Asymmetric Synthesis of Trifluoroethyl-based, Chiral 3-Benzoxy-1- and -2-Phenyl-quinazolinones of Biomedicinal Interests by Radical Type Cross Coupling to Olefins

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Supporting Information

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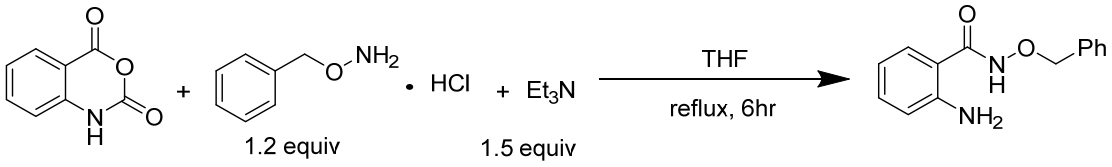
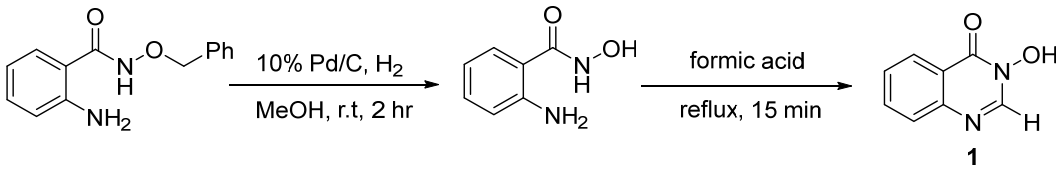
Experimental procedures for the preparation of 3-hydroxy-quinazolin(di)ones as radical tarpping agents

2-Amino-*N*-(benzyloxy)benzamide[1a]



In a 100-mL three-necked flask was placed *N*-carboxyaminobenzenecarboxylic anhydride (1.63 g, 10.0 mmol) and *O*-benzylhydroxylamine hydrochloride (1.93 g, 12.0 mmol, 1.2 equiv) in anhydrous THF (20 mL). Triethylamine (2.1 mL, 15.0 mmol, 1.5 equiv) was then added. The resulting mixture was stirred under reflux for 18 h and the quenched with sat. aqueous NH_4Cl solution (20 mL) at ambient temperature. The reaction mixture was extracted with ethyl acetate (20 mL × 3). The combined organic layer was dried over $MgSO_4$ (1.5 g), filtered, and evaporated. The crude product was purified by column chromatography on silica gel (ethyl acetate/hexanes, 1/3) to obtain 1.99 g (82% yield) of 2-mino-*N*-(benzyloxy)benzamide: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.44 (s, 1H), 7.48-7.30 (m, 6H), 7.16 (td, *J* = 7.8, 1.4 Hz, 1H), 6,73 (dd, *J* = 8.2, 1.0 Hz), 6.49 (td, *J* = 7.8, 1.0 Hz), 6.30 (s, 2H), 4.90 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 167.7, 150.1, 136.6, 132.6, 129.3, 128.8, 128.7, 128.2, 116.8, 115.1, 112.8, 77.4; TLC R_f 0.25 (EtOAc/hexanes, 1/3); HRMS (FD) $[M]^+$ Calcd for $C_{14}H_{14}N_2O_2$: 242.1050, found: 242.1051.

3-Hydroxyquinazolin-4(3H)-one 1[1a,b]

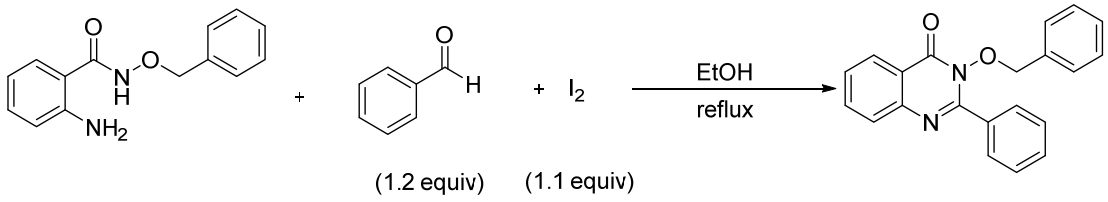


1

To a 100-mL double-necked flask was placed 2-amino-*N*-(benzyloxy)benzamide (1.34 g, 5.5 mmol) in methanol (50 mL). Ten percent Pd/C catalyst (52.3 mg) was then added. The reaction mixture was degassed with argon and then introduced hydrogen gas for 2 min. The reaction flask was kept

under a hydrogen gas balloon at ambient temperature for 2 h with stirring with complete reaction as evidenced by TLC analysis. The reaction mixture was passed through a short plug of Celite and the filtrate was concentrated under reduced pressure to provide 743.2 mg of crude 2-amino-*N*-hydroxybenzamide. The crude product was placed in a 25-mL double-necked flask in formic acid (3 mL). The reaction mixture was stirred under reflux for 15 min. Deionized water (15 mL) was then added and the reaction mixture was kept boiling for another 15 min and gradually cooled to ambient temperature to induce precipitation of the product. The solid was collected by filtration through a sintered glass funnel and rinsed with deionized water (20 mL). The wet crude product was recrystallized from acetone. (30 mL) to give 394.6 mg of **1** in 44% yield: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.91 (s, 1H), 8.54 (s, 1H), 8.18 (d, *J* = 8.0 Hz, 1H), 7.83 (td, *J* = 8.2, 1.2 Hz, 1H), 7.72 (d, *J* = 8.2 Hz, 1H), 7.57 (td, *J* = 8.0, 1.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.3, 146.9, 145.9, 134.0, 127.5, 127.0, 125.9, 122.5; TLC R_f 0.19 (Hexanes/EtOAc, 1/3); HRMS (FI) $[M]^+$ Calcd for $C_8H_6N_2O_2$: 162.0424, found: 162.0425.

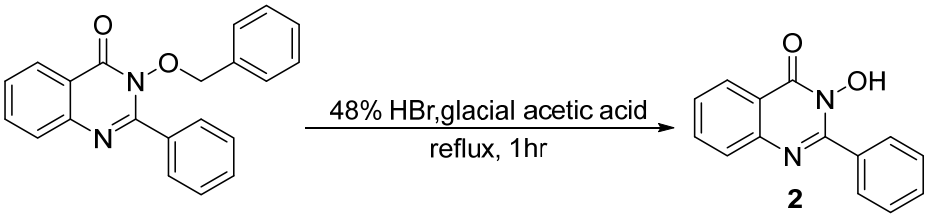
3-(Benzyloxy)-2-phenyl-quinazolin-4(3H)-one[2]



In a 100-mL three-necked flask was placed 2-amino-*N*-benzyloxy-benzamide (2.18 g, 9.0 mmol) and dissolve it in ethanol (30 mL). Iodine (2.51 g, 9.9 mmol, 1.1 equiv) was added and benzaldehyde (1.1 mL, 10.8 mmol, 1.2 equiv) was injected. The reaction mixture was stirred at ambient temperature for 2 h and then quenched by adding sat. aqueous sodium thiosulfate (9 mL). The reaction mixture was extracted with ethyl acetate (25 mL×3). The combined organic layer dried over $MgSO_4$ (1.5 g), filtered, and evaporated. The crude residue was purified by column chromatography on silica gel

(EtOAc/hexanes, 1/8) to give 1.48 g (50% yield) of 3-(benzyloxy)-2-phenylquinazolin-4(3H)-one: ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 (dd, *J* = 7.9, Hz, 1H), 7.90 (t, *J* = 7.6 Hz, 1H), 7.76 (d, *J* = 7.3 Hz, 3H), 7.62 (q, *J* = 6.8 Hz, 2H), 7.53 (t, *J* = 7.7 Hz, 2H), 7.32 (t, *J* = 7.2 Hz, 1H), 7.25 (t, *J* = 7.4 Hz, 2H), 6,94 (d, *J* = 7.4 Hz, 2H), 4.93 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.3, 153.7, 146.1, 134.6, 133.1, 132.3, 130.4, 129.5, 129.3, 129.0, 128.3, 127.9, 127.7, 127.1, 126.2, 122.4, 77.7; TLC R_f 0.17 (EtOAc/hexanes, 1/8); HRMS (FD) $[M]^+$ Calcd for $C_{21}H_{16}N_2O_2$:328.1217, found:328.1226.

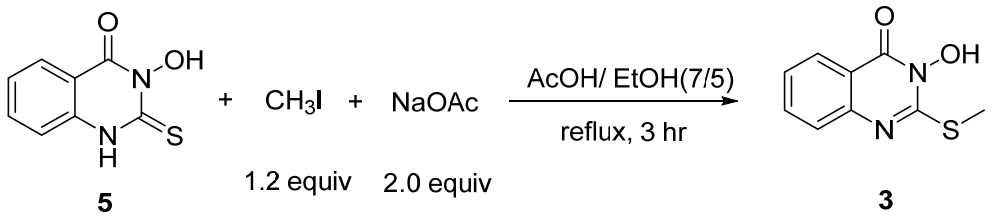
3-Hydroxy-2-phenyl-quinazolin-4(3H)-one 2[3]



2

In a 100-mL double-necked flask was placed 3-(benzyloxy)-2-phenylquinazolin-4(3H)-one (328.4 mg, 1.0 mmol) in glacial acetic acid (2 mL). The reaction was heated to reflux with stirring for 3 min to reach a homogeneous state and 48% hydrobromic acid (2 mL) was added. After having been stirred for1 h, the reaction mixture was cooled to ambient temperature. Deionized water (20 mL) was added to quench the reaction and to induce precipitation of the product. The solid was collected by passing thru a sintered glass and the rinsed with deionized water (30 mL). The resulting wet crude product was recrystallized from acetone (10 mL) to obtain 162.0 mg (68%) of 2 as a white solid: ^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (s, 1H) 8.20 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.87-7.81 (m, 3H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.60-7.47 (m, 4H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.3, 153.3, 146.2, 134.2, 132.8, 130.3, 129.4, 127.9, 127.5, 126.8, 125.9, 121.4; TLC R_f 0.77 (EtOAc/hexanes, 1/1); HRMS (FD) $[M]^+$ Calcd for $C_{14}H_{10}N_2O_2$:238.0748, found:238.0741.

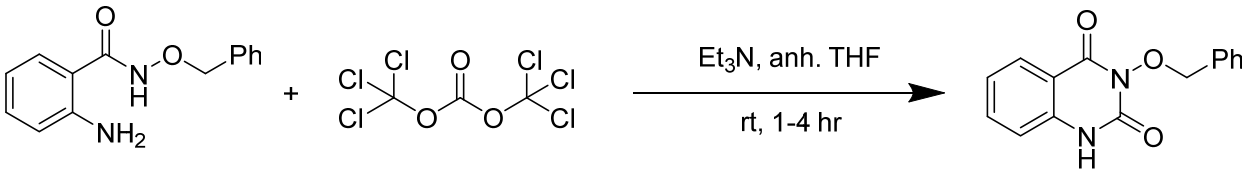
3-Hydroxy-2-(methylthio)quinazolin-4(3H)-one 3[4]



5 **3**

To a 50-mL double-necked flask was placed **5** (972.3 mg, 5.0 mmol) and anhydrous sodium acetate (828.2 mg, 10.0 mmol, 2.0 equiv) in glacial acetic acid/ethanol (7/5) mixed solvent (12 mL). The reaction mixture was heated to reflux till completely homogeneous and then returned to ambient temperature. Iodomethane (382.2 μL, 6.0 mmol, 1.2 equiv) was added and the resulting reaction mixture was stirred under reflux for 3 h. The reaction mixture was gradually cooled to ambient temperature and concentrated to remove EtOH by rotatory evaporation. Deionized water (30 mL) was added to induce product precipitation. The crude product was washed with deionized water (30 mL) and the wet solid was recrystallized from acetone (40 mL) to give 994.2 mg (96% yield) of **3** as a white solid: ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.11 (s, 1H), 8.08 (d, J = 7.6 Hz, 1H), 7.78 (t, J = 7.6 Hz, 1H), 7.59 (d, J = 8.2 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 157.8, 157.3, 146.3, 134.2, 126.1, 126.1, 125.5, 119.9, 13.2; TLC R_f 0.38 (MeOH/EtOAc, 1/10); HRMS (FD) $[M]^+$ Calcd for $C_9H_8N_2O_2S$: 208.0301, found: 208.0303.

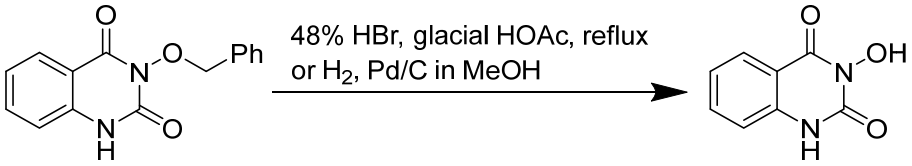
3-(Benzyloxy)quinazoline-2,4(1H,3H)-dione[2]



In a 50-mL, two-necked, round-bottomed flask was placed 2-amino-*N*-benzyloxy-benzamide (726.8 mg, 3.0 mmol) and triphosgene (356.1mg, 1.2 mmol, 0.4 equiv) in anhydrous tetrahydrofuran (30 mL). Triethylamine (1.04 mL, 7.5 mol, 2.5 equiv) was added dropwise. The resulting reaction mixture was stirred at ambient temperature for 1h and then quenched with H_2O (80 mL). The resulting

white solid was collected and then washed consecutively with H_2O (2 × 250 mL) and acetone (50 mL). The wet solid was dried under vacuum to give 579.5 mg (72% yield) of ***N*-Bn-QuizOn** as a white solid: ^{1}H NMR (400 MHz, d_6-DMSO) δ 11.66 (s, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.8 Hz, 1H), 7.57 (d, *J* = 6.6 Hz, 2H), 7.41 (d, *J* = 6.6 Hz, 3H), 7.26-7.20 (m, 2H), 5.10 (s, 2H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 159.0, 148.0, 138.7, 135.0, 134.5, 129.4, 128.8, 128.3, 127.2, 122.6, 115.4, 114.4, 77.5; R_f 0.26 (EtOAc/hexanes, 1/2); HRMS (FD) Calcd for $C_{15}H_{12}N_2O_3$: 268.0842, found: 268.0846.

3-Hydroxyquinazoline-2,4(1H,3H)-dione 4[1a,3]

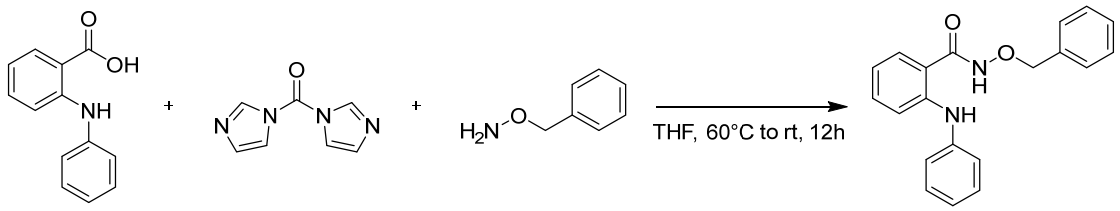


In a 25-mL, two-necked, round-bottomed flask was placed *N*-Bn-QuizOn (804.8 mg, 3.0 mmol) and hydrobromic acid (48%, 6 mL) in glacial acetic acid (6 mL). the resulting reaction mixture was heated to reflux for 4-5 h. The resulting solution was gradually cooled to ambient temperature and then quenched with water (50 mL). The resulting precipitate was collected by filtration and the solid was washed with water (10 mL). The wet solid was dried in vacuo and then recrystallized from MeOH (? mL) to give 272 mg (51% yield) of *N*-OH-**QuizOn** as a white solid:

In a 250-mL, round-bottomed flask was placed *N*-Bn-**QuizOn** (804.8 mg, 3.0 mmol) and Pd/C (10 wt% loading, 15.9 mg, 5 mol%) in MeOH (90 mL). The reaction flask was then topped with a H_2 gas balloon. After three cycles of rotavap. evacuation/H_2-gas saturation, the reaction mixture was kept stiiring under H2 at ambient temperature for1h. The reaction mixture was then passed through a shot plug of Celite (2.8 g) and the Celite pad was washed with MeOH (? mL). The combined filtrates were concentrated by rotary evaporation to give 375 mg (70% yield) of *N*-OH-**QuizOn** as a white solid: ^{1}H NMR (400 MHz, d_6-DMSO) δ 11.55 (s, 1H), 10.58 (s, 1H), 7.94 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.65 (td, *J*

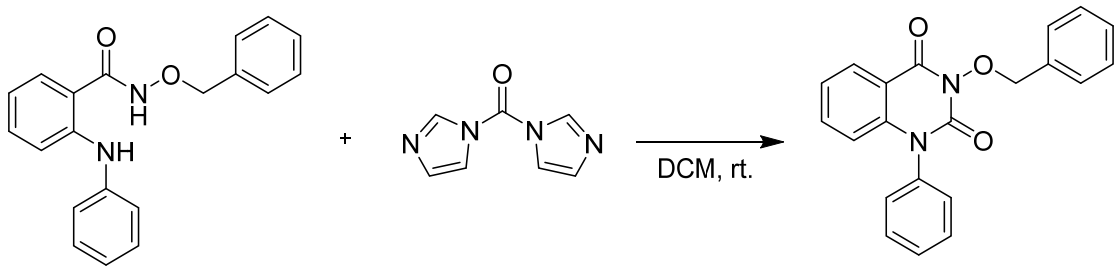
= 7.8, 1.4 Hz, 1H), 7.24-7.18 (m, 2H); ^{13}C NMR (100 MHz, d_6-DMSO) δ 159.4, 148.7, 138.3, 134.7, 127.1, 122.5, 115.3, 114.1; R_f 0.33 (CH_3OH/CH_2Cl_2, 1/6).

_N_-(Benzyloxy)-2-(phenylamino)benzamide[4a]



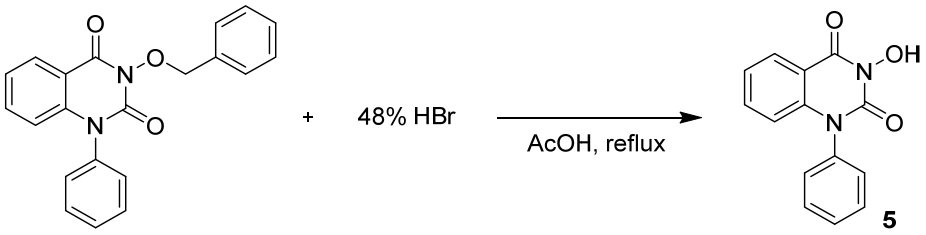
In a 100-mL double-necked bottle was placed Fenamic acid (2.1 g, 10 mmol) in anhydrous THF (15 mL) followed by addition of 1,1'-carbonyldiimidazole (1.8 g, 11 mL, 1.1 equiv). The reaction mixture was stirred at 60 °C for 20 min after which *O*-benzylhydroxylamine (1.5 g, 12 mmol, 1.2 equiv) was added through syringe. The reaction mixture was stirred at ambient temperature for 12 h and then concentrated. The resulting residue was treated with 1*N* aqueous hydrochloric acid (15 mL) and then extracted with ether (20 mL × 3). The combined organic layer was washed with sat. aqueous $NaHCO_3$ (15 mL×3), dried (MgSO4), filtered, evaporated. The crude product was recrystallized from ether/*n*-hexane mixture to obtain 1.7 g (53% yield) of *N*-(Benzyloxy)-2-(phenylamino)benzamide: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.96 (s, 1H), 8.82 (s, 1H), 7.46-7.25 (m, 10H), 7.19 (s, 1H), 7.17 (s, 1H), 7.04 (t, J = 7.3 Hz, 1H), 6.70 (t, J = 7.5 Hz, 1H), 5.01 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 168.3, 145.6, 141.2, 135.2, 132.7, 129.3, 128.7, 128.6, 127.5, 122.7, 120.9, 117.9, 115.5, 115.4, 78.4; TLC R_f 0.30 (EtOAc/hexanes, 1/2); HRMS (ESI) $[M+Na]^+$ Calcd for $C_{20}H_{18}N_2Na_1O_2$: 341.1266, found: 341.1267.

3-(Benzyloxy)-1-phenylquinazoline-2,4(1H,3H)-dione[4b]



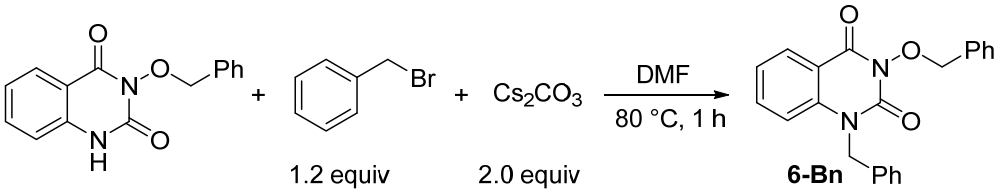
In a 250-m flask wwas placed *N*-(benzyloxy)-2-(phenylamino)benzamide (2.2 g, 7.0 mmol) and 1,1′- carbonyldiimidazole (2.5 g, 14.0 mmol, 2.0 equiv) in CH_2Cl_2 (70 mL). The reaction mixture was stirred at ambient temperature for 12 h. The mixture was concentrated to 30% of its original volume and then washed with aqueous 1*N* HCl solution (15 mL× 3). The remaining organic layer was concentrated by rotatory evaporation to give 1.89 g (yield 55% yield) of 3-(benzyloxy)-1-phenylquinazoline-2,4(1H,3H)-dione: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.67-7.40 (m, 11H), 7.33 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 8.4 Hz, 1H), 5.16 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.5, 148.2, 140.9, 136.2, 135.0, 134.4, 130.2, 129.5, 129.3, 128.9, 128.4, 127.6, 123.1, 115.4, 115.1, 77.5; TLC R_f 0.11 (EtOAc/hexanes, 1/2); HRMS (ESI) $[M+Na]^+$ Calcd for $C_{21}H_{16}N_2Na_1O_3$: 367.1059, found: 367.1059.

3-Hydroxy-1-phenylquinazoline-2,4(1H,3H)-dione 5[3]



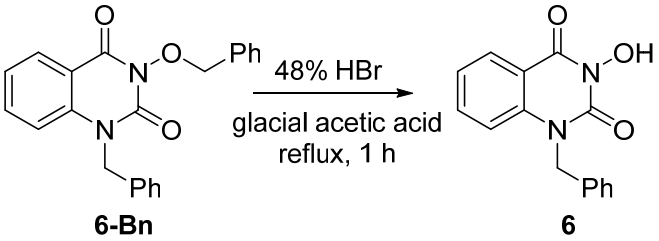
In a 100-mL double-necked flask was placed 3-(benzyloxy)-1-phenylquinazoline-2,4(1H,3H)-dione (1.7 g, 5.0 mmol) in glacial acetic acid (10 mL). The mixture was heated till dissolution of the substrate and 48% hydrobromic acid (5.0 mL) was then added. After having been stirred under reflux for 2.5 h, the reaction mixture was quenched with deionized water (50 mL) to induce precipitation of the product out. The collected solid was sequentially washed with deionized water (30 mL×3) and n-hexane (30 mL×3), and then dried under vacuum to obtain 720 mg (57% yield) of **5** as a white solid: ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.85 (s, 1H), δ 8.10 (dd, *J* = 6.6, 1.3 Hz, 1H), δ 7.65-7.56 (m, 2H), δ 7.48-7.46 (m, 2H), δ 7.29 (t, *J* = 7.5Hz, 1H), δ 6.44 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 158.8, 149.0, 140.5, 136.4, 134.7, 130.2, 129.3, 127.5, 123.0, 115.3, 114.8; TLC R_f 0.61 (EtOAc/hexanes, 1/1); HRMS (ESI) $[M+Na]^+$ Calcd for $C_{14}H_{10}N_2Na_1O_3$: 277.0589, found: 277.0587.

1-Benzyl-3-(benzyloxy)quinazoline-2,4(1H,3H)-dione 6-Bn[5]



In a a 50-mL double-necked flask was placed 3-(benzyloxy)quinazoline-2,4(1H,3H)-dione (537.8 mg, 2.0 mmol) in *N*,*N*-dimethylformamide (DMF, 10 mL). Cesium carbonate (1321.4 mg, 4.0 mmol, 2.0 equiv) and benzyl bromide (286.3 μL, 1.2 mmol, 1.2 equiv) were added. After having been stirred at 80 °C for 1 h, the reaction was quenched with deionized water (30 mL) at ambient temperature. A copious amount of white solid was formed. The mixture was filtered through a suction funnel and the solid was rinsed with deionized water (30 mL). The collected solid was re-dissolved in acetone (40 mL) and concentrated by rotatory evaporation to remove acetone and the remaining DMF to obtain 586.9 mg (82% yield) of 6-Bn as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 (dd, *J* = 7.8, 1.4 Hz 1H), 7.65-7.63 (m, 2H), 7.55 (td, *J* = 8.4, 1.6 Hz, 1H), 7.40-7.38 (m, 3H), 7.35-7.31 (m, 2H), 7.29 (m, 1H), 7.26-7.19 (m, 3H), 7.11 (d, *J* = 8.4 Hz, 1H), 5.37 (s, 2H), 5.29 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 149.6, 139.2, 135.2, 133.7, 130.2, 129.1, 129.0, 128.9, 128.4, 127.8, 126.5, 123.4, 115.9, 114.7, 78.4, 47.4; TLC R_f 0.48 (EtOAc/hexanes, 1/1); HRMS (ESI) $[M+Na]^+$ Calcd for $C_{22}H_{18}N_2O_3Na$: 381.1215, found: 381.1209.

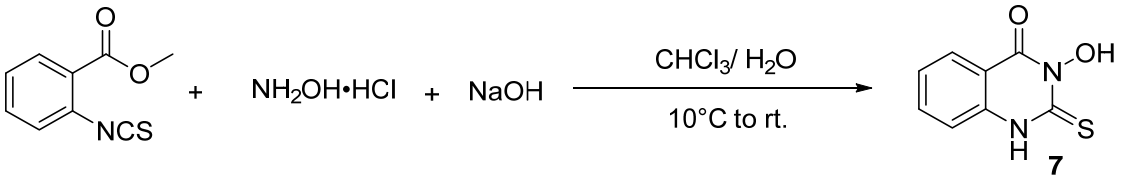
1-Benzyl-3-hydroxyquinazoline-2,4(1H,3H)-dione 6[3]



In a 25-mL two-necked flask was placed **6-Bn** (360.2 mg, 1.0 mmol) in glacial acetic acid (2 mL). The reaction mixture was heated to reflux in an oil bath and became homogeneous after 3 min. Hydrobromic acid (48%, 2 mL) was then added. After having been stirred for 1 h, the reaction

gradually cooled to ambient temperature. Deionized water (15 mL) was added to quench the reaction. The product precipitated out as a white solid. The solid was suction-filtered and washed with deionized water (30 mL). The wet solid was recrystallized from acetone (15 mL) to obtain 171.7 mg (64% yield) of **6**: ^{1}H NMR (400 MHz, DMSO-d$_6$) δ 10.86 (s, 1H), 8.08 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.67 (t, *J* = 8.4, 1H), 7.35-7.26 (m, 7H), 5.39 (s, 2H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 158.5, 149.8, 138.6, 136.1, 134.9, 128.7, 127.7, 127.3, 126.4, 123.1, 115.2, 115.1, 46.4; TLC R_f 0.19 (hexanes/EtOAc, 1/2); HRMS (ESI) $[M+Na]^+$ Calcd for $C_{15}H_{12}N_2O_3$+Na: 291.0746, found: 291.1070

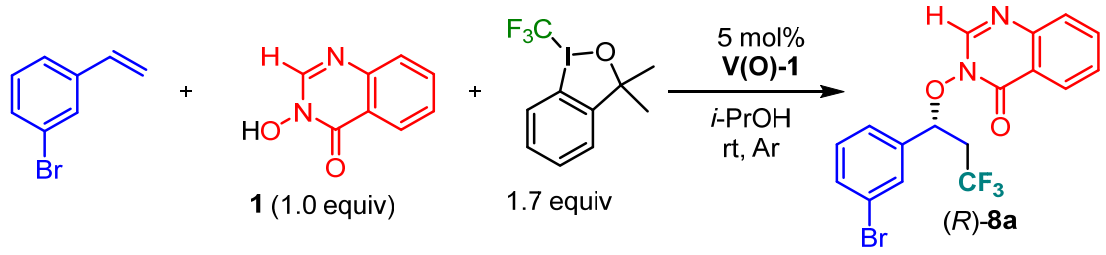
3-Hydroxy-2-thioxo-2,3-dihydroquinazolin-4(1H)-one 7[6]



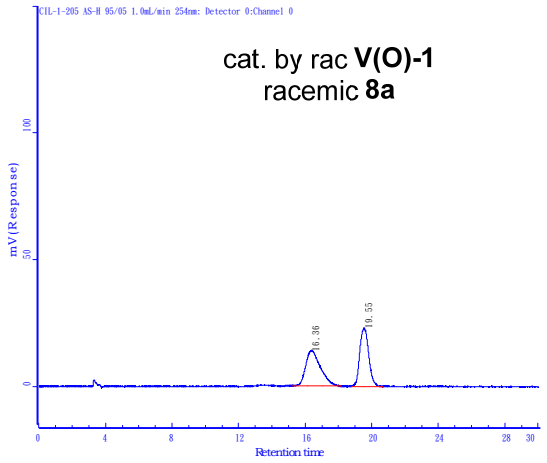
A solution of methyl 2-isothiocyanatobenzoate (956.3 mg, 5.0 mmol, 1.0 equiv) in chloroform (2 mL) was added at 5-10 °C to a stirred solution of NH_2OH•HCl (384.5 mg, 5.5 mmol, 1.1 equiv) and NaOH (234 mg, 5.5 mmol, 1.1 equiv) in water (10 mL). After 20 minutes added chloroform (5 mL) and water (20 mL) to let reaction dissolved. The reaction mixture was stirred at room temperature for 2 h. The precipitate that formed was filtered off, washed with water (10 mL) and hexane (20 mL), and dried to give a colorless solid: 732.4 mg (76%)^{1}H NMR (400 MHz, DMSO-d$_6$) δ 12.96 (s, 1H), 11.26 (s, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.73 (t, *J* = 7.2 Hz, 1H), 7.39 (d, *J* = 8.2 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d$_6$) δ 172.7, 156.6, 138.7, 135.1, 127.0, 124.3, 115.9, 115.8; R_f 0.22 (MeOH/CH_2Cl_2, 1/5); HRMS (ESI) $[M+Na]^+$ Calcd for $C_8H_6N_2O_2S$+Na: 217.0048, found: 217.0061

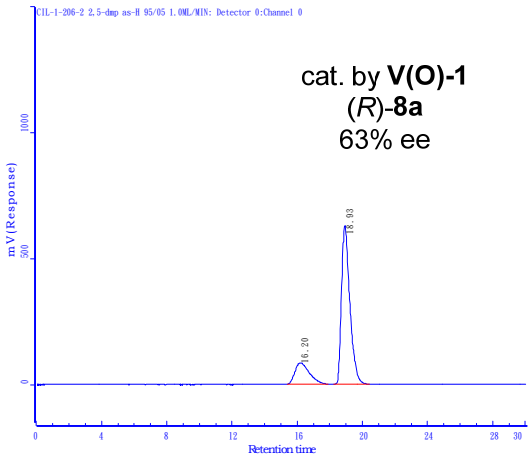
Representative catalytic procedure by V(O)-1

(*R*)-3-(1-(3-Bromophenyl)-3,3,3-trifluoropropoxy)quinazolin-4(3H)-one 8a



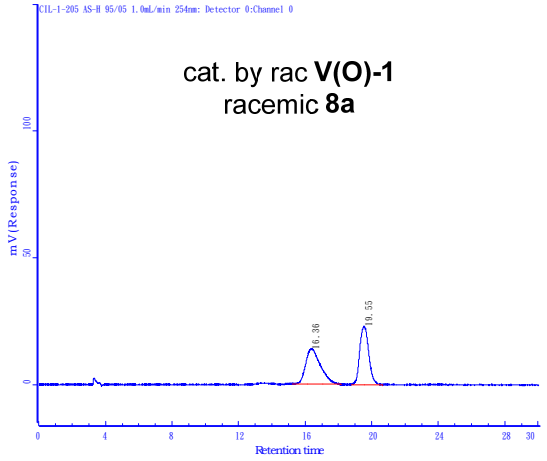
To an oven dried reaction tube (1.5 cm OD × 15.0 cm height) was placed **V(O)-1** (10.3 mg, 0.02 mmol, 5 mol%) and 2-H-Quiz **1** (65.3 mg, 0.4 mmol) in anhydrous *i*-PrOH (degassed by Ar, 2 mL) followed by addition of 3-bromo-styrene (52.7 μL, 0.4 mmol, 1.0 equiv) thru a microsyringe under Ar atmosphere. A solution of Togni reagent (225.9 mg, 0.68 mmol, 1.7 equiv) in anhydrous *i*-PrOH (1+1 mL) was added. The resulting reaction mixture was stirred at ambient temperature for 68 h and was concentrated by rotatory evaporation. The crude mixture was purified by flash column chromatography (EtOAc/ hexanes, 1/4) on silica gel to give 127.2 mg (71% yield) of **8a** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.31 (dd, J = 8.0, 1.4 Hz 1H), 7.75 (td, J = 7.6, 1.6 Hz, 1H), 7.64-7.62 (m, 2H), 7.55-7.50 (m, 3H), 7.30-7.23 (m, 2H), 5.76 (t, J = 6.6 Hz, 1H), 3.24-3.11 (m, 1H), 2.84-2.71 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.4, 146.6, 144.0, 137.7, 134.6, 133.6, 130.9, 130.8, 127.9, 127.6, 126.8, 124.7 (q, $^{1}J_{C\text{-}F}$ = 275.3 Hz), 123.5, 123.3, 81.3, 39.0 (q, $^{2}J_{C\text{-}F}$ = 29.5 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.96 (s, 3F); TLC R_f 0.25 (EtOAc/Hexanes, 1/4); HRMS (FD) $[M]^+$ Calcd for $C_{17}H_{12}F_3N_2O_2Br$: 412.0029, found: 412.0030; HPLC analysis from racemic product: t_R 16.4 min (*S*), 19.5 min (*R*) (Chiralpak AS-H, *i*-PrOH/hexane, 5/95, 1.0 ml/min, λ = 254 nm); For the reaction catalyzed by **V(O)-1**: t_R 16.2 min (minor, 18.4%), 18.9 min (major, 81.6%) for 63 % ee (*R*); $[\alpha]_D^{30}$ +301.4 (*c* 0.48, $CHCl_3$) for 63% ee (*R*); For the reaction catalyzed by **V(O)-2** (51.1 mg, 31% yield): t_R 25.4 min (major, 83.2%), 33.0 min (minor, 16.8%); $[\alpha]_D^{29}$ -313.7 (*c* 0.25, $CHCl_3$) for 66 % ee (*S*); For racemic synthesis catalyzed by racemic **V(O)-1** in *i*-PrOH: 75% yield (134.3 mg, 68h).

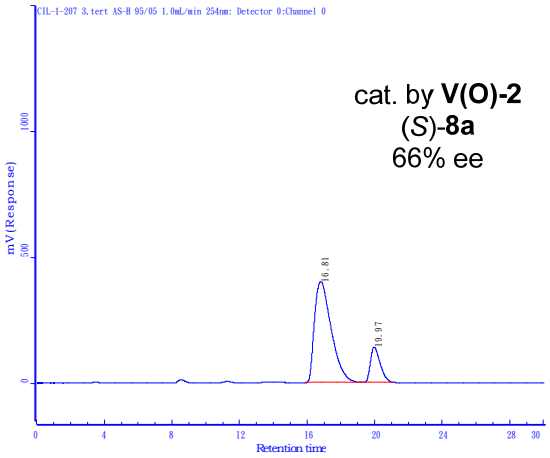




#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		16.362	871.91	49.93	0.00
1		19.549	874.48	50.07	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		16.201	5085.47	18.36	0.00
1		18.929	22610.92	81.64	0.00



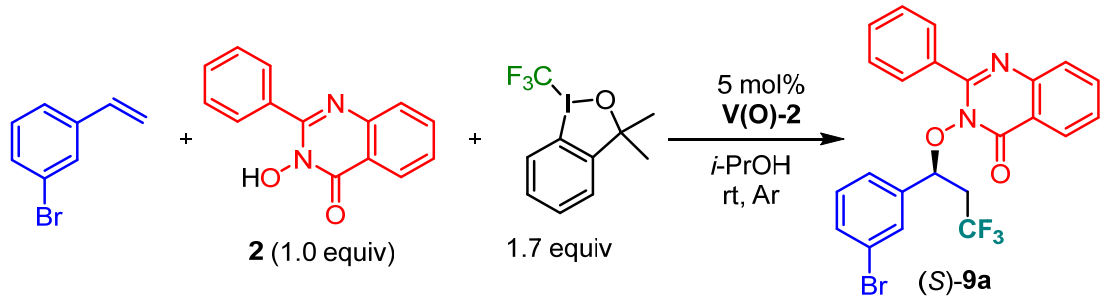


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		16.362	871.91	49.93	0.00
1		19.549	874.48	50.07	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		16.807	27530.51	83.20	0.00
1		19.966	5560.15	16.80	0.00

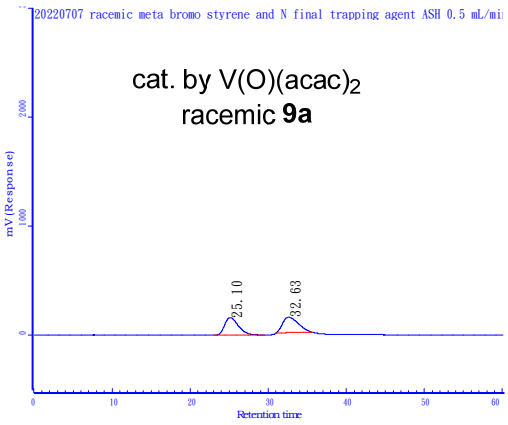
Representative catalytic procedure by V(O)-2

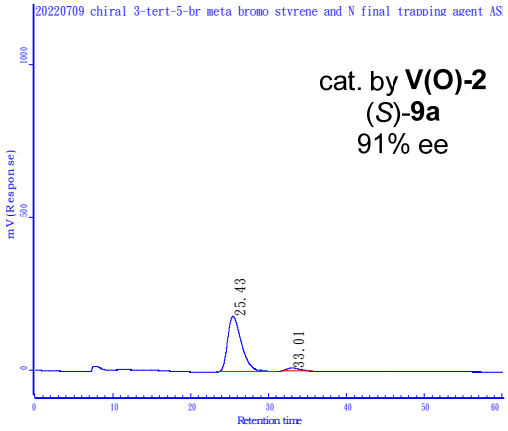
(*S*)-3-(1-(3-Bromophenyl)-3,3,3-trifluoropropoxy)-2-phenylquinazolin-4(3H)-one 9a



In an oven dried reaction tube (1.5 cm OD × 15.0 cm height) was placed **V(O)-2** (9.3 mg, 0.02

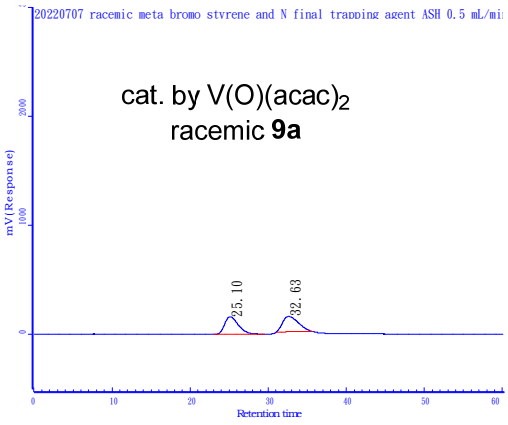
mmol, 5 mol%) and 2-Ph-Quiz **2** (95.5 mg, 0.4 mmol, 1.0 equiv) in anhydrous *i*-PrOH (degassed by Ar, 2 mL) followed by addition of 3-bromo-styrene (73 μL, 0.56 mmol, 1.4 equiv) thru a microsyringe under Ar atmosphere. A solution of Togni reagent (224.6 mg, 0.68 mmol, 1.7 equiv) in anhydrous *i*-PrOH (1+1 mL) was added. The resulting reaction mixture was stirred at ambient temperature for 92 h and was concentrated by rotatory evaporation. The crude mixture was purified by flash column chromatography (EtOAc/ hexanes, 1/10) on silica gel to give 54.8 mg (28%) of (*S*)-**9a** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.77 (td, *J* = 7.6, 1.5 Hz, 1H), 7.70 (d, *J* = 7.9 Hz, 1H), 7.56-7.49 (m, 4H), 7.46-7.40 (m, 2H), 7.35 (d, *J* = 8.4 Hz, 1H), 6.94 (t, *J* = 7.9 Hz, 1H), 6.81-6.73 (m, 2H), 5.66 (t, *J* = 6.7 Hz, 1H), 3.10-2.91 (m, 1H), 2.67-2.49 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 153.5, 146.3, 136.4, 134.6, 133.0, 132.3, 130.9, 130.7, 129.9, 129.6, 128.1, 128.0, 127.4, 127.1, 126.7, 124.7 (q, $^{1}J_{C\text{-}F}$ = 277.2 Hz), 122.7, 122.1, 80.4, 38.1 (q, $^{2}J_{C\text{-}F}$ = 29.6 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.01 (s, 3F); TLC R_f 0.19 (CH_2Cl_2/Hexanes, 1/4); HRMS (FD) $[M]^+$ Calcd for $C_{23}H_{16}F_3N_2O_2Br$: 488.0236, found: 488.0354; HPLC analysis from racemic product: t_R 25.1 min (*S*), 32.6 min (*R*) (Chiralpak AS-H, *i*-PrOH/hexane, 1/99, 0.5 ml/min, λ = 254 nm); From the reaction catalyzed by **V(O)-2**: t_R 25.4 min (major, 95.6%), 33.0 min (minor, 4.4%) for 91.2 % ee (*S*); $[\alpha]_D^{22}$ +122.4 (*c* 1.0, $CHCl_3$) for 91% ee (*R*); From the reaction catalyzed by **V(O)-1** (88.1mg, 45% yield, 84h): t_R 26.5 min (minor, 24.9%), 32.8 min (major, 75.1%) for 50 % ee (*R*); For racemic synthesis catalyzed by racemic **V(O)-1** in *i*-PrOH: 31% yield (60.7 mg, 92h).

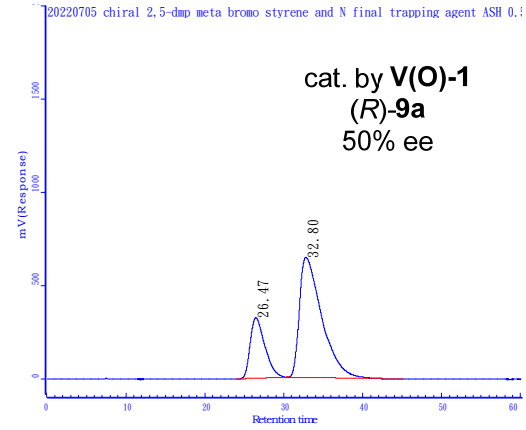




#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		25.103	19442.05	49.71	0.00
1		32.626	19671.63	50.29	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		25.434	22367.08	95.60	0.00
1		33.011	1029.88	4.40	0.00

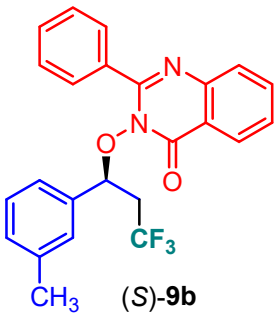




#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		25.103	19442.05	49.71	0.00
1		32.626	19671.63	50.29	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		26.468	41803.19	24.88	0.00
1		32.804	126238.69	75.12	0.00

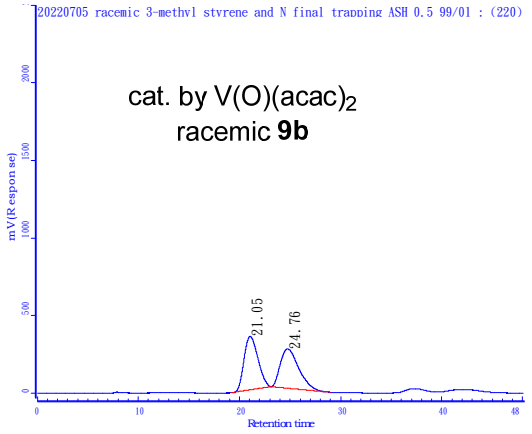
(*S*)-2-Phenyl-3-(3,3,3-trifluoro-1-(*m*-tolyl)propoxy)quinazolin-4(3H)-one 9b



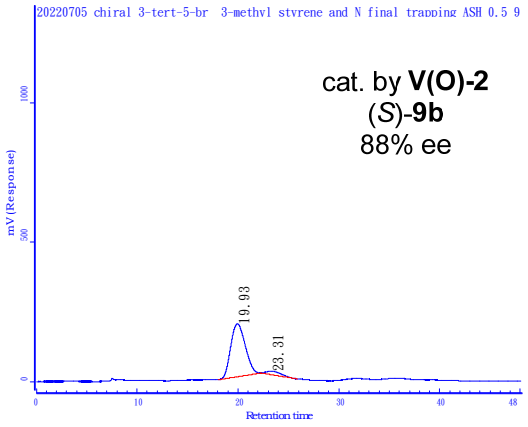
(*S*)-**9b**

Data for **9b**: 61.5 mg, 31% yield, 108h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.34 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.74 (td, *J* = 7.8, 1.4 Hz, 1H), 7.68 (d, *J* = 7.5 Hz, 1H), 7.54-7.45 (m, 4H), 7.40 (t, *J* = 7.8 Hz, 2H), 7.02 (d, *J* = 7.6 Hz, 1H), 6.93 (t, *J* = 7.6 Hz, 1H), 6.57 (d, *J* = 7.6 Hz, 1H), 6.47 (s, 1H), 5.72 (t, *J* = 6.7 Hz, 1H), 3.05-2.90 (m, 1H), 2.70-2.51 (m, 1H) 2.07 (s, 3H); ^{13}C NMR ($CDCl_3$) δ 158.4, 153.7, 146.3, 142.7, 138.1, 134.4, 133.9, 132.7, 130.6, 130.3, 129.8, 128.7, 128.2, 127.8, 126.9, 126.7, 125.9, 125.0 (q, $^{1}J_{C\text{-}F}$ = 277.6 Hz), 122.1, 80.8, 38.0 (q, $^{2}J_{C\text{-}F}$ = 29.3 Hz), 21.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.15 (s, 3F); TLC R_f 0.44 (EtOAc/Hexanes, 1/6); HRMS (FD)

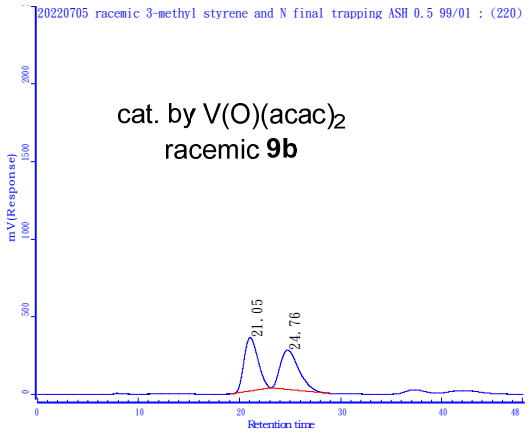
$[M]^+$ Calcd for $C_{24}H_{19}F_3N_2O_2$: 424.14041, found: 424.14078; HPLC analysis from racemic product: t_R 21.1 min (*S*), 24.8 min (*R*) (Chiralpak AS-H, *i*-PrOH/hexane, 1/99, 0.5 ml/min, λ = 254 nm); From the reaction catalyzed by **V(O)-2**: t_R 19.9 min (major, 93.8%), 23.3 min (minor, 6.2%); $[\alpha]_D^{22}$ +111.5 (*c* 1.0, $CHCl_3$) for 88% ee (*S*); From the reactiuon catalyzed by **V(O)-1** (118.2 mg, 60% yield, 70h): t_R 21.1 min (minor, 27.3%), 24.6 min (major, 72.7%) for 45% ee (*R*).



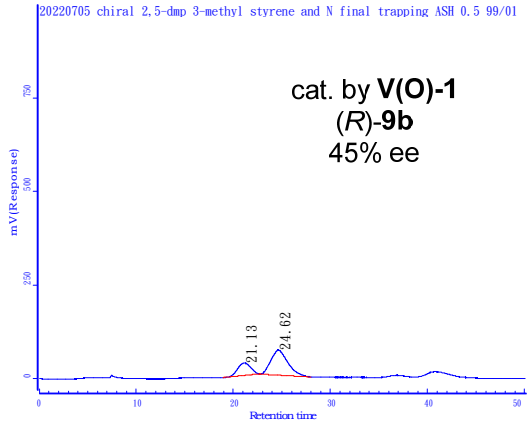
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		21.051	32834.79	50.39	0.00
1		24.762	32321.23	49.61	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.932	19084.85	93.75	0.00
1		23.311	1273.37	6.25	0.00

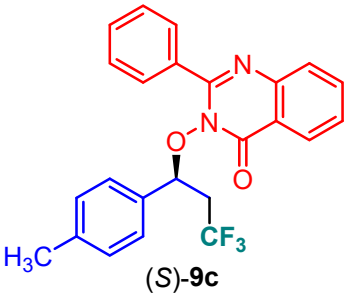


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		21.051	32834.79	50.39	0.00
1		24.762	32321.23	49.61	0.00



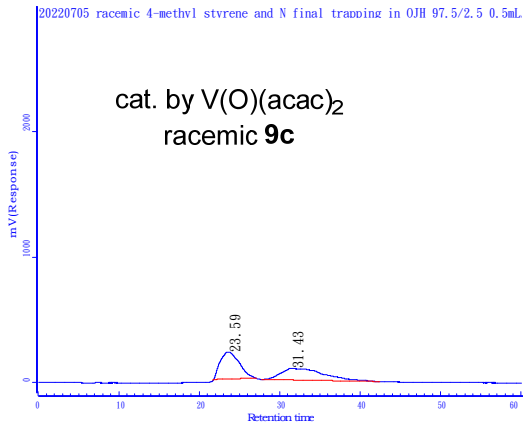
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		21.128	3056.77	27.33	0.00
1		24.624	8129.88	72.67	0.00

(*S*)-2-Phenyl-3-(3,3,3-trifluoro-1-(*p*-tolyl)propoxy)quinazolin-4(3H)-one 9c

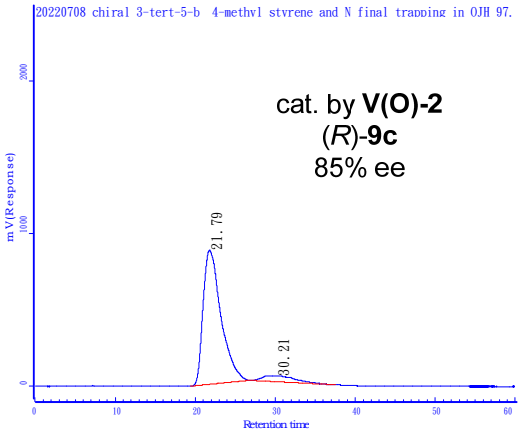


(*S*)-**9c**

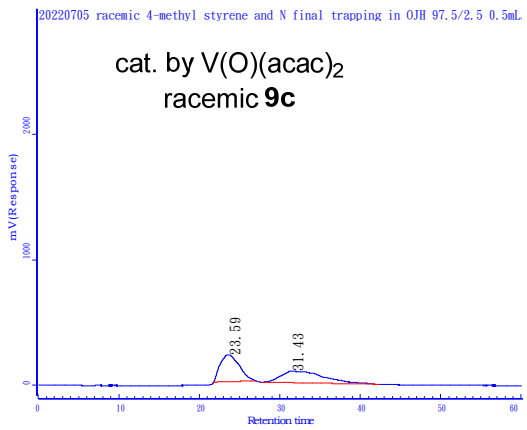
Data for **9c**: 107.3 mg, 55% yield, 92h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.33 (d, *J* = 7.8 Hz, 1H), 7.74 (td, *J* = 7.7, 1.2 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.53-7.44 (m, 4H), 7.38 (t, *J* = 7.7 Hz, 2H), 6.82 (d, *J* = 7.9 Hz, 2H), 6.62 (d, *J* = 7.9 Hz, 2H), 5.67 (t, *J* = 6.7 Hz, 1H), 3.05-2.90 (m, 1H), 2.68-2.52 (m, 1H) 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 153.7, 146.3, 139.7, 134.4, 132.7, 131.0, 130.3, 129.8, 129.1, 128.3, 127.9, 127.7, 126.9, 126.7, 125.0 (q, $^{1}J_{C\text{-}F}$ = 277.4 Hz), 122.2, 80.7, 38.0 (q, $^{2}J_{C\text{-}F}$ = 29.8 Hz), 21.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.10 (s, 3F); TLC R_f 0.36 (EtOAc/Hexanes, 1/6); HRMS (FD) $[M]^+$ Calcd for $C_{24}H_{19}F_3N_2O_2$: 424.14041, found: 424.14026; HPLC analysis from racemic product: t_R 23.6 min (*S*), 31.4 min (*R*) (Chiralpak OJ-H, *i*-PrOH/hexane, 2.5/97.5, 0.5 ml/min, λ = 254 nm); From the reaction catalyzed by **V(O)-2**: t_R 19.9 min (major, 93.8%), 23.3 min (minor, 6.2%); $[\alpha]_D^{22}$ +108.3 (*c* 1.0, $CHCl_3$) for 85% ee (*S*); From the reactiuon catalyzed by **V(O)-1** (137.1 mg, 70% yield, 52h): t_R 22.4 min (minor, 37.1%), 29.7 min (major, 62.9%) for 26% ee (*R*).

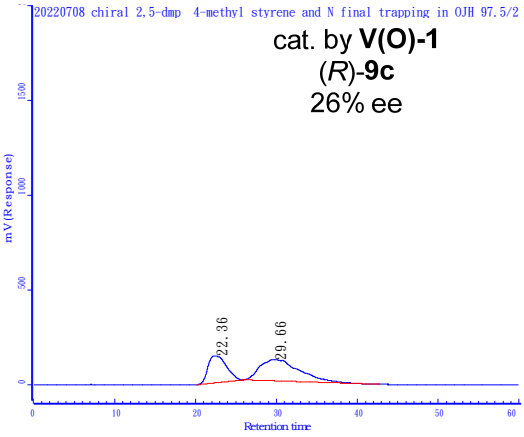


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		23.588	35243.57	50.43	0.00
1		31.427	34638.60	49.57	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		21.786	136480.56	92.57	0.00
1		30.214	10949.51	7.43	0.00

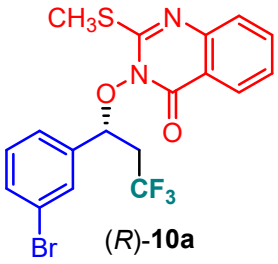




#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		23.588	35243.57	50.43	0.00
1		31.427	34638.60	49.57	0.00

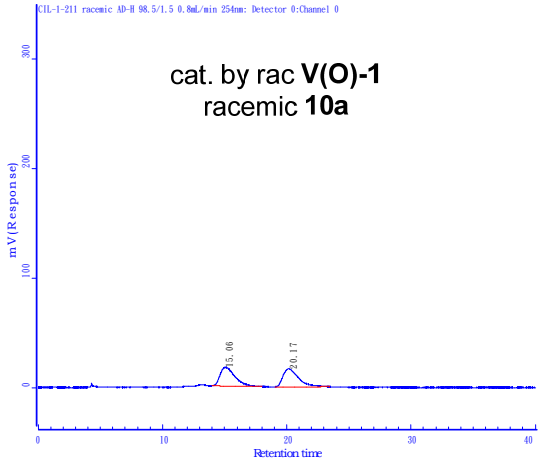
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		22.361	22673.62	37.10	0.00
1		29.662	38437.98	62.90	0.00

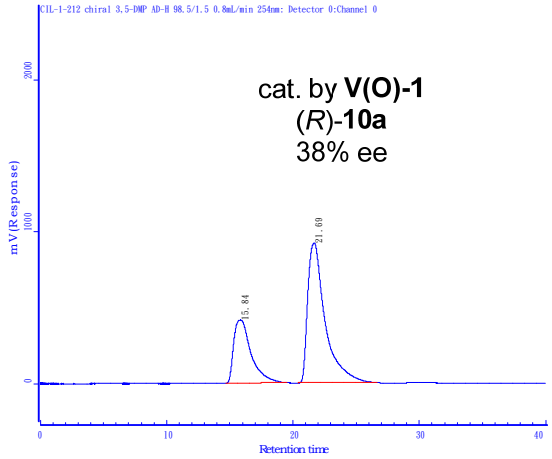
(*R*)-3-(1-(3-Bromophenyl)-3,3,3-trifluoropropoxy)-2-(methylthio)quinazolin-4(3H)-one 10a



(*R*)-**10a**

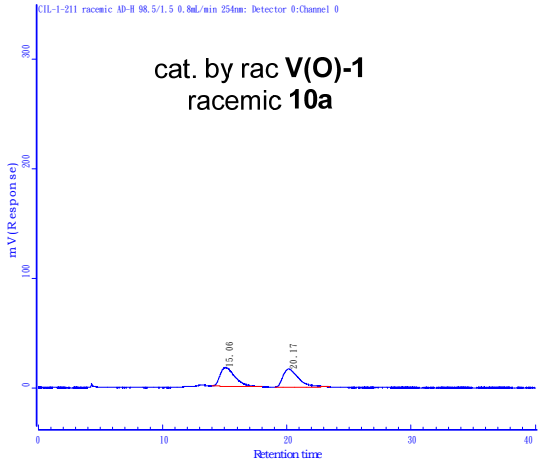
Data for **10a**: 114.7mg, 62% yield, 30h: ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.0 Hz, 1H), 7.70 (s, 1H), 7.68 (d, *J* = 7.6 Hz, 1H), 7.53 (d, *J* = 8.2 Hz, 1H), 7.49 (d, *J* = 8.2 Hz, 1H), 7.41-7.37 (m, 2H), 7.20 (t, *J* = 8.0 Hz, 1H), 5.98 (dd, *J* = 8.0, 5.4 Hz, 1H), 3.25-3.15 (m, 1H), 2.98-2.87 (m, 1H), 2.52 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 156.5, 146.5, 137.0, 133.2, 131.6, 130.1, 127.5, 126.8, 126.4, 125.8, 124.8 (q, $^{1}J_{C\text{-}F}$ = 275.4 Hz), 122.5, 120.5, 81.1 (q, $^{3}J_{C\text{-}F}$ = 2.4 Hz, 38.3 (q, $^{2}J_{C\text{-}F}$ = 28.8 Hz), 13.8; ^{19}F NMR (471 MHz, $CDCl_3$) δ -62.83 (s, 3F); TLC R_f 0.25 (EtOAc/hexanes, 1/20); HRMS (FD) $[M]^+$ Calcd for $C_{18}H_{14}N_2O_2F_3BrS$: 457.9906, found: 457.9897; HPLC analysis from racemic product: t_R 15.1 min (*S*), 20.2 min (*R*) (Chiralpak AS-H, *i*-PrOH/hexane, 1.5/98.5, 0.8 ml/min, λ = 254 nm); For the reaction catalyzed by **V(O)-1**: t_R 15.8 min (minor, 31.0%), 21.7 min (major, 69.0%); $[\alpha]_D^{29}$ +60.1 (*c* 0.42, $CHCl_3$) for 38% ee (*R*); For the reaction catalyzed by **V(O)-2** (71.2 mg, 39% yield, 50h): t_R 15.4 min (major, 75.0%), 21.4 min (minor, 25.0%); $[\alpha]_D^{29}$ -77.2 (*c* 0.14, $CHCl_3$) for 50% ee (*S*); For racemic synthesis catalyzed by racemic **V(O)-1** in *i*-PrOH: 62% yield (114.3 mg, 30h).

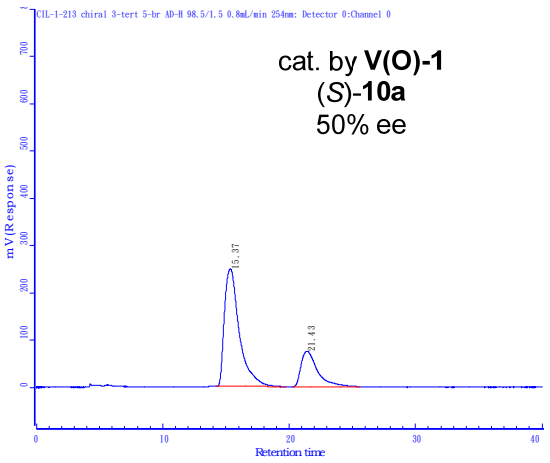




#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.056	1428.16	50.07	0.00
1		20.171	1424.13	49.93	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.837	39710.54	31.01	0.00
1		21.687	88349.59	68.99	0.00



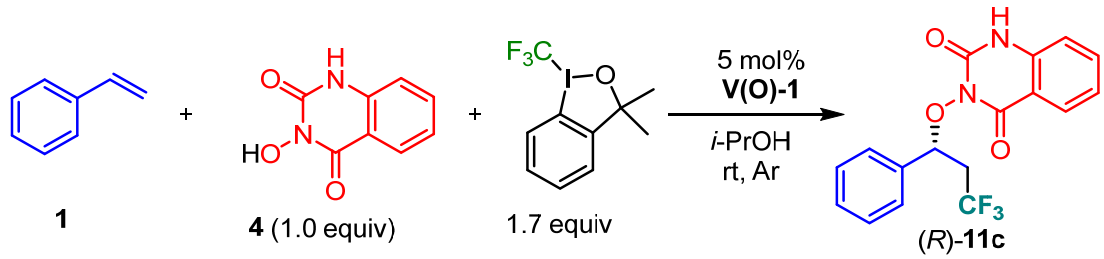


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.056	1428.16	50.07	0.00
1		20.171	1424.13	49.93	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.368	20268.12	74.98	0.00
1		21.429	6763.41	25.02	0.00

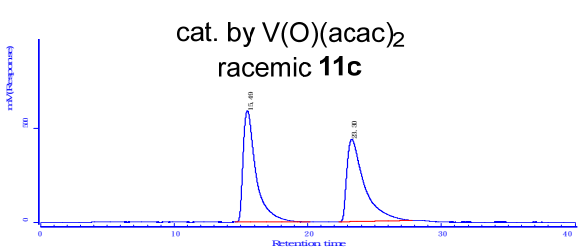
Representative catalytic procedure by V(O)-1

3-(3,3,3-Trifluoro-1-phenylpropoxy)quinazoline-2,4(1H,3H)-dione 11c

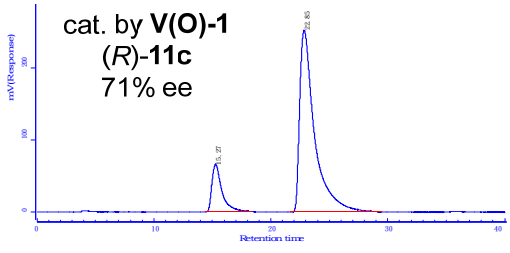


To an oven dried reaction tube (1.5 cm OD × 15.0 cm height) was placed **V(O)-1** (9.3 mg, 0.019 mmol, 4.5 mol%) and **4** (71.3 mg, 0.4 mmol, 1.0 equiv) in anhydrous *i*-PrOH (degassed by Ar, 2 mL)

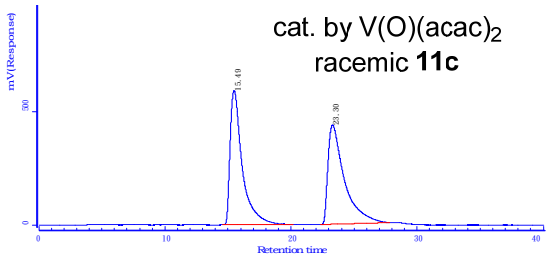
followed by addition of styrene (45.8 μL, 0.4 mmol) thru a microsyringe under Ar atmosphere. A solution of Togni reagent (224.5 mg, 0.68 mmol, 1.7 equiv) in anhydrous *i*-PrOH (1+1 mL) was added. The resulting reaction mixture was stirred at ambient temperature for 51 h and was concentrated by rotatory evaporation. The crude mixture was purified by flash column chromatography (EtOAc/ hexanes, 1/2) on silica gel to give 122.7 mg (84%) of **11c** as a white solid: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.25 (s, 1H), 8.06 (d, J = 7.8 Hz, 1H), 7.62 (td, J = 7.2, 1.2 Hz, 1H), 7.52-7.50 (m, 2H), 7.32-7.30 (m, 3H), 7.24 (t, J = 7.2 Hz, 1H), 7.08 (d, J = 8.2 Hz, 1H), 5.80 (t, J = 6.4 Hz, 1H), 3.30-3.16 (m, 1H), 2.93-2.80 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 150.2, 137.5, 135.6, 135.3, 129.8, 128.5, 128.4, 128.3, 125.2 (q, $^{1}J_{C\text{-}F}$ = 275.3 Hz), 123.7, 115.3, 114.6, 81.6, 39.0 (q, $^{2}J_{C\text{-}F}$ = 28.7 Hz); ^{19}F NMR (471 MHz, $CDCl_3$): δ -63.2 (s, 3F); R_f 0.25 (EtOAc/hexanes, 1/2); HRMS (FD) $[M+H]^+$ Calcd for $C_{17}H_{14}F_3N_2O_3$: 351.0951, found: 351.0954; HPLC analysis from racemic product: t_R 15.5 min (*S*), 23.3 min (*R*) (Chiralpak AD-H, *i*-PrOH/*n*-hexane, 12/88, 0.8 mL/min, λ = 254 nm); For the reaction reaction catalysed by **V(O)-1**: HPLC t_R 15.3 min (major, 14.7%), 22.8 min (minor, 85.3%) for 71 %ee (*R*); For the reaction reaction catalysed by **V(O)-2** (120 h, 105.3 mg, 75%): HPLC t_R 15.5 min (major, 87.5%), 23.4 min (minor, 12.5%) for 75 %ee (*S*). Racemic reaction catalyzed by $V(O)(acac)_2$ in CH_3CN in 5h: 48.9 mg, 34% yield.



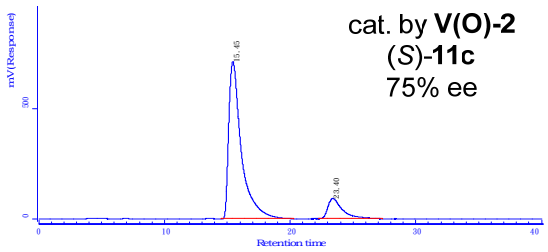
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.488	39716.10	50.05	0.00
1		23.298	39634.96	49.95	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.272	3816.13	14.69	0.00
1		22.849	22163.39	85.31	0.00

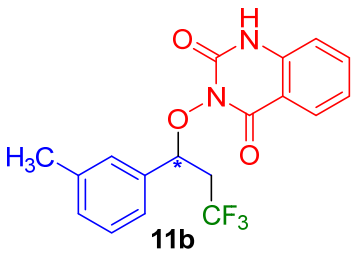


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.488	39716.10	50.05	0.00
1		23.298	39634.96	49.95	0.00



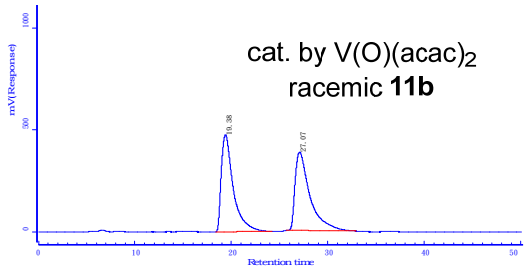
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.449	49345.80	87.46	0.00
1		23.405	7072.98	12.54	0.00

3-(3,3,3-Trifluoro-1-(m-tolyl)propoxy)quinazoline-2,4(1H,3H)-dione 11b

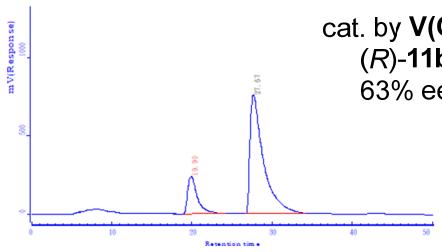


11b

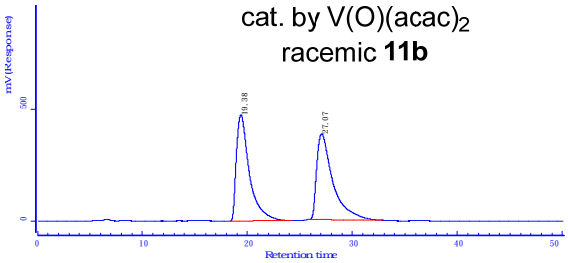
White solid; Yield: 84%/54% (122.7/78.8 mg, 10 mol% cat. **V(O)-1**/5 mol% cat. **V(O)-2**, 38/48 h); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.51 (s, 1H), 8.07 (d, J = 8.0 Hz, 1H), 7.62 (td, J = 7.8, 1.2 Hz, 1H), 7.33-7.31 (m, 2H), 7.25 (d, J = 7.8 Hz, 1H), 7.20 (t, J = 8.2 Hz, 1H), 7.14-7.11 (m, 2H), 5.75 (t, J = 6.4 Hz, 1H), 3.28-3.15 (m, 1H), 2.92-2.79 (m, 1H), 2.29 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 150.4, 138.1, 137.6, 135.7, 135.3, 130.5, 129. 0, 128.3, 125.5, 125.3 (q, $^{1}J_{C\text{-}F}$ = 275.4 Hz), 123.7, 115.4, 114.7, 81.7, 39.1 (q, $^{2}J_{C\text{-}F}$ = 28.6 Hz), 21.3; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.08 (s, 3F); R_f 0.25 (EtOAc/Hexanes, 1/2); HRMS (ESI) $[M]^+$ Calcd for $C_{18}H_{15}F_3N_2O_3$: 364.1029, found: 364.1026; HPLC analysis from racemic product: t_R 19.4 min (*S*), 27.1 min (*R*) (Chiralpak AD-H, *i*-PrOH/n-hexane, 10/90, 0.6 ml/min, λ = 254 nm). For the reaction reaction catalyzed by **V(O)-1**: t_R 19.9 min (minor, 18.5%), 27.7 min (major, 81.5%); $[\alpha]_D^{25}$ +122.5 (*c*, 0.74, $CHCl_3$) for 63% ee (*R*); For the reaction catalyzed by **V(O)-2** (54% yield, 48 h): t_R 19.7 min (major, 84.0%), 27.8 min (minor, 16.0%) for 68% ee (*S*). For racemic synthesis by $V(O)(acac)_2$ in CH_3CN: 30.1% (43.9 mg, 96 h).



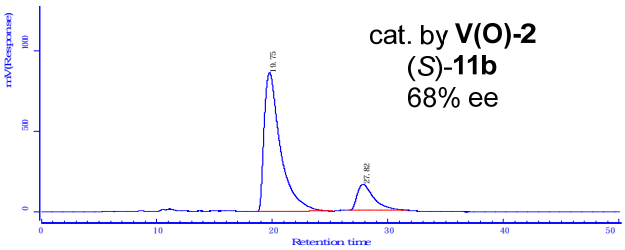
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.375	41164.82	50.00	0.00
1		27.069	41157.93	50.00	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.902	20130.70	18.52	0.00
1		27.671	88548.41	81.48	0.00

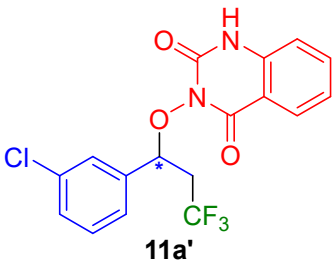


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.375	41164.82	50.00	0.00
1		27.069	41157.93	50.00	0.00



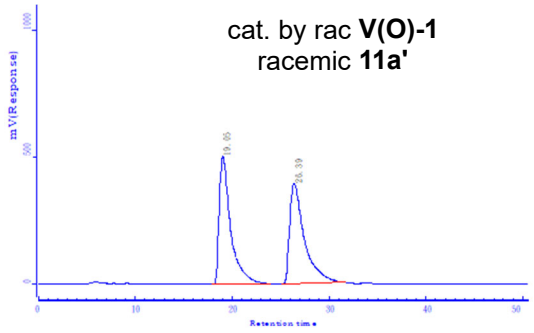
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.746	83838.64	84.01	0.00
1		27.824	15962.32	15.99	0.00

(*R*)-3-(1-(3-Chlorophenyl)-3,3,3-trifluoropropoxy)quinazoline-2,4(1H,3H)-dione 11a'

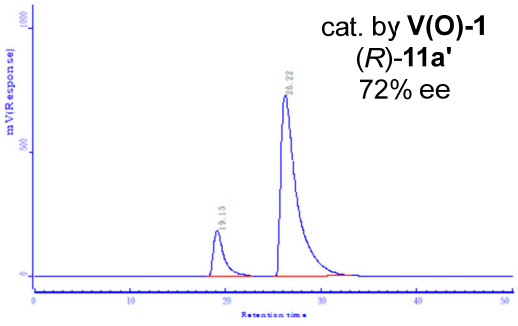


11a'

White solid; Yield: 83.1% (127.9 mg, 18h); ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.48 (s, 1H), 8.08 (d, J = 8.0 Hz, 1H), 7.65 (td, J = 7.8, 1.0 Hz, 1H), 7.57 (s, 1H), 7.40 (d, J = 7.2 Hz, 1H), 7.33-7.30 (m, 1H), 7.29-7.27 (m, 1H), 7.62-7.24 (m, 1H), 7.12 (d, J = 8.0 Hz, 1H), 5.71 (t, J = 6.6 Hz, 1H), 3.27-3.14 (m, 1H), 2.89-2.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 150.3, 138.0, 137.5, 135.5, 134.3, 129.9, 129.8, 128.5, 128.4, 126.6, 125.0 (q, $^{1}J_{C\text{-}F}$ = 275.4 Hz), 123.9, 115.5, 114.6, 81.2, 39.2 (q, $^{2}J_{C\text{-}F}$ = 28.9 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.08 (s, 3F); R_f 0.25 (EtOAc/Hexanes, 1/2); HRMS (FD) $[M]^+$ Calcd for $C_{17}H_{12}F_3N_2O_3Cl$: 384.0483, found: 384.0480; HPLC analysis from racemic product: t_R 19.05 min (*S*), 26.40 min (*R*) (Chiralpak AD-H, *i*-PrOH/hexane, 12/88, 0.6 ml/min, λ = 254 nm). For the reaction catalyzed by **V(O)-1**: t_R 19.13 min (minor, 14.1%), 26.22 min (major, 85.9%); $[\alpha]_D^{30}$ +124.0 (*c*, 1.0, $CHCl_3$) for 72% ee (*R*); 74.3% yield (114.3 mg, 18h) for racemic synthesis catalyzed by racemic **V(O)-1**.

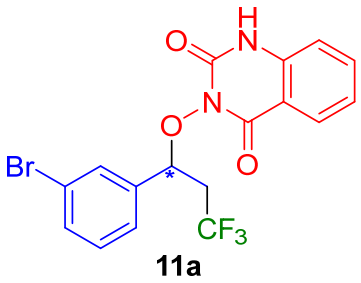


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.052	41641.29	50.02	0.00
1		26.395	41601.52	49.98	0.00



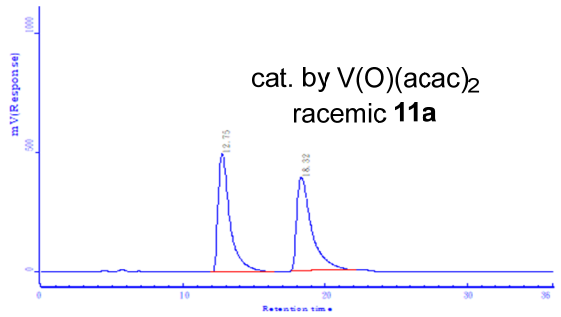
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.126	13951.66	14.08	0.00
1		26.221	85135.70	85.92	0.00

(*R*)-3-(1-(3-Bromophenyl)-3,3,3-trifluoropropoxy)quinazoline-2,4(1H,3H)-dione 11a

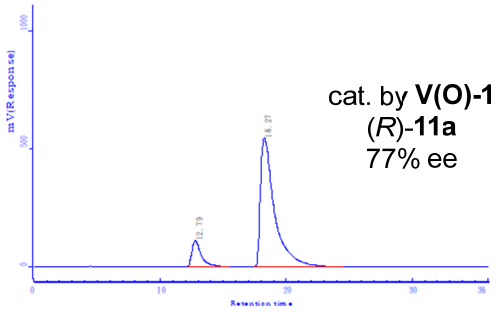


11a

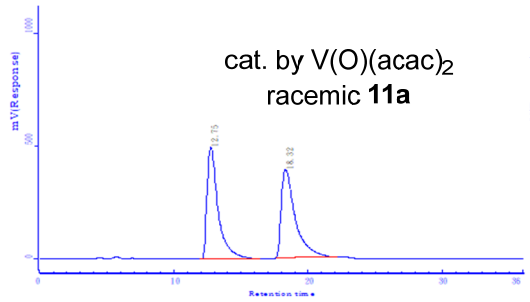
White solid; Yield 88% (144.2 mg, 43h); Data for **10a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.49 (s, 1H), 8.08 (d, *J* = 7.8 Hz, 1H), 7.62 (td, *J* = 7.2, 1.4 Hz, 1H), 7.48-7.45 (m, 2H), 7.26 (t, *J* = 8.0 Hz, 1H), 7.21 (t, *J* = 7.8 Hz, 1H), 7.13 (d, *J* = 8.2 Hz, 1H), 5.70 (t, *J* = 6.6 Hz, 1H), 3.27-3.14 (m, 1H), 2.89-2.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 150.3, 138.2, 137.6, 135.5, 132.8, 131.4, 130.0, 128.4, 127.0, 125.0 (q, $^{1}J_{C\text{-}F}$ = 275.3 Hz), 123.9, 122.4, 115.6, 114.6, 81.1, 39.2 (q, $^{2}J_{C\text{-}F}$ = 28.8 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.05 (s, 3F); R_f 0.25 (EtOAc/Hexanes, 1/2); HRMS (FD) $[M]^+$ Calcd for $C_{17}H_{12}F_3N_2O_3Br$: 427.9978, found: 427.9976; HPLC analysis from racemic product: t_R 12.8 min (*S*), 18.3 min (*R*) (Chiralpak AD-H, *i*-PrOH/hexane, 14/86, 0.8 ml/min, λ = 254 nm). For the reaction reaction catalyzed by **V(O)-1**: t_R 12.8 min (minor, 11.7%), 18.3 min (major, 88.3%); $[\alpha]_D^{24}$ +65.9 (*c*, 1.0, $CHCl_3$) for 77% ee (*R*). For the reaction catalyzed by **V(O)-2** (53% yield, 120h): t_R 12.9 min (major, 86.9%), 18.7 min (major, 13.1%) for 74% ee (*S*); For racemic synthesis catalyzed by $V(O)(acac)_2$ in CH_3CN: 30.6% yield (52.5 mg, 17h).



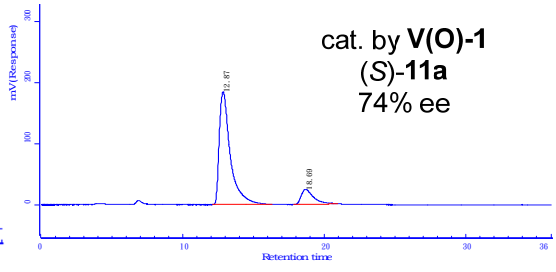
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.747	28170.73	50.00	0.00
1		18.316	28165.17	50.00	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.787	5602.01	11.74	0.00
1		18.272	42121.59	88.26	0.00



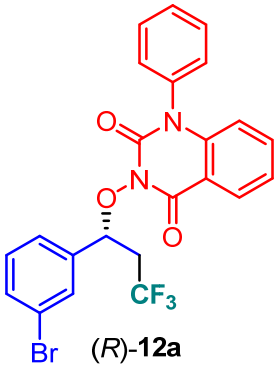
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.747	28170.73	50.00	0.00
1		18.316	28165.17	50.00	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.868	10002.91	86.94	0.00
1		18.695	1502.72	13.06	0.00

Representative catalytic procedure by V(O)-1

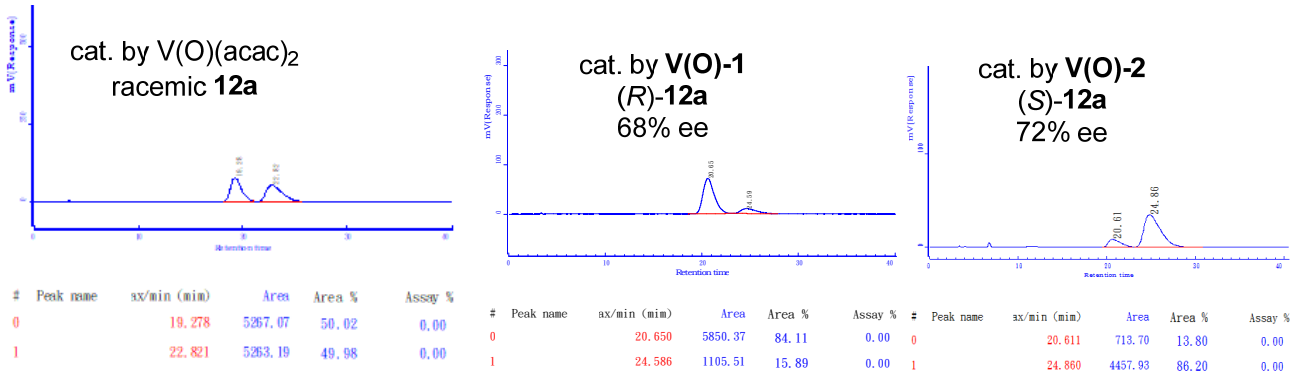
(*R*)-3-(1-(3-Bromophenyl)-3,3,3-trifluoropropoxy)-1-phenylquinazoline-2,4(1H,3H)-dione 12a



(*R*)-**12a**

Data for **12a**: 187.3 mg, 93% yield, 18h: ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.18 (dd, J = 7.9, 1.4, 1H), 7.66 (t, J = 1.8 Hz, 1H), 7.61-7.43 (m, 6H), 7.28-7.19 (m, 4H), 6.50 (d, J = 8.4 Hz, 1H), 5.78 (t, J = 6.5 Hz, 1H), 3.25-3.12 (m, 1H), 2.91-2.78 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$): δ 158.9, 148.9, 140.6, 138.0, 135.6, 134.9, 132.7, 131.5, 130.4, 130.4, 130.1, 129.7, 128.9, 128.8, 128.6, 127.0, 125.0 (q, $^{1}J_{C\text{-}F}$ = 279.0 Hz), 123.6, 122.2, 115.6, 114.8, 80.7 (q, $^{3}J_{C\text{-}F}$ = 3.0 Hz), 38.9 (q, $^{2}J_{C\text{-}F}$ = 28.7 Hz); ^{19}F NMR (471 MHz, $CDCl_3$): δ -62.98 (s, 3F); TLC R_f 0.30 (EtOAc/hexanes, 1/6); HRMS (FD) $[M]^+$ Calcd for $C_{23}H_{16}BrF_3N_2O_3$: 504.0291, found: 504.0287; HPLC analysis from racemic product: t_R 19.3 min (*R*), 22.8 min (*S*); From the reaction catalyzed by **V(O)-1**: t_R 20.65 min (major, 84.1%), 24.59 min (minor, 15.9%) (Chiralpak AS-H, *i*-PrOH/*n*-hexane, 05/95, 1.0 mL/min, λ = 254 nm); $[\alpha]_D^{22}$ +108.4 (*c* 1.0, $CHCl_3$) for 68% ee (*R*); From the reaction

catalyzed by **V(O)-2** in EtOH (46% yield, 96 h): t_R 20.6 min (minor, 13.8%), 24.9 min (major, 86.2%) for 72% ee (*S*).

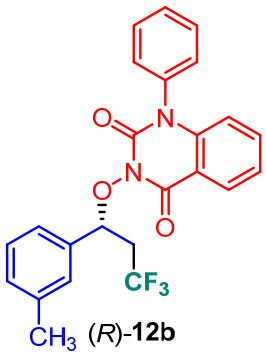


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		19.278	5267.07	50.02	0.00
1		22.821	5263.19	49.98	0.00

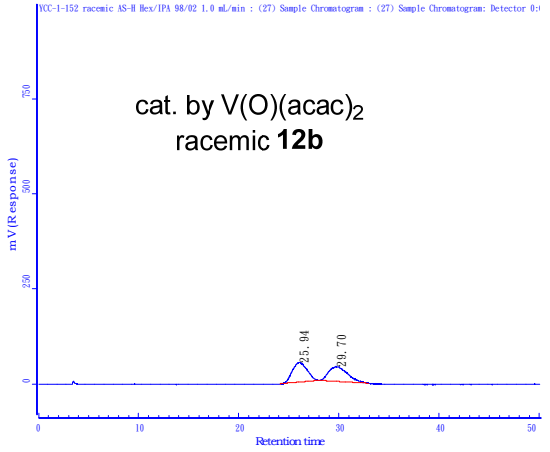
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		20.650	5850.37	84.11	0.00
1		24.586	1105.51	15.89	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		20.611	713.70	13.80	0.00
1		24.860	4457.93	86.20	0.00

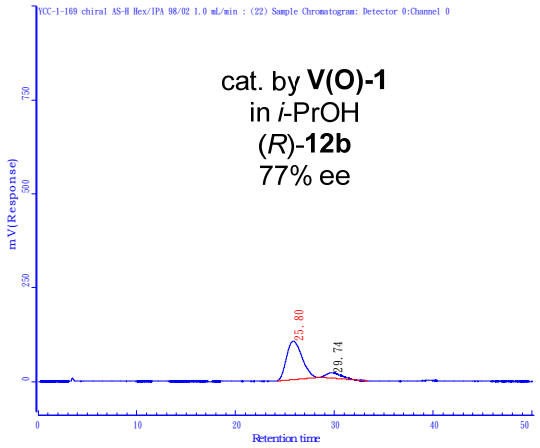
(*R*)-1-Phenyl-3-(3,3,3-trifluoro-1-(*m*-tolyl)propoxy)quinazoline-2,4(1H,3H)-dione 12b



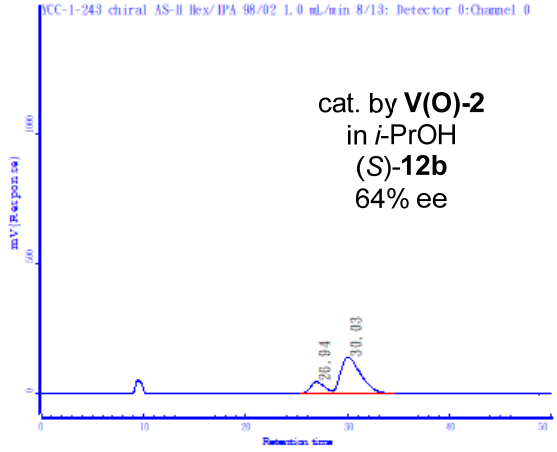
Data for **12b**: 104.2 mg, 59% yield, 17h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (dd, *J* = 7.9, 1.0 Hz, 1H), 7.60-7.15 (m, 11H), 6.48 (d, *J* = 8.7 Hz, 1H), 5.83 (t, *J* = 6.2 Hz, 1H), 3.25-3.15 (m, 1H), 2.93-2.83 (m, 1H), 2.32 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.0, 140.6, 138.0, 135.7, 135.5, 134.8, 130.4, 129.6, 129.2, 128.9, 128.9, 128.6, 128.3, 125.6, 125.3 ($^1J_{C\text{-}F}$ = 277.2 Hz), 123.4, 115.5, 114.9, 81.4 ($^3J_{C\text{-}F}$ = 2.9 Hz), 38.9 ($^2J_{C\text{-}F}$ = 28.5 Hz), 21.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.2 (s, 3F); TLC R_f0.28 (EtOAc/hexanes, 1/6);HRMS (FD) Calcd for $C_{24}H_{19}F_3N_2O_3$: 440.1353, found: 440.1359; HPLC from racemic product: t_R 19.3 min (*R*), 22.8 min (*S*); From the reaction catalyzed by **V(O)-1**: t_R 25.80 min (major, 88.6%), 29.74 min (minor, 11.4%) (Chiralpak AS-H, *i*-PrOH/*n*-hexane, 2/98, 1.0 mL/min, λ = 254 nm); $[\alpha]_D^{22}$ +72.6 (*c* 1.0, $CHCl_3$) for 77% ee (*R*); From the reaction catalyzed by **V(O)-2** in *i*-PrOH (56% yield, 130h): t_R 26.9 min (minor, 18%), 30.0 min (major, 82%) for 64% ee (*S*); From the reaction catalyzed by **V(O)-2** in EtOH (54% yield, 24h): t_R 27.1 min (minor, 12.3%), 30.5 min (major, 87.7%) for 75.4% ee (*S*).



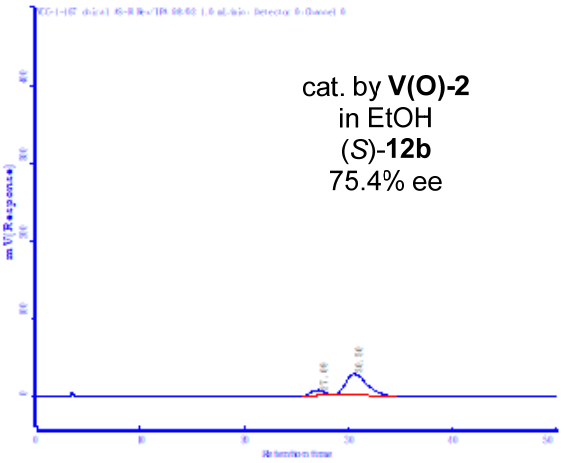
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		25.943	5225.68	50.80	0.00
1		29.696	5061.21	49.20	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		25.804	11159.31	88.58	0.00
1		29.744	1438.38	11.42	0.00

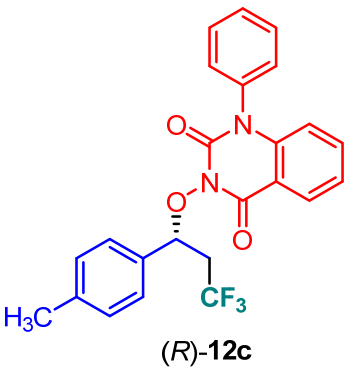


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		26.942	4246.58	17.94	0.00
1		30.030	19418.90	82.06	0.00



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		27.093	513.06	12.29	0.00
1		30.500	3660.08	87.71	0.00

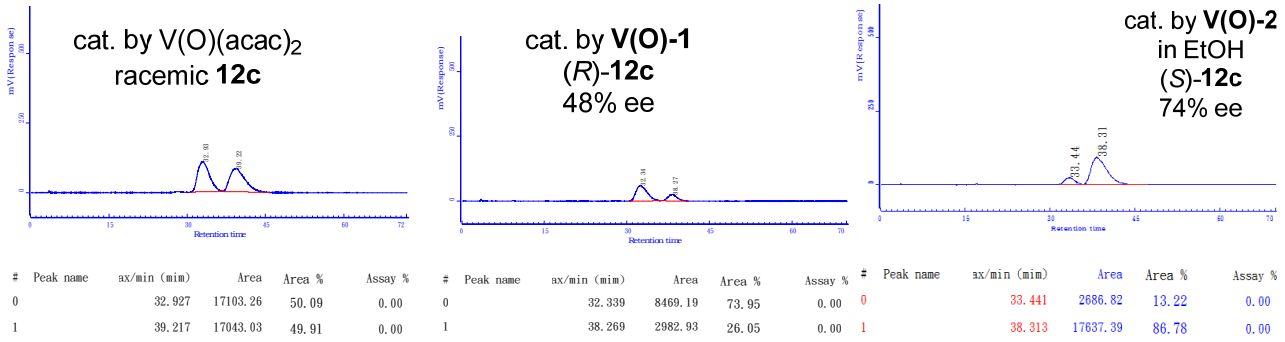
(*R*)-1-Phenyl-3-(3,3,3-trifluoro-1-(*p*-tolyl)propoxy)quinazoline-2,4(1H,3H)-dione 12c



(*R*)-**12c**

Data for **12c**: 104.5 mg, 80% yield, 24h: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, J = 7.9, 1.1 Hz, 1H), 7.60-7.11 (m, 11 H), 6.47 (d, J = 8.3 Hz, 1H), 5.83 (t, J = 6.4 Hz, 1H), 3.26-3.13 (m, 1H), 2.94-2.80 (m, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 148.9, 140.6, 139.6, 135.7, 134.7, 132.5, 130.4, 129.6, 129.0, 128.9, 128.6, 125.3 ($^{1}J_{C\text{-}F}$ = 276.9 Hz), 123.4, 115.5, 114.9, 81.1, 38.8 ($^{2}J_{C\text{-}F}$ = 28.6 Hz), 21.2; ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.1 (s, 3F); TLC R_f 0.27 (EtOAc/hexanes, 1/6); HRMS (FD) Calcd for

$C_{24}H_{19}F_3N_2O_3$: 440.1353, found: 440.1340; HPLC analysis form racemic product: t_R 32.93 min (*R*), 39.22 min (*S*) (Chiralpak AS-H, *i*-PrOH/*n*-hexane, 2/98, 1.0 mL/min, λ = 254 nm); From the reaction catalyzed by **V(O)-1**: t_R 32.34 min (major, 74%), 38.27 min (minor, 26%); $[\alpha]_D^{22}$ +112.9 (*c* 1.0, $CHCl_3$) for 48% ee (*R*); From the reaction catalyzed by **V(O)-2** in EtOH (64% yield, 96 h): t_R 33.4 min (minor, 13.2%), 38.3 min (major, 86.8%) for 74% ee (*S*).

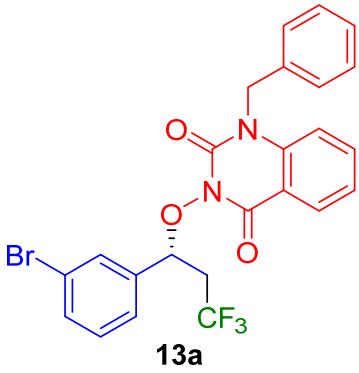


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		32.927	17103.26	50.09	0.00
1		39.217	17043.03	49.91	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		32.339	8469.19	73.95	0.00
1		38.269	2982.93	26.05	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		33.441	2686.82	13.22	0.00
1		38.313	17637.39	86.78	0.00

(*R*)-1-Benzyl-3-(1-(3-bromophenyl)-3,3,3-trifluoropropoxy)quinazoline-2,4(1H,3H)-dione 13a

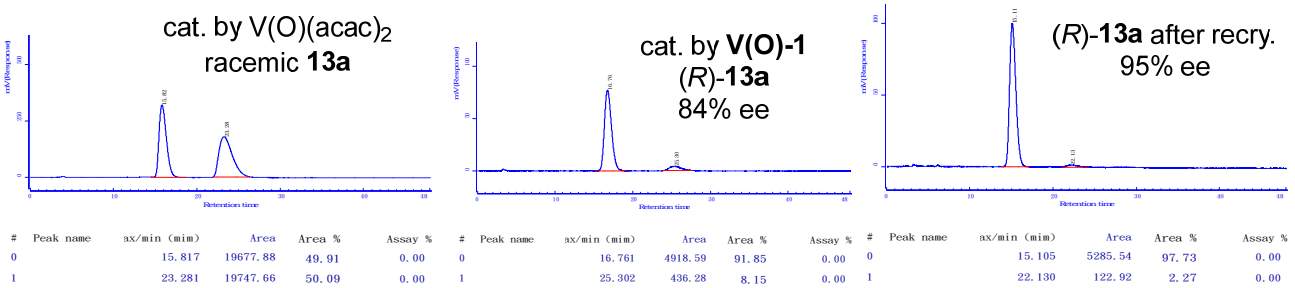


13a

White solid; Yield 96/82% (198.6 mg for 0.4 mmol scale in EtOH or *i*-PrOH, 26h/44h); Data for **13a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 7.8, 1.4 Hz 1H), 7.67 (t, *J* = 1.8 Hz, 1H), 7.54-7.49 (m, 3H), 7.33-7.28 (m, 3H), 7.25-7.20 (m, 2H), 7.04-7.01 (m, 3H), 5.82 (t, *J* = 6.4 Hz, 1H), 5.39 (d, *J* = 16.4 Hz, 1H), 5.16 (d, *J* = 16.4 Hz, 1H), 3.27-3.14 (m, 1H), 2.91-2.78 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.0, 149.8, 139.2, 138.1, 135.5, 135.1, 133.0, 131.9, 130.2, 129.2, 129.2, 128.0, 127.4, 126.4, 125.2 (q, $^1J_{C\text{-}F}$ = 275.5 Hz), 123.7, 122.5, 115.6, 114.8, 80.7, 47.5, 39.2 (q, $^2J_{C\text{-}F}$ = 28.8 Hz); ^{19}F NMR (471 Hz, $CDCl_3$) δ -63.1 (s, 3F); TLC R_f 0.25 (EtOAc/hexanes, 1/4); HRMS (FD) Calcd for $C_{24}H_{18}BrF_3N_2O_3$: 518.0447, found: 518.0455.

For racemic synthesis catalyzed by $V(O)(acac)_2$ in CH_3CN: 26% yield (53.6 mg, 17h): HPLC analysis from racemic product: t_R 15.8min (*R*), 23.3 min (*S*) (Chiralpak AS-H, *i*-PrOH/hexane, 10/90, 1.0 ml/min, λ = 254 nm); For the reaction catalyzed by **V(O)-1**: t_R 16.8 min (major, 91.9%), 25.3 min

(minor, 8.1%); $[\alpha]_D^{25}$ +108.0 (*c*, 1.0, $CHCl_3$) for 84% ee (*R*); X-ray crystallographic analysis was done for recrystallized (*R*)-**13a** (95% ee) from a mixed solvent of *n*-hexane/acetone (1/2.5).

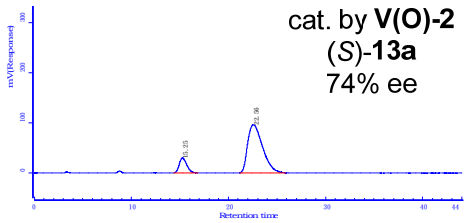


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.817	19677.88	49.91	0.00
1		23.281	19747.66	50.09	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		16.761	4918.59	91.85	0.00
1		25.302	436.28	8.15	0.00

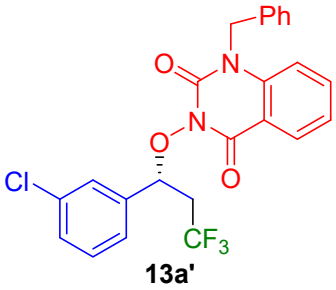
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.105	5285.54	97.73	0.00
1		22.130	122.92	2.27	0.00

For the reaction catalyzed by **V(O)-2**: Yield 45% (93 mg, 120h); t_R 15.3 min (minor, 13.1%), 22.6 min (major, 86.9%) for 74% ee (*S*).



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		15.250	1535.81	13.14	0.00
1		22.556	10156.28	86.86	0.00

(*R*)-1-Benzyl-3-(1-(3-chlorophenyl)-3,3,3-trifluoropropoxy)quinazoline-2,4(1H,3H)-dione 13a′

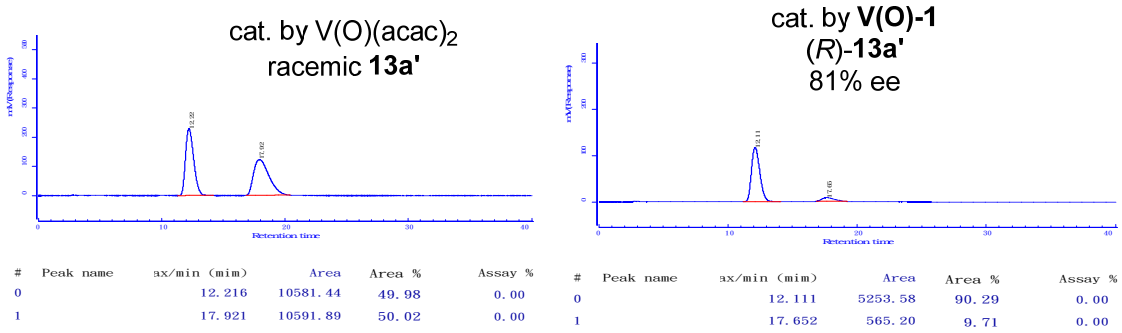


13a'

White solid; Yield: 82.5% (156.7 mg, 65h); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17 (dd, *J* = 7.8, 1.4 Hz 1H), 7.53-7.49 (m, 3H), 7.46 (d, *J* = 7.6 Hz, 1H), 7.36-7.24 (m, 5H), 7.21 (t, *J* = 7.8 Hz, 2H), 7.04-7.01 (m, 3H), 5.83 (t, *J* = 6.4 Hz, 1H), 5.39 (d, *J* = 16.4 Hz, 1H), 5.16 (d, *J* = 16.4 Hz, 1H), 3.27-3.14 (m, 1H), 2.92-2.79 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 149.6, 139.0, 137.7, 135.3, 135.0, 134.3, 129.9, 129.8, 129.0, 128.9, 128.8, 127.8, 126.8, 126.2, 125.0 (q, $^1J_{C\text{-}F}$ = 275.4 Hz), 123.5, 115.4, 114.6, 80.6 (q, $^3J_{C\text{-}F}$ = 2.5 Hz), 47.3, 39.0 (q, $^2J_{C\text{-}F}$ = 28.8 Hz); ^{19}F NMR (471 MHz, $CDCl_3$) δ -63.1 (s, 3F); R_f 0.25 (EtOAc/Hexanes, 1/4); HRMS (FD) $[M]^+$ Calcd for $C_{24}H_{18}F_3N_2O_3Cl$: 474.0953, found: 474.0949.

For racemic synthesis catalyzed by $V(O)(acac)_2$ in CH_3CN: 23% yield (43.7 mg, 18h); HPLC analysis from racemic product: t_R 12.22 min (*R*), 17.92 min (*R*) (Chiralpak AS-H, *i*-PrOH/hexane, 10/90, 1.2 ml/min, λ = 254 nm); For the reaction catalyzed by **V(O)-1**: t_R 12.11 min (major, 92.3%),

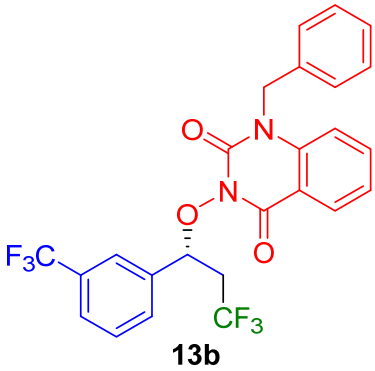
17.65 min (minor, 9.7%); $[\alpha]_D^{30}$ +112.6 (*c*, 1.0, $CHCl_3$) for 81% ee (*R*).



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.216	10581.44	49.98	0.00
1		17.921	10591.89	50.02	0.00

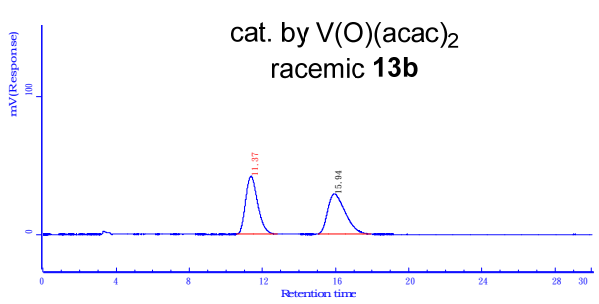
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.111	5253.58	90.29	0.00
1		17.652	565.20	9.71	0.00

(*R*)-1-Benzyl-3-(3,3,3-trifluoro-1-(3-(trifluoromethyl)phenyl)propoxy)quinazoline-2,4(1H,3H)-dione 13b

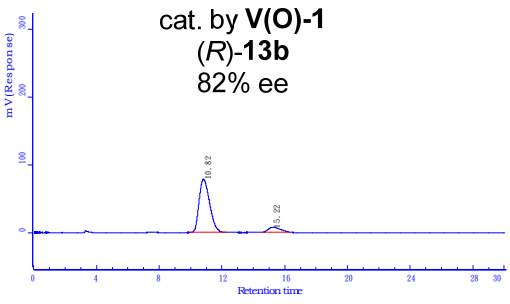


13b

White solid; Yield 88% (178.3 mg, 46h); Data for **13b**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.80-7.83 (m, 2H), 7.63 (d, *J* = 7.9 Hz, 1H), 7.53-7.48 (m, 2H), 7.30-7.24 (m, 3H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.05-7.01 (m, 3H), 5.91 (t, *J* = 6.7 Hz, 1H), 5.35 (d, *J* = 16.4 Hz, 1H), 5.19 (d, *J* = 16.4 Hz, 1H), 3.30-3.20 (m, 1H), 2.94-2.84 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.8, 149.6, 139.0, 136.8, 135.4, 134.9, 132.0, 130.8 (q, $^2J_{C-F}$ = 32.4 Hz), 129.0, 129.0, 127.8, 126.5 (q, $^3J_{C-F}$ = 3.3 Hz), 126.1, 125.5 (q, $^3J_{C-F}$ = 3.3 Hz), 125.0 (q, $^1J_{C-F}$ = 275.4 Hz), 123.7 (q, $^1J_{C-F}$ = 271.0 Hz), 123.5, 115.3, 114.7, 80.6 (q, $^3J_{C-F}$ = 2.3 Hz), 47.4, 39.0 (q, $^2J_{C-F}$ = 28.9 Hz); ^{19}F NMR (471 Hz, $CDCl_3$) δ -62.69 (s, 3F), -63.02 (s, 3F); TLC R_f 0.25 (EtOAc/hexanes, 1/5); HRMS (FD) Calcd for $C_{25}H_{18}N_2O_3F_6$: 508.1216, found: 508.1213; HPLC analysis from racemic product: t_R 11.4 min (*R*), 15.9 min (*S*) (Chiralpak AS-H, *i*-PrOH/hexane, 7/93, 1.0 ml/min, λ = 254 nm). For the reaction catalyzed by **V(O)-1**: t_R 10.8 min (major, 91.0%), 15.2 min (minor, 9.0%); $[\alpha]_D^{30}$ +119.9 (*c*, 1.0, $CHCl_3$) for 82% ee (*R*). For racemic synthesis catalyzed by V(O)(acac)$_2$ in CH_3CN: 27% yield (54.9 mg, 20h).

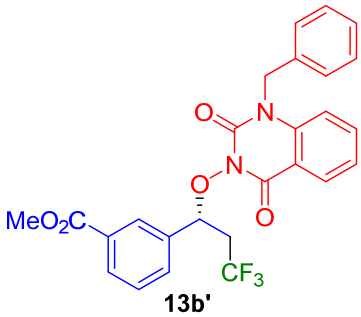


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		11.369	1938.19	50.00	0.00
1		15.937	1937.94	50.00	0.00



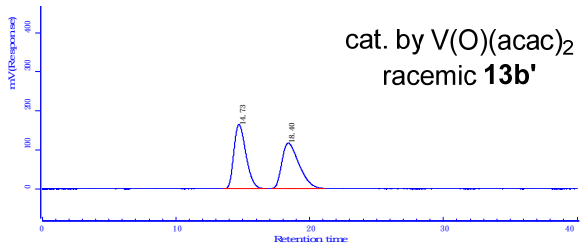
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		10.818	3640.50	90.98	0.00
1		15.222	361.05	9.02	0.00

Methyl (*R*)-3-(1-((1-Benzyl-2,4-dioxo-1,4-dihydroquinazolin-3(2H)-yl)oxy)-3,3,3-trifluoropropyl) -benzoate 13b'

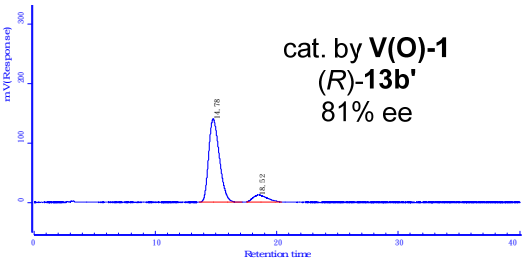


13b'

White solid; Yield 90% (180.1 mg, 46h); Data for **13b'**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.16-8.13 (m, 2H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.81 (d, *J* = 7.8 Hz, 1H), 7.51-7.42 (m, 2H), 7.26-7.24 (m, 3H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 8.4 Hz, 1H), 6.97-6.95 (m, 2H), 5.90 (t, *J* = 6.6 Hz, 1H), 5.36 (d, *J* = 16.4 Hz, 1H), 5.11 (d, *J* = 16.4 Hz, 1H), 3.87 (s, 3H), 3.22-3.19 (m, 1H), 2.97-2.83 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 158.7, 149.5, 138.9, 136.1, 135.3, 134.9, 133.1, 130.9, 130.3, 129.8, 128.9, 128.6, 127.7, 126.1, 125.2 (q, $^{1}J_{C\text{-}F}$ = 275.3 Hz), 123.4, 115.3, 114.6, 80.8, 52.1, 47.2, 38.9 (q, $^{2}J_{C\text{-}F}$ = 28.8 Hz); ^{19}F NMR (471 Hz, $CDCl_3$) δ -62.99 (s, 3F); TLC R_f 0.25 (EtOAc/hexanes, 1/2); HRMS (FD) $[M]^+$ Calcd for $C_{26}H_{21}N_2O_5F_3$: 498.1398, found: 498.1397; HPLC analysis from racemic product: t_R 14.7 min (*R*), 18.4 min (*S*) (Chiralpak AS-H, *i*-PrOH/hexane, 15/85, 1.2 ml/min, λ = 254 nm). For the reaction catalyzed by **V(O)-1**: t_R 14.8 min (major, 90.4%), 18.5 min (minor, 9.6%); $[\alpha]_D^{30}$ +137.1 (*c*, 1.0, $CHCl_3$) for 81% ee (*R*). For racemic synthesis catalyzed by $V(O)(acac)_2$ in CH_3CN: 28% yield (55.8 mg, 17h).

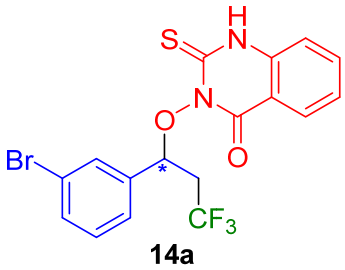


#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		14.725	10274.04	49.96	0.00
1		18.399	10289.90	50.04	0.00



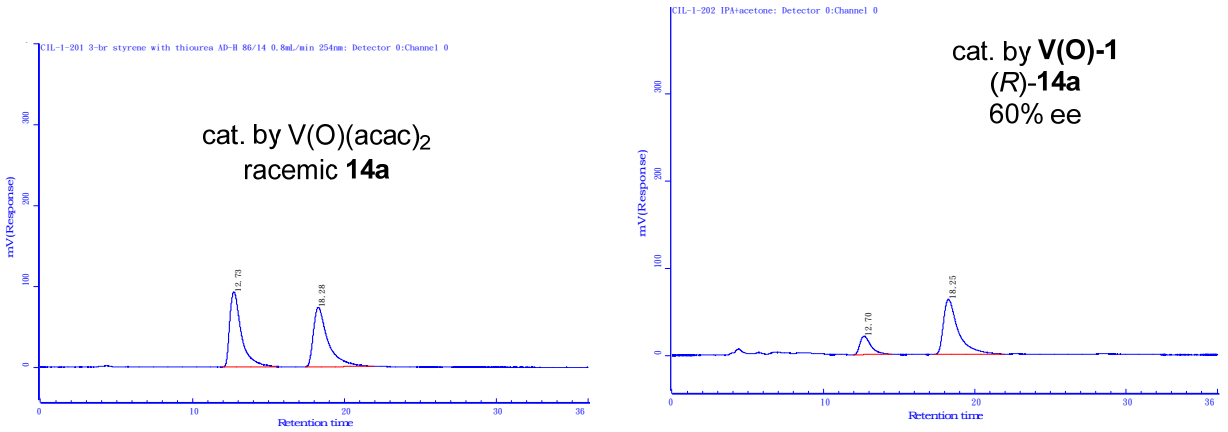
#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		14.779	8581.88	90.44	0.00
1		18.523	906.99	9.56	0.00

3-(1-(3-bromophenyl)-3,3,3-trifluoropropoxy)-2-thioxo-2,3-dihydroquinazolin-4(1H)-one 14a



14a

White solid; Yield 4.3% (7.4 mg for 0.4 mmol scale in acetone/*i*-PrOH 0.5/4 mL, 48 h); Data for **14a**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.83 (s, 1H), 8.09 (d, J = 7.8 Hz, 1H), 7.71 (t, J = 1.6 Hz, 1H), 7.67-7.63 (m, 1H), 7.49-7.45 (m, 2H), 7.26 (t, J = 7.8 Hz, 1H), 7.21 (t, J = 7.8 Hz, 1H), 7.09 (d, J = 8.0 Hz, 1H), 5.71 (t, J = 6.6 Hz, 1H), 3.26-3.13 (m, 1H), 2.89-2.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 149.9, 138.2, 137.5, 135.5, 132.9, 131.4, 130.0, 128.5, 127.0, 125.0 (q, $^{1}J_{C\text{-}F}$ = 275.3 Hz), 123.9, 122.4, 115.4, 114.6, 81.1, 39.2 (q, $^{2}J_{C\text{-}F}$ = 28.8 Hz); ^{19}F NMR (471 Hz, $CDCl_3$) δ -63.1 (s, 3F); TLC R_f 0.25 (EtOAc/hexanes, 1/2); HRMS (FD) Calcd for $C_{17}H_{12}BrF_3N_2O_2S$: 443.9798, found: 443.9803; HPLC analysis from racemic product: t_R 12.7 min (*S*), 18.3 min (*R*) (Chiralpak AD-H, *i*-PrOH/hexane, 14/86, 0.8 ml/min, λ = 254 nm). For the reaction catalyzed by **V(O)-1**: t_R 12.7 min (minor, 20.0%), 18.3 min (major, 80.0%) for 60% ee (*R*); $[\alpha]_D^{25}$ +90.0 (*c*, 0.06, $CHCl_3$) for 60% ee (*R*). For racemic synthesis catalyzed by $V(O)(acac)_2$ in CH_3CN: 7.4% yield (13.2 mg, 30h).



#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.731	4989.25	50.12	0.00
1		18.277	4965.15	49.88	0.00

#	Peak name	ax/min (mim)	Area	Area %	Assay %
0		12.704	1058.35	19.99	0.00
1		18.254	4237.18	80.01	0.00

Figure S1: X-ray crystal structure of (*R*)-**12a** (CCDC 2215699) in Platon drawing (ellipsoids are shown at 50% probability level)

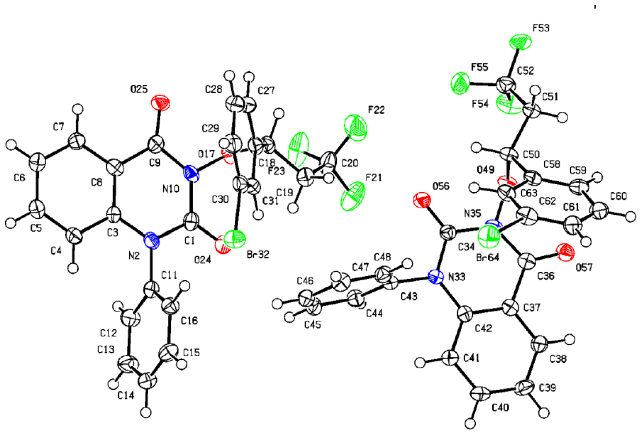


Table S1 Crystal data and structure refinement for (*R*)-12a (2208117lt2_auto)**.**

Identification code	2208117lt2_auto
Empirical formula	$C_{46}H_{32}Br_2F_6N_4O_6$
Formula weight	1010.57
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	10.22560(11)
b/Å	20.67971(18)
c/Å	10.38564(11)
α/°	90
β/°	110.7384(12)

γ/°	90
Volume/Å^3	2053.88(4)
Z	2
ρ_{calc}g/cm^3	1.634
μ/mm^{-1}	3.239
F(000)	1016.0
Crystal size/mm^3	0.14 × 0.09 × 0.03
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.552 to 134.146
Index ranges	-11 ≤ h ≤ 12, -24 ≤ k ≤ 24, -12 ≤ l ≤ 12
Reflections collected	23889
Independent reflections	7328 [R_{int} = 0.0235, R_{sigma} = 0.0223]
Data/restraints/parameters	7328/1/577
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R_1 = 0.0378, wR_2 = 0.1058
Final R indexes [all data]	R_1 = 0.0384, wR_2 = 0.1065
Largest diff. peak/hole / e Å^{-3}	1.99/-0.55
Flack parameter	-0.016(8)

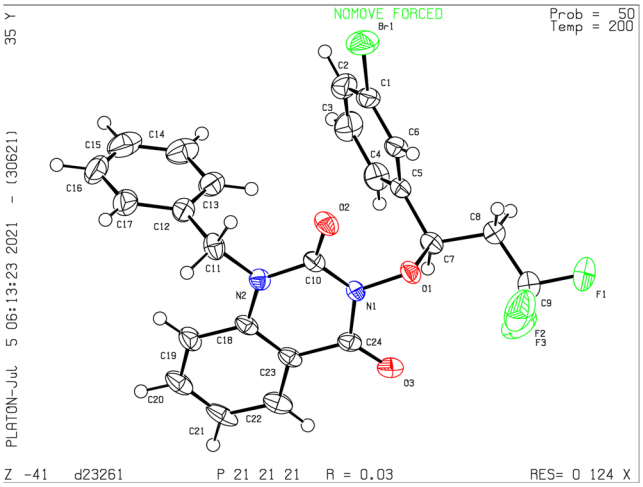


Figure S2. X-ray crystal structure of (*R*)-**13a** (CCDC 2094844) in Platon drawing (ellipsoids are shown at 50% probability level)

Selected data for X-ray crystal structure of (*R*)-**13a**

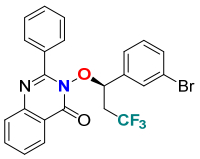
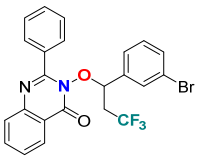
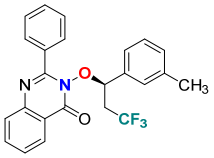
Crystal data and structural refinement for (*R*)-13a: $C_{24}H_{18}BrF_3N_2O_3$, *Mr* = 519.3, prism, space group P 21 21 21, a = 9.0260(3) Å, b = 13.0929(5) Å, c = 18.3842(7) Å, α = 90.0, β = 90, γ = 90, *V* = 2172.58(14) $Å^3$, Z = 4, ρ_{calcd} = 1.588 Mgm^{-3}, *T* = 200(2) K, Bruker Kappa CCD diffractometer, Mo K_α radiation (λ = 0.71073), μ = 1.948 mm^{-1}. The structure was solved by SHELXL-86 (Sheldrick, 1986) Solver. All non-hydrogen atoms were refined anisotropically (SHELXS-97; Sheldrick, 1997). Final block-diagonal matrix least-square refinement on F^2 with all 3835 reflections and 298 variables converged to *R*1 ($I > 2\sigma(I)$) = 0.0327, *w*R2 (all data) = 0.0759 and GOF = 0.940. Absolute structure parameter 0.023(8).

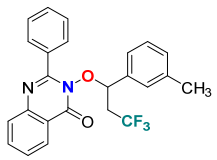
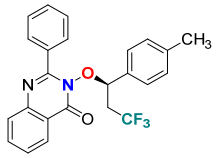
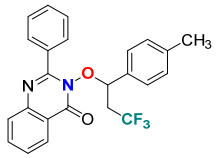
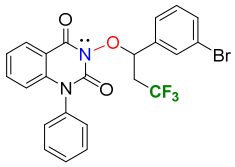
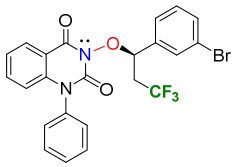
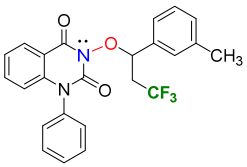
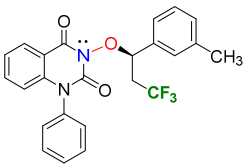
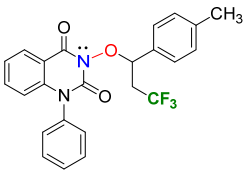
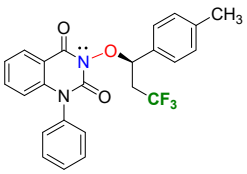
EGFR-TK inhibition results:

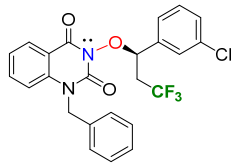
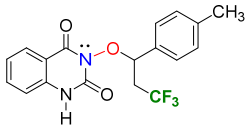
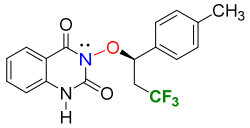
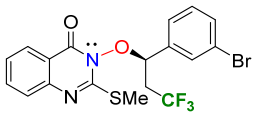
Preliminary EGFR-TK inhibition test results for our compounds at single point analyses at 1 μM concentrations are attached at the end. These results are compiled as a Table in SI as shown below: Project #: SSBK13429_63766 (samples 1-15; on Oct. 28); SSBK13429_64251 (sample 1 on Dec. 16); Test Compound Concentration: 1,000 nM; [ATP] Tested: Km app

Kinase Tested: EGFR (ErbB1); Kinase lot#: PV3872/2281133

Table S2: EGFR-TK inhibition results

Sample name	structure	Sample number in the paper	% Inhibition Point 1/point 2	% inhibition mean
sample1		(*R*)-**9a** (*S*)-**9a**	-3/-2	-3 -3
sample2		Racemic-**9a**	0/-5	-3
sample3		(*R*)-**9b** (*S*)-**9b**	-4/-6	-5 -10

sample4		Racemic-**9b**	-8/-7	-8
sample5		(*R*)-**9c** (*S*)-**9c**	-2/-2	-2 -2
sample6		Racemic-**9c**	-3/-2	-2
sample7		Racemic-**12a**	0/-1	-1
sample8		(*R*)-**12a** (*S*)-**12a**	-5/-3	-4 2 (predicted)
sample9		Racemic-**12b**	-5/-5	-5
sample10		(*R*)-**12b** (*S*)-**12b**	-17/1 ----	-8 -2 (predicted)
sample11		Racemic-**12c**	-5/-4	-4
sample12		(*R*)-**12c** (*S*)-**12b**	-6/-3	-4 -4

sample13		(*R*)-**13a'**	-4/-2	-3
sample14		Racemic-**11a'**	-4/1	-1
sample15		(*R*)-**11a'** (*S*)-**11a'**	-4/2	-1 -1
sample 1		(*R*)-**10a**	3/5	4

The data in green are calculated from the data of the (*R*) and racemic products In general, EGFR-TK inhibition activity profile is in the order of (*S*) 1-Ph (IC_{50}: 25 μM) > 2-H > 2-Ph in the quinazoline moieties and in the order of *m*-Cl/Br > *p*-Me > *m*-Me in the styrene substrate units. Notably, (*R*)-**10a** (2-SMe and *m*-Br) showed discernible EGFR-TK inhibition activity whose IC_{50} is estimated to be around 10-12.5 μM.

Experimental References:

(S1) (a) Deore, R. R.; Chen, G. S.; Chang, P.-T.; Chern, T.-R.; Lai, S.-Y.; Chuang, M.-H.; Lin, J.-H.; Kung, F.-L.; Chen, C.-S.; Chiou, C.-T.; Chern, J.-W. Discovery of *N*-Arylalkyl-3-hydroxy-4-oxo-3,4-dihydroquinazolin-2-carboxamide Derivatives as HCV NS5B Polymerase Inhibitors. *ChemMedChem* **2012**, *7*, 850–860. (b) Tanaka, K.; Matsuo, K.; Nakanishi, A.; Kataoka, Y.; Takase, K.; Otsuki, S. *Chem. & Pharm. Bull.* **1988**, *36*, 2323–2330.

(S2) Cheng, R.; Guo, T.; Zhang-Negrerie, D.; Du, Y.; Zhao, K. One-Pot Synthesis of Quinazolinones From Anthranilamides And Aldehydes via *P*-Toluenesulfonic Acid Catalyzed Cyclocondensation and Phenyliodine Diacetate Mediated Oxidative Dehydrogenation. *Synthesis* **2013**, *45*, 2998–3006.

(S3) (a) Falsini, M.; Squarcialupi, L.; Catarzi, D.; Varano, F.; Betti, M.; Di Cesare Mannelli, L.; Tenci, B.; Ghelardini, C.; Tanc, M.; Angeli, A.; Supuran, C. T.; Colotta, V. 3-Hydroxy-1H-quinazoline-2,4-

dione as a new scaffold to develop potent and selective inhibitors of the tumor-associated carbonic anhydrases IX and XII. *J. Med. Chem.* **2017**, *60*, 6428–6439. (b) Kang, D.; Zhang, H.; Zhou, Z.; Huang, B.; Naesens, L.; Zhan, P.; Liu, X. First Discovery of Novel 3-Hydroxy-Quinazoline-2,4(1H,3H)-Diones as Specific Anti-Vaccinia And Adenovirus Agents via 'Privileged Scaffold' Refining Approach. *Bioorg. Med. Chem. Lett.* **2016**, *26*, 5182–5186.

(S4) (a) Geffken, D.; Koellner, M. A. Oxalylierung Von *N*-Phenylanthranilo-*O*-Alkylhydroxam-säuren zu 4-Alkoxy-2,3,4,5-Tetrahydro-1H-1,4-Benzodiazepin-2,3,5-Trionen. Z. *fur Naturforsch. – B: Chem*. Sci. **2005**, *60*, 337−340. (b) Domagala, John Michael; Ellsworth, Edmund L.; Huang, L.; Renau, T. E.; Singh, R.; Stier, M. A. WO9921840 A1 **1999**.

(S5) Tang, J.; Maddali, K.; Dreis, C. D.; Sham, Y. Y.; Vince, R.; Pommier, Y.; Wang, Z. 3-Hydroxy-pyrimidine-2,4-diones as an Inhibitor Scaffold of HIV Integrase. *J. Med. Chem*. **2011**, *2*, 63−67.

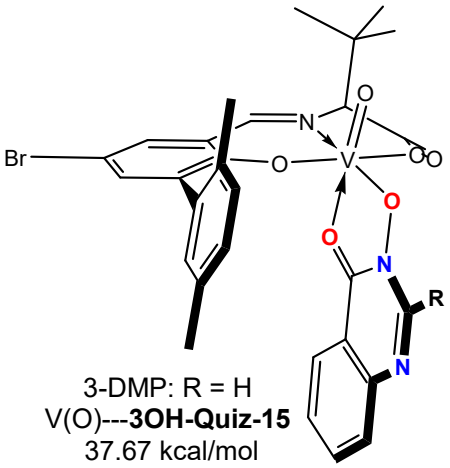
(S6) Khokhlov, P. S.; Osipov, V. N.; Roshchin, A.V. 3-Hydroxy- and 3-Alkoxy-2-Sulfanylquinazolin-4(3*H*)-Ones: Synthesis and Reactions with Alkylating and Acylating Agents. *Russ. Chem. Bull.* **2011**, *60*, 153–156.

Theoretical calculation:

Optimized geometry: The structure of a chemical sample corresponding to an energy minimum by using Scigress program. The structure of the chemical sample is refined by performing an optimize geometry calculation in Mechanics using Augmented MM3 parameters. The sandwich structure optimizations were done by performing an optimize geometry calculation in Mechanics using Augmented MM2 parameters.

Representative Cartesian coordinates

Figure S4



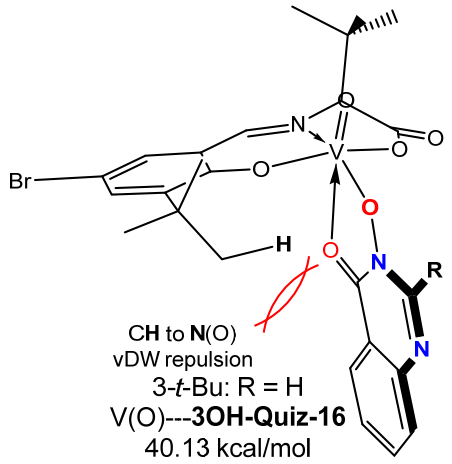
3-DMP: R = H
V(O)---**3OH-Quiz-15**
37.67 kcal/mol

Total number of atoms: 67 for 3-DMP: R = H: **V(O)---3OH-Quiz-15**

O	1	6.73873	-6.11915	-2.10071
Br	2	3.88336	-8.26748	-9.22057
V	3	5.55584	-5.10638	-2.78859
O	4	4.74563	-4.81818	-1.03396
O	5	2.73769	-5.11288	-0.073871
O	6	6.39121	-5.39113	-4.52495
N	7	4.24996	-6.56281	-2.92489
H	8	5.852	-8.29955	-1.2635
H	9	2.35456	-9.28569	-2.24777
H	10	2.38779	-6.76036	-2.07229
H	11	3.09999	-7.8136	-4.0403
H	12	3.19443	-8.18126	-6.34802
H	13	5.42615	-7.32532	0.18678
H	14	2.97377	-7.3866	1.04438
H	15	1.66333	-7.98343	-0.029932
H	16	2.77054	-9.13702	0.774775
H	17	4.10056	-9.41344	-2.66628
H	18	3.46182	-10.2591	-1.23456

H	19	6.19221	-6.42207	-8.89175
H	20	5.25227	-9.10562	0.212011
C	21	3.59611	-5.52296	-0.822372
C	22	5.12598	-8.20318	-0.427088
C	23	2.72266	-8.14558	0.27112
C	24	3.38269	-9.31685	-1.82225
C	25	3.95095	-7.11369	-4.03839
C	26	4.62273	-6.88652	-5.34354
C	27	3.6782	-8.0794	-0.944277
C	28	3.45169	-6.75014	-1.73742
C	29	4.08148	-7.53685	-6.46117
C	30	4.64213	-7.37893	-7.72423
C	31	5.75126	-6.56021	-7.89083
C	32	6.31486	-5.91395	-6.79087
C	33	5.76929	-6.09106	-5.50975
O	34	4.258	-3.8774	-3.57387
O	35	6.71952	-3.55148	-2.59304
C	36	4.6695	-2.74358	-3.61814
N	37	5.92263	-2.4335	-3.15244
C	38	7.47458	-5.01892	-7.00436
C	39	6.35527	-1.09525	-3.24398
C	40	4.49912	-0.339831	-4.14949
C	41	3.89948	-1.60773	-4.15365
C	42	3.76651	0.73737	-4.65308
C	43	2.47318	0.557795	-5.14737
C	44	1.89138	-0.70907	-5.14352
C	45	2.60503	-1.79728	-4.64483
H	46	7.37567	-0.942876	-2.85604
H	47	4.21717	1.74361	-4.65808
H	48	1.90955	1.42079	-5.54059
H	49	0.868394	-0.849741	-5.53183
H	50	2.14642	-2.80031	-4.63705
N	51	5.68208	-0.114375	-3.70937
C	52	7.29566	-3.85883	-7.76375
C	53	8.34269	-2.96225	-7.98823
C	54	9.59455	-3.24314	-7.44061
C	55	9.79019	-4.40125	-6.69104
C	56	8.74199	-5.30137	-6.46908

C	57	8.10482	-1.71742	-8.80445
H	58	10.4378	-2.55187	-7.60355
C	59	9.02943	-6.56034	-5.68687
H	60	6.30066	-3.63662	-8.18324
H	61	10.7891	-4.61089	-6.27381
H	62	7.89738	-1.97553	-9.86683
H	63	7.23247	-1.14568	-8.41637
H	64	8.98177	-1.03276	-8.79149
H	65	8.32179	-7.38275	-5.9306
H	66	8.96754	-6.36925	-4.59251
H	67	10.0514	-6.94551	-5.90026



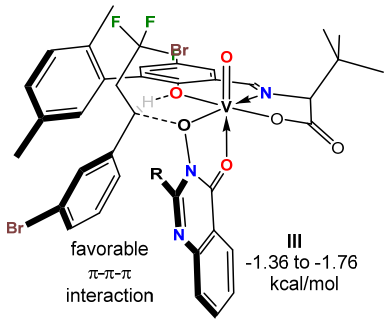
Total number of atoms: 63; for 3-*t*-Bu: R = H: **V(O)---3OH-Quiz-16**

O	1	-9.659336	1.797626	2.127046
Br	2	-16.811954	2.813393	-1.338457
V	3	-10.024867	0.893162	0.732303
O	4	-8.194422	1.113654	0.081715
O	5	-7.132976	2.020316	-1.678004
O	6	-11.844519	0.703528	1.406472
N	7	-10.377574	2.494479	-0.337559
C	8	-8.043286	2.069887	-0.881647
C	9	-8.322933	4.41988	1.090048
C	10	-7.586466	5.032671	-1.221773
C	11	-9.918575	5.505432	-0.490072
C	12	-11.558538	2.820453	-0.698855
C	13	-12.830293	2.196559	-0.248407
C	14	-8.766082	4.480191	-0.386292
C	15	-9.201025	3.079991	-0.931968

C	16	-14.000412	2.661073	-0.859163
C	17	-15.241238	2.160993	-0.491969
C	18	-15.331261	1.183259	0.4902
C	19	-14.183162	0.690297	1.128053
C	20	-12.924117	1.222132	0.763367
O	21	-10.431136	-0.2242	-0.816365
O	22	-9.571693	-0.768099	1.652041
C	23	-10.23081	-1.395096	-0.601871
N	24	-9.779994	-1.815812	0.6242
C	25	-14.321308	-0.391773	2.203636
C	26	-9.54327	-3.192647	0.810356
C	27	-10.145026	-3.782419	-1.221053
C	28	-10.43529	-2.462169	-1.595965
C	29	-10.331252	-4.792923	-2.166791
C	30	-10.798673	-4.498513	-3.449008
C	31	-11.08865	-3.181832	-3.80368
C	32	-10.905783	-2.158026	-2.876093
N	33	-9.716254	-4.112544	-0.058693
C	34	-13.739633	0.089862	3.555184
C	35	-15.791765	-0.787494	2.494914
C	36	-13.608381	-1.691682	1.761671
H	37	-11.131097	-1.114866	-3.154888
H	38	-9.170927	4.164301	1.761477
H	39	-7.517525	3.670506	1.255652
H	40	-7.929108	5.402194	1.434899
H	41	-7.825196	5.050329	-2.308903
H	42	-6.660305	4.431448	-1.090322
H	43	-7.330581	6.075302	-0.927649
H	44	-10.301892	5.592685	-1.53123
H	45	-10.774748	5.241586	0.169406
H	46	-9.586818	6.522188	-0.182268
H	47	-11.648488	3.64261	-1.426859
H	48	-9.435288	3.225341	-2.012648
H	49	-13.947015	3.435373	-1.641435
H	50	-16.332149	0.807498	0.748641
H	51	-10.104255	-5.837379	-1.895776
H	52	-10.939057	-5.309802	-4.183485
H	53	-11.459296	-2.95002	-4.816486

H	54	-14.210108	1.044753	3.880884
H	55	-12.641897	0.257104	3.525659
H	56	-13.91854	-0.655018	4.362384
H	57	-16.394094	0.074979	2.860064
H	58	-15.850713	-1.567316	3.287038
H	59	-16.298332	-1.214447	1.60007
H	60	-14.000322	-2.057975	0.786219
H	61	-12.511018	-1.56617	1.647277
H	62	-13.756559	-2.508144	2.503392
H	63	-9.175706	-3.435738	1.820707

Figure S5 for R = H



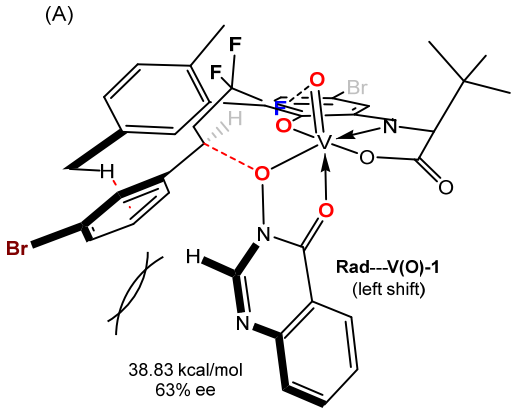
Total number of atoms: 87

C	1	-5.915243	1.654716	-0.123429
F	2	-4.219972	3.084721	0.853296
F	3	-6.330921	3.814627	0.833511
F	4	-5.164406	3.762307	-1.073491
C	5	-5.396961	3.074249	0.11045
C	6	-5.209255	-1.523195	-2.246461
C	7	-5.640979	-2.841375	-2.400084
C	8	-6.529722	-3.39596	-1.480361
C	9	-6.977025	-2.61477	-0.413628
C	10	-6.534319	-1.297151	-0.266652
C	11	-5.130677	0.736701	-1.046837
C	12	-5.633888	-0.727296	-1.175525
O	13	-2.512363	3.008522	-1.456179
Br	14	-3.885763	1.982587	-8.982528
V	15	-2.221992	1.359263	-1.807802
O	16	-0.582012	1.405857	-0.764667
O	17	1.550357	0.769885	-1.014079
O	18	-3.851356	1.372177	-2.909682

N	19	-0.978024	1.836481	-3.240824
Br	20	-8.191016	-3.344698	0.839911
C	21	0.57227	1.330851	-1.454501
C	22	0.439455	4.368686	-1.947979
C	23	2.606355	3.262997	-2.51421
C	24	1.064546	3.965614	-4.32785
C	25	-1.380037	1.882501	-4.4413
C	26	-2.607014	1.760899	-4.996393
C	27	1.115066	3.367838	-2.90597
C	28	0.447285	1.965094	-2.844928
C	29	-2.656817	1.8912	-6.392706
C	30	-3.854948	1.797678	-7.098669
C	31	-5.03452	1.570184	-6.396209
C	32	-4.994078	1.444126	-5.006214
C	33	-3.797937	1.531715	-4.271995
O	34	-1.868931	-0.539922	-2.102673
O	35	-3.51279	0.699949	-0.4785
C	36	-2.251547	-1.273195	-1.217086
N	37	-3.044041	-0.695229	-0.237004
C	38	-6.174462	1.238622	-4.399799
C	39	-3.419473	-1.462329	0.804685
C	40	-2.408342	-3.26334	-0.011654
C	41	-1.939187	-2.588434	-1.145063
C	42	-2.120479	-4.624293	0.126273
C	43	-1.379639	-5.291969	-0.852001
C	44	-0.918021	-4.605627	-1.977389
C	45	-1.195425	-3.246047	-2.129868
N	46	-3.094126	-2.682599	0.883034
C	47	-6.867286	2.295804	-3.795585
C	48	-8.088523	2.021544	-3.172021
C	49	-8.62503	0.73292	-3.177724
C	50	-7.96032	-0.314431	-3.818256
C	51	-6.731151	-0.04388	-4.425368
C	52	-8.567814	-1.692262	-3.84725
C	53	-6.333077	3.705674	-3.839849
H	54	-7.892202	-2.441526	-4.318347
H	55	-4.882391	1.162736	-2.080831
H	56	-6.902256	-0.723401	0.57176

H	57	-5.986737	1.193449	0.887213
H	58	-6.947081	1.73214	-0.537704
H	59	-4.521606	-1.127934	-2.981567
H	60	-5.292688	-3.432693	-3.238975
H	61	-6.86685	-4.417704	-1.609138
H	62	-0.614294	4.568442	-2.243805
H	63	0.442709	4.002328	-0.896904
H	64	0.96235	5.352095	-1.95106
H	65	3.142196	2.523243	-3.151534
H	66	2.739897	2.963288	-1.451253
H	67	3.131147	4.239106	-2.629262
H	68	1.513968	3.274428	-5.076544
H	69	0.024028	4.204648	-4.642832
H	70	1.629782	4.923645	-4.389177
H	71	-0.547039	2.03335	-5.145631
H	72	1.022305	1.287944	-3.522028
H	73	-1.752899	2.073622	-6.963361
H	74	-5.981725	1.497601	-6.919279
H	75	-2.474434	-5.172248	0.992253
H	76	-1.16172	-6.348062	-0.736875
H	77	-0.343075	-5.130243	-2.732139
H	78	-0.834027	-2.721139	-3.005724
H	79	-8.640527	2.81781	-2.686658
H	80	-9.578297	0.546479	-2.696974
H	81	-6.196482	-0.841162	-4.927229
H	82	-9.516834	-1.672597	-4.429408
H	83	-8.793596	-2.037091	-2.812983
H	84	-6.453053	4.112106	-4.869362
H	85	-6.87544	4.380948	-3.140091
H	86	-5.252254	3.746264	-3.580918
H	87	-4.06846	-1.06664	1.602237

Figure S6:



Total number of atoms: 87

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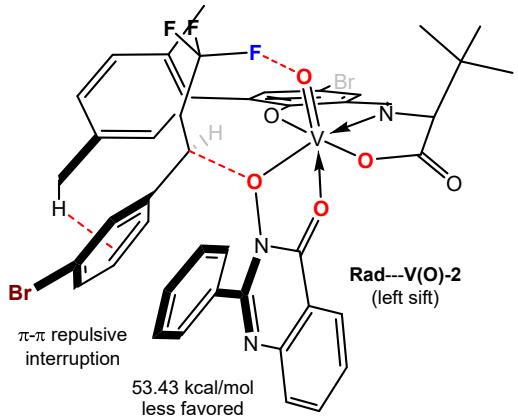
F	4	-4.644022	4.059367	0.091208
C	5	-4.331493	3.170257	1.110632
C	6	-5.973427	-0.889321	-1.566698
C	7	-6.737866	-2.047369	-1.699604
C	8	-7.557589	-2.465197	-0.655267
C	9	-7.589864	-1.72671	0.524952
C	10	-6.80275	-0.582883	0.665369
C	11	-5.083438	1.119664	-0.254032
C	12	-5.982646	-0.144036	-0.382744
O	13	-2.761431	2.925458	-1.790743
Br	14	-3.301081	1.169628	-9.419549
V	15	-2.290487	1.313662	-2.063241
O	16	-0.838594	1.473211	-0.766726
O	17	1.390706	1.220263	-0.761856
O	18	-3.713376	1.170239	-3.384536
N	19	-0.932572	1.871712	-3.363285
Br	20	-8.700614	-2.287584	1.9586
C	21	0.39672	1.619056	-1.326402
C	22	-0.109343	4.579535	-2.080081
C	23	2.25156	3.757359	-2.187932
C	24	0.972794	4.136048	-4.285071
C	25	-1.087563	1.780591	-4.630266
C	26	-2.343682	1.462183	-5.361091
C	27	0.848426	3.62989	-2.829231

C	28	0.358597	2.142185	-2.772725
C	29	-2.281726	1.448068	-6.76112
C	30	-3.413909	1.182073	-7.524138
C	31	-4.631179	0.946466	-6.898403
C	32	-4.722228	0.964046	-5.506101
C	33	-3.573215	1.205438	-4.733595
O	34	-1.781574	-0.542542	-2.366042
O	35	-3.483822	0.619146	-0.66319
C	36	-2.205473	-1.278915	-1.510441
N	37	-3.039482	-0.804232	-0.529433
C	38	-6.044128	0.728671	-4.881599
C	39	-3.346966	-1.681433	0.535467
C	40	-2.342338	-3.436572	-0.325137
C	41	-1.86543	-2.708655	-1.42305
C	42	-2.024023	-4.794262	-0.245392
C	43	-1.252361	-5.409337	-1.232775
C	44	-0.781749	-4.669547	-2.316704
C	45	-1.088618	-3.313786	-2.414103
N	46	-3.043967	-2.920323	0.614399
C	47	-6.682435	1.715229	-4.112378
C	48	-7.933028	1.43693	-3.550711
C	49	-8.565891	0.216946	-3.779465
C	50	-7.960782	-0.751359	-4.580561
C	51	-6.69908	-0.484823	-5.1169
C	52	-8.651676	-2.063584	-4.853825
C	53	-6.10414	3.098564	-3.930474
H	54	-7.920858	-2.888453	-5.010155
H	55	-5.295143	1.806348	-1.096858
H	56	-6.84295	-0.029093	1.615678
H	57	-4.885292	1.244283	1.891765
H	58	-6.239852	2.193225	1.21278
H	59	-5.333871	-0.577583	-2.407634
H	60	-6.692131	-2.631391	-2.633885
H	61	-8.170748	-3.374824	-0.766074
H	62	-1.105189	4.629509	-2.572172
H	63	-0.26566	4.26865	-1.023175
H	64	0.287653	5.619461	-2.057201
H	65	2.97502	3.0409	-2.63831

H	66	2.231741	3.574825	-1.090854
H	67	2.673133	4.777919	-2.329002
H	68	1.621894	3.471478	-4.898727
H	69	-0.01652	4.215054	-4.787817
H	70	1.423278	5.152915	-4.322304
H	71	-0.202502	1.978162	-5.255194
H	72	1.101838	1.537734	-3.344429
H	73	-1.327081	1.651092	-7.274045
H	74	-5.53253	0.757733	-7.503058
H	75	-2.387805	-5.387021	0.610518
H	76	-1.010787	-6.483027	-1.152109
H	77	-0.167806	-5.154812	-3.094723
H	78	-0.71965	-2.72558	-3.271195
H	79	-8.44139	2.199773	-2.938387
H	80	-9.558398	0.026392	-3.339068
H	81	-6.207588	-1.24997	-5.739191
H	82	-9.282713	-1.992198	-5.767596
H	83	-9.310847	-2.363984	-4.008732
H	84	-6.905805	3.867318	-3.866801
H	85	-5.507667	3.164804	-2.994903
H	86	-5.446627	3.394635	-4.777104
H	87	-3.938663	-1.208005	1.334146



Total number of atoms: 97

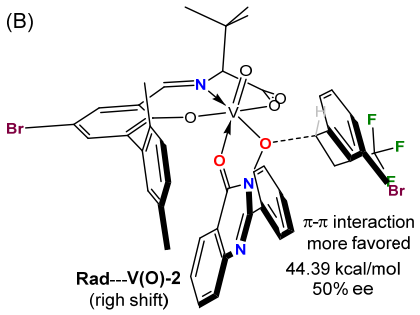
C	1	-5.564381	1.485704	0.709957
F	2	-3.364533	2.363022	1.230627
F	3	-5.136449	3.299977	2.206512
F	4	-4.758064	3.662077	0.038043
C	5	-4.696743	2.696945	1.033911

C	6	-5.924359	-1.193834	-2.081838
C	7	-6.686773	-2.320358	-2.386762
C	8	-7.668214	-2.757909	-1.502072
C	9	-7.871647	-2.066	-0.31101
C	10	-7.089233	-0.954618	0.003196
C	11	-5.188298	0.716542	-0.543951
C	12	-6.095687	-0.503854	-0.876449
O	13	-2.757883	2.684904	-1.552092
Br	14	-2.888106	1.54862	-9.390789
V	15	-2.314274	1.107889	-2.007612
O	16	-0.918541	1.067647	-0.642365
O	17	1.311816	0.838822	-0.557352
O	18	-3.670677	1.174605	-3.404236
N	19	-0.891814	1.799739 -	.166957
Br	20	-9.205086	-2.651891	0.906701
C	21	0.340045	1.295696	-1.116277
C	22	-0.145665	4.329488	1.491221
C	23	2.221829	3.537865	-1.635502
C	24	0.997223	4.176736	-3.703648
C	25	-0.972066	1.828202	-4.443873
C	26	-2.180999	1.572638	-5.27172
C	27	0.839212	3.487297	-2.329211
C	28	0.364363	2.002102	-2.482342
C	29	-2.032661	1.64737	-6.662962
C	30	-3.117872	1.44793	-7.509254
C	31	-4.37489	1.194282	-6.97566
C	32	-4.551785	1.126474	-5.592817
C	33	-3.450146	1.299321	-4.737563
O	34	-1.883437	-0.725004	-2.488624
O	35	-3.5307	0.203354	-0.766853
C	36	-2.368796	-1.567574	-1.77041
N	37	-3.194382	-1.264	-0.705904
C	38	-5.912626	0.876553	-5.065081
C	39	-3.660195	-2.313022	0.131126
C	40	-2.803289	-3.910693	-1.142537
C	41	-2.169669	-3.006987	-2.001845
C	42	-2.640452	-5.276477	-1.38398
C	43	-1.87466	-5.729317	-2.459898

C	44	-1.250355	-4.815966	-3.307644
C	45	-1.400354	-3.44923	-3.081912
N	46	-3.487868	-3.556219	-0.121335
C	47	-6.572239	1.813522	-4.252314
C	48	-7.855318	1.51992	-3.777594
C	49	-8.501781	0.341329	-4.142478
C	50	-7.877964	-0.568647	-4.996116
C	51	-6.581848	-0.293616	-5.439285
C	52	-8.590749	-1.825237	-5.427688
C	53	-5.985195	3.16861	-3.935778
H	54	-7.876559	-2.644384	-5.666575
H	55	-5.282001	1.433121	-1.381474
H	56	-7.264303	-0.443657	0.962232
H	57	-5.536215	0.804124	1.586398
H	58	-6.619132	1.835384	0.62169
H	59	-5.157364	-0.863999	-2.800755
H	60	-6.511542	-2.862541	-3.331121
H	61	-8.275171	-3.645112	-1.746343
H	62	-1.120565	4.456512	-2.009909
H	63	-0.344256	3.873909	-0.495816
H	64	0.252147	5.352382	-1.306308
H	65	2.965776	2.892764	-2.154556
H	66	2.171783	3.209823	-0.574122
H	67	2.63568	4.571167	-1.6262
H	68	1.682588	3.610161	-4.373063
H	69	0.023503	.295023	-4.227972
H	70	1.421523	.20021	-3.597057
H	71	-0.054621	2.088043	-4.995891
H	72	1.142119	1.48058	-3.088166
H	73	-1.0456	1.866973	-7.101464
H	74	-5.239335	1.058307	-7.646292
H	75	-3.117578	-6.006139	-0.709145
H	76	-1.75598	-6.812172	-2.634687
H	77	-0.641791	-5.172775	-4.155775
H	78	-0.916301	-2.723736	-3.75736
H	79	-8.378928	2.242804	-3.130284
H	80	-9.520418	0.140134	-3.771618
H	81	-6.075735	-1.017051	-6.099307

H	82	-9.203529	-1.635989	-6.336997
H	83	-9.271204	-2.204154	-4.632856
H	84	-6.775806	3.950376	-3.894948
H	85	-5.471928	3.165782	-2.949719
H	86	-5.251371	3.501225	-4.702249
C	87	-4.207879	-1.949712	1.461653
C	88	-5.254284	-2.690653	2.023282
C	89	-3.649034	-0.90351	2.205455
C	90	-4.153226	-0.578511	3.464807
C	91	-5.222004	-1.297918	3.995487
C	92	-5.769866	-2.35728	3.275288
H	93	-5.688098	-3.540437	1.469732
H	94	-2.788517	-0.337752	1.809723
H	95	-3.70176	0.245946	4.042523
H	96	-5.622947	-1.039596	4.990028
H	97	-6.607052	-2.937762	3.698472

(B)



Total Number of atoms: 97

C	1	-3.313861	-0.209945	1.344002
F	2	-2.221362	1.54134	2.607276
F	3	-2.20087	-0.529668	3.446342
F	4	-4.091808	0.656716	3.465168
C	5	-2.96129	0.371227	2.71181
C	6	-6.320236	2.059818	0.30834
C	7	-7.672875	2.27588	0.570482
C	8	-8.385932	1.362694	1.34356
C	9	-7.740218	0.232374	1.840635
C	10	-6.391073	0.009545	1.562316
C	11	-4.147727	0.748618	0.51003
C	12	-5.660743	0.924887	0.794054
O	13	-3.44534	2.795704	-2.021493
Br	14	-1.810859	0.10389	-9.462666

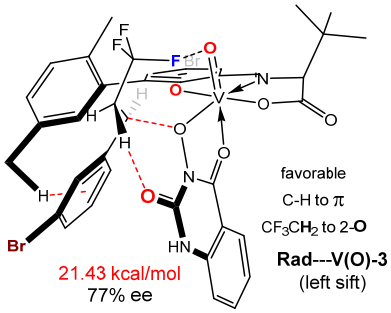
V	15	-2.598568	1.336411	-2.247229
O	16	-1.433588	1.726329	-0.728188
O	17	0.733793	2.117919	-0.303938
O	18	-3.716918	0.991081	-3.799788
N	19	-1.181359	2.19854	-3.293337
Br	20	-8.704347	-1.011537	2.90426
C	21	-0.209468	2.234422	-1.053373
C	22	-1.266481	5.012087	-1.943564
C	23	1.210201	4.786354	-1.672861
C	24	0.211286	4.855993	-3.949756
C	25	-1.040463	2.007961	-4.55245
C	26	-1.976937	1.285727	-5.456647
C	27	-0.006089	4.329226	-2.513039
C	28	-0.124317	2.769355	-2.492965
C	29	-1.568939	1.067149	-6.779208
C	30	-2.39199	0.396413	-7.679429
C	31	-3.635839	-0.069377	-7.270283
C	32	-4.065961	0.149893	-5.9622
C	33	-3.250812	0.849329	-5.063346
O	34	-1.696127	-0.374856	-2.4726
O	35	-3.886542	0.325754	-1.161789
C	36	-2.404171	-1.301598	-2.166957
N	37	-3.639847	-1.086623	-1.604414
C	38	-5.383017	-0.369729	-5.539288
C	39	-4.54083	-2.186838	-1.543261
C	40	-2.988897	-3.680156	-2.088046
C	41	-2.026715	-2.707719	-2.369326
C	42	-2.642757	-5.021441	-2.263892
C	43	-1.364973	-5.380635	-2.697408
C	44	-0.416009	-4.396812	-2.971712
C	45	-0.74606	-3.052983	-2.807704
N	46	-4.182595	-3.404605	-1.720223
C	47	-6.50106	0.473232	-5.458837
C	48	-7.736354	-0.068611	-5.090151
C	49	-7.860168	-1.42471	-4.794225
C	50	-6.747865	-2.265622	-4.852946
C	51	-5.516446	-1.726188	-5.232099
C	52	-6.868215	-3.726445	-4.501832

C	53	-6.393875	1.94428	-5.777732
H	54	-5.950203	-4.101857	-3.997878
H	55	-3.657113	1.74082	0.504427
H	56	-5.909519	-0.893125	1.967502
H	57	-2.363342	-0.441209	0.811718
H	58	-3.835739	-1.185035	1.46554
H	59	-5.767068	2.799754	-0.293709
H	60	-8.17572	3.173618	0.172818
H	61	-9.452906	1.537586	1.558976
H	62	-2.154747	4.835715	-2.588324
H	63	-1.510093	4.651007	-0.919718
H	64	-1.134401	6.115202	-1.876669
H	65	2.144841	4.270469	-1.988256
H	66	1.067257	4.592971	-0.587055
H	67	1.389808	5.879861	-1.777038
H	68	1.099264	4.387694	-4.430496
H	69	-0.67016	4.669633	-4.6021
H	70	0.381257	5.955894	-3.957125
H	71	-0.120467	2.395835	-5.018447
H	72	0.833091	2.376187	-2.908988
H	73	-0.581033	1.420527	-7.116567
H	74	-4.286498	-0.612173	-7.975712
H	75	-3.391981	-5.80548	-2.064354
H	76	-1.107648	-6.445327	-2.830394
H	77	0.592838	-4.680456	-3.316433
H	78	0.002299	-2.270572	-3.018423
H	79	-8.625636	0.579809	-5.026497
H	80	-8.841465	-1.829938	-4.496726
H	81	-4.631272	-2.381157	-5.285506
H	82	-7.028274	-4.33904	-5.416593
H	83	-7.720994	-3.915828	-3.812571
H	84	-7.39289	2.419915	-5.892628
H	85	-5.860165	2.48865	-4.96734
H	86	-5.841481	2.116504	-6.727988
C	87	-5.982374	-1.927972	-1.286533
C	88	-6.763211	-2.890854	-0.63369
C	89	-8.128683	-2.690023	-0.435471
C	90	-8.736815	-1.526162	-0.898758

C	91	-7.975513	-0.564909	-1.558262
C	92	-6.610179	-0.768101	-1.756479
H	93	-6.303447	-3.827031	-0.275045
H	94	-8.729321	-3.456413	0.082797
H	95	-9.817523	-1.368035	-0.746682
H	96	-8.454976	0.351388	-1.940973
H	97	-6.041545	-0.01466	-2.325266

Figure S7:

(A)

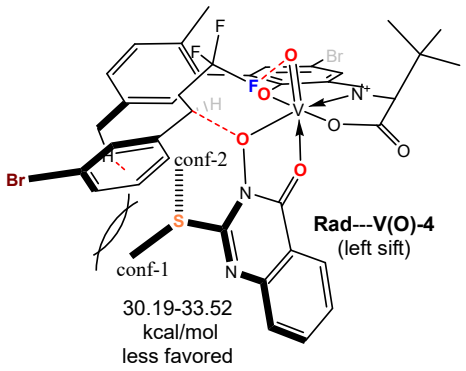


Total number of atoms: 88

C	1	-4.938664	1.775598	1.276846
F	2	-2.537073	1.663376	1.632549
F	3	-3.735092	3.046741	2.90603
F	4	-3.382398	3.552555	0.76379
C	5	-3.64315	2.500683	1.630775
C	6	-6.083029	-0.730702	-1.480419
C	7	-7.037271	-1.726803	-1.682307
C	8	-8.064742	-1.90625	-0.760966
C	9	-8.118385	-1.093459	0.368235
C	10	-7.145899	-0.116251	0.582449
C	11	-4.993875	1.142677	-0.105414
C	12	-6.107262	0.078468	-0.338349
O	13	-2.871883	2.837154	-1.838917
Br	14	-3.254676	1.039601	-9.45773
V	15	-2.330129	1.243428	-2.087327
O	16	-0.894192	1.482989	-0.784984
O	17	1.345327	1.344226	-0.757844
O	18	-3.732301	1.033626	-3.423986
N	19	-0.983803	1.844307	-3.381196
Br	20	-9.517073	-1.327569	1.630328

C	21	0.337563	1.686751	-1.334205
C	22	-0.330855	4.612064	-2.144452
C	23	2.073249	3.922252	-2.197298
C	24	0.812634	4.19279	-4.321691
C	25	-1.116247	1.726344	-4.64804
C	26	-2.351604	1.361245	-5.389548
C	27	0.691514	3.704183	-2.859711
C	28	0.285512	2.192021	-2.784996
C	29	-2.272591	1.344369	-6.788421
C	30	-3.388947	1.054576	-7.564255
C	31	-4.610427	0.808407	-6.951687
C	32	-4.718113	0.826814	-5.559969
C	33	-3.579195	1.070667	-4.772826
O	34	-1.745879	-0.593211	-2.34822
O	35	-3.498003	0.501719	-0.69033
C	36	-2.134367	-1.344594	-1.487233
N	37	-3.005854	-0.911335	-0.504186
C	38	-6.05274	0.603019	-4.958403
C	39	-3.424622	-1.666218	0.587063
C	40	-2.123868	-3.531813	-0.351127
C	41	-1.684292	-2.745954	-1.415517
C	42	-1.701712	-4.864546	-0.267591
C	43	-0.850269	-5.396929	-1.236675
C	44	-0.412548	-4.601196	-2.295096
C	45	-0.828787	-3.273257	-2.387369
N	46	-2.985066	-2.973244	0.633528
C	47	-6.693293	1.593832	-4.195351
C	48	-7.973149	1.342716	-3.688626
C	49	-8.633028	0.148598	-3.968523
C	50	-8.021727	-0.82514	-4.758443
C	51	-6.730385	-0.58893	-5.236035
C	52	-8.739063	-2.110167	-5.085155
C	53	-6.090844	2.958885	-3.962851
H	54	-8.028091	-2.955998	-5.216112
H	55	-5.137126	1.963596	-0.8356
H	56	-7.211625	0.502853	1.490072
H	57	-5.098977	0.995488	2.053725
H	58	-5.783261	2.495478	1.382654

H	59	-5.289525	-0.603952	-2.233149
H	60	-6.979066	-2.368984	-2.57676
H	61	-8.825557	-2.685964	-0.928922
H	62	-1.317356	4.601145	-2.656993
H	63	-0.492108	4.307329	-1.086631
H	64	0.009146	5.671853	-2.129145
H	65	2.844753	3.242454	-2.624009
H	66	2.044237	3.754113	-1.098229
H	67	2.437497	4.963677	-2.34632
H	68	1.508154	3.556634	-4.913647
H	69	-0.169701	4.207478	-4.842798
H	70	1.205816	5.233026	-4.370037
H	71	-0.233119	1.95584	-5.265027
H	72	1.065813	1.62236	-3.342476
H	73	-1.317126	1.56857	-7.290009
H	74	-5.503664	0.614067	-7.567923
H	75	-2.039733	-5.497123	0.569203
H	76	-0.518491	-6.446775	-1.16351
H	77	0.265454	-5.020762	-3.057448
H	78	-0.477658	-2.644887	-3.223416
H	79	-8.481969	2.108931	-3.080643
H	80	-9.648156	-0.018755	-3.572292
H	81	-6.23908	-1.356826	-5.855746
H	82	-9.320228	-2.006775	-6.028246
H	83	-9.4492	-2.400542	-4.279273
H	84	-6.873426	3.749764	-3.954809
H	85	-5.566695	3.002082	-2.983393
H	86	-5.363005	3.242804	-4.754267
O	87	-4.139101	-1.240613	1.461614
H	88	-3.327515	-3.508945	1.446132



Total number of atoms: 91

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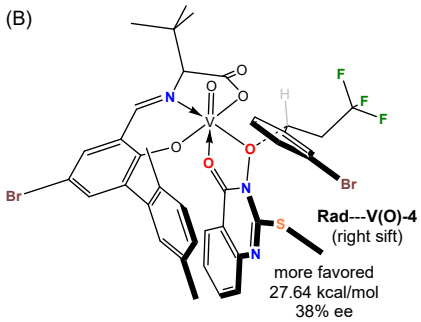
F	3	-3.929689	3.270214	2.749378
F	4	-3.506635	3.711819	0.607251
C	5	-3.747092	2.680914	1.503608
C	6	-5.903269	-0.870829	-1.484338
C	7	-6.838177	-1.888173	-1.669945
C	8	-7.927791	-1.999612	-0.811226
C	9	-8.063722	-1.095603	0.239009
C	10	-7.110735	-0.096573	0.440139
C	11	-4.919003	1.119971	-0.1989
C	12	-6.008306	0.028344	-0.416391
O	13	-2.787891	2.839788	-1.788131
Br	14	-3.340149	1.073135	-9.434409
V	15	-2.260254	1.251566	-2.091004
O	16	-0.792811	1.450291	-0.817302
O	17	1.447016	1.315382	-0.852477
O	18	-3.697536	1.081904	-3.394392
N	19	-0.94841	1.889039	-3.401828
Br	20	-9.545691	-1.235439	1.416381
C	21	0.423748	1.67259	-1.392137
C	22	-0.290457	4.622922	-2.111956
C	23	2.116081	3.94876	-2.205611
C	24	0.83127	4.264976	-4.310669
C	25	-1.110309	1.793077	-4.667645
C	26	-2.357525	1.418505	-5.385876
C	27	0.729645	3.739583	-2.860303
C	28	0.333298	2.223819	-2.824679
C	29	-2.307264	1.399159	-6.786266

C	30	-3.436381	1.094724	-7.538375
C	31	-4.642416	0.833482	-6.901016
C	32	-4.721478	0.854903	-5.507558
C	33	-3.571126	1.120169	-4.745534
O	34	-1.685066	-0.573122	-2.44298
O	35	-3.387442	0.469822	-0.676882
C	36	-2.034622	-1.344639	-1.586147
N	37	-2.860358	-0.93801	-0.562923
C	38	-6.036394	0.609	-4.872952
C	39	-3.064729	-1.85613	0.505491
C	40	-1.96616	-3.521193	-0.453849
C	41	-1.588546	-2.745825	-1.551727
C	42	-1.548593	-4.853059	-0.407176
C	43	-0.773383	-5.396481	-1.433005
C	44	-0.401747	-4.608524	-2.521165
C	45	-0.808929	-3.277004	-2.582422
N	46	-2.663142	-3.069974	0.516902
C	47	-6.678397	1.594898	-4.105151
C	48	-7.934852	1.319302	-3.554589
C	49	-8.572959	0.105364	-3.798252
C	50	-7.963073	-0.862735	-4.596575
C	51	-6.692328	-0.602362	-5.115683
C	52	-8.660379	-2.166566	-4.891292
C	53	-6.103215	2.97875	-3.918401
H	54	-7.935416	-3.001395	-5.016128
H	55	-5.064589	1.887152	-0.983441
H	56	-7.244906	0.595418	1.285539
H	57	-5.15938	1.142348	1.952651
H	58	-5.860089	2.549637	1.122075
H	59	-5.06467	-0.794135	-2.194438
H	60	-6.719178	-2.596505	-2.507012
H	61	-8.674327	-2.795468	-0.968247
H	62	-1.279976	4.625249	-2.618795
H	63	-0.443886	4.286454	-1.06267
H	64	0.047258	5.682426	-2.067388
H	65	2.887434	3.285512	-2.657297
H	66	2.098343	3.751233	-1.111263
H	67	2.472175	4.995969	-2.330009

H	68	1.52645	3.650047	-4.925115
H	69	-0.15651	4.281932	-4.821685
H	70	1.213303	5.310113	-4.336775
H	71	-0.243597	2.041456	-5.300262
H	72	1.103326	1.677101	-3.418225
H	73	-1.364701	1.631251	-7.307992
H	74	-5.544926	0.622538	-7.498163
H	75	-1.830721	-5.480908	0.454341
H	76	-0.448328	-6.449114	-1.379236
H	77	0.215732	-5.035623	-3.329485
H	78	-0.513819	-2.64881	-3.439853
H	79	-8.445143	2.081631	-2.94284
H	80	-9.5714	-0.081169	-3.369768
H	81	-6.199583	-1.366479	-5.73908
H	82	-9.254479	-2.090566	-5.828895
H	83	-9.355736	-2.455762	-4.072128
H	84	-6.906171	3.74772	-3.872915
H	85	-5.524482	3.048977	-2.972089
H	86	-5.430896	3.273091	-4.753722
S	87	-4.029687	-1.412122	1.962729
C	88	-5.255964	-2.684425	2.320353
H	89	-4.741702	-3.637055	2.573878
H	90	-5.902836	-2.837167	1.429181
H	91	-5.879447	-2.357523	3.180786

(B)



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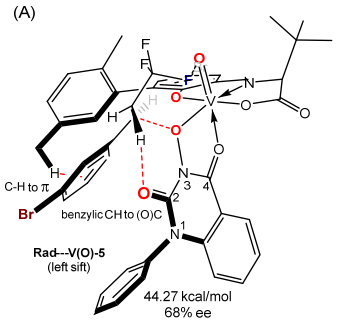
F	2	-1.89918	3.00542	1.27747
F	3	-1.10022	1.18573	2.30022
F	4	-3.15756	1.91245	2.77468
C	5	-2.24392	1.74375	1.74317

C	6	-6.56455	1.8772	0.122636
C	7	-7.83923	1.70322	0.660472
C	8	-8.02428	0.854613	1.74863
C	9	-6.92599	0.197198	2.29802
C	10	-5.65121	0.379379	1.7608
C	11	-4.05357	1.42077	0.009521
C	12	-5.45444	1.20512	0.646865
O	13	-4.79408	3.24071	-2.43329
Br	14	-7.42862	0.257781	-9.41693
V	15	-3.94103	1.96633	-3.17039
O	16	-2.23628	2.74185	-2.62003
O	17	-0.409935	3.65244	-3.55369
O	18	-5.64116	1.23267	-3.74389
N	19	-3.68175	3.01814	-4.80388
Br	20	-7.16296	-0.954613	3.78836
C	21	-1.60694	3.47547	-3.5859
C	22	-3.51004	5.887	-3.49912
C	23	-1.44873	6.18717	-4.88587
C	24	-3.64784	5.83085	-5.9899
C	25	-4.30158	2.75569	-5.89604
C	26	-5.39857	1.76377	-6.08849
C	27	-2.78531	5.41476	-4.77662
C	28	-2.51847	3.8722	-4.76364
C	29	-5.84736	1.51821	-7.39268
C	30	-6.85154	0.583978	-7.63813
C	31	-7.41091	-0.134738	-6.58675
C	32	-6.99069	0.107885	-5.27985
C	33	-6.02159	1.08629	-5.03133
O	34	-2.97834	0.499408	-4.00894
O	35	-4.09853	0.775351	-1.61173
C	36	-3.10895	-0.537429	-3.41082
N	37	-3.74467	-0.571367	-2.19041
C	38	-7.52633	-0.702964	-4.164
C	39	-4.1066	-1.85634	-1.69776
C	40	-3.00162	-2.98217	-3.25043
C	41	-2.65328	-1.82701	-3.95109
C	42	-2.5762	-4.21464	-3.74969
C	43	-1.8183	-4.28903	-4.91974

C	44	-1.48117	-3.12576	-5.61035
C	45	-1.90094	-1.88808	-5.12685
N	46	-3.70645	-2.96867	-2.18479
C	47	-8.32535	-0.136714	-3.15827
C	48	-8.72964	-0.931517	-2.08035
C	49	-8.36418	-2.27366	-2.00565
C	50	-7.58612	-2.84962	-3.01076
C	51	-7.1745	-2.05317	-4.08184
C	52	-7.17206	-4.29727	-2.94227
C	53	-8.78418	1.29958	-3.22195
H	54	-7.69823	-4.89538	-3.71918
H	55	-3.89395	2.4878	-0.236401
H	56	-4.80352	-0.149044	2.22235
H	57	-2.0042	0.749412	-0.151914
H	58	-2.96686	-0.17545	1.02018
H	59	-6.44357	2.54981	-0.740232
H	60	-8.70059	2.23491	0.221294
H	61	-9.03264	0.711744	2.17087
H	62	-4.53862	5.47085	-3.43435
H	63	-2.96416	5.59397	-2.57494
H	64	-3.61271	6.99507	-3.47864
H	65	-0.842305	5.83905	-5.75212
H	66	-0.824319	6.08006	-3.97208
H	67	-1.6188	7.27834	-5.02495
H	68	-3.1868	5.51295	-6.95187
H	69	-4.67367	5.40315	-5.94102
H	70	-3.77058	6.93591	-6.03978
H	71	-3.97118	3.29127	-6.80036
H	72	-1.93783	3.64801	-5.68928
H	73	-5.39481	2.05662	-8.24116
H	74	-8.1815	-0.898827	-6.78095
H	75	-2.84472	-5.13961	-3.21328
H	76	-1.48724	-5.27023	-5.30039
H	77	-0.882979	-3.18417	-6.53565
H	78	-1.63582	-0.964981	-5.66943
H	79	-9.34645	-0.496317	-1.27678
H	80	-8.69132	-2.87872	-1.14383
H	81	-6.53381	-2.49326	-4.86364

H	82	-7.40336	-4.7523	-1.9536
H	83	-6.07789	-4.41041	-3.1096
H	84	-9.73109	1.45296	-2.65852
H	85	-8.02394	1.98279	-2.78403
H	86	-8.97624	1.62637	-4.26781
S	87	-5.12053	-2.04966	-0.222228
C	88	-4.41374	-3.27165	0.897914
H	89	-4.37651	-4.26149	0.39256
H	90	-3.38632	-2.9585	1.18573
H	91	-5.0489	-3.34376	1.80755

Figure S9:



Total number of atoms: 98

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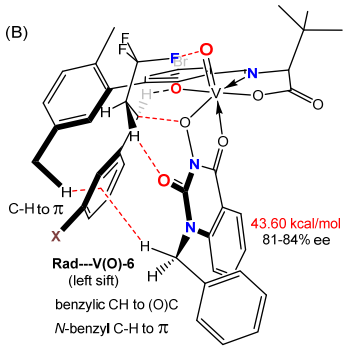
F	4	-5.08455	3.71984	-0.123454
C	5	-4.82812	2.81505	0.898723
C	6	-5.99301	-1.1093	-2.17136
C	7	-6.67555	-2.29014	-2.46014
C	8	-7.47751	-2.88594	-1.49079
C	9	-7.57847	-2.29915	-0.23164
C	10	-6.88399	-1.12449	0.057908
C	11	-5.2731	0.788018	-0.610972
C	12	-6.07858	-0.510018	-0.910233
O	13	-2.82437	2.81133	-1.75597
Br	14	-3.10915	1.91601	-9.52729
V	15	-2.36143	1.22612	-2.16518
O	16	-0.958455	1.24385	-0.806292
O	17	1.26198	0.922033	-0.756366
O	18	-3.73127	1.23344	-3.54923

N	19	-0.947539	1.8842	-3.35494
Br	20	-8.65779	-3.11414	1.10092
C	21	0.299338	1.40539	-1.30873
C	22	-0.119905	4.43007	-1.7578
C	23	2.22968	3.5802	-1.91002
C	24	0.998278	4.20432	-3.97595
C	25	-1.05457	1.92712	-4.62939
C	26	-2.28786	1.72032	-5.43363
C	27	0.837702	3.54758	-2.58582
C	28	0.324425	2.07104	-2.69503
C	29	-2.17767	1.8645	-6.82301
C	30	-3.28744	1.71588	-7.64787
C	31	-4.53109	1.44256	-7.09311
C	32	-4.66828	1.30245	-5.7116
C	33	-3.54181	1.41896	-4.88004
O	34	-1.87175	-0.60241	-2.61301
O	35	-3.60265	0.401783	-0.88542
C	36	-2.27663	-1.40702	-1.80971
N	37	-3.11422	-1.01928	-0.78087
C	38	-6.01435	1.03462	-5.15703
C	39	-3.5131	-1.82022	0.280384
C	40	-2.34955	-3.686	-0.866802
C	41	-1.87261	-2.82323	-1.85161
C	42	-1.94008	-5.02482	-0.880208
C	43	-1.09576	-5.49314	-1.88824
C	44	-0.641927	-4.62662	-2.8816
C	45	-1.02597	-3.28685	-2.86253
N	46	-3.19801	-3.16379	0.148314
C	47	-6.65412	1.94943	-4.30463
C	48	-7.91995	1.63684	-3.79737
C	49	-8.56614	0.458023	-4.16246
C	50	-7.96083	-0.43204	-5.04999
C	51	-6.6841	-0.134452	-5.53292
C	52	-8.67299	-1.69259	-5.47073
C	53	-6.05768	3.29659	-3.97253
H	54	-7.96065	-2.47858	-5.80675
H	55	-5.43156	1.50715	-1.43767
H	56	-6.9699	-0.694671	1.06771

H	57	-5.33349	0.833703	1.55403
H	58	-6.66675	1.70905	0.75202
H	59	-5.36076	-0.657056	-2.95117
H	60	-6.57739	-2.75179	-3.45686
H	61	-8.0205	-3.81743	-1.72041
H	62	-1.10418	4.55006	-2.26057
H	63	-0.304387	4.01129	-0.74373
H	64	0.29376	5.45365	-1.6162
H	65	2.95176	2.90778	-2.42554
H	66	2.1867	3.27434	-0.841709
H	67	2.66735	4.60355	-1.92706
H	68	1.65252	3.60114	-4.64458
H	69	0.021324	4.34988	-4.48716
H	70	1.46092	5.2135	-3.89581
H	71	-0.143312	2.17013	-5.19837
H	72	1.07866	1.51218	-3.29753
H	73	-1.20215	2.1029	-7.27743
H	74	-5.41617	1.34884	-7.74378
H	75	-2.27121	-5.72514	-0.09668
H	76	-0.779515	-6.55022	-1.89485
H	77	0.029714	-4.99728	-3.67478
H	78	-0.654912	-2.59886	-3.64088
H	79	-8.42834	2.34188	-3.11894
H	80	-9.56965	0.239114	-3.76152
H	81	-6.19137	-0.840362	-6.22132
H	82	-9.3706	-1.48748	-6.31291
H	83	-9.26729	-2.12399	-4.63461
H	84	-6.84843	4.06779	-3.83886
H	85	-5.47239	3.2563	-3.02853
H	86	-5.38466	3.66827	-4.77616
O	87	-4.12814	-1.3946	1.23
C	88	-3.83727	-4.07464	1.02824
C	89	-3.34348	-4.2814	2.31653
C	90	-3.97773	-5.19026	3.16413
C	91	-5.09408	-5.89838	2.71687
C	92	-5.57591	-5.70377	1.42209
C	93	-4.94339	-4.79469	0.574705
H	94	-2.46152	-3.7183	2.6628

H	95	-3.59968	-5.34547	4.18878
H	96	-5.59877	-6.61244	3.38941
H	97	-6.45878	-6.26418	1.07098
H	98	-5.31854	-4.63756	-0.44939



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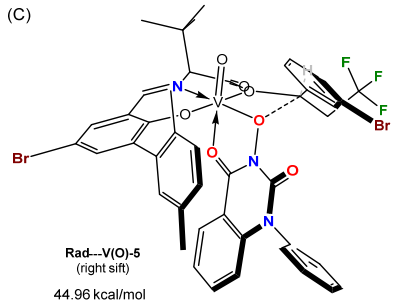
F	3	-6.3481	4.839899	3.0309
F	4	-6.0391	4.6668	0.8278
C	5	-5.8177	4.0238	2.0388
C	6	-6.5596	-0.4831	-0.2498
C	7	-7.1001	-1.7659	-0.3218
C	8	-7.8381	-2.2692	0.7456
C	9	-8.0298	-1.4798	1.877199
C	10	-7.4807	-0.1993	1.9489
C	11	-6.0523	1.7179	0.956799
C	12	-6.7283	0.3166	0.886
O	13	-3.421	3.5764	-0.3612
Br	14	-4.0976	0.9566	-7.8316
V	15	-3.094	1.917099	-0.547
O	16	-1.6273	2.039099	0.7371
O	17	0.5861	1.6737	0.7703
O	18	-4.5195	1.840299	-1.869
N	19	-1.6977	2.2569	-1.8824
Br	20	-9.023	-2.1656	3.341799
C	21	-0.3851	2.081199	0.173699
C	22	-0.7288	5.010599	-0.8687
C	23	1.580099	4.0478	-0.8249
C	24	0.376	4.2874	-2.9857

C	25	-1.8513	2.0416	-3.1352
C	26	-3.1232	1.731299	-3.8421
C	27	0.188	3.9374	-1.4914
C	28	-0.3929	2.4936	-1.3087
C	29	-3.0608	1.5159	-5.225
C	30	-4.2125	1.251799	-5.96
C	31	-5.45	1.2262	-5.3282
C	32	-5.5388	1.450499	-3.9543
C	33	-4.3729	1.6824	-3.2072
O	34	-2.7754	0.004199	-0.7188
O	35	-4.3372	1.4001	0.882299
C	36	-3.1953	-0.6225	0.2238
N	37	-3.917	-0.0057	1.22
C	38	-6.8709	1.4466	-3.3082
C	39	-4.279	-0.5738	2.432
C	40	-3.4574	-2.6999	1.5285
C	41	-2.9624	-2.0643	0.3882
C	42	-3.2598	-4.0826	1.6444
C	43	-2.5784	-4.7965	0.6569
C	44	-2.0857	-4.1417	-0.4689
C	45	-2.2815	-2.7703	-0.6074
O	46	-4.7402	0.089599	3.330899
N	47	-4.1475	-1.9566	2.5416
C	48	-7.3868	2.598499	-2.6923
C	49	-8.6242	2.5291	-2.0439
C	50	-9.3591	1.3462	-2.0324
C	51	-8.8789	0.211	-2.6859
C	52	-7.6371	0.2766	-3.3236
C	53	-9.6883	-1.0608	-2.6791
C	54	-6.6775	3.930299	-2.7561
C	55	-4.7417	-2.6455	3.692799
C	56	-3.9264	-4.4997	5.208299
C	57	-2.9965	-5.0412	6.095199
C	58	-1.8584	-4.3158	6.4412
C	59	-1.6584	-3.0445	5.9068
C	60	-2.5904	-2.5027	5.022
C	61	-3.7244	-3.232	4.6472
H	62	-9.1041	-1.9307	-3.0531

H	63	-5.4386	-3.4394	3.340699
H	64	-5.3846	-1.9624	4.2916
H	65	-6.1943	2.2481	-0.0039
H	66	-7.6289	0.3922	2.865499
H	67	-6.2375	2.1815	3.066399
H	68	-7.5755	2.779999	2.046799
H	69	-5.9624	-0.1119	-1.0969
H	70	-6.9338	-2.3832	-1.2209
H	71	-8.2609	-3.2859	0.6918
H	72	-1.7045	5.073199	-1.3984
H	73	-0.9349	4.81	0.205999
H	74	-0.2679	6.022	-0.9282
H	75	2.2716	3.2535	-1.1854
H	76	1.5235	3.9708	0.2831
H	77	2.0625	5.026	-1.0474
H	78	0.9996	3.5303	-3.5119
H	79	-0.5939	4.3685	-3.5237
H	80	0.8849	5.2695	-3.1109
H	81	-0.9526	2.1144	-3.7683
H	82	0.3114	1.7999	-1.8255
H	83	-2.0902	1.555299	-5.746
H	84	-6.3657	1.040899	-5.9134
H	85	-3.6311	-4.6393	2.516499
H	86	-2.4262	-5.8836	0.769799
H	87	-1.5467	-4.7063	-1.2486
H	88	-1.9027	-2.2508	-1.5041
H	89	-9.0342	3.4244	-1.5476
H	90	-10.3338	1.3135	-1.5178
H	91	-7.2395	-0.6211	-3.8243
H	92	-10.5892	-0.9595	-3.3241
H	93	-10.0321	-1.3119	-1.6508
H	94	-7.4003	4.776	-2.7614
H	95	-6.0085	4.071799	-1.8796
H	96	-6.0614	4.033099	-3.6765
H	97	-4.8283	-5.0816	4.954299
H	98	-3.1642	-6.0419	6.5275
H	99	-1.1229	-4.7424	7.1434
H	100	-0.7638	-2.4633	6.1872

H 101 -2.4251 -1.491 4.6149

(C)



Total number of atoms: 98

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F	3	-2.7653	0.029002	3.78422
F	4	-4.57482	1.29161	3.43709
C	5	-3.37577	0.879962	2.87155
C	6	-6.34353	2.30485	-0.295636
C	7	-7.72109	2.51707	-0.34736
C	8	-8.57817	1.70747	0.394325
C	9	-8.04759	0.6914	1.18629
C	10	-6.66936	0.483642	1.23796
C	11	-4.25811	1.08036	0.51527
C	12	-5.79727	1.27908	0.484098
O	13	-3.13228	2.89677	-1.86423
Br	14	-2.13558	0.578533	-9.4945
V	15	-2.46202	1.36319	-2.17294
O	16	-1.20527	1.56614	-0.692723
O	17	1.00701	1.73192	-0.362734
O	18	-3.66886	1.1631	-3.68105
N	19	-1.02437	2.15479	-3.24546
Br	20	-9.20682	-0.414583	2.20605
C	21	0.044935	1.97768	-1.05488
C	22	-0.76328	4.88634	-1.69811
C	23	1.69129	4.41192	-1.63274
C	24	0.545624	4.73261	-3.81651
C	25	-0.975576	2.06238	-4.52202
C	26	-2.01375	1.48029	-5.41624
C	27	0.379764	4.12763	-2.40384

C	28	0.113845	2.58578	-2.46767
C	29	-1.69484	1.34145	-6.77318
C	30	-2.59968	0.772629	-7.66402
C	31	-3.82718	0.309448	-7.20587
C	32	-4.17214	0.449071	-5.86072
C	33	-3.2882	1.08757	-4.97844
O	34	-1.7913	-0.425195	-2.53944
O	35	-3.78789	0.458089	-1.0467
C	36	-2.57237	-1.28695	-2.21408
N	37	-3.69883	-0.980686	-1.47326
C	38	-5.43685	-0.149028	-5.37414
C	39	-4.70494	-1.86917	-1.12407
C	40	-3.37525	-3.62241	-2.26308
C	41	-2.40588	-2.69031	-2.63076
C	42	-3.24615	-4.94476	-2.7045
C	43	-2.14648	-5.32697	-3.47434
C	44	-1.17347	-4.3907	-3.82057
C	45	-1.30512	-3.06697	-3.4051
N	46	-4.48063	-3.1905	-1.4778
C	47	-6.44235	0.609751	-4.75245
C	48	-7.58375	-0.040347	-4.26935
C	49	-7.75202	-1.41378	-4.4333
C	50	-6.77577	-2.16965	-5.08227
C	51	-5.62256	-1.52606	-5.53469
C	52	-6.94044	-3.65235	-5.3001
C	53	-6.37098	2.11258	-4.62728
H	54	-6.09177	-4.2184	-4.85509
H	55	-3.73135	2.05309	0.470811
H	56	-6.28016	-0.325477	1.8745
H	57	-2.58971	-0.145674	1.14846
H	58	-4.16714	-0.758859	1.68553
H	59	-5.6805	2.95478	-0.889474
H	60	-8.13181	3.32563	-0.975407
H	61	-9.66721	1.87447	0.35426
H	62	-1.70553	4.84688	-2.28631
H	63	-0.974711	4.47709	-0.685374
H	64	-0.51443	5.96337	-1.5677
H	65	2.54722	3.83596	-2.05076

H	66	1.60821	4.15756	-0.553447
H	67	1.96814	5.48892	-1.68181
H	68	1.35124	4.2234	-4.39147
H	69	-0.392431	4.67231	-4.41118
H	70	0.816387	5.81113	-3.76653
H	71	-0.053678	2.41137	-5.01408
H	72	1.01112	2.13369	-2.95214
H	73	-0.710693	1.67019	-7.14523
H	74	-4.52805	-0.177587	-7.90369
H	75	-4.00858	-5.70025	-2.45695
H	76	-2.04904	-6.37213	-3.81455
H	77	-0.306789	-4.6938	-4.43249
H	78	-0.544503	-2.32288	-3.69591
H	79	-8.37249	0.542128	-3.76489
H	80	-8.66755	-1.89751	-4.0548
H	81	-4.83489	-2.12551	-6.01986
H	82	-6.97449	-3.89104	-6.38644
H	83	-7.87756	-4.04309	-4.84513
H	84	-7.37163	2.5764	-4.77424
H	85	-6.01102	2.41337	-3.6186
H	86	-5.69545	2.56894	-5.3838
C	87	-5.43097	-4.14682	-1.03071
C	88	-5.09701	-5.03489	-0.006672
C	89	-6.03024	-5.97633	0.428457
C	90	-7.29396	-6.02908	-0.160911
C	91	-7.62774	-5.14145	-1.18405
C	92	-6.69486	-4.20068	-1.61891
H	93	-4.10124	-4.98383	0.462894
H	94	-5.77238	-6.67371	1.24331
H	95	-8.03418	-6.76822	0.189253
H	96	-8.63101	-5.1758	-1.64136
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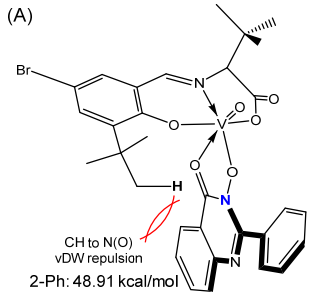
O	98	-5.69872	-1.52952	-0.528493

Figure S10:



Total number of atoms: 73

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Br	2	-16.879627	3.293322	-1.095626
V	3	-10.156735	0.822623	0.709251
O	4	-8.293484	1.063385	0.172891
O	5	-7.191651	1.891952	-1.599335
O	6	-12.009493	0.576433	1.259757
N	7	-10.458853	2.437923	-0.356487
C	8	-8.112162	1.983514	-0.818661
C	9	-8.486177	4.362512	1.121812
C	10	-7.572107	4.903533	-1.144519
C	11	-9.930123	5.462384	-0.589035
C	12	-11.625214	2.82033	-0.707899
C	13	-12.923728	2.269864	-0.240799
C	14	-8.82272	4.403419	-0.383159
C	15	-9.259014	3.001398	-0.926116
C	16	-14.073716	2.87294	-0.763144
C	17	-15.336884	2.449401	-0.376633
C	18	-15.470259	1.410794	0.535444
C	19	-14.344272	0.776915	1.080855
C	20	-13.060243	1.227775	0.695761
O	21	-10.430013	-0.346991	-0.826467
O	22	-9.758534	-0.869843	1.567602
C	23	-10.230425	-1.523035	-0.612063
N	24	-9.834063	-2.005421	0.617371
C	25	-14.531519	-0.371472	2.077871
C	26	-9.632179	-3.390453	0.829738
C	27	-10.193629	-3.899987	-1.258335
C	28	-10.409973	-2.567411	-1.633343
C	29	-10.375549	-4.893812	-2.222402

C	30	-10.759592	-4.570514	-3.524837
C	31	-10.969668	-3.239756	-3.882142
C	32	-10.797273	-2.233037	-2.933964
N	33	-9.82739	-4.264055	-0.085854
C	34	-13.848313	-0.059005	3.431775
C	35	-16.017957	-0.657046	2.415141
C	36	-13.962166	-1.687599	1.49582
C	37	-9.151251	-3.852541	2.160952
C	38	-8.308487	-3.064234	2.955937
C	39	-7.863085	-3.521388	4.196414
C	40	-9.511415	-5.123152	2.630183
C	41	-9.06659	-5.582147	3.869908
C	42	-8.244392	-4.779374	4.656669
H	43	-10.965766	-1.179305	-3.213092
H	44	-9.382807	4.128536	1.735862
H	45	-7.70547	3.605292	1.35578
H	46	-8.103081	5.345177	1.477506
H	47	-7.731345	4.893787	-2.24622
H	48	-6.673049	4.285962	-0.927913
H	49	-7.313287	5.948467	-0.861438
H	50	-10.24777	5.525984	-1.653932
H	51	-10.831556	5.252275	0.02779
H	52	-9.580384	6.477272	-0.294905
H	53	-11.680277	3.652929	-1.42704
H	54	-9.459139	3.130618	-2.015886
H	55	-13.985744	3.699914	-1.486473
H	56	-16.487916	1.102617	0.815537
H	57	-10.206806	-5.948989	-1.950445
H	58	-10.893593	-5.369712	-4.273601
H	59	-11.271595	-2.984093	-4.911994
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H	61	-12.741638	0.004298	3.361501
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H	65	-16.603318	-0.96375	1.519057
H	66	-14.440983	-1.940192	0.522936
H	67	-12.865869	-1.646496	1.320088

H	68	-14.140194	-2.545588	2.182046
H	69	-7.959312	-2.080375	2.604045
H	70	-7.196989	-2.890435	4.808888
H	71	-10.159189	-5.774942	2.020153
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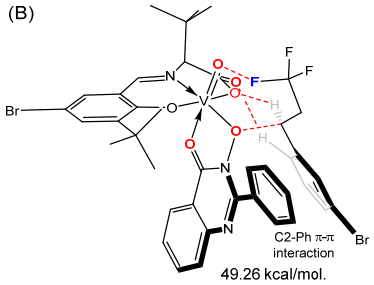

Total number of atoms: 93

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C	4	6.919579	1.053798	-0.914724
C	5	5.554528	1.249269	-0.716135
C	6	4.699679	0.150116	-0.700259
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C	8	7.097441	-2.790815	-1.316395
C	9	6.578667	-1.343003	-1.107974
O	10	6.718976	-5.913477	-2.186401
H	11	8.511805	-0.351577	-1.26515
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Br	13	3.758921	-8.800725	-9.048691
V	14	5.427642	-5.056176	-2.8902
O	15	4.616772	-4.741539	-1.140629
O	16	2.744925	-5.25258	-0.016641
O	17	6.186694	-5.441387	-4.642364
N	18	4.269542	-6.636985	-2.907274
H	19	6.125532	-8.080962	-1.188551
H	20	5.149137	2.263638	-0.56642
H	21	3.617402	0.292949	-0.539246
H	22	4.520307	-1.991635	-0.865282
C	23	9.084458	-3.406208	0.108712

H	24	2.767691	-9.5225	-2.090318
H	25	2.471385	-6.987348	-1.965014
H	26	3.18259	-8.031543	-3.903607
H	27	3.171928	-8.522089	-6.171129
H	28	9.176828	-2.29337	-1.745164
H	29	5.598109	-7.112324	0.231574
H	30	3.177228	-7.451606	1.127838
H	31	1.944038	-8.252101	0.09529
H	32	3.203103	-9.221458	0.91968
H	33	4.510933	-9.442202	-2.533714
H	34	4.001593	-10.313941	-1.06578
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C	38	5.400634	-8.042007	-0.346863
C	39	3.018943	-8.263127	0.384212
C	40	3.796773	-9.409537	-1.681494
C	41	3.967289	-7.262246	-3.981973
C	42	4.562649	-7.077232	-5.333849
C	43	3.943263	-8.115989	-0.848019
C	44	3.541062	-6.851422	-1.679252
C	45	4.01599	-7.842062	-6.370028
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C	47	5.595833	-6.914448	-7.928306
C	48	6.174575	-6.131977	-6.918287
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O	50	4.002502	-4.012256	-3.706499
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C	52	4.372002	-2.916759	-4.049342
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C	58	3.277447	0.138252	-5.888634
C	59	1.935571	-0.147682	-6.148052
C	60	1.383103	-1.356014	-5.726055
C	61	2.173868	-2.275443	-5.039633

C	62	7.53241	-0.91436	-4.325461
H	63	3.710037	1.090477	-6.237564
H	64	1.312726	0.58112	-6.694146
H	65	0.32382	-1.584039	-5.934009
H	66	1.740706	-3.231309	-4.700133
H	67	6.572043	-3.485395	-0.635844
F	68	8.455382	-4.5061	0.676878
F	69	8.890961	-2.323936	0.956597
F	70	10.447019	-3.676513	0.095487
N	71	5.312771	-0.470732	-5.014229
C	72	6.922565	-3.742971	-7.134717
C	73	7.889077	-5.401472	-8.700189
H	74	8.224213	-6.445551	-8.894809
C	75	7.916121	0.432542	-4.285057
C	76	9.262604	0.79272	-4.239315
C	77	10.248599	-0.190426	-4.256956
C	78	8.535922	-1.889814	-4.368898
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H	82	10.662462	-2.312925	-4.368908
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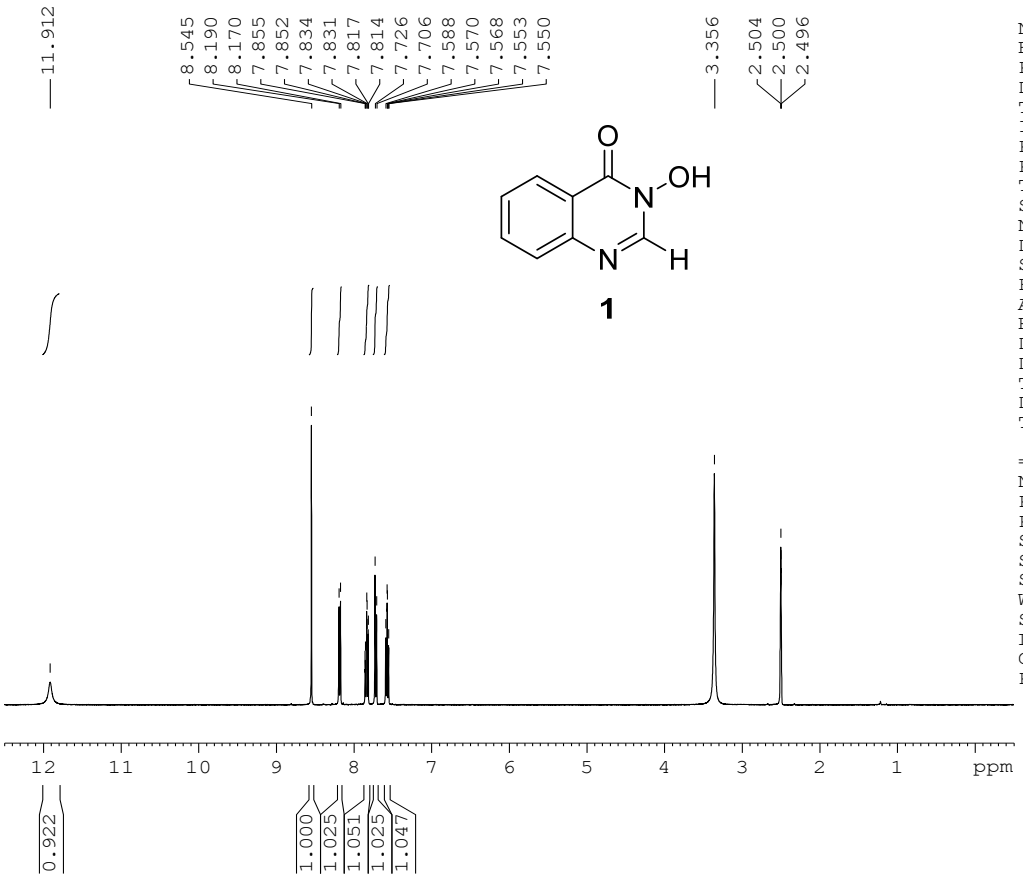
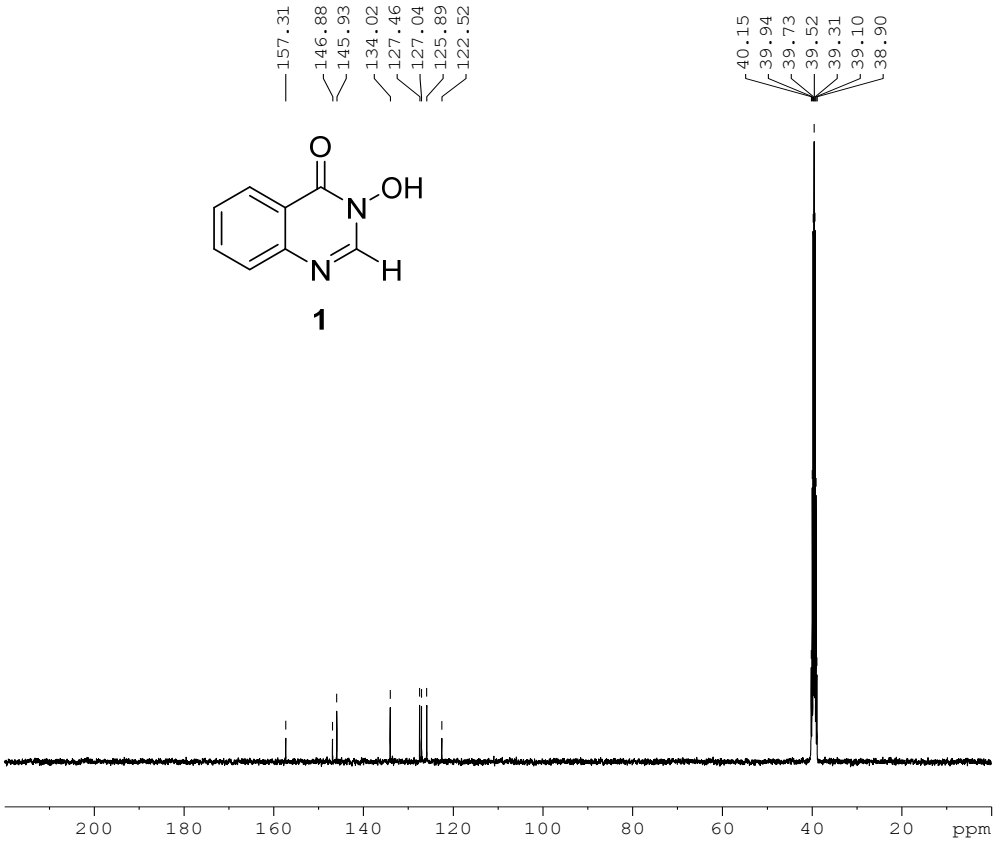
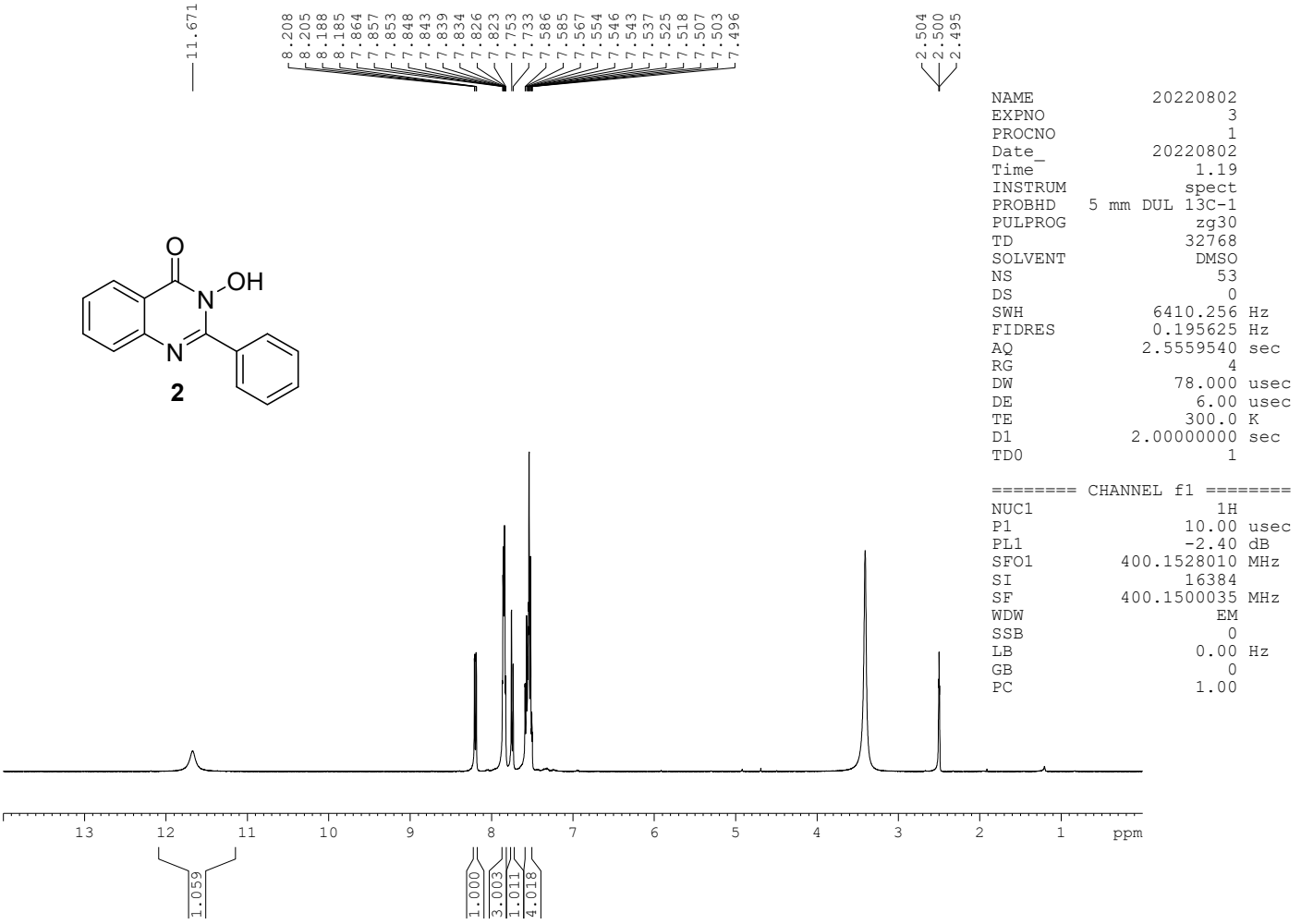
H	84	9.546607	1.857678	-4.192432
C	85	8.566393	-5.499603	-6.329979
H	86	6.095614	-3.502404	-7.840054
H	87	6.560637	-3.492512	-6.116538
H	88	7.762735	-3.048959	-7.361159
H	89	7.130859	-5.130545	-9.468814
H	90	8.768769	-4.746415	-8.89038
H	91	8.867197	-6.570725	-6.371056
H	92	8.373573	-5.253883	-5.264688
H	93	9.454219	-4.899198	-6.629711



NAME	NHOH N=C
EXPNO	1
PROCNO	1
Date_	20210427
Time	12.10
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500035 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	NHOH N=C
EXPNO	2
PROCNO	1
Date_	20210427
Time	12.14
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	200
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178431 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00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7.843
7.839
7.834
7.826
7.823
7.753
7.733
7.586
7.585
7.567
7.554
7.546
7.543
7.537
7.525
7.518
7.507
7.503
7.496
2.504
2.500
2.495
O
N
OH
N
2
NAME 20220802
EXPNO 3
PROCNO 1
Date_ 20220802
Time 1.19
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 53
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500035 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
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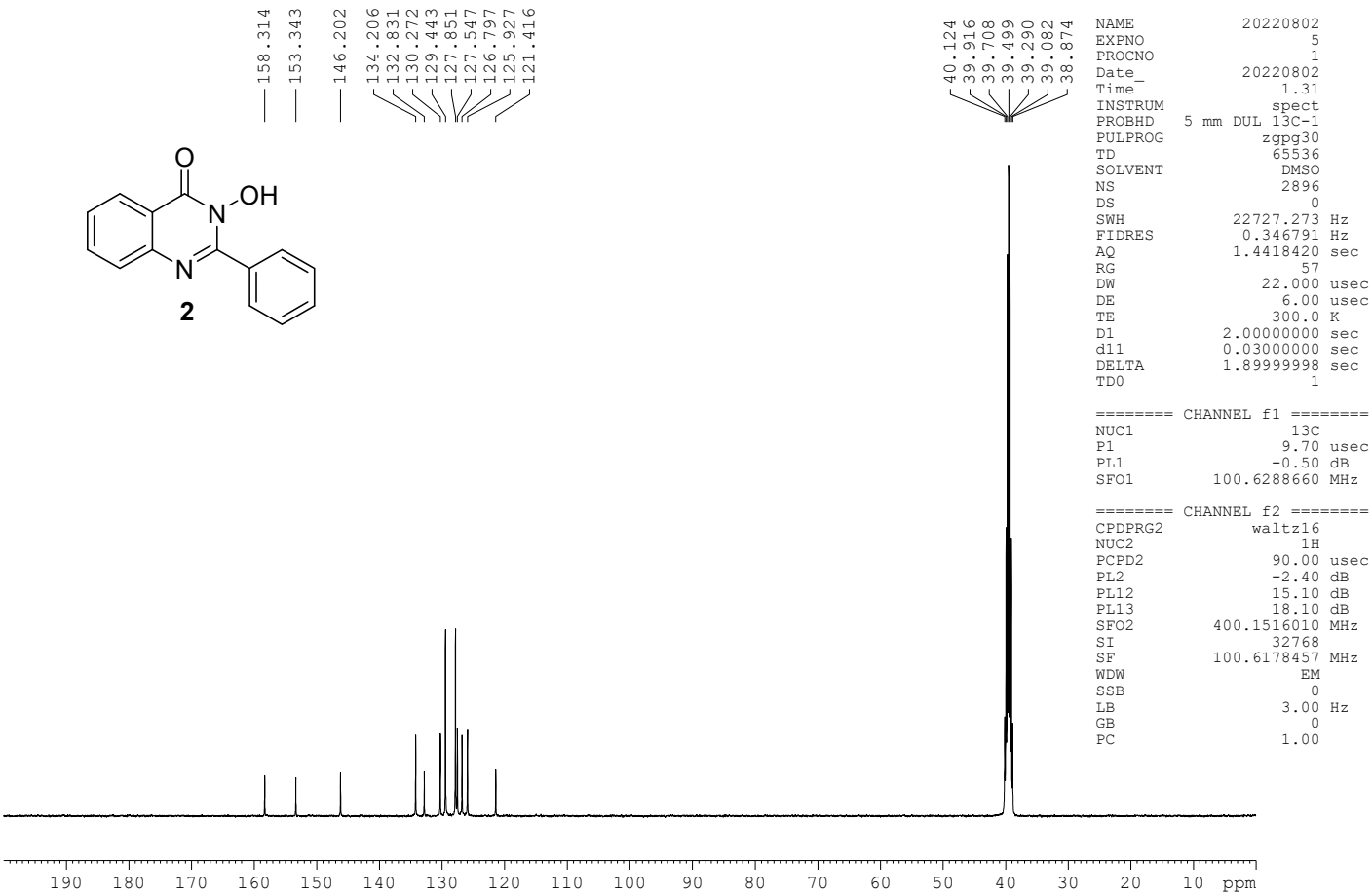
1.000
3.003
1.011
4.018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130.272
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127.851
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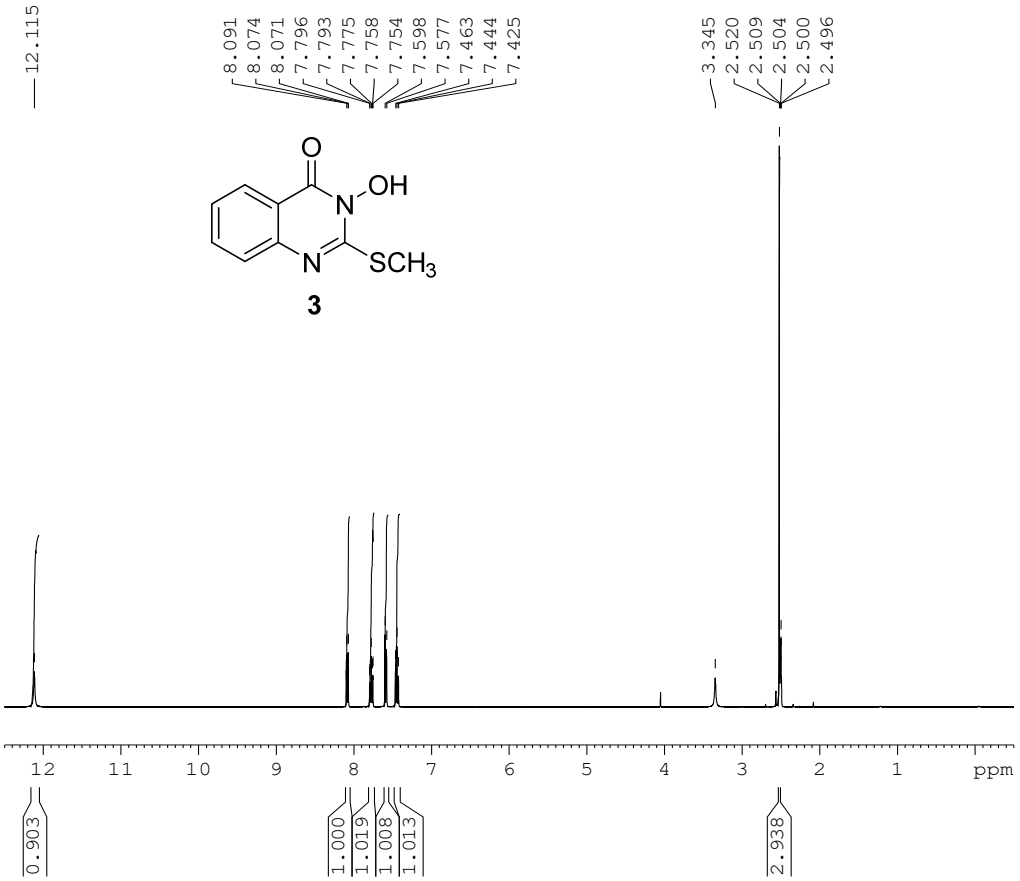
126.797
125.927
121.416
40.124
39.916
39.708
39.499
39.290
39.082
38.874
O
N
OH
N
2
NAME 20220802
EXPNO 5
PROCNO 1
Date_ 20220802
Time 1.31
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2896
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
PL12 15.10 dB
PL13 18.10 dB
SFO2 400.1516010 MHz
SI 32768
SF 100.6178457 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm




```
NAME                 s-ch3
EXPNO                   10
PROCNO                   1
Date_             20210510
Time                 21.04
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   32768
SOLVENT               DMSO
NS                       8
DS                       0
SWH               6410.256 Hz
FIDRES            0.195625 Hz
AQ                2.5559540 sec
RG                       4
DW                  78.000 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -2.40 dB
SFO1           400.1528010 MHz
SI                   16384
SF             400.1500031 MHz
WDW                     EM
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
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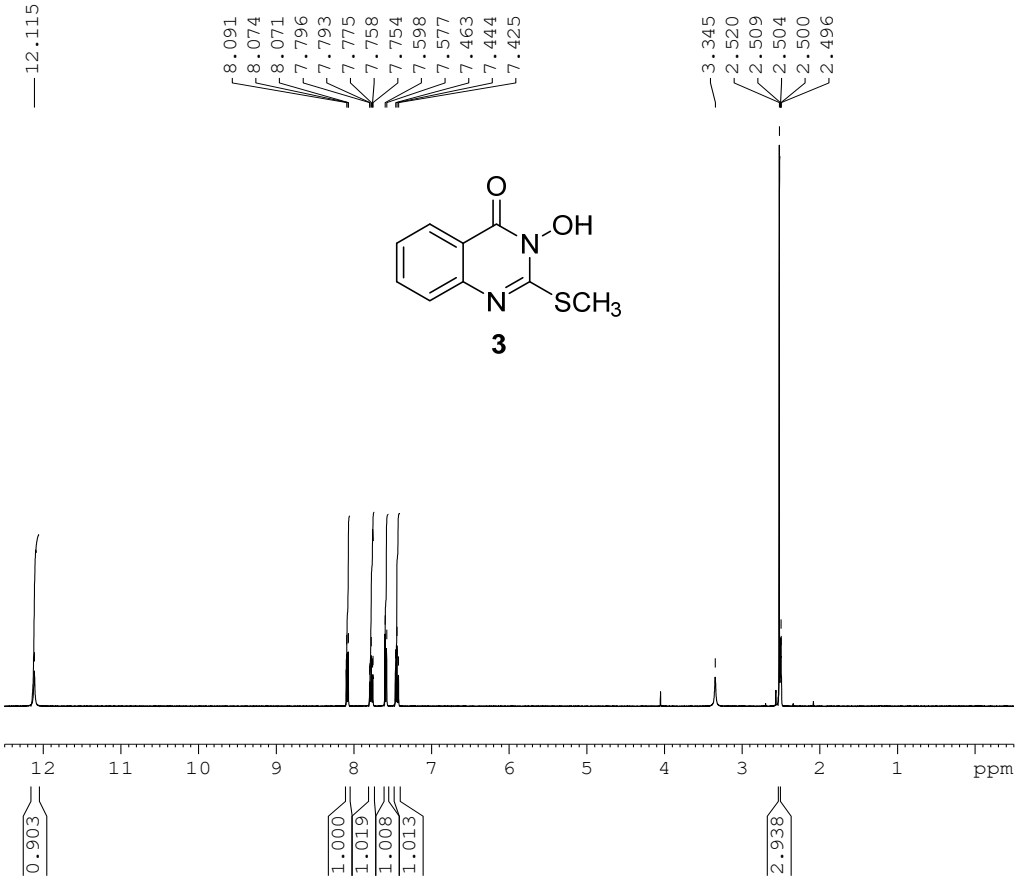


```
NAME                 s-ch3
EXPNO                   10
PROCNO                   1
Date_             20210510
Time                 21.04
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   32768
SOLVENT               DMSO
NS                       8
DS                       0
SWH               6410.256 Hz
FIDRES            0.195625 Hz
AQ                2.5559540 sec
RG                       4
DW                  78.000 usec
DE                   6.00 usec
TE                  300.0 K
D1               2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -2.40 dB
SFO1           400.1528010 MHz
SI                   16384
SF             400.1500031 MHz
WDW                     EM
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
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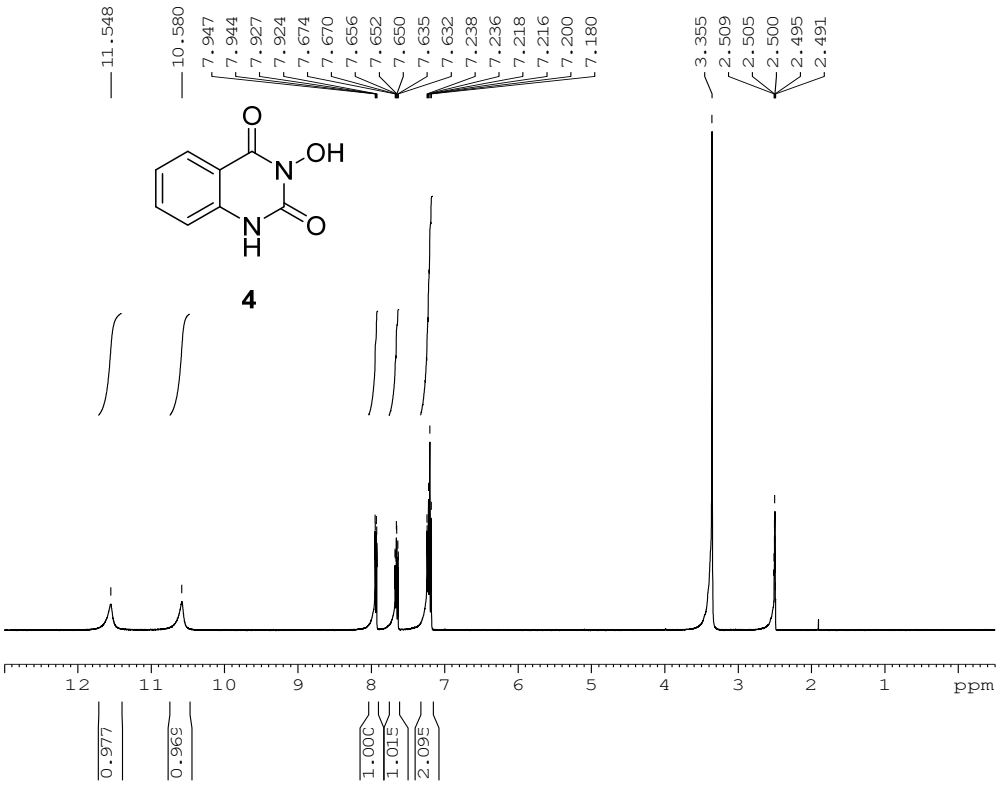


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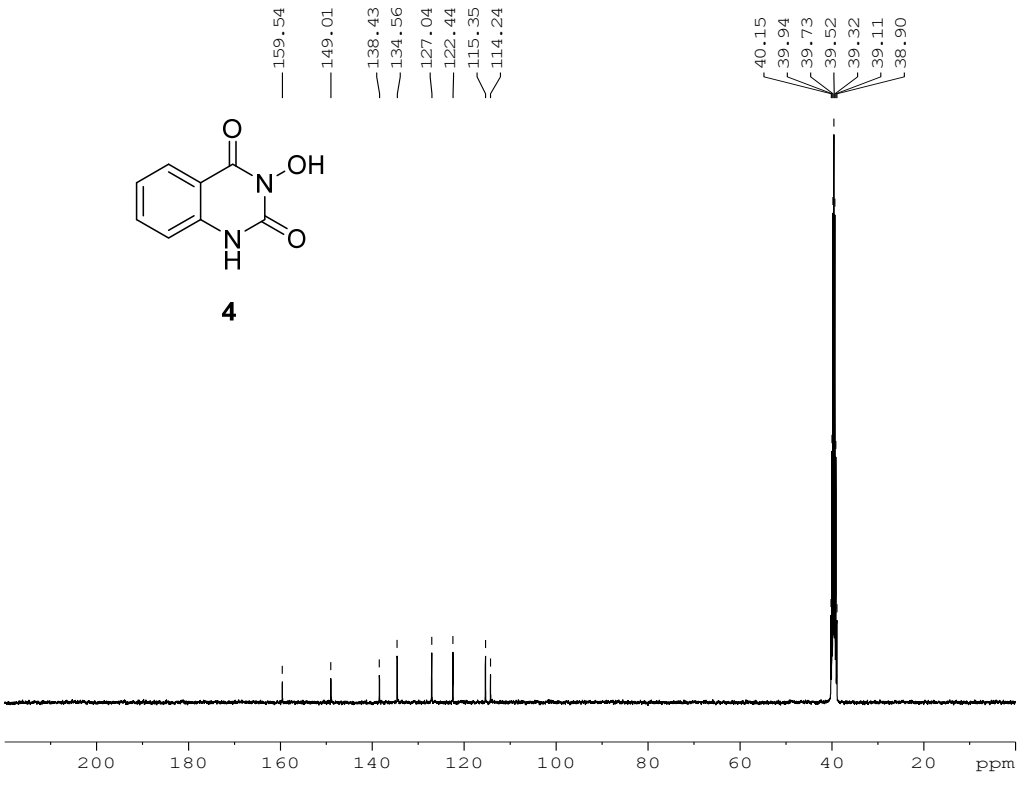
EXPNO                   1
PROCNO                  1
Date_            20201015
Time                11.38
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT              DMSO
NS                     28
DS                      0
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  10.00 usec
PL1                 -2.40 dB
SFO1         400.1528010 MHz
SI                  16384
SF           400.1500023 MHz
WDW                    EM
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

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NAME            CIL-1-132
EXPNO                   6
PROCNO                  1
Date_            20201012
Time                21.11
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                    196
DS                      0
SWH             22727.273 Hz
FIDRES           0.346791 Hz
AQ               1.4418420 sec
RG                     57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                   9.70 usec
PL1                 -0.50 dB
SFO1         100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               90.00 usec
PL2                 -2.40 dB
PL12                15.10 dB
PL13                18.10 dB
SFO2         400.1516010 MHz
SI                  32768
SF           100.6178403 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
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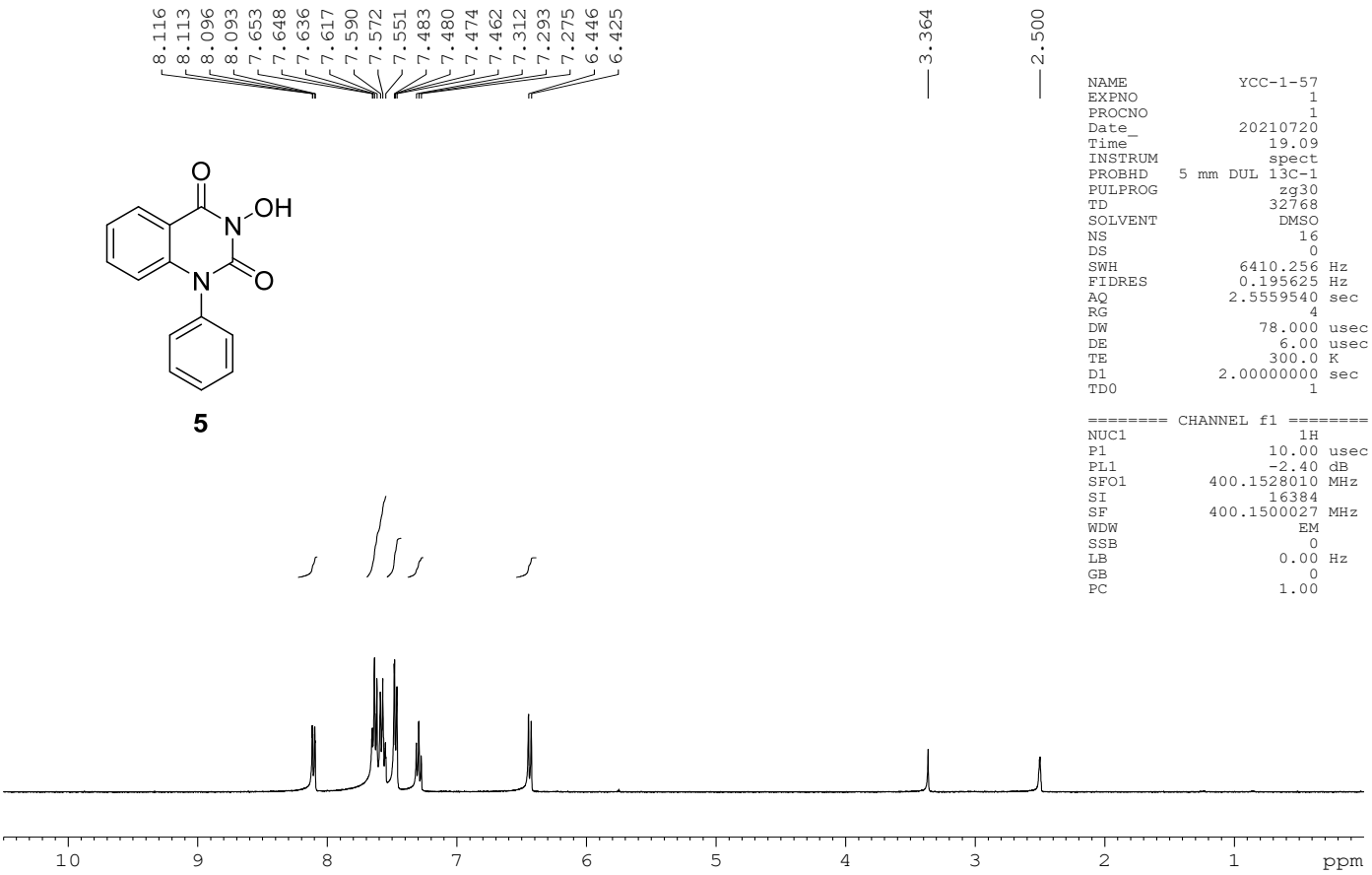
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7.293
7.275
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6.425
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O
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NAME YCC-1-57
EXPNO 1
PROCNO 1
Date_ 20210720
Time 19.09
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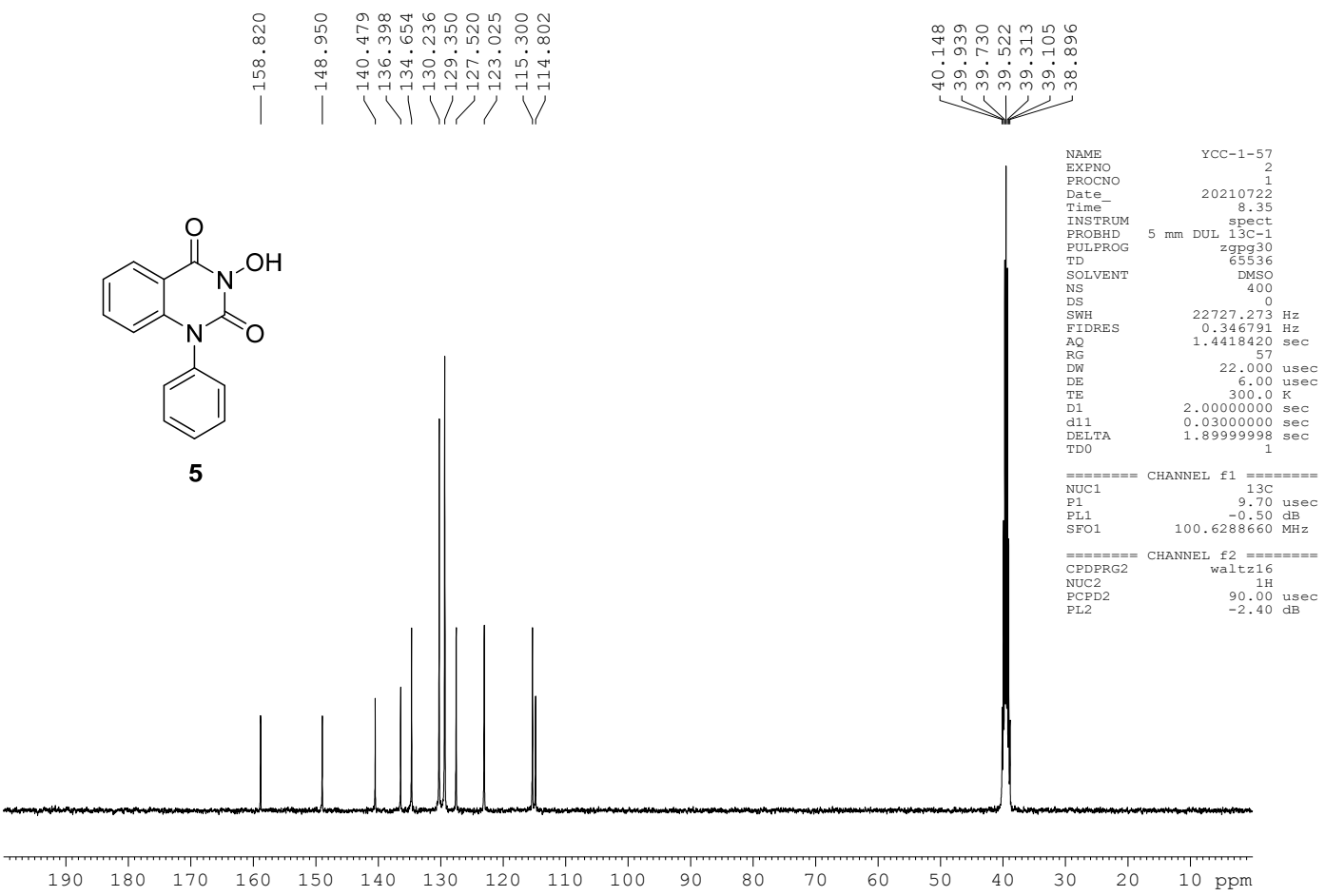
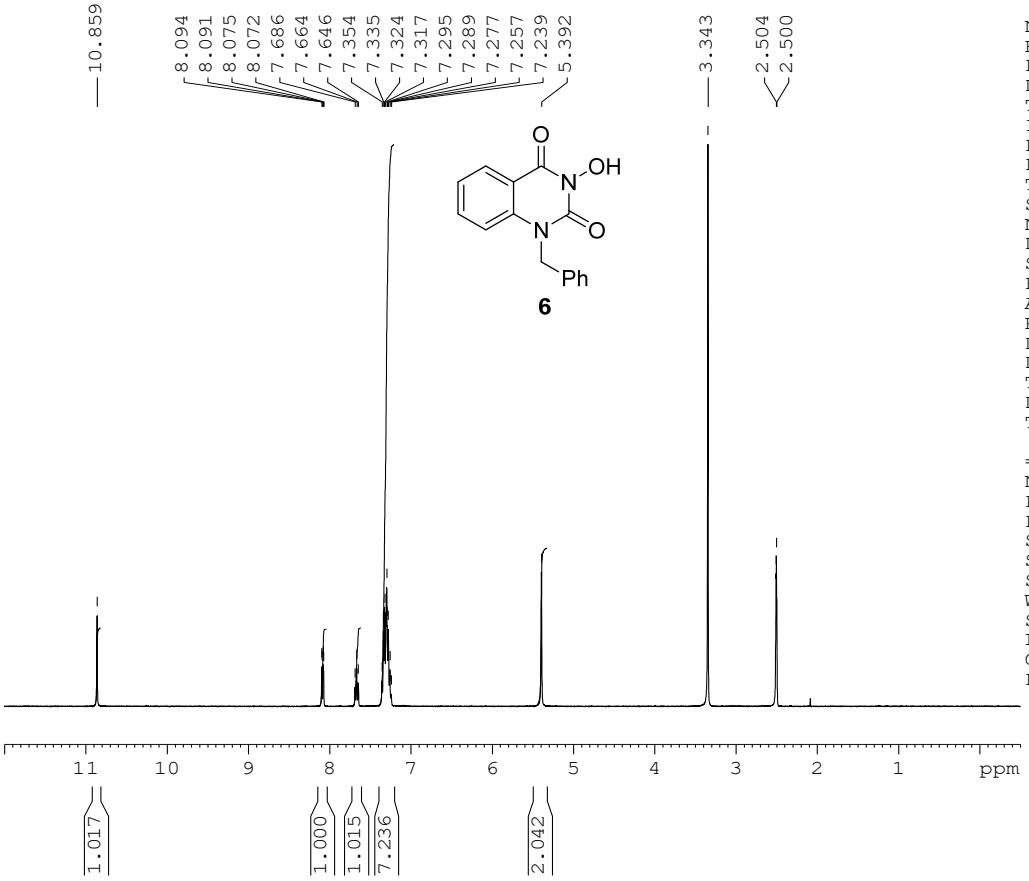
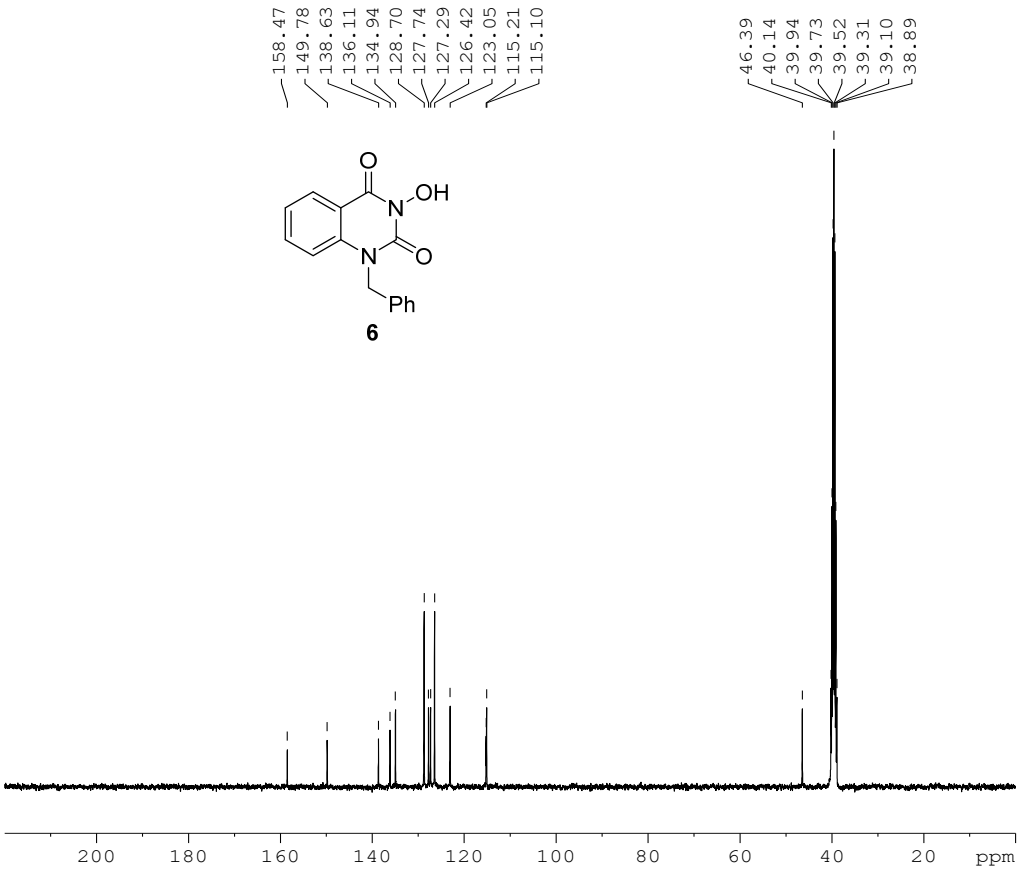
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500027 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 ppm
1.037
4.146
1.990
1.010
1.000

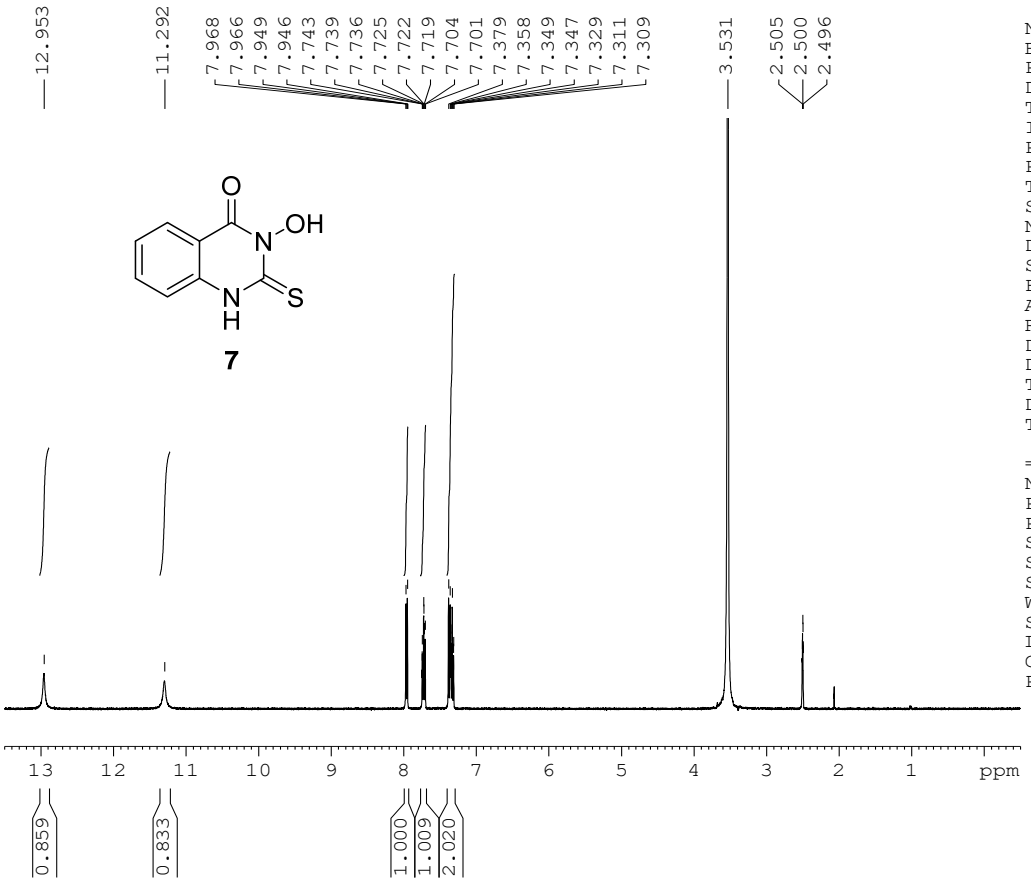

158.820
148.950
140.479
136.398
134.654
130.236
129.350
127.520
123.025
115.300
114.802
40.148
39.939
39.730
39.522
39.313
39.105
38.896
OH
N
O
5
NAME YCC-1-57
EXPNO 2
PROCNO 1
Date_ 20210722
Time 8.35
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 400
DS 0
SWH 22727.273 Hz
FIDRES 0.346791 Hz
AQ 1.4418420 sec
RG 57
DW 22.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.70 usec
PL1 -0.50 dB
SFO1 100.6288660 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -2.40 dB
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm



NAME	CIL-1-185
EXPNO	5
PROCNO	1
Date_	20210224
Time	19.57
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	24
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500027 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00

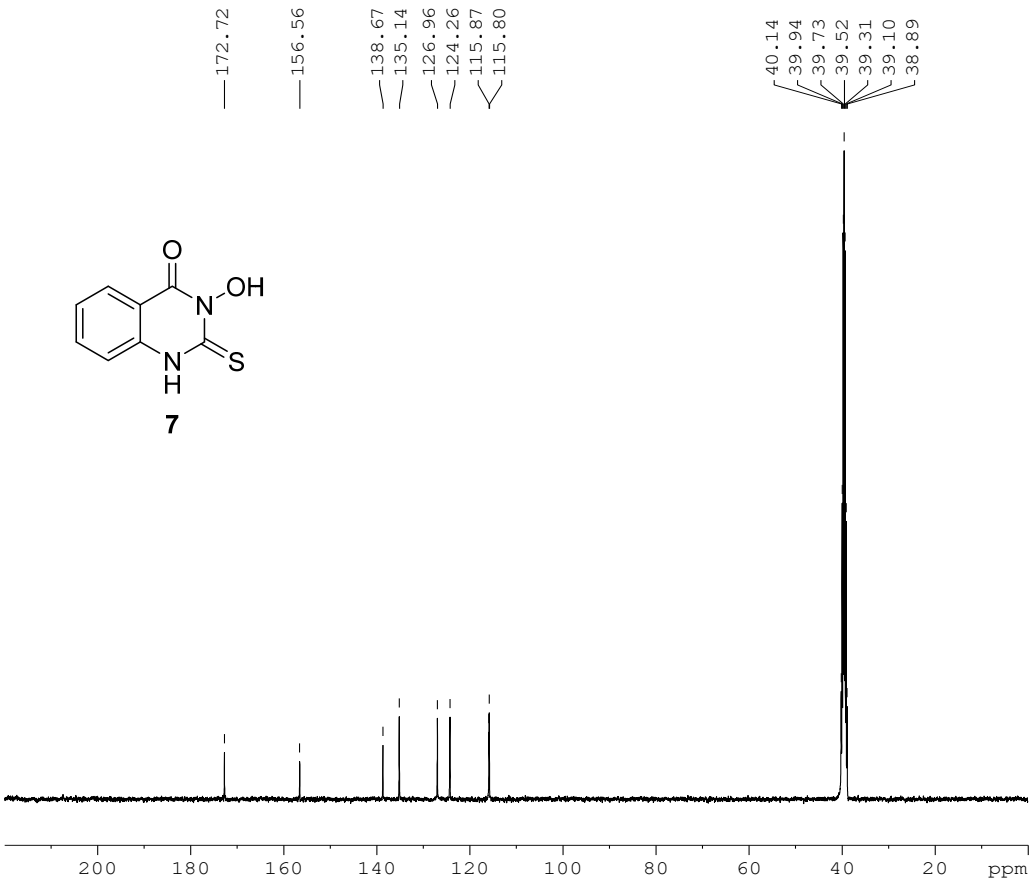


NAME	CIL-1-185
EXPNO	4
PROCNO	1
Date_	20210222
Time	21.06
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	400
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178466 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00




```
NAME                NHS-OH
EXPNO                    8
PROCNO                   1
Date_             20210509
Time                 17.39
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG               zg30
TD                   32768
SOLVENT                DMSO
NS                       10
DS                        0
SWH               6410.256 Hz
FIDRES               0.195625 Hz
AQ                2.5559540 sec
RG                       4
DW                  78.000 usec
DE                   6.00 usec
TE                  300.0 K
D1                2.00000000 sec
TD0                      1

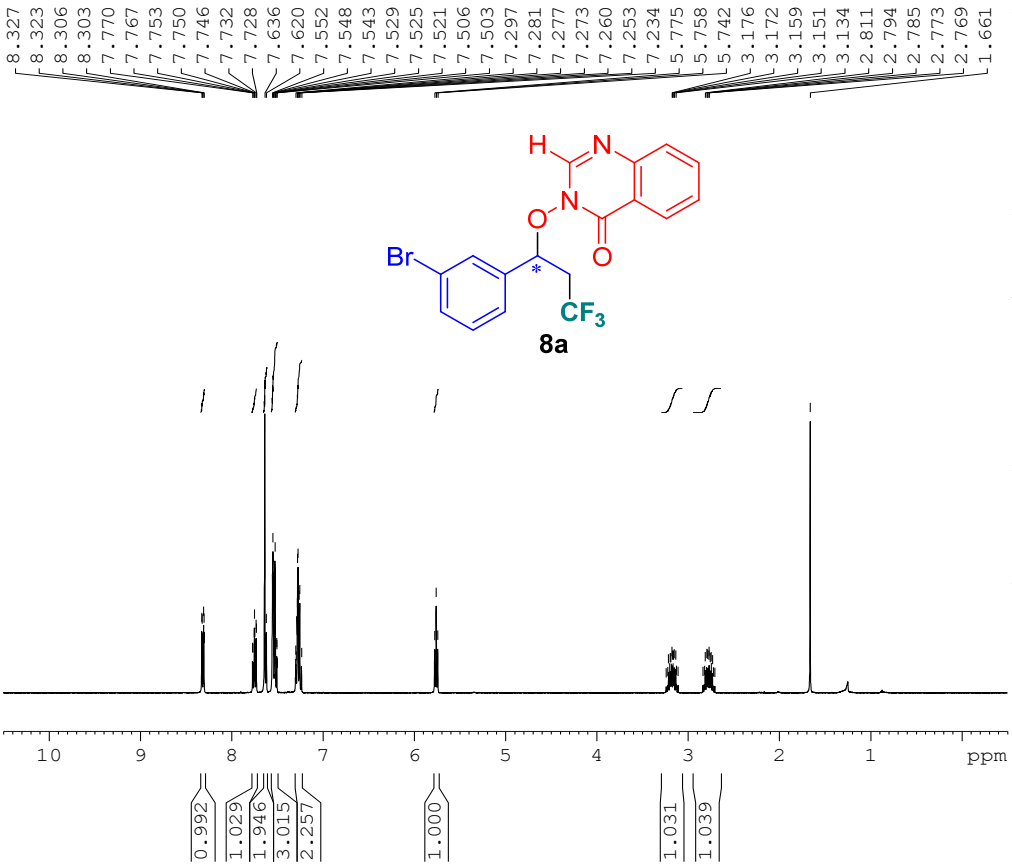
======== CHANNEL f1 ========
NUC1                    1H
P1                   10.00 usec
PL1                  -2.40 dB
SFO1          400.1528010 MHz
SI                   16384
SF            400.1500039 MHz
WDW                     EM
SSB                      0
LB                   0.00 Hz
GB                       0
PC                    1.00
```



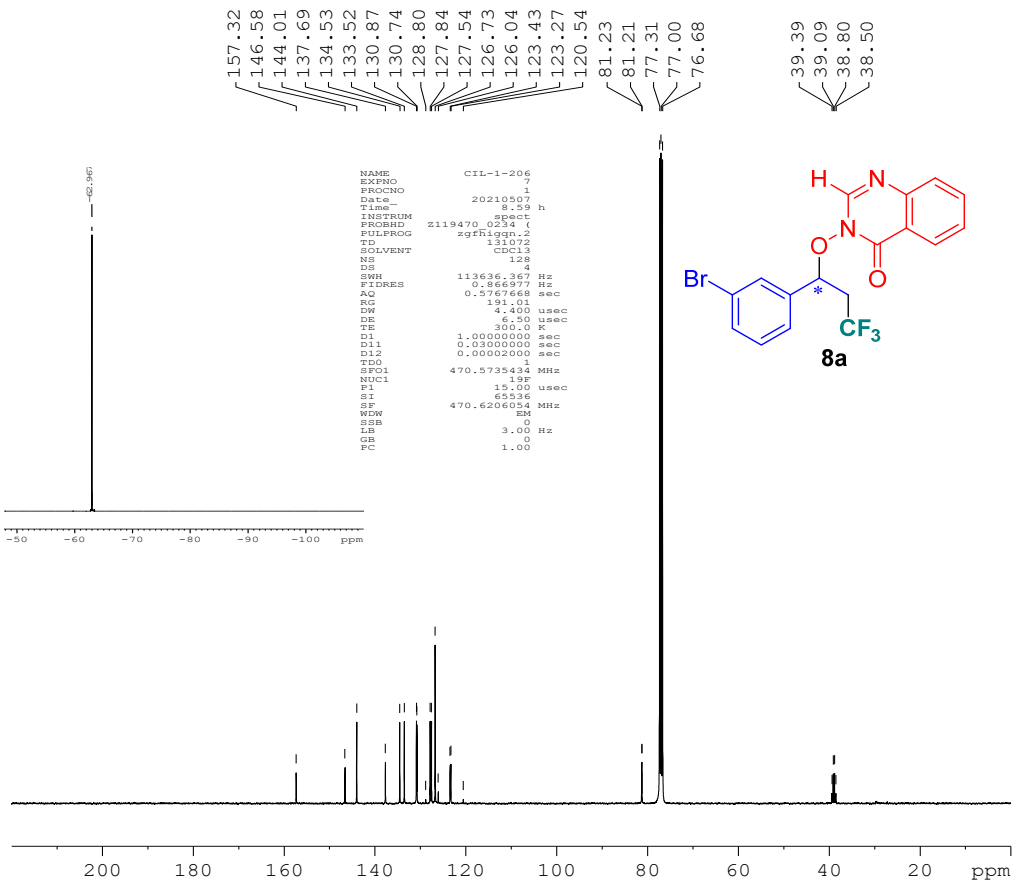

```
NAME              CIL-1-174
EXPNO                    10
PROCNO                    1
Date_             20210201
Time                 21.12
INSTRUM              spect
PROBHD    5 mm DUL 13C-1
PULPROG             zgpg30
TD                   65536
SOLVENT                DMSO
NS                      720
DS                        0
SWH              22727.273 Hz
FIDRES               0.346791 Hz
AQ                1.4418420 sec
RG                       57
DW                  22.000 usec
DE                   6.00 usec
TE                  300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                   13C
P1                    9.70 usec
PL1                  -0.50 dB
SFO1          100.6288660 MHz

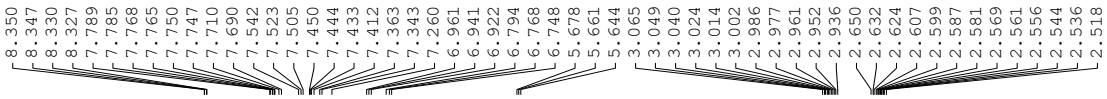
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2                90.00 usec
PL2                  -2.40 dB
PL12                 15.10 dB
PL13                 18.10 dB
SFO2          400.1516010 MHz
SI                   32768
SF            100.6178450 MHz
WDW                     EM
SSB                      0
LB                   3.00 Hz
GB                       0
PC                    1.00
```

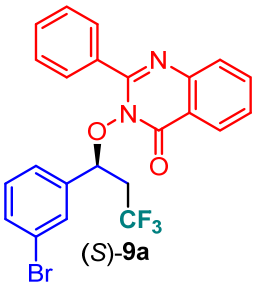


NAME	CIL-1-206
EXPNO	3
PROCNO	1
Date_	20210506
Time	11.47
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zg30
TD	32768
SOLVENT	CDCl3
NS	16
DS	0
SWH	6410.256 Hz
FIDRES	0.195625 Hz
AQ	2.5559540 sec
RG	4
DW	78.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-2.40 dB
SFO1	400.1528010 MHz
SI	16384
SF	400.1500092 MHz
WDW	EM
SSB	0
LB	0.00 Hz
GB	0
PC	1.00



NAME	CIL-1-206
EXPNO	5
PROCNO	1
Date_	20210507
Time	23.55
INSTRUM	spect
PROBHD	5 mm DUL 13C-1
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10000
DS	0
SWH	22727.273 Hz
FIDRES	0.346791 Hz
AQ	1.4418420 sec
RG	57
DW	22.000 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.70 usec
PL1	-0.50 dB
SFO1	100.6288660 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	90.00 usec
PL2	-2.40 dB
PL12	15.10 dB
PL13	18.10 dB
SFO2	400.1516010 MHz
SI	32768
SF	100.6178013 MHz
WDW	EM
SSB	0
LB	3.00 Hz
GB	0
PC	1.00

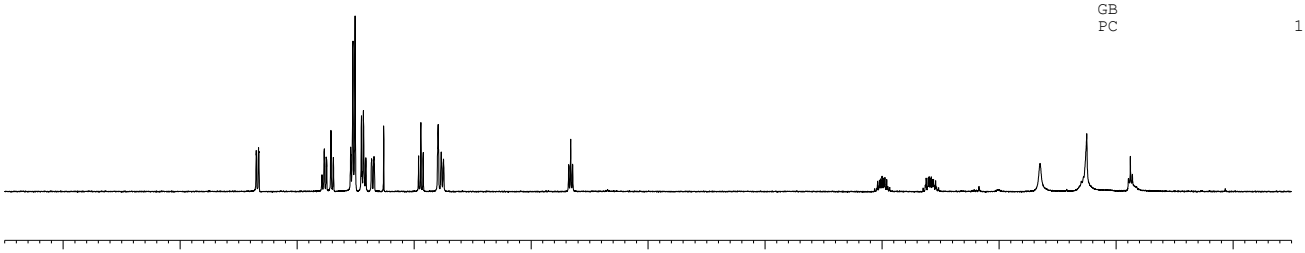


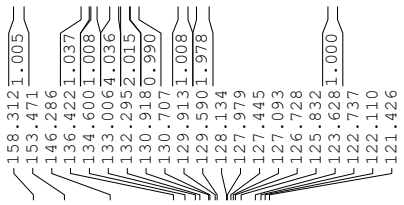


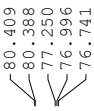
(*S*)-**9a**

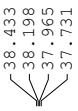
```
NAME                 2021129
EXPNO                      3
PROCNO                     1
Date_               20211229
Time                   14.29
INSTRUM                spect
PROBHD    5 mm DUL 13C-1
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                       16
DS                        0
SWH                6410.256 Hz
FIDRES                0.195625 Hz
AQ                 2.5559540 sec
RG                        4
DW                   78.000 usec
DE                    6.00 usec
TE                   300.0 K
D1                 2.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    10.00 usec
PL1                   -2.40 dB
SFO1           400.1528010 MHz
SI                    16384
SF             400.1500092 MHz
WDW                      EM
SSB                       0
LB                    0.00 Hz
GB                        0
PC                    1.00
```

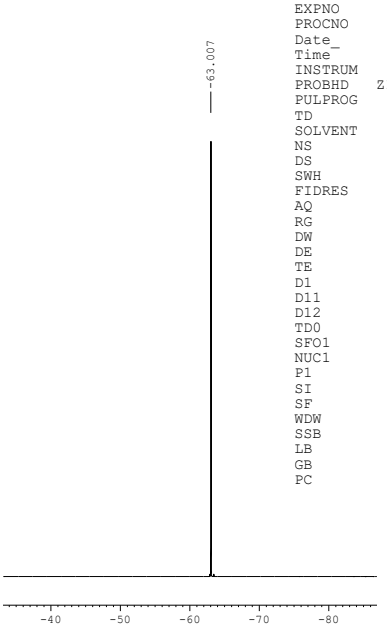


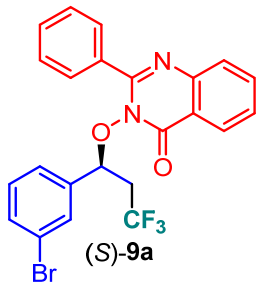






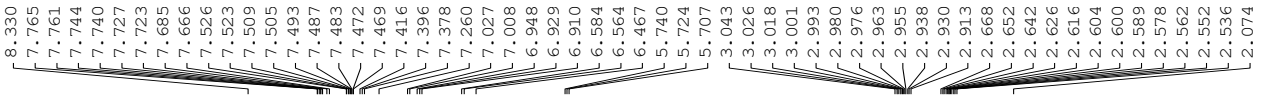

```
NAME          chem211230.001
EXPNO                      3
PROCNO                     1
Date_               20211229
Time                  16.06 h
INSTRUM                spect
PROBHD    Z119470_0234 (
PULPROG          zgfhigqn.2
TD                    131072
SOLVENT               CDCl3
NS                      128
DS                        4
SWH               113636.367 Hz
FIDRES                0.866977 Hz
AQ                 0.5767668 sec
RG                   191.01
DW                    4.400 usec
DE                    6.50 usec
TE                   299.2 K
D1                 1.00000000 sec
D11                0.03000000 sec
D12                0.00002000 sec
TD0                        1
SFO1           470.5735434 MHz
NUC1                      19F
P1                   15.00 usec
SI                    65536
SF             470.6206054 MHz
WDW                      EM
SSB                       0
LB                    3.00 Hz
GB                        0
PC                    1.00
```

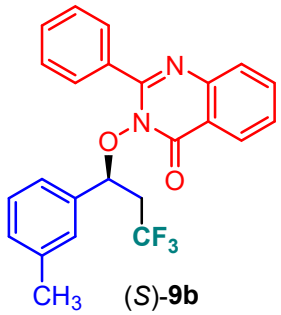




(*S*)-**9a**

```
NAME          chem211230.001
EXPNO                      2
PROCNO                     2
Date_               20211230
Time                  13.18 h
INSTRUM                spect
PROBHD    Z119470_0234 (
PULPROG               zgpg30
TD                     32768
SOLVENT               CDCl3
NS                      2485
DS                        0
SWH                29761.904 Hz
FIDRES                0.908261 Hz
AQ                 0.5505524 sec
RG                   191.01
DW                   16.800 usec
DE                    6.50 usec
TE                   299.9 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                        1
SFO1           125.7785374 MHz
NUC1                      13C
P1                   10.00 usec
SI                    32768
SF             125.7653353 MHz
WDW                      EM
SSB                       0
LB                    2.00 Hz
GB                        0
PC                    1.00
```

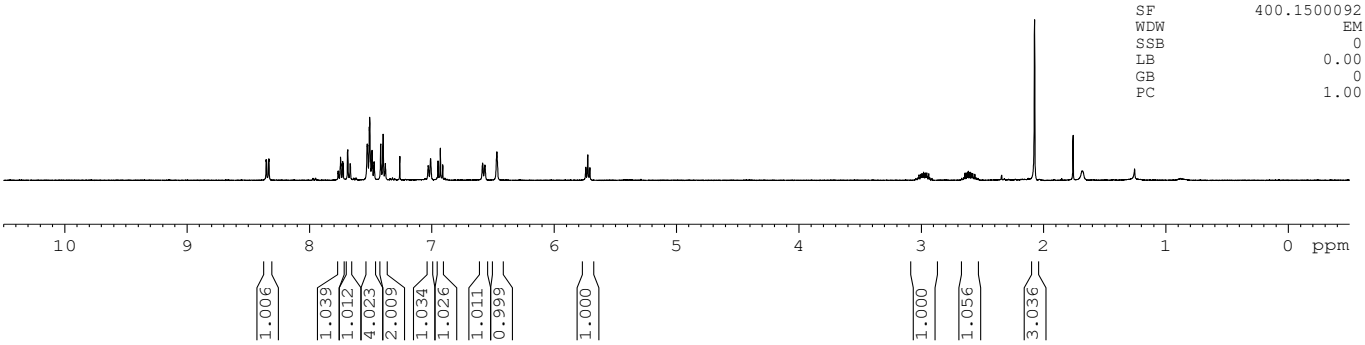


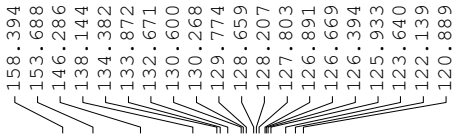


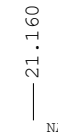
(*S*)-**9b**

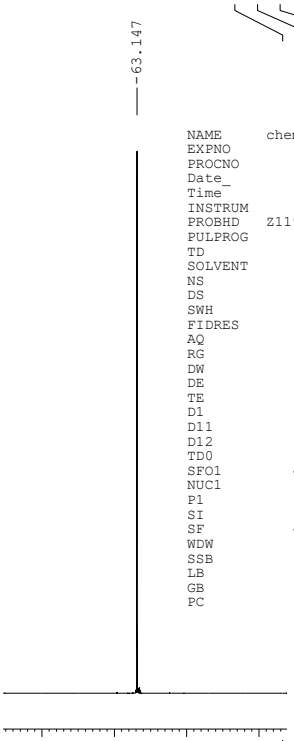
```
NAME            20220728
EXPNO                  6
PROCNO                 1
Date_           20220728
Time                6.27
INSTRUM            spect
PROBHD    5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    13
DS                     0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              2.5559540 sec
RG                     4
DW                78.000 usec
DE                 6.00 usec
TE                300.0 K
D1              2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -2.40 dB
SFO1          400.1528010 MHz
SI                 16384
SF            400.1500092 MHz
WDW                   EM
SSB                    0
LB                0.00 Hz
GB                     0
PC                1.00
```

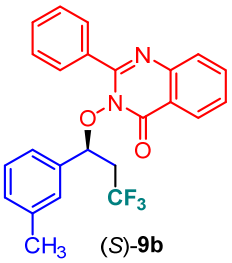









```
NAME      chem220728.003
EXPNO                  2
PROCNO                 1
Date_           20220728
Time              14.43 h
INSTRUM            spect
PROBHD    Z119470_0234 (
PULPROG      zgfhigqn.2
TD                131072
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ              0.5767668 sec
RG                191.01
DW                 4.400 usec
DE                 6.50 usec
TE                299.6 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                    1
SFO1          470.5735434 MHz
NUC1                 19F
P1                15.00 usec
SI                 65536
SF            470.6206054 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```

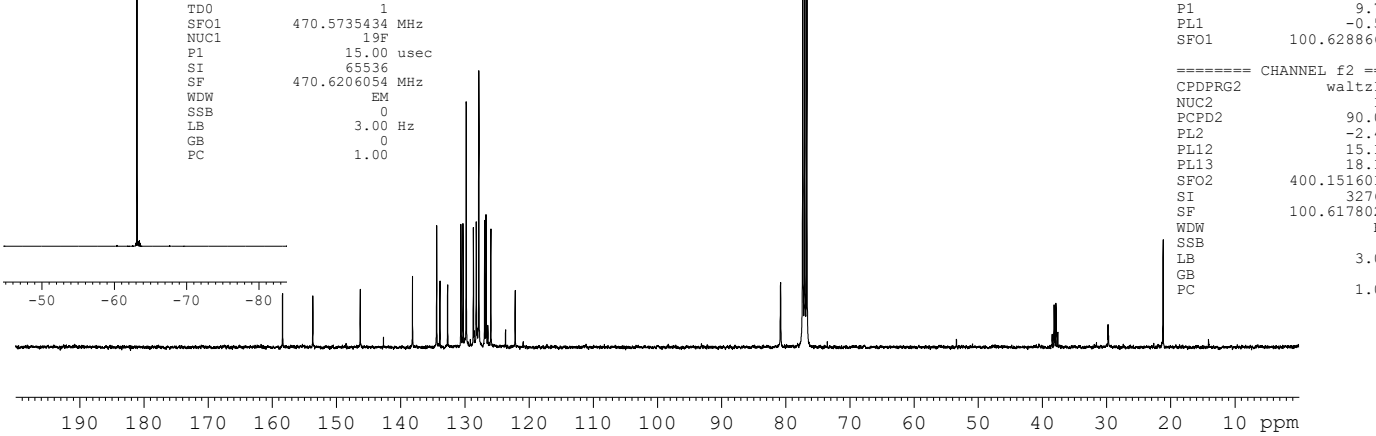


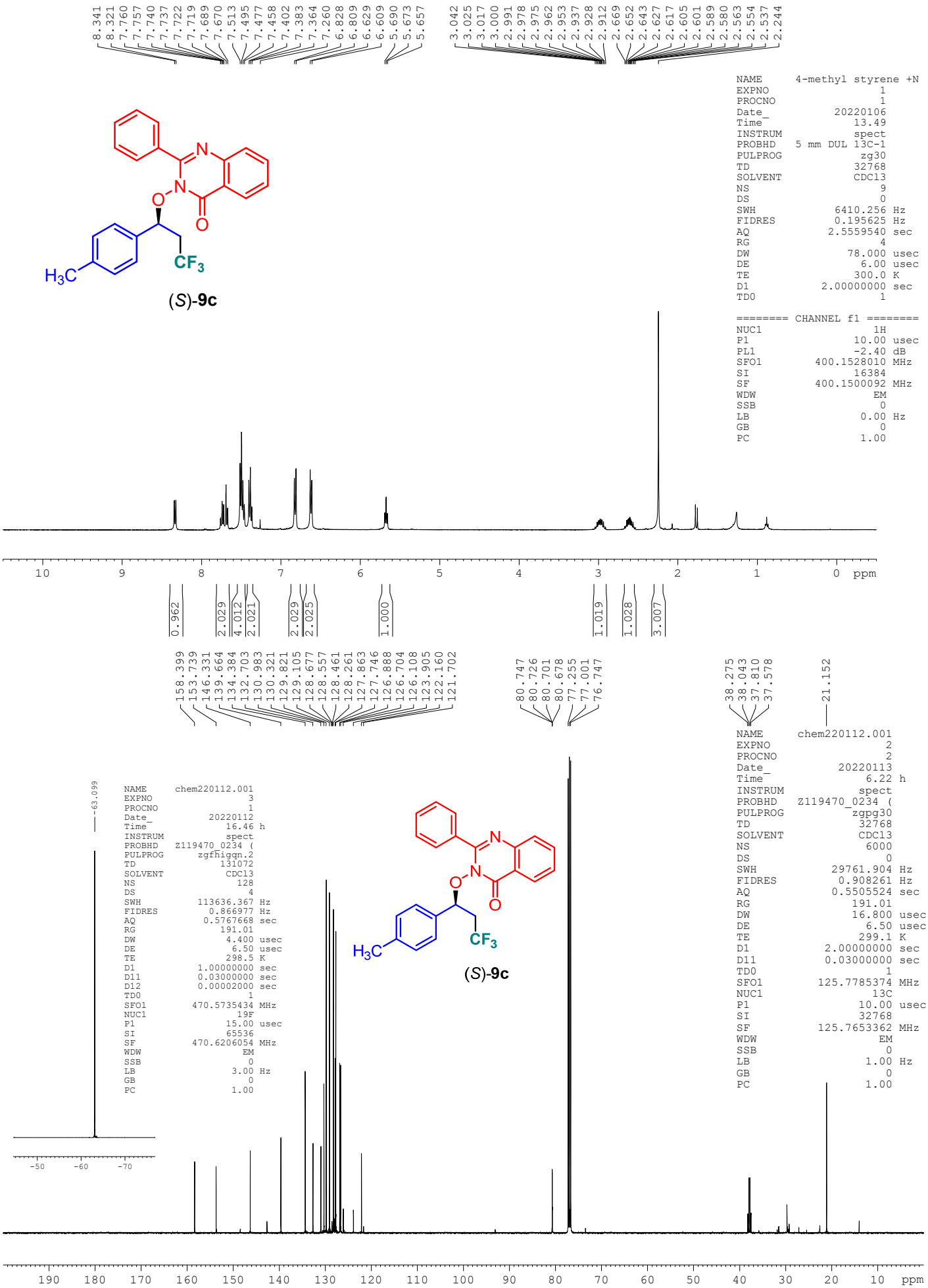
(*S*)-**9b**

```
NAME            20220728
EXPNO                  3
PROCNO                 1
Date_           20220728
Time                2.55
INSTRUM            spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  2400
DS                     0
SWH            22727.273 Hz
FIDRES          0.346791 Hz
AQ              1.4418420 sec
RG                    57
DW                22.000 usec
DE                 6.00 usec
TE                300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.70 usec
PL1               -0.50 dB
SFO1          100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2               -2.40 dB
PL12              15.10 dB
PL13              18.10 dB
SFO2          400.1516010 MHz
SI                 32768
SF            100.6178025 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```

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8.321
7.760
7.757
7.740
7.737
7.722
7.719
7.689
7.670
7.513
7.495
7.477
7.458
7.402
7.383
7.364
7.260
6.828
6.809
6.629
6.609
5.690
5.673
5.657
3.042
3.025
3.017
3.000
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2.978
2.975
2.962
2.953
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2.928
2.912
2.669
2.652
2.643
2.627
2.617
2.605
2.601
2.589
2.580
2.563
2.554
2.537
2.244
NAME 4-methyl styrene +N
EXPNO 1
PROCNO 1
Date_ 20220106
Time 13.49
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 9
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500092 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
N
N
O
O
H3C
CF3
(S)-9c
10
9
8
7
6
5
4
3
2
1
0 ppm
0.962
2.029
4.012
2.021
2.029
2.025
1.000
1.019
1.028
3.007
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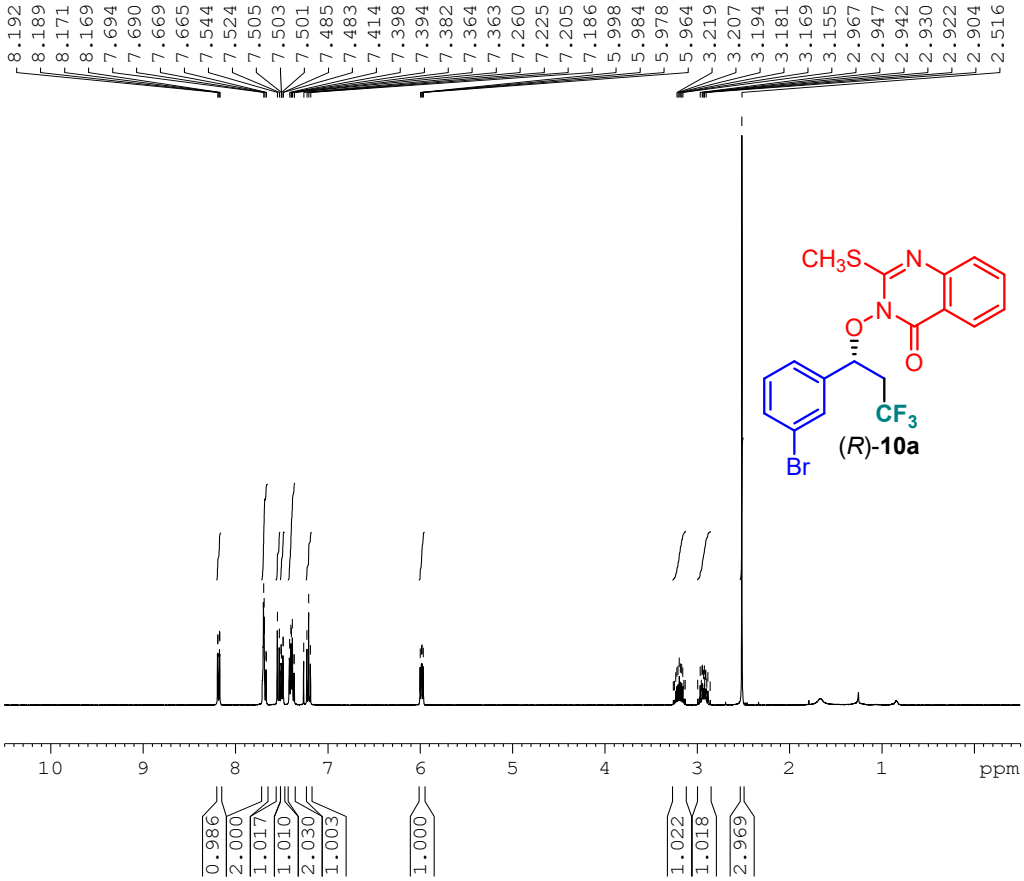
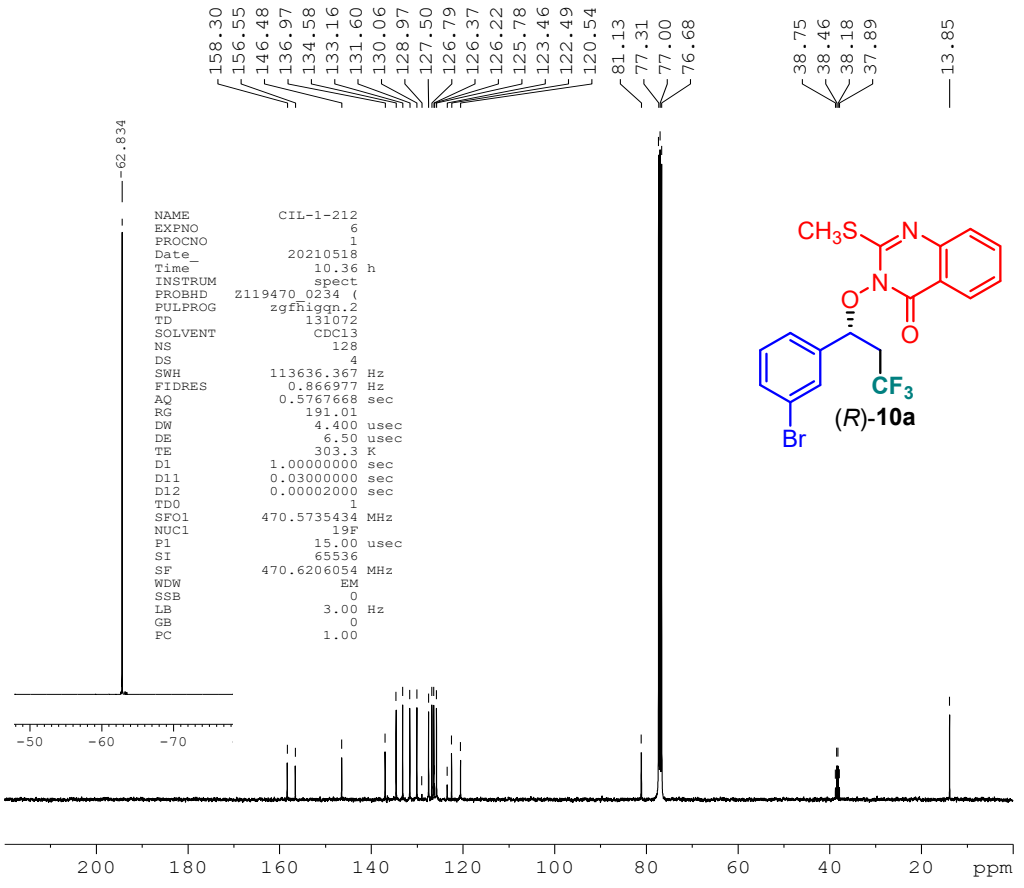
-63.099
NAME chem220112.001
EXPNO 3
PROCNO 1
Date_ 20220112
Time 16.46 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 191.01
DW 4.400 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5735434 MHz
NUC1 19F
P1 15.00 usec
SI 65536
SF 470.6206054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
-50
-60
-70
NAME chem220112.001
EXPNO 2
PROCNO 2
Date_ 20220113
Time 6.22 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 6000
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653362 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
N
N
O
O
H3C
CF3
(S)-9c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10 ppm




```
NAME            CIL-1-212
EXPNO                   3
PROCNO                  1
Date_            20210518
Time                20.20
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      0
SWH           6410.256 Hz
FIDRES        0.195625 Hz
AQ            2.5559540 sec
RG                      4
DW              78.000 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1        400.1528010 MHz
SI                  16384
SF          400.1500092 MHz
WDW                   EM
SSB                    0
LB                0.00 Hz
GB                     0
PC                1.00
```

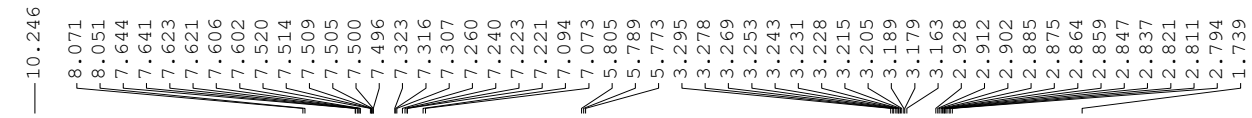


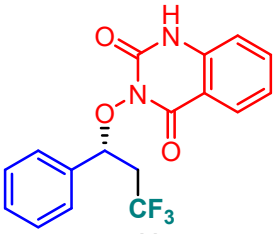

```
NAME            CIL-1-212
EXPNO                   6
PROCNO                  1
Date_            20210518
Time              10.36 h
INSTRUM             spect
PROBHD   Z119470_0234 (
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                    128
DS                      4
SWH          113636.367 Hz
FIDRES         0.866977 Hz
AQ             0.5767668 sec
RG                191.01
DW                4.400 usec
DE                6.50 usec
TE                303.3 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                     1
SFO1        470.5735434 MHz
NUC1                  19F
P1                15.00 usec
SI                  65536
SF          470.6206054 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```

```
NAME            CIL-1-212
EXPNO                   4
PROCNO                  1
Date_            20210518
Time                20.21
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  11000
DS                      0
SWH          22727.273 Hz
FIDRES         0.346791 Hz
AQ             1.4418420 sec
RG                     57
DW              22.000 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.70 usec
PL1               -0.50 dB
SFO1        100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2             90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2        400.1516010 MHz
SI                  32768
SF          100.6178006 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```

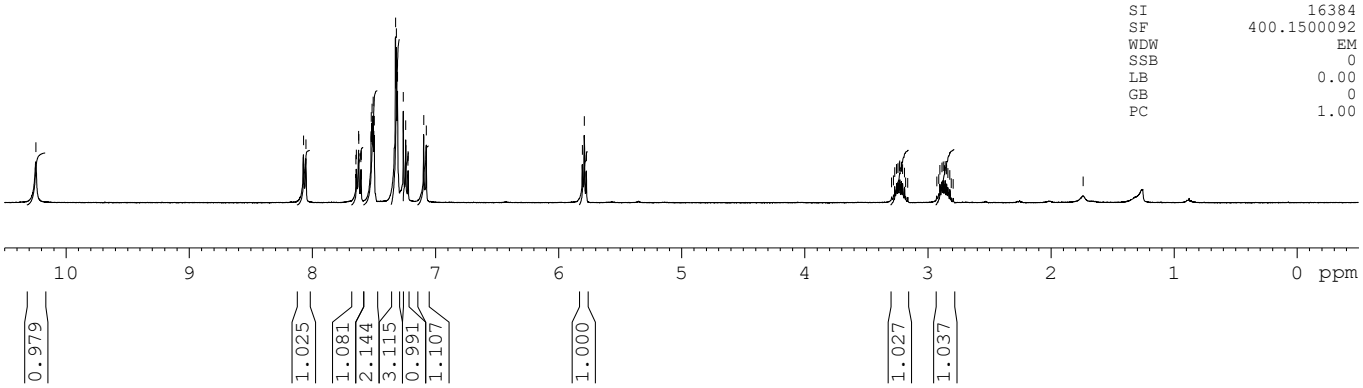


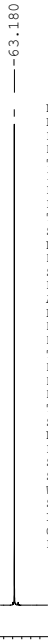


(*R*)-**11c**

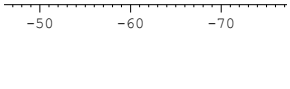
```
NAME            CIL-1-137
EXPNO                   4
PROCNO                  1
Date_            20201020
Time                20.07
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
TD0                     1

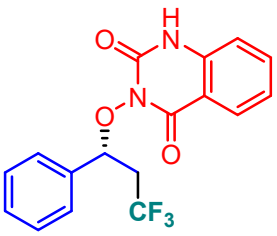
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1          400.1528010 MHz
SI                  16384
SF            400.1500092 MHz
WDW                    EM
SSB                     0
LB                 0.00 Hz
GB                      0
PC                   1.00
```






```
NAME            CIL-1-137
EXPNO                   8
PROCNO                  1
Date_            20201029
Time              15.40 h
INSTRUM             spect
PROBHD   Z119470_0234 (
PULPROG      zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                    128
DS                      4
SWH            113636.367 Hz
FIDRES           0.866977 Hz
AQ               0.5767668 sec
RG                 191.01
DW                  4.400 usec
DE                  6.50 usec
TE                299.8 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1
SFO1           470.5735434 MHz
NUC1                  19F
P1                 15.00 usec
SI                  65536
SF             470.6206054 MHz
WDW                    EM
SSB                     0
LB                  3.00 Hz
GB                      0
PC                   1.00
```



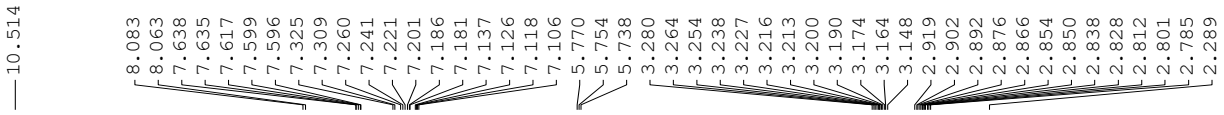


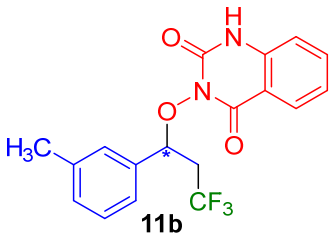
(*R*)-**11c**

```
NAME            CIL-1-137
EXPNO                   6
PROCNO                  1
Date_            20201021
Time                23.58
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   8000
DS                      0
SWH            22727.273 Hz
FIDRES           0.346791 Hz
AQ               1.4418420 sec
RG                     57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1          100.6288660 MHz

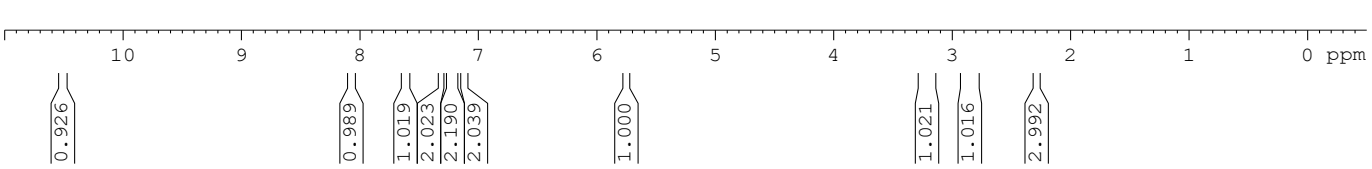
======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2          400.1516010 MHz
SI                  32768
SF            100.6178000 MHz
WDW                    EM
SSB                     0
LB                  3.00 Hz
GB                      0
PC                   1.00
```

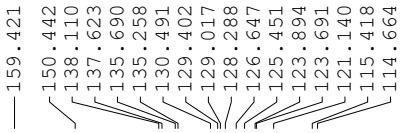


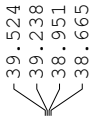


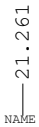

```
NAME            CIL-1-156
EXPNO                   1
PROCNO                  1
Date_            20201204
Time                19.21
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1          400.1528010 MHz
SI                  16384
SF            400.1500092 MHz
WDW                    EM
SSB                     0
LB                 0.00 Hz
GB                      0
PC                   1.00
```

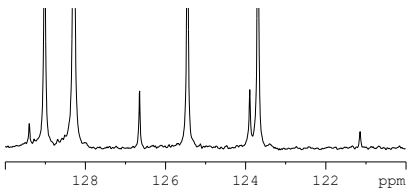


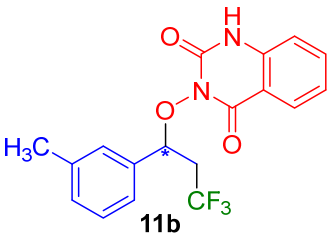







```
NAME            CIL-1-153
EXPNO                   7
PROCNO                  1
Date_            20201129
Time               14.37 h
INSTRUM             spect
PROBHD    Z119470_0234 (
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                    128
DS                      4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ              0.5767668 sec
RG                 191.01
DW                  4.400 usec
DE                  6.50 usec
TE                 299.8 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1
SFO1          470.5735434 MHz
NUC1                  19F
P1                 15.00 usec
SI                  65536
SF            470.6206054 MHz
WDW                    EM
SSB                     0
LB                 3.00 Hz
GB                      0
PC                   1.00
```

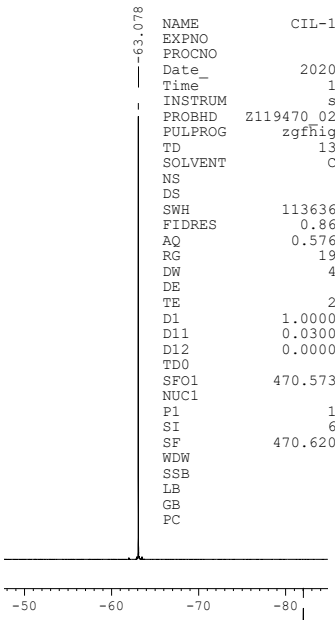


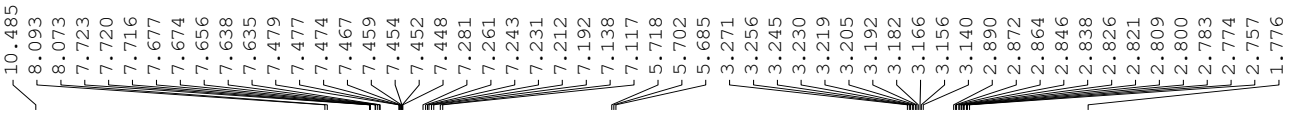


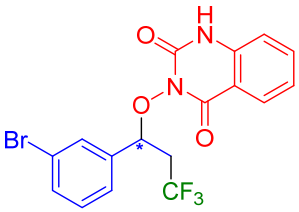

```
NAME            CIL-1-156
EXPNO                   3
PROCNO                  1
Date_            20201205
Time               23.46
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   9200
DS                      0
SWH           22727.273 Hz
FIDRES          0.346791 Hz
AQ              1.4418420 sec
RG                     57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1          100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2          400.1516010 MHz
SI                  32768
SF            100.6178013 MHz
WDW                    EM
SSB                     0
LB                 3.00 Hz
GB                      0
PC                   1.00
```



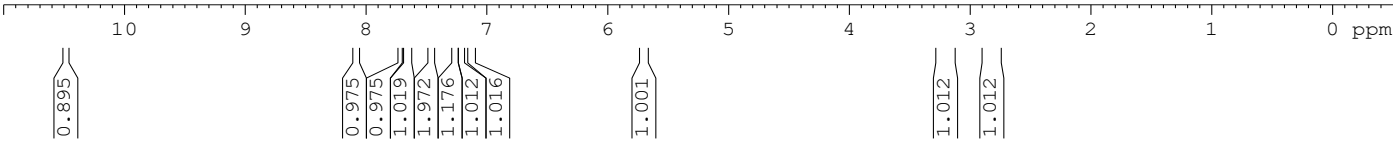


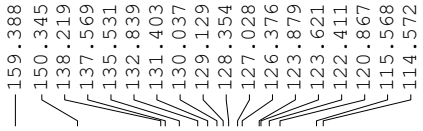


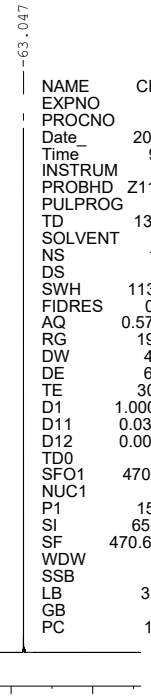
11a

```
NAME            CIL-1-148
EXPNO                   1
PROCNO                  1
Date_            20201116
Time                20.13
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     40
DS                      0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
TD0                     1

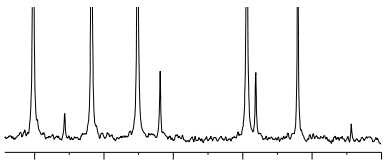
======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1          400.1528010 MHz
SI                  16384
SF            400.1500092 MHz
WDW                    EM
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

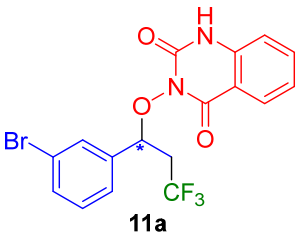







```
NAME            CIL-1-148
EXPNO                   7
PROCNO                  1
Date_            20201117
Time                9.55 h
INSTRUM             spect
PROBHD   Z119470_0234 (
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT             CDCl3
NS                    128
DS                      4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ              0.5767668 sec
RG                 191.01
DW                  4.400 usec
DE                  6.50 usec
TE                 300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1
SFO1          470.5735434 MHz
NUC1                  19F
P1                 15.00 usec
SI                  65536
SF            470.6206054 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```



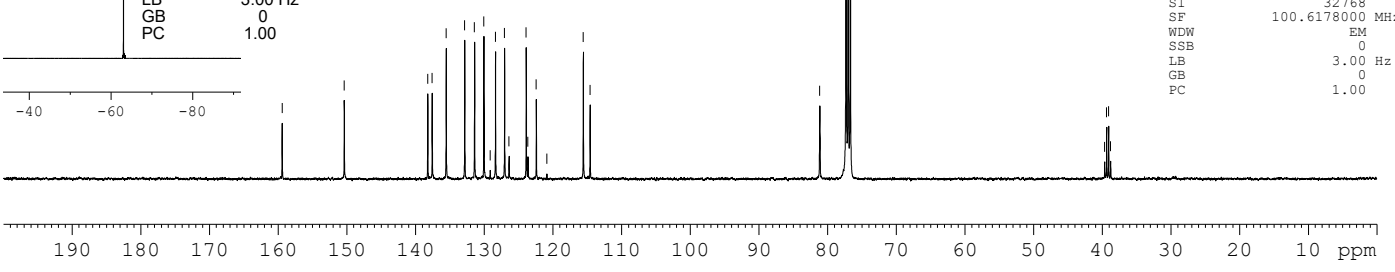


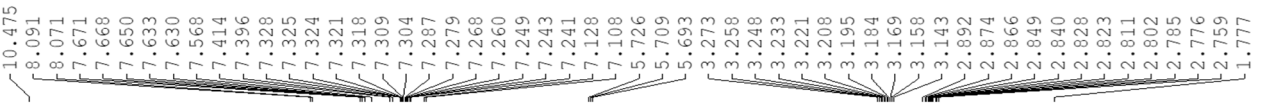
11a

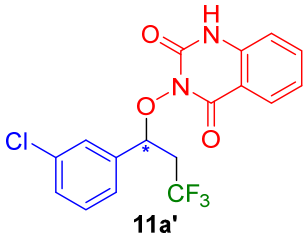
```
NAME            CIL-1-147
EXPNO                   4
PROCNO                  1
Date_            20201118
Time                0.01
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    9000
DS                      0
SWH            22727.273 Hz
FIDRES          0.346791 Hz
AQ              1.4418420 sec
RG                     57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1          100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2          400.1516010 MHz
SI                  32768
SF            100.6178000 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```



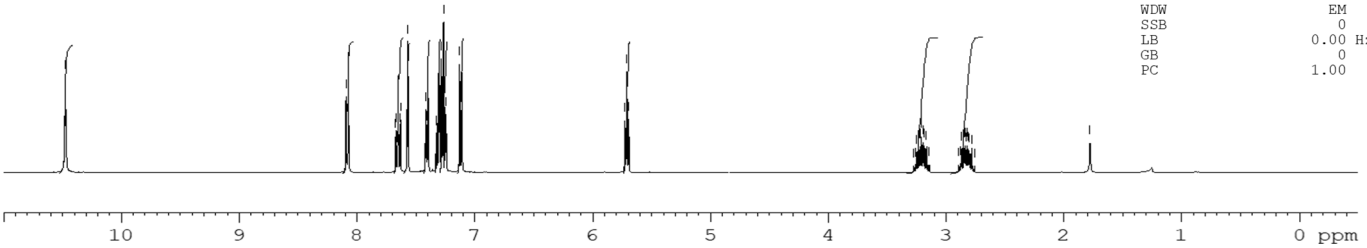


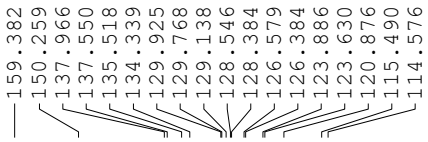


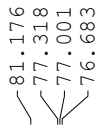
11a'

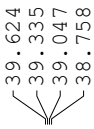
```
NAME          CIL-1-153
EXPNO                 2
PROCNO                1
Date_          20201123
Time              21.29
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                  100
DS                    0
SWH          6410.256 Hz
FIDRES       0.195625 Hz
AQ           2.5559540 sec
RG                    4
DW              78.000 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
TD0                   1

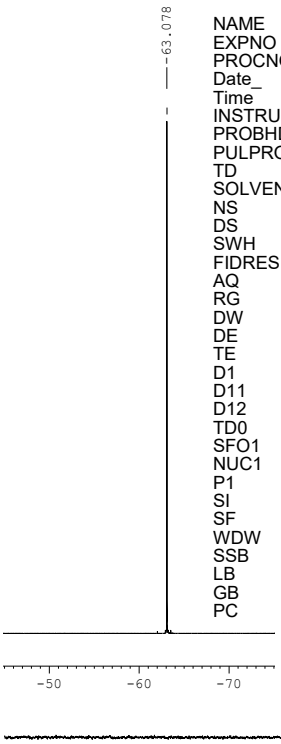
======== CHANNEL f1 ========
NUC1                 1H
P1                10.00 usec
PL1               -2.40 dB
SFO1        400.1528010 MHz
SI                16384
SF          400.1500096 MHz
WDW                  EM
SSB                   0
LB               0.00 Hz
GB                    0
PC                 1.00
```



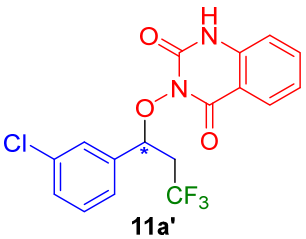









```
NAME          CIL-1-153
EXPNO                 7
PROCNO                1
Date_          20201125
Time             14.37 h
INSTRUM           spect
PROBHD   Z119470_0234 (
PULPROG      zgfhigqn.2
TD               131072
SOLVENT            CDCl3
NS                  128
DS                    4
SWH          113636.367 Hz
FIDRES         0.866977 Hz
AQ             0.5767668 sec
RG                191.01
DW                4.400 usec
DE                6.50 usec
TE                299.8 K
D1           1.00000000 sec
D11          0.03000000 sec
D12          0.00002000 sec
TD0                   1
SFO1        470.5735434 MHz
NUC1                19F
P1               15.00 usec
SI                65536
SF          470.6206054 MHz
WDW                  EM
SSB                   0
LB               3.00 Hz
GB                    0
PC                 1.00
```

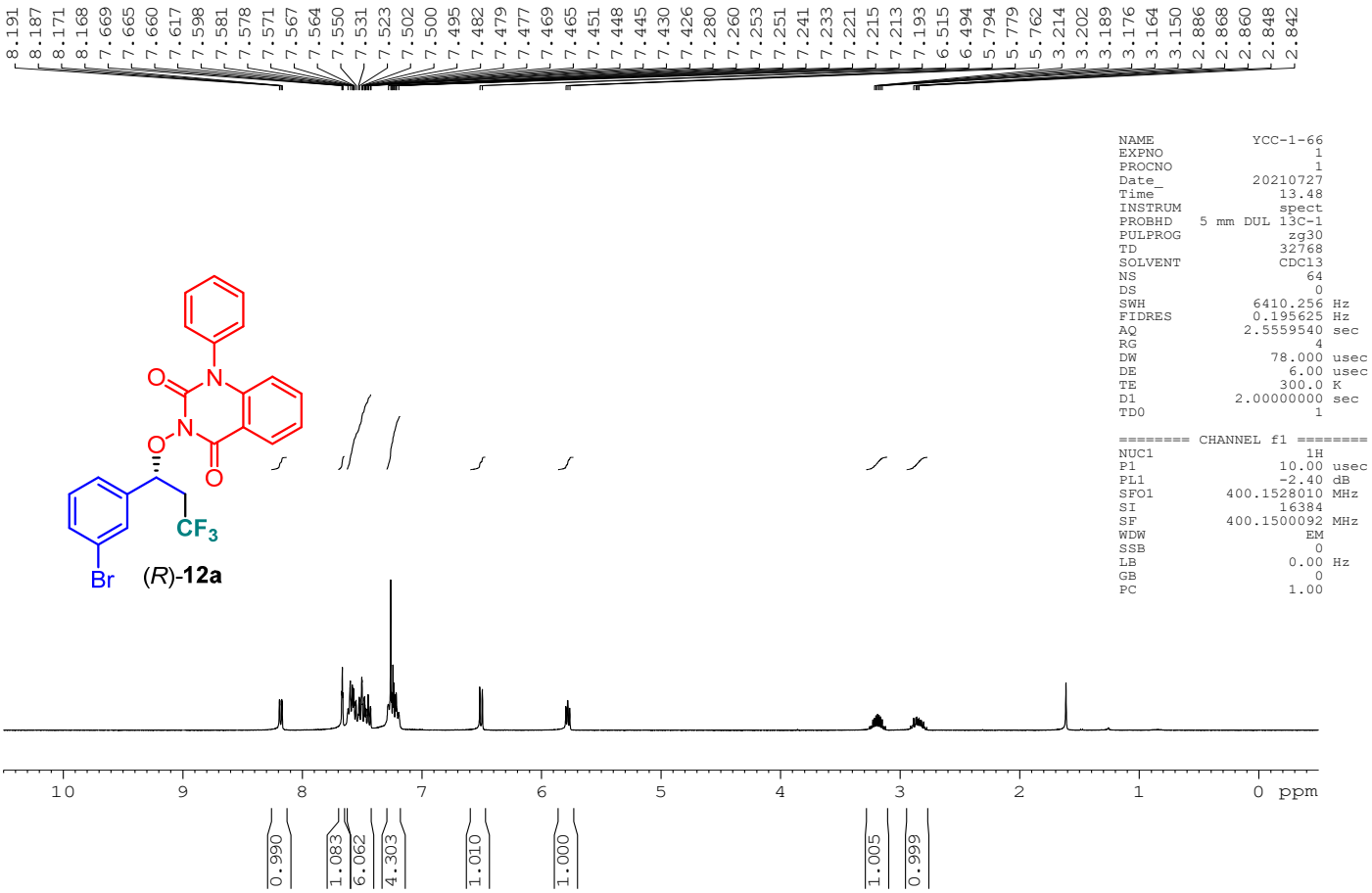


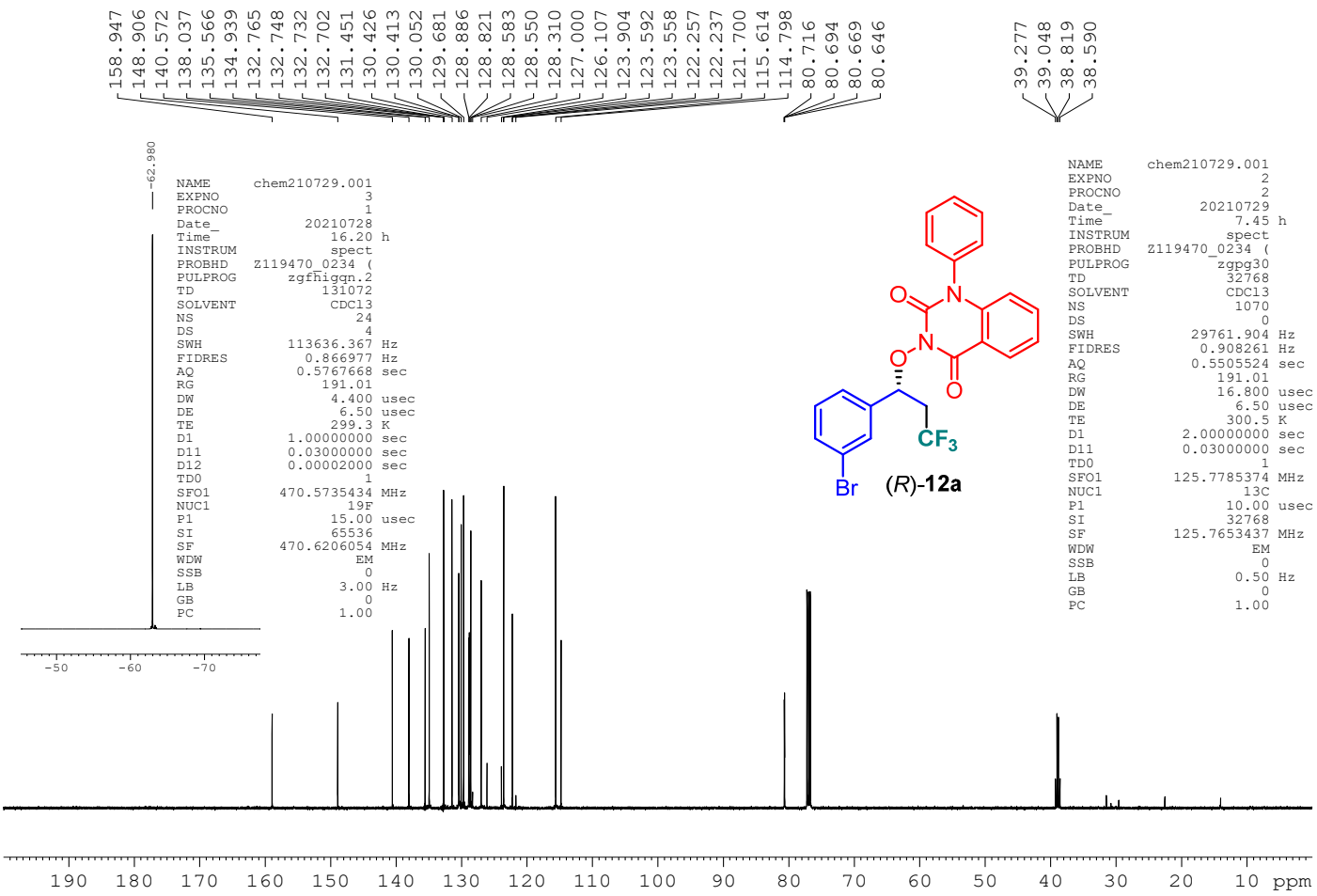
11a'

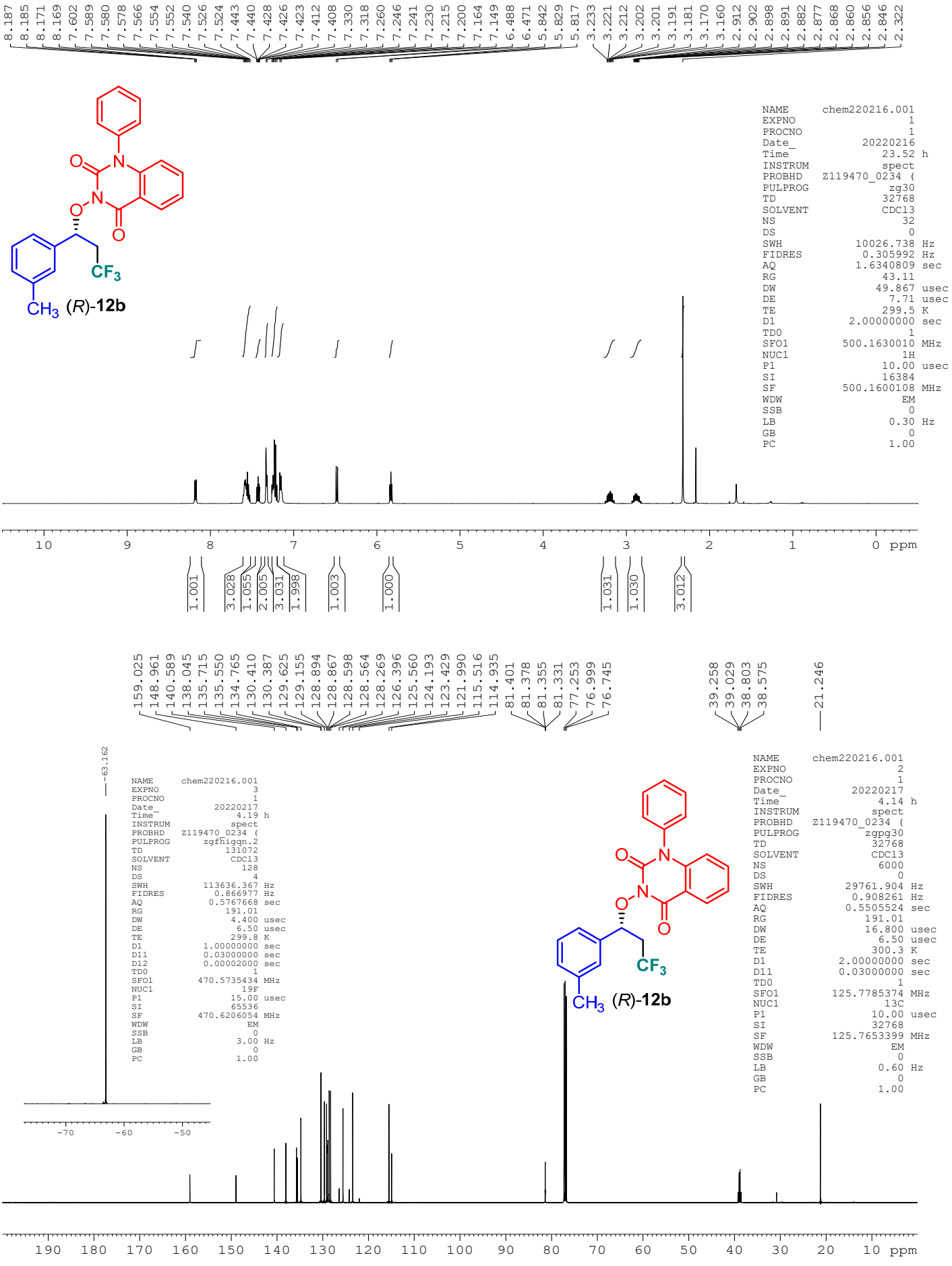
```
NAME          CIL-1-153
EXPNO                 4
PROCNO                1
Date_          20201124
Time              0.05
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 8000
DS                    0
SWH          22727.273 Hz
FIDRES        0.346791 Hz
AQ            1.4418420 sec
RG                   57
DW              22.000 usec
DE               6.00 usec
TE              300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

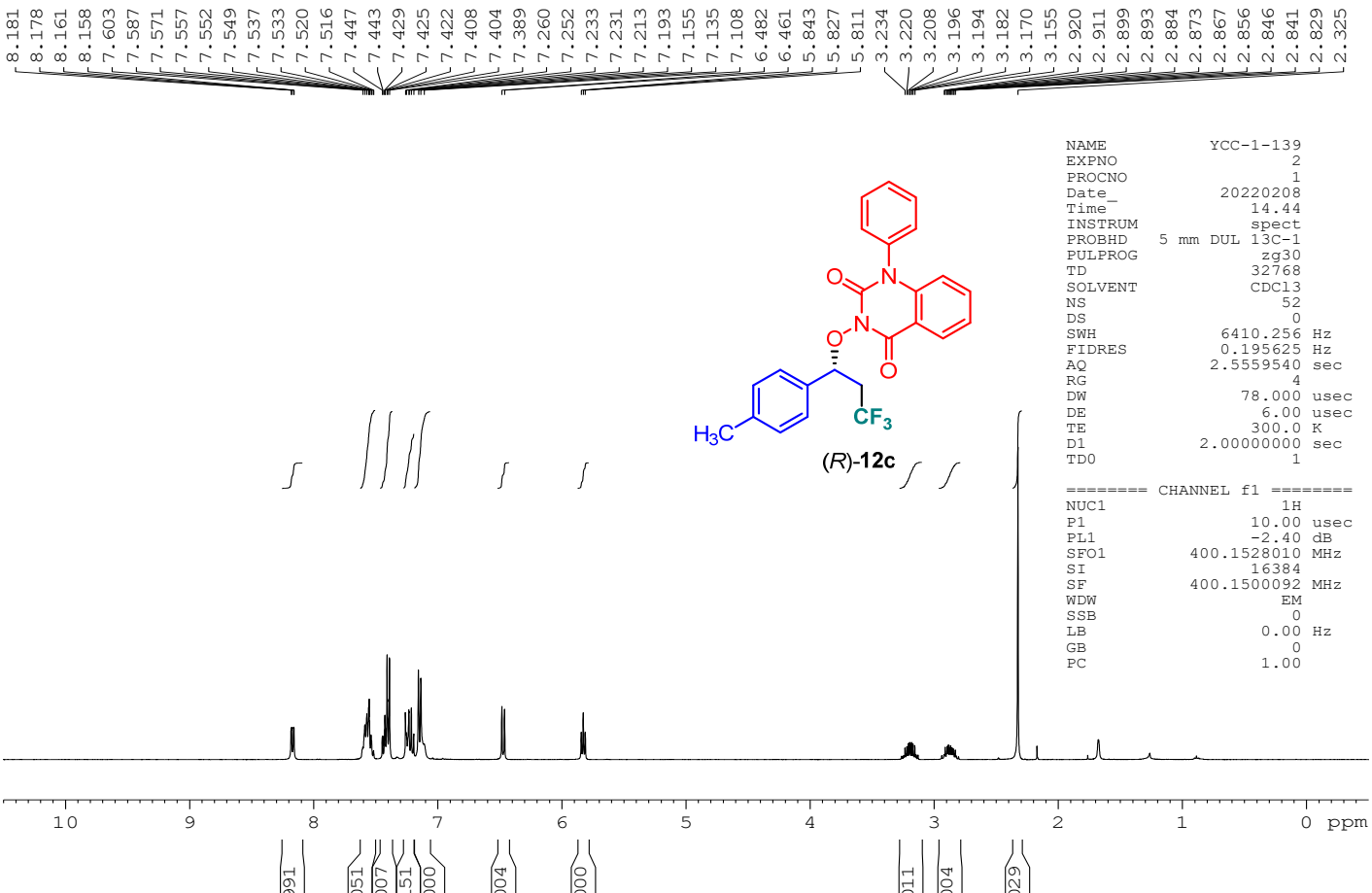
======== CHANNEL f1 ========
NUC1                13C
P1                9.70 usec
PL1              -0.50 dB
SFO1        100.6288660 MHz

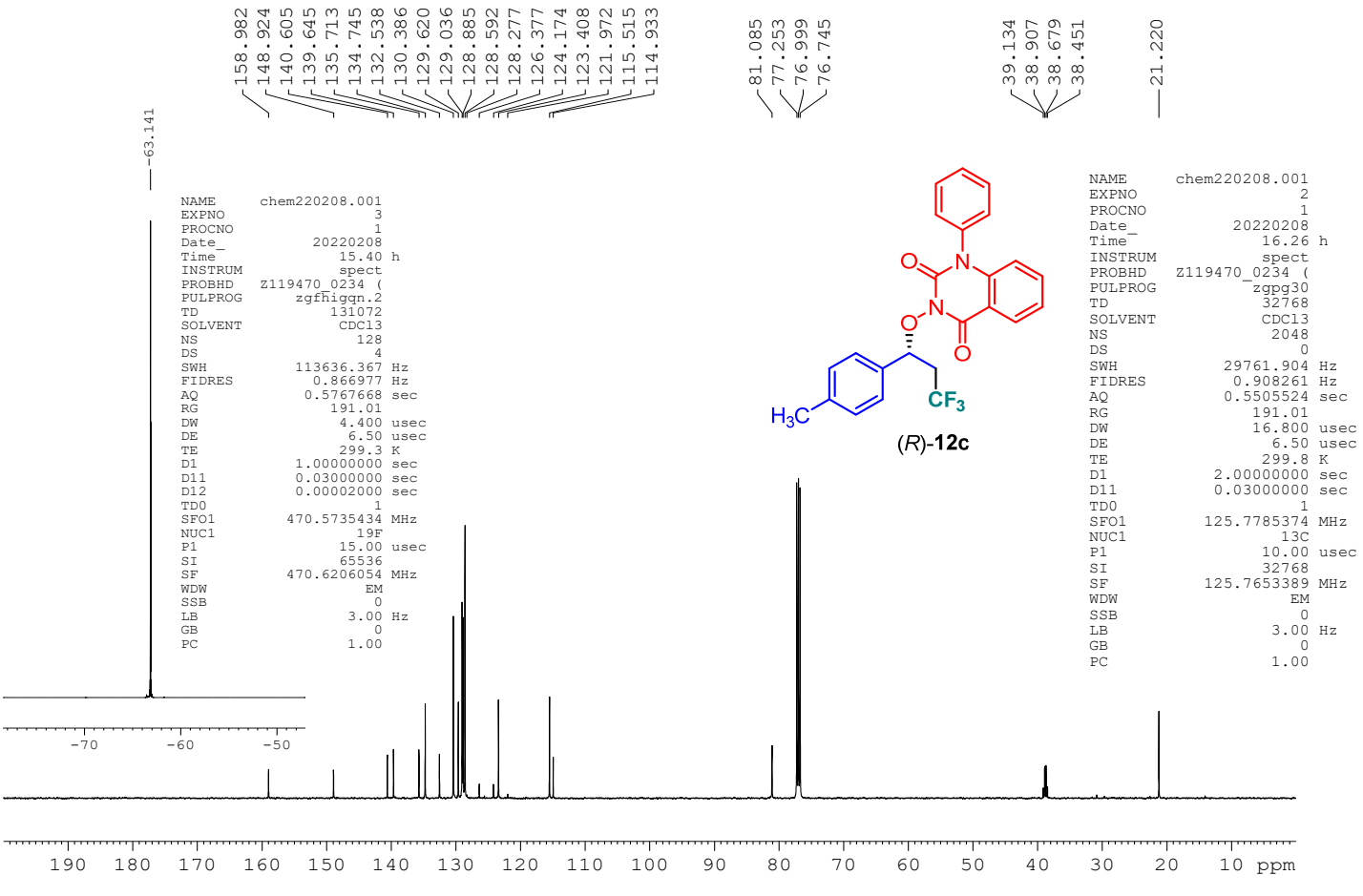
======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             90.00 usec
PL2               -2.40 dB
PL12              15.10 dB
PL13              18.10 dB
SFO2        400.1516010 MHz
SI                32768
SF          100.6177993 MHz
WDW                  EM
SSB                   0
LB               3.00 Hz
GB                    0
PC                 1.00
```

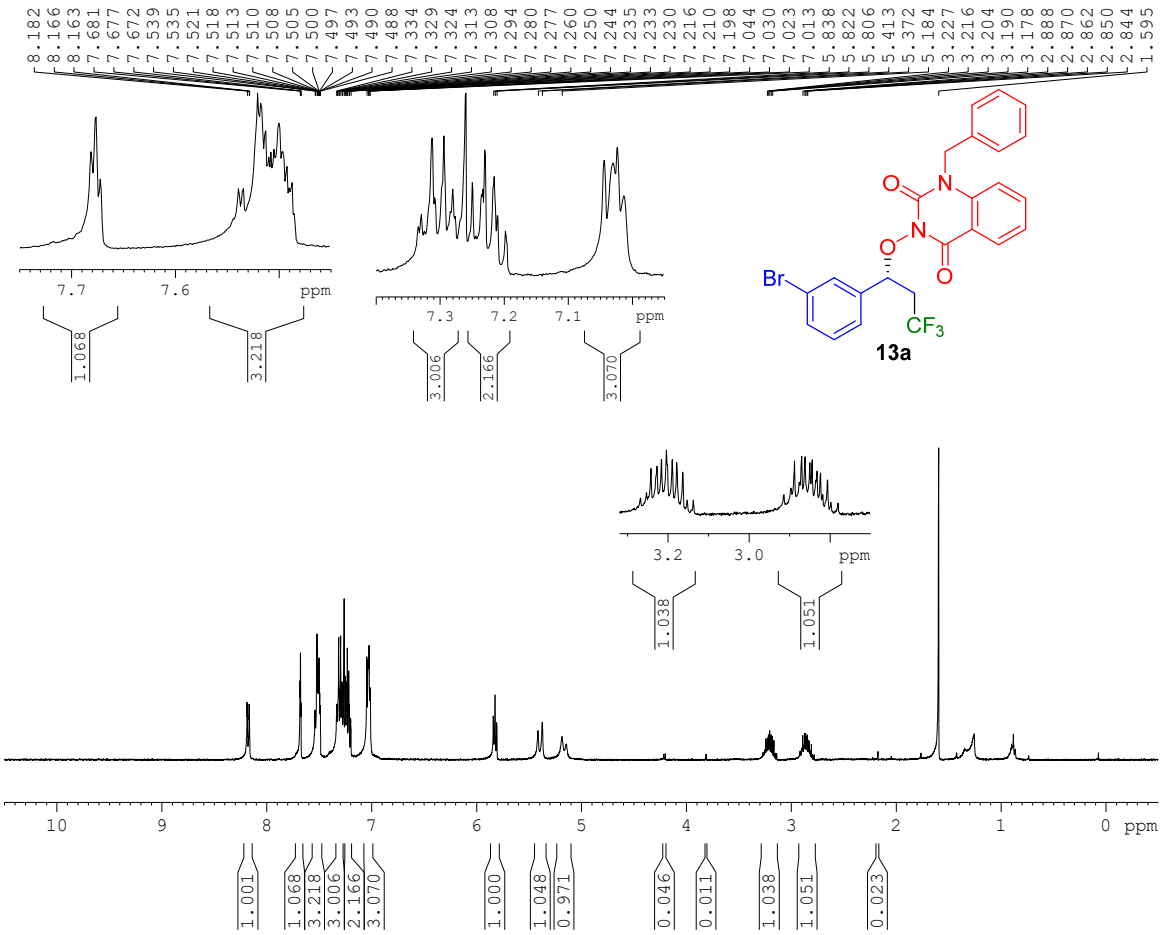

8.191 8.187 8.171 8.168 7.669 7.665 7.660 7.617 7.598 7.581 7.578 7.571 7.567 7.564 7.550 7.531 7.523 7.502 7.500 7.495 7.482 7.479 7.477 7.469 7.465 7.451 7.448 7.445 7.430 7.426 7.280 7.260 7.253 7.251 7.241 7.233 7.221 7.215 7.213 7.193 6.515 6.494 5.794 5.779 5.762 3.214 3.202 3.189 3.176 3.164 3.150 2.886 2.868 2.860 2.848 2.842
NAME YCC-1-66
EXPNO 1
PROCNO 1
Date_ 20210727
Time_ 13.48
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500092 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
CF3
Br
(R)-12a
10 9 8 7 6 5 4 3 2 1 0 ppm
0.990 1.083 6.062 4.303 1.010 1.000 1.005 0.999


158.947 148.906 140.572 138.037 135.566 134.939 132.765 132.748 132.732 132.702 131.451 130.426 130.413 130.052 129.681 128.886 128.821 128.583 128.550 128.310 127.000 126.107 123.904 123.592 123.558 122.257 122.237 121.700 115.614 114.798 80.716 80.694 80.669 80.646 39.277 39.048 38.819 38.590
-62.980
NAME chem210729.001
EXPNO 3
PROCNO 1
Date_ 20210728
Time 16.20 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 24
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 191.01
DW 4.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5735434 MHz
NUC1 19F
P1 15.00 usec
SI 65536
SF 470.6206054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
-50 -60 -70
NAME chem210729.001
EXPNO 2
PROCNO 2
Date_ 20210729
Time 7.45 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 1070
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653437 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00
CF3
Br
(R)-12a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.187 8.185 8.171 8.169 8.602 7.589 7.580 7.578 7.566 7.554 7.552 7.540 7.526 7.524 7.443 7.440 7.428 7.426 7.423 7.412 7.408 7.330 7.318 7.260 7.246 7.241 7.230 7.215 7.200 7.164 7.149 6.488 6.471 5.842 5.829 5.817 3.233 3.221 3.212 3.202 3.201 3.191 3.181 3.170 3.160 2.912 2.902 2.898 2.891 2.882 2.877 2.868 2.860 2.856 2.846 2.322
CF3
CH3 (R)-12b
NAME chem220216.001
EXPNO 1
PROCNO 1
Date_ 20220216
Time 23.52 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 32
DS 0
SWH 10026.738 Hz
FIDRES 0.305992 Hz
AQ 1.6340809 sec
RG 43.11
DW 49.867 usec
DE 7.71 usec
TE 299.5 K
D1 2.00000000 sec
TD0 1
SFO1 500.1630010 MHz
NUC1 1H
P1 10.00 usec
SI 16384
SF 500.1600108 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
1.001 3.028 1.055 2.005 3.031 1.998 1.003 1.000 1.031 1.030 3.012
159.025 148.961 140.589 138.045 135.715 135.550 134.765 130.410 130.387 129.625 129.155 128.894 128.867 128.598 128.564 128.269 126.396 125.560 124.193 123.429 121.990 115.516 114.935 81.401 81.378 81.355 81.331 77.253 76.999 76.745 39.258 39.029 38.803 38.575 21.246
-63.162
NAME chem220216.001
EXPNO 3
PROCNO 1
Date_ 20220217
Time 4.19 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 191.01
DW 4.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5735434 MHz
NUC1 19F
P1 15.00 usec
SI 65536
SF 470.6206054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
-70 -60 -50
CF3
CH3 (R)-12b
NAME chem220216.001
EXPNO 2
PROCNO 1
Date_ 20220217
Time 4.14 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 6000
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653399 MHz
WDW EM
SSB 0
LB 0.60 Hz
GB 0
PC 1.00
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

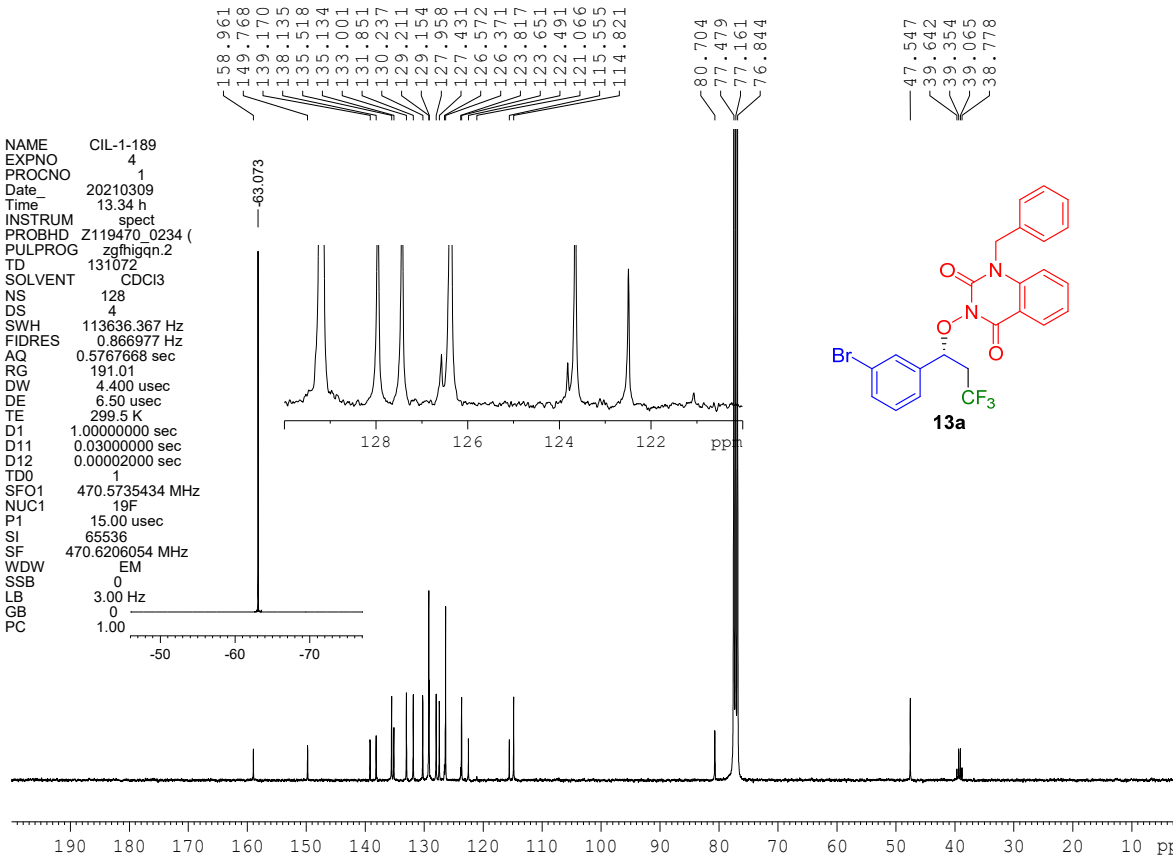

8.181 8.178 8.161 8.158 8.603 7.587 7.571 7.557 7.552 7.549 7.537 7.533 7.520 7.516 7.447 7.443 7.429 7.425 7.422 7.408 7.404 7.389 7.260 7.252 7.233 7.231 7.213 7.193 7.155 7.135 7.108 6.482 6.461 5.843 5.827 5.811 3.234 3.220 3.208 3.196 3.194 3.182 3.170 3.155 2.920 2.911 2.899 2.893 2.884 2.873 2.867 2.856 2.846 2.841 2.829 2.325
NAME YCC-1-139
EXPNO 2
PROCNO 1
Date_ 20220208
Time 14.44
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 52
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500092 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
(R)-12c
10 9 8 7 6 5 4 3 2 1 0 ppm
0.991 3.051 3.007 2.151 3.000 1.004 1.000 1.011 1.004 3.029


158.982 148.924 140.605 139.645 135.713 134.745 132.538 130.386 129.620 129.036 128.885 128.592 128.277 126.377 124.174 123.408 121.972 115.515 114.933
81.085 77.253 76.999 76.745
39.134 38.907 38.679 38.451
21.220
-63.141
NAME chem220208.001
EXPNO 3
PROCNO 1
Date_ 20220208
Time 15.40 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 128
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 191.01
DW 4.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5735434 MHz
NUC1 19F
P1 15.00 usec
SI 65536
SF 470.6206054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
(R)-12c
NAME chem220208.001
EXPNO 2
PROCNO 1
Date_ 20220208
Time 16.26 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 2048
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 299.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653389 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
-70 -60 -50
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm




```
NAME            CIL-1-187
EXPNO                   5
PROCNO                  1
Date_            20210302
Time                17.34
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     36
DS                      0
SWH              6410.256 Hz
FIDRES           0.195625 Hz
AQ               2.5559540 sec
RG                      4
DW                 78.000 usec
DE                  6.00 usec
TE                 300.0 K
D1               2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -2.40 dB
SFO1          400.1528010 MHz
SI                  16384
SF            400.1500086 MHz
WDW                    EM
SSB                     0
LB                 0.00 Hz
GB                      0
PC                   1.00
```

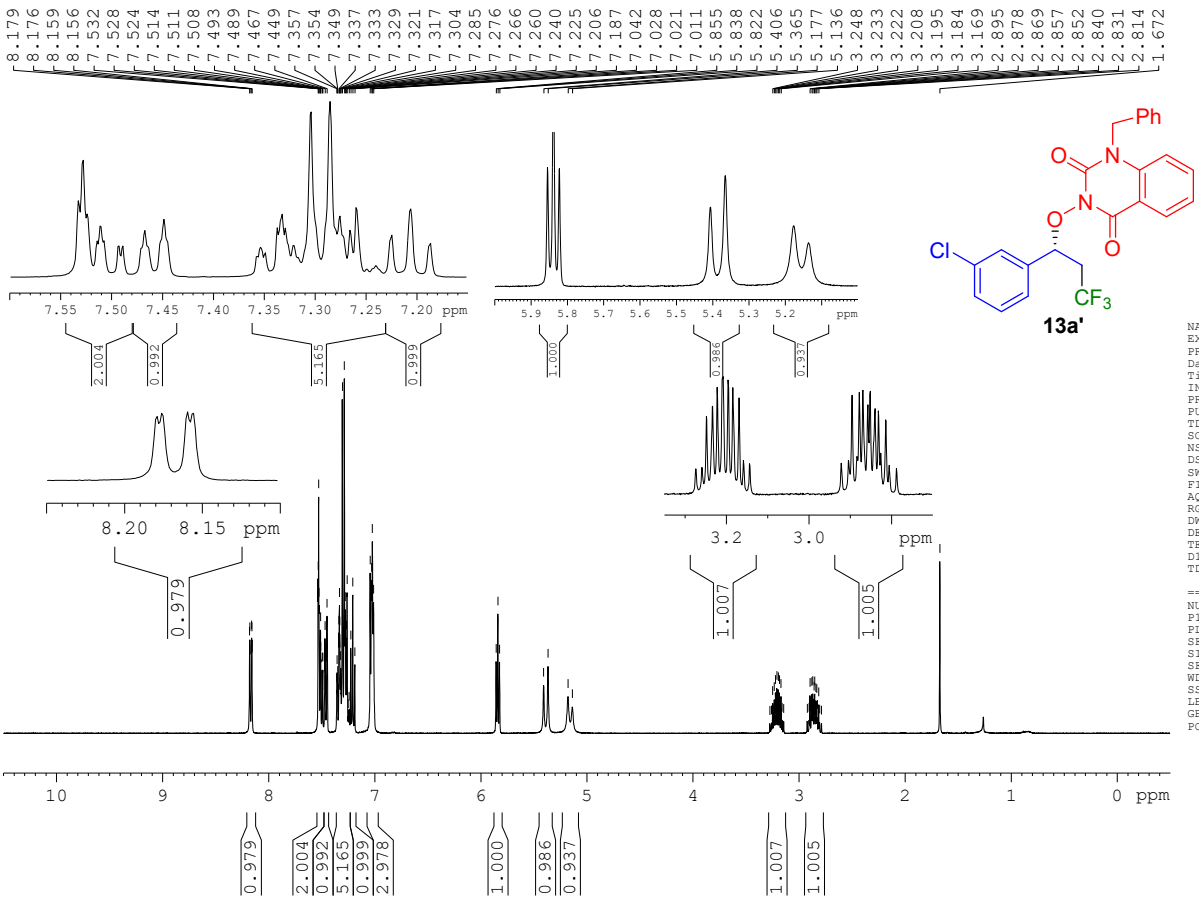


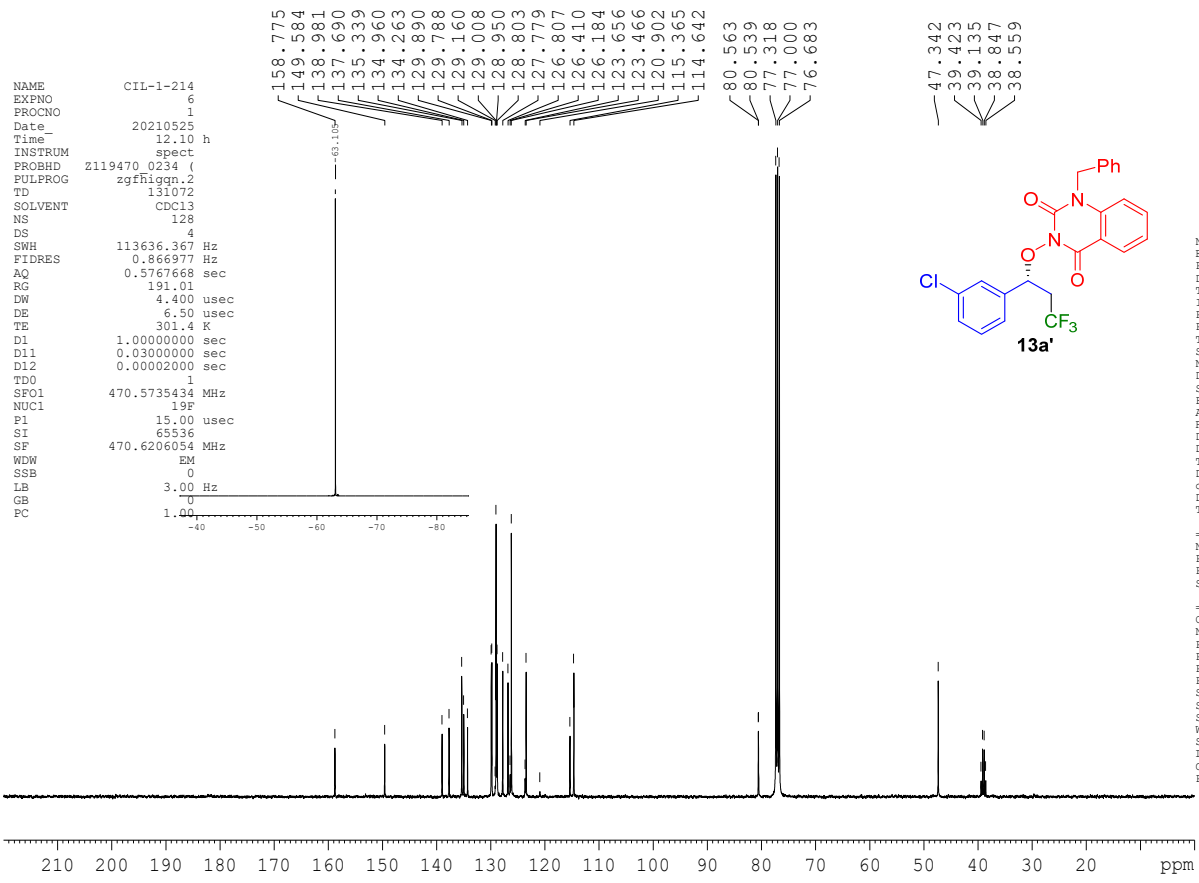

```
NAME            CIL-1-189
EXPNO                   4
PROCNO                  1
Date_            20210309
Time               13.34 h
INSTRUM             spect
PROBHD   Z119470_0234 (
PULPROG          zgfhigqn.2
TD                  131072
SOLVENT              CDCl3
NS                     128
DS                       4
SWH             113636.367 Hz
FIDRES            0.866977 Hz
AQ                0.5767668 sec
RG                   191.01
DW                  4.400 usec
DE                  6.50 usec
TE                  299.5 K
D1              1.00000000 sec
D11             0.03000000 sec
D12             0.00002000 sec
TD0                     1
SFO1           470.5735434 MHz
NUC1                  19F
P1                 15.00 usec
SI                  65536
SF            470.6206054 MHz
WDW                    EM
SSB                     0
LB                 3.00 Hz
GB                      0
PC                   1.00
```

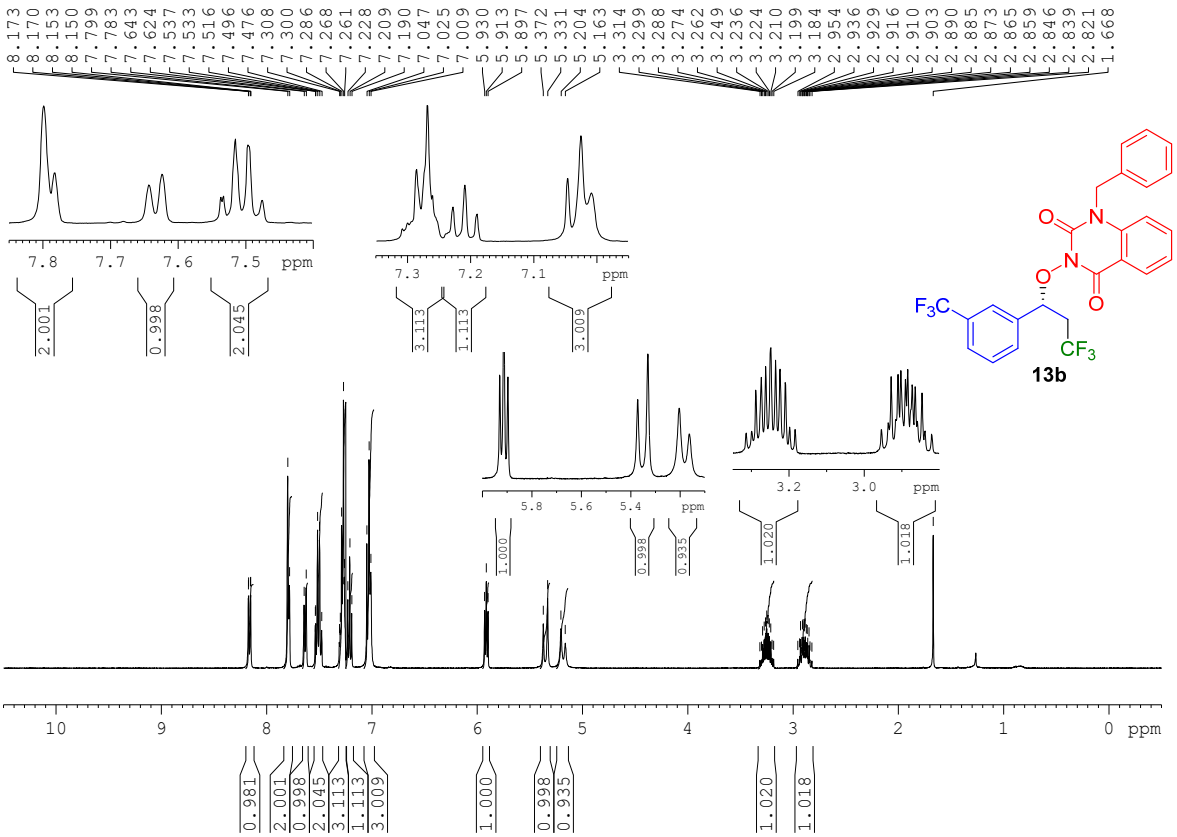
```
NAME            CIL-1-187
EXPNO                  10
PROCNO                  1
Date_            20210306
Time                 0.07
INSTRUM             spect
PROBHD   5 mm DUL 13C-1
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    9600
DS                       0
SWH             22727.273 Hz
FIDRES           0.346791 Hz
AQ               1.4418420 sec
RG                      57
DW                 22.000 usec
DE                  6.00 usec
TE                 300.0 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                     1

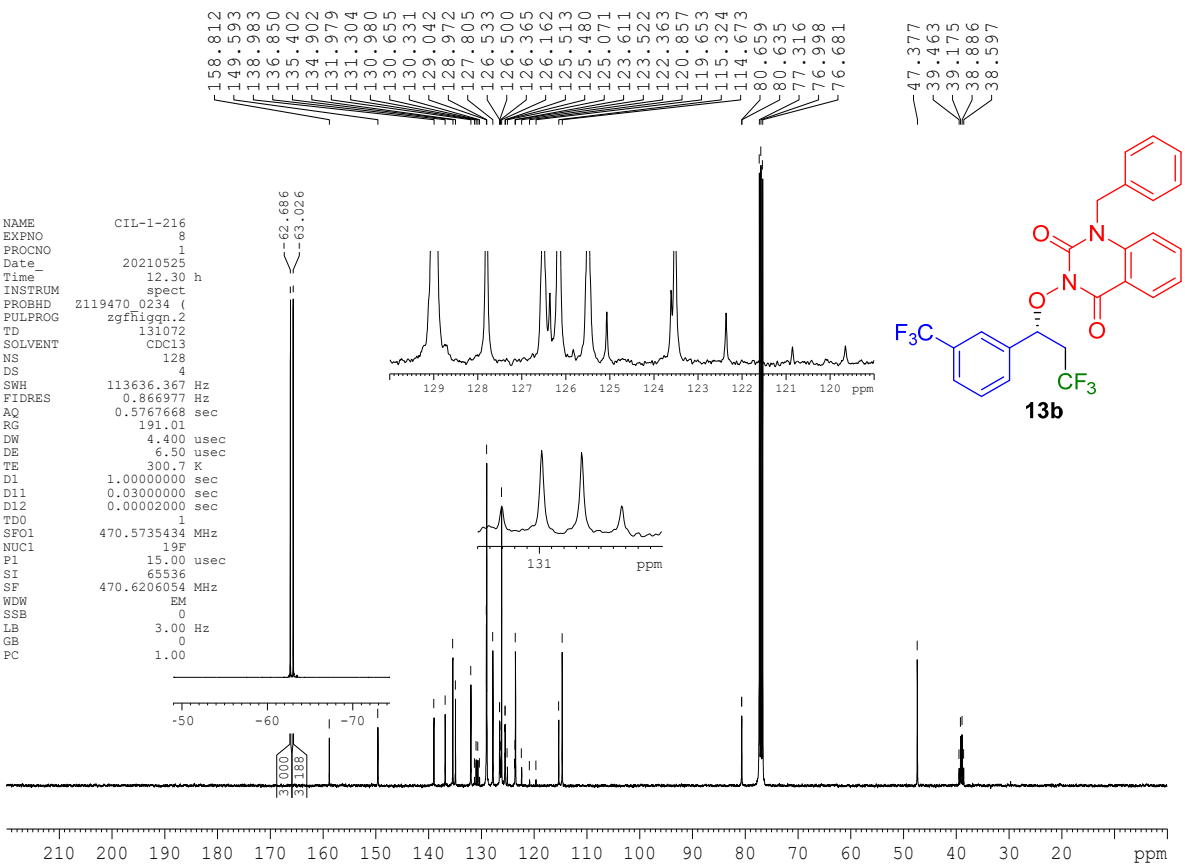
======== CHANNEL f1 ========
NUC1                   13C
P1                  9.70 usec
PL1                -0.50 dB
SFO1          100.6288660 MHz

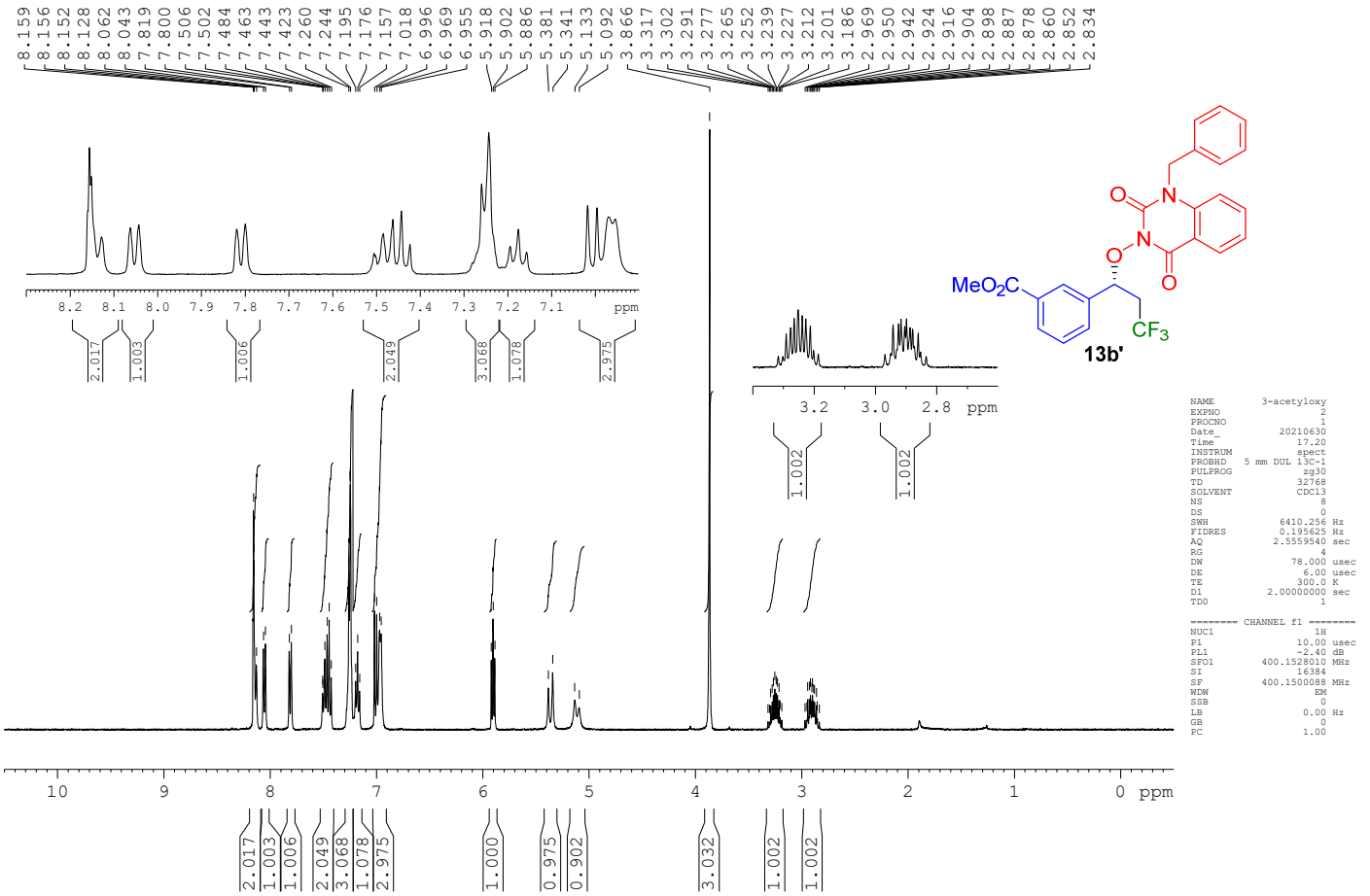
======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              90.00 usec
PL2                -2.40 dB
PL12               15.10 dB
PL13               18.10 dB
SFO2          400.1516010 MHz
SI                  32768
SF            100.6177839 MHz
WDW                    EM
SSB                     0
LB                 3.00 Hz
GB                      0
PC                   1.00
```


13a'


13a'

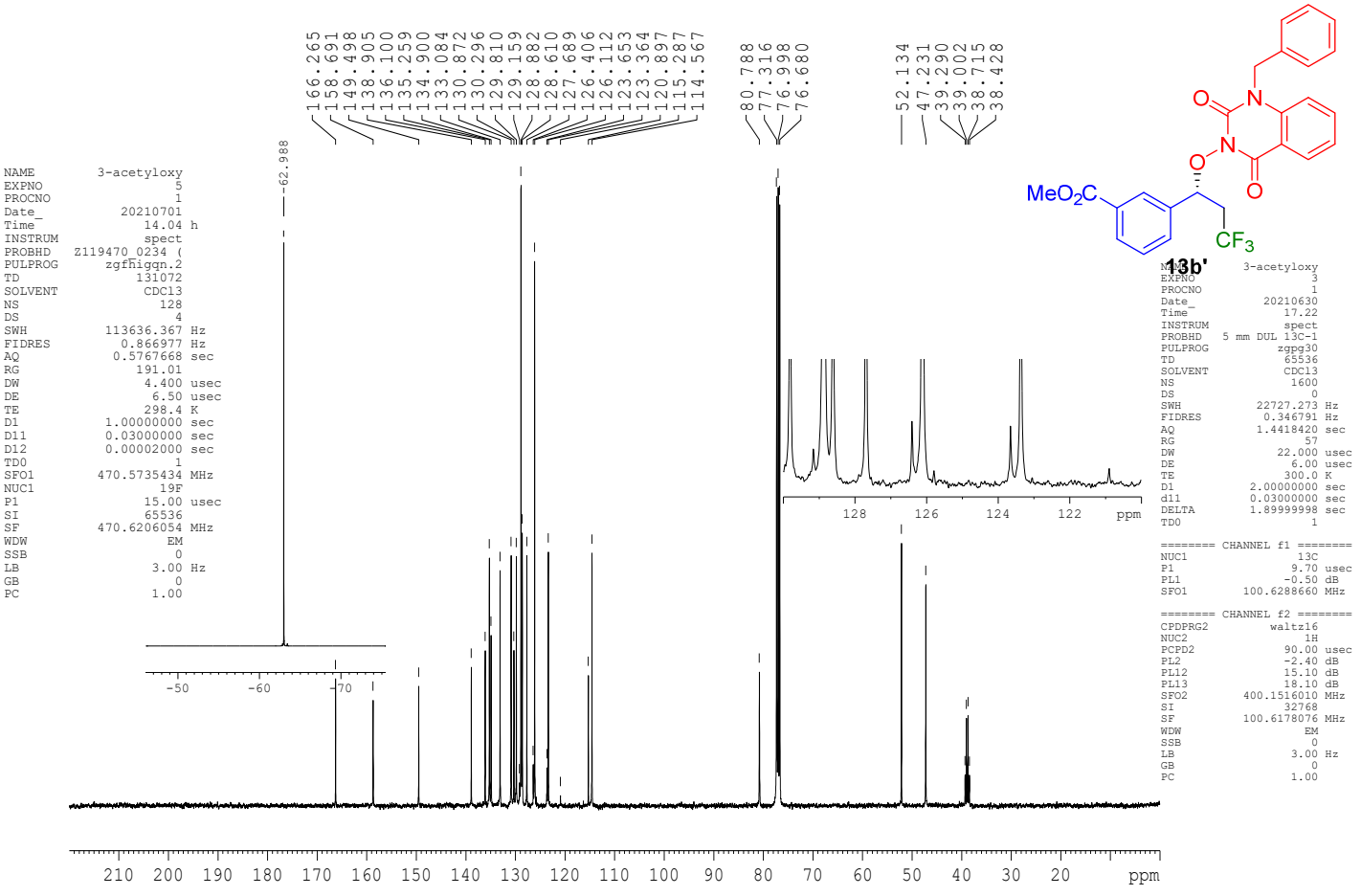

13b


13b




```
NAME          3-acetyloxy
EXPNO                   2
PROCNO                  1
Date_            20210630
Time                17.20
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                     8
DS                     0
SWH             6410.256 Hz
FIDRES          0.195625 Hz
AQ              2.5559540 sec
RG                     4
DW                78.000 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.00 usec
PL1               -2.40 dB
SFO1         400.1528010 MHz
SI                 16384
SF           400.1500088 MHz
WDW                   EM
SSB                    0
LB                0.00 Hz
GB                     0
PC                1.00
```

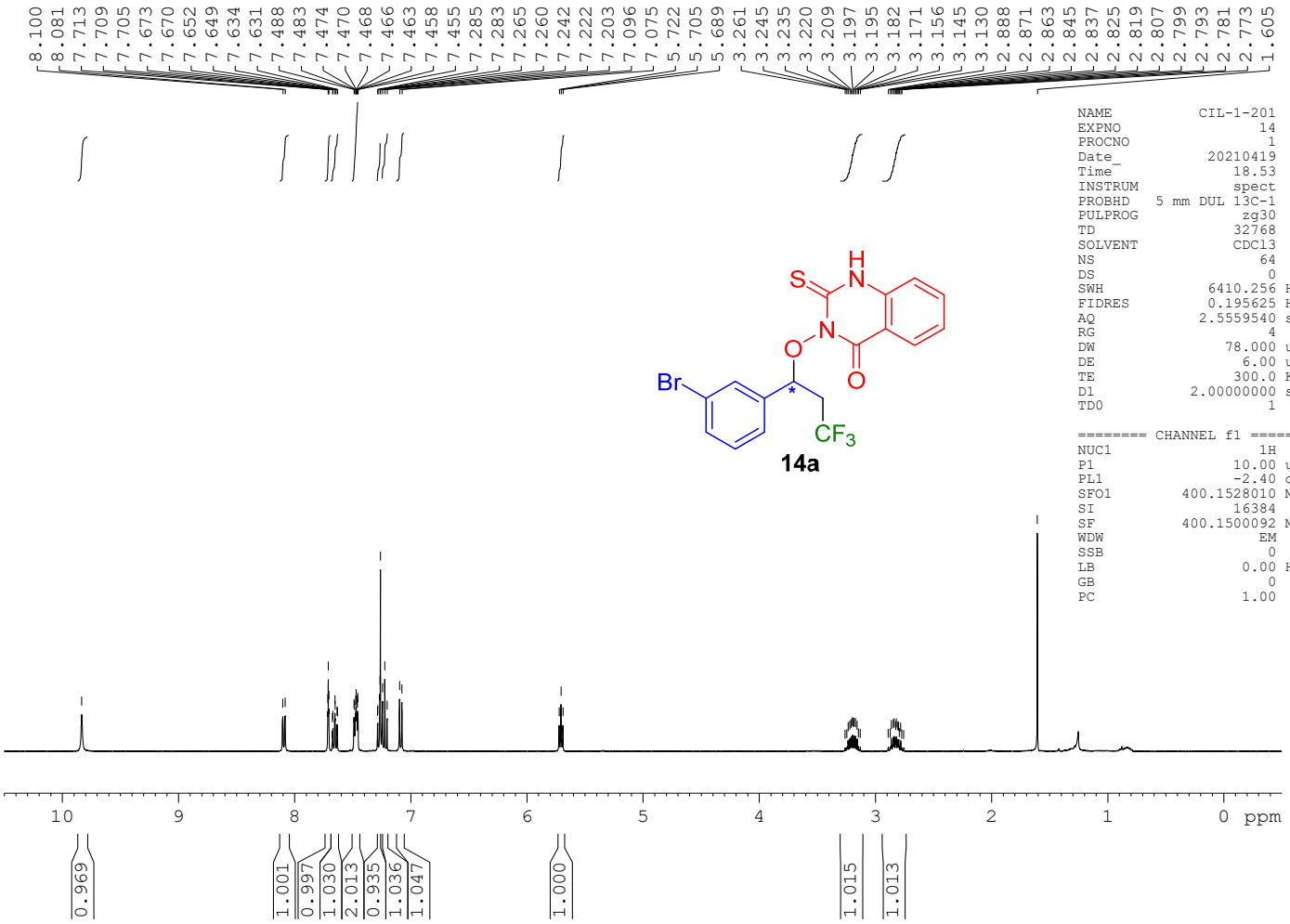


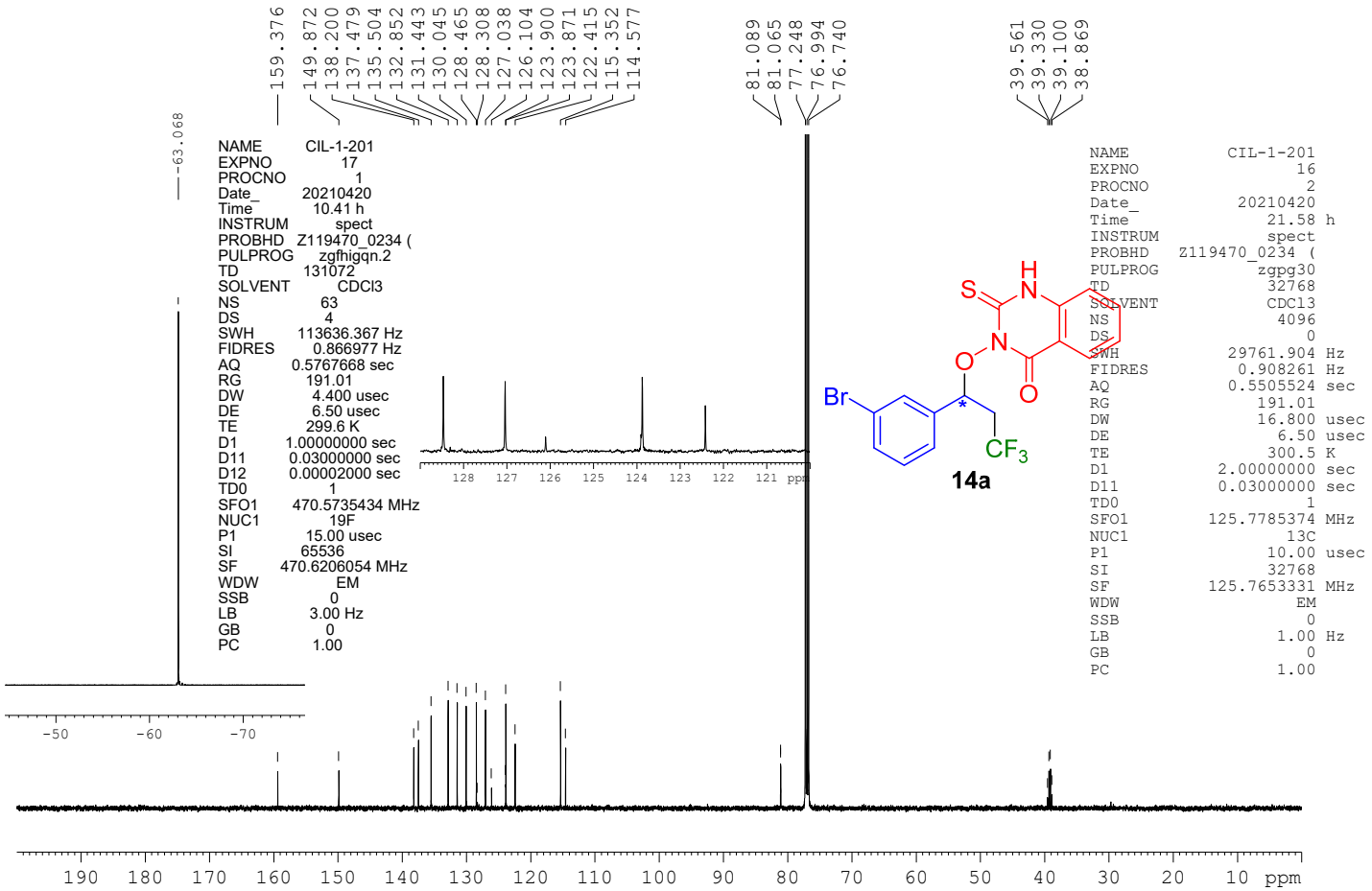

```
NAME          3-acetyloxy
EXPNO                   5
PROCNO                  1
Date_            20210701
Time               14.04 h
INSTRUM             spect
PROBHD    Z119470_0234 (
PULPROG       zgfhigqn.2
TD                 131072
SOLVENT            CDCl3
NS                   128
DS                     4
SWH           113636.367 Hz
FIDRES          0.866977 Hz
AQ              0.5767668 sec
RG                191.01
DW                 4.400 usec
DE                 6.50 usec
TE                298.4 K
D1             1.00000000 sec
D11            0.03000000 sec
D12            0.00002000 sec
TD0                    1
SFO1         470.5735434 MHz
NUC1                  19F
P1                15.00 usec
SI                 65536
SF           470.6206054 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```

```
NAME          3-acetyloxy
EXPNO                   3
PROCNO                  1
Date_            20210630
Time                17.22
INSTRUM             spect
PROBHD    5 mm DUL 13C-1
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1600
DS                     0
SWH            22727.273 Hz
FIDRES          0.346791 Hz
AQ              1.4418420 sec
RG                    57
DW                22.000 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.70 usec
PL1               -0.50 dB
SFO1         100.6288660 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             90.00 usec
PL2               -2.40 dB
PL12              15.10 dB
PL13              18.10 dB
SFO2         400.1516010 MHz
SI                 32768
SF           100.6178076 MHz
WDW                   EM
SSB                    0
LB                3.00 Hz
GB                     0
PC                1.00
```


8.100 8.081 7.713 7.709 7.705 7.673 7.670 7.652 7.649 7.634 7.631 7.488 7.483 7.474 7.470 7.468 7.466 7.463 7.458 7.455 7.285 7.283 7.265 7.260 7.242 7.222 7.203 7.096 7.075 5.722 5.705 5.689
3.261 3.245 3.235 3.220 3.209 3.197 3.195 3.182 3.171 3.156 3.145 3.130 2.888 2.871 2.863 2.845 2.837 2.825 2.819 2.807 2.799 2.793 2.781 2.773 1.605
NAME CIL-1-201
EXPNO 14
PROCNO 1
Date_ 20210419
Time 18.53
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 64
DS 0
SWH 6410.256 Hz
FIDRES 0.195625 Hz
AQ 2.5559540 sec
RG 4
DW 78.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.00 usec
PL1 -2.40 dB
SFO1 400.1528010 MHz
SI 16384
SF 400.1500092 MHz
WDW EM
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
14a
10 9 8 7 6 5 4 3 2 1 0 ppm
0.969 1.001 0.997 1.030 2.013 0.935 1.036 1.047 1.000 1.015 1.013


159.376 149.872 138.200 137.479 135.504 132.852 131.443 130.045 128.465 128.308 127.038 126.104 123.900 123.871 122.415 115.352 114.577
81.089 81.065 77.248 76.994 76.740
39.561 39.330 39.100 38.869
-63.068
NAME CIL-1-201
EXPNO 17
PROCNO 1
Date_ 20210420
Time 10.41 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgfhigqn.2
TD 131072
SOLVENT CDCl3
NS 63
DS 4
SWH 113636.367 Hz
FIDRES 0.866977 Hz
AQ 0.5767668 sec
RG 191.01
DW 4.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
SFO1 470.5735434 MHz
NUC1 19F
P1 15.00 usec
SI 65536
SF 470.6206054 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00
NAME CIL-1-201
EXPNO 16
PROCNO 2
Date_ 20210420
Time 21.58 h
INSTRUM spect
PROBHD Z119470_0234 (
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 4096
DS 0
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 191.01
DW 16.800 usec
DE 6.50 usec
TE 300.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7785374 MHz
NUC1 13C
P1 10.00 usec
SI 32768
SF 125.7653331 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
14a
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm