

## Supplementary Materials

# Synthesis of Functionalized 3*H*-pyrrolo-[1,2,3-*de*] Quinoxalines via Gold-Catalyzed Intramolecular Hydroamination of Alkynes

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## Contents

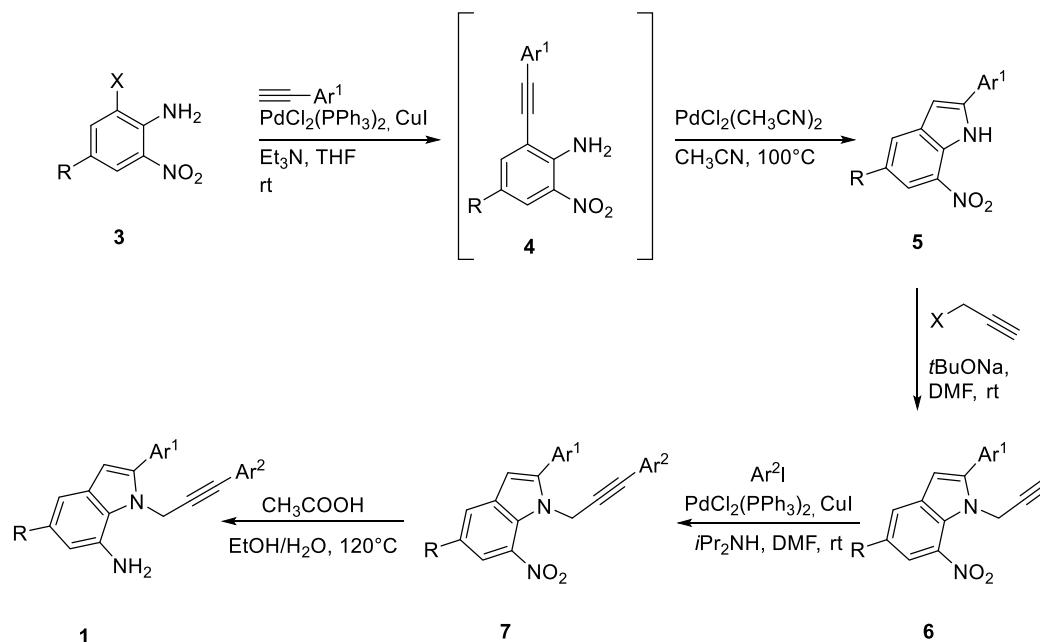
<b>1. SYNTHETIC PROCEDURES FOR STARTING MATERIALS .....</b>	<b>3</b>
1.1 General procedure for the preparation of substituted 1-(3-arylprop-2-yn-1-yl)-2-aryl-1 <i>H</i> -indol-7-amine <b>1</b> .....	3
1.1.a. Typical procedure for the preparation of 5- substituted-7-nitro-2-phenyl-1 <i>H</i> -indole <b>5</b> .....	3
1.1.b. Typical procedure for the preparation of substituted 7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1 <i>H</i> -indoles <b>6</b> .....	4
1.1.c. Typical procedure for the preparation of substituted 1-(3-arylprop-2-yn-1-yl)-7-nitro-2-phenyl-1 <i>H</i> -indoles <b>7</b> .....	4
1.1.d. Typical procedure for the synthesis of substituted 1-(3-arylprop-2-yn-1-yl)-2-aryl-1 <i>H</i> -indol-7-amine <b>1</b> .....	5
1.2. General procedure for the preparation of 1-(4-(3-(7-amino-5-methyl-2,3-diphenyl-1 <i>H</i> -indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one <b>11</b> .....	5
<b>2. PROCEDURE FOR THE SYNTHESIS OF COMPOUND 9d .....</b>	<b>7</b>
<b>3. CHARACTERIZATION DATA OF STARTING MATERIALS .....</b>	<b>9</b>
3.1 Characterization data of 5-substituted 7-nitro-2-aryl-1 <i>H</i> -indole <b>5</b> .....	9
3.2 Characterization data of 7-nitro-2-aryl-1-(prop-2-yn-1-yl)-1 <i>H</i> -indole <b>6</b> .....	9

3.3 Characterization data of 7-nitro-2-aryl-1-(3-phenylprop-2-yn-1-yl)-1 <i>H</i> -indole <b>7</b> .....	11
3.4 Characterization data of 2-aryl-1-(3-phenylprop-2-yn-1-yl)-1 <i>H</i> -indol-7-amines <b>1</b> .....	15
<b>4. REFERENCES</b> .....	<b>18</b>
<b>5. HF CALCULATION ON ISOMERS 2a and 2'a</b> .....	<b>19</b>
<b>6. COPIES OF NMR SPECTRA</b>	<b>198</b>

## 1. SYNTHETIC PROCEDURES FOR STARTING MATERIALS

### 1.1 General procedure for the preparation of substituted 1-(3-arylprop-2-yn-1-yl)-2-aryl-1H-indol-7-amine **1**

Starting materials **1** were prepared according to literature procedures through the four-step sequence of reactions depicted in scheme S1.

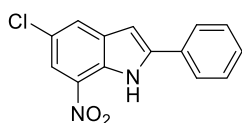


**Scheme S1.** Preparation of starting materials **1**

#### 1.1.a. Typical procedure for the preparation of 5- substituted-7-nitro-2-phenyl-1H-indole **5**

##### STEP 1: synthesis of 5-chloro-7-nitro-2-phenyl-1H-indole **5a**

In a 100 ml two-necked round bottom flask, equipped with a magnetic stirring bar,  $\text{PdCl}_2(\text{PPh}_3)_2$  (0.329 g, 0.469 mmol, 0.04 equiv.) and  $\text{CuI}$  (0.045 g, 0.234 mmol, 0.02 equiv.) were dissolved in 36.0 mL of THF and 1.56 mL of  $\text{Et}_3\text{N}$  at room temperature and under a nitrogen atmosphere. Then, 2-iodo-4-chloro-6-nitroaniline (3.5 g, 11.74 mmol, 1.0 equiv.) was added and, dropwise, phenylacetylene (1.93 mL, 17.61 mmol, 1.5 equiv.). The solution was stirred for 2h. After this time, the reaction mixture was diluted with  $\text{Et}_2\text{O}$ , and washed with a saturated solution of  $\text{NH}_4\text{Cl}$ ,  $\text{NaHCO}_3$ , and brine. The organic layer was separated, dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The residue, containing 4-chloro-2-nitro-6-(phenylethynyl)aniline **4a**, was transferred with 60 mL of MeCN in a two-necked 100-mL round bottom flask equipped with a condenser, and a magnetic stirring bar, then  $\text{PdCl}_2(\text{CH}_3\text{CN})_2$  was added. The solution was stirred for 2.5 h at 100 °C. After this time, the mixture was cooled to room temperature, concentrated under reduced pressure, purified by chromatography on  $\text{SiO}_2$  (25-40  $\mu\text{m}$ ), eluting with an 92/8 (v/v) *n*-hexane-AcOEt mixture ( $R_f$  = 0.26) to obtain 5-chloro-7-nitro-2-phenyl-1H-indole **5a** (2.57 g, 80 % yield).

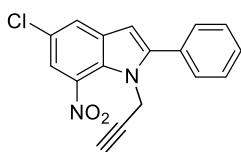


**5-chloro-7-nitro-2-phenyl-1H-indole **5a****: yield: 80%; orange solid; mp: 164 - 166 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  10.07 (bs, 1 H), 8.11 (d,  $J$  = 1.5 Hz, 1 H), 7.93 - 7.88 (m, 1 H), 7.74 (d,  $J$  = 7.8 Hz, 1 H), 7.53 (t,  $J$

= 7.3 Hz, 2 H), 7.45 (t,  $J$  = 7.3 Hz, 2 H), 6.90 (d,  $J$  = 2.4 Hz, 1 H), 5.05 (d,  $J$  = 2.4 Hz, 2 H), 2.20 (t,  $J$  = 2.4 Hz, 1 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  142.0 (C), 133.7 (C), 133.5 (C), 130.4 (C), 129.34 (CH), 129.27 (CH), 128.8 (C), 127.6 (CH), 125.7 (CH), 125.1 (C), 118.7 (CH), 100.1 (CH).

1.1.b. Typical procedure for the preparation of substituted 7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indoles 6  
STEP 2: synthesis of 5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6a

A 250 mL round bottom flask, equipped with a magnetic stirring bar, was charged with  $\text{tBuONa}$  (1.35 g, 14.02 mmol, 1.5 equiv) and 90 mL of anhydrous DMF. The reaction mixture was cooled at  $0^\circ\text{C}$  and 5-chloro-7-nitro-2-phenyl-1H-indole (2.4 g, 9.35 mmol, 1.0 equiv) was added dropwise. Then, propargyl bromide (1.21 mL, 14.02 mmol, 1.5 equiv) was added and the solution was warmed to room temperature and stirred for 6 h. After this time, the reaction mixture was diluted with  $\text{Et}_2\text{O}$  and washed with saturated solution of  $\text{NaHCO}_3$  and brine. The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The residue was purified by chromatography on  $\text{SiO}_2$  (25-40  $\mu\text{m}$ ), eluting with an 96/4 (v/v)  $n$ -hexane-AcOEt mixture ( $R_f$  = 0.25) to obtain 5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole **6a** (2.324 g, 80 % yield).

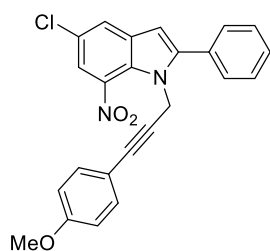


**5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6a:** 80 % yield; brown solid; mp  $103 - 104^\circ\text{C}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J$  = 1.9 Hz, 1 H), 7.87 (d,  $J$  = 1.9 Hz, 1 H), 7.58-7.50 (m, 5 H), 6.70 (s, 1 H), 5.05 (d,  $J$  = 2.4 Hz, 2 H), 2.20 (t,  $J$  = 2.4 Hz, 1 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  146.8 (C), 137.3 (C), 134.3 (C), 130.6 (C), 129.6 (CH), 129.4 (CH), 129.1 (CH), 127.1 (C), 126.0 (CH), 125.2 (C), 119.8 (CH), 104.1 (CH), 77.1 (C), 74.4 (CH), 37.1 ( $\text{CH}_2$ ).

1.1.c. Typical procedure for the preparation of substituted 1-(3-arylprop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indoles 7

STEP 3: synthesis of 5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7c

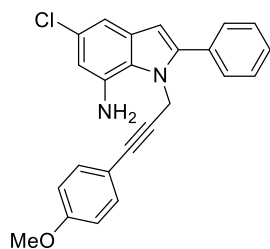
In a two-necked 50-mL round bottom flask, equipped with a magnetic stirring bar,  $\text{PdCl}_2(\text{PPh}_3)_2$  (0.084 g, 0.119 mmol, 0.04 equiv.) and  $\text{CuI}$  (0.011 g, 0.0597 mmol, 0.02 equiv.) were dissolved in 12.3 mL of  $i\text{Pr}_2\text{NH}$  and 6.1 mL of DMF at room temperature and under nitrogen; then, 4-iodoanisole (0.839 g, 3.584 mmol, 1.2 equiv.) and 5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole (0.928 g, 2.98 mmol, 1.0 equiv.) were added and the resulting mixture was stirred for 24 h. After this time, the mixture was diluted with  $\text{Et}_2\text{O}$  and washed with a saturated solution of  $\text{NH}_4\text{Cl}$ , a saturated solution of  $\text{NaHCO}_3$ , and with brine. The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The residue was purified by chromatography on  $\text{SiO}_2$  (25-40  $\mu\text{m}$ ), eluting with a 93/7 (v/v)  $n$ -hexane/AcOEt mixture ( $R_f$  = 0.27) to obtain 5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole **7c** (0.860 g, 70% yield).



**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7c:** 70 % yield; yellow solid; mp 133 - 134 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.91 (d,  $J$  = 1.9 Hz, 1 H), 7.87 (d,  $J$  = 1.9 Hz, 1 H), 7.60 - 7.50 (m, 5 H), 7.21 (d,  $J$  = 8.8 Hz, 2 H), 6.78 (d,  $J$  = 8.8 Hz, 2 H), 6.70 (s, 1 H), 5.23 (s, 2 H), 3.78 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  159.9 (C), 146.7 (C), 138.2 (C), 137.5 (C), 134.2 (C), 133.2 (CH), 130.8 (C), 129.6 (CH), 129.3 (CH), 129.0 (CH), 127.1 (C), 125.8 (CH), 124.9 (C), 119.6 (CH), 113.8 (CH), 103.8 (CH), 86.1 (C), 80.9 (C), 55.2 ( $\text{CH}_3$ ), 38.2 ( $\text{CH}_2$ ).

**1.1.d. Typical procedure for the synthesis of substituted 1-(3-arylprop-2-yn-1-yl)-2-aryl-1H-indol-7-amine 1**  
**STEP 4: synthesis of 5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1c**

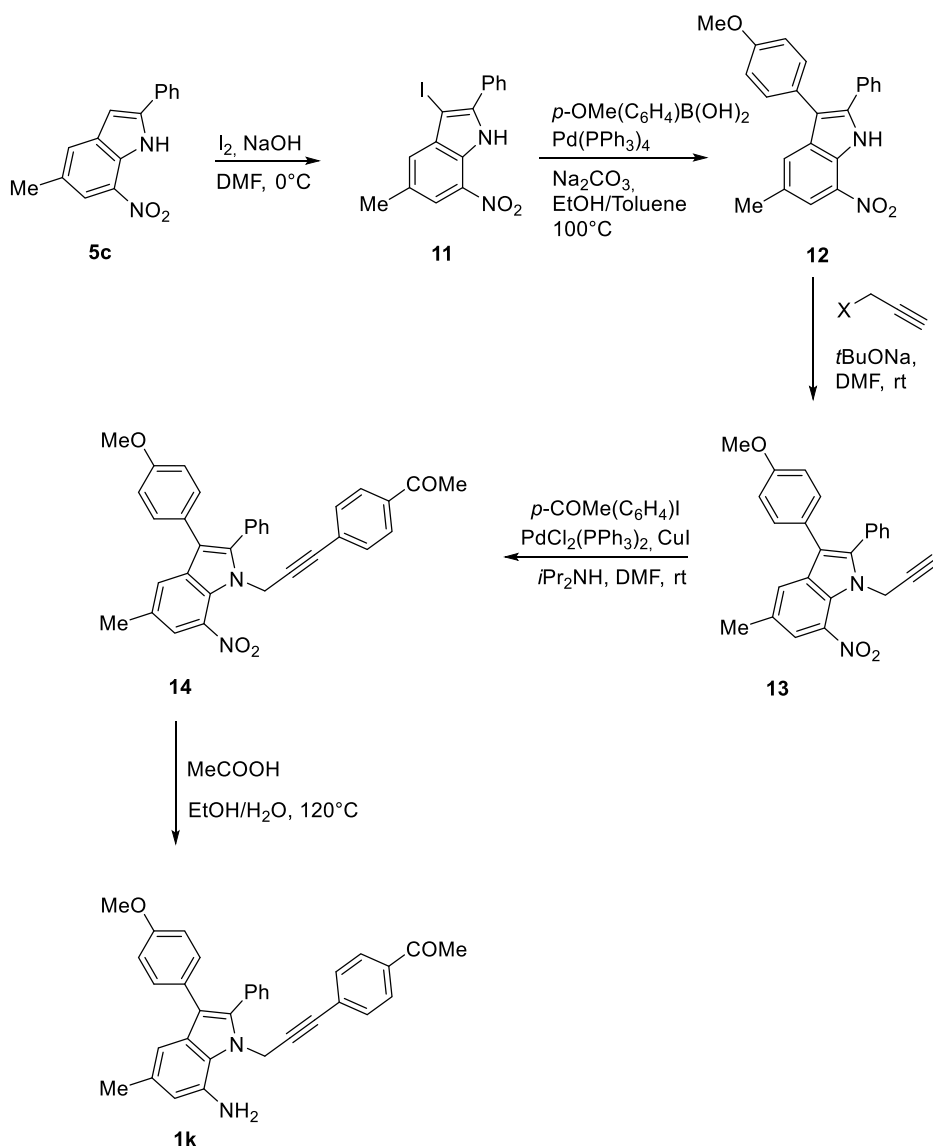
In a 50 mL Carousel Tube Reactor (Radely Discovery Technology), equipped with a magnetic stirring bar, 5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole (0.180 g, 0.431 mmol, 1.0 equiv.) was added to a solution of EtOH/ $\text{H}_2\text{O}$  (3:1) and stirred at 120°C for 10 minutes. Then, 51  $\mu\text{l}$  of acetic acid and 72 mg of Fe (0) (0.431 mmol, 1.0 equiv.) were added in three portions every 15 minutes. The reaction mixture was then stirred for 2 hours before being cooled at room temperature, and concentrated under reduced pressure. Subsequently, the mixture was diluted with Et $_2\text{O}$  and washed with a saturated solution of  $\text{NaHCO}_3$ , and with brine. The organic layer was dried over  $\text{Na}_2\text{SO}_4$ , filtered, and concentrated under reduced pressure. The residue was purified by filtration on a pad of celite eluting with DCM to obtain 5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine **1a** (0.140 g, 85% yield)



**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1c:** 85% yield; orange solid; mp 91 - 92 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.71 - 7.68 (m, 2 H), 7.55 - 7.49 (m, 2 H), 7.48 - 7.44 (m, 1 H), 7.42 (d,  $J$  = 8.8 Hz, 2 H), 7.09 (d,  $J$  = 1.8 Hz, 1 H), 6.89 (d,  $J$  = 8.8 Hz, 2H), 6.54 (d,  $J$  = 1.8 Hz, 1 H), 6.47 (s, 1 H), 5.17 (s, 2 H), 4.35 (bs, 2 H), 3.84 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  160.1 (C), 143.2 (C), 134.0 (C), 133.2 (CH), 131.9 (C), 130.8 (C), 129.3 (CH), 128.7 (CH), 128.3 (CH), 127.1 (C), 126.3 (C), 114.1 (CH), 113.8 (C), 111.3 (CH), 110.1 (CH), 102.4 (CH), 86.6 (C), 84.9 (C), 55.3 ( $\text{CH}_3$ ), 36.5 ( $\text{CH}_2$ ).

**1.2. General procedure for the preparation of 1-(4-(3-(7-amino-5-methyl-2,3-diphenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1l**

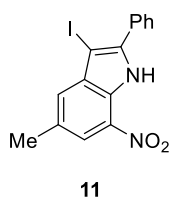
Starting material 1l was prepared according to literature procedures from 5-methyl-7-nitro-2-phenyl-1H-indole through the sequence of reactions depicted in scheme S2.



## Scheme S2. Preparation of starting materials **1k**

### STEP 1: synthesis of 3-iodo-5-methyl-7-nitro-2-phenyl-1H-indole

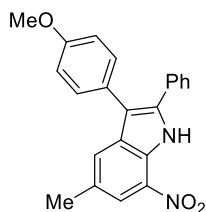
To a solution of 5-methyl-7-nitro-2-phenyl-1H-indole **5c** (1.0 g, 3.982 mmol, 1.0 equiv.) in DMF (8.0 mL) KOH (0.671 g, 11.94 mmol, 3.0 equiv.) was added at 0°C and the resulting mixture was stirred for 10 minutes before a solution of iodine (1.061 g, 4.181 mmol, 1.05 equiv.) in DMF (10.0 mL) was added dropwise over 5 minutes. After 1 h, the mixture was poured into a saturated solution of NH<sub>4</sub>Cl and Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> to precipitate the product. The solid material was filtered off, solubilized in Et<sub>2</sub>O, washed with water and dried over Na<sub>2</sub>SO<sub>4</sub>. After filtration, the mixture was concentrated under reduced pressure to give of 3-iodo-5-methyl-7-nitro-2-phenyl-1H-indole as an orange powder (0.97 g, 65% yield).



**3-iodo-5-methyl-7-nitro-2-phenyl-1H-indole 11:** 65% yield; orange solid; mp: 143-145 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 10.06 (bs, 1 H), 8.07 (s, 1 H), 7.88-7.82 (m, 2 H), 7.67 (s, 1 H), 7.61-7.47 (m, 3 H), 2.59 (s, 3 H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 140.6 (C), 135.3 (C), 132.4 (C), 131.0 (C), 130.3 (C), 129.9 (CH), 129.4 (CH), 128.9 (CH), 128.6 (C), 128.5 (CH), 121.0 (CH), 58.4 (C), 21.2 (CH<sub>3</sub>).

STEP 2: synthesis of 5-methyl-7-nitro-2,3-diphenyl-1H-indole

In a three-necked round bottom flask, equipped with a condenser and magnetic stirring bar, [Pd(PPh<sub>3</sub>)<sub>4</sub>] (115.4 mg, 0.10 mmol, 0.05 equiv.) was dissolved at room temperature in 25 mL of EtOH/Toluene (2:1) under argon; then, 3-iodo-5-methyl-7-nitro-2-phenyl-1H-indole (0.756 g, 2.0 mmol, 1.0 equiv.), 4-methoxyphenylboronic acid (0.912 g, 6.0 mmol, 3.0 equiv.), and Na<sub>2</sub>CO<sub>3</sub> (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<sub>2</sub>Cl<sub>2</sub> and washed with brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, and concentrated under reduced pressure. The residue was purified by chromatography on SiO<sub>2</sub> (25-40 μm), eluting with an 80/20 (v/v) *n*-hexane-AcOEt mixture (R<sub>f</sub> = 0.22) to obtain the desired product (0.609 g, 85% yield)



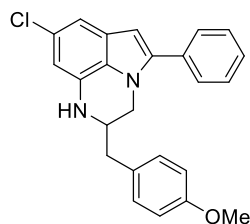
12

**3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1H-indole 12:** 85% yield; yellow solid; mp: 133-135 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 9.89 (bs, 1 H), 8.03 (s, 1 H), 7.75 (s, 1 H), 7.53-7.46 (m, 2 H), 7.43-7.31 (m, 5 H), 6.99 (d, *J* = 8.7 Hz, 1 H), 3.89 (s, 3 H), 2.52 (s, 3 H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 158.7 (C), 136.1 (C), 133.1 (C), 132.3 (C), 131.5 (C), 131.3 (CH), 129.6 (C), 128.9 (CH), 128.7 (C), 128.4 (CH), 128.1 (CH), 127.9 (CH), 125.9 (C), 120.3 (CH), 115.0 (C), 114.3 (CH), 55.3 (CH<sub>3</sub>), 21.1 (CH<sub>3</sub>).

STEPS 3 – 5 were carried out with procedures described in paragraphs 2.1b -d

## 2. PROCEDURE FOR THE SYNTHESIS OF COMPOUND 9d

A flame dried 50 mL Carousel Tube Reactor (Radely Discovery Technology), equipped with a magnetic stirring bar, was charged with 8-chloro-2-(4-methoxybenzyl)-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline **2c** (50.0 mg, 0.13 mmol, 1.0 equiv) dissolved in anhydrous 2 mL of THF under argon. Then, a solution of LiAlH<sub>4</sub> 2 M in THF (108 μL, 0.26 mmol, 2.0 equiv.) was added at 0°C and the mixture was stirred for 15 minutes at 80°C. After this time, the mixture was diluted with Et<sub>2</sub>O and washed with a saturated NaHCO<sub>3</sub> solution and brine. The organic layer was dried over Na<sub>2</sub>SO<sub>4</sub>, filtered, concentrated under reduced pressure. The resulting residue was purified by chromatography on SiO<sub>2</sub> (25-40 μm), eluting with a 93/7 (v/v) *n*-hexane/AcOEt mixture (R<sub>f</sub> = 0.27) to obtain 8-chloro-2-(4-methoxybenzyl)-5-phenyl-2,3-dihydro-1H-pyrrolo[1,2,3-*de*]quinoxaline (49.5 mg, 98 % yield).

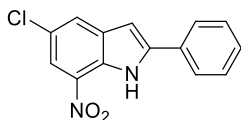


**8-chloro-2-(4-methoxybenzyl)-5-phenyl-2,3-dihydro-1H-pyrrolo[1,2,3-*de*]quinoxaline 9d:** 98 % yield; brown oil;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ): 7.53-7.42 (m, 4 H), 7.44-7.35 (m, 3 H), 7.08 (d,  $J = 1.8$  Hz, 1 H), 6.93 (d,  $J = 8.8$  Hz, 2 H), 6.48 (s, 1 H), 6.47 (d,  $J = 1.8$  Hz, 1 H), 4.76 (bs, 1 H), 4.45 - 4.33 (m, 2 H), 3.84 (s, 3 H), 3.74-3.64 (m, 1 H), 2.45-2.28 (m, 2 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  159.2 (C), 143.7 (C), 136.6 (C), 135.9 (C), 132.7 (C), 131.7 (C), 129.3 (CH), 128.6 (CH), 128.1 (CH), 127.7 (CH), 127.4 (C), 126.2 (C), 114.2 (CH), 110.4 (CH), 108.5 (CH), 103.4 (CH), 62.4 (CH), 55.4 ( $\text{CH}_3$ ), 46.6 ( $\text{CH}_2$ ), 38.6 ( $\text{CH}_2$ ).

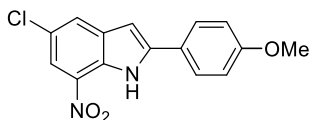


### 3. CHARACTERIZATION DATA OF STARTING MATERIALS

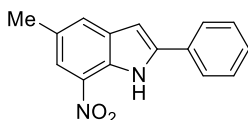
#### 3.1 Characterization data of 5-substituted 7-nitro-2-aryl-1H-indole 5



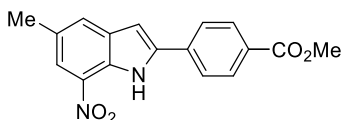
**5-chloro-7-nitro-2-phenyl-1H-indole 5a** 80 % yield; orange solid; mp: 164 - 166 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 10.07 (bs, 1 H), 8.11 (d, *J* = 1.5 Hz, 1 H), 7.93 - 7.88 (m, 1 H), 7.74 (d, *J* = 7.8 Hz, 1 H), 7.53 (t, *J* = 7.3 Hz, 2 H), 7.45 (t, *J* = 7.3 Hz, 2 H), 6.90 (d, *J* = 2.4 Hz, 1 H), 5.05 (d, *J* = 2.4 Hz, 2 H), 2.20 (t, *J* = 2.4 Hz, 1 H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 142.0 (C), 133.7 (C), 133.5 (C), 130.4 (C), 129.34 (CH), 129.27 (CH), 128.8 (C), 127.6 (CH), 125.7 (CH), 125.1 (C), 118.7 (CH), 100.1 (CH).



**5-chloro-2-(4-methoxyphenyl)-7-nitro-1H-indole 5b**: 72 % yield; yellow - orange solid; mp: 196 - 198 °C; <sup>1</sup>H NMR (400.13 MHz) (DMSO- *d*<sub>6</sub>): δ 11.78 (bs, 1 H), 8.13 (d, *J* = 1.3 Hz, 1 H), 8.05 (d, *J* = 1.3 Hz, 1 H), 8.01 (d, *J* = 8.7 Hz, 2 H), 7.12 (d, *J* = 8.7 Hz, 2 H), 7.1 (s, 1 H), 3.89 (s, 3 H); <sup>13</sup>C NMR (100.6 MHz) (DMSO- *d*<sub>6</sub>): δ 160.3 (C), 143.8 (C), 134.6 (C), 133.0 (C), 128.8 (CH), 128.7 (C), 127.0 (CH), 123.6 (C), 123.3 (C), 117.5 (CH), 114.7 (CH), 99.9 (CH), 55.8 (CH<sub>3</sub>).

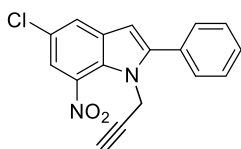


**5-methyl-7-nitro-2-phenyl-1H-indole 5c**: 97 % yield; yellow solid; mp 172 - 174 °C <sup>[1]</sup>; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 9.87 (s, 1H), 7.88 (s, 1H), 7.73–7.57 (m, 3H), 7.56–7.24 (m, 3H), 6.78 (s, 1H), 2.47 (s, 3H); <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>) δ 140.5 (C), 133.04 (C), 132.3 (C), 131.0 (C), 129.5 (C), 129.2 (CH), 128.8 (C), 128.8 (CH), 128.7 (CH), 125.5 (CH), 119.9 (CH), 100.0 (CH), 21.1 (CH<sub>3</sub>).

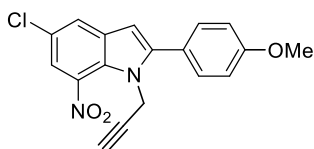


**methyl 4-(5-methyl-7-nitro-1H-indol-2-yl)benzoate 5d** 98 % yield; yellow solid; mp: 244 - 246 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 9.96 (s, 1H), 8.08 (d, *J* = 8.2 Hz, 2H), 7.93 (s, 1H), 7.72 (d, *J* = 8.7 Hz, 3H), 6.90 (d, *J* = 1.7 Hz, 1H), 3.89 (s, 3H), 2.46 (s, 3H); <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>) δ 166.5 (C), 139.1 (C), 135.1 (C), 132.8 (C), 132.5 (C), 130.5 (CH), 129.9 (C), 129.9 (C), 129.1 (CH), 125.2 (CH), 120.7 (CH), 101.7 (CH), 52.3 (CH<sub>3</sub>), 21.1 (CH<sub>3</sub>).

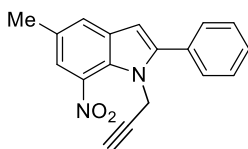
#### 3.2 Characterization data of 7-nitro-2-aryl-1-(prop-2-yn-1-yl)-1H-indole 6



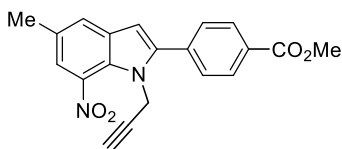
**5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6a:** 80 % yield; brown solid; mp: 114 - 116 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 7.92 (d, *J* = 1.9 Hz, 1 H), 7.87 (d, *J* = 1.9 Hz, 1 H), 7.58-7.50 (m, 5 H), 6.70 (s, 1 H), 5.05 (d, *J* = 2.4 Hz, 2 H), 2.20 (t, *J* = 2.4 Hz, 1 H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 160.6 (C), 147.1 (C), 137.3 (C), 134.5 (C), 131.4 (CH), 126.7 (C), 126.3 (CH), 124.4 (C), 122.6 (C), 119.3 (CH), 115.1 (CH), 104.0 (CH), 78.0 (C), 77.5 (CH), 55.8 (CH<sub>3</sub>), 37.2 (CH<sub>2</sub>).



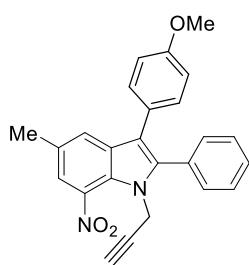
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(prop-2-yn-1-yl)-1H-indole 6b:** 50 % yield; yellow solid; mp: 146 - 148 °C; <sup>1</sup>H NMR (400.13 MHz) (DMSO *d*<sub>6</sub>): δ 8.12 (d, *J* = 1.7 Hz, 1 H), 7.96 (d, *J* = 1.7 Hz, 1 H), 7.56 (d, *J* = 8.6 Hz, 2 H), 7.14 (d, *J* = 8.6 Hz, 2 H), 6.80 (s, 1 H), 4.97 (d, *J* = 2.4 Hz, 2 H), 3.85 (s, 1 H), 3.33 - 3.30 (m, 1 H); <sup>13</sup>C NMR (100.6 MHz) (DMSO *d*<sub>6</sub>): δ 160.5 (C), 146.8 (C), 137.2 (C), 134.4 (C), 130.9 (CH), 125.7 (CH), 125.1 (C), 122.8 (C), 119.5 (CH), 114.7 (C), 114.5 (CH), 103.5 (CH), 77.2 (C), 74.4 (CH), 55.45 (CH<sub>3</sub>), 37.1 (CH<sub>2</sub>).



**5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6c:** 88 % yield; brown solid; mp: 94 - 96 °C; <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>) δ 7.63 (s, 1H), 7.53 (s, 1H), 7.49-7.10 (m, 5H), 6.50 (s, 1H), 4.90 (d, *J* = 2.3 Hz, 2H), 2.35 (s, 3H), 1.98 (t, *J* = 2.3 Hz, 1H). <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 145.6 (C), 137.1 (C), 133.7 (C), 131.3 (C), 129.9 (C), 129.6 (CH), 129.0 (CH), 129.0 (CH), 127.4 (C), 127.1 (CH), 121.2 (CH), 104.3 (CH), 77.68 (C), 73.93 (C), 36.94 (CH<sub>2</sub>), 20.83 (CH<sub>3</sub>).

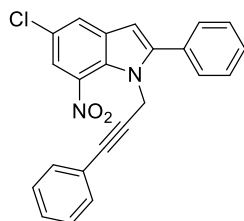


**methyl 4-(5-methyl-7-nitro-1-(prop-2-yn-1-yl)-1H-indol-2-yl)benzoate 6d:** 63 % yield; orange solid; mp 166 - 164 °C; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 8.20 (d, *J* = 8.5 Hz, 2 H), 7.82 (s, 1 H), 7.74 (s, 1 H), 8.20 (d, *J* = 8.5 Hz, 2 H), 7.61 (d, *J* = 8.5 Hz, 2 H), 6.75 (s, 1 H), 5.05 (d, *J* = 2.4 Hz, 2 H), 3.99 (s, 3 H), 2.54 (s, 3 H), 2.17 (t, *J* = 2.4 Hz, 2 H); <sup>13</sup>C NMR (100.6 MHz) (400.13 MHz): δ 166.5 (C), 144.5 (C), 137.2 (C), 135.6 (C), 133.5 (C), 130.4 (C), 130.2 (C), 130.1 (CH), 129.3 (CH), 127.8 (C), 127.3 (CH), 121.8 (CH), 105.4 (CH), 77.3 (C), 74.0 (CH), 52.4 (CH<sub>3</sub>), 37.1 (CH<sub>2</sub>), 20.8 (CH<sub>3</sub>).

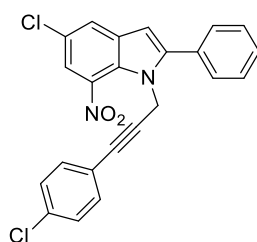


**5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 13:** 70 % yield; orange liquid;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.72 (d,  $J$  = 0.9 Hz, 1H), 7.66 (d,  $J$  = 0.9 Hz, 1H), 7.30 (m, 5H), 7.12–7.02 (m, 2H), 6.85–6.72 (m, 2H), 4.89 (d,  $J$  = 2.5 Hz, 2H), 3.73 (s, 3H), 2.43 (s, 3H), 2.10 (t,  $J$  = 2.4 Hz, 1H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  158.3 (C), 141.1 (C), 137.0 (C), 133.4 (C), 131.2 (CH), 131.1 (CH), 130.4 (C), 129.9 (C), 128.8 (CH), 128.7 (CH), 126.2 (C), 126.0 (CH), 125.7 (C), 121.5 (CH), 117.1 (C), 113.9 (CH), 77.8 (C), 73.8 (C), 55.2 ( $\text{CH}_3$ ), 36.6 ( $\text{CH}_2$ ), 20.9 ( $\text{CH}_3$ ).

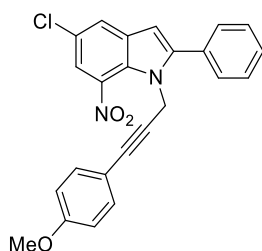
### 3.3 Characterization data of 7-nitro-2-aryl-1-(3-phenylprop-2-yn-1-yl)-1H-indole 7



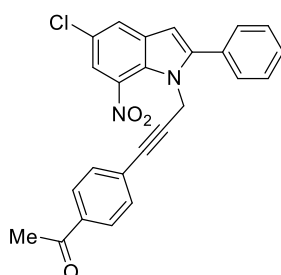
**5-chloro-7-nitro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indole 7a:** 73 % yield; yellow - orange solid; mp 152 - 153  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J$  = 1.9 Hz, 1 H), 7.88 (d,  $J$  = 1.9 Hz, 1 H), 7.61 - 7.52 (m, 5 H), 7.32 - 7.22 (m, 5 H), 6.72 (s, 1 H), 5.26 (s, 2 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  146.8 (C), 137.5 (C), 134.2 (C), 131.7 (CH), 130.8 (C), 129.6 (CH), 129.3 (CH), 129.0 (CH), 128.7 (CH), 128.2 (CH), 127.1 (C), 125.9 (CH), 125.0 (C), 121.7 (C), 119.7 (CH), 103.9 (CH), 86.1 (C), 82.2 (C), 38.1 ( $\text{CH}_2$ ).



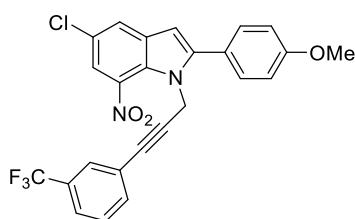
**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7b:** 73 % yield; orange solid; mp 109 - 110  $^{\circ}\text{C}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.91 (d,  $J$  = 1.7 Hz, 1 H), 7.88 (d,  $J$  = 1.7 Hz, 1 H), 7.62 - 7.50 (m, 5 H), 7.26 - 7.17 (m, 4 H), 6.72 (s, 1 H), 5.24 (s, 2 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  146.8 (C), 137.4 (C), 134.9 (C), 134.2 (C), 133.0 (CH), 130.7 (C), 129.6 (CH), 129.4 (CH), 129.0 (CH), 128.6 (CH), 127.1 (C), 126.0 (CH), 125.1 (C), 120.2 (C), 119.7 (CH), 103.9 (CH), 85.1 (C), 83.3 (C), 38.0 ( $\text{CH}_2$ ).



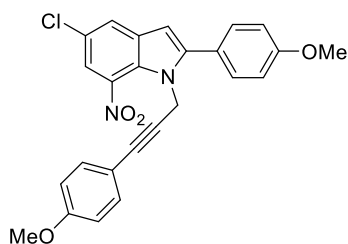
**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7c:** 70 % yield; yellow solid; mp 133 - 134 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.91 (d,  $J$  = 1.9 Hz, 1 H), 7.87 (d,  $J$  = 1.9 Hz, 1 H), 7.60 - 7.50 (m, 5 H), 7.21 (d,  $J$  = 8.8 Hz, 2 H), 6.78 (d,  $J$  = 8.8 Hz, 2 H), 6.70 (s, 1 H), 5.23 (s, 2 H), 3.78 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  159.9 (C), 146.7 (C), 138.2 (C), 137.5 (C), 134.2 (C), 133.2 (CH), 130.8 (C), 129.6 (CH), 129.3 (CH), 129.0 (CH), 127.1 (C), 125.8 (CH), 124.9 (C), 119.6 (CH), 113.8 (CH), 103.8 (CH), 86.1 (C), 80.9 (C), 55.2 ( $\text{CH}_3$ ), 38.2 ( $\text{CH}_2$ ).



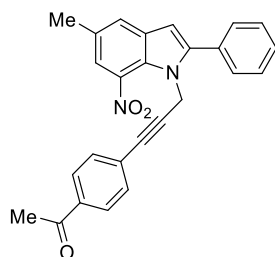
**1-(4-(3-(5-chloro-7-nitro-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7d:** 52 % yield; brown solid; mp 133 - 134 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.92 (d,  $J$  = 1.9 Hz, 1 H), 7.90 (d,  $J$  = 1.9 Hz, 1 H), 7.84 (d,  $J$  = 8.5 Hz, 2 H), 7.60 - 7.53 (m, 5 H), 7.36 (d,  $J$  = 8.5 Hz, 2 H), 6.73 (s, 1 H), 5.27 (s, 2 H), 2.58 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  197.2 (C), 146.8 (C), 137.4 (C), 136.6 (C), 134.2 (C), 131.9 (CH), 130.6 (C), 129.6 (CH), 129.4 (CH), 129.1 (CH), 128.1 (CH), 127.1 (C), 126.5 (C), 126.0 (CH), 125.2 (C), 119.7 (CH), 104.0 (CH), 85.4 (C), 85.3 (C), 38.0 ( $\text{CH}_2$ ), 26.6 ( $\text{CH}_3$ ).



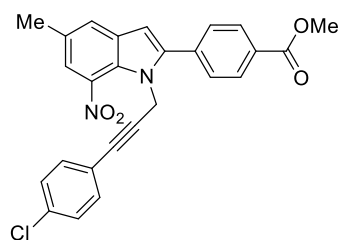
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indole 7e:** 47 % yield; yellow - orange solid; mp 86 - 87 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.90 (d,  $J$  = 1.8 Hz, 1 H), 7.87 (d,  $J$  = 1.8 Hz, 1 H), 7.57 - 7.44 (m, 5 H), 7.40 (t,  $J$  = 7.6 Hz, 1 H), 7.10 (d,  $J$  = 8.6 Hz, 2 H), 6.67 (s, 1 H), 5.24 (s, 2 H), 3.92 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  160.5 (C), 146.7 (C), 137.3 (C), 135.0 (CH), 134.3 (C), 131.0 (CH), 130.8 (q,  $J_{\text{CF}}$  = 33 Hz, C), 128.8 (CH), 128.5 (q,  $J_{\text{CF}}$  = 4.0 Hz, CH), 126.9 (C), 125.7 (CH), 125.3 (q,  $J_{\text{CF}}$  = 4.0 Hz, CH), 125.1 (C), 123.5 (q,  $J_{\text{CF}}$  = 273 Hz, C), 122.9 (C), 122.7 (C), 119.4 (CH), 114.5 (CH), 103.4 (CH), 84.4 (C), 84.0 (C), 55.4 ( $\text{CH}_3$ ), 37.8 ( $\text{CH}_2$ );  $^{19}\text{F}$  NMR (376.5 MHz) ( $\text{CDCl}_3$ ):  $\delta$  -63.0.



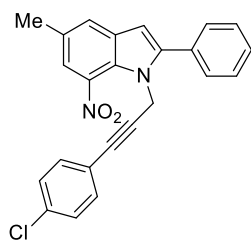
**5-chloro-2-(4-methoxyphenyl)-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-1H-indole 7f:** 60 % yield; yellow - orange solid; mp 112 - 113 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.86 (d,  $J$  = 1.8 Hz, 1 H), 7.85 (d,  $J$  = 1.8 Hz, 1 H), 7.50 (d,  $J$  = 8.6 Hz, 2 H), 7.22 (d,  $J$  = 8.6 Hz, 2 H), 7.08 (d,  $J$  = 8.7 Hz, 2 H), 6.78 (d,  $J$  = 8.7 Hz, 2 H), 6.64 (s, 1 H), 5.20 (s, 2H), 3.92 (s, 3H), 3.78 (s, 3H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  160.4 (C), 159.9 (C), 146.7 (C), 137.4 (C), 134.3 (C), 133.2 (CH), 131.0 (CH), 127.0 (C), 125.6 (CH), 124.9 (C), 123.1 (C), 119.3 (CH), 114.5 (CH), 113.9 (C), 113.8 (CH), 103.2 (CH), 86.0 (C), 81.1 (C), 55.5 ( $\text{CH}_3$ ), 55.2 ( $\text{CH}_3$ ), 38.1 ( $\text{CH}_2$ ).



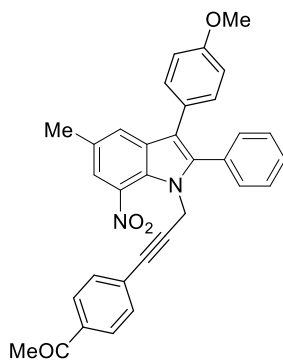
**1-(4-(3-(5-methyl-7-nitro-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7g:** 73 % yield; yellow solid; mp 109 - 110 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.72 (d,  $J$  = 8.5 Hz, 2 H), 7.69 (s, 1 H), 7.63 (s, 1 H), 7.52 - 7.38 (m, 5 H), 7.22 (d,  $J$  = 8.5 Hz, 2 H), 6.60 (s, 1 H), 5.18 (s, 2 H), 2.47 (s, 3 H), 2.44 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  197.3 (C), 145.5 (C), 137.2 (C), 136.5 (C), 133.6 (C), 131.9 (CH), 131.3 (C), 129.8 (C), 129.6 (CH), 129.0 (CH), 128.9 (CH), 128.0 (CH), 127.3 (C), 127.0 (CH), 126.9 (C), 121.1 (CH), 104.1 (CH), 86.1 (C), 84.8 (C), 38.4 ( $\text{CH}_2$ ), 26.7 ( $\text{CH}_3$ ), 20.9 ( $\text{CH}_3$ ).



**methyl 4-(1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-1H-indol-2-yl)benzoate 7h:** 58 % yield; yellow solid; mp 150 - 151 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  8.21 (d,  $J$  = 8.5 Hz, 2 H), 7.80 (s, 1 H), 7.73 (s, 1 H), 7.66 (d,  $J$  = 8.5 Hz, 2 H), 7.23 - 7.17 (m, 4 H), 6.76 (s, 1 H), 5.23 (s, 2 H), 4.00 (s, 3 H), 2.53 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  166.5 (C), 144.3 (C), 137.3 (C), 135.6 (C), 134.7 (C), 133.4 (C), 133.0 (CH), 130.2 (C), 130.16 (CH), 130.13 (C), 129.4 (CH), 128.5 (CH), 127.8 (C), 127.2 (CH), 121.6 (CH), 120.3 (C), 105.1 (CH), 84.8 (C), 83.4 (C), 52.4 (CH), 38.0 ( $\text{CH}_2$ ), 20.8 ( $\text{CH}_3$ ).

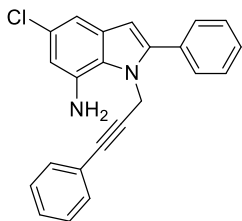


**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-2-phenyl-1H-indole 7i:** 63 % yield; yellow-orange solid; mp 122 - 123 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.78 (s, 1 H), 7.72 (s, 1 H), 7.62 - 7.42 (m, 5 H), 7.24 - 7.17 (m, 4 H), 6.69 (s, 1 H), 5.24 (s, 2 H), 2.53 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  145.5 (C), 137.2 (C), 134.6 (C), 133.5 (C), 133.0 (CH), 131.3 (C), 129.8 (C), 129.6 (CH), 128.96 (CH), 128.94 (CH), 128.5 (CH), 127.2 (C), 127.0 (CH), 121.1 (CH), 120.5 (C), 104.1 (CH), 84.6 (C), 83.8 (C), 37.8 ( $\text{CH}_2$ ), 20.8 ( $\text{CH}_3$ ).

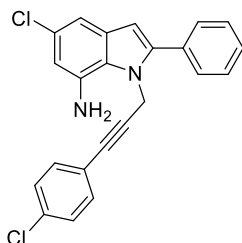


**1-(4-(3-(3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 14:** 92 % yield; yellow solid; mp: 200 - 202 °C;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.85 (d,  $J$  = 8.3 Hz, 2 H), 7.81 (s, 1 H), 7.76 (s, 1 H), 7.49 - 7.35 (m, 7 H), 7.19 (d,  $J$  = 8.7 Hz, 2 H), 6.89 (d,  $J$  = 8.7 Hz, 2 H), 5.20 (s, 2 H), 3.83 (s, 3 H), 2.58 (s, 3 H), 2.52 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  197.3 (C), 158.3 (C), 140.9 (C), 137.1 (C), 136.5 (C), 133.3 (C), 131.9 (CH), 131.2 (CH), 131.1 (CH), 129.8 (CH), 128.9 (CH), 128.8 (CH), 128.1 (C), 127.0 (C), 126.2 (C), 126.0 (CH), 125.7 (C), 121.4 (CH), 116.9 (C), 114.0 (CH), 104.1 (C), 86.3 (C), 84.8 (CH), 55.2 ( $\text{CH}_3$ ), 37.6 ( $\text{CH}_2$ ), 26.6 ( $\text{CH}_3$ ), 55.2 ( $\text{CH}_3$ ), 20.9 ( $\text{CH}_3$ ).

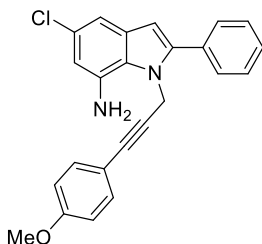
### 3.4 Characterization data of 2-aryl-1-(3-phenylprop-2-yn-1-yl)-1H-indol-7-amines 1



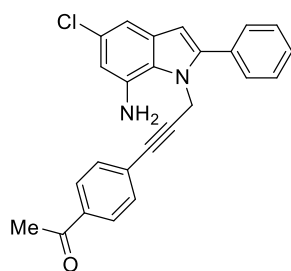
**5-chloro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indol-7-amine 1a:** 60% yield; brown oil;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.68 (d,  $J$  = 8.8 Hz, 2 H), 7.56 - 7.43 (m, 5 H), 7.41 - 7.34 (m, 3 H), 7.01 (d,  $J$  = 1.6 Hz, 1 H), 6.47 (s, 1 H), 6.50 (d,  $J$  = 1.6 Hz, 1 H), 5.19 (s, 2 H), 4.33 (bs, 2 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  143.2 (C), 134.0 (C), 131.8 (C), 131.7 (CH), 130.9 (C), 129.3 (CH), 129.0 (CH), 128.8 (CH), 128.49 (CH), 128.43 (CH), 127.2 (C), 126.4 (C), 121.8 (C), 111.4 (CH), 110.3 (CH), 102.5 (CH), 86.5 (C), 86.2 (C), 36.5 ( $\text{CH}_2$ ).



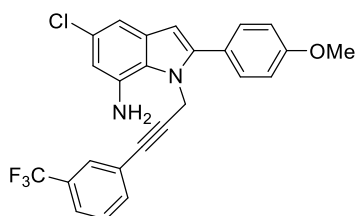
**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1b:** 55% yield; yellow - orange solid; mp 109 - 110  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.60 - 7.64 (m, 2 H), 7.56 - 7.45 (m, 3 H), 7.41 (d,  $J$  = 8.6 Hz, 2 H), 7.34 (d,  $J$  = 8.6 Hz, 2 H), 7.11 (d,  $J$  = 1.9 Hz, 1 H), 6.56 (d,  $J$  = 1.9 Hz, 1 H), 6.48 (s, 1 H), 5.19 (s, 2 H), 4.27 (bs, 2 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  143.3 (C), 135.1 (C), 133.9 (C), 132.9 (CH), 131.8 (C), 130.9 (C), 129.3 (CH), 128.87 (CH), 128.83 (CH), 128.5 (CH), 127.2 (C), 126.5 (C), 120.3 (C), 111.6 (CH), 110.5 (CH), 102.7 (CH), 87.2 (C), 85.4 (C), 36.4 ( $\text{CH}_2$ ).



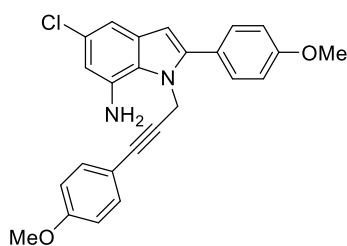
**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1c:** 85 % yield; yellow-orange solid; mp 91 - 92  $^\circ\text{C}$ ;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.69 (d,  $J$  = 7.2 Hz, 2 H), 7.52 (t,  $J$  = 7.5 Hz, 2 H), 7.48 - 7.40 (m, 3 H), 6.99 (d,  $J$  = 1.8 Hz, 1 H), 7.00 (d,  $J$  = 1.9 Hz, 1 H), 6.89 (d,  $J$  = 8.8 Hz, 2 H), 6.55 (d,  $J$  = 1.9 Hz, 1 H), 6.46 (s, 1 H), 5.17 (s, 2 H), 4.35 (bs, 2 H), 3.8 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  160.1 (C), 143.2 (C), 134.0 (C), 133.2 (CH), 131.9 (C), 130.8 (C), 129.3 (CH), 128.7 (CH), 128.3 (CH), 127.1 (C), 126.3 (C), 114.1 (CH), 113.8 (C), 111.3 (CH), 110.1 (CH), 102.4 (CH), 86.6 (C), 84.9 (C), 55.3 ( $\text{CH}_3$ ), 36.6 ( $\text{CH}_2$ ).



**1-(4-(3-(7-amino-5-chloro-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1d:** 81 % yield; brown solid; mp 80 - 81 °C;  $^1\text{H}$  NMR (400.13 MHz) (DMSO  $d_6$ ):  $\delta$  7.90 (d,  $J_1 = 8.4$  Hz, 2 H), 7.60 (d,  $J = 7.6$  Hz, 2 H), 7.55 (t,  $J = 7.5$  Hz, 2 H), 7.48- 7.44 (m, 3 H), 6.71 (s, 1 H), 6.46 (s, 1 H), 6.40 (d,  $J = 1.1$  Hz, 1 H), 5.31 (s, 2 H), 4.89 (bs, 2 H), 2.55 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) (DMSO  $d_6$ ):  $\delta$  197.7 (C), 142.7 (C), 136.8 (C), 134.9 (C), 132.6 (C), 132.1 (CH), 131.0 (C), 130.5 (C), 129.4 (CH), 129.2 (CH), 128.9 (CH), 128.8 (CH), 127.6 (C), 126.7 (C), 112.2 (CH), 110.8 (CH), 104.4 (CH), 90.2 (C), 84.0 (C), 36.3 (CH<sub>2</sub>), 27.2 (CH<sub>3</sub>).

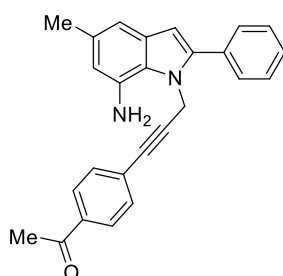


**5-chloro-2-(4-methoxyphenyl)-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indol-7-amine 1e:** 93 % yield; brown solid; mp 101 - 102 °C;  $^1\text{H}$  NMR (400.13 MHz) (CDCl<sub>3</sub>):  $\delta$  7.73 (s, 1 H), 7.67 - 7.61 (m, 2 H), 7.58 (d,  $J = 8.6$  Hz, 2 H), 7.5 (t,  $J = 7.8$  Hz, 1 H), 7.09 (d,  $J = 1.5$  Hz, 1 H), 7.06 (d,  $J = 8.6$  Hz, 2 H), 6.55 (d,  $J = 1.5$  Hz, 1 H), 6.42 (s, 1 H), 5.20 (s, 2 H), 4.21 (bs, 2 H), 3.90 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) (CDCl<sub>3</sub>):  $\delta$  159.9 (C), 143.2 (C), 134.9 (CH), 133.7 (C), 131.2 (q,  $J_{CF} = 32$  Hz, C), 131.0 (C), 130.7 (CH), 129.1 (CH), 128.5 (q,  $J_{CF} = 4$  Hz, CH), 127.0 (C), 126.4 (C), 125.8 (q,  $J_{CF} = 4$  Hz, CH), 124.1 (C), 123.5 (q,  $J_{CF} = 273$  Hz, C), 122.8 (CH), 114.3 (CH), 111.5 (CH), 110.4 (CH), 102.1 (CH), 87.9 (C), 84.7 (C), 55.4 (CH<sub>3</sub>), 36.3 (CH<sub>2</sub>);  $^{19}\text{F}$  NMR (376.5 MHz) (CDCl<sub>3</sub>):  $\delta$  -62.6.

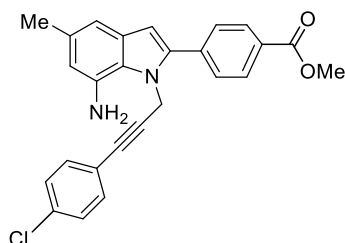


**5-chloro-2-(4-methoxyphenyl)-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-1H-indol-7-amine 1f:** 95 % yield; brown solid; mp 105 - 106 °C;  $^1\text{H}$  NMR (400.13 MHz) (CDCl<sub>3</sub>):  $\delta$  7.61 (d,  $J = 8.6$  Hz, 2 H), 7.42 (d,  $J = 8.4$  Hz, 2 H), 7.09 - 7.02 (m, 3 H), 6.88 (d,  $J = 8.4$  Hz, 2 H), 6.52 (d,  $J = 1.4$  Hz, 2 H), 6.39 (s, 1 H), 5.15 (s, 2 H), 4.33 (bs, 2 H), 3.89 (s, 3 H), 3.85 (s, 3 H);  $^{13}\text{C}$  NMR (100.6 MHz) (CDCl<sub>3</sub>):  $\delta$  160.1 (C), 159.8 (C), 143.1 (C), 134.0 (C), 133.2 (CH), 130.9 (C), 130.6 (CH), 126.9 (C), 126.2 (C), 124.3 (C), 120.4 (C), 114.2 (CH), 114.1 (CH), 111.2 (CH), 109.9 (CH), 101.7 (CH), 86.4 (C), 85.0 (C), 55.4 (CH<sub>3</sub>), 55.3 (CH<sub>2</sub>), 36.5 (CH<sub>2</sub>).

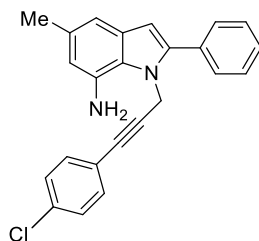




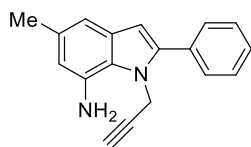
**1-(4-(3-(7-amino-5-methyl-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1g:** 70 % yield; yellow - orange solid; mp 83 - 84 °C; <sup>1</sup>H NMR (400.13 MHz, CDCl<sub>3</sub>) δ 7.84 (d, *J* = 8.2 Hz, 2H), 7.58 (d, *J* = 7.3 Hz, 2H), 7.50–7.30 (m, 5H), 6.85 (s, 1H), 6.38–6.35 (m, 2H), 5.15 (s, 2H), 4.04 (s, 2H), 2.53 (s, 3H), 2.29 (s, 3H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 197.2 (C), 142.4 (C), 136.7 (C), 132.5 (C), 132.4 (C), 131.9 (CH), 131.0 (C), 130.7 (C), 129.3 (CH), 128.7 (CH), 128.3 (CH), 128.1 (CH), 127.4 (C), 126.9 (C), 112.4 (CH), 112.3 (CH), 102.9 (CH), 90.0 (C), 85.2 (C), 36.5 (CH<sub>2</sub>), 26.7 (CH<sub>3</sub>), 21.3 (CH<sub>3</sub>).



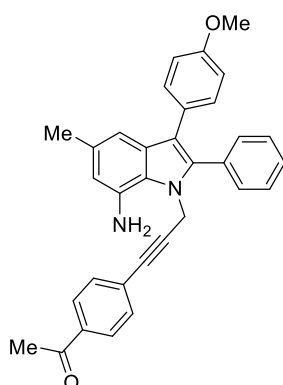
**methyl 4-(7-amino-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-1H-indol-2-yl)benzoate 1h:** 63 % yield; red wax; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 8.08 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 8.5 Hz, 2H), 7.28 (m, 4H), 6.85 (s, 1H), 6.46 (s, 1H), 6.36 (d, *J* = 1.0 Hz, 1H), 5.10 (s, 2H), 4.06 (s, 2H), 3.88 (s, 3H), 2.29 (s, 3H); <sup>13</sup>C NMR (100.6 MHz, CDCl<sub>3</sub>) δ 166.8 (C), 141.3 (C), 136.8 (C), 135.1 (C), 133.0 (CH), 132.7 (C), 131.2 (C), 130.5 (C), 130.0 (CH), 129.4 (C), 128.9 (CH), 128.9 (CH), 128.1 (C), 120.4 (C), 112.8 (CH), 112.4 (CH), 104.0 (CH), 87.4 (C), 85.3 (C), 52.3 (CH<sub>3</sub>), 36.6 (CH<sub>2</sub>), 21.3 (CH<sub>3</sub>).



**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-2-phenyl-1H-indol-7-amine 1i:** 57 % yield; brown wax; <sup>1</sup>H NMR (400.13 MHz) (CDCl<sub>3</sub>): δ 7.57 (d, *J* = 8.0 Hz, 2H), 7.40 (t, *J* = 8.0, 7.0 Hz, 2H), 7.37–7.27 (m, 3H), 7.23 (d, *J* = 8.5 Hz, 2H), 6.84 (s, 1H), 6.37–6.33 (m, 1H), 5.10 (s, 2H), 4.05 (s, 2H), 2.28 (s, 3H); <sup>13</sup>C NMR (100.6 MHz) (CDCl<sub>3</sub>): δ 142.3 (C), 135.0 (C), 133.0 (CH), 132.6 (C), 132.5 (C), 130.9 (C), 130.6 (C), 129.3 (CH), 128.8 (CH), 128.7 (CH), 128.1 (CH), 127.4 (C), 120.6 (C), 112.3 (CH), 112.2 (CH), 102.7 (CH), 87.8 (C), 85.0 (C), 36.4 (CH<sub>2</sub>), 21.3 (CH<sub>3</sub>).



**5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1H-indol-7-amine 1j:** 43 % yield; brown wax;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.55 (d,  $J$  = 7.1 Hz, 2H), 7.42–7.31 (m, 3H), 6.83 (s, 1H), 6.35 - 6.33 (m, 2H), 4.89 (d,  $J$  = 2.4 Hz, 2H), 4.00 (s, 2H), 2.52 (t,  $J$  = 2.4 Hz, 1H), 2.28 (s, 3H).  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ): 142.4 (C), 132.5 (C), 132.4 (C), 130.9 (C), 130.6 (C), 129.3 (CH), 128.7 (CH), 128.1 (CH), 112.4 (CH), 112.3 (CH), 102.8 (CH), 81.9 (C), 74.4 (C), 35.7 ( $\text{CH}_2$ ), 21.3 ( $\text{CH}_3$ ).



**1-(4-(3-(7-amino-3-(4-methoxyphenyl)-5-methyl-2-phenyl-1H-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1k:** 57 % yield; brown wax;  $^1\text{H}$  NMR (400.13 MHz) ( $\text{CDCl}_3$ ):  $\delta$  7.84 (d,  $J$  = 8.4 Hz, 2H), 7.45 (d,  $J$  = 8.4 Hz, 2H), 7.38–7.29 (m, 5H), 7.12 (d,  $J$  = 8.7 Hz, 2H), 6.93 (s, 1H), 6.76 (d,  $J$  = 8.8 Hz, 2H), 6.40 (s, 1H), 5.10 (s, 2H), 4.05 (m, 2H), 3.72 (s, 3H), 2.53 (s, 3H), 2.28 (s, 3H);  $^{13}\text{C}$  NMR (100.6 MHz) ( $\text{CDCl}_3$ ):  $\delta$  197.2 (C), 157.7 (C), 138.1 (C), 136.7 (C), 132.5 (C), 131.9 (CH), 131.5 (C), 131.3 (CH), 131.1 (CH), 130.1 (C), 128.5 (CH), 128.3 (CH), 128.1 (CH), 127.5 (C), 127.0 (C), 126.3 (C), 115.8 (C), 113.7 (CH), 112.9 (CH), 111.3 (CH), 89.9 (C), 85.0 (C), 55.2 ( $\text{CH}_3$ ), 36.3 ( $\text{CH}_2$ ), 26.7 ( $\text{CH}_3$ ), 21.4 ( $\text{CH}_3$ ).

#### 4. REFERENCES

[1] Sanz R., Guilarte V., Pérez A., Straightforward selective preparation of nitro- or amino-indoles from 2-halonitroanilines and alkynes. First synthesis of 7-amino-5-nitroindoles, *Tetrahedron Lett.*, **2009**, 50, 4423-4426, doi.org/10.1016/j.tetlet.2009.05.027.

## 5. HF CALCULATION ON ISOMERS 2a and 2'a

### Compound 2a

```
+-----+
---+
| 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: WF3654
Executables used: D:\TITAN
Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF3654
```

```
Input file comments:
Molecule001
This file created by Spartan
```

```
basis set:          6-31G**
net molecular charge: 0
multiplicity:       1
```

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number of basis functions....          465
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Input geometry:

	angstroms		
atom	x	y	z
N1	-0.1550260000	0.4374990000	1.1210390000
N2	-1.0086730000	-2.3256400000	1.1332130000
C4	-1.1860510000	-0.0350800000	1.9315790000
C5	-0.0104550000	-1.9237530000	0.4028750000
C6	-1.6456290000	-1.3760560000	1.9632780000
C7	-1.7070180000	1.0262900000	2.7388420000
C13	0.7199200000	-2.8803430000	-0.5063790000
H4	-3.1185930000	-2.6496450000	2.9223950000
C8	-2.7656460000	0.7093510000	3.5969080000
C11	-0.9132890000	2.1852800000	2.3994340000

H7	-3.2133600000	1.4833470000	4.2359600000
C9	-3.2381490000	-0.5972350000	3.6279590000
H8	-4.0721010000	-0.8455450000	4.3029390000
C10	-2.7017240000	-1.6349910000	2.8394980000
C12	0.0268720000	1.8011420000	1.4273890000
C2	1.0263770000	2.6560040000	0.8075810000
H13	1.8204060000	-2.6663390000	-0.4286580000
C14	0.2610050000	-2.7449900000	-1.9177470000
H15	0.5612370000	-3.9425620000	-0.1705390000
C15	-0.5895550000	-2.5433530000	-4.5760680000
C16	1.1246910000	-2.2456410000	-2.8988340000
C17	-1.0320590000	-3.1444790000	-2.2771670000
C18	-1.4542200000	-3.0419090000	-3.6012120000
C19	0.6998040000	-2.1465450000	-4.2231290000
H16	2.1442750000	-1.9343460000	-2.6271240000
H17	-1.7134540000	-3.5365780000	-1.5059970000
H18	-2.4719630000	-3.3556810000	-3.8767030000
H19	1.3846780000	-1.7555640000	-4.9897570000
H20	-0.9239070000	-2.4642400000	-5.6207450000
C1	0.5776390000	-0.5062530000	0.3222060000
H5	1.6528730000	-0.5444960000	0.6633050000
H6	0.5619750000	-0.1829560000	-0.7593680000
C3	2.9246780000	4.3652120000	-0.3378590000
C26	1.7455110000	3.5549090000	1.6101580000
C27	1.2625130000	2.6251890000	-0.5732690000
C28	2.2088580000	3.4770190000	-1.1402160000
C29	2.6895760000	4.4036320000	1.0366540000
H1	1.5580180000	3.5843390000	2.6943120000
H2	0.6891520000	1.9402470000	-1.2156630000
H3	2.3868000000	3.4502800000	-2.2254160000
H9	3.2505630000	5.1053430000	1.6714530000
H10	3.6710440000	5.0358360000	-0.7881560000
H25	-1.0275920000	3.1833010000	2.8110280000

Molecular weight: 322.15 amu

Stoichiometry: C23N2H18

Molecular Point Group: C1

Point Group used: C1

nuclear repulsion energy..... 1952.777623249 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: 3.218E-04

number of canonical orbitals..... 462

end of program onee

start of program hfig  
 initial wavefunction generated automatically from atomic  
 wavefunctions

Irreducible representation No Symm	Total no orbitals 462	No of occupied orbitals Shell_1 Shell_2 ...		
-----		85		
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	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	88	88	88	90	84
73							
grid # 2	104	112	97	95	98	98	92
118							
grid # 3	214	229	199	184	197	196	170
223							
grid # 4	391	414	331	322	327	347	304
232							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
90							
grid # 2	97	95	118	97	118	97	97
98							
grid # 3	186	182	224	184	222	186	191
195							
grid # 4	332	341	234	329	231	332	331
341							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	89	89
89							
grid # 2	110	100	112	97	96	96	97
97							

grid # 3	210	195	216	187	186	185	186
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185

grid # 4	215	342	223	331	330	331	331
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330

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
------	-----	-----	-----	-----	-----	----	----

H6

grid # 1	72	72	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	112	114	118	118	118	90	112
----------	-----	-----	-----	-----	-----	----	-----

102

grid # 3	214	217	224	223	224	167	216
----------	-----	-----	-----	-----	-----	-----	-----

205

grid # 4	221	223	232	231	232	299	217
----------	-----	-----	-----	-----	-----	-----	-----

206

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	89	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	96	96	97	97	115	111
----------	----	----	----	----	----	-----	-----

118

grid # 3	187	184	186	186	186	218	212
----------	-----	-----	-----	-----	-----	-----	-----

224

grid # 4	332	330	330	329	330	224	217
----------	-----	-----	-----	-----	-----	-----	-----

232

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3521
grid # 2	118	118	115	4498
grid # 3	224	224	219	8672
grid # 4	232	232	222	12443

end of program grid

start of program rwr  
end of program rwr

start of program scf

number of electrons.....	170
number of alpha electrons....	85
number of beta electrons.....	85
number of orbitals, total....	462
number of core orbitals.....	85
number of open shell orbs....	0
number of occupied orbitals..	85
number of virtual orbitals...	377

```

number of hamiltonians..... 1
number of shells..... 1
SCF type: HF

```

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	5	M	-987.21080013367		3.9E-03	9.8E-02
etot	2	Y	Y	6	M	-989.98476104696	2.8E+00	1.7E-03	5.5E-02
etot	3	Y	Y	6	M	-990.27640419982	2.9E-01	7.8E-04	2.7E-02
etot	4	N	Y	2	U	-990.34536478481	6.9E-02	3.8E-04	1.5E-02
etot	5	Y	Y	6	M	-990.35620931742	1.1E-02	1.0E-03	1.0E-02
etot	6	N	Y	2	U	-990.36578188544	9.6E-03	1.2E-04	2.2E-03
etot	7	Y	Y	6	M	-990.36633784606	5.6E-04	4.0E-05	5.6E-04
etot	8	Y	Y	6	M	-990.36641184175	7.4E-05	1.2E-05	2.3E-04
etot	9	N	Y	2	U	-990.36623705176	-1.7E-04	5.8E-06	1.1E-04
etot	10	Y	Y	6	M	-990.36624305181	6.0E-06	4.9E-06	5.8E-05
etot	11	Y	N	6	M	-990.36624587679	2.8E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

```

(A) Nuclear repulsion..... 1952.77762324898
(E) Total one-electron terms..... -5223.87627037117
(I) Total two-electron terms..... 2280.73240124540
(L) Electronic energy..... -2943.14386912577 (E+I)
(N) Total energy..... -990.36624587679 (A+L)

```

```

SCFE: SCF energy: HF      -990.36624587679 hartrees  iterations:
11

```

```

HOMO energy:      -0.26238
LUMO energy:       0.08458

```

Orbital energies:

```

-15.61225  -15.57394  -11.30699  -11.29988  -11.28257  -11.26176
-11.25976  -11.25489  -11.25065  -11.24883  -11.24706  -11.24570
-11.24527  -11.24438  -11.24359  -11.24267  -11.24138  -11.24124
-11.23937  -11.23733  -11.22956  -11.22835  -11.22767  -11.22333
-11.22233  -1.30891   -1.23521  -1.15989  -1.15811  -1.13132
-1.07044   -1.06879   -1.03483  -1.01840  -1.01489  -1.01367
-0.96165   -0.95090   -0.92391  -0.85859  -0.83575  -0.83045
-0.82627   -0.79990   -0.78600  -0.76574  -0.72486  -0.71505
-0.69233   -0.69090   -0.66232  -0.65281  -0.64039  -0.63511
-0.63125   -0.61793   -0.61598  -0.61045  -0.59401  -0.58832
-0.58652   -0.58354   -0.57683  -0.55347  -0.54722  -0.54082
-0.53565   -0.51410   -0.50599  -0.49981  -0.49872  -0.49409
-0.49103   -0.48832   -0.48378  -0.47850  -0.42632  -0.40843
-0.36790   -0.34360   -0.34155  -0.33783  -0.32751  -0.27573
-0.26238    0.08458    0.11895    0.13358    0.13414    0.14570

```

0.17403 0.20148 0.21421 0.22686 0.23450

end of program scf

start of program der1a  
end of program der1a

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

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-3.240872E-02	9.749688E-03	3.179943E-02
2	N2	3.994841E-02	1.589784E-02	-2.744144E-02
3	C4	-4.648588E-03	1.109702E-02	6.253104E-03
4	C5	-3.592959E-02	-8.241299E-03	3.439027E-02
5	C6	2.414258E-03	2.916011E-02	4.891493E-03
6	C7	2.172547E-02	-2.498377E-02	-2.655680E-02
7	C13	1.776470E-02	-2.489095E-02	2.423915E-02
8	H4	8.099431E-03	1.571016E-02	-2.748483E-03
9	C8	-8.989727E-03	2.813047E-03	8.737148E-03
10	C11	2.073446E-02	-1.403474E-02	-2.135011E-02
11	H7	5.617432E-03	-1.253712E-02	-8.781297E-03
12	C9	-1.066947E-02	1.935235E-03	1.014118E-02
13	H8	1.338669E-02	4.465009E-03	-1.056642E-02
14	C10	7.534698E-03	-9.961889E-03	-9.389467E-03
15	C12	-4.116184E-02	-1.291056E-02	3.163420E-02
16	C2	1.304881E-02	8.436034E-03	-7.725578E-03
17	H13	-2.288695E-02	-5.875229E-03	-2.856836E-03
18	C14	-3.001289E-05	9.115626E-04	-2.375293E-02
19	H15	2.454104E-03	2.667852E-02	-3.093814E-03
20	C15	-8.755934E-04	1.284549E-03	-8.246274E-03
21	C16	1.904926E-03	8.743392E-04	-2.548369E-04
22	C17	-5.241454E-03	-1.814770E-03	2.230640E-03
23	C18	-7.258278E-03	-2.346623E-03	-2.041341E-04
24	C19	3.649640E-03	3.130199E-03	-7.320720E-03
25	H16	-1.529594E-02	-5.126618E-03	-3.849080E-03
26	H17	1.141142E-02	6.616599E-03	-1.234182E-02
27	H18	1.586235E-02	4.779575E-03	4.278800E-03
28	H19	-1.052798E-02	-5.951830E-03	1.156894E-02
29	H20	5.229882E-03	-1.242672E-03	1.606278E-02
30	C1	2.113894E-02	9.772674E-03	-1.632786E-02
31	H5	-2.245682E-02	-6.894493E-04	-1.106135E-02
32	H6	4.269849E-03	-1.216673E-02	2.603804E-02



33	C3	5.645640E-03	4.899727E-03	-3.657363E-03
34	C26	4.904907E-04	2.576969E-03	4.717966E-03
35	C27	-4.000485E-04	-2.665549E-03	-5.344084E-03
36	C28	1.194079E-03	-8.729806E-04	-7.925486E-03
37	C29	2.773262E-03	5.466727E-03	5.063842E-03
38	H1	3.964567E-03	-1.650721E-03	-1.828743E-02
39	H2	8.982905E-03	1.280343E-02	1.060548E-02
40	H3	-2.910655E-03	4.951888E-04	1.678907E-02
41	H9	-8.627735E-03	-1.102210E-02	-9.843115E-03
42	H10	-1.152274E-02	-1.049380E-02	6.921504E-03
43	H25	2.708121E-03	-9.050340E-03	-6.693826E-03
-----				
	total	1.123978E-04	1.024489E-03	7.424633E-04

end of program der1b

start of program geopt 1

geometry optimization step 1

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000165

Cos(theta): 0.8700386

Final level shift: -9.0459602E-02

gradient maximum: 5.6400E-02 . ( 4.5000E-04 )

gradient rms: 1.1269E-02 . ( 3.0000E-04 )

step size: 0.30001 trust radius: 0.30000

displacement maximum: 7.9070E-02 . ( 1.8000E-03 )

displacement rms: 2.3571E-02 . ( 1.2000E-03 )

predicted energy change: -2.2790E-02 geom step: 3.0001E-

01 full step: 3.0001E-01

molecular structure not yet converged...

center of mass moved by:

x: 1.7900E-03 y: 7.9249E-03 z: 5.2280E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.1851238607	0.4641584805	1.1496398783
N2	-0.9624306185	-2.2803275995	1.1391335864
C4	-1.1923369589	-0.0180925749	1.9481977188
C5	0.0003838455	-1.8866472314	0.4304247849
C6	-1.6131242204	-1.3444054000	1.9677332987
C7	-1.7143322129	1.0107834641	2.7508560527
C13	0.6888484121	-2.8743700008	-0.4705903976

H4	-3.0326107871	-2.6499595048	2.8909113274
C8	-2.7758076385	0.6768625265	3.6172856202
C11	-0.9256685288	2.1808482739	2.4168546928
H7	-3.2270829119	1.4262828740	4.2504106118
C9	-3.2256779072	-0.6251283660	3.6377251029
H8	-4.0393570567	-0.8900121801	4.2984882981
C10	-2.6561623240	-1.6393208618	2.8310281808
C12	-0.0161416855	1.8156812458	1.4563175807
C2	1.0081011308	2.6662618384	0.8151804166
H13	1.7673251388	-2.7356321765	-0.3960304160
C14	0.2466641767	-2.7462605278	-1.9265734159
H15	0.4459377797	-3.8754027525	-0.1219375680
C15	-0.5453795077	-2.5531842005	-4.6103164906
C16	1.1228101928	-2.2821169158	-2.9004344929
C17	-1.0389296276	-3.1210357258	-2.3122887225
C18	-1.4308521122	-3.0220378034	-3.6483671644
C19	0.7311661555	-2.1855070811	-4.2360240634
H16	2.1179862862	-2.0041675136	-2.6156208078
H17	-1.7271848709	-3.4681454408	-1.5658608400
H18	-2.4200252396	-3.2868875229	-3.9394618092
H19	1.4207969829	-1.8273231853	-4.9765738859
H20	-0.8415814914	-2.4643443665	-5.6434658446
C1	0.5813167973	-0.4636626778	0.3433044617
H5	1.6400268303	-0.4816687726	0.6523424559
H6	0.5606286448	-0.1702832088	-0.7202931642
C3	2.9112386307	4.3243859975	-0.3688081175
C26	1.7641520157	3.5436729388	1.5963361301
C27	1.2174113891	2.6356426600	-0.5675864813
C28	2.1639530001	3.4567854144	-1.1533354185
C29	2.7066639823	4.3656913408	1.0056564678
H1	1.6123726912	3.5626682239	2.6583667114
H2	0.6171678014	1.9866834111	-1.1807727574
H3	2.3092217370	3.4311451005	-2.2201183904
H9	3.2922168597	5.0359612586	1.6129911517
H10	3.6489292197	4.9615184331	-0.8293143894
H25	-1.0462406649	3.1705625677	2.8156287502

nuclear repulsion energy..... 1960.025589350 hartrees

-----  
 / end of geometry optimization iteration 1 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.977E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	87	88	88	92	84
73							
grid # 2	103	112	95	95	96	101	92
118							
grid # 3	214	227	197	186	193	197	164
223							
grid # 4	393	413	326	321	328	351	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
93							
grid # 2	97	94	118	97	118	97	96
100							
grid # 3	184	184	223	184	222	185	195
197							
grid # 4	328	336	226	331	224	332	319
344							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	89	89
89							
grid # 2	109	100	109	97	96	96	97
97							
grid # 3	211	195	214	184	184	184	186
182							
grid # 4	216	340	216	328	328	330	331
328							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	72
69							
grid # 2	112	115	118	118	118	90	112
102							
grid # 3	213	216	223	222	223	166	217
205							
grid # 4	214	215	224	222	223	294	219
207							

number of gridpoints:		C3	C26	C27	C28	C29	H1	H2
H3	atom							
73	grid # 1	89	87	87	89	89	72	70
118	grid # 2	97	97	96	97	97	115	111
222	grid # 3	185	181	183	184	184	218	213
224	grid # 4	329	328	330	328	328	217	210

number of gridpoints:				
atom	H9	H10	H25	total
grid # 1	73	73	72	3523
grid # 2	118	118	115	4494
grid # 3	223	223	219	8635
grid # 4	224	224	222	12295

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g		RMS	maximum
	t	p	i	c	r		density	DIIS
	e	d	i	u	i	energy	change	error
	r	t	s	t	d	total energy	change	
etot	1	N	N	2	U	-990.37561875819	2.2E-04	5.2E-03
etot	2	Y	Y	6	M	-990.38629314976	1.1E-02	2.1E-03
etot	3	N	Y	2	U	-990.38722199985	9.3E-04	7.2E-04
etot	4	Y	Y	6	M	-990.38736835388	1.5E-04	3.4E-04
etot	5	Y	Y	6	M	-990.38740323781	3.5E-05	1.3E-04
etot	6	Y	Y	6	M	-990.38740916528	5.9E-06	4.7E-05
etot	7	Y	N	6	M	-990.38741265890	3.5E-06	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1960.02558935013	
(E)	Total one-electron terms.....	-5238.29315543660	
(I)	Total two-electron terms.....	2287.88015342757	
(L)	Electronic energy.....	-2950.41300200903	(E+I)
(N)	Total energy.....	-990.38741265890	(A+L)

SCFE: SCF energy: HF -990.38741265890 hartrees iterations:

HOMO energy: -0.26625  
LUMO energy: 0.09232

Orbital energies:

-15.60805	-15.56700	-11.29787	-11.29337	-11.27638	-11.25511
-11.25341	-11.25179	-11.24692	-11.24146	-11.24113	-11.24000
-11.23941	-11.23867	-11.23797	-11.23592	-11.23504	-11.23469
-11.23278	-11.23229	-11.22657	-11.22384	-11.22377	-11.21820
-11.21692	-1.31817	-1.24994	-1.16238	-1.15889	-1.13461
-1.07262	-1.06754	-1.03658	-1.02296	-1.01802	-1.01474
-0.96749	-0.95529	-0.93114	-0.85928	-0.83758	-0.83378
-0.83067	-0.80421	-0.79354	-0.76882	-0.73077	-0.71744
-0.69958	-0.69803	-0.66500	-0.65657	-0.64316	-0.63792
-0.63536	-0.62308	-0.61992	-0.61392	-0.59697	-0.59327
-0.58930	-0.58645	-0.57884	-0.55677	-0.55072	-0.54533
-0.54289	-0.51775	-0.50819	-0.50301	-0.50024	-0.49594
-0.49263	-0.49143	-0.48732	-0.48017	-0.42932	-0.40604
-0.36912	-0.34308	-0.34234	-0.33503	-0.33025	-0.28019
-0.26625	0.09232	0.12603	0.13625	0.13684	0.14868
0.17722	0.20851	0.22157	0.23301	0.24218	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-9.539155E-03	2.745592E-03	1.044822E-02
2	N2	-2.673465E-03	1.727028E-03	2.906341E-03
3	C4	-1.885556E-04	1.245403E-02	3.193744E-03
4	C5	2.271285E-03	6.211561E-03	1.516907E-03
5	C6	-6.464198E-03	7.479387E-03	7.554108E-03
6	C7	8.793345E-03	-1.029557E-02	-9.843759E-03
7	C13	-5.471678E-04	-7.069051E-03	-5.718790E-03
8	H4	1.852086E-03	3.212933E-03	-7.082379E-04
9	C8	4.338852E-03	4.033060E-03	-3.262937E-03
10	C11	1.606909E-03	-1.006096E-02	-6.249112E-03
11	H7	9.730113E-04	-2.564706E-03	-1.338833E-03
12	C9	-5.458253E-04	-4.327700E-03	-5.240229E-04

13	H8	2.968983E-03	5.464179E-04	-2.555816E-03
14	C10	4.804096E-03	2.217867E-04	-3.885245E-03
15	C12	-7.171547E-03	-3.974109E-03	7.707933E-03
16	C2	9.332330E-04	2.740879E-04	-3.181994E-03
17	H13	-2.015010E-03	-1.526317E-03	-1.690651E-03
18	C14	3.524810E-03	-3.916218E-04	-2.663166E-03
19	H15	1.889224E-03	3.787146E-03	1.319866E-03
20	C15	-1.027612E-03	6.505881E-05	3.781739E-04
21	C16	-4.116869E-03	-8.483180E-04	-5.317073E-03
22	C17	-1.277121E-04	3.725580E-03	-1.022516E-02
23	C18	8.848389E-03	3.067855E-03	9.831513E-03
24	C19	3.253650E-03	-3.767333E-04	8.365422E-03
25	H16	4.090188E-03	1.430527E-03	-2.015014E-04
26	H17	-2.307131E-03	-1.447538E-03	4.755238E-04
27	H18	-8.359663E-03	-3.799457E-03	-4.288966E-04
28	H19	2.299917E-03	9.846778E-04	-2.783170E-04
29	H20	-1.387235E-03	-1.403497E-03	2.321291E-03
30	C1	3.683293E-03	3.676776E-03	-8.195002E-03
31	H5	-9.851720E-03	-8.517076E-04	-2.436073E-03
32	H6	1.473065E-03	-4.295533E-03	1.252041E-02
33	C3	3.914041E-04	-3.266543E-04	4.963776E-04
34	C26	-2.384326E-03	-3.429782E-03	-4.918934E-03
35	C27	-1.975575E-03	-5.180976E-04	5.429357E-03
36	C28	1.047866E-03	1.965373E-03	9.943780E-04
37	C29	2.585439E-03	2.168460E-03	-3.629454E-03
38	H1	4.052696E-04	7.061260E-05	1.388971E-03
39	H2	5.731526E-04	1.449645E-03	2.603645E-05
40	H3	3.735787E-05	-1.572279E-04	8.376755E-04
41	H9	-9.939832E-04	-7.438282E-04	-2.855378E-04
42	H10	-1.057111E-03	-6.022944E-04	1.457865E-03
43	H25	1.116333E-03	-1.534056E-03	-1.866734E-03
-----				
	total	1.027296E-03	7.528330E-04	-2.351347E-04

end of program derlb

start of program geopt 2

geometry optimization step 2

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001262

Cos(theta): 0.4522028

Final level shift: -7.1431608E-03

energy change: -2.1167E-02 . ( 5.0000E-05 )

gradient maximum: 2.0310E-02 . ( 4.5000E-04 )

gradient rms: 3.9611E-03 . ( 3.0000E-04 )  
 step size: 0.29998 trust radius: 0.30000  
 displacement maximum: 1.2227E-01 . ( 1.8000E-03 )  
 displacement rms: 2.3569E-02 . ( 1.2000E-03 )  
 predicted energy change: -3.7426E-03 geom step: 2.9998E-  
 01 full step: 2.9998E-01  
 molecular structure not yet converged...

center of mass moved by:

x: -9.2535E-03 y: 3.1123E-03 z: 1.4212E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2322091003	0.4425447477	1.1722376588
N2	-1.0170271355	-2.2784648229	1.1730995628
C4	-1.2206159278	-0.0226657246	1.9837450839
C5	-0.0448348209	-1.9052512670	0.4751983779
C6	-1.6507777180	-1.3371163143	2.0094539253
C7	-1.7024716670	0.9919018866	2.7899381630
C13	0.6283020713	-2.9170533017	-0.4248611566
H4	-3.0346295842	-2.6472027368	2.9359624232
C8	-2.7497248744	0.6679486212	3.6759761067
C11	-0.9219400908	2.1551243638	2.4291375123
H7	-3.1822925194	1.4081076944	4.3208527754
C9	-3.2122659889	-0.6338983252	3.7021230748
H8	-4.0092368660	-0.8922566392	4.3712351952
C10	-2.6664125428	-1.6434906978	2.8798451206
C12	-0.0462186113	1.7852092098	1.4609796706
C2	0.9639603762	2.6172556086	0.7603660644
H13	1.7049014864	-2.8504962231	-0.3042157835
C14	0.2872845063	-2.7186247711	-1.9011082558
H15	0.3111604572	-3.8957135626	-0.0910075502
C15	-0.3637160763	-2.3879002288	-4.5957973831
C16	1.2521389896	-2.2939910017	-2.8167452985
C17	-1.0099224983	-2.9730715129	-2.3497803317
C18	-1.3345315137	-2.8115555909	-3.6881685682
C19	0.9281516443	-2.1274223633	-4.1580106912
H16	2.2689730521	-2.0919467686	-2.4900654971
H17	-1.7651731246	-3.3056021719	-1.6519350479
H18	-2.3449269541	-3.0307603123	-4.0214737620
H19	1.6928080246	-1.7993395561	-4.8496324883
H20	-0.6146895035	-2.2677049661	-5.6318950361
C1	0.5593460744	-0.4968540721	0.4025037161
H5	1.5835558214	-0.5417582018	0.7564692615
H6	0.6038790034	-0.2150061772	-0.6400473898
C3	2.8215489000	4.2490688071	-0.5283409458
C26	1.8492457635	3.4064361869	1.4997536269
C27	1.0238745658	2.6583201916	-0.6349113427
C28	1.9515451393	3.4616543589	-1.2728168602
C29	2.7672368925	4.2206654051	0.8601900607
H1	1.8310545892	3.3653506796	2.5769048131

H2	0.3330469792	2.0787631427	-1.2253750449
H3	1.9815361995	3.4802193197	-2.3500591580
H9	3.4413282681	4.8236548923	1.4492434236
H10	3.5316247441	4.8745490259	-1.0248311658
H25	-1.0230567326	3.1472274108	2.8145615026

nuclear repulsion energy..... 1967.210994655 hartrees

-----  
/ end of geometry optimization iteration 2 /  
-----

end of program geopt

start of program onee  
smallest eigenvalue of S: 2.843E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	84	88	87	89	84
73							
grid # 2	104	112	96	95	97	97	92
118							
grid # 3	214	227	196	186	189	198	163
223							
grid # 4	391	413	320	320	324	348	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	186	222	184	194
196							
grid # 4	330	331	226	331	223	327	316
343							

number of gridpoints:



atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	88	89
grid # 2	109	101	109	97	96	96	97
grid # 3	211	195	214	184	185	184	185
grid # 4	214	342	212	329	329	328	328

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
grid # 1	72	73	73	73	73	82	70
grid # 2	113	115	118	118	118	88	109
grid # 3	214	215	223	222	224	165	217
grid # 4	221	215	224	222	224	290	217

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
grid # 1	89	89	88	89	89	72	71
grid # 2	97	95	96	97	97	115	114
grid # 3	185	182	185	184	184	218	214
grid # 4	328	328	330	328	329	218	210

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3517
grid # 2	118	118	115	4490
grid # 3	223	223	220	8640
grid # 4	223	224	224	12258

end of program grid

start of program rwr  
recomputing RWR matrix 1 grid: 4  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i	total energy	energy	change	error
	r	t	s	t	d		change		
etot	1	N	N	2	U	-990.33510685770		3.7E-04	3.1E-02
etot	2	Y	Y	6	M	-990.38314472816	4.8E-02	1.8E-04	1.2E-02
etot	3	N	Y	2	U	-990.38935537066	6.2E-03	5.3E-05	3.1E-03
etot	4	Y	Y	6	M	-990.38969679674	3.4E-04	2.3E-05	1.1E-03
etot	5	Y	Y	6	M	-990.38977611385	7.9E-05	7.6E-06	2.8E-04
etot	6	N	Y	2	U	-990.38979109239	1.5E-05	3.0E-06	6.9E-05
etot	7	Y	N	6	M	-990.38979365506	2.6E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1967.21099465467	
(E)	Total one-electron terms.....	-5252.71557057016	
(I)	Total two-electron terms.....	2295.11478226043	
(L)	Electronic energy.....	-2957.60078830974	(E+I)
(N)	Total energy.....	-990.38979365506	(A+L)

SCFE: SCF energy: HF -990.38979365506 hartrees iterations:

7

HOMO energy: -0.26875  
LUMO energy: 0.09679

Orbital energies:

-15.60440	-15.56408	-11.29484	-11.28605	-11.27171	-11.25310
-11.25060	-11.24821	-11.24599	-11.24090	-11.23981	-11.23932
-11.23928	-11.23863	-11.23847	-11.23780	-11.23743	-11.23721
-11.23472	-11.23260	-11.22506	-11.21958	-11.21917	-11.21594
-11.21230	-1.32371	-1.25138	-1.16194	-1.15811	-1.13746
-1.07380	-1.06529	-1.03784	-1.02261	-1.01706	-1.01675
-0.97106	-0.95358	-0.93345	-0.86016	-0.83584	-0.83204
-0.82722	-0.80690	-0.79592	-0.76979	-0.73260	-0.71689
-0.70107	-0.69646	-0.66553	-0.65782	-0.64254	-0.63657
-0.63323	-0.62328	-0.62039	-0.61546	-0.59597	-0.59273
-0.59071	-0.58733	-0.57653	-0.55793	-0.55254	-0.54806
-0.54230	-0.51743	-0.50677	-0.50276	-0.50055	-0.49573
-0.49322	-0.49115	-0.48789	-0.48019	-0.42914	-0.40421
-0.36715	-0.34259	-0.34204	-0.33775	-0.32820	-0.28241
-0.26875	0.09679	0.12767	0.13691	0.13716	0.14724
0.17920	0.20956	0.22641	0.23420	0.24136	

end of program scf

start of program derla  
end of program derla

```

start of program rwr
recomputing RwR matrix 1      grid: 4
end of program rwr

```

```

start of program der1b

```

```

forces (hartrees/bohr) : total

```

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	1.305964E-03	-1.677270E-03	-2.594790E-03
2	N2	-7.405171E-03	-1.586511E-03	6.320733E-03
3	C4	3.028731E-03	1.790473E-03	-3.798228E-04
4	C5	7.226851E-03	4.524737E-03	-7.098855E-03
5	C6	2.476199E-04	-3.135427E-03	2.297075E-04
6	C7	-2.330886E-03	2.478329E-03	3.273788E-04
7	C13	2.227097E-04	1.311746E-03	-4.798910E-03
8	H4	-1.002454E-03	-3.214195E-03	-8.533394E-05
9	C8	2.159221E-03	-4.853058E-03	-3.527892E-03
10	C11	-3.302127E-03	-1.233147E-03	3.282272E-03
11	H7	-7.362198E-04	1.749372E-03	1.319340E-03
12	C9	3.320533E-03	4.276770E-03	-1.934309E-03
13	H8	-1.912353E-03	-7.144657E-04	1.822387E-03
14	C10	8.315593E-04	4.548646E-03	7.271826E-04
15	C12	4.548962E-03	-1.450949E-03	-2.371630E-03
16	C2	-9.938152E-04	7.535157E-04	1.267906E-03
17	H13	1.386542E-03	-4.258552E-04	9.927676E-04
18	C14	2.299989E-03	-7.682804E-05	1.238775E-03
19	H15	1.984307E-04	-8.884950E-04	-8.118002E-04
20	C15	-6.451323E-04	-1.027048E-03	4.774511E-03
21	C16	-2.632256E-04	-3.149773E-04	3.356515E-03
22	C17	1.008954E-03	6.183636E-05	-1.888416E-03
23	C18	1.484312E-04	-5.973317E-04	-2.098115E-03
24	C19	-1.156244E-03	-3.591191E-04	4.042049E-04
25	H16	-7.120642E-03	-2.020923E-03	-6.701640E-04
26	H17	3.236541E-03	1.487269E-03	-1.213183E-03
27	H18	7.301887E-03	2.526935E-03	1.127166E-03
28	H19	-4.266701E-03	-1.422013E-03	1.600621E-03
29	H20	-5.797366E-04	3.861398E-04	-2.246165E-03
30	C1	-5.155529E-03	-8.921110E-04	1.159786E-03
31	H5	2.282436E-03	2.852896E-04	2.405521E-03
32	H6	-2.782347E-04	1.257850E-03	-1.502622E-03
33	C3	-3.641709E-03	-3.629131E-03	3.069671E-03
34	C26	-2.578335E-03	-3.574081E-03	-3.583493E-04
35	C27	-8.629869E-04	-1.384270E-03	3.235411E-03
36	C28	1.635804E-03	2.327281E-03	9.648920E-04
37	C29	8.904502E-04	7.644047E-04	-3.194343E-03
38	H1	-1.706450E-03	-2.318215E-04	-2.241600E-03
39	H2	4.690082E-04	6.810360E-04	2.172640E-03
40	H3	8.078606E-04	8.518771E-04	1.530140E-03

41	H9	-1.100102E-03	-1.113211E-03	-2.495881E-03
42	H10	3.825774E-03	3.254866E-03	-2.412596E-03
43	H25	-2.808875E-04	1.593320E-03	4.916000E-04
-----				
	total	1.065317E-03	1.089457E-03	-1.036505E-04

end of program derlb

start of program geopt 3

geometry optimization step 3

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000236

Cos(theta): 0.4953472

Final level shift: -1.6630388E-02

energy change: -2.3810E-03 . ( 5.0000E-05 )

gradient maximum: 9.9076E-03 . ( 4.5000E-04 )

gradient rms: 2.3236E-03 . ( 3.0000E-04 )

step size: 0.29975 trust radius: 0.30000

displacement maximum: 1.0837E-01 . ( 1.8000E-03 )

displacement rms: 2.3551E-02 . ( 1.2000E-03 )

predicted energy change: -2.9446E-03 geom step: 2.9975E-

01 full step: 2.9975E-01

molecular structure not yet converged...

center of mass moved by:

x: 4.5379E-03 y: 1.6225E-03 z: -1.0573E-02

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2064093151	0.4564334872	1.1449569640
N2	-0.9777143120	-2.2675882391	1.1401282031
C4	-1.2067896365	-0.0074822023	1.9347114372
C5	0.0100178696	-1.8812418506	0.4407932188
C6	-1.6301115836	-1.3290633316	1.9647297688
C7	-1.7180530931	1.0023503931	2.7134818099
C13	0.7013842690	-2.8816737324	-0.4740592873
H4	-3.0216327063	-2.6539904306	2.8557401227
C8	-2.7796853502	0.6766421222	3.5699349035
C11	-0.9469746435	2.1651389329	2.3678165600
H7	-3.2396438255	1.4178307697	4.2013122414
C9	-3.2317902692	-0.6316840549	3.6015379272

H8	-4.0475645815	-0.8929676898	4.2526147254
C10	-2.6592479127	-1.6425581119	2.8070396413
C12	-0.0282154727	1.7951337785	1.4350689770
C2	0.9934644979	2.6280168532	0.7795619441
H13	1.7730430366	-2.7575478083	-0.4156955215
C14	0.2865859920	-2.7249268767	-1.9051731340
H15	0.4713121897	-3.8629015133	-0.0943843922
C15	-0.5615655542	-2.4619627032	-4.5190042806
C16	1.1125815133	-2.1862381413	-2.8583626252
C17	-0.9661916103	-3.1291782413	-2.2777042664
C18	-1.3890096252	-3.0026868085	-3.5700862667
C19	0.6893320833	-2.0524259860	-4.1584209800
H16	2.0979129012	-1.8591107039	-2.5945051992
H17	-1.6160289056	-3.5619217481	-1.5421987308
H18	-2.3733434532	-3.3581172536	-3.8357831773
H19	1.3434543159	-1.6264018218	-4.8889259482
H20	-0.9021702747	-2.3804723563	-5.5318037396
C1	0.5974414175	-0.4754948750	0.3889408228
H5	1.6054220101	-0.5235796038	0.7857568676
H6	0.6751609178	-0.1866596432	-0.6452941877
C3	2.9244707837	4.2594570176	-0.3923566804
C26	1.7907979932	3.4485799055	1.5329596121
C27	1.1713262529	2.6405355796	-0.5729922605
C28	2.1366910125	3.4439199169	-1.1538018568
C29	2.7452329284	4.2656384654	0.9532276351
H1	1.6745334301	3.4364257238	2.5857229416
H2	0.5529801450	2.0327292614	-1.1904461656
H3	2.2687279040	3.4308993892	-2.2062196320
H9	3.3448720185	4.8980738147	1.5650329855
H10	3.6696029435	4.8876836769	-0.8403675527
H25	-1.0676334116	3.1643232144	2.7358050805

nuclear repulsion energy..... 1978.365603056 hartrees

-----  
 / end of geometry optimization iteration 3 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.790E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:								
	atom	N1	N2	C4	C5	C6	C7	C13
H4								
73	grid # 1	96	102	86	88	90	88	84
118	grid # 2	104	112	95	95	99	96	92
224	grid # 3	214	227	194	188	192	198	164
223	grid # 4	389	414	321	321	322	344	298

number of gridpoints:								
	atom	C8	C11	H7	C9	H8	C10	C12
C2								
88	grid # 1	89	87	73	87	73	89	86
99	grid # 2	97	94	118	97	118	97	94
191	grid # 3	185	184	223	185	222	184	195
339	grid # 4	331	331	226	330	223	326	320

number of gridpoints:								
	atom	H13	C14	H15	C15	C16	C17	C18
C19								
87	grid # 1	69	93	69	87	86	87	87
97	grid # 2	109	101	109	97	96	96	97
182	grid # 3	211	191	213	182	182	181	182
327	grid # 4	209	339	212	325	327	327	328

number of gridpoints:								
	atom	H16	H17	H18	H19	H20	C1	H5
H6								
69	grid # 1	72	72	73	73	73	82	70
103	grid # 2	113	114	118	118	118	87	108
204	grid # 3	213	215	222	221	223	163	217
202	grid # 4	213	214	223	222	224	290	217

number of gridpoints:								
	atom	C3	C26	C27	C28	C29	H1	H2
H3								

grid # 1	89	87	86	87	87	72	70
73							
grid # 2	97	96	96	97	97	115	113
118							
grid # 3	182	181	182	182	183	217	213
222							
grid # 4	328	326	327	327	324	216	210
222							

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3497
grid # 2	118	118	115	4486
grid # 3	222	222	219	8597
grid # 4	223	223	222	12205

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.32090183004		4.0E-04	2.7E-02
etot	2	Y	Y	6	M	-990.37602444074	5.5E-02	1.9E-04	1.1E-02
etot	3	N	Y	2	U	-990.38279174353	6.8E-03	5.6E-05	2.9E-03
etot	4	Y	Y	6	M	-990.38330673990	5.1E-04	2.8E-05	1.2E-03
etot	5	Y	Y	6	M	-990.38339751676	9.1E-05	7.9E-06	2.7E-04
etot	6	N	Y	2	U	-990.38336351948	-3.4E-05	3.5E-06	8.1E-05
etot	7	Y	N	6	M	-990.38336784090	4.3E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1978.36560305571	
(E)	Total one-electron terms.....	-5274.81755689824	
(I)	Total two-electron terms.....	2306.06858600163	
(L)	Electronic energy.....	-2968.74897089661	(E+I)
(N)	Total energy.....	-990.38336784090	(A+L)

SCFE: SCF energy: HF -990.38336784090 hartrees iterations:

7

HOMO energy: -0.26814  
LUMO energy: 0.09639

Orbital energies:

-15.60547	-15.56550	-11.29770	-11.28619	-11.27078	-11.25022
-11.24528	-11.24450	-11.23825	-11.23745	-11.23449	-11.23301
-11.23221	-11.23109	-11.23069	-11.23034	-11.22948	-11.22838
-11.22673	-11.22459	-11.22253	-11.21876	-11.21686	-11.21593
-11.21192	-1.32742	-1.24676	-1.17463	-1.17229	-1.14078
-1.07809	-1.07260	-1.04756	-1.02329	-1.02291	-1.02144
-0.97578	-0.95637	-0.93529	-0.86214	-0.84435	-0.83597
-0.83375	-0.80916	-0.79677	-0.77365	-0.73422	-0.72183
-0.70571	-0.70299	-0.66886	-0.65951	-0.64726	-0.64126
-0.63446	-0.62424	-0.62327	-0.61823	-0.59835	-0.59393
-0.59044	-0.58890	-0.58373	-0.56063	-0.55582	-0.54996
-0.54261	-0.52147	-0.51054	-0.50427	-0.50252	-0.49989
-0.49515	-0.49181	-0.48895	-0.48236	-0.42870	-0.40579
-0.37068	-0.34887	-0.34027	-0.33992	-0.33265	-0.28268
-0.26814	0.09639	0.13129	0.13834	0.14272	0.15301
0.18158	0.21027	0.22587	0.23576	0.24199	

end of program scf

start of program derla

end of program derla

start of program rwr

end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	2.088108E-03	-1.816608E-03	-3.641703E-03
2	N2	1.359145E-02	2.603072E-03	-9.392358E-03
3	C4	4.660404E-04	-1.020443E-02	-2.510234E-03
4	C5	-1.216198E-02	-6.585574E-03	6.161446E-03
5	C6	7.087680E-03	-4.398158E-04	-6.447246E-03
6	C7	-3.899426E-03	5.933573E-03	2.324081E-03
7	C13	3.821605E-03	5.890252E-03	1.357044E-02
8	H4	2.973135E-04	4.132462E-04	7.230307E-05
9	C8	-6.397915E-03	-7.377681E-03	4.298384E-03
10	C11	3.207322E-03	5.420828E-03	1.334689E-03
11	H7	6.085201E-04	2.998135E-05	-7.440425E-04
12	C9	-3.822426E-04	8.286041E-03	2.243006E-03
13	H8	2.340008E-04	7.691603E-04	4.906764E-04
14	C10	-1.938760E-03	-6.468270E-04	1.244062E-03
15	C12	-6.102382E-03	-1.064691E-03	1.815286E-03
16	C2	-8.753000E-03	-6.468478E-03	1.178688E-02



17	H13	5.162556E-03	1.641355E-03	3.634586E-03
18	C14	3.407200E-03	-1.591991E-03	8.898751E-03
19	H15	-2.336800E-03	-4.255029E-03	-1.094404E-03
20	C15	-8.884359E-03	-7.898080E-04	-1.509099E-02
21	C16	1.333100E-02	6.137570E-03	1.627549E-03
22	C17	-1.655284E-02	-9.413400E-03	8.281097E-03
23	C18	-2.099264E-02	-9.634396E-03	-4.550000E-03
24	C19	1.119810E-02	6.856261E-03	-8.067226E-03
25	H16	4.778835E-03	6.395915E-04	1.815445E-03
26	H17	-2.269290E-03	-3.734078E-04	2.039251E-03
27	H18	1.898389E-03	2.441004E-03	-7.736249E-04
28	H19	4.019581E-03	1.995855E-03	-3.556696E-03
29	H20	5.225823E-04	1.660109E-03	-3.684042E-03
30	C1	-1.526528E-04	-1.293907E-03	5.029993E-03
31	H5	3.804775E-03	3.806220E-04	3.734436E-04
32	H6	1.802152E-04	1.858511E-03	-4.200778E-03
33	C3	1.062426E-02	8.644818E-03	-1.207225E-02
34	C26	1.147070E-02	1.162699E-02	1.033083E-02
35	C27	4.957450E-03	-1.858617E-04	-2.536308E-02
36	C28	-9.660113E-03	-1.041083E-02	-8.949314E-03
37	C29	-5.181304E-03	-1.111879E-03	2.398876E-02
38	H1	-3.259171E-04	1.476531E-03	1.312592E-02
39	H2	-4.697105E-03	-3.791650E-03	-6.595315E-03
40	H3	-5.870500E-04	-1.164633E-03	-1.251753E-02
41	H9	4.371697E-03	4.237461E-03	6.763454E-03
42	H10	1.379739E-03	7.800523E-04	-2.571094E-03
43	H25	-3.342425E-04	-4.287707E-04	6.210274E-04
-----				
	total	8.991054E-04	6.732157E-04	4.943495E-05

end of program derlb

start of program geopt 4

geometry optimization step 4

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 3 \*\*

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000460

Cos(theta): 0.3075896

Final level shift: -4.9937562E-03

energy change: 6.4258E-03 . ( 5.0000E-05 )

gradient maximum: 9.9076E-03 . ( 4.5000E-04 )

gradient rms: 2.3236E-03 . ( 3.0000E-04 )

step size: 0.29978 trust radius: 0.30000  
 displacement maximum: 1.5805E-01 . ( 1.8000E-03 )  
 displacement rms: 2.3553E-02 . ( 1.2000E-03 )  
 predicted energy change: -1.5876E-03 geom step: 2.9978E-01  
 full step: 2.9978E-01  
 molecular structure not yet converged...

center of mass moved by:

x: -2.4980E-16 y: -3.4694E-17 z: -6.1062E-16

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2605037549	0.4125439612	1.1900034197
N2	-1.0201882848	-2.3117451892	1.2286465763
C4	-1.2291547382	-0.0501813353	2.0213210471
C5	-0.0584840655	-1.9323738777	0.5045877913
C6	-1.6433405541	-1.3707651498	2.0724302477
C7	-1.7196322432	0.9707097685	2.8115399710
C13	0.6123641543	-2.9395135162	-0.4045486213
H4	-3.0004875650	-2.6843033639	3.0337672096
C8	-2.7502677659	0.6466074665	3.7128944205
C11	-0.9641692572	2.1368330189	2.4248916539
H7	-3.1870956384	1.3938929758	4.3523390576
C9	-3.1923609494	-0.6577264470	3.7717764284
H8	-3.9791920871	-0.9171763497	4.4577173169
C10	-2.6430824576	-1.6735110866	2.9607130298
C12	-0.0894151548	1.7589272383	1.4540514090
C2	0.8975931598	2.5804167511	0.7178403216
H13	1.6900885460	-2.9175445528	-0.2351375024
C14	0.3269913213	-2.6769735270	-1.8741990189
H15	0.2546697460	-3.9228910664	-0.1143387386
C15	-0.2180137009	-2.2191864228	-4.5767173828
C16	1.3496559462	-2.4227648804	-2.7664884238
C17	-0.9764471114	-2.6992027704	-2.3557447632
C18	-1.2462393835	-2.4742543646	-3.6931624843
C19	1.0776231861	-2.1937356607	-4.1071135875
H16	2.3658535888	-2.4078532060	-2.4199820995
H17	-1.7766859001	-2.8933381124	-1.6738564557
H18	-2.2487902734	-2.4928964715	-4.0444386495
H19	1.8875121812	-1.9993966839	-4.7814773829
H20	-0.4271057620	-2.0495195336	-5.6159740449
C1	0.5363502956	-0.5262371704	0.4297996206
H5	1.5569005697	-0.5698600523	0.8077454585
H6	0.5969268301	-0.2400532601	-0.6132951547
C3	2.7366658910	4.1635728363	-0.6570139302
C26	1.8494198086	3.3298911691	1.4147477126
C27	0.8738252674	2.6383115327	-0.6774631325
C28	1.7919425574	3.4195085202	-1.3586689873
C29	2.7597734096	4.1195096692	0.7311384976
H1	1.8863612505	3.2798815381	2.4949515492
H2	0.1256541849	2.0873284863	-1.2299565889

H3	1.7610423948	3.4526209625	-2.4364084657
H9	3.4896654651	4.6919589348	1.2854978074
H10	3.4478987066	4.7719686917	-1.1860693938
H25	-1.0742926529	3.1373751310	2.7923517727

nuclear repulsion energy..... 1974.668059347 hartrees

-----  
 / end of geometry optimization iteration 4 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.817E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	87	88	90	88	84
73							
grid # 2	104	112	95	95	99	98	92
118							
grid # 3	214	227	195	186	191	200	164
224							
grid # 4	389	414	320	320	324	347	299
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	84
92							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	184	222	184	195
196							
grid # 4	330	330	226	331	223	327	321
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							

grid # 1	69	91	69	89	88	86	89
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87

grid # 2	110	100	110	97	96	96	97
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96

grid # 3	210	196	218	182	183	183	183
----------	-----	-----	-----	-----	-----	-----	-----

182

grid # 4	215	342	217	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
------	-----	-----	-----	-----	-----	----	----

H6

grid # 1	73	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	113	115	118	118	118	88	109
----------	-----	-----	-----	-----	-----	----	-----

105

grid # 3	214	216	222	221	223	165	217
----------	-----	-----	-----	-----	-----	-----	-----

208

grid # 4	213	214	223	222	224	290	217
----------	-----	-----	-----	-----	-----	-----	-----

206

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	89	88	89	89	73	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
----------	----	----	----	----	----	-----	-----

118

grid # 3	185	182	185	184	184	218	216
----------	-----	-----	-----	-----	-----	-----	-----

223

grid # 4	330	328	329	328	329	219	214
----------	-----	-----	-----	-----	-----	-----	-----

223

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	73	3516
grid # 2	118	118	115	4495
grid # 3	223	224	221	8642
grid # 4	224	224	224	12258

end of program grid

start of program rwr  
end of program rwr

start of program scf

i	u	d	i	g		
t	p	i	c	r		
e	d	i	u	i	energy	RMS maximum density DIIS

	r	t	s	t	d	total energy	change	change	error
etot	1	N	N	2	U	-990.14145563547		7.8E-04	3.9E-02
etot	2	Y	Y	6	M	-990.35861329482	2.2E-01	3.9E-04	1.6E-02
etot	3	N	Y	2	U	-990.38809039062	2.9E-02	1.2E-04	3.9E-03
etot	4	Y	Y	6	M	-990.38982038619	1.7E-03	4.1E-05	1.2E-03
etot	5	Y	Y	6	M	-990.39009100052	2.7E-04	1.6E-05	3.2E-04
etot	6	N	Y	2	U	-990.39013660923	4.6E-05	5.8E-06	1.0E-04
etot	7	Y	Y	6	M	-990.39013977366	3.2E-06	2.4E-06	3.6E-05
etot	8	Y	N	6	M	-990.39014043744	6.6E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1974.66805934711	
(E)	Total one-electron terms.....	-5267.59739614095	
(I)	Total two-electron terms.....	2302.53919635640	
(L)	Electronic energy.....	-2965.05819978455	(E+I)
(N)	Total energy.....	-990.39014043744	(A+L)

SCFE: SCF energy: HF -990.39014043744 hartrees iterations:

8

HOMO energy: -0.26872  
LUMO energy: 0.09755

Orbital energies:

-15.60449	-15.56529	-11.29607	-11.28604	-11.27093	-11.25222
-11.25039	-11.24527	-11.24459	-11.24123	-11.24070	-11.24044
-11.24005	-11.23923	-11.23844	-11.23434	-11.23294	-11.23235
-11.23098	-11.22932	-11.22452	-11.21957	-11.21815	-11.21574
-11.21231	-1.32548	-1.24923	-1.16438	-1.16096	-1.13857
-1.07363	-1.06865	-1.03835	-1.02173	-1.02055	-1.01749
-0.97069	-0.95517	-0.93360	-0.86029	-0.83635	-0.83387
-0.83017	-0.80766	-0.79576	-0.76982	-0.73217	-0.71750
-0.70155	-0.70000	-0.66622	-0.65729	-0.64350	-0.63778
-0.63371	-0.62436	-0.62014	-0.61563	-0.59577	-0.59197
-0.59045	-0.58757	-0.58039	-0.55733	-0.55239	-0.54828
-0.54513	-0.51672	-0.50646	-0.50304	-0.50031	-0.49689
-0.49432	-0.49097	-0.48728	-0.48190	-0.42913	-0.40459
-0.36595	-0.34214	-0.34166	-0.33817	-0.33118	-0.28287
-0.26872	0.09755	0.12906	0.13686	0.13760	0.14839
0.17922	0.20764	0.22771	0.23529	0.24258	

end of program scf

start of program derla  
end of program derla

start of program rwr

end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	1.722647E-04	-1.371273E-03	-2.097232E-03
2	N2	2.307619E-03	2.645434E-04	-1.429536E-03
3	C4	9.233719E-04	-1.909727E-03	-3.397651E-04
4	C5	-2.472205E-03	-1.364835E-03	1.074612E-03
5	C6	9.104396E-04	-8.696098E-04	-8.667630E-04
6	C7	-2.264358E-03	1.987665E-03	9.229630E-04
7	C13	1.704094E-05	-1.512183E-03	1.932501E-03
8	H4	-1.303564E-04	-3.601330E-04	6.584231E-05
9	C8	-2.402673E-04	-8.558610E-04	6.577247E-04
10	C11	1.082298E-03	1.304216E-03	5.319032E-04
11	H7	2.368012E-04	2.173179E-04	-3.217904E-04
12	C9	5.433283E-04	1.494368E-03	-2.250984E-04
13	H8	-7.318402E-06	9.919423E-05	2.294528E-04
14	C10	-3.416522E-04	-3.416849E-04	3.024806E-05
15	C12	5.998397E-04	6.585509E-04	7.717878E-04
16	C2	1.338325E-03	2.564232E-03	7.609119E-04
17	H13	-2.445629E-03	3.019296E-04	-7.005633E-04
18	C14	-1.006014E-03	-2.287806E-03	2.671755E-03
19	H15	3.635537E-04	1.884244E-03	-9.943853E-04
20	C15	2.027062E-03	2.500076E-04	-2.559217E-03
21	C16	2.727088E-03	1.063025E-03	-3.560983E-03
22	C17	-9.564304E-04	-6.952268E-05	-1.579709E-04
23	C18	2.482024E-03	-4.635361E-04	6.616306E-03
24	C19	5.817905E-03	2.160421E-04	-5.459483E-04
25	H16	2.531985E-03	4.057878E-04	1.288178E-04
26	H17	-4.824063E-03	-1.082739E-03	2.997523E-03
27	H18	-1.047403E-02	-7.737787E-04	-2.242630E-03
28	H19	2.831240E-03	6.714518E-04	-2.296848E-03
29	H20	2.548070E-04	7.177312E-04	-1.647014E-03
30	C1	4.326349E-04	1.117342E-03	1.134530E-03
31	H5	3.099164E-04	3.869422E-04	-1.953429E-05
32	H6	-4.484517E-05	5.228931E-04	6.438714E-04
33	C3	-2.488043E-03	-2.181722E-03	6.024058E-04
34	C26	-2.683586E-03	-2.958448E-03	1.442213E-03
35	C27	2.666601E-04	-4.104175E-04	1.506358E-03
36	C28	2.305602E-03	2.215407E-03	4.983410E-04
37	C29	8.628620E-04	7.523044E-04	-1.843323E-03
38	H1	-1.674844E-03	-2.410790E-04	-4.984929E-03
39	H2	2.525584E-03	1.790540E-03	2.833707E-03
40	H3	8.433839E-04	7.493248E-04	2.107534E-03
41	H9	-2.068308E-03	-1.653712E-03	-2.587104E-03
42	H10	8.221141E-05	1.717202E-04	-7.402267E-04
43	H25	-1.315526E-04	-2.308952E-04	-4.026906E-05

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total      5.423385E-04    8.678193E-04   -3.982191E-05

```

end of program derlb

start of program geopt 5

geometry optimization step 5

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001034

Cos(theta): 0.4746771

Final level shift: -1.8111015E-02

energy change: -3.4678E-04 . ( 5.0000E-05 )

gradient maximum: 1.0656E-02 . ( 4.5000E-04 )

gradient rms: 2.1734E-03 . ( 3.0000E-04 )

step size: 0.29956 trust radius: 0.30000

displacement maximum: 1.2495E-01 . ( 1.8000E-03 )

displacement rms: 2.3536E-02 . ( 1.2000E-03 )

predicted energy change: -2.7815E-03 geom step: 2.9956E-

01 full step: 2.9956E-01

molecular structure not yet converged...

center of mass moved by:

x: 8.1464E-03 y: 6.0566E-03 z: -8.7285E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2292024469	0.4427015271	1.1628880103
N2	-0.9782568628	-2.2878207032	1.1779266582
C4	-1.2094337002	-0.0303642055	1.9757531149
C5	-0.0161249279	-1.9029247248	0.4674816553
C6	-1.6194223744	-1.3523145475	2.0109279641
C7	-1.7211646352	0.9868621882	2.7632723068
C13	0.6544591552	-2.9143021590	-0.4408657883
H4	-2.9999077625	-2.6718770241	2.9344446436
C8	-2.7718199836	0.6572998838	3.6401084653
C11	-0.9491404552	2.1543222696	2.4120276559
H7	-3.2211900614	1.4029180697	4.2716980948
C9	-3.2132989134	-0.6466971041	3.6786741679
H8	-4.0163262814	-0.9105012423	4.3442732707
C10	-2.6416683415	-1.6597368984	2.8743855662
C12	-0.0562922792	1.7860587709	1.4560571753

C2	0.9488951143	2.6311226377	0.7701830808
H13	1.7281674582	-2.8468821058	-0.3270846920
C14	0.2937960086	-2.7261589105	-1.9088007454
H15	0.3445375745	-3.8922911028	-0.1088900635
C15	-0.4402906415	-2.3952792758	-4.5794029238
C16	1.2395116030	-2.3428910048	-2.8630371971
C17	-1.0270889510	-2.9533277298	-2.3085099819
C18	-1.3921717180	-2.7920309200	-3.6337066705
C19	0.8788052648	-2.1725843519	-4.1956505663
H16	2.2638244085	-2.1880678707	-2.5683467508
H17	-1.7675239977	-3.2630084538	-1.5767242550
H18	-2.4257099259	-2.9929594166	-3.9302355350
H19	1.6217050002	-1.8773108746	-4.9256653884
H20	-0.7280733175	-2.2675932286	-5.6111620858
C1	0.5821138301	-0.4915229124	0.4118188533
H5	1.5989978845	-0.5325329495	0.8024327801
H6	0.6562234427	-0.2012124645	-0.6287278123
C3	2.8551861345	4.2505727705	-0.4749461088
C26	1.7771405951	3.4522098043	1.5201834275
C27	1.0866007330	2.6404146539	-0.6152847579
C28	2.0341472297	3.4391158849	-1.2329113044
C29	2.7192766740	4.2587160999	0.9026633710
H1	1.6846480152	3.4442277353	2.5858043452
H2	0.4363216332	2.0366757013	-1.2116377193
H3	2.1295952060	3.4333746931	-2.3030217836
H9	3.3514260736	4.8860237979	1.4956835722
H10	3.5921450310	4.8707133033	-0.9544874007
H25	-1.0689547267	3.1499012113	2.7877233660

nuclear repulsion energy..... 1967.972340116 hartrees

/ end of geometry optimization iteration 5 /

end of program geopt

start of program onee  
smallest eigenvalue of S: 2.829E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							



grid # 1	95	102	87	88	90	90	84
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73

grid # 2	103	112	95	95	99	98	92
----------	-----	-----	----	----	----	----	----

118

grid # 3	212	227	195	188	190	199	163
----------	-----	-----	-----	-----	-----	-----	-----

224

grid # 4	386	413	321	320	321	348	300
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12

C2

grid # 1	89	87	73	87	73	89	86
----------	----	----	----	----	----	----	----

92

grid # 2	97	94	118	97	118	97	95
----------	----	----	-----	----	-----	----	----

100

grid # 3	184	185	223	184	222	184	195
----------	-----	-----	-----	-----	-----	-----	-----

195

grid # 4	328	330	226	331	223	327	320
----------	-----	-----	-----	-----	-----	-----	-----

340

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18

C19

grid # 1	69	93	69	89	88	88	89
----------	----	----	----	----	----	----	----

89

grid # 2	109	100	110	97	96	96	97
----------	-----	-----	-----	----	----	----	----

96

grid # 3	211	198	213	185	185	184	185
----------	-----	-----	-----	-----	-----	-----	-----

184

grid # 4	210	342	212	330	329	328	329
----------	-----	-----	-----	-----	-----	-----	-----

329

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5

H6

grid # 1	72	72	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	115	114	118	118	118	88	110
----------	-----	-----	-----	-----	-----	----	-----

104

grid # 3	214	215	223	222	224	163	217
----------	-----	-----	-----	-----	-----	-----	-----

206

grid # 4	214	215	232	223	224	292	217
----------	-----	-----	-----	-----	-----	-----	-----

204

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2

H3

grid # 1	89	87	88	89	89	72	70
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	113
----------	----	----	----	----	----	-----	-----

118

grid # 3	184	182	184	184	185	217	213
----------	-----	-----	-----	-----	-----	-----	-----

222

grid # 4	328	327	329	327	328	215	211
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3518
grid # 2	118	118	115	4493
grid # 3	222	223	219	8634
grid # 4	224	224	223	12248

end of program grid

start of program rwr  
end of program rwr

start of program scf

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

etot	1	N	N	2	U	-990.30892225319		4.4E-04	2.7E-02
etot	2	Y	Y	6	M	-990.37951017403	7.1E-02	2.2E-04	1.1E-02
etot	3	N	Y	2	U	-990.38894674829	9.4E-03	6.5E-05	2.8E-03
etot	4	Y	Y	6	M	-990.38948696771	5.4E-04	2.2E-05	8.5E-04
etot	5	Y	Y	6	M	-990.38957252266	8.6E-05	9.0E-06	2.1E-04
etot	6	N	Y	2	U	-990.38957720340	4.7E-06	3.0E-06	4.3E-05
etot	7	Y	N	6	M	-990.38957709405	-1.1E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1967.97234011558	
(E)	Total one-electron terms.....	-5254.19895519368	
(I)	Total two-electron terms.....	2295.83703798405	
(L)	Electronic energy.....	-2958.36191720963	(E+I)
(N)	Total energy.....	-990.38957709405	(A+L)

SCFE: SCF energy: HF -990.38957709405 hartrees iterations:  
7

HOMO energy: -0.26884  
LUMO energy: 0.09597

Orbital energies:

-15.60543	-15.56487	-11.29622	-11.28765	-11.27212	-11.25108
-11.25053	-11.24792	-11.24652	-11.23892	-11.23891	-11.23883

-11.23801	-11.23777	-11.23716	-11.23711	-11.23637	-11.23587
-11.23553	-11.23260	-11.22496	-11.22078	-11.21925	-11.21651
-11.21329	-1.32543	-1.25168	-1.16443	-1.15738	-1.13804
-1.07535	-1.06529	-1.04001	-1.02194	-1.01727	-1.01663
-0.97152	-0.95322	-0.93415	-0.85977	-0.83914	-0.83253
-0.82686	-0.80677	-0.79549	-0.77050	-0.73321	-0.71759
-0.70203	-0.69559	-0.66640	-0.65820	-0.64265	-0.63725
-0.63362	-0.62320	-0.62133	-0.61564	-0.59719	-0.59253
-0.59025	-0.58763	-0.57566	-0.55800	-0.55276	-0.54852
-0.54404	-0.51815	-0.50817	-0.50261	-0.50009	-0.49525
-0.49276	-0.49132	-0.48786	-0.48039	-0.42993	-0.40500
-0.36914	-0.34440	-0.34069	-0.33787	-0.32708	-0.28199
-0.26884	0.09597	0.12827	0.13658	0.13747	0.14798
0.17910	0.21010	0.22715	0.23493	0.24011	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	1.630734E-03	4.147837E-04	-2.328007E-04
2	N2	-4.394325E-03	-1.352038E-03	2.472753E-03
3	C4	-1.011245E-03	1.568492E-03	3.045752E-05
4	C5	4.998187E-03	1.221166E-03	-4.075432E-03
5	C6	-2.039398E-03	-4.311267E-04	1.780415E-03
6	C7	6.101085E-05	-2.060345E-04	7.720866E-04
7	C13	4.203179E-04	3.755701E-03	-3.272974E-03
8	H4	5.925810E-05	2.078679E-04	8.546451E-05
9	C8	1.534280E-03	-1.965932E-04	-1.082552E-03
10	C11	-1.931759E-03	-9.908874E-04	6.215361E-04
11	H7	-1.775814E-04	1.464387E-04	1.739668E-04
12	C9	7.213503E-04	-1.263375E-03	-1.016812E-03
13	H8	1.282530E-04	-1.587411E-04	7.876069E-06
14	C10	-2.470540E-04	1.260490E-03	7.692993E-04
15	C12	1.453405E-03	1.325890E-03	-3.933628E-03
16	C2	-1.019141E-03	-2.748754E-03	-8.869362E-04
17	H13	4.139215E-03	1.790964E-04	9.518011E-04
18	C14	-1.890313E-03	5.889275E-04	-2.220388E-03
19	H15	-5.789694E-04	-2.664568E-03	1.096563E-03
20	C15	-1.086856E-03	-8.299807E-04	2.186525E-03

21	C16	-5.200446E-03	-1.943274E-03	4.012439E-03
22	C17	1.011256E-03	-1.508706E-04	6.361840E-04
23	C18	-3.123879E-03	-7.158290E-04	-6.583892E-03
24	C19	-7.063939E-03	-2.062728E-03	8.090705E-04
25	H16	-2.103718E-04	4.707942E-04	8.553744E-04
26	H17	5.839874E-03	2.613085E-03	-4.175018E-03
27	H18	1.242488E-02	3.786442E-03	1.561713E-03
28	H19	-3.859295E-03	-1.242690E-03	3.275097E-03
29	H20	2.965080E-04	-4.598800E-04	1.965477E-03
30	C1	1.066212E-04	-1.197430E-03	2.415771E-04
31	H5	-6.245271E-04	-2.326934E-04	4.699059E-05
32	H6	-9.647908E-05	1.200227E-04	3.096240E-06
33	C3	2.194370E-03	2.154896E-03	1.522594E-03
34	C26	2.819150E-03	2.857859E-03	-7.306075E-04
35	C27	-1.348596E-04	-3.131549E-04	-4.776516E-04
36	C28	-2.416145E-03	-2.441204E-03	-9.400507E-04
37	C29	-1.201260E-03	-6.874415E-04	9.218558E-06
38	H1	7.430163E-04	7.420055E-04	4.313428E-03
39	H2	-2.921308E-03	-2.500431E-03	-3.182915E-03
40	H3	-1.090762E-03	-7.223903E-04	-1.231965E-03
41	H9	2.552610E-03	2.455616E-03	3.038091E-03
42	H10	7.688328E-05	2.110463E-04	6.463850E-04
43	H25	1.247264E-05	2.472986E-04	8.043307E-05
-----				
	total	9.037392E-04	8.158031E-04	-7.771103E-05

end of program derlb

start of program geopt 6

geometry optimization step 6

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3005785

Cos(theta): 0.4030506

Final level shift: -1.2859045E-02

energy change: 5.6334E-04 . ( 5.0000E-05 )

gradient maximum: 1.2826E-02 . ( 4.5000E-04 )

gradient rms: 2.6475E-03 . ( 3.0000E-04 )

step size: 0.30039 trust radius: 0.30000

displacement maximum: 1.4866E-01 . ( 1.8000E-03 )

displacement rms: 2.3601E-02 . ( 1.2000E-03 )

predicted energy change: -2.6208E-03 geom step: 3.0039E-

01 full step: 3.0039E-01

molecular structure not yet converged...

center of mass moved by:

x: -7.0070E-03 y: 3.1695E-03 z: -3.9849E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2431388835	0.4556736239	1.1723735471
N2	-1.0052221025	-2.2638064326	1.1711775865
C4	-1.2354149005	-0.0068382249	1.9686217617
C5	-0.0219368988	-1.8840112724	0.4769055945
C6	-1.6547168498	-1.3251930492	1.9985456785
C7	-1.7404984224	1.0066322943	2.7505185979
C13	0.6709126692	-2.8977538263	-0.4172186213
H4	-3.0356419670	-2.6439761971	2.9042709974
C8	-2.7930706857	0.6804961350	3.6197611198
C11	-0.9650101197	2.1686595222	2.4024960703
H7	-3.2425652691	1.4227454725	4.2536593268
C9	-3.2422765659	-0.6233719281	3.6535786031
H8	-4.0458719809	-0.8841748627	4.3157805202
C10	-2.6766502685	-1.6346558742	2.8502873309
C12	-0.0710715297	1.7970748741	1.4546947917
C2	0.9503376395	2.6145402001	0.7646068978
H13	1.7459317870	-2.8218826796	-0.2973025660
C14	0.3175412762	-2.7210862854	-1.8808548888
H15	0.3721363370	-3.8731171893	-0.0645970713
C15	-0.4054882560	-2.4055350093	-4.5510673450
C16	1.2049840844	-2.1961843098	-2.8003720449
C17	-0.9385119890	-3.0863025612	-2.3151953733
C18	-1.2985482642	-2.9334100012	-3.6363835117
C19	0.8468309784	-2.0394783637	-4.1317416864
H16	2.1814549757	-1.8985296468	-2.4799685659
H17	-1.6351318329	-3.4951433926	-1.6093012692
H18	-2.2805077802	-3.2390864388	-3.9568211189
H19	1.5442219641	-1.6284067831	-4.8322649240
H20	-0.6918667664	-2.2895583892	-5.5817584789
C1	0.5775477845	-0.4792363854	0.4348181138
H5	1.5772891761	-0.5317014840	0.8498355316
H6	0.6798600143	-0.1840634649	-0.5932120927
C3	2.8710077594	4.1851297153	-0.5136427992
C26	1.9198910499	3.2990087678	1.5101069134
C27	0.9496482049	2.7305127321	-0.6306199707
C28	1.9063251470	3.5077111519	-1.2645504751
C29	2.8739200353	4.0827381339	0.8755772877
H1	1.9381200101	3.2016452634	2.5905377595
H2	0.1888699186	2.2286821548	-1.2204008413
H3	1.8906486427	3.5909148714	-2.3446780704
H9	3.6213149051	4.5998757976	1.4699197044
H10	3.6131544908	4.7887646367	-1.0058448436
H25	-1.0749029726	3.1646160247	2.7777097600

nuclear repulsion energy..... 1972.328492632 hartrees

-----  
/ end of geometry optimization iteration 6 /  
-----

end of program geopt

start of program onee

smallest eigenvalue of S: 2.771E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	95	102	85	88	89	88	84
73							
grid # 2	103	112	95	95	97	96	92
118							
grid # 3	212	227	194	188	190	198	164
224							
grid # 4	387	415	320	320	327	345	300
223							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	193
196							
grid # 4	330	330	226	329	223	326	316
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	87	89
89							
grid # 2	110	101	109	97	96	96	97
96							

grid # 3	211	191	213	182	183	182	184
182							
grid # 4	213	338	212	327	327	327	327
327							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	70
69							
grid # 2	113	115	118	118	118	87	108
103							
grid # 3	214	215	222	221	222	162	217
208							
grid # 4	214	215	224	223	224	290	215
205							

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	89	88	89	89	73	71
73							
grid # 2	97	95	96	97	97	115	115
118							
grid # 3	186	184	185	185	185	218	218
222							
grid # 4	331	328	330	328	329	219	215
222							

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	73	3516
grid # 2	118	118	115	4486
grid # 3	223	224	221	8628
grid # 4	224	224	224	12242

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			
	t	p	i	c	r			
	e	d	i	u	i			
	r	t	s	t	d	total energy	energy change	RMS density change maximum DIIS error
etot	1	N	N	2	U	-990.31135910434		4.3E-04 4.0E-02
etot	2	Y	Y	6	M	-990.37781182905	6.6E-02	2.3E-04 1.6E-02

etot	3	N	Y	2	U	-990.38806340056	1.0E-02	6.8E-05	3.7E-03
etot	4	Y	Y	6	M	-990.38873042054	6.7E-04	2.3E-05	1.0E-03
etot	5	Y	Y	6	M	-990.38880803844	7.8E-05	9.7E-06	2.1E-04
etot	6	N	Y	2	U	-990.38880825493	2.2E-07	3.3E-06	4.7E-05
etot	7	Y	N	6	M	-990.38881016479	1.9E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1972.32849263240	
(E)	Total one-electron terms.....	-5262.93232379671	
(I)	Total two-electron terms.....	2300.21502099953	
(L)	Electronic energy.....	-2962.71730279719	(E+I)
(N)	Total energy.....	-990.38881016479	(A+L)

SCFE: SCF energy: HF      -990.38881016479 hartrees      iterations:  
7

HOMO energy:      -0.26932  
LUMO energy:      0.09840

Orbital energies:

-15.60367	-15.56424	-11.29601	-11.28477	-11.26958	-11.25339
-11.24904	-11.24380	-11.24330	-11.24251	-11.24217	-11.24206
-11.24138	-11.24062	-11.23899	-11.23339	-11.23226	-11.23184
-11.22993	-11.22656	-11.22352	-11.21808	-11.21636	-11.21470
-11.21091	-1.32713	-1.24880	-1.16550	-1.15964	-1.13970
-1.07482	-1.06839	-1.03820	-1.02143	-1.02048	-1.01816
-0.97093	-0.95526	-0.93500	-0.86046	-0.83462	-0.83327
-0.83082	-0.80788	-0.79619	-0.76992	-0.73305	-0.71766
-0.70058	-0.69957	-0.66673	-0.65810	-0.64423	-0.63655
-0.63289	-0.62318	-0.62001	-0.61738	-0.59598	-0.59206
-0.59102	-0.58737	-0.58058	-0.55931	-0.55282	-0.54918
-0.54135	-0.51709	-0.50650	-0.50245	-0.50066	-0.49748
-0.49337	-0.49087	-0.48836	-0.48092	-0.42887	-0.40467
-0.36567	-0.34214	-0.34177	-0.33713	-0.33161	-0.28300
-0.26932	0.09840	0.12812	0.13581	0.14035	0.14932
0.17951	0.20872	0.22741	0.23483	0.24185	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b



forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	2.996888E-03	-1.092300E-03	-5.075419E-03
2	N2	2.902098E-03	9.995089E-05	-2.104699E-03
3	C4	5.384872E-04	-5.237104E-03	-1.331028E-03
4	C5	-2.465605E-03	-1.986060E-03	6.611523E-04
5	C6	4.699496E-03	-2.649344E-03	-4.655830E-03
6	C7	-3.021900E-03	4.173873E-03	3.348288E-03
7	C13	1.016495E-03	3.817286E-03	3.204766E-03
8	H4	-8.333256E-04	-1.623874E-03	3.098643E-04
9	C8	-2.602591E-03	-3.503070E-03	1.654229E-03
10	C11	-1.632059E-03	4.019113E-03	2.604804E-03
11	H7	-3.480026E-04	8.474685E-04	4.877169E-04
12	C9	2.348395E-04	3.465178E-03	6.491069E-04
13	H8	-1.358836E-03	-2.713855E-04	1.230370E-03
14	C10	-2.396643E-03	4.501606E-04	2.552408E-03
15	C12	4.320330E-03	-4.826731E-04	-1.817665E-03
16	C2	4.569580E-03	4.725283E-03	-7.136536E-05
17	H13	2.265698E-03	1.215287E-03	1.281866E-03
18	C14	4.469088E-03	5.048013E-04	5.703955E-03
19	H15	-8.762473E-04	-2.464998E-03	-1.072243E-03
20	C15	-8.066367E-03	-2.185489E-03	-6.728433E-03
21	C16	3.580633E-03	2.454246E-03	-1.704632E-03
22	C17	-1.006307E-02	-3.935131E-03	-1.505949E-03
23	C18	-8.697968E-03	-3.668085E-03	-2.236322E-03
24	C19	7.507799E-03	2.895454E-03	4.149845E-03
25	H16	5.818461E-03	8.205617E-04	1.129787E-03
26	H17	-2.640653E-03	-8.339735E-04	1.123124E-03
27	H18	3.887211E-04	9.312185E-04	7.660585E-05
28	H19	3.923565E-03	1.582982E-03	-1.724279E-03
29	H20	2.529764E-05	3.214141E-05	1.544815E-05
30	C1	-2.579334E-03	-1.237971E-03	4.679537E-03
31	H5	3.899026E-03	3.218813E-04	1.595166E-03
32	H6	1.944755E-04	2.244129E-03	-6.101903E-03
33	C3	-4.312188E-03	-3.167459E-03	1.263702E-03
34	C26	-3.044044E-03	-3.147202E-03	-9.892063E-05
35	C27	-2.661653E-04	-6.060645E-04	2.329980E-03
36	C28	4.226828E-03	3.422783E-03	1.485505E-03
37	C29	3.350305E-04	-9.021500E-06	-3.264345E-03
38	H1	-2.026984E-03	-3.716618E-06	-7.193914E-03
39	H2	4.612104E-03	2.770042E-03	5.079830E-03
40	H3	1.355729E-03	4.917203E-04	5.686416E-03
41	H9	-4.759377E-03	-2.903258E-03	-5.357919E-03
42	H10	-3.207912E-04	-1.602736E-04	-6.972213E-04
43	H25	-5.459823E-04	8.909836E-04	6.012465E-04
total		1.022540E-03	1.008090E-03	1.626298E-04

end of program der1b

start of program geopt 7

geometry optimization step 7

reading input hessian of dimension 129  
in five columns format

reading input hessian of dimension 129  
in five columns format

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001756

Cos(theta): 0.3481846

Final level shift: -5.8225096E-03

energy change: 7.6693E-04 . ( 5.0000E-05 )

gradient maximum: 1.7603E-02 . ( 4.5000E-04 )

gradient rms: 3.4045E-03 . ( 3.0000E-04 )

step size: 0.29981 trust radius: 0.30000

displacement maximum: 1.6540E-01 . ( 1.8000E-03 )

displacement rms: 2.3556E-02 . ( 1.2000E-03 )

predicted energy change: -2.5296E-03 geom step: 2.9981E-

01 full step: 2.9981E-01

molecular structure not yet converged...

center of mass moved by:

x: -3.4490E-03

y: -8.1566E-03

z: 4.8314E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2623089590	0.4311251804	1.1716991713
N2	-1.0180143788	-2.2950059180	1.2042298173
C4	-1.2360309063	-0.0332939736	1.9960257998
C5	-0.0491760452	-1.9161106272	0.4898652496
C6	-1.6476617970	-1.3546394568	2.0462415395
C7	-1.7230911186	0.9831467707	2.7922374034
C13	0.6280306553	-2.9273737531	-0.4121209218
H4	-2.9937724088	-2.6736769475	3.0115780294
C8	-2.7457092522	0.6539618582	3.6975262155
C11	-0.9667588878	2.1493399444	2.4114356404
H7	-3.1781071145	1.3980009698	4.3414501000
C9	-3.1860027373	-0.6506742671	3.7535912964
H8	-3.9650269465	-0.9130115590	4.4450494557
C10	-2.6416558807	-1.6625876251	2.9369875099
C12	-0.0857743078	1.7755955971	1.4454283139
C2	0.9164503009	2.6009974180	0.7343857052
H13	1.7123800183	-2.8842131896	-0.2571412082

C14	0.3088978040	-2.7056385440	-1.8863538501
H15	0.2866736531	-3.9117867885	-0.0961463804
C15	-0.2973622557	-2.3040914497	-4.5907098684
C16	1.3065628895	-2.3700351452	-2.7900211464
C17	-0.9983945440	-2.8282694144	-2.3525013671
C18	-1.2991393561	-2.6286610044	-3.6904363154
C19	1.0036021505	-2.1732391689	-4.1341691423
H16	2.3304900741	-2.2499797277	-2.4490130079
H17	-1.7797248649	-3.0692236040	-1.6584418267
H18	-2.3091793966	-2.7128159017	-4.0314102359
H19	1.7931017057	-1.9116780263	-4.8188293061
H20	-0.5306398208	-2.1492911389	-5.6298028759
C1	0.5501654299	-0.5106191206	0.4295419250
H5	1.5613035628	-0.5554938071	0.8239873713
H6	0.6303048976	-0.2234538860	-0.6093977434
C3	2.8015088368	4.1881714110	-0.5810245152
C26	1.8234927411	3.3659516372	1.4559907329
C27	0.9590649824	2.6466221398	-0.6560625455
C28	1.8988761714	3.4310895081	-1.3074873104
C29	2.7564483373	4.1586935309	0.8023034085
H1	1.8043237458	3.3261495512	2.5316351329
H2	0.2432097047	2.0877393438	-1.2297362427
H3	1.9178440967	3.4562601140	-2.3820556926
H9	3.4514125005	4.7412314670	1.3756845720
H10	3.5280434798	4.7976541261	-1.0885472588
H25	-1.0762728724	3.1476511252	2.7825837903

nuclear repulsion energy..... 1971.760476131 hartrees

/ end of geometry optimization iteration 7 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.799E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	96	102	87	88	89	88	84

73

grid # 2	104	112	95	95	97	98	92
118							
grid # 3	214	227	195	187	190	199	164
224							
grid # 4	388	414	320	320	327	348	301
224							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	84
92							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	184	222	184	195
195							
grid # 4	330	331	226	329	223	326	321
343							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	87	89
88							
grid # 2	110	100	110	97	96	96	97
96							
grid # 3	211	194	215	183	183	183	184
183							
grid # 4	216	340	217	327	329	329	328
327							

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	73	73	73	73	82	70
69							
grid # 2	114	114	118	118	118	88	108
105							
grid # 3	214	216	222	222	223	164	217
207							
grid # 4	214	215	224	222	224	290	217
204							

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	88	88	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	184	182	184	184	184	217	214
222							

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grid # 4      328      327      329      327      328      217      212
224

```

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3512
grid # 2	118	118	115	4492
grid # 3	222	223	220	8629
grid # 4	224	224	224	12258

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.30270768203		4.6E-04	3.1E-02
etot	2	Y	Y	6	M	-990.37847298562	7.6E-02	2.4E-04	1.2E-02
etot	3	N	Y	2	U	-990.38974615112	1.1E-02	7.3E-05	3.0E-03
etot	4	Y	Y	6	M	-990.39043838018	6.9E-04	2.1E-05	7.2E-04
etot	5	Y	Y	6	M	-990.39051259464	7.4E-05	9.9E-06	1.8E-04
etot	6	N	Y	2	U	-990.39052152447	8.9E-06	3.4E-06	8.4E-05
etot	7	Y	N	6	M	-990.39052390496	2.4E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.76047613143	
(E)	Total one-electron terms.....	-5261.77830707936	
(I)	Total two-electron terms.....	2299.62730704297	
(L)	Electronic energy.....	-2962.15100003639	(E+I)
(N)	Total energy.....	-990.39052390496	(A+L)

```

SCFE: SCF energy: HF      -990.39052390496 hartrees   iterations:
7

```

HOMO energy: -0.26911  
LUMO energy: 0.09715

Orbital energies:

-15.60451	-15.56524	-11.29616	-11.28590	-11.27118	-11.25063
-11.25053	-11.24661	-11.24537	-11.24207	-11.23978	-11.23885
-11.23840	-11.23770	-11.23689	-11.23687	-11.23575	-11.23433
-11.23300	-11.23088	-11.22421	-11.21944	-11.21799	-11.21554

-11.21243	-1.32546	-1.24901	-1.16385	-1.16049	-1.13916
-1.07447	-1.06674	-1.04044	-1.02137	-1.01939	-1.01613
-0.97215	-0.95419	-0.93387	-0.86020	-0.83767	-0.83371
-0.82913	-0.80726	-0.79554	-0.77026	-0.73264	-0.71762
-0.70168	-0.69844	-0.66645	-0.65787	-0.64274	-0.63728
-0.63416	-0.62358	-0.62128	-0.61619	-0.59608	-0.59210
-0.59055	-0.58653	-0.57915	-0.55835	-0.55307	-0.54811
-0.54314	-0.51759	-0.50730	-0.50317	-0.50057	-0.49639
-0.49350	-0.49125	-0.48704	-0.48151	-0.42958	-0.40467
-0.36720	-0.34424	-0.34058	-0.33732	-0.32999	-0.28301
-0.26911	0.09715	0.12930	0.13663	0.13689	0.14839
0.17926	0.20825	0.22812	0.23474	0.24177	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	1.716334E-03	-1.943601E-03	-3.246573E-03
2	N2	1.508741E-03	7.372569E-04	-8.449564E-04
3	C4	1.732777E-03	-2.550928E-03	-1.144846E-04
4	C5	-2.258395E-03	-1.157807E-03	1.364650E-03
5	C6	3.010108E-03	-1.559524E-03	-2.676497E-03
6	C7	-2.119800E-03	2.378055E-03	8.088183E-05
7	C13	7.949520E-04	-3.166784E-03	1.193967E-03
8	H4	-5.137608E-04	-1.262150E-03	5.166284E-05
9	C8	-1.260196E-03	-1.009633E-03	7.377051E-04
10	C11	1.581835E-03	1.944482E-03	1.100216E-03
11	H7	-2.844006E-04	7.476233E-04	4.649418E-04
12	C9	3.021764E-04	2.034644E-03	3.016599E-04
13	H8	-9.191824E-04	-1.596108E-04	8.422822E-04
14	C10	-2.885543E-04	-3.647628E-05	3.084839E-04
15	C12	-1.002256E-04	1.528865E-04	8.546479E-05
16	C2	-1.824596E-03	-8.798194E-04	7.008701E-05
17	H13	-5.907107E-03	4.474195E-05	-1.786917E-03
18	C14	2.117880E-03	2.467810E-04	1.794266E-03
19	H15	1.613655E-03	3.598184E-03	-1.510856E-03
20	C15	3.515496E-03	5.380807E-04	1.351633E-03
21	C16	3.599045E-03	1.791191E-03	-2.863792E-03
22	C17	6.384644E-04	6.449569E-04	-1.226921E-03

23	C18	3.274344E-03	3.831445E-04	3.904487E-03
24	C19	3.397778E-03	6.246062E-04	2.548436E-04
25	H16	-6.033188E-03	-1.648501E-03	-2.241051E-03
26	H17	-2.244134E-03	-1.119039E-03	1.633890E-03
27	H18	-5.095790E-03	-1.462176E-03	-5.193377E-04
28	H19	-7.132674E-04	-3.366359E-04	6.699522E-05
29	H20	5.473843E-04	5.484700E-05	2.894166E-04
30	C1	-2.121480E-03	9.323276E-04	7.055723E-04
31	H5	1.935195E-03	3.195981E-04	1.225099E-03
32	H6	1.335999E-04	6.505389E-04	-1.350591E-03
33	C3	2.237467E-04	7.332118E-04	8.228264E-04
34	C26	2.934216E-03	2.259092E-03	1.769155E-03
35	C27	1.749225E-03	1.423862E-03	-2.428323E-03
36	C28	-3.039822E-03	-2.449444E-03	-8.296198E-04
37	C29	-1.534705E-03	-1.836397E-03	1.746854E-03
38	H1	1.639685E-04	5.612689E-04	-9.703912E-04
39	H2	-6.178164E-04	-7.198783E-04	-5.945158E-04
40	H3	-2.726356E-04	-1.448398E-04	-7.139410E-04
41	H9	1.428431E-03	1.266800E-03	1.288079E-03
42	H10	1.793635E-04	8.168534E-05	1.338084E-04
43	H25	-2.945761E-04	3.841792E-04	3.416161E-04
-----				
	total	6.550833E-04	1.090803E-03	1.177413E-05

end of program derlb

start of program geopt 8

geometry optimization step 8

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001625

Cos(theta): 0.3290489

Final level shift: -3.2712361E-03

energy change: -1.7137E-03 . ( 5.0000E-05 )

gradient maximum: 6.5993E-03 . ( 4.5000E-04 )

gradient rms: 1.5880E-03 . ( 3.0000E-04 )

step size: 0.30014 trust radius: 0.30000

displacement maximum: 1.3289E-01 . ( 1.8000E-03 )

displacement rms: 2.3581E-02 . ( 1.2000E-03 )

predicted energy change: -1.1454E-03 geom step: 3.0014E-

01 full step: 3.0014E-01

molecular structure not yet converged...

center of mass moved by:

x: 1.4339E-03 y: 3.9888E-03 z: 1.3736E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2427301136	0.4133581705	1.1722777583
N2	-1.0454939928	-2.3112638158	1.1699656111
C4	-1.2161957562	-0.0597207232	2.0064760689
C5	-0.0696132821	-1.9370852449	0.4798595573
C6	-1.6544570973	-1.3757803348	2.0263648965
C7	-1.6847856453	0.9623542639	2.8316875226
C13	0.5944122868	-2.9384071474	-0.4387964649
H4	-3.0378534973	-2.6801972707	2.9787940568
C8	-2.7195283903	0.6400467042	3.7315827985
C11	-0.8978500352	2.1256728813	2.4741738095
H7	-3.1321827458	1.3838331907	4.3903874062
C9	-3.1856697575	-0.6615094865	3.7551713096
H8	-3.9748299789	-0.9205218030	4.4383849881
C10	-2.6599327111	-1.6753768988	2.9171144248
C12	-0.0449844390	1.7563976980	1.4791878795
C2	0.9261767262	2.6151140566	0.7518235711
H13	1.6652174605	-2.8719758706	-0.3024610873
C14	0.2876181649	-2.7034242241	-1.9136085293
H15	0.2724733448	-3.9275784756	-0.1477724137
C15	-0.2818249606	-2.3156026969	-4.6110105067
C16	1.3116920078	-2.5254385140	-2.8427232568
C17	-1.0214564856	-2.6804795857	-2.3448902825
C18	-1.3074367587	-2.4976491583	-3.6888738098
C19	1.0337227845	-2.3208152467	-4.1837294462
H16	2.3428974456	-2.5809231360	-2.5252940373
H17	-1.8180053491	-2.8390751217	-1.6358051292
H18	-2.3411635228	-2.5448754781	-4.0117834742
H19	1.8504547007	-2.2045671815	-4.8863974827
H20	-0.5093223464	-2.1903514419	-5.6550411487
C1	0.5725384418	-0.5359270224	0.4467237410
H5	1.5825600909	-0.6025572202	0.8639586010
H6	0.6849443477	-0.2439441492	-0.5977493705
C3	2.7427643680	4.2718109037	-0.5786007634
C26	1.7583262170	3.4655134300	1.4748050376
C27	1.0258000879	2.6093370968	-0.6475070512
C28	1.9286490508	3.4252015088	-1.3062477428
C29	2.6507103176	4.2926508665	0.8143808905
H1	1.7064457766	3.4685024593	2.5540630146
H2	0.3832676468	1.9769465517	-1.2258047756
H3	1.9981625157	3.3991783059	-2.3867378260
H9	3.2735304395	4.9523138350	1.3873712355
H10	3.4343293803	4.9068564617	-1.0932588436
H25	-0.9916197529	3.1137132967	2.8763314713



nuclear repulsion energy..... 1966.909747028 hartrees

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/ end of geometry optimization iteration 8 /  
-----

end of program geopt

start of program onee

smallest eigenvalue of S: 2.927E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	86	88	88	90	84
73							
grid # 2	104	112	94	95	101	98	92
118							
grid # 3	215	228	195	186	189	198	163
223							
grid # 4	388	413	323	321	327	351	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
91							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	185	222	184	194
195							
grid # 4	329	331	226	331	224	328	318
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	90	69	89	87	88	88
88							
grid # 2	107	98	111	97	96	96	97
97							

grid # 3	209	195	218	183	184	184	184
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182

grid # 4	207	339	213	329	329	330	331
----------	-----	-----	-----	-----	-----	-----	-----

330

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
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H6

grid # 1	73	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	114	115	118	118	118	90	110
----------	-----	-----	-----	-----	-----	----	-----

105

grid # 3	214	215	223	222	224	166	217
----------	-----	-----	-----	-----	-----	-----	-----

205

grid # 4	213	215	223	222	224	293	220
----------	-----	-----	-----	-----	-----	-----	-----

207

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	89	88	89	89	72	70
----------	----	----	----	----	----	----	----

73

grid # 2	97	96	96	97	97	115	113
----------	----	----	----	----	----	-----	-----

118

grid # 3	186	182	185	184	186	217	213
----------	-----	-----	-----	-----	-----	-----	-----

222

grid # 4	330	327	328	327	330	217	210
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3513
grid # 2	118	118	115	4497
grid # 3	223	223	219	8634
grid # 4	223	223	222	12263

end of program grid

start of program rwr  
end of program rwr

start of program scf

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

etot	1	N	N	2	U	-990.33991144147		3.6E-04	2.8E-02
etot	2	Y	Y	6	M	-990.38172607361	4.2E-02	1.8E-04	1.1E-02

etot	3	N	Y	2	U	-990.38813338998	6.4E-03	5.5E-05	2.7E-03
etot	4	Y	Y	6	M	-990.38854871108	4.2E-04	2.2E-05	8.5E-04
etot	5	Y	Y	6	M	-990.38862044730	7.2E-05	8.4E-06	1.6E-04
etot	6	N	Y	2	U	-990.38863299439	1.3E-05	3.2E-06	5.7E-05
etot	7	Y	N	6	M	-990.38863307052	7.6E-08	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1966.90974702809	
(E)	Total one-electron terms.....	-5252.08828716800	
(I)	Total two-electron terms.....	2294.78990706939	
(L)	Electronic energy.....	-2957.29838009861	(E+I)
(N)	Total energy.....	-990.38863307052	(A+L)

SCFE: SCF energy: HF      -990.38863307052 hartrees      iterations:  
7

HOMO energy:      -0.26918  
LUMO energy:      0.09483

Orbital energies:

-15.60546	-15.56553	-11.29617	-11.28888	-11.27440	-11.25323
-11.25291	-11.24932	-11.24466	-11.23989	-11.23899	-11.23849
-11.23820	-11.23781	-11.23695	-11.23662	-11.23581	-11.23470
-11.23345	-11.22918	-11.22676	-11.22253	-11.22247	-11.21821
-11.21580	-1.32205	-1.25283	-1.16216	-1.16049	-1.13639
-1.07414	-1.06661	-1.03656	-1.02137	-1.01847	-1.01697
-0.96944	-0.95479	-0.93227	-0.85933	-0.83776	-0.83195
-0.82823	-0.80624	-0.79536	-0.76922	-0.73264	-0.71663
-0.70030	-0.69768	-0.66473	-0.65767	-0.64239	-0.63624
-0.63253	-0.62481	-0.62019	-0.61335	-0.59730	-0.59249
-0.58848	-0.58801	-0.57615	-0.55734	-0.55154	-0.54848
-0.54556	-0.51729	-0.50702	-0.50198	-0.49950	-0.49588
-0.49449	-0.49099	-0.48779	-0.47966	-0.42997	-0.40493
-0.36948	-0.34394	-0.33991	-0.33752	-0.32983	-0.28137
-0.26918	0.09483	0.12818	0.13771	0.13869	0.14741
0.17628	0.20896	0.22759	0.23471	0.23973	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-3.608445E-03	2.818146E-03	4.387853E-03
2	N2	-8.257060E-03	-1.291490E-03	6.873558E-03
3	C4	2.927401E-04	9.089283E-03	2.291217E-03
4	C5	1.159396E-02	4.274925E-03	-1.002984E-02
5	C6	-2.111425E-03	3.526585E-03	5.173623E-03
6	C7	3.146159E-03	-4.915515E-03	-4.361290E-03
7	C13	1.197140E-03	3.152175E-03	-4.853313E-03
8	H4	6.158857E-05	2.208153E-04	-3.754693E-04
9	C8	3.232912E-03	-4.388872E-03	-3.687738E-03
10	C11	-2.930359E-03	-7.516295E-03	-1.095850E-03
11	H7	-5.246514E-04	-5.339326E-04	3.142423E-05
12	C9	2.211024E-03	7.245822E-04	-2.076187E-03
13	H8	-9.756688E-05	-4.122068E-04	2.025975E-04
14	C10	2.685113E-04	4.837745E-03	1.404553E-03
15	C12	1.505465E-03	8.606128E-04	-3.784882E-03
16	C2	4.596320E-04	-4.228012E-03	-4.301454E-03
17	H13	4.376286E-03	-2.059499E-03	1.720359E-03
18	C14	1.184396E-02	2.108409E-03	5.874802E-03
19	H15	-6.450204E-04	-1.250607E-03	1.770200E-03
20	C15	-5.854112E-03	1.356985E-04	-5.815791E-04
21	C16	3.009072E-03	-1.664308E-03	4.118831E-03
22	C17	-8.790402E-03	-1.738000E-03	-6.298458E-03
23	C18	-4.719041E-03	-2.976537E-03	-2.898018E-03
24	C19	3.419037E-03	-2.514676E-03	-7.224967E-04
25	H16	-2.647010E-03	1.940020E-03	9.827487E-04
26	H17	7.504203E-04	1.171925E-03	-1.479661E-03
27	H18	6.000360E-03	3.165718E-03	-3.106612E-04
28	H19	-5.276927E-03	3.874991E-04	2.823860E-03
29	H20	-6.458594E-04	6.314977E-04	1.160412E-04
30	C1	4.753900E-04	-1.944511E-03	-4.062617E-03
31	H5	-3.832564E-03	-2.580860E-04	-2.786851E-04
32	H6	-7.710760E-04	-1.574150E-03	5.124757E-03
33	C3	-8.483867E-04	5.126358E-04	1.028467E-02
34	C26	-3.375860E-04	6.706250E-04	2.040083E-04
35	C27	-2.580503E-03	-2.382582E-03	7.317669E-03
36	C28	-4.311198E-04	-1.818641E-03	-1.976063E-03
37	C29	3.356317E-04	9.286614E-04	-7.586848E-03
38	H1	4.426202E-04	2.672569E-04	-4.159578E-03
39	H2	-3.082192E-03	-2.219428E-03	-4.993021E-04
40	H3	-1.537561E-03	6.603144E-05	5.377819E-03
41	H9	2.343965E-03	1.305606E-03	1.437853E-04
42	H10	3.434594E-03	3.036993E-03	3.538105E-04
43	H25	3.444813E-05	5.165315E-04	-1.111761E-03
total		9.060454E-04	6.626275E-04	4.644130E-05

end of program der1b

start of program geopt 9

geometry optimization step 9

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 8 \*\*

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3007076

Cos(theta): 0.3121536

Final level shift: -6.2152375E-03

energy change: 1.8908E-03 . ( 5.0000E-05 )

gradient maximum: 6.5993E-03 . ( 4.5000E-04 )

gradient rms: 1.5880E-03 . ( 3.0000E-04 )

step size: 0.29990 trust radius: 0.30000

displacement maximum: 1.3848E-01 . ( 1.8000E-03 )

displacement rms: 2.3562E-02 . ( 1.2000E-03 )

predicted energy change: -1.2255E-03 geom step: 2.9990E-

01 full step: 2.9990E-01

molecular structure not yet converged...

center of mass moved by:

x: -7.4940E-16

y: 2.6368E-16

z: -8.3267E-16

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2112213224	0.4759821970	1.1509370987
N2	-0.9304654889	-2.2596315619	1.1557263606
C4	-1.2007566870	-0.0050996186	1.9468199390
C5	0.0308354325	-1.8599684763	0.4447847412
C6	-1.5893298383	-1.3330206181	1.9833821552
C7	-1.7559182331	1.0130893177	2.7060893243
C13	0.7195427103	-2.8544750054	-0.4654951884
H4	-2.9732939203	-2.6636627946	2.8871238361
C8	-2.8165407677	0.6740276669	3.5624798977
C11	-0.9876468060	2.1851605542	2.3748675911
H7	-3.2934365683	1.4196419607	4.1781118649
C9	-3.2309842879	-0.6335021660	3.6104914752
H8	-4.0426550097	-0.9068067006	4.2655024799
C10	-2.6247327918	-1.6447328748	2.8300957907
C12	-0.0663221250	1.8221726220	1.4414763503
C2	0.9615610706	2.6573510475	0.7929901780
H13	1.7804240263	-2.7291419038	-0.3977998181

C14	0.2904550036	-2.7194671495	-1.9078212042
H15	0.4874628272	-3.8353817165	-0.1033936907
C15	-0.5195728220	-2.5100998311	-4.5600986738
C16	1.1731723675	-2.2603581915	-2.8876463572
C17	-1.0114333568	-3.0801698853	-2.2799362236
C18	-1.4107209530	-2.9767515754	-3.5926183840
C19	0.7731816258	-2.1547371391	-4.2060163333
H16	2.1848694620	-1.9871622113	-2.6169976829
H17	-1.6947814125	-3.4329355076	-1.5285602629
H18	-2.3991425622	-3.2559857461	-3.8614828367
H19	1.4638084288	-1.7938641349	-4.9522904025
H20	-0.8298119621	-2.4271286947	-5.5831759553
C1	0.6128319456	-0.4474688200	0.4042533197
H5	1.6225608382	-0.4852424998	0.8284411699
H6	0.7094088190	-0.1466392262	-0.6361783628
C3	2.9218539781	4.2333037928	-0.3978184205
C26	1.8547642164	3.3951618772	1.5732849714
C27	1.0554555784	2.7250390584	-0.5942672449
C28	2.0276025330	3.5107060596	-1.1848132236
C29	2.8296541634	4.1778589369	0.9812369472
H1	1.7838933136	3.3413965331	2.6388352230
H2	0.3516514934	2.1776688845	-1.2016643395
H3	2.0892544843	3.5634944072	-2.2542289962
H9	3.5239664473	4.7363520807	1.5935527668
H10	3.6885398335	4.8392355334	-0.8576710935
H25	-1.1255993547	3.1803096411	2.7475409393

nuclear repulsion energy..... 1969.045876041 hartrees

/ end of geometry optimization iteration 9 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.808E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	95	102	84	87	89	90	84

73

grid # 2	104	112	95	95	101	98	92
118							
grid # 3	212	227	193	187	192	198	163
224							
grid # 4	386	414	324	320	324	350	294
224							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
90							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	184	223	184	222	184	195
194							
grid # 4	328	332	226	328	223	330	317
341							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	87	89
89							
grid # 2	108	100	109	97	96	96	97
97							
grid # 3	211	196	214	186	184	182	183
184							
grid # 4	210	341	212	329	328	326	329
327							

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	70
69							
grid # 2	114	115	118	118	118	90	108
104							
grid # 3	213	215	223	222	223	164	217
206							
grid # 4	214	215	223	223	224	293	219
208							

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	87	87	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	185	181	182	184	185	217	213
223							

grid # 4        330        328        330        327        328        216        212  
224

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3507
grid # 2	118	118	115	4495
grid # 3	223	223	220	8625
grid # 4	224	224	224	12249

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.19143961399		6.9E-04	5.1E-02
etot	2	Y	Y	6	M	-990.36304368943	1.7E-01	3.6E-04	2.1E-02
etot	3	N	Y	2	U	-990.38756589331	2.5E-02	1.1E-04	4.9E-03
etot	4	Y	Y	6	M	-990.38902919237	1.5E-03	3.0E-05	1.2E-03
etot	5	Y	Y	6	M	-990.38919073874	1.6E-04	1.6E-05	3.2E-04
etot	6	N	Y	2	U	-990.38919602691	5.3E-06	5.3E-06	8.1E-05
etot	7	Y	Y	6	M	-990.38919546120	-5.7E-07	2.6E-06	3.1E-05
etot	8	Y	N	6	M	-990.38919647219	1.0E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1969.04587604074	
(E)	Total one-electron terms.....	-5256.35681247047	
(I)	Total two-electron terms.....	2296.92173995754	
(L)	Electronic energy.....	-2959.43507251293	(E+I)
(N)	Total energy.....	-990.38919647219	(A+L)

SCFE: SCF energy: HF        -990.38919647219 hartrees        iterations:  
8

HOMO energy:        -0.26840

LUMO energy:        0.09701

Orbital energies:

-15.60534	-15.56470	-11.29636	-11.28875	-11.27084	-11.25072
-11.25052	-11.24617	-11.24576	-11.24057	-11.23986	-11.23892
-11.23842	-11.23745	-11.23597	-11.23589	-11.23480	-11.23326



-11.23202	-11.22987	-11.22361	-11.22021	-11.21809	-11.21556
-11.21238	-1.32578	-1.25026	-1.16340	-1.15935	-1.13851
-1.07486	-1.06779	-1.03915	-1.02304	-1.01954	-1.01789
-0.96974	-0.95431	-0.93406	-0.86044	-0.83631	-0.83390
-0.82845	-0.80772	-0.79588	-0.77036	-0.73270	-0.71782
-0.70108	-0.69798	-0.66655	-0.65810	-0.64342	-0.63833
-0.63434	-0.62250	-0.62043	-0.61751	-0.59675	-0.59349
-0.59179	-0.58934	-0.57738	-0.55766	-0.55188	-0.54826
-0.54421	-0.51763	-0.50773	-0.50313	-0.50021	-0.49540
-0.49235	-0.49068	-0.48759	-0.48192	-0.42965	-0.40506
-0.36691	-0.34326	-0.34192	-0.33901	-0.32575	-0.28176
-0.26840	0.09701	0.12789	0.13689	0.13892	0.14831
0.17873	0.20902	0.22650	0.23488	0.24146	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-1.847904E-03	1.350870E-03	1.372186E-03
2	N2	8.004859E-04	-1.184322E-03	-1.290199E-03
3	C4	-2.990647E-03	1.894084E-03	-1.153339E-03
4	C5	-1.267694E-03	-1.405869E-03	2.168808E-03
5	C6	-3.781687E-03	1.063700E-03	1.466086E-03
6	C7	3.701565E-03	-2.358705E-03	9.208506E-04
7	C13	-6.358814E-03	5.686112E-03	1.117194E-03
8	H4	7.566979E-04	2.267632E-03	4.118942E-04
9	C8	3.487603E-04	4.660037E-03	1.792745E-03
10	C11	-4.761810E-04	-4.721753E-05	-2.385896E-03
11	H7	6.406881E-04	-9.788330E-04	-1.030604E-03
12	C9	-1.838024E-03	-6.112861E-03	1.573878E-04
13	H8	1.321968E-03	2.841587E-04	-1.158728E-03
14	C10	-9.988378E-04	-2.699473E-03	-2.337905E-04
15	C12	-3.644818E-04	5.292972E-04	1.985804E-03
16	C2	4.214487E-03	2.571180E-03	2.054306E-03
17	H13	1.220174E-02	2.129938E-03	9.413491E-04
18	C14	-1.971814E-03	-2.257252E-04	-1.000693E-02
19	H15	-2.739856E-03	-7.545521E-03	3.261445E-03
20	C15	-3.750255E-04	-1.032296E-03	2.979952E-03
21	C16	3.971553E-04	-1.694801E-03	1.180222E-02

22	C17	1.081296E-02	3.319375E-03	5.677630E-03
23	C18	1.275942E-02	5.331517E-03	-6.004976E-03
24	C19	-6.135291E-03	-1.513302E-04	-5.275360E-03
25	H16	-3.575445E-03	-1.293270E-03	1.989000E-04
26	H17	-2.282103E-04	-2.076355E-04	5.184705E-04
27	H18	-1.003847E-02	-2.388316E-03	-4.271375E-03
28	H19	-1.686569E-03	-1.077089E-03	1.228071E-03
29	H20	-1.715323E-03	-1.767050E-04	-2.514137E-03
30	C1	6.153916E-03	1.649965E-03	1.097077E-03
31	H5	-3.027084E-03	-3.480673E-04	-3.342055E-03
32	H6	-1.486703E-04	-3.556652E-04	2.982007E-03
33	C3	1.936388E-06	2.107970E-04	-5.988076E-03
34	C26	-4.239919E-03	-2.750183E-03	-4.310837E-03
35	C27	-6.213987E-04	-7.833312E-05	4.417728E-04
36	C28	4.704144E-03	3.029595E-03	2.767092E-03
37	C29	2.147902E-03	1.746275E-03	9.650488E-04
38	H1	-4.030953E-04	-8.930180E-04	4.530742E-03
39	H2	1.885956E-03	1.855455E-03	5.925202E-04
40	H3	5.723930E-04	3.930392E-04	-2.575663E-03
41	H9	-2.986811E-03	-2.049155E-03	-1.829814E-03
42	H10	-2.808888E-03	-1.906220E-03	-3.199569E-05
43	H25	3.854478E-04	-1.625851E-04	-2.576043E-04
-----				
	total	1.181474E-03	8.498306E-04	-2.298122E-04

end of program der1b

start of program geopt 10

geometry optimization step 10

[ turning on trust-radius adjustment ]

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 8 \*\*

energy change: 1.3274E-03 . ( 5.0000E-05 )

gradient maximum: 6.5993E-03 . ( 4.5000E-04 )

gradient rms: 1.5880E-03 . ( 3.0000E-04 )

step size: 0.12023 trust radius: 0.15000

displacement maximum: 4.6109E-02 . ( 1.8000E-03 )

displacement rms: 9.4462E-03 . ( 1.2000E-03 )

predicted energy change: -6.6309E-04 geom step: 1.2023E-

01 full step: 1.2023E-01

molecular structure not yet converged...

center of mass moved by:

x: 5.8287E-16 y: 2.6368E-16 z: 5.5511E-17

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2503467923	0.4313387940	1.1728975667
N2	-0.9922353568	-2.3008642645	1.2068479080
C4	-1.2177846926	-0.0412413961	2.0027340636
C5	-0.0328950456	-1.9152046665	0.4874677885
C6	-1.6207580303	-1.3658403732	2.0516318574
C7	-1.7256576704	0.9802469690	2.7898913510
C13	0.6345154182	-2.9213500262	-0.4256979858
H4	-2.9784638181	-2.6865579845	3.0093481473
C8	-2.7573880472	0.6486468955	3.6876420923
C11	-0.9686088796	2.1508712541	2.4150585939
H7	-3.2011472190	1.3958055134	4.3235415609
C9	-3.1880965526	-0.6579308626	3.7452763889
H8	-3.9761108933	-0.9234283427	4.4292771187
C10	-2.6259600579	-1.6723713900	2.9368264804
C12	-0.0840044705	1.7791562074	1.4502481760
C2	0.9094340782	2.6151448582	0.7396605597
H13	1.7117184108	-2.8786891597	-0.2812033952
C14	0.3106147337	-2.6930411706	-1.8952436050
H15	0.2973278585	-3.9045733242	-0.1220199652
C15	-0.3176308144	-2.3047012879	-4.5894802502
C16	1.3058774411	-2.4094783712	-2.8200443949
C17	-1.0094991762	-2.7875081323	-2.3386183614
C18	-1.3208168237	-2.5954695037	-3.6744560256
C19	0.9966496806	-2.2130779832	-4.1595138305
H16	2.3268560103	-2.3606962160	-2.4970780760
H17	-1.7899818400	-3.0122134213	-1.6310120439
H18	-2.3448732588	-2.6750402869	-4.0018765889
H19	1.7816422461	-2.0017592358	-4.8628995476
H20	-0.5601115265	-2.1562329340	-5.6282763720
C1	0.5677714222	-0.5074561645	0.4336493303
H5	1.5802783124	-0.5505269015	0.8402390685
H6	0.6558736629	-0.2175416456	-0.6088435807
C3	2.8070428603	4.1983759363	-0.5604794150
C26	1.7923657031	3.4110711813	1.4677798769
C27	0.9824585662	2.6308465889	-0.6519969273
C28	1.9254954757	3.4145041743	-1.2967484498
C29	2.7309857208	4.2007778211	0.8223821304
H1	1.7459445767	3.3977291757	2.5379712574
H2	0.2862125744	2.0466037166	-1.2287363733
H3	1.9713578203	3.4151297035	-2.3708451625
H9	3.4096713505	4.8073562604	1.3990774035
H10	3.5437855062	4.8042079101	-1.0617698905
H25	-1.0891245347	3.1494999185	2.7854402047

nuclear repulsion energy..... 1970.392406452 hartrees

-----  
/ end of geometry optimization iteration 10 /

-----  
end of program geopt

start of program onee  
smallest eigenvalue of S: 2.841E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	87	88	90	89	84
73							
grid # 2	103	112	95	95	99	97	92
118							
grid # 3	213	227	195	187	191	200	163
224							
grid # 4	389	414	323	320	321	351	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	195
195							
grid # 4	328	331	226	331	223	329	318
342							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	88	89
89							
grid # 2	109	100	110	97	96	96	97
96							
grid # 3	210	197	216	183	184	183	184
183							
grid # 4	213	342	213	327	329	327	327
329							

```

number of gridpoints:
  atom      H16      H17      H18      H19      H20      C1      H5
H6
  grid # 1      73      73      73      73      73      82      70
69
  grid # 2     113     115     118     118     118      89     110
104
  grid # 3     214     216     223     222     224     165     217
207
  grid # 4     214     214     224     223     224     293     219
206

```

```

number of gridpoints:
  atom      C3      C26      C27      C28      C29      H1      H2
H3
  grid # 1      89      88      88      89      89      72      71
73
  grid # 2      97      95      96      97      97     115     114
118
  grid # 3     184     182     184     184     185     217     212
223
  grid # 4     329     328     329     327     329     216     212
224

```

```

number of gridpoints:
  atom      H9      H10      H25      total
grid # 1      73      73      72     3519
grid # 2     118     118     115     4492
grid # 3     222     223     220     8636
grid # 4     224     224     224    12260

```

end of program grid

```

start of program rwr
end of program rwr

```

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.29802142608		4.7E-04	3.6E-02
etot	2	Y	Y	6	M	-990.37914076540	8.1E-02	2.4E-04	1.5E-02
etot	3	N	Y	2	U	-990.39011714517	1.1E-02	7.3E-05	3.6E-03
etot	4	Y	Y	6	M	-990.39075170470	6.3E-04	1.8E-05	8.3E-04
etot	5	Y	Y	6	M	-990.39080716088	5.5E-05	9.2E-06	2.4E-04
etot	6	N	Y	2	U	-990.39081625073	9.1E-06	3.2E-06	6.3E-05

etot 7 Y N 6 M -990.39082059817 4.3E-06 0.0E+00 0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1970.39240645220	
(E)	Total one-electron terms.....	-5259.04946585476	
(I)	Total two-electron terms.....	2298.26623880439	
(L)	Electronic energy.....	-2960.78322705037	(E+I)
(N)	Total energy.....	-990.39082059817	(A+L)

SCFE: SCF energy: HF -990.39082059817 hartrees iterations:  
7

HOMO energy: -0.26884  
LUMO energy: 0.09625

Orbital energies:

-15.60520	-15.56542	-11.29634	-11.28757	-11.27197	-11.25137
-11.25137	-11.24663	-11.24624	-11.24028	-11.24014	-11.23939
-11.23864	-11.23804	-11.23717	-11.23626	-11.23525	-11.23435
-11.23339	-11.23131	-11.22496	-11.22092	-11.21941	-11.21652
-11.21351	-1.32467	-1.25038	-1.16266	-1.16009	-1.13785
-1.07415	-1.06682	-1.03876	-1.02160	-1.01902	-1.01676
-0.97049	-0.95423	-0.93360	-0.85986	-0.83666	-0.83382
-0.82912	-0.80693	-0.79529	-0.76986	-0.73238	-0.71725
-0.70084	-0.69840	-0.66614	-0.65779	-0.64278	-0.63724
-0.63391	-0.62371	-0.62052	-0.61551	-0.59631	-0.59205
-0.59042	-0.58760	-0.57799	-0.55757	-0.55200	-0.54823
-0.54488	-0.51728	-0.50751	-0.50254	-0.49998	-0.49565
-0.49359	-0.49112	-0.48733	-0.48118	-0.42972	-0.40500
-0.36774	-0.34301	-0.34117	-0.33775	-0.32916	-0.28213
-0.26884	0.09625	0.12876	0.13660	0.13709	0.14832
0.17835	0.20865	0.22790	0.23513	0.24117	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----

1	N1	3.176707E-04	-7.109467E-05	1.405262E-05
2	N2	-1.075429E-03	-2.083377E-04	7.417913E-04
3	C4	-9.732657E-04	1.912845E-03	4.219490E-04
4	C5	9.390608E-04	-3.118005E-04	-6.400202E-04
5	C6	-1.872859E-03	6.288692E-04	1.567042E-03
6	C7	8.574249E-04	-1.220477E-03	-4.534514E-04
7	C13	4.990676E-05	2.619141E-04	-1.067732E-03
8	H4	2.212391E-04	7.436348E-04	4.175358E-05
9	C8	9.716663E-04	1.126067E-03	-2.443932E-04
10	C11	-3.058807E-04	-1.016420E-03	-2.792513E-05
11	H7	2.030616E-04	-3.912862E-04	-4.531555E-04
12	C9	3.885238E-04	-1.817448E-03	-8.541092E-04
13	H8	5.647280E-04	1.033803E-04	-4.236539E-04
14	C10	1.787747E-04	1.629413E-04	-1.130833E-04
15	C12	-2.993285E-04	9.293299E-04	-8.305882E-04
16	C2	2.106919E-03	3.714443E-04	1.529857E-03
17	H13	-8.453989E-06	-1.369249E-05	-3.866099E-04
18	C14	-2.620975E-03	-8.478820E-04	-2.750261E-04
19	H15	1.703486E-04	2.476269E-04	5.668823E-04
20	C15	1.348587E-03	3.170487E-04	-3.143626E-04
21	C16	-3.287963E-03	-8.576557E-04	-7.679380E-04
22	C17	9.274778E-04	5.528706E-04	2.811386E-05
23	C18	-2.653106E-04	-1.756854E-04	1.189448E-03
24	C19	-2.378424E-03	-1.170097E-03	5.057107E-05
25	H16	3.742774E-03	1.309982E-03	7.701638E-04
26	H17	6.077310E-04	2.216130E-04	-3.997413E-04
27	H18	1.487305E-03	2.292942E-04	4.715166E-04
28	H19	5.016746E-04	5.351337E-04	-4.906618E-04
29	H20	3.420834E-04	-6.617536E-05	7.707523E-04
30	C1	1.310155E-03	1.015916E-03	-6.323303E-04
31	H5	-1.427620E-03	-7.688246E-05	-7.480952E-04
32	H6	-2.814998E-05	-3.196540E-04	2.202996E-03
33	C3	-1.512850E-03	-7.323179E-04	-2.557105E-03
34	C26	-1.040007E-03	-4.215451E-04	-2.994571E-03
35	C27	2.310941E-04	6.193161E-04	-3.498692E-04
36	C28	1.620128E-03	8.085342E-04	2.072791E-03
37	C29	2.143792E-04	-9.341659E-05	4.237368E-04
38	H1	-3.535759E-05	-1.816722E-04	3.011021E-03
39	H2	6.170067E-04	4.683717E-04	1.307347E-04
40	H3	-3.642736E-05	2.655682E-04	-5.930004E-04
41	H9	-9.794912E-04	-8.053914E-04	-4.013531E-04
42	H10	-1.162548E-03	-8.092648E-04	1.701950E-04
43	H25	1.251612E-04	-4.338929E-04	-3.335687E-04
-----		-----	-----	-----
total		7.345388E-04	7.896115E-04	-1.769761E-04

end of program derlb

start of program geopt 11

geometry optimization step 11

```

reading input hessian of dimension    129
  in five columns format
reading input hessian of dimension    129
  in five columns format
reading input hessian of dimension    129
  in five columns format

```

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0750415

Cos(theta): 0.6886741

Final level shift: -2.7962975E-02

```

energy change:          -2.9669E-04 . ( 5.0000E-05 )
gradient maximum:       3.8324E-03 . ( 4.5000E-04 )
gradient rms:           8.9140E-04 . ( 3.0000E-04 )
step size: 0.07504 trust radius: 0.07500
displacement maximum:   2.2233E-02 . ( 1.8000E-03 )
displacement rms:       5.8958E-03 . ( 1.2000E-03 )
predicted energy change: -3.7189E-04 geom step: 7.5041E-
02 full step: 7.5041E-02
molecular structure not yet converged...

```

center of mass moved by:

x: -1.1335E-03 y: -2.5596E-03 z: -2.5985E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2525386544	0.4310493893	1.1683995301
N2	-1.0138740281	-2.2939256517	1.1975942074
C4	-1.2252479678	-0.0341646614	1.9952733135
C5	-0.0436572270	-1.9157862179	0.4851284149
C6	-1.6413071326	-1.3541973725	2.0405928362
C7	-1.7145415536	0.9821590281	2.7923186325
C13	0.6288624322	-2.9244715472	-0.4211405469
H4	-2.9999644294	-2.6702187494	2.9946387869
C8	-2.7426672956	0.6546811637	3.6920735521
C11	-0.9497183169	2.1459198615	2.4208127750
H7	-3.1762743134	1.3992173904	4.3355281353
C9	-3.1879856910	-0.6483570844	3.7409436743
H8	-3.9728895093	-0.9095416004	4.4272694645
C10	-2.6429704192	-1.6600851796	2.9242590216
C12	-0.0716241692	1.7744356070	1.4512907646
C2	0.9269144697	2.6056206604	0.7453112864
H13	1.7074422886	-2.8817125614	-0.2753663900
C14	0.3076938336	-2.7045928872	-1.8905668910
H15	0.2923378719	-3.9050788522	-0.1052980764
C15	-0.3053244872	-2.3158522487	-4.5878771164
C16	1.3069751907	-2.4063165422	-2.8077883962
C17	-1.0079025385	-2.8063076055	-2.3422753578



C18	-1.3113854749	-2.6134522525	-3.6776129076
C19	1.0025465289	-2.2143970874	-4.1491423166
H16	2.3309432563	-2.3188574629	-2.4786269976
H17	-1.7917111891	-3.0332743005	-1.6406619581
H18	-2.3295554842	-2.6925171880	-4.0106917005
H19	1.7907633063	-1.9834667927	-4.8460183616
H20	-0.5422240742	-2.1661899720	-5.6255384105
C1	0.5644095491	-0.5120677085	0.4353968420
H5	1.5708233822	-0.5629812851	0.8428439319
H6	0.6581057935	-0.2218487346	-0.5998173568
C3	2.7889171356	4.2151427700	-0.5660685035
C26	1.8162112152	3.3890211368	1.4702869848
C27	0.9775928654	2.6431062201	-0.6456130349
C28	1.9045321762	3.4402657775	-1.2949648747
C29	2.7395960663	4.1914658022	0.8181678154
H1	1.7871549220	3.3588554939	2.5468422945
H2	0.2728790876	2.0718618690	-1.2204641568
H3	1.9264167737	3.4627840599	-2.3698183664
H9	3.4212751180	4.7898184578	1.3932077598
H10	3.5069237148	4.8342820442	-1.0716438394
H25	-1.0577771051	3.1427356635	2.7959918279

nuclear repulsion energy..... 1971.488097852 hartrees

/ end of geometry optimization iteration 11 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.800E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	86	88	89	88	84
73							
grid # 2	103	112	95	95	98	98	92
118							
grid # 3	214	227	195	186	190	199	164
224							

grid # 4	389	414	322	321	325	347	300
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12

C2

grid # 1	89	86	73	87	73	89	86
----------	----	----	----	----	----	----	----

92

grid # 2	97	94	118	97	118	97	94
----------	----	----	-----	----	-----	----	----

100

grid # 3	184	184	223	184	222	184	194
----------	-----	-----	-----	-----	-----	-----	-----

195

grid # 4	330	331	226	329	223	326	317
----------	-----	-----	-----	-----	-----	-----	-----

343

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18

C19

grid # 1	69	91	69	89	88	88	89
----------	----	----	----	----	----	----	----

89

grid # 2	110	100	110	97	96	96	97
----------	-----	-----	-----	----	----	----	----

96

grid # 3	211	196	214	183	184	183	184
----------	-----	-----	-----	-----	-----	-----	-----

183

grid # 4	214	340	215	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5

H6

grid # 1	72	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	114	115	118	118	118	88	110
----------	-----	-----	-----	-----	-----	----	-----

104

grid # 3	214	216	222	222	224	163	217
----------	-----	-----	-----	-----	-----	-----	-----

207

grid # 4	214	214	224	223	224	292	217
----------	-----	-----	-----	-----	-----	-----	-----

202

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2

H3

grid # 1	89	89	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
----------	----	----	----	----	----	-----	-----

118

grid # 3	185	182	184	185	184	217	214
----------	-----	-----	-----	-----	-----	-----	-----

222

grid # 4	328	327	331	327	328	217	212
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3516
grid # 2	118	118	115	4493
grid # 3	223	223	220	8631
grid # 4	224	224	224	12247

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.38859773819		8.1E-05	3.6E-03
etot	2	Y	Y	4	M	-990.39048554750	1.9E-03	3.8E-05	1.4E-03
etot	3	Y	Y	4	M	-990.39075521604	2.7E-04	1.1E-05	3.8E-04
etot	4	N	Y	1	U	-990.39078219283	2.7E-05	6.5E-06	1.5E-04
etot	5	Y	Y	4	M	-990.39078684366	4.7E-06	1.8E-06	3.2E-05
etot	6	Y	N	4	M	-990.39078874833	1.9E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.48809785247	
(E)	Total one-electron terms.....	-5261.23708829039	
(I)	Total two-electron terms.....	2299.35820168958	
(L)	Electronic energy.....	-2961.87888660080	(E+I)
(N)	Total energy.....	-990.39078874833	(A+L)

SCFE: SCF energy: HF      -990.39078874833 hartrees      iterations:  
6

HOMO energy:      -0.26900  
LUMO energy:      0.09681

Orbital energies:

-15.60450	-15.56520	-11.29613	-11.28583	-11.27124	-11.25060
-11.25060	-11.24629	-11.24564	-11.24013	-11.23934	-11.23862
-11.23812	-11.23741	-11.23665	-11.23611	-11.23489	-11.23442
-11.23272	-11.23078	-11.22433	-11.21958	-11.21829	-11.21571
-11.21257	-1.32518	-1.24924	-1.16401	-1.16055	-1.13914
-1.07477	-1.06714	-1.04013	-1.02193	-1.01901	-1.01706
-0.97170	-0.95432	-0.93398	-0.86039	-0.83766	-0.83356
-0.82897	-0.80722	-0.79561	-0.77030	-0.73280	-0.71772
-0.70154	-0.69847	-0.66672	-0.65798	-0.64297	-0.63737

-0.63423	-0.62375	-0.62103	-0.61586	-0.59622	-0.59244
-0.59059	-0.58747	-0.57852	-0.55830	-0.55278	-0.54840
-0.54412	-0.51758	-0.50739	-0.50284	-0.50056	-0.49599
-0.49355	-0.49122	-0.48722	-0.48146	-0.42973	-0.40470
-0.36763	-0.34405	-0.34100	-0.33769	-0.32924	-0.28262
-0.26900	0.09681	0.12911	0.13706	0.13737	0.14842
0.17898	0.20870	0.22842	0.23520	0.24150	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	7.004627E-04	-5.345029E-04	-8.693736E-04
2	N2	1.325105E-03	4.490218E-04	-1.207276E-03
3	C4	6.466353E-04	-1.748891E-03	-5.276414E-04
4	C5	-1.583901E-03	-5.770104E-05	1.464054E-03
5	C6	2.273493E-03	-1.141576E-03	-2.212237E-03
6	C7	-6.504121E-04	1.484241E-03	1.389573E-04
7	C13	-1.049263E-04	-1.124955E-03	1.171673E-03
8	H4	-4.026407E-04	-9.691760E-04	-5.464798E-05
9	C8	-9.303924E-04	-6.391797E-04	4.551451E-04
10	C11	6.920090E-04	1.520404E-03	3.671516E-04
11	H7	-7.863954E-05	4.226999E-04	2.440591E-04
12	C9	-2.025401E-04	1.476436E-03	5.741089E-04
13	H8	-5.400360E-04	-1.340263E-04	4.904071E-04
14	C10	-7.800840E-05	-1.362858E-04	6.780081E-04
15	C12	-2.323231E-04	-3.858693E-04	8.130474E-04
16	C2	-1.650918E-03	-1.050059E-03	-4.870314E-04
17	H13	-1.249323E-03	3.298007E-04	-3.456024E-04
18	C14	3.372735E-04	3.524076E-05	-8.065477E-04
19	H15	3.415639E-04	3.736382E-04	-5.501722E-04
20	C15	-7.211408E-05	-4.291507E-04	1.165413E-03
21	C16	1.485377E-04	5.669822E-04	3.571922E-04
22	C17	9.294633E-04	4.954721E-05	8.698192E-04
23	C18	1.506381E-03	3.791037E-04	-2.957498E-04
24	C19	1.342766E-03	5.454351E-04	-6.709570E-04
25	H16	-1.552766E-03	-6.560598E-04	-2.441234E-04
26	H17	1.700841E-04	-9.802381E-05	1.903320E-04
27	H18	-1.365794E-03	-2.753192E-04	-2.401760E-04

28	H19	-6.056477E-04	-1.969351E-04	3.560983E-04
29	H20	-1.099160E-04	1.214393E-04	-7.279111E-04
30	C1	-1.851382E-03	-1.238949E-04	1.290145E-03
31	H5	1.574782E-03	1.314021E-04	1.035441E-03
32	H6	3.969414E-04	6.577154E-04	-2.503026E-03
33	C3	1.115385E-03	1.071782E-03	1.756491E-03
34	C26	1.717762E-03	1.497857E-03	2.251613E-03
35	C27	3.012996E-04	7.204426E-04	-9.322043E-04
36	C28	-1.972431E-03	-1.672589E-03	-1.659435E-03
37	C29	-8.471681E-04	-7.644455E-04	8.396384E-04
38	H1	2.871811E-04	2.205505E-04	-1.629586E-03
39	H2	-7.152317E-04	-9.510178E-04	-5.023593E-04
40	H3	1.101136E-05	-8.687548E-05	-4.894680E-04
41	H9	1.039112E-03	8.927797E-04	5.902413E-04
42	H10	7.541013E-04	6.428744E-04	-3.083269E-04
43	H25	-2.161468E-04	5.428347E-04	2.594211E-04
-----				
	total	5.986926E-04	9.556962E-04	9.460540E-05

end of program derlb

start of program geopt 12

geometry optimization step 12

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0381814

Cos(theta): 0.6358626

Final level shift: -2.2947896E-02

energy change: 3.1850E-05 \* ( 5.0000E-05 )

gradient maximum: 3.7159E-03 . ( 4.5000E-04 )

gradient rms: 7.8551E-04 . ( 3.0000E-04 )

step size: 0.03818 trust radius: 0.03750

displacement maximum: 1.1555E-02 . ( 1.8000E-03 )

displacement rms: 2.9998E-03 . ( 1.2000E-03 )

predicted energy change: -1.3809E-04 geom step: 3.8181E-

02 full step: 3.8181E-02

molecular structure not yet converged...

center of mass moved by:

x: 4.5426E-04 y: 8.1147E-04 z: -6.7642E-04

new geometry:

angstroms

atom	x	y	z
N1	-0.2481100487	0.4334566292	1.1690590843
N2	-1.0032005669	-2.2934581620	1.1949409475
C4	-1.2219414340	-0.0343838020	1.9923563545
C5	-0.0339796710	-1.9120602342	0.4839591872
C6	-1.6327378826	-1.3563177585	2.0371288910
C7	-1.7214706152	0.9842720805	2.7832559656
C13	0.6387689584	-2.9205192316	-0.4241415240
H4	-2.9960643356	-2.6736608684	2.9862523038
C8	-2.7543266162	0.6556694707	3.6773710238
C11	-0.9567330317	2.1503186557	2.4169640341
H7	-3.1942470497	1.4021628828	4.3154141299
C9	-3.1938710405	-0.6480229029	3.7284797792
H8	-3.9830026483	-0.9107663027	4.4110346409
C10	-2.6387220303	-1.6617110159	2.9180186584
C12	-0.0739060768	1.7781436478	1.4520699323
C2	0.9254724195	2.6102272532	0.7486369541
H13	1.7151095547	-2.8707079086	-0.2840967415
C14	0.3101739106	-2.7047976511	-1.8919547337
H15	0.3108881878	-3.9021230759	-0.1082165064
C15	-0.3249288630	-2.3285963028	-4.5840286299
C16	1.2990880581	-2.4022115814	-2.8172990363
C17	-1.0064246650	-2.8179513158	-2.3322450242
C18	-1.3210023891	-2.6315174078	-3.6652839004
C19	0.9856382061	-2.2157562838	-4.1570604658
H16	2.3222336572	-2.3129300127	-2.4940718207
H17	-1.7807423369	-3.0503320668	-1.6229685692
H18	-2.3412419940	-2.7221754401	-3.9894950791
H19	1.7641119017	-1.9818956103	-4.8615237321
H20	-0.5712857690	-2.1834408899	-5.6215168996
C1	0.5743863458	-0.5077215009	0.4405346425
H5	1.5783628755	-0.5595077770	0.8633906677
H6	0.6828551014	-0.2141085169	-0.5964581000
C3	2.7976584351	4.2167944296	-0.5536768887
C26	1.8195941604	3.3876491689	1.4793453416
C27	0.9766033142	2.6525116204	-0.6445526402
C28	1.9079513036	3.4480386227	-1.2902513713
C29	2.7477220187	4.1880060271	0.8321252429
H1	1.7898857173	3.3527087763	2.5543504826
H2	0.2700912980	2.0817515541	-1.2208892319
H3	1.9329210192	3.4750874837	-2.3661874570
H9	3.4352847020	4.7809146017	1.4097776804
H10	3.5220132279	4.8352318702	-1.0559521854
H25	-1.0710358057	3.1480250996	2.7899724688

nuclear repulsion energy..... 1971.062170283 hartrees

/ end of geometry optimization iteration 12 /

end of program geopt

```

start of program onee
smallest eigenvalue of S:      2.810E-04
number of canonical orbitals.....      461
end of program onee

```

```

start of program probe
end of program probe

```

```

start of program grid

```

```

number of gridpoints:
  atom      N1      N2      C4      C5      C6      C7      C13
H4
  grid # 1      95      102      87      87      90      89      84
73
  grid # 2      103      112      95      95      99      98      92
118
  grid # 3      214      227      195      187      191      199      163
224
  grid # 4      385      414      321      320      323      348      299
224

```

```

number of gridpoints:
  atom      C8      C11      H7      C9      H8      C10      C12
C2
  grid # 1      89      86      73      87      73      89      86
92
  grid # 2      97      94      118      97      118      97      94
100
  grid # 3      184      185      223      184      222      184      194
195
  grid # 4      328      331      226      331      223      329      317
343

```

```

number of gridpoints:
  atom      H13      C14      H15      C15      C16      C17      C18
C19
  grid # 1      69      91      69      89      88      87      89
89
  grid # 2      109      100      110      97      96      96      97
96
  grid # 3      211      196      214      183      184      182      184
183
  grid # 4      214      340      213      327      327      327      327
327

```

```

number of gridpoints:
  atom      H16      H17      H18      H19      H20      C1      H5
H6

```

grid # 1	72	73	73	73	73	82	70
grid # 2	114	114	118	118	118	88	109
grid # 3	214	216	222	221	224	164	217
grid # 4	214	214	224	223	224	292	219

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
grid # 1	89	88	88	89	89	72	71
grid # 2	97	95	96	97	97	115	114
grid # 3	185	182	184	185	185	217	213
grid # 4	328	327	330	328	328	217	212

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3515
grid # 2	118	118	115	4491
grid # 3	223	224	220	8634
grid # 4	224	224	224	12246

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.39028009303		4.3E-05	2.4E-03
etot	2	Y	Y	4	M	-990.39078089231	5.0E-04	1.8E-05	5.5E-04
etot	3	Y	Y	4	M	-990.39083518771	5.4E-05	4.9E-06	1.2E-04
etot	4	Y	N	4	M	-990.39084155577	6.4E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.06217028341
(E)	Total one-electron terms.....	-5260.39454868744
(I)	Total two-electron terms.....	2298.94153684826



(L) Electronic energy..... -2961.45301183918 (E+I)  
 (N) Total energy..... -990.39084155577 (A+L)

SCFE: SCF energy: HF -990.39084155577 hartrees iterations:  
 4

HOMO energy: -0.26906  
 LUMO energy: 0.09673

Orbital energies:

-15.60462	-15.56496	-11.29644	-11.28704	-11.27124	-11.25104
-11.25071	-11.24585	-11.24537	-11.24021	-11.23959	-11.23927
-11.23874	-11.23808	-11.23742	-11.23573	-11.23438	-11.23415
-11.23269	-11.23001	-11.22431	-11.22021	-11.21853	-11.21599
-11.21287	-1.32532	-1.24973	-1.16308	-1.16069	-1.13877
-1.07464	-1.06716	-1.03922	-1.02184	-1.01901	-1.01724
-0.97091	-0.95440	-0.93382	-0.86015	-0.83698	-0.83354
-0.82928	-0.80716	-0.79551	-0.77003	-0.73266	-0.71746
-0.70102	-0.69855	-0.66633	-0.65789	-0.64293	-0.63722
-0.63387	-0.62365	-0.62070	-0.61586	-0.59633	-0.59238
-0.59043	-0.58757	-0.57842	-0.55802	-0.55233	-0.54821
-0.54447	-0.51739	-0.50720	-0.50256	-0.50022	-0.49593
-0.49341	-0.49120	-0.48742	-0.48125	-0.42975	-0.40484
-0.36746	-0.34335	-0.34121	-0.33758	-0.32931	-0.28234
-0.26906	0.09673	0.12890	0.13698	0.13758	0.14860
0.17856	0.20869	0.22823	0.23521	0.24124	

end of program scf

start of program der1a  
 end of program der1a

start of program rwr  
 end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	2.227998E-04	3.002457E-04	-7.633866E-04
2	N2	8.313377E-04	6.278822E-05	-8.329915E-04
3	C4	-2.749466E-04	-4.216903E-04	-5.263447E-07
4	C5	-6.186970E-04	-7.144881E-04	3.670361E-04
5	C6	2.786252E-04	3.974446E-05	-3.989161E-04
6	C7	9.204291E-05	2.064961E-04	1.809267E-04
7	C13	-2.647782E-04	7.202521E-04	7.337563E-04

8	H4	4.755602E-05	2.153163E-04	1.133755E-04
9	C8	-3.968861E-04	6.246385E-04	6.455230E-04
10	C11	1.871446E-05	4.167742E-04	-1.449800E-04
11	H7	4.661710E-05	-2.622866E-05	2.075457E-05
12	C9	-4.135986E-04	-8.043030E-04	2.383556E-04
13	H8	9.219046E-05	1.817128E-05	-3.487273E-05
14	C10	-5.487297E-04	-5.031939E-04	3.007736E-04
15	C12	4.545402E-04	3.326283E-05	3.764629E-06
16	C2	3.716824E-04	4.474287E-04	-1.073648E-03
17	H13	6.660705E-04	2.713936E-04	-4.580298E-05
18	C14	-9.524221E-06	-1.503978E-05	-1.155393E-04
19	H15	-2.589289E-04	-4.741291E-04	1.596626E-04
20	C15	-3.296994E-04	-8.513451E-05	-3.637118E-04
21	C16	5.059299E-04	2.273868E-04	1.343442E-04
22	C17	1.784530E-04	6.295302E-06	3.790300E-04
23	C18	4.746219E-04	1.823099E-04	-5.954331E-04
24	C19	-1.022632E-04	1.979797E-04	6.156296E-05
25	H16	3.316220E-04	-1.320570E-04	5.700000E-06
26	H17	-4.687600E-04	-9.797374E-05	2.750276E-04
27	H18	-1.205098E-03	-6.438215E-05	-3.681211E-04
28	H19	4.370449E-04	-4.587109E-06	-2.768543E-05
29	H20	1.076385E-05	-4.651129E-05	2.680799E-04
30	C1	1.139672E-03	1.536346E-04	3.587566E-04
31	H5	-4.346405E-04	-9.406025E-07	-3.907024E-04
32	H6	-1.517462E-04	-9.902310E-05	3.357495E-04
33	C3	1.185490E-04	2.269726E-04	5.102438E-04
34	C26	-2.577180E-06	8.957851E-05	-5.609457E-05
35	C27	1.261047E-04	2.099169E-04	7.317389E-04
36	C28	2.097073E-04	1.577945E-04	1.716548E-04
37	C29	3.597928E-05	-6.029637E-05	-9.796868E-04
38	H1	9.699556E-05	7.995279E-05	-5.711064E-04
39	H2	8.836115E-05	-5.681230E-05	5.451637E-05
40	H3	-2.236567E-05	-8.217920E-05	5.481682E-04
41	H9	-1.316816E-04	3.301862E-05	-1.580912E-04
42	H10	-5.437240E-04	-3.859753E-04	3.434680E-04
43	H25	-4.214022E-06	-3.049285E-05	3.941865E-06
-----				
total		6.931218E-04	8.159137E-04	2.461458E-05

end of program derlb

start of program geopt 13

geometry optimization step 13

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0192086  
Cos(theta): 0.7007821

Final level shift: -6.0023224E-02

energy change: -5.2807E-05 . ( 5.0000E-05 )  
gradient maximum: 1.3227E-03 . ( 4.5000E-04 )  
gradient rms: 3.7901E-04 . ( 3.0000E-04 )  
step size: 0.01921 trust radius: 0.01875  
displacement maximum: 6.9080E-03 . ( 1.8000E-03 )  
displacement rms: 1.5092E-03 . ( 1.2000E-03 )  
predicted energy change: -4.3542E-05 geom step: 1.9209E-  
02 full step: 1.9209E-02  
molecular structure not yet converged...

center of mass moved by:

x: -2.9109E-04 y: 4.6312E-04 z: 3.9301E-04

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2488255692	0.4322339843	1.1698872896
N2	-1.0058226391	-2.2950440448	1.1945544518
C4	-1.2229240041	-0.0361424909	1.9939013709
C5	-0.0365007616	-1.9141015496	0.4855354067
C6	-1.6347093114	-1.3580296563	2.0375911084
C7	-1.7199951420	0.9823189968	2.7870807318
C13	0.6348421100	-2.9216660268	-0.4233610698
H4	-2.9973932708	-2.6761090969	2.9877417657
C8	-2.7524946331	0.6532233934	3.6829849331
C11	-0.9547024201	2.1488365611	2.4190560905
H7	-3.1905897249	1.3985912480	4.3231430452
C9	-3.1932086574	-0.6517690880	3.7325641745
H8	-3.9812949477	-0.9149495298	4.4155551603
C10	-2.6401022769	-1.6646647698	2.9195236102
C12	-0.0728836370	1.7767980278	1.4534342970
C2	0.9248616477	2.6094547063	0.7465477863
H13	1.7116541383	-2.8719037968	-0.2842566294
C14	0.3090127646	-2.7017285669	-1.8919217197
H15	0.3057087418	-3.9036615388	-0.1088356875
C15	-0.3181517155	-2.3211174476	-4.5844573536
C16	1.3022806045	-2.4054300452	-2.8151364504
C17	-1.0074098438	-2.8056006886	-2.3339389563
C18	-1.3187367817	-2.6172398029	-3.6681293975
C19	0.9926701615	-2.2159193741	-4.1546871043
H16	2.3260666979	-2.3274211924	-2.4914155295
H17	-1.7860704955	-3.0349791182	-1.6266254226
H18	-2.3425831130	-2.7043182588	-3.9940814180
H19	1.7761371458	-1.9889515630	-4.8563274949
H20	-0.5618666539	-2.1757307323	-5.6219403179
C1	0.5740559454	-0.5100177170	0.4417086690
H5	1.5784350739	-0.5618273663	0.8611698811

H6	0.6798161828	-0.2186286872	-0.5959096950
C3	2.7946536701	4.2153968164	-0.5592303079
C26	1.8165501131	3.3931684312	1.4740306347
C27	0.9780419294	2.6451051479	-0.6454457865
C28	1.9082602778	3.4400244963	-1.2927166344
C29	2.7429412688	4.1934511473	0.8251154766
H1	1.7882002850	3.3627714017	2.5482192846
H2	0.2755486666	2.0683734653	-1.2209902818
H3	1.9348576060	3.4600611274	-2.3678965230
H9	3.4273881104	4.7918441078	1.4013512856
H10	3.5166904418	4.8328913912	-1.0628356014
H25	-1.0679447669	3.1461658281	2.7930681050

nuclear repulsion energy..... 1971.091366916 hartrees

/ end of geometry optimization iteration 13 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.824E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	87	87	90	90	84
73							
grid # 2	103	112	95	95	99	98	92
118							
grid # 3	214	227	195	187	191	199	163
224							
grid # 4	389	414	321	320	323	347	299
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							

grid # 3	184	185	223	184	222	184	194
----------	-----	-----	-----	-----	-----	-----	-----

196

grid # 4	329	331	226	331	223	329	317
----------	-----	-----	-----	-----	-----	-----	-----

341

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
------	-----	-----	-----	-----	-----	-----	-----

C19

grid # 1	69	93	69	89	88	88	89
----------	----	----	----	----	----	----	----

89

grid # 2	109	100	110	97	96	96	97
----------	-----	-----	-----	----	----	----	----

96

grid # 3	210	195	214	183	184	183	184
----------	-----	-----	-----	-----	-----	-----	-----

183

grid # 4	214	340	213	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
------	-----	-----	-----	-----	-----	----	----

H6

grid # 1	72	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	114	115	118	118	118	88	110
----------	-----	-----	-----	-----	-----	----	-----

104

grid # 3	214	216	223	222	224	164	217
----------	-----	-----	-----	-----	-----	-----	-----

207

grid # 4	214	214	224	223	224	293	217
----------	-----	-----	-----	-----	-----	-----	-----

205

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	88	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
----------	----	----	----	----	----	-----	-----

118

grid # 3	185	182	184	184	185	217	213
----------	-----	-----	-----	-----	-----	-----	-----

223

grid # 4	328	328	329	328	328	217	212
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3520
grid # 2	118	118	115	4493
grid # 3	223	223	220	8634
grid # 4	224	224	224	12246

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i	energy	energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.39066938504		2.3E-05	1.1E-03
etot	2	Y	Y	4	M	-990.39082701468	1.6E-04	1.1E-05	4.2E-04
etot	3	Y	Y	4	M	-990.39084593688	1.9E-05	3.2E-06	1.1E-04
etot	4	Y	N	4	M	-990.39084898231	3.0E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.09136691580	
(E)	Total one-electron terms.....	-5260.45116671076	
(I)	Total two-electron terms.....	2298.96895081265	
(L)	Electronic energy.....	-2961.48221589810	(E+I)
(N)	Total energy.....	-990.39084898231	(A+L)

SCFE: SCF energy: HF      -990.39084898231 hartrees      iterations:  
4

HOMO energy:      -0.26909  
LUMO energy:      0.09670

Orbital energies:

-15.60482	-15.56511	-11.29607	-11.28679	-11.27163	-11.25115
-11.25090	-11.24617	-11.24561	-11.23984	-11.23956	-11.23889
-11.23843	-11.23775	-11.23701	-11.23573	-11.23460	-11.23444
-11.23276	-11.23041	-11.22479	-11.22011	-11.21902	-11.21611
-11.21311	-1.32505	-1.25012	-1.16329	-1.16072	-1.13844
-1.07455	-1.06701	-1.03926	-1.02193	-1.01882	-1.01722
-0.97108	-0.95429	-0.93372	-0.86021	-0.83691	-0.83360
-0.82903	-0.80715	-0.79555	-0.77004	-0.73267	-0.71741
-0.70115	-0.69841	-0.66628	-0.65791	-0.64291	-0.63702
-0.63380	-0.62376	-0.62069	-0.61579	-0.59625	-0.59229
-0.59055	-0.58752	-0.57825	-0.55807	-0.55233	-0.54821
-0.54447	-0.51744	-0.50724	-0.50258	-0.50023	-0.49595
-0.49354	-0.49120	-0.48746	-0.48116	-0.42969	-0.40485
-0.36758	-0.34333	-0.34129	-0.33767	-0.32932	-0.28244
-0.26909	0.09670	0.12895	0.13716	0.13754	0.14851
0.17843	0.20872	0.22830	0.23522	0.24111	

end of program scf

start of program der1a

end of program derla

start of program rwr

end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
---	---	-----	-----	-----
1	N1	4.528739E-04	-2.150721E-04	-7.189734E-04
2	N2	-5.179471E-04	-3.795031E-05	3.540438E-04
3	C4	1.453513E-04	-6.415916E-05	2.186439E-05
4	C5	7.956954E-04	-7.125645E-05	-6.055630E-04
5	C6	1.674864E-04	-8.425208E-05	-1.081652E-04
6	C7	-2.512909E-04	2.681225E-04	1.706745E-04
7	C13	2.264142E-04	5.762714E-04	8.823663E-05
8	H4	-6.045948E-05	-1.622022E-04	5.346281E-05
9	C8	-9.811810E-06	-6.163186E-04	-1.033681E-04
10	C11	-3.140914E-04	-5.043245E-07	3.741302E-04
11	H7	-7.779658E-05	9.048357E-05	3.931211E-05
12	C9	2.767482E-04	5.658957E-04	-1.033924E-04
13	H8	-1.429809E-04	-1.901601E-05	1.548469E-04
14	C10	-7.750078E-05	3.688975E-04	2.521305E-04
15	C12	4.616740E-04	5.257927E-06	-2.829912E-04
16	C2	2.944823E-04	2.233180E-04	5.568139E-04
17	H13	4.427948E-04	6.578201E-05	1.726383E-04
18	C14	1.282378E-04	-1.306465E-04	5.130233E-04
19	H15	-1.131664E-04	-2.810631E-04	-3.533440E-05
20	C15	-5.253545E-04	1.215568E-05	-8.190267E-05
21	C16	1.228580E-04	-7.128547E-05	5.101624E-04
22	C17	-7.451867E-04	-2.526086E-04	2.209580E-04
23	C18	-1.326991E-03	-2.850276E-04	-7.335060E-04
24	C19	-1.692902E-04	6.245857E-06	-3.167455E-04
25	H16	3.328469E-04	1.496603E-04	2.129530E-04
26	H17	3.554518E-04	1.287242E-04	-1.716810E-04
27	H18	1.486137E-03	2.577115E-04	2.009026E-04
28	H19	1.714175E-05	8.756748E-05	-1.598401E-04
29	H20	3.361176E-05	4.889786E-05	-2.258726E-04
30	C1	-2.352300E-04	1.325569E-04	1.607766E-04
31	H5	-2.663504E-05	8.592286E-06	1.148176E-04
32	H6	-4.109229E-05	8.430998E-05	1.882357E-04
33	C3	-4.420181E-04	-1.741977E-04	-2.983395E-04
34	C26	-2.316693E-04	-2.309980E-04	-1.002232E-04
35	C27	-8.113392E-05	-3.491728E-05	-1.261326E-04
36	C28	2.378795E-04	1.576131E-04	7.887497E-05
37	C29	1.155601E-04	5.628839E-05	2.498595E-04
38	H1	-1.391838E-04	-3.540240E-05	1.268414E-04
39	H2	6.131107E-05	1.420514E-04	1.187152E-04

40	H3	5.722184E-05	1.176396E-04	-1.489399E-04
41	H9	-1.997639E-04	-2.093410E-04	-2.637846E-04
42	H10	2.310080E-04	2.058152E-04	-3.046466E-04
43	H25	-5.723237E-05	6.307406E-05	-1.828532E-05
-----				
	total	6.569597E-04	8.467135E-04	2.658720E-05

end of program derlb

start of program geopt 14

geometry optimization step 14

reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0108550

Cos(theta): 0.7082419

Final level shift: -3.0472439E-02

energy change: -7.4265E-06 \* ( 5.0000E-05 )  
gradient maximum: 1.4699E-03 . ( 4.5000E-04 )  
gradient rms: 2.7737E-04 \* ( 3.0000E-04 )  
step size: 0.01085 trust radius: 0.01000  
displacement maximum: 4.5549E-03 . ( 1.8000E-03 )  
displacement rms: 8.5285E-04 \* ( 1.2000E-03 )  
predicted energy change: -1.5366E-05 geom step: 1.0855E-02  
full step: 1.0855E-02  
molecular structure not yet converged...

center of mass moved by:

x: 2.3234E-04 y: -3.9719E-04 z: 1.1836E-04

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2476098628	0.4319499494	1.1700896461
N2	-1.0050850757	-2.2950871682	1.1949182325
C4	-1.2225555532	-0.0359392069	1.9934979632
C5	-0.0345337388	-1.9145591457	0.4863206158
C6	-1.6345629750	-1.3576518558	2.0372932256
C7	-1.7207638142	0.9827487410	2.7857085019
C13	0.6372167911	-2.9214974519	-0.4226269266
H4	-2.9991767135	-2.6746254046	2.9867461727
C8	-2.7544283972	0.6541992122	3.6802520196



C11	-0.9547075557	2.1487129569	2.4185234965
H7	-3.1936858699	1.4000793918	4.3191782963
C9	-3.1953417522	-0.6499826706	3.7301011813
H8	-3.9846205275	-0.9126483273	4.4122075724
C10	-2.6412076664	-1.6632555907	2.9184523073
C12	-0.0714118196	1.7763193928	1.4539254438
C2	0.9267126827	2.6085697080	0.7475086448
H13	1.7145636018	-2.8715088035	-0.2838423517
C14	0.3089199593	-2.7020981095	-1.8909152593
H15	0.3081077662	-3.9039526830	-0.1083403583
C15	-0.3215924809	-2.3201267580	-4.5836616469
C16	1.3004540244	-2.3992437756	-2.8137797881
C17	-1.0077278059	-2.8118948597	-2.3339058106
C18	-1.3203617236	-2.6227459376	-3.6680394462
C19	0.9888784831	-2.2093360982	-4.1534576988
H16	2.3240667900	-2.3146888619	-2.4895233992
H17	-1.7849137076	-3.0449393883	-1.6268919447
H18	-2.3419771432	-2.7122708466	-3.9947783125
H19	1.7707403444	-1.9764961643	-4.8551652860
H20	-0.5656277175	-2.1736956496	-5.6211053749
C1	0.5760456600	-0.5105838268	0.4433549677
H5	1.5800429573	-0.5626136306	0.8641513090
H6	0.6825437933	-0.2189447287	-0.5941242795
C3	2.7951744578	4.2145617192	-0.5601377830
C26	1.8187572576	3.3915699332	1.4744469707
C27	0.9785171969	2.6447421378	-0.6446715605
C28	1.9082206454	3.4396720163	-1.2930044553
C29	2.7448249516	4.1917280945	0.8244421729
H1	1.7902754511	3.3610162274	2.5486052296
H2	0.2747696491	2.0686681731	-1.2192937084
H3	1.9337718424	3.4605773143	-2.3682340620
H9	3.4301063300	4.7894624992	1.3997519889
H10	3.5171655374	4.8322369654	-1.0645143063
H25	-1.0688078963	3.1463685995	2.7914697600

nuclear repulsion energy..... 1971.109269844 hartrees

/ end of geometry optimization iteration 14 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.820E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	87	87	90	90	84
73							
grid # 2	103	112	95	95	99	98	92
118							
grid # 3	214	227	195	187	191	199	163
224							
grid # 4	389	414	322	320	323	347	299
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	194
195							
grid # 4	329	331	226	331	223	329	317
341							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	88	89
89							
grid # 2	110	100	110	97	96	96	97
96							
grid # 3	211	197	214	183	184	183	184
183							
grid # 4	214	340	213	327	327	327	327
327							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	73	73	73	73	82	70
69							
grid # 2	114	115	118	118	118	88	110
104							
grid # 3	214	216	223	222	224	164	217
207							
grid # 4	214	214	224	223	224	293	217
205							

number of gridpoints:

	atom	C3	C26	C27	C28	C29	H1	H2
H3								
	grid # 1	89	88	88	89	89	72	71
73								
	grid # 2	97	95	96	97	97	115	114
118								
	grid # 3	185	182	184	185	185	217	213
223								
	grid # 4	328	328	329	328	328	217	212
224								

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3518
grid # 2	118	118	115	4494
grid # 3	223	224	220	8638
grid # 4	224	224	224	12247

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.39080246980		1.4E-05	9.2E-04
etot	2	Y	Y	4	M	-990.39085334491	5.1E-05	6.4E-06	3.6E-04
etot	3	Y	Y	4	M	-990.39085990967	6.6E-06	2.0E-06	9.6E-05
etot	4	Y	N	4	M	-990.39085924579	-6.6E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.10926984366	
(E)	Total one-electron terms.....	-5260.48968808571	
(I)	Total two-electron terms.....	2298.98955899626	
(L)	Electronic energy.....	-2961.50012908945	(E+I)
(N)	Total energy.....	-990.39085924579	(A+L)

SCFE: SCF energy: HF -990.39085924579 hartrees iterations:  
4

HOMO energy: -0.26901  
LUMO energy: 0.09668

Orbital energies:

-15.60463	-15.56524	-11.29626	-11.28681	-11.27141	-11.25098
-11.25089	-11.24604	-11.24583	-11.23989	-11.23981	-11.23902
-11.23846	-11.23783	-11.23708	-11.23595	-11.23451	-11.23447
-11.23271	-11.23045	-11.22455	-11.22026	-11.21879	-11.21610
-11.21302	-1.32494	-1.24990	-1.16327	-1.16057	-1.13849
-1.07446	-1.06705	-1.03929	-1.02190	-1.01890	-1.01702
-0.97103	-0.95434	-0.93367	-0.86016	-0.83696	-0.83361
-0.82905	-0.80707	-0.79550	-0.76999	-0.73262	-0.71741
-0.70112	-0.69838	-0.66629	-0.65789	-0.64288	-0.63712
-0.63384	-0.62367	-0.62072	-0.61582	-0.59621	-0.59233
-0.59050	-0.58743	-0.57834	-0.55809	-0.55227	-0.54820
-0.54435	-0.51743	-0.50724	-0.50258	-0.50021	-0.49593
-0.49348	-0.49117	-0.48739	-0.48119	-0.42972	-0.40488
-0.36749	-0.34336	-0.34123	-0.33760	-0.32929	-0.28245
-0.26901	0.09668	0.12894	0.13711	0.13740	0.14856
0.17846	0.20869	0.22827	0.23519	0.24116	

end of program scf

start of program derla

end of program derla

start of program rwr

end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	3.594168E-04	-3.247900E-04	-4.707368E-04
2	N2	1.456478E-04	1.299541E-04	-1.590589E-04
3	C4	1.259234E-04	-1.305667E-04	-7.187211E-05
4	C5	-3.678037E-05	-4.521296E-05	1.199478E-04
5	C6	5.984738E-05	-1.658855E-04	-5.162803E-05
6	C7	-6.725914E-05	2.139092E-04	6.314595E-05
7	C13	-3.445068E-05	1.086910E-04	1.095968E-04
8	H4	1.233470E-05	-3.123613E-05	3.656539E-05
9	C8	-2.053567E-05	3.892458E-05	6.619510E-05
10	C11	-3.836909E-05	2.069748E-04	1.279422E-04
11	H7	-2.571961E-06	9.001533E-05	2.737180E-05
12	C9	4.406467E-05	-4.942249E-05	-3.711664E-05
13	H8	-1.489958E-05	3.325105E-06	5.832352E-05
14	C10	-2.354330E-05	2.627673E-05	4.444407E-05
15	C12	1.173535E-04	8.037980E-05	-1.135315E-05
16	C2	3.023010E-05	1.143481E-04	1.144053E-04
17	H13	4.746262E-05	8.375568E-05	4.709878E-06

18	C14	-2.570906E-04	-7.682341E-05	2.962546E-05
19	H15	4.472624E-05	-6.375860E-05	-2.023663E-05
20	C15	1.891440E-04	6.801696E-05	-1.397037E-04
21	C16	8.780006E-05	7.855990E-05	-3.361955E-05
22	C17	7.344717E-05	-2.688328E-05	3.500123E-04
23	C18	-2.375303E-04	-1.002662E-04	-2.346247E-05
24	C19	3.475516E-05	4.269829E-05	-7.942340E-05
25	H16	-1.546063E-05	-3.301204E-05	-2.106096E-05
26	H17	6.240769E-05	4.272218E-05	5.193411E-05
27	H18	2.079249E-04	6.398798E-05	5.979060E-05
28	H19	-1.512320E-05	-2.486948E-05	-5.670209E-05
29	H20	3.073742E-05	1.633282E-05	-8.591535E-05
30	C1	-1.156034E-04	1.492051E-04	1.091582E-04
31	H5	-1.311443E-04	5.783864E-05	4.118251E-05
32	H6	4.583649E-05	3.741885E-05	1.991567E-04
33	C3	-1.431507E-04	-3.099268E-05	-1.181485E-04
34	C26	4.632667E-05	6.386637E-05	-1.655493E-04
35	C27	1.736270E-05	4.420336E-05	-2.361738E-04
36	C28	3.924001E-05	3.200689E-05	1.369748E-04
37	C29	1.549265E-05	1.514235E-05	4.802569E-05
38	H1	-3.310335E-05	2.030411E-05	1.784773E-04
39	H2	9.751055E-05	8.306954E-05	8.534773E-05
40	H3	2.527376E-05	2.668486E-05	-9.347572E-05
41	H9	-9.749903E-05	-4.736787E-05	-9.930280E-05
42	H10	-2.819321E-06	2.249804E-05	-7.816079E-05
43	H25	-1.728472E-05	5.798267E-05	1.449746E-05
-----				
	total	6.560473E-04	8.680061E-04	2.412989E-05

end of program der1b

start of program geopt 15

geometry optimization step 15

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0143612

Cos(theta): 0.4919231

Final level shift: -2.7000810E-02

energy change: -1.0263E-05 \* ( 5.0000E-05 )

gradient maximum: 4.0569E-04 \* ( 4.5000E-04 )

gradient rms: 1.0457E-04 \* ( 3.0000E-04 )

step size: 0.01436 trust radius: 0.01414

displacement maximum: 8.4903E-03 . ( 1.8000E-03 )

displacement rms: 1.1283E-03 \* ( 1.2000E-03 )  
 predicted energy change: -7.4859E-06 geom step: 1.4361E-  
 02 full step: 1.4361E-02  
 molecular structure not yet converged...

center of mass moved by:  
 x: 2.6501E-05 y: -2.4923E-04 z: 6.1267E-05

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2463607370	0.4314193906	1.1710338958
N2	-1.0035424221	-2.2955233045	1.1947806590
C4	-1.2216235933	-0.0368540479	1.9940347638
C5	-0.0326064789	-1.9145180546	0.4866450499
C6	-1.6331040260	-1.3588415492	2.0376289344
C7	-1.7214275643	0.9821252034	2.7857401080
C13	0.6387952323	-2.9207111820	-0.4230303496
H4	-2.9983933254	-2.6759482577	2.9865390107
C8	-2.7554322781	0.6531437848	3.6795071530
C11	-0.9556687926	2.1484771315	2.4194464699
H7	-3.1957362911	1.3993275357	4.3177668929
C9	-3.1954005477	-0.6509580953	3.7294178623
H8	-3.9851392350	-0.9139827639	4.4112945459
C10	-2.6402354285	-1.6642884757	2.9184542048
C12	-0.0716231059	1.7762215315	1.4549835704
C2	0.9257296648	2.6089482628	0.7484190091
H13	1.7160363204	-2.8699892414	-0.2843745120
C14	0.3092857777	-2.7015111760	-1.8910420198
H15	0.3107659365	-3.9038972276	-0.1098048464
C15	-0.3210182211	-2.3198001555	-4.5845563047
C16	1.3026267989	-2.4078132613	-2.8158087619
C17	-1.0093417649	-2.8017601438	-2.3324540938
C18	-1.3215507168	-2.6128445964	-3.6669555125
C19	0.9912426335	-2.2182211833	-4.1556558124
H16	2.3277109198	-2.3309831513	-2.4925549566
H17	-1.7872243266	-3.0262248434	-1.6238607485
H18	-2.3426567575	-2.6932803270	-3.9926346211
H19	1.7741739528	-1.9932912445	-4.8591528825
H20	-0.5645529054	-2.1734405864	-5.6223463359
C1	0.5782555737	-0.5107568800	0.4460053859
H5	1.5811573473	-0.5631828239	0.8704649311
H6	0.6880840404	-0.2177615274	-0.5909622482
C3	2.7922215595	4.2150771119	-0.5617697159
C26	1.8178585798	3.3922403513	1.4746958238
C27	0.9762379671	2.6449102789	-0.6443115909
C28	1.9050145102	3.4399273512	-1.2938231691
C29	2.7430458157	4.1923393067	0.8232302794
H1	1.7893807507	3.3619023049	2.5491513072
H2	0.2718921784	2.0685313456	-1.2175644237
H3	1.9300026211	3.4609305987	-2.3692287604
H9	3.4287854490	4.7902046058	1.3973483110

H10	3.5140165769	4.8329081285	-1.0672737690
H25	-1.0711083010	3.1462171349	2.7921150838

nuclear repulsion energy..... 1971.034696625 hartrees

-----  
/ end of geometry optimization iteration 15 /  
-----

end of program geopt

start of program onee  
smallest eigenvalue of S: 2.821E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
grid # 1		96	102	87	87	90	89	84
73								
grid # 2		103	112	95	95	99	98	92
118								
grid # 3		214	227	195	187	191	199	163
224								
grid # 4		388	414	321	320	322	348	299
224								

number of gridpoints:

	atom	C8	C11	H7	C9	H8	C10	C12
C2								
grid # 1		89	86	73	87	73	89	86
92								
grid # 2		97	94	118	97	118	97	94
100								
grid # 3		184	185	223	184	222	184	194
195								
grid # 4		328	331	226	331	223	329	317
343								

number of gridpoints:

	atom	H13	C14	H15	C15	C16	C17	C18
C19								
grid # 1		69	91	69	89	88	88	89
89								

grid # 2	109	100	110	97	96	96	97
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96

grid # 3	210	196	214	183	184	183	184
----------	-----	-----	-----	-----	-----	-----	-----

183

grid # 4	214	340	213	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
------	-----	-----	-----	-----	-----	----	----

H6

grid # 1	72	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	114	115	118	118	118	88	109
----------	-----	-----	-----	-----	-----	----	-----

104

grid # 3	214	216	222	222	224	164	217
----------	-----	-----	-----	-----	-----	-----	-----

207

grid # 4	214	214	224	223	224	293	219
----------	-----	-----	-----	-----	-----	-----	-----

205

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	88	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
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118

grid # 3	185	182	183	185	185	217	213
----------	-----	-----	-----	-----	-----	-----	-----

223

grid # 4	328	327	329	327	328	217	212
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
------	----	-----	-----	-------

grid # 1	73	73	72	3517
grid # 2	118	118	115	4492
grid # 3	222	224	220	8633
grid # 4	224	224	224	12246

end of program grid

start of program rwr  
end of program rwr

start of program scf

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



etot	1	N	N	1	U	-990.39072743546		2.7E-05	1.6E-03
etot	2	Y	Y	4	M	-990.39084046479	1.1E-04	1.0E-05	6.3E-04
etot	3	Y	Y	4	M	-990.39085660547	1.6E-05	2.9E-06	1.5E-04
etot	4	Y	N	4	M	-990.39085842189	1.8E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.03469662474	
(E)	Total one-electron terms.....	-5260.33898399291	
(I)	Total two-electron terms.....	2298.91342894628	
(L)	Electronic energy.....	-2961.42555504663	(E+I)
(N)	Total energy.....	-990.39085842189	(A+L)

SCFE: SCF energy: HF      -990.39085842189 hartrees      iterations:  
4

HOMO energy:      -0.26904  
LUMO energy:      0.09663

Orbital energies:

-15.60476	-15.56511	-11.29628	-11.28688	-11.27173	-11.25112
-11.25088	-11.24616	-11.24601	-11.23993	-11.23979	-11.23905
-11.23848	-11.23784	-11.23711	-11.23607	-11.23466	-11.23444
-11.23292	-11.23053	-11.22458	-11.22023	-11.21899	-11.21606
-11.21326	-1.32501	-1.24984	-1.16321	-1.16033	-1.13852
-1.07453	-1.06701	-1.03926	-1.02190	-1.01887	-1.01693
-0.97093	-0.95430	-0.93367	-0.86015	-0.83703	-0.83361
-0.82898	-0.80705	-0.79545	-0.77000	-0.73261	-0.71741
-0.70108	-0.69829	-0.66635	-0.65790	-0.64282	-0.63719
-0.63386	-0.62365	-0.62070	-0.61581	-0.59629	-0.59238
-0.59044	-0.58747	-0.57825	-0.55807	-0.55220	-0.54819
-0.54450	-0.51739	-0.50722	-0.50256	-0.50019	-0.49584
-0.49341	-0.49117	-0.48733	-0.48121	-0.42975	-0.40483
-0.36754	-0.34337	-0.34122	-0.33756	-0.32914	-0.28243
-0.26904	0.09663	0.12889	0.13707	0.13733	0.14845
0.17836	0.20861	0.22838	0.23520	0.24116	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-2.481303E-04	2.161363E-04	3.038174E-05
2	N2	2.836382E-04	-2.499438E-05	-2.728610E-04
3	C4	-5.332666E-05	1.576006E-04	1.308833E-04
4	C5	-3.595149E-04	-1.387013E-04	2.963041E-04
5	C6	2.019594E-05	1.908855E-04	2.396059E-05
6	C7	2.466402E-04	-1.423657E-04	-1.552636E-04
7	C13	-1.276988E-04	5.612039E-06	6.448695E-05
8	H4	8.439654E-05	1.557089E-04	3.881350E-05
9	C8	1.165608E-05	5.058858E-04	1.509718E-04
10	C11	1.471085E-04	-4.822498E-05	-3.124871E-04
11	H7	5.901722E-05	-5.856555E-05	-6.083047E-05
12	C9	-2.081620E-04	-4.628287E-04	1.114154E-04
13	H8	1.113241E-04	3.132659E-05	-7.909427E-05
14	C10	-1.274255E-04	-2.859290E-04	1.870702E-05
15	C12	-5.235787E-06	8.359514E-05	2.010785E-04
16	C2	2.011226E-05	1.154169E-04	-3.679946E-04
17	H13	1.231949E-04	6.717329E-05	-9.936772E-05
18	C14	-2.239323E-04	1.957682E-04	-5.369846E-04
19	H15	3.610993E-06	-2.367943E-05	1.405502E-04
20	C15	4.528455E-04	8.163430E-06	3.393146E-04
21	C16	-5.301138E-05	-4.748777E-05	2.288187E-04
22	C17	9.188483E-04	1.208919E-04	1.826117E-04
23	C18	1.202191E-03	1.978553E-04	5.774334E-05
24	C19	-4.165740E-04	-3.910772E-05	-2.787547E-04
25	H16	-3.998587E-04	2.166071E-05	-1.106724E-04
26	H17	-1.196398E-04	-1.085782E-04	1.297513E-04
27	H18	-9.010150E-04	-1.633065E-04	-2.194062E-04
28	H19	-1.346353E-04	2.261628E-05	1.123854E-04
29	H20	4.154382E-06	-5.819682E-06	1.013341E-04
30	C1	5.219134E-04	1.699161E-04	-4.100770E-06
31	H5	-3.070221E-04	-1.084423E-05	-1.892583E-04
32	H6	6.403176E-05	-1.027693E-04	3.230711E-04
33	C3	1.449365E-04	1.660298E-04	1.228439E-04
34	C26	-3.787139E-07	5.421162E-05	-1.973404E-04
35	C27	1.942710E-05	4.496688E-05	2.562209E-04
36	C28	-4.419795E-05	-3.799500E-05	5.523642E-05
37	C29	-1.078932E-06	-5.617927E-06	-2.284443E-04
38	H1	8.125850E-05	7.200215E-05	-6.136742E-05
39	H2	4.595660E-05	3.363527E-05	-2.715897E-05
40	H3	-3.156831E-05	-9.218442E-06	3.647842E-06
41	H9	3.691536E-05	8.898917E-05	2.667129E-05
42	H10	-2.160082E-04	-1.433661E-04	1.416099E-04
43	H25	3.817919E-05	-4.036847E-05	-5.326570E-05
total		6.631381E-04	8.262798E-04	3.416091E-05

end of program der1b

start of program geopt 16

geometry optimization step 16

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 15 \*\*

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0104342

Cos(theta): 0.4965050

Final level shift: -2.6262214E-02

energy change: 8.2390E-07 # ( 5.0000E-05 )

gradient maximum: 4.0569E-04 \* ( 4.5000E-04 )

gradient rms: 1.0457E-04 \* ( 3.0000E-04 )

step size: 0.01043 trust radius: 0.01000

displacement maximum: 6.0223E-03 . ( 1.8000E-03 )

displacement rms: 8.1979E-04 \* ( 1.2000E-03 )

predicted energy change: -4.8790E-06 geom step: 1.0434E-

02 full step: 1.0434E-02

\*\*\*\*\*

\*\* Geometry optimization complete \*\*

\*\*\*\*\*

center of mass moved by:

x: 0.0000E+00

y: -6.8695E-16

z: 3.8858E-16

final geometry:

	angstroms		
atom	x	y	z
N1	-0.2476098628	0.4319499494	1.1700896461
N2	-1.0050850757	-2.2950871682	1.1949182325
C4	-1.2225555532	-0.0359392069	1.9934979632
C5	-0.0345337388	-1.9145591457	0.4863206158
C6	-1.6345629750	-1.3576518558	2.0372932256
C7	-1.7207638142	0.9827487410	2.7857085019
C13	0.6372167911	-2.9214974519	-0.4226269266
H4	-2.9991767135	-2.6746254046	2.9867461727
C8	-2.7544283972	0.6541992122	3.6802520196
C11	-0.9547075557	2.1487129569	2.4185234965
H7	-3.1936858699	1.4000793918	4.3191782963
C9	-3.1953417522	-0.6499826706	3.7301011813
H8	-3.9846205275	-0.9126483273	4.4122075724
C10	-2.6412076664	-1.6632555907	2.9184523073
C12	-0.0714118196	1.7763193928	1.4539254438
C2	0.9267126827	2.6085697080	0.7475086448
H13	1.7145636018	-2.8715088035	-0.2838423517

C14	0.3089199593	-2.7020981095	-1.8909152593
H15	0.3081077662	-3.9039526830	-0.1083403583
C15	-0.3215924809	-2.3201267580	-4.5836616469
C16	1.3004540244	-2.3992437756	-2.8137797881
C17	-1.0077278059	-2.8118948597	-2.3339058106
C18	-1.3203617236	-2.6227459376	-3.6680394462
C19	0.9888784831	-2.2093360982	-4.1534576988
H16	2.3240667900	-2.3146888619	-2.4895233992
H17	-1.7849137076	-3.0449393883	-1.6268919447
H18	-2.3419771432	-2.7122708466	-3.9947783125
H19	1.7707403444	-1.9764961643	-4.8551652860
H20	-0.5656277175	-2.1736956496	-5.6211053749
C1	0.5760456600	-0.5105838268	0.4433549677
H5	1.5800429573	-0.5626136306	0.8641513090
H6	0.6825437933	-0.2189447287	-0.5941242795
C3	2.7951744578	4.2145617192	-0.5601377830
C26	1.8187572576	3.3915699332	1.4744469707
C27	0.9785171969	2.6447421378	-0.6446715605
C28	1.9082206454	3.4396720163	-1.2930044553
C29	2.7448249516	4.1917280945	0.8244421729
H1	1.7902754511	3.3610162274	2.5486052296
H2	0.2747696491	2.0686681731	-1.2192937084
H3	1.9337718424	3.4605773143	-2.3682340620
H9	3.4301063300	4.7894624992	1.3997519889
H10	3.5171655374	4.8322369654	-1.0645143063
H25	-1.0688078963	3.1463685995	2.7914697600

nuclear repulsion energy..... 1971.109269844 hartrees

/ end of geometry optimization iteration 16 /

end of program geopt

start of program post  
 Writing a SPARTAN archive file  
 end of program post

Total cpu seconds      user:      1761.812      user+sys:      1761.812

## Compound 2'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: WF3654  
Executables used: D:\TITAN  
Temporary files : C:\Users\gfabr\AppData\Local\Temp\WF3654

Input file comments:  
Molecule001  
This file created by Spartan

basis set: 6-31G\*\*  
net molecular charge: 0  
multiplicity: 1

number of basis functions.... 465

Input geometry:

	angstroms		
atom	x	y	z
N1	-0.1550260000	0.4374990000	1.1210390000
N2	-1.0086730000	-2.3256400000	1.1332130000
C4	-1.1860510000	-0.0350800000	1.9315790000
C5	-0.0104550000	-1.9237530000	0.4028750000
C6	-1.6456290000	-1.3760560000	1.9632780000
C7	-1.7070180000	1.0262900000	2.7388420000
C13	0.7199200000	-2.8803430000	-0.5063790000
H4	-3.1185930000	-2.6496450000	2.9223950000
C8	-2.7656460000	0.7093510000	3.5969080000
C11	-0.9132890000	2.1852800000	2.3994340000
H7	-3.2133600000	1.4833470000	4.2359600000
C9	-3.2381490000	-0.5972350000	3.6279590000

H8	-4.0721010000	-0.8455450000	4.3029390000
C10	-2.7017240000	-1.6349910000	2.8394980000
C12	0.0268720000	1.8011420000	1.4273890000
C2	1.0263770000	2.6560040000	0.8075810000
H13	1.8204060000	-2.6663390000	-0.4286580000
C14	0.2610050000	-2.7449900000	-1.9177470000
H15	0.5612370000	-3.9425620000	-0.1705390000
C15	-0.5895550000	-2.5433530000	-4.5760680000
C16	1.1246910000	-2.2456410000	-2.8988340000
C17	-1.0320590000	-3.1444790000	-2.2771670000
C18	-1.4542200000	-3.0419090000	-3.6012120000
C19	0.6998040000	-2.1465450000	-4.2231290000
H16	2.1442750000	-1.9343460000	-2.6271240000
H17	-1.7134540000	-3.5365780000	-1.5059970000
H18	-2.4719630000	-3.3556810000	-3.8767030000
H19	1.3846780000	-1.7555640000	-4.9897570000
H20	-0.9239070000	-2.4642400000	-5.6207450000
C1	0.5776390000	-0.5062530000	0.3222060000
H5	1.6528730000	-0.5444960000	0.6633050000
H6	0.5619750000	-0.1829560000	-0.7593680000
C3	2.9246780000	4.3652120000	-0.3378590000
C26	1.7455110000	3.5549090000	1.6101580000
C27	1.2625130000	2.6251890000	-0.5732690000
C28	2.2088580000	3.4770190000	-1.1402160000
C29	2.6895760000	4.4036320000	1.0366540000
H1	1.5580180000	3.5843390000	2.6943120000
H2	0.6891520000	1.9402470000	-1.2156630000
H3	2.3868000000	3.4502800000	-2.2254160000
H9	3.2505630000	5.1053430000	1.6714530000
H10	3.6710440000	5.0358360000	-0.7881560000
H25	-1.0275920000	3.1833010000	2.8110280000

Molecular weight: 322.15 amu

Stoichiometry: C23N2H18

Molecular Point Group: C1

Point Group used: C1

nuclear repulsion energy..... 1952.777623249 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: 3.218E-04

number of canonical orbitals..... 462

end of program onee

start of program hfig  
 initial wavefunction generated automatically from atomic  
 wavefunctions

Irreducible representation No Symm	Total no orbitals 462	No of occupied orbitals		
		Shell_1	Shell_2	...
-----		85		
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	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	88	88	88	90	84
73							
grid # 2	104	112	97	95	98	98	92
118							
grid # 3	214	229	199	184	197	196	170
223							
grid # 4	391	414	331	322	327	347	304
232							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
90							
grid # 2	97	95	118	97	118	97	97
98							
grid # 3	186	182	224	184	222	186	191
195							
grid # 4	332	341	234	329	231	332	331
341							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	89	89
89							
grid # 2	110	100	112	97	96	96	97
97							
grid # 3	210	195	216	187	186	185	186
185							

grid # 4	215	342	223	331	330	331	331
----------	-----	-----	-----	-----	-----	-----	-----

330

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
------	-----	-----	-----	-----	-----	----	----

H6

grid # 1	72	72	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	112	114	118	118	118	90	112
----------	-----	-----	-----	-----	-----	----	-----

102

grid # 3	214	217	224	223	224	167	216
----------	-----	-----	-----	-----	-----	-----	-----

205

grid # 4	221	223	232	231	232	299	217
----------	-----	-----	-----	-----	-----	-----	-----

206

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	89	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	96	96	97	97	115	111
----------	----	----	----	----	----	-----	-----

118

grid # 3	187	184	186	186	186	218	212
----------	-----	-----	-----	-----	-----	-----	-----

224

grid # 4	332	330	330	329	330	224	217
----------	-----	-----	-----	-----	-----	-----	-----

232

number of gridpoints:

atom	H9	H10	H25	total
------	----	-----	-----	-------

grid # 1	73	73	72	3521
----------	----	----	----	------

grid # 2	118	118	115	4498
----------	-----	-----	-----	------

grid # 3	224	224	219	8672
----------	-----	-----	-----	------

grid # 4	232	232	222	12443
----------	-----	-----	-----	-------

end of program grid

start of program rwr

end of program rwr

start of program scf

number of electrons.....	170
number of alpha electrons....	85
number of beta electrons.....	85
number of orbitals, total....	462
number of core orbitals.....	85
number of open shell orbs....	0
number of occupied orbitals..	85
number of virtual orbitals...	377
number of hamiltonians.....	1
number of shells.....	1



SCF type: HF

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change	change	
etot	1	N	N	5	M	-987.21080013367		3.9E-03	9.8E-02
etot	2	Y	Y	6	M	-989.98476104696	2.8E+00	1.7E-03	5.5E-02
etot	3	Y	Y	6	M	-990.27640419982	2.9E-01	7.8E-04	2.7E-02
etot	4	N	Y	2	U	-990.34536478481	6.9E-02	3.8E-04	1.5E-02
etot	5	Y	Y	6	M	-990.35620931742	1.1E-02	1.0E-03	1.0E-02
etot	6	N	Y	2	U	-990.36578188544	9.6E-03	1.2E-04	2.2E-03
etot	7	Y	Y	6	M	-990.36633784606	5.6E-04	4.0E-05	5.6E-04
etot	8	Y	Y	6	M	-990.36641184175	7.4E-05	1.2E-05	2.3E-04
etot	9	N	Y	2	U	-990.36623705176	-1.7E-04	5.8E-06	1.1E-04
etot	10	Y	Y	6	M	-990.36624305181	6.0E-06	4.9E-06	5.8E-05
etot	11	Y	N	6	M	-990.36624587679	2.8E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1952.77762324898	
(E)	Total one-electron terms.....	-5223.87627037117	
(I)	Total two-electron terms.....	2280.73240124540	
(L)	Electronic energy.....	-2943.14386912577	(E+I)
(N)	Total energy.....	-990.36624587679	(A+L)

SCFE: SCF energy: HF      -990.36624587679 hartrees      iterations:  
11

HOMO energy:      -0.26238  
LUMO energy:      0.08458

Orbital energies:

-15.61225	-15.57394	-11.30699	-11.29988	-11.28257	-11.26176
-11.25976	-11.25489	-11.25065	-11.24883	-11.24706	-11.24570
-11.24527	-11.24438	-11.24359	-11.24267	-11.24138	-11.24124
-11.23937	-11.23733	-11.22956	-11.22835	-11.22767	-11.22333
-11.22233	-1.30891	-1.23521	-1.15989	-1.15811	-1.13132
-1.07044	-1.06879	-1.03483	-1.01840	-1.01489	-1.01367
-0.96165	-0.95090	-0.92391	-0.85859	-0.83575	-0.83045
-0.82627	-0.79990	-0.78600	-0.76574	-0.72486	-0.71505
-0.69233	-0.69090	-0.66232	-0.65281	-0.64039	-0.63511
-0.63125	-0.61793	-0.61598	-0.61045	-0.59401	-0.58832
-0.58652	-0.58354	-0.57683	-0.55347	-0.54722	-0.54082
-0.53565	-0.51410	-0.50599	-0.49981	-0.49872	-0.49409
-0.49103	-0.48832	-0.48378	-0.47850	-0.42632	-0.40843
-0.36790	-0.34360	-0.34155	-0.33783	-0.32751	-0.27573
-0.26238	0.08458	0.11895	0.13358	0.13414	0.14570
0.17403	0.20148	0.21421	0.22686	0.23450	

end of program scf

start of program derla  
end of program derla

start of program rwr  
recomputing Rwr matrix    2        grid:    4  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-3.240872E-02	9.749688E-03	3.179943E-02
2	N2	3.994841E-02	1.589784E-02	-2.744144E-02
3	C4	-4.648588E-03	1.109702E-02	6.253104E-03
4	C5	-3.592959E-02	-8.241299E-03	3.439027E-02
5	C6	2.414258E-03	2.916011E-02	4.891493E-03
6	C7	2.172547E-02	-2.498377E-02	-2.655680E-02
7	C13	1.776470E-02	-2.489095E-02	2.423915E-02
8	H4	8.099431E-03	1.571016E-02	-2.748483E-03
9	C8	-8.989727E-03	2.813047E-03	8.737148E-03
10	C11	2.073446E-02	-1.403474E-02	-2.135011E-02
11	H7	5.617432E-03	-1.253712E-02	-8.781297E-03
12	C9	-1.066947E-02	1.935235E-03	1.014118E-02
13	H8	1.338669E-02	4.465009E-03	-1.056642E-02
14	C10	7.534698E-03	-9.961889E-03	-9.389467E-03
15	C12	-4.116184E-02	-1.291056E-02	3.163420E-02
16	C2	1.304881E-02	8.436034E-03	-7.725578E-03
17	H13	-2.288695E-02	-5.875229E-03	-2.856836E-03
18	C14	-3.001289E-05	9.115626E-04	-2.375293E-02
19	H15	2.454104E-03	2.667852E-02	-3.093814E-03
20	C15	-8.755934E-04	1.284549E-03	-8.246274E-03
21	C16	1.904926E-03	8.743392E-04	-2.548369E-04
22	C17	-5.241454E-03	-1.814770E-03	2.230640E-03
23	C18	-7.258278E-03	-2.346623E-03	-2.041341E-04
24	C19	3.649640E-03	3.130199E-03	-7.320720E-03
25	H16	-1.529594E-02	-5.126618E-03	-3.849080E-03
26	H17	1.141142E-02	6.616599E-03	-1.234182E-02
27	H18	1.586235E-02	4.779575E-03	4.278800E-03
28	H19	-1.052798E-02	-5.951830E-03	1.156894E-02
29	H20	5.229882E-03	-1.242672E-03	1.606278E-02
30	C1	2.113894E-02	9.772674E-03	-1.632786E-02
31	H5	-2.245682E-02	-6.894493E-04	-1.106135E-02
32	H6	4.269849E-03	-1.216673E-02	2.603804E-02
33	C3	5.645640E-03	4.899727E-03	-3.657363E-03
34	C26	4.904907E-04	2.576969E-03	4.717966E-03

35	C27	-4.000485E-04	-2.665549E-03	-5.344084E-03
36	C28	1.194079E-03	-8.729806E-04	-7.925486E-03
37	C29	2.773262E-03	5.466727E-03	5.063842E-03
38	H1	3.964567E-03	-1.650721E-03	-1.828743E-02
39	H2	8.982905E-03	1.280343E-02	1.060548E-02
40	H3	-2.910655E-03	4.951888E-04	1.678907E-02
41	H9	-8.627735E-03	-1.102210E-02	-9.843115E-03
42	H10	-1.152274E-02	-1.049380E-02	6.921504E-03
43	H25	2.708121E-03	-9.050340E-03	-6.693826E-03
-----				
	total	1.123978E-04	1.024489E-03	7.424633E-04

end of program derlb

start of program geopt 1

geometry optimization step 1

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000165

Cos(theta): 0.8700386

Final level shift: -9.0459602E-02

gradient maximum: 5.6400E-02 . ( 4.5000E-04 )

gradient rms: 1.1269E-02 . ( 3.0000E-04 )

step size: 0.30001 trust radius: 0.30000

displacement maximum: 7.9070E-02 . ( 1.8000E-03 )

displacement rms: 2.3571E-02 . ( 1.2000E-03 )

predicted energy change: -2.2790E-02 geom step: 3.0001E-

01 full step: 3.0001E-01

molecular structure not yet converged...

center of mass moved by:

x: 1.7900E-03 y: 7.9249E-03 z: 5.2280E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.1851238607	0.4641584805	1.1496398783
N2	-0.9624306185	-2.2803275995	1.1391335864
C4	-1.1923369589	-0.0180925749	1.9481977188
C5	0.0003838455	-1.8866472314	0.4304247849
C6	-1.6131242204	-1.3444054000	1.9677332987
C7	-1.7143322129	1.0107834641	2.7508560527
C13	0.6888484121	-2.8743700008	-0.4705903976
H4	-3.0326107871	-2.6499595048	2.8909113274
C8	-2.7758076385	0.6768625265	3.6172856202

C11	-0.9256685288	2.1808482739	2.4168546928
H7	-3.2270829119	1.4262828740	4.2504106118
C9	-3.2256779072	-0.6251283660	3.6377251029
H8	-4.0393570567	-0.8900121801	4.2984882981
C10	-2.6561623240	-1.6393208618	2.8310281808
C12	-0.0161416855	1.8156812458	1.4563175807
C2	1.0081011308	2.6662618384	0.8151804166
H13	1.7673251388	-2.7356321765	-0.3960304160
C14	0.2466641767	-2.7462605278	-1.9265734159
H15	0.4459377797	-3.8754027525	-0.1219375680
C15	-0.5453795077	-2.5531842005	-4.6103164906
C16	1.1228101928	-2.2821169158	-2.9004344929
C17	-1.0389296276	-3.1210357258	-2.3122887225
C18	-1.4308521122	-3.0220378034	-3.6483671644
C19	0.7311661555	-2.1855070811	-4.2360240634
H16	2.1179862862	-2.0041675136	-2.6156208078
H17	-1.7271848709	-3.4681454408	-1.5658608400
H18	-2.4200252396	-3.2868875229	-3.9394618092
H19	1.4207969829	-1.8273231853	-4.9765738859
H20	-0.8415814914	-2.4643443665	-5.6434658446
C1	0.5813167973	-0.4636626778	0.3433044617
H5	1.6400268303	-0.4816687726	0.6523424559
H6	0.5606286448	-0.1702832088	-0.7202931642
C3	2.9112386307	4.3243859975	-0.3688081175
C26	1.7641520157	3.5436729388	1.5963361301
C27	1.2174113891	2.6356426600	-0.5675864813
C28	2.1639530001	3.4567854144	-1.1533354185
C29	2.7066639823	4.3656913408	1.0056564678
H1	1.6123726912	3.5626682239	2.6583667114
H2	0.6171678014	1.9866834111	-1.1807727574
H3	2.3092217370	3.4311451005	-2.2201183904
H9	3.2922168597	5.0359612586	1.6129911517
H10	3.6489292197	4.9615184331	-0.8293143894
H25	-1.0462406649	3.1705625677	2.8156287502

nuclear repulsion energy..... 1960.025589350 hartrees

/ end of geometry optimization iteration 1 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.977E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	87	88	88	92	84
73							
grid # 2	103	112	95	95	96	101	92
118							
grid # 3	214	227	197	186	193	197	164
223							
grid # 4	393	413	326	321	328	351	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
93							
grid # 2	97	94	118	97	118	97	96
100							
grid # 3	184	184	223	184	222	185	195
197							
grid # 4	328	336	226	331	224	332	319
344							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	89	89
89							
grid # 2	109	100	109	97	96	96	97
97							
grid # 3	211	195	214	184	184	184	186
182							
grid # 4	216	340	216	328	328	330	331
328							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	72
69							
grid # 2	112	115	118	118	118	90	112
102							
grid # 3	213	216	223	222	223	166	217
205							
grid # 4	214	215	224	222	223	294	219
207							

number of gridpoints:

	atom	C3	C26	C27	C28	C29	H1	H2
H3								
73	grid # 1	89	87	87	89	89	72	70
118	grid # 2	97	97	96	97	97	115	111
222	grid # 3	185	181	183	184	184	218	213
224	grid # 4	329	328	330	328	328	217	210

number of gridpoints:

	atom	H9	H10	H25	total
grid # 1		73	73	72	3523
grid # 2		118	118	115	4494
grid # 3		223	223	219	8635
grid # 4		224	224	222	12295

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.37561875819		2.2E-04	5.2E-03
etot	2	Y	Y	6	M	-990.38629314976	1.1E-02	8.4E-05	2.1E-03
etot	3	N	Y	2	U	-990.38722199985	9.3E-04	3.1E-05	7.2E-04
etot	4	Y	Y	6	M	-990.38736835388	1.5E-04	1.3E-05	3.4E-04
etot	5	Y	Y	6	M	-990.38740323781	3.5E-05	5.6E-06	1.3E-04
etot	6	Y	Y	6	M	-990.38740916528	5.9E-06	2.4E-06	4.7E-05
etot	7	Y	N	6	M	-990.38741265890	3.5E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1960.02558935013	
(E)	Total one-electron terms.....	-5238.29315543660	
(I)	Total two-electron terms.....	2287.88015342757	
(L)	Electronic energy.....	-2950.41300200903	(E+I)
(N)	Total energy.....	-990.38741265890	(A+L)

SCFE: SCF energy: HF -990.38741265890 hartrees iterations:

7

HOMO energy: -0.26625  
LUMO energy: 0.09232

Orbital energies:

-15.60805	-15.56700	-11.29787	-11.29337	-11.27638	-11.25511
-11.25341	-11.25179	-11.24692	-11.24146	-11.24113	-11.24000
-11.23941	-11.23867	-11.23797	-11.23592	-11.23504	-11.23469
-11.23278	-11.23229	-11.22657	-11.22384	-11.22377	-11.21820
-11.21692	-1.31817	-1.24994	-1.16238	-1.15889	-1.13461
-1.07262	-1.06754	-1.03658	-1.02296	-1.01802	-1.01474
-0.96749	-0.95529	-0.93114	-0.85928	-0.83758	-0.83378
-0.83067	-0.80421	-0.79354	-0.76882	-0.73077	-0.71744
-0.69958	-0.69803	-0.66500	-0.65657	-0.64316	-0.63792
-0.63536	-0.62308	-0.61992	-0.61392	-0.59697	-0.59327
-0.58930	-0.58645	-0.57884	-0.55677	-0.55072	-0.54533
-0.54289	-0.51775	-0.50819	-0.50301	-0.50024	-0.49594
-0.49263	-0.49143	-0.48732	-0.48017	-0.42932	-0.40604
-0.36912	-0.34308	-0.34234	-0.33503	-0.33025	-0.28019
-0.26625	0.09232	0.12603	0.13625	0.13684	0.14868
0.17722	0.20851	0.22157	0.23301	0.24218	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-9.539155E-03	2.745592E-03	1.044822E-02
2	N2	-2.673465E-03	1.727028E-03	2.906341E-03
3	C4	-1.885556E-04	1.245403E-02	3.193744E-03
4	C5	2.271285E-03	6.211561E-03	1.516907E-03
5	C6	-6.464198E-03	7.479387E-03	7.554108E-03
6	C7	8.793345E-03	-1.029557E-02	-9.843759E-03
7	C13	-5.471678E-04	-7.069051E-03	-5.718790E-03
8	H4	1.852086E-03	3.212933E-03	-7.082379E-04
9	C8	4.338852E-03	4.033060E-03	-3.262937E-03
10	C11	1.606909E-03	-1.006096E-02	-6.249112E-03
11	H7	9.730113E-04	-2.564706E-03	-1.338833E-03
12	C9	-5.458253E-04	-4.327700E-03	-5.240229E-04
13	H8	2.968983E-03	5.464179E-04	-2.555816E-03
14	C10	4.804096E-03	2.217867E-04	-3.885245E-03

15	C12	-7.171547E-03	-3.974109E-03	7.707933E-03
16	C2	9.332330E-04	2.740879E-04	-3.181994E-03
17	H13	-2.015010E-03	-1.526317E-03	-1.690651E-03
18	C14	3.524810E-03	-3.916218E-04	-2.663166E-03
19	H15	1.889224E-03	3.787146E-03	1.319866E-03
20	C15	-1.027612E-03	6.505881E-05	3.781739E-04
21	C16	-4.116869E-03	-8.483180E-04	-5.317073E-03
22	C17	-1.277121E-04	3.725580E-03	-1.022516E-02
23	C18	8.848389E-03	3.067855E-03	9.831513E-03
24	C19	3.253650E-03	-3.767333E-04	8.365422E-03
25	H16	4.090188E-03	1.430527E-03	-2.015014E-04
26	H17	-2.307131E-03	-1.447538E-03	4.755238E-04
27	H18	-8.359663E-03	-3.799457E-03	-4.288966E-04
28	H19	2.299917E-03	9.846778E-04	-2.783170E-04
29	H20	-1.387235E-03	-1.403497E-03	2.321291E-03
30	C1	3.683293E-03	3.676776E-03	-8.195002E-03
31	H5	-9.851720E-03	-8.517076E-04	-2.436073E-03
32	H6	1.473065E-03	-4.295533E-03	1.252041E-02
33	C3	3.914041E-04	-3.266543E-04	4.963776E-04
34	C26	-2.384326E-03	-3.429782E-03	-4.918934E-03
35	C27	-1.975575E-03	-5.180976E-04	5.429357E-03
36	C28	1.047866E-03	1.965373E-03	9.943780E-04
37	C29	2.585439E-03	2.168460E-03	-3.629454E-03
38	H1	4.052696E-04	7.061260E-05	1.388971E-03
39	H2	5.731526E-04	1.449645E-03	2.603645E-05
40	H3	3.735787E-05	-1.572279E-04	8.376755E-04
41	H9	-9.939832E-04	-7.438282E-04	-2.855378E-04
42	H10	-1.057111E-03	-6.022944E-04	1.457865E-03
43	H25	1.116333E-03	-1.534056E-03	-1.866734E-03
-----				
	total	1.027296E-03	7.528330E-04	-2.351347E-04

end of program der1b

start of program geopt 2

geometry optimization step 2

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001262

Cos(theta): 0.4522028

Final level shift: -7.1431608E-03

energy change: -2.1167E-02 . ( 5.0000E-05 )

gradient maximum: 2.0310E-02 . ( 4.5000E-04 )

gradient rms: 3.9611E-03 . ( 3.0000E-04 )

step size: 0.29998 trust radius: 0.30000



displacement maximum: 1.2227E-01 . ( 1.8000E-03 )  
 displacement rms: 2.3569E-02 . ( 1.2000E-03 )  
 predicted energy change: -3.7426E-03 geom step: 2.9998E-  
 01 full step: 2.9998E-01  
 molecular structure not yet converged...

center of mass moved by:

x: -9.2535E-03 y: 3.1123E-03 z: 1.4212E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2322091003	0.4425447477	1.1722376588
N2	-1.0170271355	-2.2784648229	1.1730995628
C4	-1.2206159278	-0.0226657246	1.9837450839
C5	-0.0448348209	-1.9052512670	0.4751983779
C6	-1.6507777180	-1.3371163143	2.0094539253
C7	-1.7024716670	0.9919018866	2.7899381630
C13	0.6283020713	-2.9170533017	-0.4248611566
H4	-3.0346295842	-2.6472027368	2.9359624232
C8	-2.7497248744	0.6679486212	3.6759761067
C11	-0.9219400908	2.1551243638	2.4291375123
H7	-3.1822925194	1.4081076944	4.3208527754
C9	-3.2122659889	-0.6338983252	3.7021230748
H8	-4.0092368660	-0.8922566392	4.3712351952
C10	-2.6664125428	-1.6434906978	2.8798451206
C12	-0.0462186113	1.7852092098	1.4609796706
C2	0.9639603762	2.6172556086	0.7603660644
H13	1.7049014864	-2.8504962231	-0.3042157835
C14	0.2872845063	-2.7186247711	-1.9011082558
H15	0.3111604572	-3.8957135626	-0.0910075502
C15	-0.3637160763	-2.3879002288	-4.5957973831
C16	1.2521389896	-2.2939910017	-2.8167452985
C17	-1.0099224983	-2.9730715129	-2.3497803317
C18	-1.3345315137	-2.8115555909	-3.6881685682
C19	0.9281516443	-2.1274223633	-4.1580106912
H16	2.2689730521	-2.0919467686	-2.4900654971
H17	-1.7651731246	-3.3056021719	-1.6519350479
H18	-2.3449269541	-3.0307603123	-4.0214737620
H19	1.6928080246	-1.7993395561	-4.8496324883
H20	-0.6146895035	-2.2677049661	-5.6318950361
C1	0.5593460744	-0.4968540721	0.4025037161
H5	1.5835558214	-0.5417582018	0.7564692615
H6	0.6038790034	-0.2150061772	-0.6400473898
C3	2.8215489000	4.2490688071	-0.5283409458
C26	1.8492457635	3.4064361869	1.4997536269
C27	1.0238745658	2.6583201916	-0.6349113427
C28	1.9515451393	3.4616543589	-1.2728168602
C29	2.7672368925	4.2206654051	0.8601900607
H1	1.8310545892	3.3653506796	2.5769048131
H2	0.3330469792	2.0787631427	-1.2253750449
H3	1.9815361995	3.4802193197	-2.3500591580

H9	3.4413282681	4.8236548923	1.4492434236
H10	3.5316247441	4.8745490259	-1.0248311658
H25	-1.0230567326	3.1472274108	2.8145615026

nuclear repulsion energy..... 1967.210994655 hartrees

/ end of geometry optimization iteration 2 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.843E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	97	102	84	88	87	89	84
73							
grid # 2	104	112	96	95	97	97	92
118							
grid # 3	214	227	196	186	189	198	163
223							
grid # 4	391	413	320	320	324	348	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	186	222	184	194
196							
grid # 4	330	331	226	331	223	327	316
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							

grid # 1	69	93	69	89	88	88	89
grid # 2	109	101	109	97	96	96	97
grid # 3	211	195	214	184	185	184	185
grid # 4	214	342	212	329	329	328	328

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
grid # 1	72	73	73	73	73	82	70
grid # 2	113	115	118	118	118	88	109
grid # 3	214	215	223	222	224	165	217
grid # 4	221	215	224	222	224	290	217

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
grid # 1	89	89	88	89	89	72	71
grid # 2	97	95	96	97	97	115	114
grid # 3	185	182	185	184	184	218	214
grid # 4	328	328	330	328	329	218	210

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3517
grid # 2	118	118	115	4490
grid # 3	223	223	220	8640
grid # 4	223	224	224	12258

end of program grid

start of program rwr  
recomputing RwR matrix 1 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	-990.33510685770		3.7E-04	3.1E-02
etot	2	Y	Y	6	M	-990.38314472816	4.8E-02	1.8E-04	1.2E-02
etot	3	N	Y	2	U	-990.38935537066	6.2E-03	5.3E-05	3.1E-03
etot	4	Y	Y	6	M	-990.38969679674	3.4E-04	2.3E-05	1.1E-03
etot	5	Y	Y	6	M	-990.38977611385	7.9E-05	7.6E-06	2.8E-04
etot	6	N	Y	2	U	-990.38979109239	1.5E-05	3.0E-06	6.9E-05
etot	7	Y	N	6	M	-990.38979365506	2.6E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1967.21099465467	
(E)	Total one-electron terms.....	-5252.71557057016	
(I)	Total two-electron terms.....	2295.11478226043	
(L)	Electronic energy.....	-2957.60078830974	(E+I)
(N)	Total energy.....	-990.38979365506	(A+L)

SCFE: SCF energy: HF -990.38979365506 hartrees iterations:

7

HOMO energy: -0.26875  
LUMO energy: 0.09679

Orbital energies:

-15.60440	-15.56408	-11.29484	-11.28605	-11.27171	-11.25310
-11.25060	-11.24821	-11.24599	-11.24090	-11.23981	-11.23932
-11.23928	-11.23863	-11.23847	-11.23780	-11.23743	-11.23721
-11.23472	-11.23260	-11.22506	-11.21958	-11.21917	-11.21594
-11.21230	-1.32371	-1.25138	-1.16194	-1.15811	-1.13746
-1.07380	-1.06529	-1.03784	-1.02261	-1.01706	-1.01675
-0.97106	-0.95358	-0.93345	-0.86016	-0.83584	-0.83204
-0.82722	-0.80690	-0.79592	-0.76979	-0.73260	-0.71689
-0.70107	-0.69646	-0.66553	-0.65782	-0.64254	-0.63657
-0.63323	-0.62328	-0.62039	-0.61546	-0.59597	-0.59273
-0.59071	-0.58733	-0.57653	-0.55793	-0.55254	-0.54806
-0.54230	-0.51743	-0.50677	-0.50276	-0.50055	-0.49573
-0.49322	-0.49115	-0.48789	-0.48019	-0.42914	-0.40421
-0.36715	-0.34259	-0.34204	-0.33775	-0.32820	-0.28241
-0.26875	0.09679	0.12767	0.13691	0.13716	0.14724
0.17920	0.20956	0.22641	0.23420	0.24136	

end of program scf

start of program derla  
end of program derla

start of program rwr

```
recomputing Rwr matrix 1      grid: 4
end of program rwr
```

```
start of program der1b
```

```
forces (hartrees/bohr) : total
```

atom	label	x	y	z
1	N1	1.305964E-03	-1.677270E-03	-2.594790E-03
2	N2	-7.405171E-03	-1.586511E-03	6.320733E-03
3	C4	3.028731E-03	1.790473E-03	-3.798228E-04
4	C5	7.226851E-03	4.524737E-03	-7.098855E-03
5	C6	2.476199E-04	-3.135427E-03	2.297075E-04
6	C7	-2.330886E-03	2.478329E-03	3.273788E-04
7	C13	2.227097E-04	1.311746E-03	-4.798910E-03
8	H4	-1.002454E-03	-3.214195E-03	-8.533394E-05
9	C8	2.159221E-03	-4.853058E-03	-3.527892E-03
10	C11	-3.302127E-03	-1.233147E-03	3.282272E-03
11	H7	-7.362198E-04	1.749372E-03	1.319340E-03
12	C9	3.320533E-03	4.276770E-03	-1.934309E-03
13	H8	-1.912353E-03	-7.144657E-04	1.822387E-03
14	C10	8.315593E-04	4.548646E-03	7.271826E-04
15	C12	4.548962E-03	-1.450949E-03	-2.371630E-03
16	C2	-9.938152E-04	7.535157E-04	1.267906E-03
17	H13	1.386542E-03	-4.258552E-04	9.927676E-04
18	C14	2.299989E-03	-7.682804E-05	1.238775E-03
19	H15	1.984307E-04	-8.884950E-04	-8.118002E-04
20	C15	-6.451323E-04	-1.027048E-03	4.774511E-03
21	C16	-2.632256E-04	-3.149773E-04	3.356515E-03
22	C17	1.008954E-03	6.183636E-05	-1.888416E-03
23	C18	1.484312E-04	-5.973317E-04	-2.098115E-03
24	C19	-1.156244E-03	-3.591191E-04	4.042049E-04
25	H16	-7.120642E-03	-2.020923E-03	-6.701640E-04
26	H17	3.236541E-03	1.487269E-03	-1.213183E-03
27	H18	7.301887E-03	2.526935E-03	1.127166E-03
28	H19	-4.266701E-03	-1.422013E-03	1.600621E-03
29	H20	-5.797366E-04	3.861398E-04	-2.246165E-03
30	C1	-5.155529E-03	-8.921110E-04	1.159786E-03
31	H5	2.282436E-03	2.852896E-04	2.405521E-03
32	H6	-2.782347E-04	1.257850E-03	-1.502622E-03
33	C3	-3.641709E-03	-3.629131E-03	3.069671E-03
34	C26	-2.578335E-03	-3.574081E-03	-3.583493E-04
35	C27	-8.629869E-04	-1.384270E-03	3.235411E-03
36	C28	1.635804E-03	2.327281E-03	9.648920E-04
37	C29	8.904502E-04	7.644047E-04	-3.194343E-03
38	H1	-1.706450E-03	-2.318215E-04	-2.241600E-03
39	H2	4.690082E-04	6.810360E-04	2.172640E-03
40	H3	8.078606E-04	8.518771E-04	1.530140E-03
41	H9	-1.100102E-03	-1.113211E-03	-2.495881E-03
42	H10	3.825774E-03	3.254866E-03	-2.412596E-03

43	H25	-2.808875E-04	1.593320E-03	4.916000E-04
-----				
	total	1.065317E-03	1.089457E-03	-1.036505E-04

end of program derlb

start of program geopt 3

geometry optimization step 3

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000236

Cos(theta): 0.4953472

Final level shift: -1.6630388E-02

energy change: -2.3810E-03 . ( 5.0000E-05 )

gradient maximum: 9.9076E-03 . ( 4.5000E-04 )

gradient rms: 2.3236E-03 . ( 3.0000E-04 )

step size: 0.29975 trust radius: 0.30000

displacement maximum: 1.0837E-01 . ( 1.8000E-03 )

displacement rms: 2.3551E-02 . ( 1.2000E-03 )

predicted energy change: -2.9446E-03 geom step: 2.9975E-

01 full step: 2.9975E-01

molecular structure not yet converged...

center of mass moved by:

x: 4.5379E-03 y: 1.6225E-03 z: -1.0573E-02

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2064093151	0.4564334872	1.1449569640
N2	-0.9777143120	-2.2675882391	1.1401282031
C4	-1.2067896365	-0.0074822023	1.9347114372
C5	0.0100178696	-1.8812418506	0.4407932188
C6	-1.6301115836	-1.3290633316	1.9647297688
C7	-1.7180530931	1.0023503931	2.7134818099
C13	0.7013842690	-2.8816737324	-0.4740592873
H4	-3.0216327063	-2.6539904306	2.8557401227
C8	-2.7796853502	0.6766421222	3.5699349035
C11	-0.9469746435	2.1651389329	2.3678165600
H7	-3.2396438255	1.4178307697	4.2013122414
C9	-3.2317902692	-0.6316840549	3.6015379272
H8	-4.0475645815	-0.8929676898	4.2526147254
C10	-2.6592479127	-1.6425581119	2.8070396413

C12	-0.0282154727	1.7951337785	1.4350689770
C2	0.9934644979	2.6280168532	0.7795619441
H13	1.7730430366	-2.7575478083	-0.4156955215
C14	0.2865859920	-2.7249268767	-1.9051731340
H15	0.4713121897	-3.8629015133	-0.0943843922
C15	-0.5615655542	-2.4619627032	-4.5190042806
C16	1.1125815133	-2.1862381413	-2.8583626252
C17	-0.9661916103	-3.1291782413	-2.2777042664
C18	-1.3890096252	-3.0026868085	-3.5700862667
C19	0.6893320833	-2.0524259860	-4.1584209800
H16	2.0979129012	-1.8591107039	-2.5945051992
H17	-1.6160289056	-3.5619217481	-1.5421987308
H18	-2.3733434532	-3.3581172536	-3.8357831773
H19	1.3434543159	-1.6264018218	-4.8889259482
H20	-0.9021702747	-2.3804723563	-5.5318037396
C1	0.5974414175	-0.4754948750	0.3889408228
H5	1.6054220101	-0.5235796038	0.7857568676
H6	0.6751609178	-0.1866596432	-0.6452941877
C3	2.9244707837	4.2594570176	-0.3923566804
C26	1.7907979932	3.4485799055	1.5329596121
C27	1.1713262529	2.6405355796	-0.5729922605
C28	2.1366910125	3.4439199169	-1.1538018568
C29	2.7452329284	4.2656384654	0.9532276351
H1	1.6745334301	3.4364257238	2.5857229416
H2	0.5529801450	2.0327292614	-1.1904461656
H3	2.2687279040	3.4308993892	-2.2062196320
H9	3.3448720185	4.8980738147	1.5650329855
H10	3.6696029435	4.8876836769	-0.8403675527
H25	-1.0676334116	3.1643232144	2.7358050805

nuclear repulsion energy..... 1978.365603056 hartrees

-----  
 / end of geometry optimization iteration 3 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.790E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	86	88	90	88	84
73							
grid # 2	104	112	95	95	99	96	92
118							
grid # 3	214	227	194	188	192	198	164
224							
grid # 4	389	414	321	321	322	344	298
223							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
88							
grid # 2	97	94	118	97	118	97	94
99							
grid # 3	185	184	223	185	222	184	195
191							
grid # 4	331	331	226	330	223	326	320
339							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	87	86	87	87
87							
grid # 2	109	101	109	97	96	96	97
97							
grid # 3	211	191	213	182	182	181	182
182							
grid # 4	209	339	212	325	327	327	328
327							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	70
69							
grid # 2	113	114	118	118	118	87	108
103							
grid # 3	213	215	222	221	223	163	217
204							
grid # 4	213	214	223	222	224	290	217
202							

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	87	86	87	87	72	70
73							



grid # 2	97	96	96	97	97	115	113
118							
grid # 3	182	181	182	182	183	217	213
222							
grid # 4	328	326	327	327	324	216	210
222							

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3497
grid # 2	118	118	115	4486
grid # 3	222	222	219	8597
grid # 4	223	223	222	12205

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.32090183004		4.0E-04	2.7E-02
etot	2	Y	Y	6	M	-990.37602444074	5.5E-02	1.9E-04	1.1E-02
etot	3	N	Y	2	U	-990.38279174353	6.8E-03	5.6E-05	2.9E-03
etot	4	Y	Y	6	M	-990.38330673990	5.1E-04	2.8E-05	1.2E-03
etot	5	Y	Y	6	M	-990.38339751676	9.1E-05	7.9E-06	2.7E-04
etot	6	N	Y	2	U	-990.38336351948	-3.4E-05	3.5E-06	8.1E-05
etot	7	Y	N	6	M	-990.38336784090	4.3E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1978.36560305571	
(E)	Total one-electron terms.....	-5274.81755689824	
(I)	Total two-electron terms.....	2306.06858600163	
(L)	Electronic energy.....	-2968.74897089661	(E+I)
(N)	Total energy.....	-990.38336784090	(A+L)

SCFE: SCF energy: HF -990.38336784090 hartrees iterations:  
7

HOMO energy: -0.26814  
LUMO energy: 0.09639

Orbital energies:

-15.60547	-15.56550	-11.29770	-11.28619	-11.27078	-11.25022
-11.24528	-11.24450	-11.23825	-11.23745	-11.23449	-11.23301
-11.23221	-11.23109	-11.23069	-11.23034	-11.22948	-11.22838
-11.22673	-11.22459	-11.22253	-11.21876	-11.21686	-11.21593
-11.21192	-1.32742	-1.24676	-1.17463	-1.17229	-1.14078
-1.07809	-1.07260	-1.04756	-1.02329	-1.02291	-1.02144
-0.97578	-0.95637	-0.93529	-0.86214	-0.84435	-0.83597
-0.83375	-0.80916	-0.79677	-0.77365	-0.73422	-0.72183
-0.70571	-0.70299	-0.66886	-0.65951	-0.64726	-0.64126
-0.63446	-0.62424	-0.62327	-0.61823	-0.59835	-0.59393
-0.59044	-0.58890	-0.58373	-0.56063	-0.55582	-0.54996
-0.54261	-0.52147	-0.51054	-0.50427	-0.50252	-0.49989
-0.49515	-0.49181	-0.48895	-0.48236	-0.42870	-0.40579
-0.37068	-0.34887	-0.34027	-0.33992	-0.33265	-0.28268
-0.26814	0.09639	0.13129	0.13834	0.14272	0.15301
0.18158	0.21027	0.22587	0.23576	0.24199	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	2.088108E-03	-1.816608E-03	-3.641703E-03
2	N2	1.359145E-02	2.603072E-03	-9.392358E-03
3	C4	4.660404E-04	-1.020443E-02	-2.510234E-03
4	C5	-1.216198E-02	-6.585574E-03	6.161446E-03
5	C6	7.087680E-03	-4.398158E-04	-6.447246E-03
6	C7	-3.899426E-03	5.933573E-03	2.324081E-03
7	C13	3.821605E-03	5.890252E-03	1.357044E-02
8	H4	2.973135E-04	4.132462E-04	7.230307E-05
9	C8	-6.397915E-03	-7.377681E-03	4.298384E-03
10	C11	3.207322E-03	5.420828E-03	1.334689E-03
11	H7	6.085201E-04	2.998135E-05	-7.440425E-04
12	C9	-3.822426E-04	8.286041E-03	2.243006E-03
13	H8	2.340008E-04	7.691603E-04	4.906764E-04
14	C10	-1.938760E-03	-6.468270E-04	1.244062E-03
15	C12	-6.102382E-03	-1.064691E-03	1.815286E-03
16	C2	-8.753000E-03	-6.468478E-03	1.178688E-02
17	H13	5.162556E-03	1.641355E-03	3.634586E-03
18	C14	3.407200E-03	-1.591991E-03	8.898751E-03

19	H15	-2.336800E-03	-4.255029E-03	-1.094404E-03
20	C15	-8.884359E-03	-7.898080E-04	-1.509099E-02
21	C16	1.333100E-02	6.137570E-03	1.627549E-03
22	C17	-1.655284E-02	-9.413400E-03	8.281097E-03
23	C18	-2.099264E-02	-9.634396E-03	-4.550000E-03
24	C19	1.119810E-02	6.856261E-03	-8.067226E-03
25	H16	4.778835E-03	6.395915E-04	1.815445E-03
26	H17	-2.269290E-03	-3.734078E-04	2.039251E-03
27	H18	1.898389E-03	2.441004E-03	-7.736249E-04
28	H19	4.019581E-03	1.995855E-03	-3.556696E-03
29	H20	5.225823E-04	1.660109E-03	-3.684042E-03
30	C1	-1.526528E-04	-1.293907E-03	5.029993E-03
31	H5	3.804775E-03	3.806220E-04	3.734436E-04
32	H6	1.802152E-04	1.858511E-03	-4.200778E-03
33	C3	1.062426E-02	8.644818E-03	-1.207225E-02
34	C26	1.147070E-02	1.162699E-02	1.033083E-02
35	C27	4.957450E-03	-1.858617E-04	-2.536308E-02
36	C28	-9.660113E-03	-1.041083E-02	-8.949314E-03
37	C29	-5.181304E-03	-1.111879E-03	2.398876E-02
38	H1	-3.259171E-04	1.476531E-03	1.312592E-02
39	H2	-4.697105E-03	-3.791650E-03	-6.595315E-03
40	H3	-5.870500E-04	-1.164633E-03	-1.251753E-02
41	H9	4.371697E-03	4.237461E-03	6.763454E-03
42	H10	1.379739E-03	7.800523E-04	-2.571094E-03
43	H25	-3.342425E-04	-4.287707E-04	6.210274E-04
-----				
	total	8.991054E-04	6.732157E-04	4.943495E-05

end of program derlb

start of program geopt 4

geometry optimization step 4

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 3 \*\*

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3000460

Cos(theta): 0.3075896

Final level shift: -4.9937562E-03

energy change: 6.4258E-03 . ( 5.0000E-05 )

gradient maximum: 9.9076E-03 . ( 4.5000E-04 )

gradient rms: 2.3236E-03 . ( 3.0000E-04 )

step size: 0.29978 trust radius: 0.30000

displacement maximum: 1.5805E-01 . ( 1.8000E-03 )

displacement rms: 2.3553E-02 . ( 1.2000E-03 )  
 predicted energy change: -1.5876E-03 geom step: 2.9978E-  
 01 full step: 2.9978E-01  
 molecular structure not yet converged...

center of mass moved by:  
 x: -2.4980E-16 y: -3.4694E-17 z: -6.1062E-16

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2605037549	0.4125439612	1.1900034197
N2	-1.0201882848	-2.3117451892	1.2286465763
C4	-1.2291547382	-0.0501813353	2.0213210471
C5	-0.0584840655	-1.9323738777	0.5045877913
C6	-1.6433405541	-1.3707651498	2.0724302477
C7	-1.7196322432	0.9707097685	2.8115399710
C13	0.6123641543	-2.9395135162	-0.4045486213
H4	-3.0004875650	-2.6843033639	3.0337672096
C8	-2.7502677659	0.6466074665	3.7128944205
C11	-0.9641692572	2.1368330189	2.4248916539
H7	-3.1870956384	1.3938929758	4.3523390576
C9	-3.1923609494	-0.6577264470	3.7717764284
H8	-3.9791920871	-0.9171763497	4.4577173169
C10	-2.6430824576	-1.6735110866	2.9607130298
C12	-0.0894151548	1.7589272383	1.4540514090
C2	0.8975931598	2.5804167511	0.7178403216
H13	1.6900885460	-2.9175445528	-0.2351375024
C14	0.3269913213	-2.6769735270	-1.8741990189
H15	0.2546697460	-3.9228910664	-0.1143387386
C15	-0.2180137009	-2.2191864228	-4.5767173828
C16	1.3496559462	-2.4227648804	-2.7664884238
C17	-0.9764471114	-2.6992027704	-2.3557447632
C18	-1.2462393835	-2.4742543646	-3.6931624843
C19	1.0776231861	-2.1937356607	-4.1071135875
H16	2.3658535888	-2.4078532060	-2.4199820995
H17	-1.7766859001	-2.8933381124	-1.6738564557
H18	-2.2487902734	-2.4928964715	-4.0444386495
H19	1.8875121812	-1.9993966839	-4.7814773829
H20	-0.4271057620	-2.0495195336	-5.6159740449
C1	0.5363502956	-0.5262371704	0.4297996206
H5	1.5569005697	-0.5698600523	0.8077454585
H6	0.5969268301	-0.2400532601	-0.6132951547
C3	2.7366658910	4.1635728363	-0.6570139302
C26	1.8494198086	3.3298911691	1.4147477126
C27	0.8738252674	2.6383115327	-0.6774631325
C28	1.7919425574	3.4195085202	-1.3586689873
C29	2.7597734096	4.1195096692	0.7311384976
H1	1.8863612505	3.2798815381	2.4949515492
H2	0.1256541849	2.0873284863	-1.2299565889
H3	1.7610423948	3.4526209625	-2.4364084657
H9	3.4896654651	4.6919589348	1.2854978074

H10	3.4478987066	4.7719686917	-1.1860693938
H25	-1.0742926529	3.1373751310	2.7923517727

nuclear repulsion energy..... 1974.668059347 hartrees

-----  
/ end of geometry optimization iteration 4 /  
-----

end of program geopt

start of program onee  
smallest eigenvalue of S: 2.817E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	97	102	87	88	90	88	84
73								
	grid # 2	104	112	95	95	99	98	92
118								
	grid # 3	214	227	195	186	191	200	164
224								
	grid # 4	389	414	320	320	324	347	299
224								

number of gridpoints:

	atom	C8	C11	H7	C9	H8	C10	C12
C2								
	grid # 1	89	86	73	87	73	89	84
92								
	grid # 2	97	94	118	97	118	97	95
100								
	grid # 3	184	185	223	184	222	184	195
196								
	grid # 4	330	330	226	331	223	327	321
343								

number of gridpoints:

	atom	H13	C14	H15	C15	C16	C17	C18
C19								
	grid # 1	69	91	69	89	88	86	89
87								

grid # 2	110	100	110	97	96	96	97
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96

grid # 3	210	196	218	182	183	183	183
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182

grid # 4	215	342	217	327	327	327	327
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327

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
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H6

grid # 1	73	73	73	73	73	82	70
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69

grid # 2	113	115	118	118	118	88	109
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105

grid # 3	214	216	222	221	223	165	217
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208

grid # 4	213	214	223	222	224	290	217
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206

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
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H3

grid # 1	89	89	88	89	89	73	71
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73

grid # 2	97	95	96	97	97	115	114
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118

grid # 3	185	182	185	184	184	218	216
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223

grid # 4	330	328	329	328	329	219	214
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223

number of gridpoints:

atom	H9	H10	H25	total
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grid # 1	73	73	73	3516
grid # 2	118	118	115	4495
grid # 3	223	224	221	8642
grid # 4	224	224	224	12258

end of program grid

start of program rwr  
end of program rwr

start of program scf

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

etot	1	N	N	2	U	-990.14145563547		7.8E-04	3.9E-02
etot	2	Y	Y	6	M	-990.35861329482	2.2E-01	3.9E-04	1.6E-02
etot	3	N	Y	2	U	-990.38809039062	2.9E-02	1.2E-04	3.9E-03
etot	4	Y	Y	6	M	-990.38982038619	1.7E-03	4.1E-05	1.2E-03
etot	5	Y	Y	6	M	-990.39009100052	2.7E-04	1.6E-05	3.2E-04
etot	6	N	Y	2	U	-990.39013660923	4.6E-05	5.8E-06	1.0E-04
etot	7	Y	Y	6	M	-990.39013977366	3.2E-06	2.4E-06	3.6E-05
etot	8	Y	N	6	M	-990.39014043744	6.6E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1974.66805934711	
(E)	Total one-electron terms.....	-5267.59739614095	
(I)	Total two-electron terms.....	2302.53919635640	
(L)	Electronic energy.....	-2965.05819978455	(E+I)
(N)	Total energy.....	-990.39014043744	(A+L)

SCFE: SCF energy: HF      -990.39014043744 hartrees      iterations:  
8

HOMO energy:      -0.26872  
LUMO energy:      0.09755

Orbital energies:

-15.60449	-15.56529	-11.29607	-11.28604	-11.27093	-11.25222
-11.25039	-11.24527	-11.24459	-11.24123	-11.24070	-11.24044
-11.24005	-11.23923	-11.23844	-11.23434	-11.23294	-11.23235
-11.23098	-11.22932	-11.22452	-11.21957	-11.21815	-11.21574
-11.21231	-1.32548	-1.24923	-1.16438	-1.16096	-1.13857
-1.07363	-1.06865	-1.03835	-1.02173	-1.02055	-1.01749
-0.97069	-0.95517	-0.93360	-0.86029	-0.83635	-0.83387
-0.83017	-0.80766	-0.79576	-0.76982	-0.73217	-0.71750
-0.70155	-0.70000	-0.66622	-0.65729	-0.64350	-0.63778
-0.63371	-0.62436	-0.62014	-0.61563	-0.59577	-0.59197
-0.59045	-0.58757	-0.58039	-0.55733	-0.55239	-0.54828
-0.54513	-0.51672	-0.50646	-0.50304	-0.50031	-0.49689
-0.49432	-0.49097	-0.48728	-0.48190	-0.42913	-0.40459
-0.36595	-0.34214	-0.34166	-0.33817	-0.33118	-0.28287
-0.26872	0.09755	0.12906	0.13686	0.13760	0.14839
0.17922	0.20764	0.22771	0.23529	0.24258	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	1.722647E-04	-1.371273E-03	-2.097232E-03
2	N2	2.307619E-03	2.645434E-04	-1.429536E-03
3	C4	9.233719E-04	-1.909727E-03	-3.397651E-04
4	C5	-2.472205E-03	-1.364835E-03	1.074612E-03
5	C6	9.104396E-04	-8.696098E-04	-8.667630E-04
6	C7	-2.264358E-03	1.987665E-03	9.229630E-04
7	C13	1.704094E-05	-1.512183E-03	1.932501E-03
8	H4	-1.303564E-04	-3.601330E-04	6.584231E-05
9	C8	-2.402673E-04	-8.558610E-04	6.577247E-04
10	C11	1.082298E-03	1.304216E-03	5.319032E-04
11	H7	2.368012E-04	2.173179E-04	-3.217904E-04
12	C9	5.433283E-04	1.494368E-03	-2.250984E-04
13	H8	-7.318402E-06	9.919423E-05	2.294528E-04
14	C10	-3.416522E-04	-3.416849E-04	3.024806E-05
15	C12	5.998397E-04	6.585509E-04	7.717878E-04
16	C2	1.338325E-03	2.564232E-03	7.609119E-04
17	H13	-2.445629E-03	3.019296E-04	-7.005633E-04
18	C14	-1.006014E-03	-2.287806E-03	2.671755E-03
19	H15	3.635537E-04	1.884244E-03	-9.943853E-04
20	C15	2.027062E-03	2.500076E-04	-2.559217E-03
21	C16	2.727088E-03	1.063025E-03	-3.560983E-03
22	C17	-9.564304E-04	-6.952268E-05	-1.579709E-04
23	C18	2.482024E-03	-4.635361E-04	6.616306E-03
24	C19	5.817905E-03	2.160421E-04	-5.459483E-04
25	H16	2.531985E-03	4.057878E-04	1.288178E-04
26	H17	-4.824063E-03	-1.082739E-03	2.997523E-03
27	H18	-1.047403E-02	-7.737787E-04	-2.242630E-03
28	H19	2.831240E-03	6.714518E-04	-2.296848E-03
29	H20	2.548070E-04	7.177312E-04	-1.647014E-03
30	C1	4.326349E-04	1.117342E-03	1.134530E-03
31	H5	3.099164E-04	3.869422E-04	-1.953429E-05
32	H6	-4.484517E-05	5.228931E-04	6.438714E-04
33	C3	-2.488043E-03	-2.181722E-03	6.024058E-04
34	C26	-2.683586E-03	-2.958448E-03	1.442213E-03
35	C27	2.666601E-04	-4.104175E-04	1.506358E-03
36	C28	2.305602E-03	2.215407E-03	4.983410E-04
37	C29	8.628620E-04	7.523044E-04	-1.843323E-03
38	H1	-1.674844E-03	-2.410790E-04	-4.984929E-03
39	H2	2.525584E-03	1.790540E-03	2.833707E-03
40	H3	8.433839E-04	7.493248E-04	2.107534E-03
41	H9	-2.068308E-03	-1.653712E-03	-2.587104E-03
42	H10	8.221141E-05	1.717202E-04	-7.402267E-04
43	H25	-1.315526E-04	-2.308952E-04	-4.026906E-05
total		5.423385E-04	8.678193E-04	-3.982191E-05



end of program der1b

start of program geopt 5

geometry optimization step 5

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001034

Cos(theta): 0.4746771

Final level shift: -1.8111015E-02

energy change: -3.4678E-04 . ( 5.0000E-05 )

gradient maximum: 1.0656E-02 . ( 4.5000E-04 )

gradient rms: 2.1734E-03 . ( 3.0000E-04 )

step size: 0.29956 trust radius: 0.30000

displacement maximum: 1.2495E-01 . ( 1.8000E-03 )

displacement rms: 2.3536E-02 . ( 1.2000E-03 )

predicted energy change: -2.7815E-03 geom step: 2.9956E-

01 full step: 2.9956E-01

molecular structure not yet converged...

center of mass moved by:

x: 8.1464E-03

y: 6.0566E-03

z: -8.7285E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2292024469	0.4427015271	1.1628880103
N2	-0.9782568628	-2.2878207032	1.1779266582
C4	-1.2094337002	-0.0303642055	1.9757531149
C5	-0.0161249279	-1.9029247248	0.4674816553
C6	-1.6194223744	-1.3523145475	2.0109279641
C7	-1.7211646352	0.9868621882	2.7632723068
C13	0.6544591552	-2.9143021590	-0.4408657883
H4	-2.9999077625	-2.6718770241	2.9344446436
C8	-2.7718199836	0.6572998838	3.6401084653
C11	-0.9491404552	2.1543222696	2.4120276559
H7	-3.2211900614	1.4029180697	4.2716980948
C9	-3.2132989134	-0.6466971041	3.6786741679
H8	-4.0163262814	-0.9105012423	4.3442732707
C10	-2.6416683415	-1.6597368984	2.8743855662
C12	-0.0562922792	1.7860587709	1.4560571753
C2	0.9488951143	2.6311226377	0.7701830808
H13	1.7281674582	-2.8468821058	-0.3270846920

C14	0.2937960086	-2.7261589105	-1.9088007454
H15	0.3445375745	-3.8922911028	-0.1088900635
C15	-0.4402906415	-2.3952792758	-4.5794029238
C16	1.2395116030	-2.3428910048	-2.8630371971
C17	-1.0270889510	-2.9533277298	-2.3085099819
C18	-1.3921717180	-2.7920309200	-3.6337066705
C19	0.8788052648	-2.1725843519	-4.1956505663
H16	2.2638244085	-2.1880678707	-2.5683467508
H17	-1.7675239977	-3.2630084538	-1.5767242550
H18	-2.4257099259	-2.9929594166	-3.9302355350
H19	1.6217050002	-1.8773108746	-4.9256653884
H20	-0.7280733175	-2.2675932286	-5.6111620858
C1	0.5821138301	-0.4915229124	0.4118188533
H5	1.5989978845	-0.5325329495	0.8024327801
H6	0.6562234427	-0.2012124645	-0.6287278123
C3	2.8551861345	4.2505727705	-0.4749461088
C26	1.7771405951	3.4522098043	1.5201834275
C27	1.0866007330	2.6404146539	-0.6152847579
C28	2.0341472297	3.4391158849	-1.2329113044
C29	2.7192766740	4.2587160999	0.9026633710
H1	1.6846480152	3.4442277353	2.5858043452
H2	0.4363216332	2.0366757013	-1.2116377193
H3	2.1295952060	3.4333746931	-2.3030217836
H9	3.3514260736	4.8860237979	1.4956835722
H10	3.5921450310	4.8707133033	-0.9544874007
H25	-1.0689547267	3.1499012113	2.7877233660

nuclear repulsion energy..... 1967.972340116 hartrees

/ end of geometry optimization iteration 5 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.829E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	95	102	87	88	90	90	84

73

grid # 2	103	112	95	95	99	98	92
118							
grid # 3	212	227	195	188	190	199	163
224							
grid # 4	386	413	321	320	321	348	300
224							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	184	222	184	195
195							
grid # 4	328	330	226	331	223	327	320
340							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	88	89
89							
grid # 2	109	100	110	97	96	96	97
96							
grid # 3	211	198	213	185	185	184	185
184							
grid # 4	210	342	212	330	329	328	329
329							

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	70
69							
grid # 2	115	114	118	118	118	88	110
104							
grid # 3	214	215	223	222	224	163	217
206							
grid # 4	214	215	232	223	224	292	217
204							

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	87	88	89	89	72	70
73							
grid # 2	97	95	96	97	97	115	113
118							
grid # 3	184	182	184	184	185	217	213
222							

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grid # 4      328      327      329      327      328      215      211
224

```

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3518
grid # 2	118	118	115	4493
grid # 3	222	223	219	8634
grid # 4	224	224	223	12248

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.30892225319		4.4E-04	2.7E-02
etot	2	Y	Y	6	M	-990.37951017403	7.1E-02	2.2E-04	1.1E-02
etot	3	N	Y	2	U	-990.38894674829	9.4E-03	6.5E-05	2.8E-03
etot	4	Y	Y	6	M	-990.38948696771	5.4E-04	2.2E-05	8.5E-04
etot	5	Y	Y	6	M	-990.38957252266	8.6E-05	9.0E-06	2.1E-04
etot	6	N	Y	2	U	-990.38957720340	4.7E-06	3.0E-06	4.3E-05
etot	7	Y	N	6	M	-990.38957709405	-1.1E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1967.97234011558	
(E)	Total one-electron terms.....	-5254.19895519368	
(I)	Total two-electron terms.....	2295.83703798405	
(L)	Electronic energy.....	-2958.36191720963	(E+I)
(N)	Total energy.....	-990.38957709405	(A+L)

SCFE: SCF energy: HF -990.38957709405 hartrees iterations:  
7

HOMO energy: -0.26884  
LUMO energy: 0.09597

Orbital energies:

-15.60543	-15.56487	-11.29622	-11.28765	-11.27212	-11.25108
-11.25053	-11.24792	-11.24652	-11.23892	-11.23891	-11.23883
-11.23801	-11.23777	-11.23716	-11.23711	-11.23637	-11.23587
-11.23553	-11.23260	-11.22496	-11.22078	-11.21925	-11.21651

-11.21329	-1.32543	-1.25168	-1.16443	-1.15738	-1.13804
-1.07535	-1.06529	-1.04001	-1.02194	-1.01727	-1.01663
-0.97152	-0.95322	-0.93415	-0.85977	-0.83914	-0.83253
-0.82686	-0.80677	-0.79549	-0.77050	-0.73321	-0.71759
-0.70203	-0.69559	-0.66640	-0.65820	-0.64265	-0.63725
-0.63362	-0.62320	-0.62133	-0.61564	-0.59719	-0.59253
-0.59025	-0.58763	-0.57566	-0.55800	-0.55276	-0.54852
-0.54404	-0.51815	-0.50817	-0.50261	-0.50009	-0.49525
-0.49276	-0.49132	-0.48786	-0.48039	-0.42993	-0.40500
-0.36914	-0.34440	-0.34069	-0.33787	-0.32708	-0.28199
-0.26884	0.09597	0.12827	0.13658	0.13747	0.14798
0.17910	0.21010	0.22715	0.23493	0.24011	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	1.630734E-03	4.147837E-04	-2.328007E-04
2	N2	-4.394325E-03	-1.352038E-03	2.472753E-03
3	C4	-1.011245E-03	1.568492E-03	3.045752E-05
4	C5	4.998187E-03	1.221166E-03	-4.075432E-03
5	C6	-2.039398E-03	-4.311267E-04	1.780415E-03
6	C7	6.101085E-05	-2.060345E-04	7.720866E-04
7	C13	4.203179E-04	3.755701E-03	-3.272974E-03
8	H4	5.925810E-05	2.078679E-04	8.546451E-05
9	C8	1.534280E-03	-1.965932E-04	-1.082552E-03
10	C11	-1.931759E-03	-9.908874E-04	6.215361E-04
11	H7	-1.775814E-04	1.464387E-04	1.739668E-04
12	C9	7.213503E-04	-1.263375E-03	-1.016812E-03
13	H8	1.282530E-04	-1.587411E-04	7.876069E-06
14	C10	-2.470540E-04	1.260490E-03	7.692993E-04
15	C12	1.453405E-03	1.325890E-03	-3.933628E-03
16	C2	-1.019141E-03	-2.748754E-03	-8.869362E-04
17	H13	4.139215E-03	1.790964E-04	9.518011E-04
18	C14	-1.890313E-03	5.889275E-04	-2.220388E-03
19	H15	-5.789694E-04	-2.664568E-03	1.096563E-03
20	C15	-1.086856E-03	-8.299807E-04	2.186525E-03
21	C16	-5.200446E-03	-1.943274E-03	4.012439E-03
22	C17	1.011256E-03	-1.508706E-04	6.361840E-04

23	C18	-3.123879E-03	-7.158290E-04	-6.583892E-03
24	C19	-7.063939E-03	-2.062728E-03	8.090705E-04
25	H16	-2.103718E-04	4.707942E-04	8.553744E-04
26	H17	5.839874E-03	2.613085E-03	-4.175018E-03
27	H18	1.242488E-02	3.786442E-03	1.561713E-03
28	H19	-3.859295E-03	-1.242690E-03	3.275097E-03
29	H20	2.965080E-04	-4.598800E-04	1.965477E-03
30	C1	1.066212E-04	-1.197430E-03	2.415771E-04
31	H5	-6.245271E-04	-2.326934E-04	4.699059E-05
32	H6	-9.647908E-05	1.200227E-04	3.096240E-06
33	C3	2.194370E-03	2.154896E-03	1.522594E-03
34	C26	2.819150E-03	2.857859E-03	-7.306075E-04
35	C27	-1.348596E-04	-3.131549E-04	-4.776516E-04
36	C28	-2.416145E-03	-2.441204E-03	-9.400507E-04
37	C29	-1.201260E-03	-6.874415E-04	9.218558E-06
38	H1	7.430163E-04	7.420055E-04	4.313428E-03
39	H2	-2.921308E-03	-2.500431E-03	-3.182915E-03
40	H3	-1.090762E-03	-7.223903E-04	-1.231965E-03
41	H9	2.552610E-03	2.455616E-03	3.038091E-03
42	H10	7.688328E-05	2.110463E-04	6.463850E-04
43	H25	1.247264E-05	2.472986E-04	8.043307E-05
-----				
	total	9.037392E-04	8.158031E-04	-7.771103E-05

end of program derlb

start of program geopt 6

geometry optimization step 6

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3005785

Cos(theta): 0.4030506

Final level shift: -1.2859045E-02

energy change: 5.6334E-04 . ( 5.0000E-05 )

gradient maximum: 1.2826E-02 . ( 4.5000E-04 )

gradient rms: 2.6475E-03 . ( 3.0000E-04 )

step size: 0.30039 trust radius: 0.30000

displacement maximum: 1.4866E-01 . ( 1.8000E-03 )

displacement rms: 2.3601E-02 . ( 1.2000E-03 )

predicted energy change: -2.6208E-03 geom step: 3.0039E-

01 full step: 3.0039E-01

molecular structure not yet converged...

center of mass moved by:

x: -7.0070E-03 y: 3.1695E-03 z: -3.9849E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2431388835	0.4556736239	1.1723735471
N2	-1.0052221025	-2.2638064326	1.1711775865
C4	-1.2354149005	-0.0068382249	1.9686217617
C5	-0.0219368988	-1.8840112724	0.4769055945
C6	-1.6547168498	-1.3251930492	1.9985456785
C7	-1.7404984224	1.0066322943	2.7505185979
C13	0.6709126692	-2.8977538263	-0.4172186213
H4	-3.0356419670	-2.6439761971	2.9042709974
C8	-2.7930706857	0.6804961350	3.6197611198
C11	-0.9650101197	2.1686595222	2.4024960703
H7	-3.2425652691	1.4227454725	4.2536593268
C9	-3.2422765659	-0.6233719281	3.6535786031
H8	-4.0458719809	-0.8841748627	4.3157805202
C10	-2.6766502685	-1.6346558742	2.8502873309
C12	-0.0710715297	1.7970748741	1.4546947917
C2	0.9503376395	2.6145402001	0.7646068978
H13	1.7459317870	-2.8218826796	-0.2973025660
C14	0.3175412762	-2.7210862854	-1.8808548888
H15	0.3721363370	-3.8731171893	-0.0645970713
C15	-0.4054882560	-2.4055350093	-4.5510673450
C16	1.2049840844	-2.1961843098	-2.8003720449
C17	-0.9385119890	-3.0863025612	-2.3151953733
C18	-1.2985482642	-2.9334100012	-3.6363835117
C19	0.8468309784	-2.0394783637	-4.1317416864
H16	2.1814549757	-1.8985296468	-2.4799685659
H17	-1.6351318329	-3.4951433926	-1.6093012692
H18	-2.2805077802	-3.2390864388	-3.9568211189
H19	1.5442219641	-1.6284067831	-4.8322649240
H20	-0.6918667664	-2.2895583892	-5.5817584789
C1	0.5775477845	-0.4792363854	0.4348181138
H5	1.5772891761	-0.5317014840	0.8498355316
H6	0.6798600143	-0.1840634649	-0.5932120927
C3	2.8710077594	4.1851297153	-0.5136427992
C26	1.9198910499	3.2990087678	1.5101069134
C27	0.9496482049	2.7305127321	-0.6306199707
C28	1.9063251470	3.5077111519	-1.2645504751
C29	2.8739200353	4.0827381339	0.8755772877
H1	1.9381200101	3.2016452634	2.5905377595
H2	0.1888699186	2.2286821548	-1.2204008413
H3	1.8906486427	3.5909148714	-2.3446780704
H9	3.6213149051	4.5998757976	1.4699197044
H10	3.6131544908	4.7887646367	-1.0058448436
H25	-1.0749029726	3.1646160247	2.7777097600

nuclear repulsion energy..... 1972.328492632 hartrees

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/ end of geometry optimization iteration 6 /

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end of program geopt

start of program onee  
smallest eigenvalue of S: 2.771E-04  
number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	95	102	85	88	89	88	84
73							
grid # 2	103	112	95	95	97	96	92
118							
grid # 3	212	227	194	188	190	198	164
224							
grid # 4	387	415	320	320	327	345	300
223							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	193
196							
grid # 4	330	330	226	329	223	326	316
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	93	69	89	88	87	89
89							
grid # 2	110	101	109	97	96	96	97
96							
grid # 3	211	191	213	182	183	182	184
182							



grid # 4	213	338	212	327	327	327	327
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number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
grid # 1	72	72	73	73	73	82	70
grid # 2	113	115	118	118	118	87	108
grid # 3	214	215	222	221	222	162	217
grid # 4	214	215	224	223	224	290	215

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
grid # 1	89	89	88	89	89	73	71
grid # 2	97	95	96	97	97	115	115
grid # 3	186	184	185	185	185	218	218
grid # 4	331	328	330	328	329	219	215

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	73	3516
grid # 2	118	118	115	4486
grid # 3	223	224	221	8628
grid # 4	224	224	224	12242

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.31135910434		4.3E-04	4.0E-02
etot	2	Y	Y	6	M	-990.37781182905	6.6E-02	2.3E-04	1.6E-02
etot	3	N	Y	2	U	-990.38806340056	1.0E-02	6.8E-05	3.7E-03
etot	4	Y	Y	6	M	-990.38873042054	6.7E-04	2.3E-05	1.0E-03

etot	5	Y	Y	6	M	-990.38880803844	7.8E-05	9.7E-06	2.1E-04
etot	6	N	Y	2	U	-990.38880825493	2.2E-07	3.3E-06	4.7E-05
etot	7	Y	N	6	M	-990.38881016479	1.9E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1972.32849263240	
(E)	Total one-electron terms.....	-5262.93232379671	
(I)	Total two-electron terms.....	2300.21502099953	
(L)	Electronic energy.....	-2962.71730279719	(E+I)
(N)	Total energy.....	-990.38881016479	(A+L)

SCFE: SCF energy: HF      -990.38881016479 hartrees      iterations:  
7

HOMO energy:      -0.26932  
LUMO energy:      0.09840

Orbital energies:

-15.60367	-15.56424	-11.29601	-11.28477	-11.26958	-11.25339
-11.24904	-11.24380	-11.24330	-11.24251	-11.24217	-11.24206
-11.24138	-11.24062	-11.23899	-11.23339	-11.23226	-11.23184
-11.22993	-11.22656	-11.22352	-11.21808	-11.21636	-11.21470
-11.21091	-1.32713	-1.24880	-1.16550	-1.15964	-1.13970
-1.07482	-1.06839	-1.03820	-1.02143	-1.02048	-1.01816
-0.97093	-0.95526	-0.93500	-0.86046	-0.83462	-0.83327
-0.83082	-0.80788	-0.79619	-0.76992	-0.73305	-0.71766
-0.70058	-0.69957	-0.66673	-0.65810	-0.64423	-0.63655
-0.63289	-0.62318	-0.62001	-0.61738	-0.59598	-0.59206
-0.59102	-0.58737	-0.58058	-0.55931	-0.55282	-0.54918
-0.54135	-0.51709	-0.50650	-0.50245	-0.50066	-0.49748
-0.49337	-0.49087	-0.48836	-0.48092	-0.42887	-0.40467
-0.36567	-0.34214	-0.34177	-0.33713	-0.33161	-0.28300
-0.26932	0.09840	0.12812	0.13581	0.14035	0.14932
0.17951	0.20872	0.22741	0.23483	0.24185	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	2.996888E-03	-1.092300E-03	-5.075419E-03
2	N2	2.902098E-03	9.995089E-05	-2.104699E-03
3	C4	5.384872E-04	-5.237104E-03	-1.331028E-03
4	C5	-2.465605E-03	-1.986060E-03	6.611523E-04
5	C6	4.699496E-03	-2.649344E-03	-4.655830E-03
6	C7	-3.021900E-03	4.173873E-03	3.348288E-03
7	C13	1.016495E-03	3.817286E-03	3.204766E-03
8	H4	-8.333256E-04	-1.623874E-03	3.098643E-04
9	C8	-2.602591E-03	-3.503070E-03	1.654229E-03
10	C11	-1.632059E-03	4.019113E-03	2.604804E-03
11	H7	-3.480026E-04	8.474685E-04	4.877169E-04
12	C9	2.348395E-04	3.465178E-03	6.491069E-04
13	H8	-1.358836E-03	-2.713855E-04	1.230370E-03
14	C10	-2.396643E-03	4.501606E-04	2.552408E-03
15	C12	4.320330E-03	-4.826731E-04	-1.817665E-03
16	C2	4.569580E-03	4.725283E-03	-7.136536E-05
17	H13	2.265698E-03	1.215287E-03	1.281866E-03
18	C14	4.469088E-03	5.048013E-04	5.703955E-03
19	H15	-8.762473E-04	-2.464998E-03	-1.072243E-03
20	C15	-8.066367E-03	-2.185489E-03	-6.728433E-03
21	C16	3.580633E-03	2.454246E-03	-1.704632E-03
22	C17	-1.006307E-02	-3.935131E-03	-1.505949E-03
23	C18	-8.697968E-03	-3.668085E-03	-2.236322E-03
24	C19	7.507799E-03	2.895454E-03	4.149845E-03
25	H16	5.818461E-03	8.205617E-04	1.129787E-03
26	H17	-2.640653E-03	-8.339735E-04	1.123124E-03
27	H18	3.887211E-04	9.312185E-04	7.660585E-05
28	H19	3.923565E-03	1.582982E-03	-1.724279E-03
29	H20	2.529764E-05	3.214141E-05	1.544815E-05
30	C1	-2.579334E-03	-1.237971E-03	4.679537E-03
31	H5	3.899026E-03	3.218813E-04	1.595166E-03
32	H6	1.944755E-04	2.244129E-03	-6.101903E-03
33	C3	-4.312188E-03	-3.167459E-03	1.263702E-03
34	C26	-3.044044E-03	-3.147202E-03	-9.892063E-05
35	C27	-2.661653E-04	-6.060645E-04	2.329980E-03
36	C28	4.226828E-03	3.422783E-03	1.485505E-03
37	C29	3.350305E-04	-9.021500E-06	-3.264345E-03
38	H1	-2.026984E-03	-3.716618E-06	-7.193914E-03
39	H2	4.612104E-03	2.770042E-03	5.079830E-03
40	H3	1.355729E-03	4.917203E-04	5.686416E-03
41	H9	-4.759377E-03	-2.903258E-03	-5.357919E-03
42	H10	-3.207912E-04	-1.602736E-04	-6.972213E-04
43	H25	-5.459823E-04	8.909836E-04	6.012465E-04
total		1.022540E-03	1.008090E-03	1.626298E-04

end of program der1b

start of program geopt 7

geometry optimization step 7

reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001756

Cos(theta): 0.3481846

Final level shift: -5.8225096E-03

energy change: 7.6693E-04 . ( 5.0000E-05 )  
gradient maximum: 1.7603E-02 . ( 4.5000E-04 )  
gradient rms: 3.4045E-03 . ( 3.0000E-04 )  
step size: 0.29981 trust radius: 0.30000  
displacement maximum: 1.6540E-01 . ( 1.8000E-03 )  
displacement rms: 2.3556E-02 . ( 1.2000E-03 )  
predicted energy change: -2.5296E-03 geom step: 2.9981E-  
01 full step: 2.9981E-01  
molecular structure not yet converged...

center of mass moved by:

x: -3.4490E-03 y: -8.1566E-03 z: 4.8314E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2623089590	0.4311251804	1.1716991713
N2	-1.0180143788	-2.2950059180	1.2042298173
C4	-1.2360309063	-0.0332939736	1.9960257998
C5	-0.0491760452	-1.9161106272	0.4898652496
C6	-1.6476617970	-1.3546394568	2.0462415395
C7	-1.7230911186	0.9831467707	2.7922374034
C13	0.6280306553	-2.9273737531	-0.4121209218
H4	-2.9937724088	-2.6736769475	3.0115780294
C8	-2.7457092522	0.6539618582	3.6975262155
C11	-0.9667588878	2.1493399444	2.4114356404
H7	-3.1781071145	1.3980009698	4.3414501000
C9	-3.1860027373	-0.6506742671	3.7535912964
H8	-3.9650269465	-0.9130115590	4.4450494557
C10	-2.6416558807	-1.6625876251	2.9369875099
C12	-0.0857743078	1.7755955971	1.4454283139
C2	0.9164503009	2.6009974180	0.7343857052
H13	1.7123800183	-2.8842131896	-0.2571412082
C14	0.3088978040	-2.7056385440	-1.8863538501
H15	0.2866736531	-3.9117867885	-0.0961463804

C15	-0.2973622557	-2.3040914497	-4.5907098684
C16	1.3065628895	-2.3700351452	-2.7900211464
C17	-0.9983945440	-2.8282694144	-2.3525013671
C18	-1.2991393561	-2.6286610044	-3.6904363154
C19	1.0036021505	-2.1732391689	-4.1341691423
H16	2.3304900741	-2.2499797277	-2.4490130079
H17	-1.7797248649	-3.0692236040	-1.6584418267
H18	-2.3091793966	-2.7128159017	-4.0314102359
H19	1.7931017057	-1.9116780263	-4.8188293061
H20	-0.5306398208	-2.1492911389	-5.6298028759
C1	0.5501654299	-0.5106191206	0.4295419250
H5	1.5613035628	-0.5554938071	0.8239873713
H6	0.6303048976	-0.2234538860	-0.6093977434
C3	2.8015088368	4.1881714110	-0.5810245152
C26	1.8234927411	3.3659516372	1.4559907329
C27	0.9590649824	2.6466221398	-0.6560625455
C28	1.8988761714	3.4310895081	-1.3074873104
C29	2.7564483373	4.1586935309	0.8023034085
H1	1.8043237458	3.3261495512	2.5316351329
H2	0.2432097047	2.0877393438	-1.2297362427
H3	1.9178440967	3.4562601140	-2.3820556926
H9	3.4514125005	4.7412314670	1.3756845720
H10	3.5280434798	4.7976541261	-1.0885472588
H25	-1.0762728724	3.1476511252	2.7825837903

nuclear repulsion energy..... 1971.760476131 hartrees

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 / end of geometry optimization iteration 7 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.799E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	87	88	89	88	84
73							
grid # 2	104	112	95	95	97	98	92
118							

grid # 3	214	227	195	187	190	199	164
224							
grid # 4	388	414	320	320	327	348	301
224							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	84
92							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	184	222	184	195
195							
grid # 4	330	331	226	329	223	326	321
343							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	87	89
88							
grid # 2	110	100	110	97	96	96	97
96							
grid # 3	211	194	215	183	183	183	184
183							
grid # 4	216	340	217	327	329	329	328
327							

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	73	73	73	73	82	70
69							
grid # 2	114	114	118	118	118	88	108
105							
grid # 3	214	216	222	222	223	164	217
207							
grid # 4	214	215	224	222	224	290	217
204							

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	88	88	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	184	182	184	184	184	217	214
222							
grid # 4	328	327	329	327	328	217	212
224							

number of gridpoints:

	atom	H9	H10	H25	total
grid # 1		73	73	72	3512
grid # 2		118	118	115	4492
grid # 3		222	223	220	8629
grid # 4		224	224	224	12258

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g		energy	RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		change	change	error
	r	t	s	t	d	total energy			
etot	1	N	N	2	U	-990.30270768203		4.6E-04	3.1E-02
etot	2	Y	Y	6	M	-990.37847298562	7.6E-02	2.4E-04	1.2E-02
etot	3	N	Y	2	U	-990.38974615112	1.1E-02	7.3E-05	3.0E-03
etot	4	Y	Y	6	M	-990.39043838018	6.9E-04	2.1E-05	7.2E-04
etot	5	Y	Y	6	M	-990.39051259464	7.4E-05	9.9E-06	1.8E-04
etot	6	N	Y	2	U	-990.39052152447	8.9E-06	3.4E-06	8.4E-05
etot	7	Y	N	6	M	-990.39052390496	2.4E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.76047613143	
(E)	Total one-electron terms.....	-5261.77830707936	
(I)	Total two-electron terms.....	2299.62730704297	
(L)	Electronic energy.....	-2962.15100003639	(E+I)
(N)	Total energy.....	-990.39052390496	(A+L)

SCFE: SCF energy: HF -990.39052390496 hartrees iterations:

7

HOMO energy: -0.26911

LUMO energy: 0.09715

Orbital energies:

-15.60451	-15.56524	-11.29616	-11.28590	-11.27118	-11.25063
-11.25053	-11.24661	-11.24537	-11.24207	-11.23978	-11.23885
-11.23840	-11.23770	-11.23689	-11.23687	-11.23575	-11.23433
-11.23300	-11.23088	-11.22421	-11.21944	-11.21799	-11.21554
-11.21243	-1.32546	-1.24901	-1.16385	-1.16049	-1.13916
-1.07447	-1.06674	-1.04044	-1.02137	-1.01939	-1.01613

-0.97215	-0.95419	-0.93387	-0.86020	-0.83767	-0.83371
-0.82913	-0.80726	-0.79554	-0.77026	-0.73264	-0.71762
-0.70168	-0.69844	-0.66645	-0.65787	-0.64274	-0.63728
-0.63416	-0.62358	-0.62128	-0.61619	-0.59608	-0.59210
-0.59055	-0.58653	-0.57915	-0.55835	-0.55307	-0.54811
-0.54314	-0.51759	-0.50730	-0.50317	-0.50057	-0.49639
-0.49350	-0.49125	-0.48704	-0.48151	-0.42958	-0.40467
-0.36720	-0.34424	-0.34058	-0.33732	-0.32999	-0.28301
-0.26911	0.09715	0.12930	0.13663	0.13689	0.14839
0.17926	0.20825	0.22812	0.23474	0.24177	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	1.716334E-03	-1.943601E-03	-3.246573E-03
2	N2	1.508741E-03	7.372569E-04	-8.449564E-04
3	C4	1.732777E-03	-2.550928E-03	-1.144846E-04
4	C5	-2.258395E-03	-1.157807E-03	1.364650E-03
5	C6	3.010108E-03	-1.559524E-03	-2.676497E-03
6	C7	-2.119800E-03	2.378055E-03	8.088183E-05
7	C13	7.949520E-04	-3.166784E-03	1.193967E-03
8	H4	-5.137608E-04	-1.262150E-03	5.166284E-05
9	C8	-1.260196E-03	-1.009633E-03	7.377051E-04
10	C11	1.581835E-03	1.944482E-03	1.100216E-03
11	H7	-2.844006E-04	7.476233E-04	4.649418E-04
12	C9	3.021764E-04	2.034644E-03	3.016599E-04
13	H8	-9.191824E-04	-1.596108E-04	8.422822E-04
14	C10	-2.885543E-04	-3.647628E-05	3.084839E-04
15	C12	-1.002256E-04	1.528865E-04	8.546479E-05
16	C2	-1.824596E-03	-8.798194E-04	7.008701E-05
17	H13	-5.907107E-03	4.474195E-05	-1.786917E-03
18	C14	2.117880E-03	2.467810E-04	1.794266E-03
19	H15	1.613655E-03	3.598184E-03	-1.510856E-03
20	C15	3.515496E-03	5.380807E-04	1.351633E-03
21	C16	3.599045E-03	1.791191E-03	-2.863792E-03
22	C17	6.384644E-04	6.449569E-04	-1.226921E-03
23	C18	3.274344E-03	3.831445E-04	3.904487E-03
24	C19	3.397778E-03	6.246062E-04	2.548436E-04



25	H16	-6.033188E-03	-1.648501E-03	-2.241051E-03
26	H17	-2.244134E-03	-1.119039E-03	1.633890E-03
27	H18	-5.095790E-03	-1.462176E-03	-5.193377E-04
28	H19	-7.132674E-04	-3.366359E-04	6.699522E-05
29	H20	5.473843E-04	5.484700E-05	2.894166E-04
30	C1	-2.121480E-03	9.323276E-04	7.055723E-04
31	H5	1.935195E-03	3.195981E-04	1.225099E-03
32	H6	1.335999E-04	6.505389E-04	-1.350591E-03
33	C3	2.237467E-04	7.332118E-04	8.228264E-04
34	C26	2.934216E-03	2.259092E-03	1.769155E-03
35	C27	1.749225E-03	1.423862E-03	-2.428323E-03
36	C28	-3.039822E-03	-2.449444E-03	-8.296198E-04
37	C29	-1.534705E-03	-1.836397E-03	1.746854E-03
38	H1	1.639685E-04	5.612689E-04	-9.703912E-04
39	H2	-6.178164E-04	-7.198783E-04	-5.945158E-04
40	H3	-2.726356E-04	-1.448398E-04	-7.139410E-04
41	H9	1.428431E-03	1.266800E-03	1.288079E-03
42	H10	1.793635E-04	8.168534E-05	1.338084E-04
43	H25	-2.945761E-04	3.841792E-04	3.416161E-04
-----				
	total	6.550833E-04	1.090803E-03	1.177413E-05

end of program derlb

start of program geopt 8

geometry optimization step 8

reading input hessian of dimension 129  
in five columns format

reading input hessian of dimension 129  
in five columns format

reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3001625

Cos(theta): 0.3290489

Final level shift: -3.2712361E-03

energy change: -1.7137E-03 . ( 5.0000E-05 )

gradient maximum: 6.5993E-03 . ( 4.5000E-04 )

gradient rms: 1.5880E-03 . ( 3.0000E-04 )

step size: 0.30014 trust radius: 0.30000

displacement maximum: 1.3289E-01 . ( 1.8000E-03 )

displacement rms: 2.3581E-02 . ( 1.2000E-03 )

predicted energy change: -1.1454E-03 geom step: 3.0014E-

01 full step: 3.0014E-01

molecular structure not yet converged...

center of mass moved by:

x: 1.4339E-03 y: 3.9888E-03 z: 1.3736E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2427301136	0.4133581705	1.1722777583
N2	-1.0454939928	-2.3112638158	1.1699656111
C4	-1.2161957562	-0.0597207232	2.0064760689
C5	-0.0696132821	-1.9370852449	0.4798595573
C6	-1.6544570973	-1.3757803348	2.0263648965
C7	-1.6847856453	0.9623542639	2.8316875226
C13	0.5944122868	-2.9384071474	-0.4387964649
H4	-3.0378534973	-2.6801972707	2.9787940568
C8	-2.7195283903	0.6400467042	3.7315827985
C11	-0.8978500352	2.1256728813	2.4741738095
H7	-3.1321827458	1.3838331907	4.3903874062
C9	-3.1856697575	-0.6615094865	3.7551713096
H8	-3.9748299789	-0.9205218030	4.4383849881
C10	-2.6599327111	-1.6753768988	2.9171144248
C12	-0.0449844390	1.7563976980	1.4791878795
C2	0.9261767262	2.6151140566	0.7518235711
H13	1.6652174605	-2.8719758706	-0.3024610873
C14	0.2876181649	-2.7034242241	-1.9136085293
H15	0.2724733448	-3.9275784756	-0.1477724137
C15	-0.2818249606	-2.3156026969	-4.6110105067
C16	1.3116920078	-2.5254385140	-2.8427232568
C17	-1.0214564856	-2.6804795857	-2.3448902825
C18	-1.3074367587	-2.4976491583	-3.6888738098
C19	1.0337227845	-2.3208152467	-4.1837294462
H16	2.3428974456	-2.5809231360	-2.5252940373
H17	-1.8180053491	-2.8390751217	-1.6358051292
H18	-2.3411635228	-2.5448754781	-4.0117834742
H19	1.8504547007	-2.2045671815	-4.8863974827
H20	-0.5093223464	-2.1903514419	-5.6550411487
C1	0.5725384418	-0.5359270224	0.4467237410
H5	1.5825600909	-0.6025572202	0.8639586010
H6	0.6849443477	-0.2439441492	-0.5977493705
C3	2.7427643680	4.2718109037	-0.5786007634
C26	1.7583262170	3.4655134300	1.4748050376
C27	1.0258000879	2.6093370968	-0.6475070512
C28	1.9286490508	3.4252015088	-1.3062477428
C29	2.6507103176	4.2926508665	0.8143808905
H1	1.7064457766	3.4685024593	2.5540630146
H2	0.3832676468	1.9769465517	-1.2258047756
H3	1.9981625157	3.3991783059	-2.3867378260
H9	3.2735304395	4.9523138350	1.3873712355
H10	3.4343293803	4.9068564617	-1.0932588436
H25	-0.9916197529	3.1137132967	2.8763314713

nuclear repulsion energy..... 1966.909747028 hartrees

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/ end of geometry optimization iteration 8 /

-----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.927E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	86	88	88	90	84
73							
grid # 2	104	112	94	95	101	98	92
118							
grid # 3	215	228	195	186	189	198	163
223							
grid # 4	388	413	323	321	327	351	300
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	87	73	87	73	89	86
91							
grid # 2	97	94	118	97	118	97	95
100							
grid # 3	184	185	223	185	222	184	194
195							
grid # 4	329	331	226	331	224	328	318
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	90	69	89	87	88	88
88							
grid # 2	107	98	111	97	96	96	97
97							
grid # 3	209	195	218	183	184	184	184
182							

```

    grid # 4      207      339      213      329      329      330      331
330

```

```

    number of gridpoints:
      atom      H16      H17      H18      H19      H20      C1      H5
H6
    grid # 1      73      73      73      73      73      82      70
69
    grid # 2      114      115      118      118      118      90      110
105
    grid # 3      214      215      223      222      224      166      217
205
    grid # 4      213      215      223      222      224      293      220
207

```

```

    number of gridpoints:
      atom      C3      C26      C27      C28      C29      H1      H2
H3
    grid # 1      89      89      88      89      89      72      70
73
    grid # 2      97      96      96      97      97      115      113
118
    grid # 3      186      182      185      184      186      217      213
222
    grid # 4      330      327      328      327      330      217      210
224

```

```

    number of gridpoints:
      atom      H9      H10      H25      total
grid # 1      73      73      72      3513
grid # 2      118      118      115      4497
grid # 3      223      223      219      8634
grid # 4      223      223      222      12263

```

end of program grid

```

start of program rwr
end of program rwr

```

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.33991144147		3.6E-04	2.8E-02
etot	2	Y	Y	6	M	-990.38172607361	4.2E-02	1.8E-04	1.1E-02
etot	3	N	Y	2	U	-990.38813338998	6.4E-03	5.5E-05	2.7E-03
etot	4	Y	Y	6	M	-990.38854871108	4.2E-04	2.2E-05	8.5E-04

etot	5	Y	Y	6	M	-990.38862044730	7.2E-05	8.4E-06	1.6E-04
etot	6	N	Y	2	U	-990.38863299439	1.3E-05	3.2E-06	5.7E-05
etot	7	Y	N	6	M	-990.38863307052	7.6E-08	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1966.90974702809	
(E)	Total one-electron terms.....	-5252.08828716800	
(I)	Total two-electron terms.....	2294.78990706939	
(L)	Electronic energy.....	-2957.29838009861	(E+I)
(N)	Total energy.....	-990.38863307052	(A+L)

SCFE: SCF energy: HF      -990.38863307052 hartrees      iterations:  
7

HOMO energy:      -0.26918  
LUMO energy:      0.09483

Orbital energies:

-15.60546	-15.56553	-11.29617	-11.28888	-11.27440	-11.25323
-11.25291	-11.24932	-11.24466	-11.23989	-11.23899	-11.23849
-11.23820	-11.23781	-11.23695	-11.23662	-11.23581	-11.23470
-11.23345	-11.22918	-11.22676	-11.22253	-11.22247	-11.21821
-11.21580	-1.32205	-1.25283	-1.16216	-1.16049	-1.13639
-1.07414	-1.06661	-1.03656	-1.02137	-1.01847	-1.01697
-0.96944	-0.95479	-0.93227	-0.85933	-0.83776	-0.83195
-0.82823	-0.80624	-0.79536	-0.76922	-0.73264	-0.71663
-0.70030	-0.69768	-0.66473	-0.65767	-0.64239	-0.63624
-0.63253	-0.62481	-0.62019	-0.61335	-0.59730	-0.59249
-0.58848	-0.58801	-0.57615	-0.55734	-0.55154	-0.54848
-0.54556	-0.51729	-0.50702	-0.50198	-0.49950	-0.49588
-0.49449	-0.49099	-0.48779	-0.47966	-0.42997	-0.40493
-0.36948	-0.34394	-0.33991	-0.33752	-0.32983	-0.28137
-0.26918	0.09483	0.12818	0.13771	0.13869	0.14741
0.17628	0.20896	0.22759	0.23471	0.23973	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-3.608445E-03	2.818146E-03	4.387853E-03
2	N2	-8.257060E-03	-1.291490E-03	6.873558E-03
3	C4	2.927401E-04	9.089283E-03	2.291217E-03
4	C5	1.159396E-02	4.274925E-03	-1.002984E-02
5	C6	-2.111425E-03	3.526585E-03	5.173623E-03
6	C7	3.146159E-03	-4.915515E-03	-4.361290E-03
7	C13	1.197140E-03	3.152175E-03	-4.853313E-03
8	H4	6.158857E-05	2.208153E-04	-3.754693E-04
9	C8	3.232912E-03	-4.388872E-03	-3.687738E-03
10	C11	-2.930359E-03	-7.516295E-03	-1.095850E-03
11	H7	-5.246514E-04	-5.339326E-04	3.142423E-05
12	C9	2.211024E-03	7.245822E-04	-2.076187E-03
13	H8	-9.756688E-05	-4.122068E-04	2.025975E-04
14	C10	2.685113E-04	4.837745E-03	1.404553E-03
15	C12	1.505465E-03	8.606128E-04	-3.784882E-03
16	C2	4.596320E-04	-4.228012E-03	-4.301454E-03
17	H13	4.376286E-03	-2.059499E-03	1.720359E-03
18	C14	1.184396E-02	2.108409E-03	5.874802E-03
19	H15	-6.450204E-04	-1.250607E-03	1.770200E-03
20	C15	-5.854112E-03	1.356985E-04	-5.815791E-04
21	C16	3.009072E-03	-1.664308E-03	4.118831E-03
22	C17	-8.790402E-03	-1.738000E-03	-6.298458E-03
23	C18	-4.719041E-03	-2.976537E-03	-2.898018E-03
24	C19	3.419037E-03	-2.514676E-03	-7.224967E-04
25	H16	-2.647010E-03	1.940020E-03	9.827487E-04
26	H17	7.504203E-04	1.171925E-03	-1.479661E-03
27	H18	6.000360E-03	3.165718E-03	-3.106612E-04
28	H19	-5.276927E-03	3.874991E-04	2.823860E-03
29	H20	-6.458594E-04	6.314977E-04	1.160412E-04
30	C1	4.753900E-04	-1.944511E-03	-4.062617E-03
31	H5	-3.832564E-03	-2.580860E-04	-2.786851E-04
32	H6	-7.710760E-04	-1.574150E-03	5.124757E-03
33	C3	-8.483867E-04	5.126358E-04	1.028467E-02
34	C26	-3.375860E-04	6.706250E-04	2.040083E-04
35	C27	-2.580503E-03	-2.382582E-03	7.317669E-03
36	C28	-4.311198E-04	-1.818641E-03	-1.976063E-03
37	C29	3.356317E-04	9.286614E-04	-7.586848E-03
38	H1	4.426202E-04	2.672569E-04	-4.159578E-03
39	H2	-3.082192E-03	-2.219428E-03	-4.993021E-04
40	H3	-1.537561E-03	6.603144E-05	5.377819E-03
41	H9	2.343965E-03	1.305606E-03	1.437853E-04
42	H10	3.434594E-03	3.036993E-03	3.538105E-04
43	H25	3.444813E-05	5.165315E-04	-1.111761E-03
total		9.060454E-04	6.626275E-04	4.644130E-05

end of program der1b

start of program geopt 9

```

geometry optimization step 9
reading input hessian of dimension 129
  in five columns format
reading input hessian of dimension 129
  in five columns format
reading input hessian of dimension 129
  in five columns format
** restarting optimization from step 8 **

```

Level shifts adjusted to satisfy step-size constraints

Step size: 0.3007076

Cos(theta): 0.3121536

Final level shift: -6.2152375E-03

```

energy change:          1.8908E-03 . ( 5.0000E-05 )
gradient maximum:       6.5993E-03 . ( 4.5000E-04 )
gradient rms:          1.5880E-03 . ( 3.0000E-04 )
step size: 0.29990 trust radius: 0.30000
displacement maximum:   1.3848E-01 . ( 1.8000E-03 )
displacement rms:       2.3562E-02 . ( 1.2000E-03 )
predicted energy change: -1.2255E-03 geom step: 2.9990E-
01 full step: 2.9990E-01
molecular structure not yet converged...

```

center of mass moved by:

x: -7.4940E-16 y: 2.6368E-16 z: -8.3267E-16

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2112213224	0.4759821970	1.1509370987
N2	-0.9304654889	-2.2596315619	1.1557263606
C4	-1.2007566870	-0.0050996186	1.9468199390
C5	0.0308354325	-1.8599684763	0.4447847412
C6	-1.5893298383	-1.3330206181	1.9833821552
C7	-1.7559182331	1.0130893177	2.7060893243
C13	0.7195427103	-2.8544750054	-0.4654951884
H4	-2.9732939203	-2.6636627946	2.8871238361
C8	-2.8165407677	0.6740276669	3.5624798977
C11	-0.9876468060	2.1851605542	2.3748675911
H7	-3.2934365683	1.4196419607	4.1781118649
C9	-3.2309842879	-0.6335021660	3.6104914752
H8	-4.0426550097	-0.9068067006	4.2655024799
C10	-2.6247327918	-1.6447328748	2.8300957907
C12	-0.0663221250	1.8221726220	1.4414763503
C2	0.9615610706	2.6573510475	0.7929901780
H13	1.7804240263	-2.7291419038	-0.3977998181
C14	0.2904550036	-2.7194671495	-1.9078212042
H15	0.4874628272	-3.8353817165	-0.1033936907

C15	-0.5195728220	-2.5100998311	-4.5600986738
C16	1.1731723675	-2.2603581915	-2.8876463572
C17	-1.0114333568	-3.0801698853	-2.2799362236
C18	-1.4107209530	-2.9767515754	-3.5926183840
C19	0.7731816258	-2.1547371391	-4.2060163333
H16	2.1848694620	-1.9871622113	-2.6169976829
H17	-1.6947814125	-3.4329355076	-1.5285602629
H18	-2.3991425622	-3.2559857461	-3.8614828367
H19	1.4638084288	-1.7938641349	-4.9522904025
H20	-0.8298119621	-2.4271286947	-5.5831759553
C1	0.6128319456	-0.4474688200	0.4042533197
H5	1.6225608382	-0.4852424998	0.8284411699
H6	0.7094088190	-0.1466392262	-0.6361783628
C3	2.9218539781	4.2333037928	-0.3978184205
C26	1.8547642164	3.3951618772	1.5732849714
C27	1.0554555784	2.7250390584	-0.5942672449
C28	2.0276025330	3.5107060596	-1.1848132236
C29	2.8296541634	4.1778589369	0.9812369472
H1	1.7838933136	3.3413965331	2.6388352230
H2	0.3516514934	2.1776688845	-1.2016643395
H3	2.0892544843	3.5634944072	-2.2542289962
H9	3.5239664473	4.7363520807	1.5935527668
H10	3.6885398335	4.8392355334	-0.8576710935
H25	-1.1255993547	3.1803096411	2.7475409393

nuclear repulsion energy..... 1969.045876041 hartrees

-----  
 / end of geometry optimization iteration 9 /  
 -----

end of program geopt

start of program onee  
 smallest eigenvalue of S: 2.808E-04  
 number of canonical orbitals..... 461  
 end of program onee

start of program probe  
 end of program probe

start of program grid

number of gridpoints:		N1	N2	C4	C5	C6	C7	C13
H4	atom							
	grid # 1	95	102	84	87	89	90	84
73								
	grid # 2	104	112	95	95	101	98	92
118								



grid # 3	212	227	193	187	192	198	163
224							
grid # 4	386	414	324	320	324	350	294
224							

number of gridpoints:							
atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
90							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	184	223	184	222	184	195
194							
grid # 4	328	332	226	328	223	330	317
341							

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	87	89
89							
grid # 2	108	100	109	97	96	96	97
97							
grid # 3	211	196	214	186	184	182	183
184							
grid # 4	210	341	212	329	328	326	329
327							

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	72	73	73	73	82	70
69							
grid # 2	114	115	118	118	118	90	108
104							
grid # 3	213	215	223	222	223	164	217
206							
grid # 4	214	215	223	223	224	293	219
208							

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	87	87	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	185	181	182	184	185	217	213
223							
grid # 4	330	328	330	327	328	216	212
224							

number of gridpoints:

	atom	H9	H10	H25	total
grid # 1		73	73	72	3507
grid # 2		118	118	115	4495
grid # 3		223	223	220	8625
grid # 4		224	224	224	12249

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g		energy	RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		change	change	error
	r	t	s	t	d	total energy			
etot	1	N	N	2	U	-990.19143961399		6.9E-04	5.1E-02
etot	2	Y	Y	6	M	-990.36304368943	1.7E-01	3.6E-04	2.1E-02
etot	3	N	Y	2	U	-990.38756589331	2.5E-02	1.1E-04	4.9E-03
etot	4	Y	Y	6	M	-990.38902919237	1.5E-03	3.0E-05	1.2E-03
etot	5	Y	Y	6	M	-990.38919073874	1.6E-04	1.6E-05	3.2E-04
etot	6	N	Y	2	U	-990.38919602691	5.3E-06	5.3E-06	8.1E-05
etot	7	Y	Y	6	M	-990.38919546120	-5.7E-07	2.6E-06	3.1E-05
etot	8	Y	N	6	M	-990.38919647219	1.0E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1969.04587604074	
(E)	Total one-electron terms.....	-5256.35681247047	
(I)	Total two-electron terms.....	2296.92173995754	
(L)	Electronic energy.....	-2959.43507251293	(E+I)
(N)	Total energy.....	-990.38919647219	(A+L)

SCFE: SCF energy: HF      -990.38919647219 hartrees      iterations:  
8

HOMO energy:      -0.26840  
LUMO energy:      0.09701

Orbital energies:

-15.60534	-15.56470	-11.29636	-11.28875	-11.27084	-11.25072
-11.25052	-11.24617	-11.24576	-11.24057	-11.23986	-11.23892
-11.23842	-11.23745	-11.23597	-11.23589	-11.23480	-11.23326
-11.23202	-11.22987	-11.22361	-11.22021	-11.21809	-11.21556
-11.21238	-1.32578	-1.25026	-1.16340	-1.15935	-1.13851

-1.07486	-1.06779	-1.03915	-1.02304	-1.01954	-1.01789
-0.96974	-0.95431	-0.93406	-0.86044	-0.83631	-0.83390
-0.82845	-0.80772	-0.79588	-0.77036	-0.73270	-0.71782
-0.70108	-0.69798	-0.66655	-0.65810	-0.64342	-0.63833
-0.63434	-0.62250	-0.62043	-0.61751	-0.59675	-0.59349
-0.59179	-0.58934	-0.57738	-0.55766	-0.55188	-0.54826
-0.54421	-0.51763	-0.50773	-0.50313	-0.50021	-0.49540
-0.49235	-0.49068	-0.48759	-0.48192	-0.42965	-0.40506
-0.36691	-0.34326	-0.34192	-0.33901	-0.32575	-0.28176
-0.26840	0.09701	0.12789	0.13689	0.13892	0.14831
0.17873	0.20902	0.22650	0.23488	0.24146	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
----	-----	-----	-----	-----
1	N1	-1.847904E-03	1.350870E-03	1.372186E-03
2	N2	8.004859E-04	-1.184322E-03	-1.290199E-03
3	C4	-2.990647E-03	1.894084E-03	-1.153339E-03
4	C5	-1.267694E-03	-1.405869E-03	2.168808E-03
5	C6	-3.781687E-03	1.063700E-03	1.466086E-03
6	C7	3.701565E-03	-2.358705E-03	9.208506E-04
7	C13	-6.358814E-03	5.686112E-03	1.117194E-03
8	H4	7.566979E-04	2.267632E-03	4.118942E-04
9	C8	3.487603E-04	4.660037E-03	1.792745E-03
10	C11	-4.761810E-04	-4.721753E-05	-2.385896E-03
11	H7	6.406881E-04	-9.788330E-04	-1.030604E-03
12	C9	-1.838024E-03	-6.112861E-03	1.573878E-04
13	H8	1.321968E-03	2.841587E-04	-1.158728E-03
14	C10	-9.988378E-04	-2.699473E-03	-2.337905E-04
15	C12	-3.644818E-04	5.292972E-04	1.985804E-03
16	C2	4.214487E-03	2.571180E-03	2.054306E-03
17	H13	1.220174E-02	2.129938E-03	9.413491E-04
18	C14	-1.971814E-03	-2.257252E-04	-1.000693E-02
19	H15	-2.739856E-03	-7.545521E-03	3.261445E-03
20	C15	-3.750255E-04	-1.032296E-03	2.979952E-03
21	C16	3.971553E-04	-1.694801E-03	1.180222E-02
22	C17	1.081296E-02	3.319375E-03	5.677630E-03
23	C18	1.275942E-02	5.331517E-03	-6.004976E-03

24	C19	-6.135291E-03	-1.513302E-04	-5.275360E-03
25	H16	-3.575445E-03	-1.293270E-03	1.989000E-04
26	H17	-2.282103E-04	-2.076355E-04	5.184705E-04
27	H18	-1.003847E-02	-2.388316E-03	-4.271375E-03
28	H19	-1.686569E-03	-1.077089E-03	1.228071E-03
29	H20	-1.715323E-03	-1.767050E-04	-2.514137E-03
30	C1	6.153916E-03	1.649965E-03	1.097077E-03
31	H5	-3.027084E-03	-3.480673E-04	-3.342055E-03
32	H6	-1.486703E-04	-3.556652E-04	2.982007E-03
33	C3	1.936388E-06	2.107970E-04	-5.988076E-03
34	C26	-4.239919E-03	-2.750183E-03	-4.310837E-03
35	C27	-6.213987E-04	-7.833312E-05	4.417728E-04
36	C28	4.704144E-03	3.029595E-03	2.767092E-03
37	C29	2.147902E-03	1.746275E-03	9.650488E-04
38	H1	-4.030953E-04	-8.930180E-04	4.530742E-03
39	H2	1.885956E-03	1.855455E-03	5.925202E-04
40	H3	5.723930E-04	3.930392E-04	-2.575663E-03
41	H9	-2.986811E-03	-2.049155E-03	-1.829814E-03
42	H10	-2.808888E-03	-1.906220E-03	-3.199569E-05
43	H25	3.854478E-04	-1.625851E-04	-2.576043E-04
-----				
total		1.181474E-03	8.498306E-04	-2.298122E-04

end of program derlb

start of program geopt 10

geometry optimization step 10

[ turning on trust-radius adjustment ]

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 8 \*\*

energy change: 1.3274E-03 . ( 5.0000E-05 )

gradient maximum: 6.5993E-03 . ( 4.5000E-04 )

gradient rms: 1.5880E-03 . ( 3.0000E-04 )

step size: 0.12023 trust radius: 0.15000

displacement maximum: 4.6109E-02 . ( 1.8000E-03 )

displacement rms: 9.4462E-03 . ( 1.2000E-03 )

predicted energy change: -6.6309E-04 geom step: 1.2023E-

01 full step: 1.2023E-01

molecular structure not yet converged...

center of mass moved by:

x: 5.8287E-16 y: 2.6368E-16 z: 5.5511E-17

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2503467923	0.4313387940	1.1728975667
N2	-0.9922353568	-2.3008642645	1.2068479080
C4	-1.2177846926	-0.0412413961	2.0027340636
C5	-0.0328950456	-1.9152046665	0.4874677885
C6	-1.6207580303	-1.3658403732	2.0516318574
C7	-1.7256576704	0.9802469690	2.7898913510
C13	0.6345154182	-2.9213500262	-0.4256979858
H4	-2.9784638181	-2.6865579845	3.0093481473
C8	-2.7573880472	0.6486468955	3.6876420923
C11	-0.9686088796	2.1508712541	2.4150585939
H7	-3.2011472190	1.3958055134	4.3235415609
C9	-3.1880965526	-0.6579308626	3.7452763889
H8	-3.9761108933	-0.9234283427	4.4292771187
C10	-2.6259600579	-1.6723713900	2.9368264804
C12	-0.0840044705	1.7791562074	1.4502481760
C2	0.9094340782	2.6151448582	0.7396605597
H13	1.7117184108	-2.8786891597	-0.2812033952
C14	0.3106147337	-2.6930411706	-1.8952436050
H15	0.2973278585	-3.9045733242	-0.1220199652
C15	-0.3176308144	-2.3047012879	-4.5894802502
C16	1.3058774411	-2.4094783712	-2.8200443949
C17	-1.0094991762	-2.7875081323	-2.3386183614
C18	-1.3208168237	-2.5954695037	-3.6744560256
C19	0.9966496806	-2.2130779832	-4.1595138305
H16	2.3268560103	-2.3606962160	-2.4970780760
H17	-1.7899818400	-3.0122134213	-1.6310120439
H18	-2.3448732588	-2.6750402869	-4.0018765889
H19	1.7816422461	-2.0017592358	-4.8628995476
H20	-0.5601115265	-2.1562329340	-5.6282763720
C1	0.5677714222	-0.5074561645	0.4336493303
H5	1.5802783124	-0.5505269015	0.8402390685
H6	0.6558736629	-0.2175416456	-0.6088435807
C3	2.8070428603	4.1983759363	-0.5604794150
C26	1.7923657031	3.4110711813	1.4677798769
C27	0.9824585662	2.6308465889	-0.6519969273
C28	1.9254954757	3.4145041743	-1.2967484498
C29	2.7309857208	4.2007778211	0.8223821304
H1	1.7459445767	3.3977291757	2.5379712574
H2	0.2862125744	2.0466037166	-1.2287363733
H3	1.9713578203	3.4151297035	-2.3708451625
H9	3.4096713505	4.8073562604	1.3990774035
H10	3.5437855062	4.8042079101	-1.0617698905
H25	-1.0891245347	3.1494999185	2.7854402047

nuclear repulsion energy..... 1970.392406452 hartrees

/ end of geometry optimization iteration 10 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.841E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	96	102	87	88	90	89	84
73								
	grid # 2	103	112	95	95	99	97	92
118								
	grid # 3	213	227	195	187	191	200	163
224								
	grid # 4	389	414	323	320	321	351	300
224								

number of gridpoints:

	atom	C8	C11	H7	C9	H8	C10	C12
C2								
	grid # 1	89	86	73	87	73	89	86
92								
	grid # 2	97	94	118	97	118	97	94
100								
	grid # 3	184	185	223	184	222	184	195
195								
	grid # 4	328	331	226	331	223	329	318
342								

number of gridpoints:

	atom	H13	C14	H15	C15	C16	C17	C18
C19								
	grid # 1	69	91	69	89	88	88	89
89								
	grid # 2	109	100	110	97	96	96	97
96								
	grid # 3	210	197	216	183	184	183	184
183								
	grid # 4	213	342	213	327	329	327	327
329								

number of gridpoints:

	atom	H16	H17	H18	H19	H20	C1	H5
H6								
69	grid # 1	73	73	73	73	73	82	70
104	grid # 2	113	115	118	118	118	89	110
207	grid # 3	214	216	223	222	224	165	217
206	grid # 4	214	214	224	223	224	293	219

number of gridpoints:

	atom	C3	C26	C27	C28	C29	H1	H2
H3								
73	grid # 1	89	88	88	89	89	72	71
118	grid # 2	97	95	96	97	97	115	114
223	grid # 3	184	182	184	184	185	217	212
224	grid # 4	329	328	329	327	329	216	212

number of gridpoints:

	atom	H9	H10	H25	total
grid # 1		73	73	72	3519
grid # 2		118	118	115	4492
grid # 3		222	223	220	8636
grid # 4		224	224	224	12260

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	2	U	-990.29802142608		4.7E-04	3.6E-02
etot	2	Y	Y	6	M	-990.37914076540	8.1E-02	2.4E-04	1.5E-02
etot	3	N	Y	2	U	-990.39011714517	1.1E-02	7.3E-05	3.6E-03
etot	4	Y	Y	6	M	-990.39075170470	6.3E-04	1.8E-05	8.3E-04
etot	5	Y	Y	6	M	-990.39080716088	5.5E-05	9.2E-06	2.4E-04
etot	6	N	Y	2	U	-990.39081625073	9.1E-06	3.2E-06	6.3E-05
etot	7	Y	N	6	M	-990.39082059817	4.3E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1970.39240645220	
(E)	Total one-electron terms.....	-5259.04946585476	
(I)	Total two-electron terms.....	2298.26623880439	
(L)	Electronic energy.....	-2960.78322705037	(E+I)
(N)	Total energy.....	-990.39082059817	(A+L)

SCFE: SCF energy: HF -990.39082059817 hartrees iterations:

7

HOMO energy: -0.26884

LUMO energy: 0.09625

Orbital energies:

-15.60520	-15.56542	-11.29634	-11.28757	-11.27197	-11.25137
-11.25137	-11.24663	-11.24624	-11.24028	-11.24014	-11.23939
-11.23864	-11.23804	-11.23717	-11.23626	-11.23525	-11.23435
-11.23339	-11.23131	-11.22496	-11.22092	-11.21941	-11.21652
-11.21351	-1.32467	-1.25038	-1.16266	-1.16009	-1.13785
-1.07415	-1.06682	-1.03876	-1.02160	-1.01902	-1.01676
-0.97049	-0.95423	-0.93360	-0.85986	-0.83666	-0.83382
-0.82912	-0.80693	-0.79529	-0.76986	-0.73238	-0.71725
-0.70084	-0.69840	-0.66614	-0.65779	-0.64278	-0.63724
-0.63391	-0.62371	-0.62052	-0.61551	-0.59631	-0.59205
-0.59042	-0.58760	-0.57799	-0.55757	-0.55200	-0.54823
-0.54488	-0.51728	-0.50751	-0.50254	-0.49998	-0.49565
-0.49359	-0.49112	-0.48733	-0.48118	-0.42972	-0.40500
-0.36774	-0.34301	-0.34117	-0.33775	-0.32916	-0.28213
-0.26884	0.09625	0.12876	0.13660	0.13709	0.14832
0.17835	0.20865	0.22790	0.23513	0.24117	

end of program scf

start of program der1a

end of program der1a

start of program rwr

end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	3.176707E-04	-7.109467E-05	1.405262E-05
2	N2	-1.075429E-03	-2.083377E-04	7.417913E-04



3	C4	-9.732657E-04	1.912845E-03	4.219490E-04
4	C5	9.390608E-04	-3.118005E-04	-6.400202E-04
5	C6	-1.872859E-03	6.288692E-04	1.567042E-03
6	C7	8.574249E-04	-1.220477E-03	-4.534514E-04
7	C13	4.990676E-05	2.619141E-04	-1.067732E-03
8	H4	2.212391E-04	7.436348E-04	4.175358E-05
9	C8	9.716663E-04	1.126067E-03	-2.443932E-04
10	C11	-3.058807E-04	-1.016420E-03	-2.792513E-05
11	H7	2.030616E-04	-3.912862E-04	-4.531555E-04
12	C9	3.885238E-04	-1.817448E-03	-8.541092E-04
13	H8	5.647280E-04	1.033803E-04	-4.236539E-04
14	C10	1.787747E-04	1.629413E-04	-1.130833E-04
15	C12	-2.993285E-04	9.293299E-04	-8.305882E-04
16	C2	2.106919E-03	3.714443E-04	1.529857E-03
17	H13	-8.453989E-06	-1.369249E-05	-3.866099E-04
18	C14	-2.620975E-03	-8.478820E-04	-2.750261E-04
19	H15	1.703486E-04	2.476269E-04	5.668823E-04
20	C15	1.348587E-03	3.170487E-04	-3.143626E-04
21	C16	-3.287963E-03	-8.576557E-04	-7.679380E-04
22	C17	9.274778E-04	5.528706E-04	2.811386E-05
23	C18	-2.653106E-04	-1.756854E-04	1.189448E-03
24	C19	-2.378424E-03	-1.170097E-03	5.057107E-05
25	H16	3.742774E-03	1.309982E-03	7.701638E-04
26	H17	6.077310E-04	2.216130E-04	-3.997413E-04
27	H18	1.487305E-03	2.292942E-04	4.715166E-04
28	H19	5.016746E-04	5.351337E-04	-4.906618E-04
29	H20	3.420834E-04	-6.617536E-05	7.707523E-04
30	C1	1.310155E-03	1.015916E-03	-6.323303E-04
31	H5	-1.427620E-03	-7.688246E-05	-7.480952E-04
32	H6	-2.814998E-05	-3.196540E-04	2.202996E-03
33	C3	-1.512850E-03	-7.323179E-04	-2.557105E-03
34	C26	-1.040007E-03	-4.215451E-04	-2.994571E-03
35	C27	2.310941E-04	6.193161E-04	-3.498692E-04
36	C28	1.620128E-03	8.085342E-04	2.072791E-03
37	C29	2.143792E-04	-9.341659E-05	4.237368E-04
38	H1	-3.535759E-05	-1.816722E-04	3.011021E-03
39	H2	6.170067E-04	4.683717E-04	1.307347E-04
40	H3	-3.642736E-05	2.655682E-04	-5.930004E-04
41	H9	-9.794912E-04	-8.053914E-04	-4.013531E-04
42	H10	-1.162548E-03	-8.092648E-04	1.701950E-04
43	H25	1.251612E-04	-4.338929E-04	-3.335687E-04
-----		-----	-----	-----
total		7.345388E-04	7.896115E-04	-1.769761E-04

end of program derlb

start of program geopt 11

geometry optimization step 11

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0750415

Cos(theta): 0.6886741

Final level shift: -2.7962975E-02

energy change: -2.9669E-04 . ( 5.0000E-05 )  
gradient maximum: 3.8324E-03 . ( 4.5000E-04 )  
gradient rms: 8.9140E-04 . ( 3.0000E-04 )  
step size: 0.07504 trust radius: 0.07500  
displacement maximum: 2.2233E-02 . ( 1.8000E-03 )  
displacement rms: 5.8958E-03 . ( 1.2000E-03 )  
predicted energy change: -3.7189E-04 geom step: 7.5041E-  
02 full step: 7.5041E-02  
molecular structure not yet converged...

center of mass moved by:

x: -1.1335E-03

y: -2.5596E-03

z: -2.5985E-03

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2525386544	0.4310493893	1.1683995301
N2	-1.0138740281	-2.2939256517	1.1975942074
C4	-1.2252479678	-0.0341646614	1.9952733135
C5	-0.0436572270	-1.9157862179	0.4851284149
C6	-1.6413071326	-1.3541973725	2.0405928362
C7	-1.7145415536	0.9821590281	2.7923186325
C13	0.6288624322	-2.9244715472	-0.4211405469
H4	-2.9999644294	-2.6702187494	2.9946387869
C8	-2.7426672956	0.6546811637	3.6920735521
C11	-0.9497183169	2.1459198615	2.4208127750
H7	-3.1762743134	1.3992173904	4.3355281353
C9	-3.1879856910	-0.6483570844	3.7409436743
H8	-3.9728895093	-0.9095416004	4.4272694645
C10	-2.6429704192	-1.6600851796	2.9242590216
C12	-0.0716241692	1.7744356070	1.4512907646
C2	0.9269144697	2.6056206604	0.7453112864
H13	1.7074422886	-2.8817125614	-0.2753663900
C14	0.3076938336	-2.7045928872	-1.8905668910
H15	0.2923378719	-3.9050788522	-0.1052980764
C15	-0.3053244872	-2.3158522487	-4.5878771164
C16	1.3069751907	-2.4063165422	-2.8077883962
C17	-1.0079025385	-2.8063076055	-2.3422753578
C18	-1.3113854749	-2.6134522525	-3.6776129076
C19	1.0025465289	-2.2143970874	-4.1491423166

H16	2.3309432563	-2.3188574629	-2.4786269976
H17	-1.7917111891	-3.0332743005	-1.6406619581
H18	-2.3295554842	-2.6925171880	-4.0106917005
H19	1.7907633063	-1.9834667927	-4.8460183616
H20	-0.5422240742	-2.1661899720	-5.6255384105
C1	0.5644095491	-0.5120677085	0.4353968420
H5	1.5708233822	-0.5629812851	0.8428439319
H6	0.6581057935	-0.2218487346	-0.5998173568
C3	2.7889171356	4.2151427700	-0.5660685035
C26	1.8162112152	3.3890211368	1.4702869848
C27	0.9775928654	2.6431062201	-0.6456130349
C28	1.9045321762	3.4402657775	-1.2949648747
C29	2.7395960663	4.1914658022	0.8181678154
H1	1.7871549220	3.3588554939	2.5468422945
H2	0.2728790876	2.0718618690	-1.2204641568
H3	1.9264167737	3.4627840599	-2.3698183664
H9	3.4212751180	4.7898184578	1.3932077598
H10	3.5069237148	4.8342820442	-1.0716438394
H25	-1.0577771051	3.1427356635	2.7959918279

nuclear repulsion energy..... 1971.488097852 hartrees

/ end of geometry optimization iteration 11 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.800E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	86	88	89	88	84
73							
grid # 2	103	112	95	95	98	98	92
118							
grid # 3	214	227	195	186	190	199	164
224							
grid # 4	389	414	322	321	325	347	300
224							

number of gridpoints:							
	atom	C8	C11	H7	C9	H8	C10
C2							C12
92	grid # 1	89	86	73	87	73	86
100	grid # 2	97	94	118	97	118	94
195	grid # 3	184	184	223	184	222	194
343	grid # 4	330	331	226	329	223	317

number of gridpoints:							
	atom	H13	C14	H15	C15	C16	C17
C19							C18
89	grid # 1	69	91	69	89	88	89
96	grid # 2	110	100	110	97	96	97
183	grid # 3	211	196	214	183	184	184
327	grid # 4	214	340	215	327	327	327

number of gridpoints:							
	atom	H16	H17	H18	H19	H20	C1
H6							H5
69	grid # 1	72	73	73	73	73	70
104	grid # 2	114	115	118	118	118	110
207	grid # 3	214	216	222	222	224	217
202	grid # 4	214	214	224	223	224	217

number of gridpoints:							
	atom	C3	C26	C27	C28	C29	H1
H3							H2
73	grid # 1	89	89	88	89	89	71
118	grid # 2	97	95	96	97	97	114
222	grid # 3	185	182	184	185	184	214
224	grid # 4	328	327	331	327	328	212

number of gridpoints:					
	atom	H9	H10	H25	total
	grid # 1	73	73	72	3516
	grid # 2	118	118	115	4493

```

grid # 3      223      223      220      8631
grid # 4      224      224      224     12247

```

end of program grid

```

start of program rwr
end of program rwr

```

start of program scf

	i	u	d	i	g		energy	RMS	maximum
	t	p	i	c	r		change	density	DIIS
	e	d	i	u	i			change	error
	r	t	s	t	d	total energy			
etot	1	N	N	1	U	-990.38859773819		8.1E-05	3.6E-03
etot	2	Y	Y	4	M	-990.39048554750	1.9E-03	3.8E-05	1.4E-03
etot	3	Y	Y	4	M	-990.39075521604	2.7E-04	1.1E-05	3.8E-04
etot	4	N	Y	1	U	-990.39078219283	2.7E-05	6.5E-06	1.5E-04
etot	5	Y	Y	4	M	-990.39078684366	4.7E-06	1.8E-06	3.2E-05
etot	6	Y	N	4	M	-990.39078874833	1.9E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

```

(A) Nuclear repulsion..... 1971.48809785247
(E) Total one-electron terms..... -5261.23708829039
(I) Total two-electron terms..... 2299.35820168958
(L) Electronic energy..... -2961.87888660080 (E+I)
(N) Total energy..... -990.39078874833 (A+L)

```

```

SCFE: SCF energy: HF      -990.39078874833 hartrees   iterations:
6

```

```

HOMO energy:      -0.26900
LUMO energy:       0.09681

```

Orbital energies:

-15.60450	-15.56520	-11.29613	-11.28583	-11.27124	-11.25060
-11.25060	-11.24629	-11.24564	-11.24013	-11.23934	-11.23862
-11.23812	-11.23741	-11.23665	-11.23611	-11.23489	-11.23442
-11.23272	-11.23078	-11.22433	-11.21958	-11.21829	-11.21571
-11.21257	-1.32518	-1.24924	-1.16401	-1.16055	-1.13914
-1.07477	-1.06714	-1.04013	-1.02193	-1.01901	-1.01706
-0.97170	-0.95432	-0.93398	-0.86039	-0.83766	-0.83356
-0.82897	-0.80722	-0.79561	-0.77030	-0.73280	-0.71772
-0.70154	-0.69847	-0.66672	-0.65798	-0.64297	-0.63737
-0.63423	-0.62375	-0.62103	-0.61586	-0.59622	-0.59244
-0.59059	-0.58747	-0.57852	-0.55830	-0.55278	-0.54840
-0.54412	-0.51758	-0.50739	-0.50284	-0.50056	-0.49599

-0.49355	-0.49122	-0.48722	-0.48146	-0.42973	-0.40470
-0.36763	-0.34405	-0.34100	-0.33769	-0.32924	-0.28262
-0.26900	0.09681	0.12911	0.13706	0.13737	0.14842
0.17898	0.20870	0.22842	0.23520	0.24150	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	7.004627E-04	-5.345029E-04	-8.693736E-04
2	N2	1.325105E-03	4.490218E-04	-1.207276E-03
3	C4	6.466353E-04	-1.748891E-03	-5.276414E-04
4	C5	-1.583901E-03	-5.770104E-05	1.464054E-03
5	C6	2.273493E-03	-1.141576E-03	-2.212237E-03
6	C7	-6.504121E-04	1.484241E-03	1.389573E-04
7	C13	-1.049263E-04	-1.124955E-03	1.171673E-03
8	H4	-4.026407E-04	-9.691760E-04	-5.464798E-05
9	C8	-9.303924E-04	-6.391797E-04	4.551451E-04
10	C11	6.920090E-04	1.520404E-03	3.671516E-04
11	H7	-7.863954E-05	4.226999E-04	2.440591E-04
12	C9	-2.025401E-04	1.476436E-03	5.741089E-04
13	H8	-5.400360E-04	-1.340263E-04	4.904071E-04
14	C10	-7.800840E-05	-1.362858E-04	6.780081E-04
15	C12	-2.323231E-04	-3.858693E-04	8.130474E-04
16	C2	-1.650918E-03	-1.050059E-03	-4.870314E-04
17	H13	-1.249323E-03	3.298007E-04	-3.456024E-04
18	C14	3.372735E-04	3.524076E-05	-8.065477E-04
19	H15	3.415639E-04	3.736382E-04	-5.501722E-04
20	C15	-7.211408E-05	-4.291507E-04	1.165413E-03
21	C16	1.485377E-04	5.669822E-04	3.571922E-04
22	C17	9.294633E-04	4.954721E-05	8.698192E-04
23	C18	1.506381E-03	3.791037E-04	-2.957498E-04
24	C19	1.342766E-03	5.454351E-04	-6.709570E-04
25	H16	-1.552766E-03	-6.560598E-04	-2.441234E-04
26	H17	1.700841E-04	-9.802381E-05	1.903320E-04
27	H18	-1.365794E-03	-2.753192E-04	-2.401760E-04
28	H19	-6.056477E-04	-1.969351E-04	3.560983E-04
29	H20	-1.099160E-04	1.214393E-04	-7.279111E-04
30	C1	-1.851382E-03	-1.238949E-04	1.290145E-03

31	H5	1.574782E-03	1.314021E-04	1.035441E-03
32	H6	3.969414E-04	6.577154E-04	-2.503026E-03
33	C3	1.115385E-03	1.071782E-03	1.756491E-03
34	C26	1.717762E-03	1.497857E-03	2.251613E-03
35	C27	3.012996E-04	7.204426E-04	-9.322043E-04
36	C28	-1.972431E-03	-1.672589E-03	-1.659435E-03
37	C29	-8.471681E-04	-7.644455E-04	8.396384E-04
38	H1	2.871811E-04	2.205505E-04	-1.629586E-03
39	H2	-7.152317E-04	-9.510178E-04	-5.023593E-04
40	H3	1.101136E-05	-8.687548E-05	-4.894680E-04
41	H9	1.039112E-03	8.927797E-04	5.902413E-04
42	H10	7.541013E-04	6.428744E-04	-3.083269E-04
43	H25	-2.161468E-04	5.428347E-04	2.594211E-04
-----				
	total	5.986926E-04	9.556962E-04	9.460540E-05

end of program derlb

start of program geopt 12

geometry optimization step 12

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0381814

Cos(theta): 0.6358626

Final level shift: -2.2947896E-02

energy change: 3.1850E-05 \* ( 5.0000E-05 )

gradient maximum: 3.7159E-03 . ( 4.5000E-04 )

gradient rms: 7.8551E-04 . ( 3.0000E-04 )

step size: 0.03818 trust radius: 0.03750

displacement maximum: 1.1555E-02 . ( 1.8000E-03 )

displacement rms: 2.9998E-03 . ( 1.2000E-03 )

predicted energy change: -1.3809E-04 geom step: 3.8181E-

02 full step: 3.8181E-02

molecular structure not yet converged...

center of mass moved by:

x: 4.5426E-04 y: 8.1147E-04 z: -6.7642E-04

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2481100487	0.4334566292	1.1690590843
N2	-1.0032005669	-2.2934581620	1.1949409475

C4	-1.2219414340	-0.0343838020	1.9923563545
C5	-0.0339796710	-1.9120602342	0.4839591872
C6	-1.6327378826	-1.3563177585	2.0371288910
C7	-1.7214706152	0.9842720805	2.7832559656
C13	0.6387689584	-2.9205192316	-0.4241415240
H4	-2.9960643356	-2.6736608684	2.9862523038
C8	-2.7543266162	0.6556694707	3.6773710238
C11	-0.9567330317	2.1503186557	2.4169640341
H7	-3.1942470497	1.4021628828	4.3154141299
C9	-3.1938710405	-0.6480229029	3.7284797792
H8	-3.9830026483	-0.9107663027	4.4110346409
C10	-2.6387220303	-1.6617110159	2.9180186584
C12	-0.0739060768	1.7781436478	1.4520699323
C2	0.9254724195	2.6102272532	0.7486369541
H13	1.7151095547	-2.8707079086	-0.2840967415
C14	0.3101739106	-2.7047976511	-1.8919547337
H15	0.3108881878	-3.9021230759	-0.1082165064
C15	-0.3249288630	-2.3285963028	-4.5840286299
C16	1.2990880581	-2.4022115814	-2.8172990363
C17	-1.0064246650	-2.8179513158	-2.3322450242
C18	-1.3210023891	-2.6315174078	-3.6652839004
C19	0.9856382061	-2.2157562838	-4.1570604658
H16	2.3222336572	-2.3129300127	-2.4940718207
H17	-1.7807423369	-3.0503320668	-1.6229685692
H18	-2.3412419940	-2.7221754401	-3.9894950791
H19	1.7641119017	-1.9818956103	-4.8615237321
H20	-0.5712857690	-2.1834408899	-5.6215168996
C1	0.5743863458	-0.5077215009	0.4405346425
H5	1.5783628755	-0.5595077770	0.8633906677
H6	0.6828551014	-0.2141085169	-0.5964581000
C3	2.7976584351	4.2167944296	-0.5536768887
C26	1.8195941604	3.3876491689	1.4793453416
C27	0.9766033142	2.6525116204	-0.6445526402
C28	1.9079513036	3.4480386227	-1.2902513713
C29	2.7477220187	4.1880060271	0.8321252429
H1	1.7898857173	3.3527087763	2.5543504826
H2	0.2700912980	2.0817515541	-1.2208892319
H3	1.9329210192	3.4750874837	-2.3661874570
H9	3.4352847020	4.7809146017	1.4097776804
H10	3.5220132279	4.8352318702	-1.0559521854
H25	-1.0710358057	3.1480250996	2.7899724688

nuclear repulsion energy..... 1971.062170283 hartrees

/ end of geometry optimization iteration 12 /

end of program geopt

start of program onee  
smallest eigenvalue of S: 2.810E-04



number of canonical orbitals..... 461  
end of program onee

start of program probe  
end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	95	102	87	87	90	89	84
73							
grid # 2	103	112	95	95	99	98	92
118							
grid # 3	214	227	195	187	191	199	163
224							
grid # 4	385	414	321	320	323	348	299
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	194
195							
grid # 4	328	331	226	331	223	329	317
343							

number of gridpoints:

atom	H13	C14	H15	C15	C16	C17	C18
C19							
grid # 1	69	91	69	89	88	87	89
89							
grid # 2	109	100	110	97	96	96	97
96							
grid # 3	211	196	214	183	184	182	184
183							
grid # 4	214	340	213	327	327	327	327
327							

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
H6							
grid # 1	72	73	73	73	73	82	70
69							

grid # 2	114	114	118	118	118	88	109
104							
grid # 3	214	216	222	221	224	164	217
207							
grid # 4	214	214	224	223	224	292	219
206							

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
H3							
grid # 1	89	88	88	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	185	182	184	185	185	217	213
223							
grid # 4	328	327	330	328	328	217	212
224							

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3515
grid # 2	118	118	115	4491
grid # 3	223	224	220	8634
grid # 4	224	224	224	12246

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.39028009303		4.3E-05	2.4E-03
etot	2	Y	Y	4	M	-990.39078089231	5.0E-04	1.8E-05	5.5E-04
etot	3	Y	Y	4	M	-990.39083518771	5.4E-05	4.9E-06	1.2E-04
etot	4	Y	N	4	M	-990.39084155577	6.4E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.06217028341	
(E)	Total one-electron terms.....	-5260.39454868744	
(I)	Total two-electron terms.....	2298.94153684826	
(L)	Electronic energy.....	-2961.45301183918	(E+I)
(N)	Total energy.....	-990.39084155577	(A+L)

SCFE: SCF energy: HF -990.39084155577 hartrees iterations:  
4

HOMO energy: -0.26906  
LUMO energy: 0.09673

Orbital energies:

-15.60462	-15.56496	-11.29644	-11.28704	-11.27124	-11.25104
-11.25071	-11.24585	-11.24537	-11.24021	-11.23959	-11.23927
-11.23874	-11.23808	-11.23742	-11.23573	-11.23438	-11.23415
-11.23269	-11.23001	-11.22431	-11.22021	-11.21853	-11.21599
-11.21287	-1.32532	-1.24973	-1.16308	-1.16069	-1.13877
-1.07464	-1.06716	-1.03922	-1.02184	-1.01901	-1.01724
-0.97091	-0.95440	-0.93382	-0.86015	-0.83698	-0.83354
-0.82928	-0.80716	-0.79551	-0.77003	-0.73266	-0.71746
-0.70102	-0.69855	-0.66633	-0.65789	-0.64293	-0.63722
-0.63387	-0.62365	-0.62070	-0.61586	-0.59633	-0.59238
-0.59043	-0.58757	-0.57842	-0.55802	-0.55233	-0.54821
-0.54447	-0.51739	-0.50720	-0.50256	-0.50022	-0.49593
-0.49341	-0.49120	-0.48742	-0.48125	-0.42975	-0.40484
-0.36746	-0.34335	-0.34121	-0.33758	-0.32931	-0.28234
-0.26906	0.09673	0.12890	0.13698	0.13758	0.14860
0.17856	0.20869	0.22823	0.23521	0.24124	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	2.227998E-04	3.002457E-04	-7.633866E-04
2	N2	8.313377E-04	6.278822E-05	-8.329915E-04
3	C4	-2.749466E-04	-4.216903E-04	-5.263447E-07
4	C5	-6.186970E-04	-7.144881E-04	3.670361E-04
5	C6	2.786252E-04	3.974446E-05	-3.989161E-04
6	C7	9.204291E-05	2.064961E-04	1.809267E-04
7	C13	-2.647782E-04	7.202521E-04	7.337563E-04
8	H4	4.755602E-05	2.153163E-04	1.133755E-04
9	C8	-3.968861E-04	6.246385E-04	6.455230E-04

10	C11	1.871446E-05	4.167742E-04	-1.449800E-04
11	H7	4.661710E-05	-2.622866E-05	2.075457E-05
12	C9	-4.135986E-04	-8.043030E-04	2.383556E-04
13	H8	9.219046E-05	1.817128E-05	-3.487273E-05
14	C10	-5.487297E-04	-5.031939E-04	3.007736E-04
15	C12	4.545402E-04	3.326283E-05	3.764629E-06
16	C2	3.716824E-04	4.474287E-04	-1.073648E-03
17	H13	6.660705E-04	2.713936E-04	-4.580298E-05
18	C14	-9.524221E-06	-1.503978E-05	-1.155393E-04
19	H15	-2.589289E-04	-4.741291E-04	1.596626E-04
20	C15	-3.296994E-04	-8.513451E-05	-3.637118E-04
21	C16	5.059299E-04	2.273868E-04	1.343442E-04
22	C17	1.784530E-04	6.295302E-06	3.790300E-04
23	C18	4.746219E-04	1.823099E-04	-5.954331E-04
24	C19	-1.022632E-04	1.979797E-04	6.156296E-05
25	H16	3.316220E-04	-1.320570E-04	5.700000E-06
26	H17	-4.687600E-04	-9.797374E-05	2.750276E-04
27	H18	-1.205098E-03	-6.438215E-05	-3.681211E-04
28	H19	4.370449E-04	-4.587109E-06	-2.768543E-05
29	H20	1.076385E-05	-4.651129E-05	2.680799E-04
30	C1	1.139672E-03	1.536346E-04	3.587566E-04
31	H5	-4.346405E-04	-9.406025E-07	-3.907024E-04
32	H6	-1.517462E-04	-9.902310E-05	3.357495E-04
33	C3	1.185490E-04	2.269726E-04	5.102438E-04
34	C26	-2.577180E-06	8.957851E-05	-5.609457E-05
35	C27	1.261047E-04	2.099169E-04	7.317389E-04
36	C28	2.097073E-04	1.577945E-04	1.716548E-04
37	C29	3.597928E-05	-6.029637E-05	-9.796868E-04
38	H1	9.699556E-05	7.995279E-05	-5.711064E-04
39	H2	8.836115E-05	-5.681230E-05	5.451637E-05
40	H3	-2.236567E-05	-8.217920E-05	5.481682E-04
41	H9	-1.316816E-04	3.301862E-05	-1.580912E-04
42	H10	-5.437240E-04	-3.859753E-04	3.434680E-04
43	H25	-4.214022E-06	-3.049285E-05	3.941865E-06
-----		-----	-----	-----
total		6.931218E-04	8.159137E-04	2.461458E-05

end of program der1b

start of program geopt 13

geometry optimization step 13

reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0192086

Cos(theta): 0.7007821

Final level shift: -6.0023224E-02

energy change: -5.2807E-05 . ( 5.0000E-05 )  
gradient maximum: 1.3227E-03 . ( 4.5000E-04 )  
gradient rms: 3.7901E-04 . ( 3.0000E-04 )  
step size: 0.01921 trust radius: 0.01875  
displacement maximum: 6.9080E-03 . ( 1.8000E-03 )  
displacement rms: 1.5092E-03 . ( 1.2000E-03 )  
predicted energy change: -4.3542E-05 geom step: 1.9209E-  
02 full step: 1.9209E-02  
molecular structure not yet converged...

center of mass moved by:

x: -2.9109E-04 y: 4.6312E-04 z: 3.9301E-04

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2488255692	0.4322339843	1.1698872896
N2	-1.0058226391	-2.2950440448	1.1945544518
C4	-1.2229240041	-0.0361424909	1.9939013709
C5	-0.0365007616	-1.9141015496	0.4855354067
C6	-1.6347093114	-1.3580296563	2.0375911084
C7	-1.7199951420	0.9823189968	2.7870807318
C13	0.6348421100	-2.9216660268	-0.4233610698
H4	-2.9973932708	-2.6761090969	2.9877417657
C8	-2.7524946331	0.6532233934	3.6829849331
C11	-0.9547024201	2.1488365611	2.4190560905
H7	-3.1905897249	1.3985912480	4.3231430452
C9	-3.1932086574	-0.6517690880	3.7325641745
H8	-3.9812949477	-0.9149495298	4.4155551603
C10	-2.6401022769	-1.6646647698	2.9195236102
C12	-0.0728836370	1.7767980278	1.4534342970
C2	0.9248616477	2.6094547063	0.7465477863
H13	1.7116541383	-2.8719037968	-0.2842566294
C14	0.3090127646	-2.7017285669	-1.8919217197
H15	0.3057087418	-3.9036615388	-0.1088356875
C15	-0.3181517155	-2.3211174476	-4.5844573536
C16	1.3022806045	-2.4054300452	-2.8151364504
C17	-1.0074098438	-2.8056006886	-2.3339389563
C18	-1.3187367817	-2.6172398029	-3.6681293975
C19	0.9926701615	-2.2159193741	-4.1546871043
H16	2.3260666979	-2.3274211924	-2.4914155295
H17	-1.7860704955	-3.0349791182	-1.6266254226
H18	-2.3425831130	-2.7043182588	-3.9940814180
H19	1.7761371458	-1.9889515630	-4.8563274949
H20	-0.5618666539	-2.1757307323	-5.6219403179
C1	0.5740559454	-0.5100177170	0.4417086690
H5	1.5784350739	-0.5618273663	0.8611698811
H6	0.6798161828	-0.2186286872	-0.5959096950
C3	2.7946536701	4.2153968164	-0.5592303079

C26	1.8165501131	3.3931684312	1.4740306347
C27	0.9780419294	2.6451051479	-0.6454457865
C28	1.9082602778	3.4400244963	-1.2927166344
C29	2.7429412688	4.1934511473	0.8251154766
H1	1.7882002850	3.3627714017	2.5482192846
H2	0.2755486666	2.0683734653	-1.2209902818
H3	1.9348576060	3.4600611274	-2.3678965230
H9	3.4273881104	4.7918441078	1.4013512856
H10	3.5166904418	4.8328913912	-1.0628356014
H25	-1.0679447669	3.1461658281	2.7930681050

nuclear repulsion energy..... 1971.091366916 hartrees

/ end of geometry optimization iteration 13 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.824E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

atom	N1	N2	C4	C5	C6	C7	C13
H4							
grid # 1	96	102	87	87	90	90	84
73							
grid # 2	103	112	95	95	99	98	92
118							
grid # 3	214	227	195	187	191	199	163
224							
grid # 4	389	414	321	320	323	347	299
224							

number of gridpoints:

atom	C8	C11	H7	C9	H8	C10	C12
C2							
grid # 1	89	86	73	87	73	89	86
92							
grid # 2	97	94	118	97	118	97	94
100							
grid # 3	184	185	223	184	222	184	194
196							

grid # 4	329	331	226	331	223	329	317
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341

number of gridpoints:							
atom	H13	C14	H15	C15	C16	C17	C18

C19

grid # 1	69	93	69	89	88	88	89
----------	----	----	----	----	----	----	----

89

grid # 2	109	100	110	97	96	96	97
----------	-----	-----	-----	----	----	----	----

96

grid # 3	210	195	214	183	184	183	184
----------	-----	-----	-----	-----	-----	-----	-----

183

grid # 4	214	340	213	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:							
atom	H16	H17	H18	H19	H20	C1	H5

H6

grid # 1	72	73	73	73	73	82	70
----------	----	----	----	----	----	----	----

69

grid # 2	114	115	118	118	118	88	110
----------	-----	-----	-----	-----	-----	----	-----

104

grid # 3	214	216	223	222	224	164	217
----------	-----	-----	-----	-----	-----	-----	-----

207

grid # 4	214	214	224	223	224	293	217
----------	-----	-----	-----	-----	-----	-----	-----

205

number of gridpoints:							
atom	C3	C26	C27	C28	C29	H1	H2

H3

grid # 1	89	88	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
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118

grid # 3	185	182	184	184	185	217	213
----------	-----	-----	-----	-----	-----	-----	-----

223

grid # 4	328	328	329	328	328	217	212
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:				
atom	H9	H10	H25	total

grid # 1	73	73	72	3520
grid # 2	118	118	115	4493
grid # 3	223	223	220	8634
grid # 4	224	224	224	12246

end of program grid

start of program rwr  
end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r				
	e	d	i	u	i		energy	density	DIIS
	r	t	s	t	d	total energy	change	change	error
etot	1	N	N	1	U	-990.39066938504		2.3E-05	1.1E-03
etot	2	Y	Y	4	M	-990.39082701468	1.6E-04	1.1E-05	4.2E-04
etot	3	Y	Y	4	M	-990.39084593688	1.9E-05	3.2E-06	1.1E-04
etot	4	Y	N	4	M	-990.39084898231	3.0E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.09136691580	
(E)	Total one-electron terms.....	-5260.45116671076	
(I)	Total two-electron terms.....	2298.96895081265	
(L)	Electronic energy.....	-2961.48221589810	(E+I)
(N)	Total energy.....	-990.39084898231	(A+L)

SCFE: SCF energy: HF -990.39084898231 hartrees iterations:

4

HOMO energy: -0.26909  
LUMO energy: 0.09670

Orbital energies:

-15.60482	-15.56511	-11.29607	-11.28679	-11.27163	-11.25115
-11.25090	-11.24617	-11.24561	-11.23984	-11.23956	-11.23889
-11.23843	-11.23775	-11.23701	-11.23573	-11.23460	-11.23444
-11.23276	-11.23041	-11.22479	-11.22011	-11.21902	-11.21611
-11.21311	-1.32505	-1.25012	-1.16329	-1.16072	-1.13844
-1.07455	-1.06701	-1.03926	-1.02193	-1.01882	-1.01722
-0.97108	-0.95429	-0.93372	-0.86021	-0.83691	-0.83360
-0.82903	-0.80715	-0.79555	-0.77004	-0.73267	-0.71741
-0.70115	-0.69841	-0.66628	-0.65791	-0.64291	-0.63702
-0.63380	-0.62376	-0.62069	-0.61579	-0.59625	-0.59229
-0.59055	-0.58752	-0.57825	-0.55807	-0.55233	-0.54821
-0.54447	-0.51744	-0.50724	-0.50258	-0.50023	-0.49595
-0.49354	-0.49120	-0.48746	-0.48116	-0.42969	-0.40485
-0.36758	-0.34333	-0.34129	-0.33767	-0.32932	-0.28244
-0.26909	0.09670	0.12895	0.13716	0.13754	0.14851
0.17843	0.20872	0.22830	0.23522	0.24111	

end of program scf

start of program derla  
end of program derla



start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
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1	N1	4.528739E-04	-2.150721E-04	-7.189734E-04
2	N2	-5.179471E-04	-3.795031E-05	3.540438E-04
3	C4	1.453513E-04	-6.415916E-05	2.186439E-05
4	C5	7.956954E-04	-7.125645E-05	-6.055630E-04
5	C6	1.674864E-04	-8.425208E-05	-1.081652E-04
6	C7	-2.512909E-04	2.681225E-04	1.706745E-04
7	C13	2.264142E-04	5.762714E-04	8.823663E-05
8	H4	-6.045948E-05	-1.622022E-04	5.346281E-05
9	C8	-9.811810E-06	-6.163186E-04	-1.033681E-04
10	C11	-3.140914E-04	-5.043245E-07	3.741302E-04
11	H7	-7.779658E-05	9.048357E-05	3.931211E-05
12	C9	2.767482E-04	5.658957E-04	-1.033924E-04
13	H8	-1.429809E-04	-1.901601E-05	1.548469E-04
14	C10	-7.750078E-05	3.688975E-04	2.521305E-04
15	C12	4.616740E-04	5.257927E-06	-2.829912E-04
16	C2	2.944823E-04	2.233180E-04	5.568139E-04
17	H13	4.427948E-04	6.578201E-05	1.726383E-04
18	C14	1.282378E-04	-1.306465E-04	5.130233E-04
19	H15	-1.131664E-04	-2.810631E-04	-3.533440E-05
20	C15	-5.253545E-04	1.215568E-05	-8.190267E-05
21	C16	1.228580E-04	-7.128547E-05	5.101624E-04
22	C17	-7.451867E-04	-2.526086E-04	2.209580E-04
23	C18	-1.326991E-03	-2.850276E-04	-7.335060E-04
24	C19	-1.692902E-04	6.245857E-06	-3.167455E-04
25	H16	3.328469E-04	1.496603E-04	2.129530E-04
26	H17	3.554518E-04	1.287242E-04	-1.716810E-04
27	H18	1.486137E-03	2.577115E-04	2.009026E-04
28	H19	1.714175E-05	8.756748E-05	-1.598401E-04
29	H20	3.361176E-05	4.889786E-05	-2.258726E-04
30	C1	-2.352300E-04	1.325569E-04	1.607766E-04
31	H5	-2.663504E-05	8.592286E-06	1.148176E-04
32	H6	-4.109229E-05	8.430998E-05	1.882357E-04
33	C3	-4.420181E-04	-1.741977E-04	-2.983395E-04
34	C26	-2.316693E-04	-2.309980E-04	-1.002232E-04
35	C27	-8.113392E-05	-3.491728E-05	-1.261326E-04
36	C28	2.378795E-04	1.576131E-04	7.887497E-05
37	C29	1.155601E-04	5.628839E-05	2.498595E-04
38	H1	-1.391838E-04	-3.540240E-05	1.268414E-04
39	H2	6.131107E-05	1.420514E-04	1.187152E-04
40	H3	5.722184E-05	1.176396E-04	-1.489399E-04
41	H9	-1.997639E-04	-2.093410E-04	-2.637846E-04

42	H10	2.310080E-04	2.058152E-04	-3.046466E-04
43	H25	-5.723237E-05	6.307406E-05	-1.828532E-05
-----				
	total	6.569597E-04	8.467135E-04	2.658720E-05

end of program derlb

start of program geopt 14

geometry optimization step 14

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0108550

Cos(theta): 0.7082419

Final level shift: -3.0472439E-02

energy change: -7.4265E-06 \* ( 5.0000E-05 )

gradient maximum: 1.4699E-03 . ( 4.5000E-04 )

gradient rms: 2.7737E-04 \* ( 3.0000E-04 )

step size: 0.01085 trust radius: 0.01000

displacement maximum: 4.5549E-03 . ( 1.8000E-03 )

displacement rms: 8.5285E-04 \* ( 1.2000E-03 )

predicted energy change: -1.5366E-05 geom step: 1.0855E-

02 full step: 1.0855E-02

molecular structure not yet converged...

center of mass moved by:

x: 2.3234E-04 y: -3.9719E-04 z: 1.1836E-04

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2476098628	0.4319499494	1.1700896461
N2	-1.0050850757	-2.2950871682	1.1949182325
C4	-1.2225555532	-0.0359392069	1.9934979632
C5	-0.0345337388	-1.9145591457	0.4863206158
C6	-1.6345629750	-1.3576518558	2.0372932256
C7	-1.7207638142	0.9827487410	2.7857085019
C13	0.6372167911	-2.9214974519	-0.4226269266
H4	-2.9991767135	-2.6746254046	2.9867461727
C8	-2.7544283972	0.6541992122	3.6802520196
C11	-0.9547075557	2.1487129569	2.4185234965
H7	-3.1936858699	1.4000793918	4.3191782963

C9	-3.1953417522	-0.6499826706	3.7301011813
H8	-3.9846205275	-0.9126483273	4.4122075724
C10	-2.6412076664	-1.6632555907	2.9184523073
C12	-0.0714118196	1.7763193928	1.4539254438
C2	0.9267126827	2.6085697080	0.7475086448
H13	1.7145636018	-2.8715088035	-0.2838423517
C14	0.3089199593	-2.7020981095	-1.8909152593
H15	0.3081077662	-3.9039526830	-0.1083403583
C15	-0.3215924809	-2.3201267580	-4.5836616469
C16	1.3004540244	-2.3992437756	-2.8137797881
C17	-1.0077278059	-2.8118948597	-2.3339058106
C18	-1.3203617236	-2.6227459376	-3.6680394462
C19	0.9888784831	-2.2093360982	-4.1534576988
H16	2.3240667900	-2.3146888619	-2.4895233992
H17	-1.7849137076	-3.0449393883	-1.6268919447
H18	-2.3419771432	-2.7122708466	-3.9947783125
H19	1.7707403444	-1.9764961643	-4.8551652860
H20	-0.5656277175	-2.1736956496	-5.6211053749
C1	0.5760456600	-0.5105838268	0.4433549677
H5	1.5800429573	-0.5626136306	0.8641513090
H6	0.6825437933	-0.2189447287	-0.5941242795
C3	2.7951744578	4.2145617192	-0.5601377830
C26	1.8187572576	3.3915699332	1.4744469707
C27	0.9785171969	2.6447421378	-0.6446715605
C28	1.9082206454	3.4396720163	-1.2930044553
C29	2.7448249516	4.1917280945	0.8244421729
H1	1.7902754511	3.3610162274	2.5486052296
H2	0.2747696491	2.0686681731	-1.2192937084
H3	1.9337718424	3.4605773143	-2.3682340620
H9	3.4301063300	4.7894624992	1.3997519889
H10	3.5171655374	4.8322369654	-1.0645143063
H25	-1.0688078963	3.1463685995	2.7914697600

nuclear repulsion energy..... 1971.109269844 hartrees

/ end of geometry optimization iteration 14 /

end of program geopt

start of program onee

smallest eigenvalue of S: 2.820E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:								
	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	96	102	87	87	90	90	84
73								
	grid # 2	103	112	95	95	99	98	92
118								
	grid # 3	214	227	195	187	191	199	163
224								
	grid # 4	389	414	322	320	323	347	299
224								

number of gridpoints:								
	atom	C8	C11	H7	C9	H8	C10	C12
C2								
	grid # 1	89	86	73	87	73	89	86
92								
	grid # 2	97	94	118	97	118	97	94
100								
	grid # 3	184	185	223	184	222	184	194
195								
	grid # 4	329	331	226	331	223	329	317
341								

number of gridpoints:								
	atom	H13	C14	H15	C15	C16	C17	C18
C19								
	grid # 1	69	91	69	89	88	88	89
89								
	grid # 2	110	100	110	97	96	96	97
96								
	grid # 3	211	197	214	183	184	183	184
183								
	grid # 4	214	340	213	327	327	327	327
327								

number of gridpoints:								
	atom	H16	H17	H18	H19	H20	C1	H5
H6								
	grid # 1	72	73	73	73	73	82	70
69								
	grid # 2	114	115	118	118	118	88	110
104								
	grid # 3	214	216	223	222	224	164	217
207								
	grid # 4	214	214	224	223	224	293	217
205								

number of gridpoints:								
	atom	C3	C26	C27	C28	C29	H1	H2
H3								

grid # 1	89	88	88	89	89	72	71
73							
grid # 2	97	95	96	97	97	115	114
118							
grid # 3	185	182	184	185	185	217	213
223							
grid # 4	328	328	329	328	328	217	212
224							

number of gridpoints:

atom	H9	H10	H25	total
grid # 1	73	73	72	3518
grid # 2	118	118	115	4494
grid # 3	223	224	220	8638
grid # 4	224	224	224	12247

end of program grid

start of program rwr

end of program rwr

start of program scf

	i	u	d	i	g			RMS	maximum
	t	p	i	c	r			density	DIIS
	e	d	i	u	i		energy	change	error
	r	t	s	t	d	total energy	change		
etot	1	N	N	1	U	-990.39080246980		1.4E-05	9.2E-04
etot	2	Y	Y	4	M	-990.39085334491	5.1E-05	6.4E-06	3.6E-04
etot	3	Y	Y	4	M	-990.39085990967	6.6E-06	2.0E-06	9.6E-05
etot	4	Y	N	4	M	-990.39085924579	-6.6E-07	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.10926984366	
(E)	Total one-electron terms.....	-5260.48968808571	
(I)	Total two-electron terms.....	2298.98955899626	
(L)	Electronic energy.....	-2961.50012908945	(E+I)
(N)	Total energy.....	-990.39085924579	(A+L)

SCFE: SCF energy: HF -990.39085924579 hartrees iterations:  
4

HOMO energy: -0.26901  
LUMO energy: 0.09668

Orbital energies:

-15.60463	-15.56524	-11.29626	-11.28681	-11.27141	-11.25098
-----------	-----------	-----------	-----------	-----------	-----------

-11.25089	-11.24604	-11.24583	-11.23989	-11.23981	-11.23902
-11.23846	-11.23783	-11.23708	-11.23595	-11.23451	-11.23447
-11.23271	-11.23045	-11.22455	-11.22026	-11.21879	-11.21610
-11.21302	-1.32494	-1.24990	-1.16327	-1.16057	-1.13849
-1.07446	-1.06705	-1.03929	-1.02190	-1.01890	-1.01702
-0.97103	-0.95434	-0.93367	-0.86016	-0.83696	-0.83361
-0.82905	-0.80707	-0.79550	-0.76999	-0.73262	-0.71741
-0.70112	-0.69838	-0.66629	-0.65789	-0.64288	-0.63712
-0.63384	-0.62367	-0.62072	-0.61582	-0.59621	-0.59233
-0.59050	-0.58743	-0.57834	-0.55809	-0.55227	-0.54820
-0.54435	-0.51743	-0.50724	-0.50258	-0.50021	-0.49593
-0.49348	-0.49117	-0.48739	-0.48119	-0.42972	-0.40488
-0.36749	-0.34336	-0.34123	-0.33760	-0.32929	-0.28245
-0.26901	0.09668	0.12894	0.13711	0.13740	0.14856
0.17846	0.20869	0.22827	0.23519	0.24116	

end of program scf

start of program derla  
end of program derla

start of program rwr  
end of program rwr

start of program derlb

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	3.594168E-04	-3.247900E-04	-4.707368E-04
2	N2	1.456478E-04	1.299541E-04	-1.590589E-04
3	C4	1.259234E-04	-1.305667E-04	-7.187211E-05
4	C5	-3.678037E-05	-4.521296E-05	1.199478E-04
5	C6	5.984738E-05	-1.658855E-04	-5.162803E-05
6	C7	-6.725914E-05	2.139092E-04	6.314595E-05
7	C13	-3.445068E-05	1.086910E-04	1.095968E-04
8	H4	1.233470E-05	-3.123613E-05	3.656539E-05
9	C8	-2.053567E-05	3.892458E-05	6.619510E-05
10	C11	-3.836909E-05	2.069748E-04	1.279422E-04
11	H7	-2.571961E-06	9.001533E-05	2.737180E-05
12	C9	4.406467E-05	-4.942249E-05	-3.711664E-05
13	H8	-1.489958E-05	3.325105E-06	5.832352E-05
14	C10	-2.354330E-05	2.627673E-05	4.444407E-05
15	C12	1.173535E-04	8.037980E-05	-1.135315E-05
16	C2	3.023010E-05	1.143481E-04	1.144053E-04
17	H13	4.746262E-05	8.375568E-05	4.709878E-06
18	C14	-2.570906E-04	-7.682341E-05	2.962546E-05
19	H15	4.472624E-05	-6.375860E-05	-2.023663E-05

20	C15	1.891440E-04	6.801696E-05	-1.397037E-04
21	C16	8.780006E-05	7.855990E-05	-3.361955E-05
22	C17	7.344717E-05	-2.688328E-05	3.500123E-04
23	C18	-2.375303E-04	-1.002662E-04	-2.346247E-05
24	C19	3.475516E-05	4.269829E-05	-7.942340E-05
25	H16	-1.546063E-05	-3.301204E-05	-2.106096E-05
26	H17	6.240769E-05	4.272218E-05	5.193411E-05
27	H18	2.079249E-04	6.398798E-05	5.979060E-05
28	H19	-1.512320E-05	-2.486948E-05	-5.670209E-05
29	H20	3.073742E-05	1.633282E-05	-8.591535E-05
30	C1	-1.156034E-04	1.492051E-04	1.091582E-04
31	H5	-1.311443E-04	5.783864E-05	4.118251E-05
32	H6	4.583649E-05	3.741885E-05	1.991567E-04
33	C3	-1.431507E-04	-3.099268E-05	-1.181485E-04
34	C26	4.632667E-05	6.386637E-05	-1.655493E-04
35	C27	1.736270E-05	4.420336E-05	-2.361738E-04
36	C28	3.924001E-05	3.200689E-05	1.369748E-04
37	C29	1.549265E-05	1.514235E-05	4.802569E-05
38	H1	-3.310335E-05	2.030411E-05	1.784773E-04
39	H2	9.751055E-05	8.306954E-05	8.534773E-05
40	H3	2.527376E-05	2.668486E-05	-9.347572E-05
41	H9	-9.749903E-05	-4.736787E-05	-9.930280E-05
42	H10	-2.819321E-06	2.249804E-05	-7.816079E-05
43	H25	-1.728472E-05	5.798267E-05	1.449746E-05
-----				
	total	6.560473E-04	8.680061E-04	2.412989E-05

end of program derlb

start of program geopt 15

geometry optimization step 15

reading input hessian of dimension 129  
in five columns format  
reading input hessian of dimension 129  
in five columns format

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0143612

Cos(theta): 0.4919231

Final level shift: -2.7000810E-02

energy change: -1.0263E-05 \* ( 5.0000E-05 )  
gradient maximum: 4.0569E-04 \* ( 4.5000E-04 )  
gradient rms: 1.0457E-04 \* ( 3.0000E-04 )  
step size: 0.01436 trust radius: 0.01414  
displacement maximum: 8.4903E-03 . ( 1.8000E-03 )  
displacement rms: 1.1283E-03 \* ( 1.2000E-03 )

predicted energy change: -7.4859E-06      geom step: 1.4361E-02  
 full step: 1.4361E-02  
 molecular structure not yet converged...

center of mass moved by:  
 x: 2.6501E-05      y: -2.4923E-04      z: 6.1267E-05

new geometry:

	angstroms		
atom	x	y	z
N1	-0.2463607370	0.4314193906	1.1710338958
N2	-1.0035424221	-2.2955233045	1.1947806590
C4	-1.2216235933	-0.0368540479	1.9940347638
C5	-0.0326064789	-1.9145180546	0.4866450499
C6	-1.6331040260	-1.3588415492	2.0376289344
C7	-1.7214275643	0.9821252034	2.7857401080
C13	0.6387952323	-2.9207111820	-0.4230303496
H4	-2.9983933254	-2.6759482577	2.9865390107
C8	-2.7554322781	0.6531437848	3.6795071530
C11	-0.9556687926	2.1484771315	2.4194464699
H7	-3.1957362911	1.3993275357	4.3177668929
C9	-3.1954005477	-0.6509580953	3.7294178623
H8	-3.9851392350	-0.9139827639	4.4112945459
C10	-2.6402354285	-1.6642884757	2.9184542048
C12	-0.0716231059	1.7762215315	1.4549835704
C2	0.9257296648	2.6089482628	0.7484190091
H13	1.7160363204	-2.8699892414	-0.2843745120
C14	0.3092857777	-2.7015111760	-1.8910420198
H15	0.3107659365	-3.9038972276	-0.1098048464
C15	-0.3210182211	-2.3198001555	-4.5845563047
C16	1.3026267989	-2.4078132613	-2.8158087619
C17	-1.0093417649	-2.8017601438	-2.3324540938
C18	-1.3215507168	-2.6128445964	-3.6669555125
C19	0.9912426335	-2.2182211833	-4.1556558124
H16	2.3277109198	-2.3309831513	-2.4925549566
H17	-1.7872243266	-3.0262248434	-1.6238607485
H18	-2.3426567575	-2.6932803270	-3.9926346211
H19	1.7741739528	-1.9932912445	-4.8591528825
H20	-0.5645529054	-2.1734405864	-5.6223463359
C1	0.5782555737	-0.5107568800	0.4460053859
H5	1.5811573473	-0.5631828239	0.8704649311
H6	0.6880840404	-0.2177615274	-0.5909622482
C3	2.7922215595	4.2150771119	-0.5617697159
C26	1.8178585798	3.3922403513	1.4746958238
C27	0.9762379671	2.6449102789	-0.6443115909
C28	1.9050145102	3.4399273512	-1.2938231691
C29	2.7430458157	4.1923393067	0.8232302794
H1	1.7893807507	3.3619023049	2.5491513072
H2	0.2718921784	2.0685313456	-1.2175644237
H3	1.9300026211	3.4609305987	-2.3692287604
H9	3.4287854490	4.7902046058	1.3973483110
H10	3.5140165769	4.8329081285	-1.0672737690



H25            -1.0711083010            3.1462171349            2.7921150838

nuclear repulsion energy..... 1971.034696625 hartrees

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/ end of geometry optimization iteration 15 /  
-----

end of program geopt

start of program onee

smallest eigenvalue of S: 2.821E-04

number of canonical orbitals..... 461

end of program onee

start of program probe

end of program probe

start of program grid

number of gridpoints:

	atom	N1	N2	C4	C5	C6	C7	C13
H4								
	grid # 1	96	102	87	87	90	89	84
73								
	grid # 2	103	112	95	95	99	98	92
118								
	grid # 3	214	227	195	187	191	199	163
224								
	grid # 4	388	414	321	320	322	348	299
224								

number of gridpoints:

	atom	C8	C11	H7	C9	H8	C10	C12
C2								
	grid # 1	89	86	73	87	73	89	86
92								
	grid # 2	97	94	118	97	118	97	94
100								
	grid # 3	184	185	223	184	222	184	194
195								
	grid # 4	328	331	226	331	223	329	317
343								

number of gridpoints:

	atom	H13	C14	H15	C15	C16	C17	C18
C19								
	grid # 1	69	91	69	89	88	88	89
89								

grid # 2	109	100	110	97	96	96	97
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96

grid # 3	210	196	214	183	184	183	184
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183

grid # 4	214	340	213	327	327	327	327
----------	-----	-----	-----	-----	-----	-----	-----

327

number of gridpoints:

atom	H16	H17	H18	H19	H20	C1	H5
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H6

grid # 1	72	73	73	73	73	82	70
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69

grid # 2	114	115	118	118	118	88	109
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104

grid # 3	214	216	222	222	224	164	217
----------	-----	-----	-----	-----	-----	-----	-----

207

grid # 4	214	214	224	223	224	293	219
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205

number of gridpoints:

atom	C3	C26	C27	C28	C29	H1	H2
------	----	-----	-----	-----	-----	----	----

H3

grid # 1	89	88	88	89	89	72	71
----------	----	----	----	----	----	----	----

73

grid # 2	97	95	96	97	97	115	114
----------	----	----	----	----	----	-----	-----

118

grid # 3	185	182	183	185	185	217	213
----------	-----	-----	-----	-----	-----	-----	-----

223

grid # 4	328	327	329	327	328	217	212
----------	-----	-----	-----	-----	-----	-----	-----

224

number of gridpoints:

atom	H9	H10	H25	total
------	----	-----	-----	-------

grid # 1	73	73	72	3517
grid # 2	118	118	115	4492
grid # 3	222	224	220	8633
grid # 4	224	224	224	12246

end of program grid

start of program rwr  
end of program rwr

start of program scf

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

etot	1	N	N	1	U	-990.39072743546		2.7E-05	1.6E-03
etot	2	Y	Y	4	M	-990.39084046479	1.1E-04	1.0E-05	6.3E-04
etot	3	Y	Y	4	M	-990.39085660547	1.6E-05	2.9E-06	1.5E-04
etot	4	Y	N	4	M	-990.39085842189	1.8E-06	0.0E+00	0.0E+00

Energy components, in hartrees:

(A)	Nuclear repulsion.....	1971.03469662474	
(E)	Total one-electron terms.....	-5260.33898399291	
(I)	Total two-electron terms.....	2298.91342894628	
(L)	Electronic energy.....	-2961.42555504663	(E+I)
(N)	Total energy.....	-990.39085842189	(A+L)

SCFE: SCF energy: HF -990.39085842189 hartrees iterations:  
4

HOMO energy: -0.26904  
LUMO energy: 0.09663

Orbital energies:

-15.60476	-15.56511	-11.29628	-11.28688	-11.27173	-11.25112
-11.25088	-11.24616	-11.24601	-11.23993	-11.23979	-11.23905
-11.23848	-11.23784	-11.23711	-11.23607	-11.23466	-11.23444
-11.23292	-11.23053	-11.22458	-11.22023	-11.21899	-11.21606
-11.21326	-1.32501	-1.24984	-1.16321	-1.16033	-1.13852
-1.07453	-1.06701	-1.03926	-1.02190	-1.01887	-1.01693
-0.97093	-0.95430	-0.93367	-0.86015	-0.83703	-0.83361
-0.82898	-0.80705	-0.79545	-0.77000	-0.73261	-0.71741
-0.70108	-0.69829	-0.66635	-0.65790	-0.64282	-0.63719
-0.63386	-0.62365	-0.62070	-0.61581	-0.59629	-0.59238
-0.59044	-0.58747	-0.57825	-0.55807	-0.55220	-0.54819
-0.54450	-0.51739	-0.50722	-0.50256	-0.50019	-0.49584
-0.49341	-0.49117	-0.48733	-0.48121	-0.42975	-0.40483
-0.36754	-0.34337	-0.34122	-0.33756	-0.32914	-0.28243
-0.26904	0.09663	0.12889	0.13707	0.13733	0.14845
0.17836	0.20861	0.22838	0.23520	0.24116	

end of program scf

start of program der1a  
end of program der1a

start of program rwr  
end of program rwr

start of program der1b

forces (hartrees/bohr) : total

atom	label	x	y	z
1	N1	-2.481303E-04	2.161363E-04	3.038174E-05
2	N2	2.836382E-04	-2.499438E-05	-2.728610E-04
3	C4	-5.332666E-05	1.576006E-04	1.308833E-04
4	C5	-3.595149E-04	-1.387013E-04	2.963041E-04
5	C6	2.019594E-05	1.908855E-04	2.396059E-05
6	C7	2.466402E-04	-1.423657E-04	-1.552636E-04
7	C13	-1.276988E-04	5.612039E-06	6.448695E-05
8	H4	8.439654E-05	1.557089E-04	3.881350E-05
9	C8	1.165608E-05	5.058858E-04	1.509718E-04
10	C11	1.471085E-04	-4.822498E-05	-3.124871E-04
11	H7	5.901722E-05	-5.856555E-05	-6.083047E-05
12	C9	-2.081620E-04	-4.628287E-04	1.114154E-04
13	H8	1.113241E-04	3.132659E-05	-7.909427E-05
14	C10	-1.274255E-04	-2.859290E-04	1.870702E-05
15	C12	-5.235787E-06	8.359514E-05	2.010785E-04
16	C2	2.011226E-05	1.154169E-04	-3.679946E-04
17	H13	1.231949E-04	6.717329E-05	-9.936772E-05
18	C14	-2.239323E-04	1.957682E-04	-5.369846E-04
19	H15	3.610993E-06	-2.367943E-05	1.405502E-04
20	C15	4.528455E-04	8.163430E-06	3.393146E-04
21	C16	-5.301138E-05	-4.748777E-05	2.288187E-04
22	C17	9.188483E-04	1.208919E-04	1.826117E-04
23	C18	1.202191E-03	1.978553E-04	5.774334E-05
24	C19	-4.165740E-04	-3.910772E-05	-2.787547E-04
25	H16	-3.998587E-04	2.166071E-05	-1.106724E-04
26	H17	-1.196398E-04	-1.085782E-04	1.297513E-04
27	H18	-9.010150E-04	-1.633065E-04	-2.194062E-04
28	H19	-1.346353E-04	2.261628E-05	1.123854E-04
29	H20	4.154382E-06	-5.819682E-06	1.013341E-04
30	C1	5.219134E-04	1.699161E-04	-4.100770E-06
31	H5	-3.070221E-04	-1.084423E-05	-1.892583E-04
32	H6	6.403176E-05	-1.027693E-04	3.230711E-04
33	C3	1.449365E-04	1.660298E-04	1.228439E-04
34	C26	-3.787139E-07	5.421162E-05	-1.973404E-04
35	C27	1.942710E-05	4.496688E-05	2.562209E-04
36	C28	-4.419795E-05	-3.799500E-05	5.523642E-05
37	C29	-1.078932E-06	-5.617927E-06	-2.284443E-04
38	H1	8.125850E-05	7.200215E-05	-6.136742E-05
39	H2	4.595660E-05	3.363527E-05	-2.715897E-05
40	H3	-3.156831E-05	-9.218442E-06	3.647842E-06
41	H9	3.691536E-05	8.898917E-05	2.667129E-05
42	H10	-2.160082E-04	-1.433661E-04	1.416099E-04
43	H25	3.817919E-05	-4.036847E-05	-5.326570E-05
total		6.631381E-04	8.262798E-04	3.416091E-05

end of program der1b

start of program geopt 16

geometry optimization step 16

reading input hessian of dimension 129

in five columns format

reading input hessian of dimension 129

in five columns format

\*\* restarting optimization from step 15 \*\*

Level shifts adjusted to satisfy step-size constraints

Step size: 0.0104342

Cos(theta): 0.4965050

Final level shift: -2.6262214E-02

energy change: 8.2390E-07 # ( 5.0000E-05 )

gradient maximum: 4.0569E-04 \* ( 4.5000E-04 )

gradient rms: 1.0457E-04 \* ( 3.0000E-04 )

step size: 0.01043 trust radius: 0.01000

displacement maximum: 6.0223E-03 . ( 1.8000E-03 )

displacement rms: 8.1979E-04 \* ( 1.2000E-03 )

predicted energy change: -4.8790E-06 geom step: 1.0434E-

02 full step: 1.0434E-02

\*\*\*\*\*

\*\* Geometry optimization complete \*\*

\*\*\*\*\*

center of mass moved by:

x: 0.0000E+00

y: -6.8695E-16

z: 3.8858E-16

final geometry:

	angstroms		
atom	x	y	z
N1	-0.2476098628	0.4319499494	1.1700896461
N2	-1.0050850757	-2.2950871682	1.1949182325
C4	-1.2225555532	-0.0359392069	1.9934979632
C5	-0.0345337388	-1.9145591457	0.4863206158
C6	-1.6345629750	-1.3576518558	2.0372932256
C7	-1.7207638142	0.9827487410	2.7857085019
C13	0.6372167911	-2.9214974519	-0.4226269266
H4	-2.9991767135	-2.6746254046	2.9867461727
C8	-2.7544283972	0.6541992122	3.6802520196
C11	-0.9547075557	2.1487129569	2.4185234965
H7	-3.1936858699	1.4000793918	4.3191782963
C9	-3.1953417522	-0.6499826706	3.7301011813
H8	-3.9846205275	-0.9126483273	4.4122075724
C10	-2.6412076664	-1.6632555907	2.9184523073
C12	-0.0714118196	1.7763193928	1.4539254438
C2	0.9267126827	2.6085697080	0.7475086448
H13	1.7145636018	-2.8715088035	-0.2838423517

C14	0.3089199593	-2.7020981095	-1.8909152593
H15	0.3081077662	-3.9039526830	-0.1083403583
C15	-0.3215924809	-2.3201267580	-4.5836616469
C16	1.3004540244	-2.3992437756	-2.8137797881
C17	-1.0077278059	-2.8118948597	-2.3339058106
C18	-1.3203617236	-2.6227459376	-3.6680394462
C19	0.9888784831	-2.2093360982	-4.1534576988
H16	2.3240667900	-2.3146888619	-2.4895233992
H17	-1.7849137076	-3.0449393883	-1.6268919447
H18	-2.3419771432	-2.7122708466	-3.9947783125
H19	1.7707403444	-1.9764961643	-4.8551652860
H20	-0.5656277175	-2.1736956496	-5.6211053749
C1	0.5760456600	-0.5105838268	0.4433549677
H5	1.5800429573	-0.5626136306	0.8641513090
H6	0.6825437933	-0.2189447287	-0.5941242795
C3	2.7951744578	4.2145617192	-0.5601377830
C26	1.8187572576	3.3915699332	1.4744469707
C27	0.9785171969	2.6447421378	-0.6446715605
C28	1.9082206454	3.4396720163	-1.2930044553
C29	2.7448249516	4.1917280945	0.8244421729
H1	1.7902754511	3.3610162274	2.5486052296
H2	0.2747696491	2.0686681731	-1.2192937084
H3	1.9337718424	3.4605773143	-2.3682340620
H9	3.4301063300	4.7894624992	1.3997519889
H10	3.5171655374	4.8322369654	-1.0645143063
H25	-1.0688078963	3.1463685995	2.7914697600

nuclear repulsion energy..... 1971.109269844 hartrees

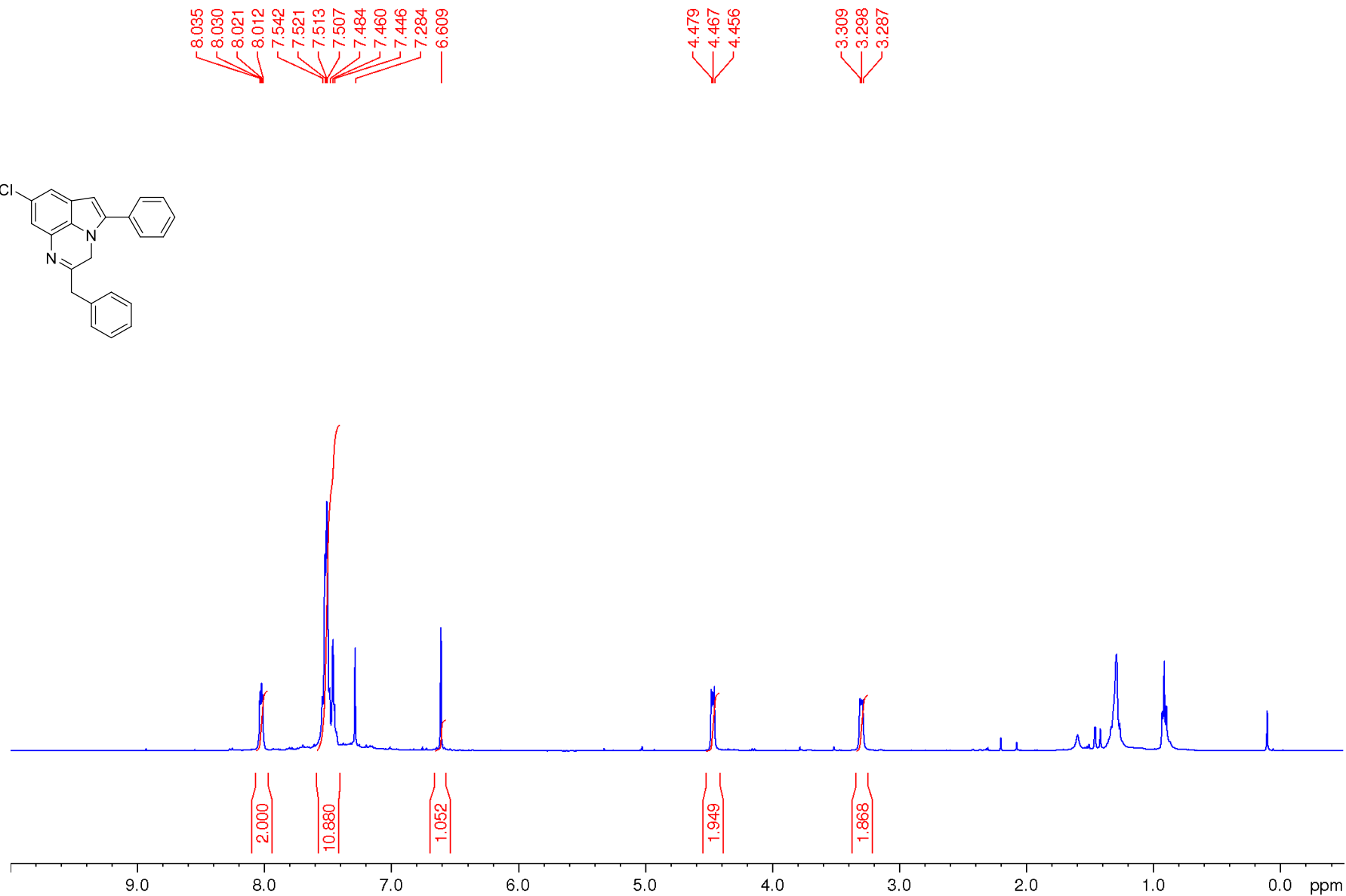
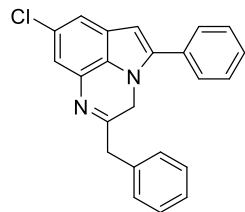
/ end of geometry optimization iteration 16 /

end of program geopt

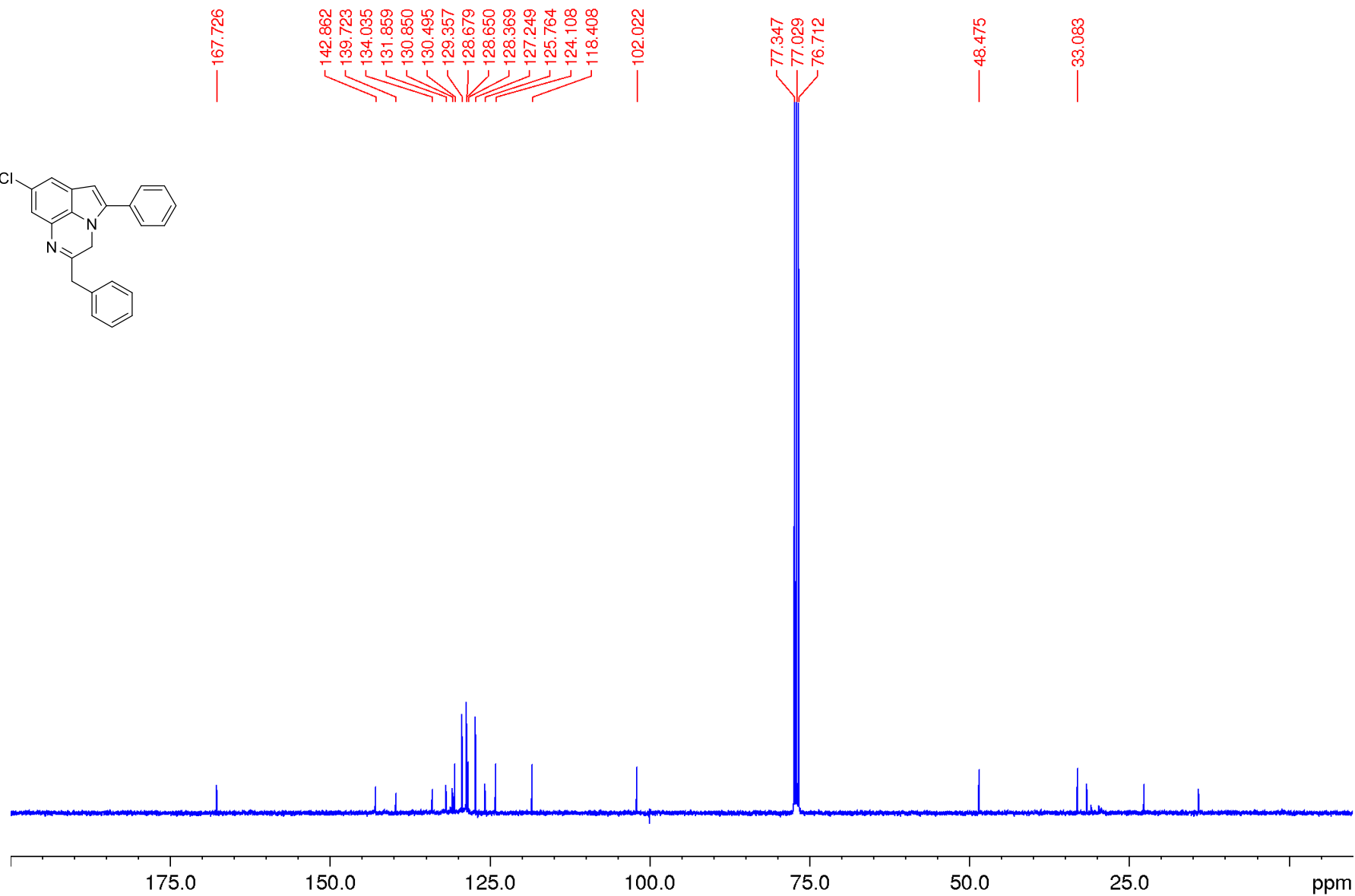
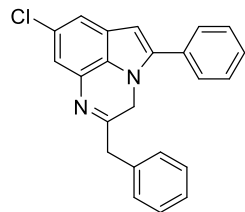
start of program post  
 Writing a SPARTAN archive file  
 end of program post

Total cpu seconds      user:      1761.812      user+sys:      1761.812

# 2-benzyl-8-chloro-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2a

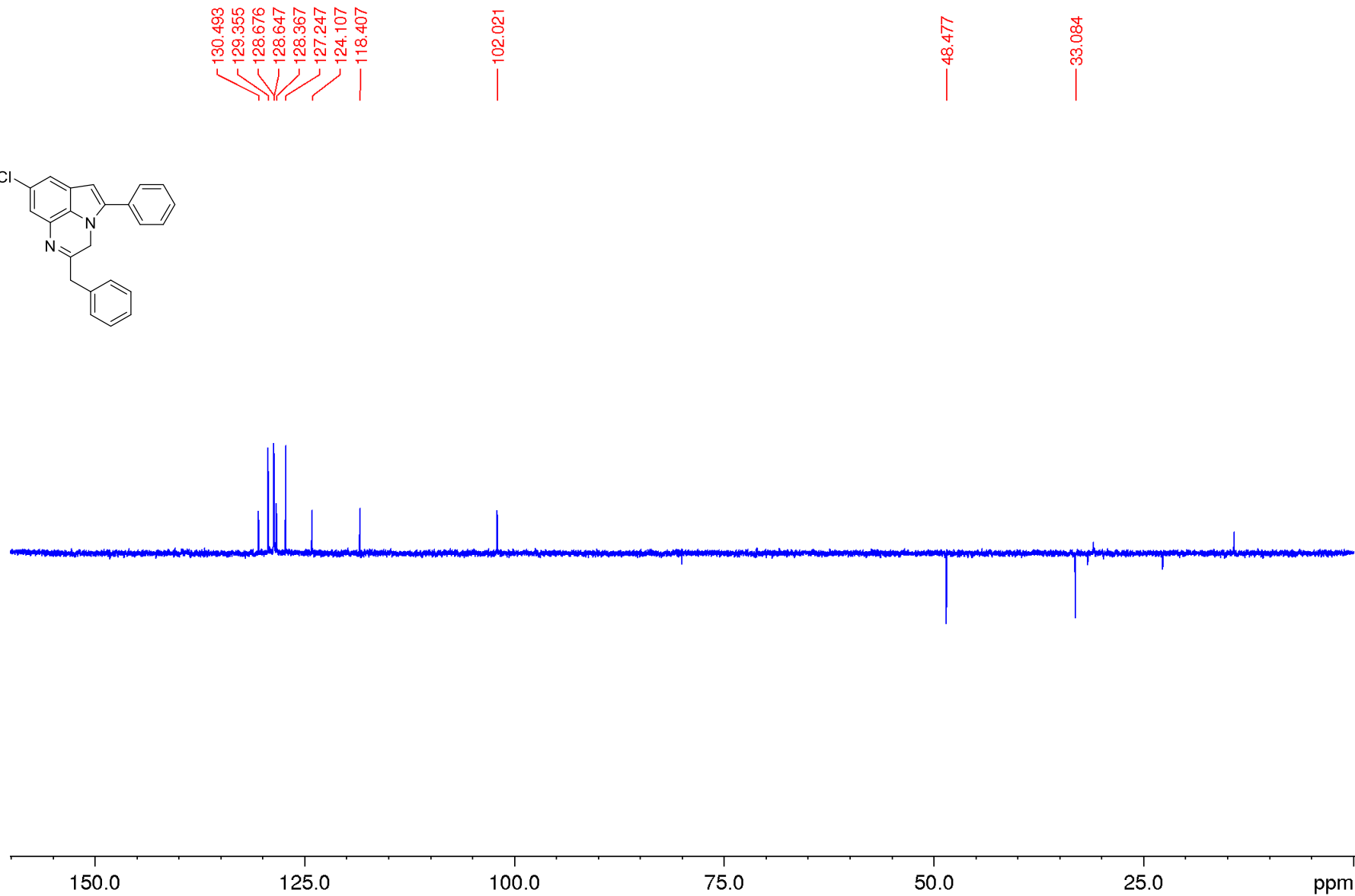
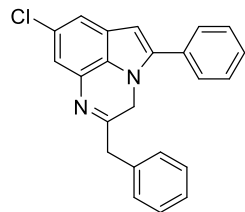


# 2-benzyl-8-chloro-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2a

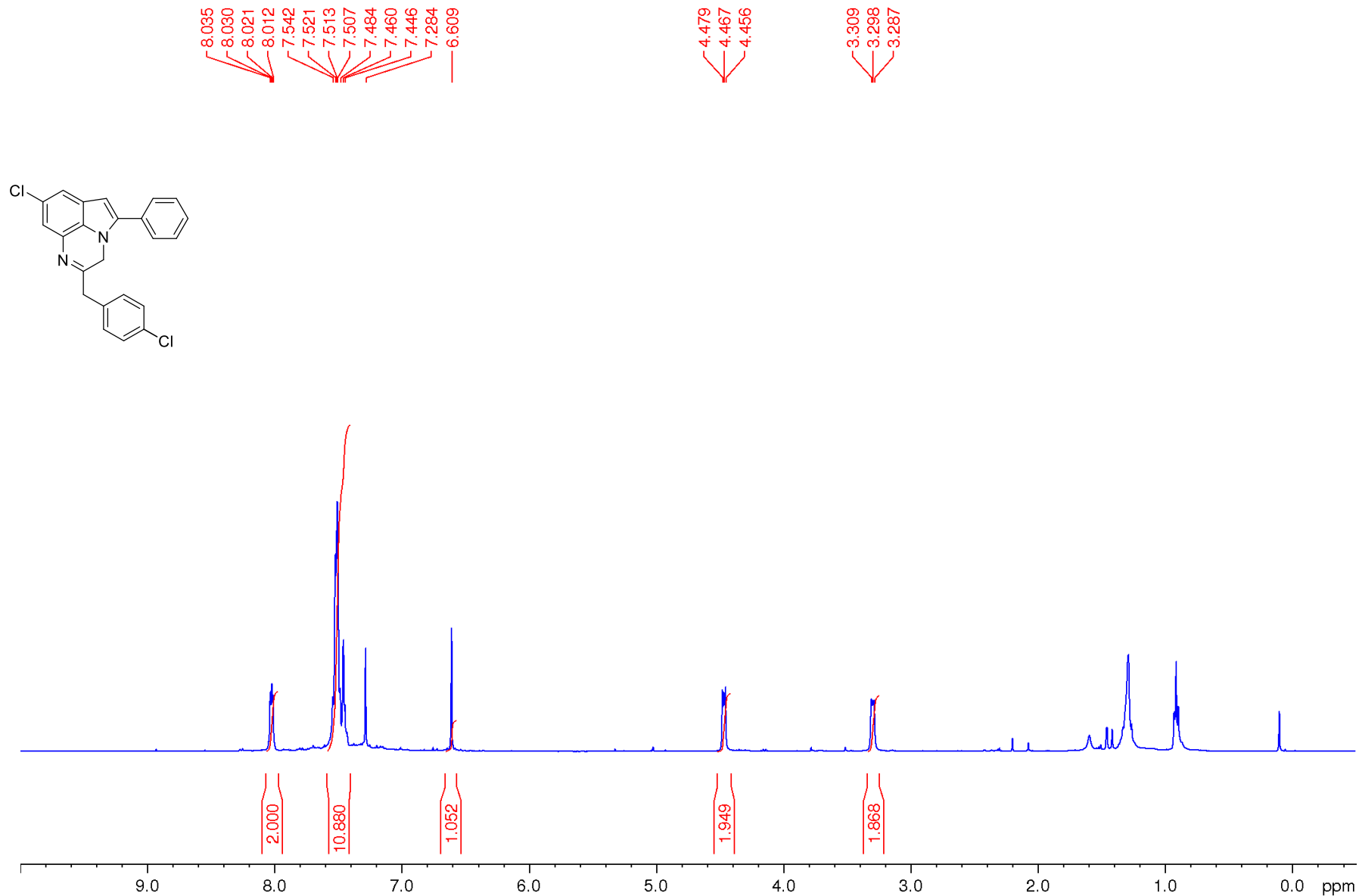




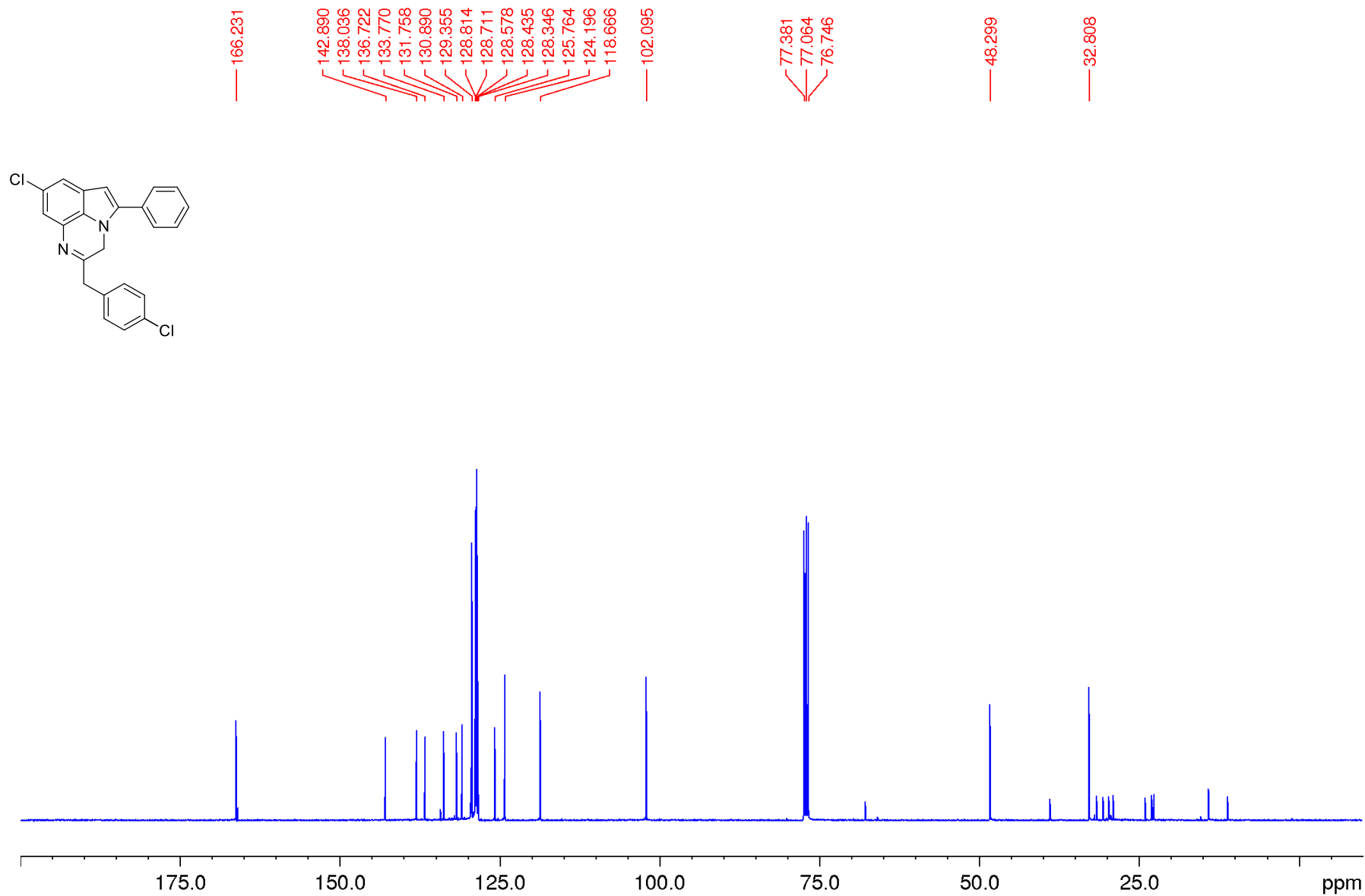
# 2-benzyl-8-chloro-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxaline 2a



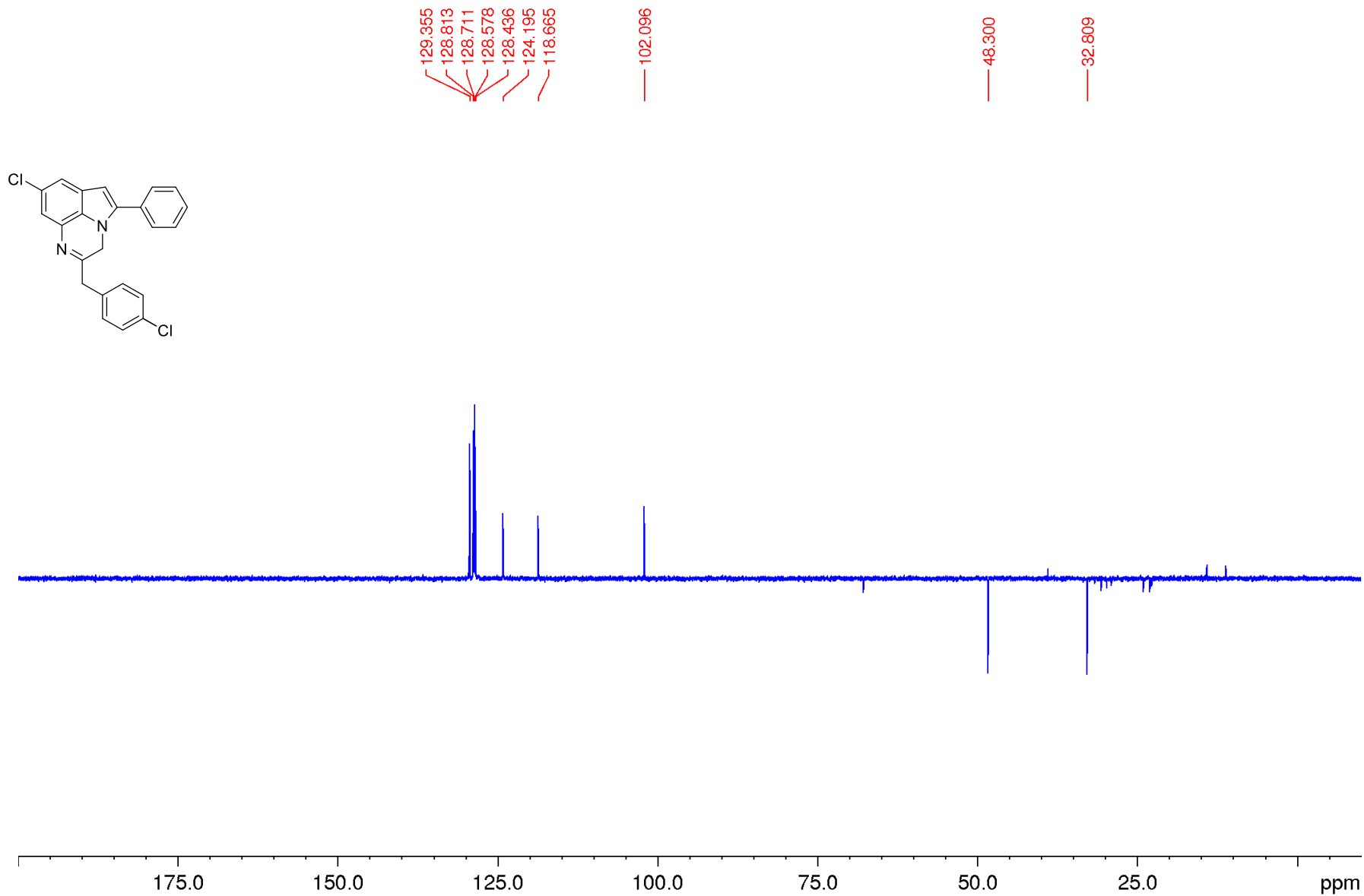
**8-chloro-2-(4-chlorobenzyl)-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2b**



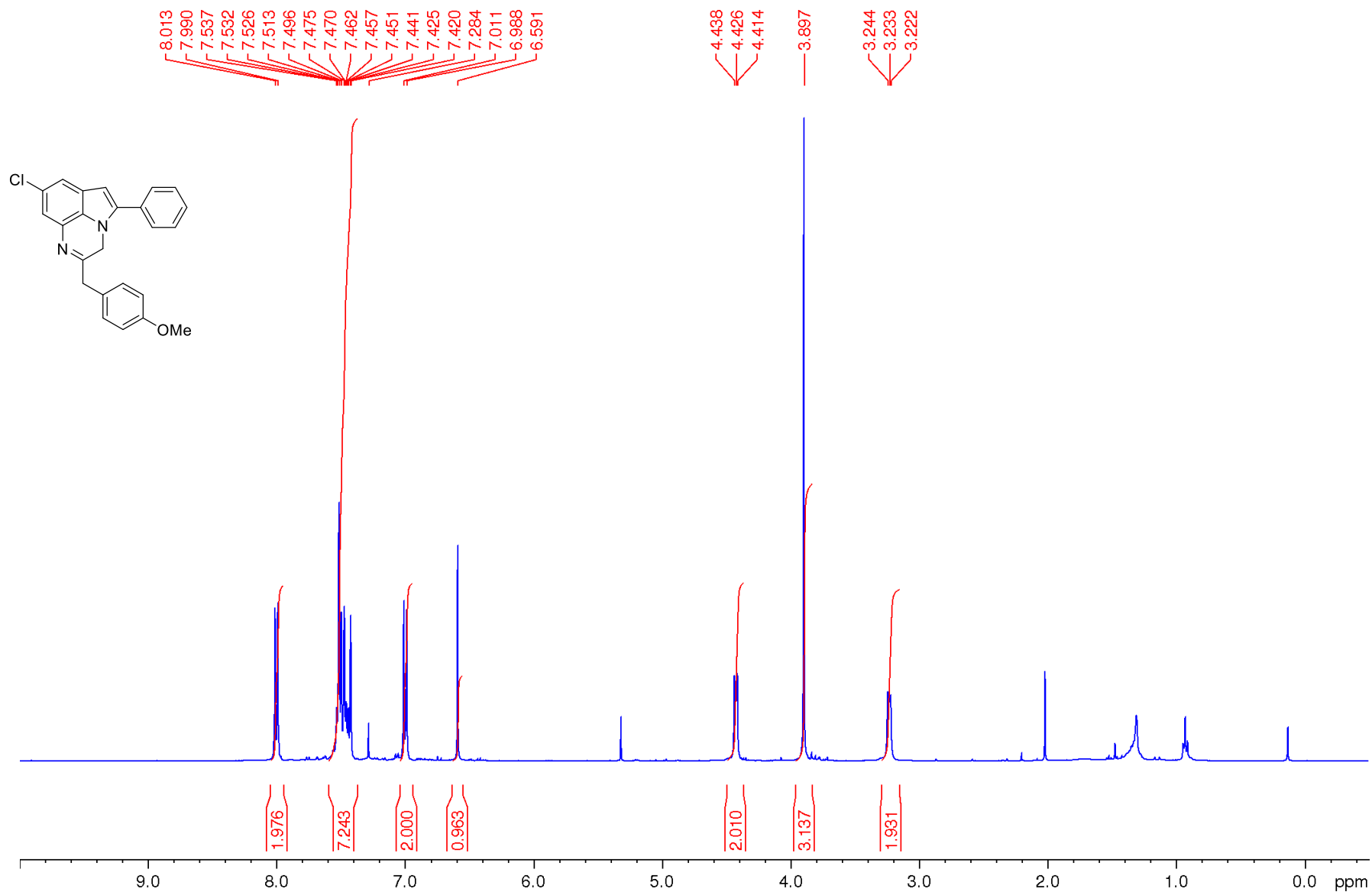
**8-chloro-2-(4-chlorobenzyl)-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2b**



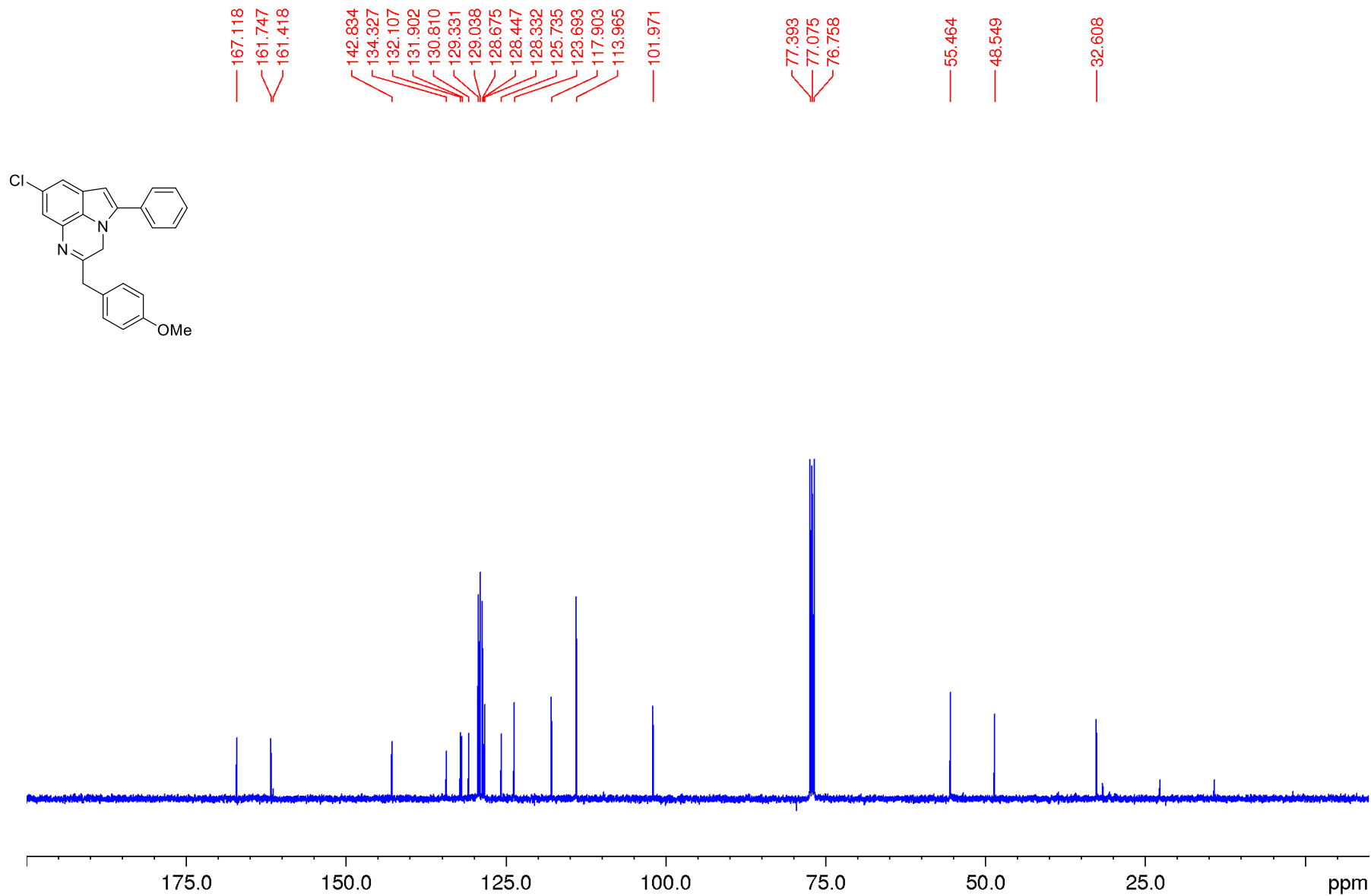
**8-chloro-2-(4-chlorobenzyl)-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2b**



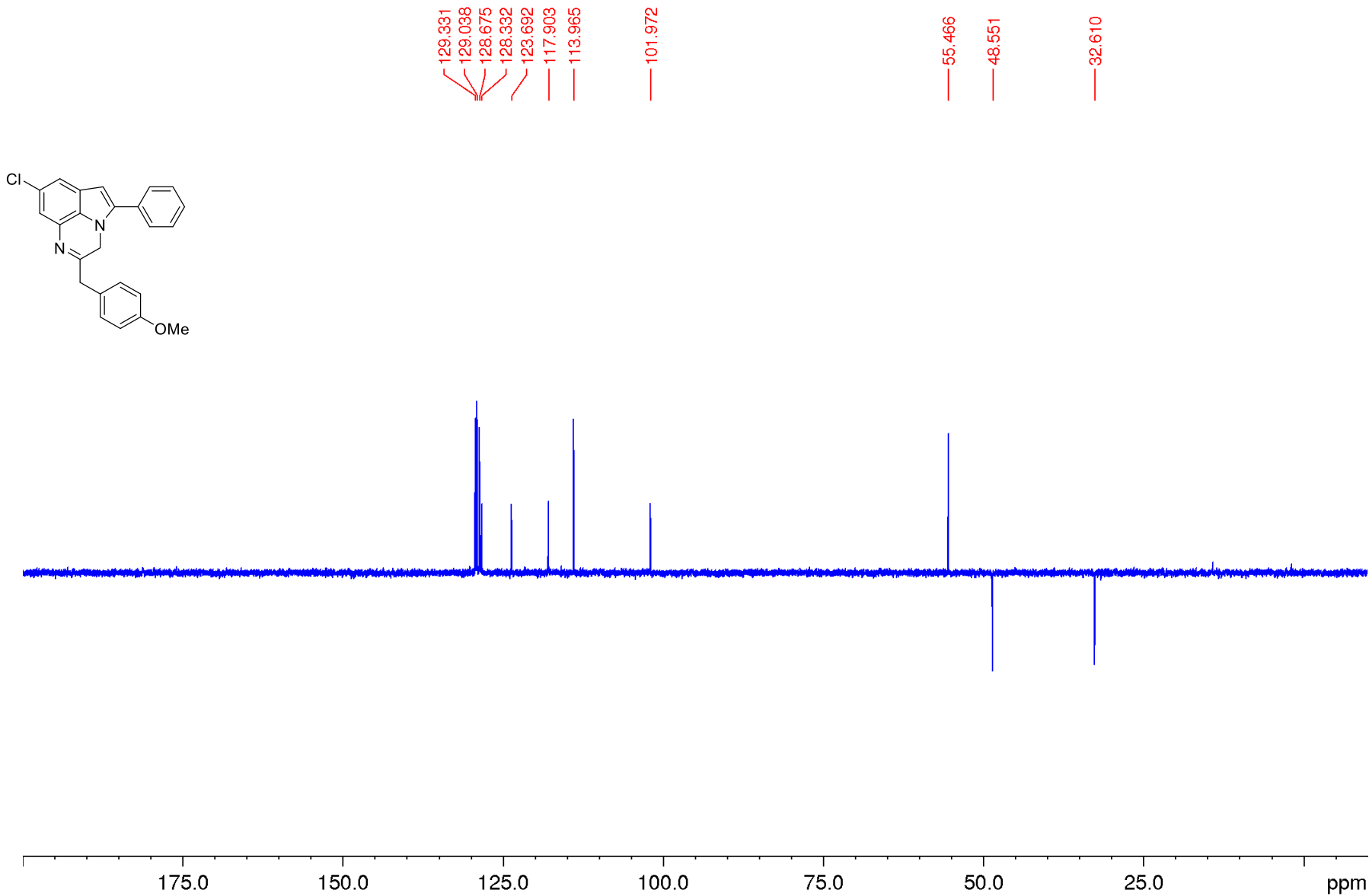
**8-chloro-2-(4-methoxybenzyl)-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2c**



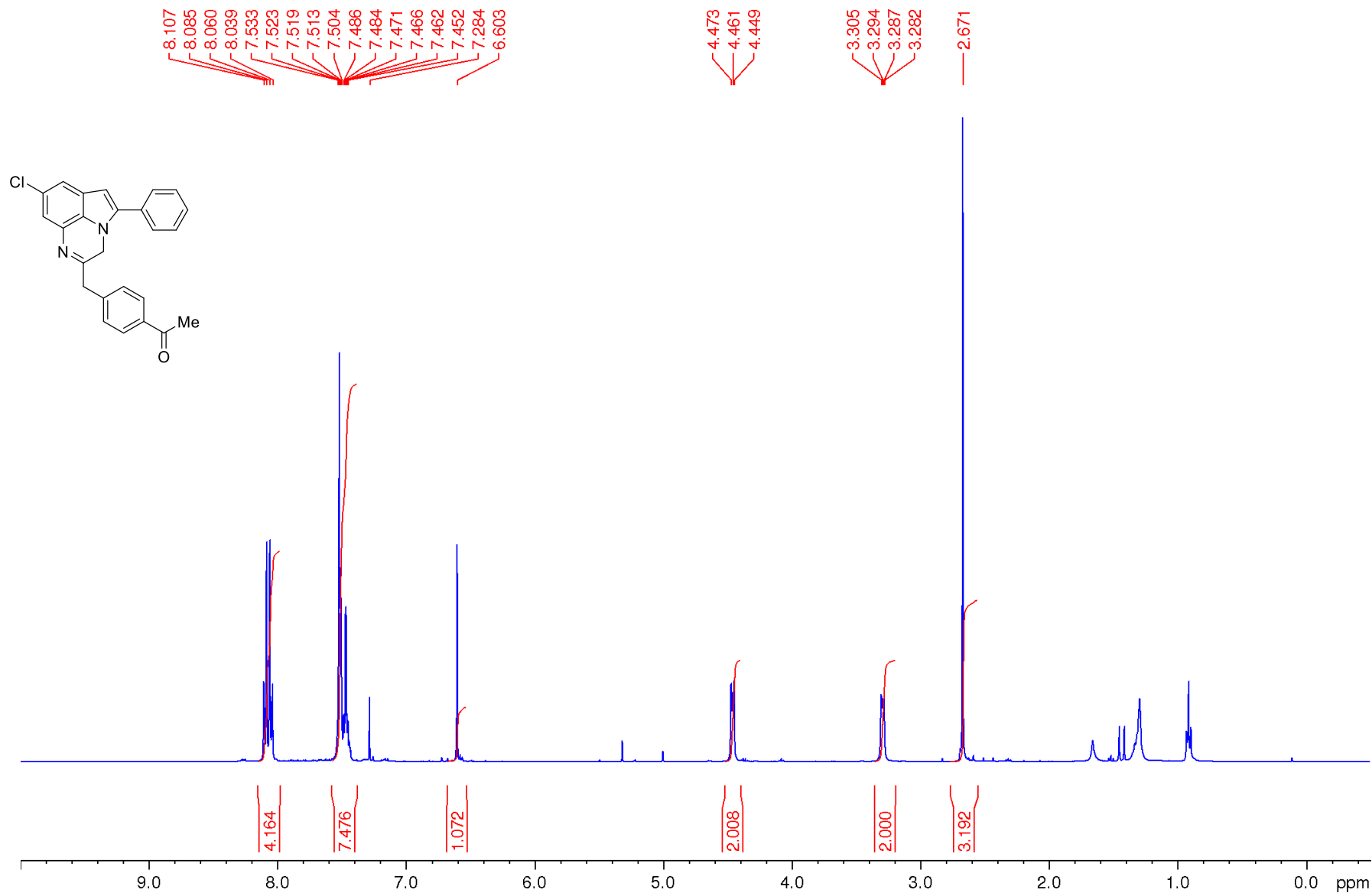
**8-chloro-2-(4-methoxybenzyl)-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxaline 2c**



**8-chloro-2-(4-methoxybenzyl)-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxaline 2c**

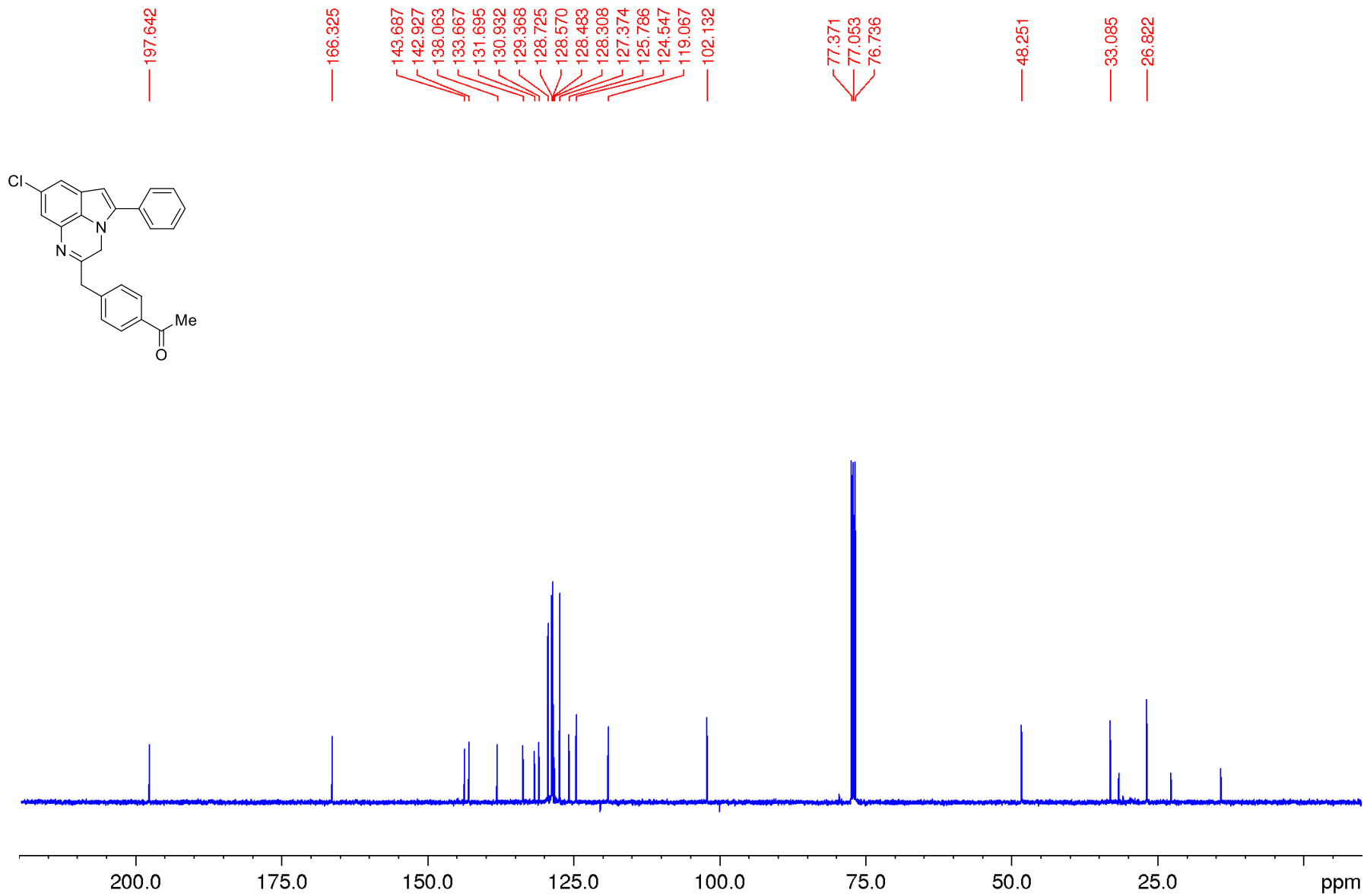


**1-(4-((8-chloro-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2d**

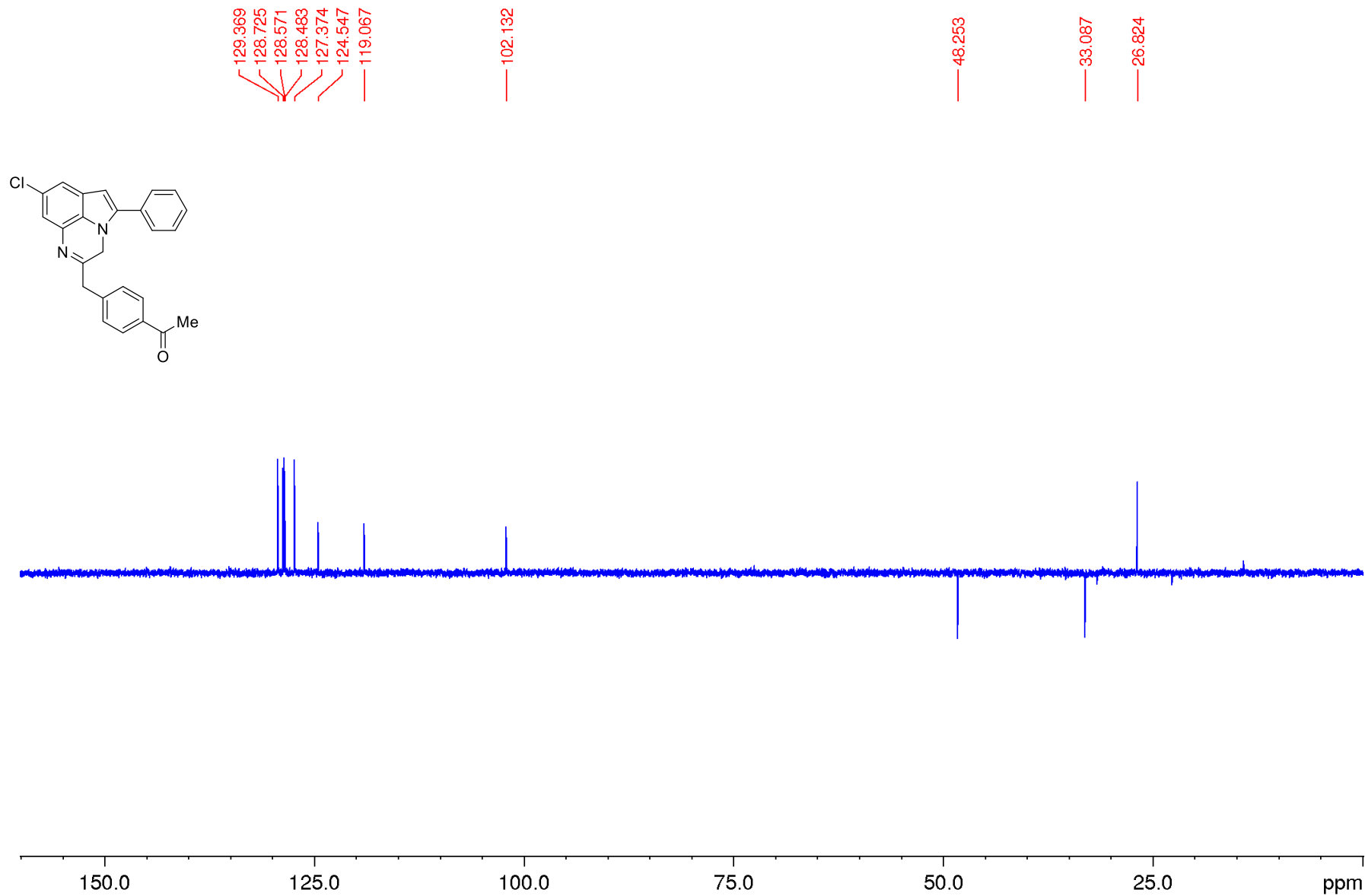




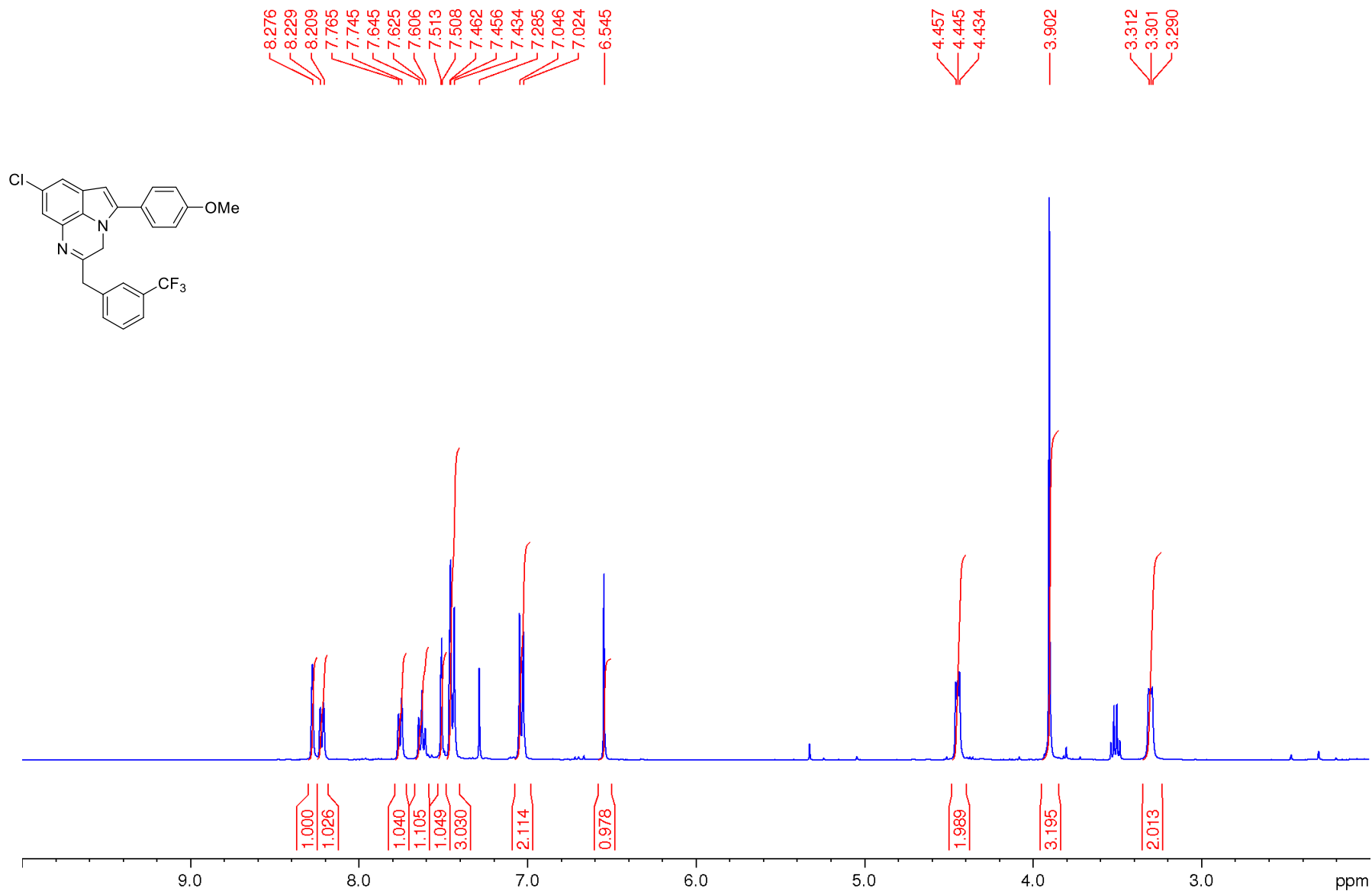
**1-(4-((8-chloro-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2d**



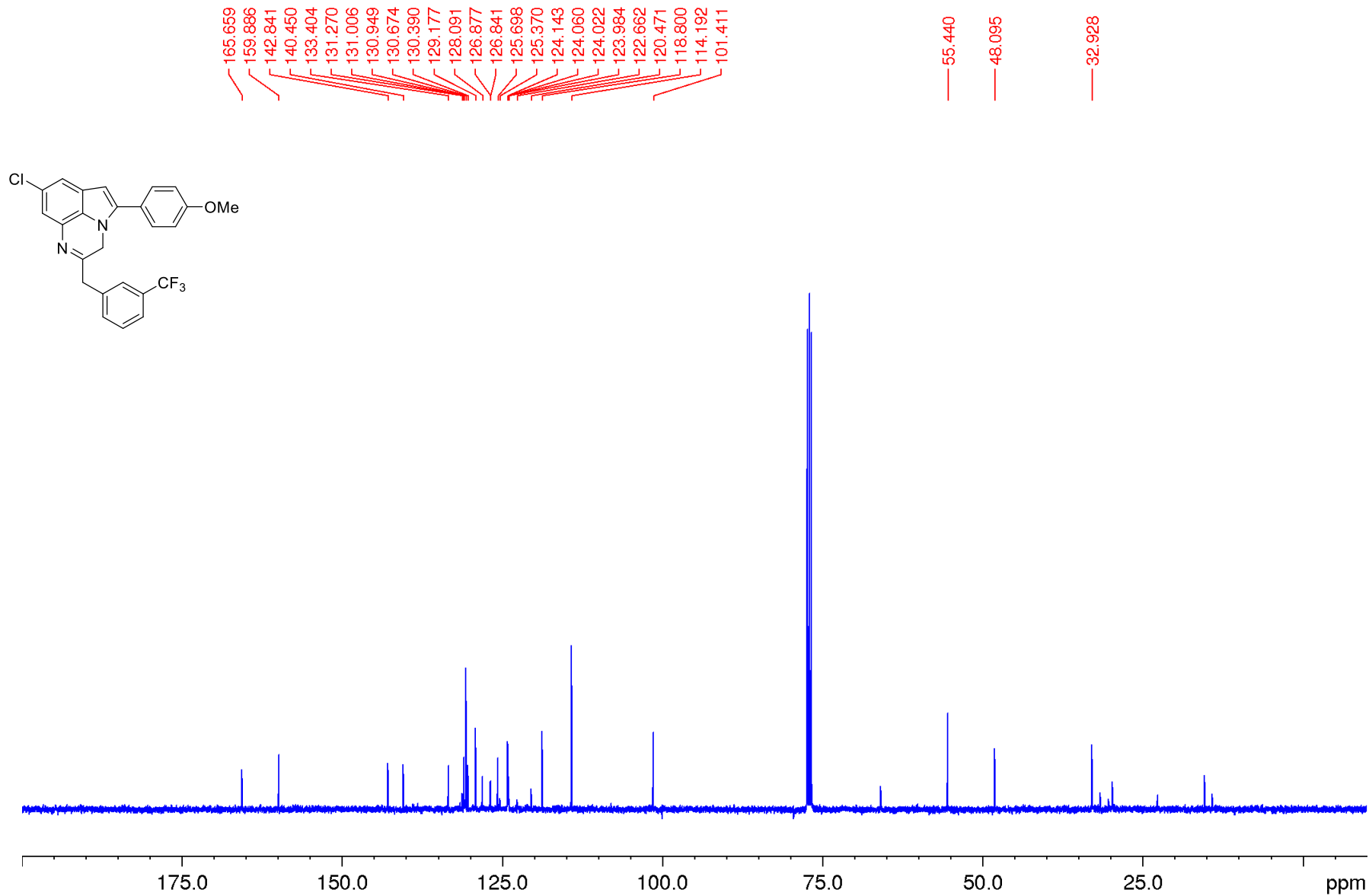
**1-(4-((8-chloro-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2d**



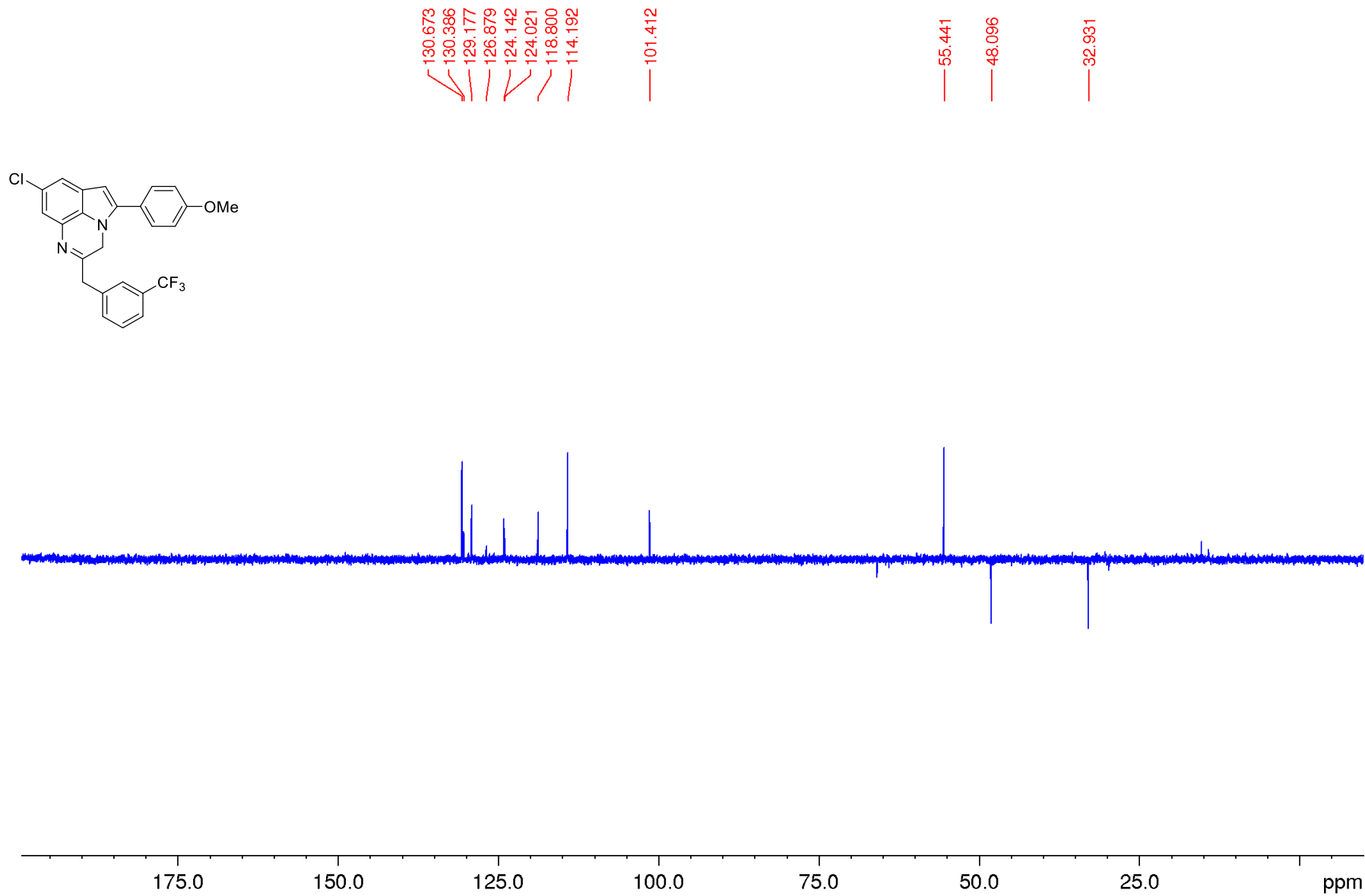
**8-chloro-5-(4-methoxyphenyl)-2-(3-(trifluoromethyl)benzyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2e**



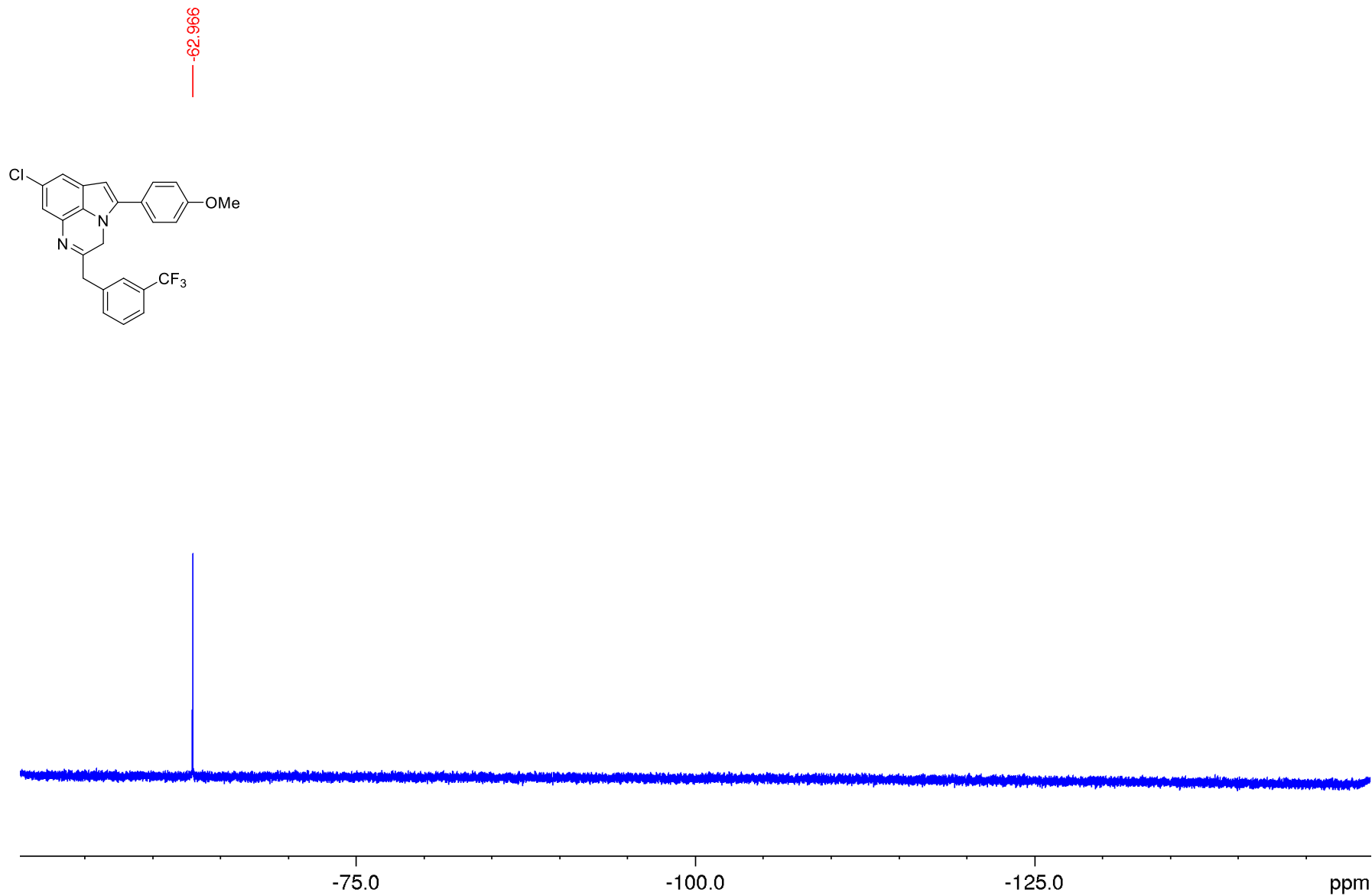
**8-chloro-5-(4-methoxyphenyl)-2-(3-(trifluoromethyl)benzyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2e**



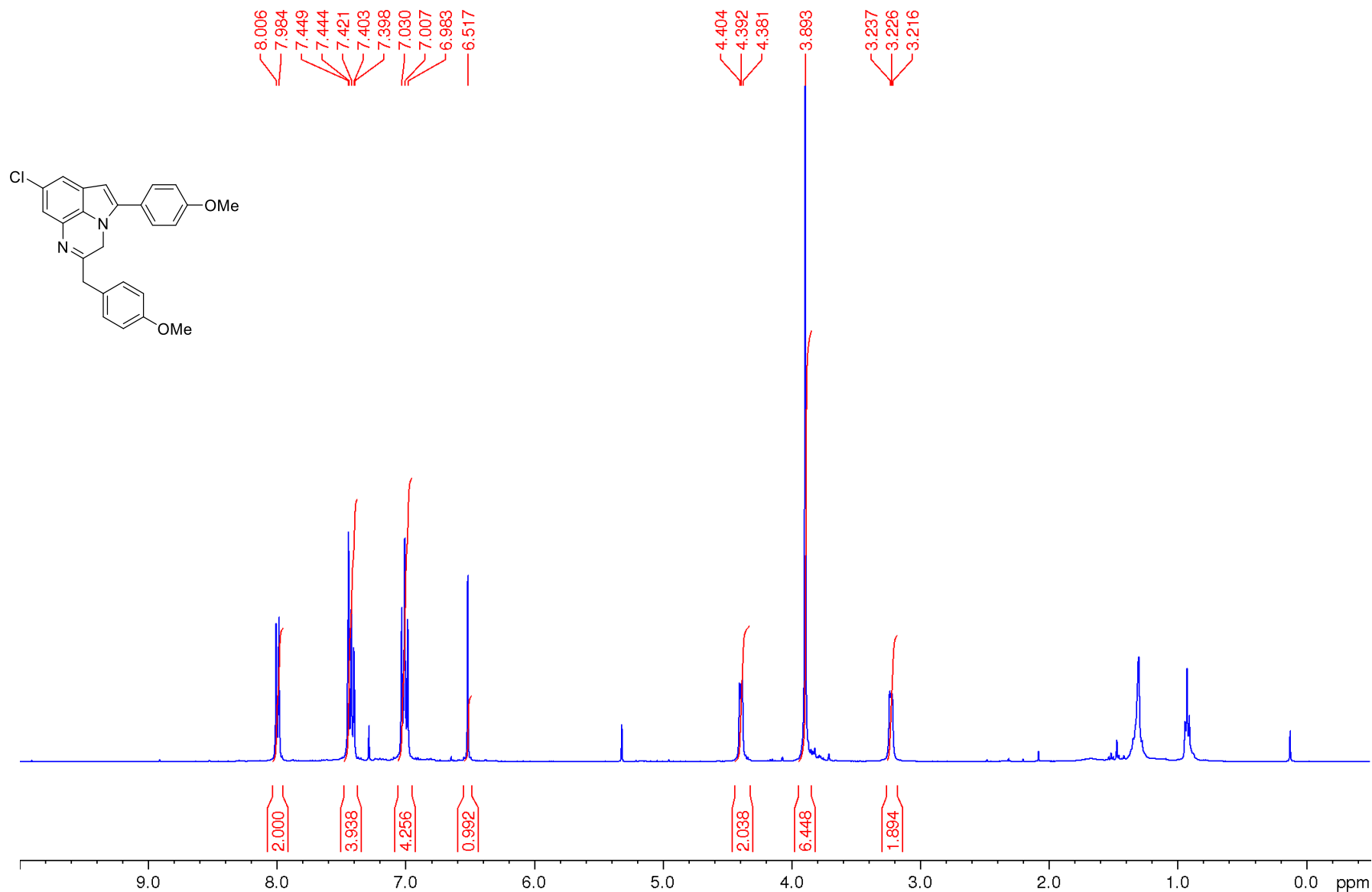
**8-chloro-5-(4-methoxyphenyl)-2-(3-(trifluoromethyl)benzyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2e**



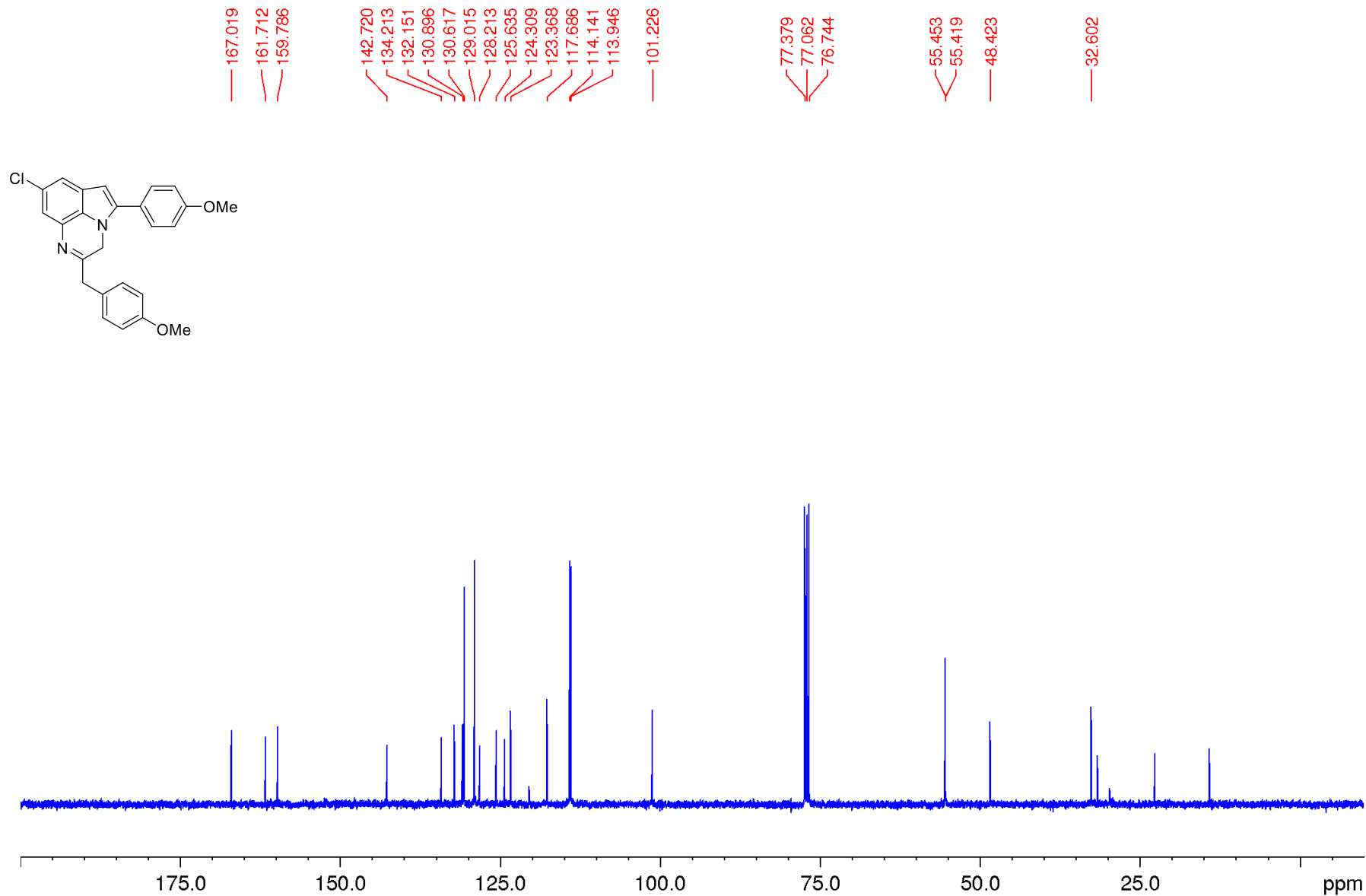
**8-chloro-5-(4-methoxyphenyl)-2-(3-(trifluoromethyl)benzyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2e**



**8-chloro-2-(4-methoxybenzyl)-5-(4-methoxyphenyl)-3H-pyrrolo[1,2,3-de]quinoxaline 2f**

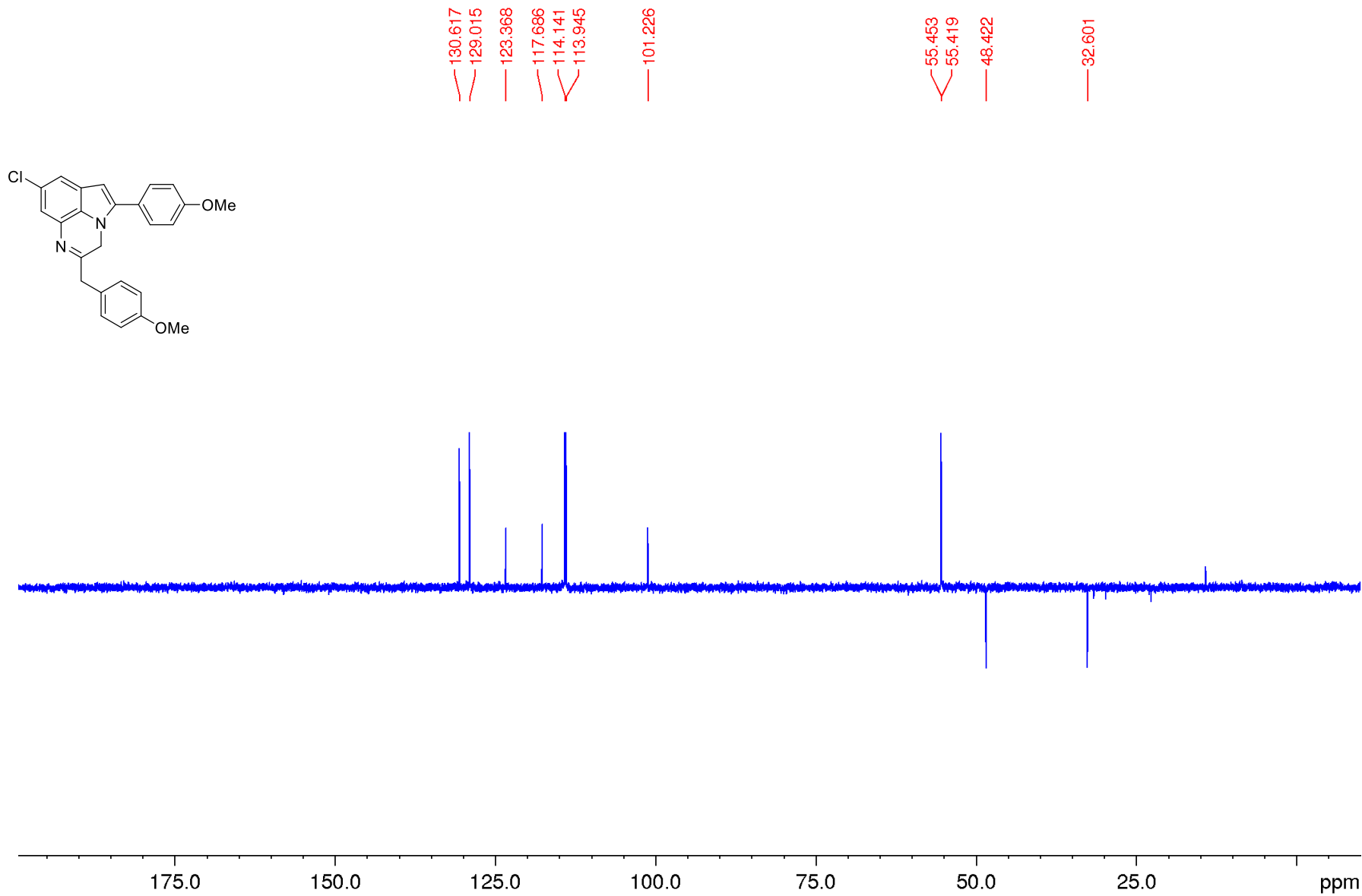


**8-chloro-2-(4-methoxybenzyl)-5-(4-methoxyphenyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2f**

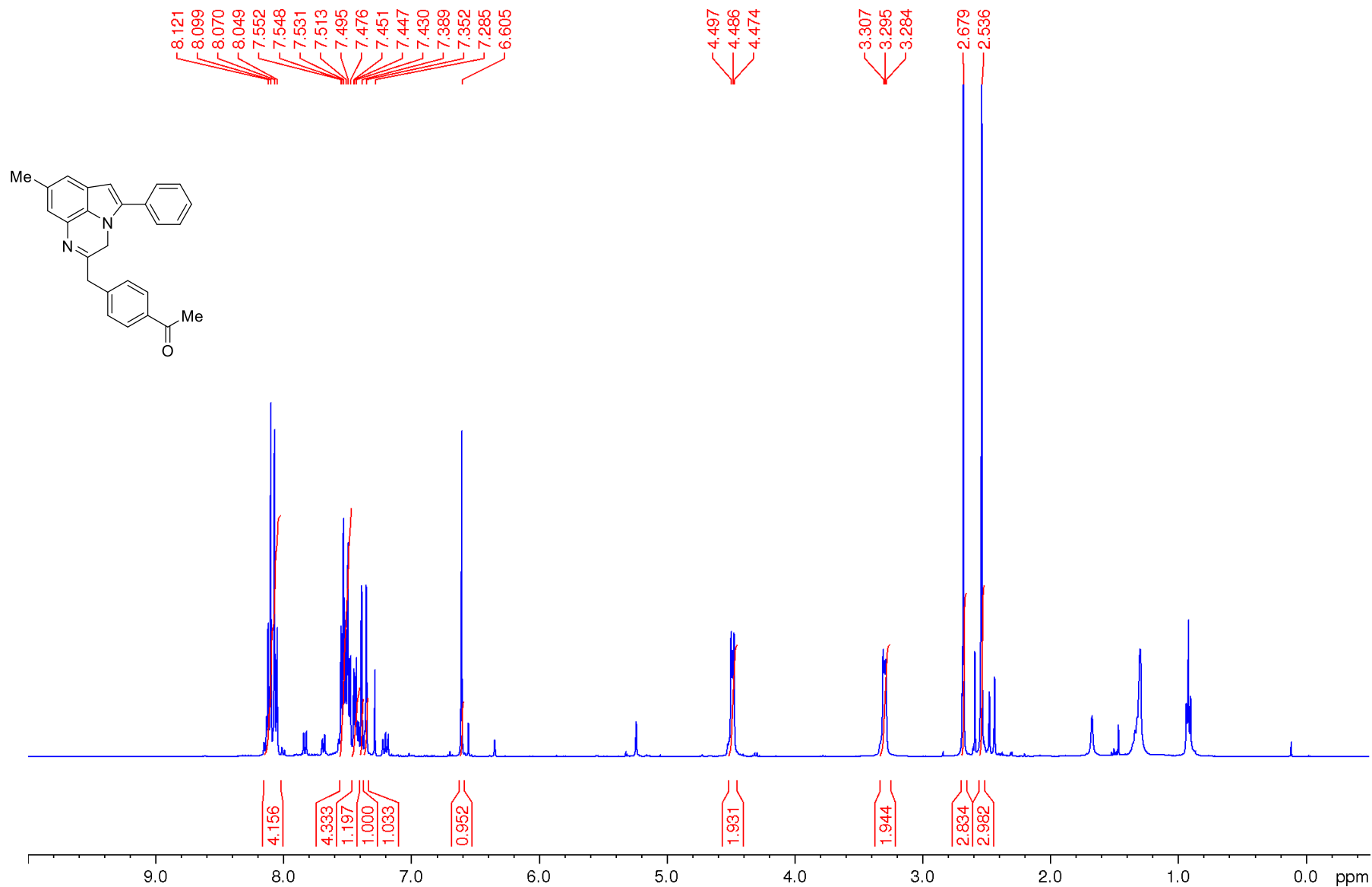




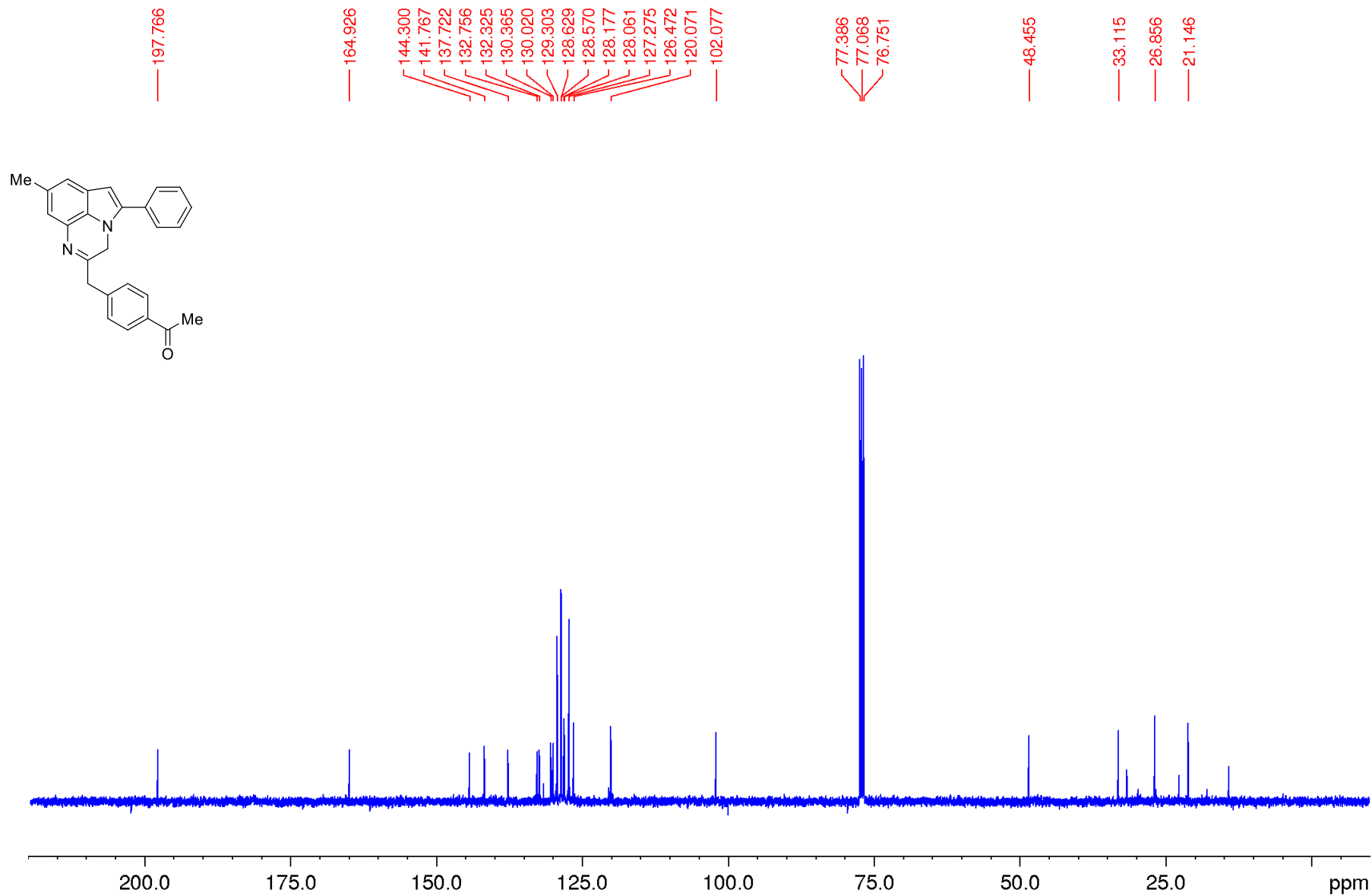
**8-chloro-2-(4-methoxybenzyl)-5-(4-methoxyphenyl)-3H-pyrrolo[1,2,3-*de*]quinoxaline 2f**



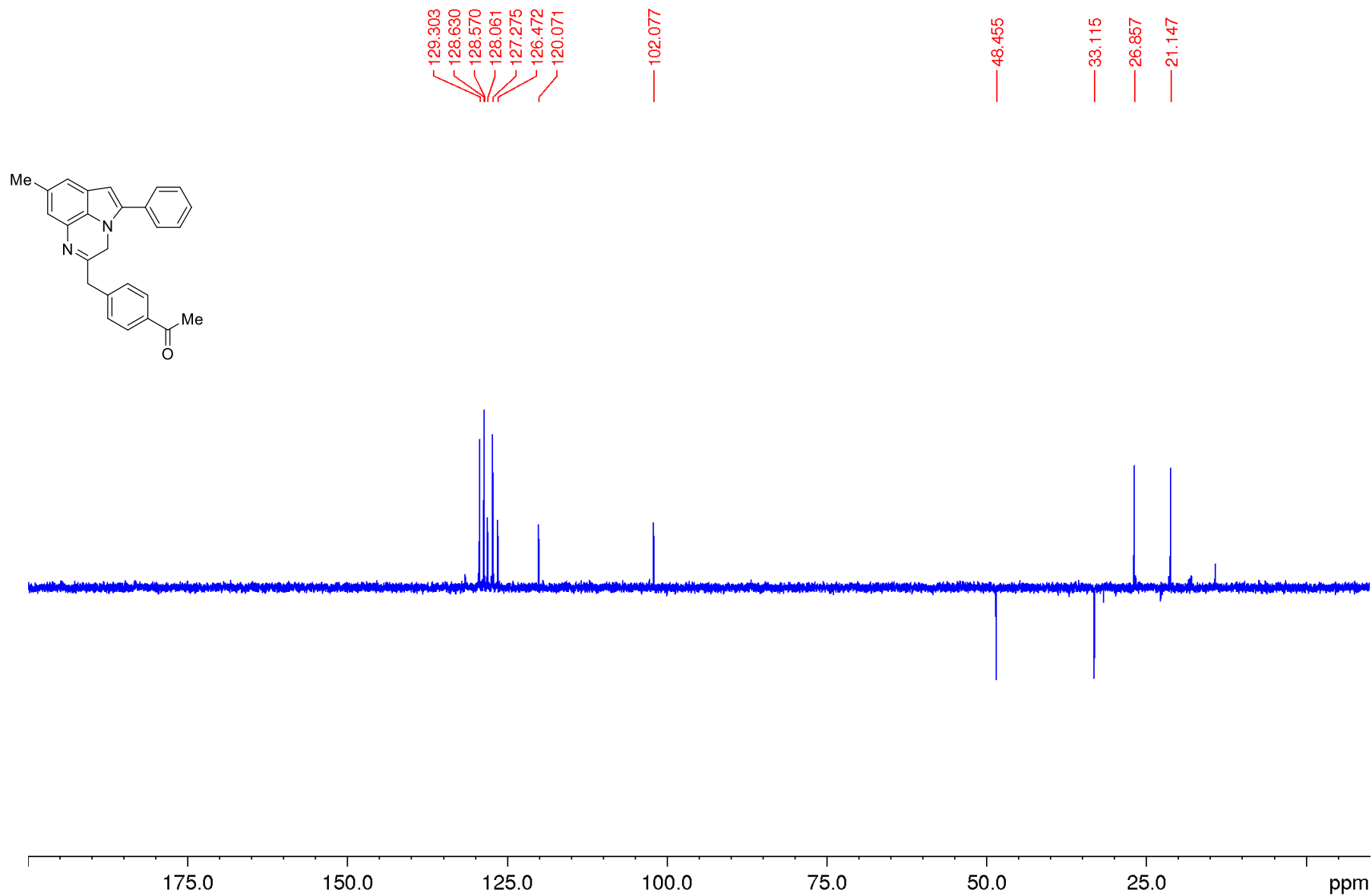
1-(4-((8-methyl-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2g



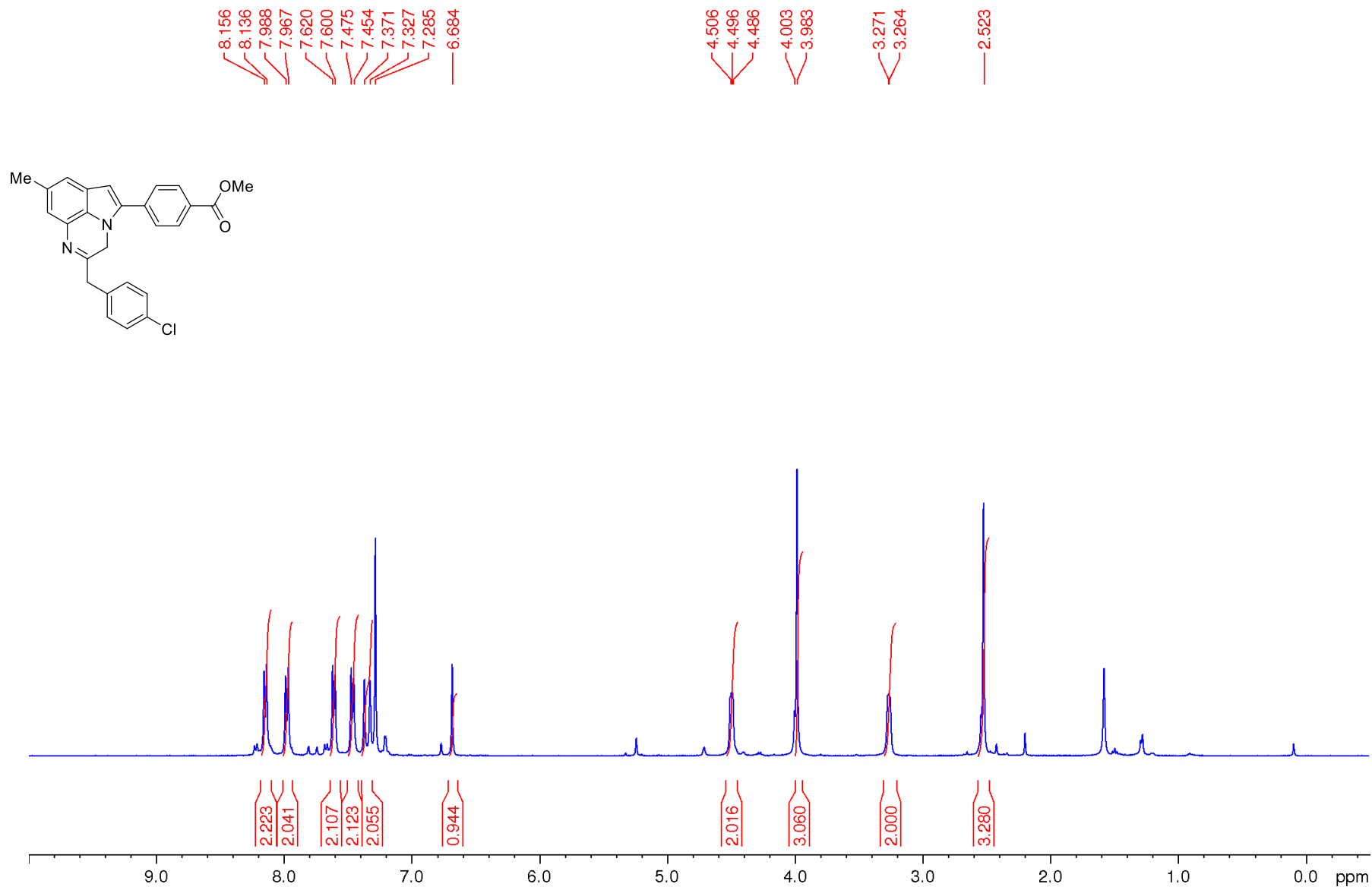
# 1-(4-((8-methyl-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2g



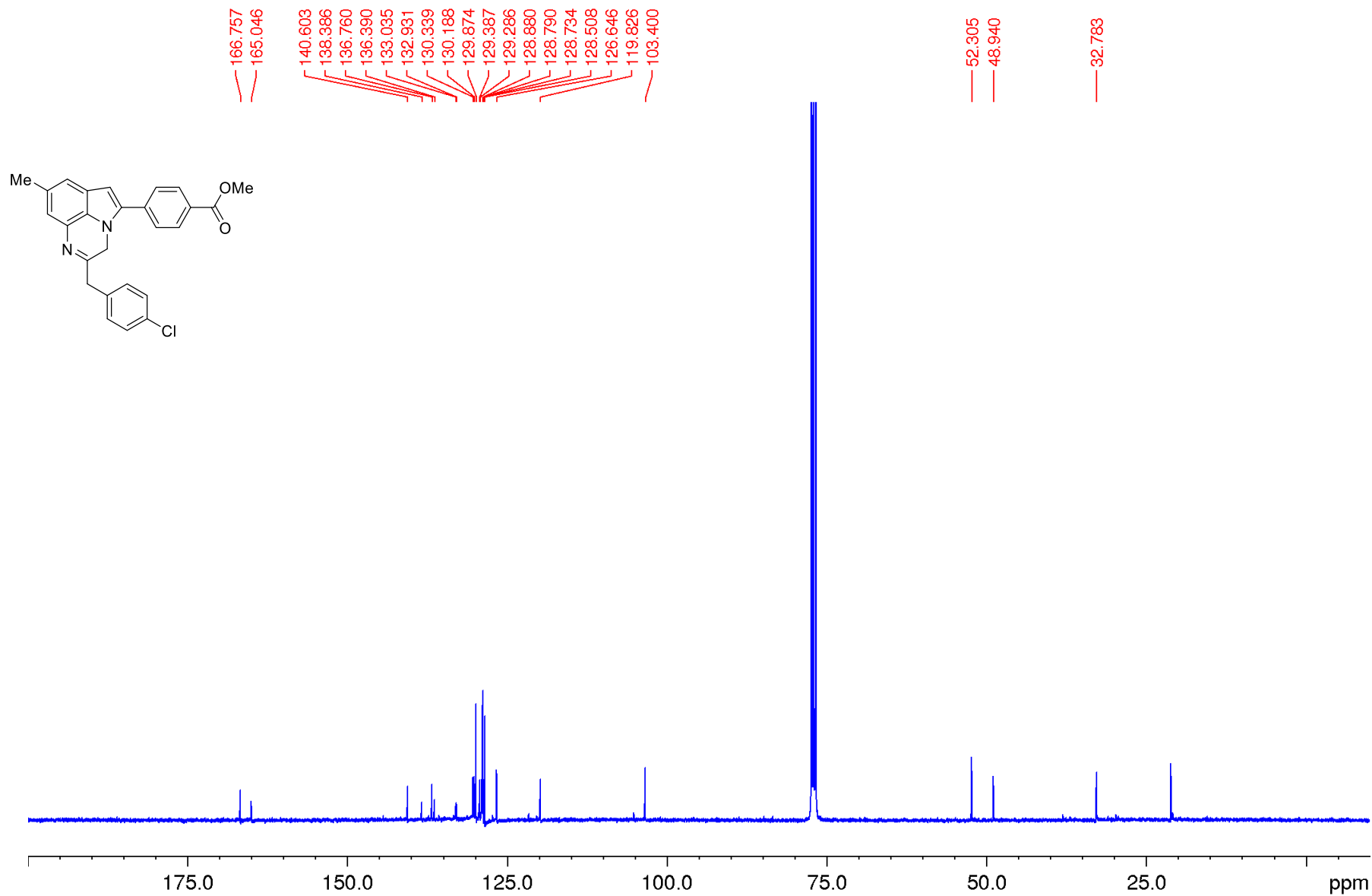
**1-(4-((8-methyl-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2g**



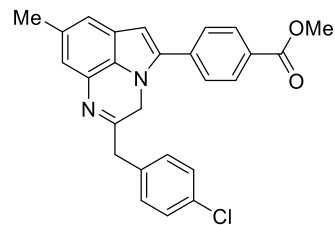
**methyl 4-(2-(4-chlorobenzyl)-8-methyl-3H-pyrrolo[1,2,3-*de*]quinoxalin-5-yl)benzoate 2h**



**methyl 4-(2-(4-chlorobenzyl)-8-methyl-3H-pyrrolo[1,2,3-*de*]quinoxalin-5-yl)benzoate 2h**



**methyl 4-(2-(4-chlorobenzyl)-8-methyl-3*H*-pyrrolo[1,2,3-*de*]quinoxalin-5-yl)benzoate 2h**



129.871  
128.878  
128.789  
128.506  
126.641

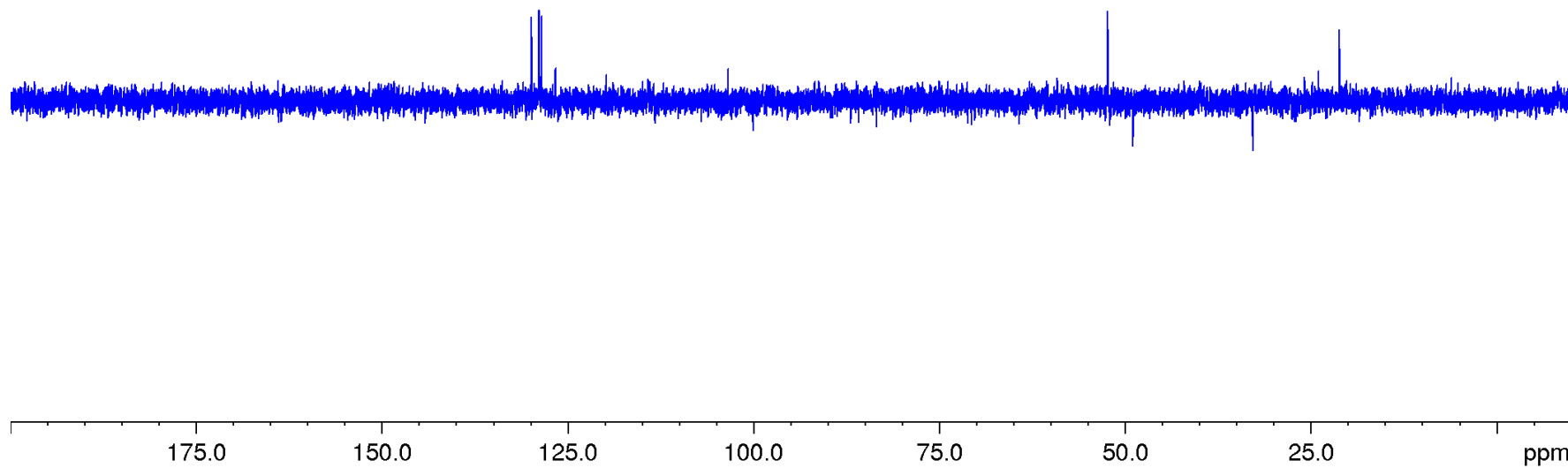
103.400

52.304

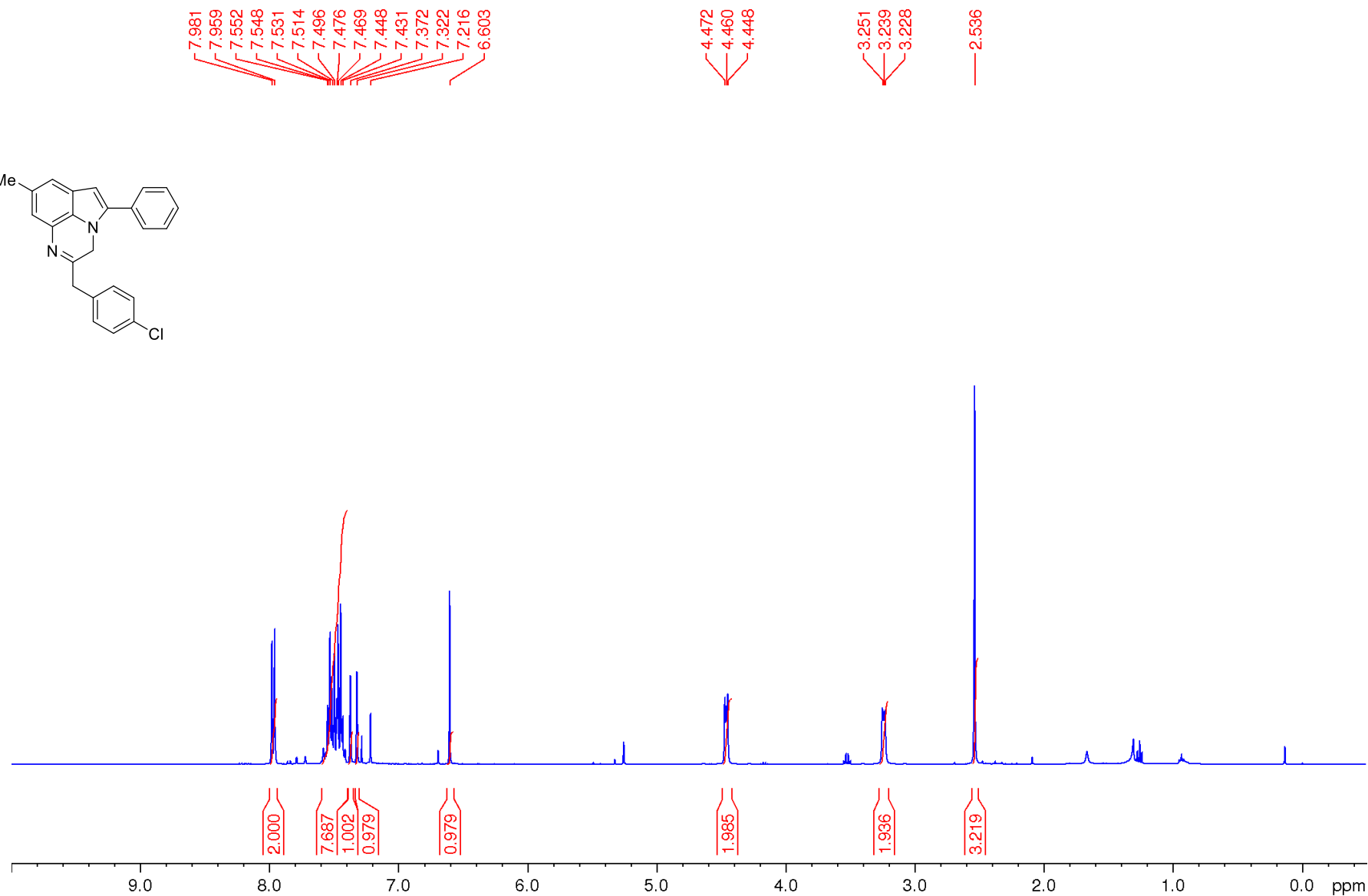
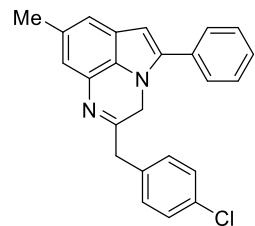
48.941

32.785

21.132

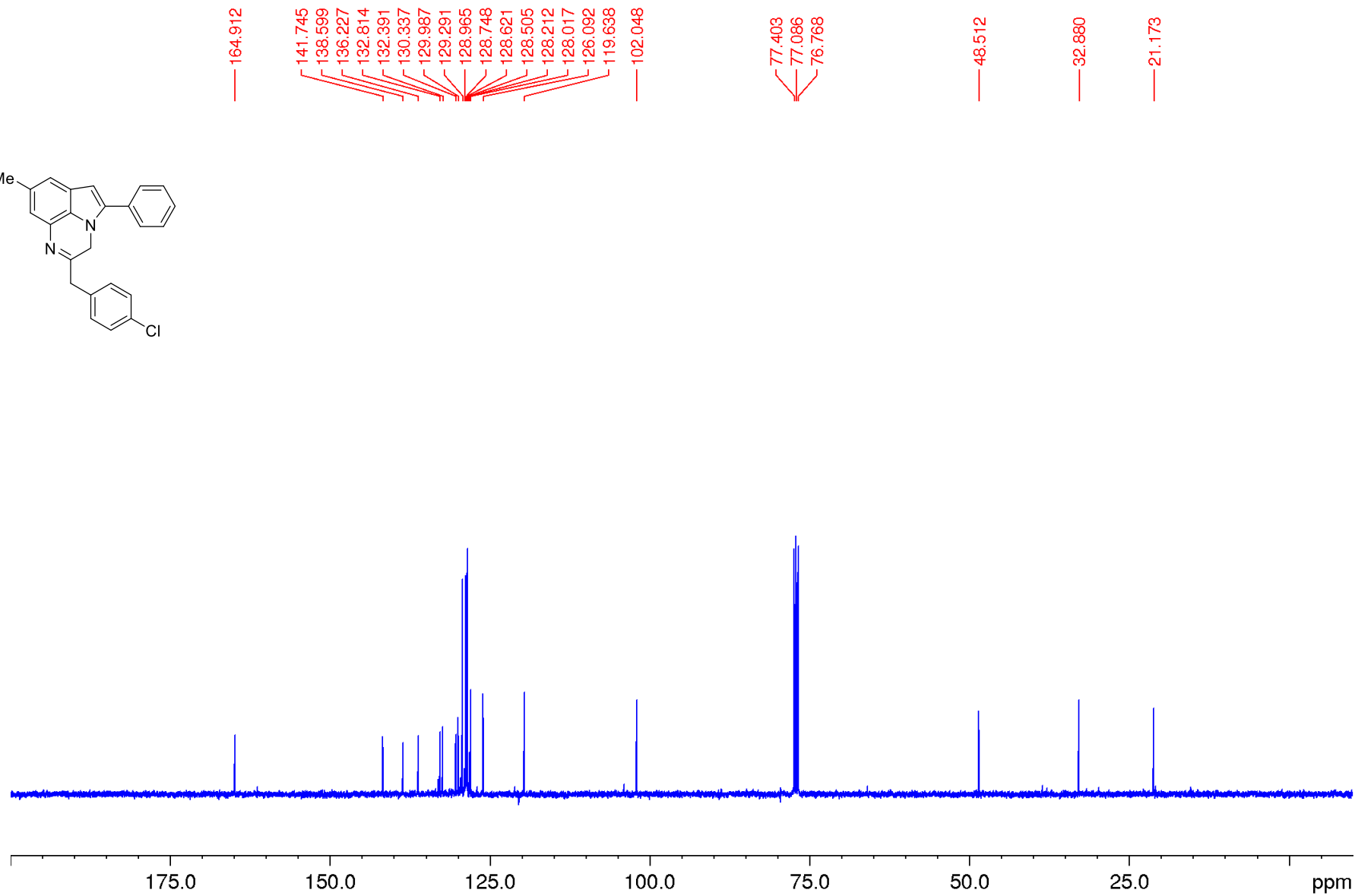
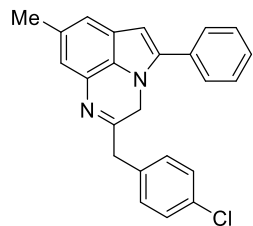


# 2-(4-chlorobenzyl)-8-methyl-5-phenyl-3H-pyrrolo[1,2,3-*de*]quinoxaline 2i

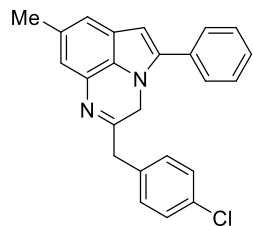




## 2-(4-chlorobenzyl)-8-methyl-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxaline 2i



**2-(4-chlorobenzyl)-8-methyl-5-phenyl-3*H*-pyrrolo[1,2,3-*de*]quinoxaline 2i**

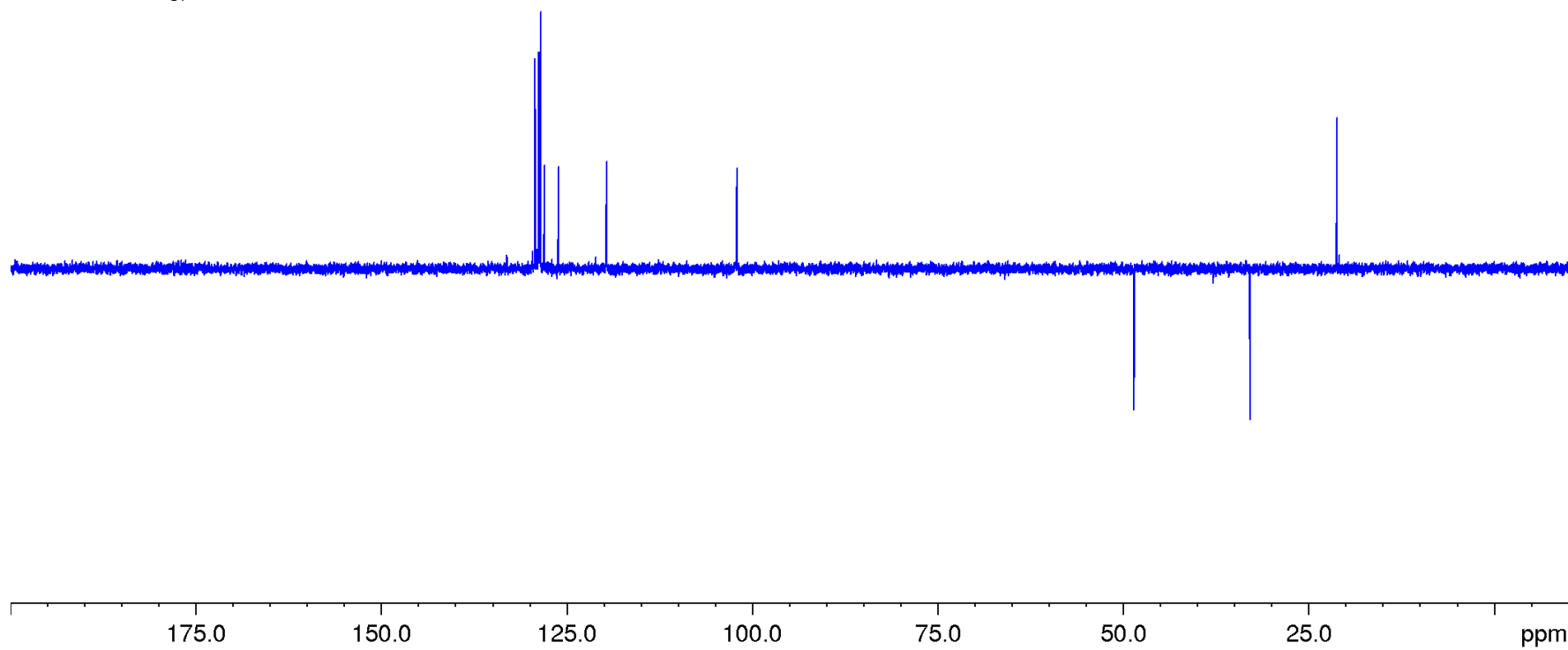


129.291  
128.747  
128.621  
128.505  
128.017  
126.091  
119.638  
102.047

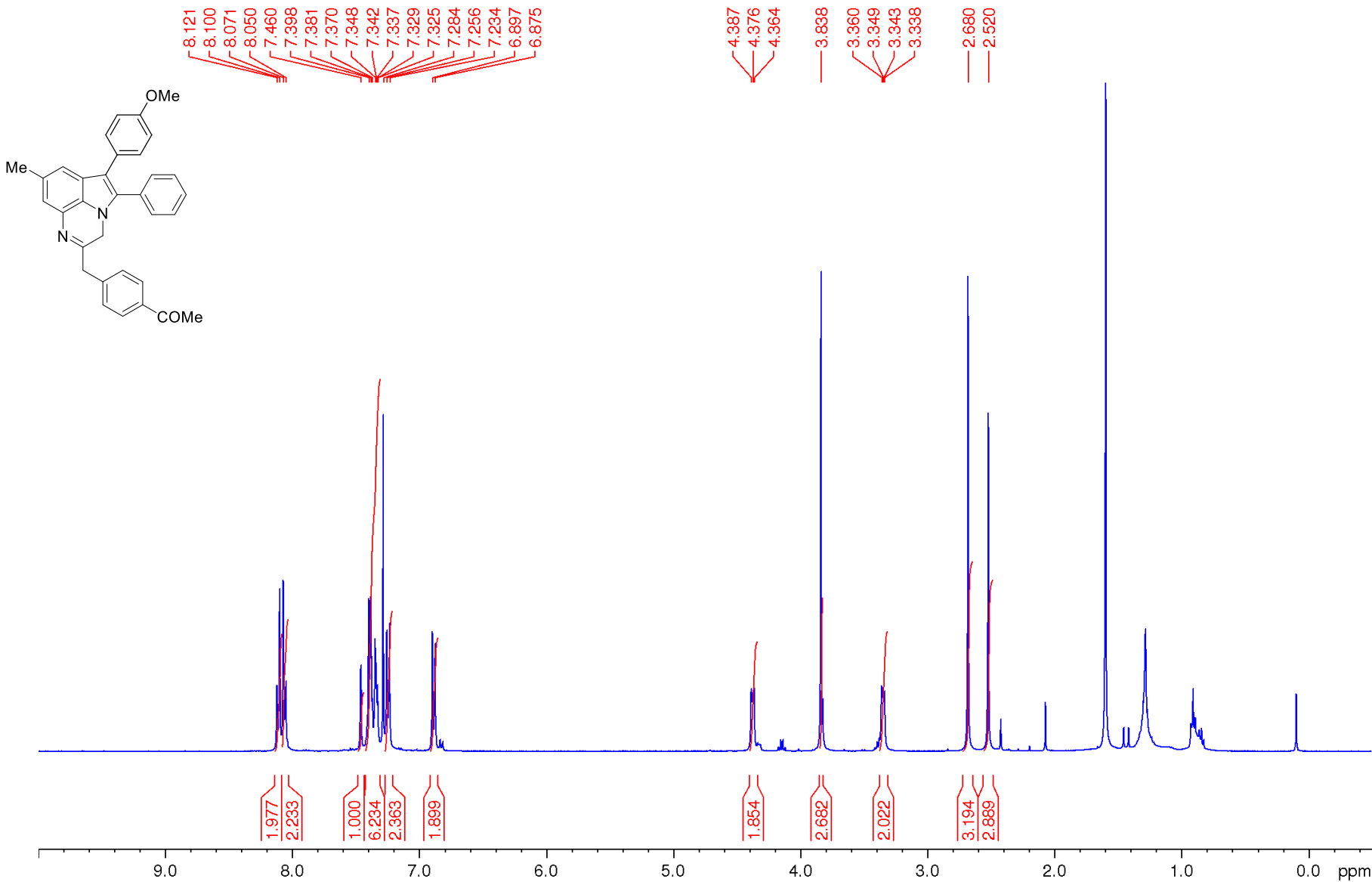
48.513

32.880

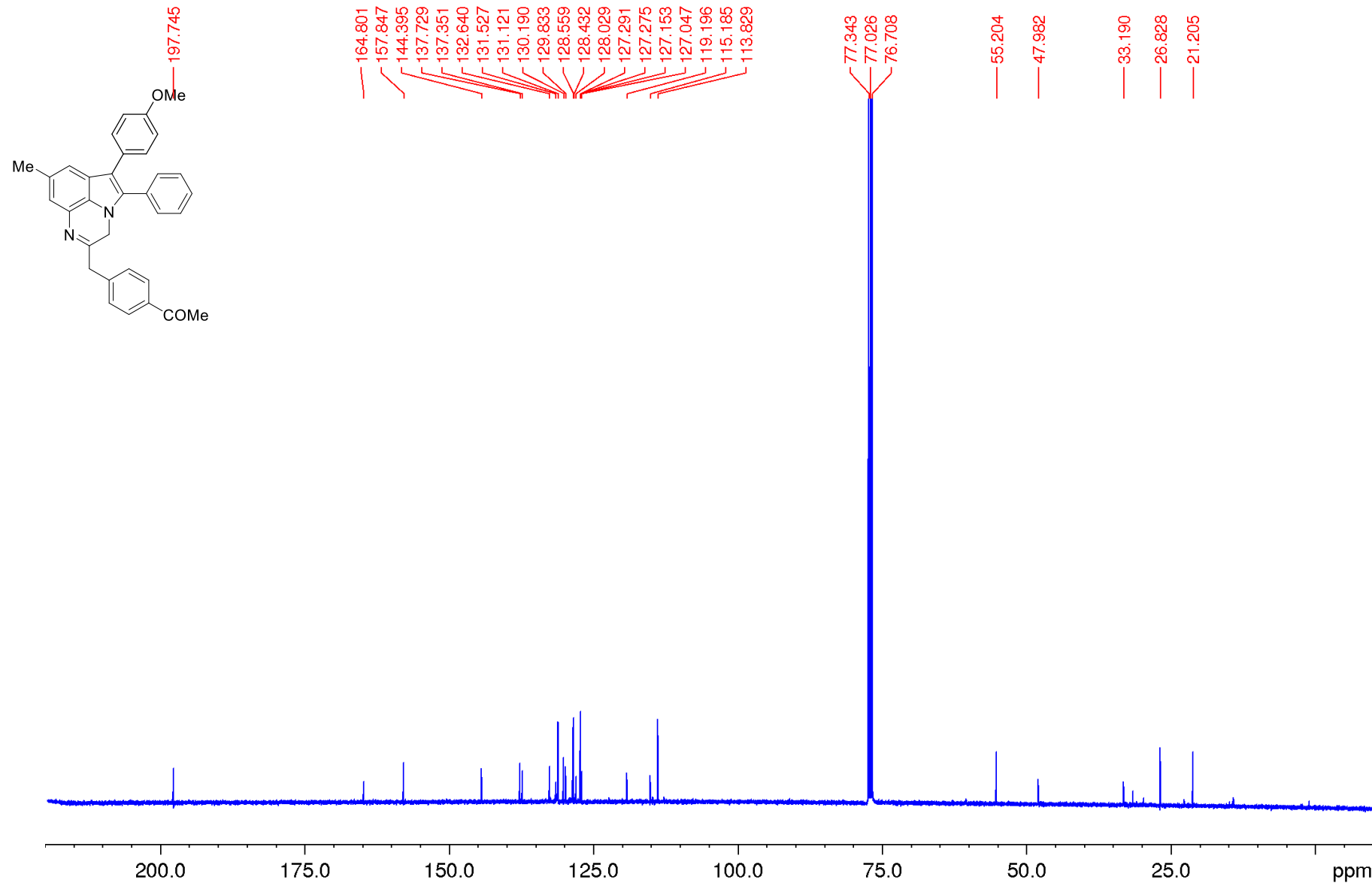
21.175



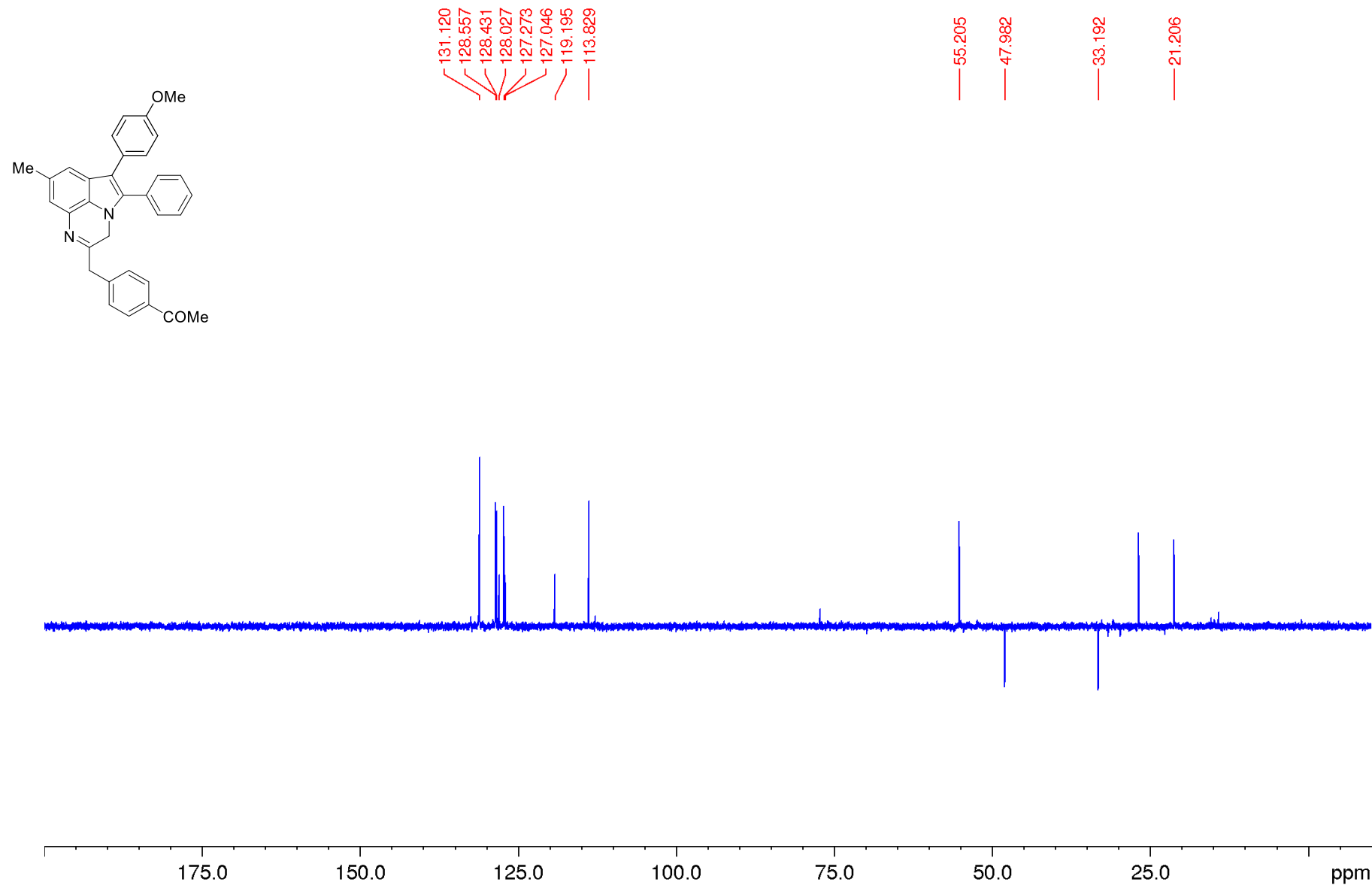
1-((4-((6-(4-methoxyphenyl)-8-methyl-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2k



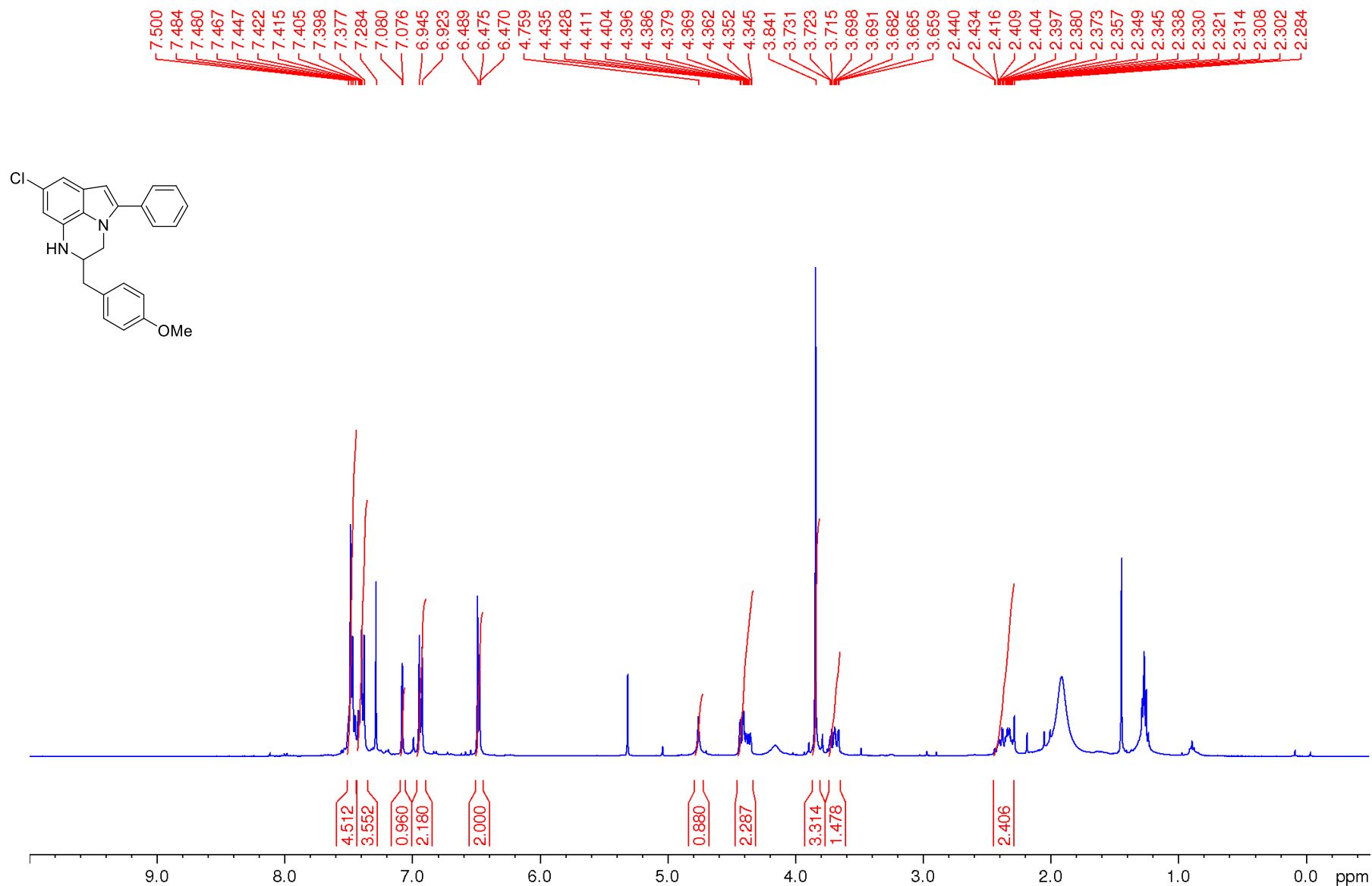
1-(4-((6-(4-methoxyphenyl)-8-methyl-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2k



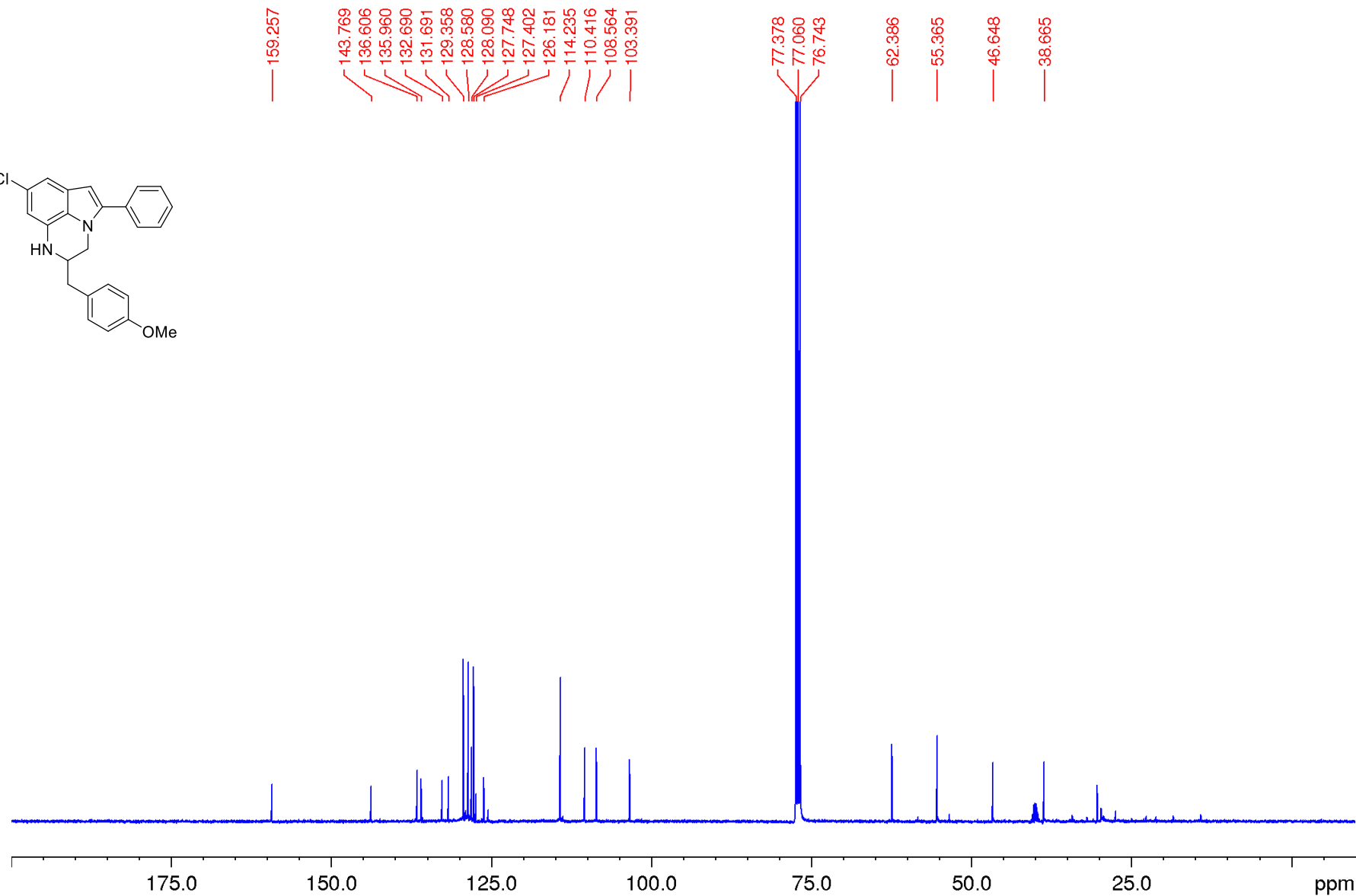
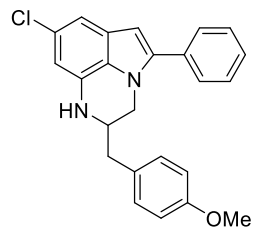
1-((4-((6-(4-methoxyphenyl)-8-methyl-5-phenyl-3H-pyrrolo[1,2,3-de]quinoxalin-2-yl)methyl)phenyl)ethan-1-one 2k



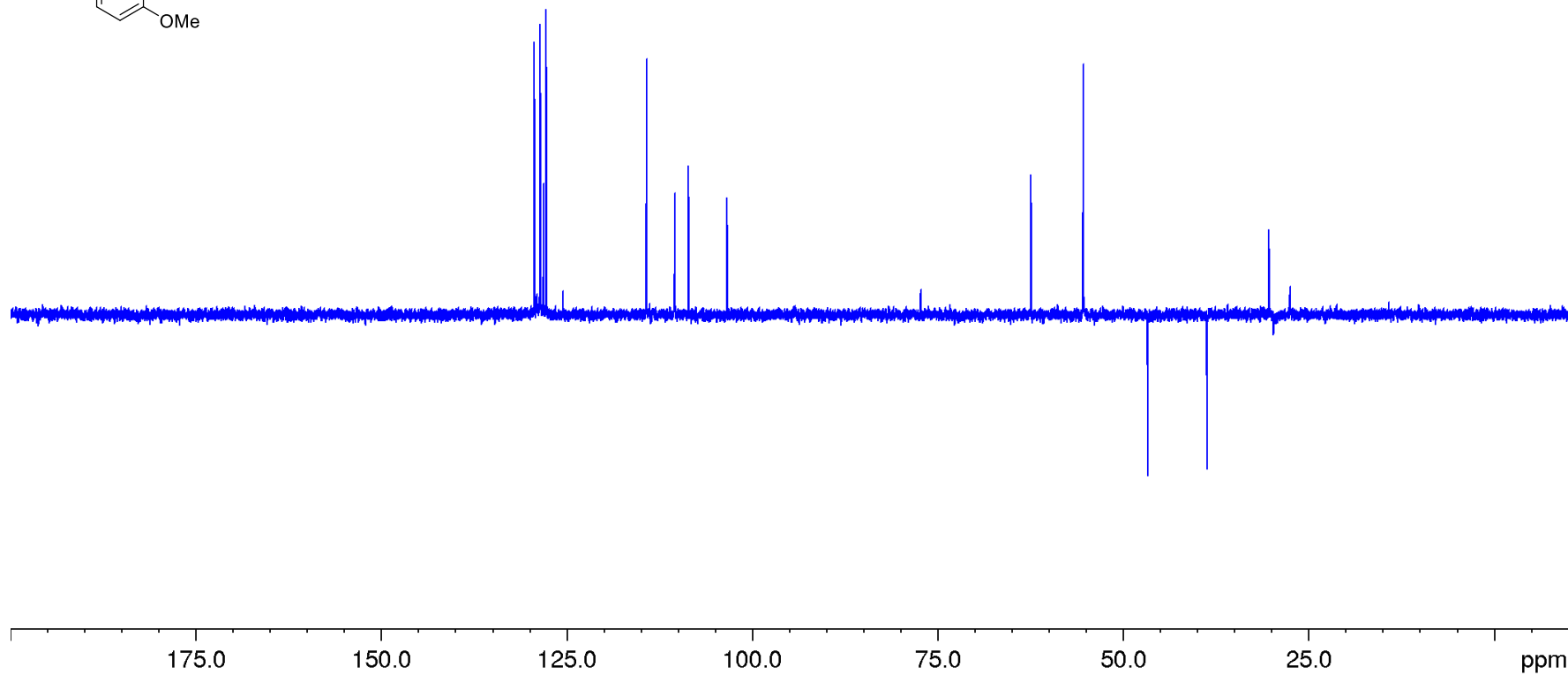
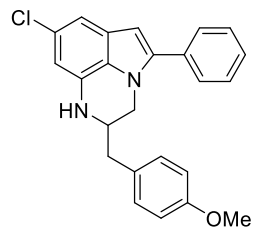
**8-chloro-2-(4-methoxybenzyl)-5-phenyl-2,3-dihydro-1H-pyrrolo[1,2,3-de]quinoxaline 9d**



**8-chloro-2-(4-methoxybenzyl)-5-phenyl-2,3-dihydro-1H-pyrrolo[1,2,3-*de*]quinoxaline 9d**



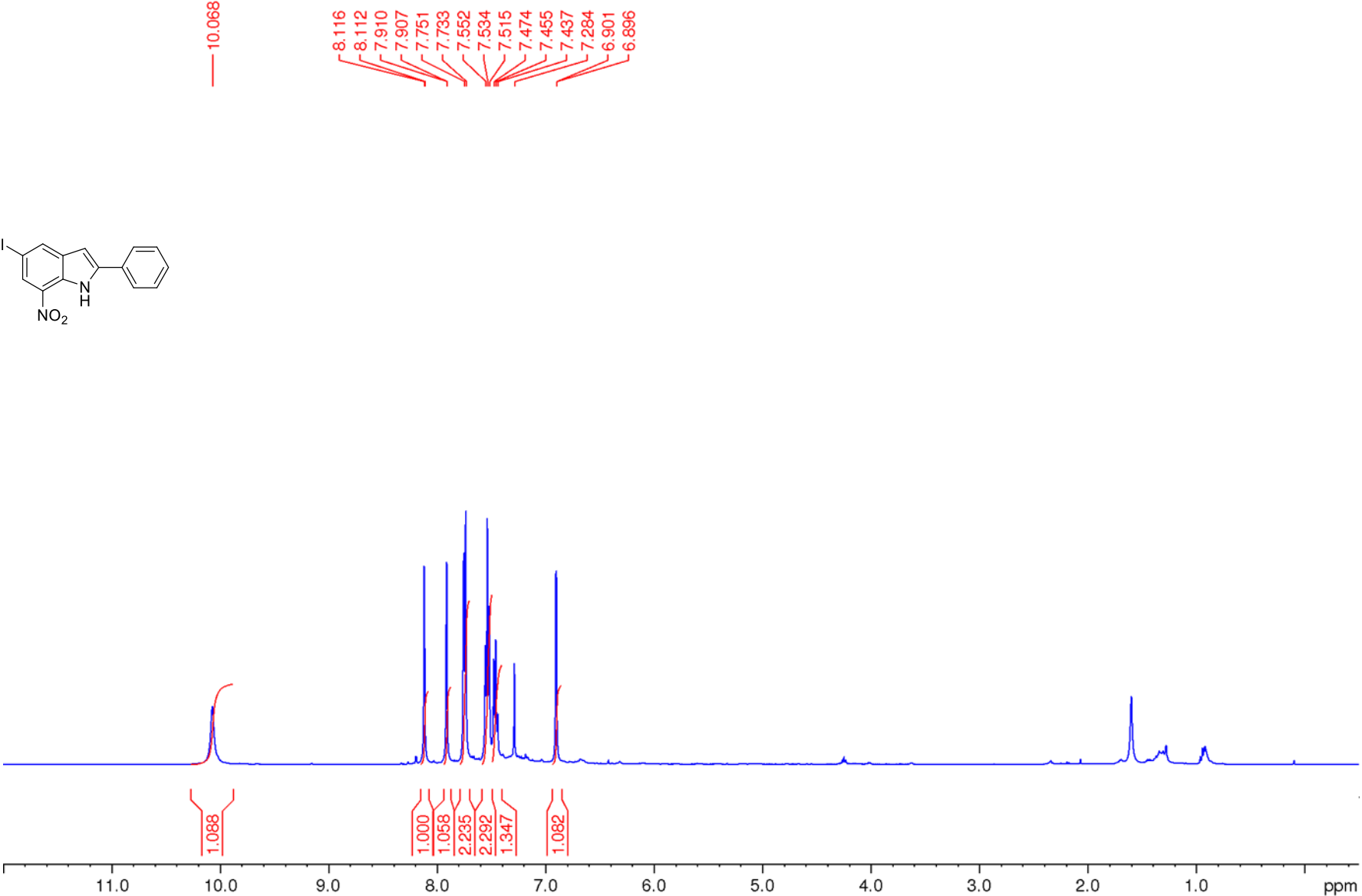
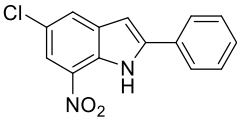
**8-chloro-2-(4-methoxybenzyl)-5-phenyl-2,3-dihydro-1H-pyrrolo[1,2,3-*de*]quinoxaline 9d**



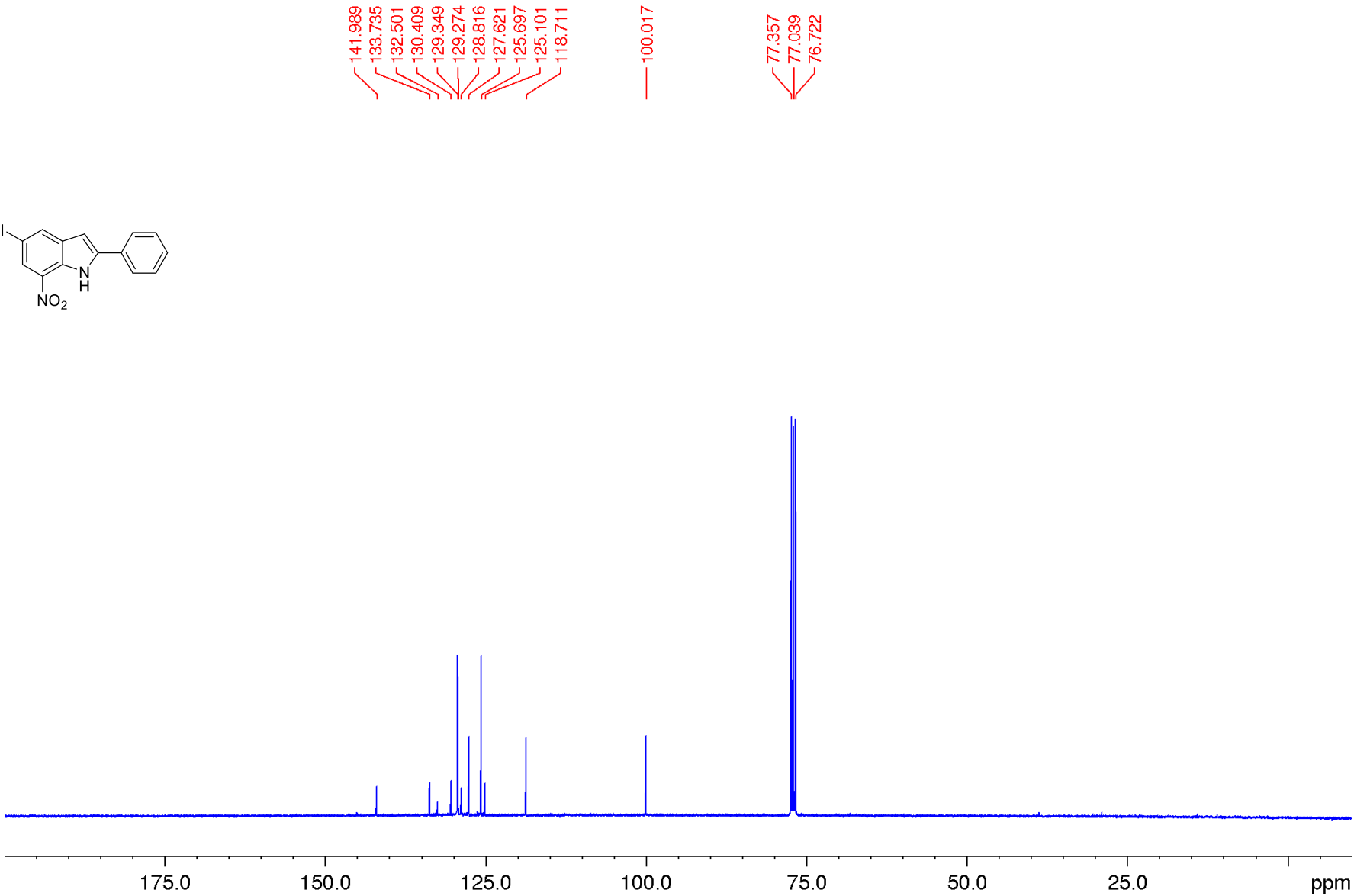
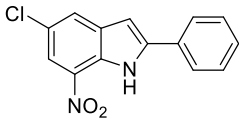




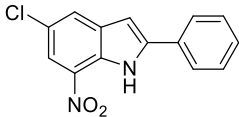
5-chloro-7-nitro-2-phenyl-1H-indole 5a



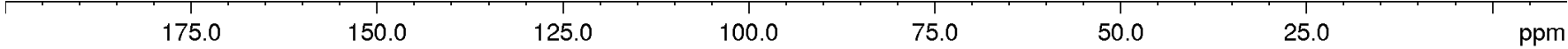
5-chloro-7-nitro-2-phenyl-1*H*-indole 5a



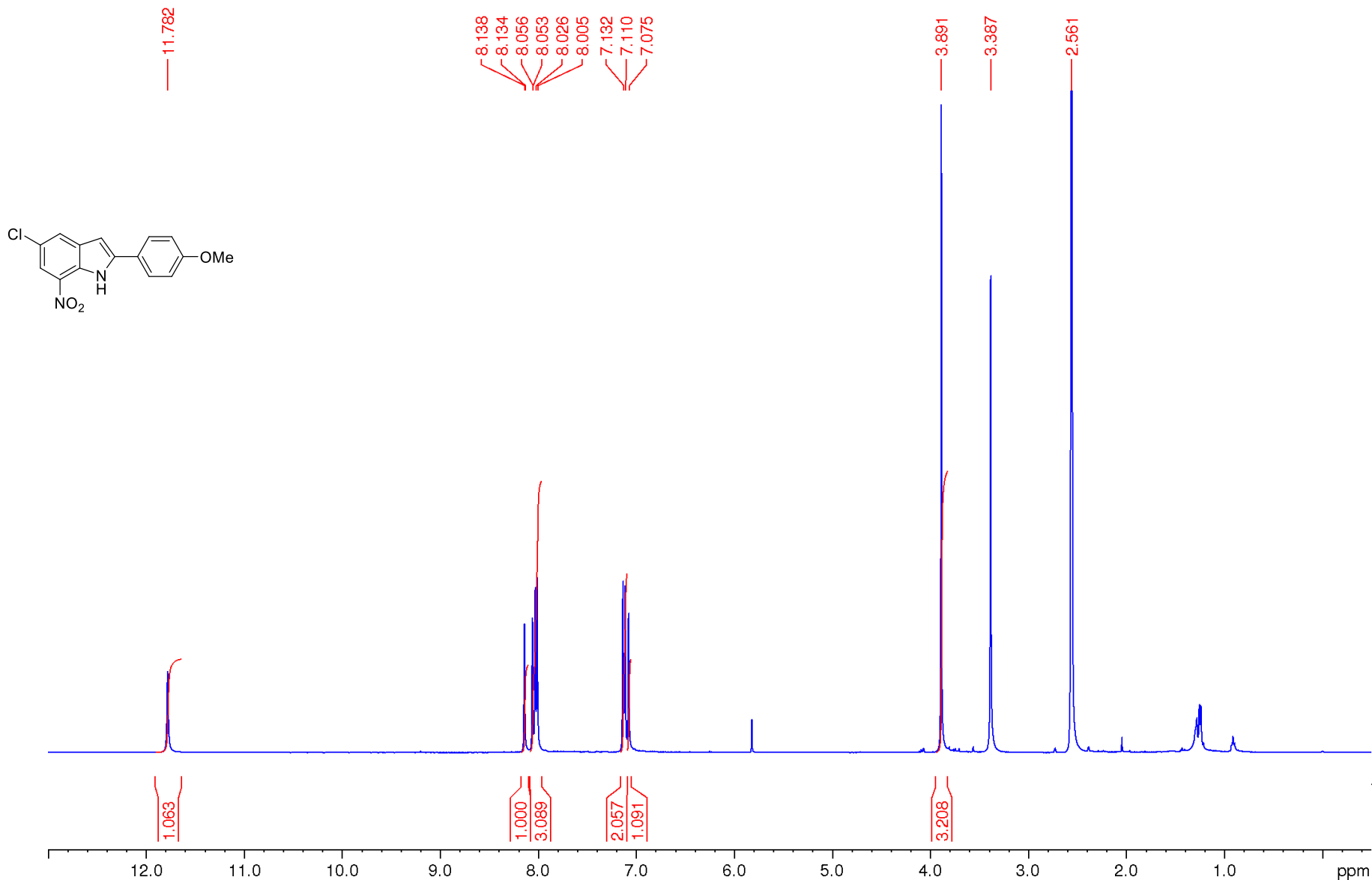
5-chloro-7-nitro-2-phenyl-1H-indole 5a



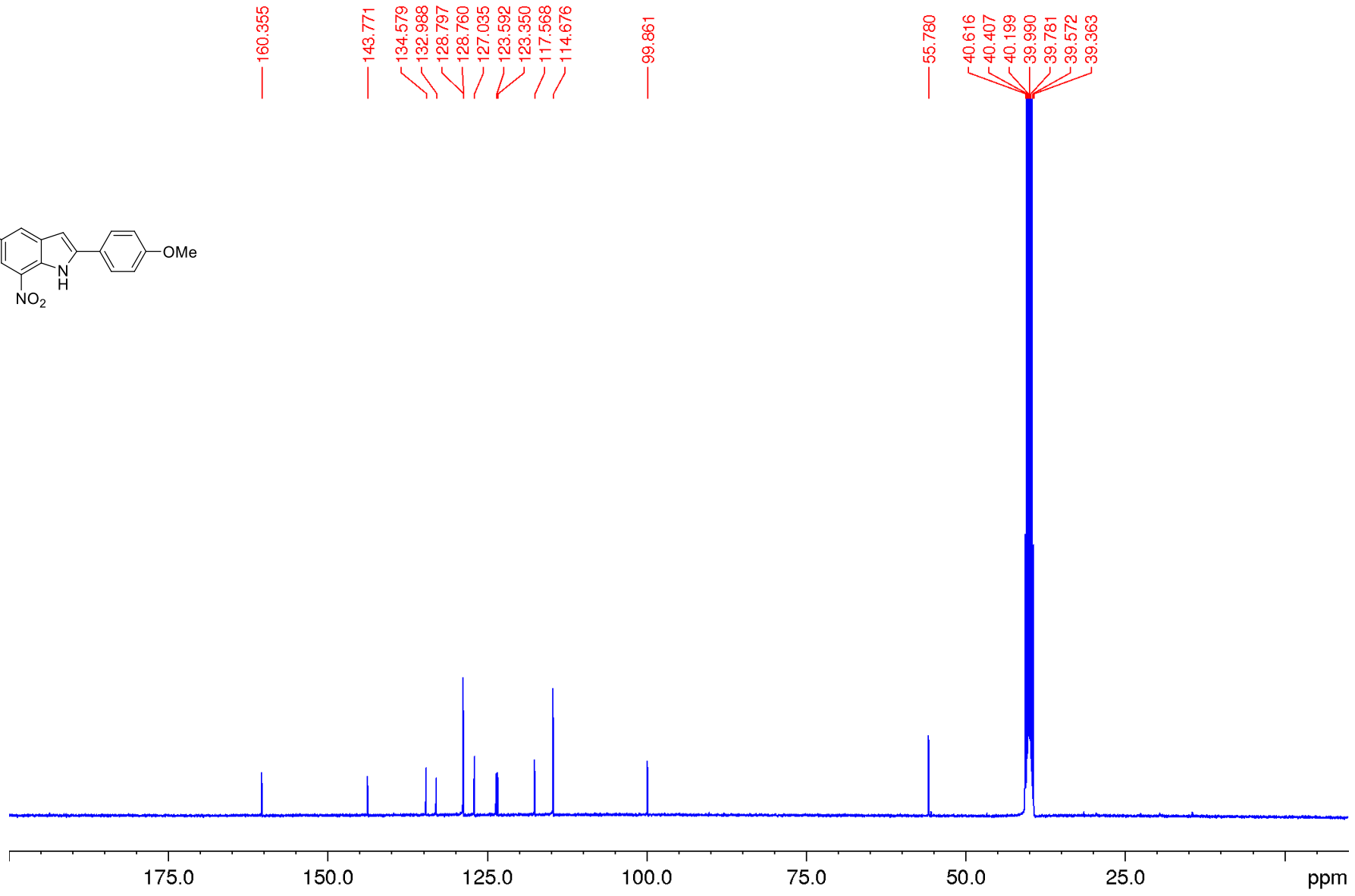
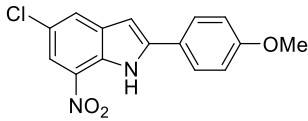
129.349  
129.273  
127.621  
125.696  
118.710  
100.016



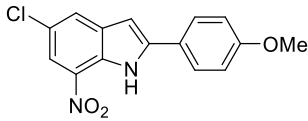
# 5-chloro-2-(4-methoxyphenyl)-7-nitro-1H-indole 5b



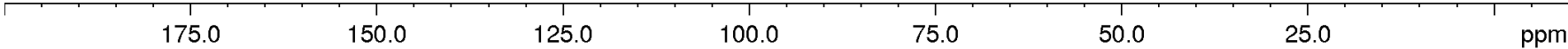
5-chloro-2-(4-methoxyphenyl)-7-nitro-1H-indole 5b



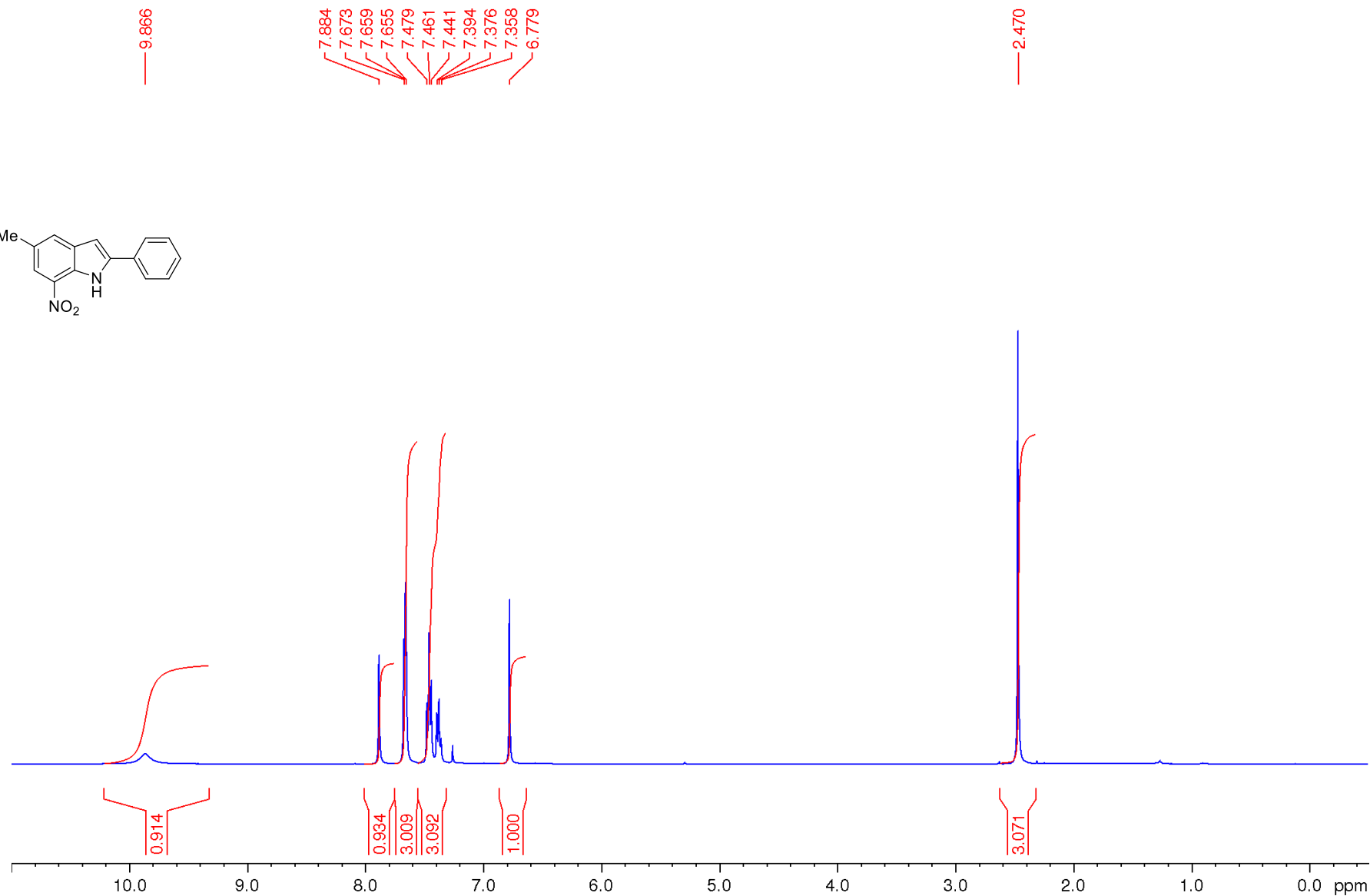
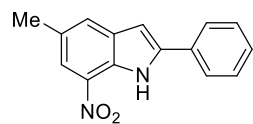
5-chloro-2-(4-methoxyphenyl)-7-nitro-1*H*-indole 5b



128.796  
127.034  
117.568  
114.675  
99.861  
55.780  
40.666  
40.457  
40.247  
40.038  
39.829

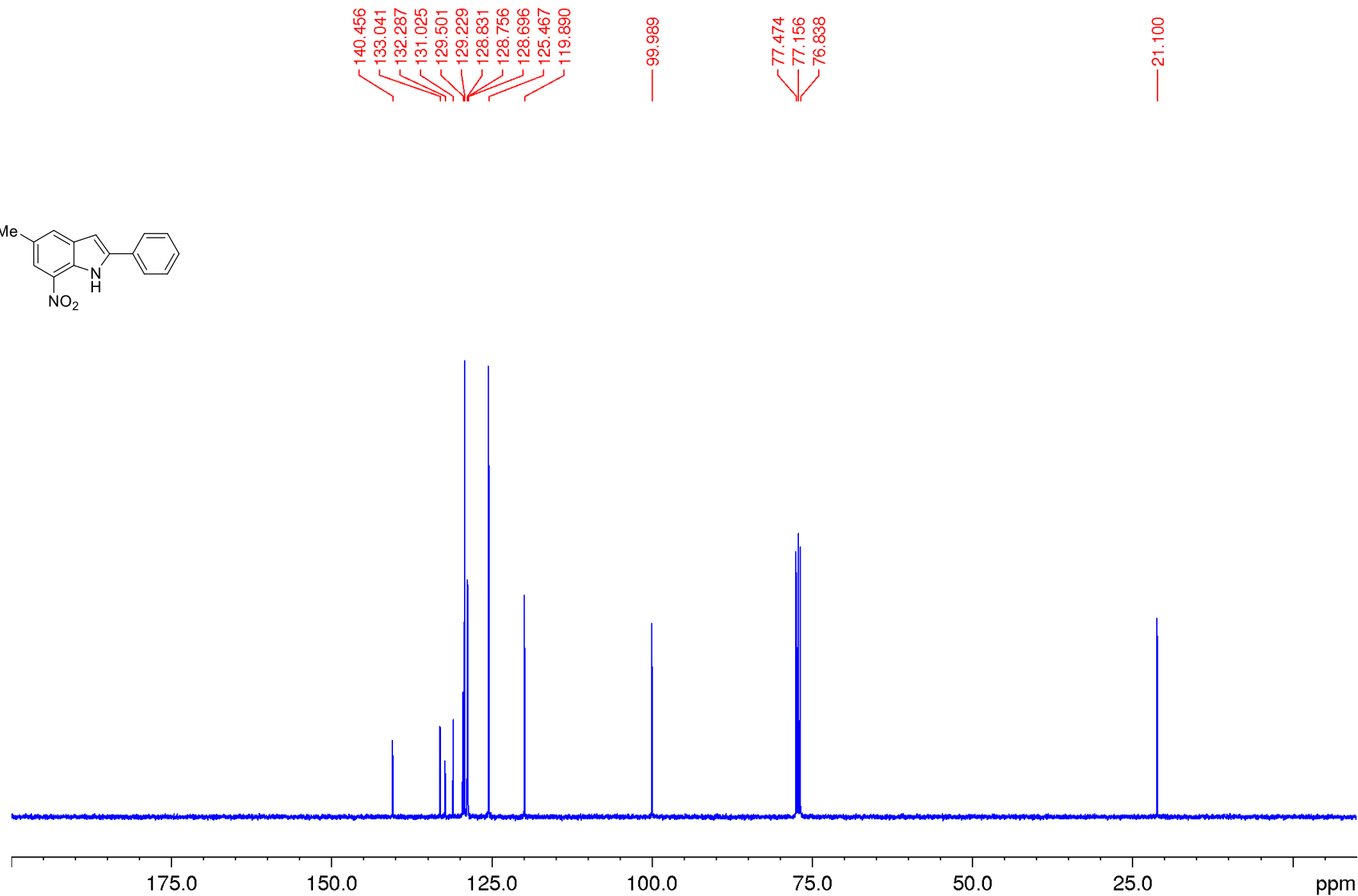
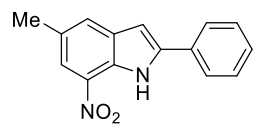


# 5-methyl-7-nitro-2-phenyl-1H-indole 5c

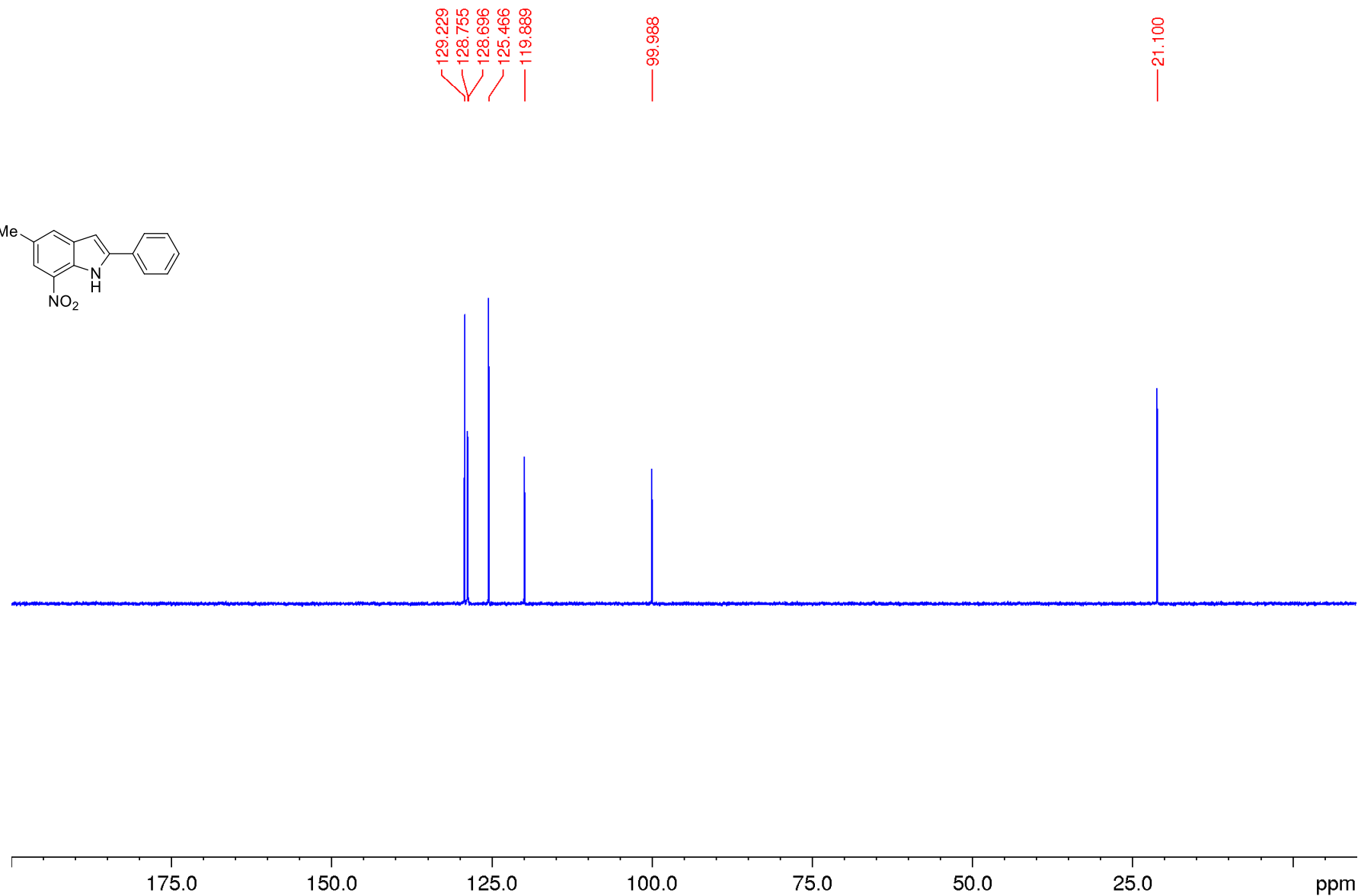
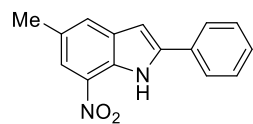




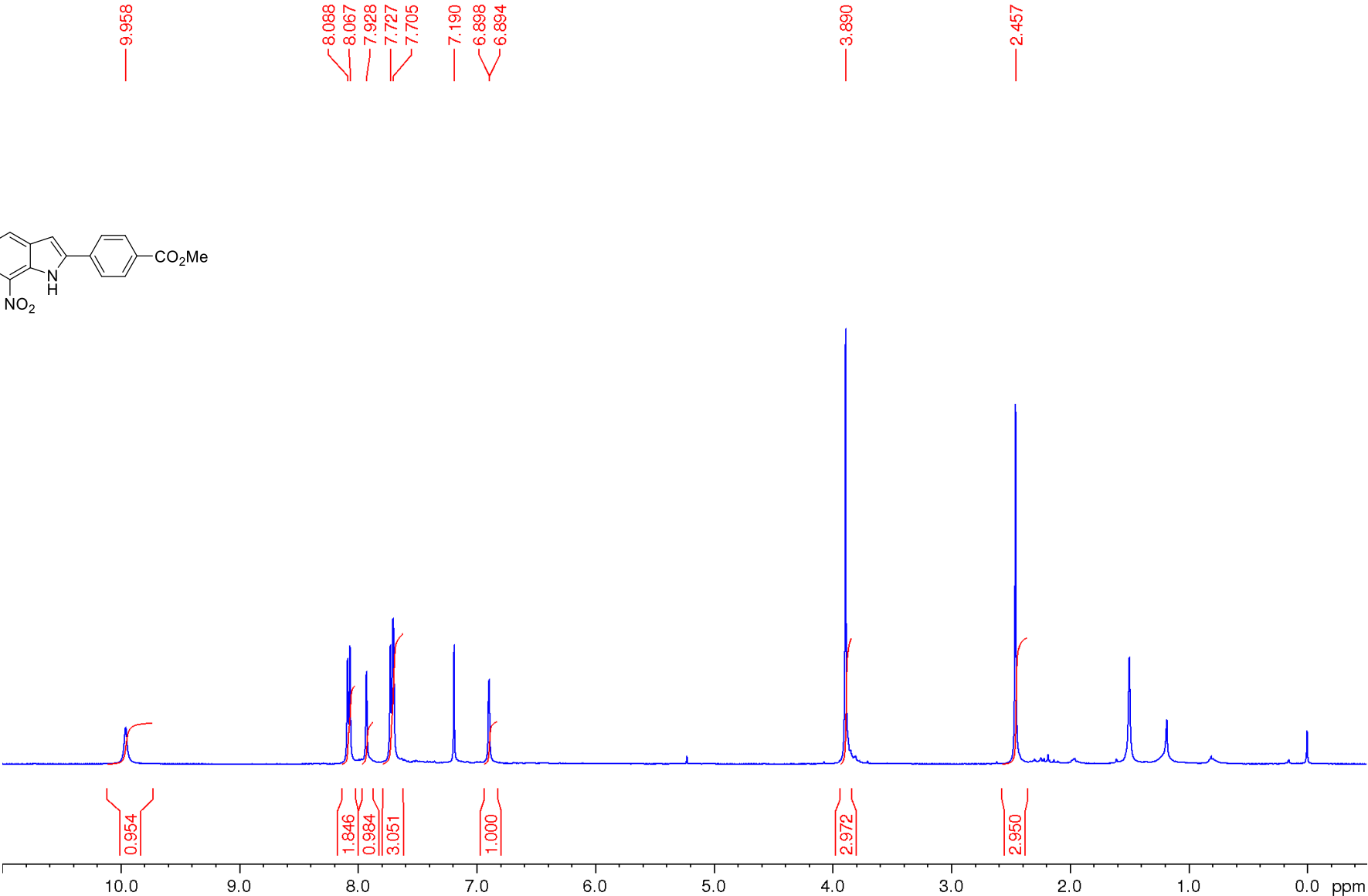
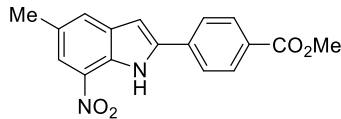
# 5-methyl-7-nitro-2-phenyl-1H-indole 5c



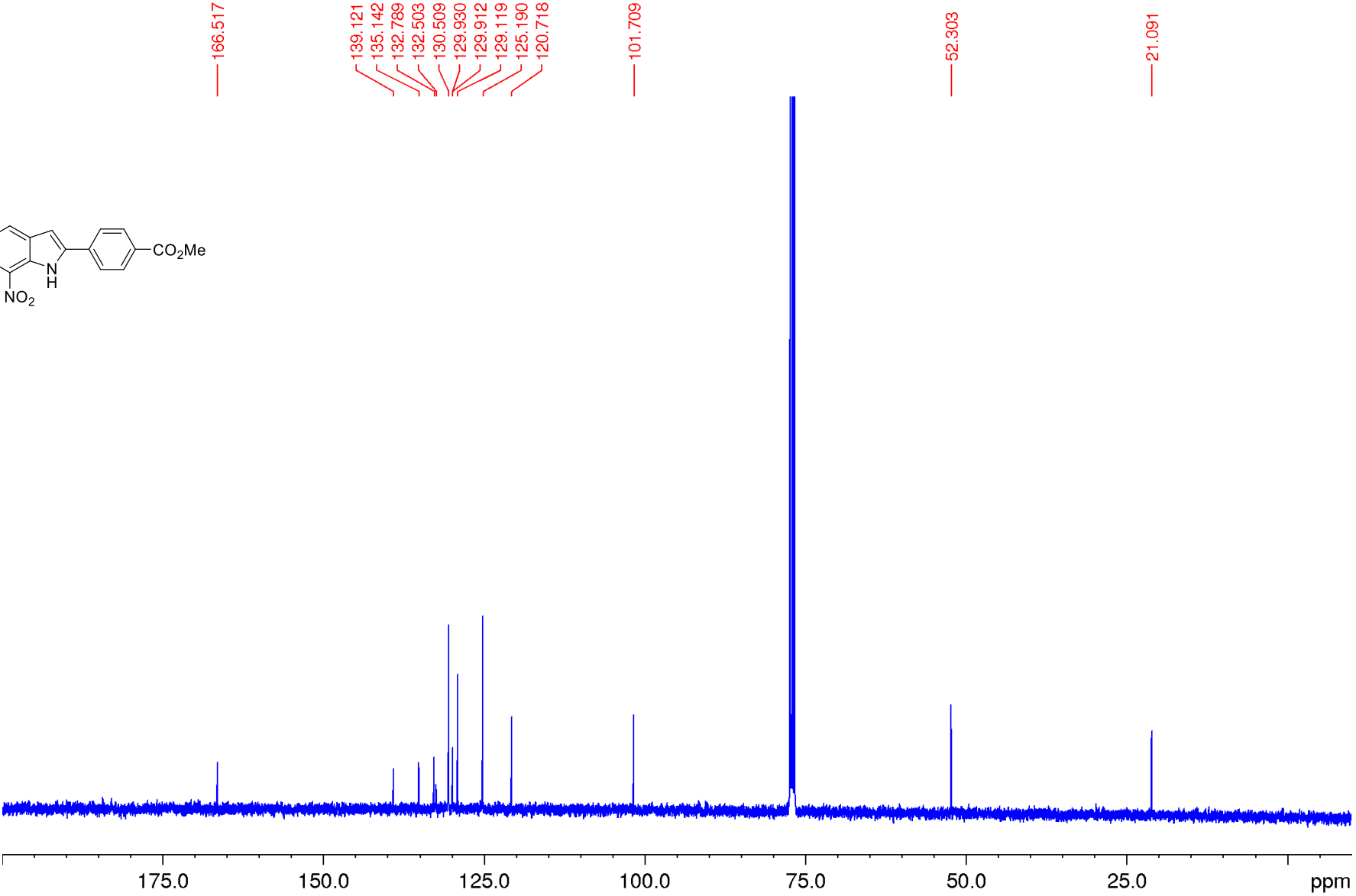
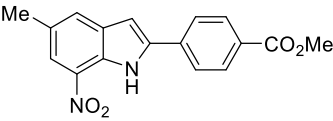
# 5-methyl-7-nitro-2-phenyl-1H-indole 5c



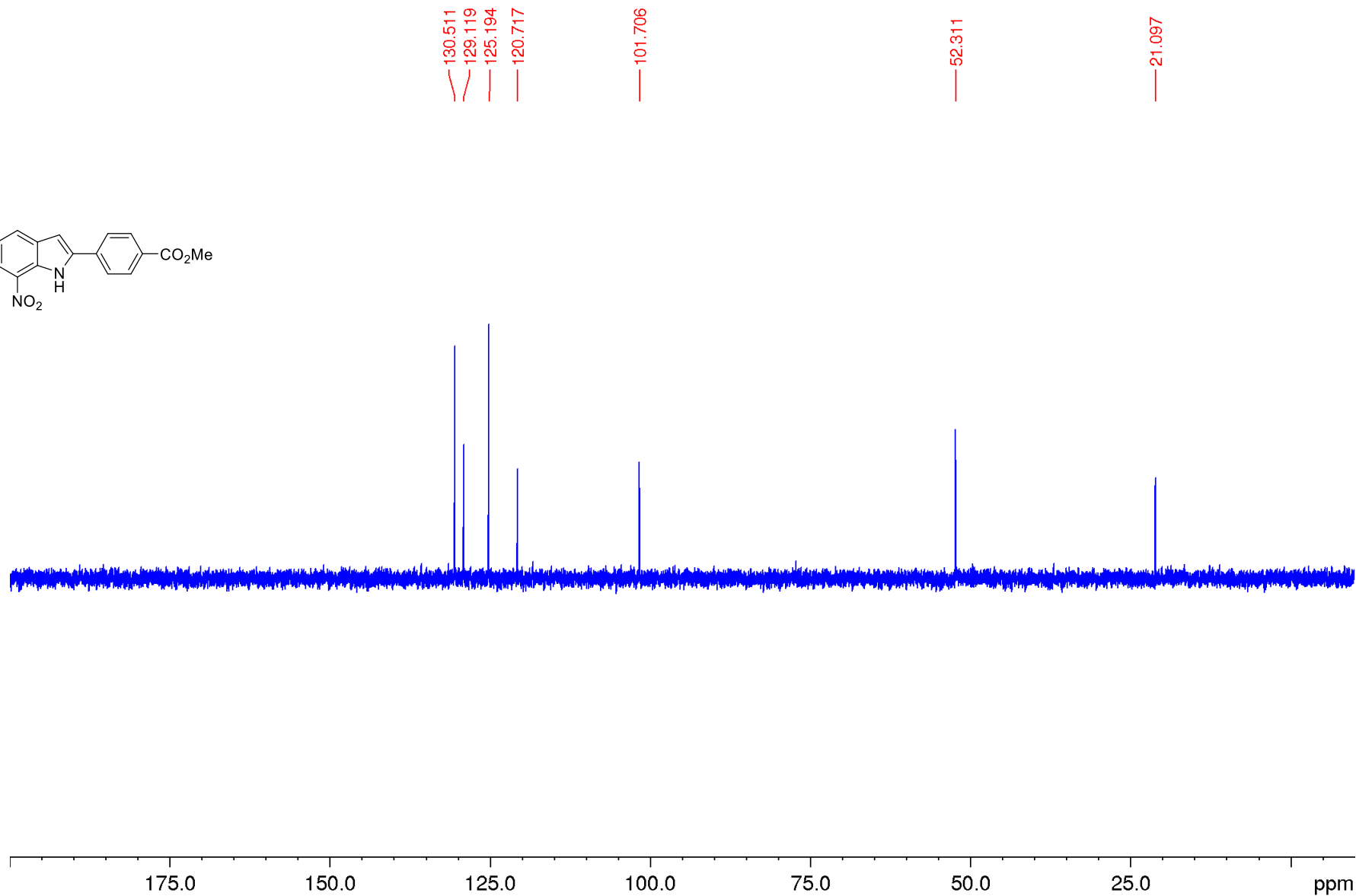
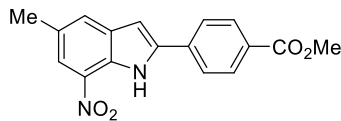
methyl 4-(5-methyl-7-nitro-1*H*-indol-2-yl)benzoate 5d



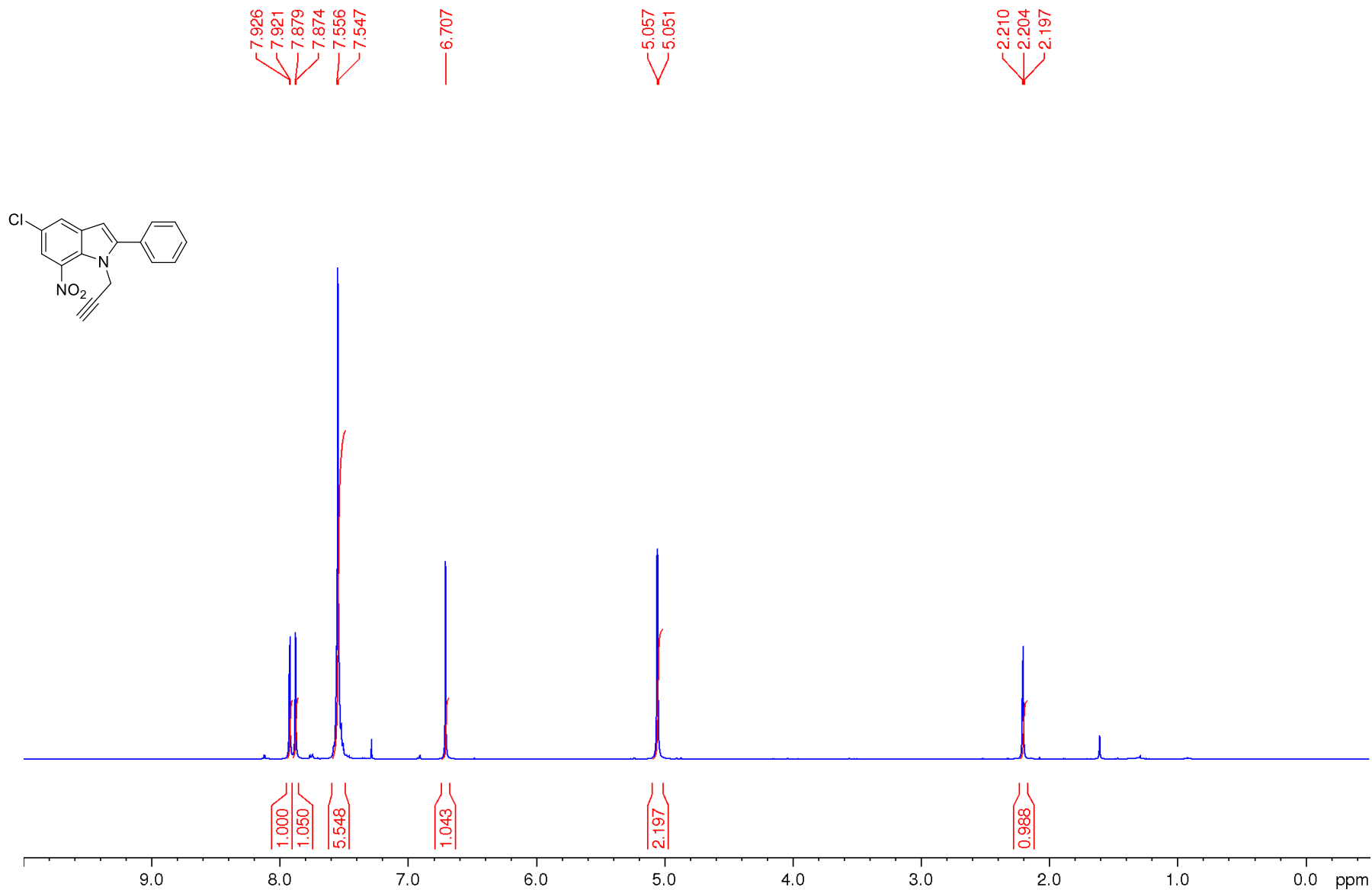
methyl 4-(5-methyl-7-nitro-1*H*-indol-2-yl)benzoate 5d



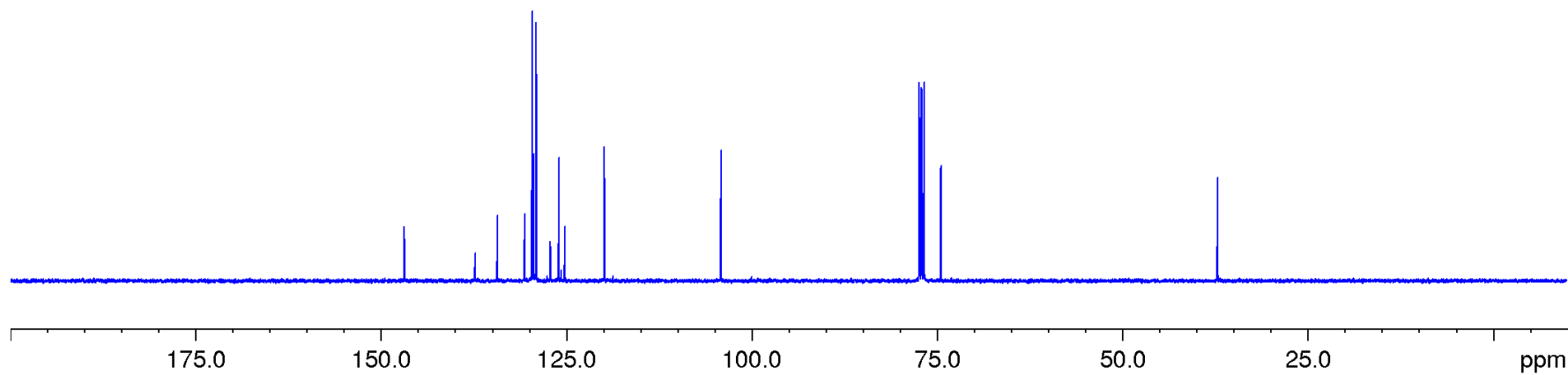
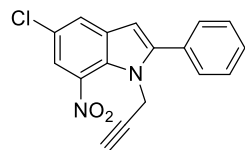
methyl 4-(5-methyl-7-nitro-1*H*-indol-2-yl)benzoate 5d



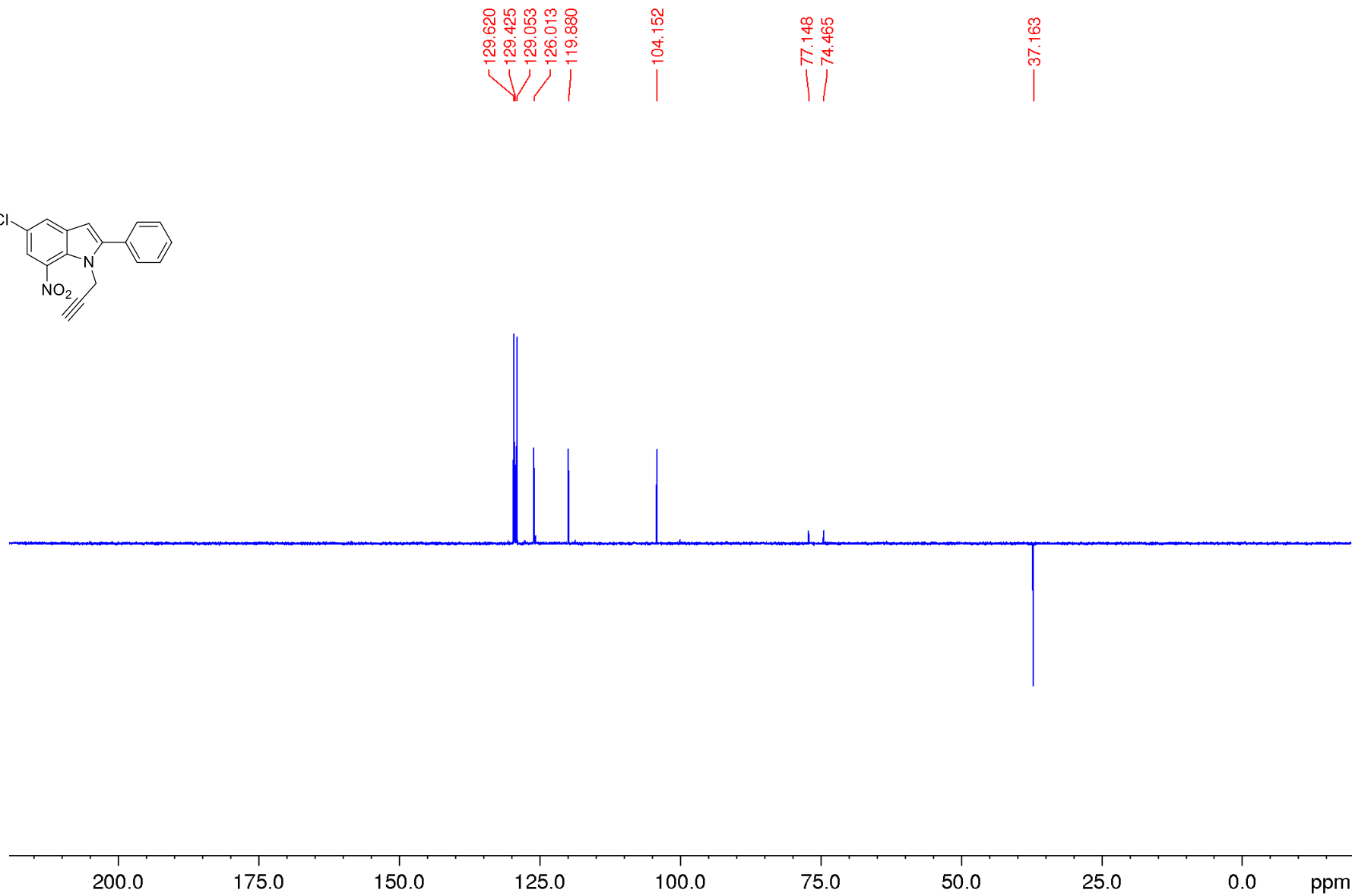
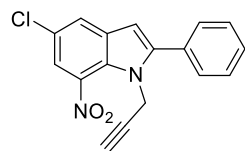
**5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6a**



**5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1*H*-indole 6a**

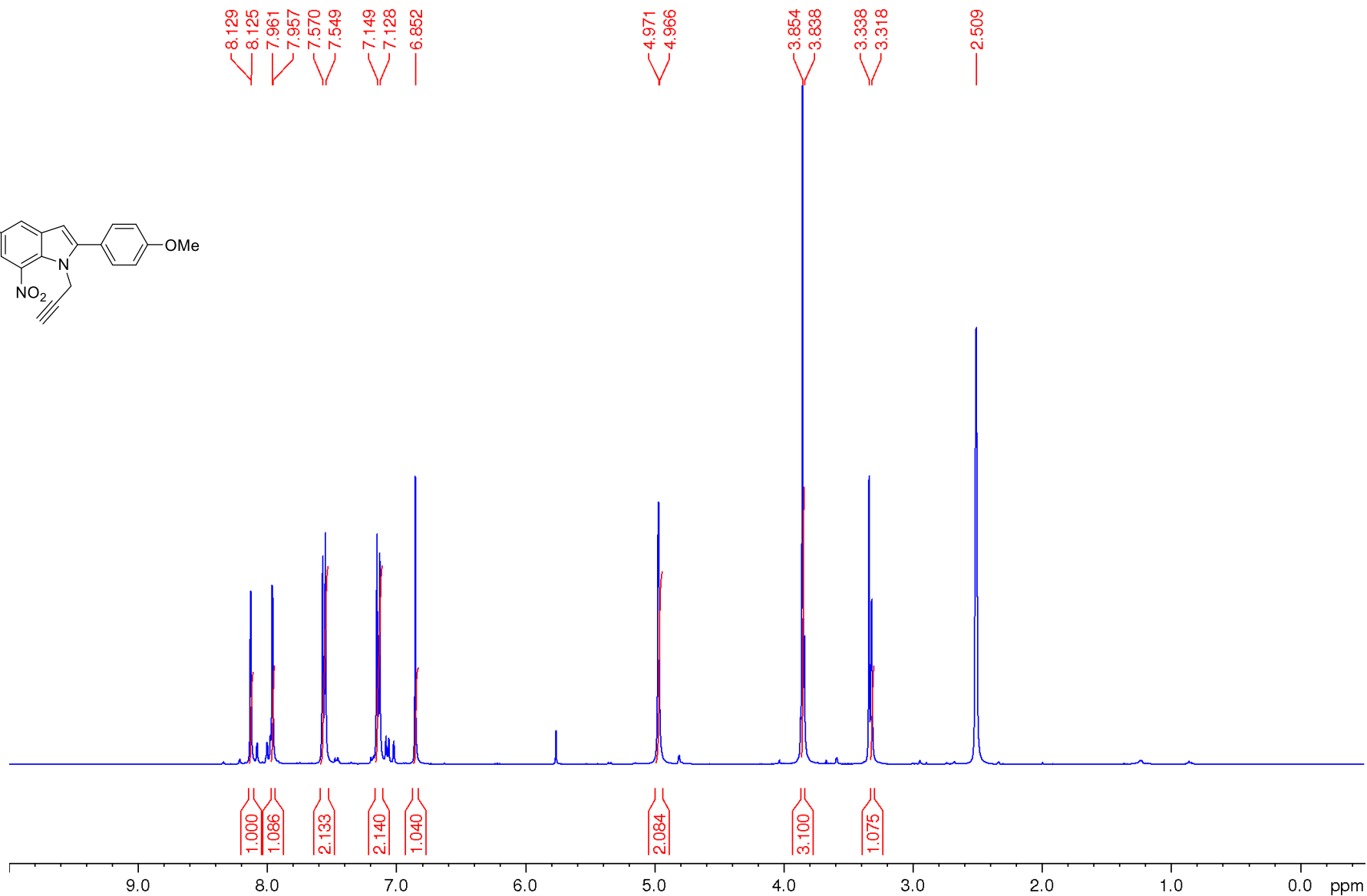
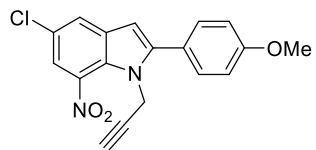


**5-chloro-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6a**

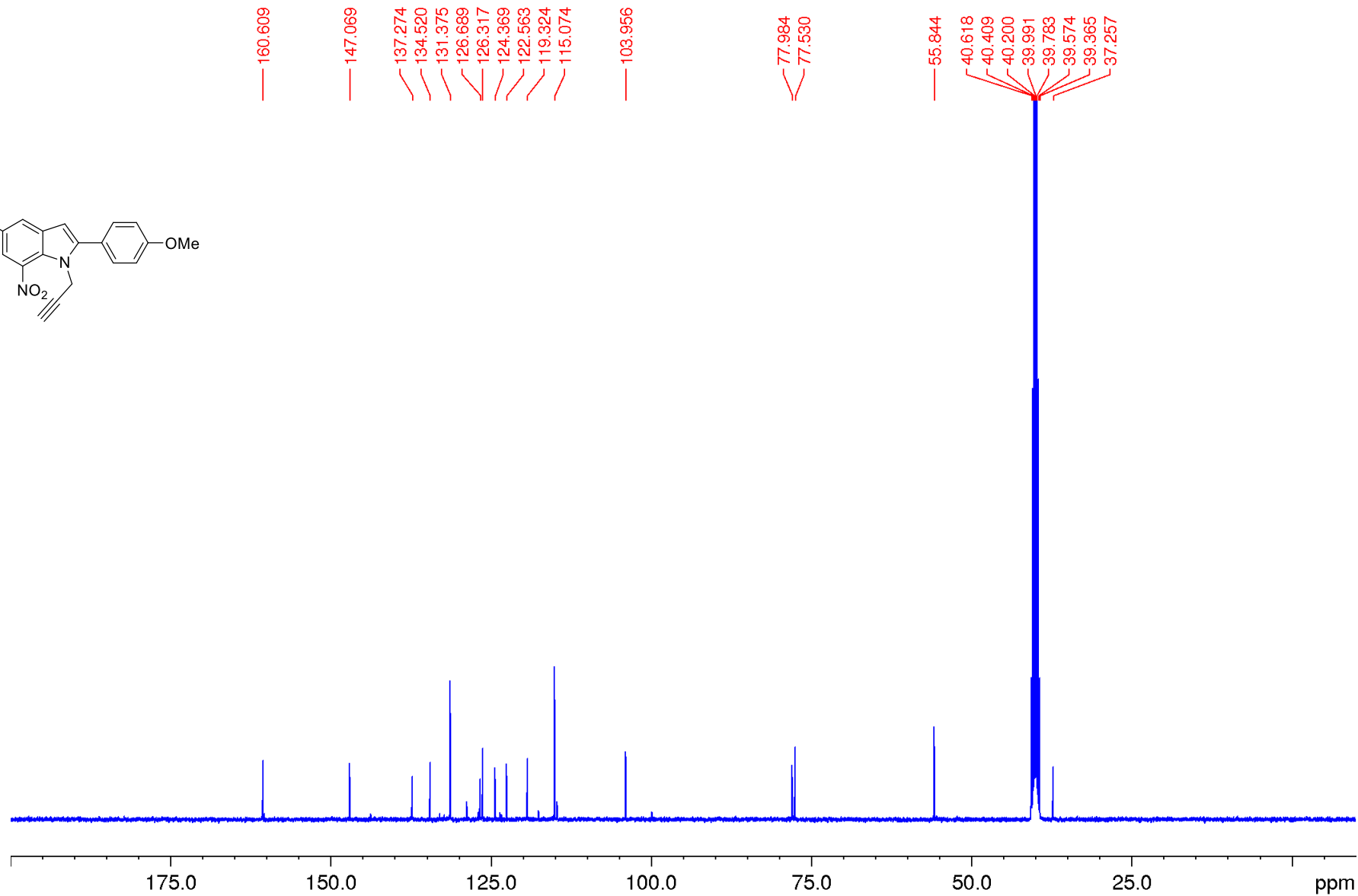
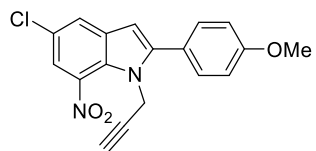




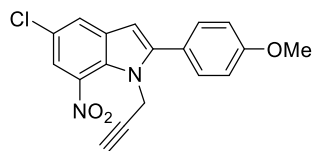
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(prop-2-yn-1-yl)-1H-indole 6b**



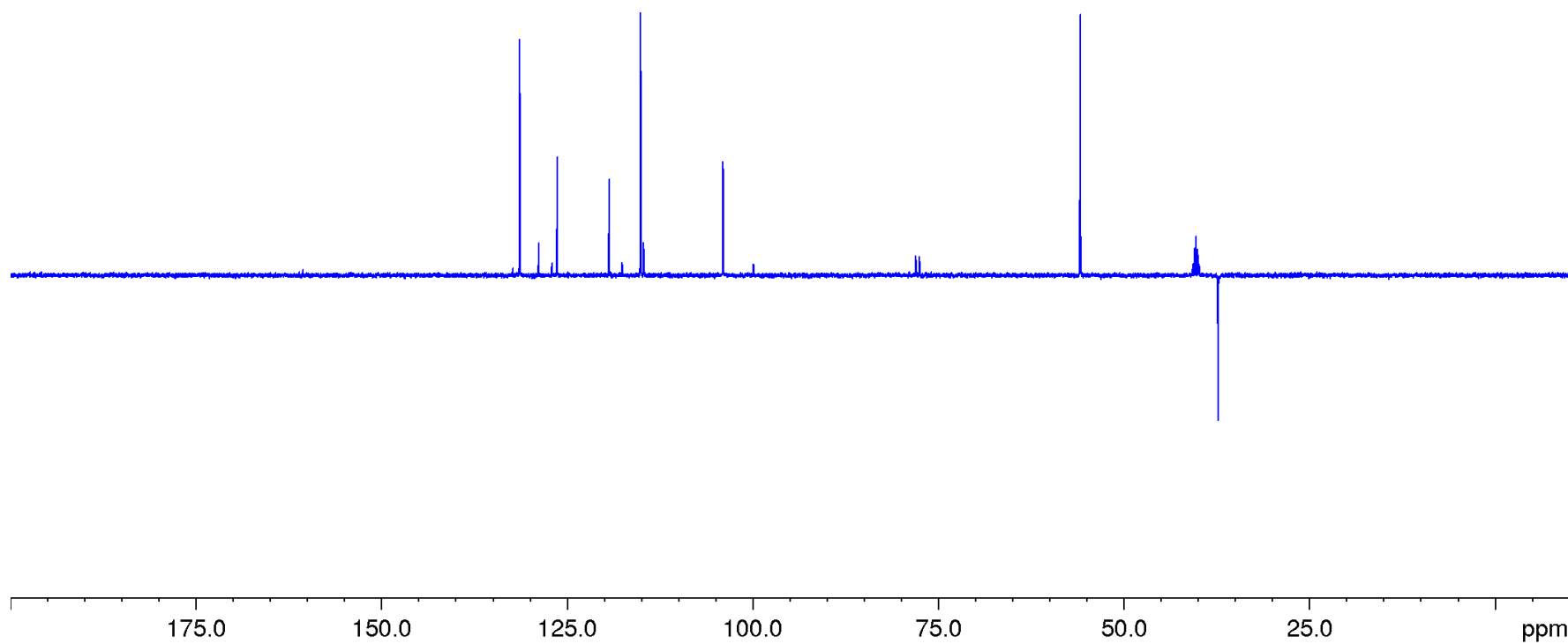
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(prop-2-yn-1-yl)-1*H*-indole 6b**



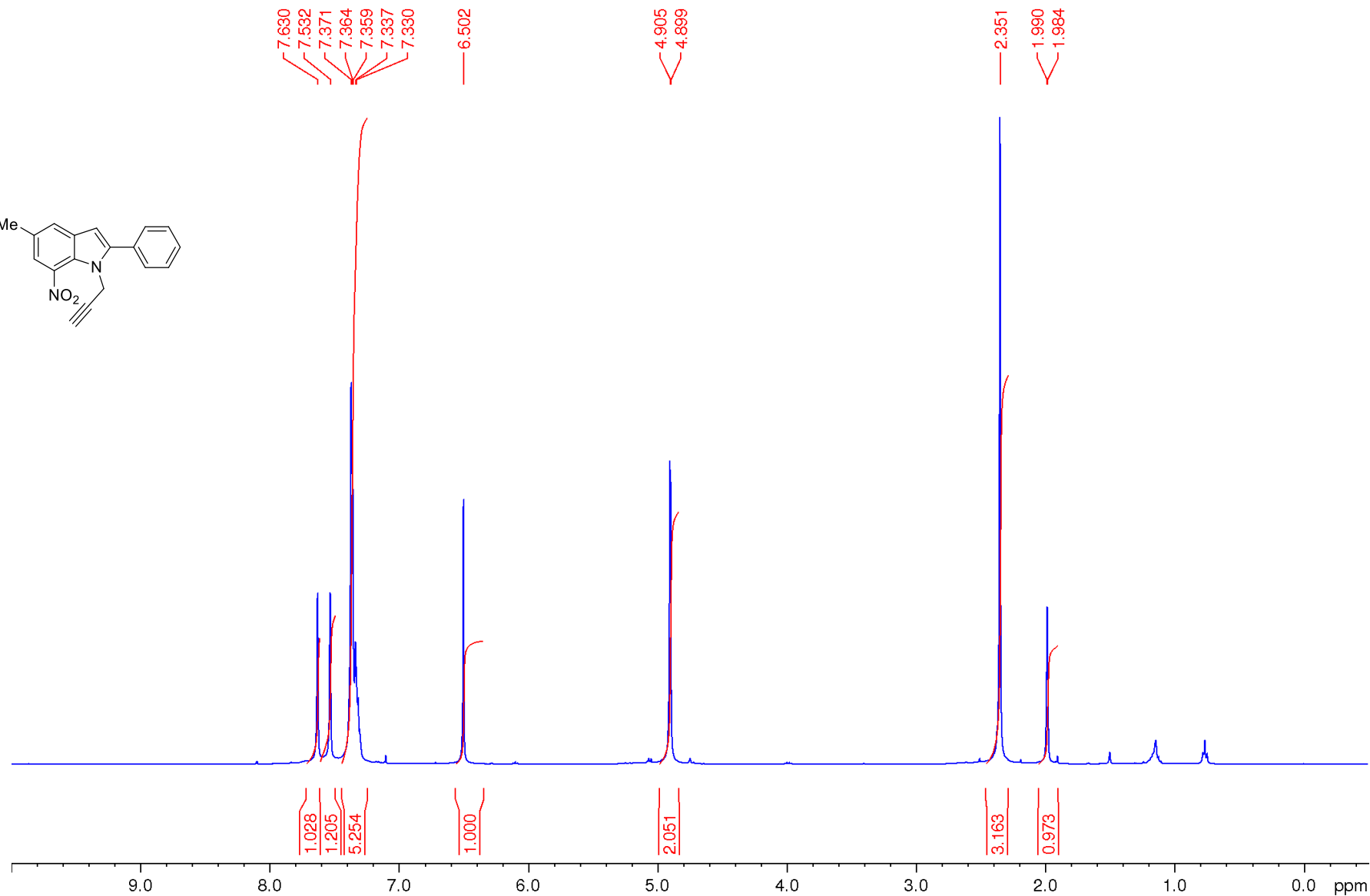
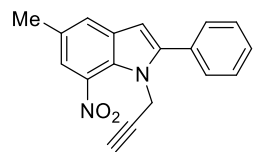
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(prop-2-yn-1-yl)-1*H*-indole 6b**



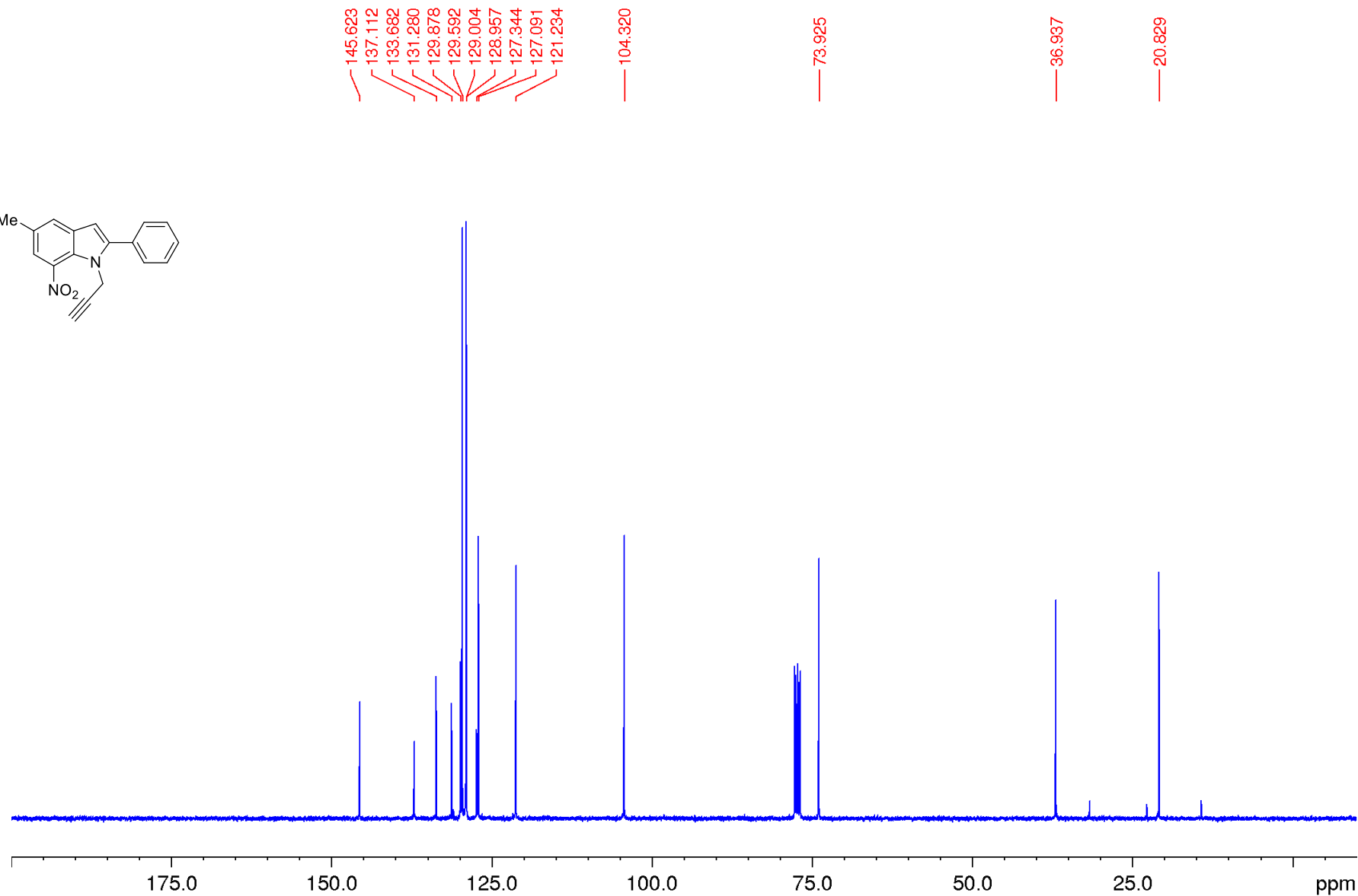
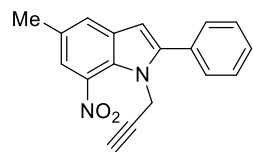
131.374  
126.317  
119.323  
115.074  
103.955  
77.984  
77.530  
55.842  
40.668  
40.457  
40.247  
40.038  
39.828  
37.256



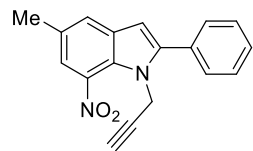
**5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6c**



# 5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6c



**5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1H-indole 6c**



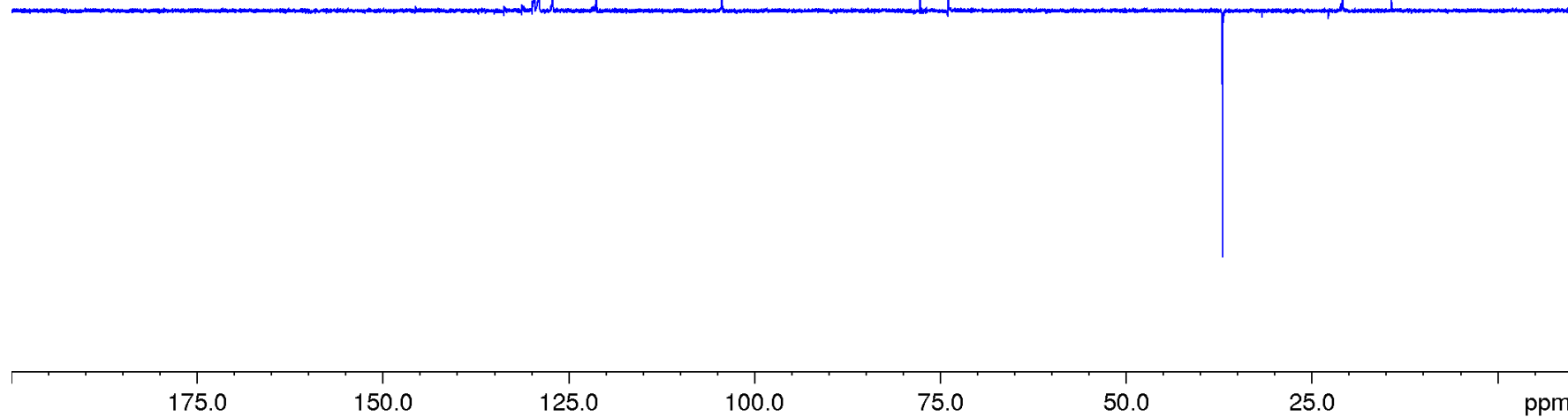
129.592  
129.004  
128.957  
127.092  
121.234

104.321

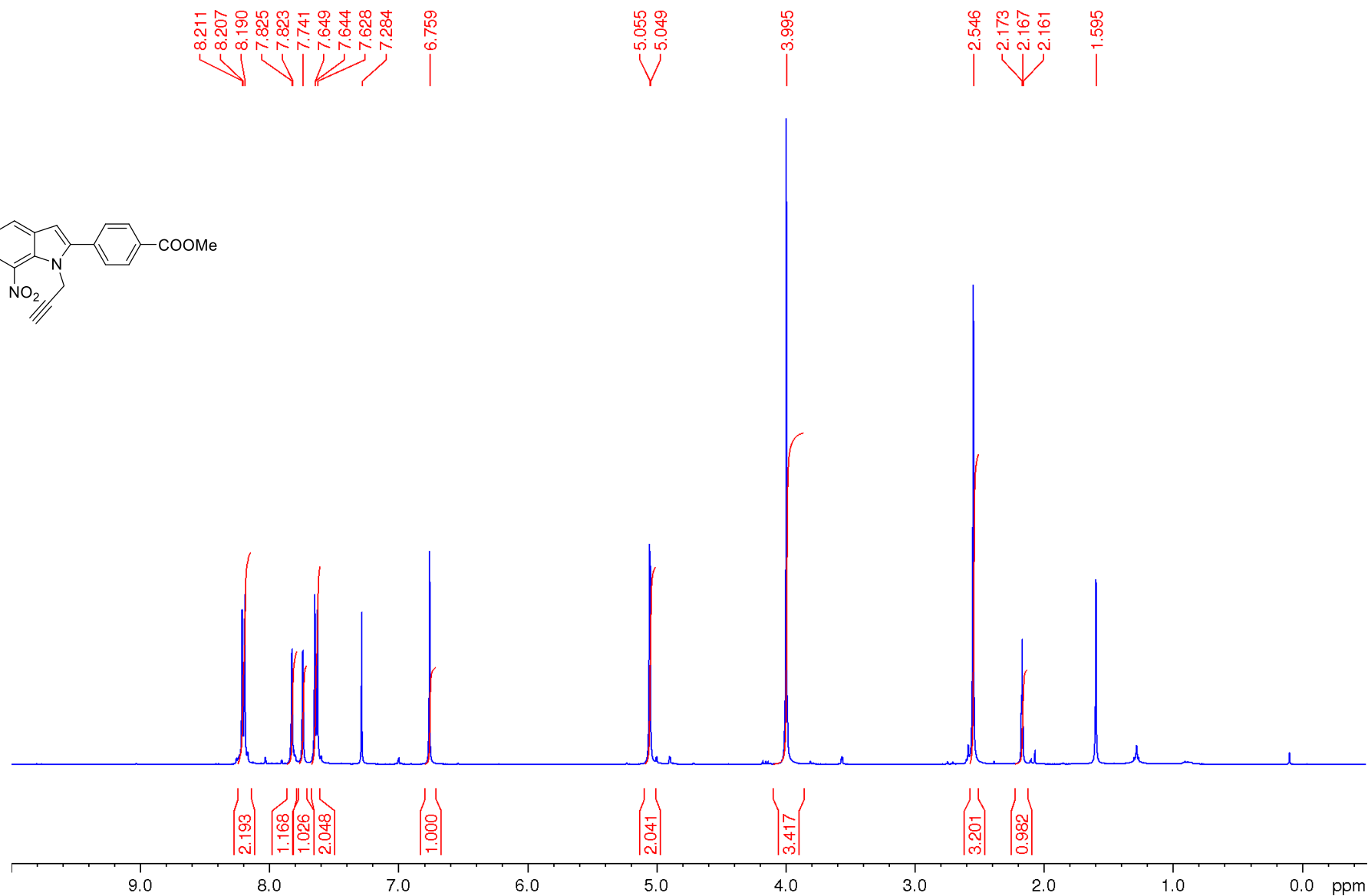
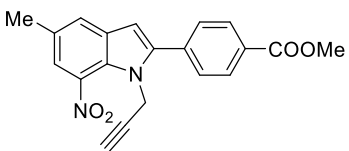
77.677  
73.920

36.938

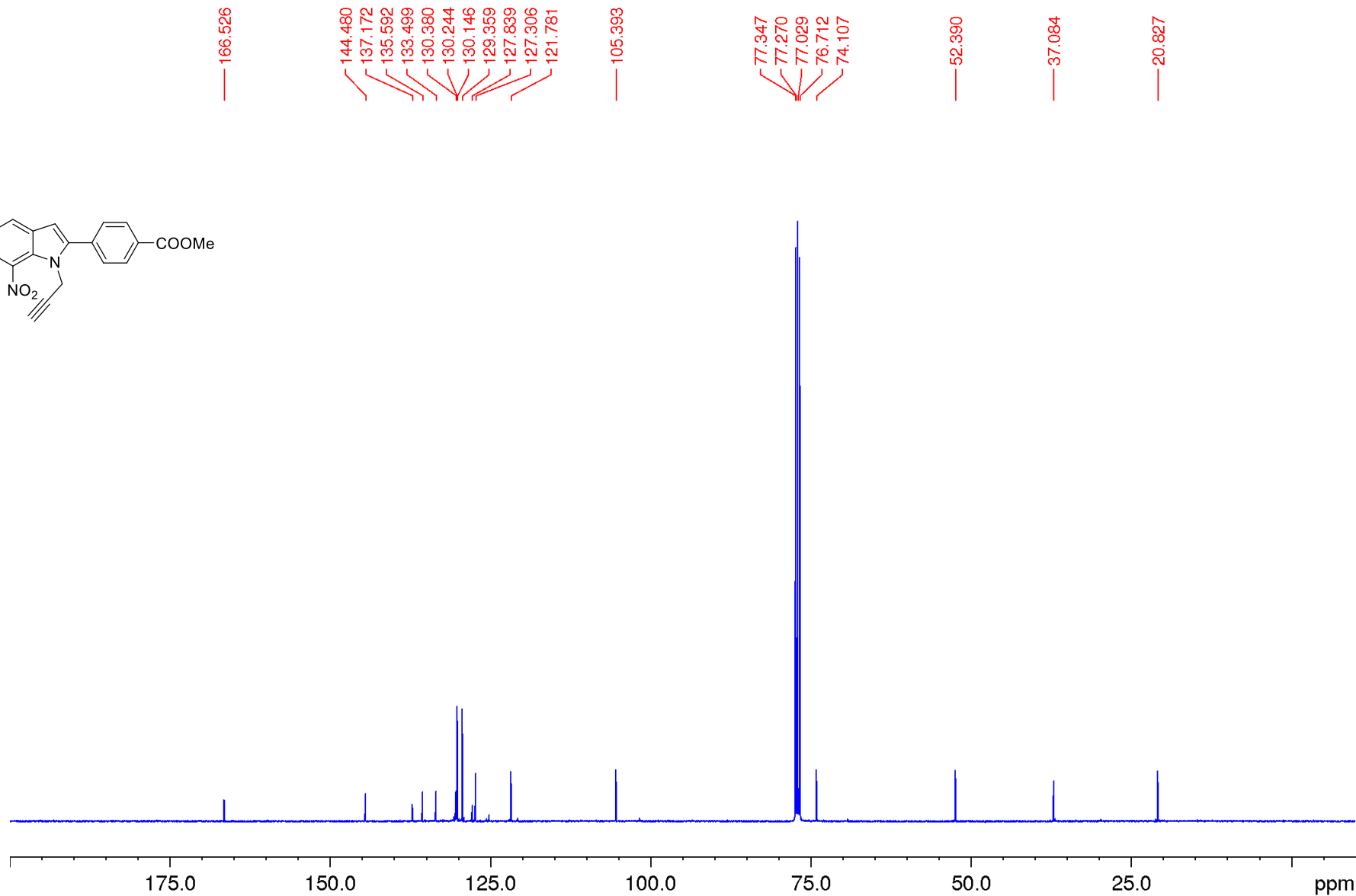
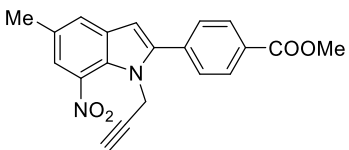
20.829



**methyl 4-(5-methyl-7-nitro-1-(prop-2-yn-1-yl)-1H-indol-2-yl)benzoate 6d**

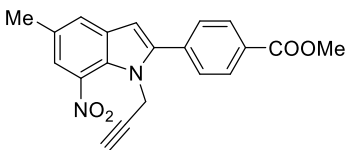


**methyl 4-(5-methyl-7-nitro-1-(prop-2-yn-1-yl)-1*H*-indol-2-yl)benzoate 6d**

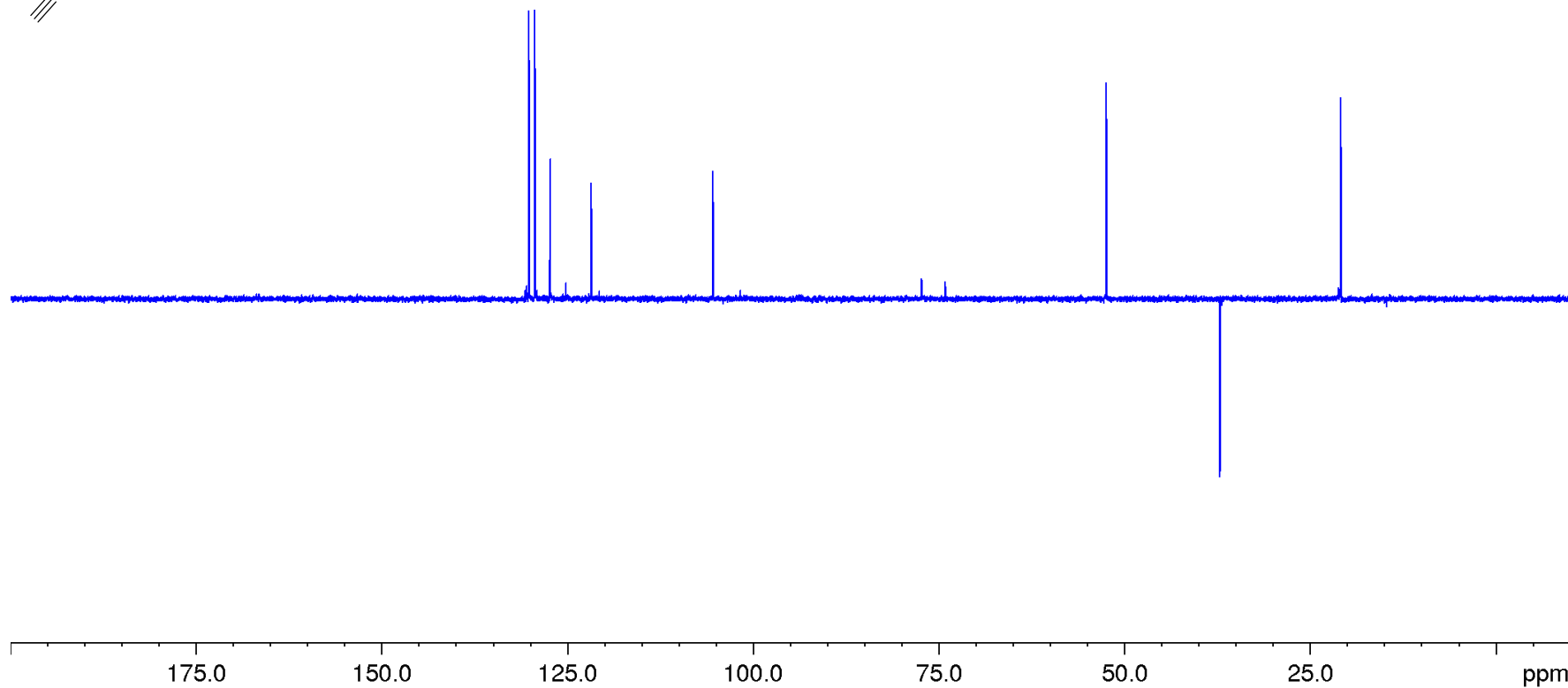




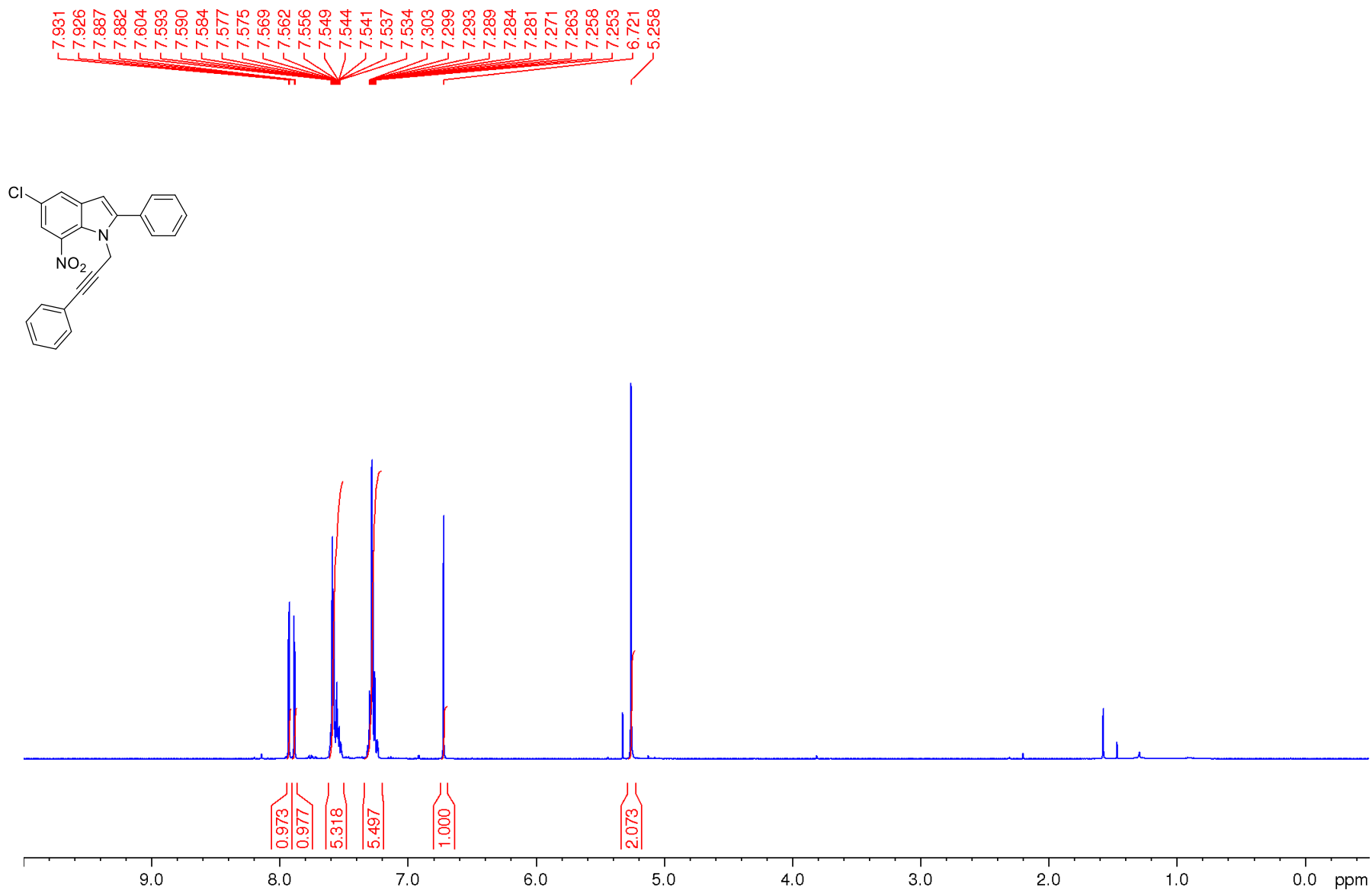
**methyl 4-(5-methyl-7-nitro-1-(prop-2-yn-1-yl)-1*H*-indol-2-yl)benzoate 6d**



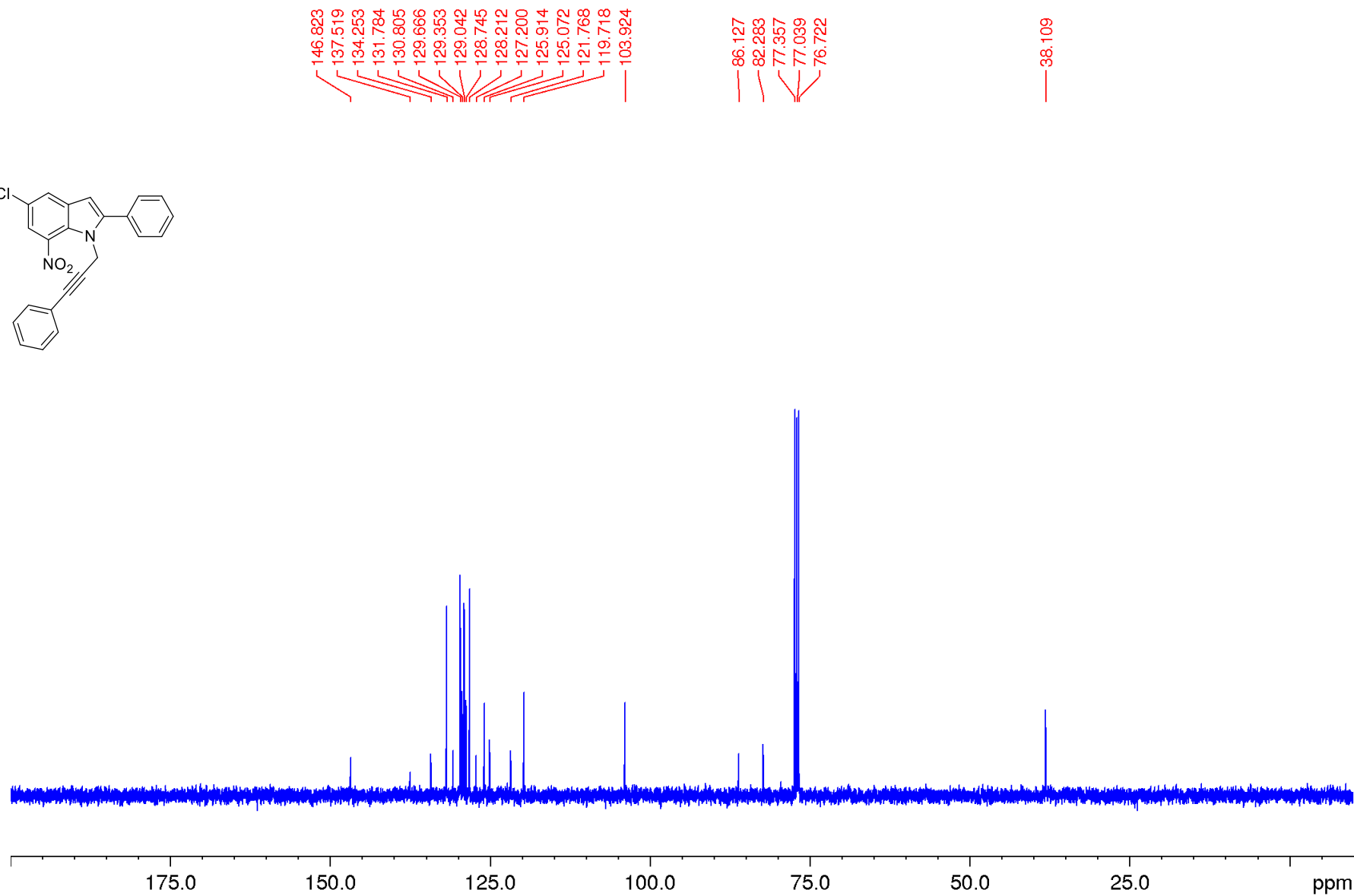
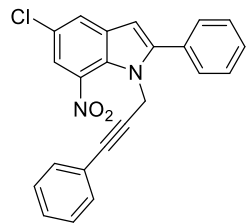
130.145  
129.358  
127.304  
121.779  
105.393  
77.269  
74.108  
52.390  
37.085  
20.827



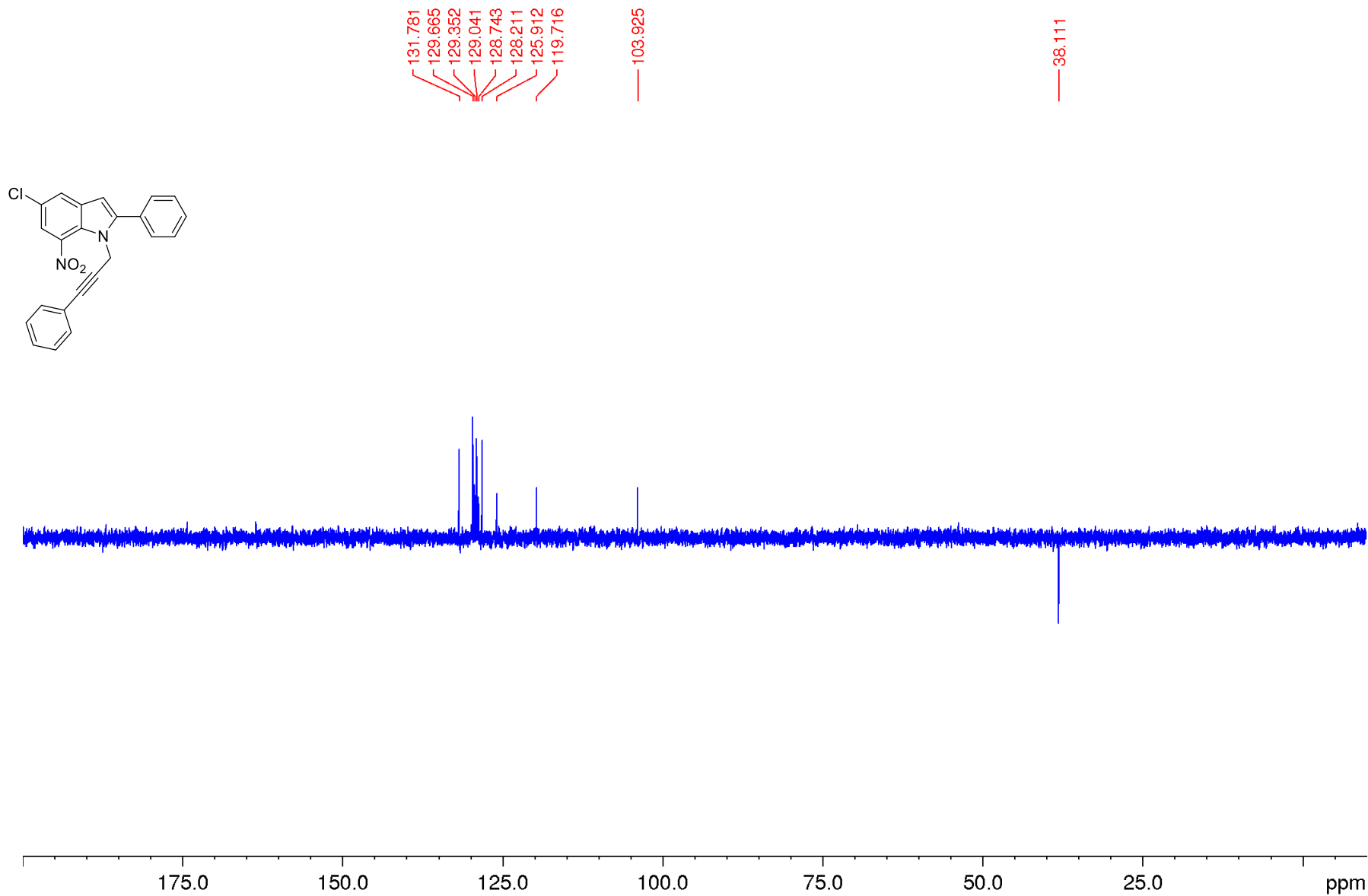
**5-chloro-7-nitro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1*H*-indole 7a**



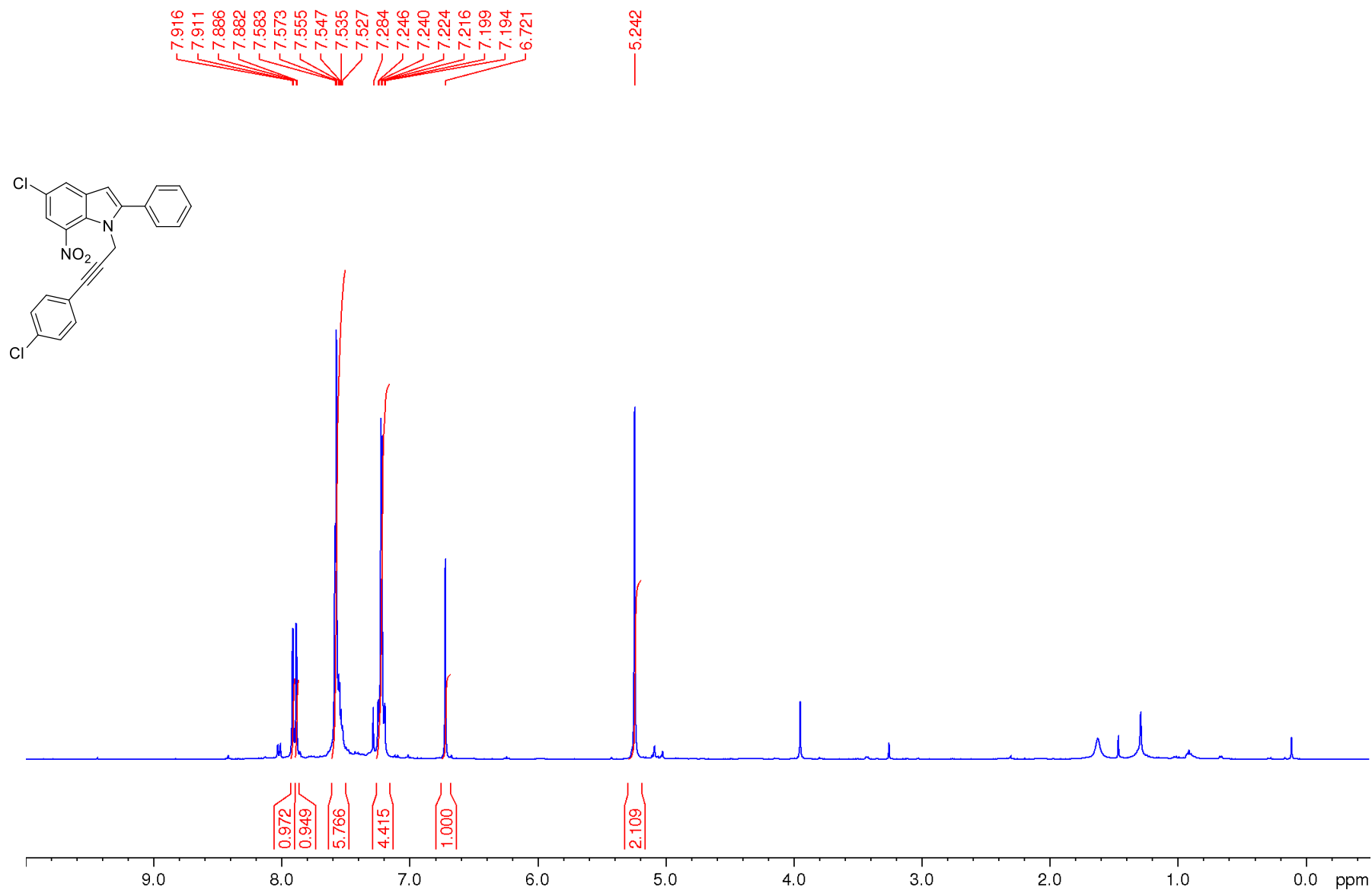
# 5-chloro-7-nitro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indole 7a



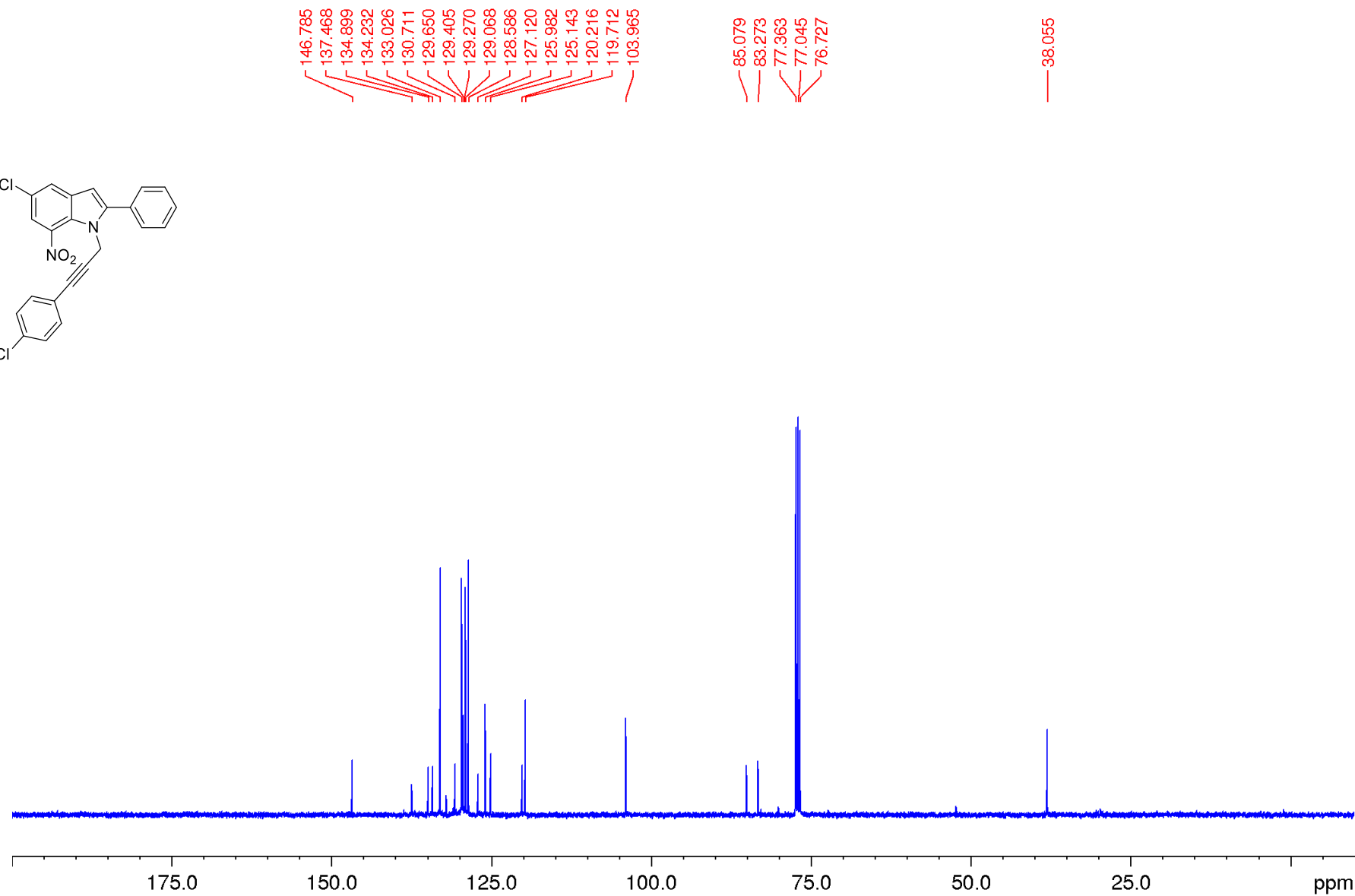
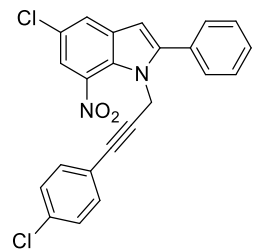
# 5-chloro-7-nitro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indole 7a



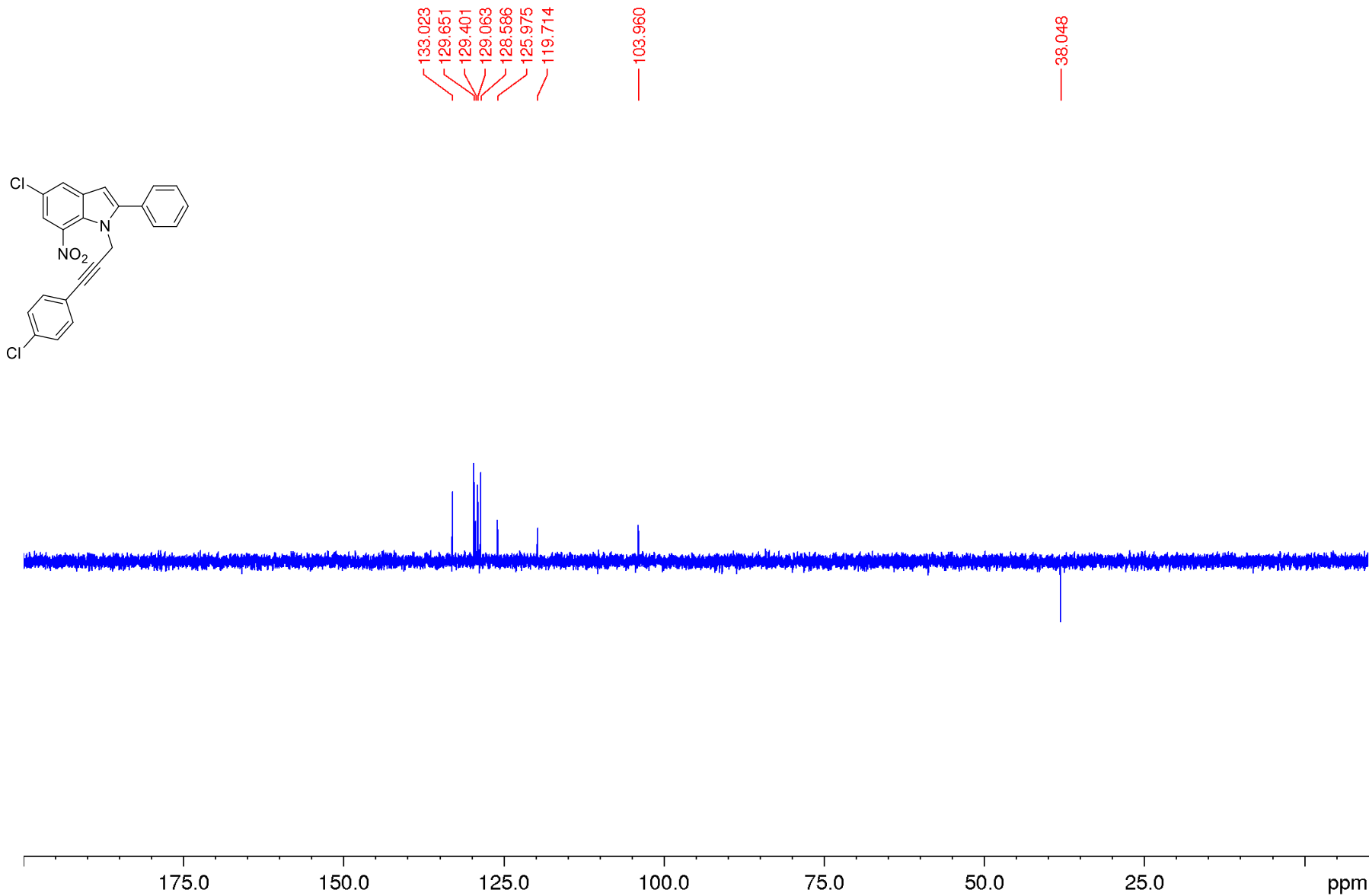
**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7b**



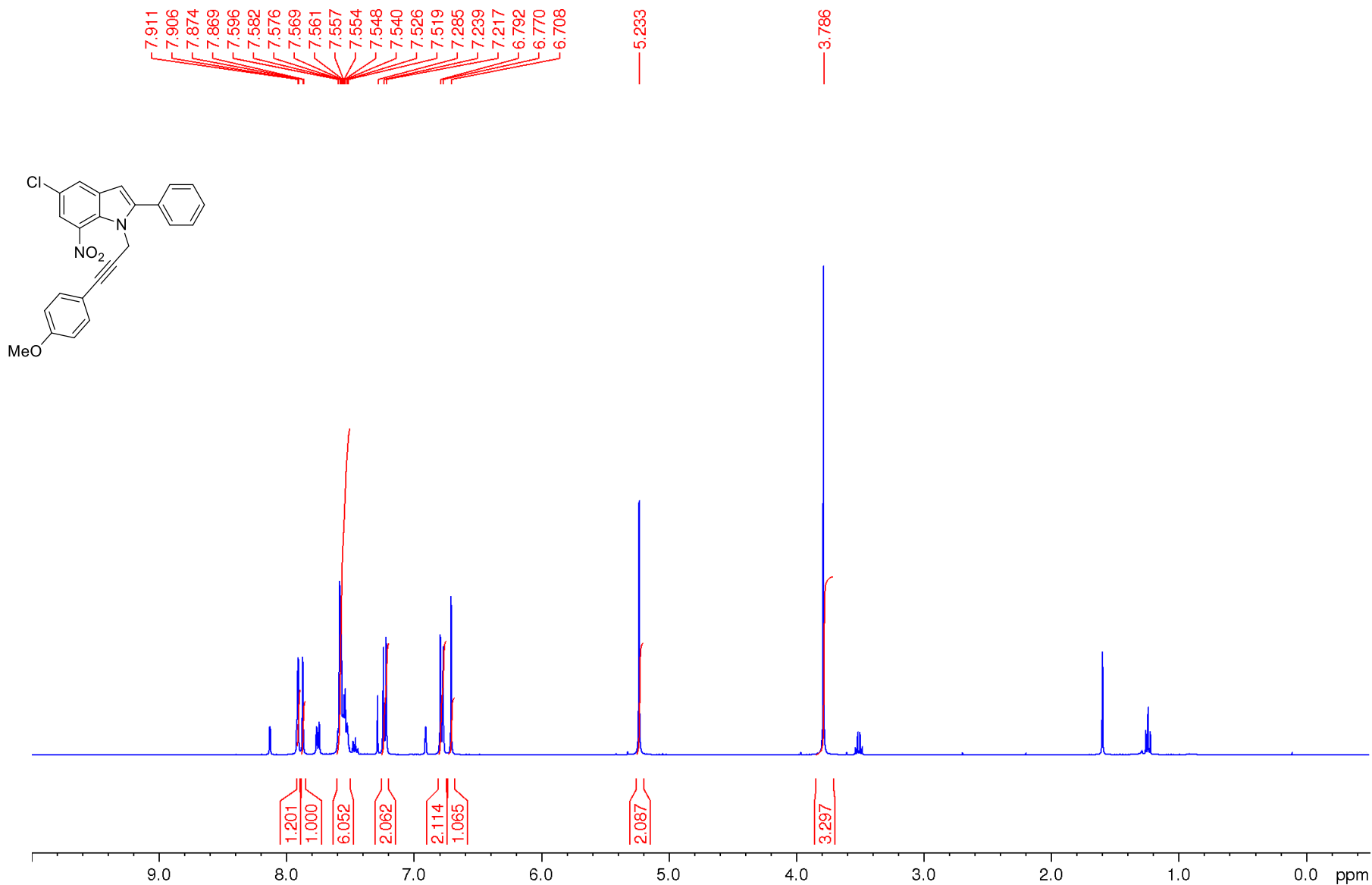
**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1*H*-indole 7b**



**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1*H*-indole 7b**

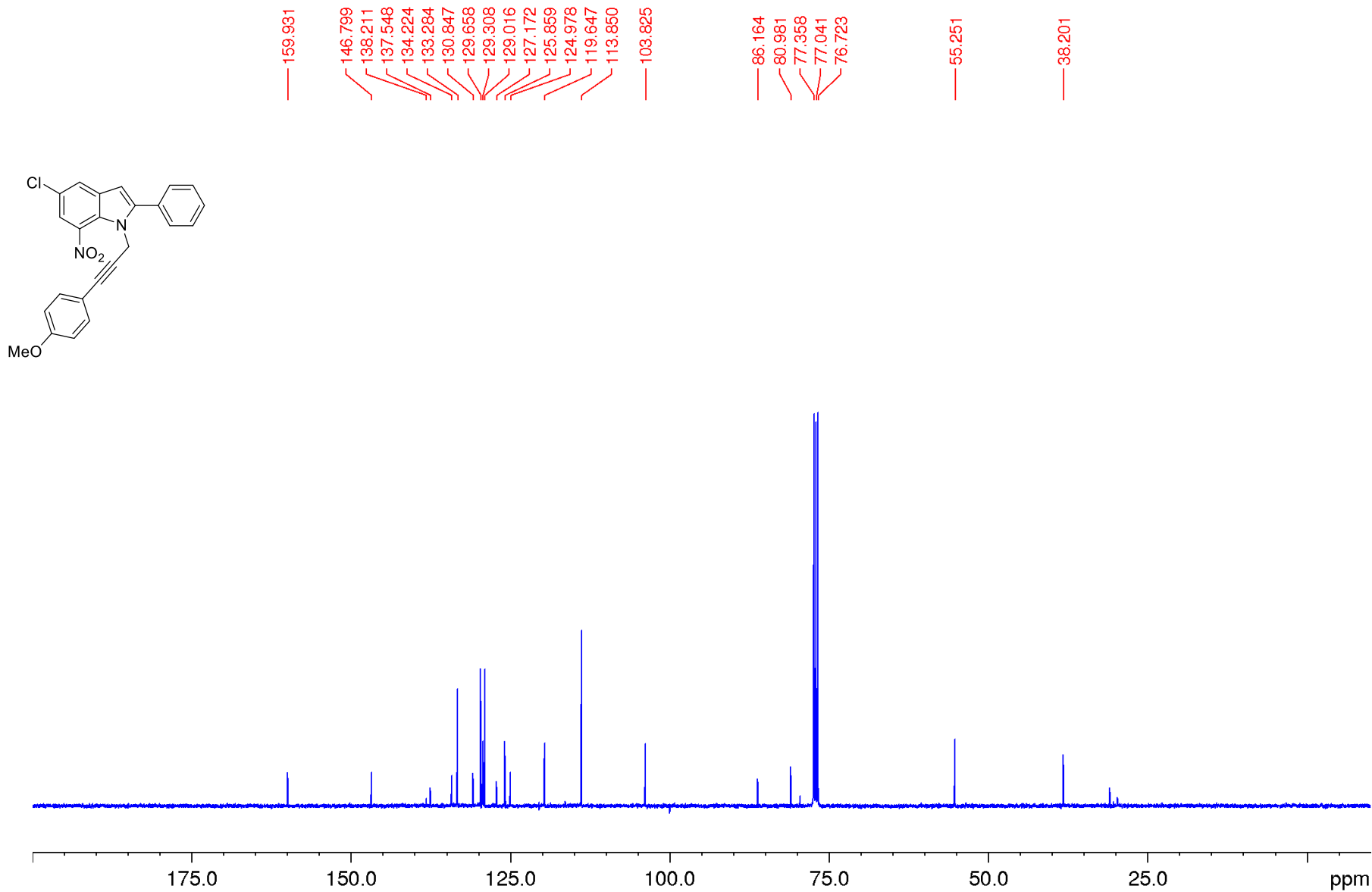


**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1H-indole 7c**

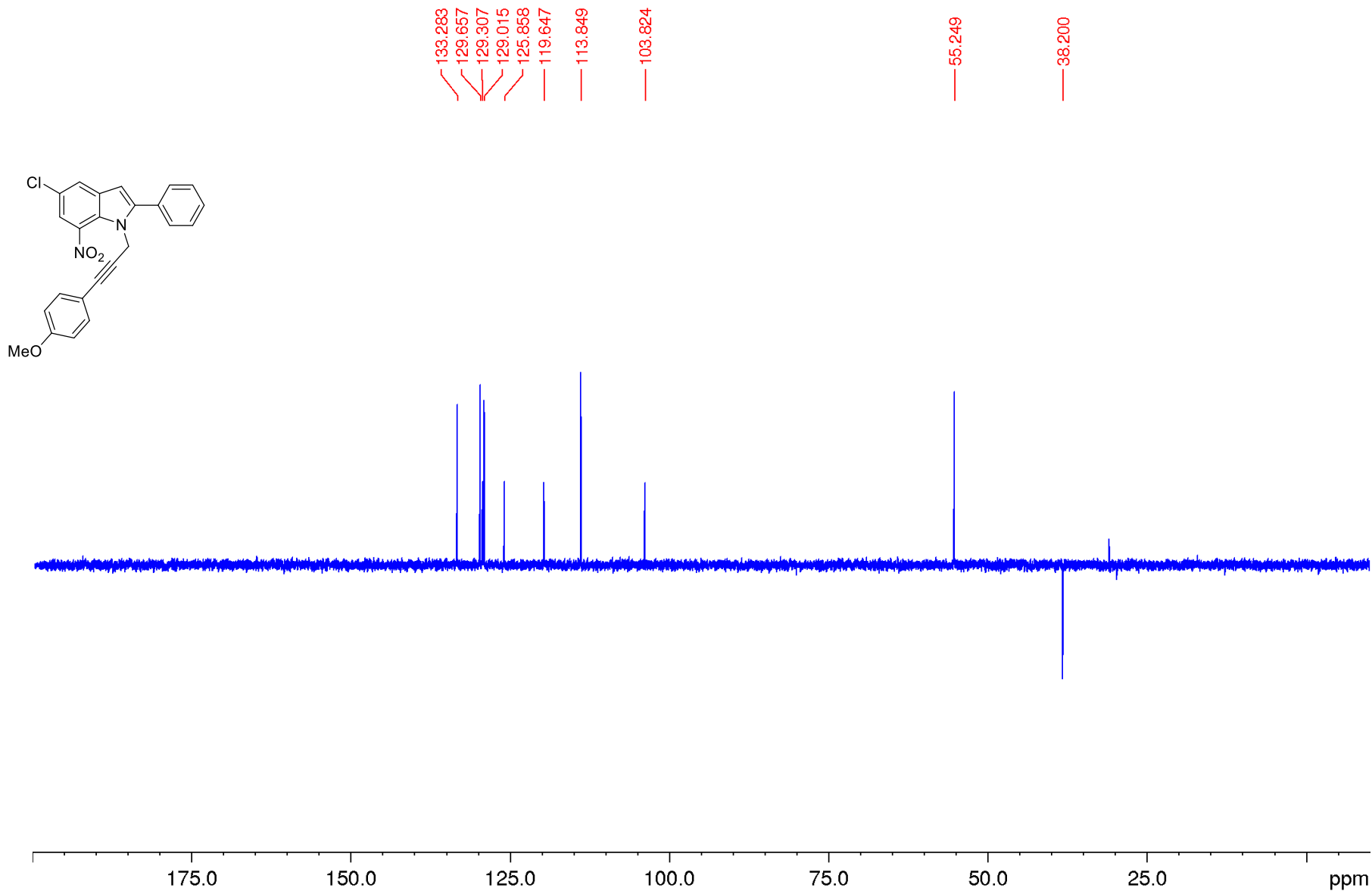




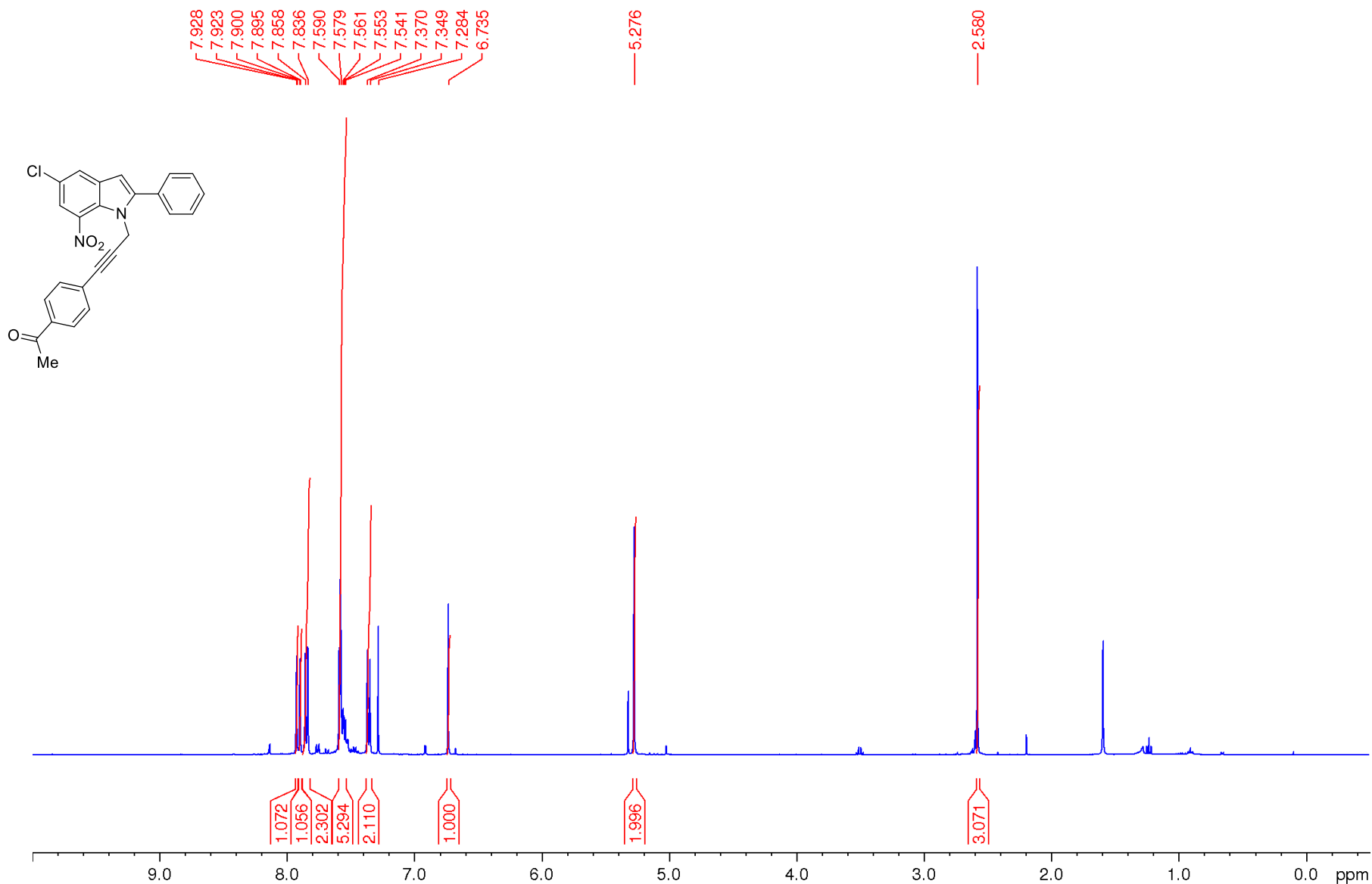
**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1*H*-indole 7c**



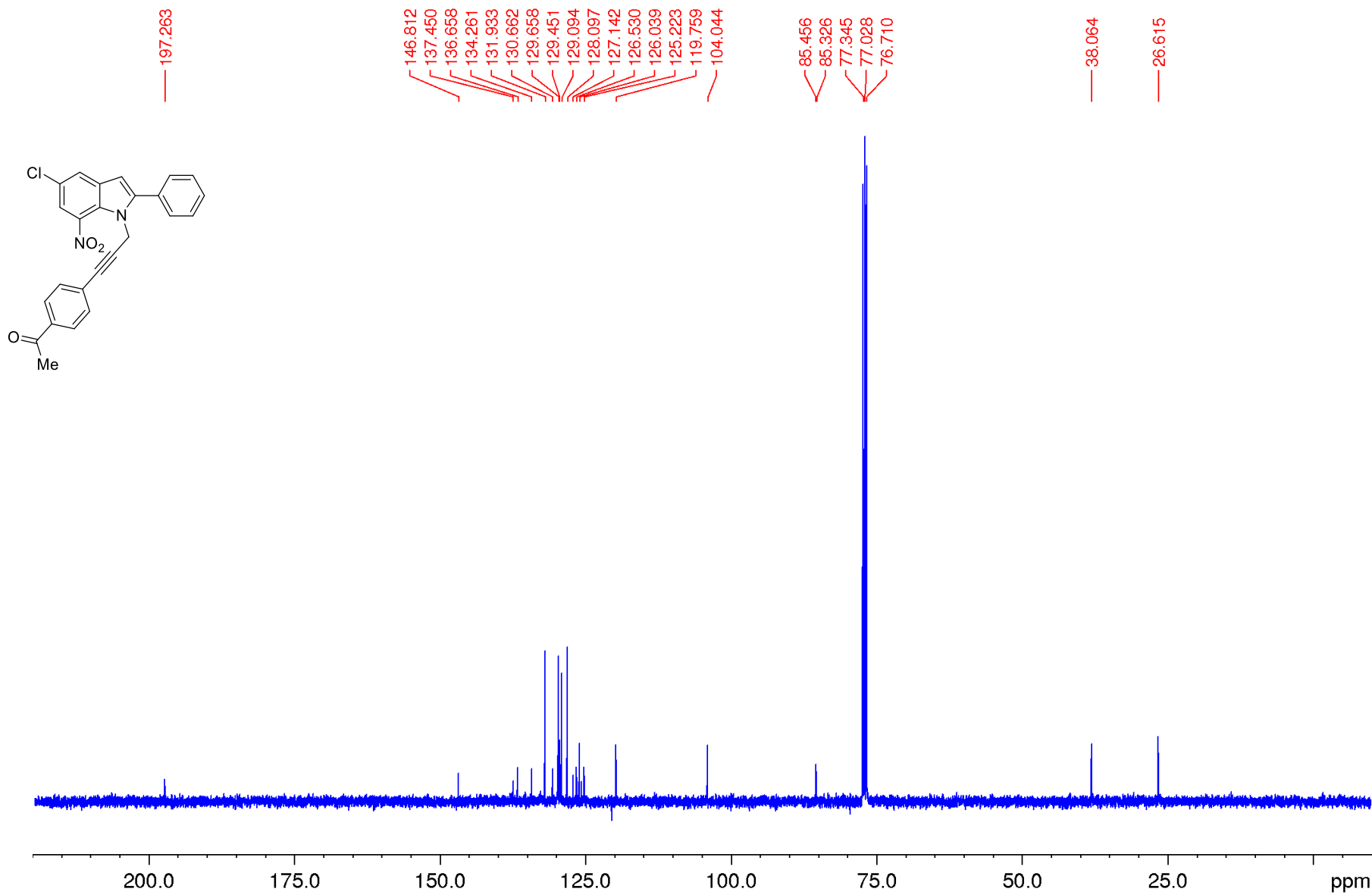
**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-2-phenyl-1*H*-indole 7c**



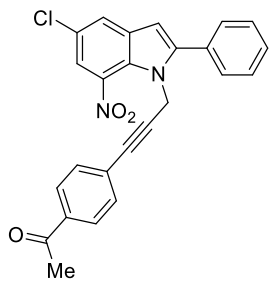
**1-(4-(3-(5-chloro-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7d**



**1-(4-(3-(5-chloro-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7d**



**1-(4-(3-(5-chloro-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7d**

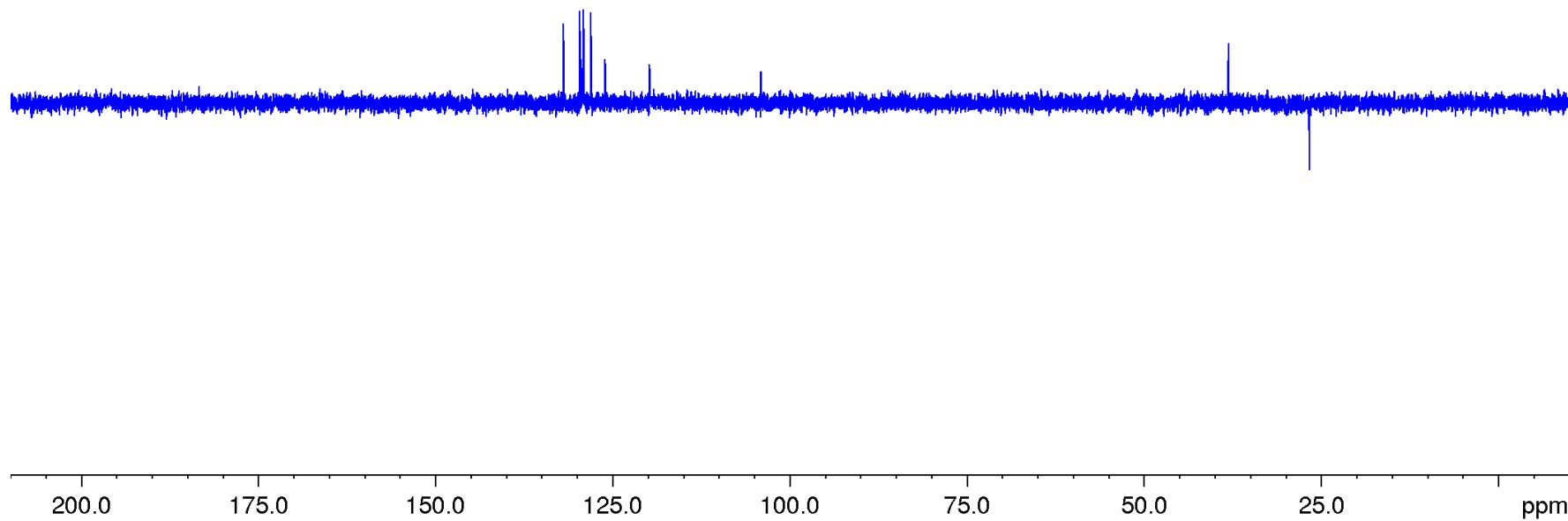


131.932  
129.657  
129.448  
129.091  
128.096  
126.035  
119.757

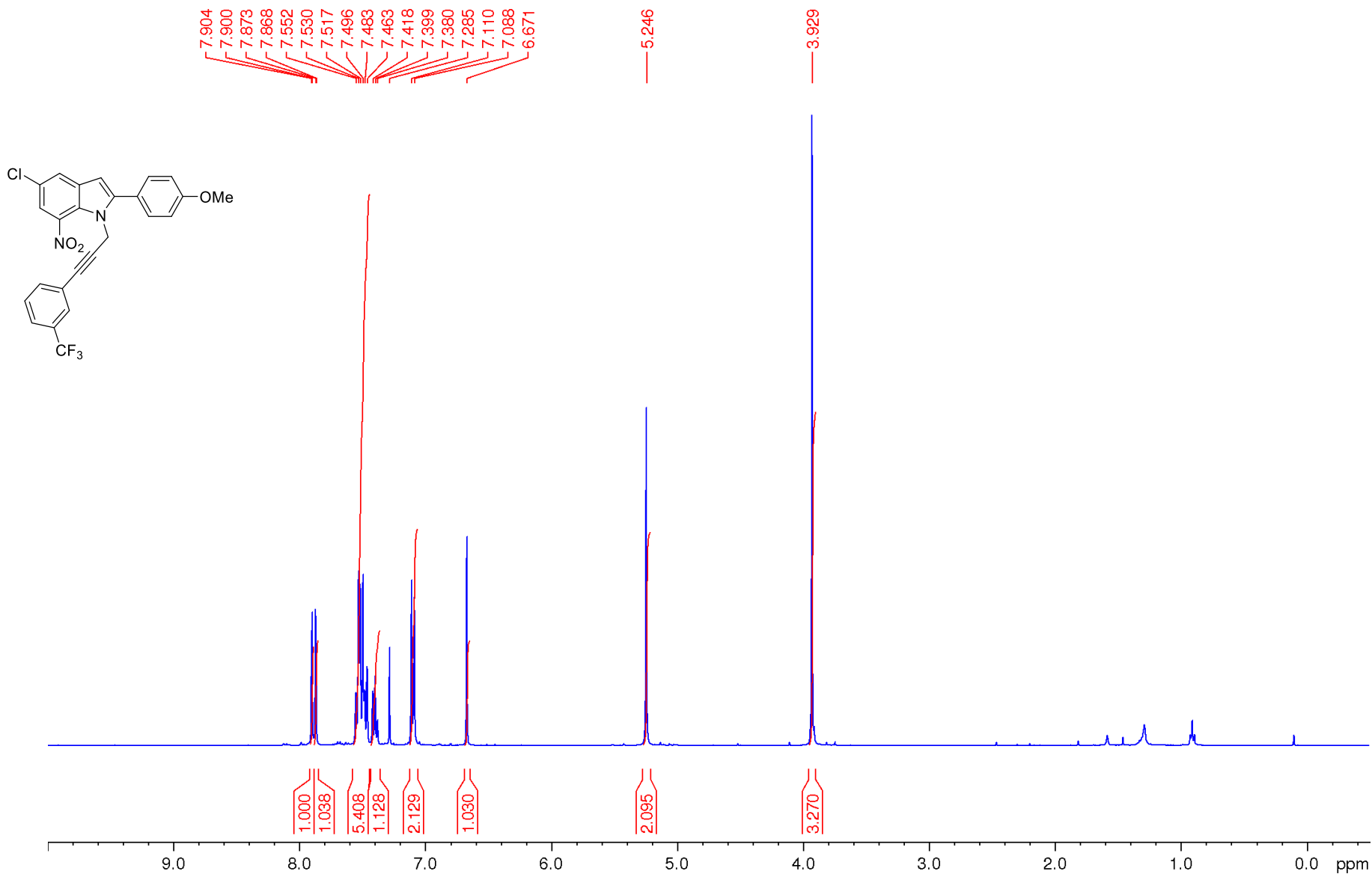
104.042

38.077

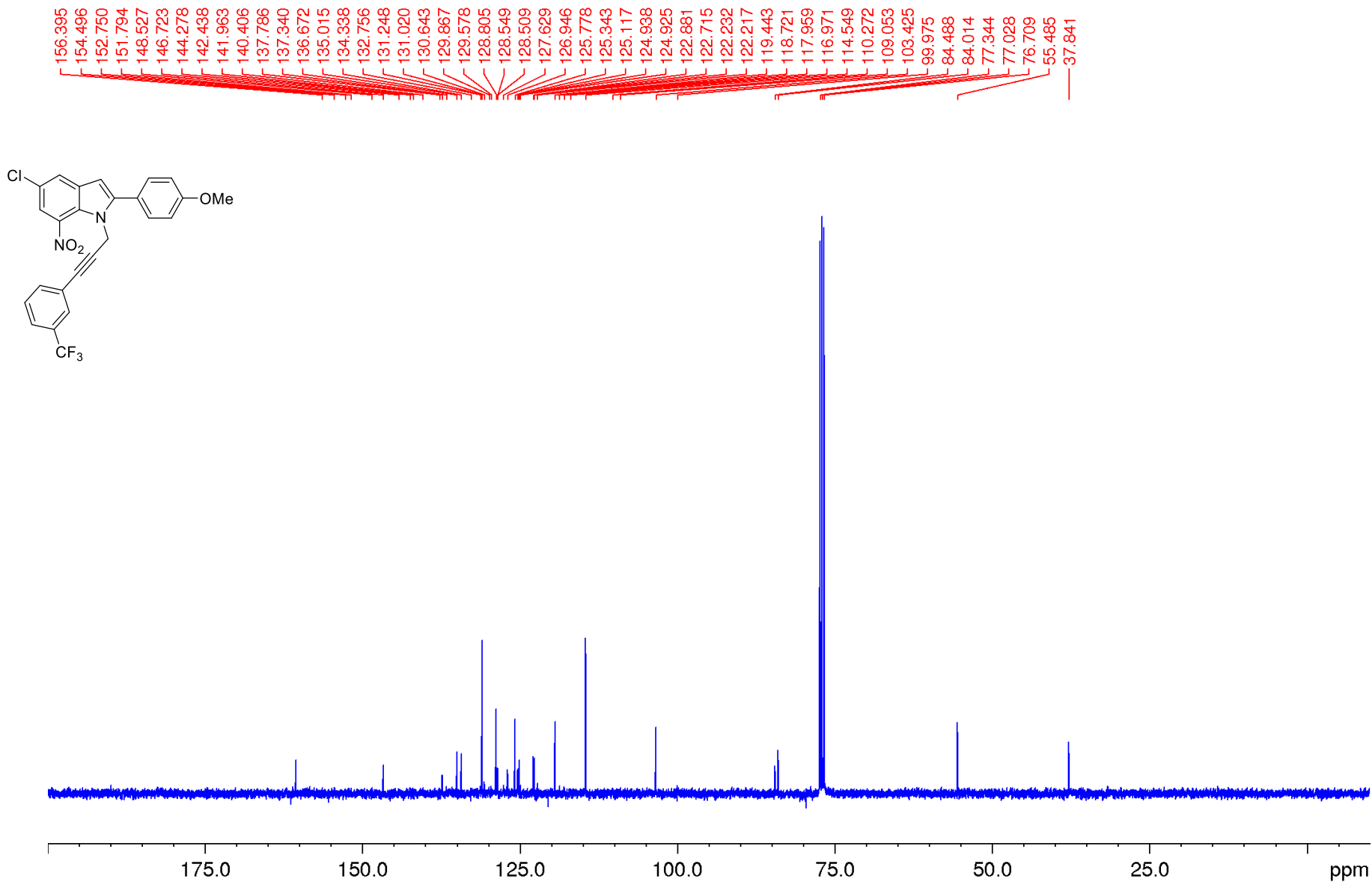
26.623



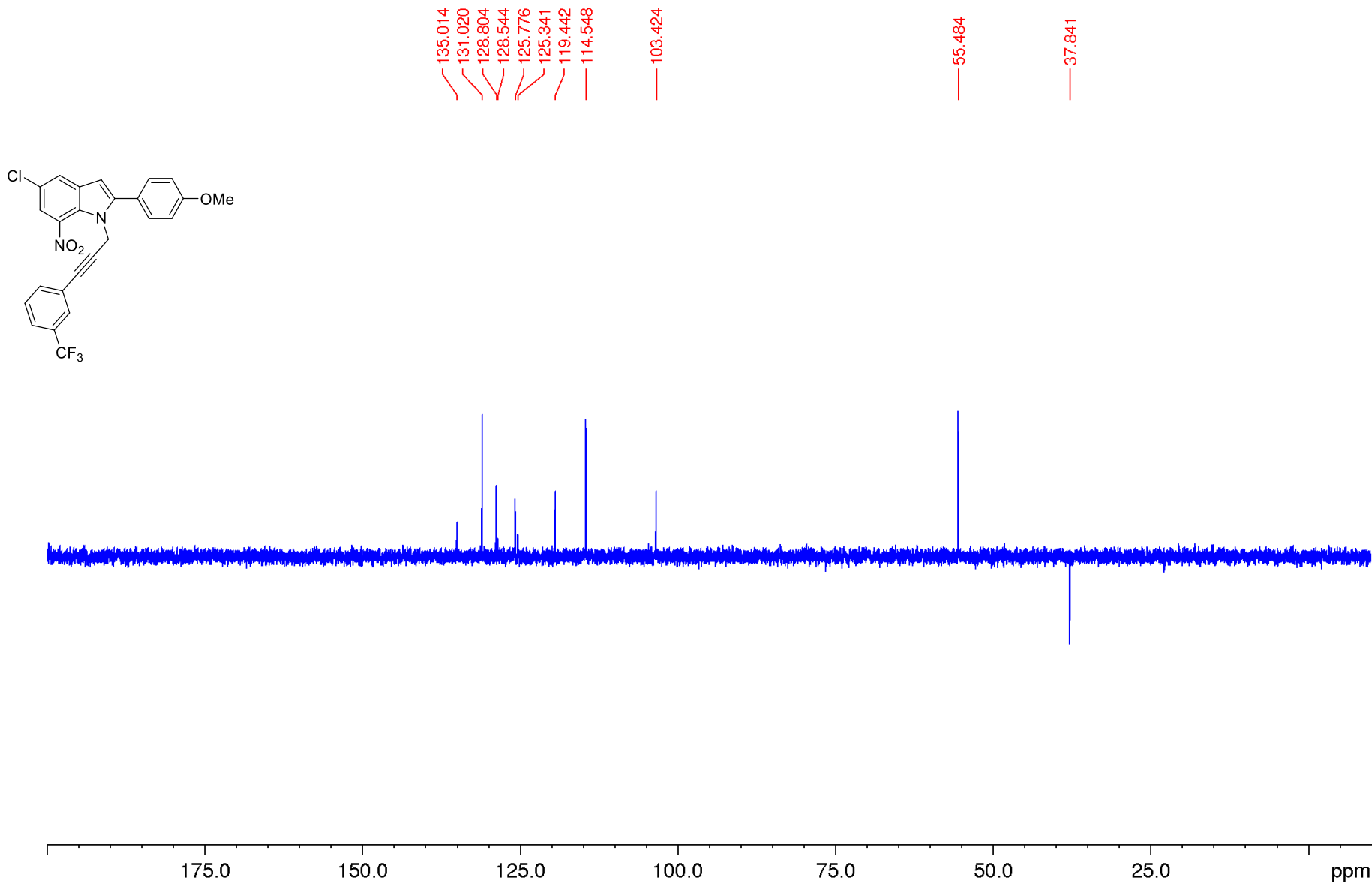
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indole 7e**



**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1*H*-indole 7e**

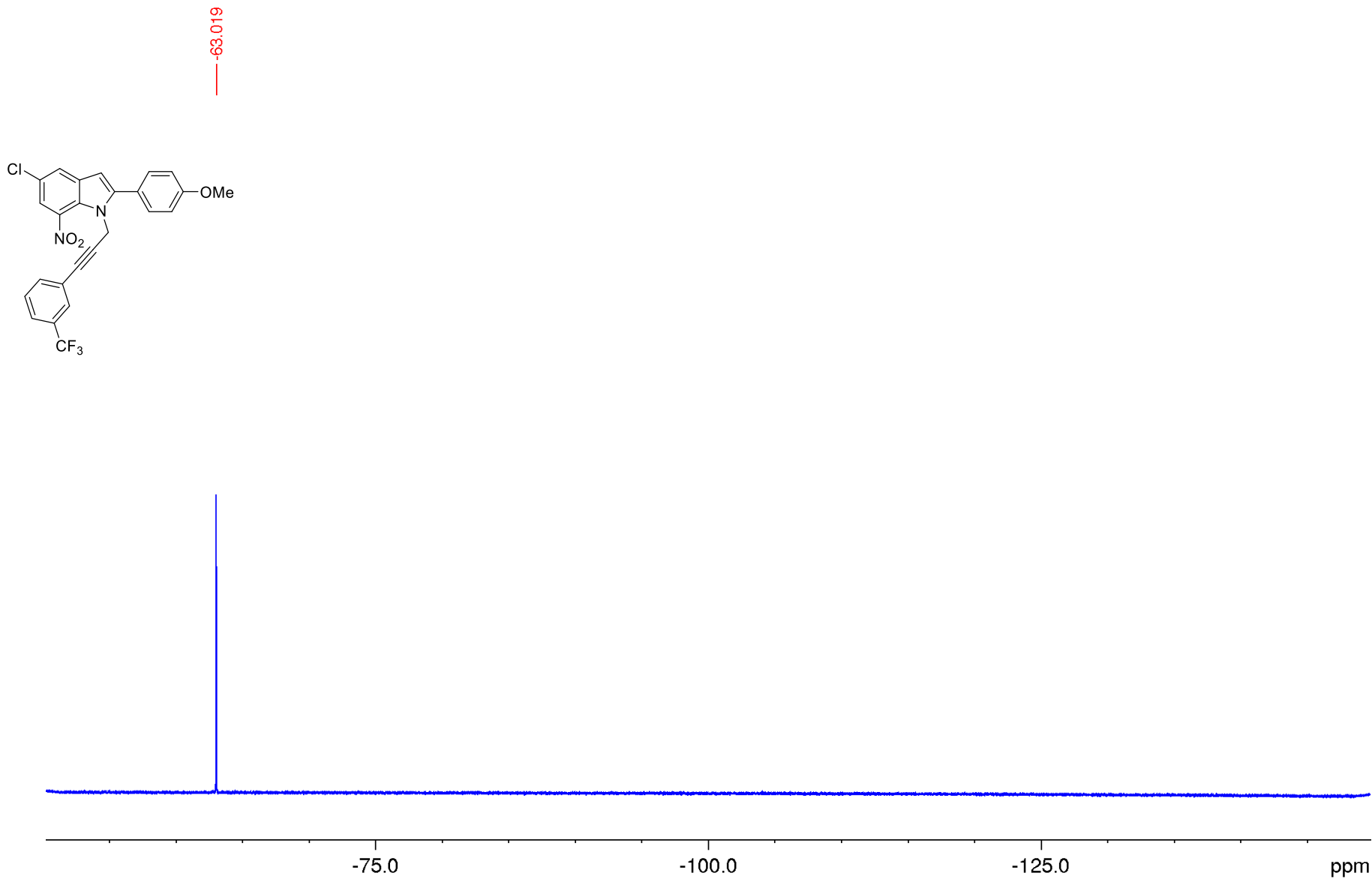


**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indole 7e**

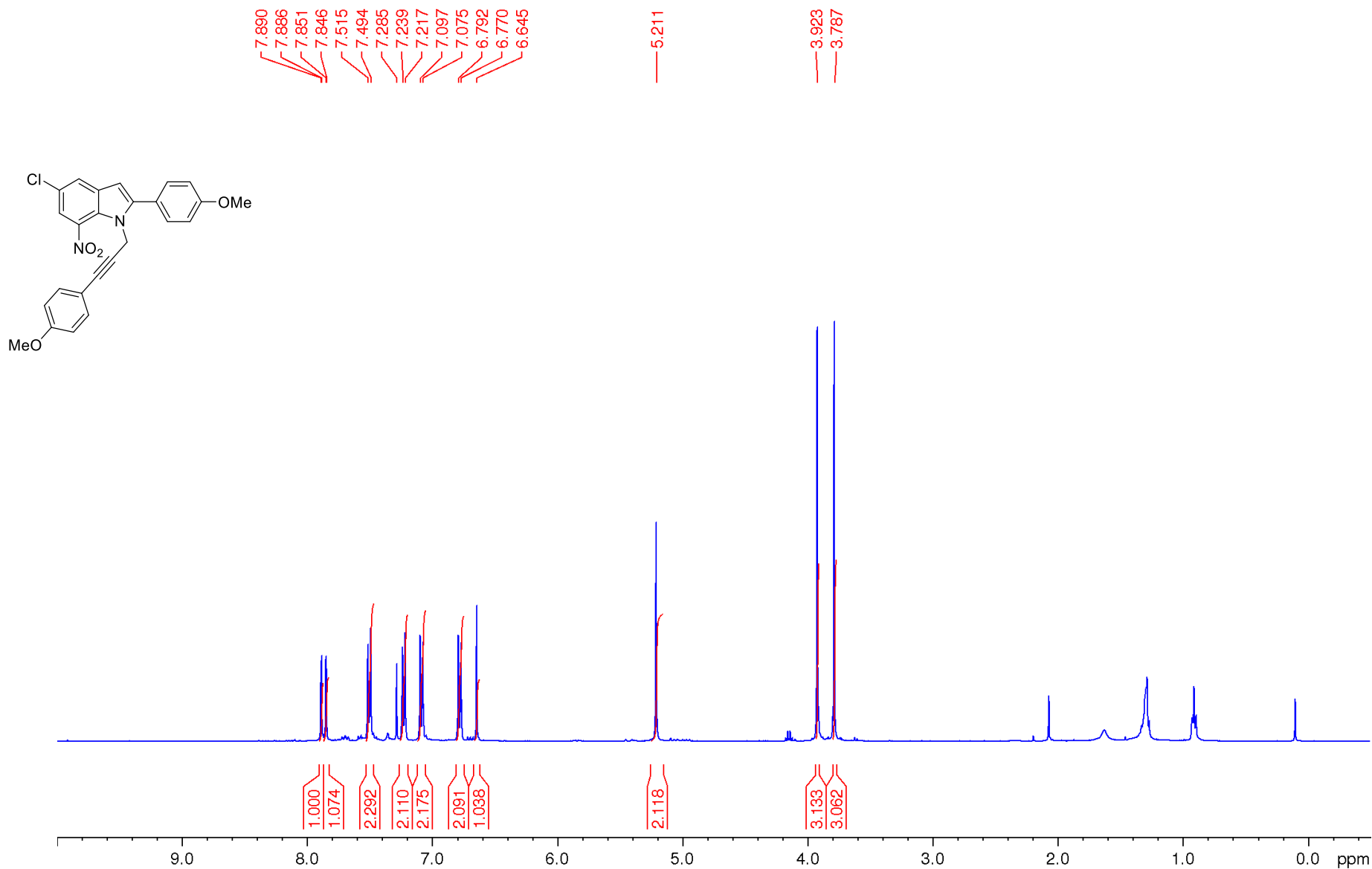




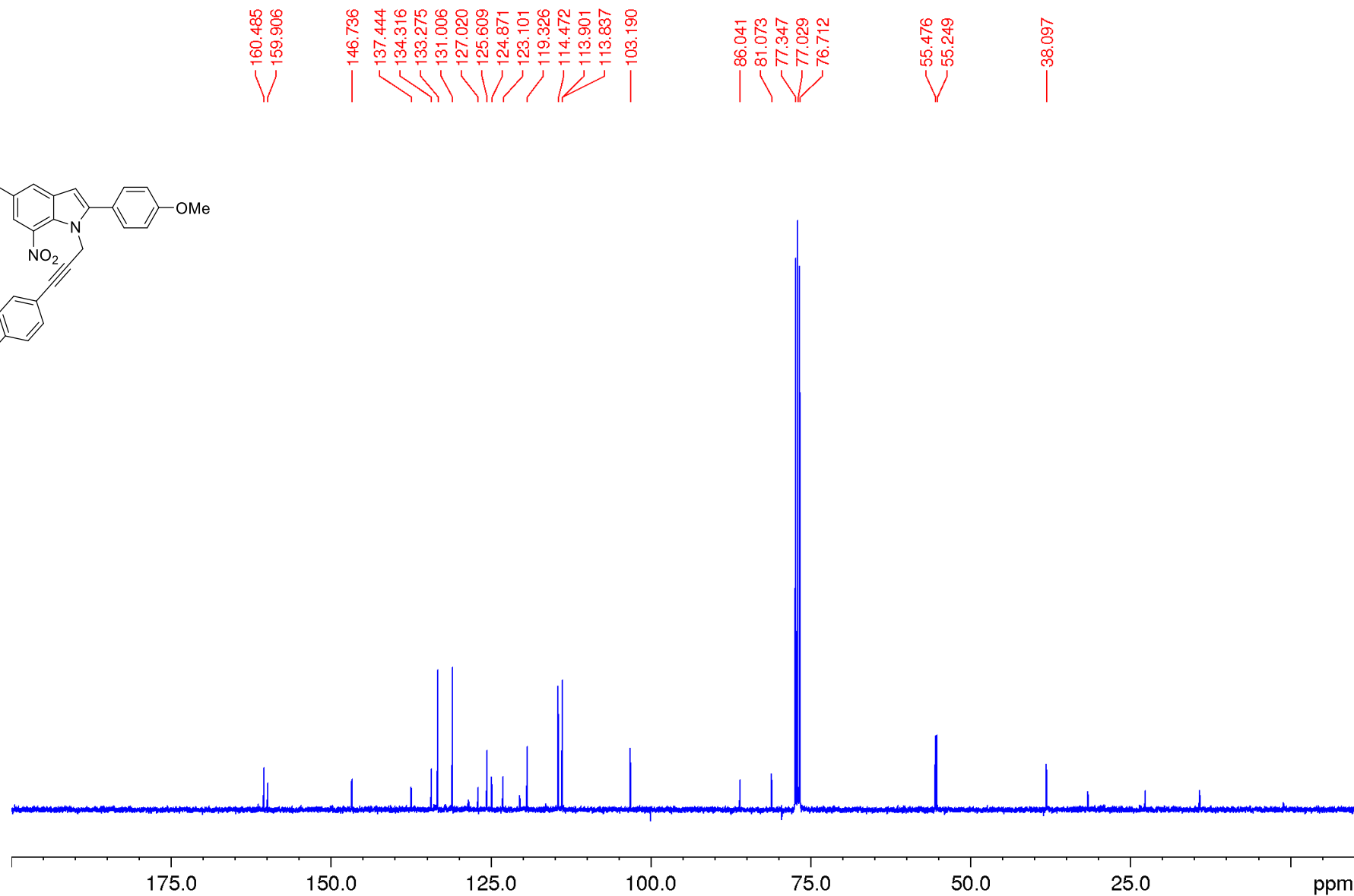
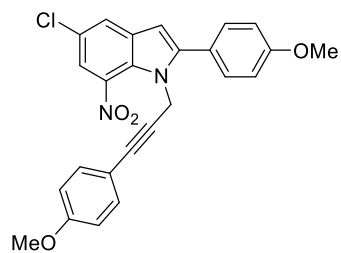
**5-chloro-2-(4-methoxyphenyl)-7-nitro-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1*H*-indole 7e**



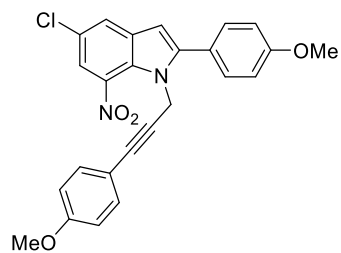
**5-chloro-2-(4-methoxyphenyl)-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-1*H*-indole 7f**



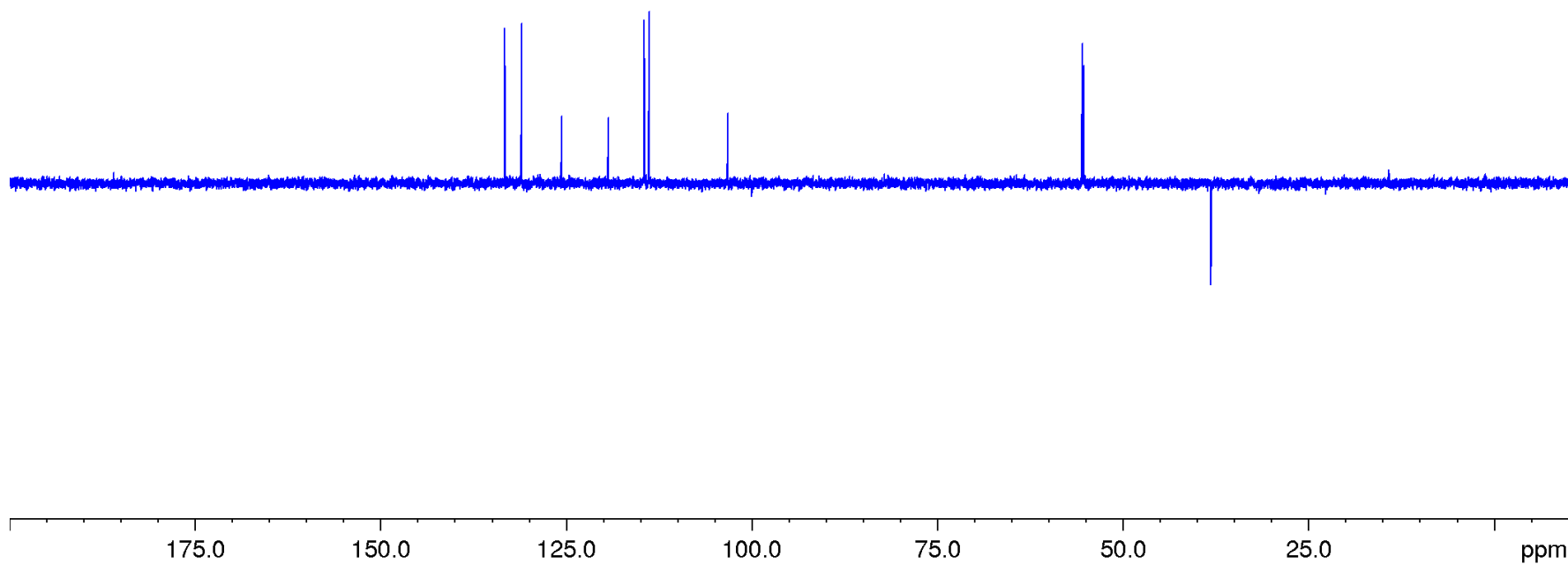
**5-chloro-2-(4-methoxyphenyl)-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-1*H*-indole 7f**



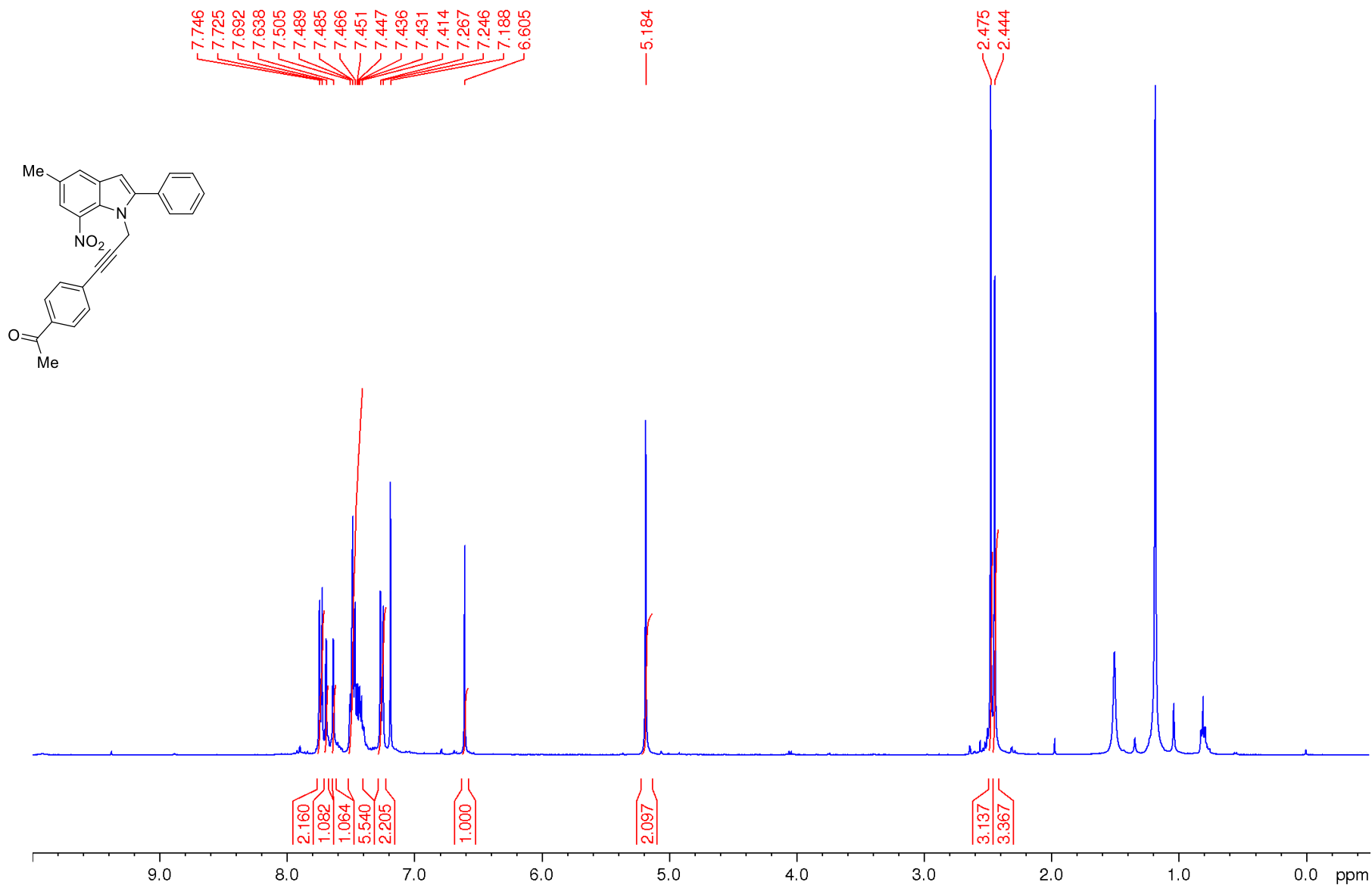
**5-chloro-2-(4-methoxyphenyl)-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-7-nitro-1*H*-indole 7f**



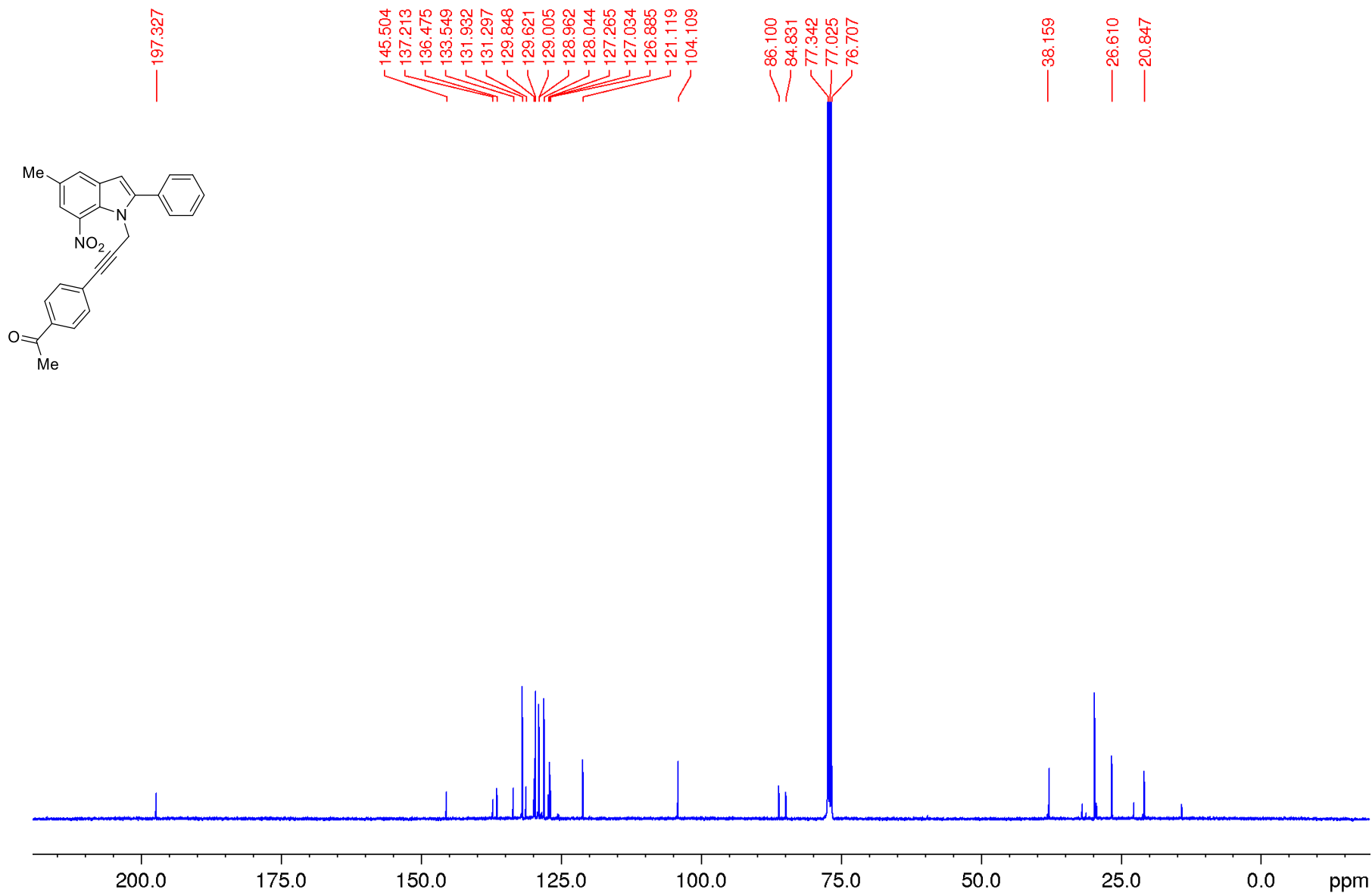
133.274  
131.005  
125.606  
119.325  
114.470  
113.836  
103.190  
55.474  
55.246  
38.095



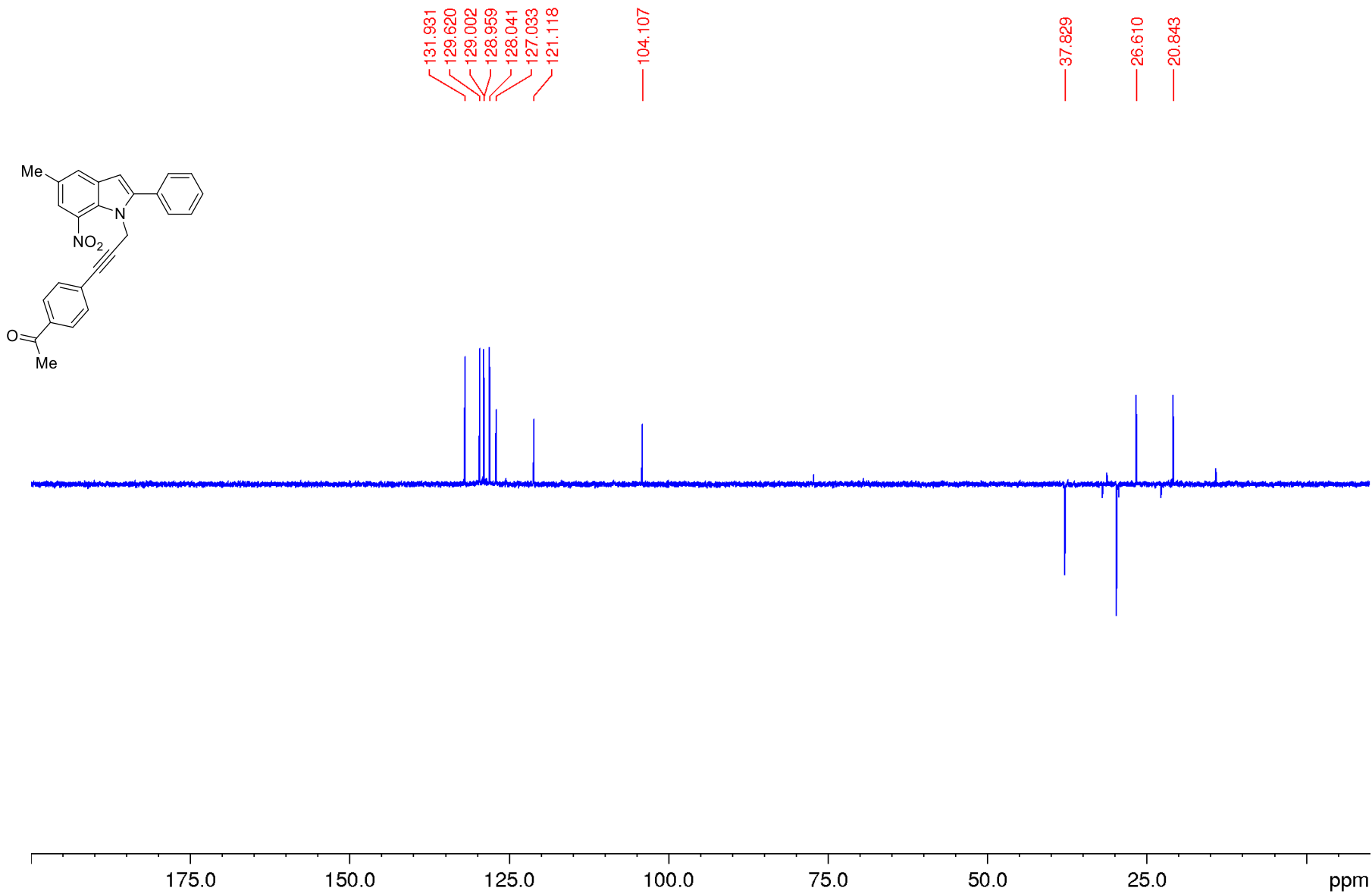
**1-(4-(3-(5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7g**



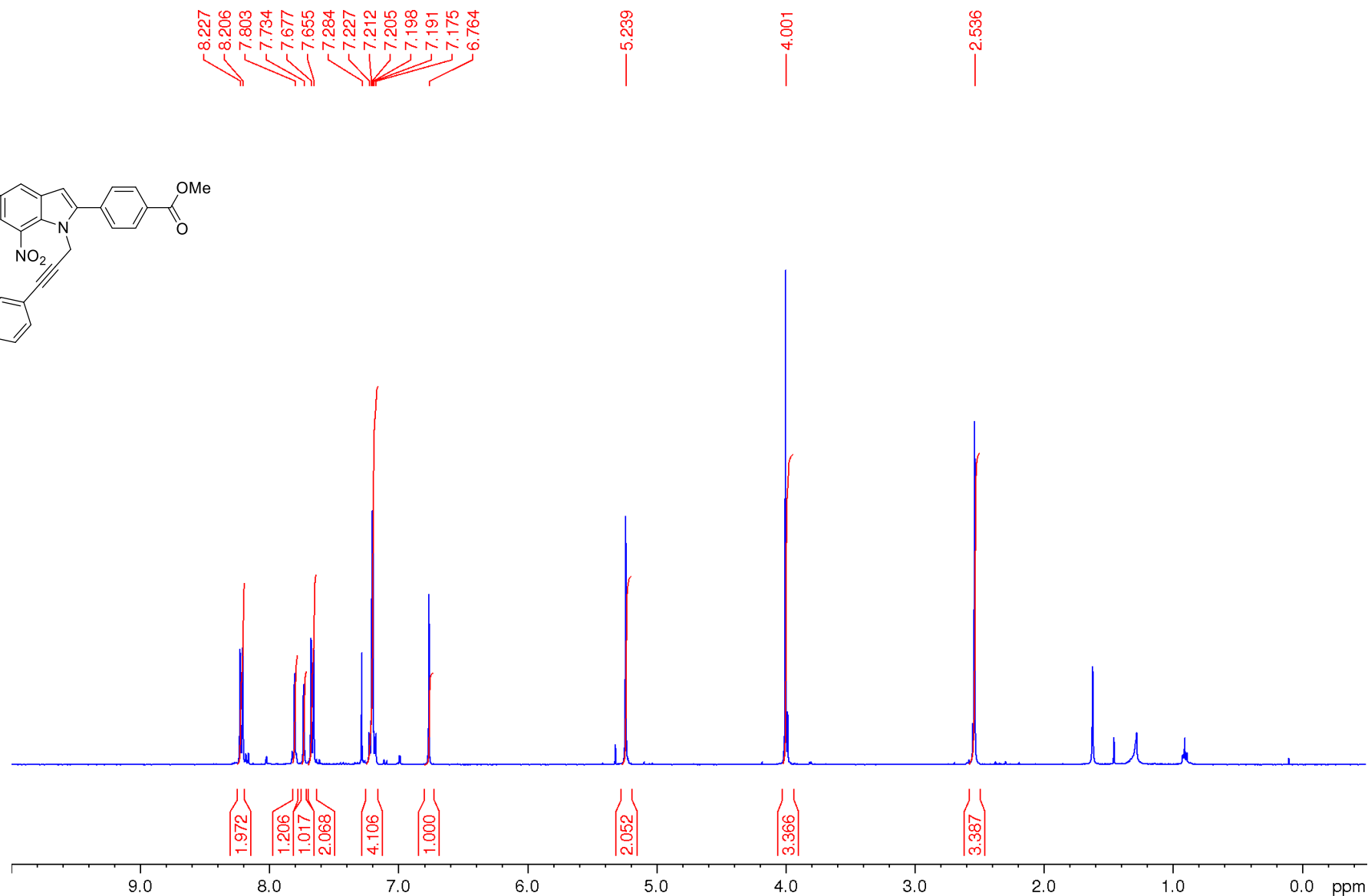
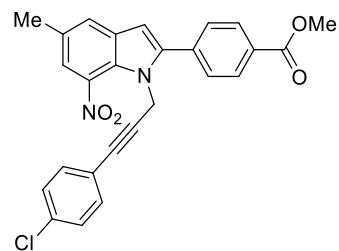
**1-(4-(3-(5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7g**



**1-(4-(3-(5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 7g**

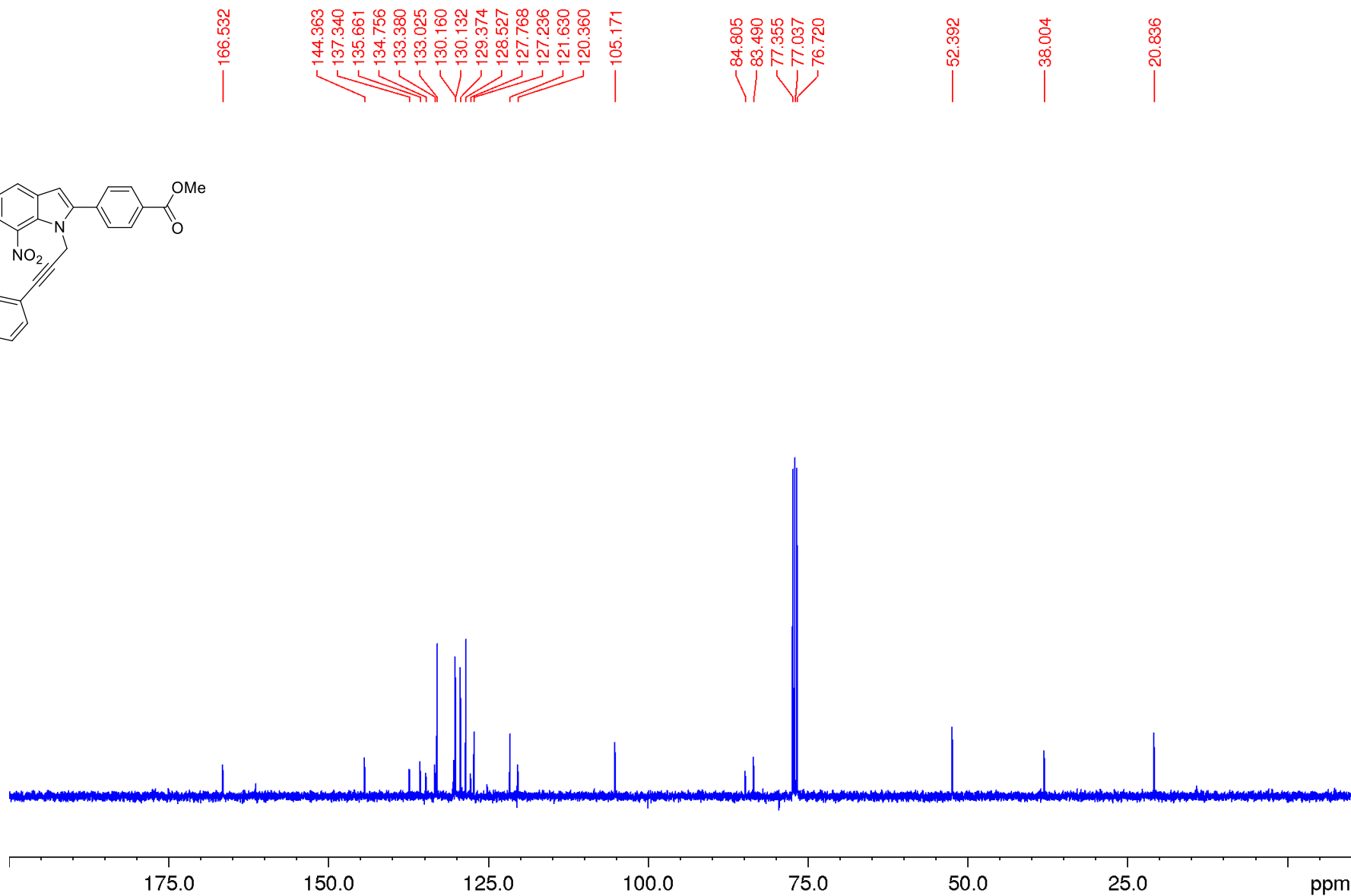
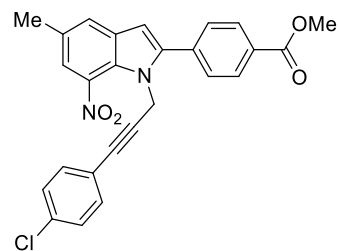


**methyl 4-(1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-1H-indol-2-yl)benzoate 7h**

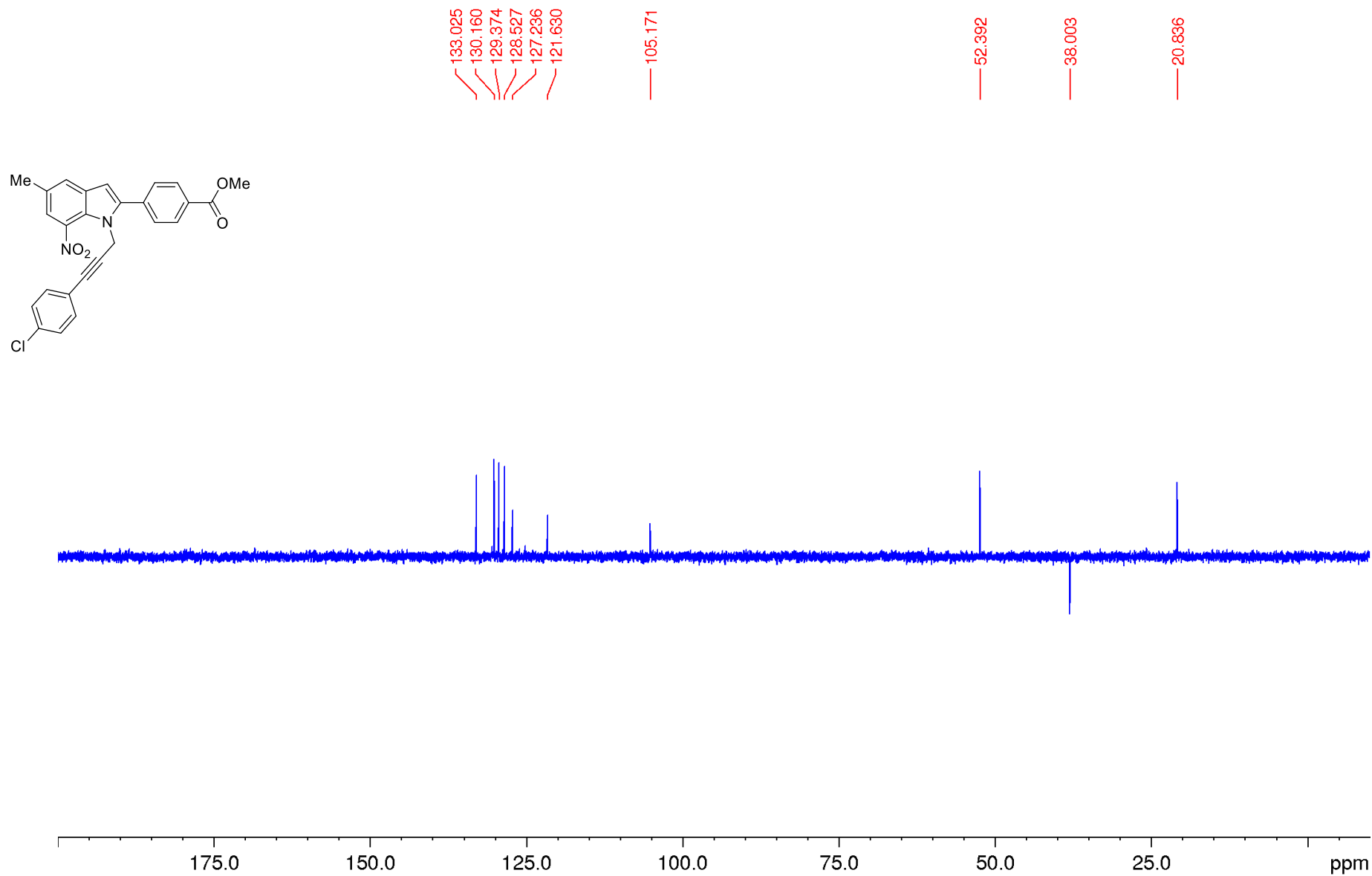




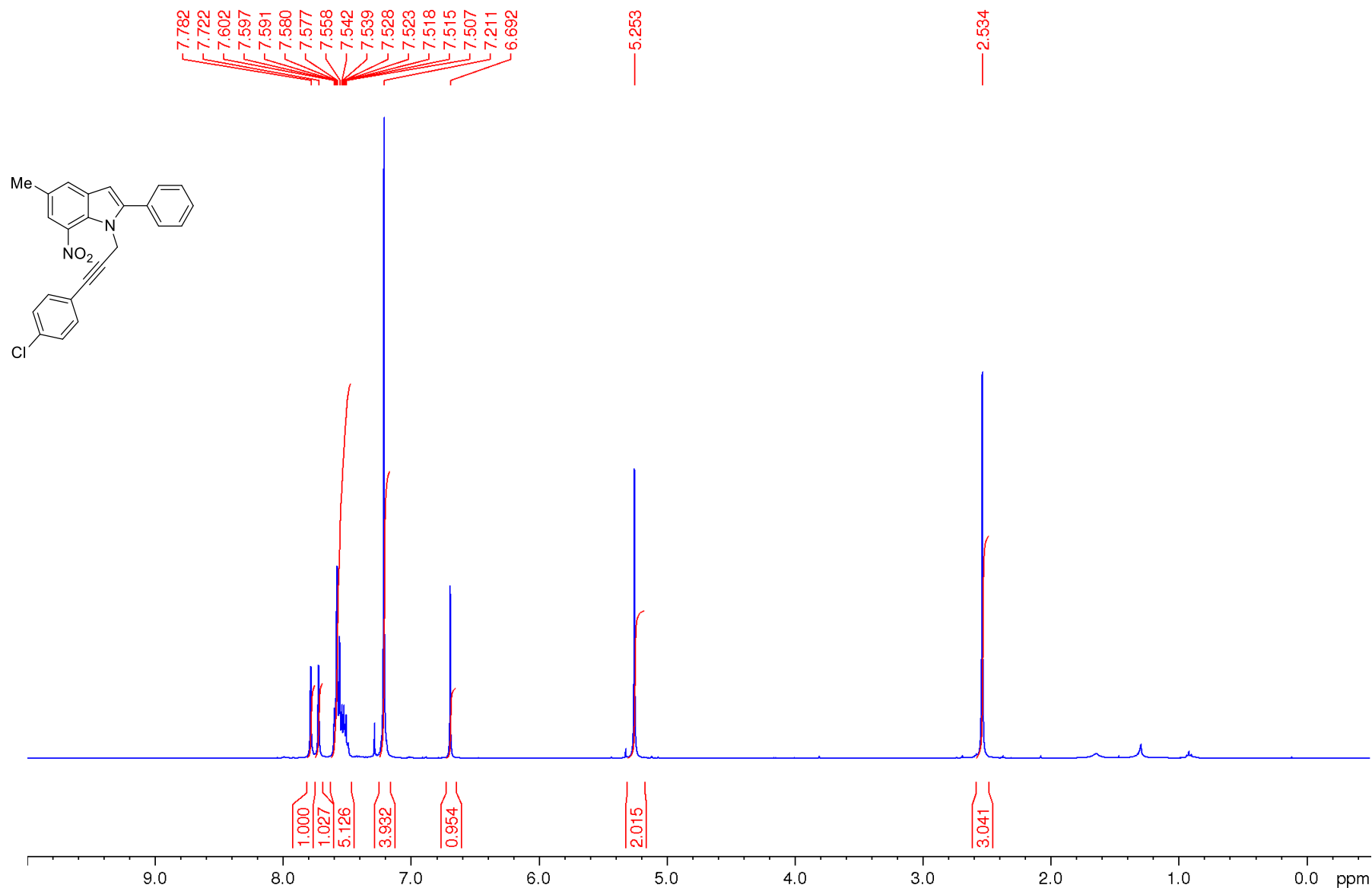
**methyl 4-(1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-1*H*-indol-2-yl)benzoate 7h**



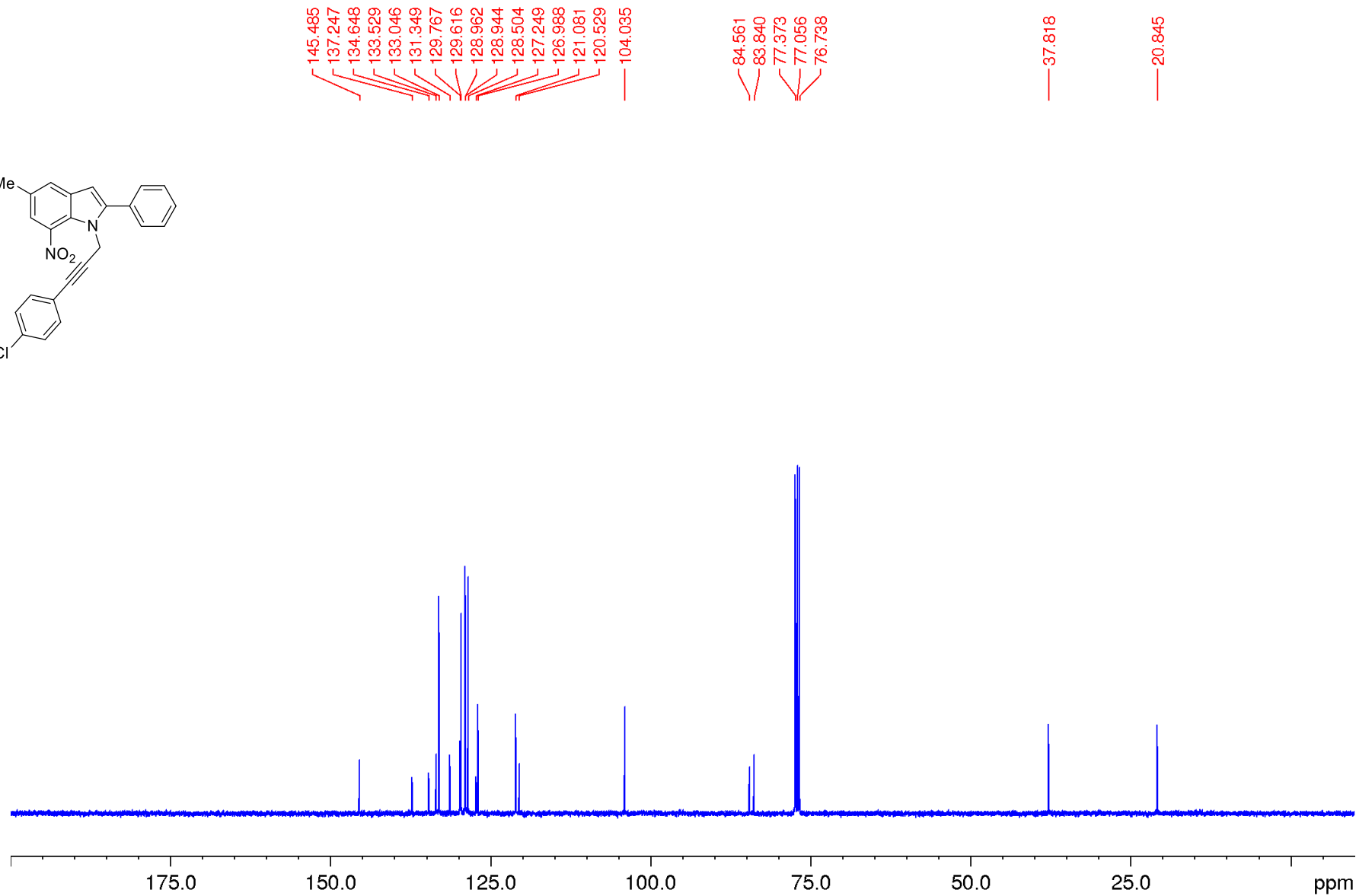
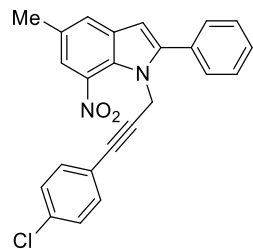
**methyl 4-(1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-1*H*-indol-2-yl)benzoate 7h**



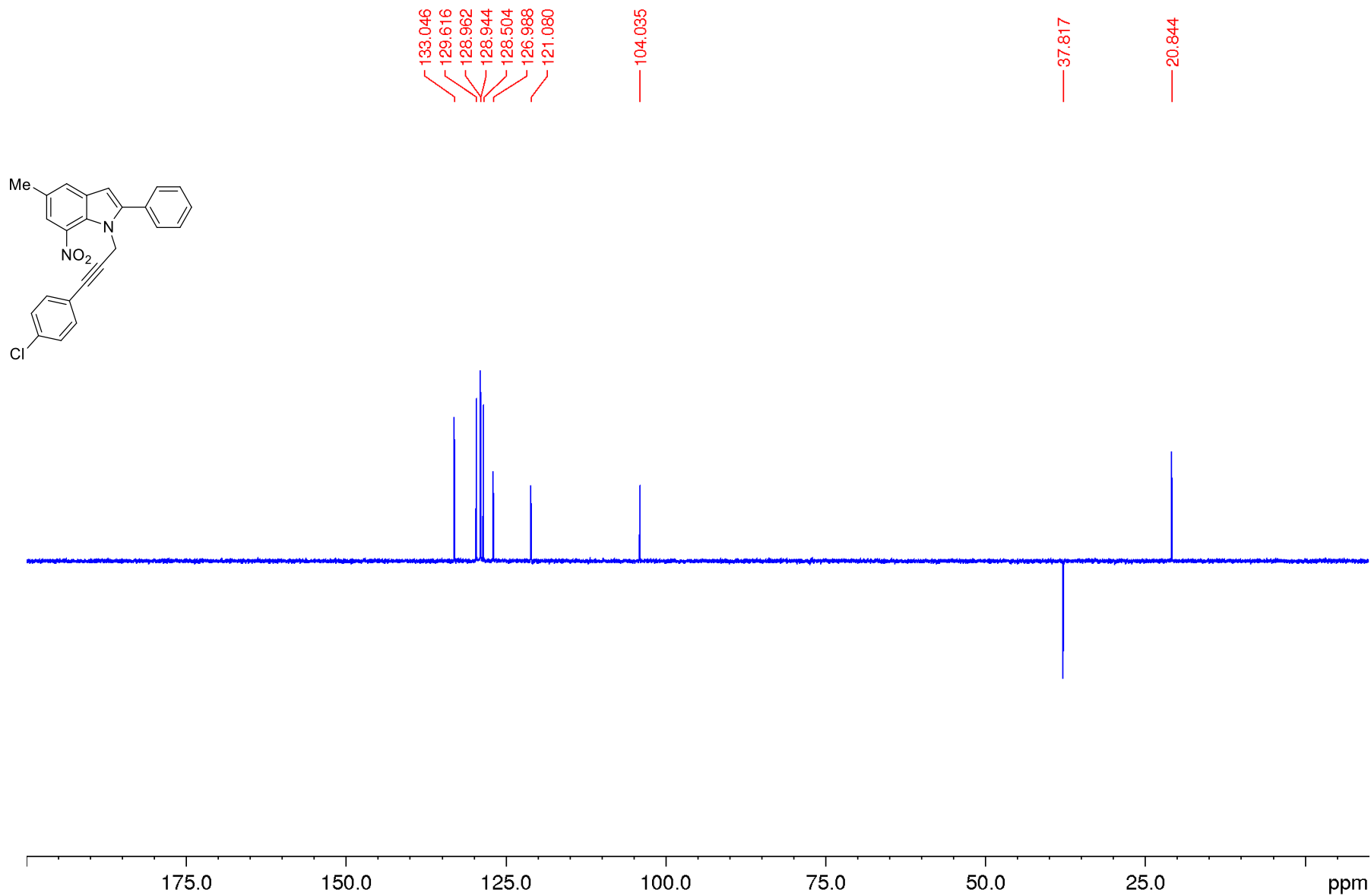
**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-2-phenyl-1*H*-indole 7i**



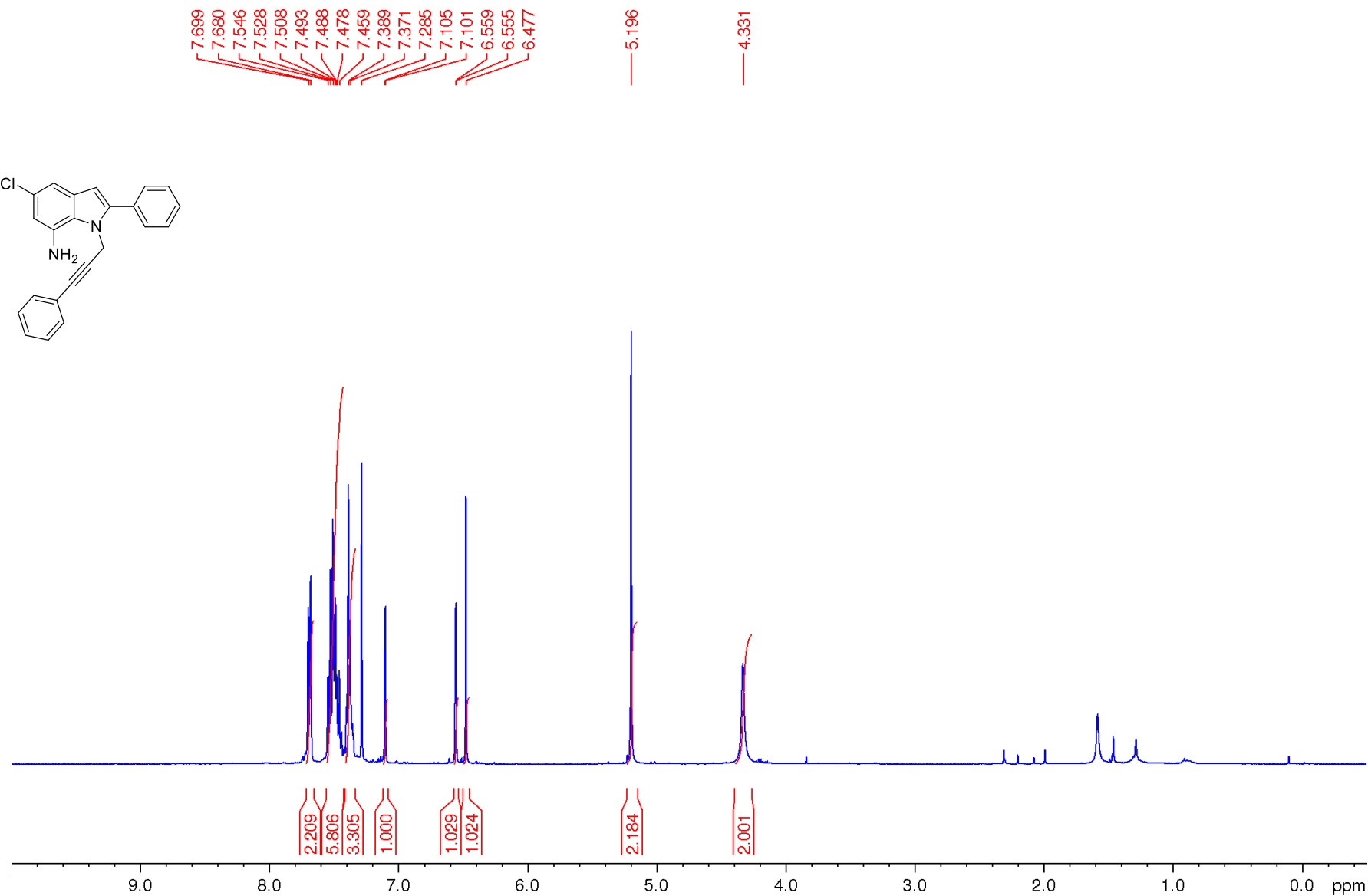
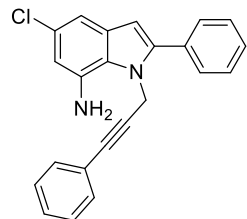
**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-2-phenyl-1*H*-indole 7i**



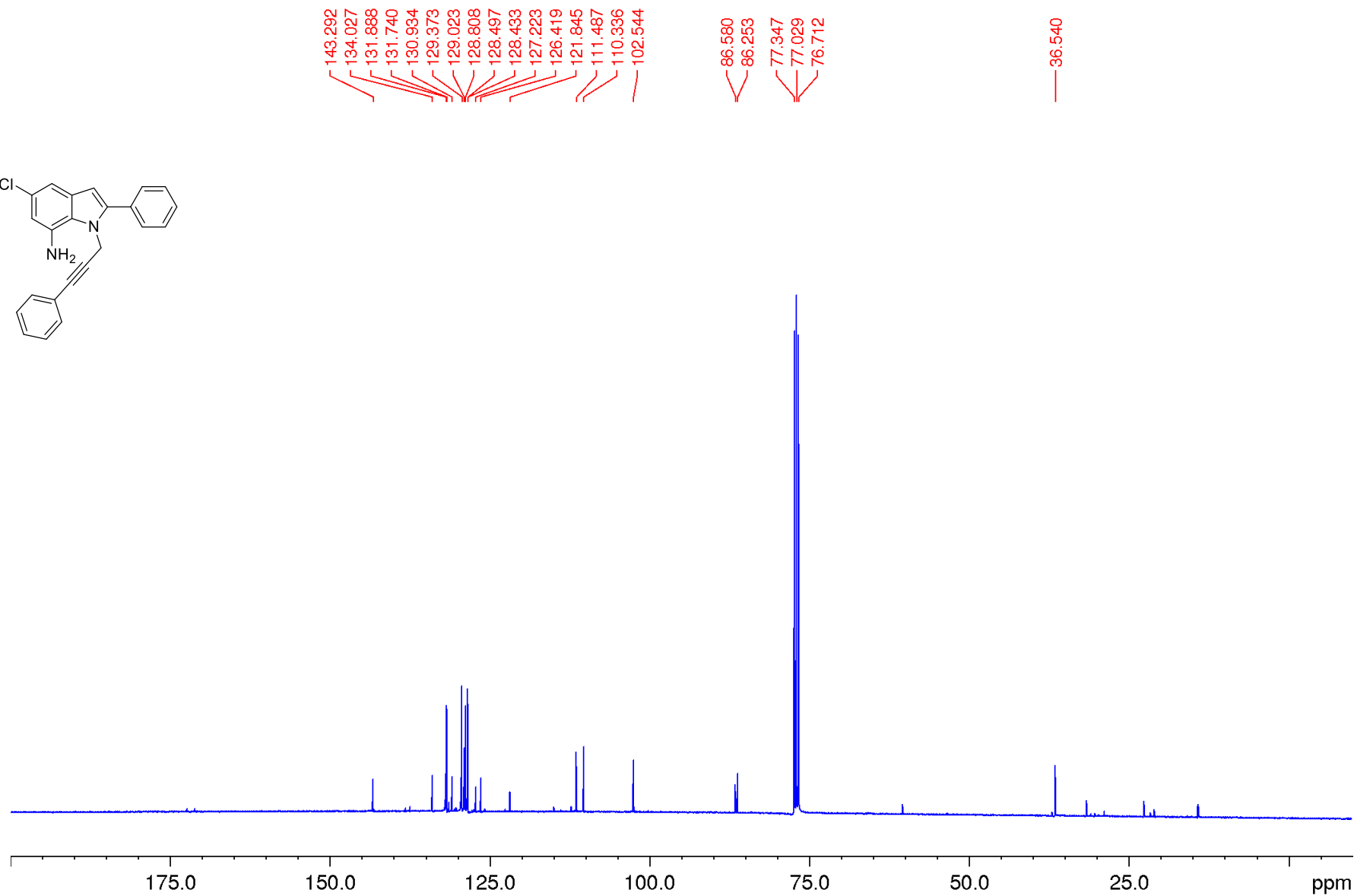
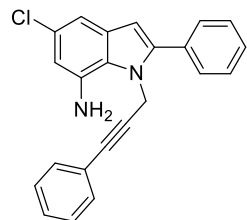
**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-7-nitro-2-phenyl-1*H*-indole 7i**



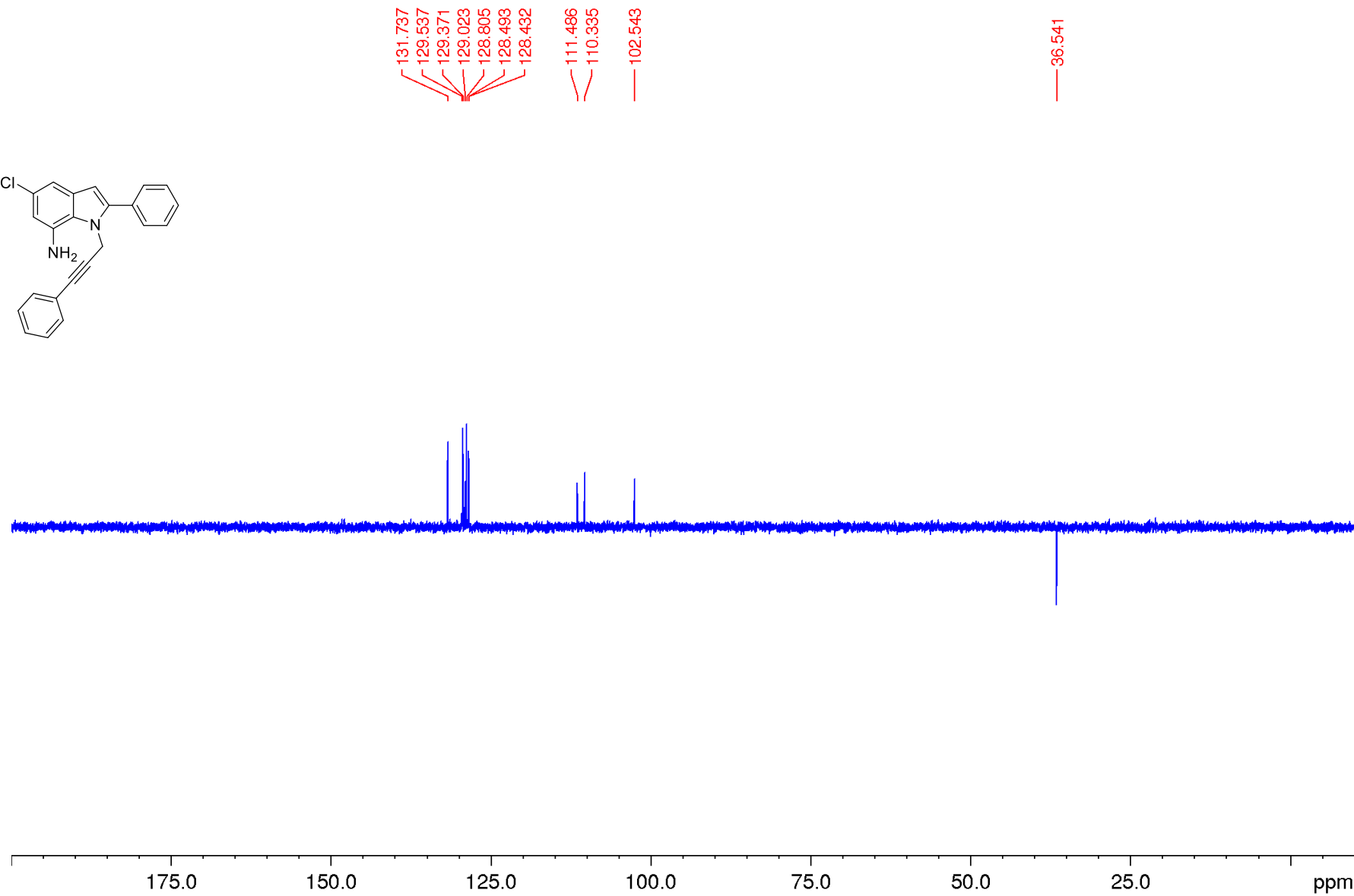
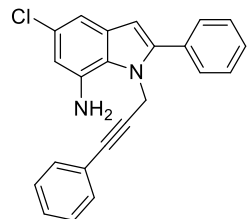
# 5-chloro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indol-7-amine 1a



# 5-chloro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1H-indol-7-amine 1a

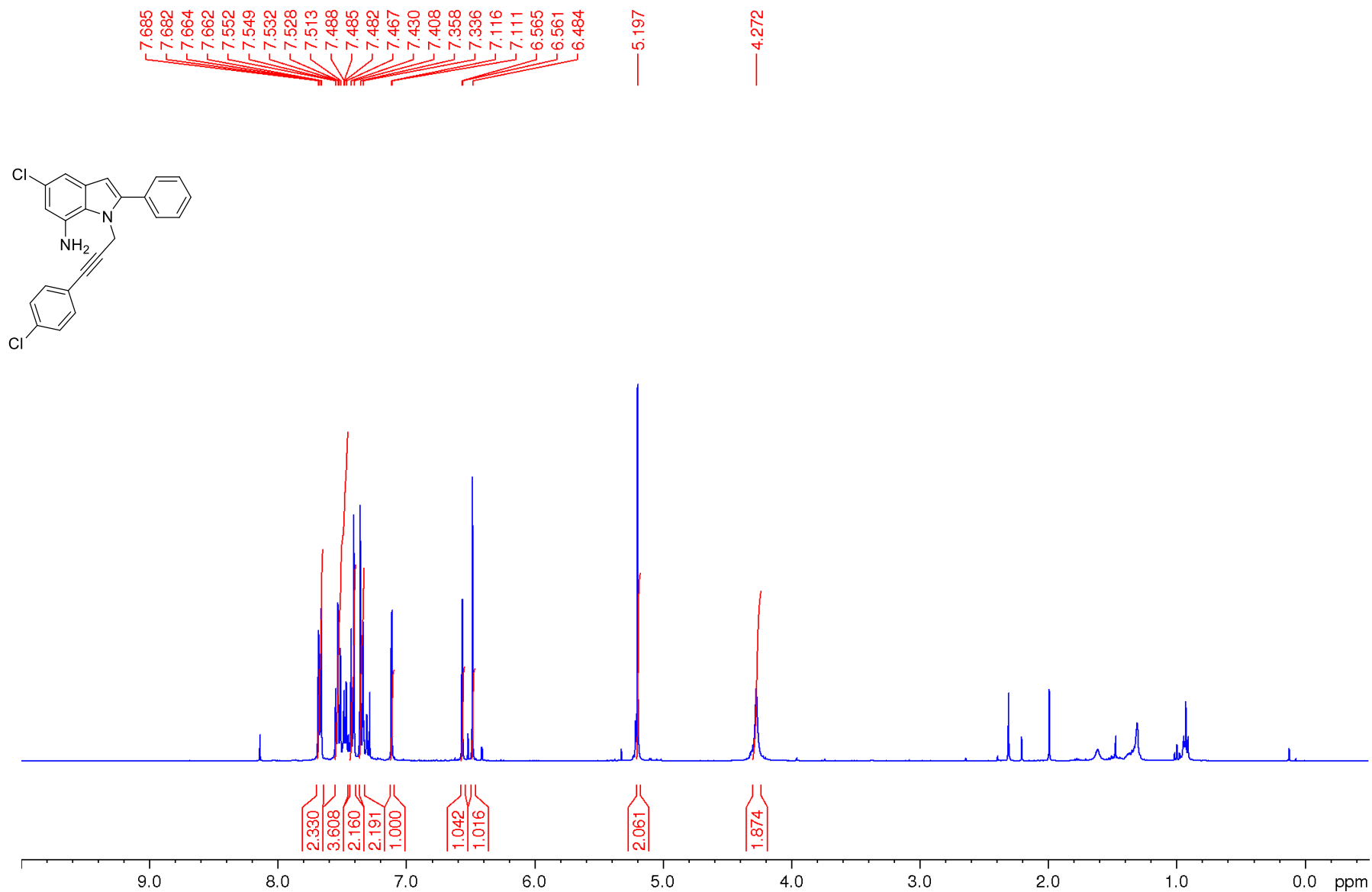


# 5-chloro-2-phenyl-1-(3-phenylprop-2-yn-1-yl)-1*H*-indol-7-amine 1a

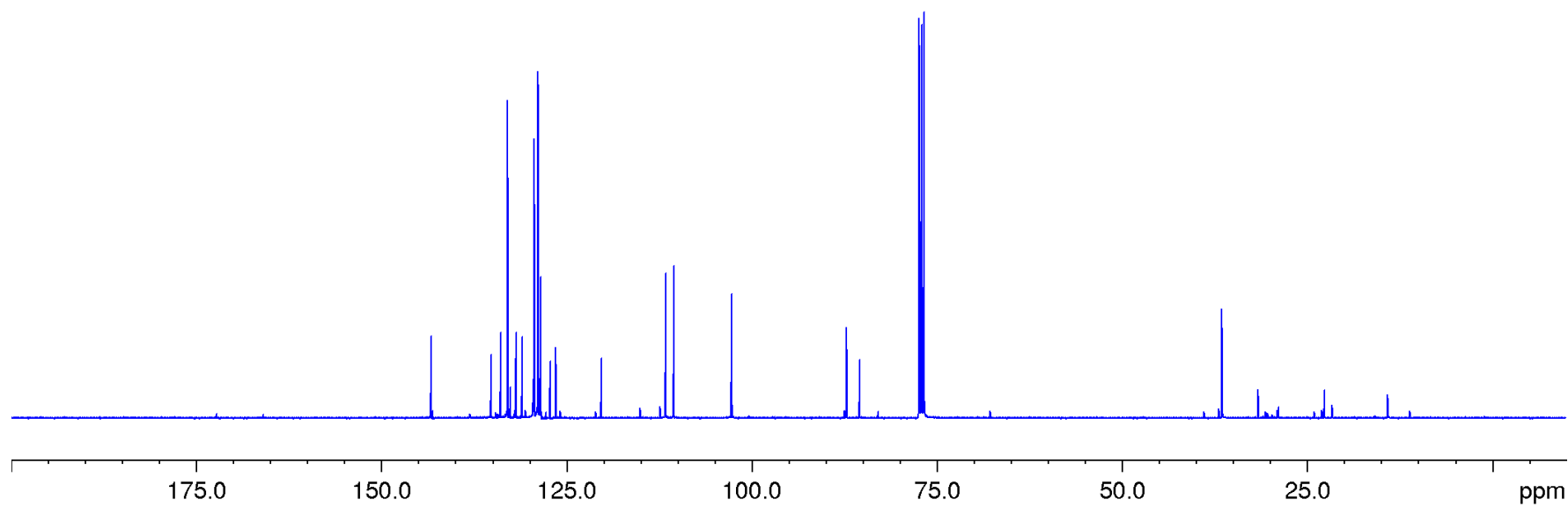
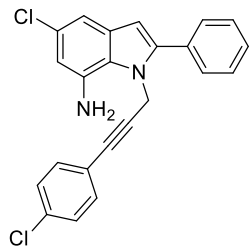




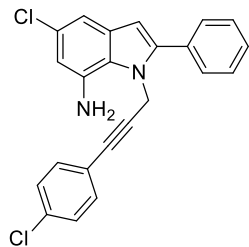
**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1b**



**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1b**



**5-chloro-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1b**

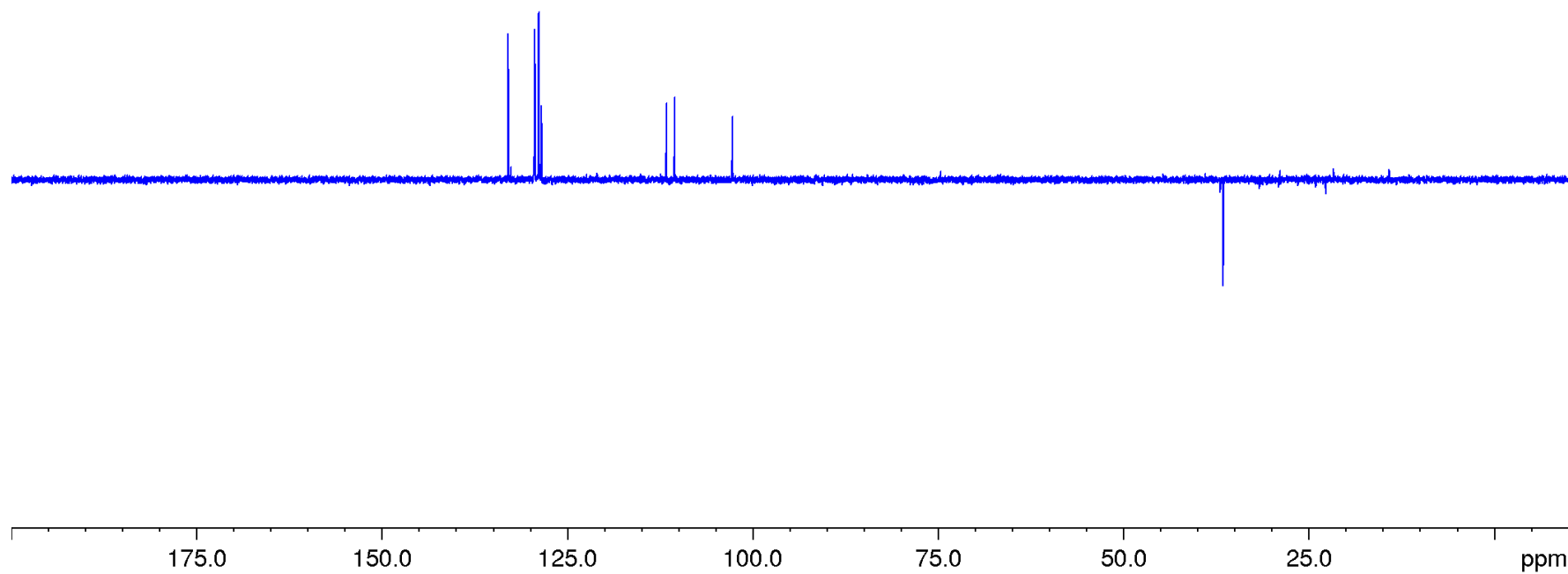


132.975  
129.364  
128.870  
128.491

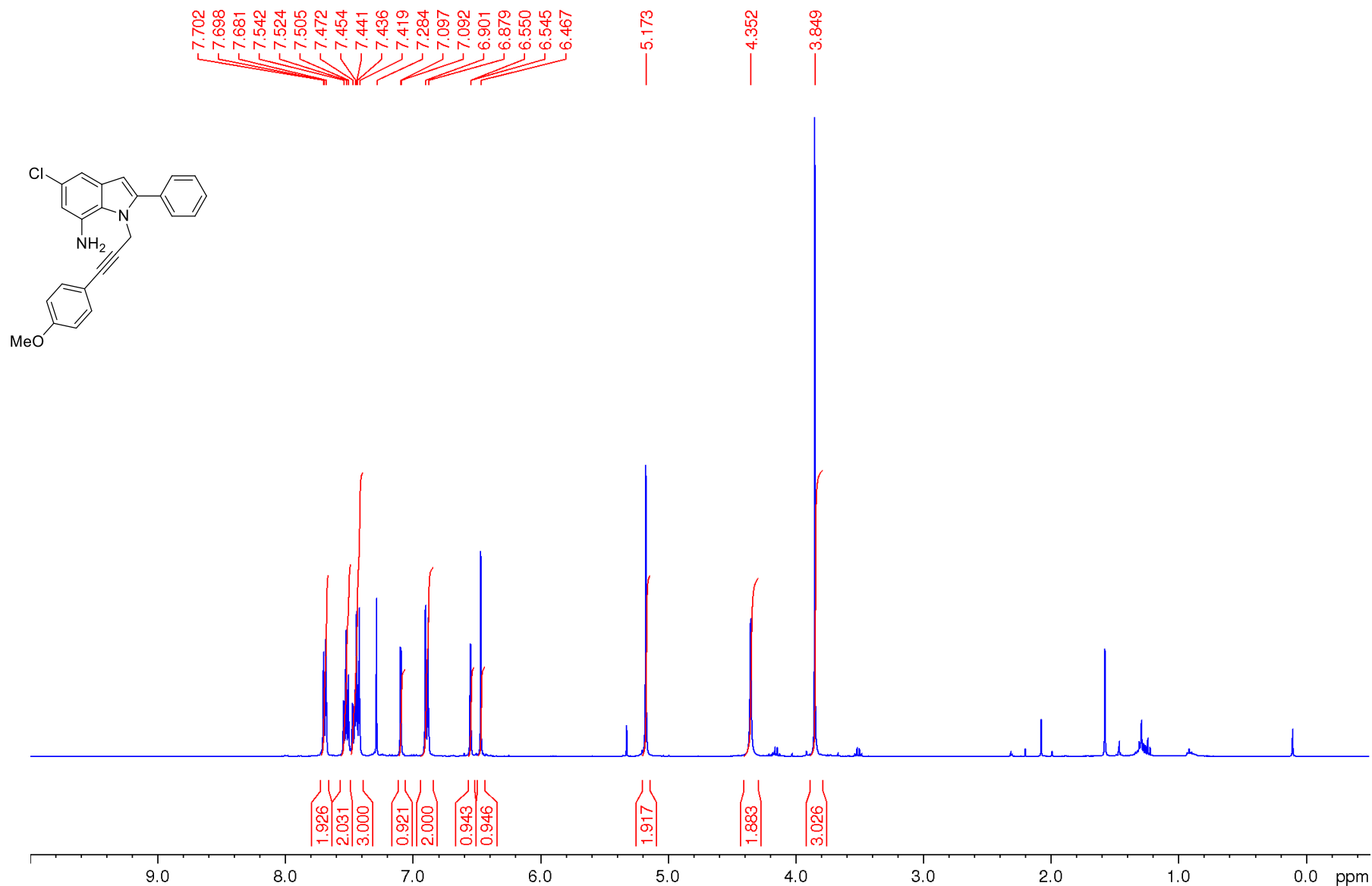
111.626  
110.518

102.720

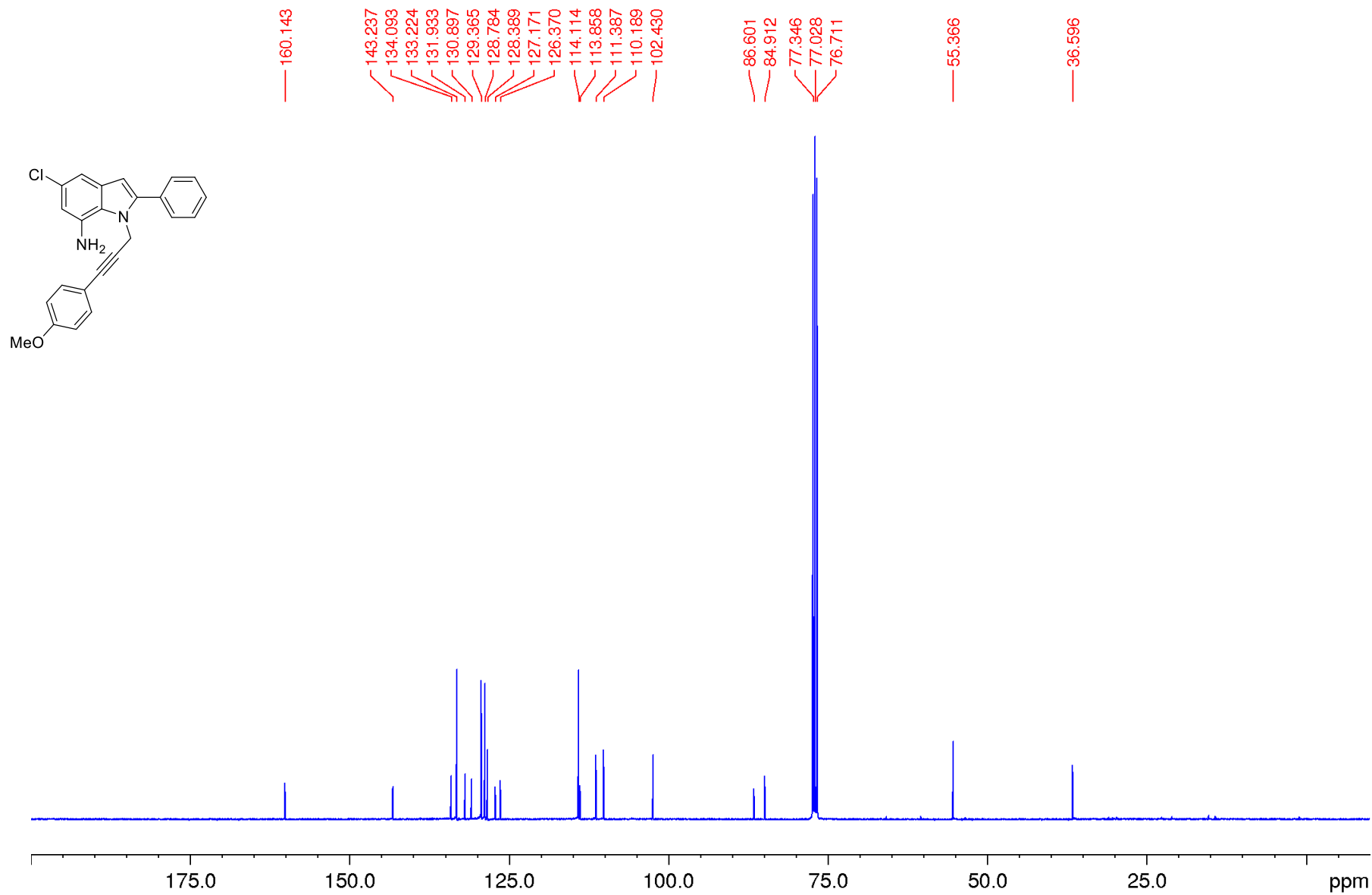
36.498



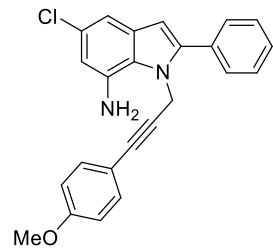
**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1c**



**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1H-indol-7-amine 1c**



**5-chloro-1-(3-(4-methoxyphenyl)prop-2-yn-1-yl)-2-phenyl-1*H*-indol-7-amine 1c**

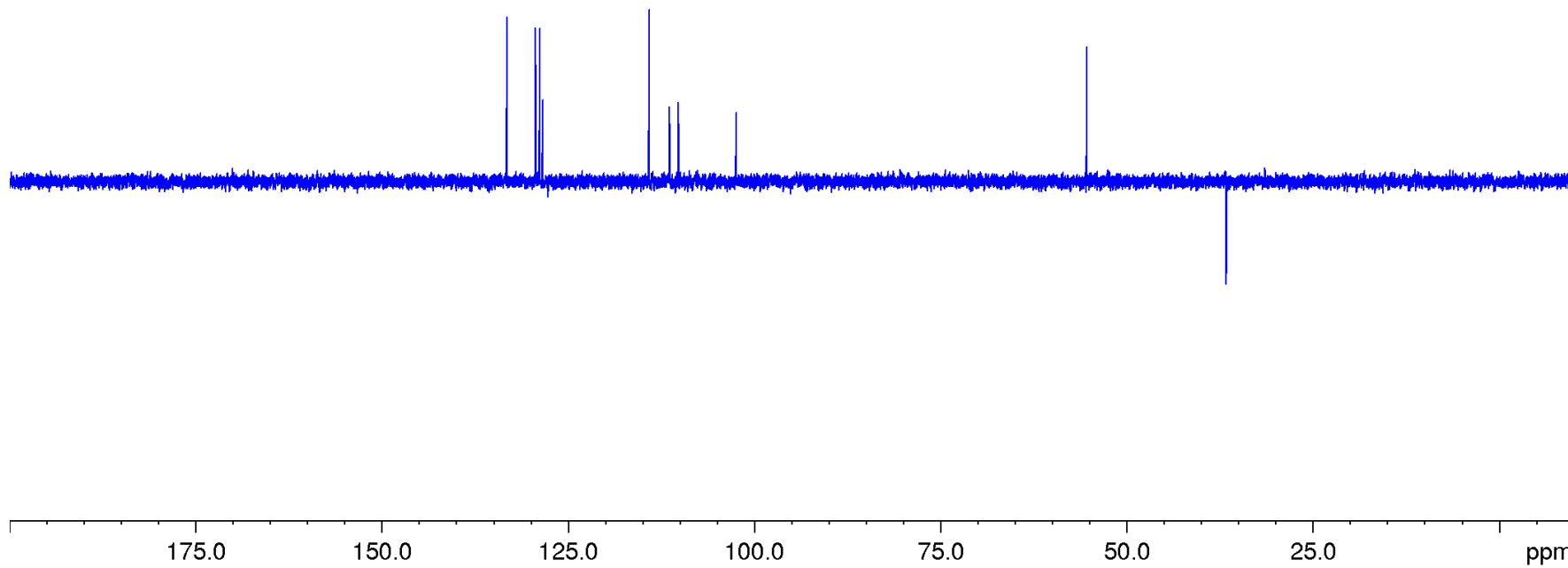


133.224  
129.365  
128.784  
128.389

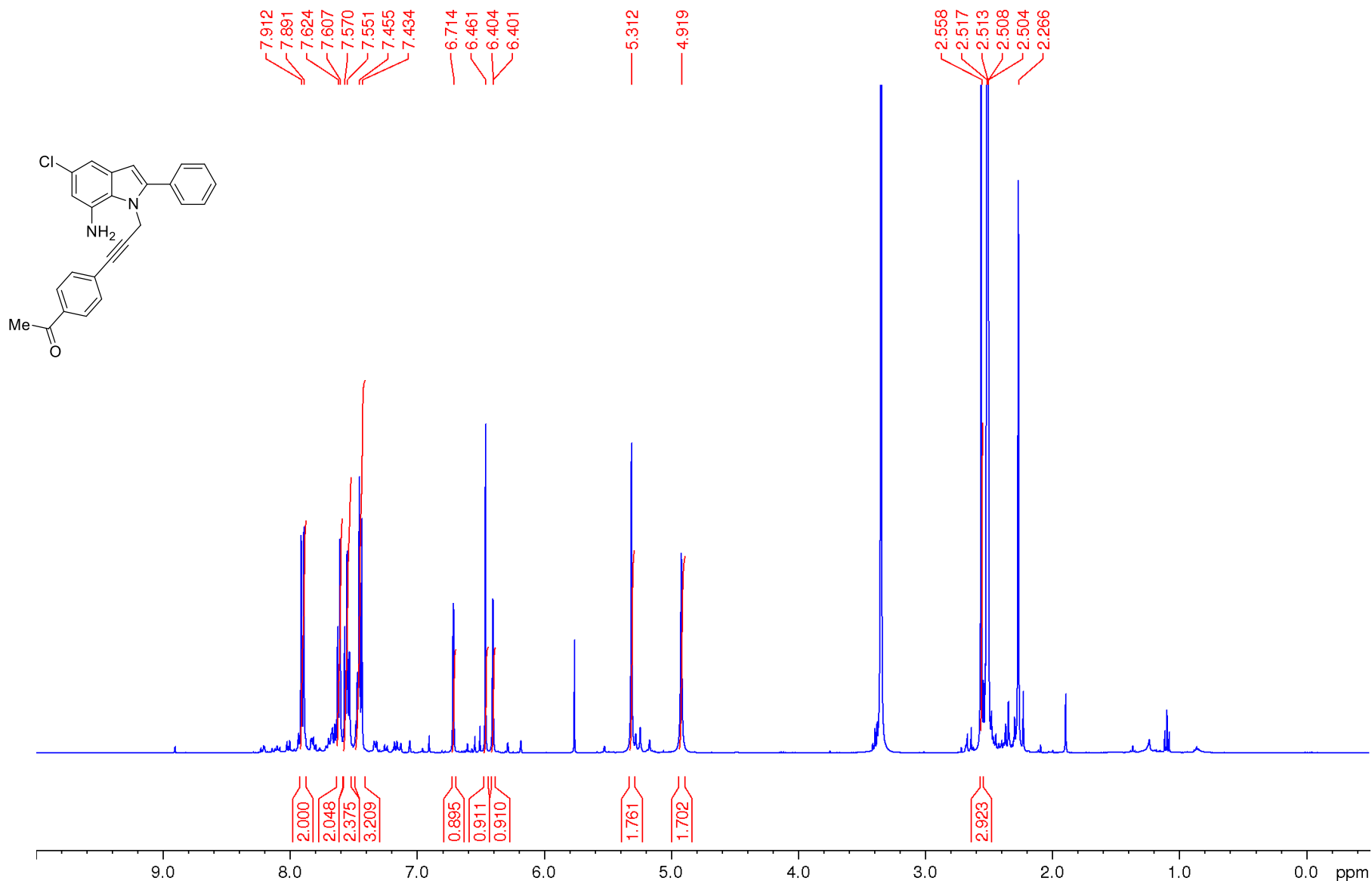
114.113  
111.387  
110.188  
102.429

55.365

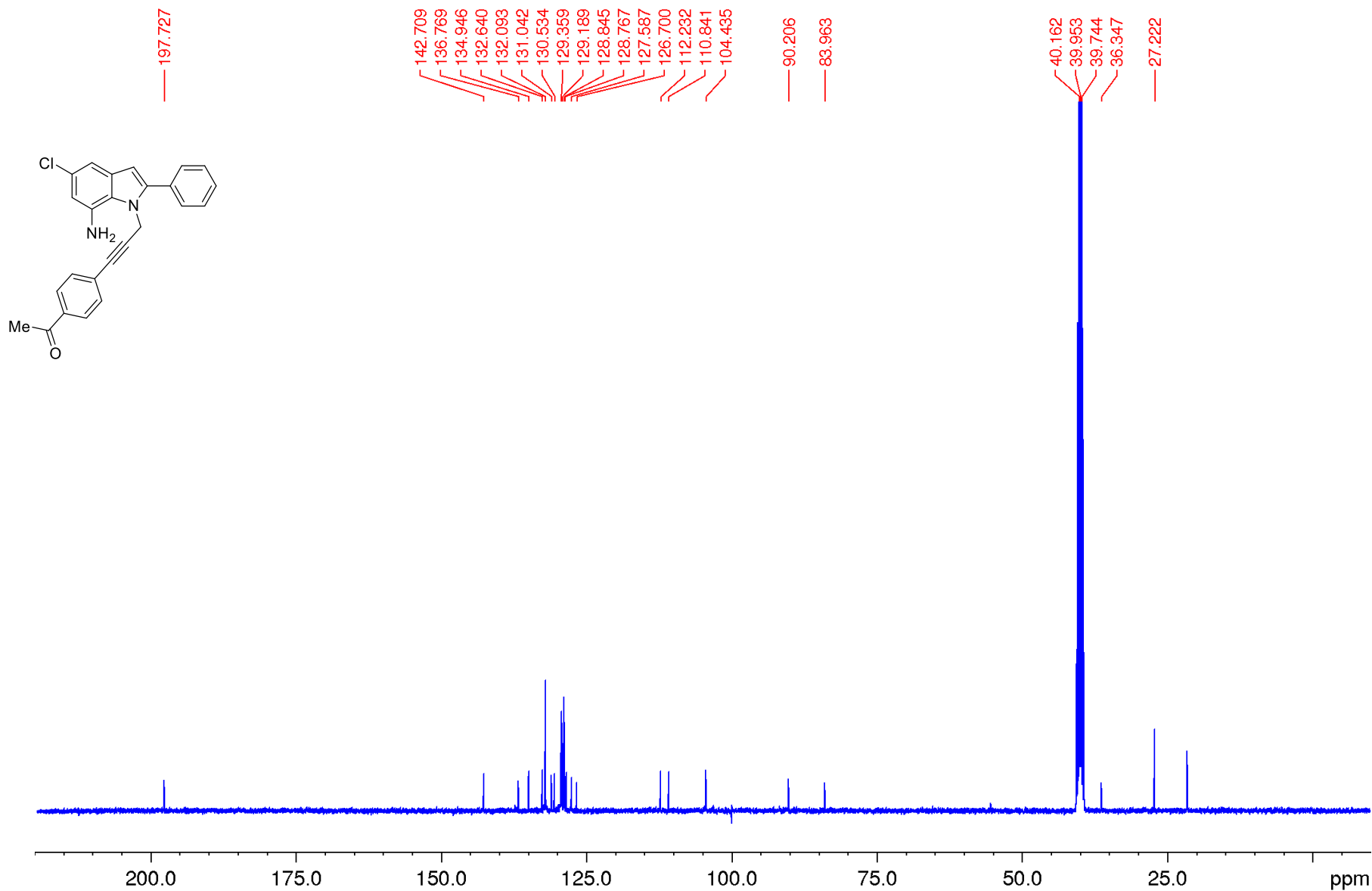
36.594



**1-(4-(3-(7-amino-5-chloro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1d**

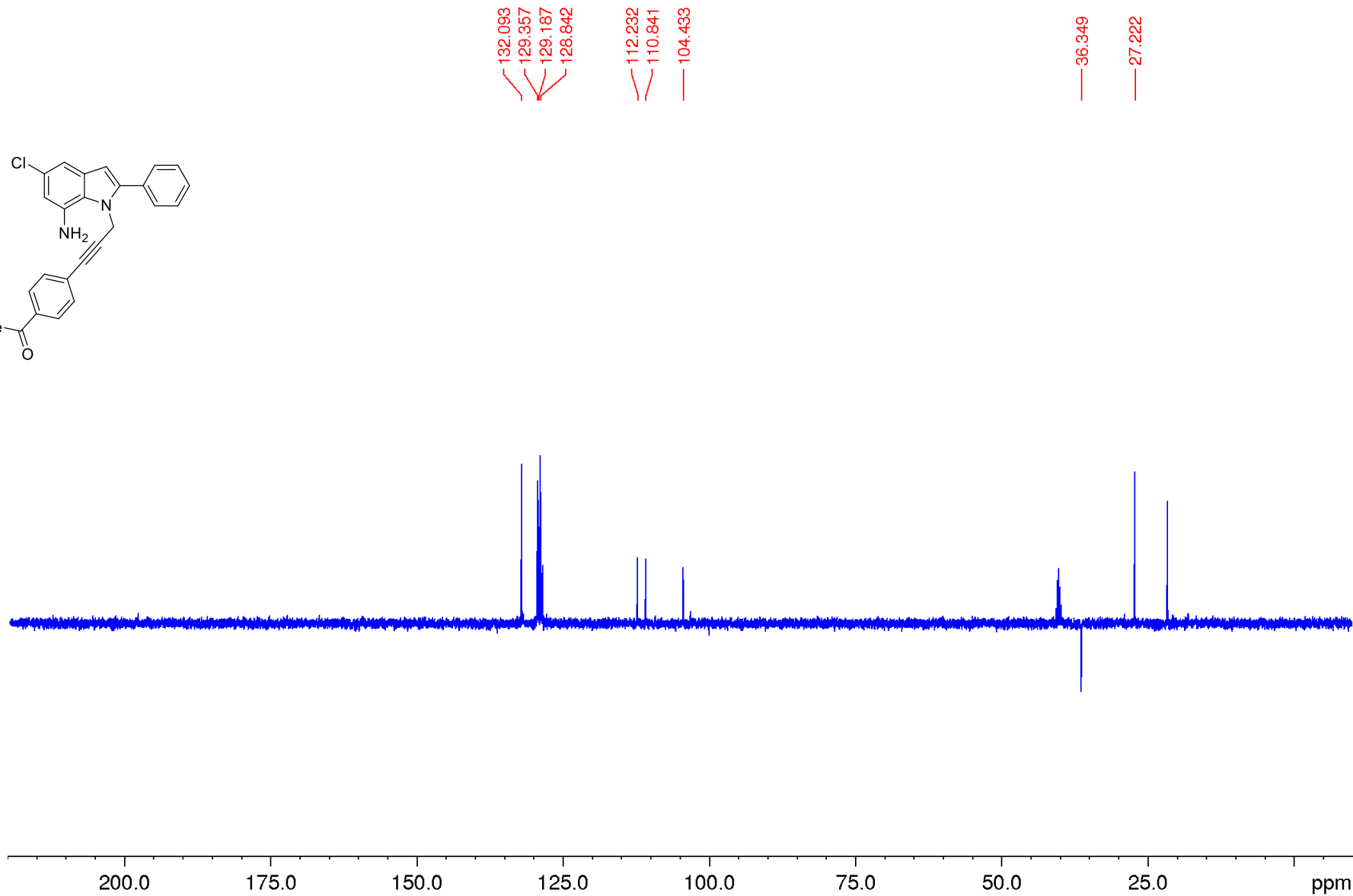
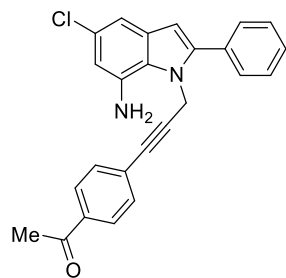


**1-(4-(3-(7-amino-5-chloro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1d**

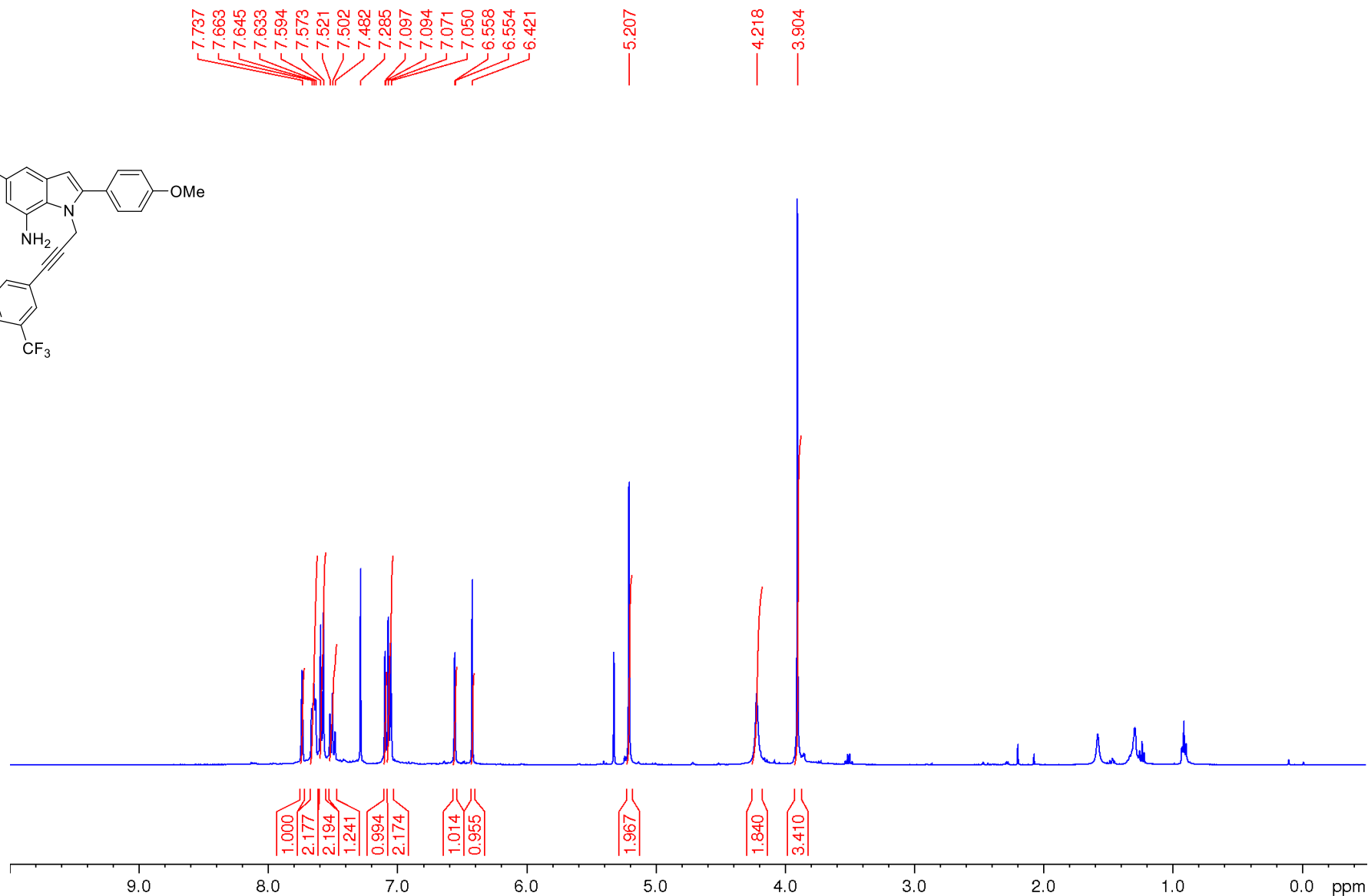
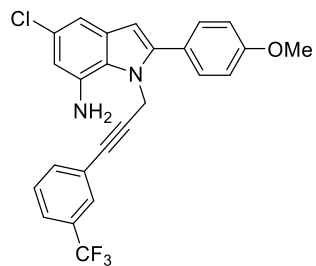




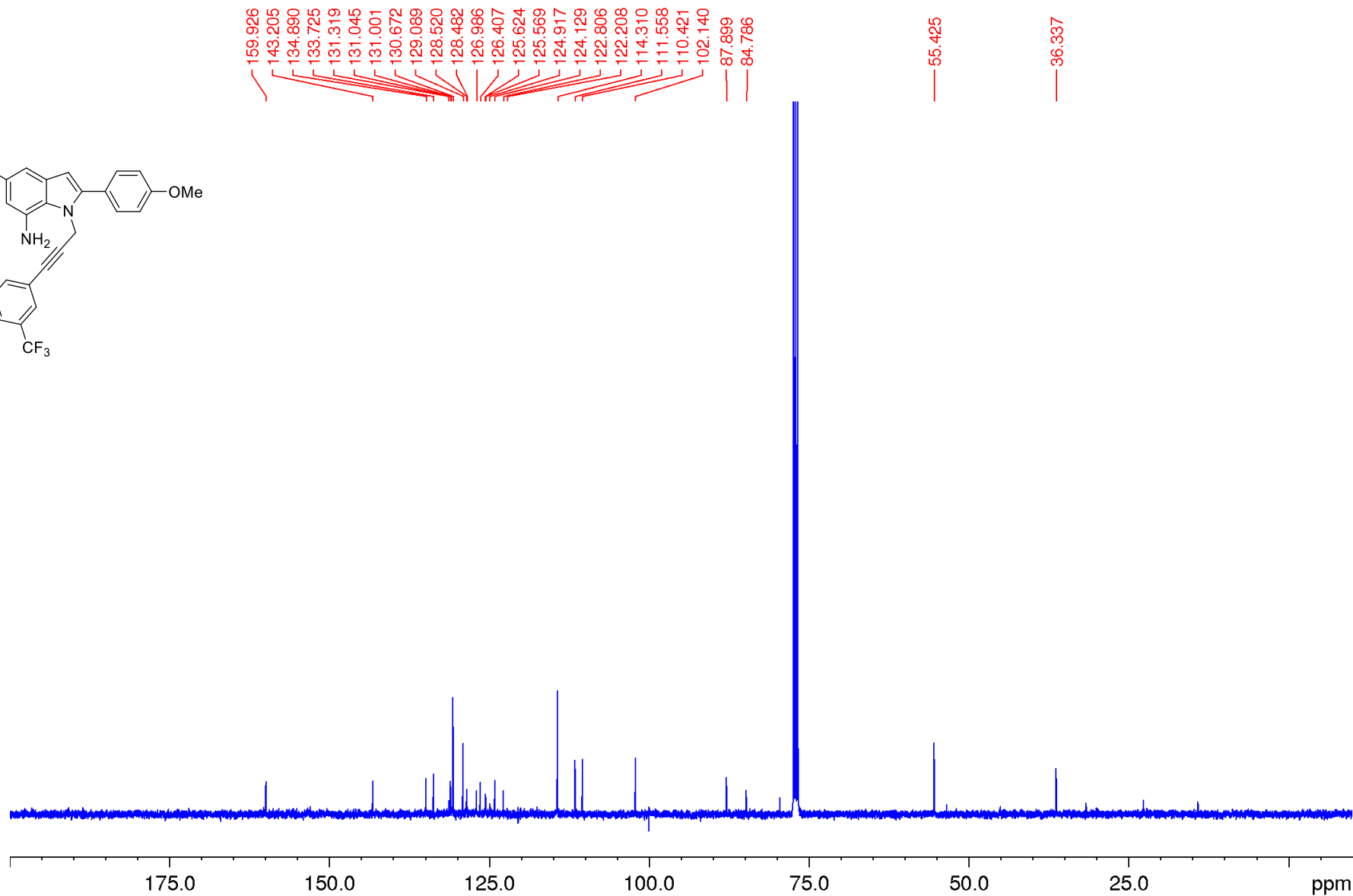
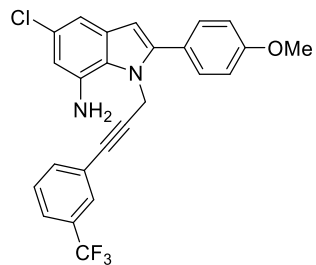
**1-(4-(3-(7-amino-5-chloro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1d**



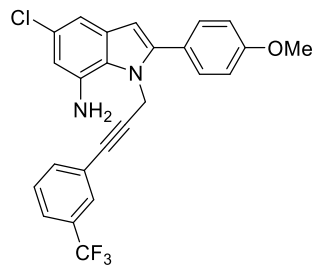
**5-chloro-2-(4-methoxyphenyl)-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indol-7-amine 1e**



**5-chloro-2-(4-methoxyphenyl)-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1H-indol-7-amine 1e**



**5-chloro-2-(4-methoxyphenyl)-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1*H*-indol-7-amine 1e**



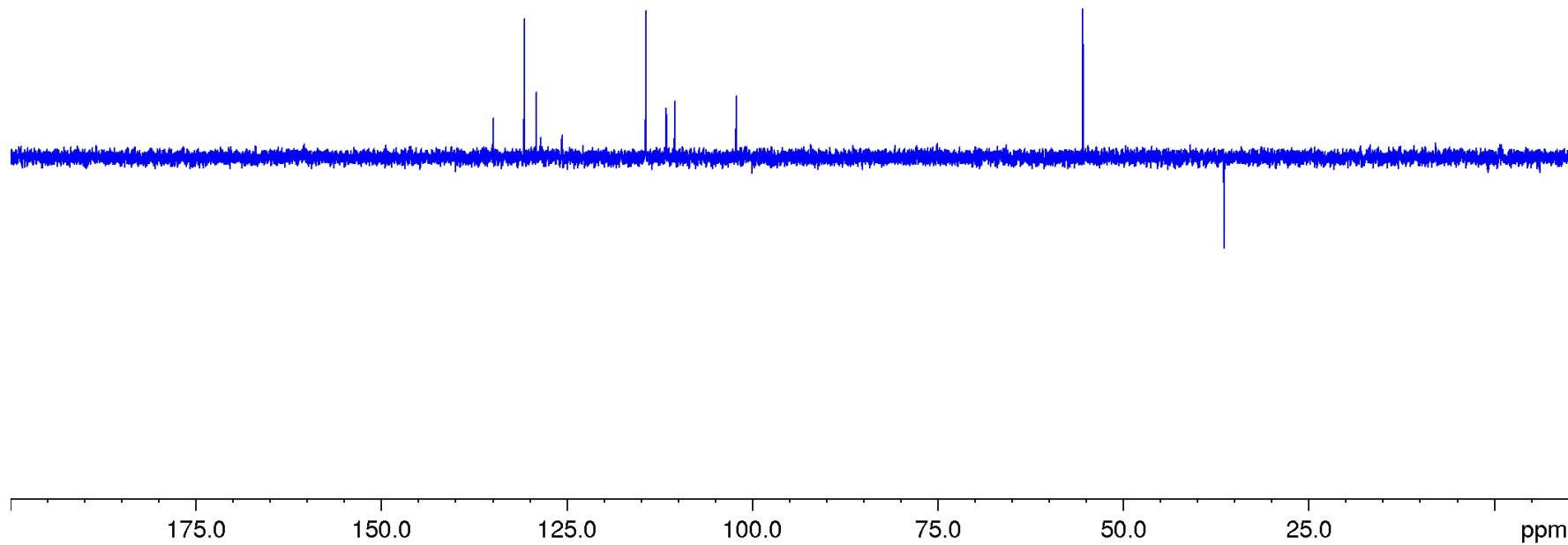
134.881  
130.672  
129.088  
128.507  
125.566

114.310  
111.557  
110.422

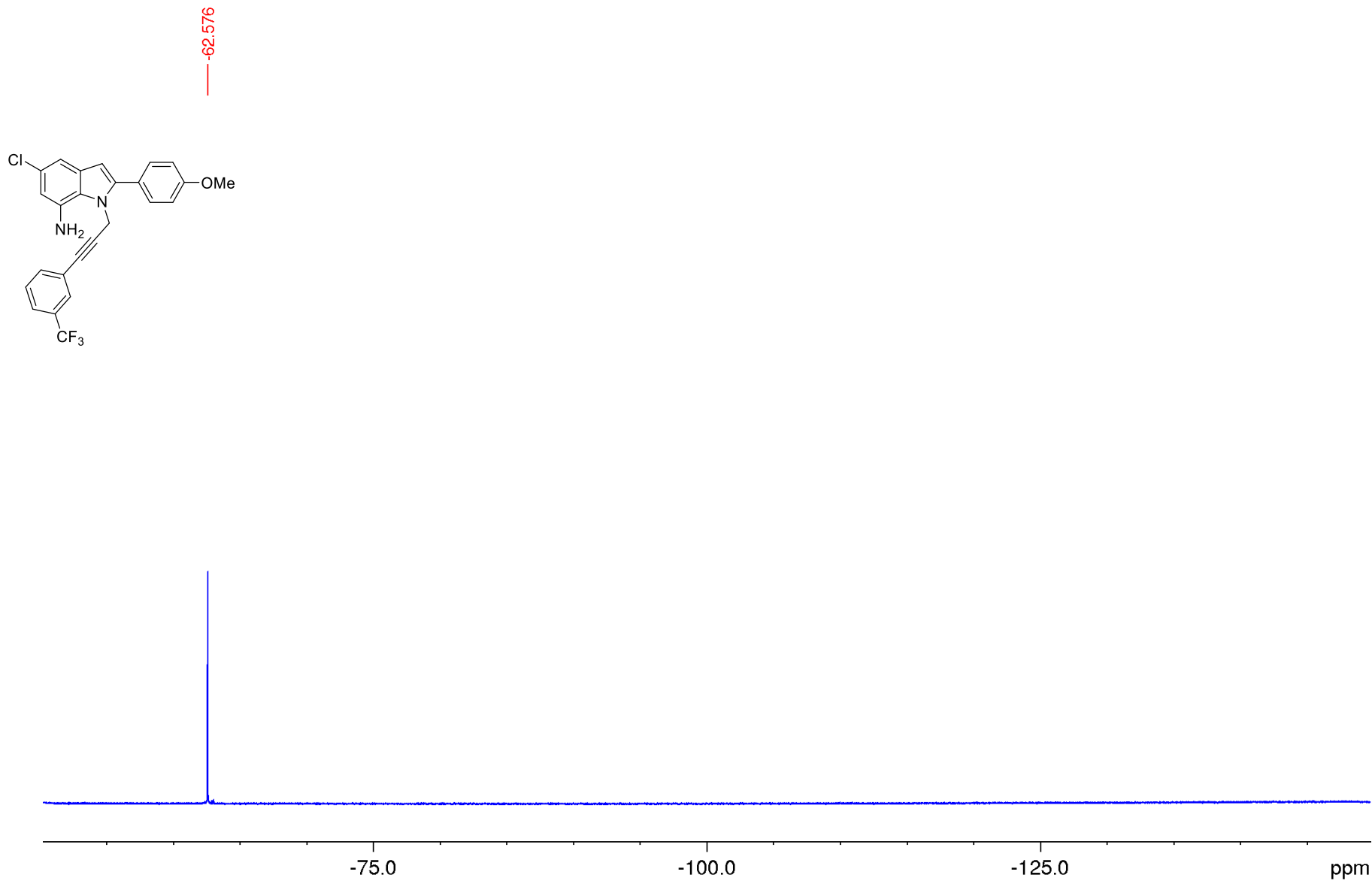
102.140

55.425

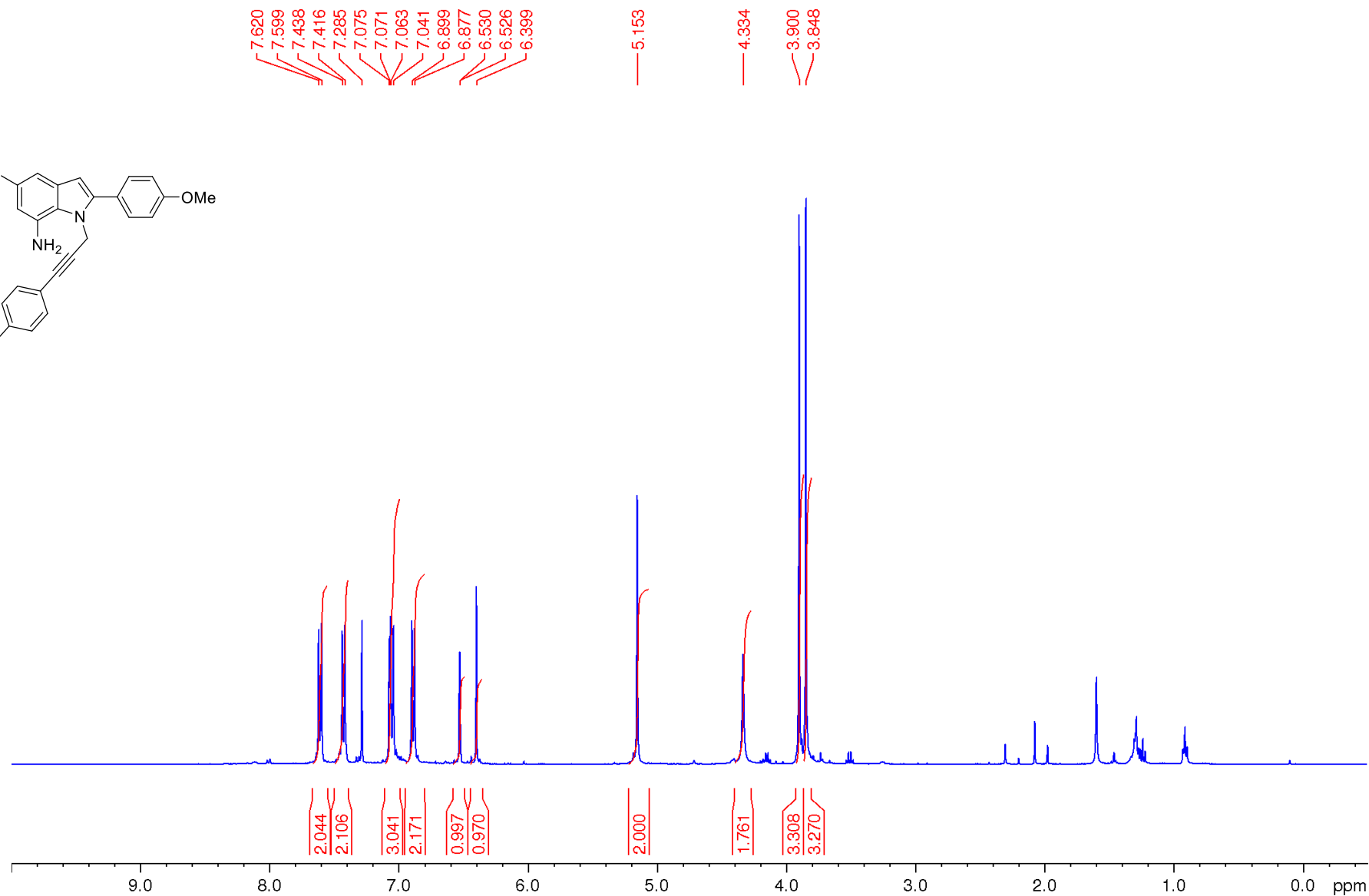
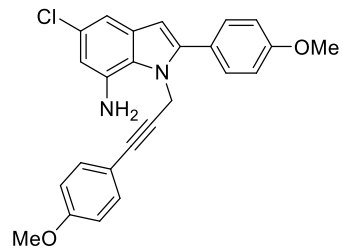
36.337



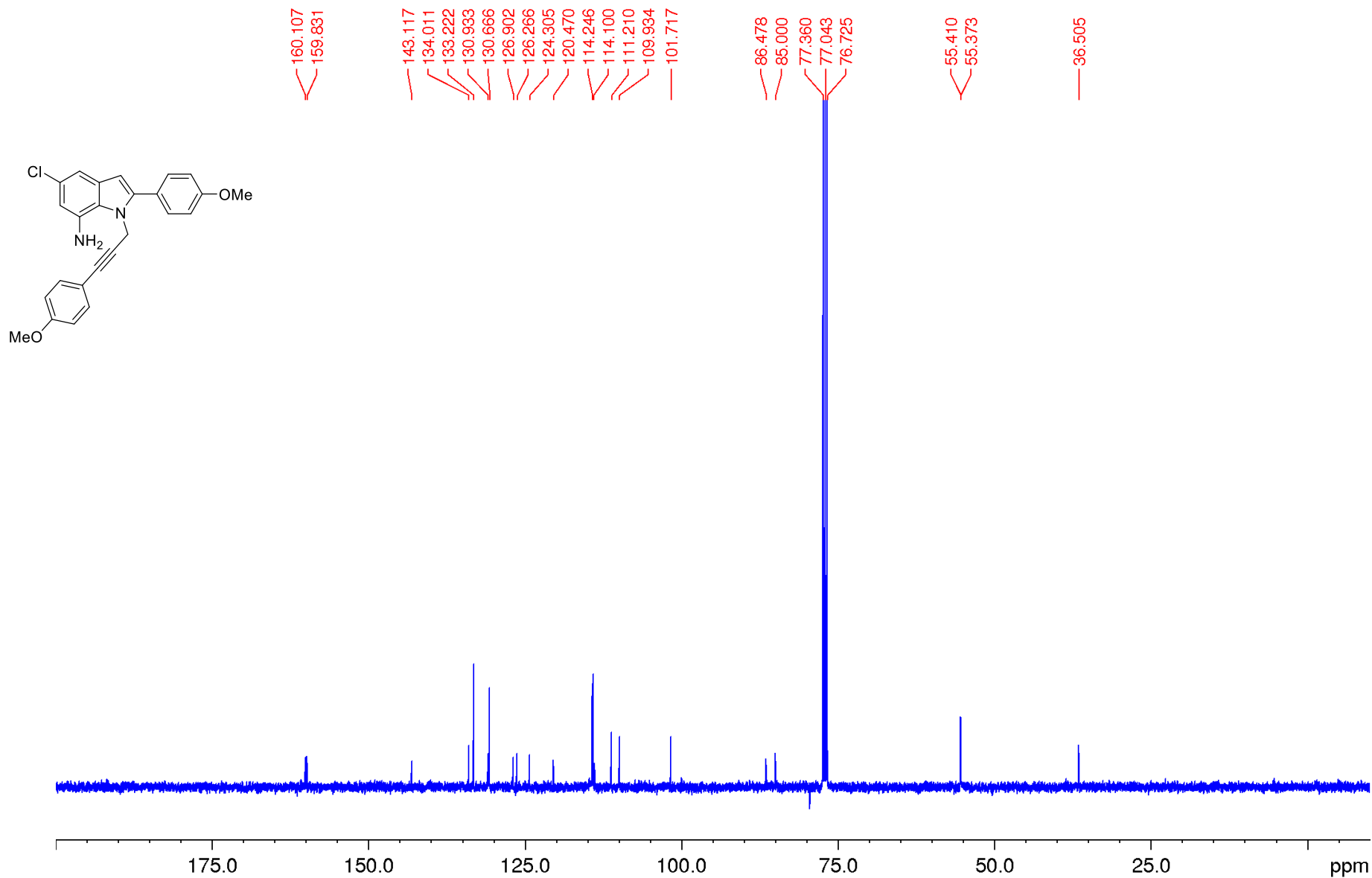
**5-chloro-2-(4-methoxyphenyl)-1-(3-(3-(trifluoromethyl)phenyl)prop-2-yn-1-yl)-1*H*-indol-7-amine 1e**



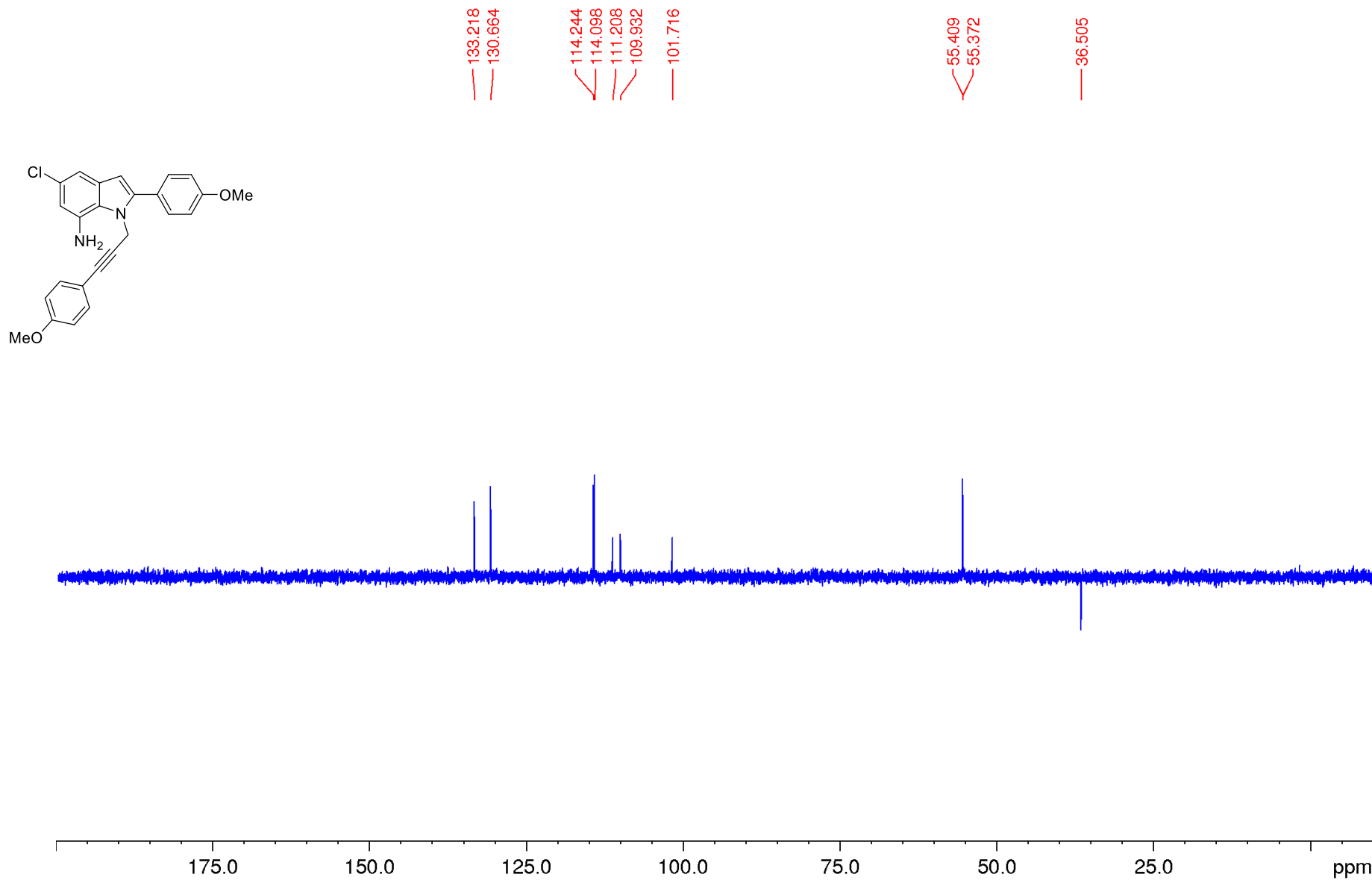
**5-cloro-2-(4-metossifenil)-1-(3-(4-metossifenil)prop-2-in-1-il)-7-ammino-1*H*-indolo amine 1f**



**5-cloro-2-(4-metossifenil)-1-(3-(4-metossifenil)prop-2-in-1-il)-7-ammino-1*H*-indolo amine 1f**

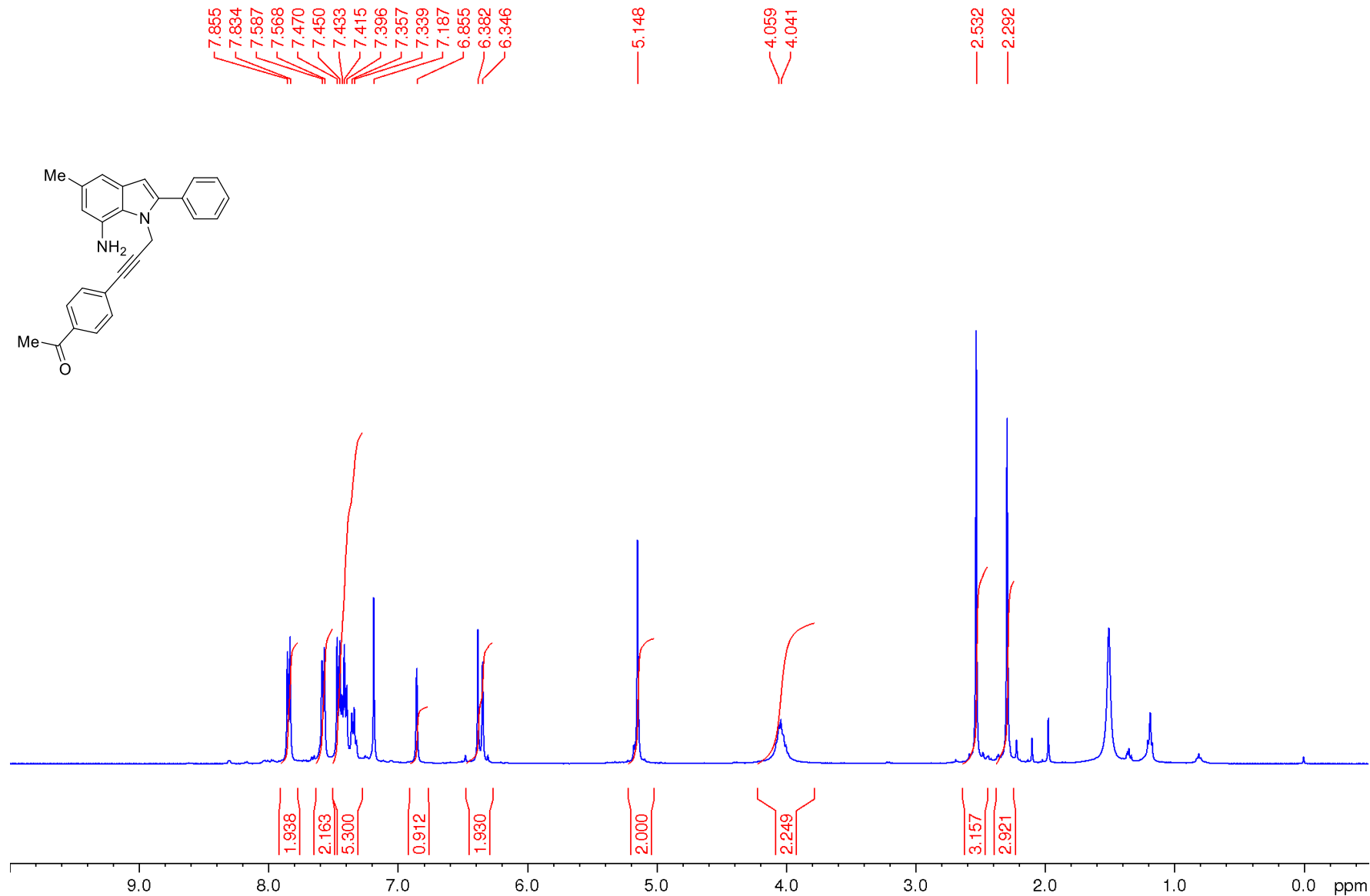
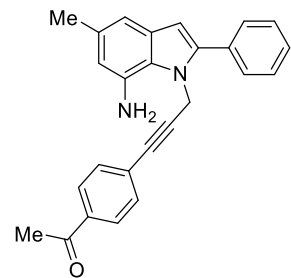


**5-cloro-2-(4-metossifenil)-1-(3-(4-metossifenil)prop-2-in-1-il)-7-ammino-1*H*-indolo amine 1f**

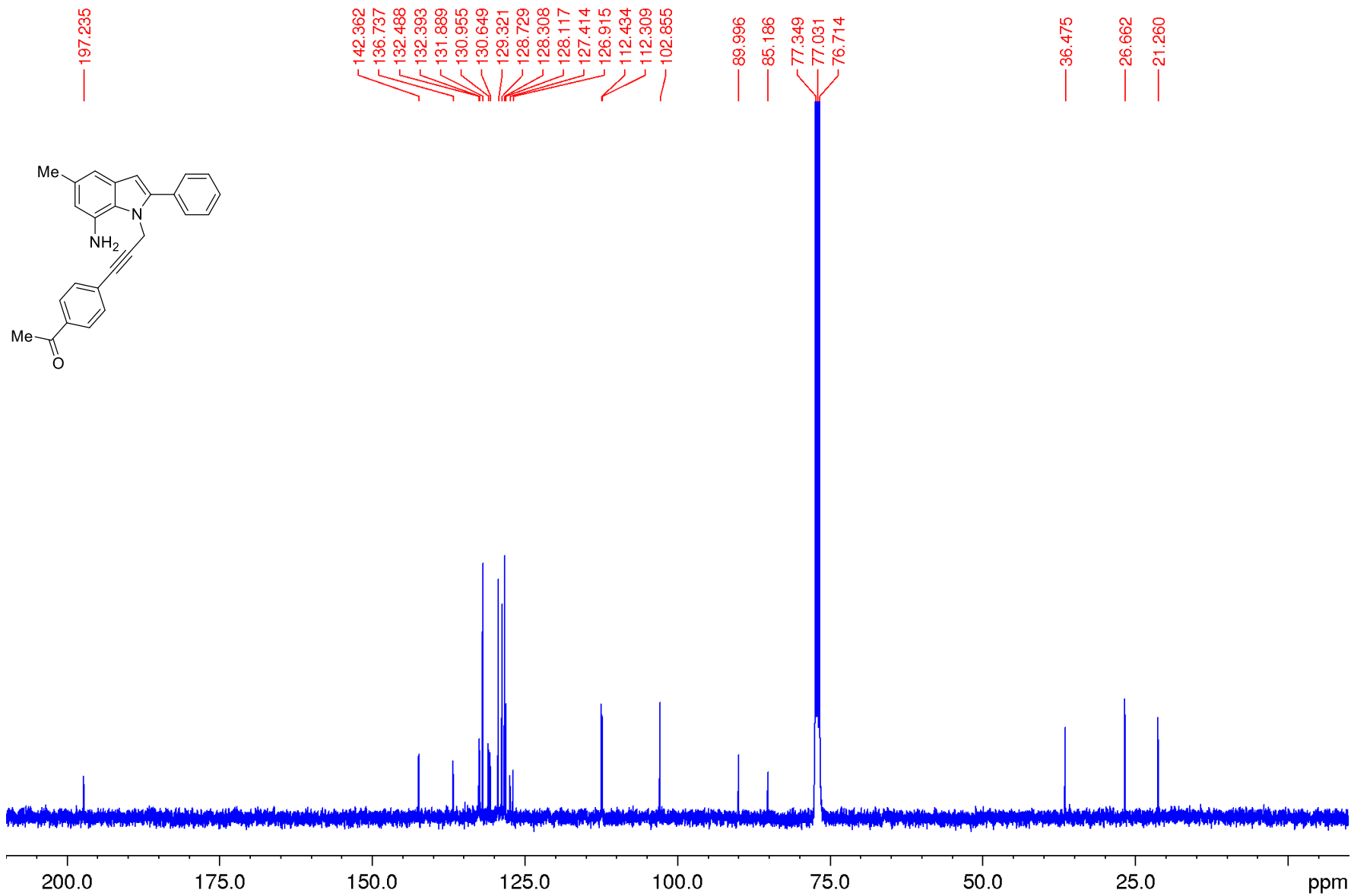




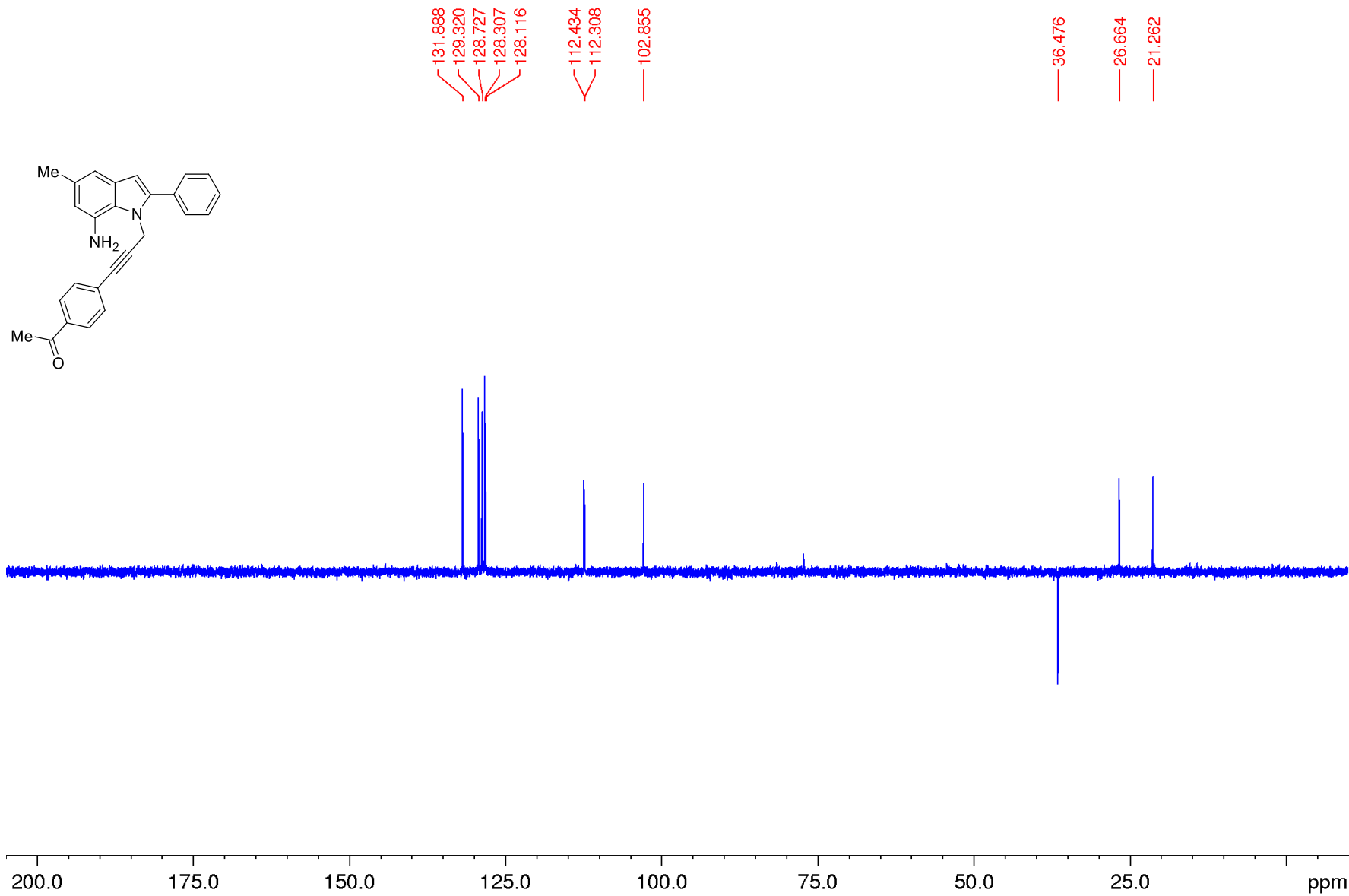
# 1-(4-(3-(7-amino-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1g



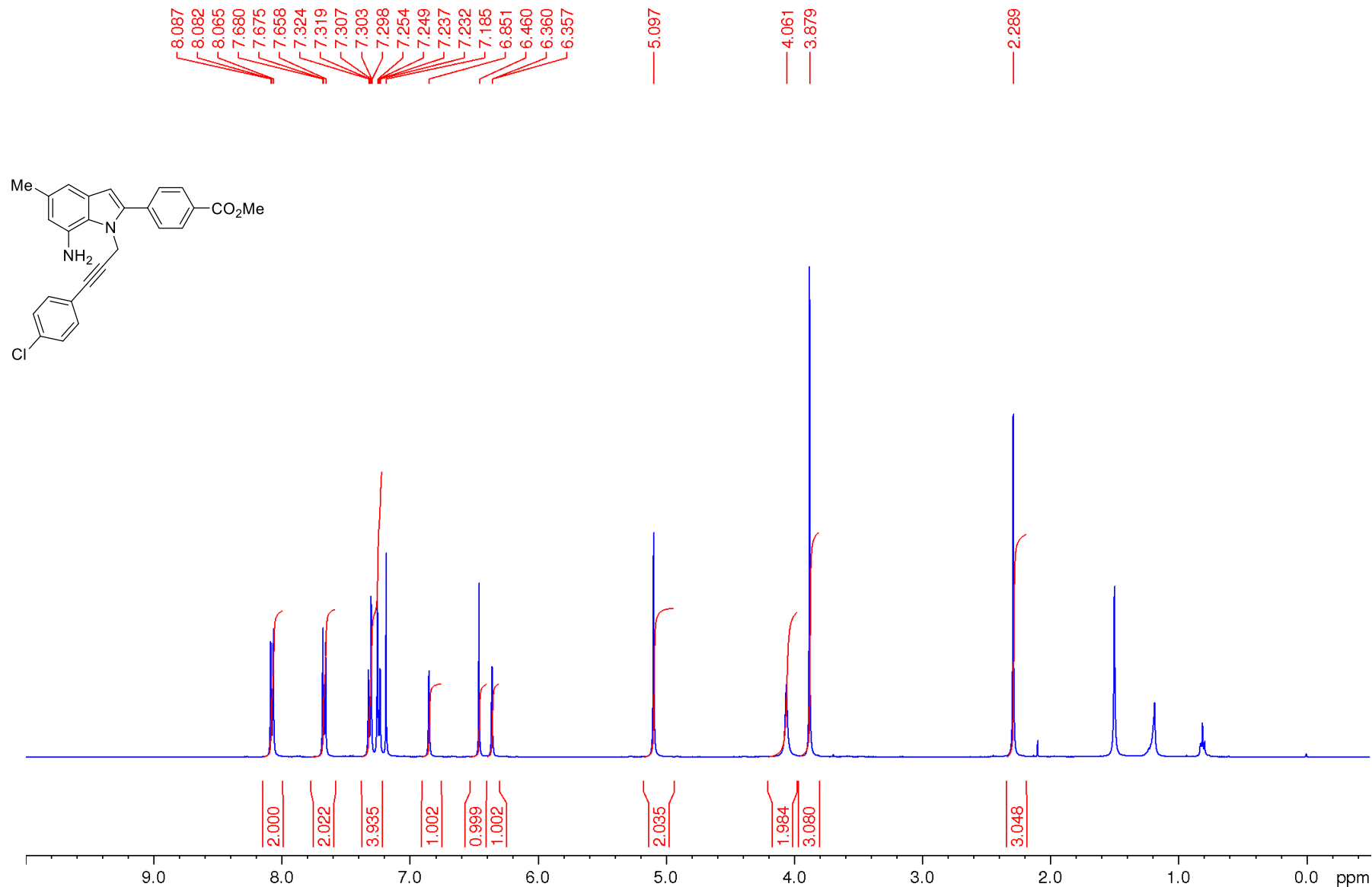
**1-(4-(3-(7-amino-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1g**



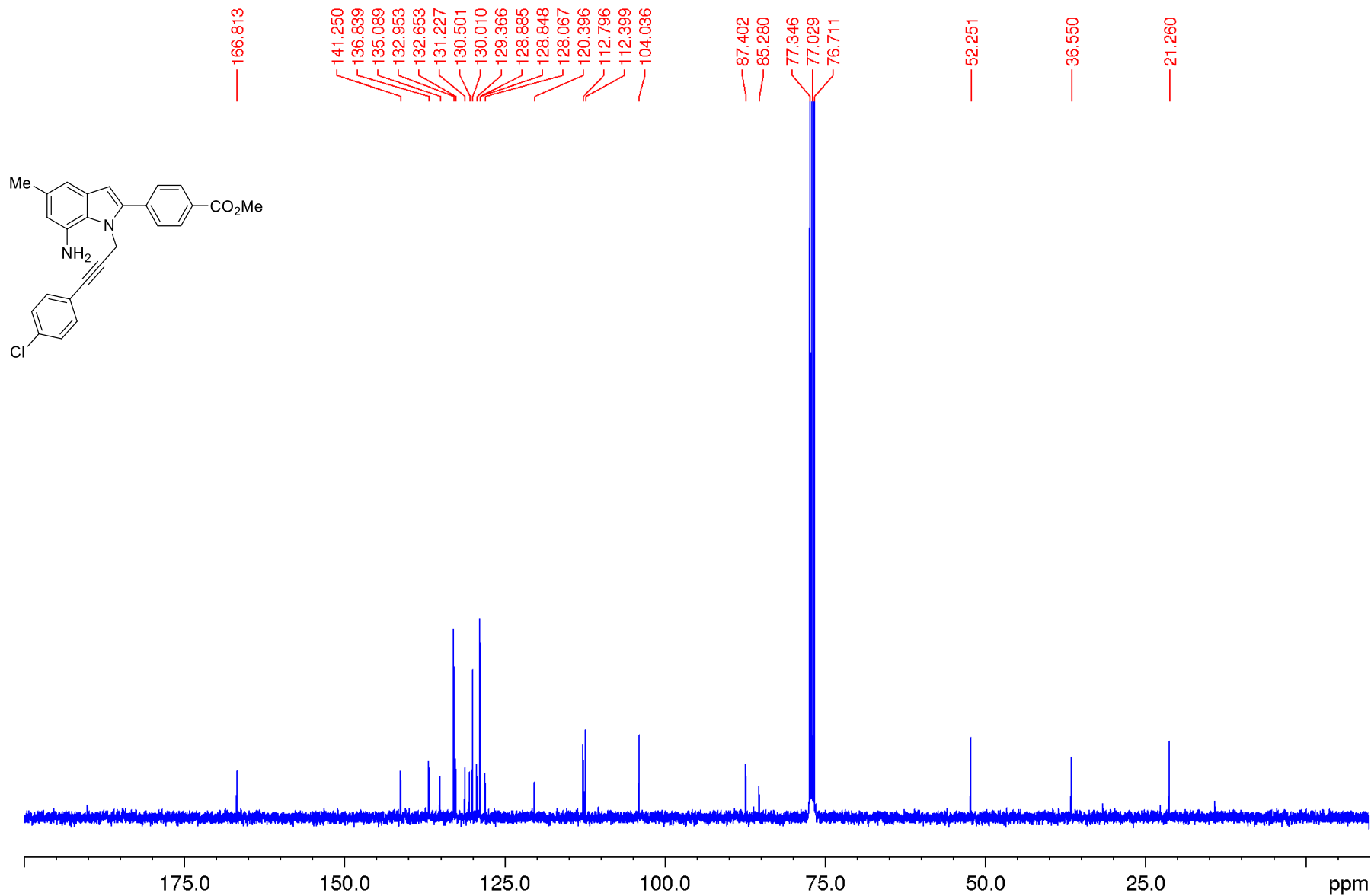
**1-(4-(3-(7-amino-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1g**



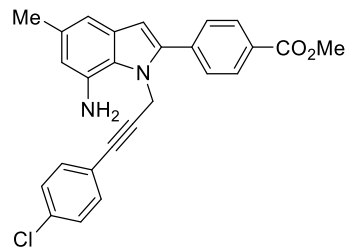
**methyl 4-(7-amino-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-1*H*-indol-2-yl)benzoate 1h**



**methyl 4-(7-amino-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-1*H*-indol-2-yl)benzoate 1h**



**methyl 4-(7-amino-1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-1*H*-indol-2-yl)benzoate 1h**



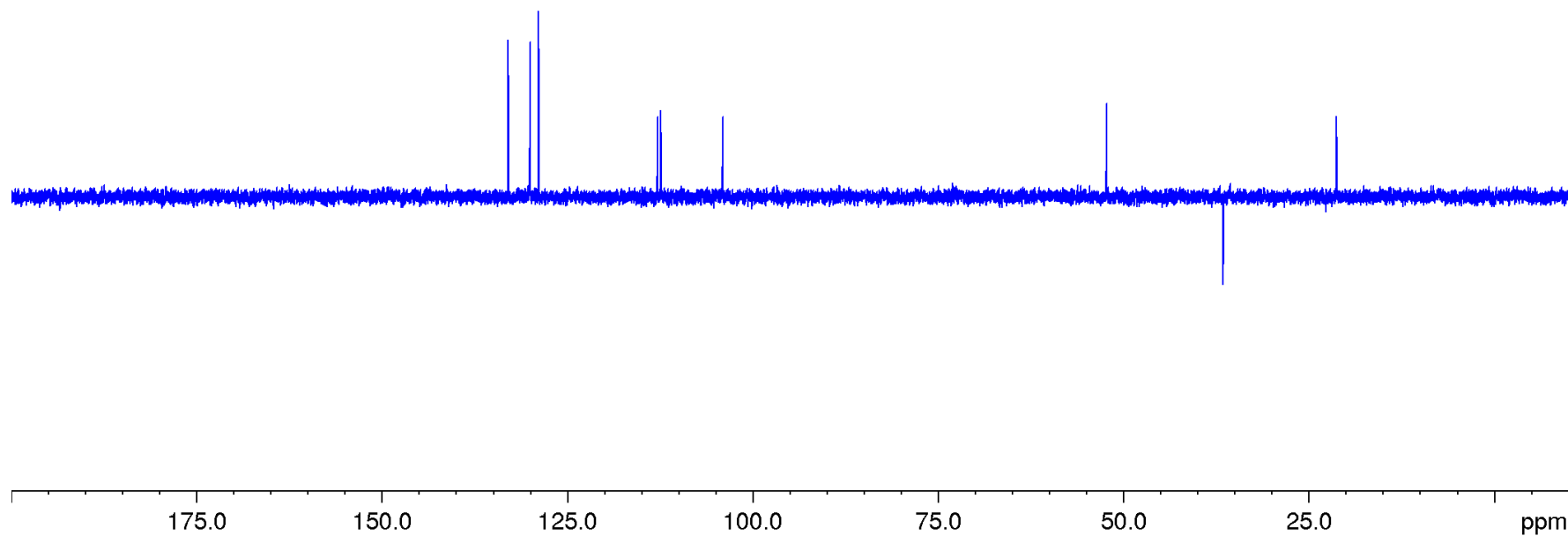
132.953  
130.010  
128.885  
128.848

112.796  
112.399  
104.036

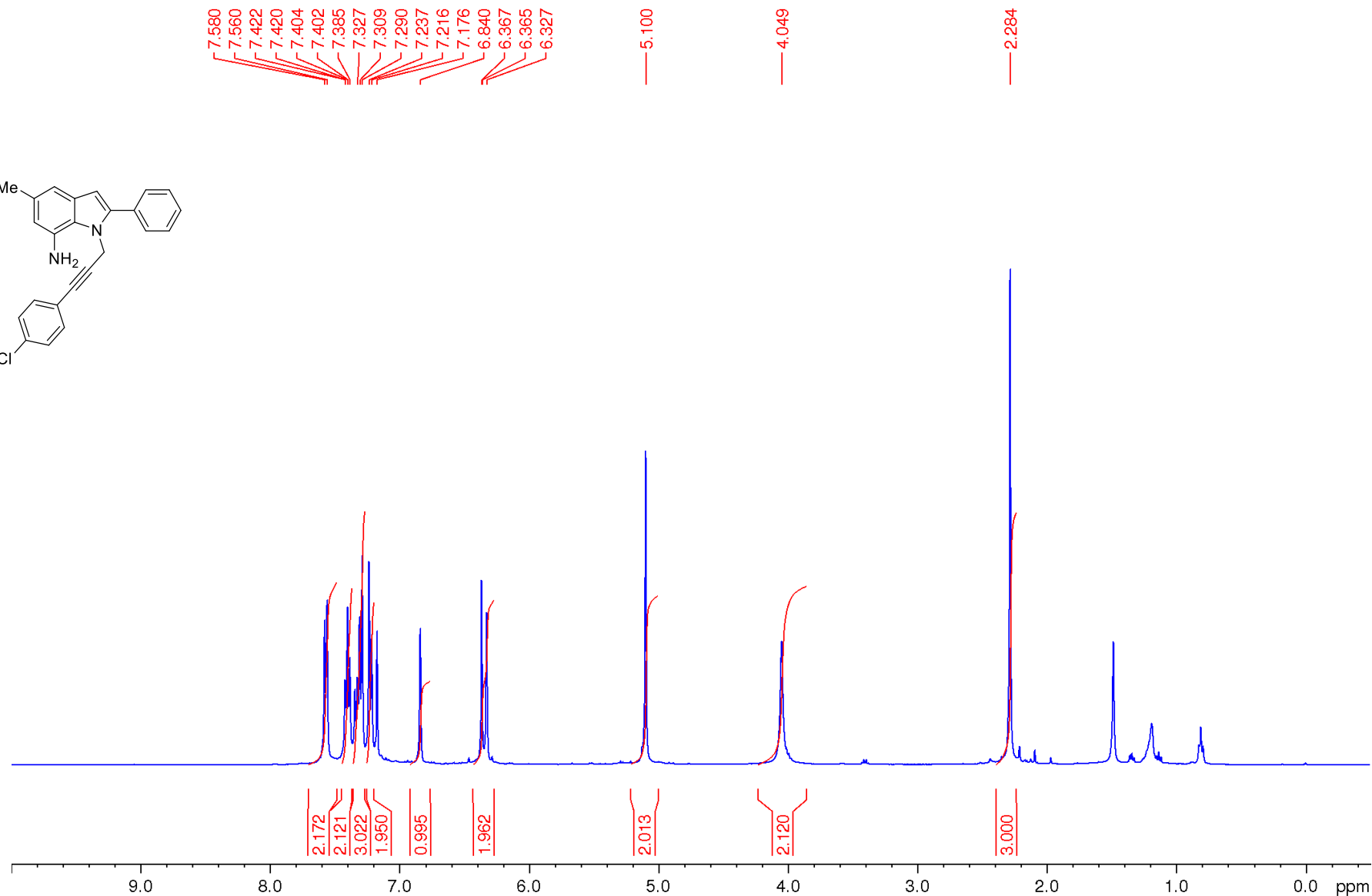
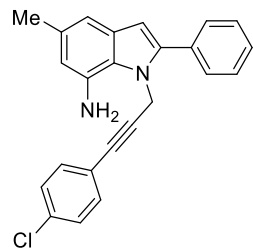
52.251

36.549

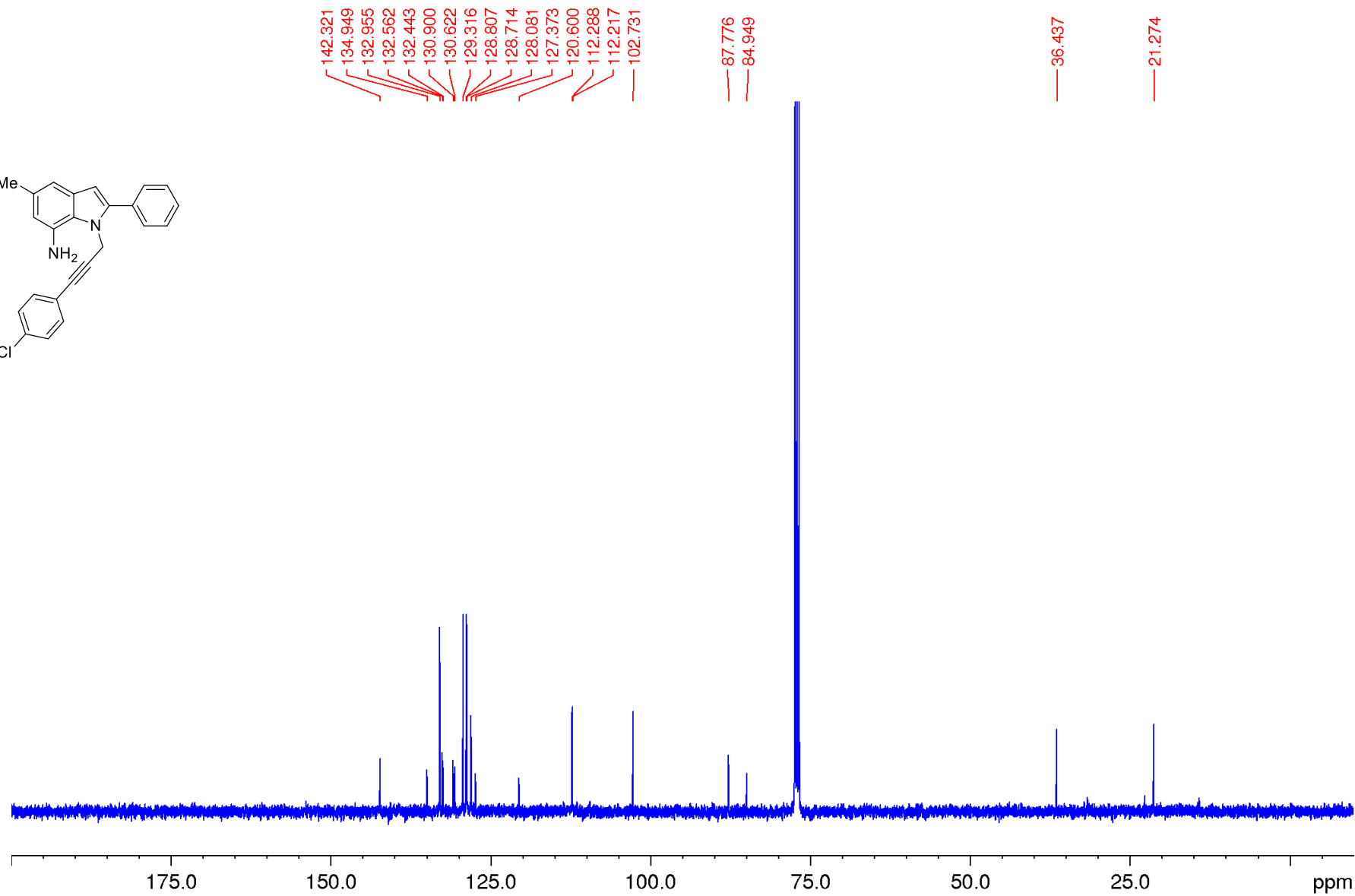
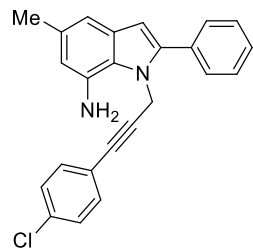
21.259



**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-2-phenyl-1*H*-indol-7-amine 1i**

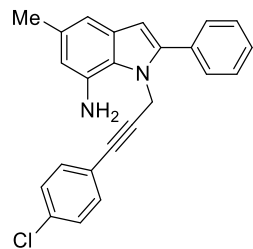


**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-2-phenyl-1*H*-indol-7-amine 1i**

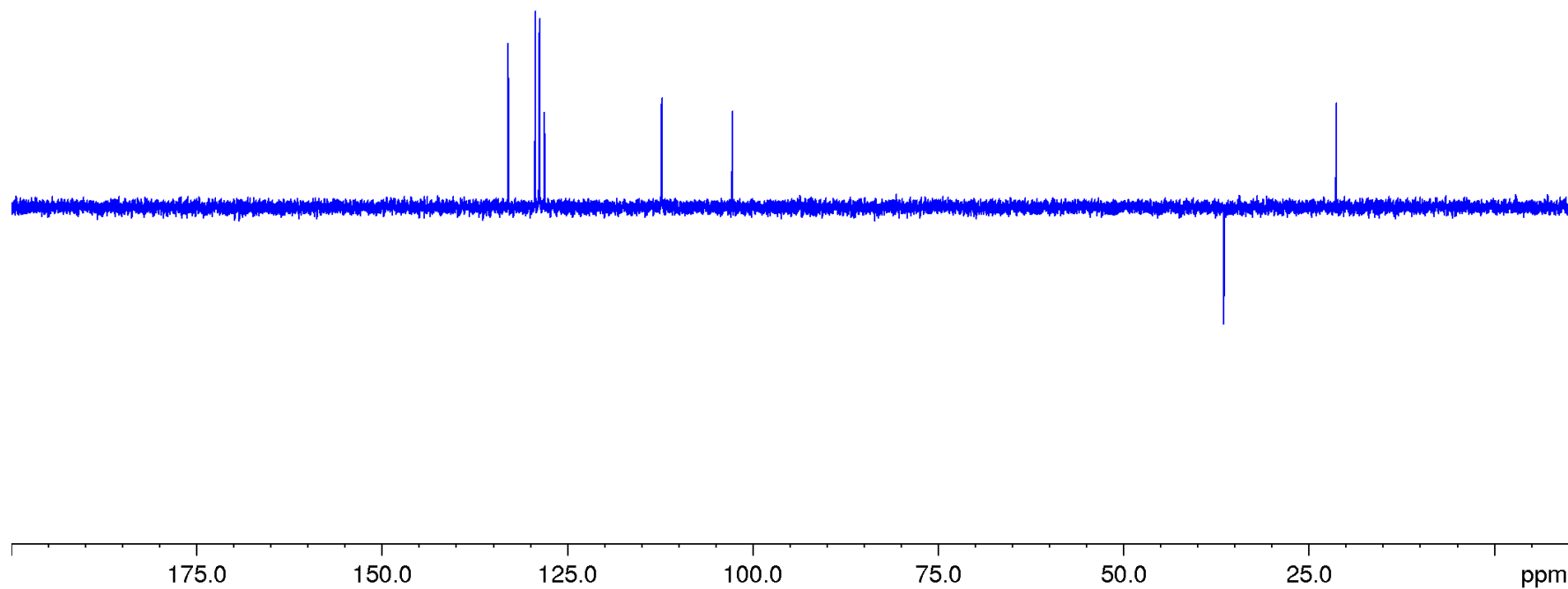




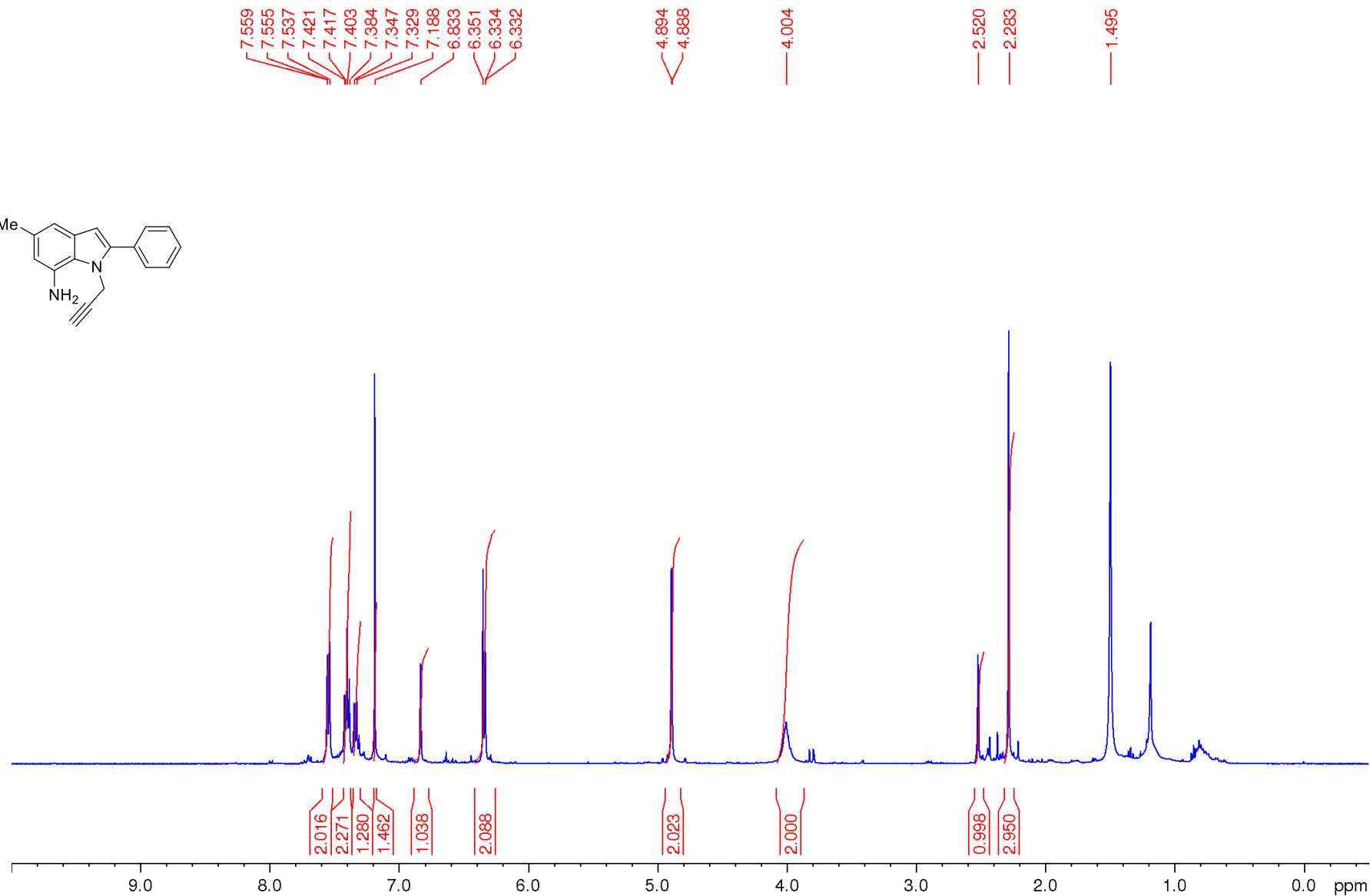
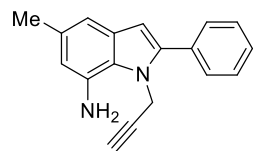
**1-(3-(4-chlorophenyl)prop-2-yn-1-yl)-5-methyl-2-phenyl-1*H*-indol-7-amine 1i**



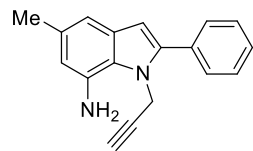
132.955  
129.315  
128.806  
128.714  
128.081  
112.287  
112.216  
102.731  
36.436  
21.273



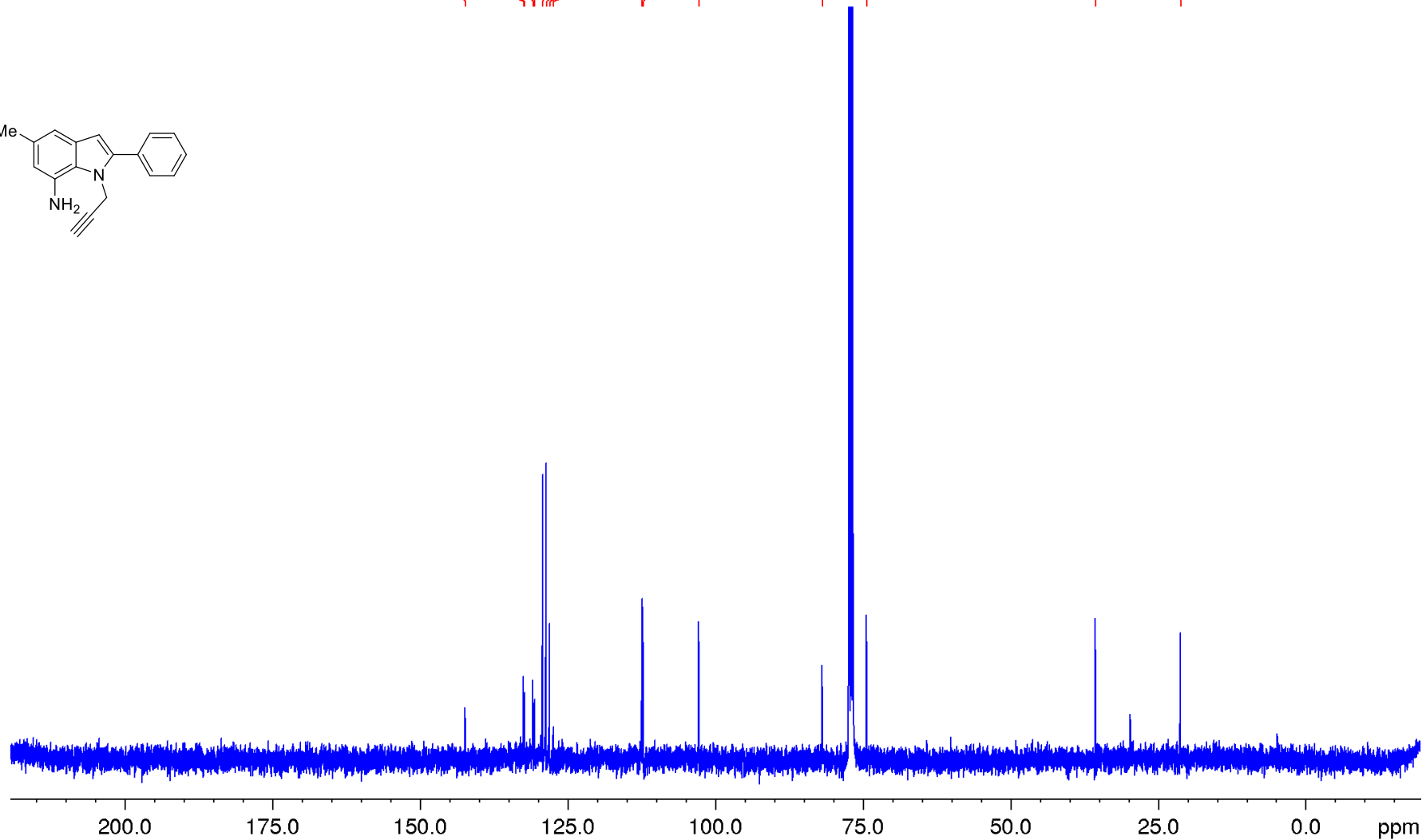
# 5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1H-indol-7-amine 1j



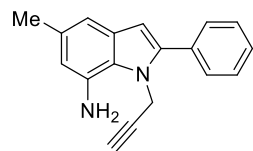
# 5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1H-indol-7-amine 1j



142.369  
132.522  
132.350  
130.899  
130.634  
129.262  
128.679  
128.065  
127.462  
112.429  
112.260  
102.798  
81.907  
74.379  
35.658  
21.243



# 5-methyl-2-phenyl-1-(prop-2-yn-1-yl)-1H-indol-7-amine 1j



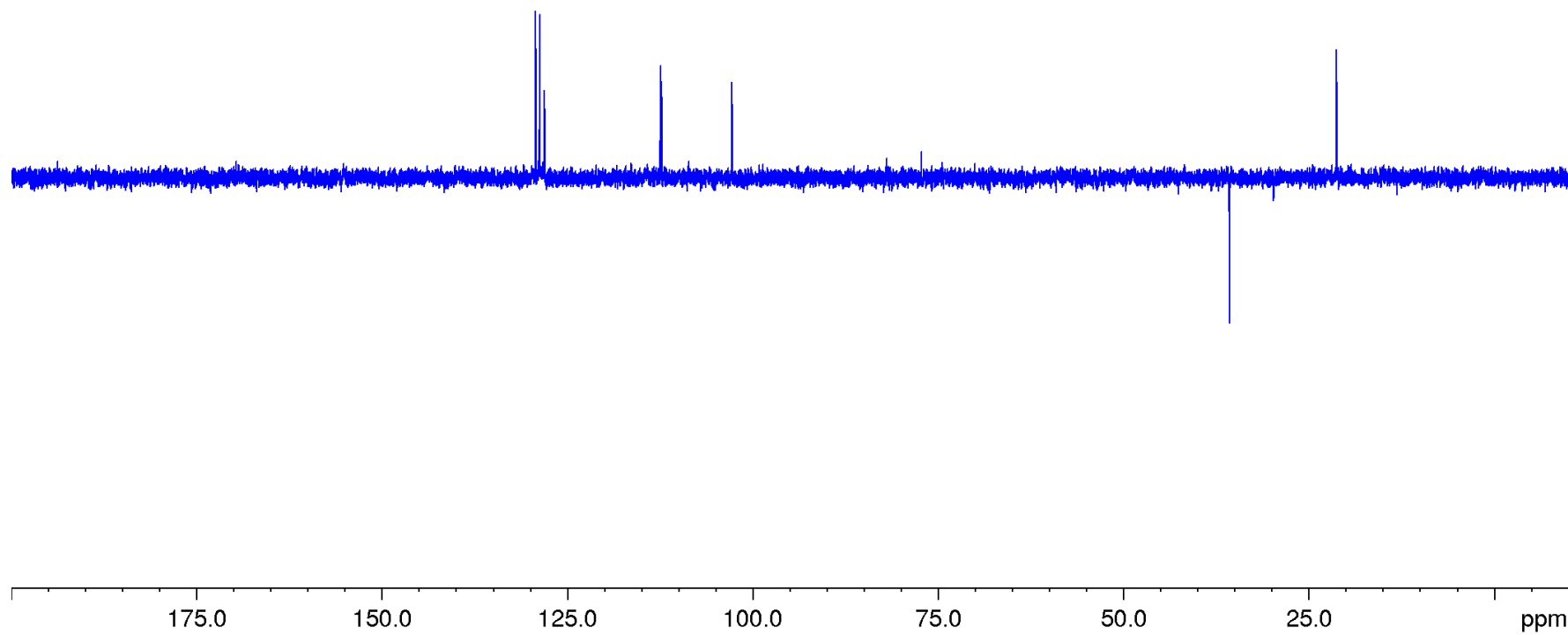
129.259  
128.676  
128.062

112.428  
112.259

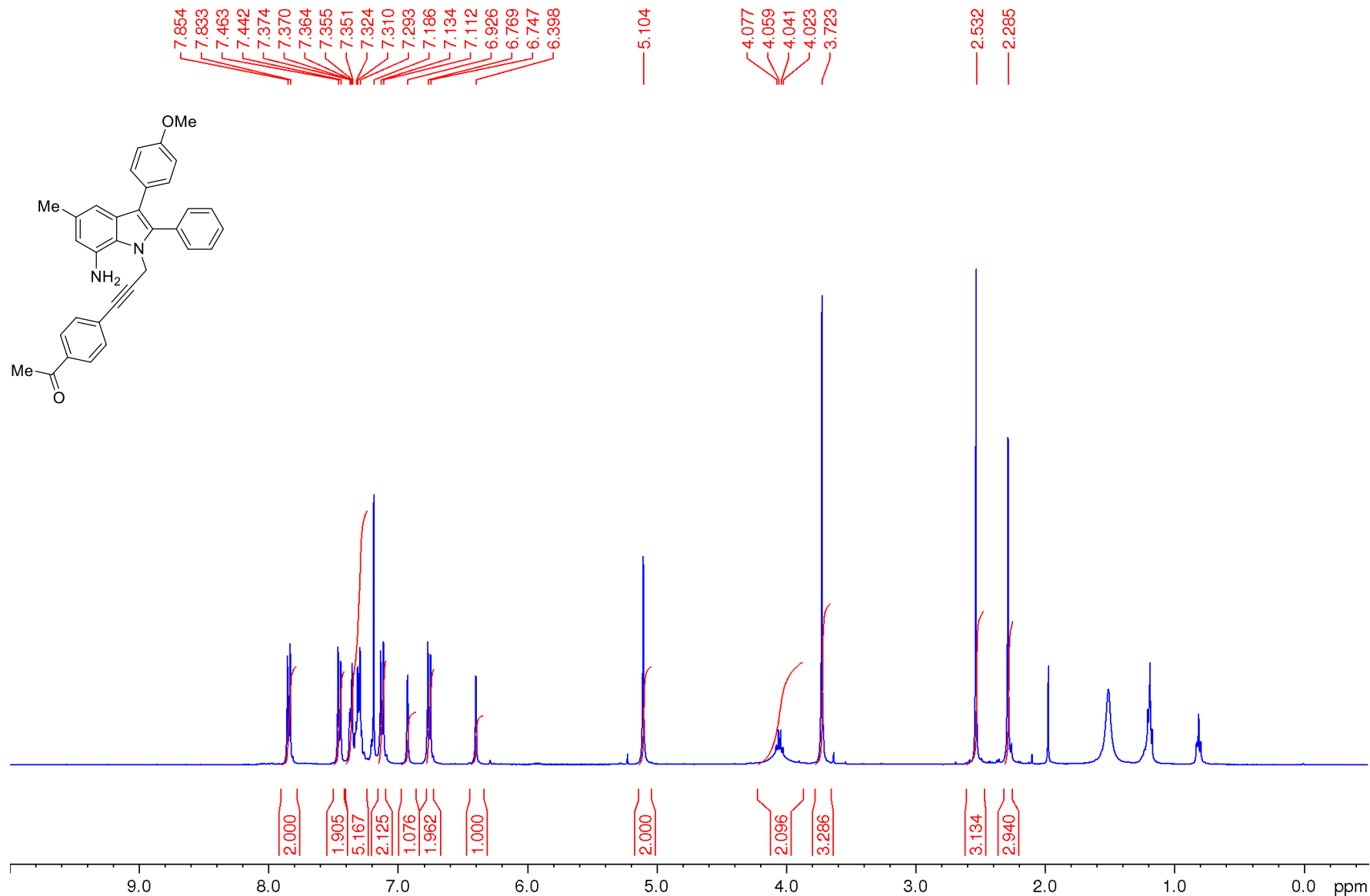
102.798

35.659

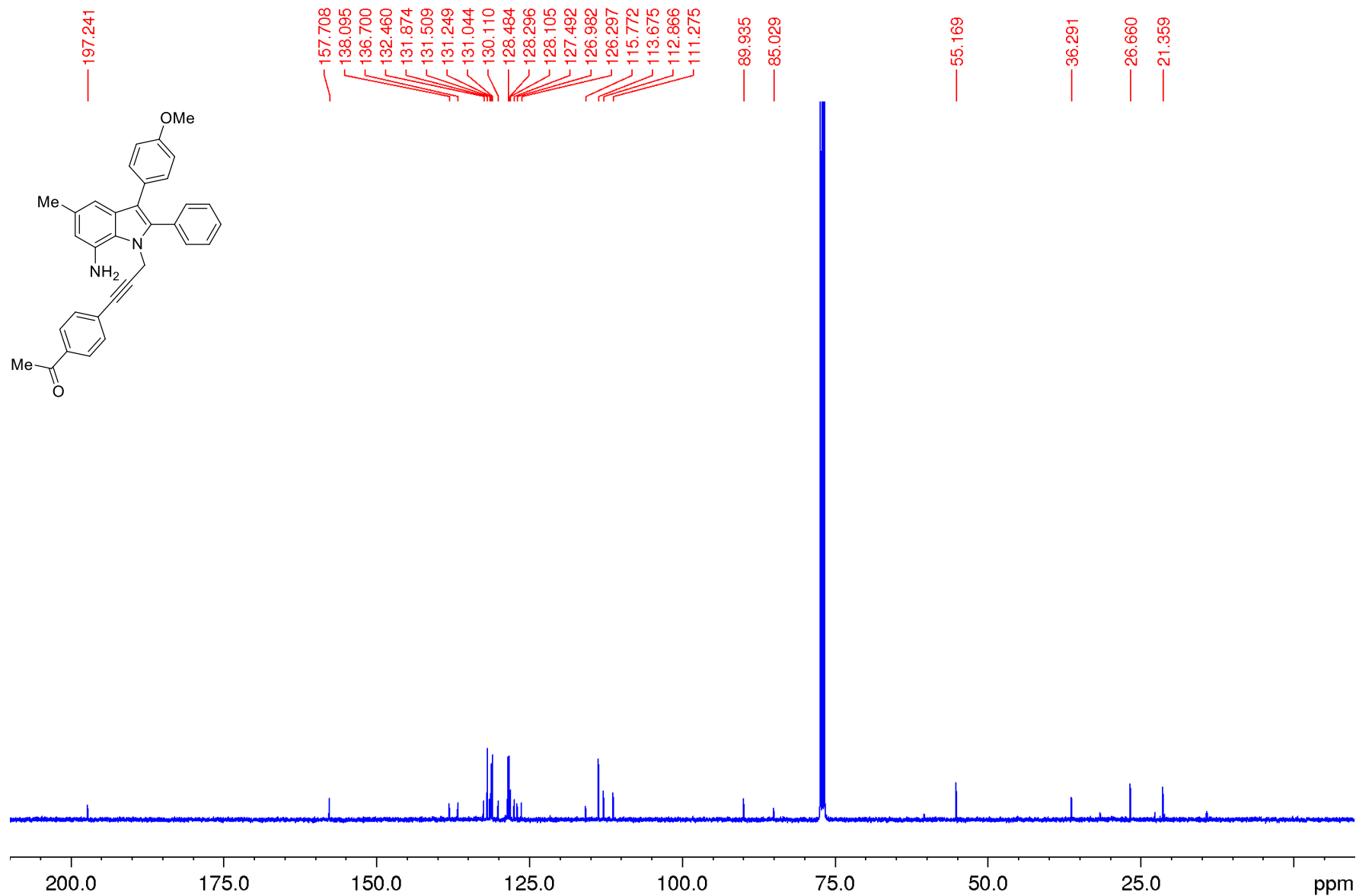
21.246



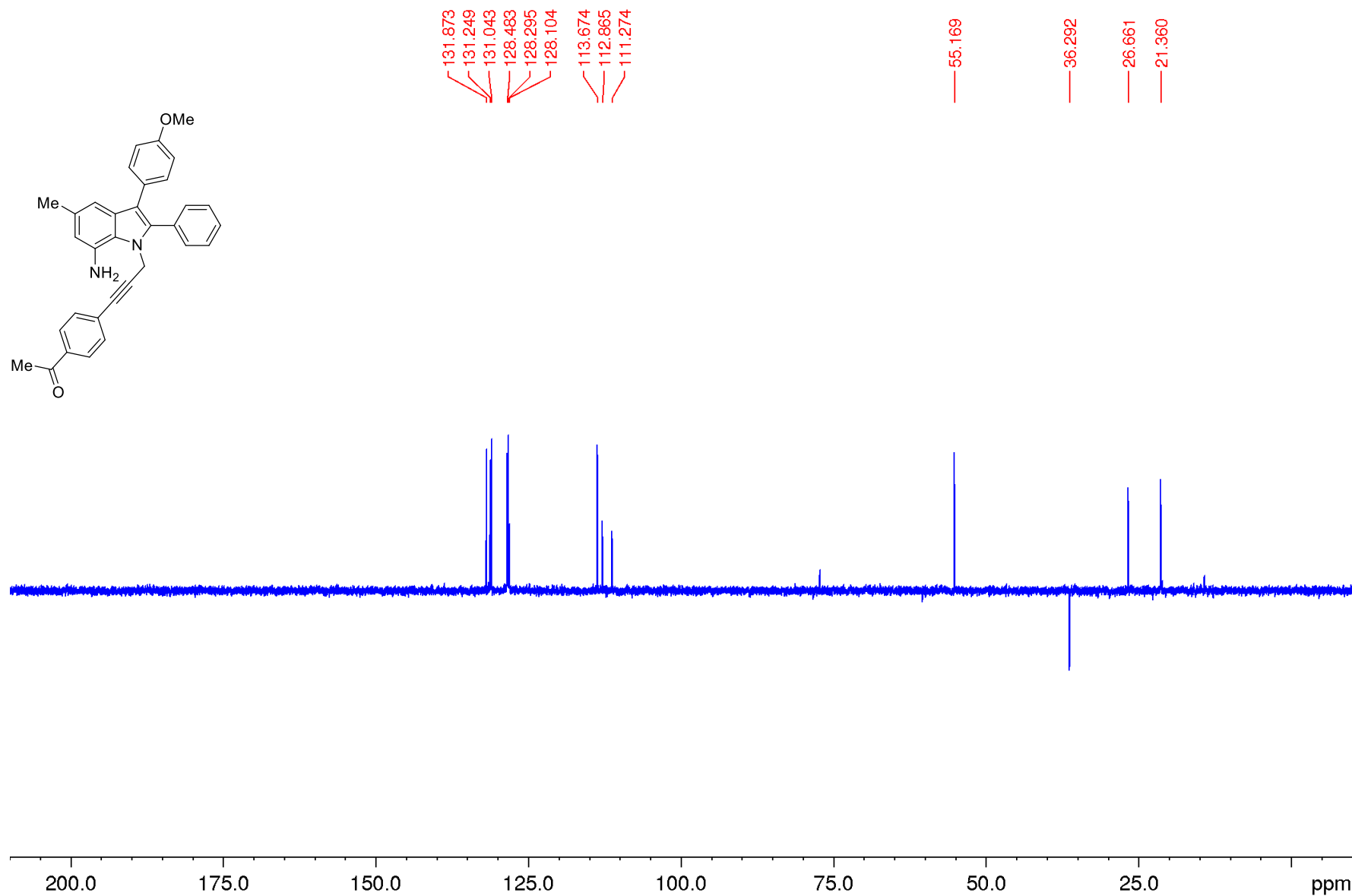
**1-(4-(3-(7-amino-3-(4-methoxyphenyl)-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1k**



**1-(4-(3-(7-amino-3-(4-methoxyphenyl)-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1k**



**1-(4-(3-(7-amino-3-(4-methoxyphenyl)-5-methyl-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 1k**

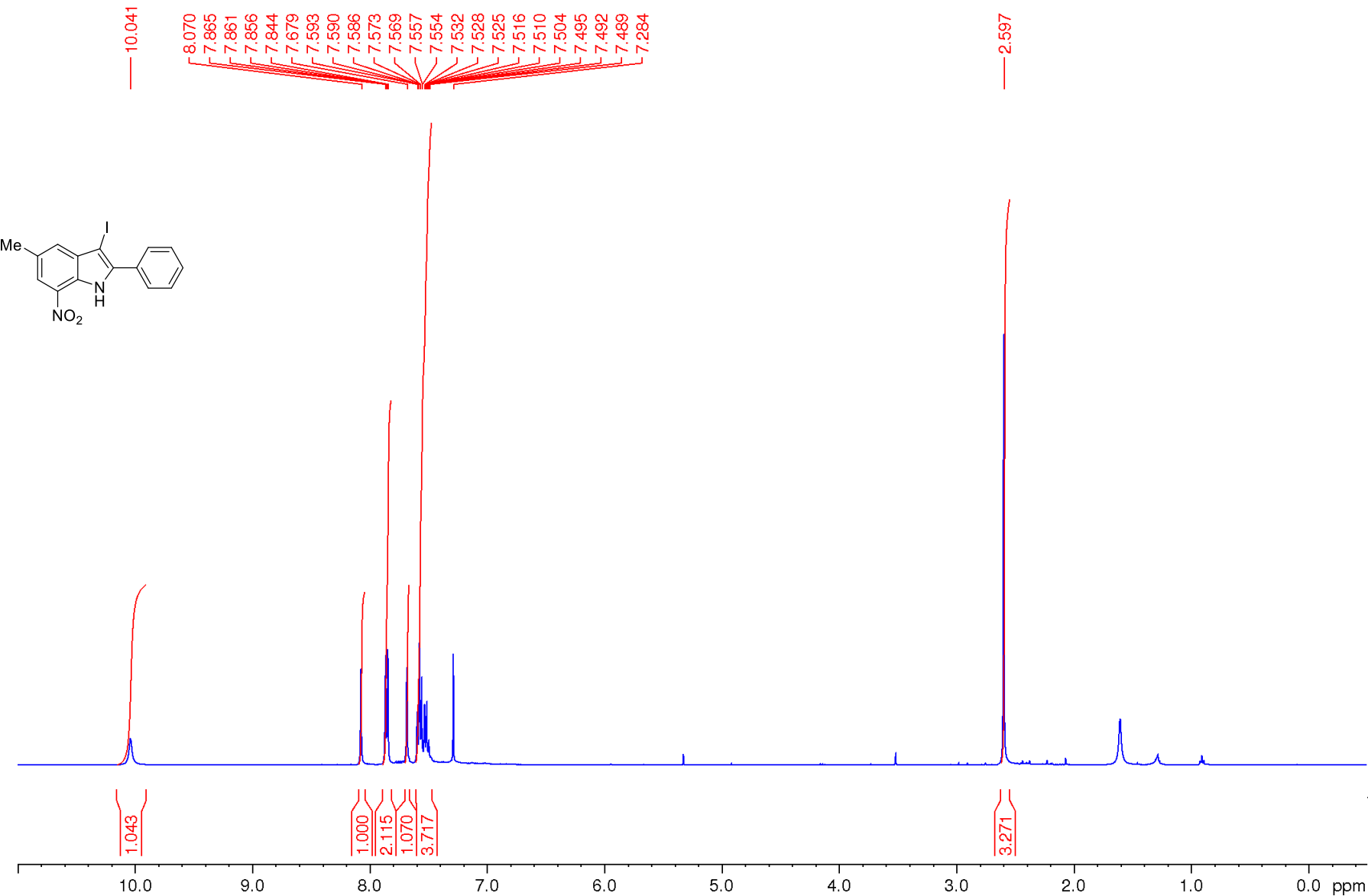




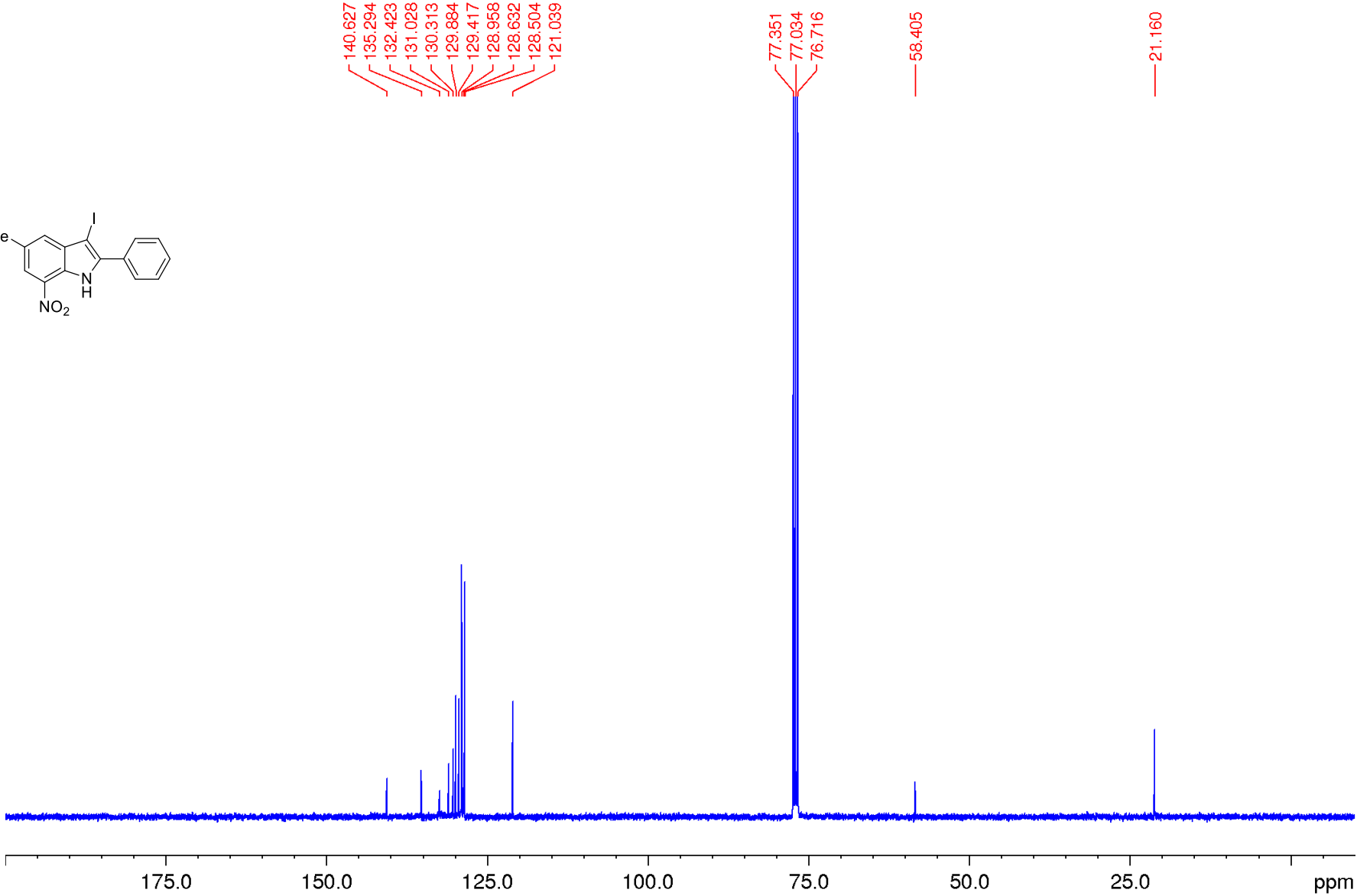
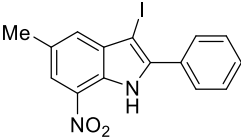




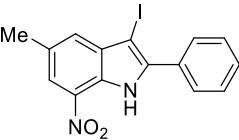
3-iodo-5-methyl-7-nitro-2-phenyl-1H-indole 11



3-iodo-5-methyl-7-nitro-2-phenyl-1*H*-indole 11

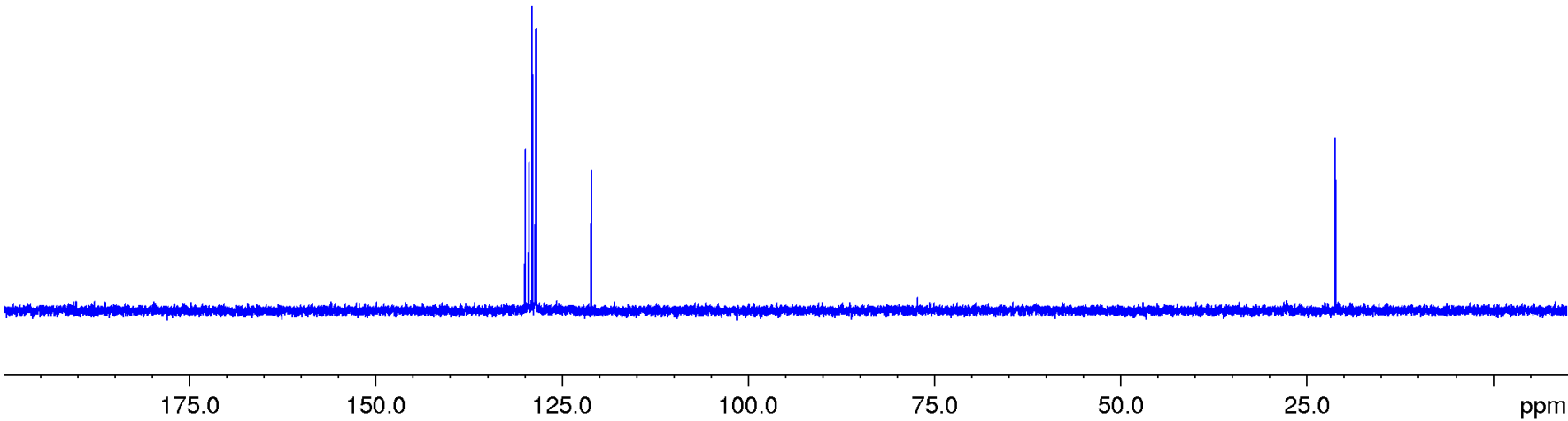


3-iodo-5-methyl-7-nitro-2-phenyl-1*H*-indole

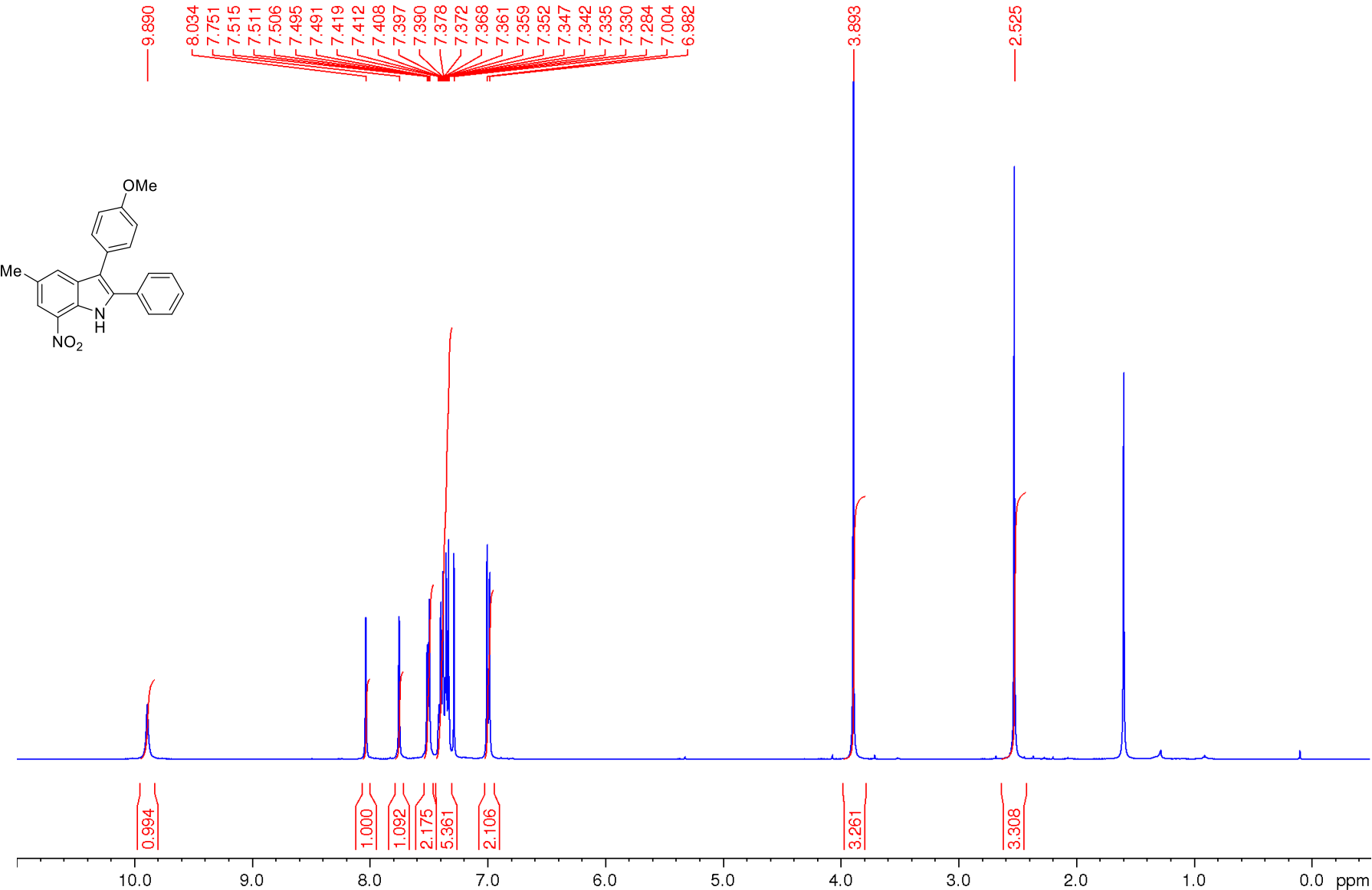


129.884  
129.417  
128.958  
128.504  
121.038

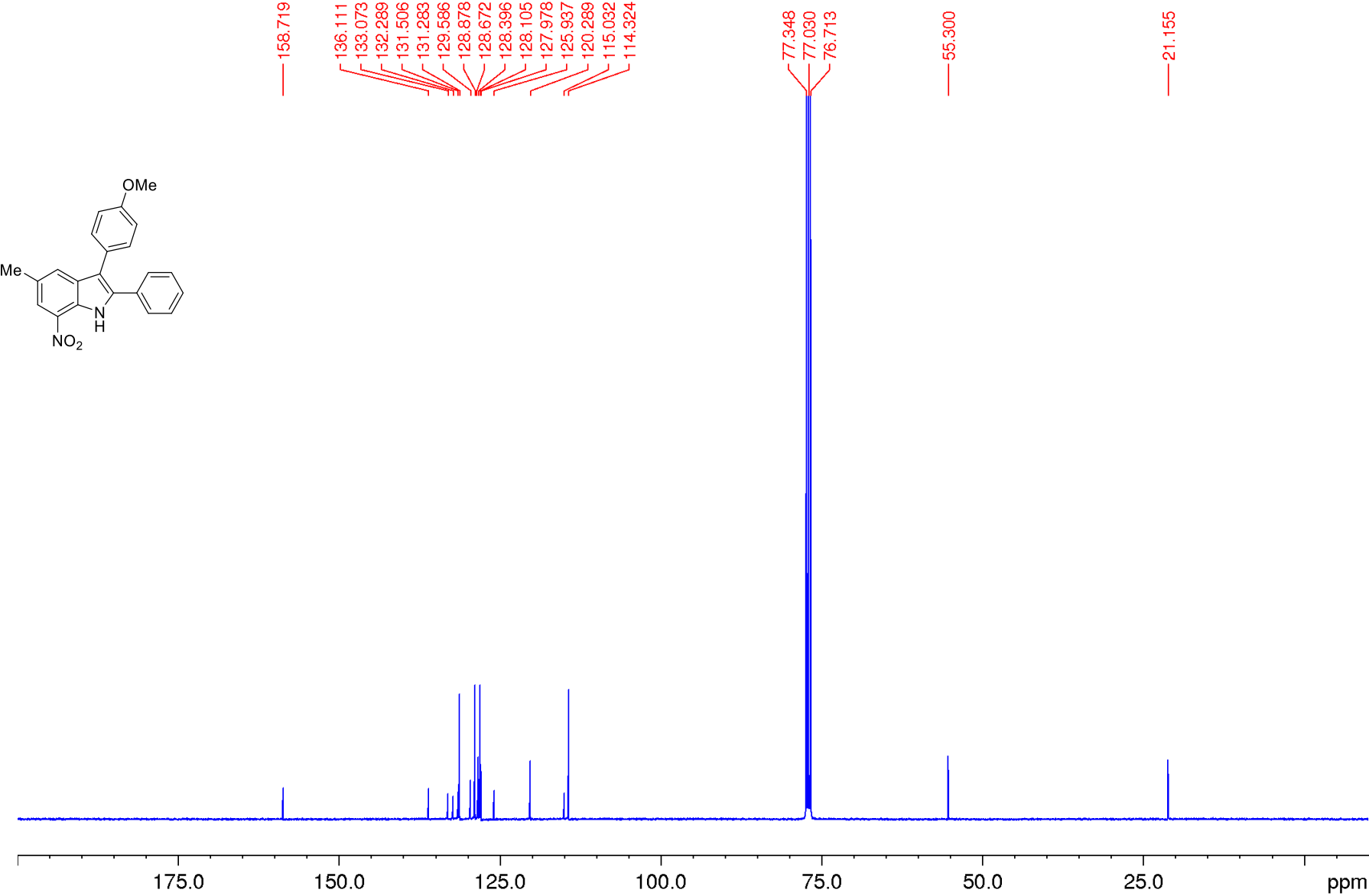
21.161



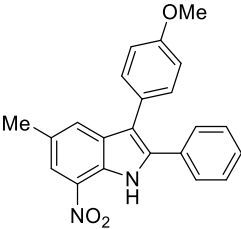
3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1H-indole 12



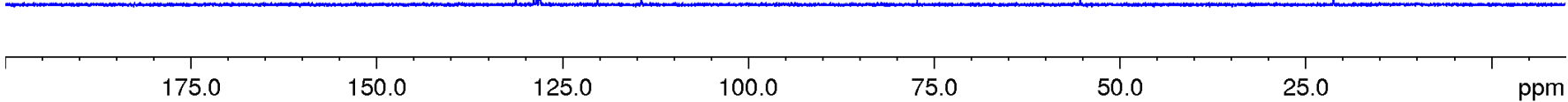
3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1H-indole 12



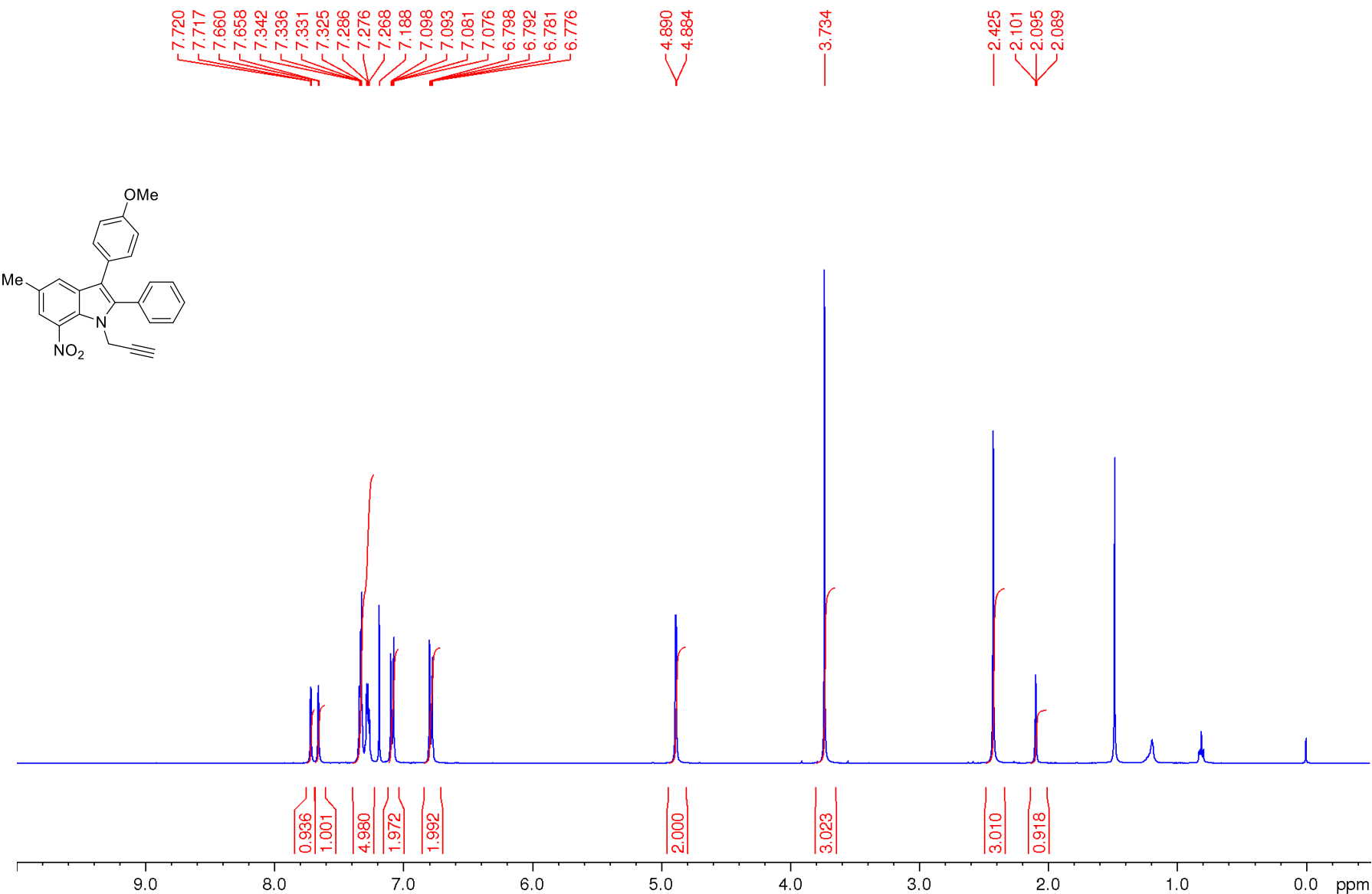
3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1H-indole 12



131.281  
128.877  
128.395  
128.104  
127.975  
120.288  
114.323  
55.299  
21.156

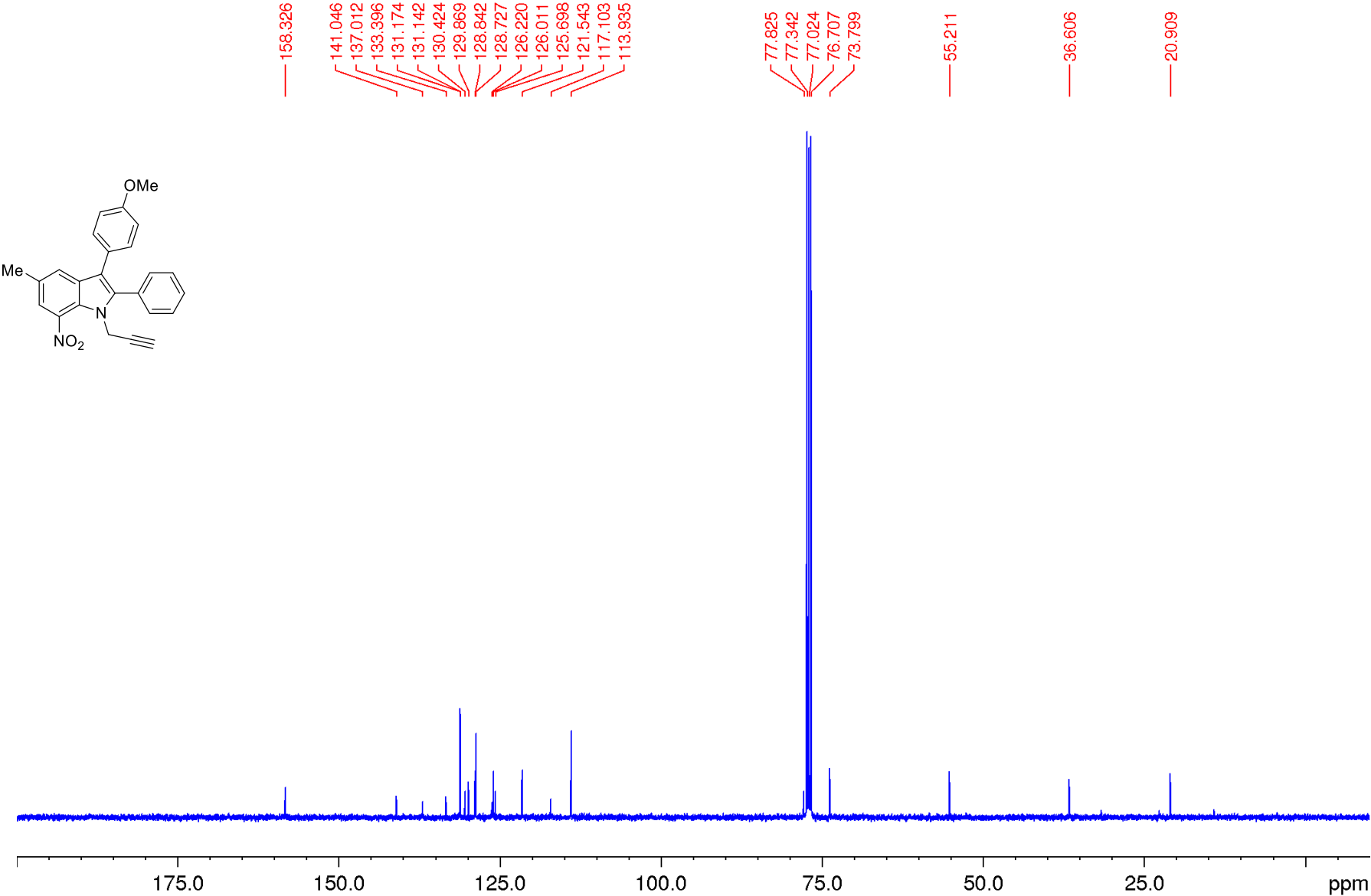


3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1*H*-indole

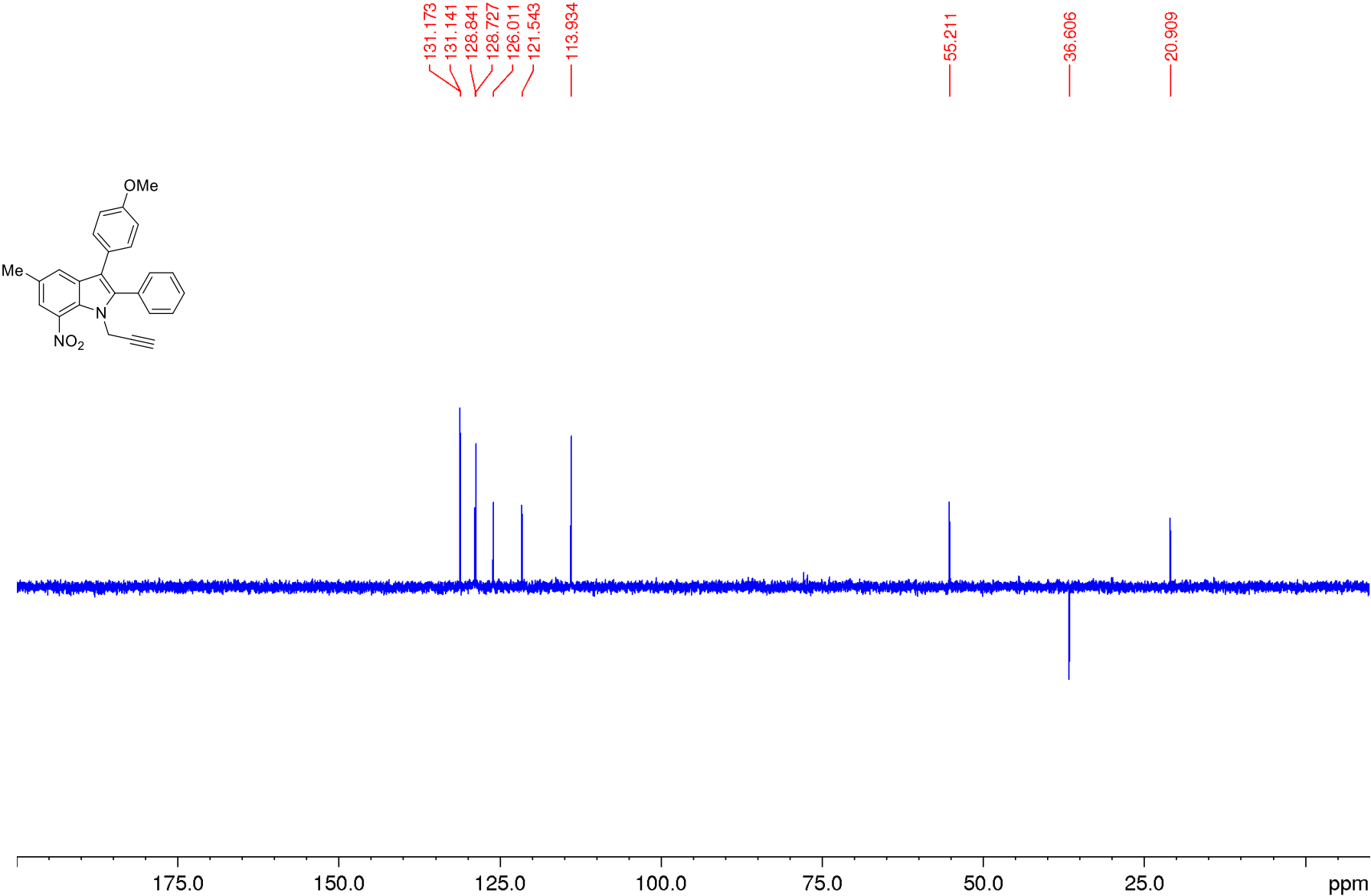




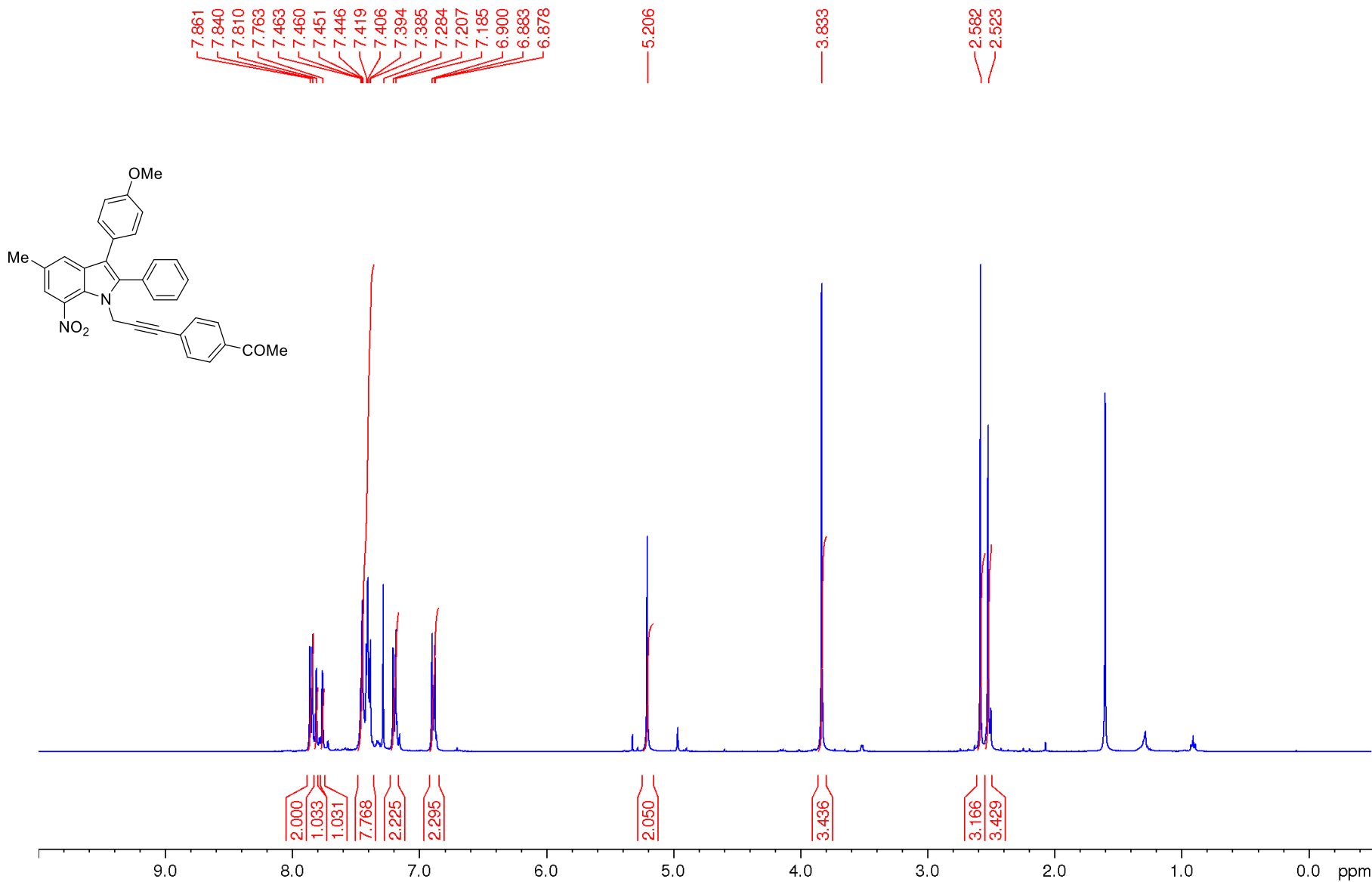
3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1*H*-indole 13



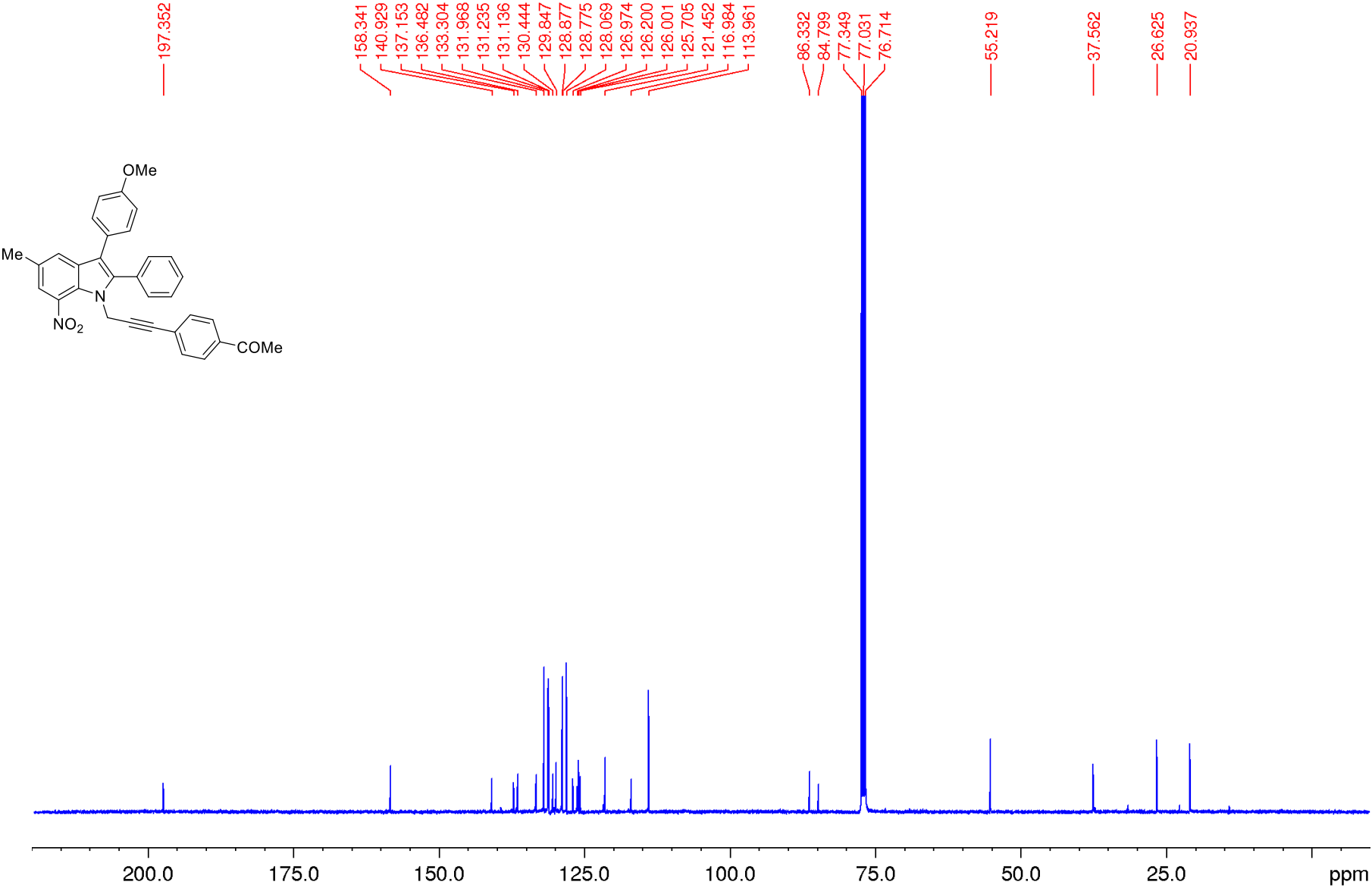
3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1-(prop-2-yn-1-yl)-1*H*-indole 13



1-(4-(3-(3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 14



1-(4-(3-(3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 14



1-(4-(3-(3-(4-methoxyphenyl)-5-methyl-7-nitro-2-phenyl-1*H*-indol-1-yl)prop-1-yn-1-yl)phenyl)ethan-1-one 14

