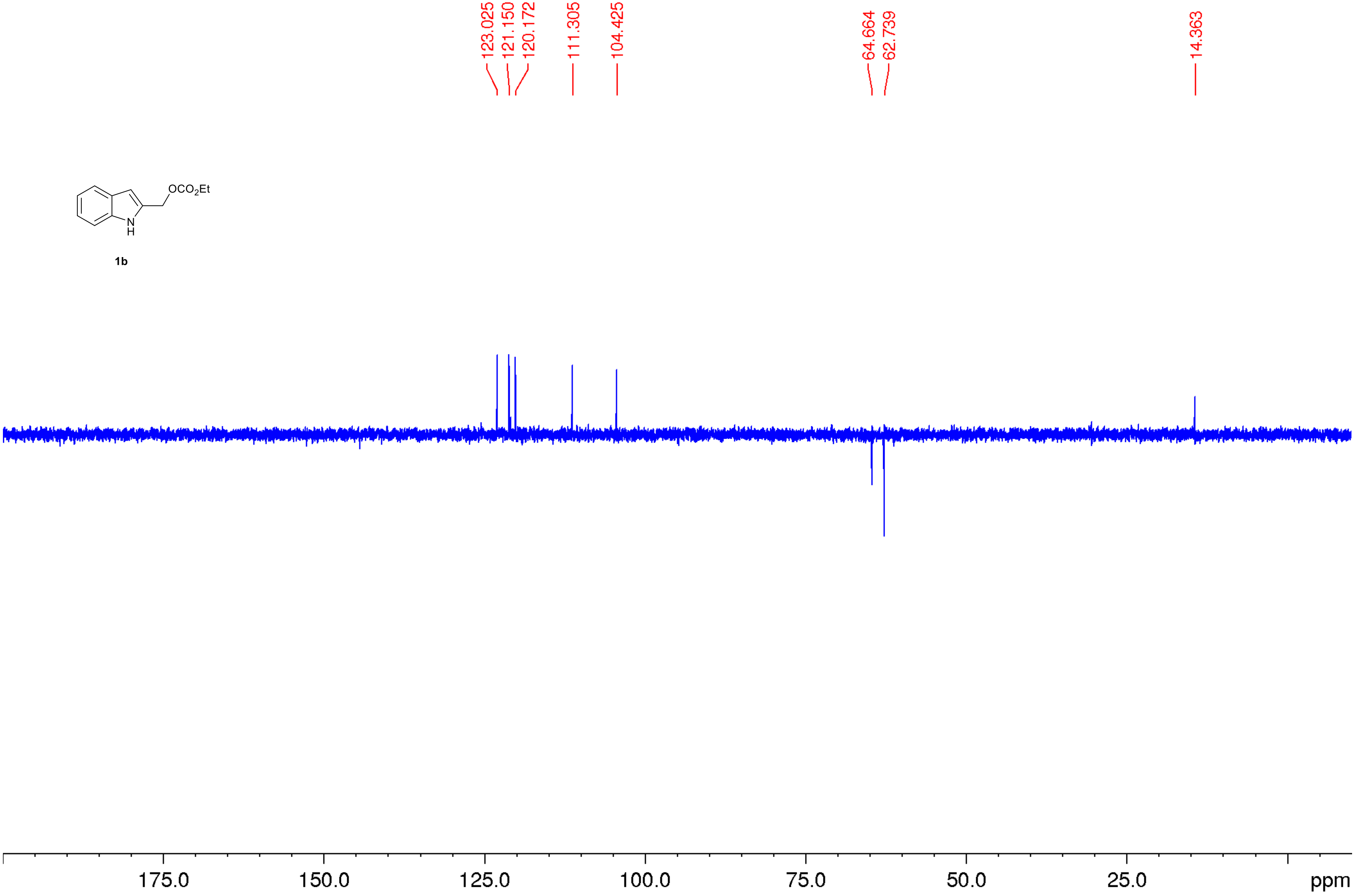
1b

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



1b

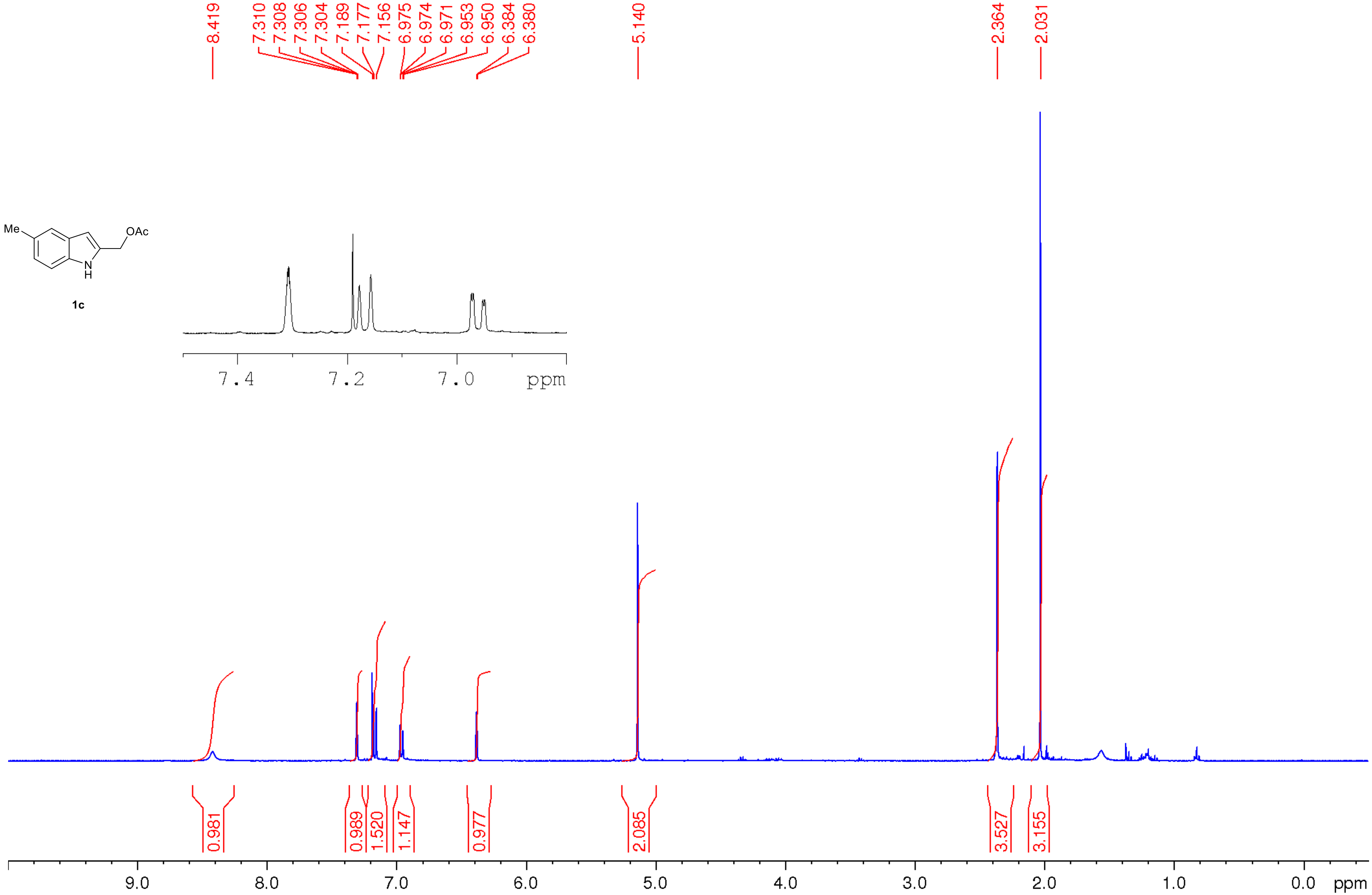
DEPT 135 NMR-spectrum ($CDCl_3$)



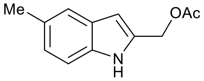
1b

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

1c



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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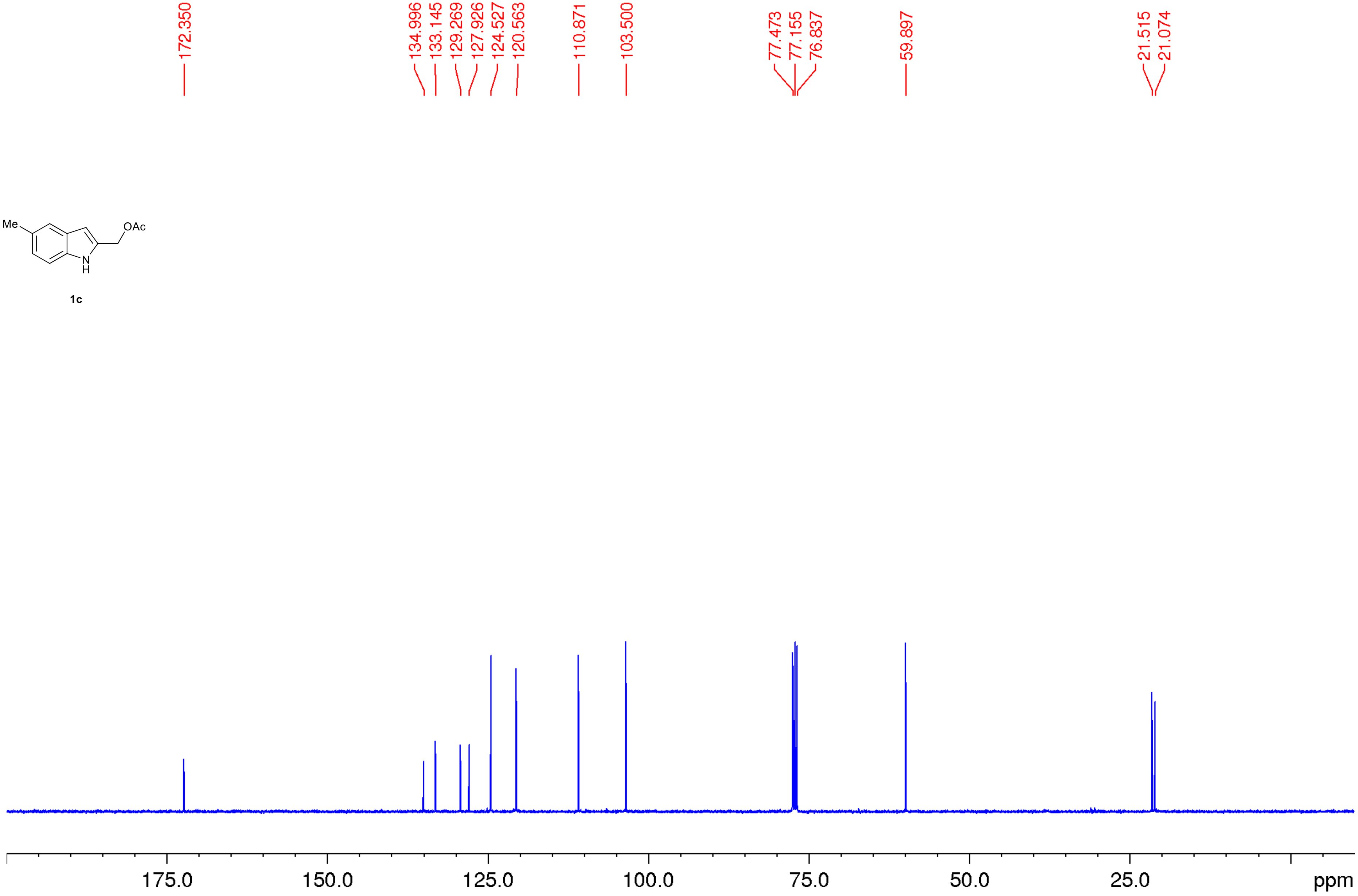
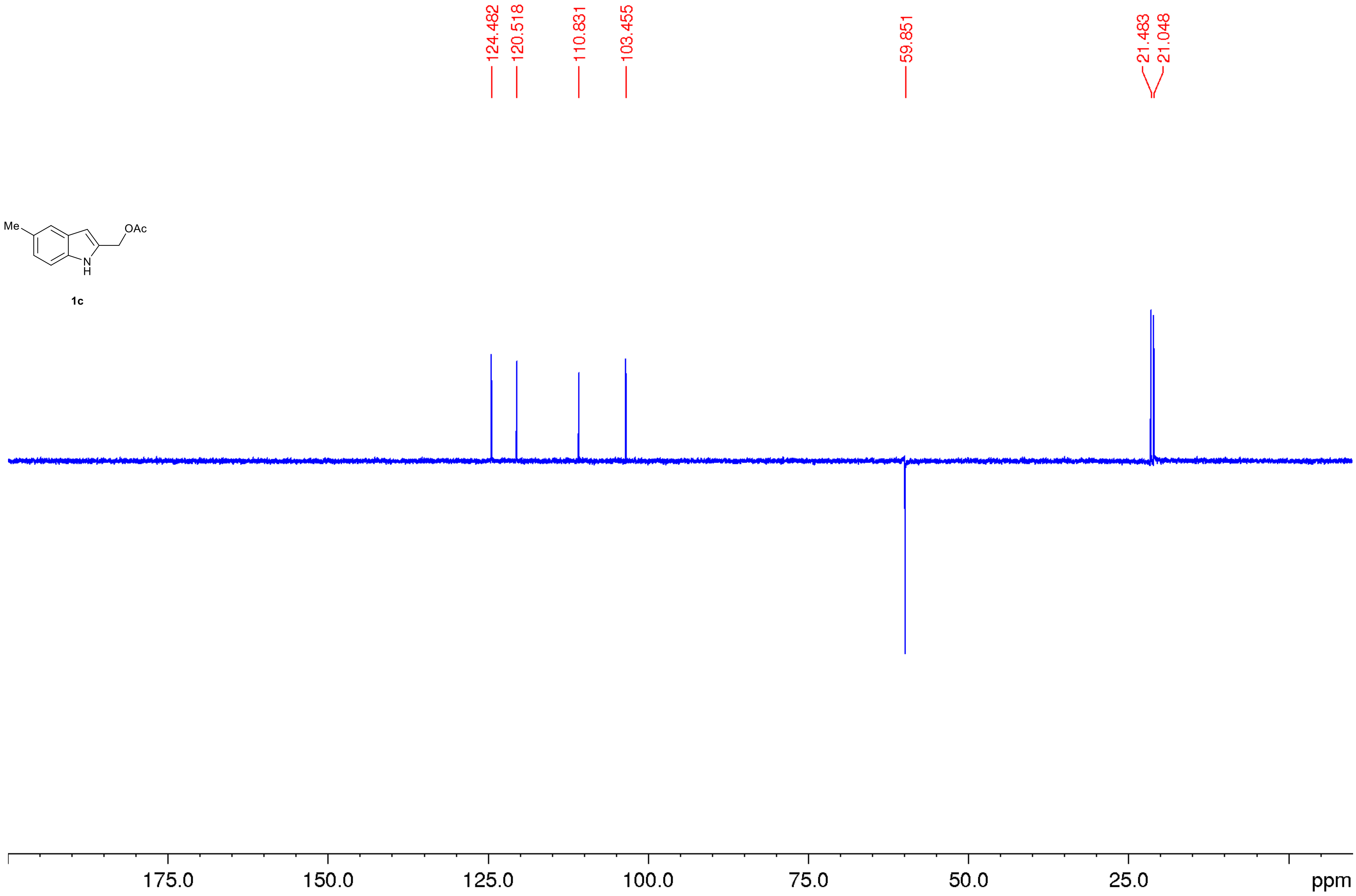


DEPT 135 NMR-spectrum ($CDCl_3$)



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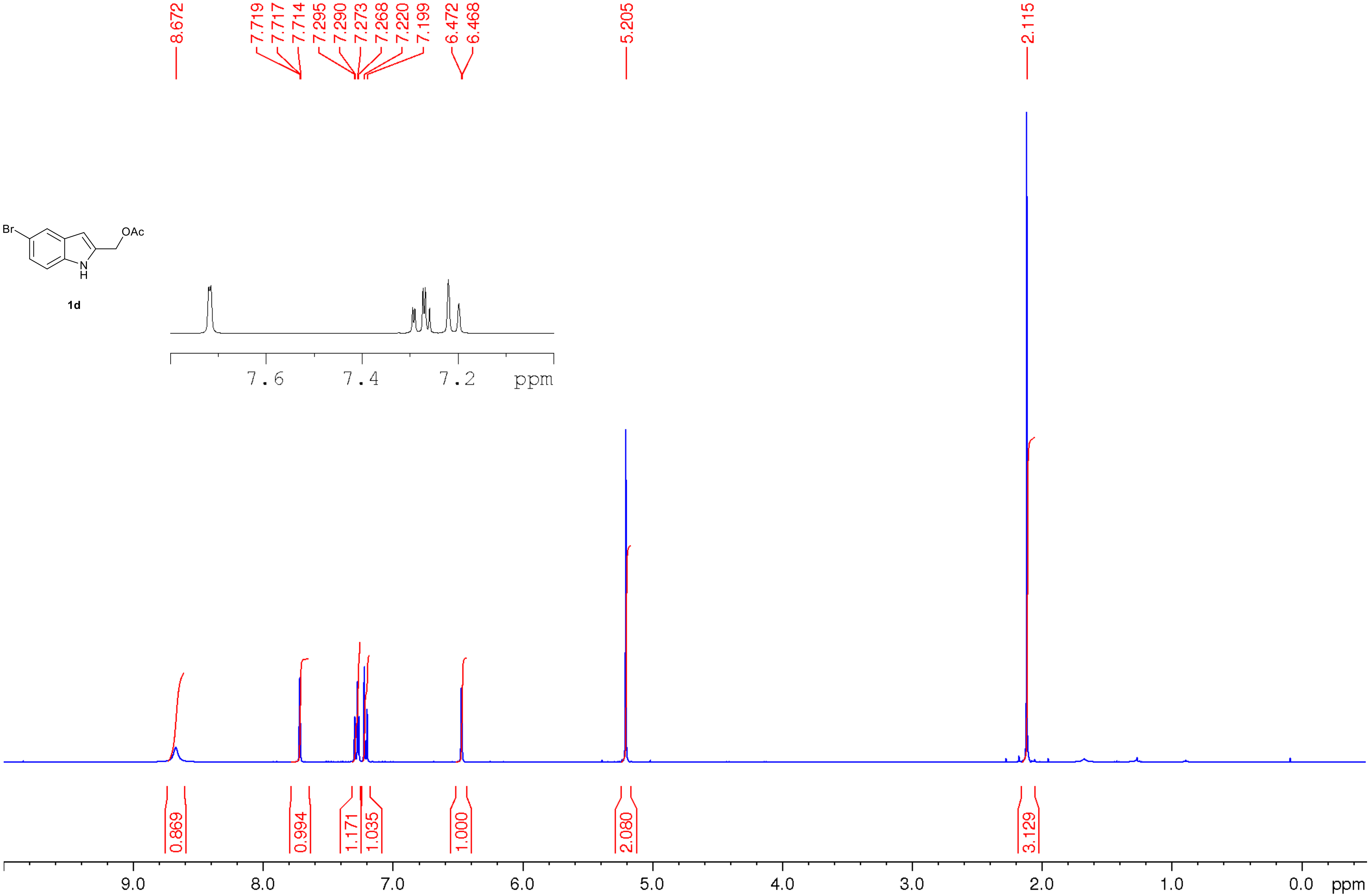
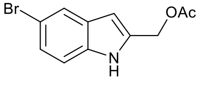


1d

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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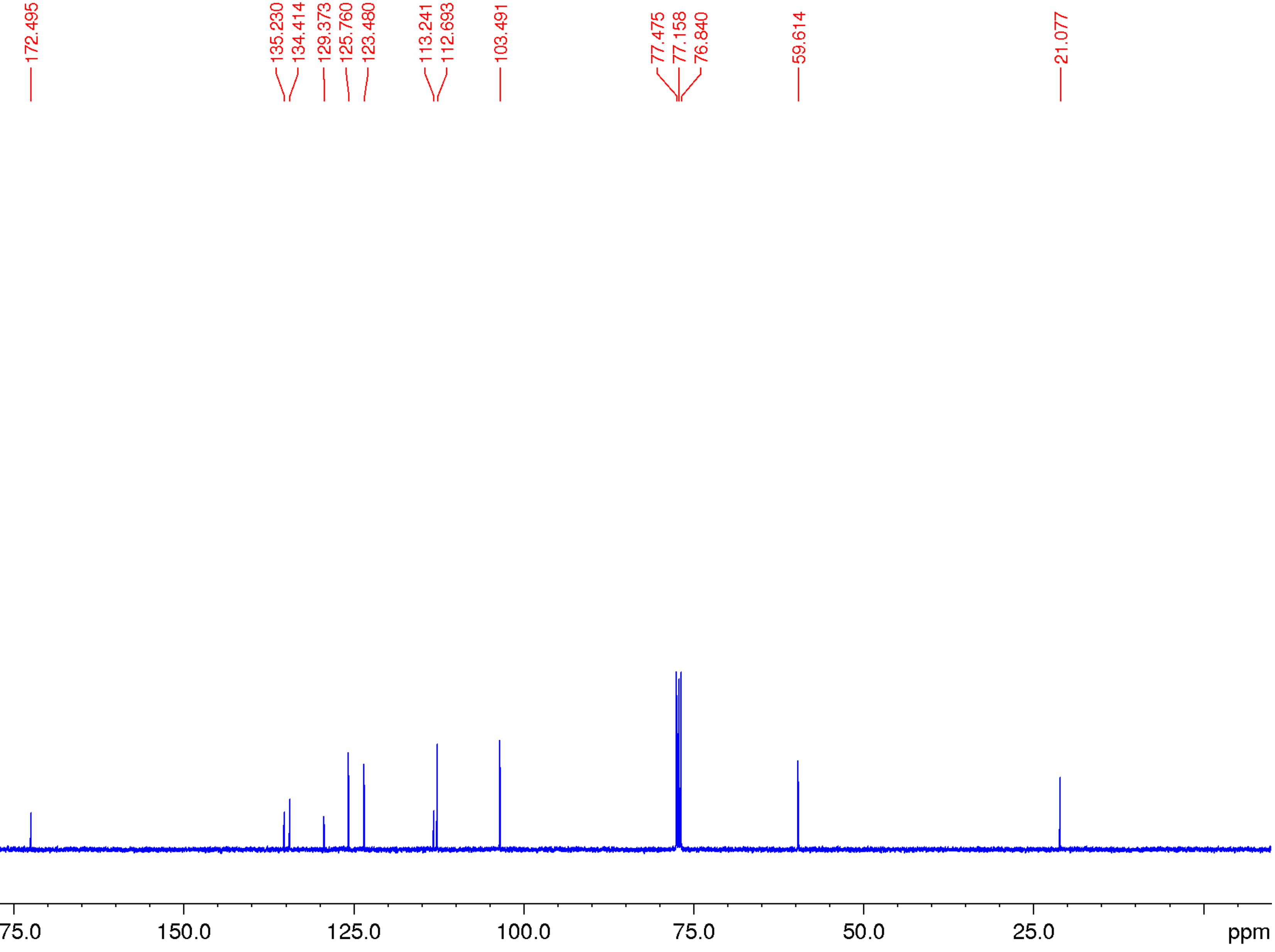
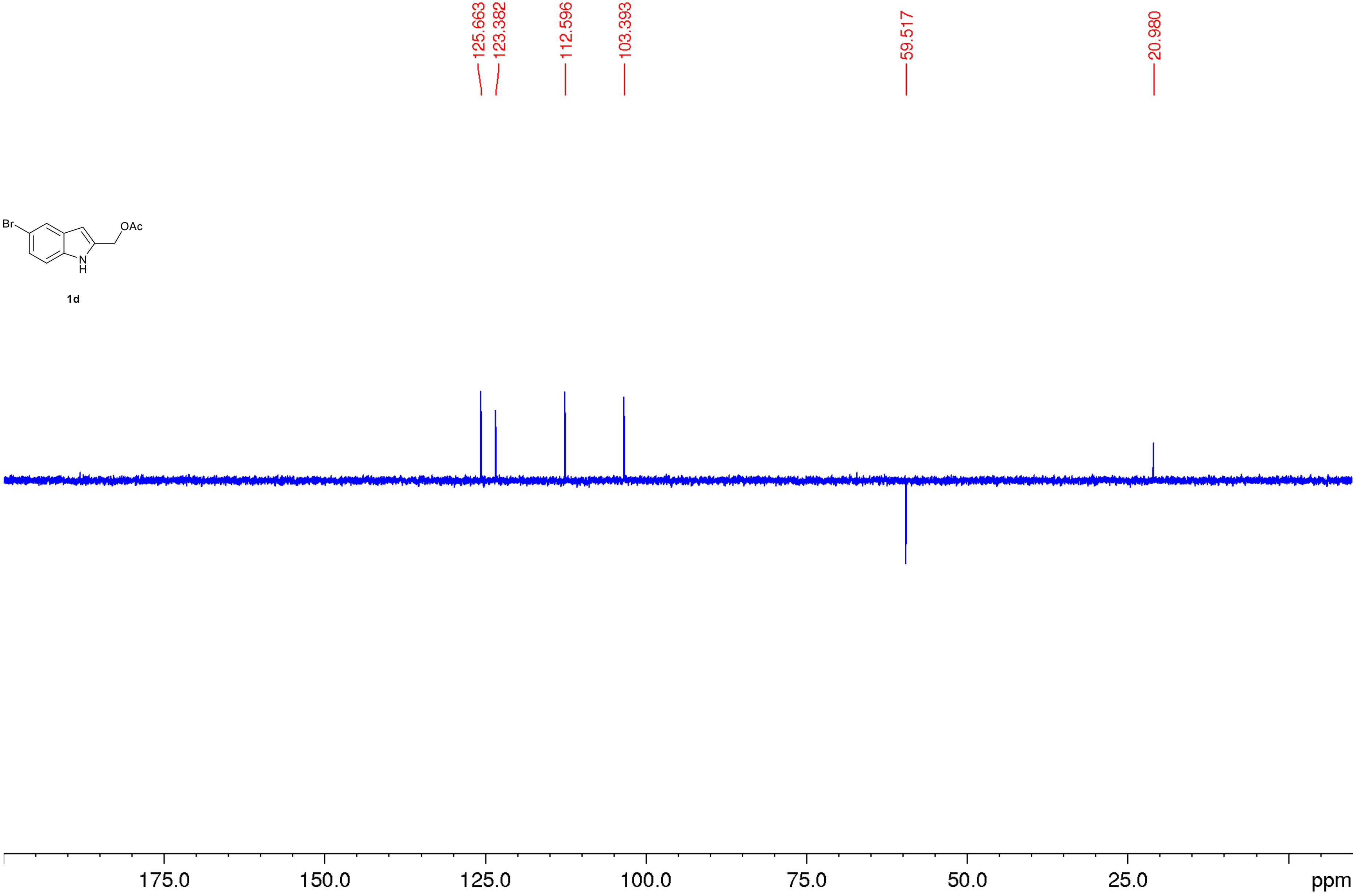


DEPT 135 NMR-spectrum ($CDCl_3$)



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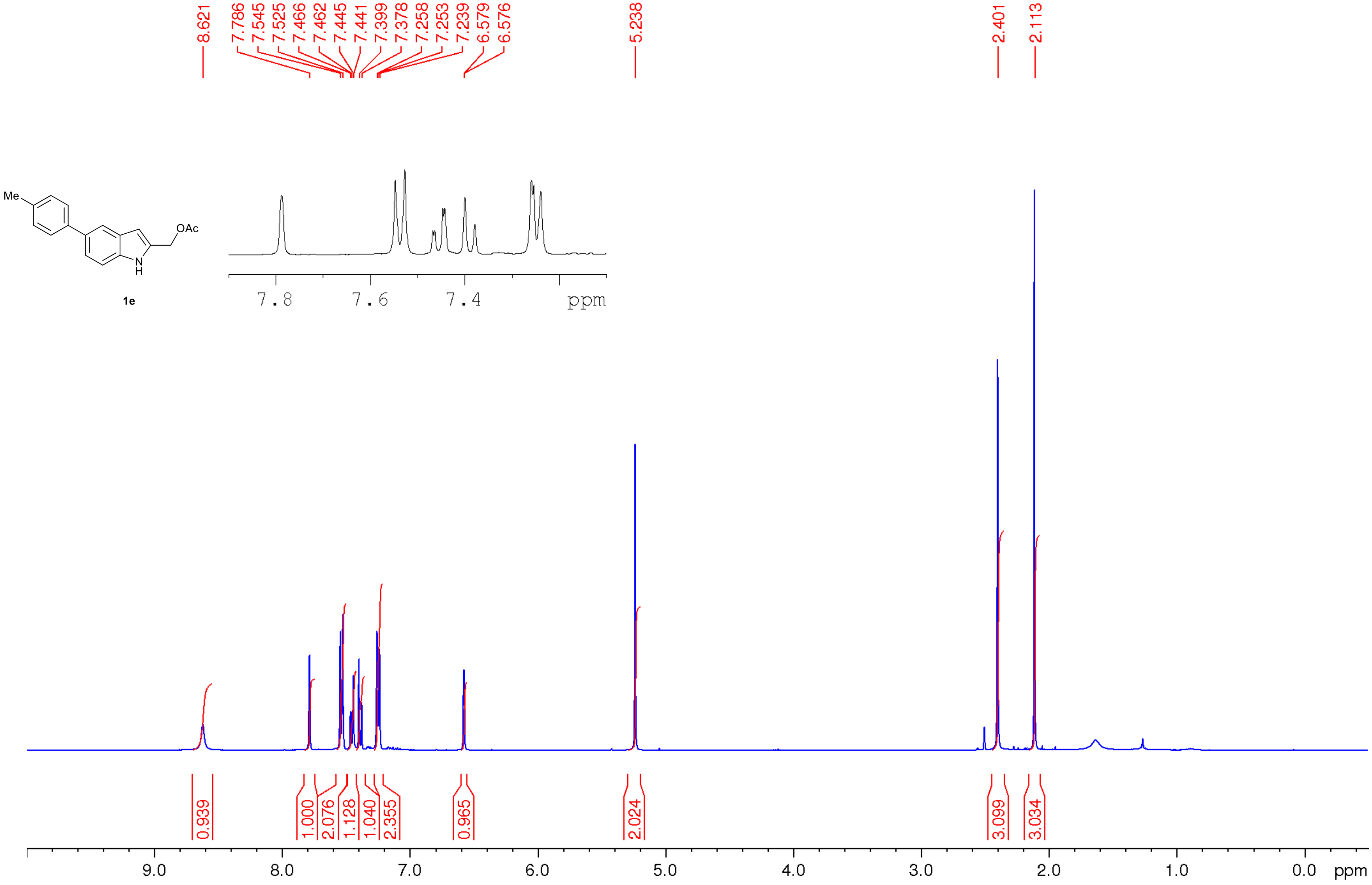
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



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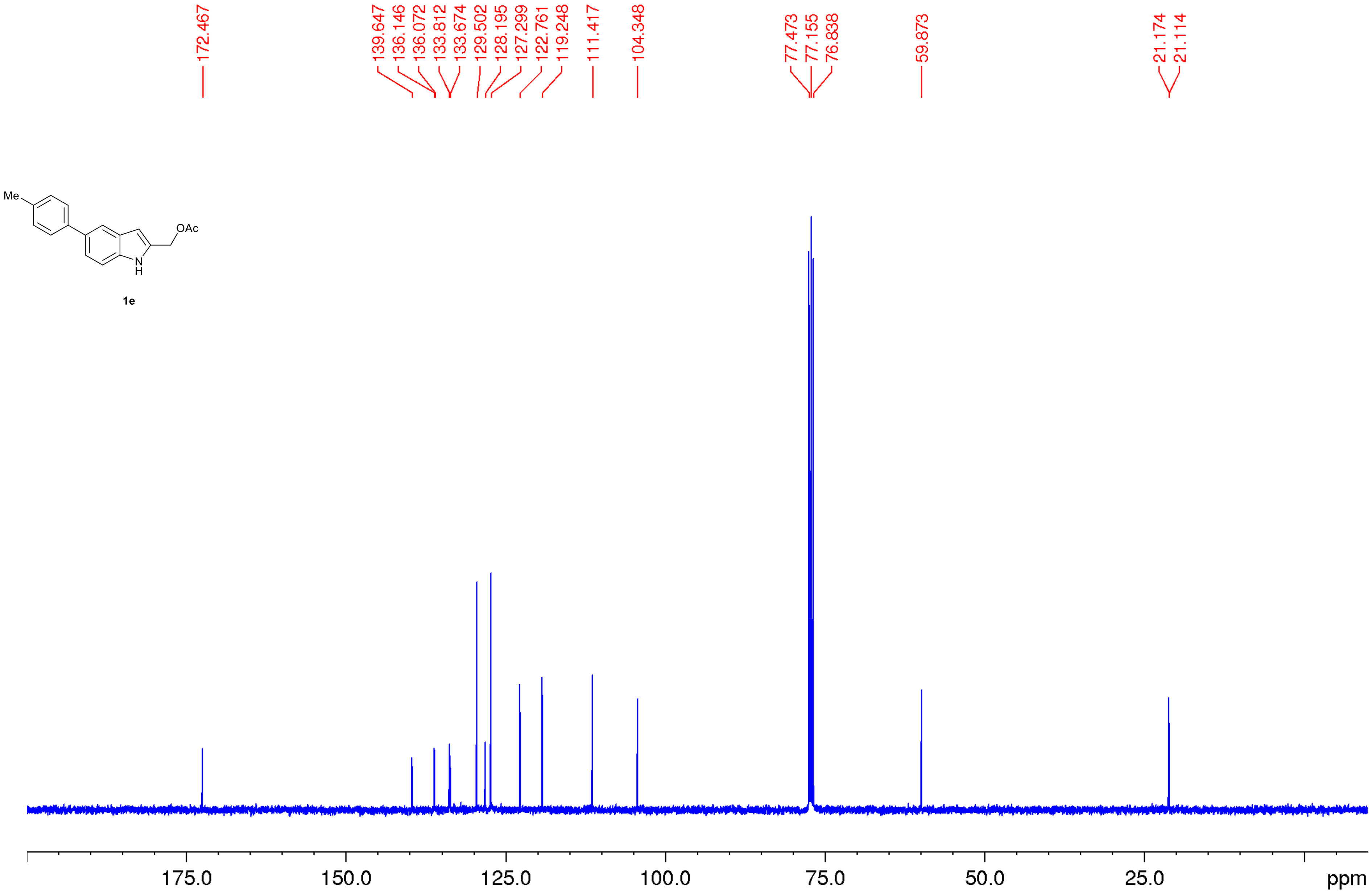
^{13}C NMR-spectrum (100 MHz, CDCl$_3$)



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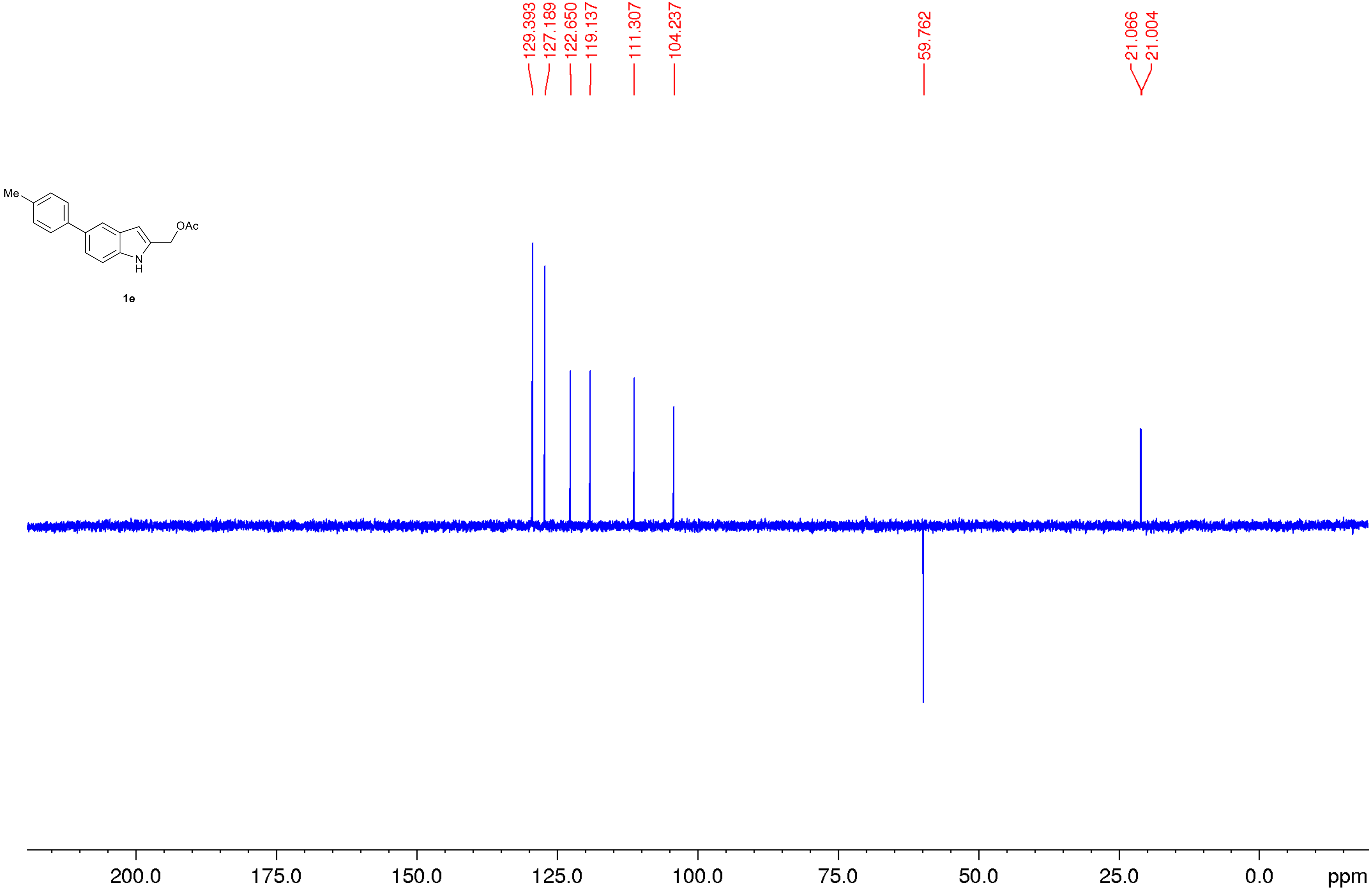
DEPT 135 NMR-spectrum ($CDCl_3$)



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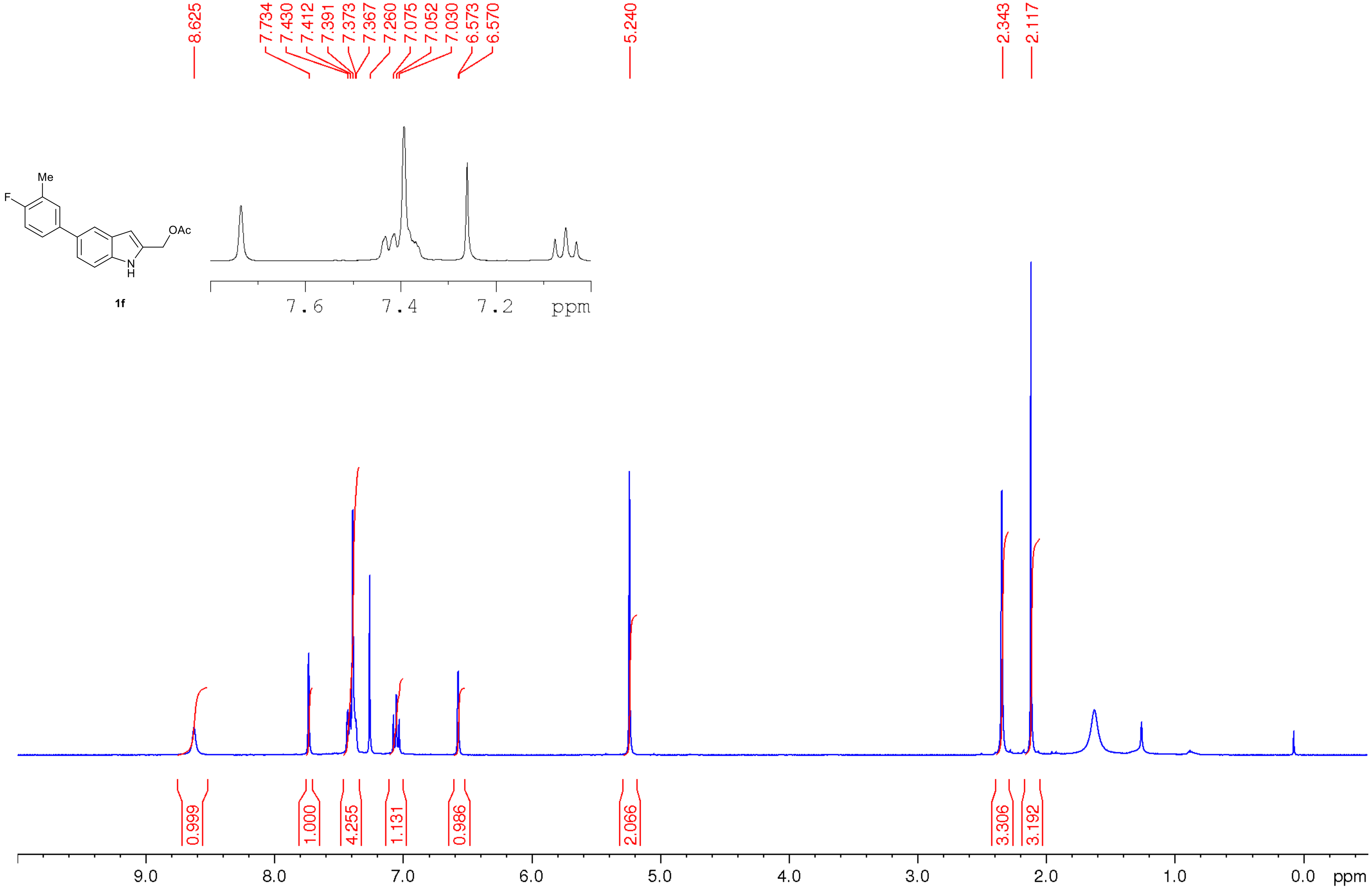
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)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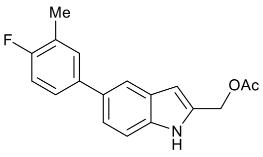
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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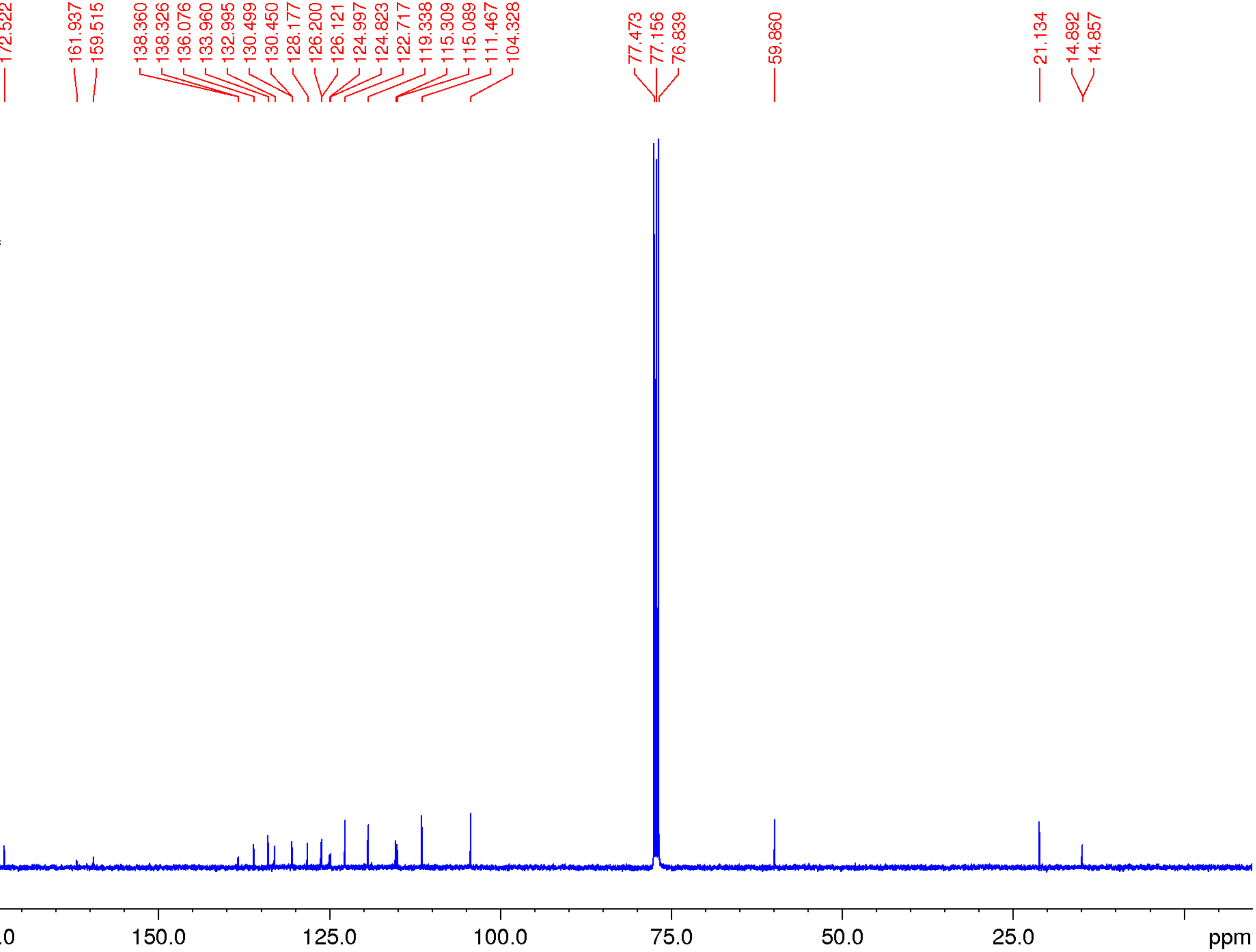
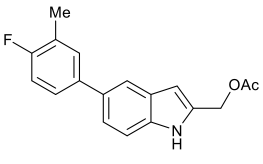


DEPT 135 NMR-spectrum ($CDCl_3$)



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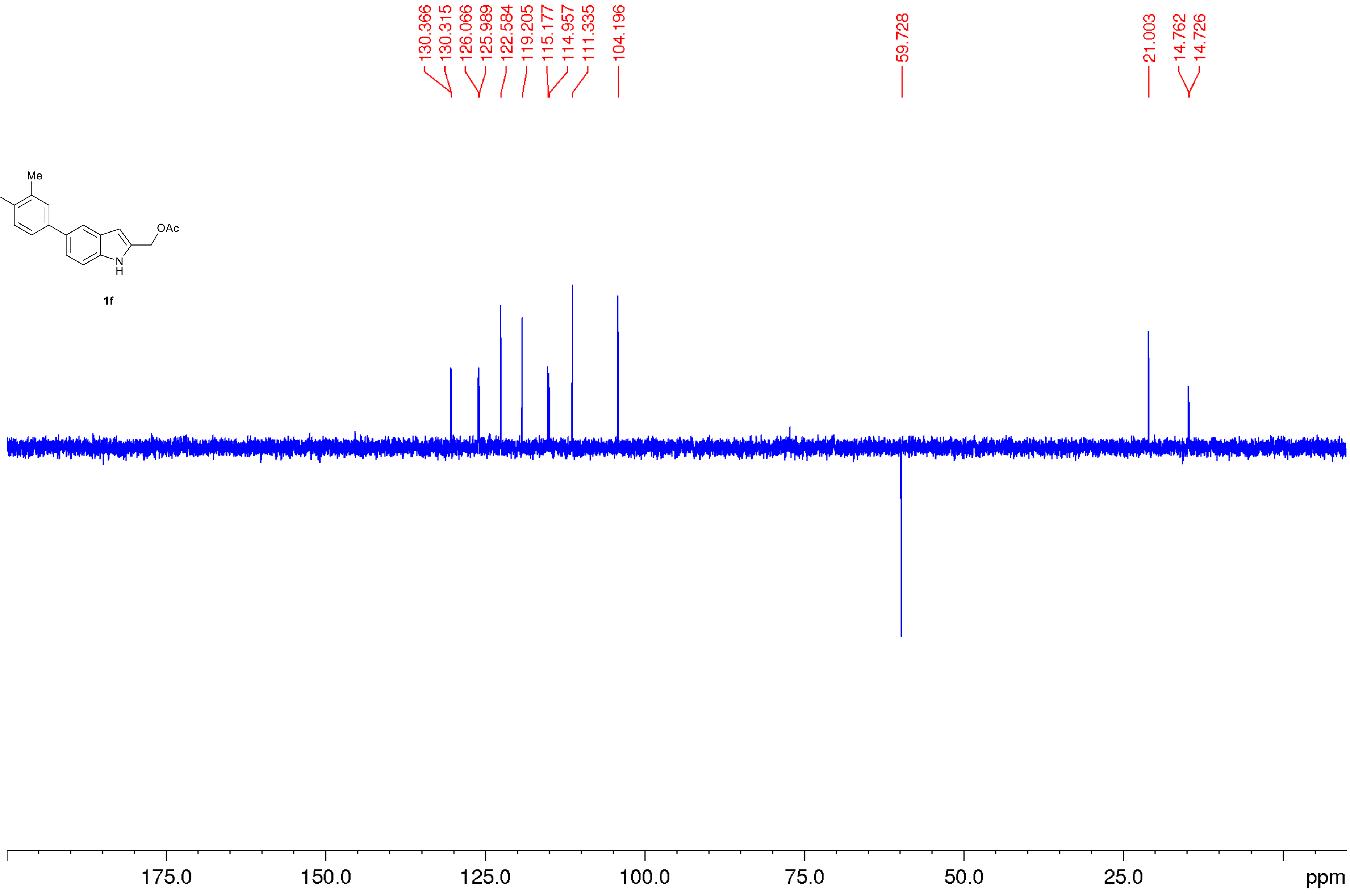
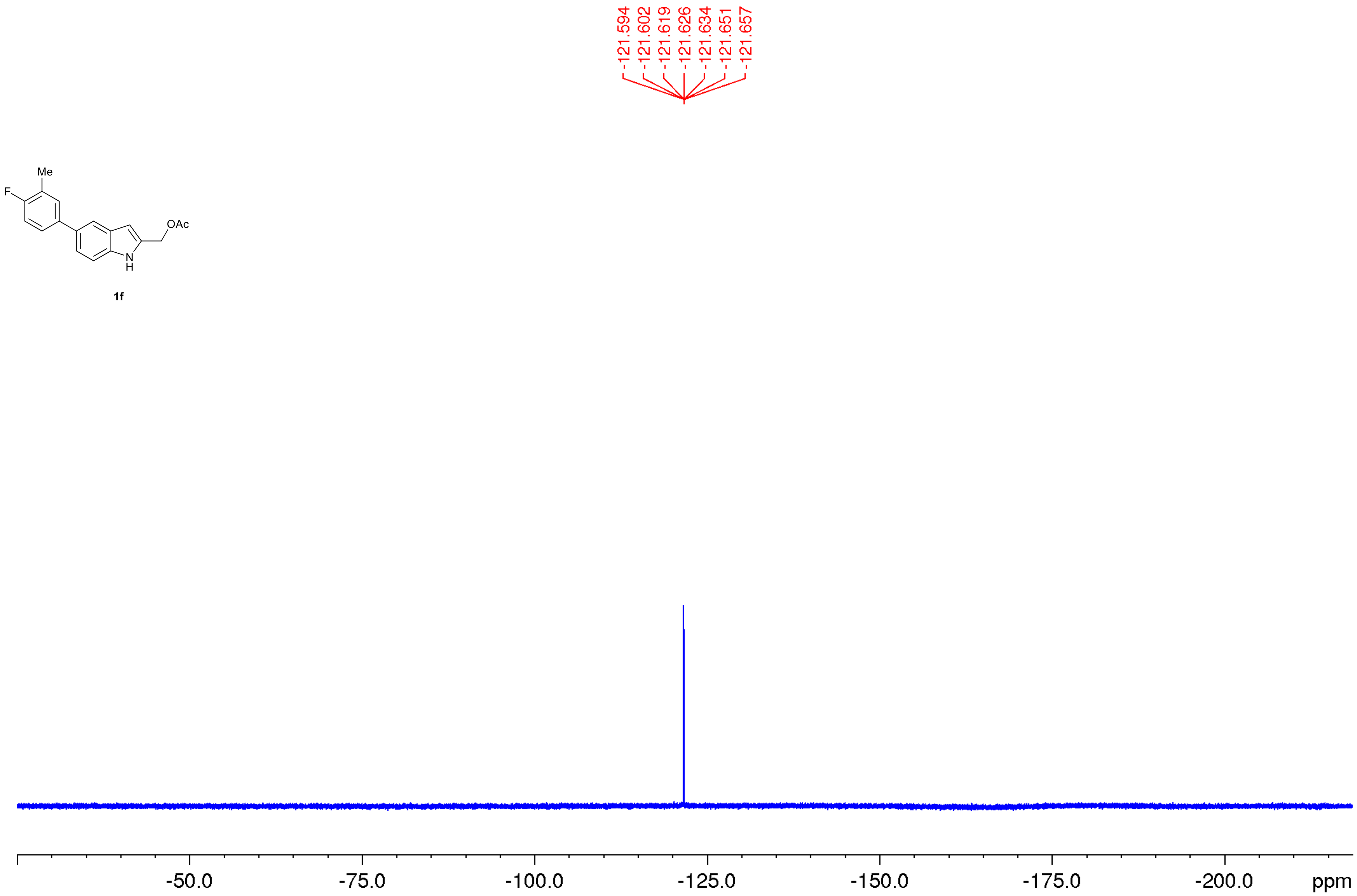
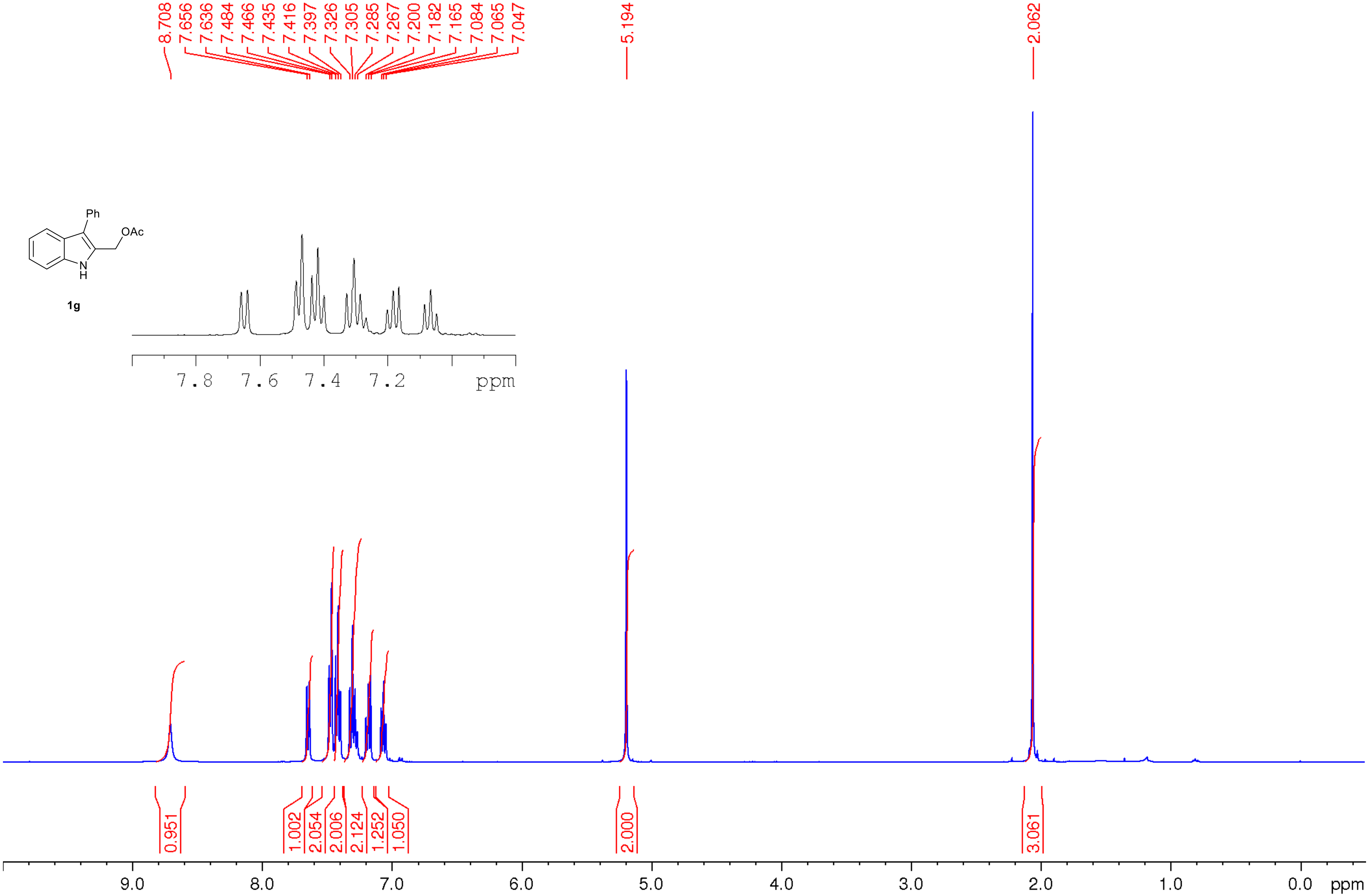


^{19}F NMR-spectrum (376.5, DMSO-d_6)



^1H NMR-spectrum (400 MHz, $CDCl_3$)

1g



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

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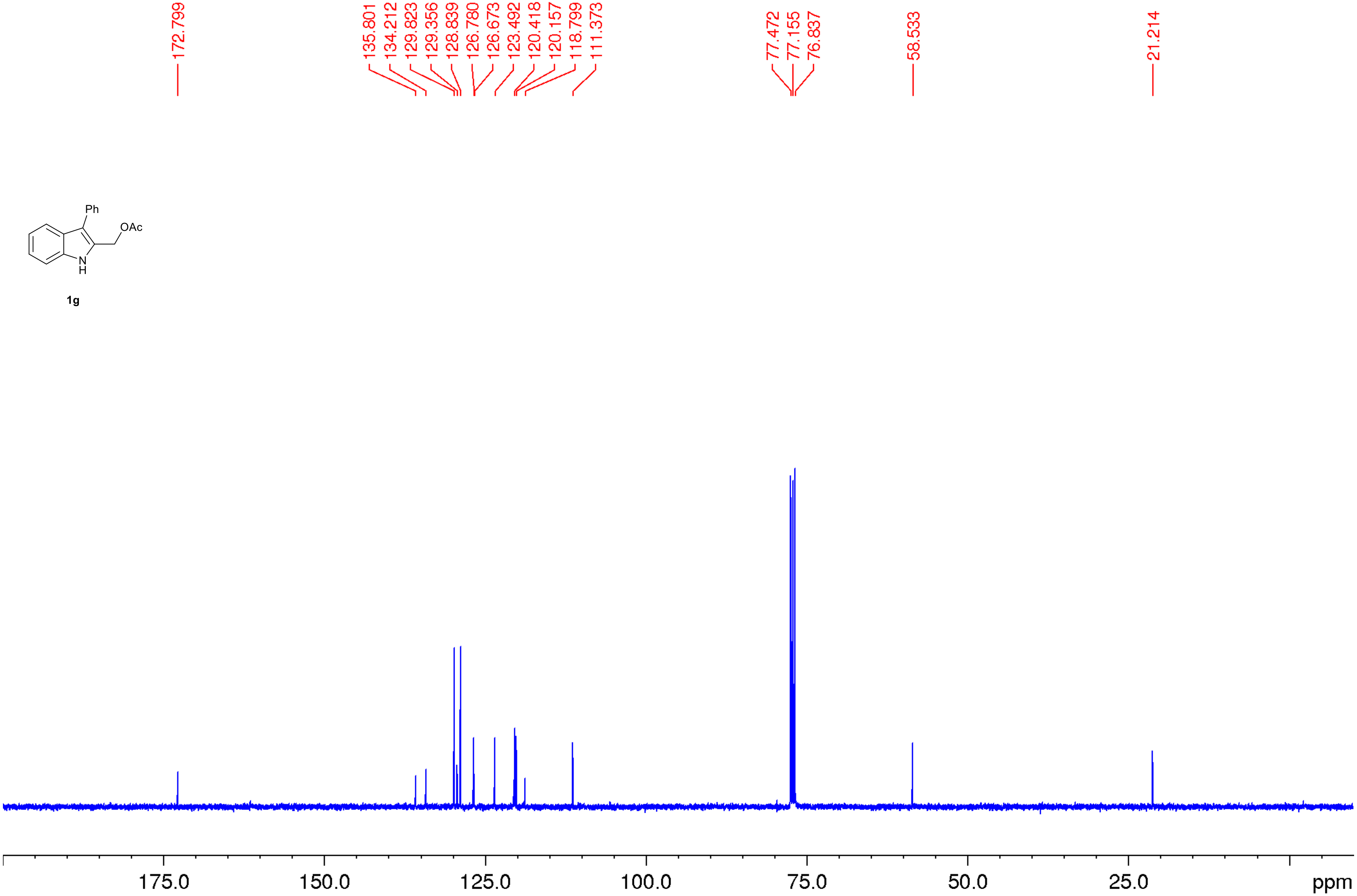
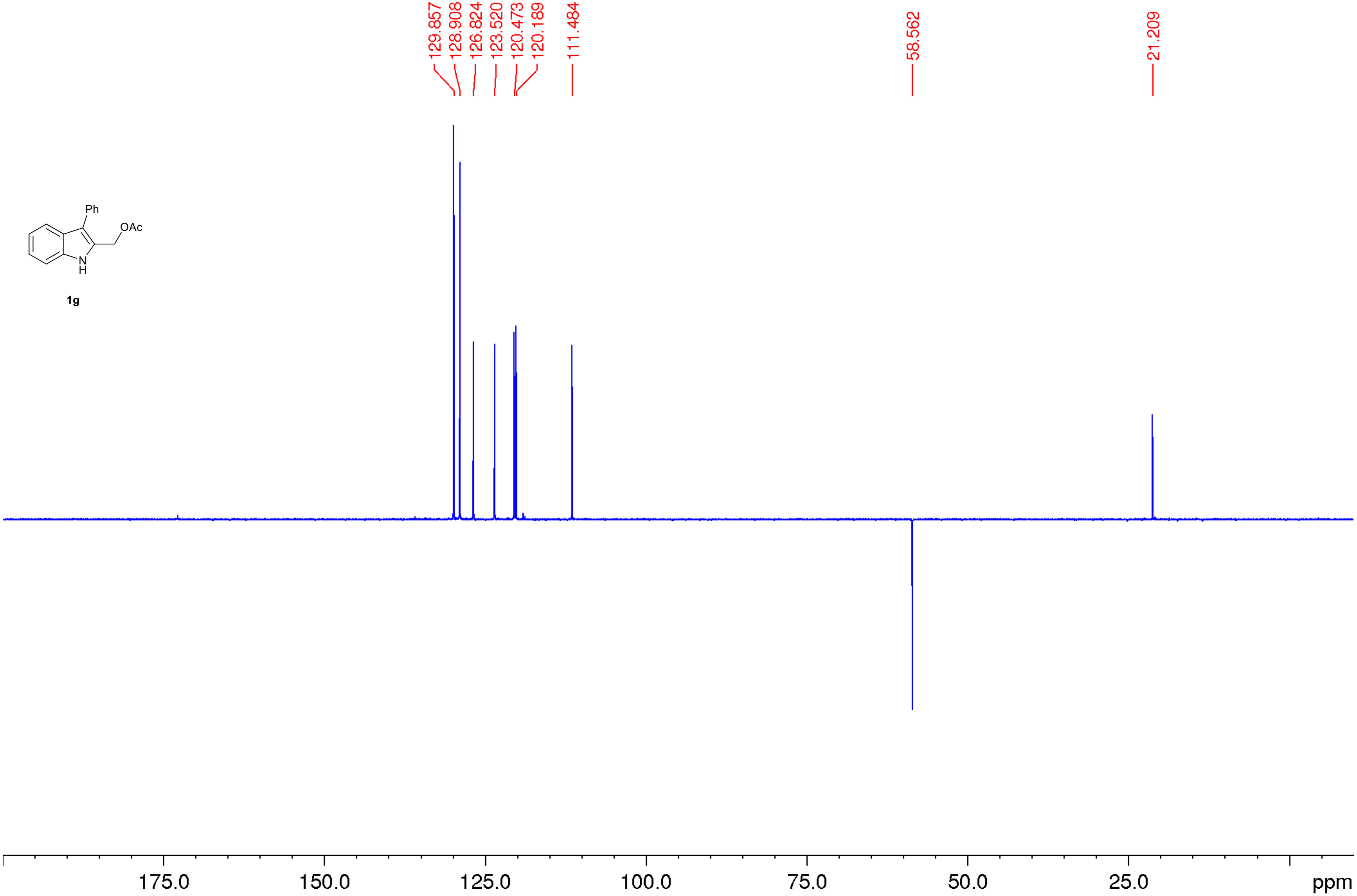
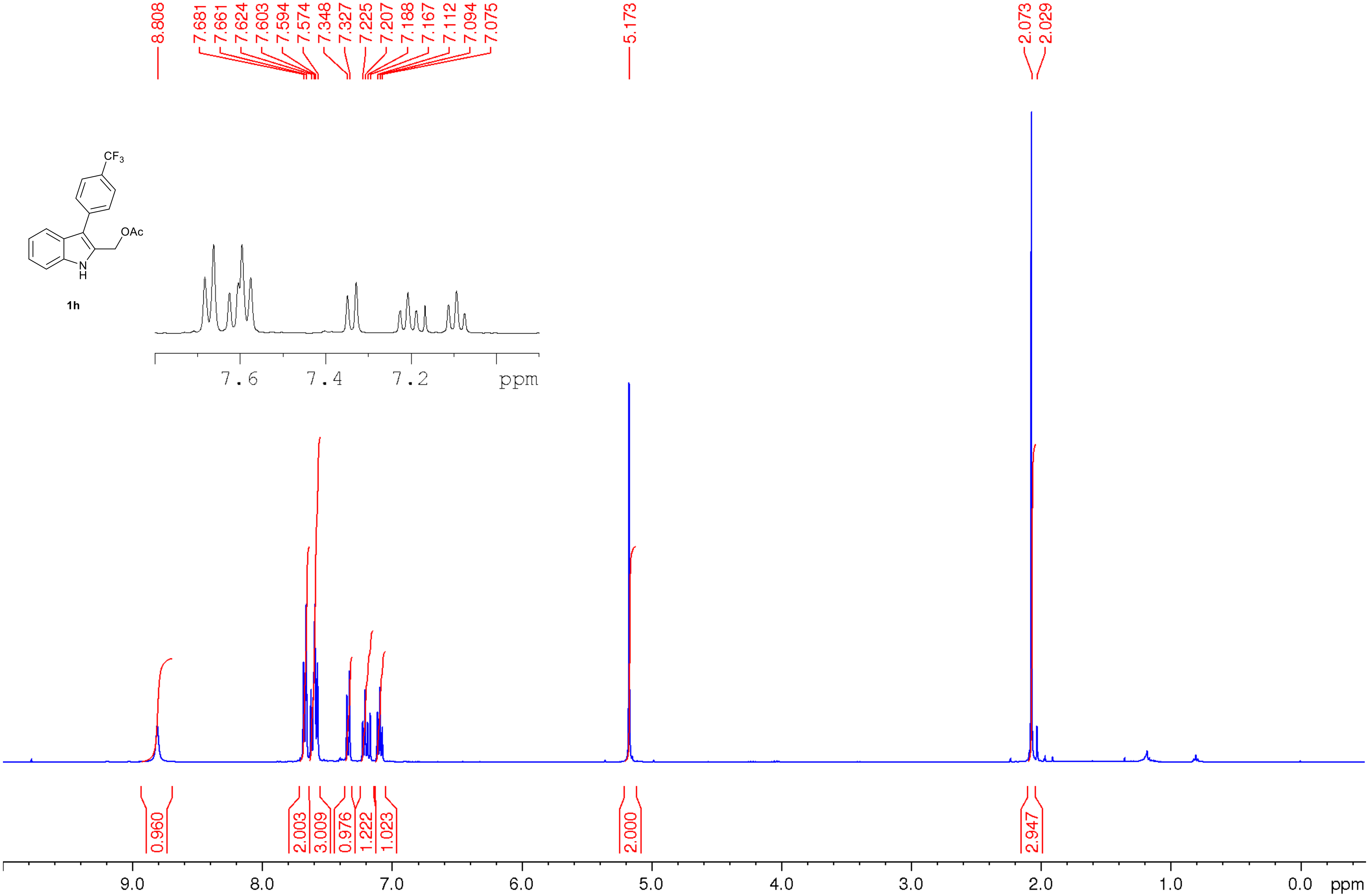


DEPT 135 NMR-spectrum ($CDCl_3$)

1g



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



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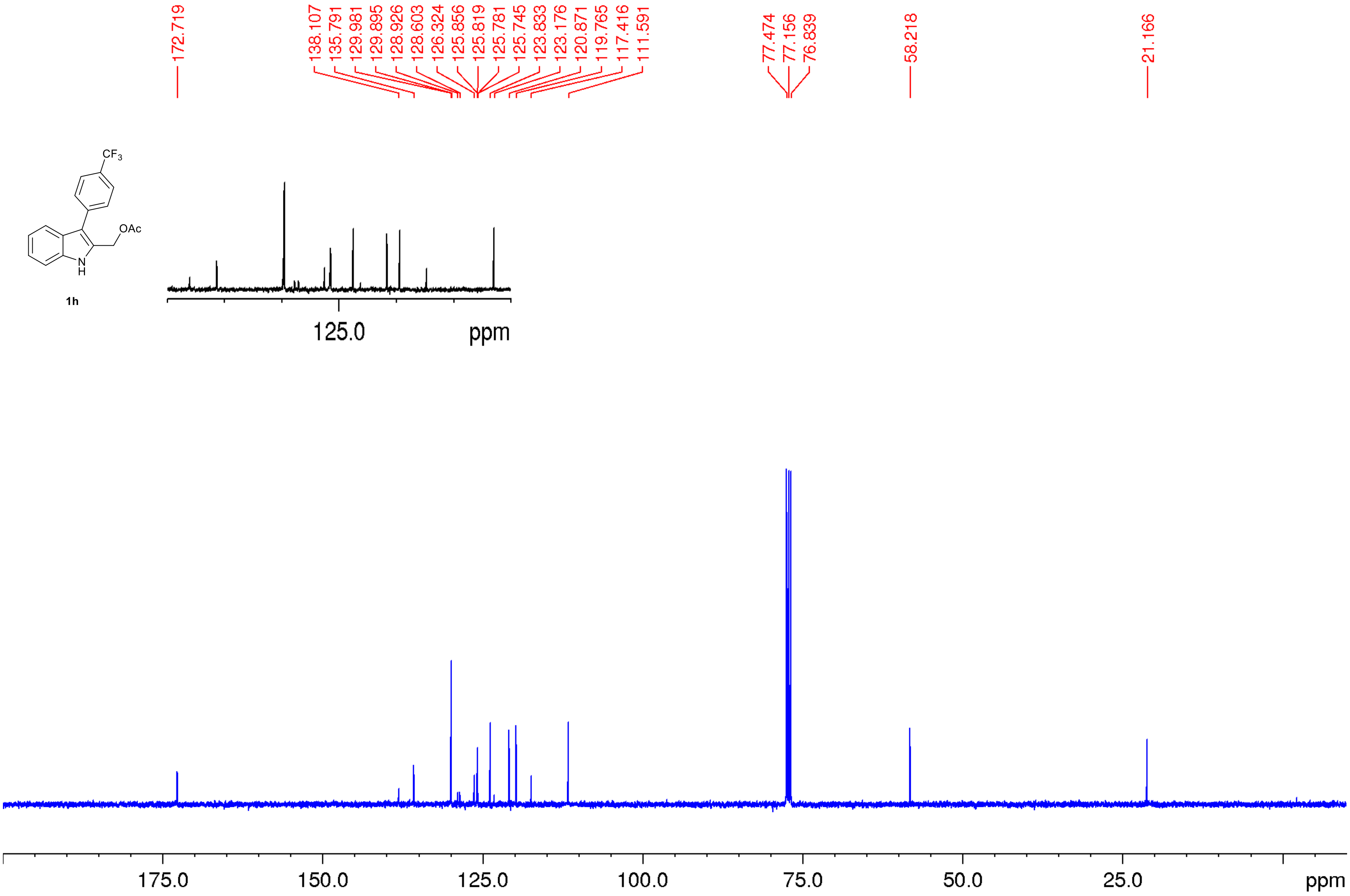
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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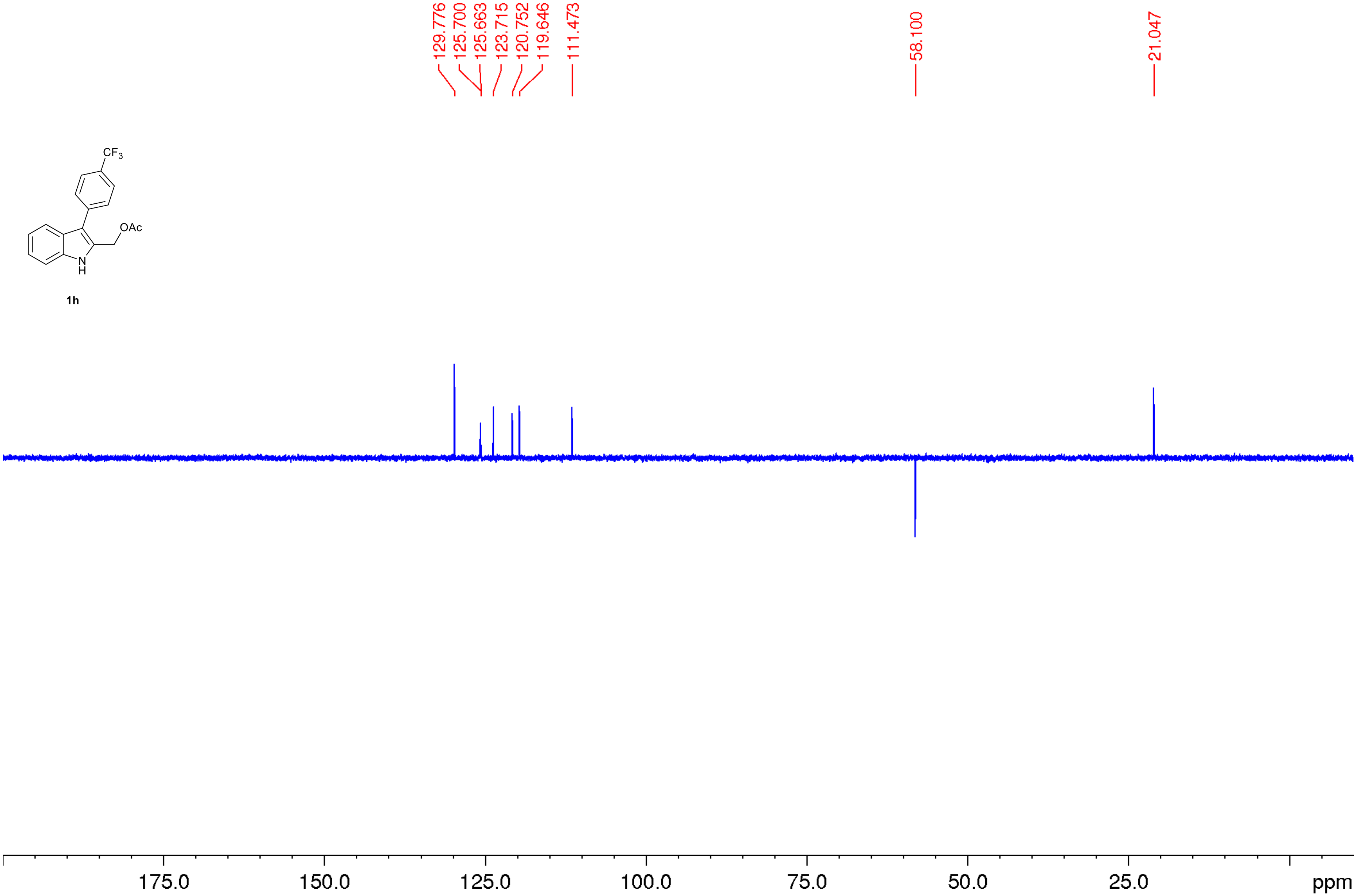
DEPT 135 NMR-spectrum ($CDCl_3$)



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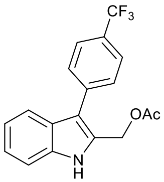
^{19}F NMR-spectrum (376.5 MHz, $CDCl_3$)



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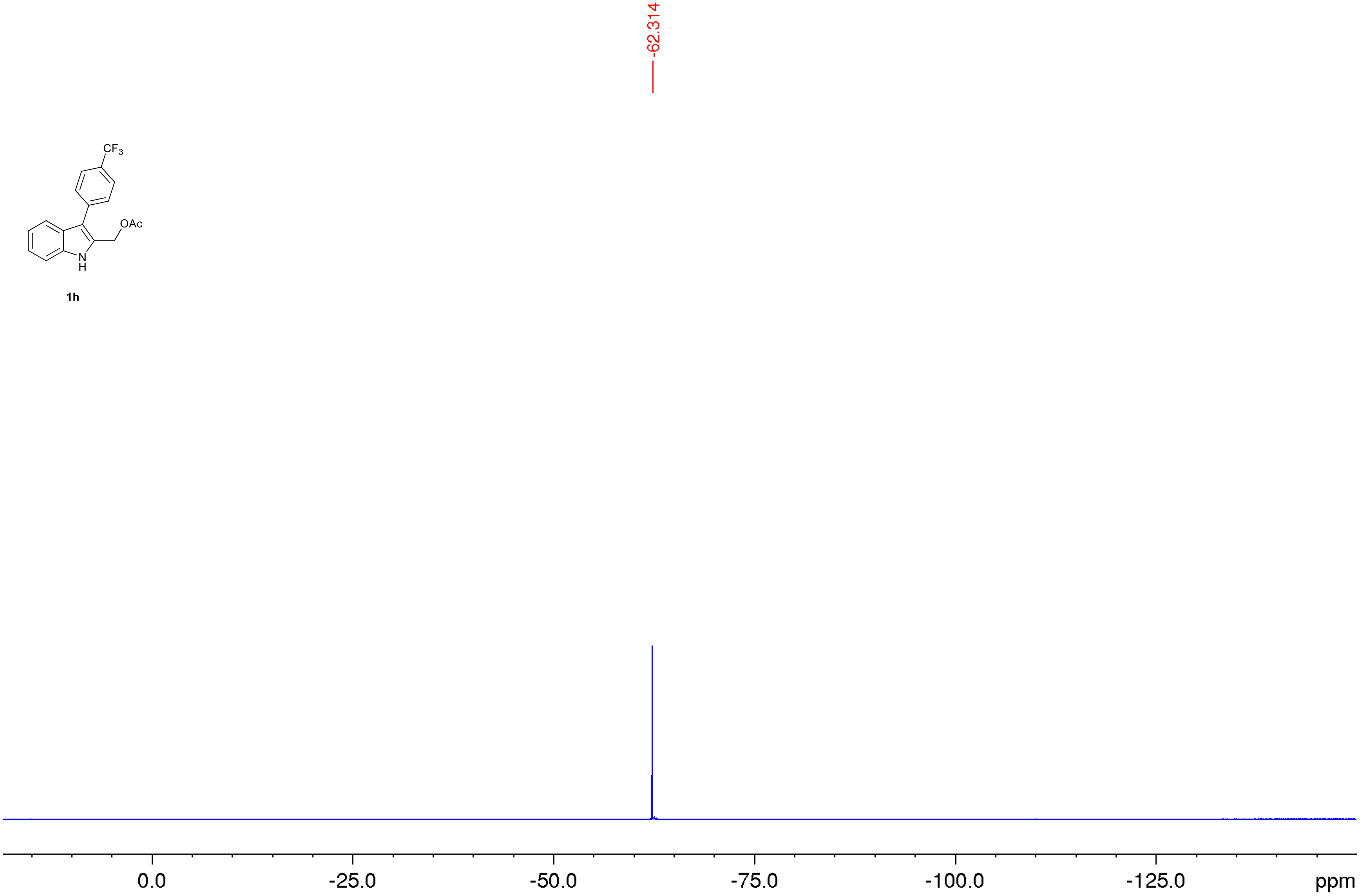
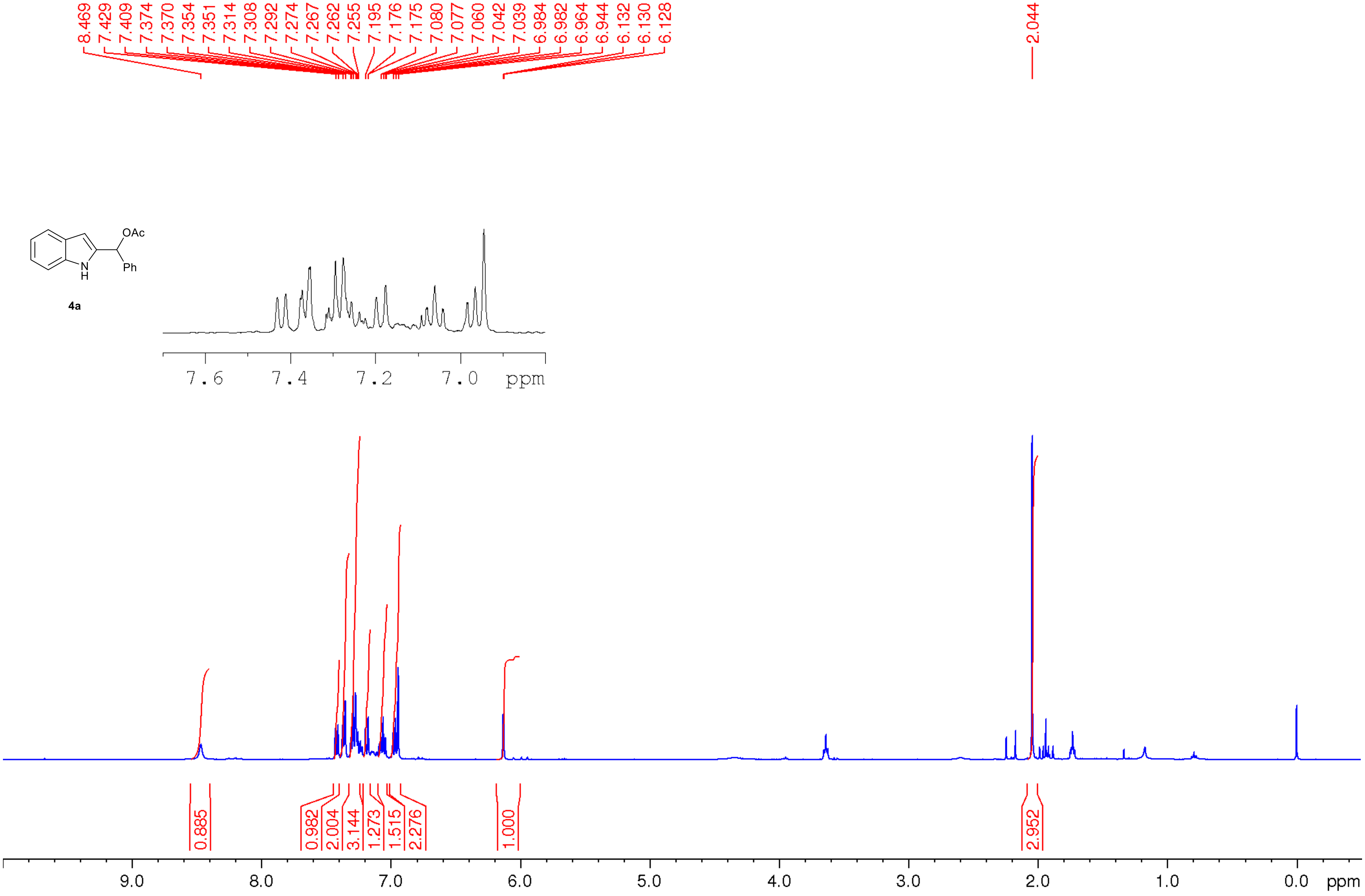
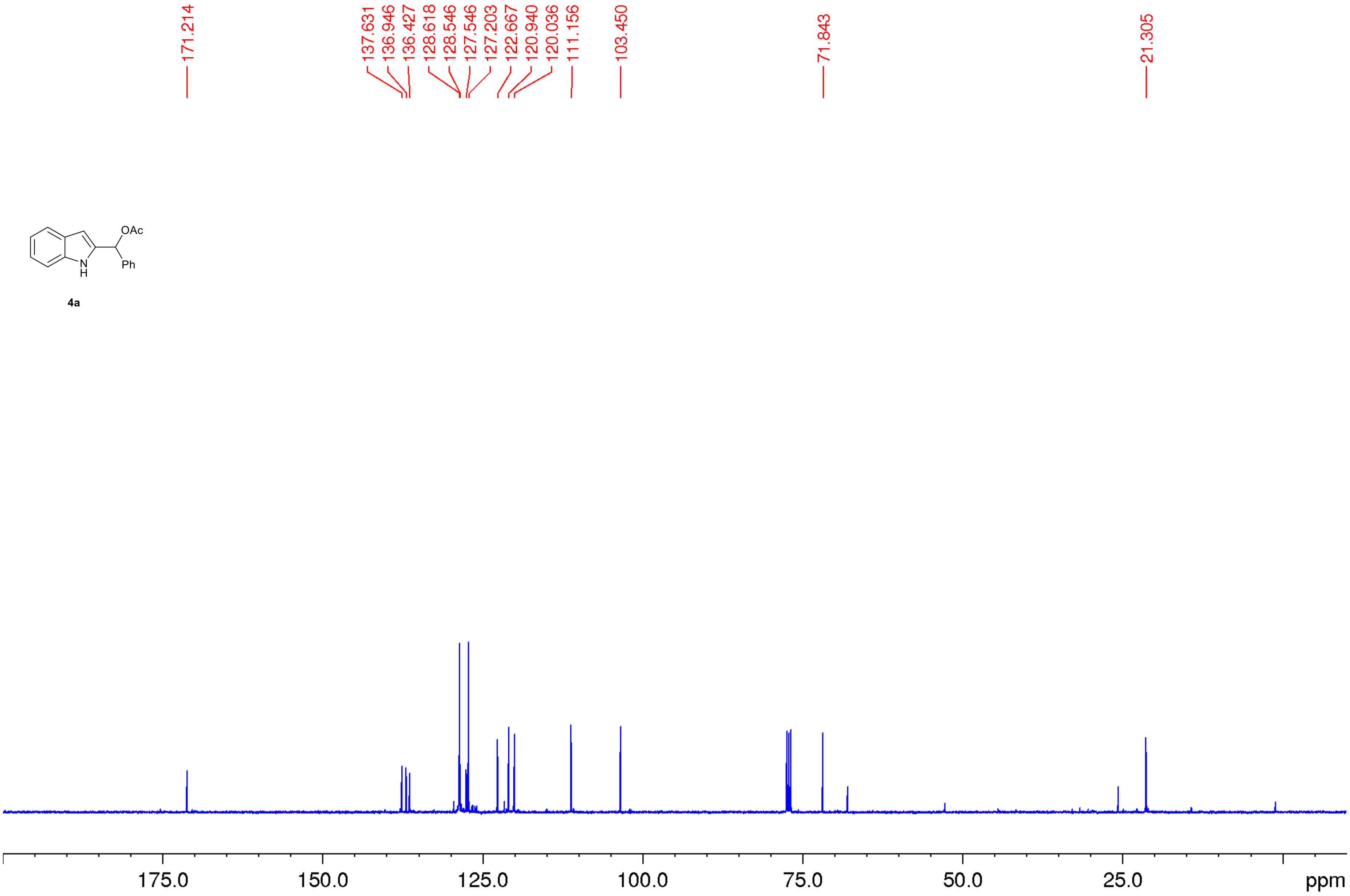


^1H NMR-spectrum (400 MHz, $CDCl_3$)


4a

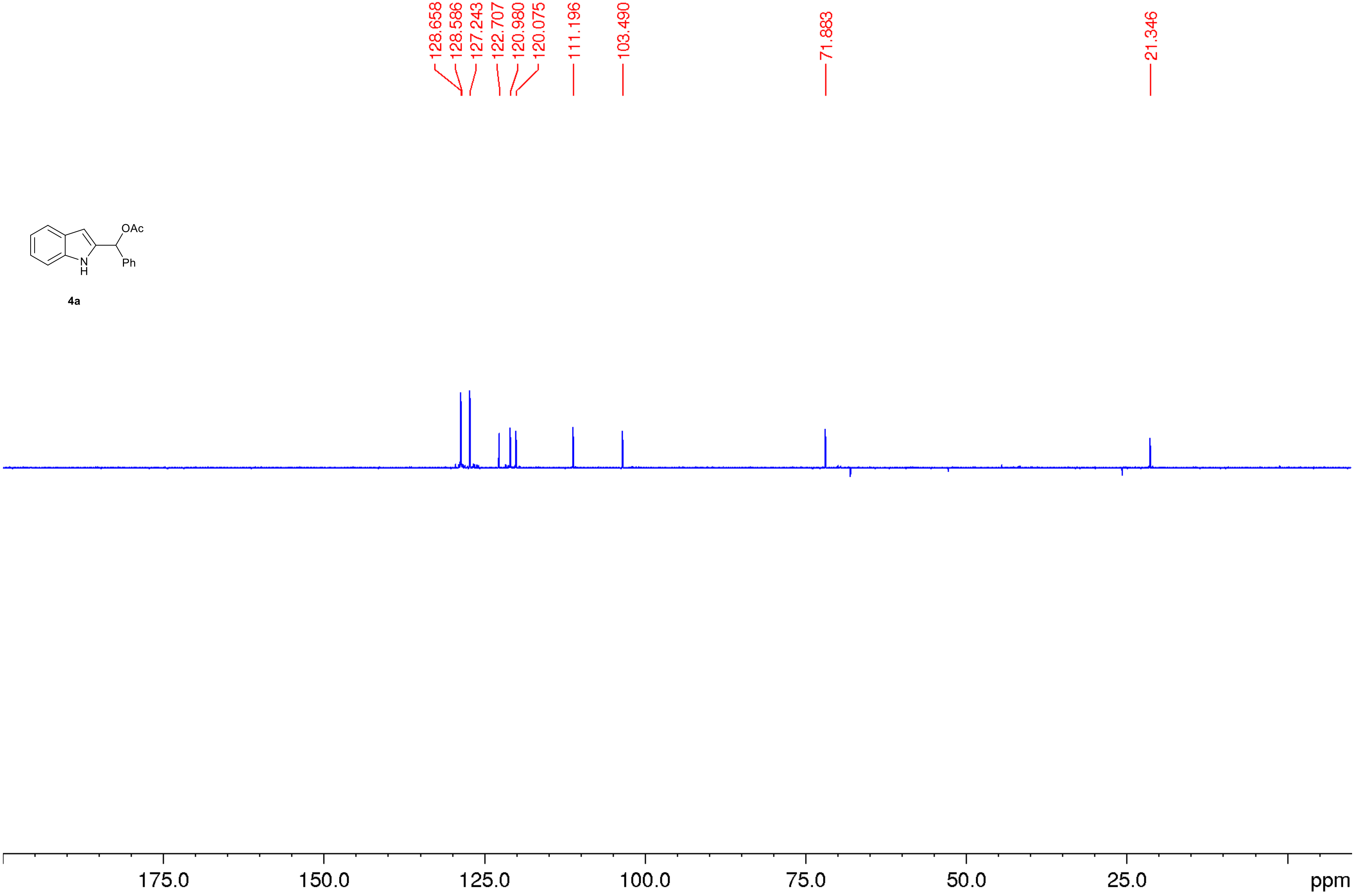
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



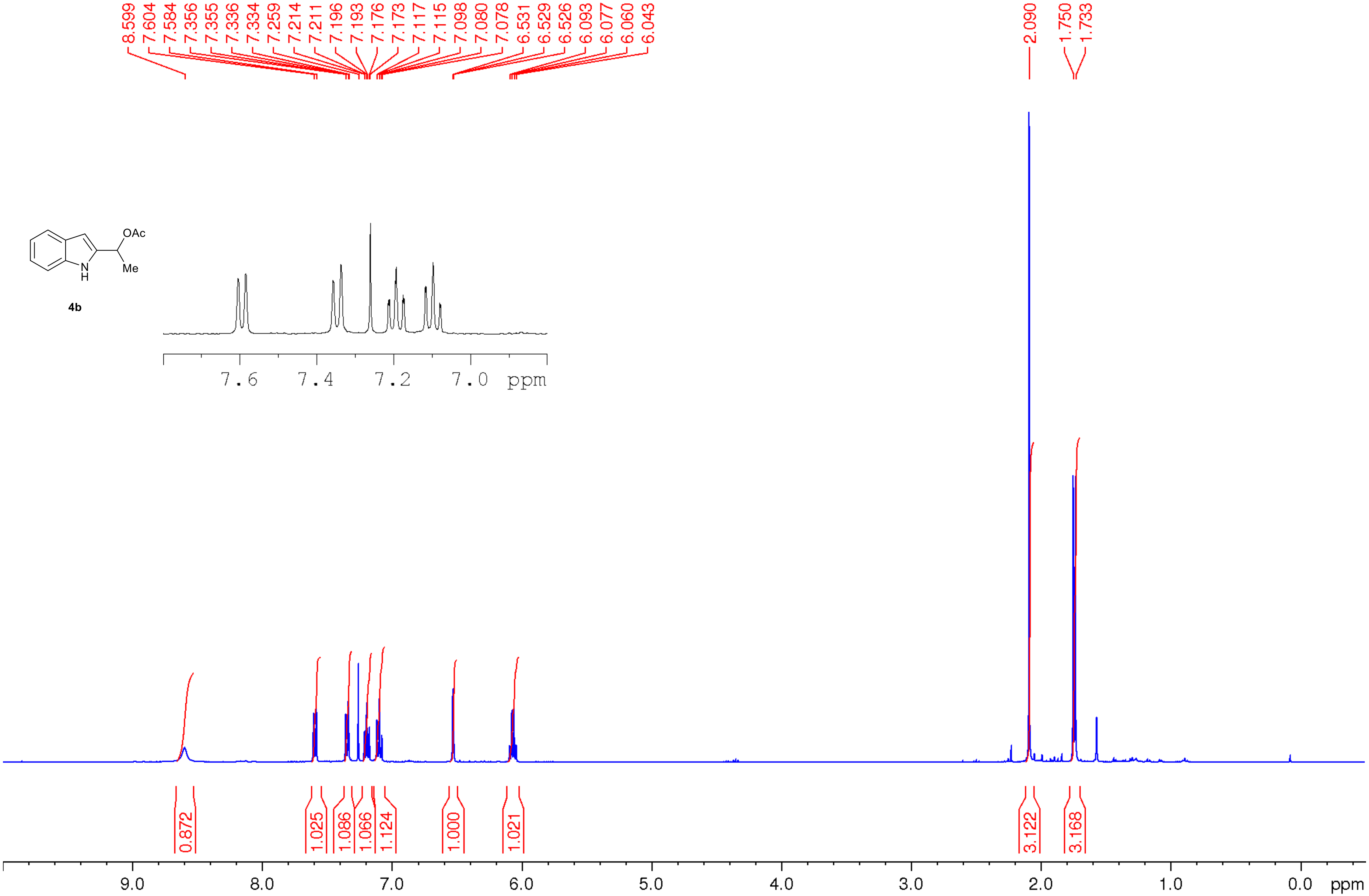
4a

DEPT 135 NMR-spectrum ($CDCl_3$)

4a

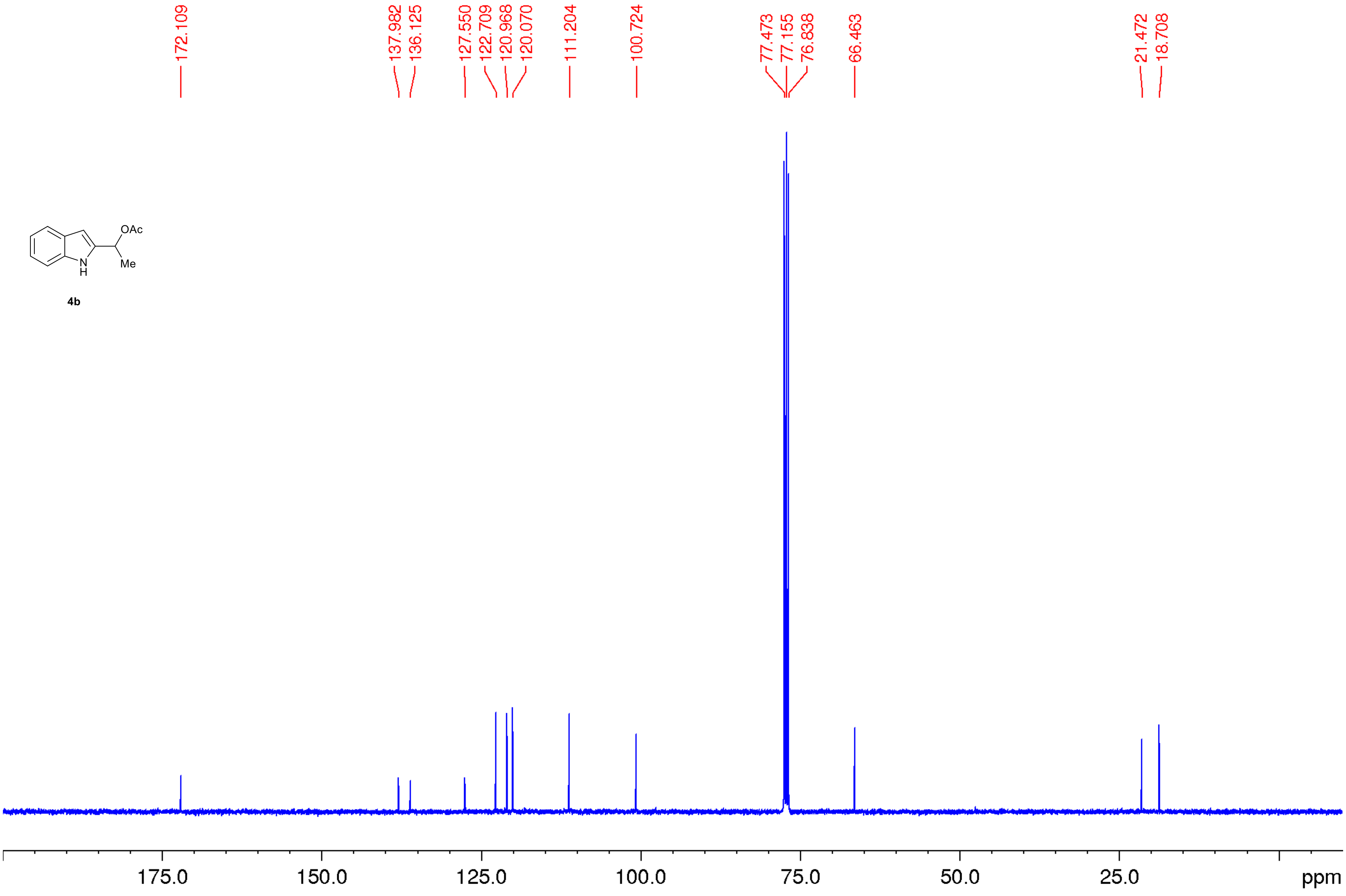


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



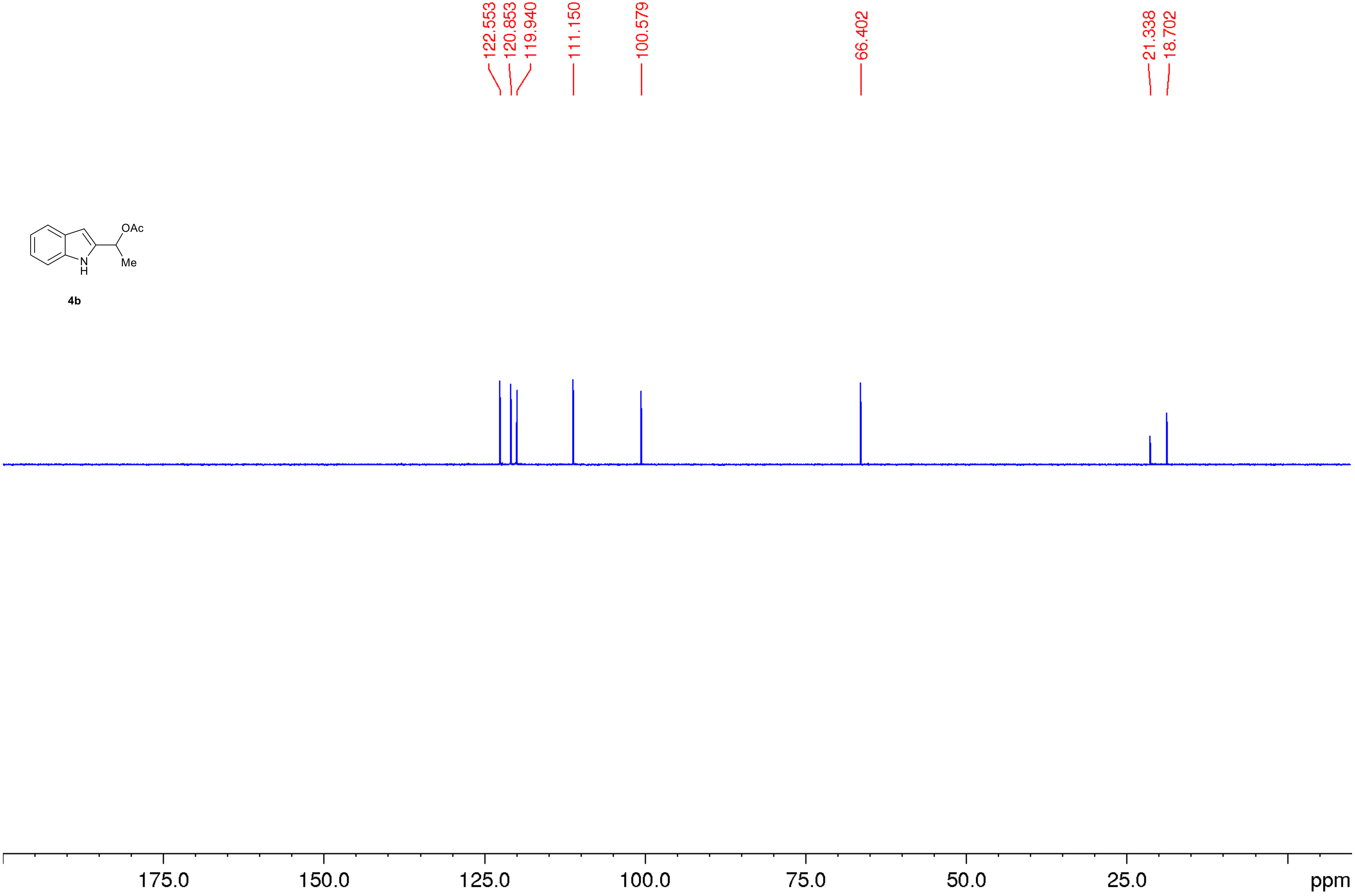
4b

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



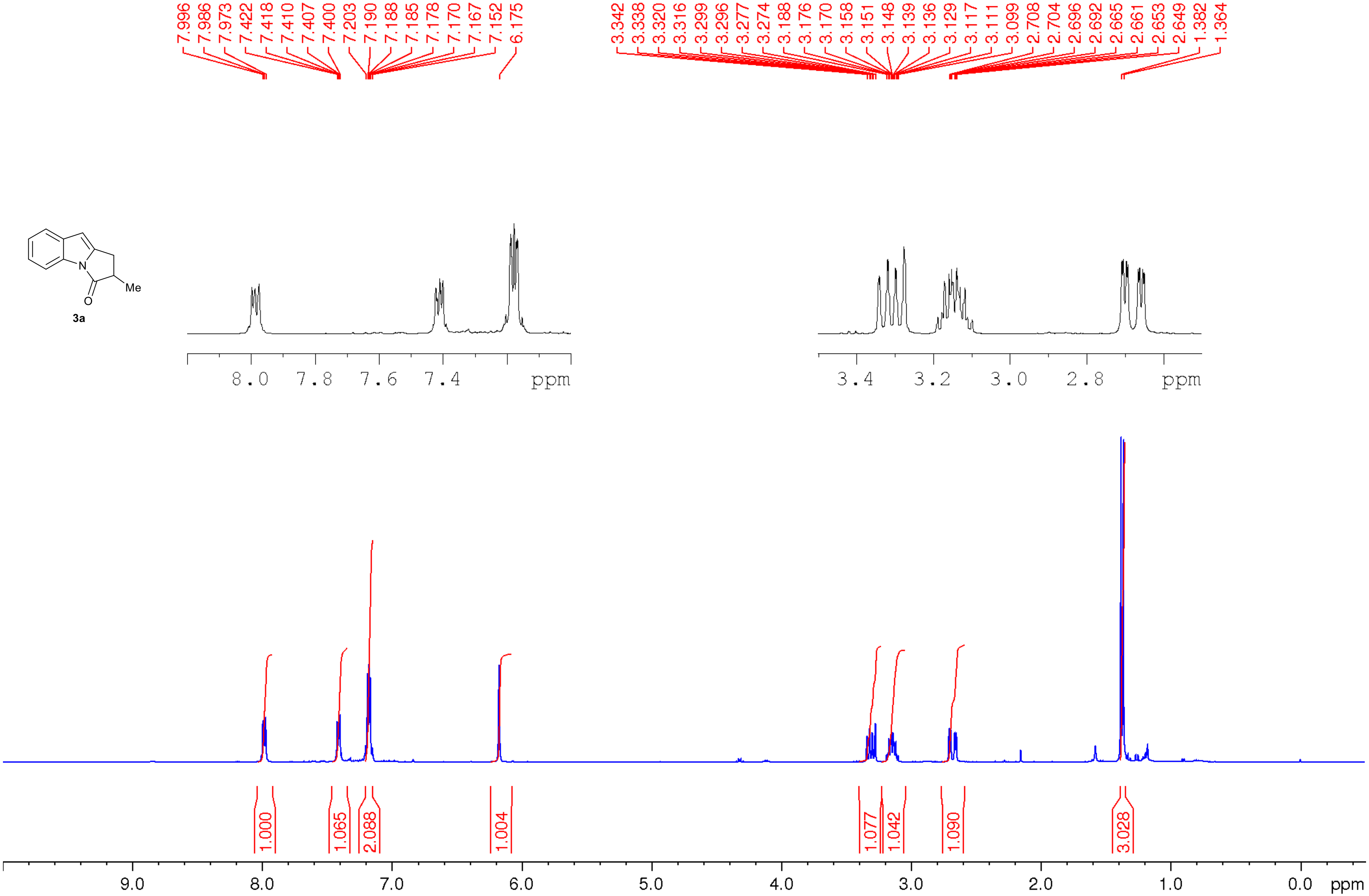
DEPT 135 NMR-spectrum ($CDCl_3$)

4b

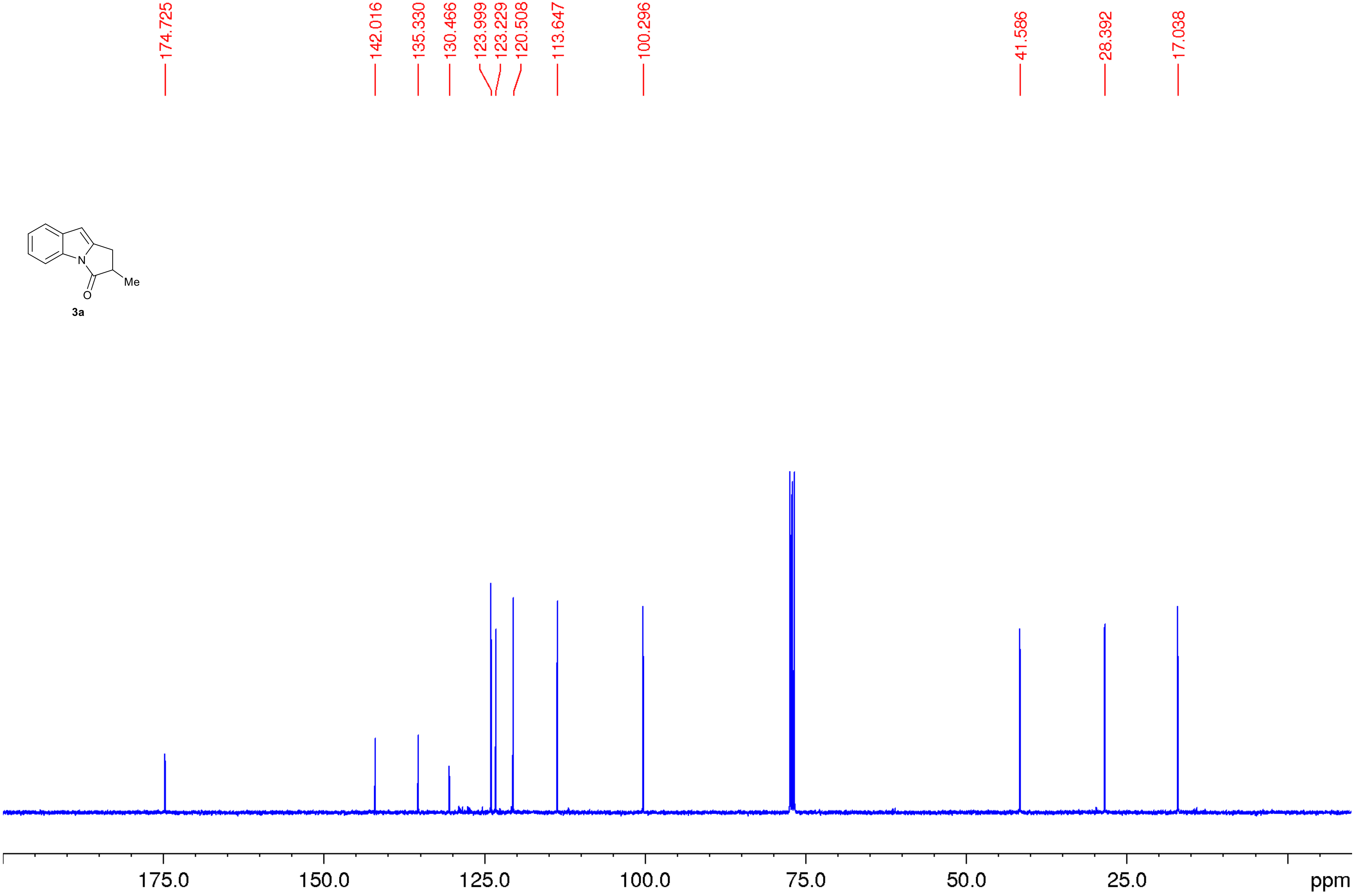


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

3a

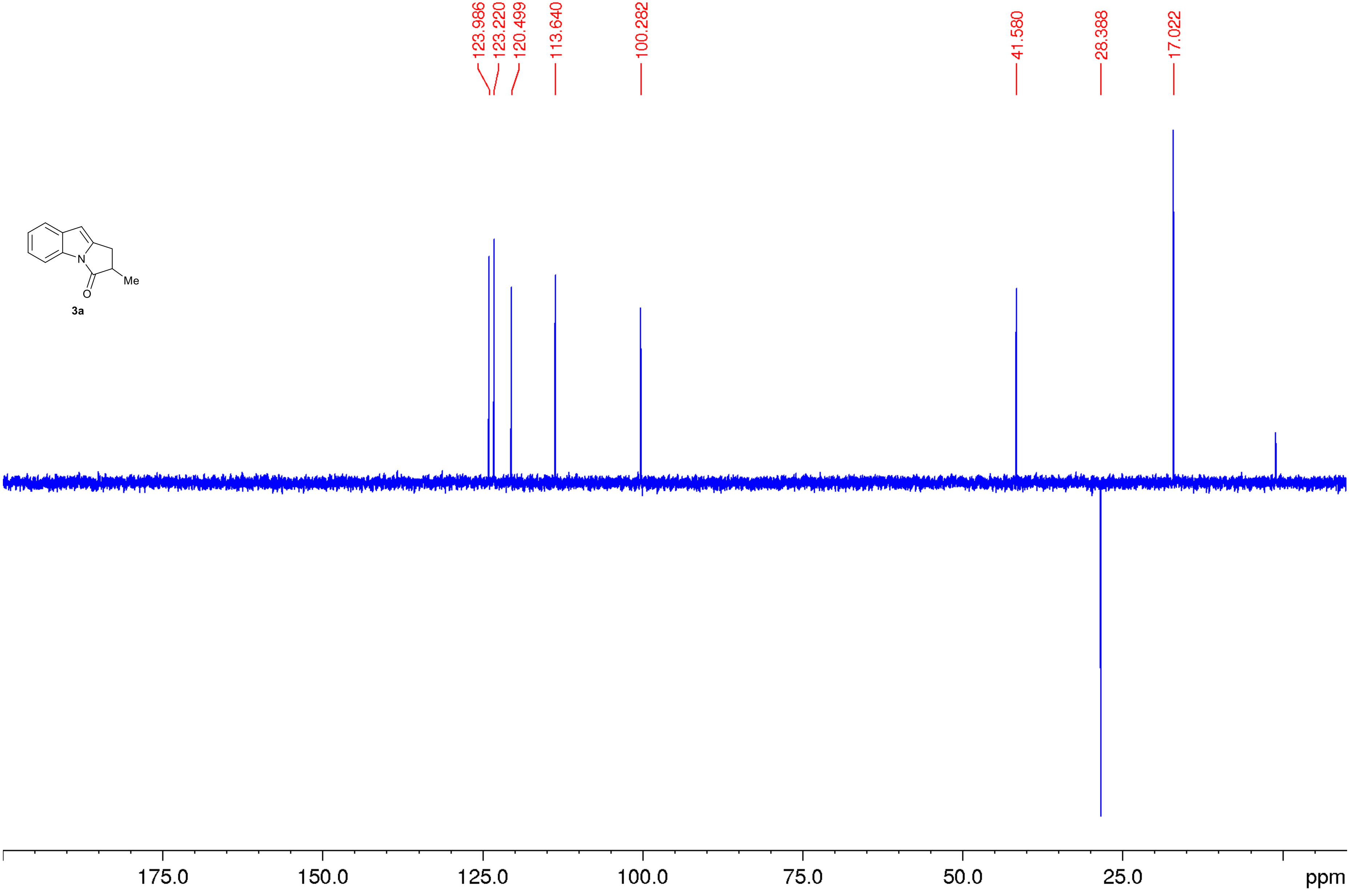


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



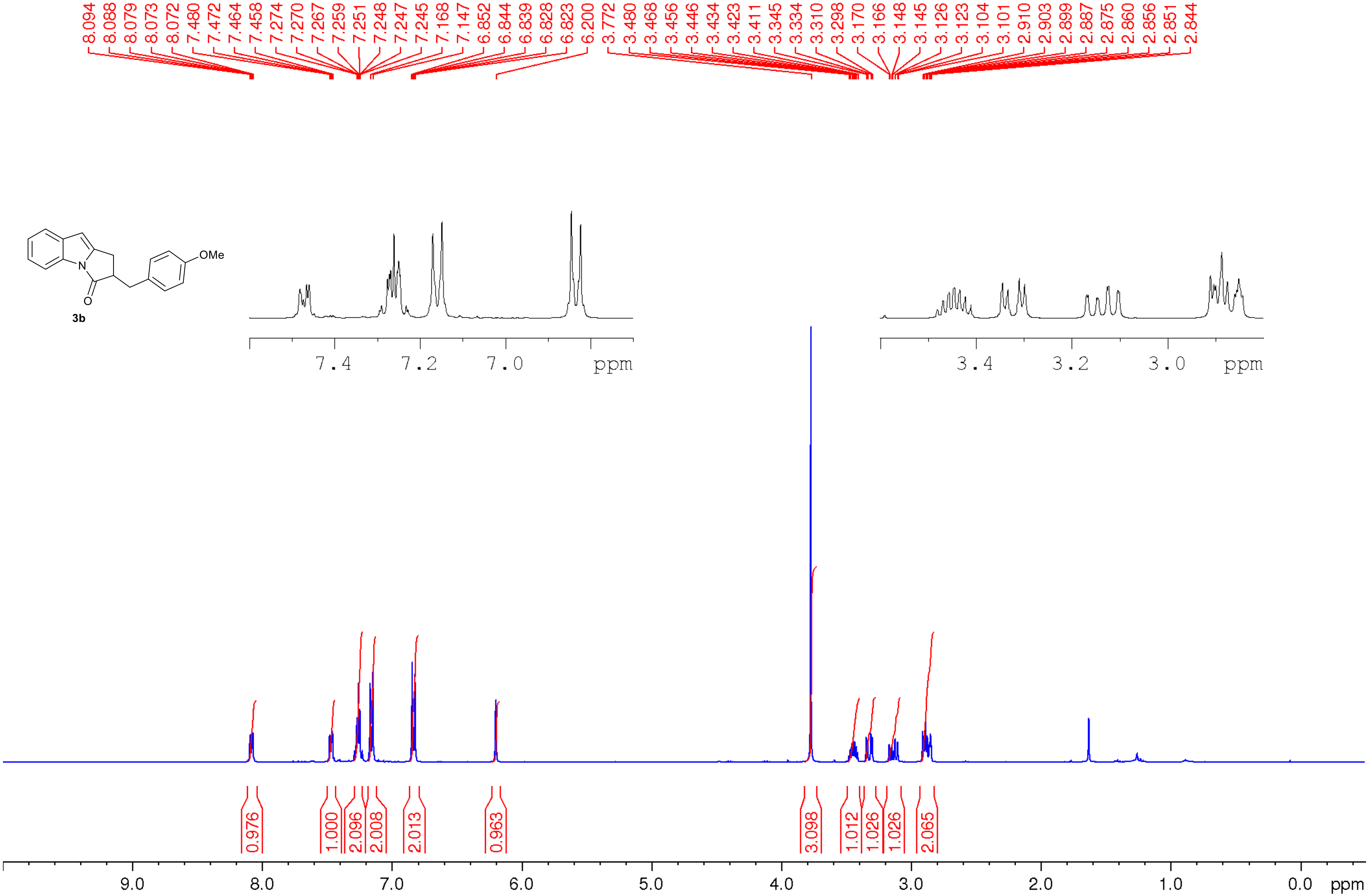
3a

DEPT 135 NMR-spectrum ($CDCl_3$)



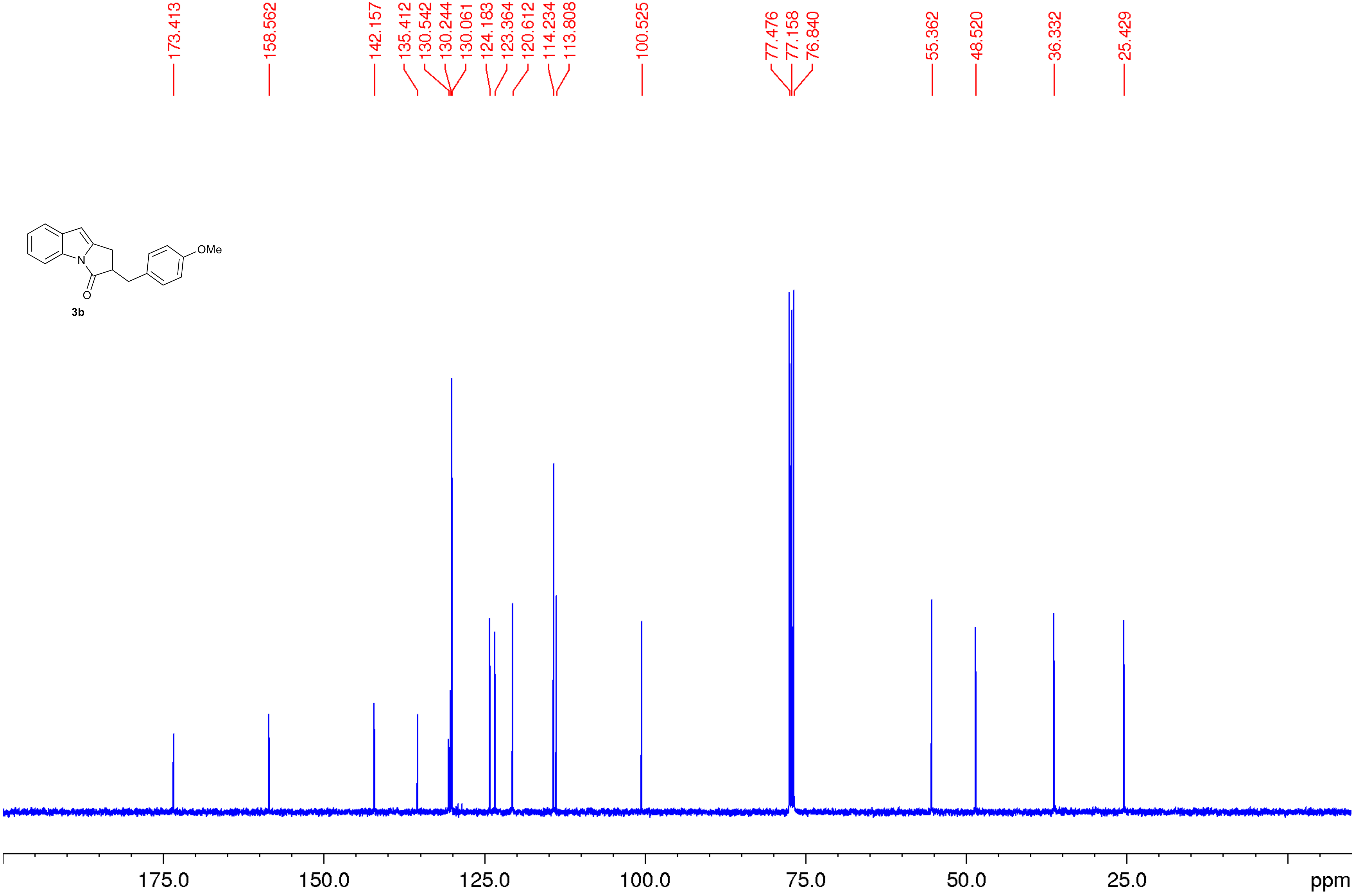
3a

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



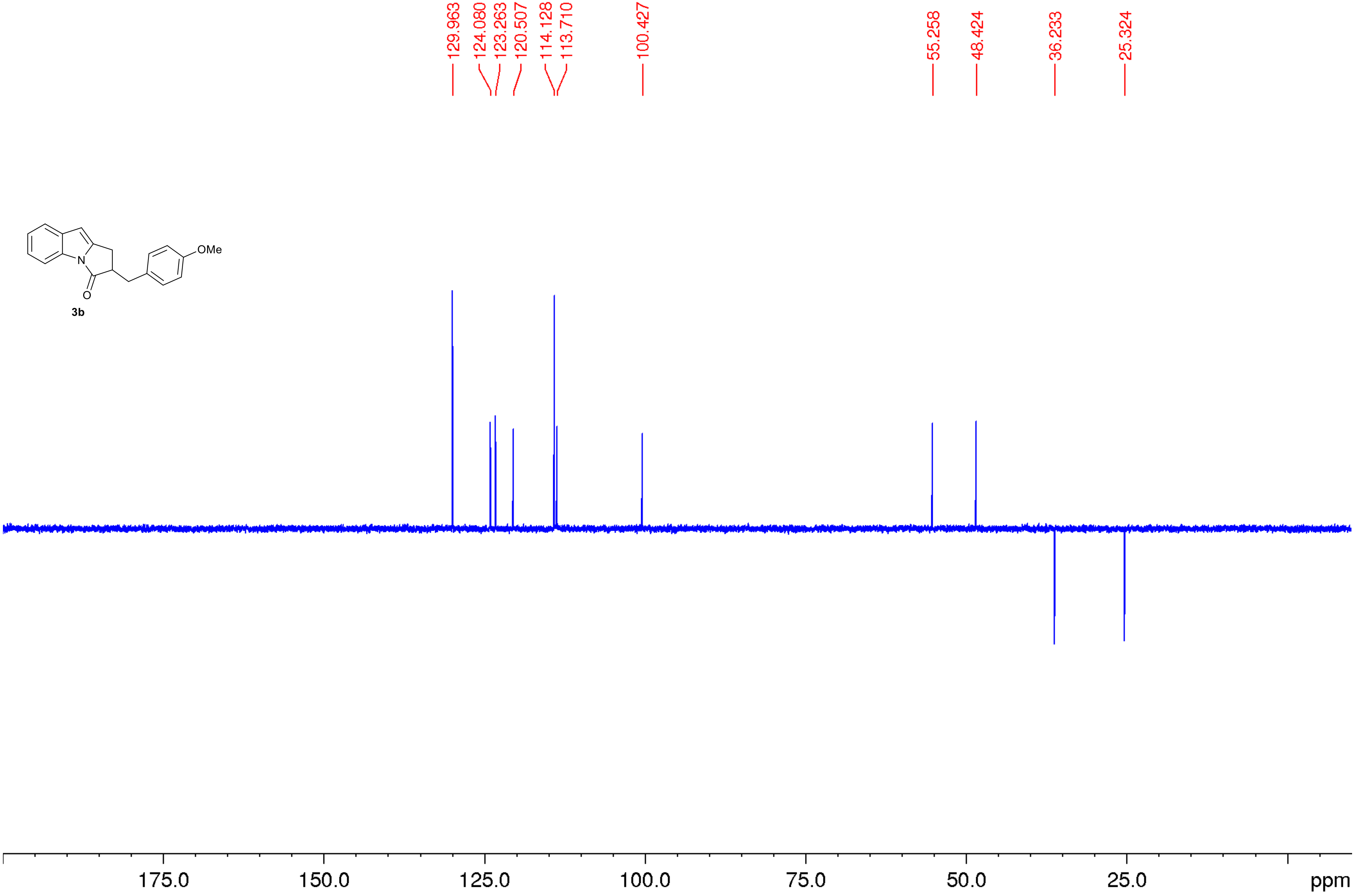
3b

^{13}C NMR-spectrum (100 MHz, CDCl$_3$)



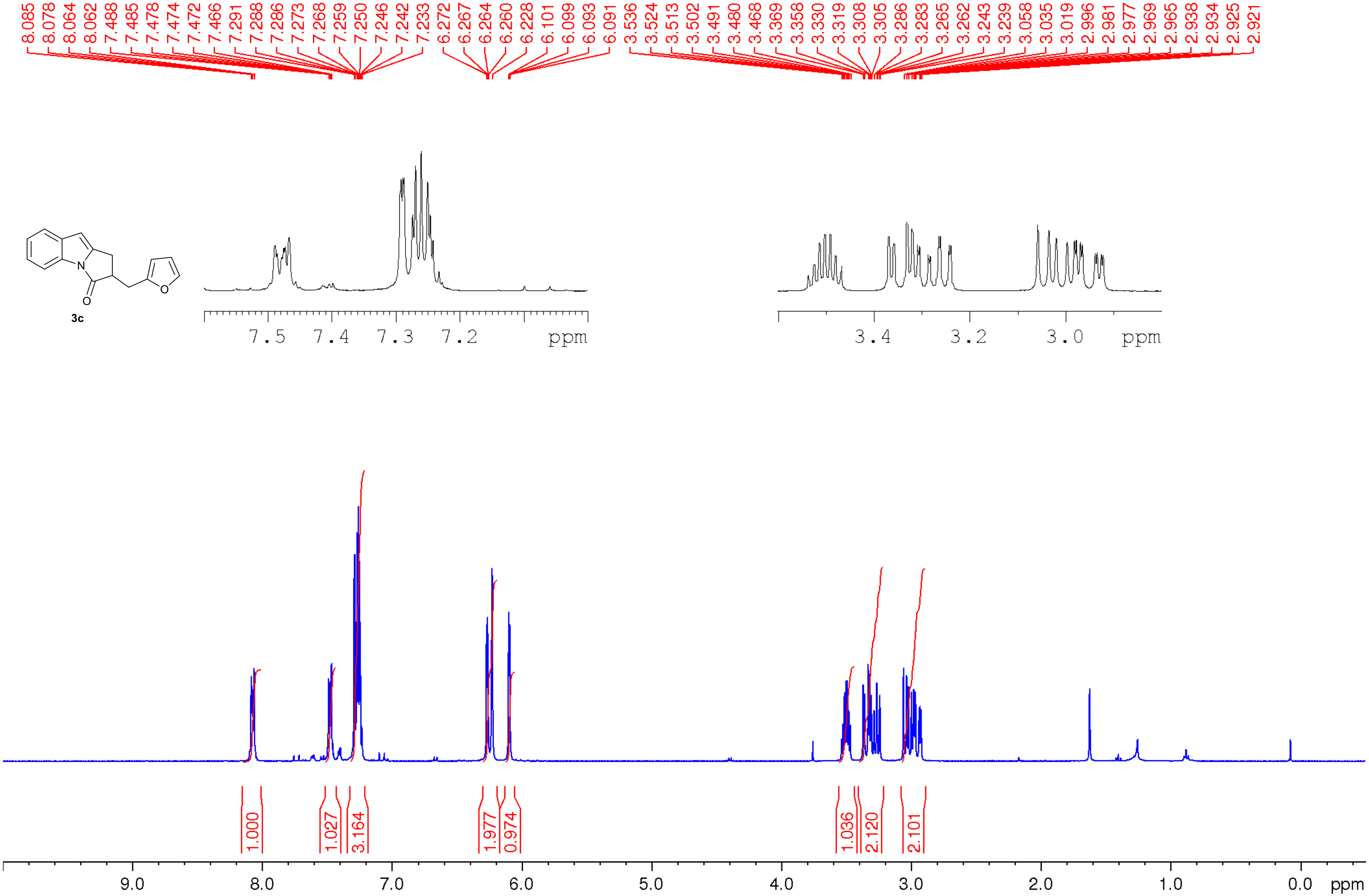
3b

DEPT 135 NMR-spectrum ($CDCl_3$)



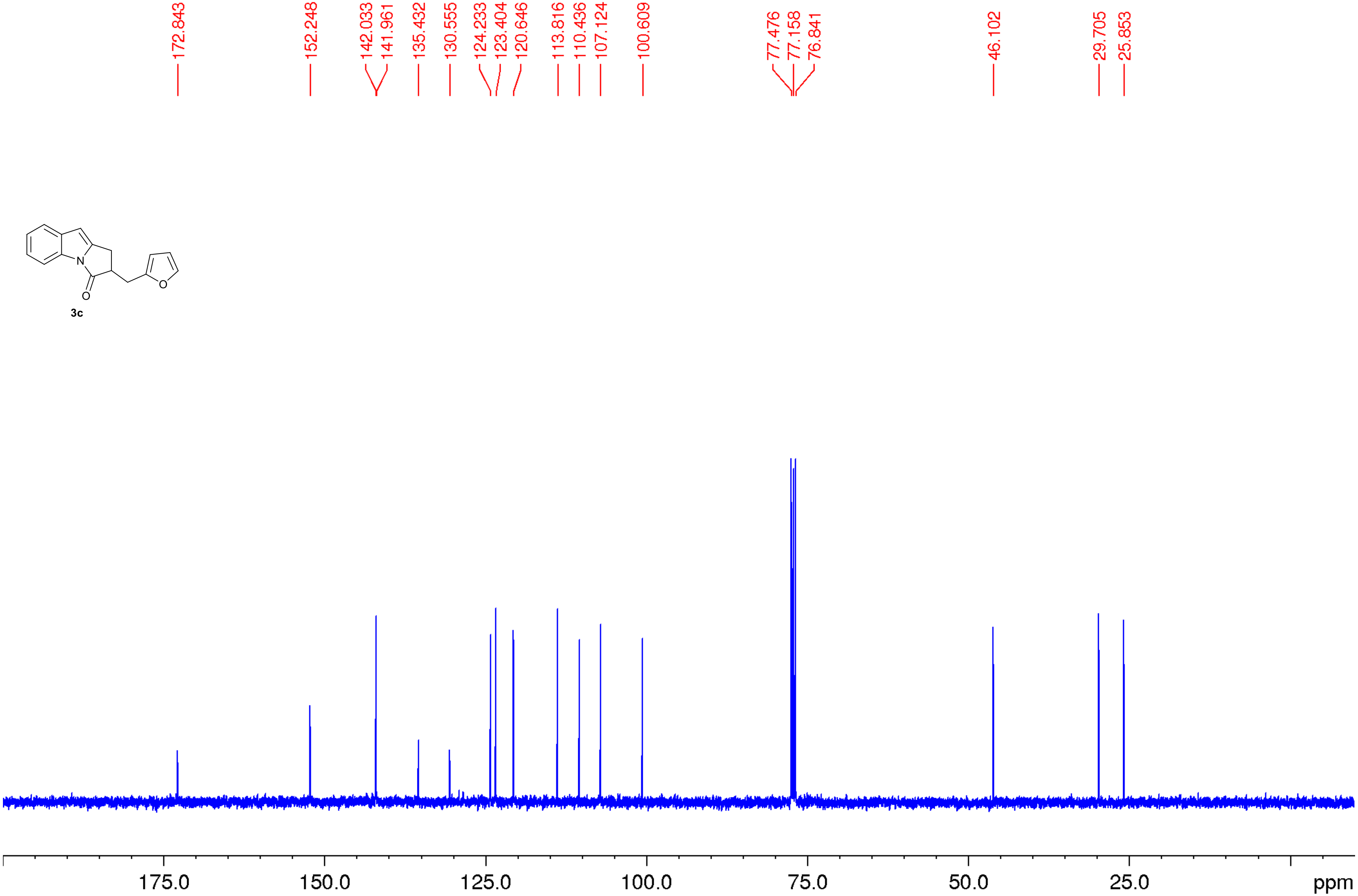
3b

^1H NMR-spectrum (400 MHz, $CDCl_3$)

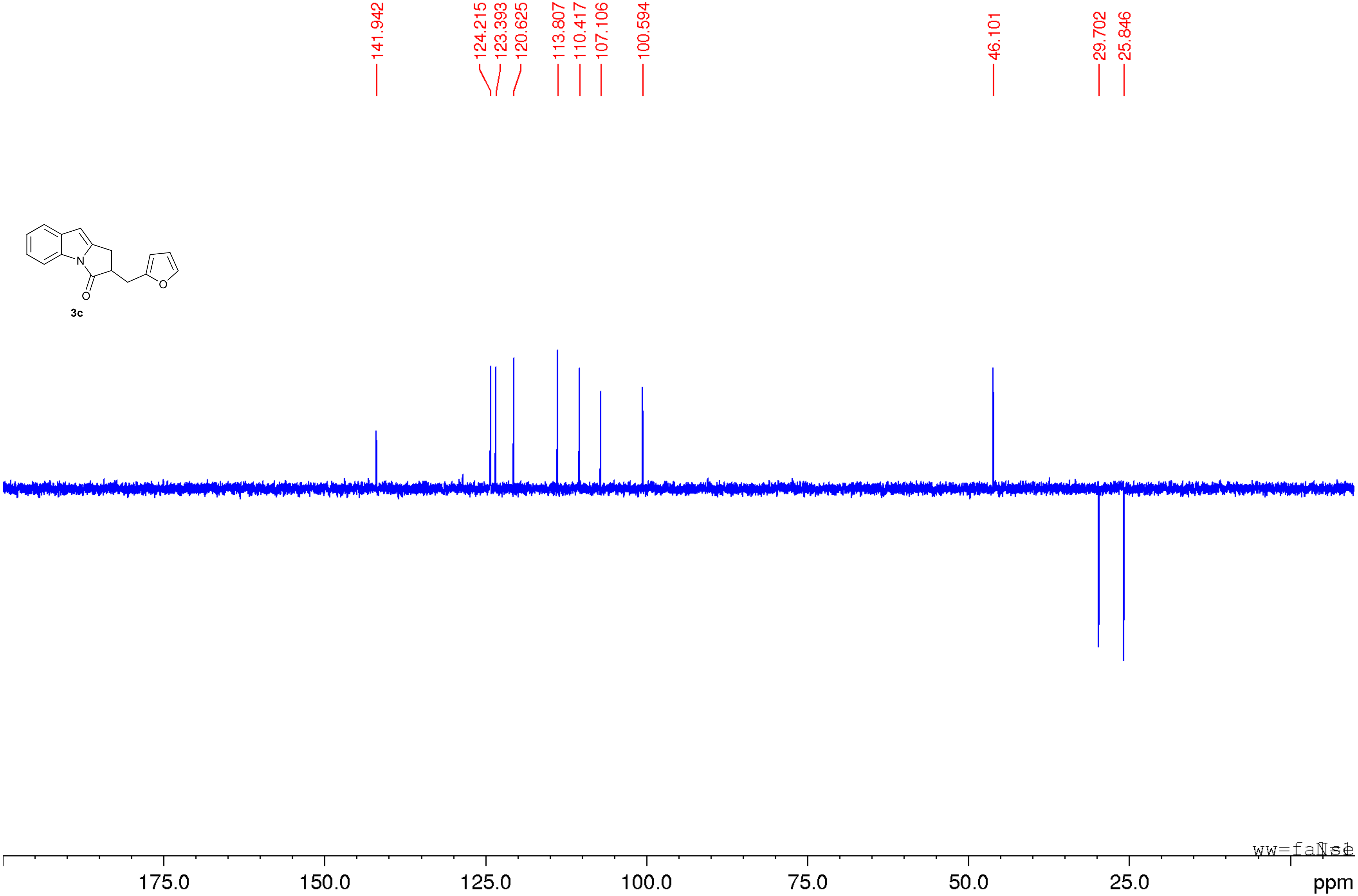


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

3c



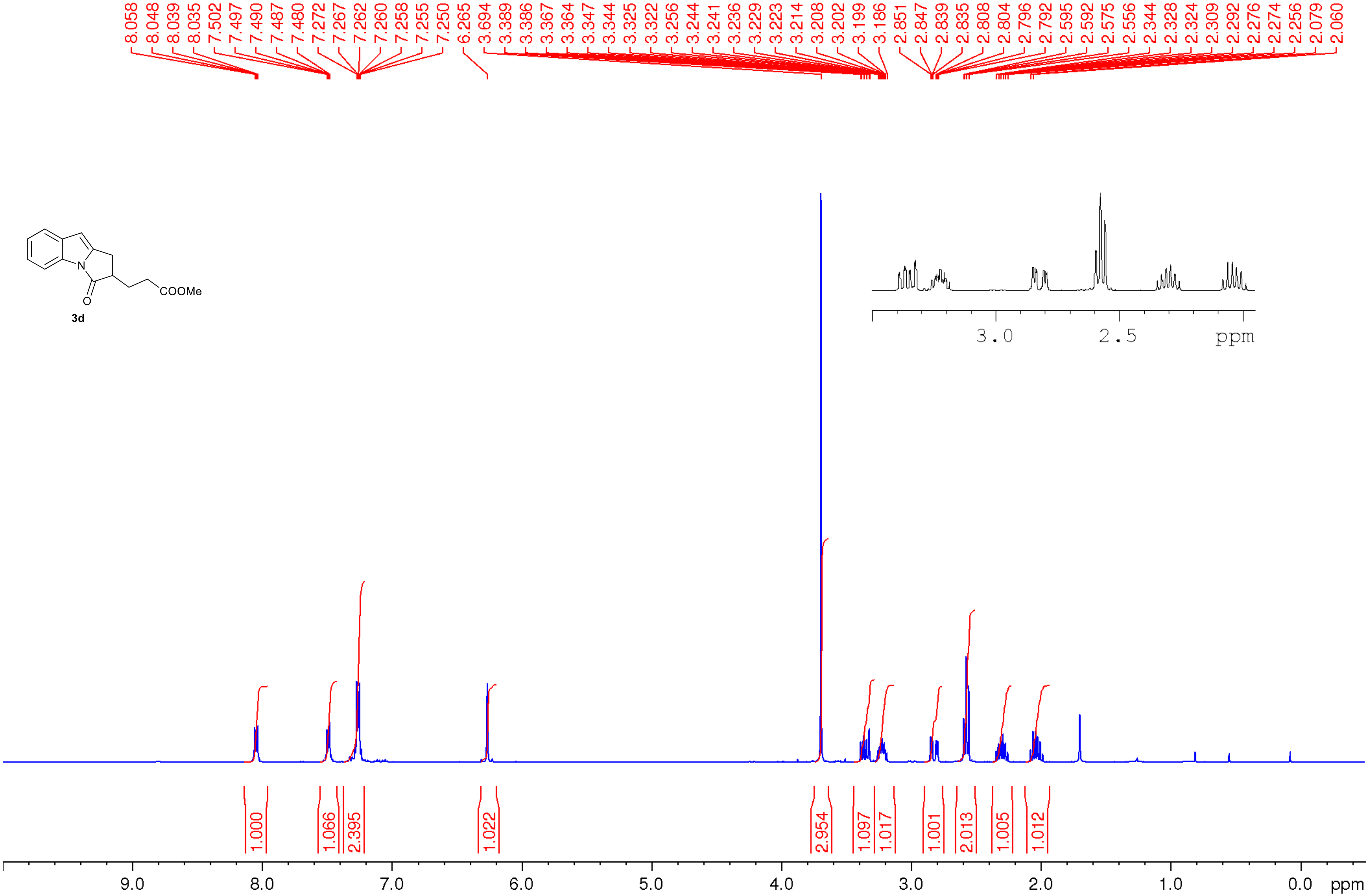
DEPT 135 NMR-spectrum ($CDCl_3$)



3c

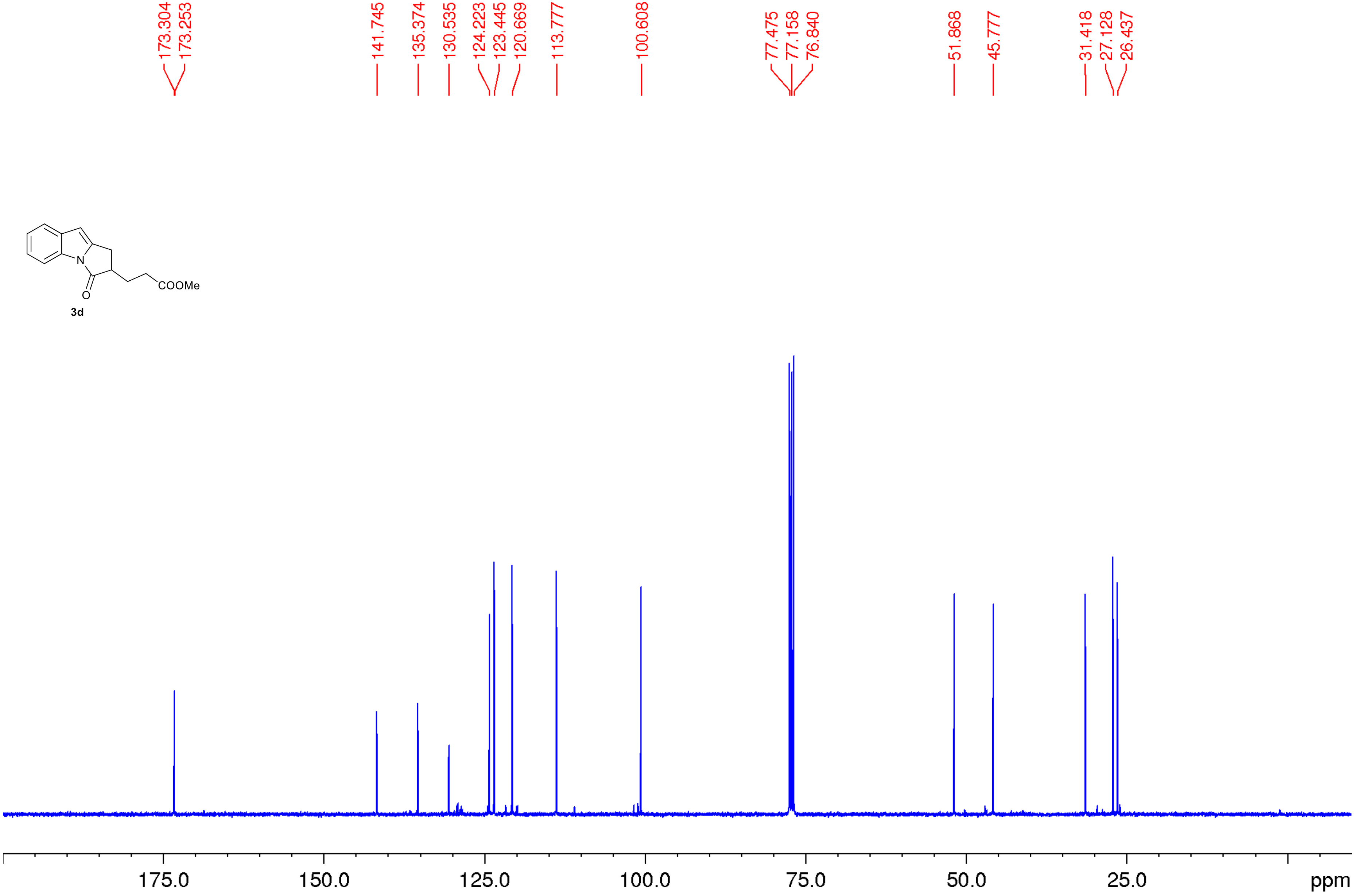
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

3d



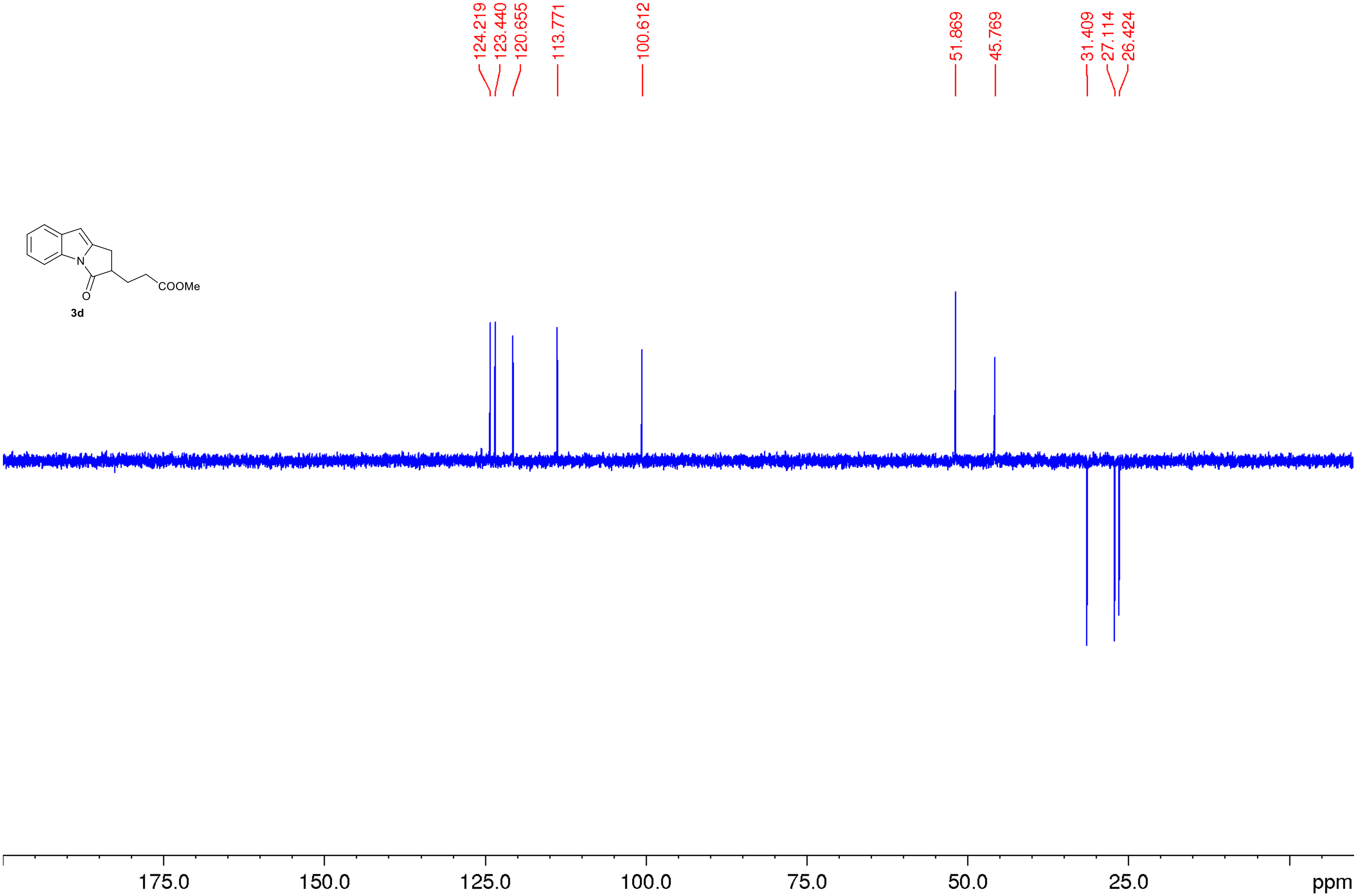
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

3d

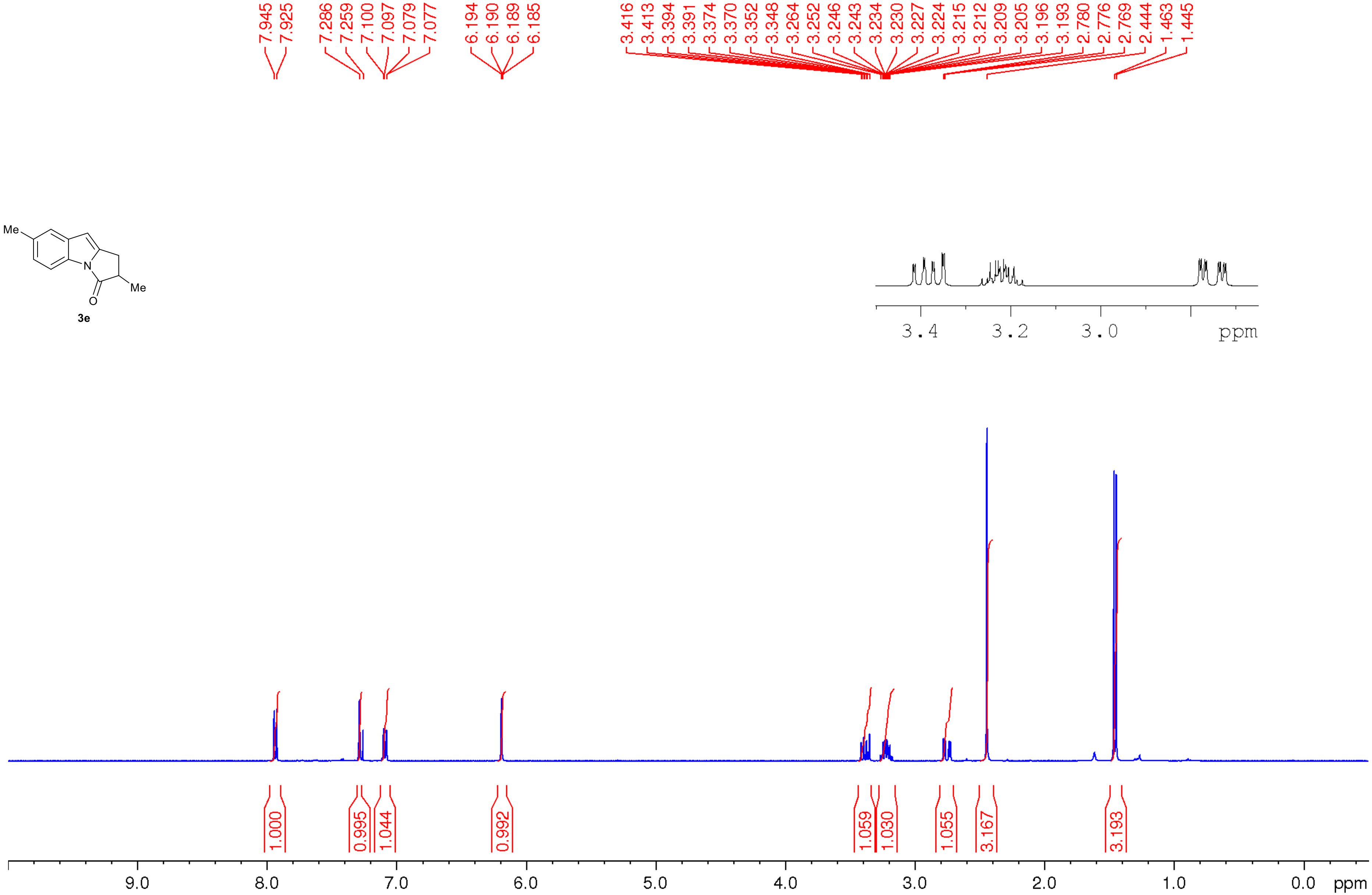


DEPT 135 NMR-spectrum ($CDCl_3$)

3d

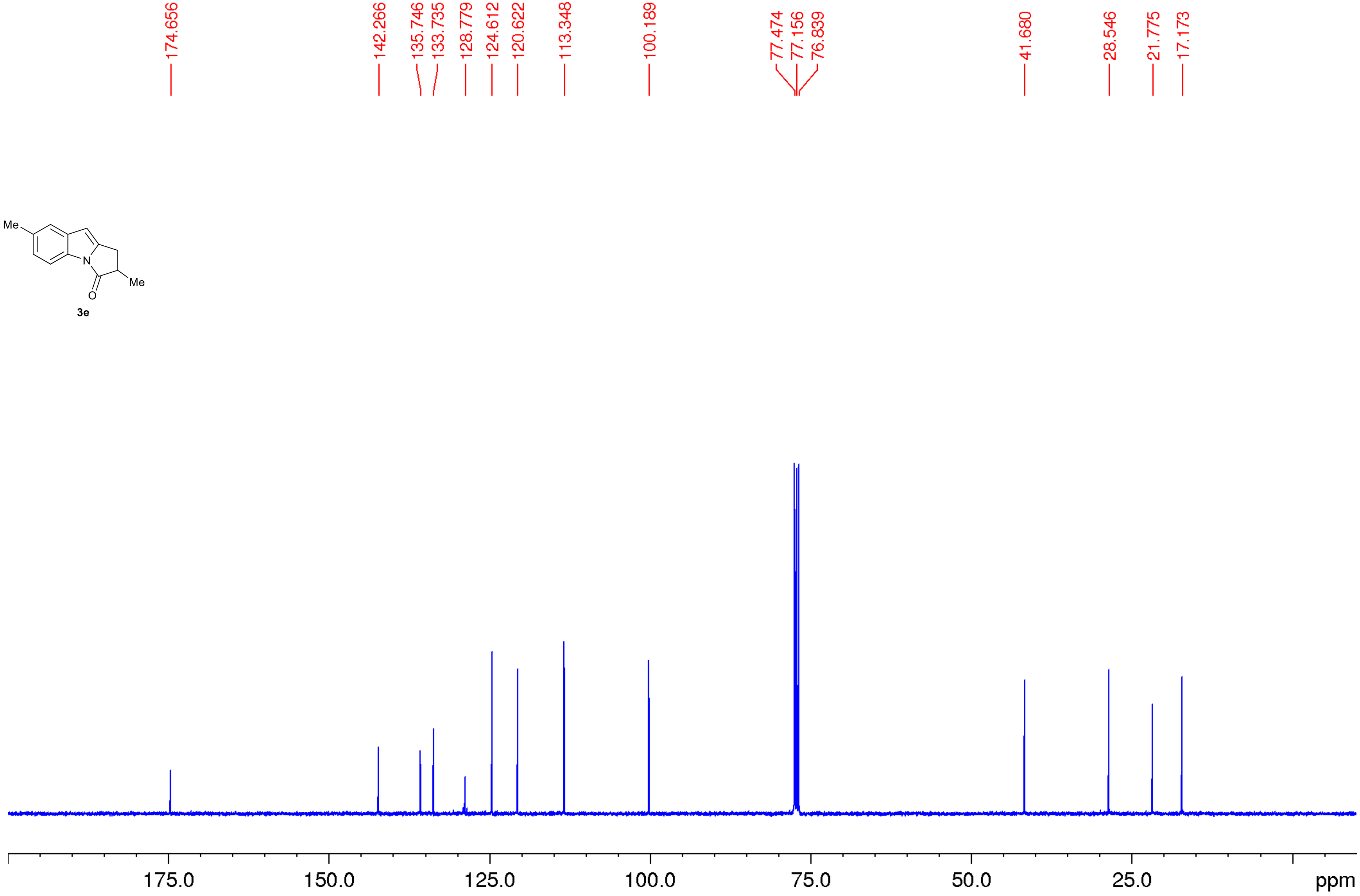


^1H NMR-spectrum (400 MHz, $CDCl_3$)



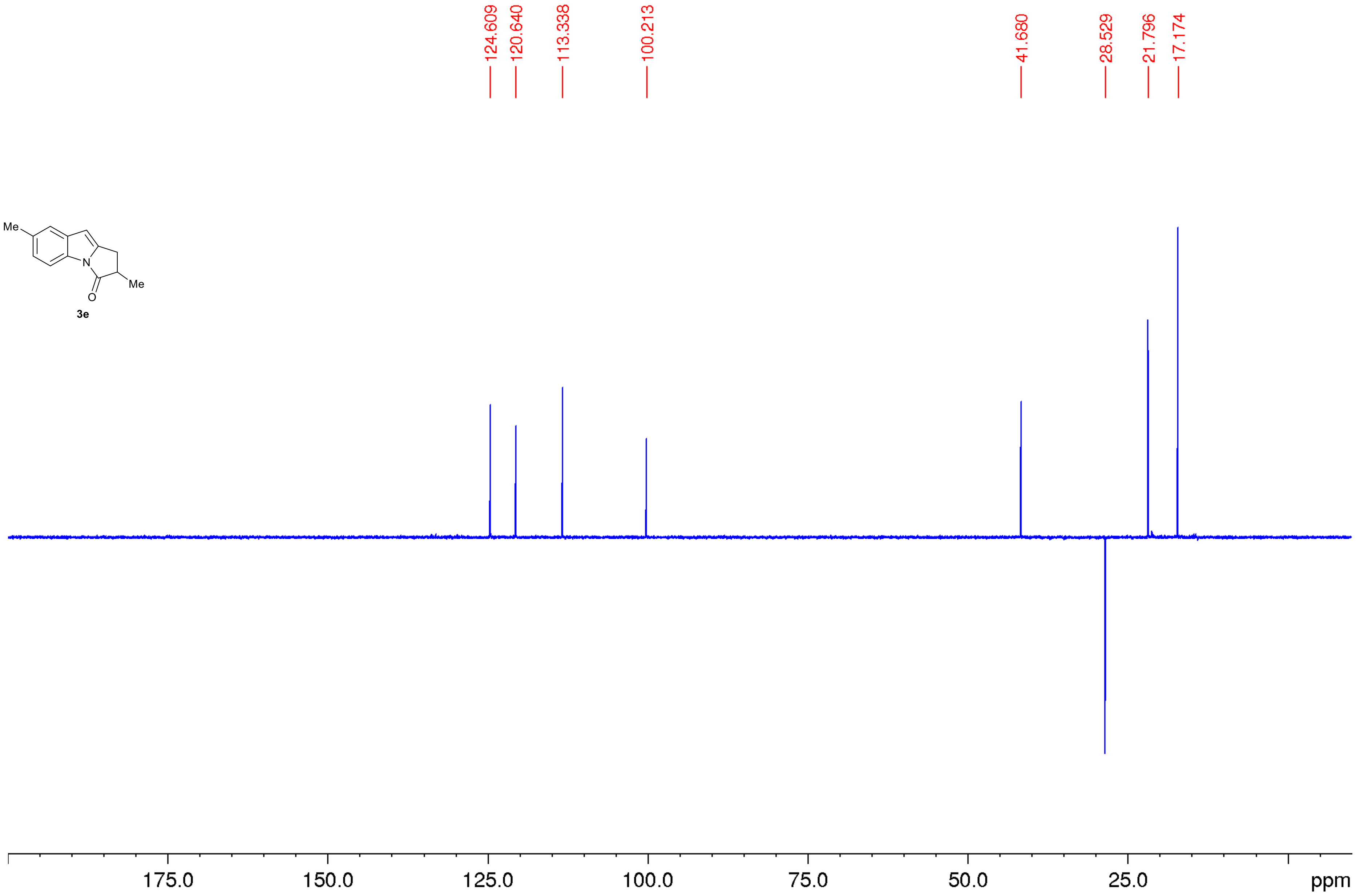
3e

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



3e

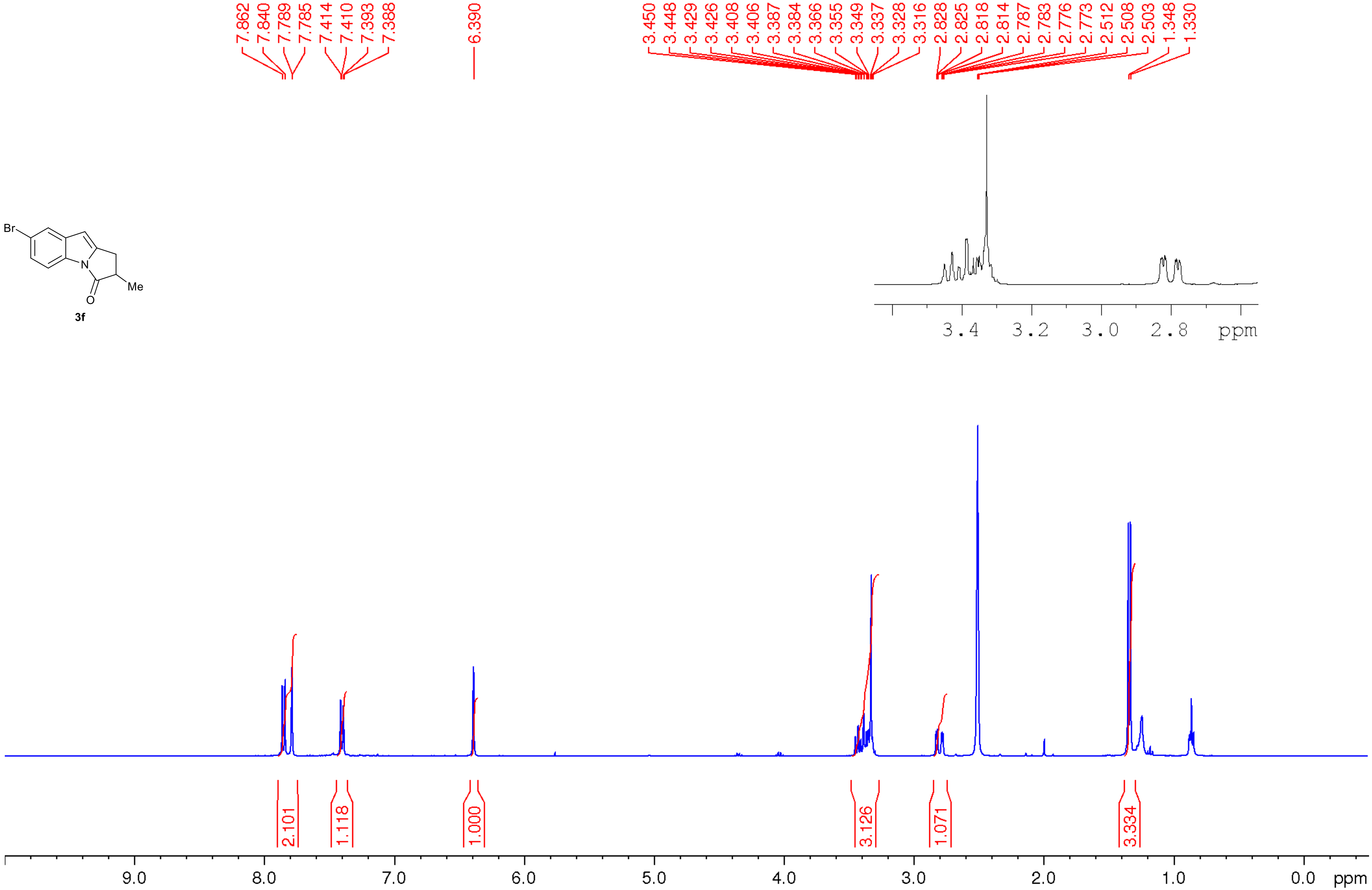
DEPT 135 NMR-spectrum ($CDCl_3$)



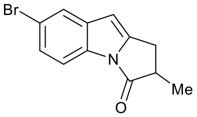
3e

^{1}H NMR-spectrum (400 MHz, DMSO-d_6)

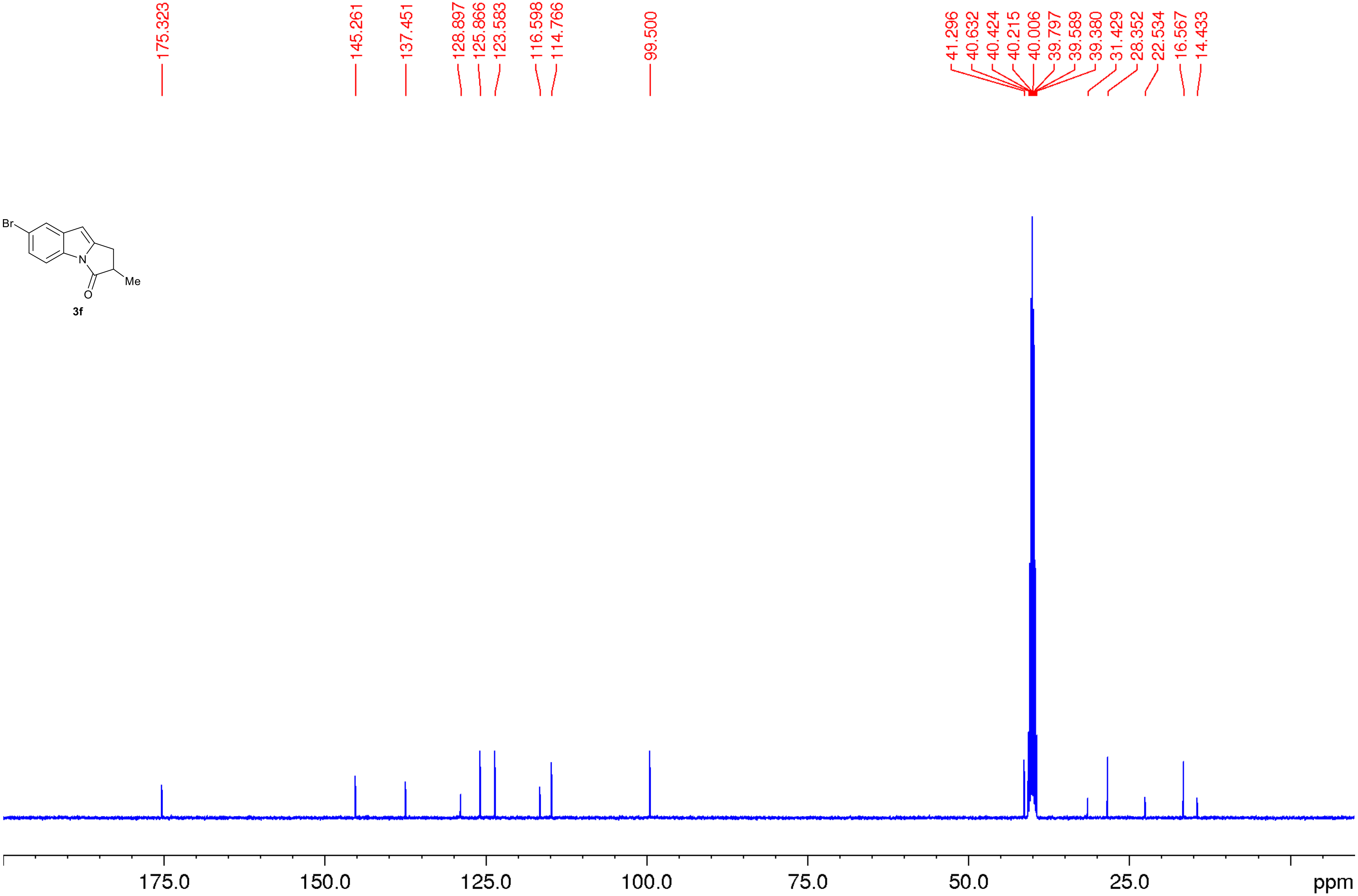
3f



^{13}C NMR-spectrum (100 MHz, DMSO-d_6)

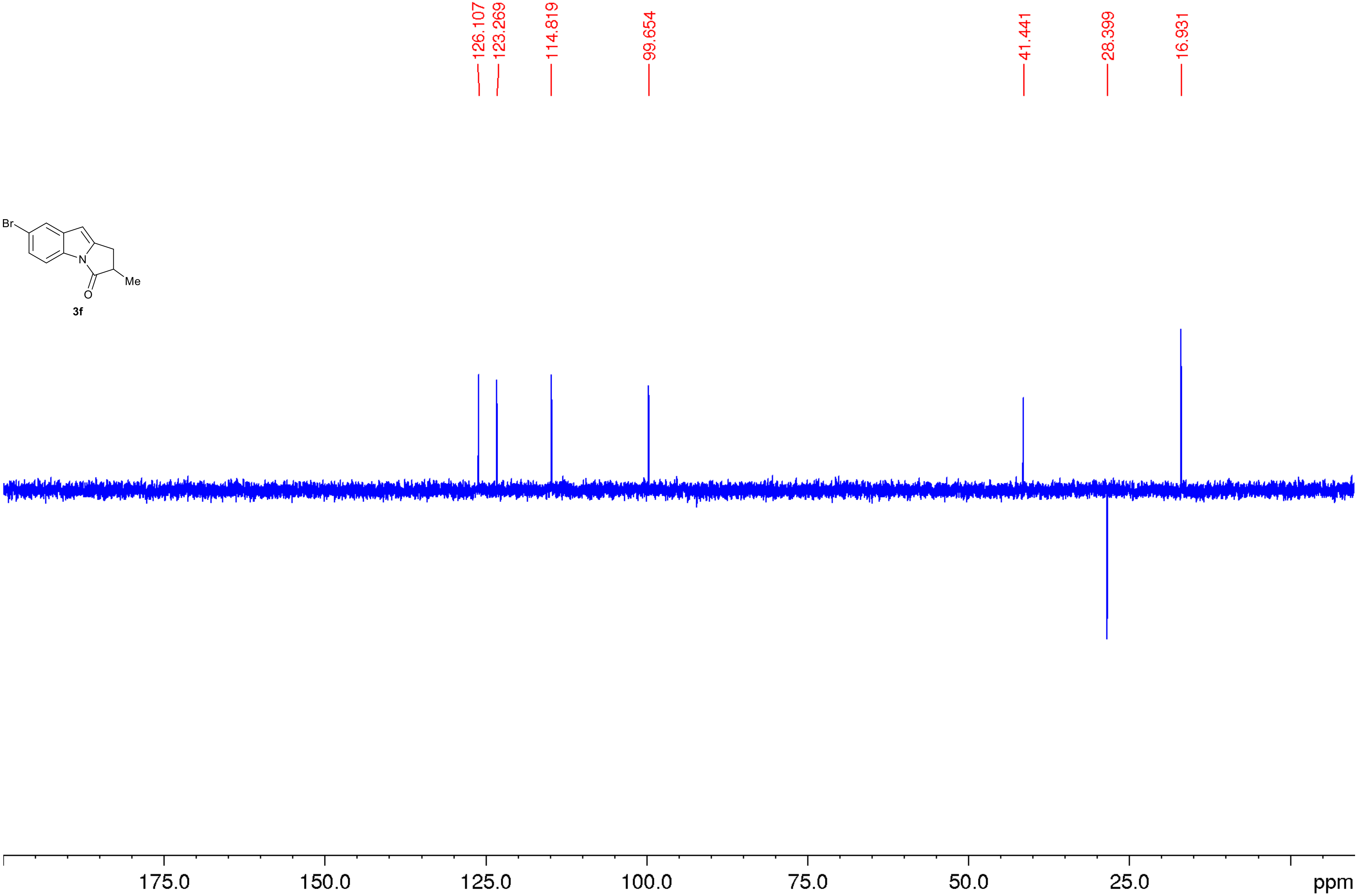


3f

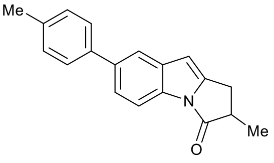


DEPT 135 NMR-spectrum (DMSO-d_6)

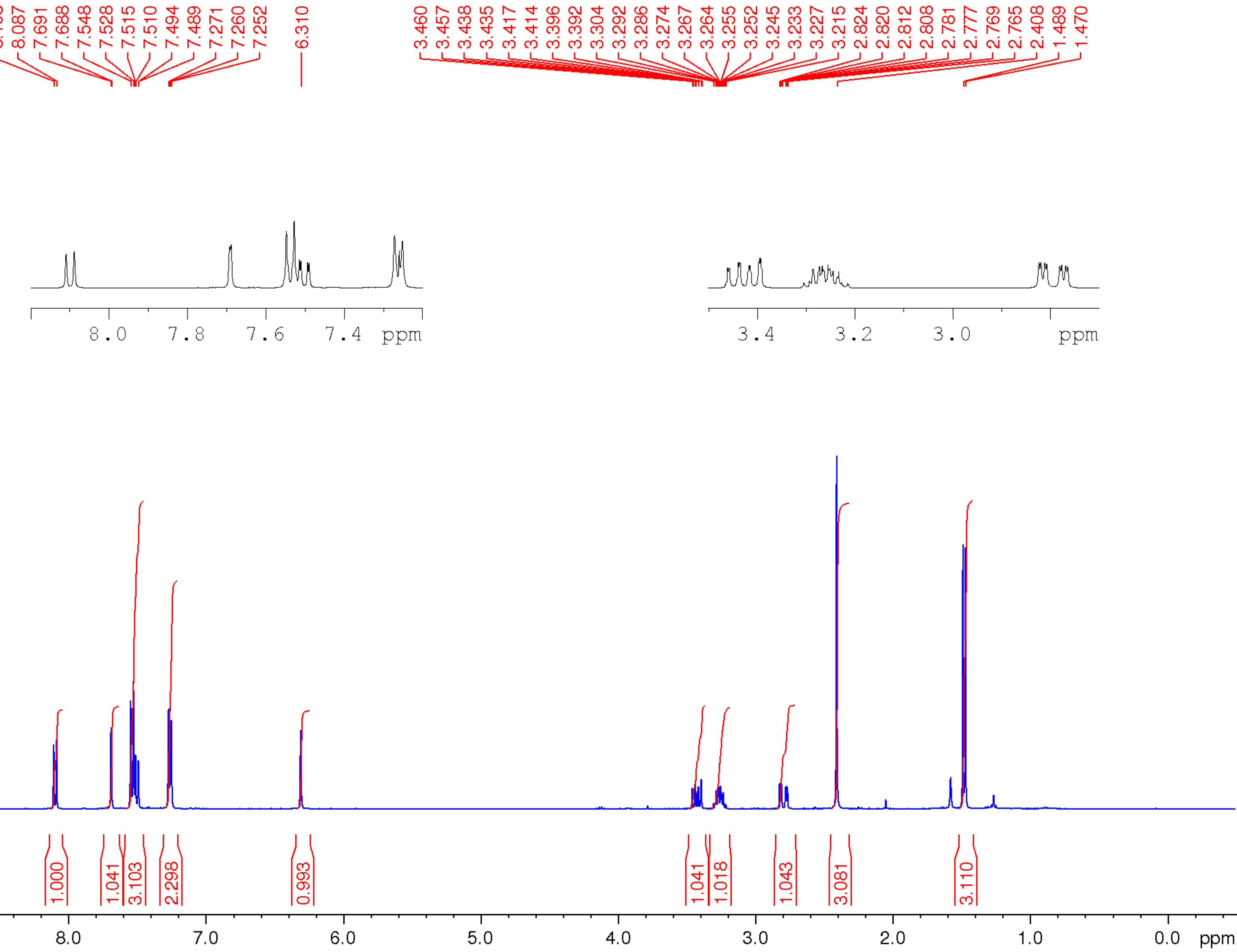
3f



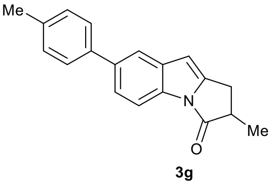
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



3g



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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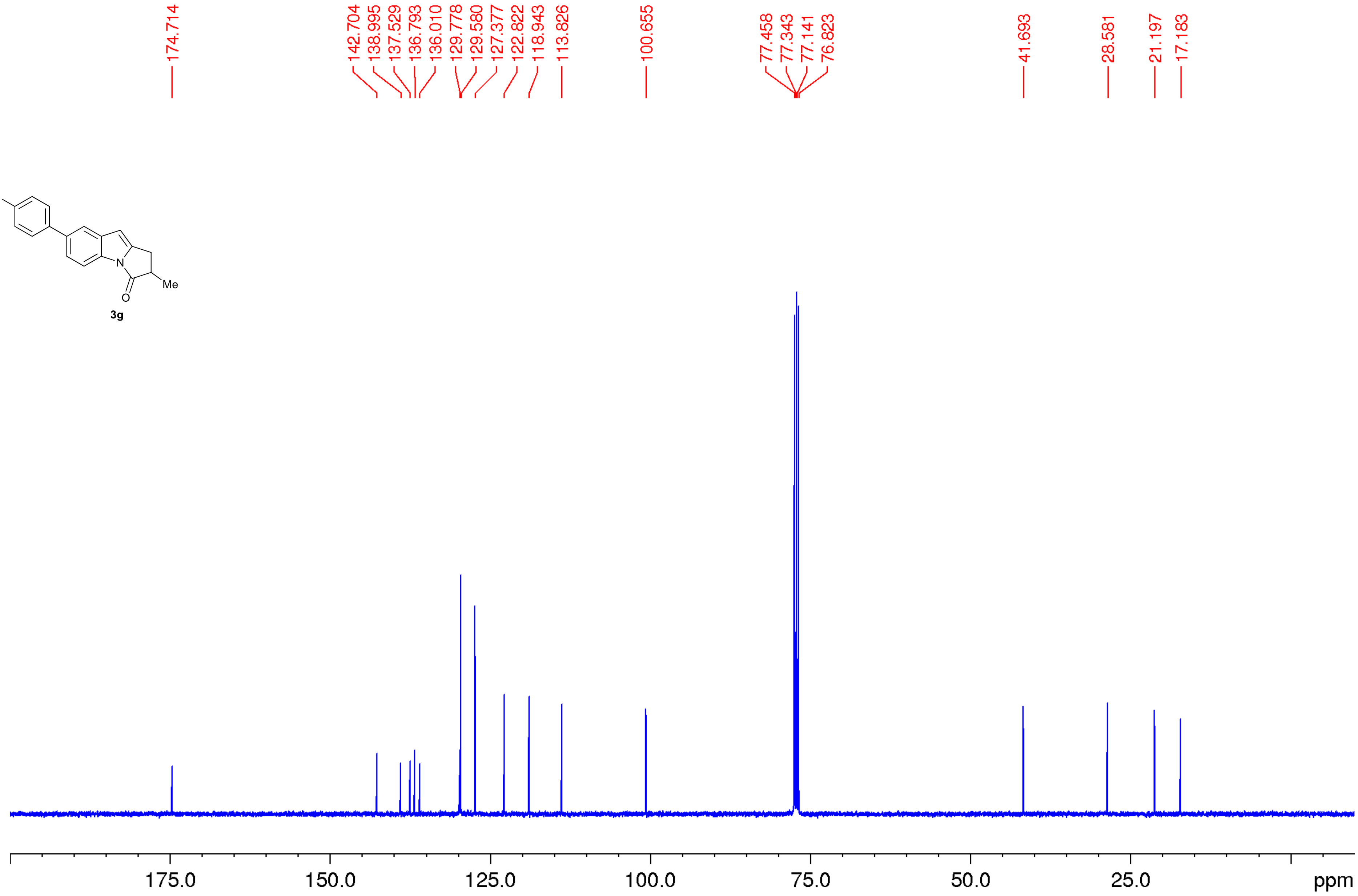
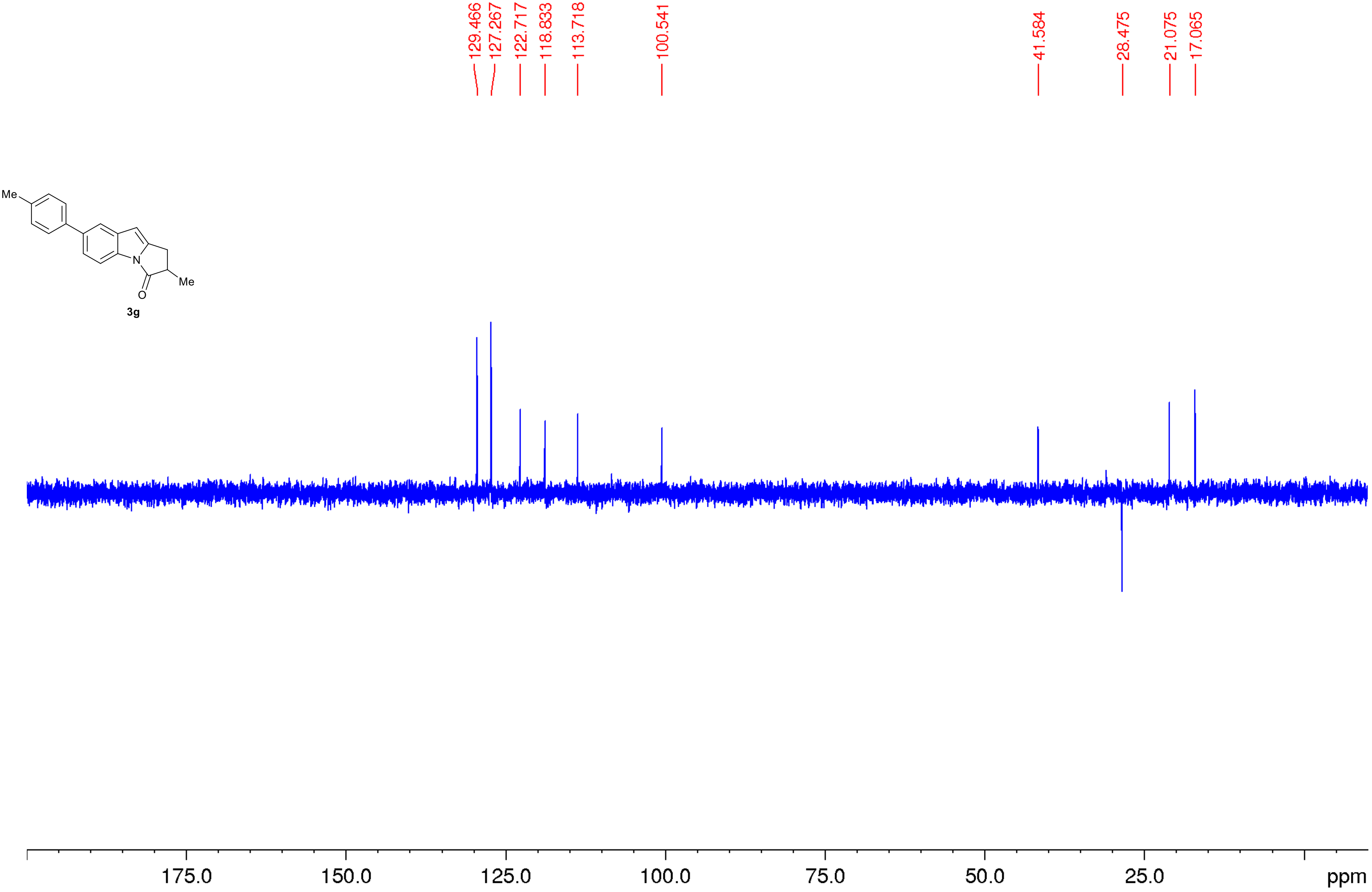
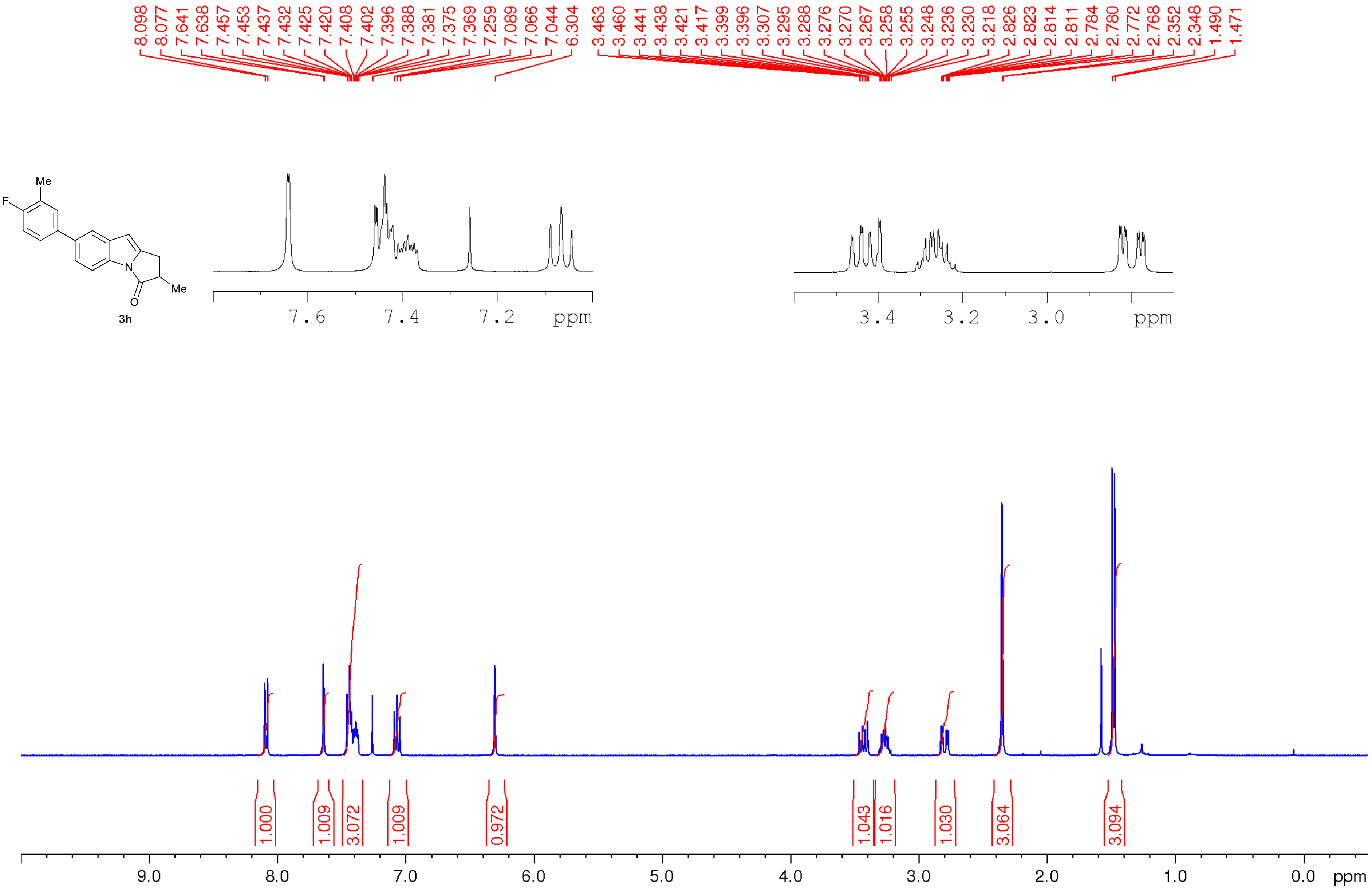


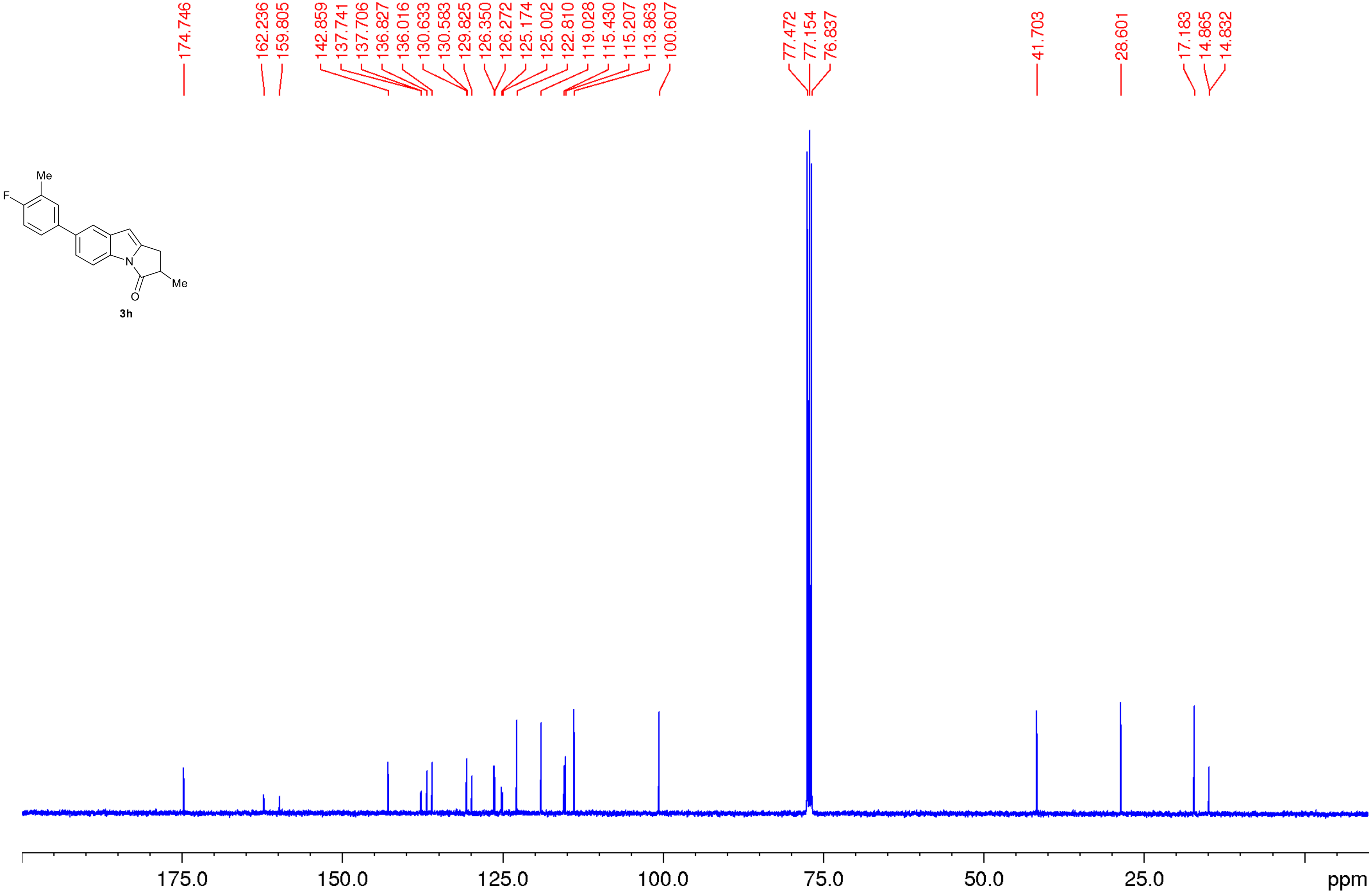
DEPT 135 NMR-spectrum (CDCl$_3$)



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



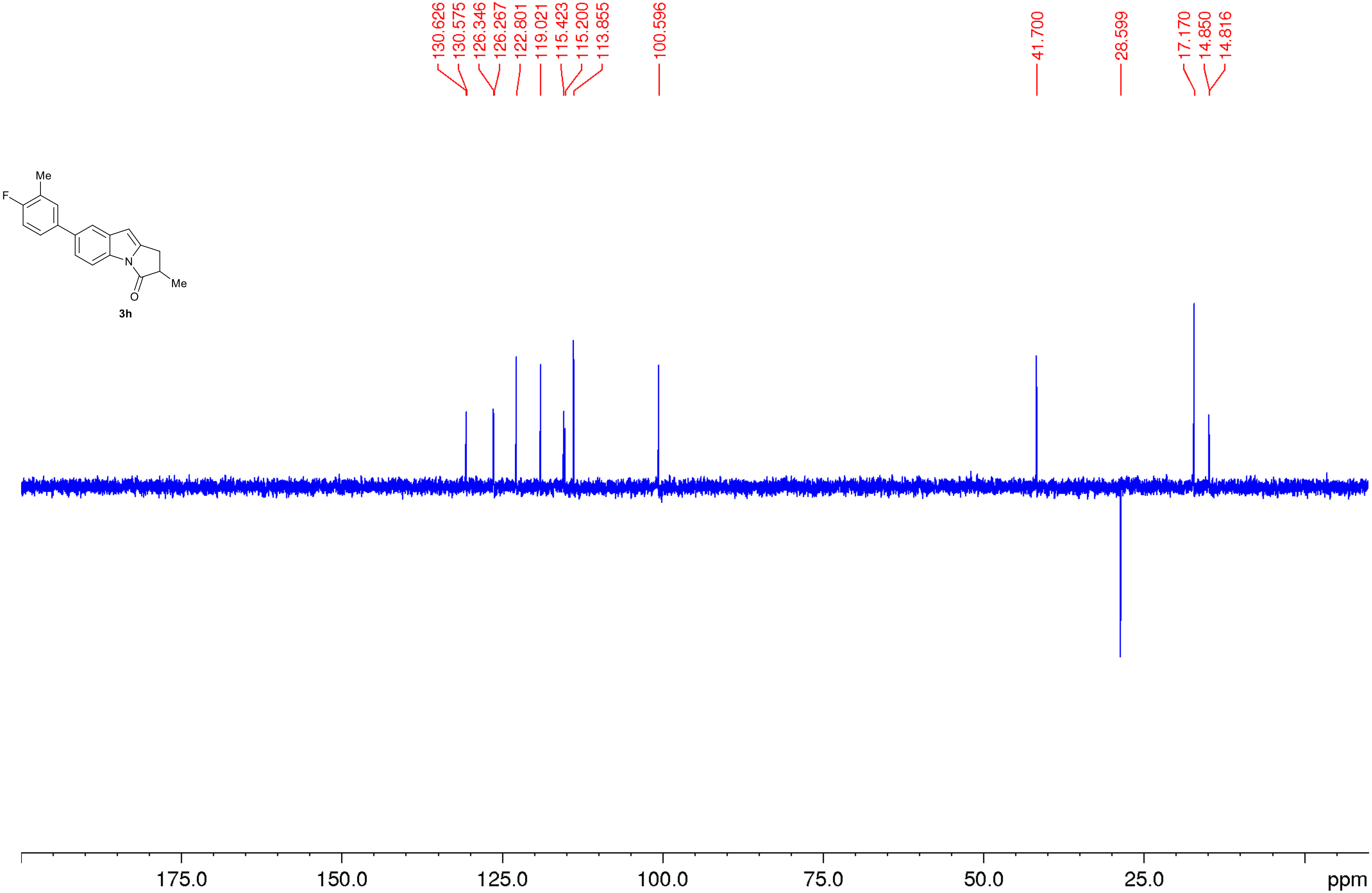
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



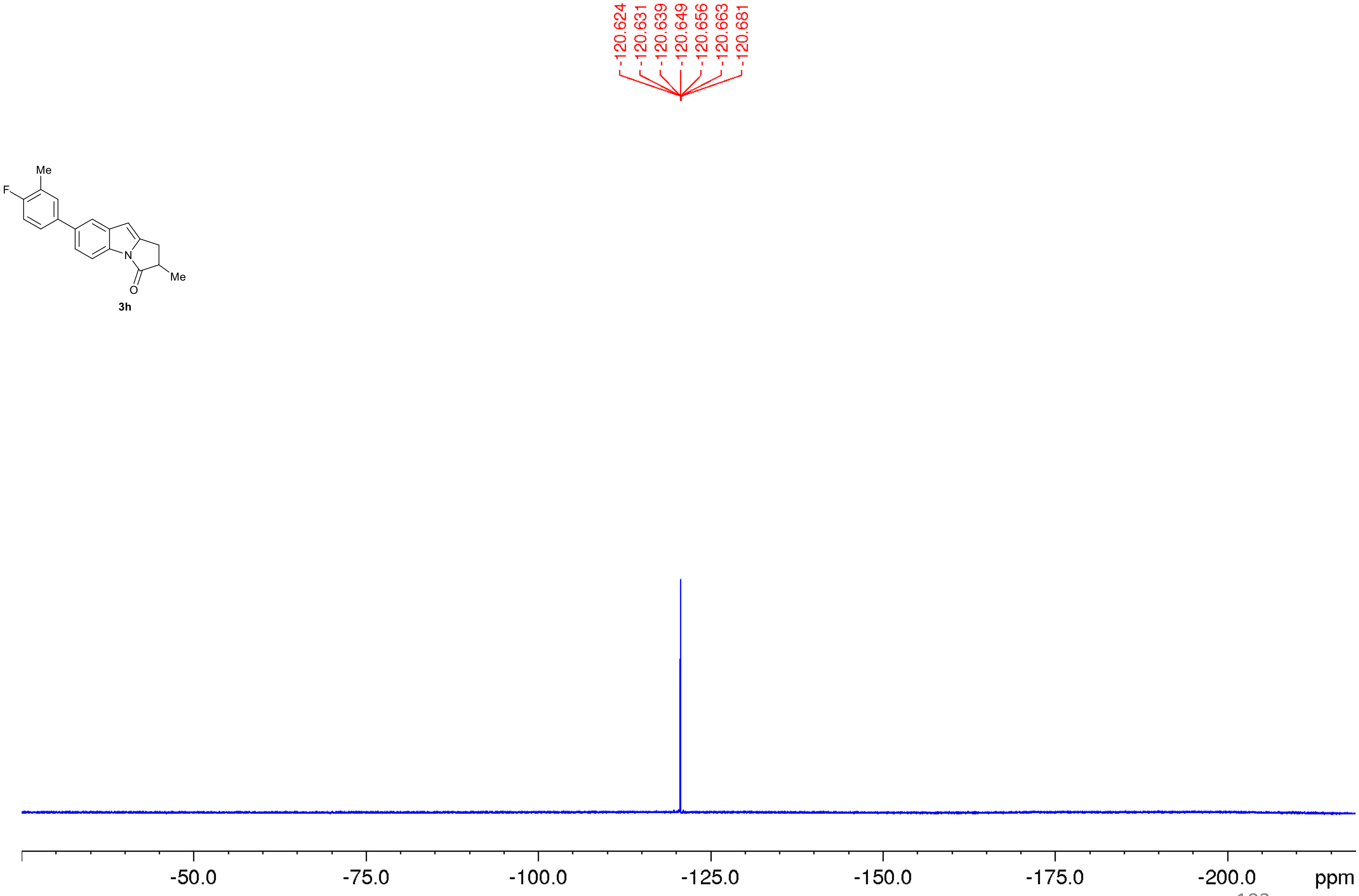
3h

DEPT 135 NMR-spectrum ($CDCl_3$)

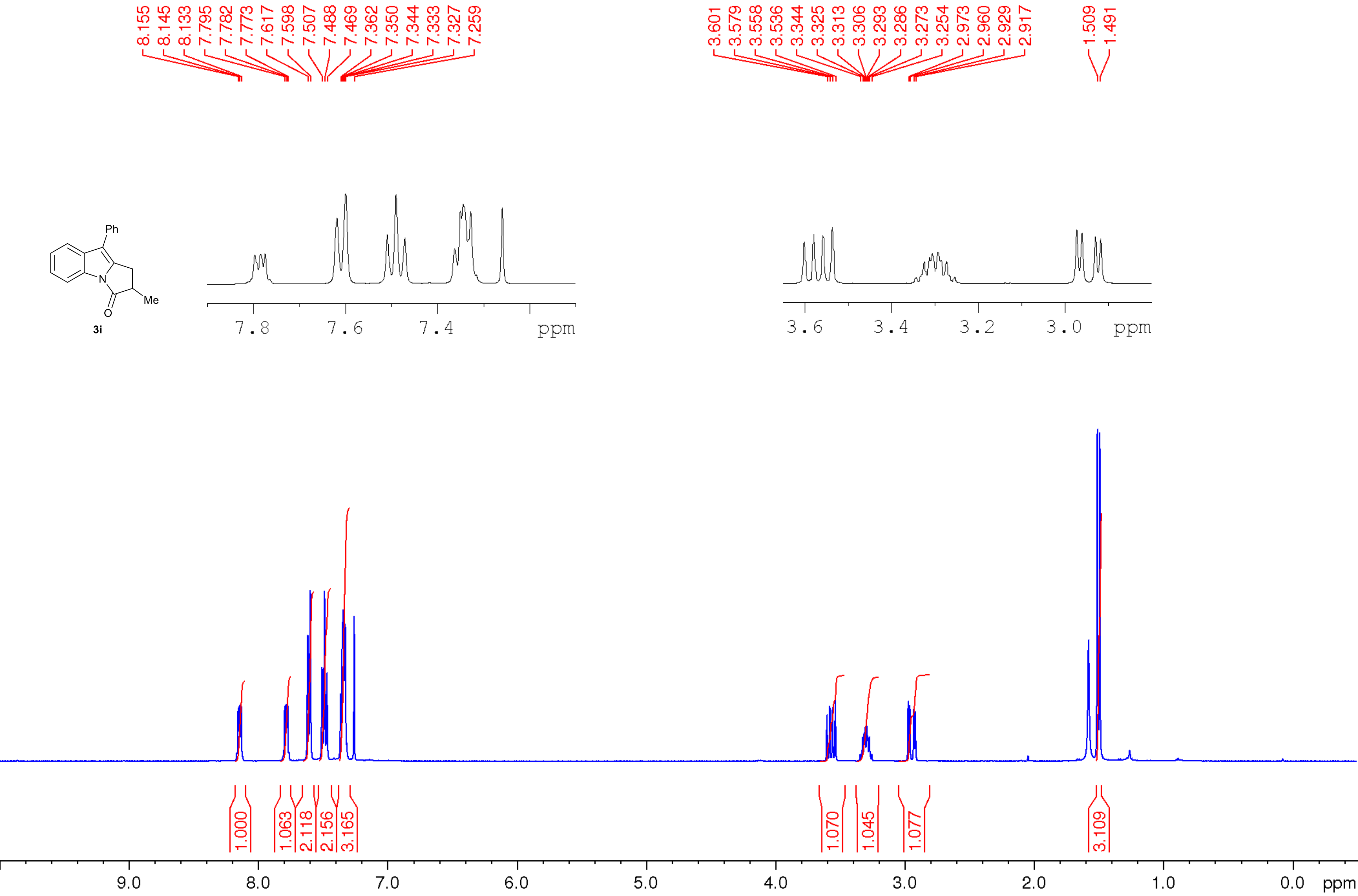
3h



^{19}F NMR-spectrum (376.5 MHz, $CDCl_3$)



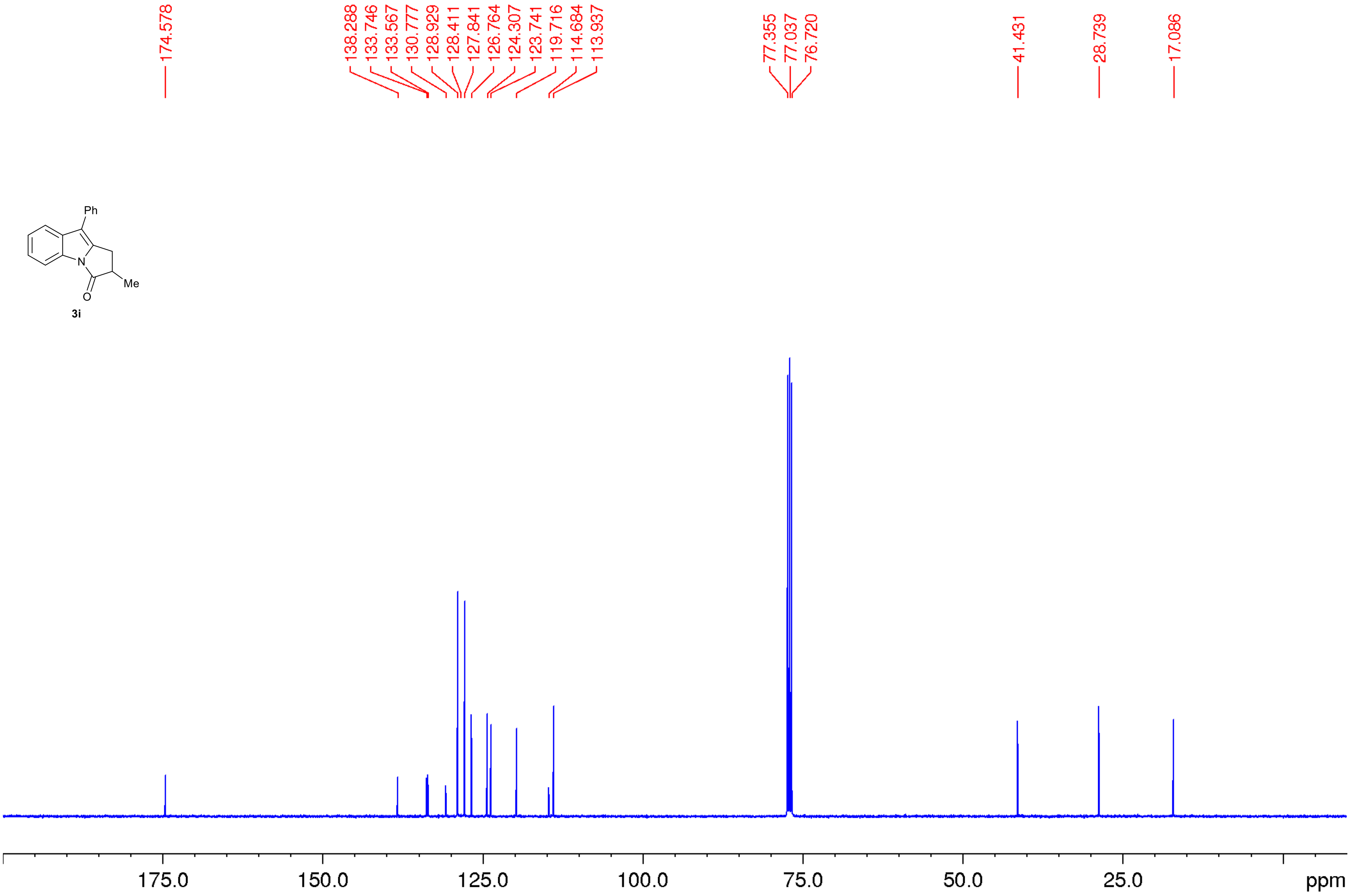
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



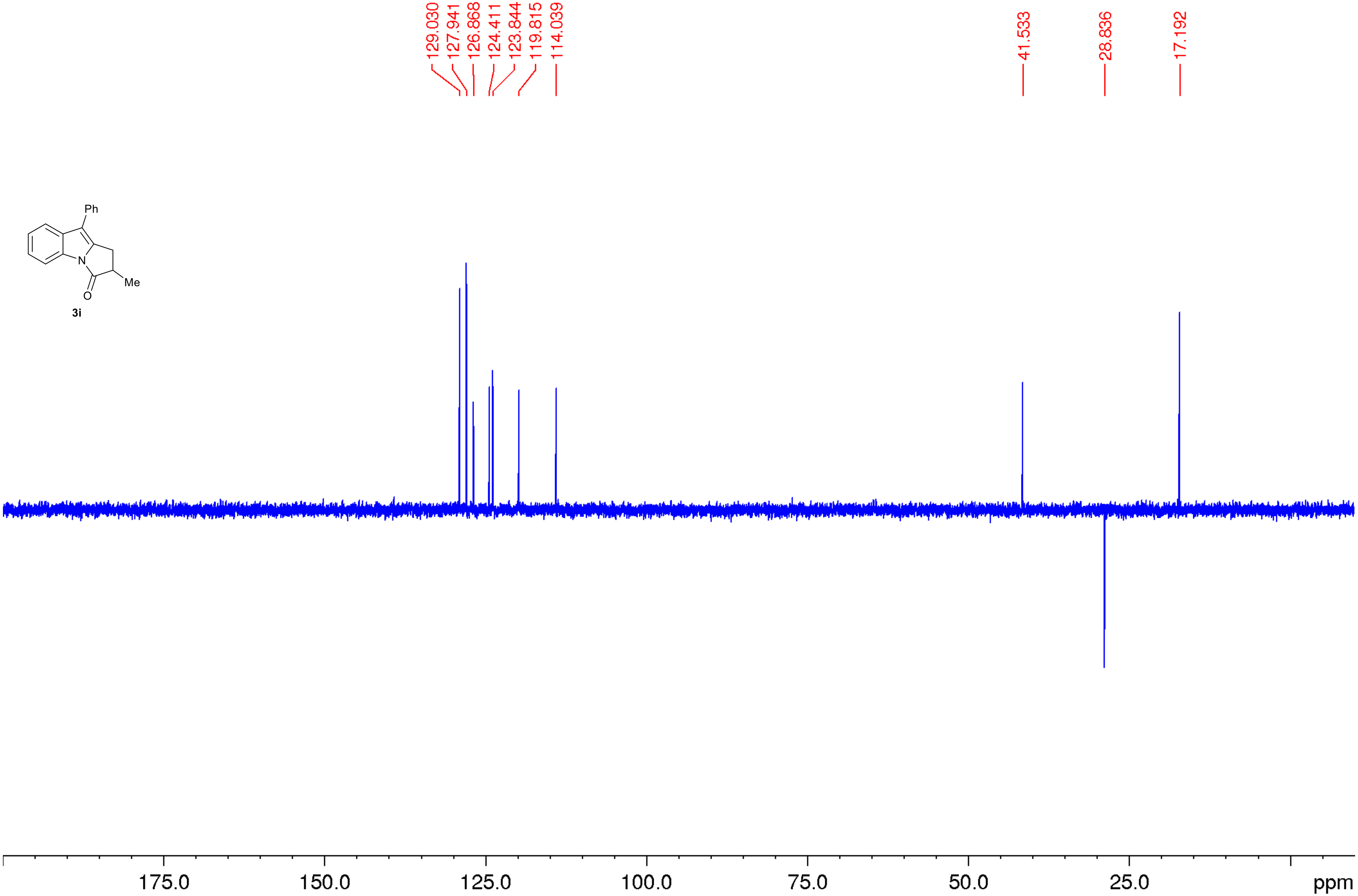
3i

^{13}C NMR-spectrum (100 MHz, CDCl$_3$)

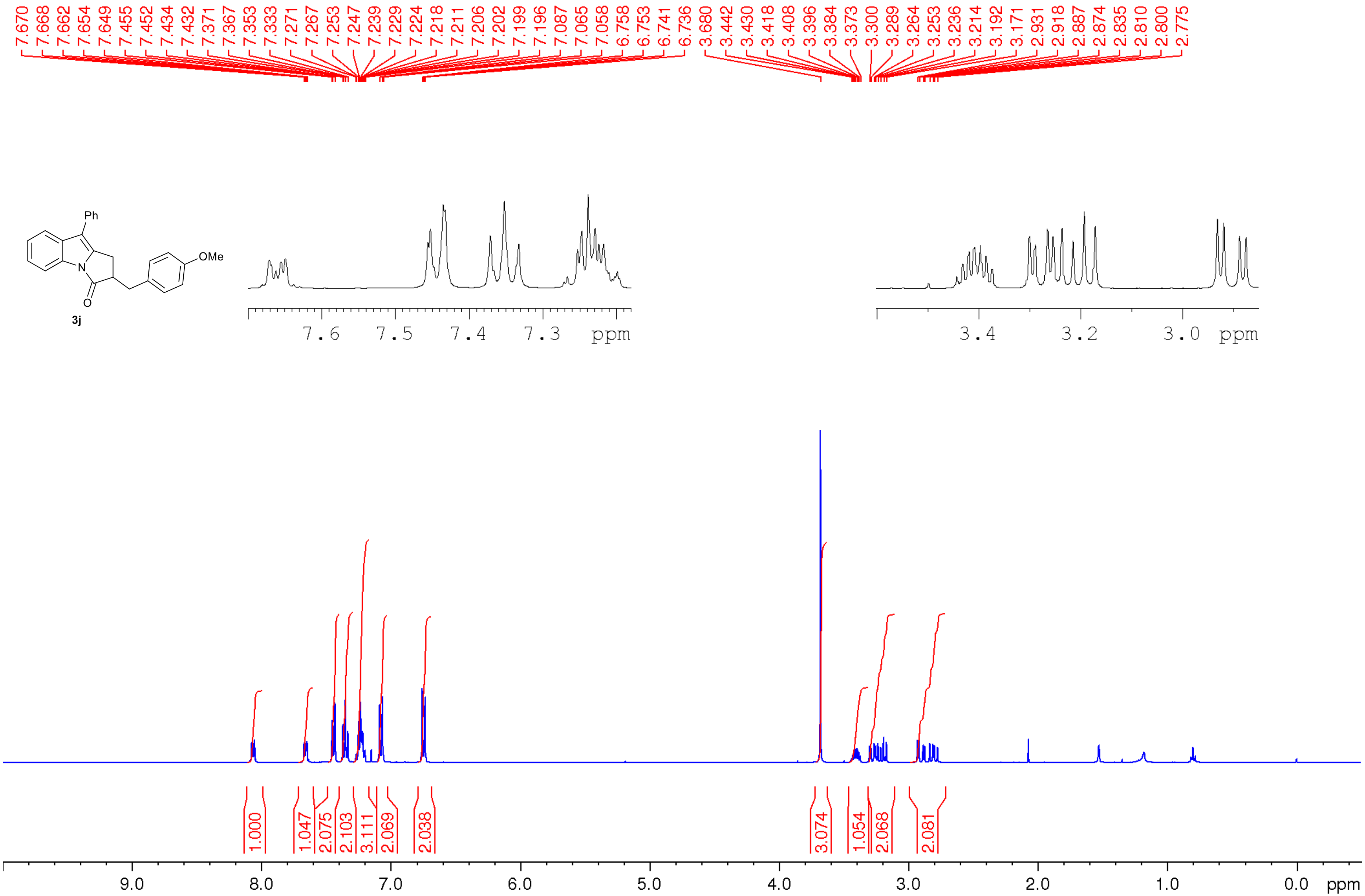
3i



DEPT 135 NMR-spectrum ($CDCl_3$)

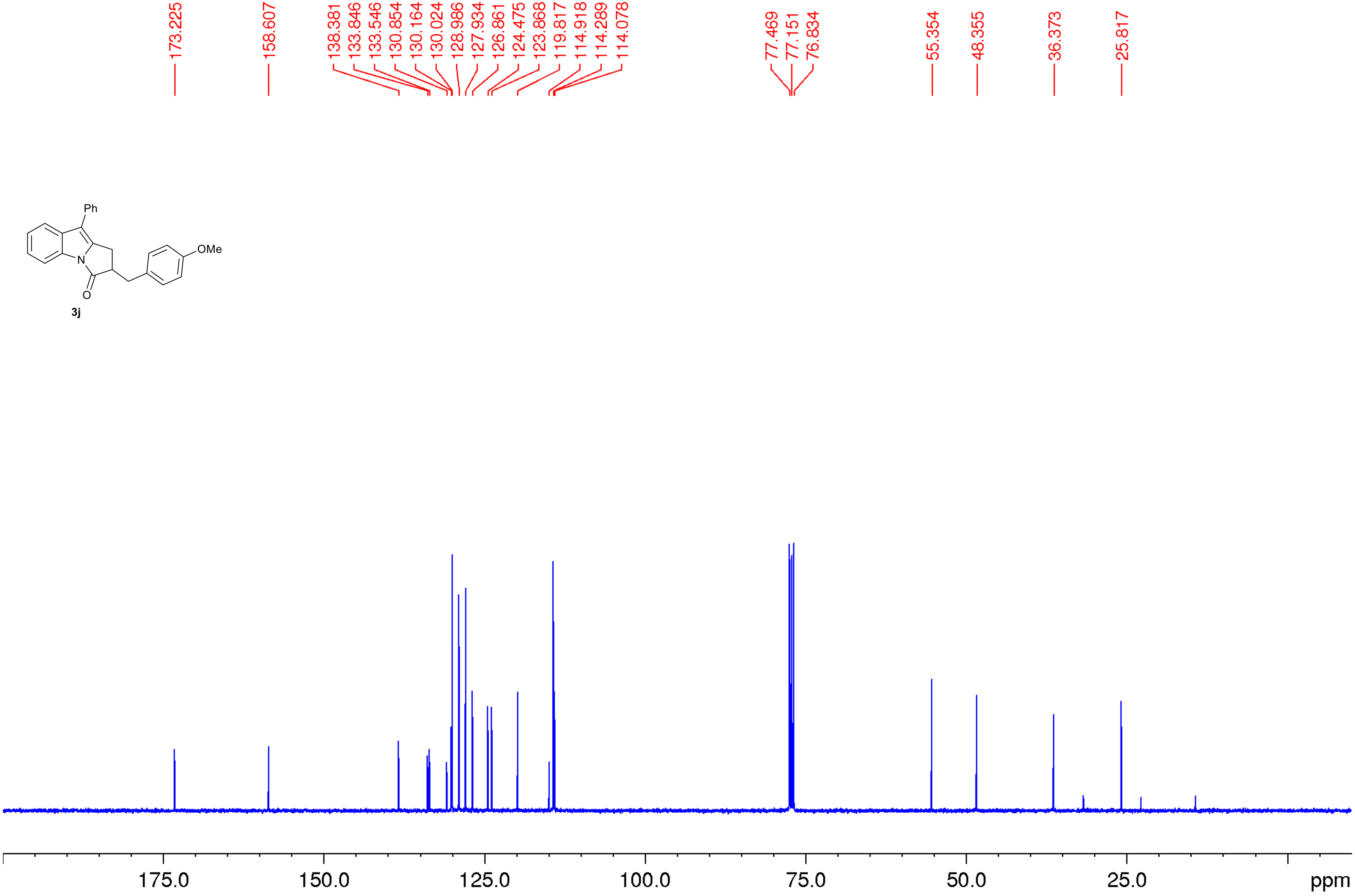

3i

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



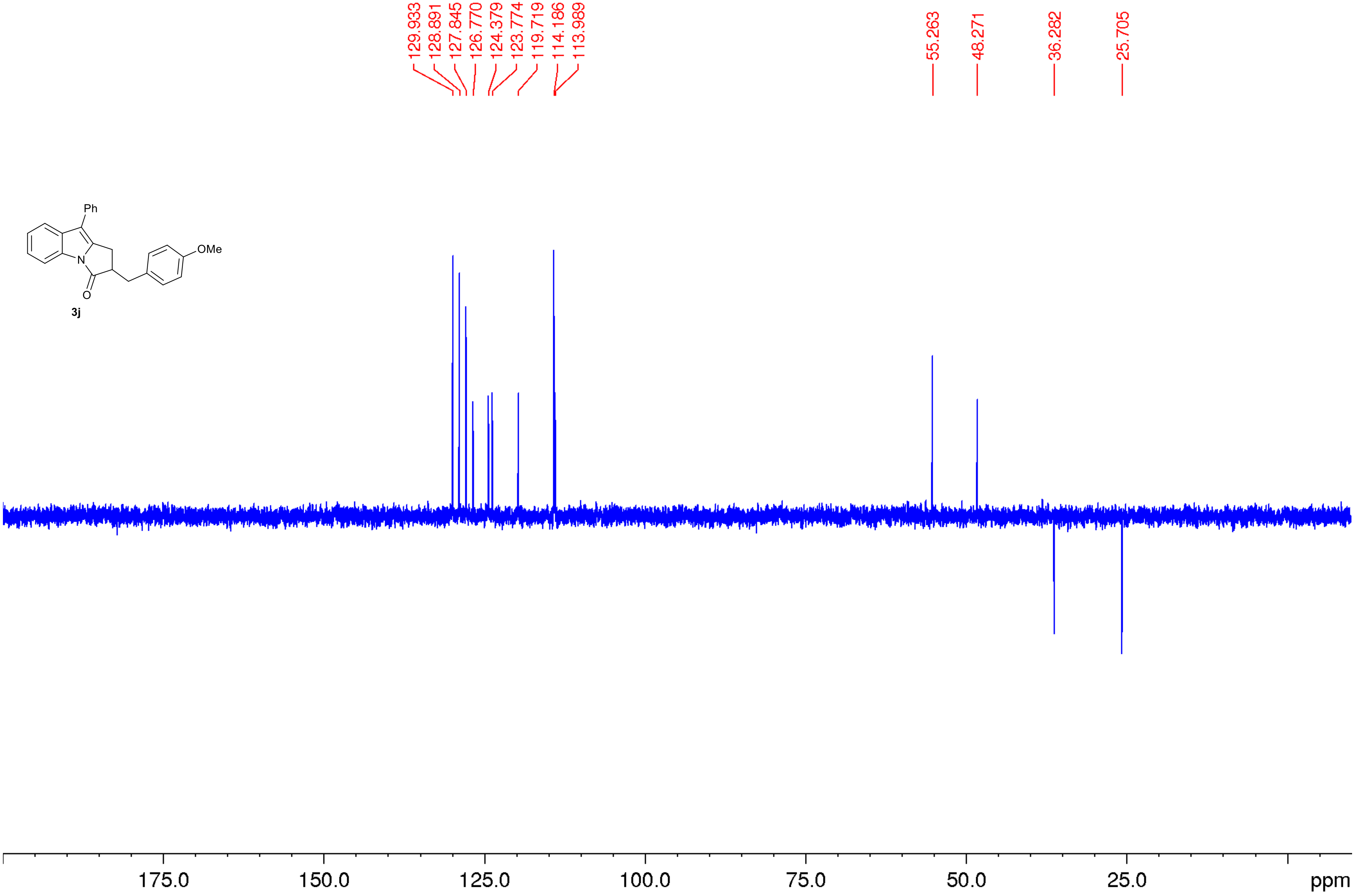
3j

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



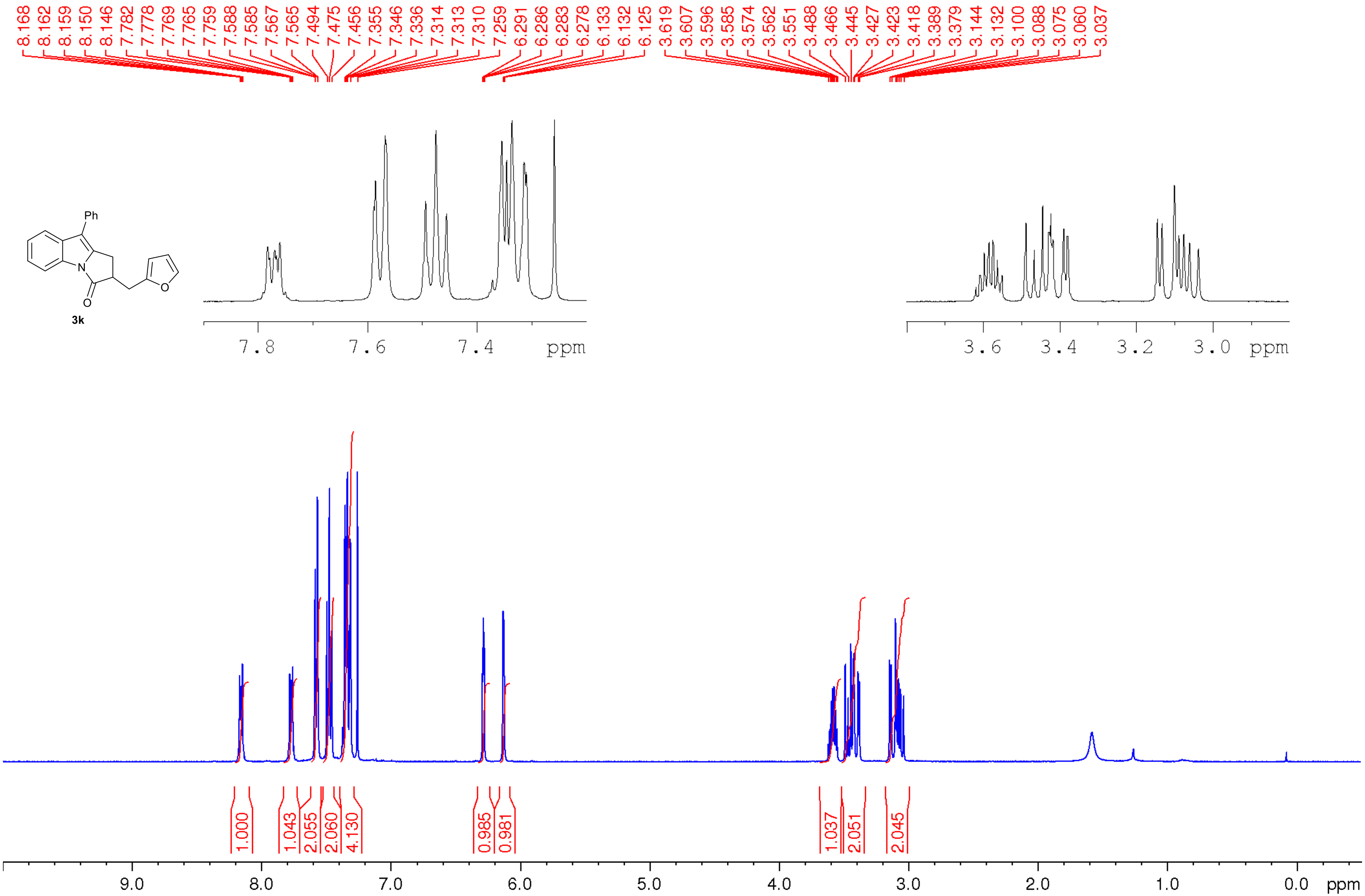
3j

DEPT 135 NMR-spectrum ($CDCl_3$)

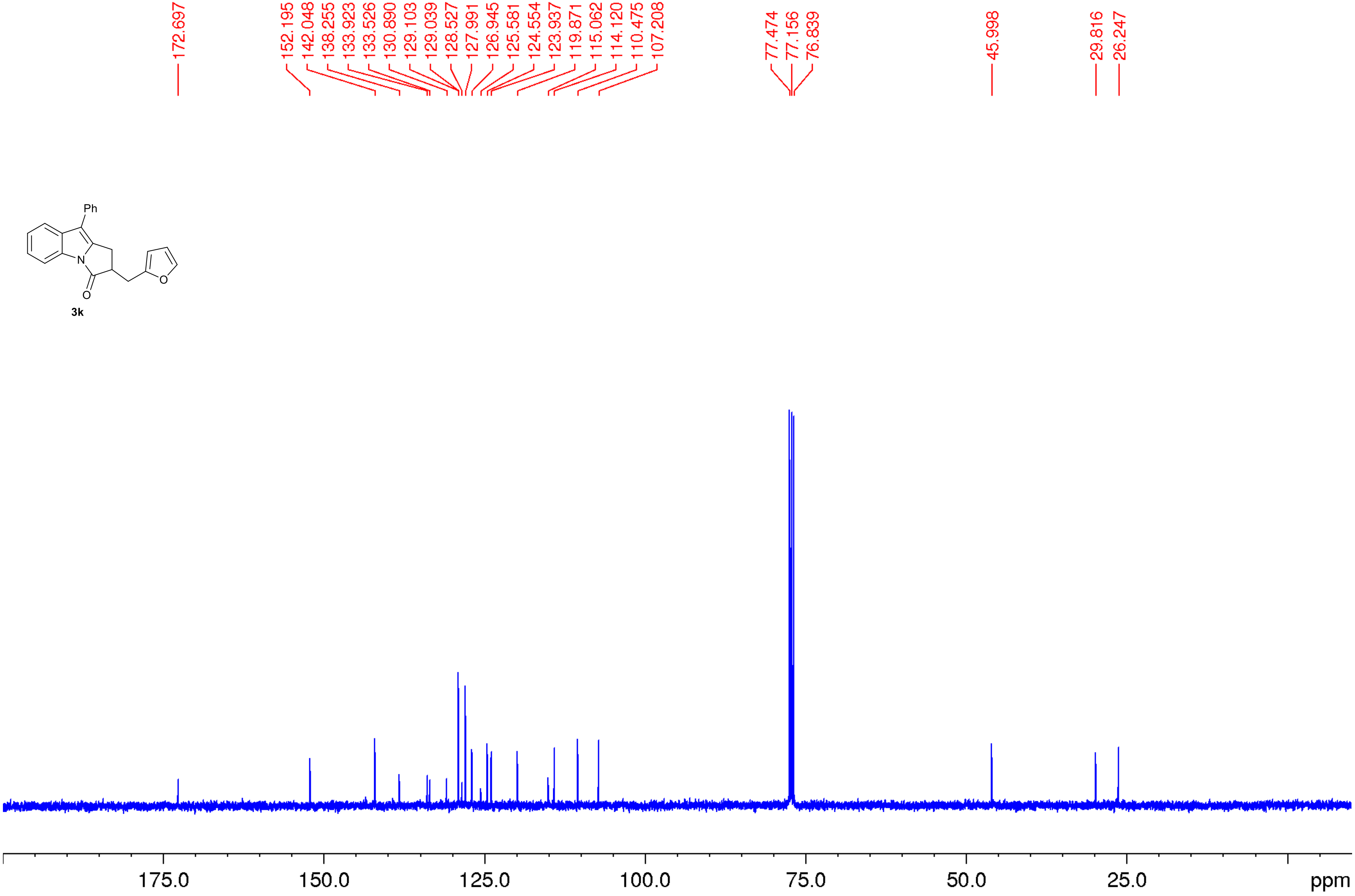


3j

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

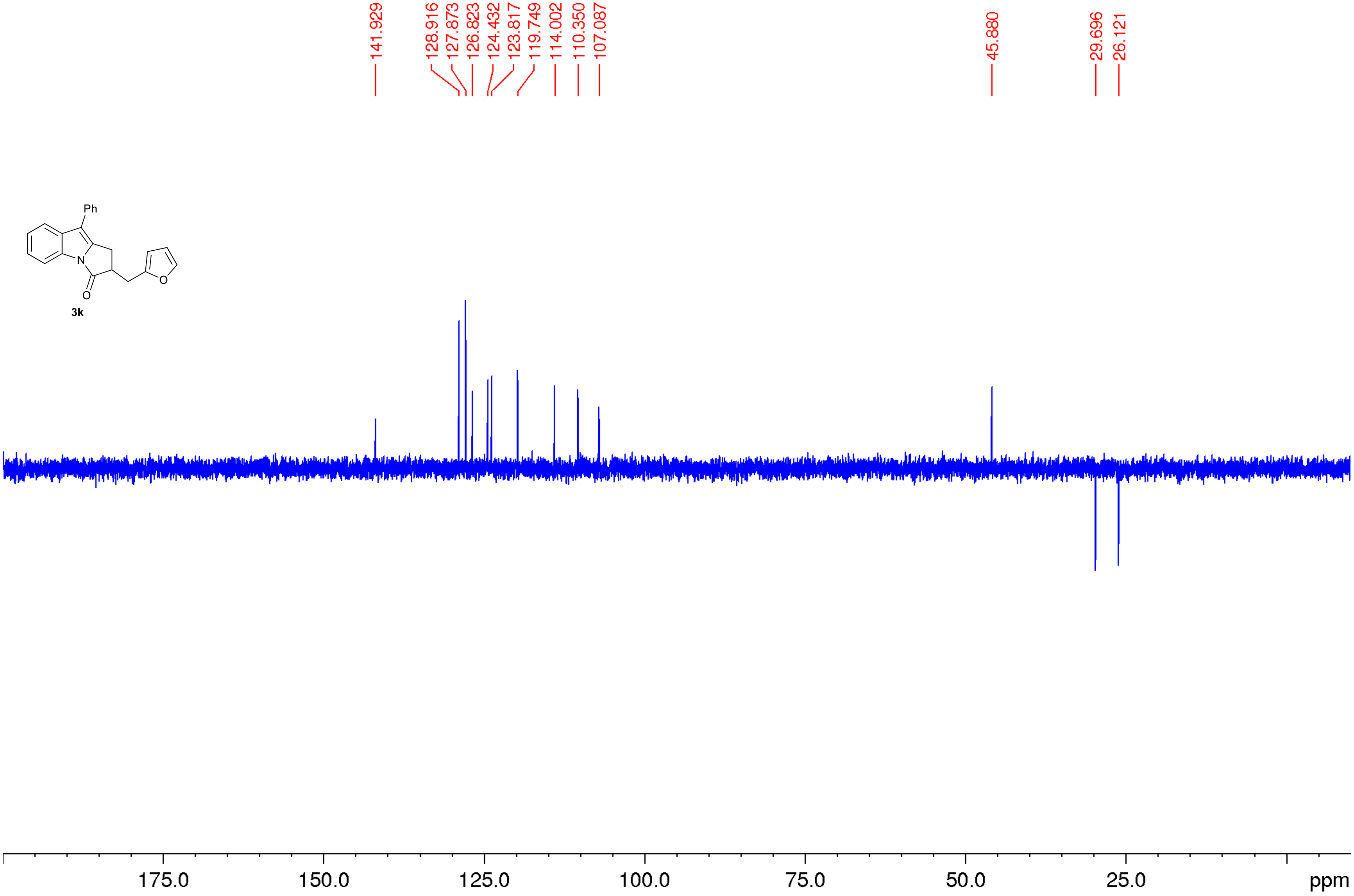


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

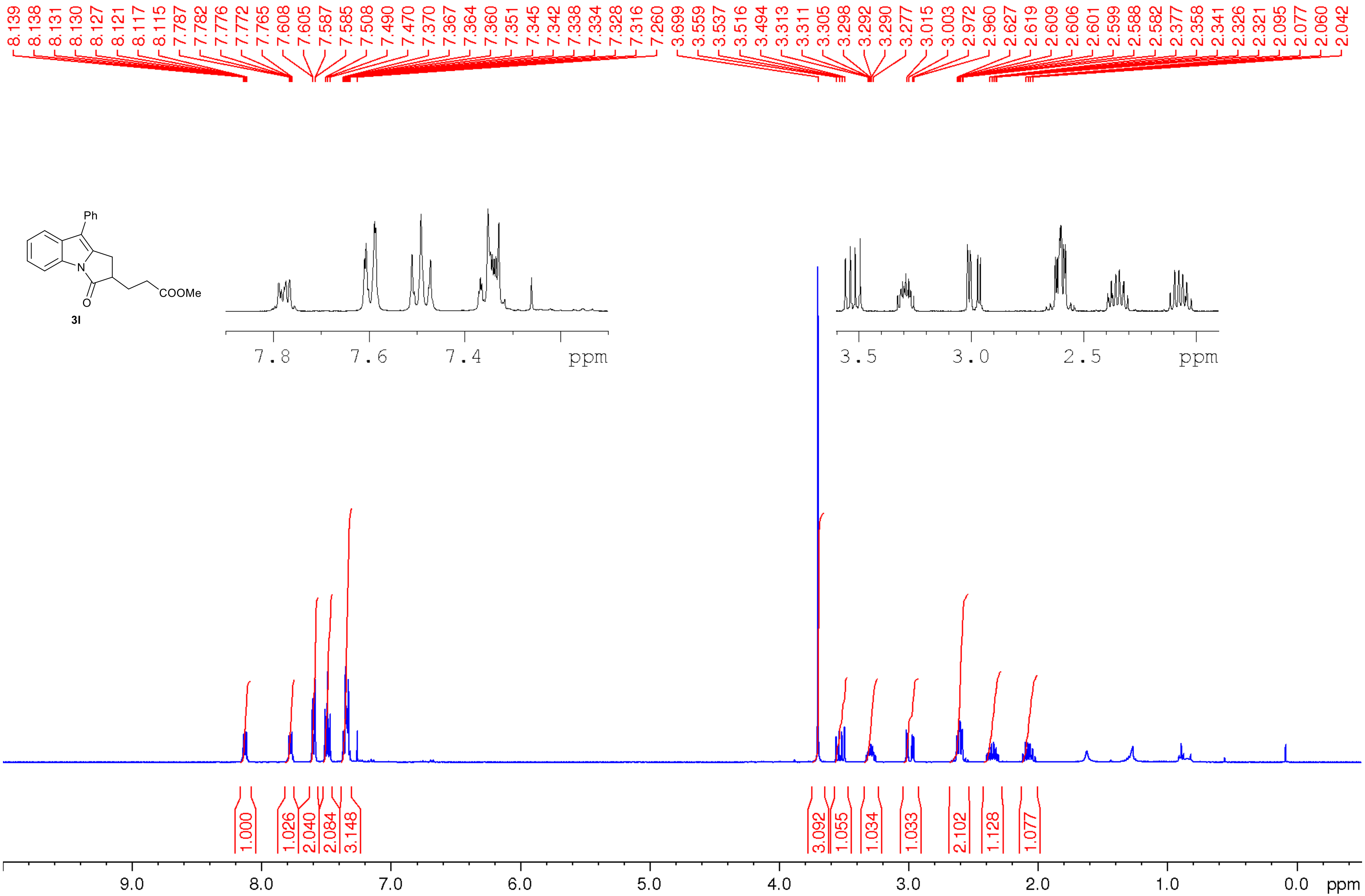


3k

DEPT 135 NMR-spectrum ($CDCl_3$)



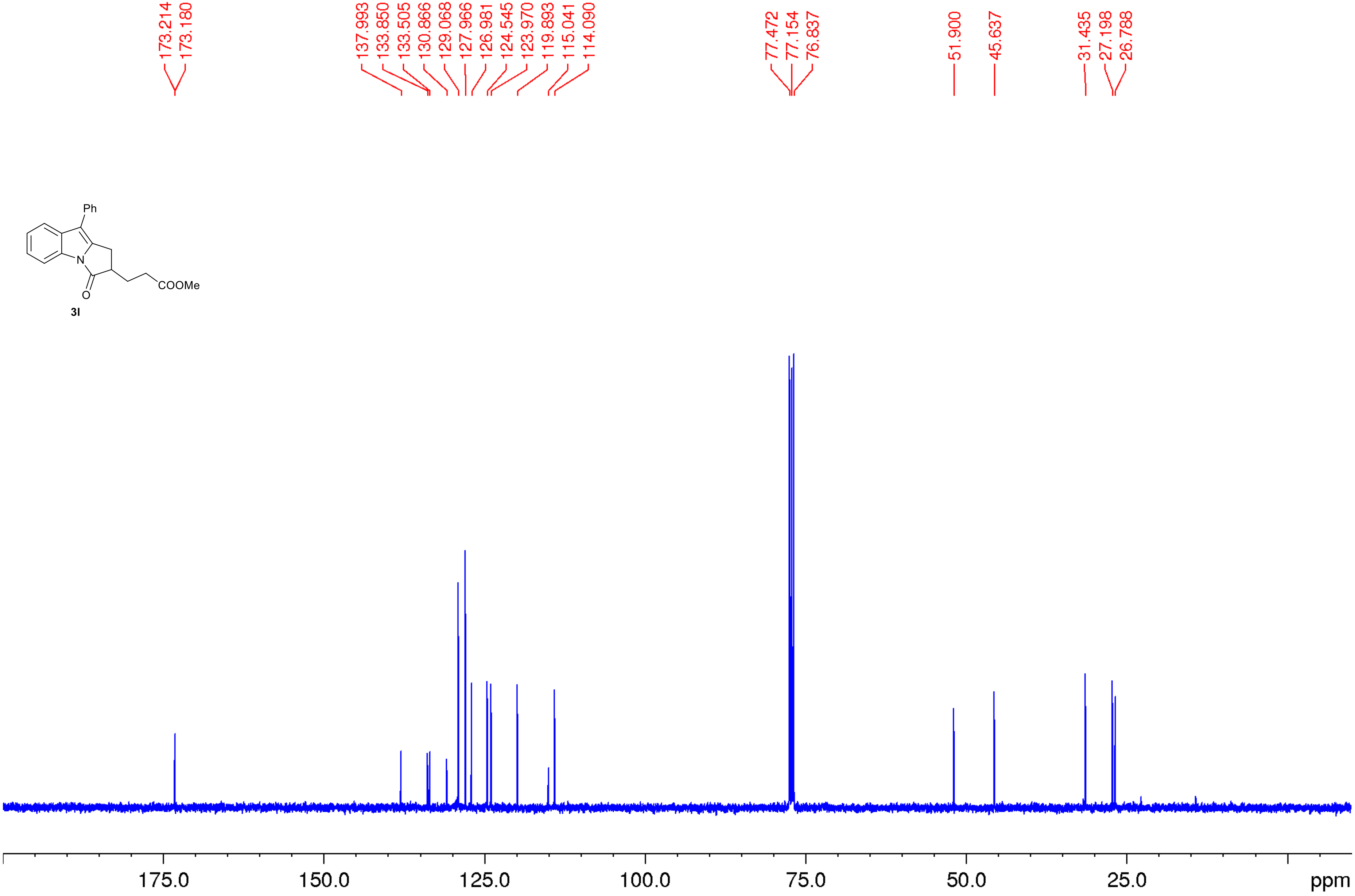
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



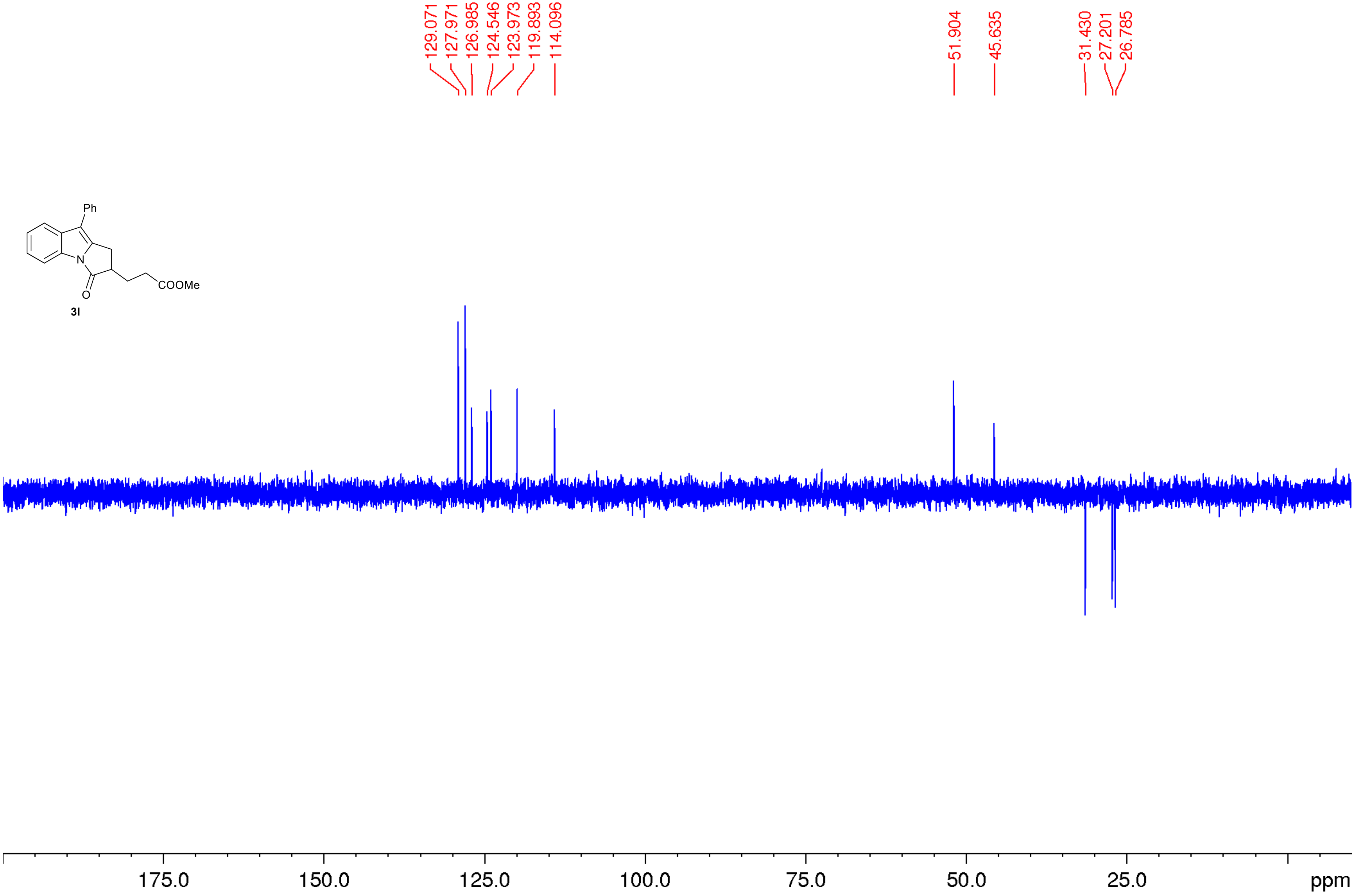
3l

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

3l

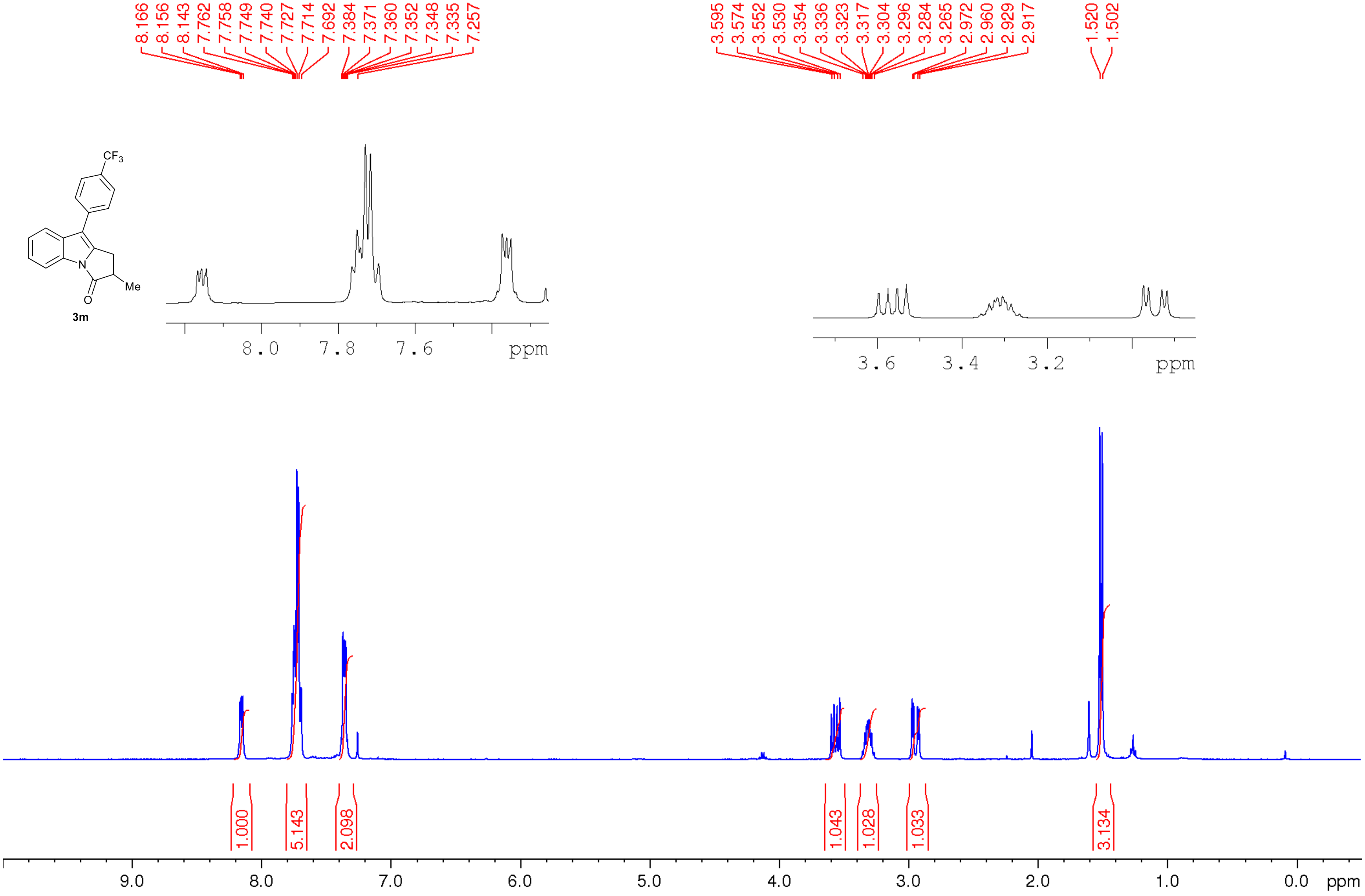


DEPT 135 NMR-spectrum ($CDCl_3$)

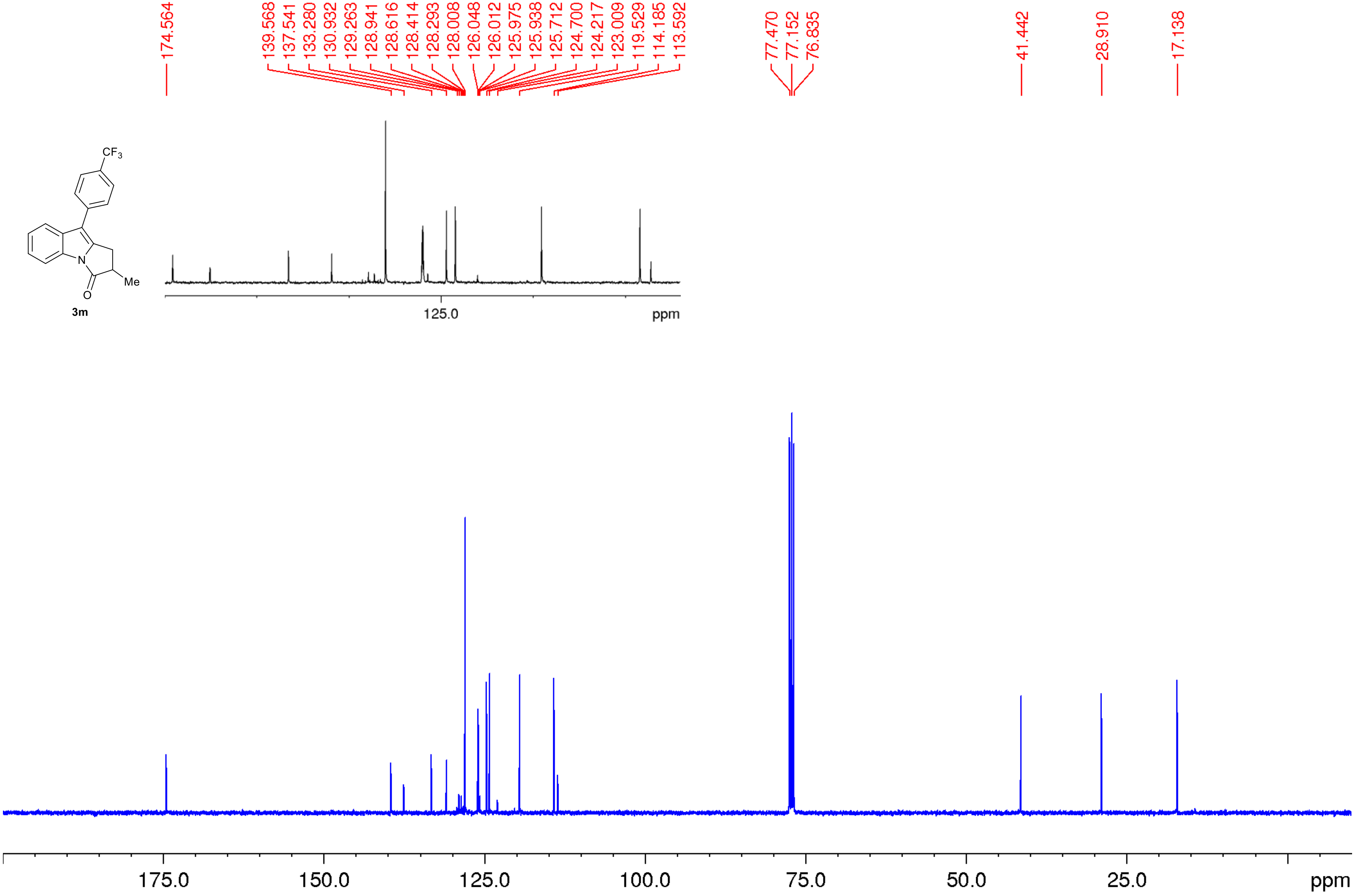


3l

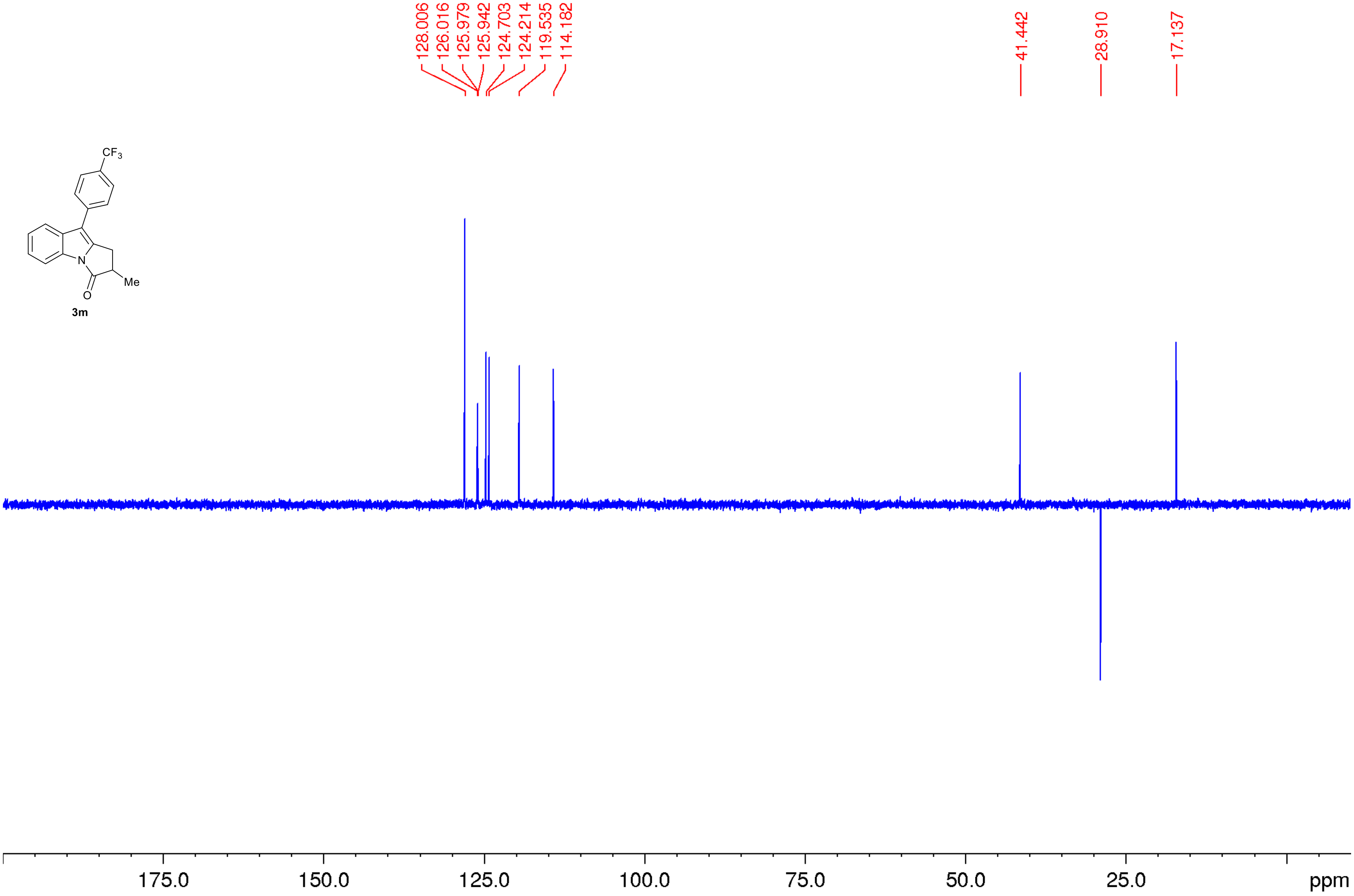
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



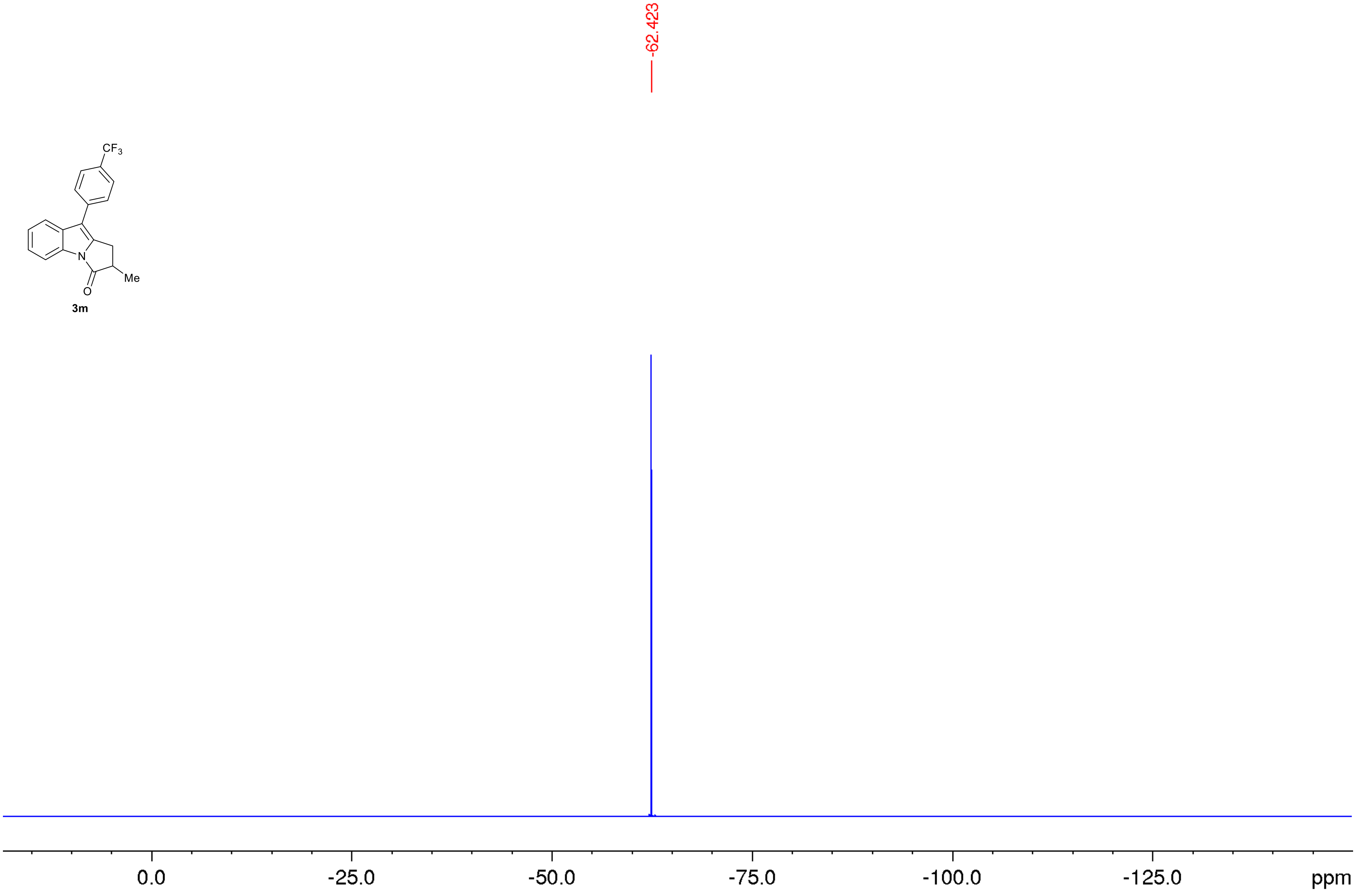
DEPT 135 NMR-spectrum ($CDCl_3$)



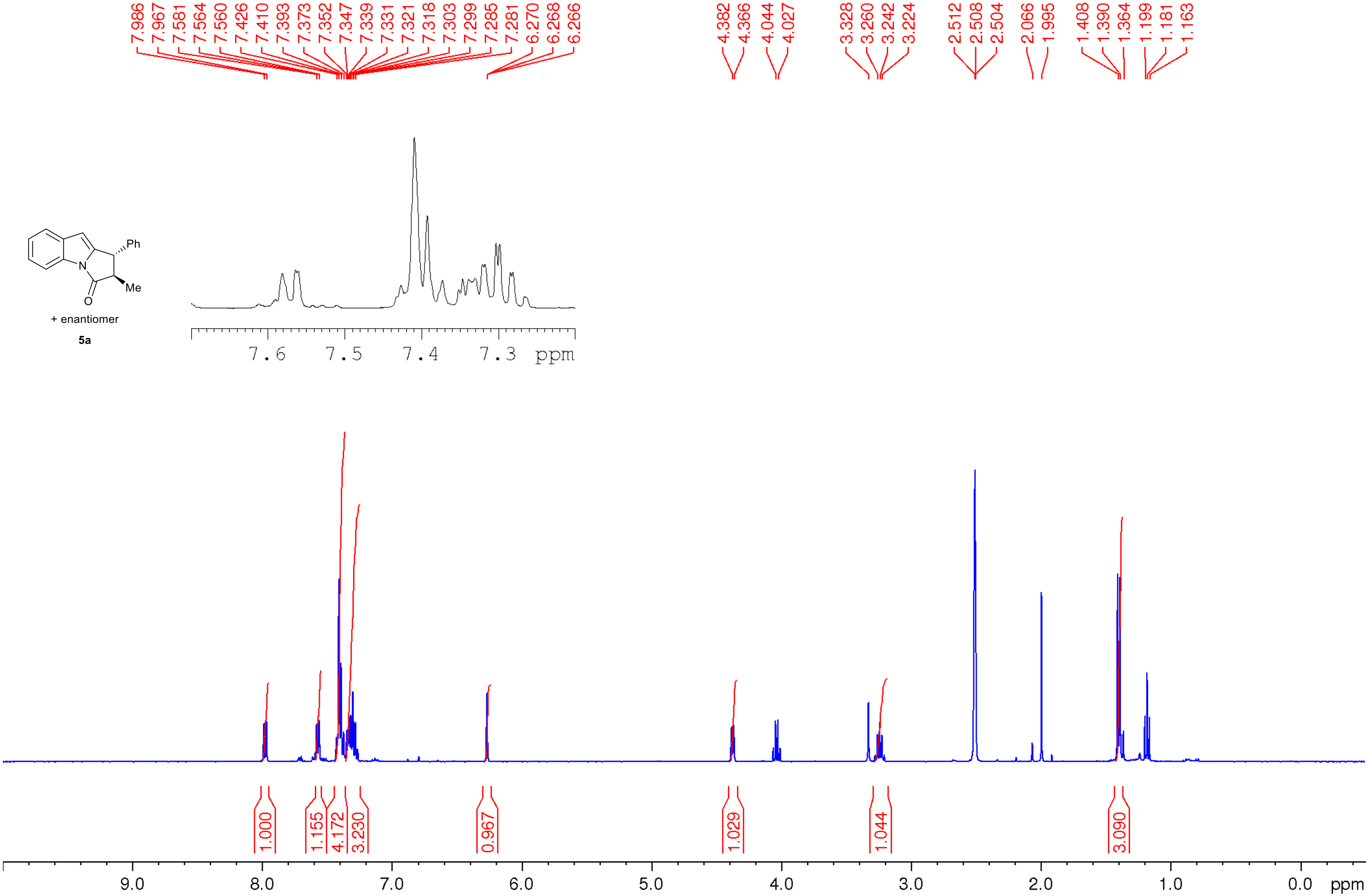
3m

^{19}F NMR-spectrum (376.5 MHz, $CDCl_3$)

3m



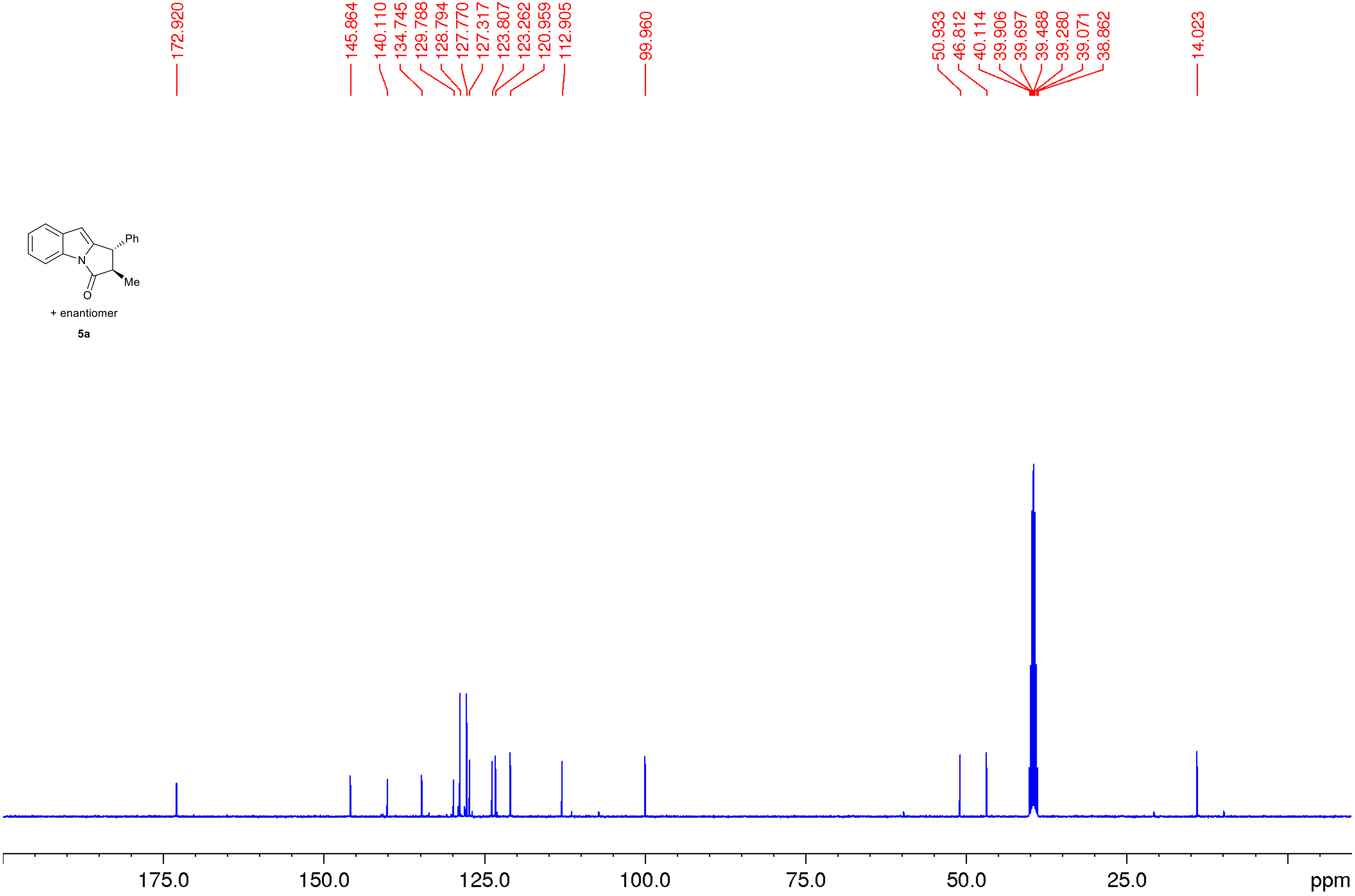
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



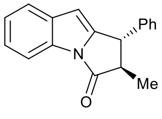
+ enantiomer

5a

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

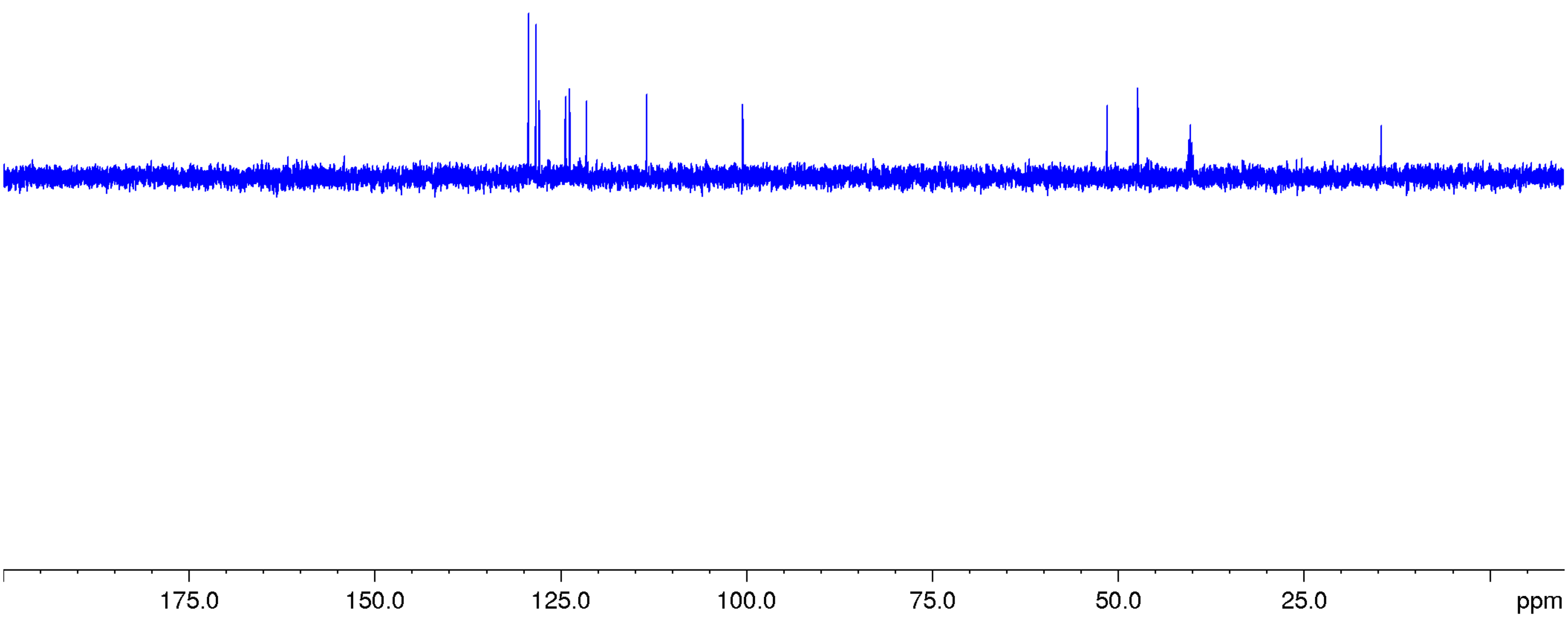


DEPT 135 NMR-spectrum ($CDCl_3$)

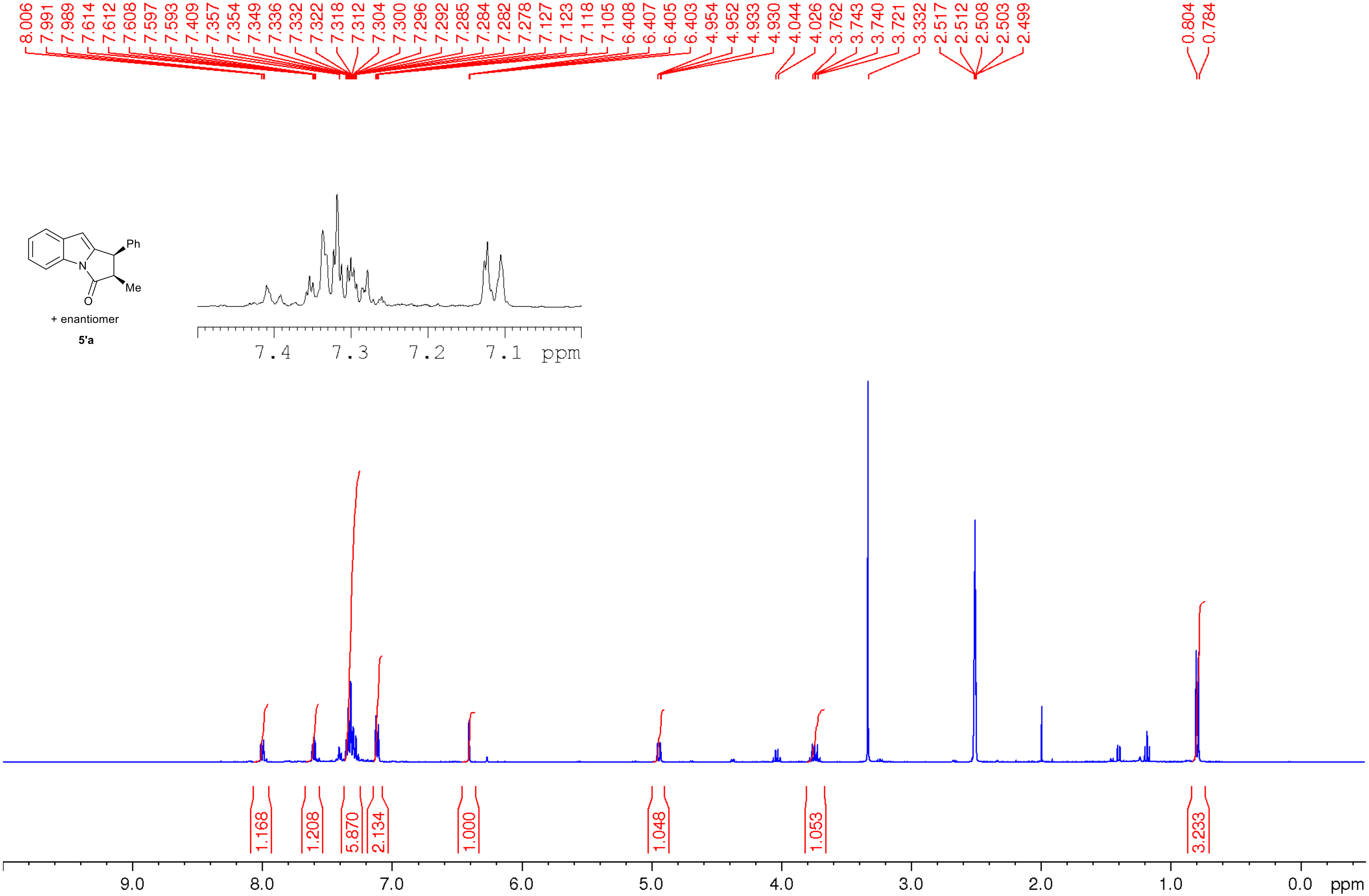


+ enantiomer

5a



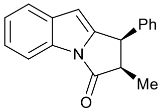
^{1}H NMR-spectrum (400 MHz, DMSO-d_6)



+ enantiomer

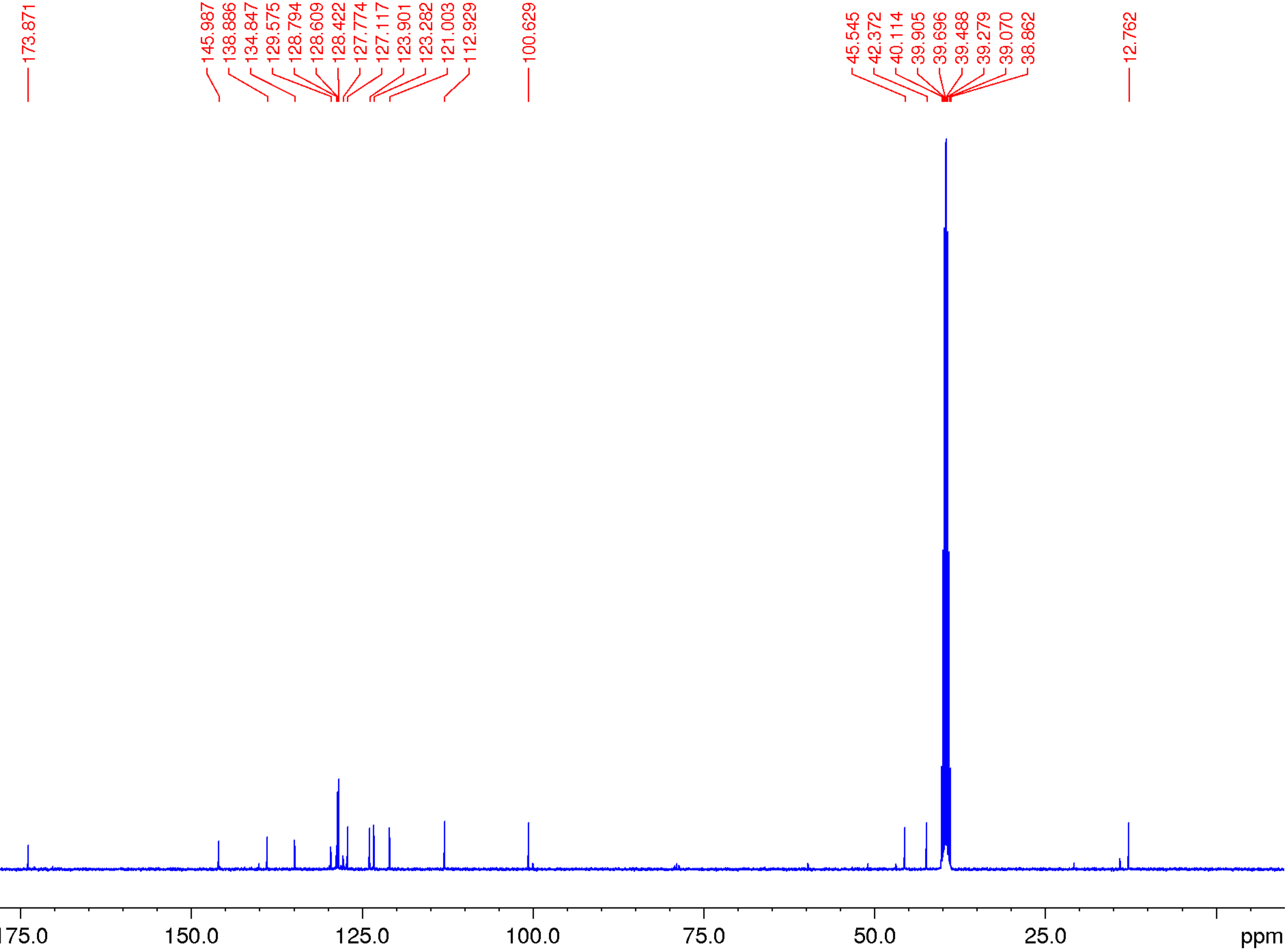
5'a

^{13}C NMR-spectrum (100 MHz, DMSO-d_6)

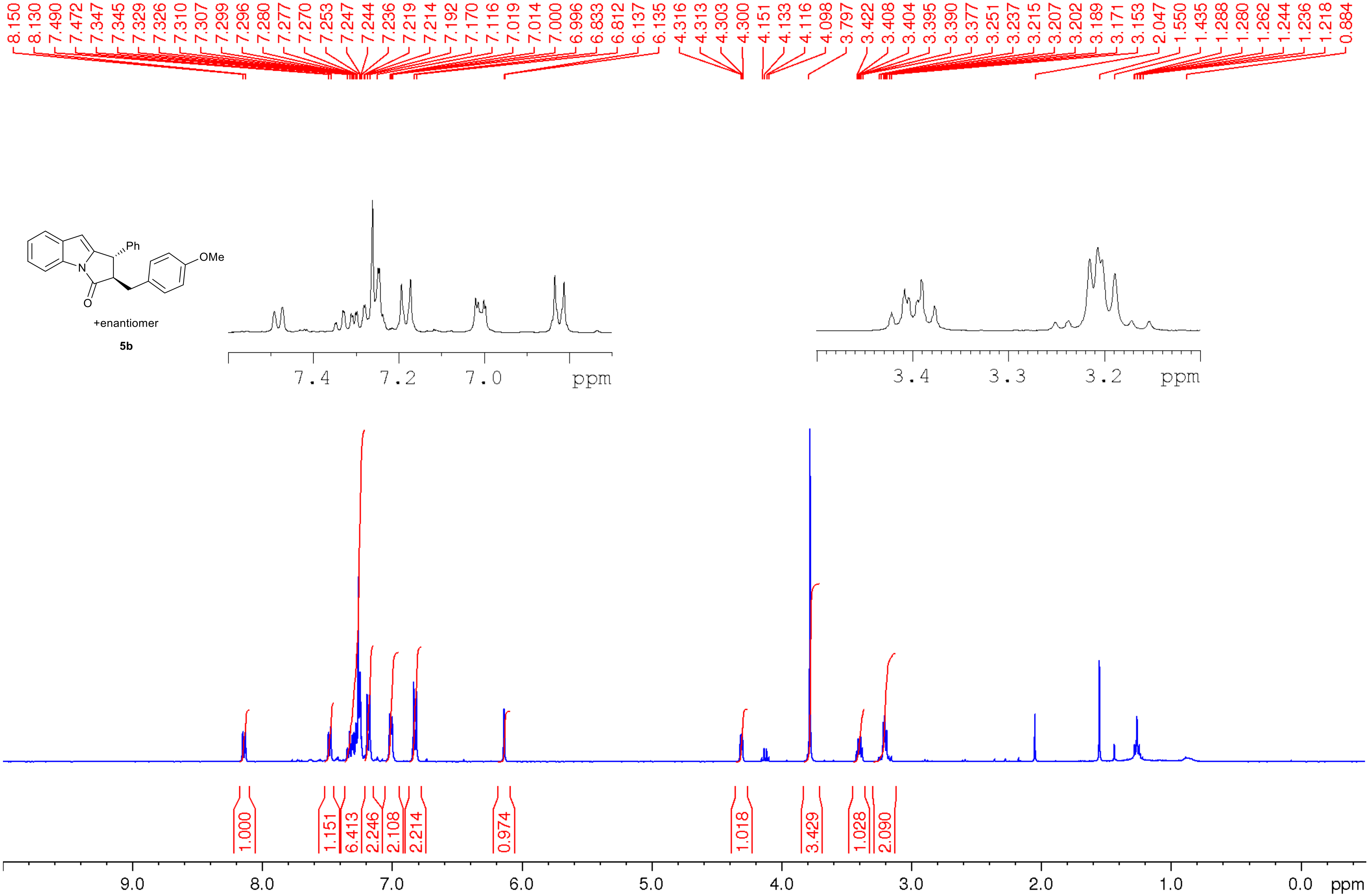


+ enantiomer

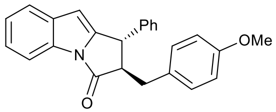
5'a



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

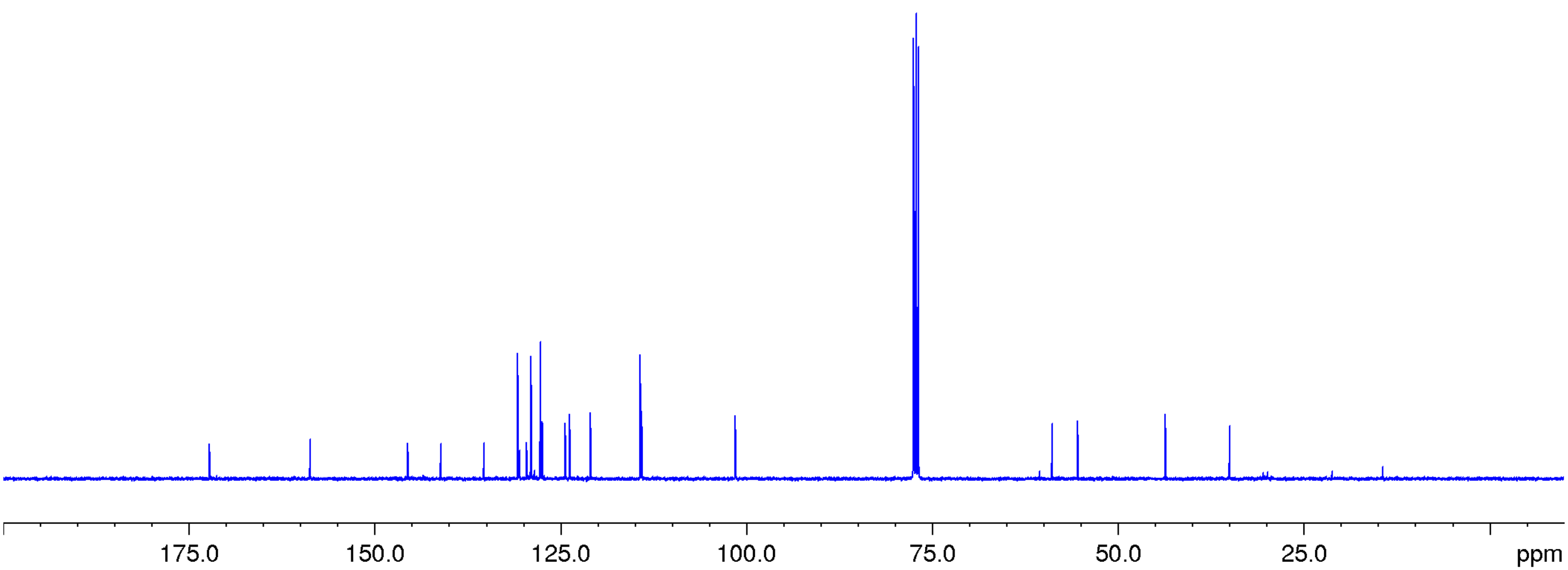


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)

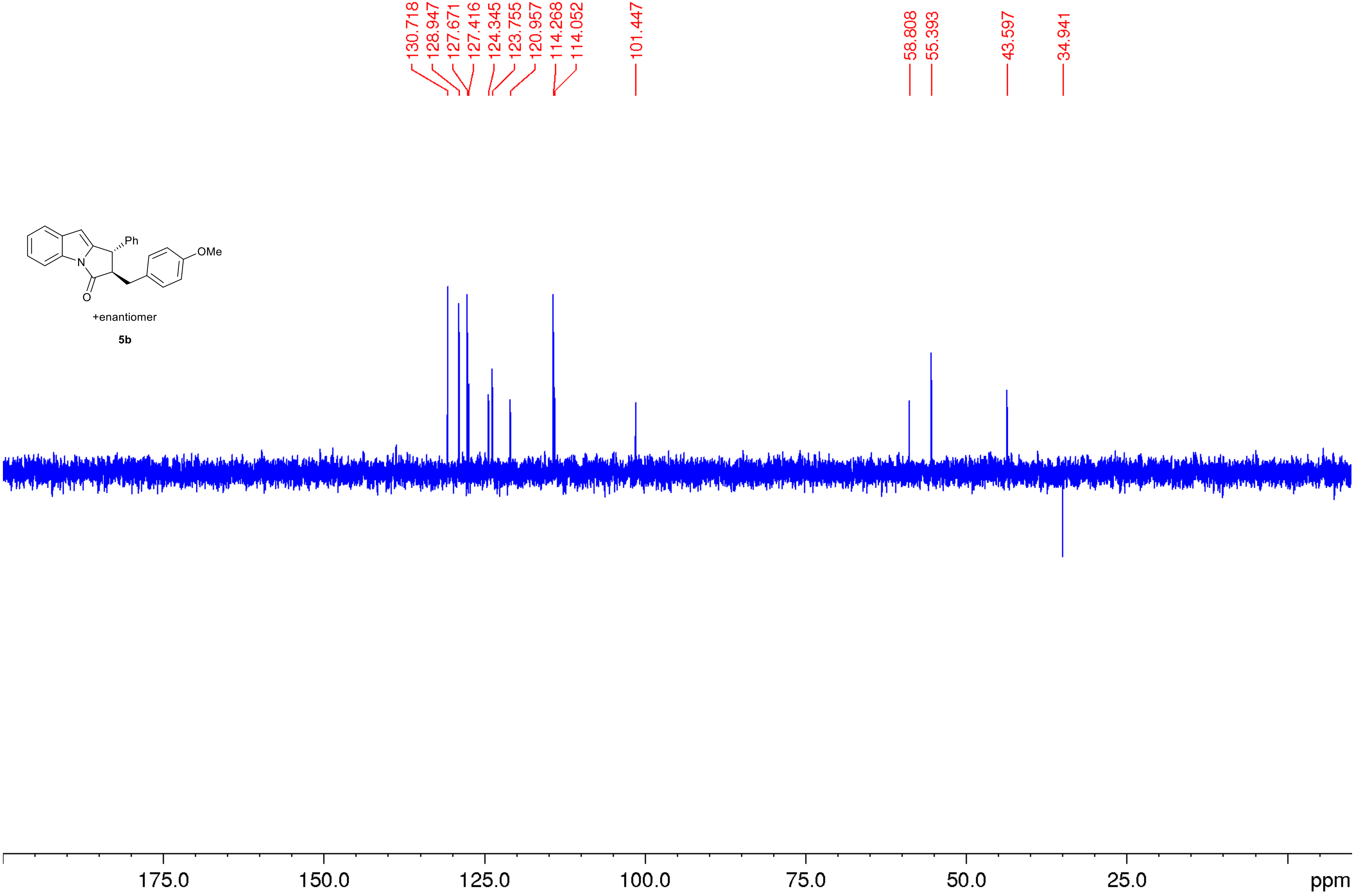


+enantiomer

5b



DEPT 135 NMR-spectrum ($CDCl_3$)



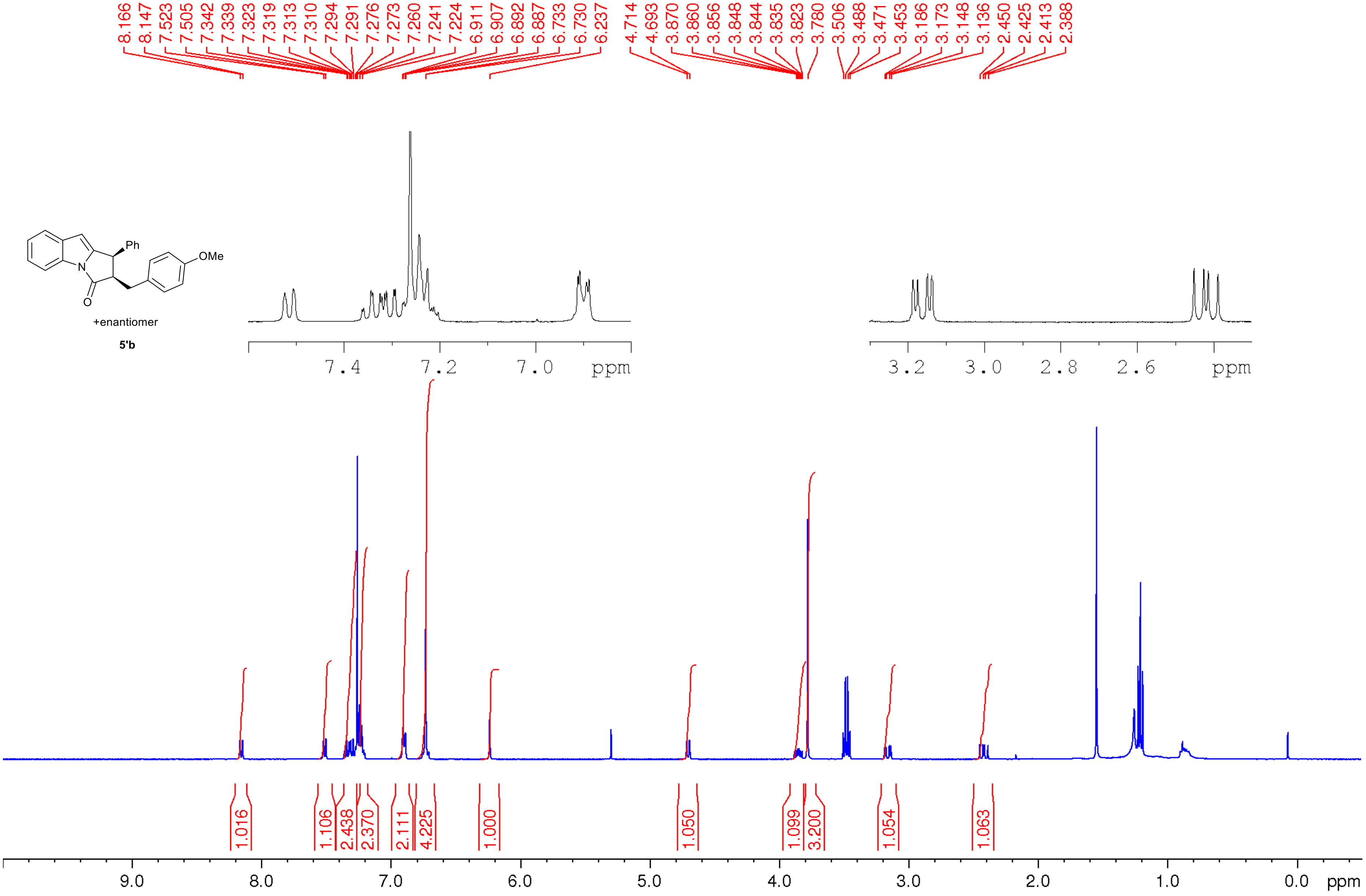
+enantiomer

5b

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

+enantiomer

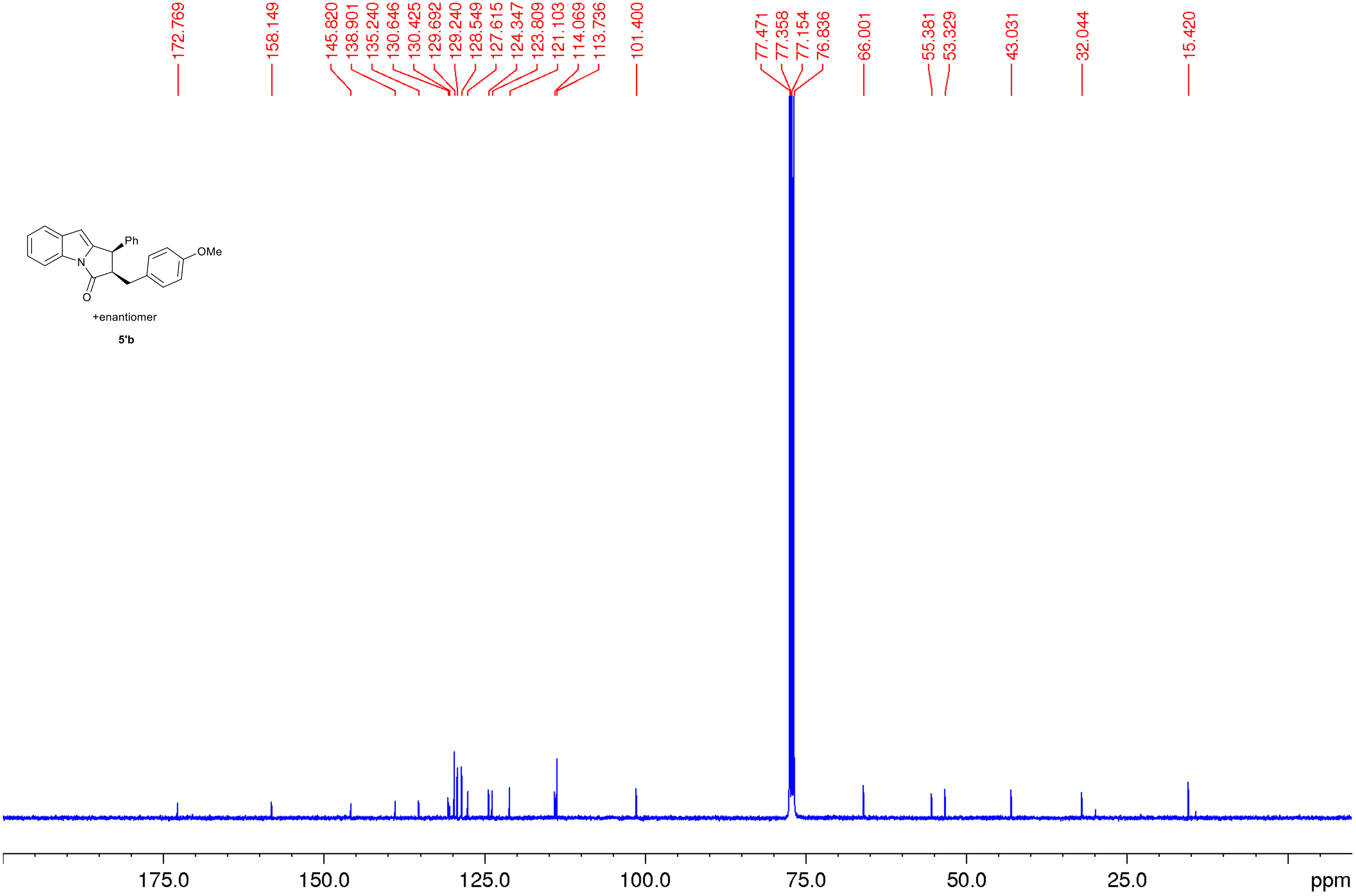
5'b



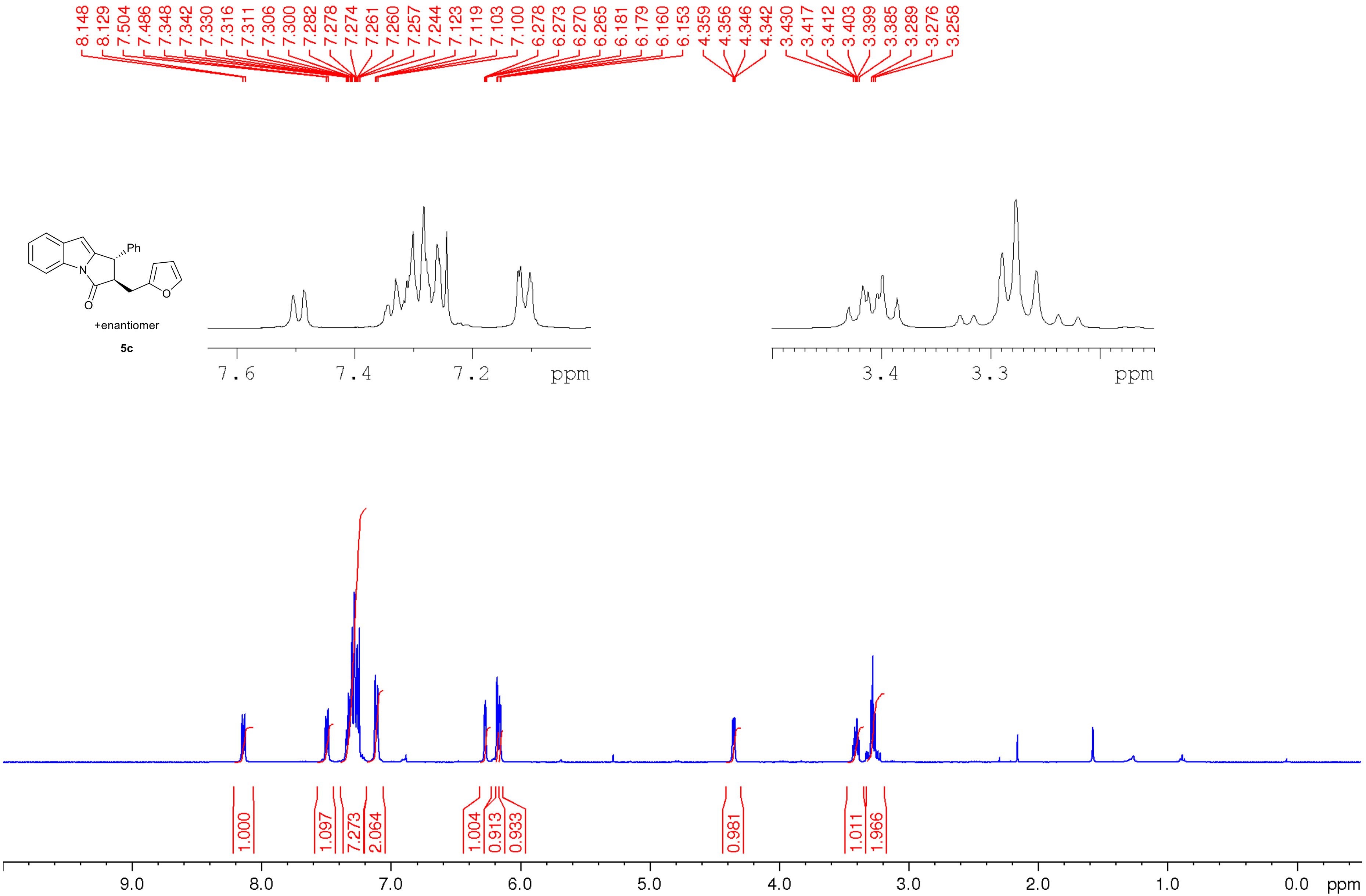
^{13}C NMR-spectrum (100 MHz, CDCl$_3$)

+enantiomer

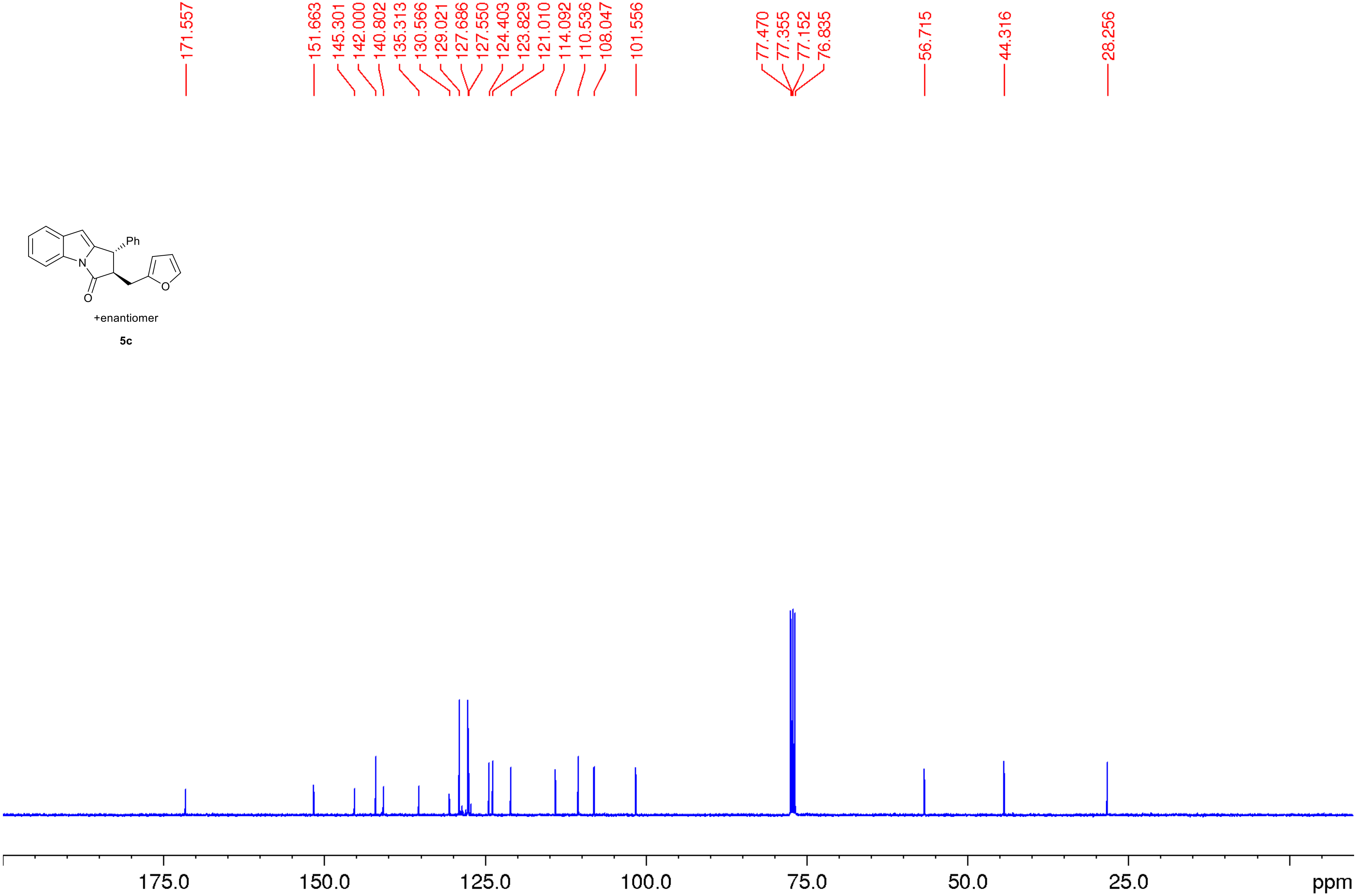
5'b



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



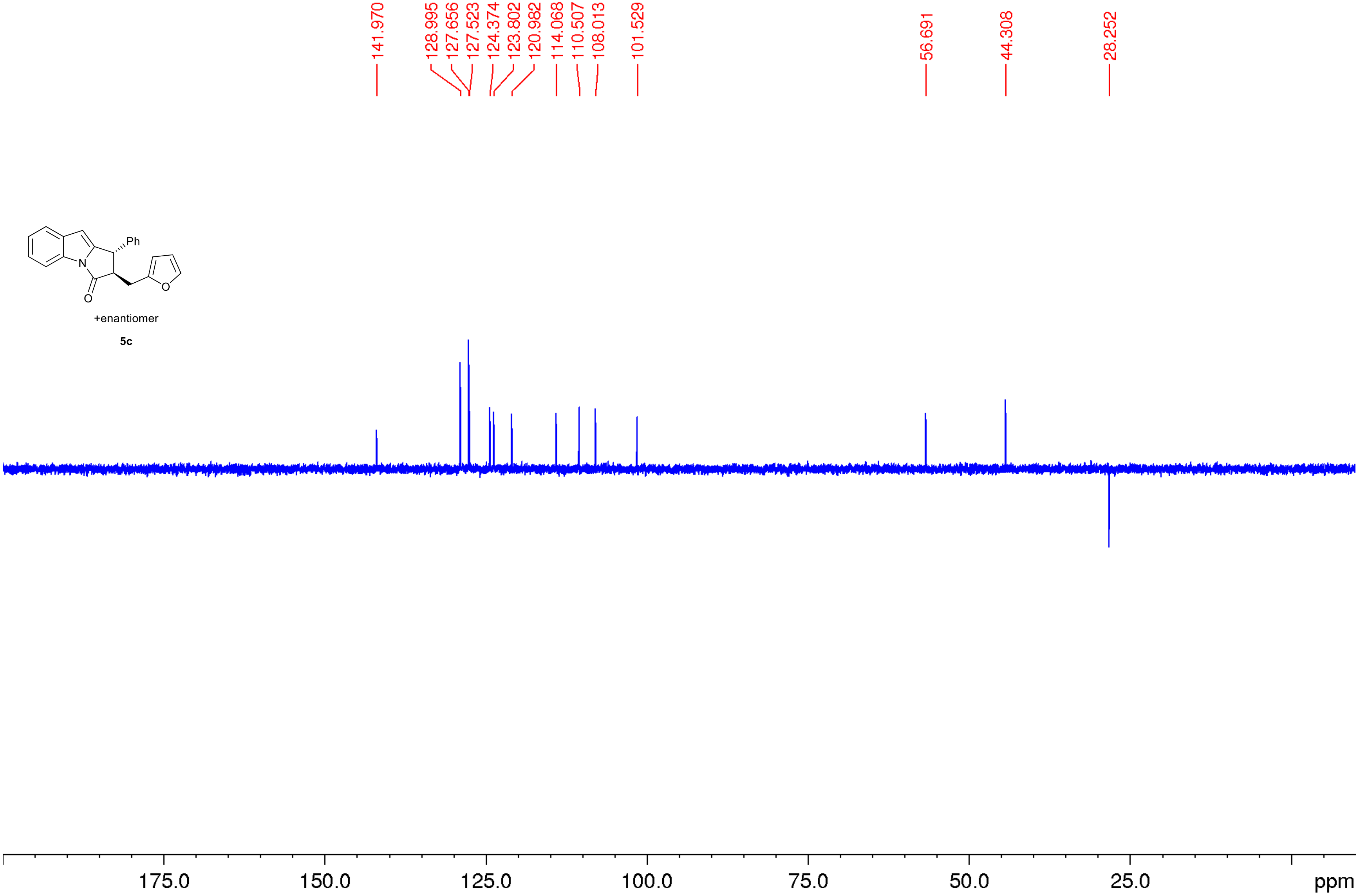
^{13}C NMR-spectrum (100 MHz, CDCl$_3$)



+enantiomer

5c

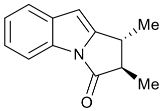
DEPT 135 NMR-spectrum ($CDCl_3$)



+enantiomer

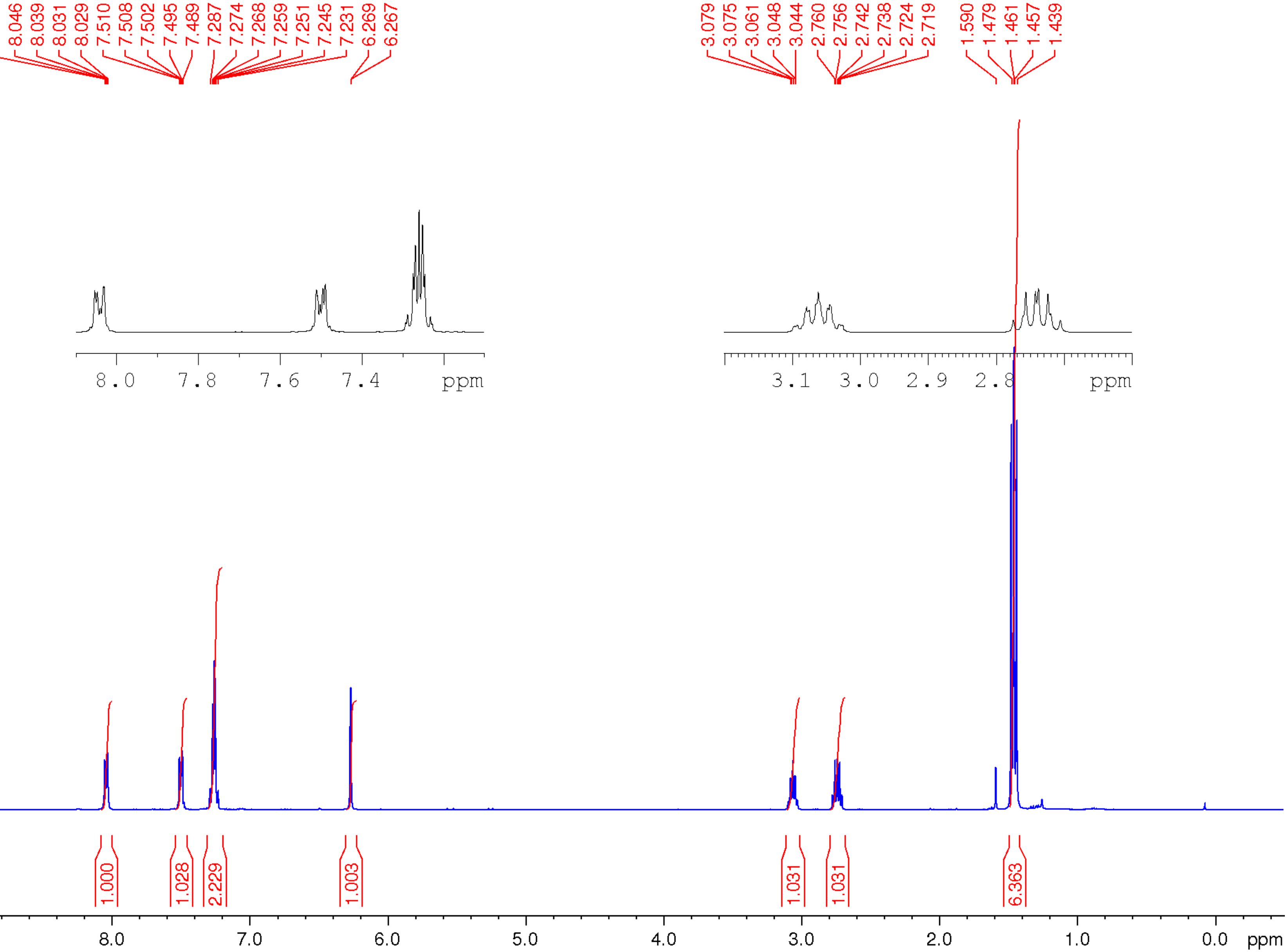
5c

^1H NMR-spectrum (400 MHz, $CDCl_3$)



+enantiomer

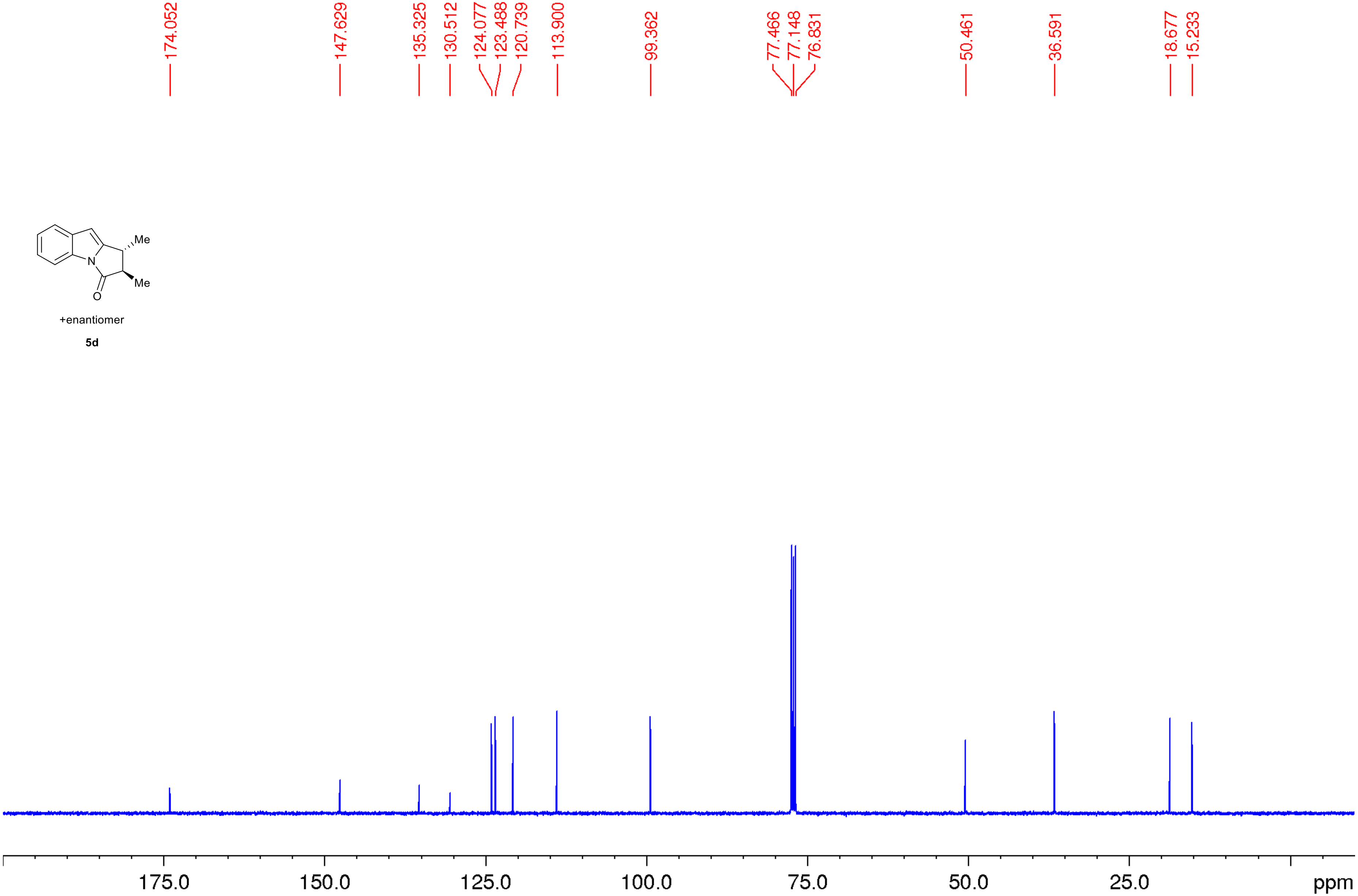
5d



^{13}C NMR-spectrum (100 MHz, CDCl$_3$)

+enantiomer

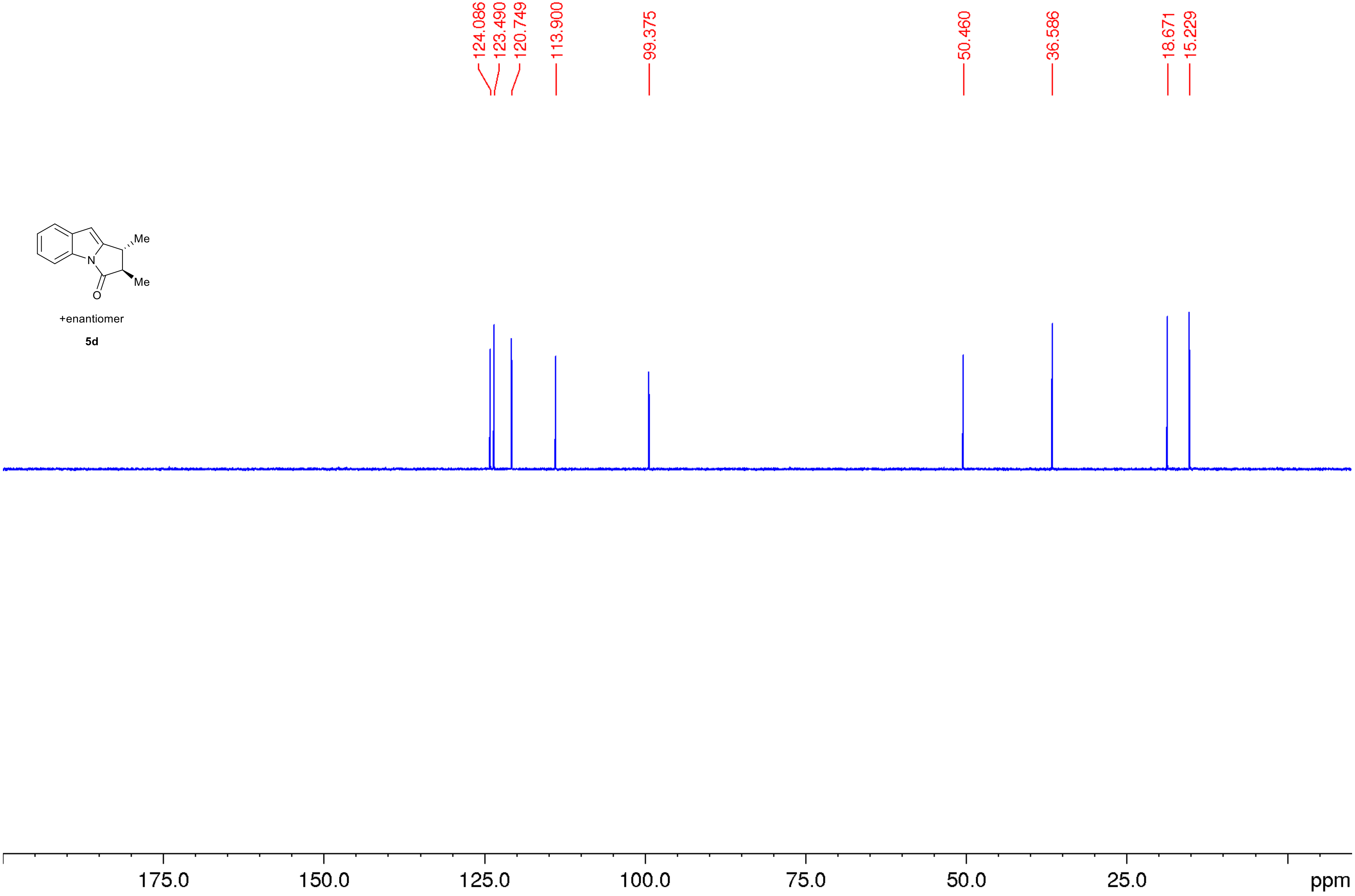
5d



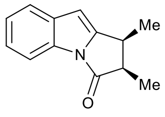
DEPT 135 NMR-spectrum ($CDCl_3$)

+enantiomer

5d

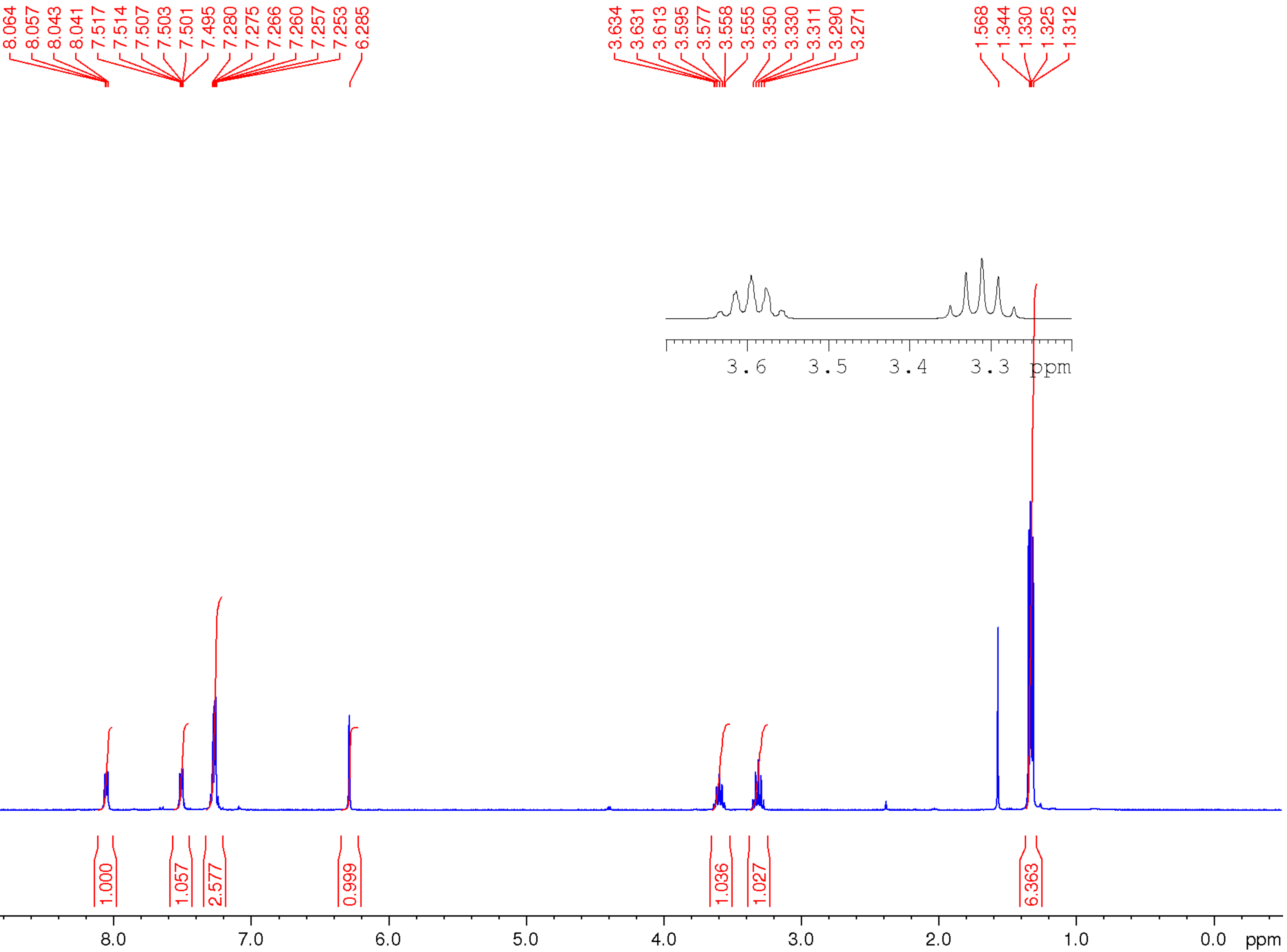


^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

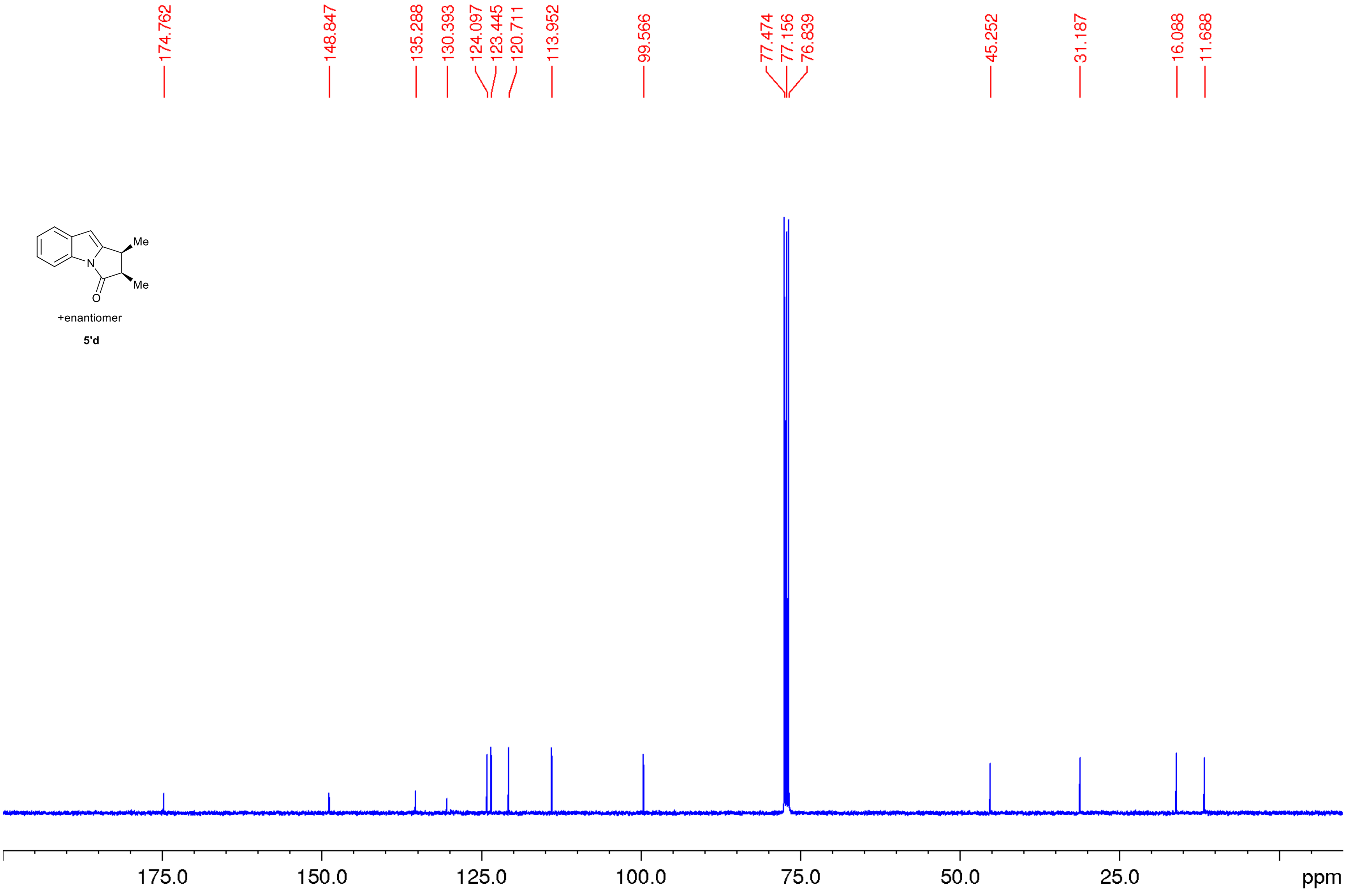


+enantiomer

5'd



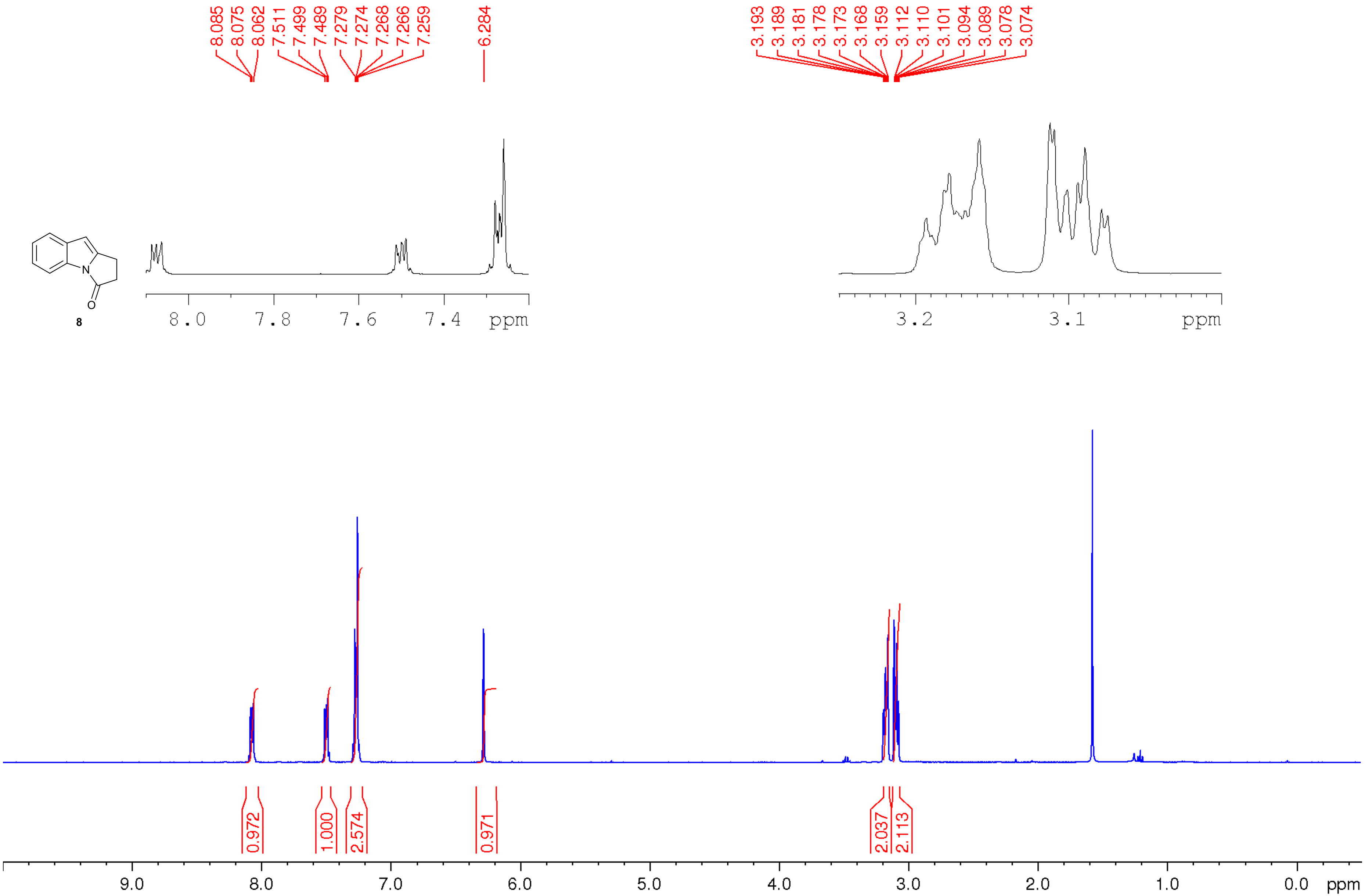
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



+enantiomer

5'd

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



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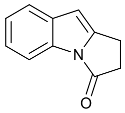
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



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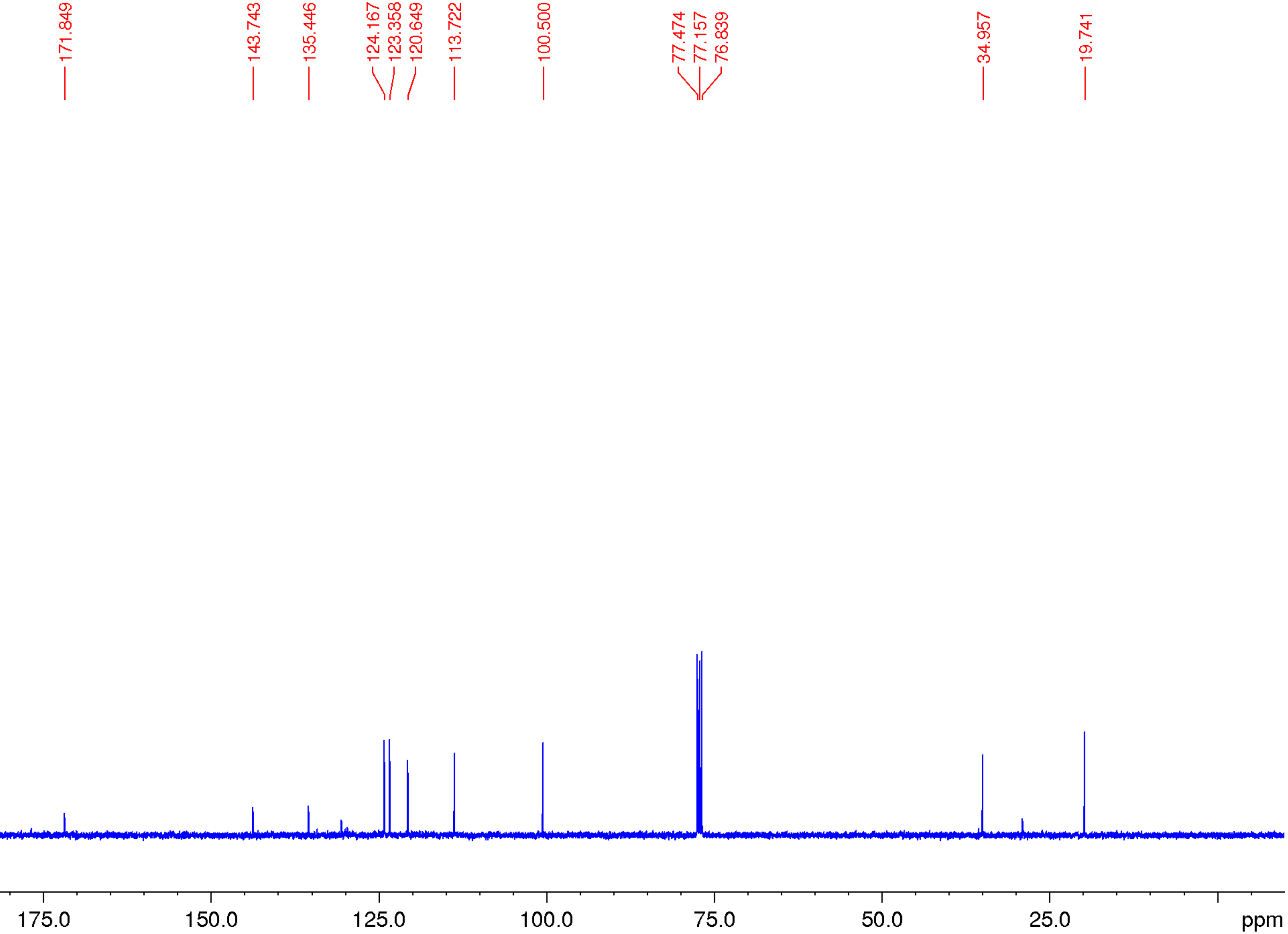
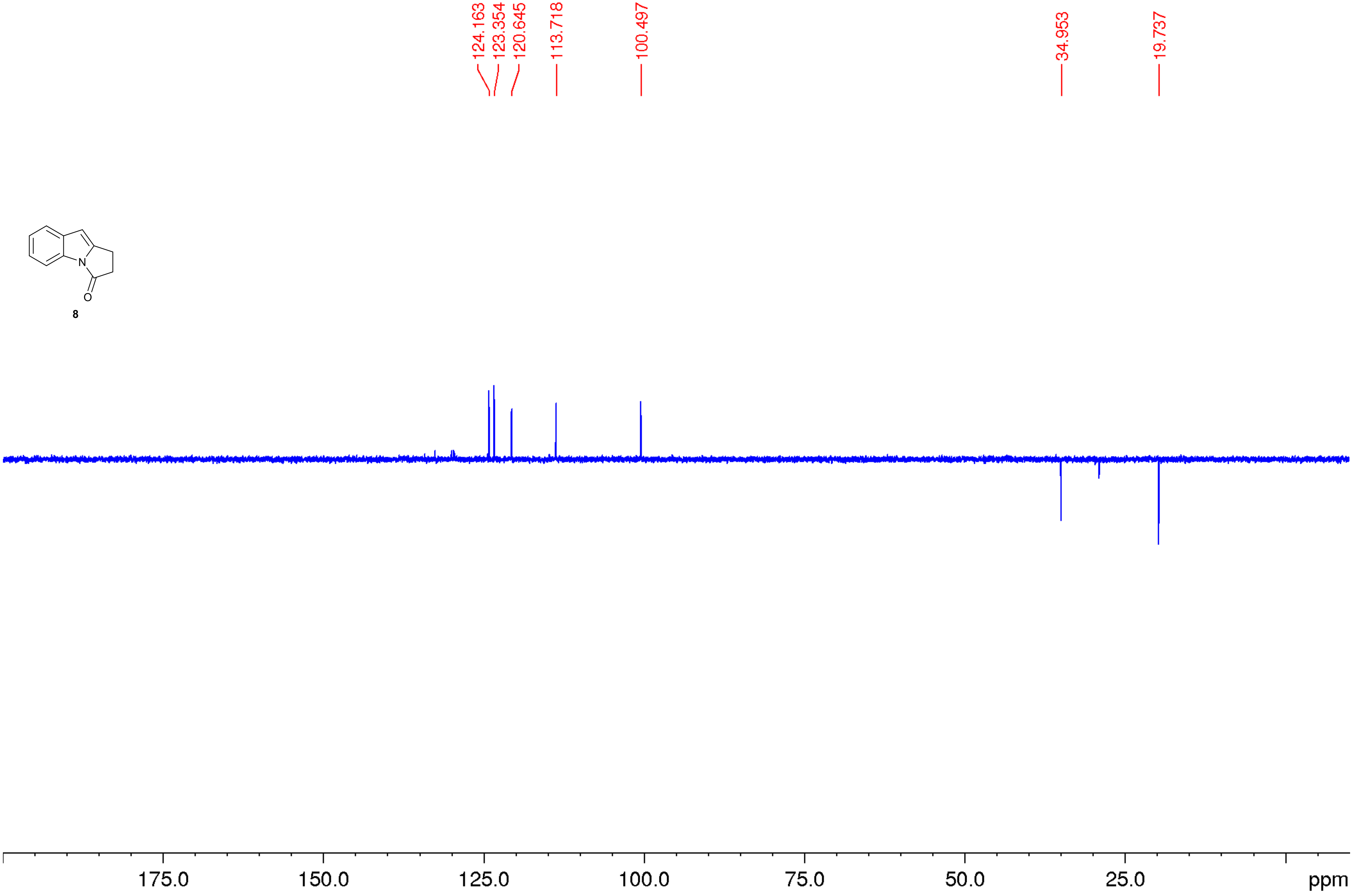
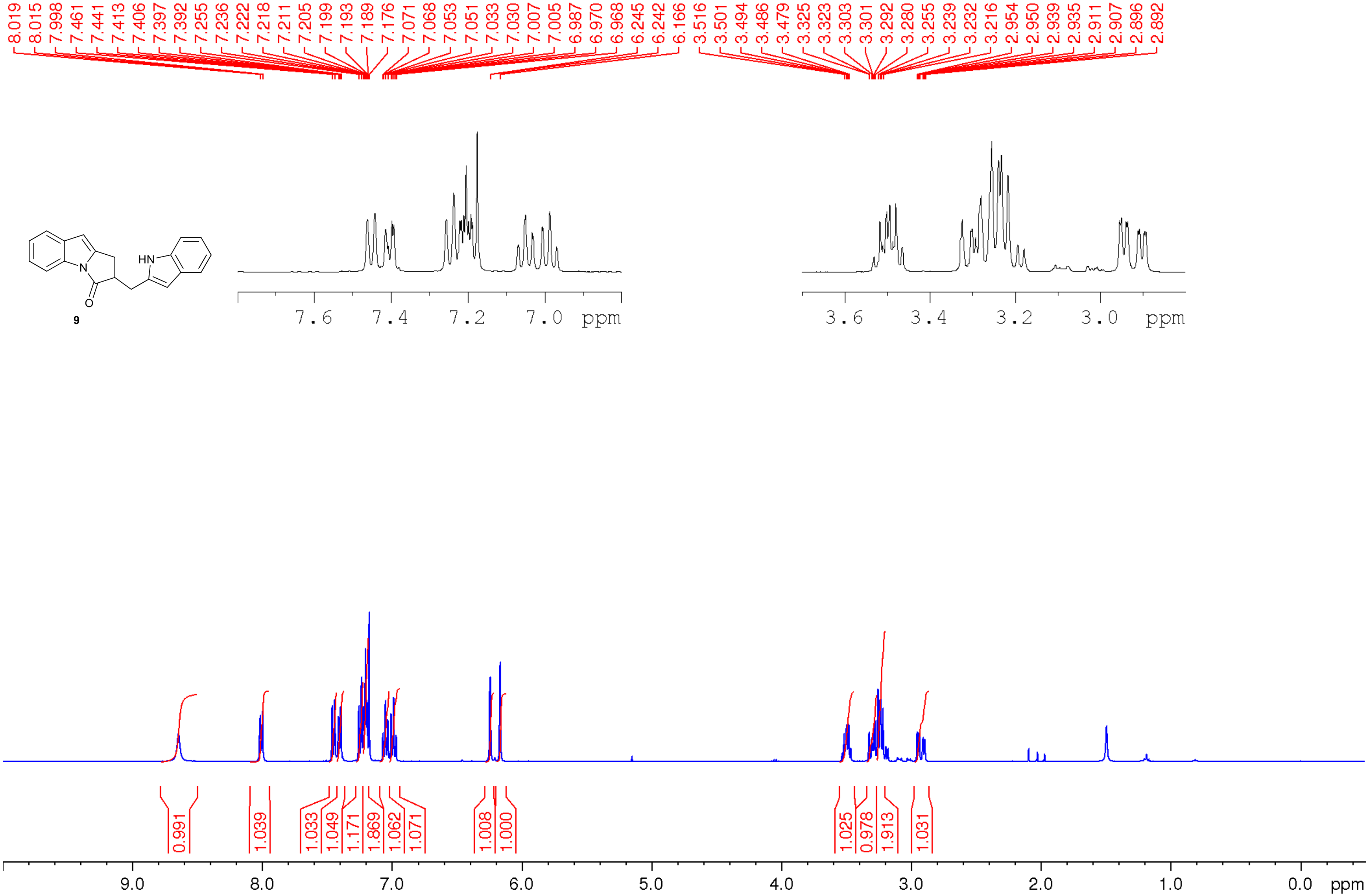


DEPT 135 NMR-spectrum ($CDCl_3$)

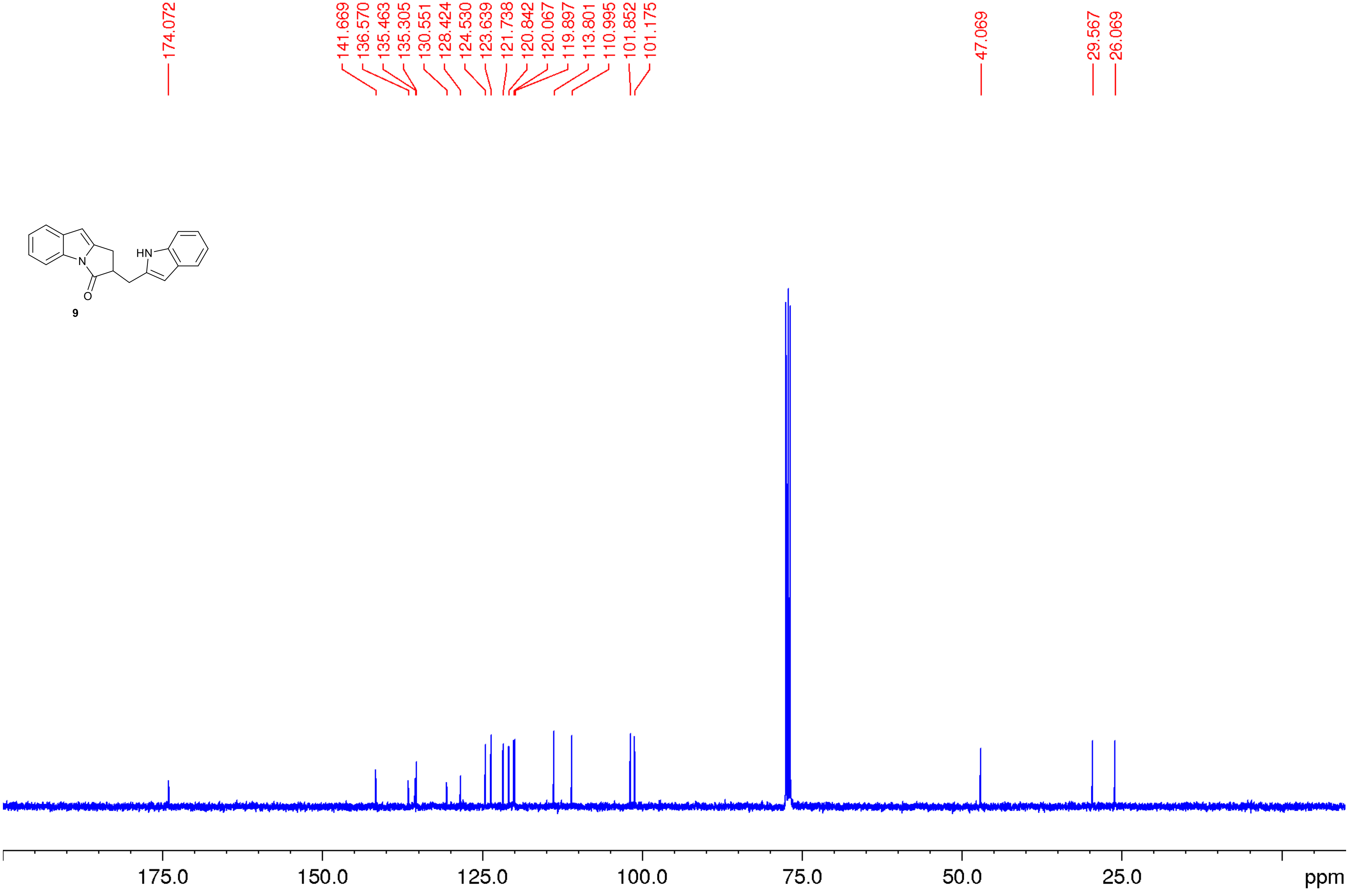
8



^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

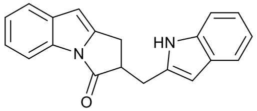


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



9

DEPT 135 NMR-spectrum ($CDCl_3$)



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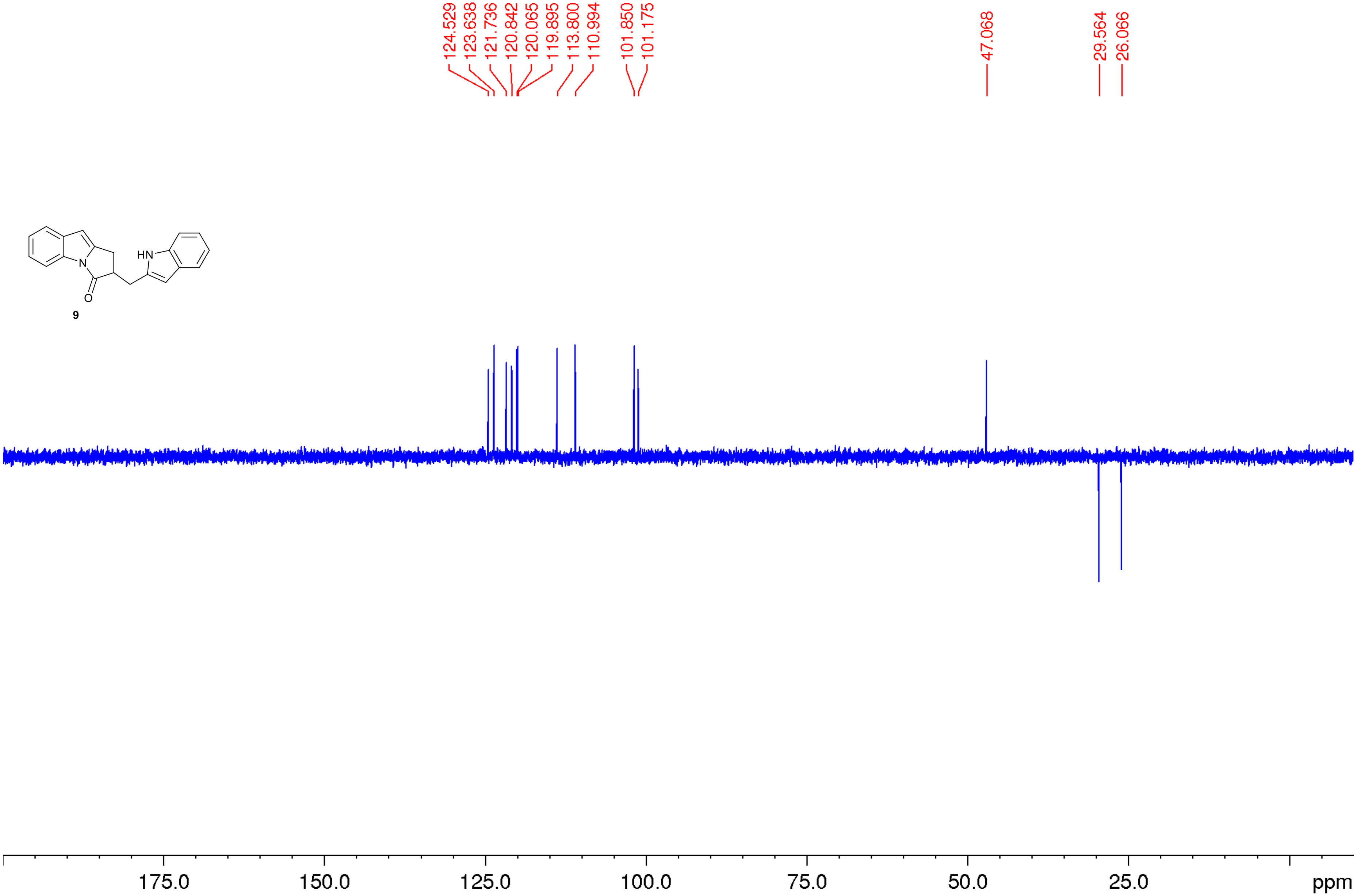
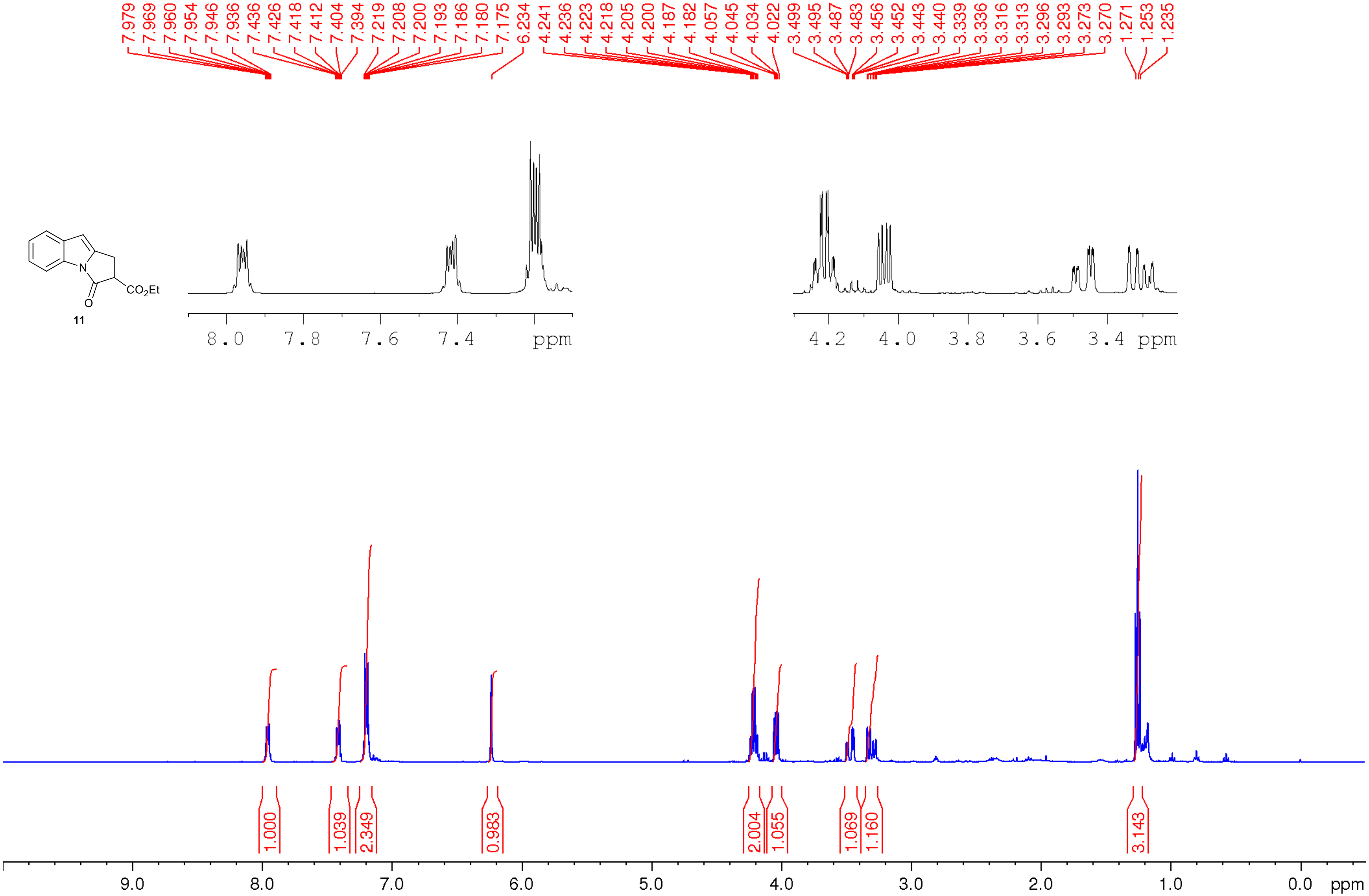
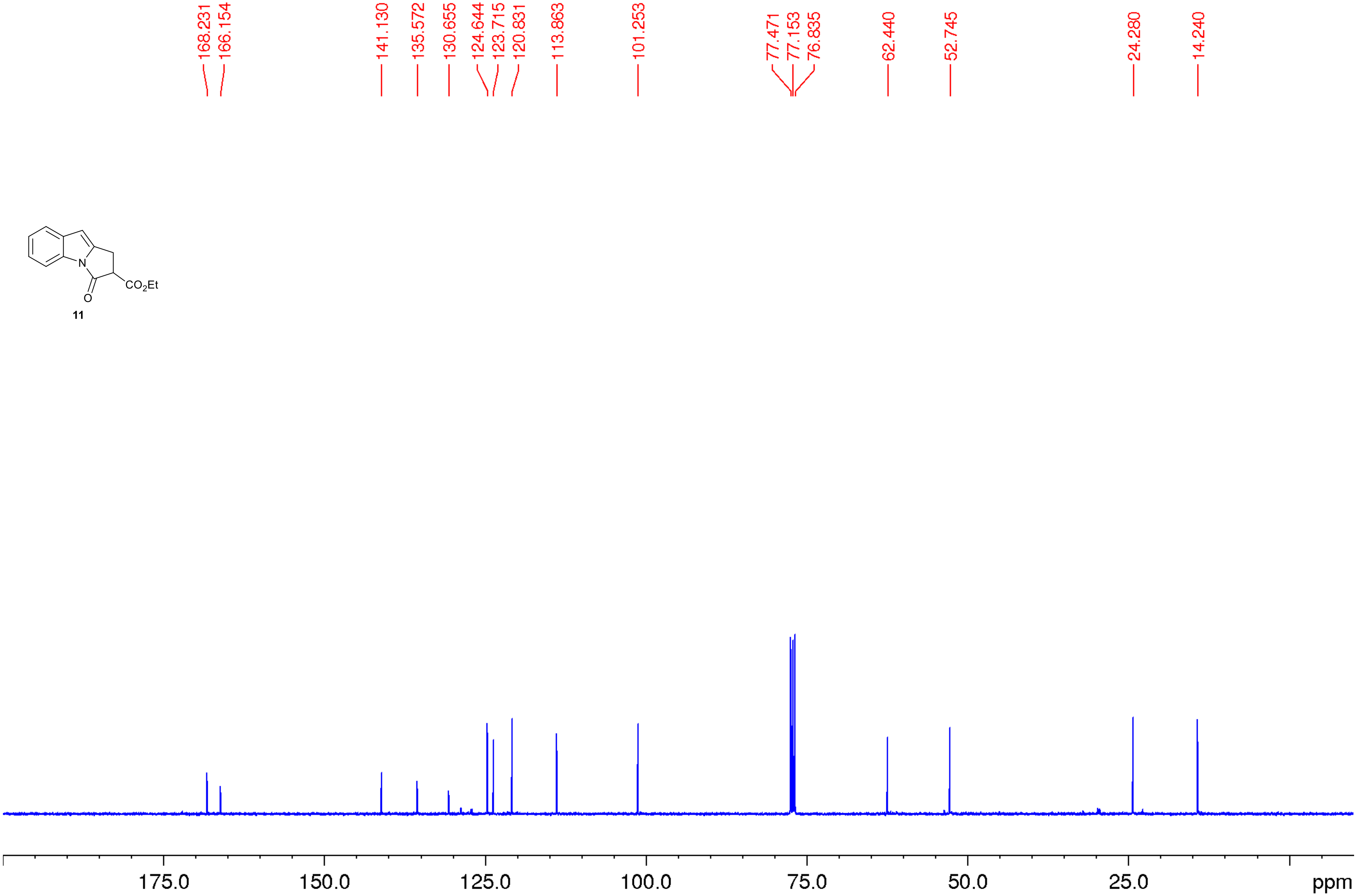


^1H NMR-spectrum (400 MHz, $CDCl_3$)



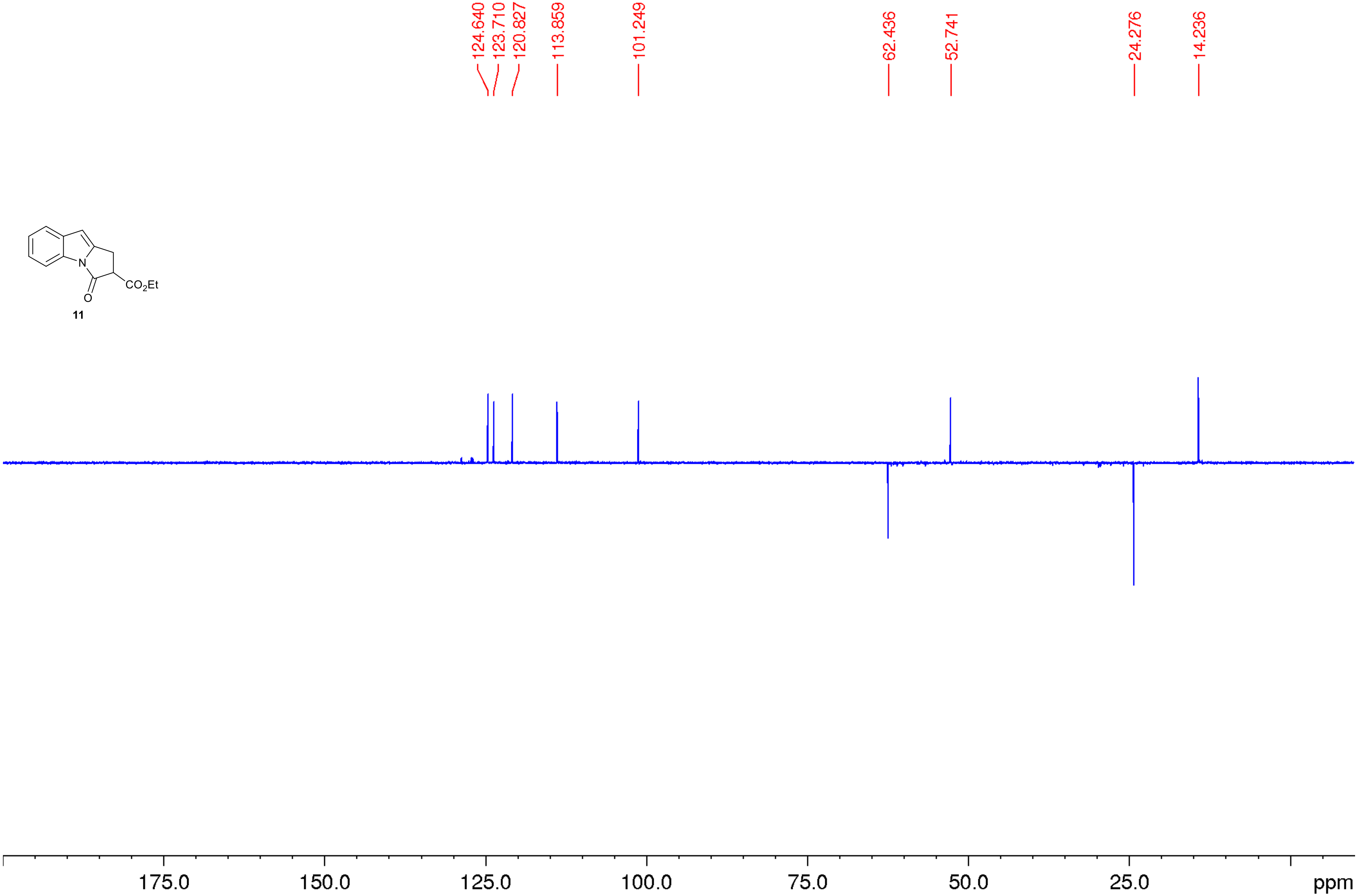
11

^{13}C NMR-spectrum (100 MHz, CDCl$_3$)



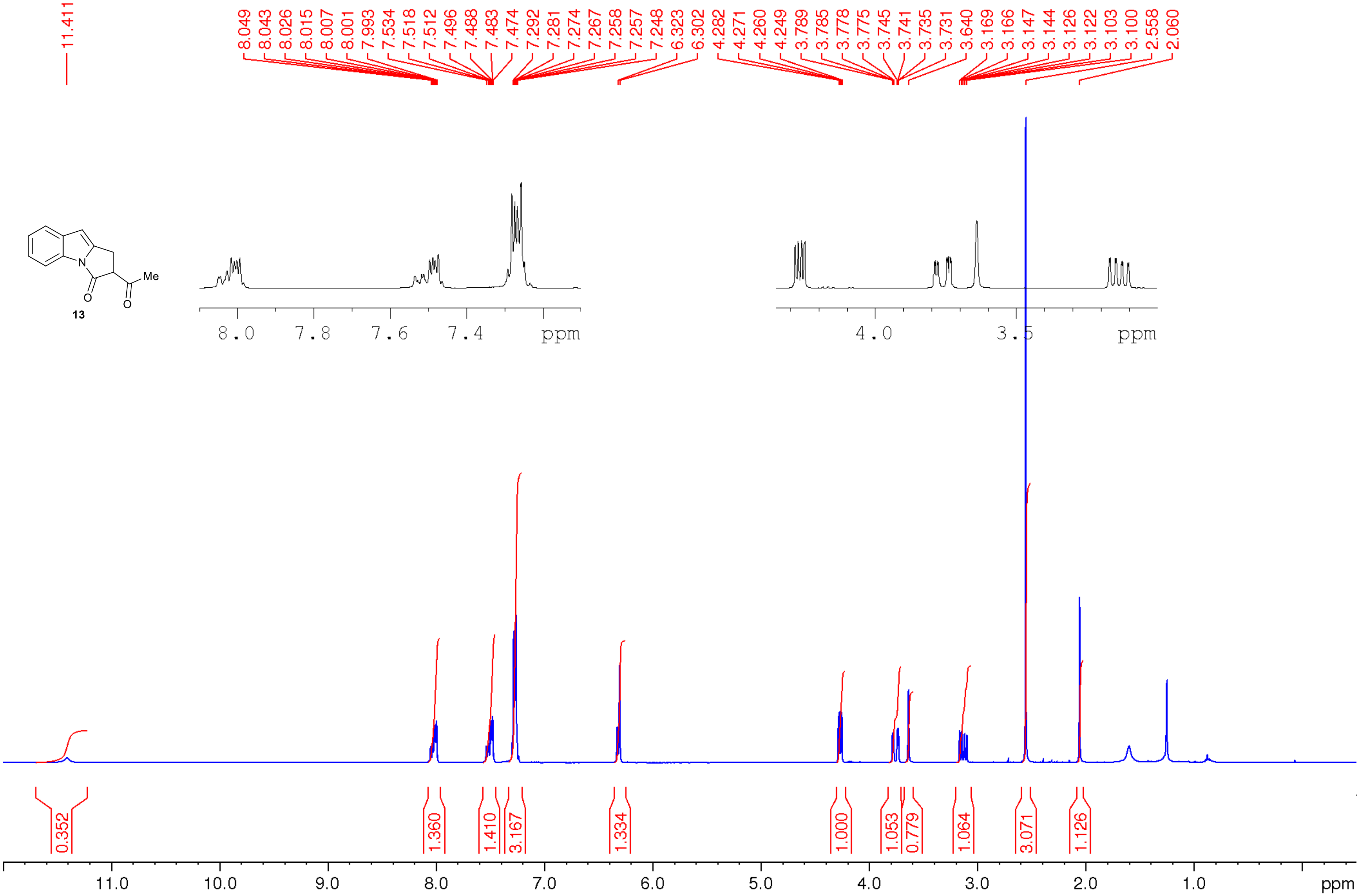
11

DEPT 135 NMR-spectrum (CDCl$_3$)

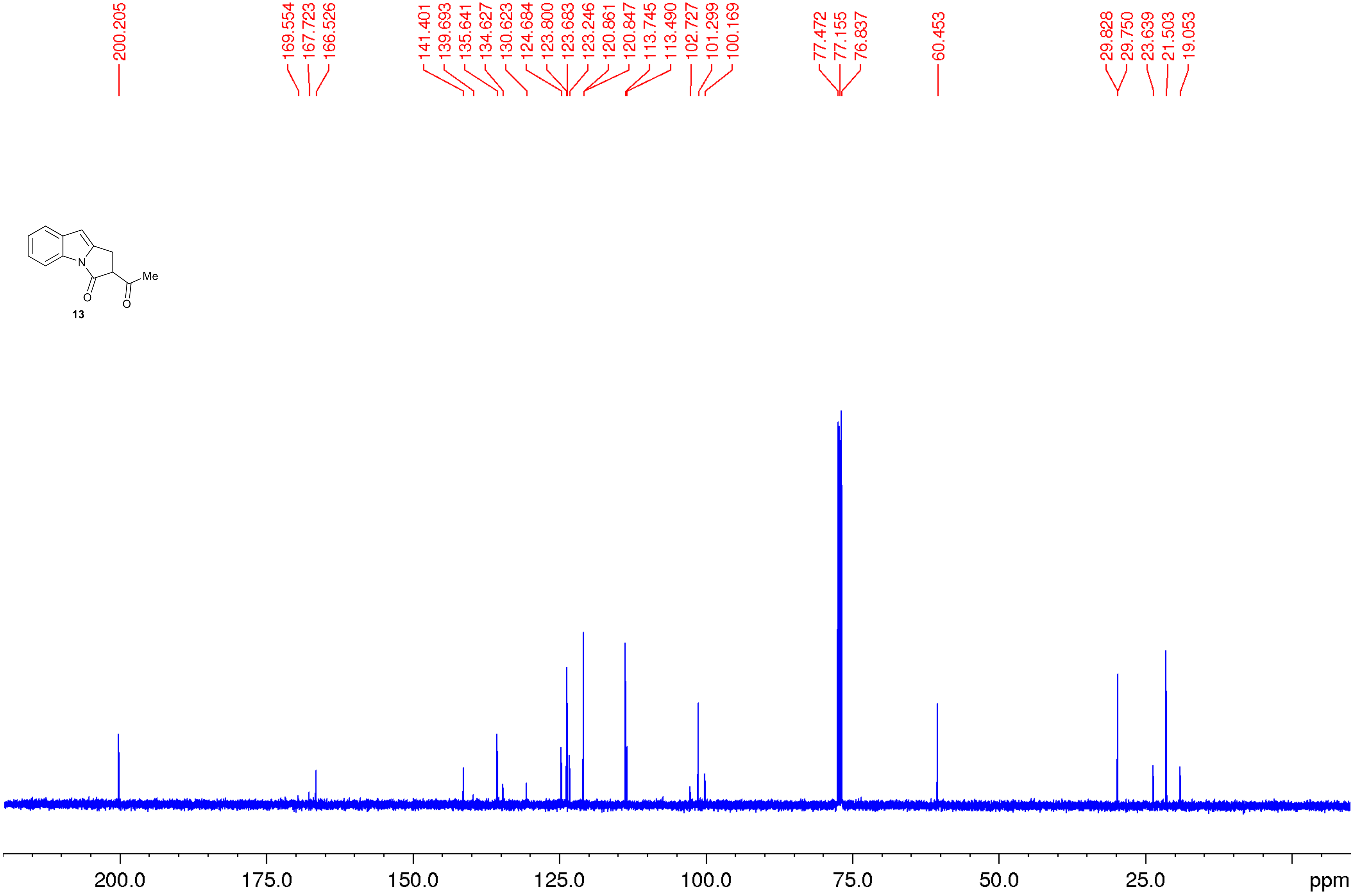


11

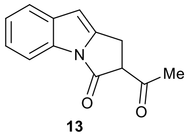
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)



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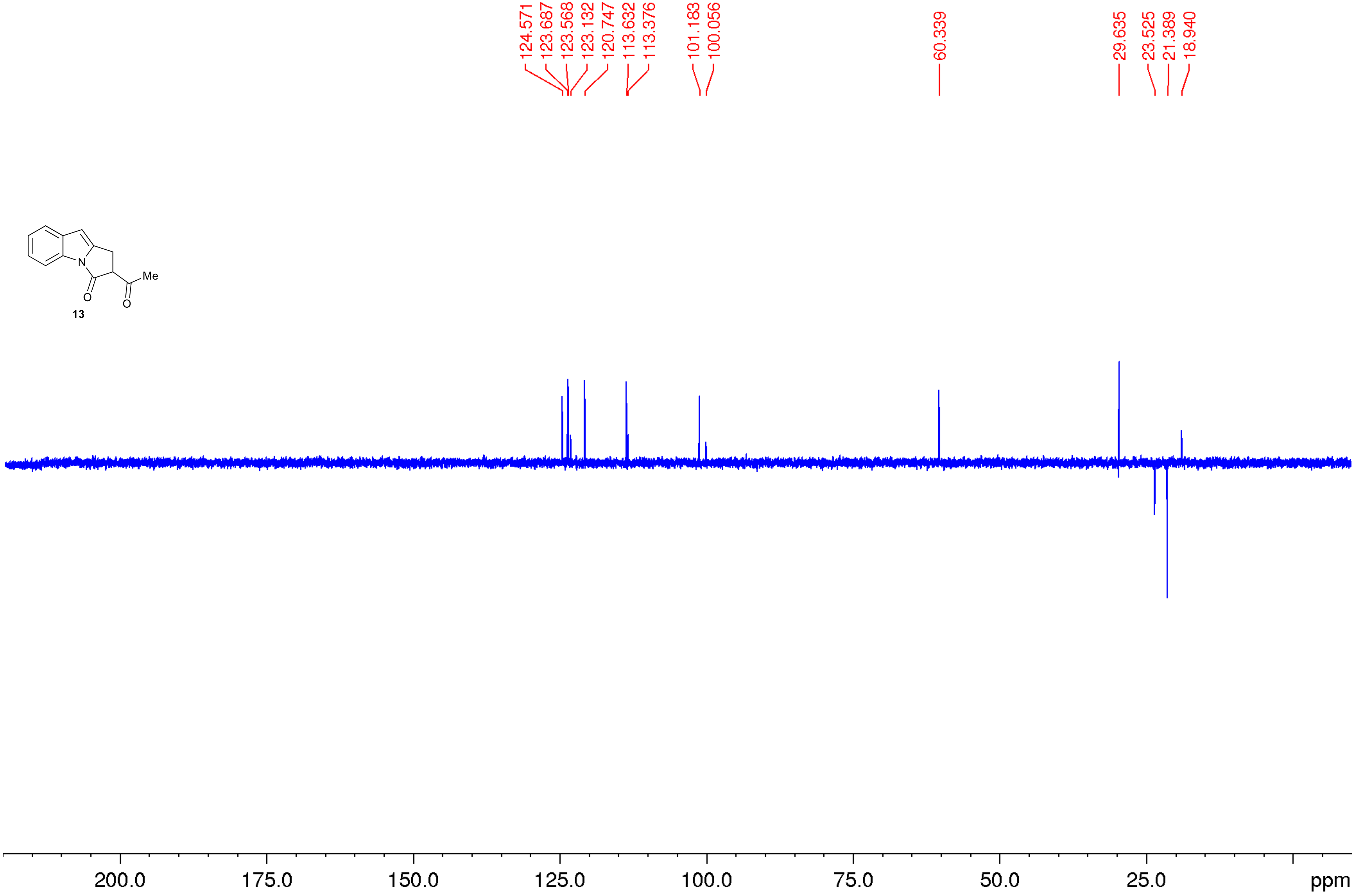
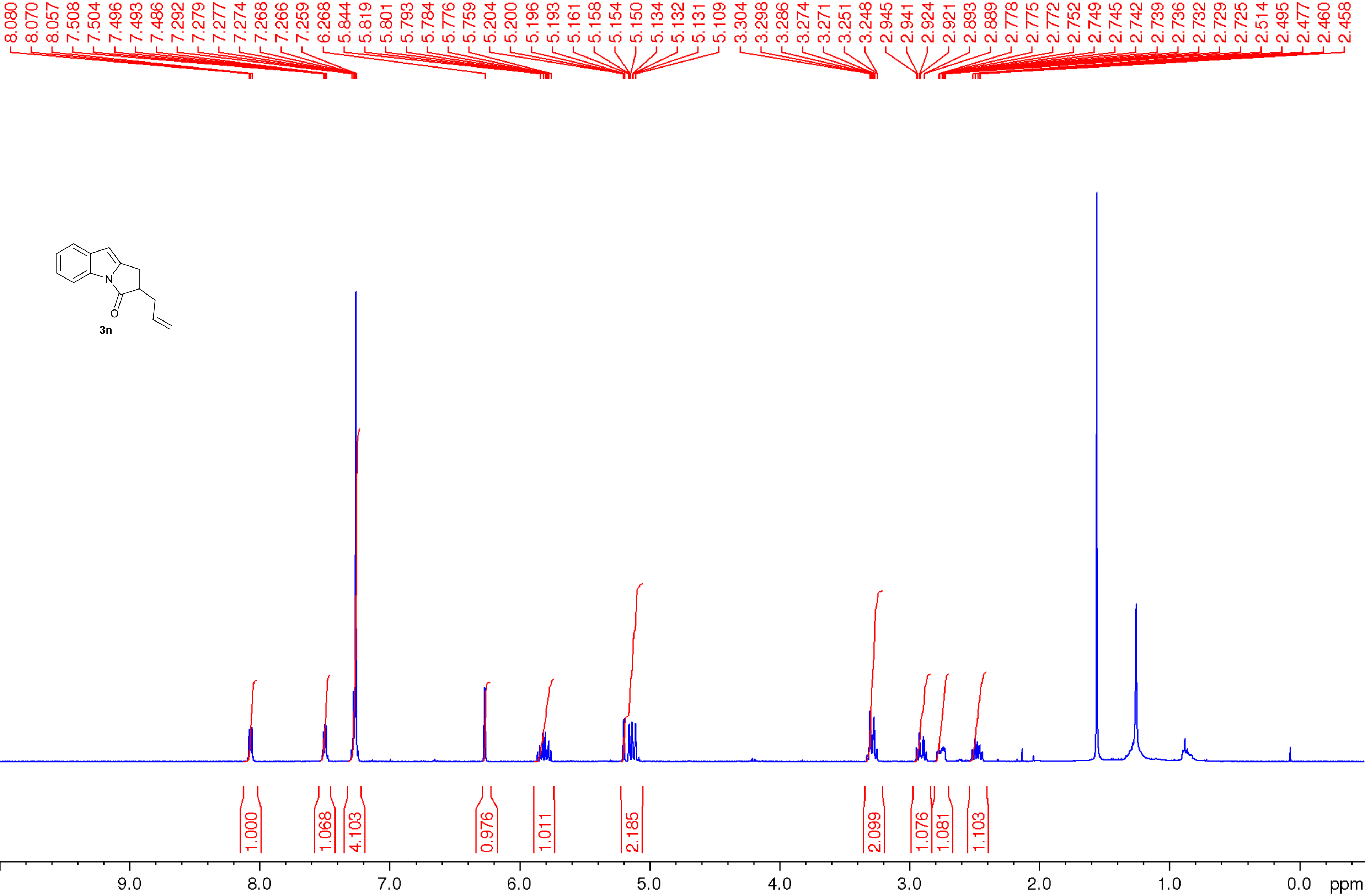
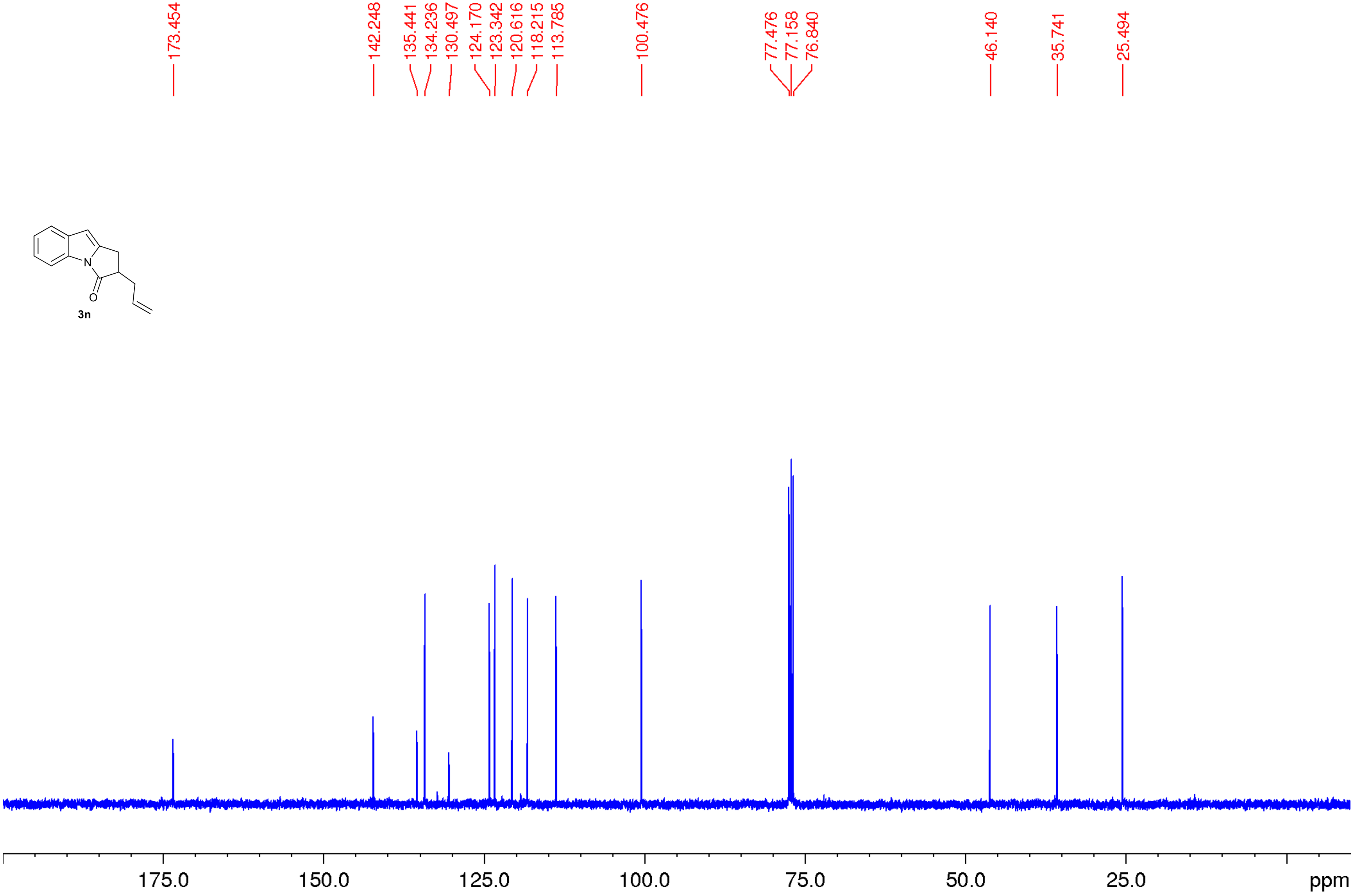


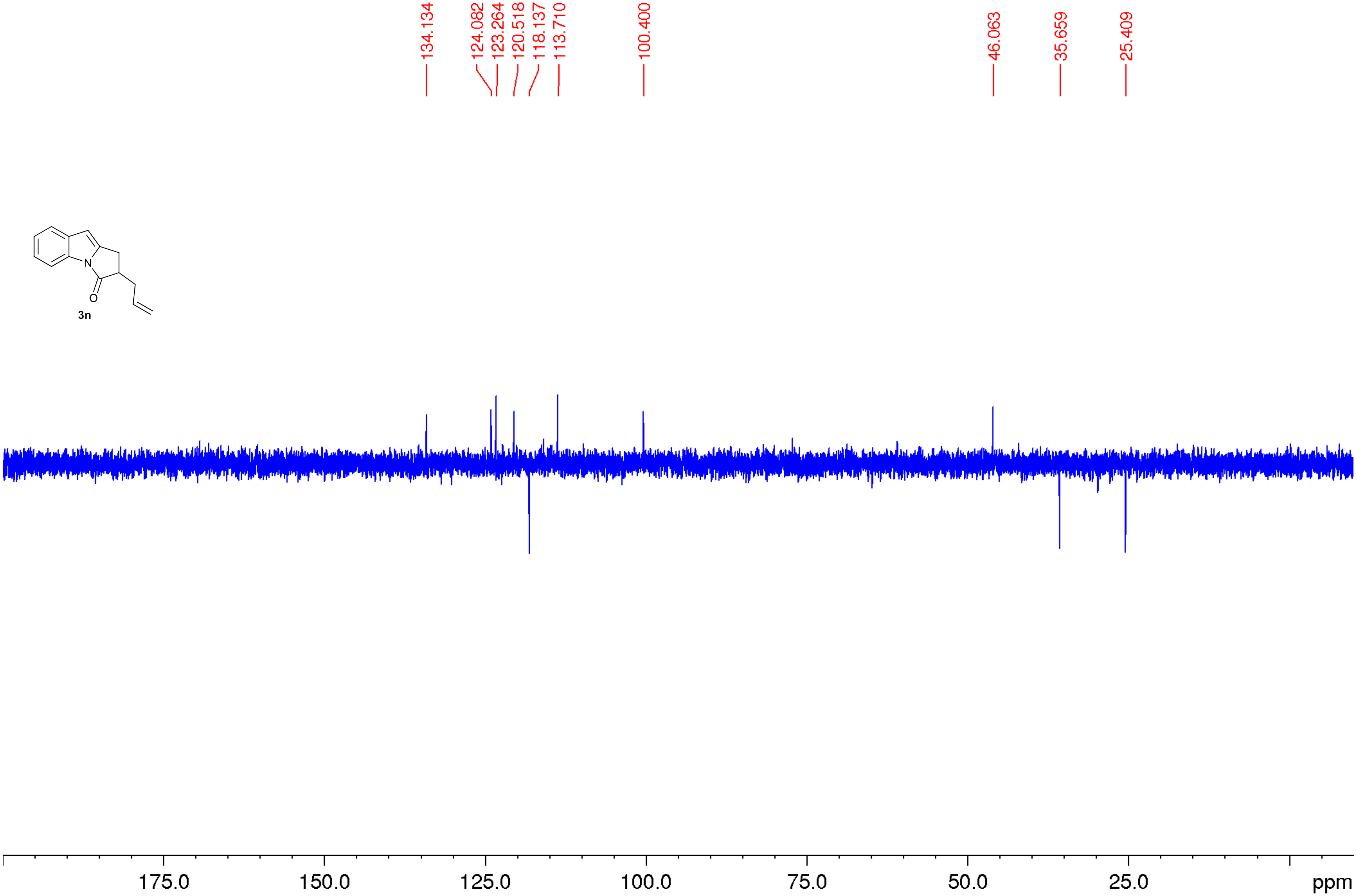
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)



^{13}C NMR-spectrum (100 MHz, CDCl$_3$)

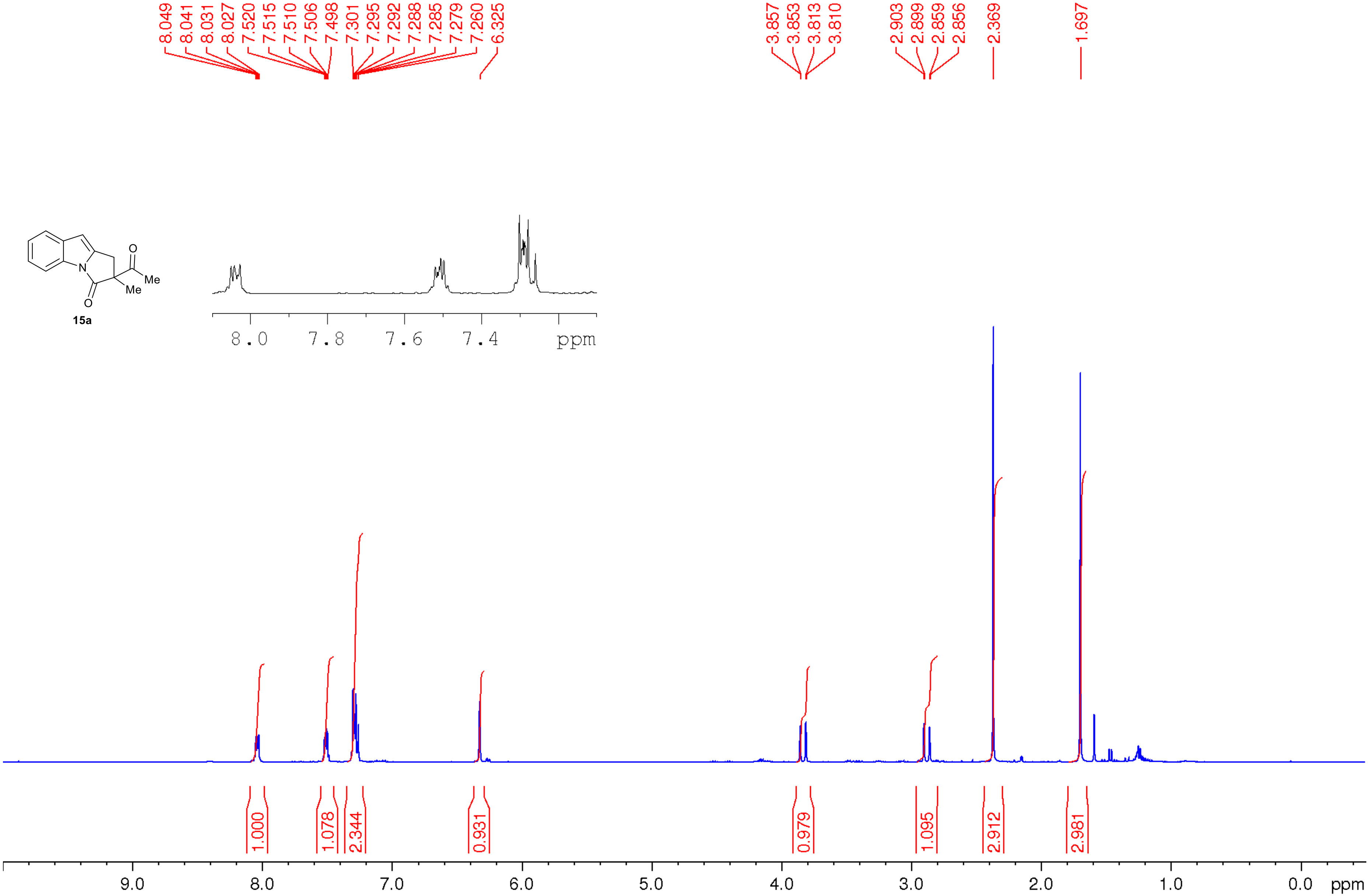

3n

DEPT 135 NMR-spectrum ($CDCl_3$)

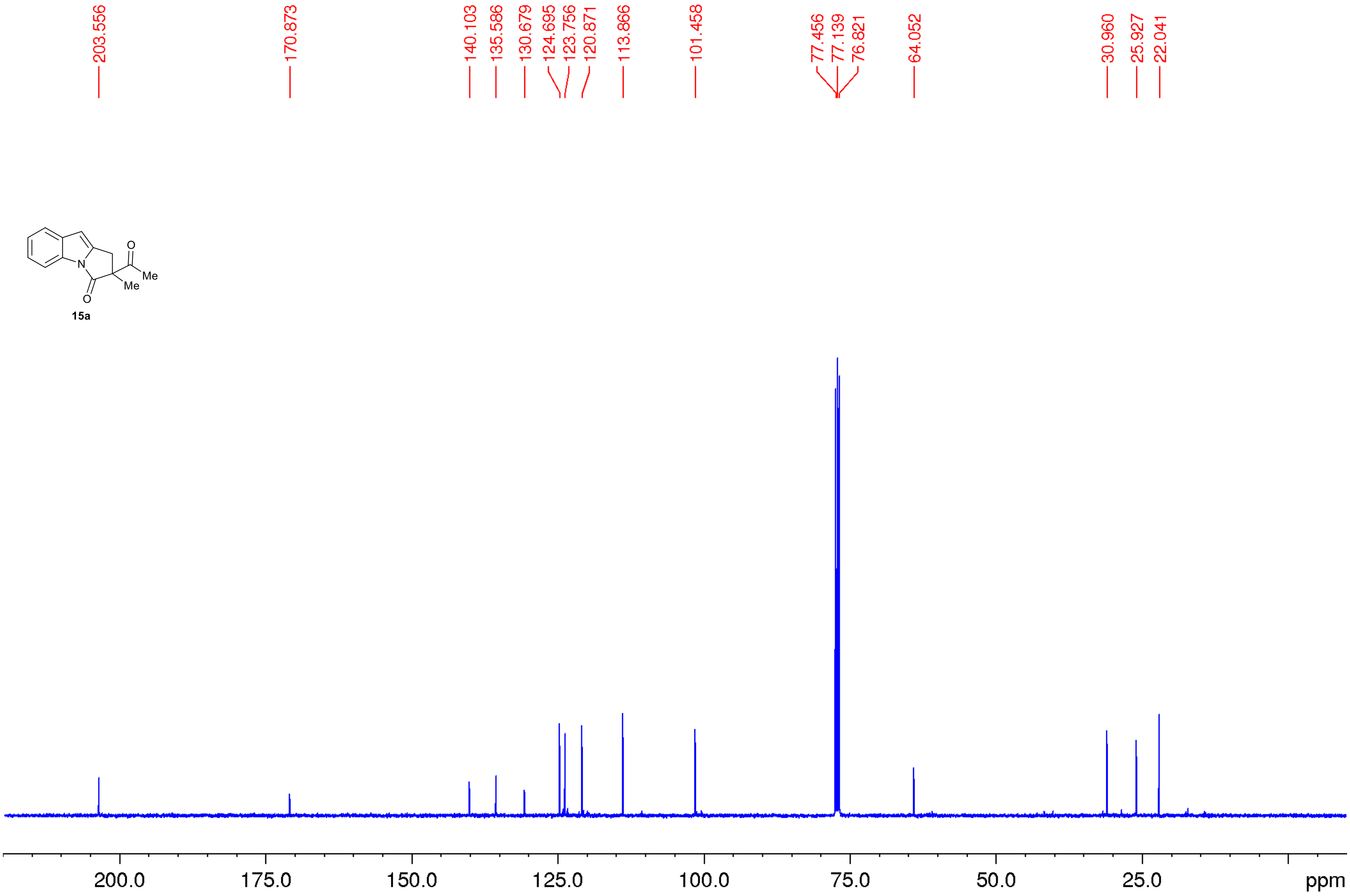


3n

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

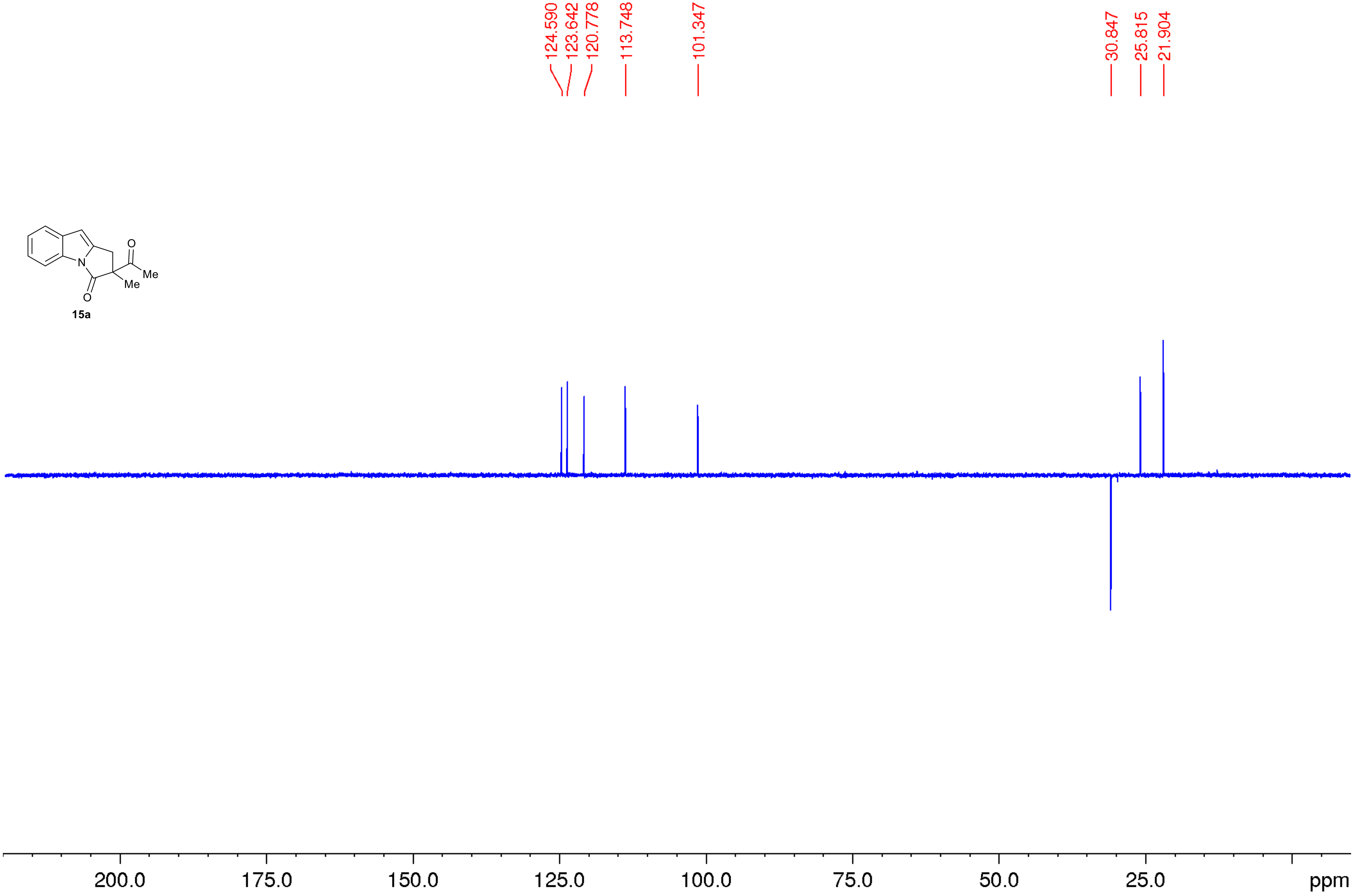


^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



15a

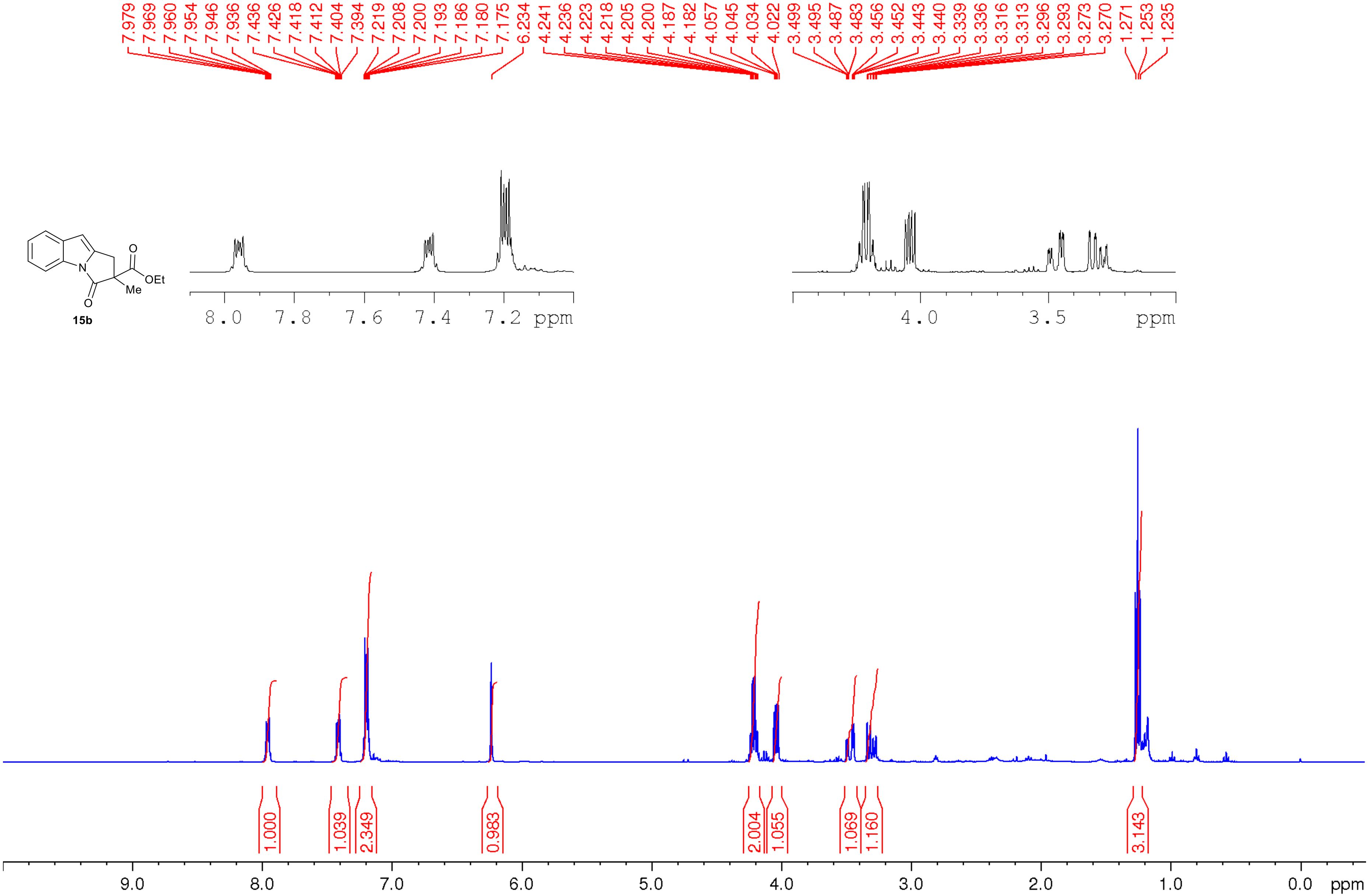
DEPT 135 NMR-spectrum ($CDCl_3$)



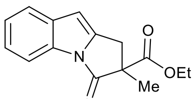
15a

^{1}H NMR-spectrum (400 MHz, $CDCl_3$)

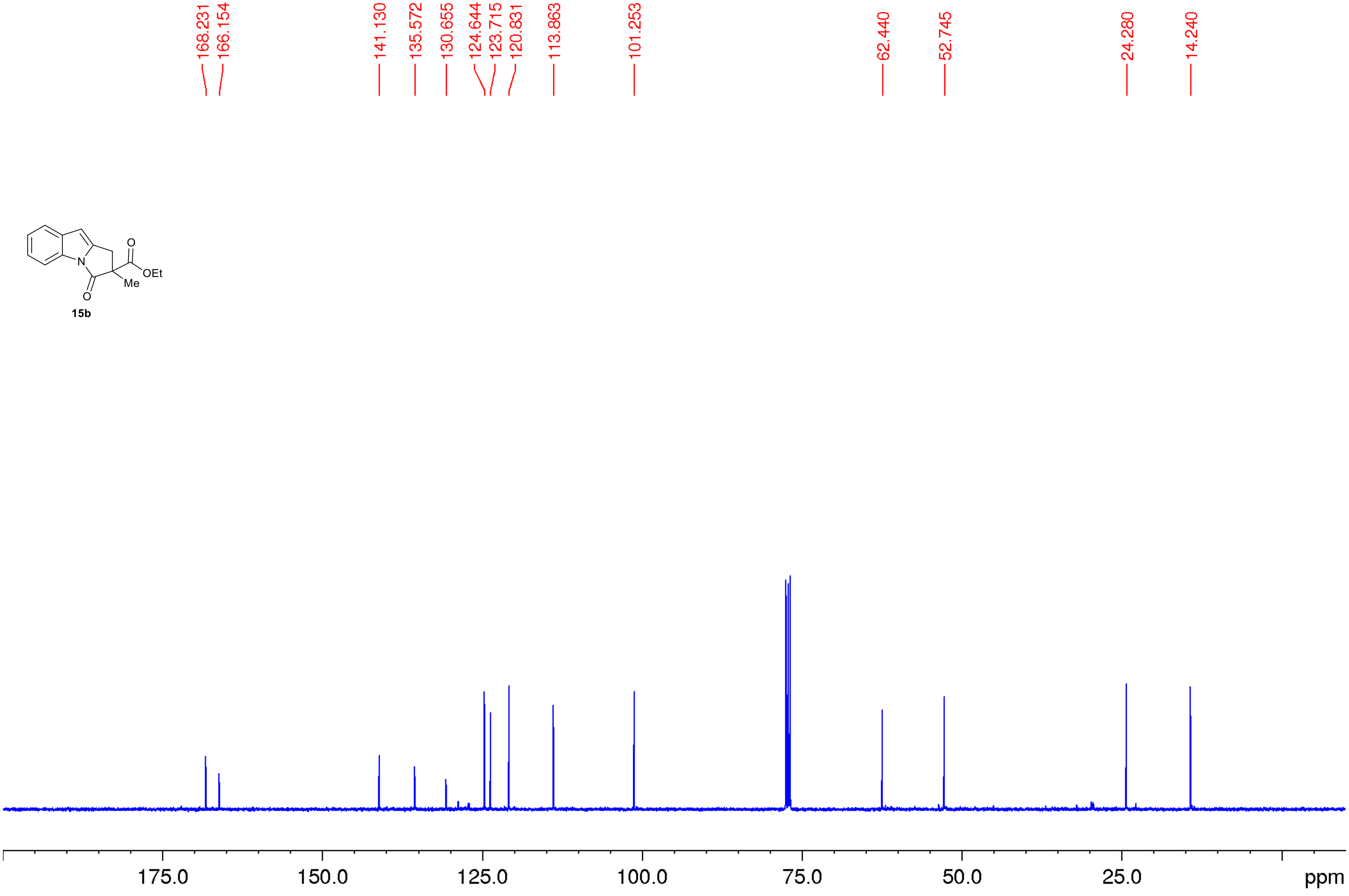
15b



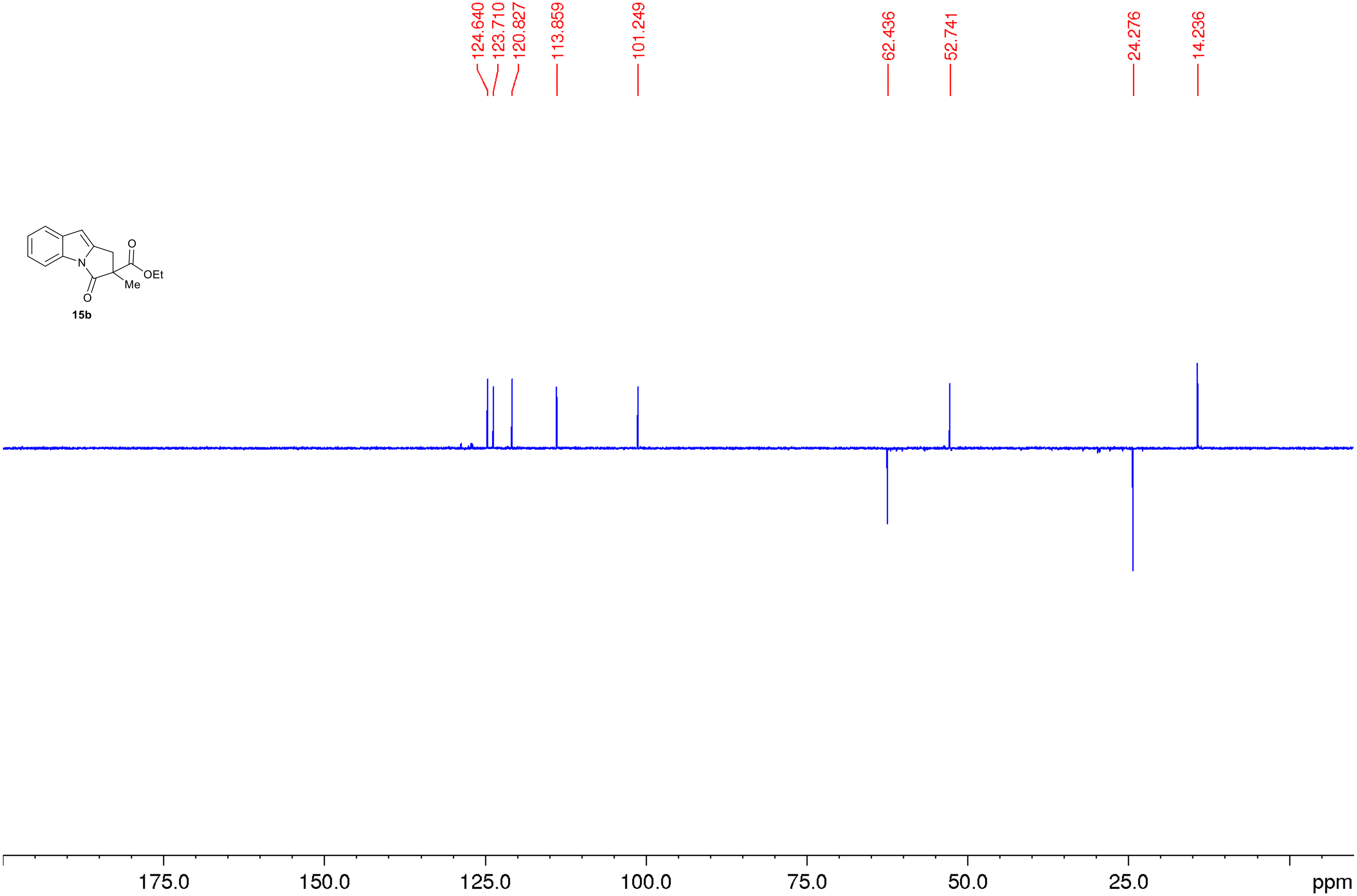
^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



15b

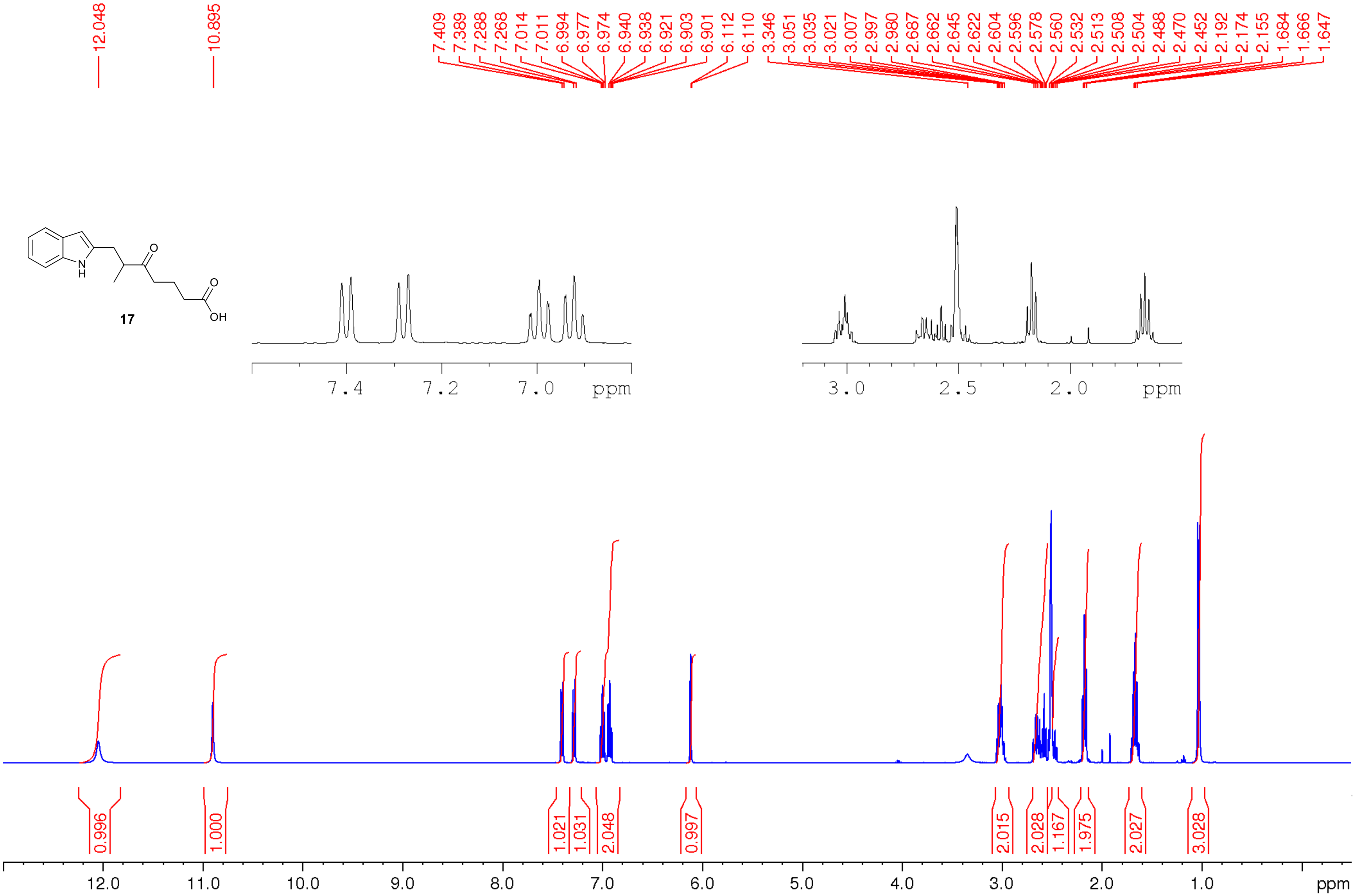


DEPT 135 NMR-spectrum ($CDCl_3$)



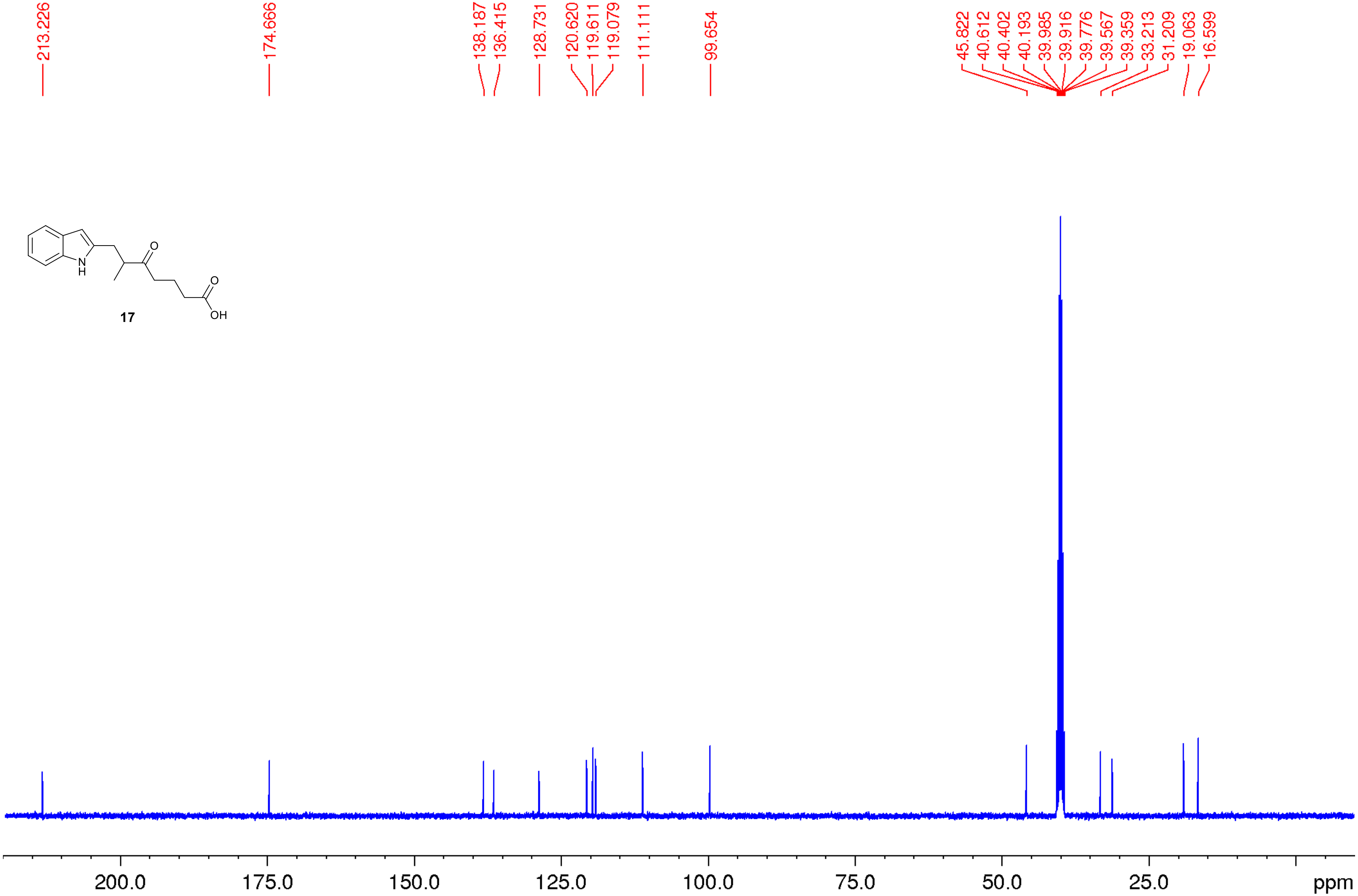
15b

^1H NMR-spectrum (400 MHz, DMSO-d_6)

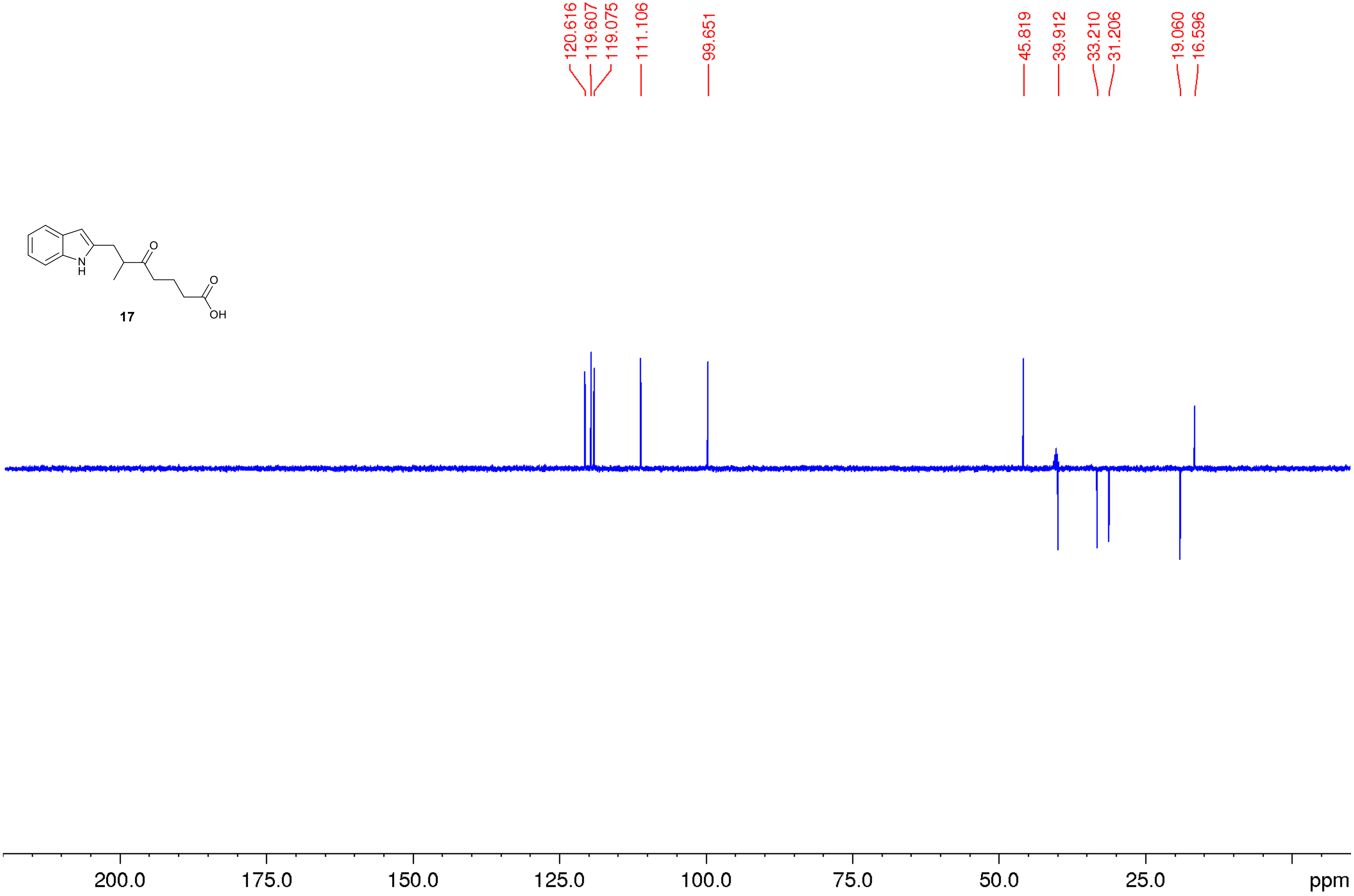


17

^{13}C NMR-spectrum (100 MHz, DMSO-d_6)

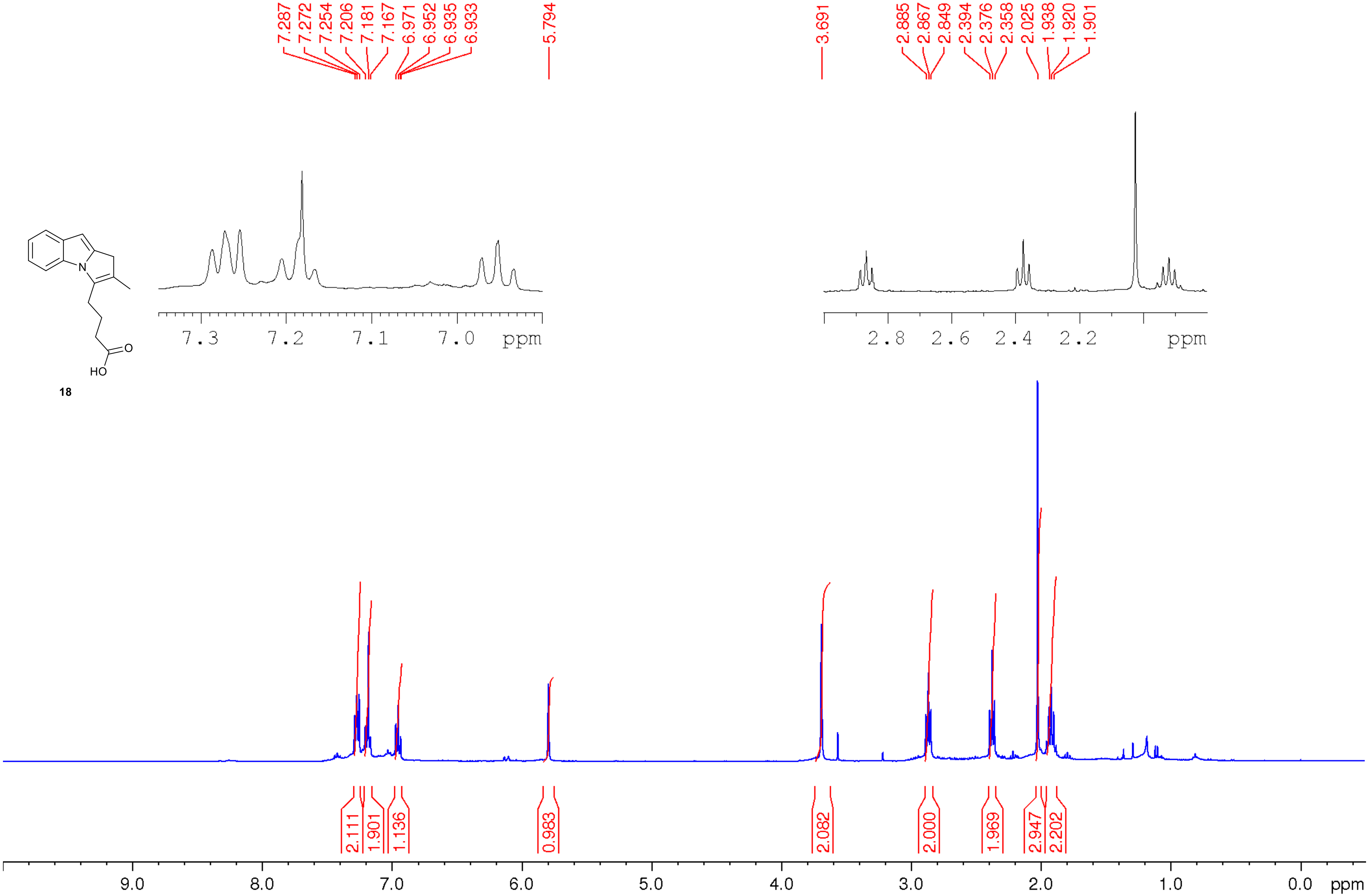


DEPT 135 NMR-spectrum (DMSO-d_6)

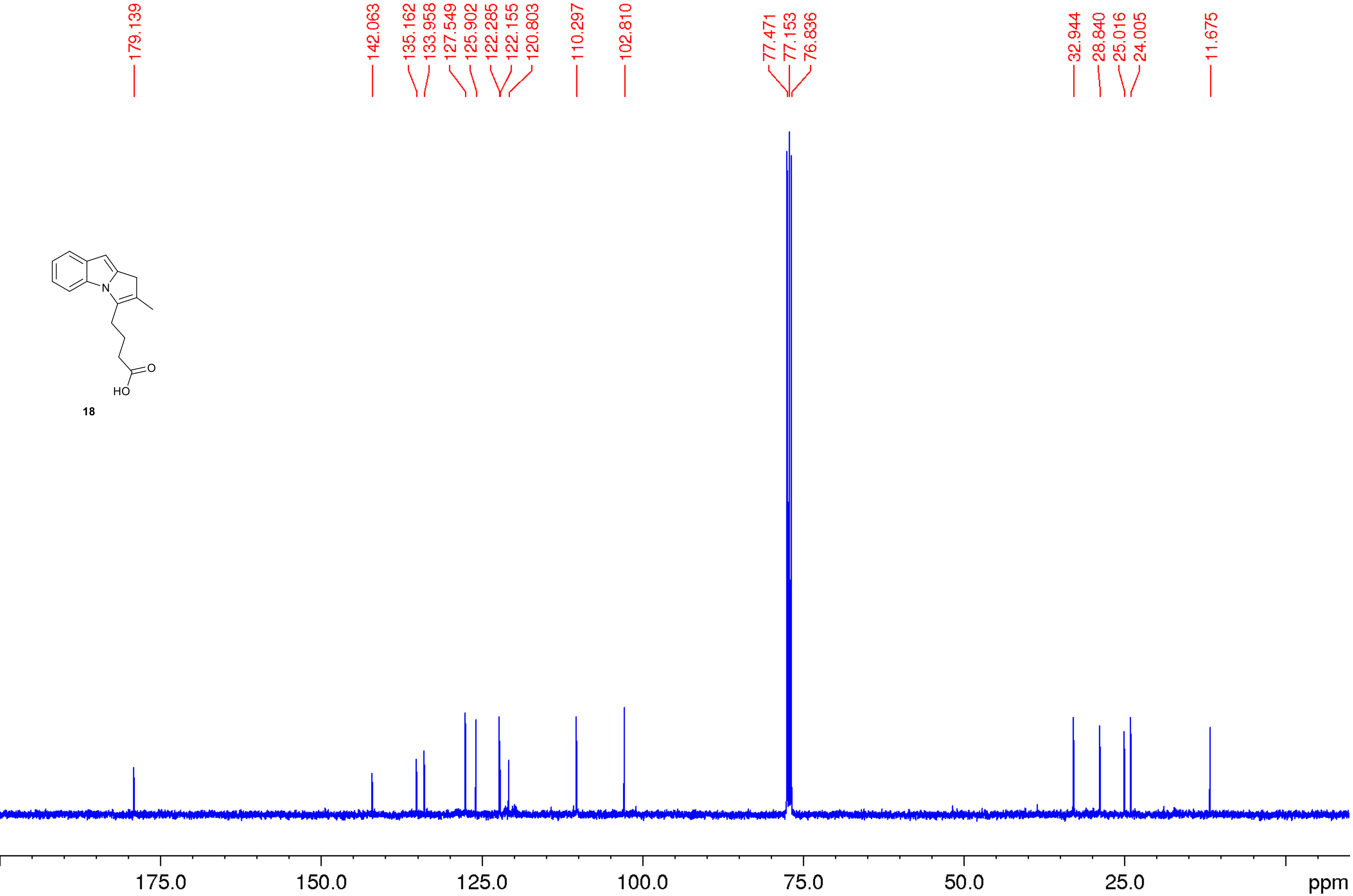


17

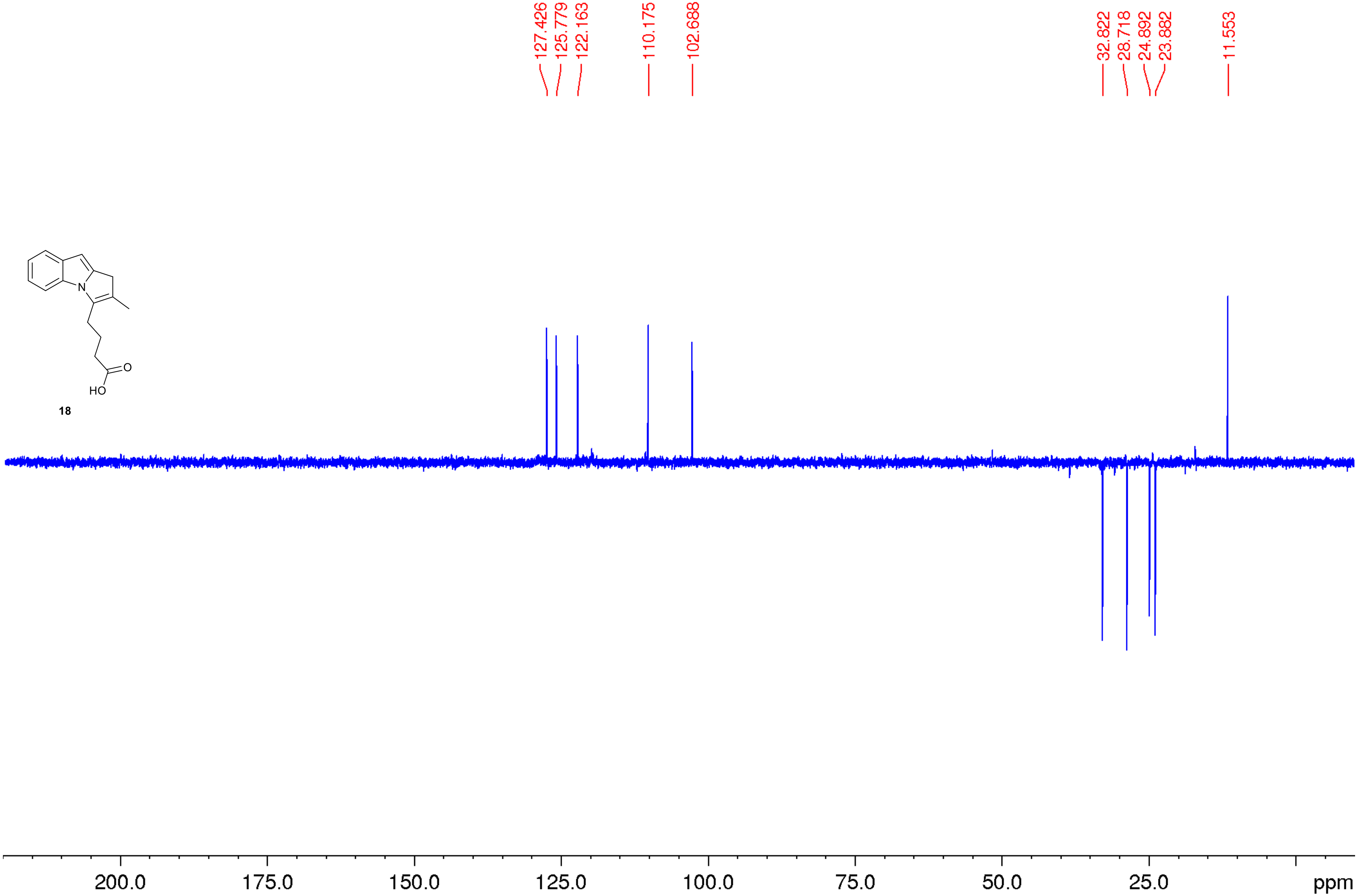
^{1}H NMR-spectrum (400 MHz, $CDCl_3$)


18

^{13}C NMR-spectrum (100 MHz, $CDCl_3$)



DEPT 135 NMR-spectrum ($CDCl_3$)

18