Supporting Information

Hydrogen Atom Transfer-Enabled Photocatalytic System for Direct Heteroarylation of C(sp^3)-H and C(sp^2)-H Bonds

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1. General Information

All reagents were purchased from commercial suppliers and used without further purification unless otherwise stated. TLC was performed on silica gel plates (GF254, 200-300 mesh) using UV light (254/366 nm) for detection. Products were purified by column chromatography using silica gel (200-300 mesh) purchased from Qing Dao Hai Yang Chemical Industry Co. The ^{1}H NMR, ^{13}C NMR, and ^{19}F NMR spectra were recorded on Bruker Avance 400 MHz or 600 MHz spectrometer at room temperature (20 ± 3°C). ^{1}H, ^{13}C, and ^{19}F chemical shifts are quoted in parts per million (ppm) downfield from TMS. High-resolution mass spectra (HRMS) were acquired using an Agilent Infinity II Q-TOF G6545 equipped with electrospray ionization (ESI) technique. Fluorescence intensities were determined using an F-7100 FL spectrophotometer.

2. Photo-reaction instrument

Photochemical reaction was carried out under visible light irradiation by a blue LED at 25 °C. RLH-18 8-position Photo Reaction System manufactured by Beijing Roger Tech Ltd was used in this system. Eight 10 W blue LED were equipped in this Photo reactor. The blue LED's energy peak wavelength is 460 nm, peak width at half-height is 18.4 nm. The reaction vessel is borosilicate glass test tube and the distance between it and the lamp is 15 mm, no filter is applied. More details are shown in Figure S1.

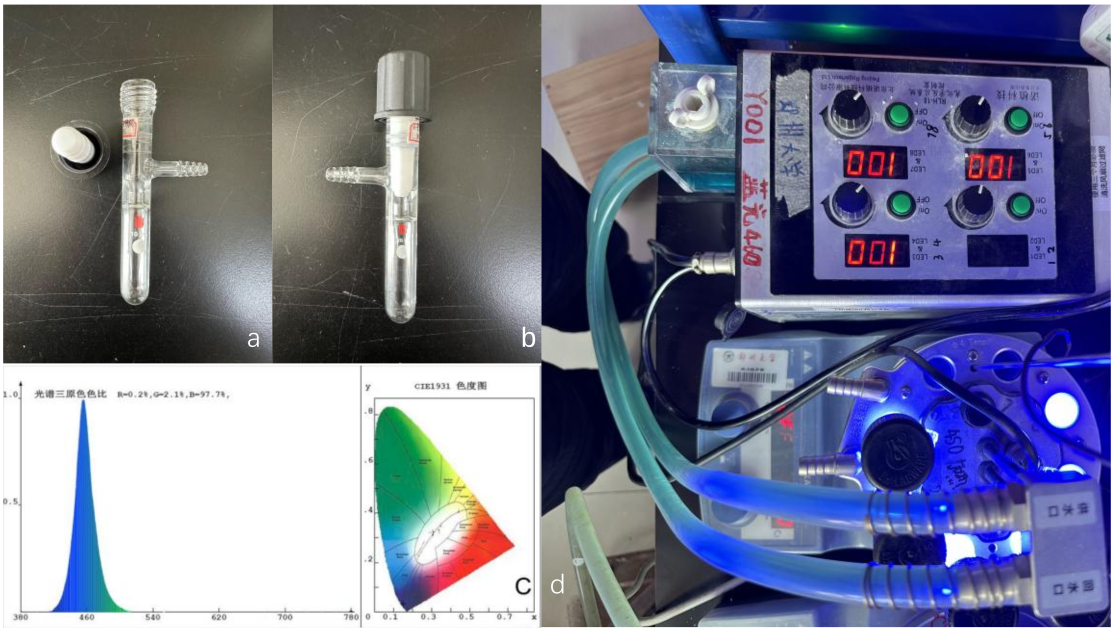
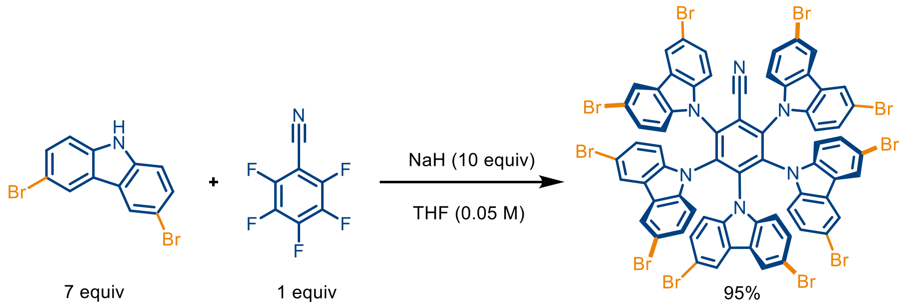


Figure S1 The visible-light irradiation instrument. **A**: 10 mL reaction tube and cap. **B**: Reaction tube assembly. **C**: spectrum of blue LED lamp. **D**: Photoreactor.

3. Procedures for the synthesis of photoredox-catalysts

3.1 Synthesis of Br-5CzBN

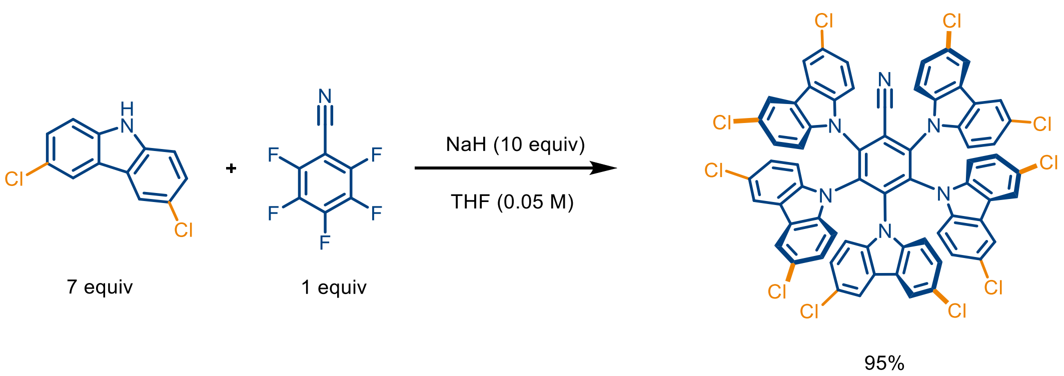


Under a nitrogen atmosphere at 0 °C, a solution of carbazole (12.5 mmol) in 40 mL of tetrahydrofuran was added dropwise to sodium hydride (NaH, 18.75 mmol). The reaction mixture was then stirred at 0 °C for 30 minutes. Subsequently, 2,3,4,5,6-pentafluorobenzonitrile (2 mmol) was introduced, and the reaction was allowed to proceed for 18 hours. Upon completion, the reaction was quenched by the addition of deionized water. The resulting mixture was subjected to vacuum filtration, and the solid residue was washed sequentially with deionized water, ethanol, and hexane. The product was then dried to yield a pure light-yellow solid, 95% yield. The final product was found to be insoluble in chloroform, ethanol, and dichloromethane, but slightly soluble in ethyl acetate (EA), dimethyl sulfoxide, and *N,N*-Dimethylformamide, The NMR sample was supplemented with EA to help dissolve.

^{1}H NMR (600 MHz, DMSO-d_6: EA = 1:5) δ 8.30 – 8.27 (m, 4H), 7.90 – 7.87 (m, 4H), 7.85 – 7.83 (m, 2H), 7.70 – 7.67 (m, 4H), 7.59 – 7.56 (m, 2H), 7.55 – 7.52 (m, 4H), 7.42 – 7.39 (m, 4H), 7.00 – 6.97 (m, 4H), 6.95 – 6.91 (m, 2H).

HRMS (ESI-TOF): m/z: $[M + K]^+$ Calcd for $C_{67}H_{30}Br_{10}N_6K^+$ 1756.3895; Found 1756.3894.

3.2 Synthesis of Cl-5CzBN

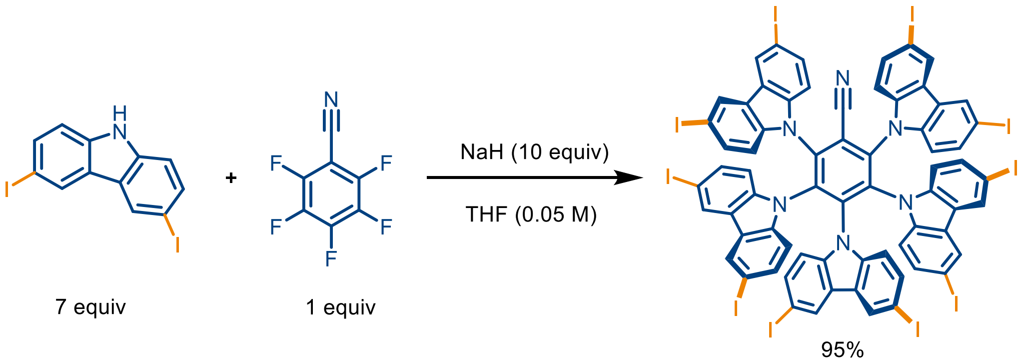


Under a nitrogen atmosphere at 0 °C, a solution of carbazole (12.5 mmol) in 40 mL of tetrahydrofuran was added dropwise to sodium hydride (NaH, 18.75 mmol). The reaction mixture was then stirred at 0 °C for 30 minutes. Subsequently, 2,3,4,5,6-pentafluorobenzonitrile (2 mmol) was introduced, and the reaction was allowed to proceed for 10 hours. Upon completion, the reaction was quenched by the addition of deionized water. The resulting mixture was subjected to vacuum filtration, and the solid residue was washed sequentially with deionized water, ethanol, and hexane. The product was then dried to yield a pure light-yellow solid, 95% yield. The final product was found to be insoluble in chloroform, ethanol, and dichloromethane, but slightly soluble in ethyl acetate (EA), dimethyl sulfoxide, and N,N-Dimethylacetamide, The NMR sample was supplemented withN,N-Dimethylacetamide to help dissolve.

1H NMR (600 MHz, DMSO-d_6 : DMA = 1 : 5) δ 8.24 – 8.21 (m, 4H), 7.83 – 7.79 (m, 10H), 7.78 – 7.78 (m, 1H), 7.76 – 7.75 (m, 2H), 7.72 – 7.68 (m, 4H), 7.33 – 7.30 (m, 4H), 6.91 – 6.88 (m, 4H), 6.86 – 6.83 (m, 1H).

HRMS (ESI-TOF): : m/z: $[M + K]^+$ Calcd for $C_{67}H_{30}Cl_{10}N_6K^+$ 1310.8990; Found 1310.8982.

3.3 Synthesis of I-5CzBN

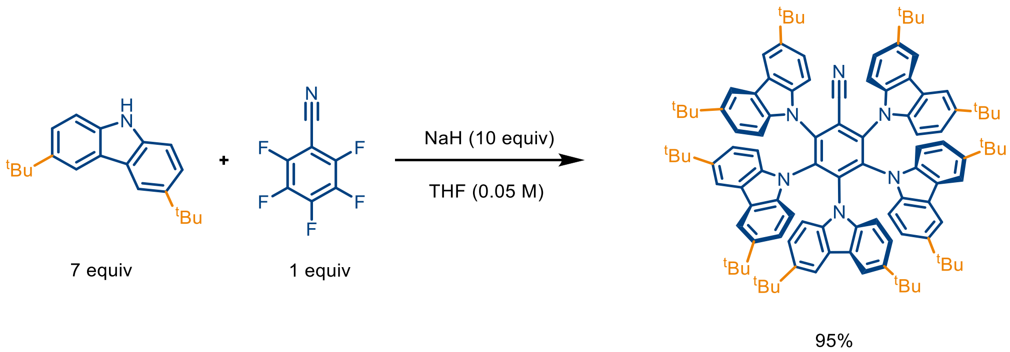


Under a nitrogen atmosphere at 0 °C, a solution of carbazole (12.5 mmol) in 40 mL of tetrahydrofuran was added dropwise to sodium hydride (NaH, 18.75 mmol). The reaction mixture was then stirred at 0 °C for 30 minutes. Subsequently, 2,3,4,5,6-pentafluorobenzonitrile (2 mmol) was introduced, and the reaction was allowed to proceed for 24 hours. Upon completion, the reaction was quenched by the addition of deionized water. The resulting mixture was subjected to vacuum filtration, and the solid residue was washed sequentially with deionized water, ethanol, and hexane. The product was then dried to yield a pure light-yellow solid, 95% yield. The final product was found to be insoluble in chloroform, ethanol, and dichloromethane, but slightly soluble in ethyl acetate (EA), dimethyl sulfoxide, and N,N-Dimethylacetamide, The NMR sample was supplemented with N,N-Dimethylacetamide to help dissolve.

^{1}H NMR (600 MHz, DMSO-d_6 : DMA = 1 : 5) δ 8.51 – 8.50 (m, 4H), 8.06 – 8.06 (m, 4H), 8.02 – 8.01 (m, 2H), 7.99 (s, 1H), 7.65 – 7.63 (m, 4H), 7.54 – 7.49 (m, 10H), 7.12 – 7.09 (m, 4H), 7.07 – 7.04 (m, 1H).

HRMS (ESI-TOF): m/z: $[M + K]^+$ Calcd for $C_{67}H_{30}I_{10}N_6K^+$ 2226.2610; Found 2226.2603.

3.4 Synthesis of ^{t}Bu-5CzBN



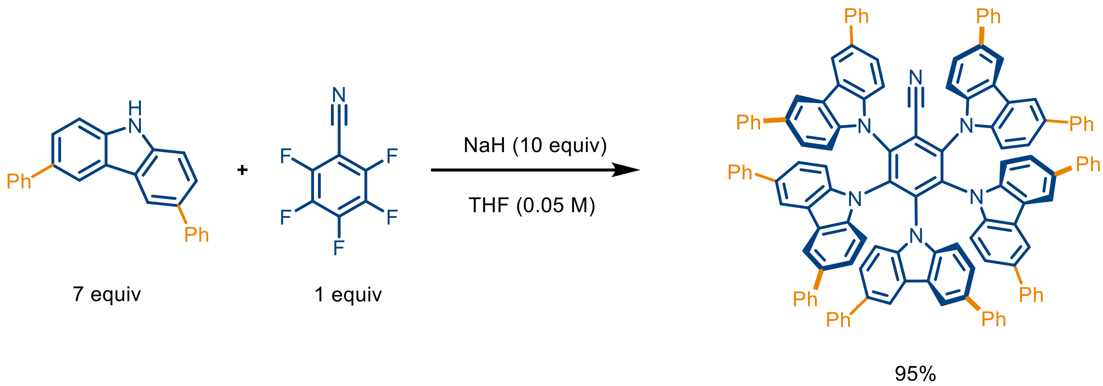
Under a nitrogen atmosphere at 0 °C, a solution of carbazole (12.5 mmol) in 40 mL of tetrahydrofuran was added dropwise to sodium hydride (NaH, 18.75 mmol). The reaction mixture was then stirred at 0 °C for 30 minutes. Subsequently, 2,3,4,5,6-pentafluorobenzonitrile (2 mmol) was introduced, and the reaction was allowed to proceed for 36 hours. Upon completion, the reaction was quenched by the addition of deionized water. Extract using ether and concentrate. Light yellow solid product was isolated by column chromatography using hexanes:ethyl acetate = 20:1 as the eluent, 95% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.61 (d, *J* = 1.4 Hz, 4H), 7.22 (d, *J* = 1.8 Hz, 6H), 7.06 (d, *J* = 8.6 Hz, 2H), 6.98 (s, 8H), 6.69 (d, *J* = 8.6 Hz, 4H), 6.63 – 6.59 (m, 2H), 6.58 – 6.53 (m, 4H), 1.35 (s, 36H), 1.25 (s, 36H), 1.14 (s, 18H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.6, 143.3, 142.9, 142.8, 140.2, 137.8, 137.4, 136.7, 136.0, 124.6, 124.4, 124.0, 122.7, 122.2, 121.7, 115.7, 115.0, 114.8, 110.6, 110.0, 109.8, 34.5, 34.2, 34.2, 31.8, 31.7, 31.6.

HRMS (ESI-TOF): m/z: [M + Na]$^{+}$ Calcd for $C_{107}H_{120}N_6Na^{+}$ 1512.9500; Found 1512.9493.

3.5 Synthesis of Ph-5CzBN



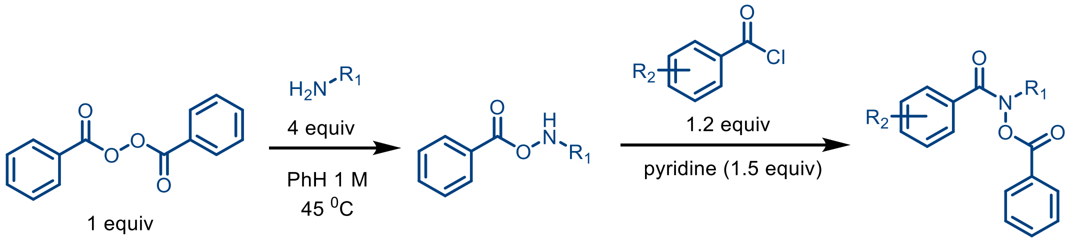
Under a nitrogen atmosphere at 0 °C, a solution of carbazole (12.5 mmol) in 40 mL of tetrahydrofuran was added dropwise to sodium hydride (NaH, 18.75 mmol). The reaction mixture was then stirred at 0 °C for 30 minutes. Subsequently, 2,3,4,5,6-pentafluorobenzonitrile (2 mmol) was introduced, and the reaction was allowed to proceed for 48 hours. Upon completion, the reaction was quenched by the addition of deionized water. Extract using ether and concentrate. Light yellow solid product was isolated by column chromatography using hexanes : ethyl acetate = 10 : 1 as the eluent, 95% yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.98 (s, 4H), 7.83 – 7.72 (m, 2H), 7.65 – 7.43 (m, 20H), 7.43 – 7.15 (m, 50H), 7.06 – 6.91 (m, 6H).

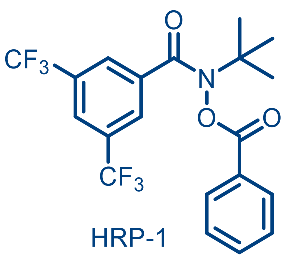
^{13}C NMR (101 MHz, Chloroform-*d*) δ 143.2, 141.5, 141.4, 141.3, 141.1, 139.5, 138.8, 138.7, 137.9, 135.3, 134.9, 134.7, 128.9, 128.8, 128.7, 128.6, 127.6, 127.4, 127.3, 127.2, 127.1, 126.9, 126.7, 125.3, 125.2, 125.1, 124.4, 124.2, 119.0, 118.4, 118.3, 111.4, 111.3, 111.2.

HRMS (ESI-TOF): m/z: $[M + Na]^+$ Calcd for $C_{127}H_{80}N_6Na^+$ 1728.6110; Found 1728.6118.

4. Procedures for the synthesis of hydrogen atom transfer reagent precursors



To a flame-dried round bottom flask with a stir bar was added benzoyl peroxide (10 mmol), which was then dissolved in benzene (15 mL). The reaction was sealed and placed under N_2. Roughly 60% of the total volume of amine was added and the reaction was heated to 45 ^{o}C for 2 hours, and changed color from cloudy white to cloudy Carolina blue. After 2 hours, the remaining amount of amine (to the total of 40 mmol) was added, and the reaction was let to stir over 12 hours. After 12 hours, the reaction was cold down to 0 ^{o}C, and pyridine (20 mmol) was added. Acyl chloride (12 mmol) was added dropwise over 10 minutes, and the mixture was allowed to warm to room temperature for 12 hours. After the reaction, the solution was washed with 1M hydrochloric acid, water, brine and dried over Na_2SO_4, concentrated, with no need for further purification, than 99% yield.



HRP-1

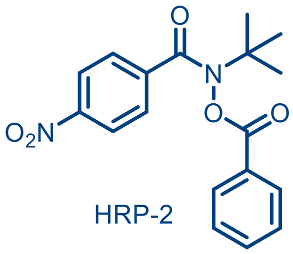
Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.04 (s, 2H), 7.84 – 7.81 (m, 2H), 7.76 (s, 1H), 7.61 – 7.57 (m, 1H), 7.42 – 7.39 (m, 2H), 1.63 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.6, 165.2, 137.8, 134.6, 131.3 (q, *J* = 33.8 Hz), 129.6, 128.8, 127.9 (q, J = 3.8 Hz), 125.8, 123.6 (q, J = 3.8 Hz), 122.8 (q, J = 273.0 Hz), 63.8, 27.5

^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.13.

HRMS (ESI-TOF): m/z: $[M + H]^+$ Calcd for $C_{20}H_{18}F_6NO_3^+$ 434.1188; Found 434.1185.m/z.



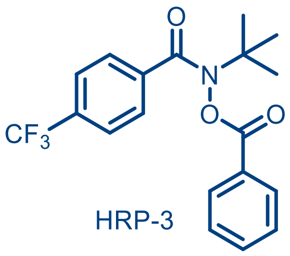
HRP-2

Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 – 7.99 (m, 2H), 7.74 – 7.70 (m, 2H), 7.64 – 7.59 (m, 2H), 7.51 – 7.45 (m, 1H), 7.33 – 7.28 (m, 2H), 1.52 (s, 11H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.0, 165.3, 148.3, 142.1, 134.6, 129.6, 128.9, 128.2, 123.1, 63.6, 27.5.

HRMS (ESI-TOF): m/z: $[M + H]^+$ Calcd for $C_{18}H_{19}N_2O_5^+$ 343.1288; Found 343.1286.



HRP-3

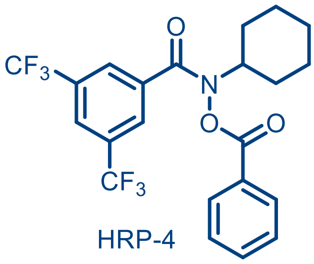
Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.80 – 7.77 (m, 2H), 7.67 – 7.63 (m, 2H), 7.59 – 7.55 (m, 1H), 7.53 – 7.50 (m, 2H), 7.41 – 7.37 (m, 2H), 1.61 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.9, 165.4, 139.6, 134.3, 131.7 (q, J = 32.7 Hz), 129.6, 128.7, 127.5, 126.3, 124.9 (q, J = 3.8 Hz), 122.7 (q, J = 271.8 Hz), 63.4, 27.6.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.01.

HRMS (ESI-TOF): m/z: $[M + H]^+$ Calcd for $C_{19}H_{19}F_3NO_3^+$ 366.1311; Found 366.1312 m/z: $[M + K]^+$ Calcd for $C_{19}H_{18}F_3NO_3K^+$ 404.0870; Found 404.0873.



HRP-4

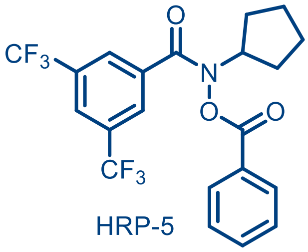
Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.72 – 7.66 (m, 3H), 7.33 – 7.31 (m, 2H), 7.29 – 7.26 (m, 1H), 7.20 – 7.15 (m, 2H), 4.67 – 4.60 (m, 1H), 2.27 – 2.17 (m, 2H), 1.98 – 1.88 (m, 4H), 1.76 – 1.68 (m, 1H), 1.50 – 1.40 (m, 2H), 1.33 – 1.24 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.0, 170.9, 140.1, 137.6, 132.5, 131.7 (q, *J* = 34.1 Hz), 128.7, 128.6, 128.2 (d, *J* = 3.9 Hz), 124.2 (q), 122.5 (q, *J* = 272.9 Hz), 59.0, 30.5, 26.3, 25.2.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.36.

HRMS (ESI-TOF): m/z: $[M + Na]^+$ Calcd for $C_{22}H_{20}F_6NO_3Na^+$ 482.1161; Found 482.1157.



HRP-5

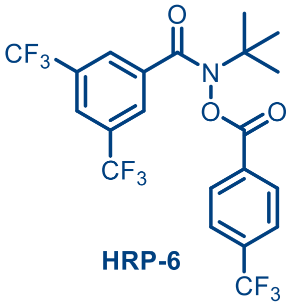
Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.75 – 7.68 (m, 3H), 7.39 – 7.35 (m, 2H), 7.33 – 7.29 (m, 1H), 7.23 – 7.18 (m, 2H), 5.08 – 4.99 (m, 1H), 2.21 – 2.13 (m, 2H), 2.12 – 2.04 (m, 2H), 2.02 – 1.94 (m, 2H), 1.70 – 1.62 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 174.0, 170.9, 140.1, 137.6, 132.5, 131.7 (q, *J* = 34.1 Hz), 128.7, 128.6, 128.2 (q, *J* = 3.9 Hz), 124.3 (q, J = 3.7 Hz), 122.5 (q, *J* = 272.9 Hz), 59.0, 30.5, 26.3, 25.2.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.36.

HRMS (ESI-TOF): m/z: $[M + K]^+$ Calcd for $C_{21}H_{17}F_6NO_3K^+$ 484.0744; Found 484.0742.



HRP-6

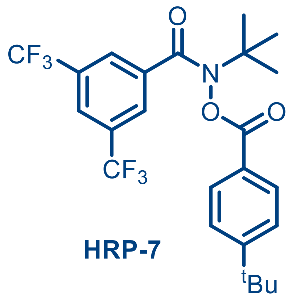
Colorless oil, yield ≥ 99%.

^{1}H NMR(600 MHz, Chloroform-*d*) δ 8.04 – 8.01 (m, 2H), 7.97 – 7.93 (m, 2H), 7.79 (s, 1H), 7.70 – 7.66 (m, 2H), 1.63 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.7, 164.1, 137.5, 136.1 (q, *J* = 33.1 Hz), 131.5 (q, *J* = 33.8 Hz), 130.0, 129.1, 127.7 (q, *J* = 3.8 Hz), 125.9 (q, *J* = 3.8 Hz), 123.8 (p, *J* = 3.8 Hz), 123.1 (q, *J* = 272.9 Hz), 122.7 (q, *J* = 273.0 Hz), 64.1, 27.5.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.21 (d, *J* = 9.0 Hz), -63.64 (d, *J* = 9.8 Hz).

HRMS (ESI-TOF): m/z: $[M + NH_4]^+$ Calcd for $C_{21}H_{20}F_9N_2O_3^+$ 519.1325; Found 519.1327; m/z: $[M + K]^+$ Calcd for $C_{21}H_{16}F_9NO_3K^+$ 540.0618; Found 540.0637



HRP-7

Colorless oil, yield ≥ 99%.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.08 (s, 2H), 7.84 – 7.76 (m, 3H), 7.50 – 7.41 (m, 2H), 1.65 (s, 9H), 1.32 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 167.7, 165.2, 158.7, 137.9 (q, *J* = 2.8 Hz), 131.3 (q, *J* = 33.9 Hz), 129.6, 128.0 (q, *J* = 3.6 Hz), 125.8, 123.6 (q, *J* = 3.7 Hz), 122.93, 122.87 (q, *J* = 272.8 Hz), 63.7, 35.2, 30.9, 27.5.

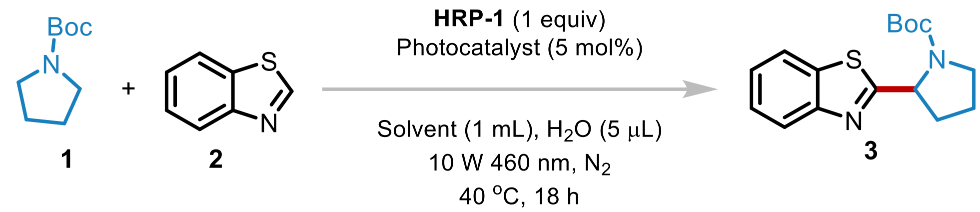
^{19}F NMR (565 MHz, Chloroform-*d*) δ -63.11.

HRMS (ESI-TOF): m/z: $[M + H]^+$ Calcd for $C_{24}H_{26}F_6NO_3^+$ 490.1811; Found 490.1817.

5. Experimental procedures

5.1 Optimization of reaction conditions

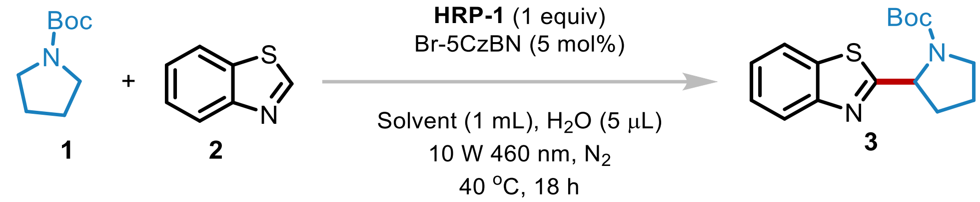
Table S1 Optimization of photocatalysts[a]



Entry	Photocatalyst	Yield of **3** (%)
1	5CzBN	31
2	Br-5CzBN	85
3	I-5CzBN	36
4	Ph-5CzBN	Trace
5	Cl-5CzBN	12
6	*t*Bu-5CzBN	10
7	$Ir(ppy)_3$	N.D.
8	4CzIPN	35
9	3CzFIPN	14
10	Eosin Y	N.D.
11	Methylene blue	16

[a]Reaction conditions: **1** (1 mmol), **2** (0.1 mmol), **HRP-1** (0.1 mmol), Photocatalyst (5 mol%), DMSO (1 mL), H_2O (5 µL), 10 W 460 nm blue LEDs, 40 °C. Isolated yields were given.

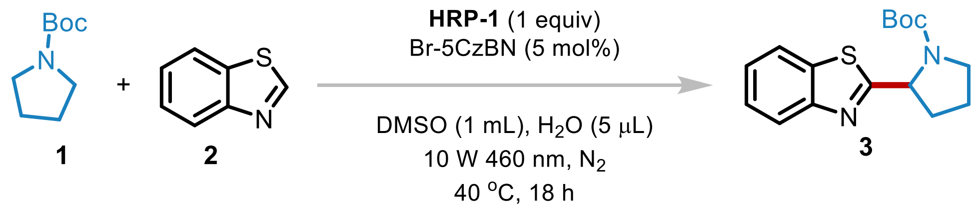
Table S2 Optimization of solvent[a]



Entry	Solvent	Yield of **3** (%)
1	DMSO	85
2	DMF	23
3	DCM	6
4	DCE	37
5	EA	4
6	MeCN	8
7	DMAc	12
8	PhCl	28
9	DMC	6
10	DEC	30
11	$PhCF_3$	45

[a]Reaction conditions: **1** (1 mmol), **2** (0.1 mmol), **HRP-1** (0.1 mmol), Br-5CzBN (5 mol%), Solvent (1 mL), H_2O (5 μL), 10 W 460 nm blue LEDs, 40 °C. Isolated yields were given.

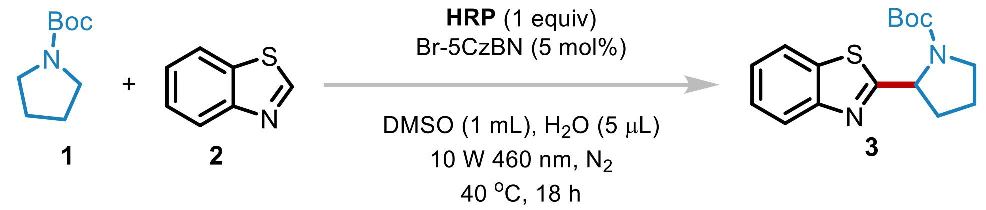
Table S3 Optimization of Reaction Conditions[a]



Entry	Reaction Conditions	Yield of **3** (%)
1	**1**:**2**=10:1	84
2	**1**:**2**=7.5:1	43
3	**1**:**2**=5:1	35
4	**1**:**2**=2.5:1	10
5	**1**:**2**=1:1	Trace
6	12 h	56
7	24 h	83
8	5 W	32
9	20 W	11
10	H_2O (10 μL)	61
11	25 °C	70
12	60 °C	79
13	No HAT Reagent	N.R.
14	No Br-5CzBN	N.R.
15	Dark	N.R.

[a]Reaction conditions: **1** (1 mmol), **2** (0.1 mmol), **HRP-1** (0.1 mmol), Br-5CzBN (5 mol%). DMSO (1 mL), H_2O (5 μL), 10 W 460 nm blue LEDs, 40 °C. Isolated yields were given.

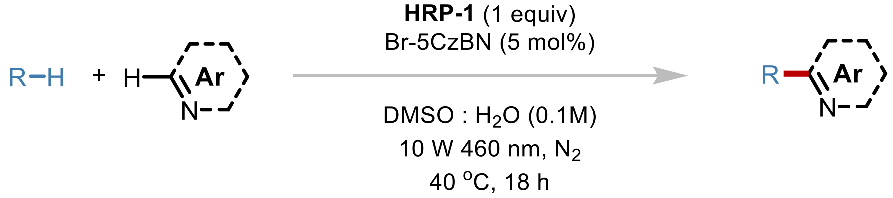
Table S4 Optimization of HRPs[a]



Entry	HAT reagents precursors	Yield of **3** (%)
1	**HRP-1**	83
2	**HRP-2**	36
3	**HRP-3**	60
4	**HRP-4**	38
5	**HRP-5**	17
6	**HRP-6**	31
7	**HRP-7**	55

[a]Reaction conditions: **1** (1 mmol), **2** (0.1 mmol), **HRP** (0.1 mmol), Br-5CzBN (5 mol%), DMSO (1 mL), H_2O (5 μL),10 W 460 nm blue LEDs, 40 °C. Isolated yields were given.

5.2 General experimental procedures for the desired products



Procedure A: In a 10 mL Schlenk tube, alkane (amine or ether) (10.0 equiv, 2.0 mmol), heteroarene (1.0 equiv, 0.2 mmol), **HRP-1** (1.0 equiv, 0.2 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (2.0 mL) and H_2O (10.0 μL), and then charging with nitrogen more than three times. The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 °C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired products.

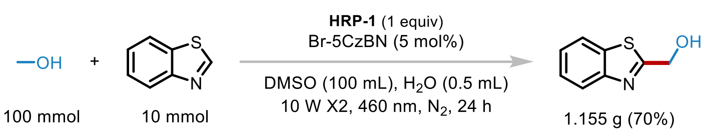
Procedure B: In a 10 mL Schlenk tube, alcohol (10.0 equiv, 2.0 mmol), heteroarene (1.0 equiv, 0.2 mmol), **HRP-1** (1.0 equiv, 0.2 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (2.0 mL) and H_2O (10.0 μL), and then charging with nitrogen more than three times.

The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 °C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired products.

Procedure C: In a 10 mL Schlenk tube, arylalkane (5.0 equiv, 1.0 mmol), heteroarene (1.0 equiv, 0.2 mmol), **HRP-1** (1.0 equiv, 0.2 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (2.0 mL) and H_2O (10.0 μL), and then charging with nitrogen more than three times. The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 °C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired products.

Procedure D: In a 10 mL Schlenk tube, aldehyde (3.0 equiv, 0.6 mmol), heteroarene (1.0 equiv, 0.2 mmol), **HRP-1** (1.0 equiv, 0.2 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (2.0 mL) and H_2O (10.0 μL), and then charging with nitrogen more than three times. The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 °C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired products.

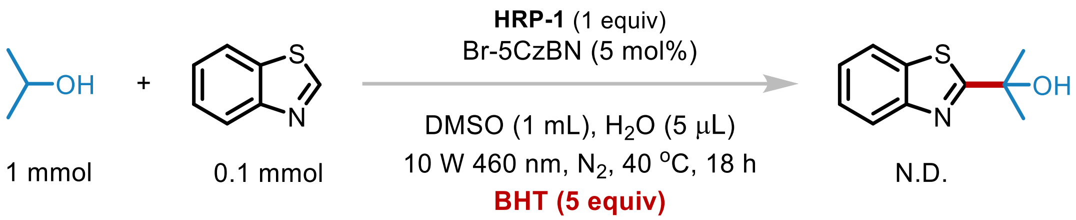
5.3 The gram-scale synthesis



In a 100 mL three-neck flask, methanol (100.0 mmol, 10.0 equiv), heteroarene (10.0 mmol, 1.0 equiv), **HRP-1** (10.0 mmol, 1.0 equiv) and Br-5CzBN (5.0 mol%) were dissolved in DMSO (100.0 mL) and H_2O (0.5 mL), and then the tube was stirred for 24 h with the irradiation of blue LED (λ = 456nm), at 40 °C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired product in 70% yield (1.155 g).

6. Mechanistic experiments

6.1 Control experiments



In a 10 mL Schlenk tube, isopropanol (10.0 equiv, 0.1 mmol), benzothiazole (1.0 equiv, 0.1 mmol), **HRP-1** (1.0 equiv, 0.1 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (1.0 mL) and H_2O (5.0 μl), Afterward, (2,6-ditert-butyl-4- methyl-phenol) (BHT, 5.0 equiv) was added in the mixture, and then charging with nitrogen more than three times. The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm). After the reaction, the yield of product was detected by TLC.

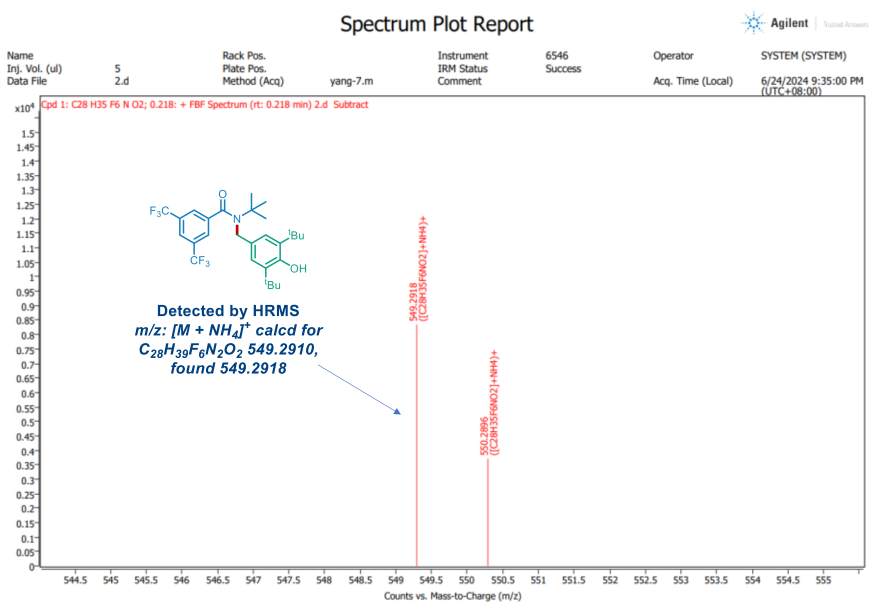


Figure S2 The HRMS analysis of reaction in the presence of BHT

In a 10 mL Schlenk tube, isopropanol (10.0 equiv, 0.1 mmol), benzothiazole (1.0 equiv, 0.1 mmol), **HRP-1** (1.0 equiv, 0.1 mmol), Br-5CzBN (5.0 mol%) were dissolved in DMSO (1.0 mL) and H_2O (5.0 μl), Afterward, (2,6-ditert-butyl-4- methyl-phenol) (TEMPO, 5.0 equiv) was added in the mixture, and then charging with nitrogen more than three times. The tube was stirred for 18 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 °C. After the reaction, the yield of product was detected by TLC.

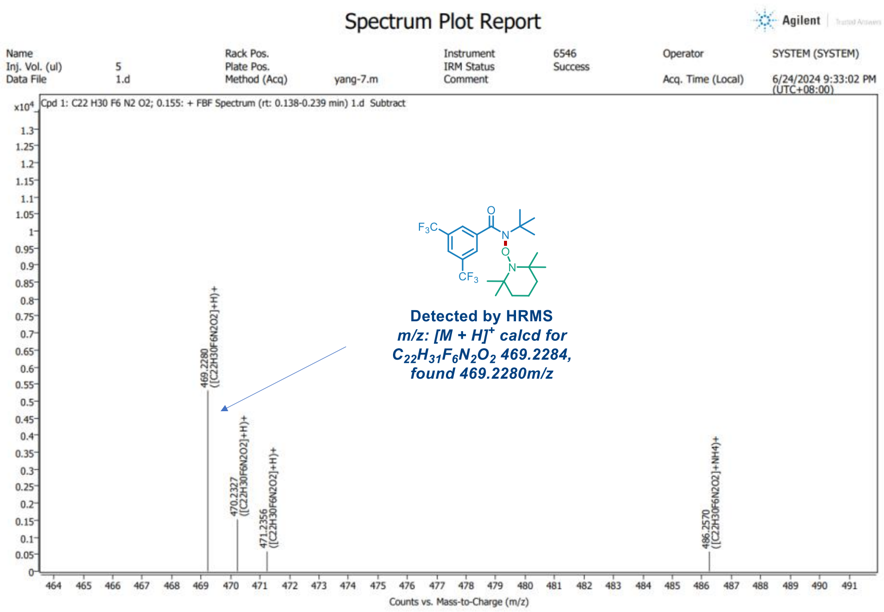


Figure S3 The HRMS analysis of reaction in the presence of TEMPO

6.2 Fluorescence quenching study

Fluorescence quenching experiments were run with a freshly prepared solution of Br-5CzBN series (5 × 10^{-5} M) in degassed anhydrous DMSO added the appropriate amount of a quencher (0.2 M) in a screw-top quartz cuvette at room temperature. After degassing the sample with a stream of N_2 for 10 minutes, the fluorescence emission was measured from 450 nm to 800 nm, at room temperature.

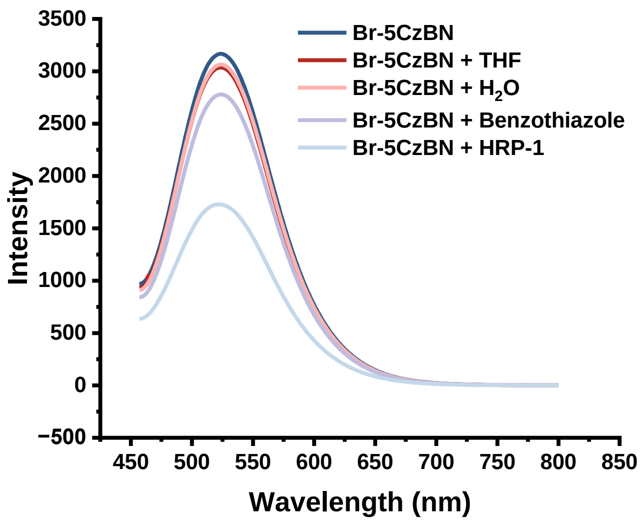


Figure S4 Substrates fluorescence quenching experiments.

Results and Discussion

It can be observed that among the various species in the reaction system, **HRP-1** exhibits the best quenching effect on Br-5CzBN*, while the other species are unable to quench Br-5CzBN*. This suggests that there is an interaction between **HRP-1** and Br-5CzBN* during the reaction process. We propose that this interaction may involve a single-electron transfer mechanism; however, further investigation is necessary to determine the extent of the interaction between HRP-1 and Br-5CzBN*.

6.3 Stern-Volmer emission quenching studies

Stern-Volmer fluorescence quenching experiments were run with freshly prepared solution of 5CzBN (5×10^{-5} M) in degassed anhydrous DMSO added the appropriate amount of a quencher (0.2 M) in a screw-top quartz cuvette at room temperature. After degassing the sample with a stream of N_2 for 10 min, the fluorescence emission was measured from 450 nm to 800 nm, at room temperature.

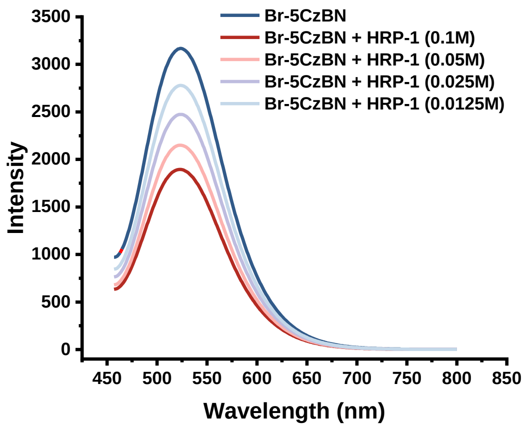


Figure S5 Concentration gradient quenching experiments.

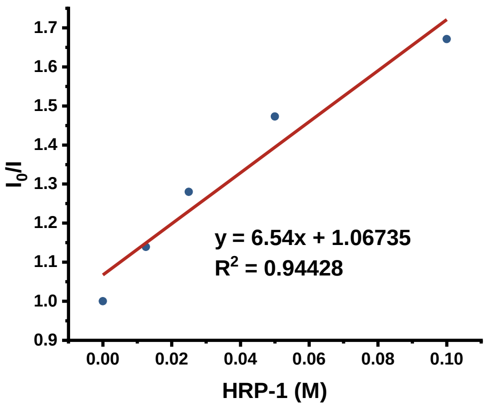


Figure S6 Stern-Volmer fluorescence quenching experiments (**R_2 = 0.94428**).

Results and Discussion

By adjusting the concentration of **HRP-1**, it is evident that the quenching intensity of Br-5CzBN* shows a positive correlation with the gradient changes in **HRP-1** concentration. This clearly indicates that the quenching effect of **HRP-1** on Br-5CzBN* results from a direct interaction. However, it still requires further experimental investigation to determine whether the quenching of sensitized Br-5CzBN* by **HRP-1** is achieved through a single electron transfer process. A comparison of the redox potentials of two species is needed for further clarification.

6.4 Measurement of Redox Potential and Oxidant Potential

Cyclic voltammetry experiments were performed in a 20 mL three-electrode cell under nitrogen atmosphere at room temperature. A steady glassy carbon disk electrode was used as the working electrode, while a platinum wire was used as the counter electrode. The reference was an SCE electrode. Tetrabutylammonium hexafluorophosphate ($TBAPF_6$) (0.1 M) was employed as the electrolyte, and DMF was employed as the solvent. The mixture was poured into the electrochemical cell in cyclic voltammetry experiments, and the scan rate was 0.10 V/s.

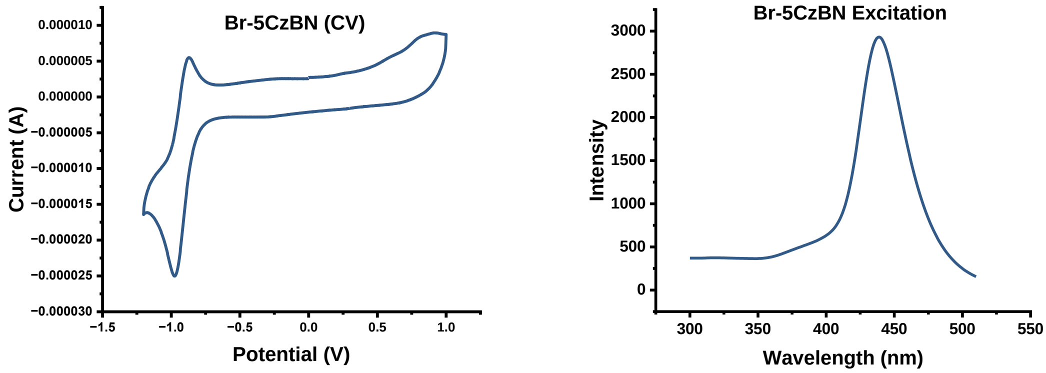


Figure S7 Cyclic voltammogram of Br-5CzBN (1 M) in DMF. **E ($PC^{•+}$/PC) = +0.94 V vs SCE** and optimal excitation wavelength.

The zero-zero vibrational state excitation energy $E_{0,0}$ of Br-5CzBN was estimated by the corresponding energy of the wavelength at optimal excitation wavelength (**438 nm**). Excited state oxidation and reduction potentials were calculated by the following approximating formulas[1]:

$E(PC^{•+}/PC^*) = E(PC^{•+}/PC) – E_{0,0}$

The excited state oxidation potentials for Br-5CzBN were thus calculated:

$E (PC^{•+}/PC^*) = E (PC^{•+}/PC) - E_{0,0} = 0.94\ V – 2.83\ V$

E ($PC^{•+}$/PC*) = –1.89 V vs SCE

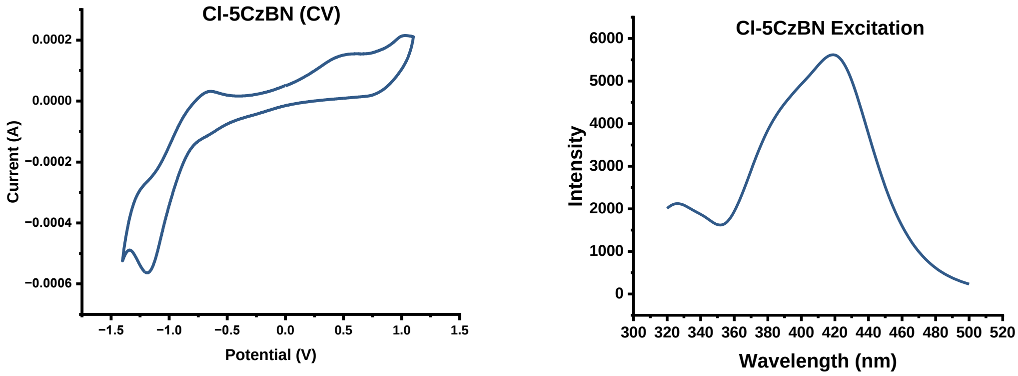


Figure S8 Cyclic voltammogram of Cl-5CzBN (1 M) in DMF. **E ($PC^{\bullet+}$/PC) = +1.02 V vs SCE** and optimal excitation wavelength.

The zero-zero vibrational state excitation energy $E_{0,0}$ of Cl-5CzBN was estimated by the corresponding energy of the wavelength at optimal excitation wavelength (**418 nm**). Excited state oxidation and reduction potentials were calculated by the following approximating formulas:

$E(PC^{\bullet+}/PC^{*}) = E(PC^{\bullet+}/PC) – E_{0,0}$

The excited state oxidation potentials for Br-5CzBN were thus calculated:

$E\ (PC^{\bullet+}/PC^{*}) = E\ (PC^{\bullet+}/PC) - E_{0,0} = 1.02\ V – 2.96\ V$

E ($PC^{\bullet+}/PC^{*}$) = –1.94 V vs SCE

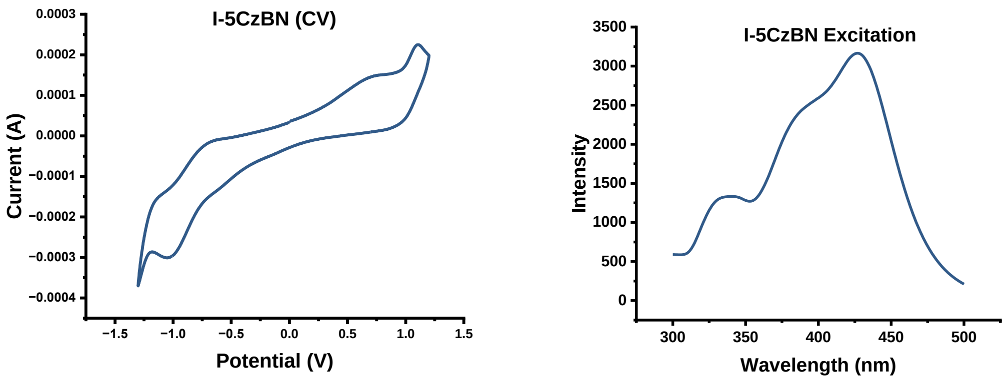


Figure S9 Cyclic voltammogram of I-5CzBN (1 M) in DMF. **E ($PC^{\bullet+}$/PC) = +1.1 V vs SCE** and optimal excitation wavelength.

The zero-zero vibrational state excitation energy $E_{0,0}$ of I-5CzBN was estimated by the corresponding energy of the wavelength at optimal excitation (**426 nm**). Excited state oxidation and reduction potentials were calculated by the following approximating formulas:

$E(PC^{\bullet+}/PC^{*}) = E(PC^{\bullet+}/PC) – E_{0,0}$

The excited state oxidation potentials for Br-5CzBN were thus calculated:

E (PC$^{\cdot+}$/PC*) = E (PC$^{\cdot+}$/PC) - $E_{0,0}$ = 1.1 V – 2.91 V

E (PC$^{\cdot+}$/PC*) = –1.81 V vs SCE

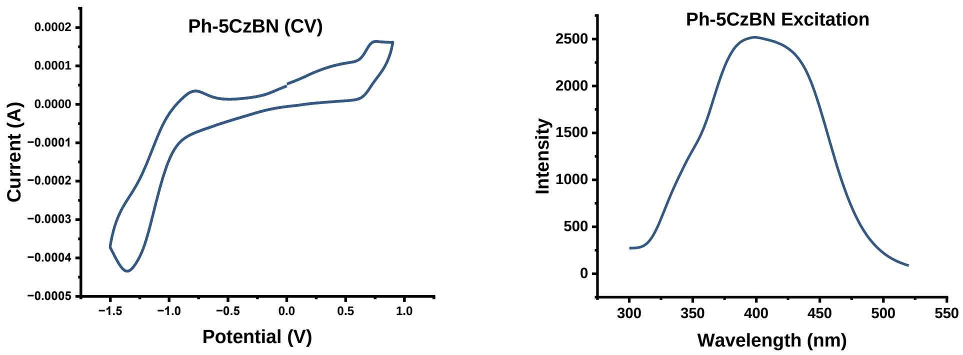


Figure S10 Cyclic voltammogram of Ph-5CzBN (1 M) in DMF. **E (PC$^{\cdot+}$/PC) = 0.77 V vs SCE** and optimal excitation wavelength.

The zero-zero vibrational state excitation energy $E_{0,0}$ of Ph-5CzBN was estimated by the corresponding energy of the wavelength at optimal excitation (**398 nm**). Excited state oxidation and reduction potentials were calculated by the following approximating formulas:

E(PC$^{\cdot+}$/PC*) = E(PC$^{\cdot+}$/PC) – $E_{0,0}$

The excited state oxidation potentials for Br-5CzBN were thus calculated:

E (PC$^{\cdot+}$/PC*) = E (PC$^{\cdot+}$/PC) - $E_{0,0}$ = 0.77 V – 3.11 V

E (PC$^{\cdot+}$/PC*) = –2.34 V vs SCE

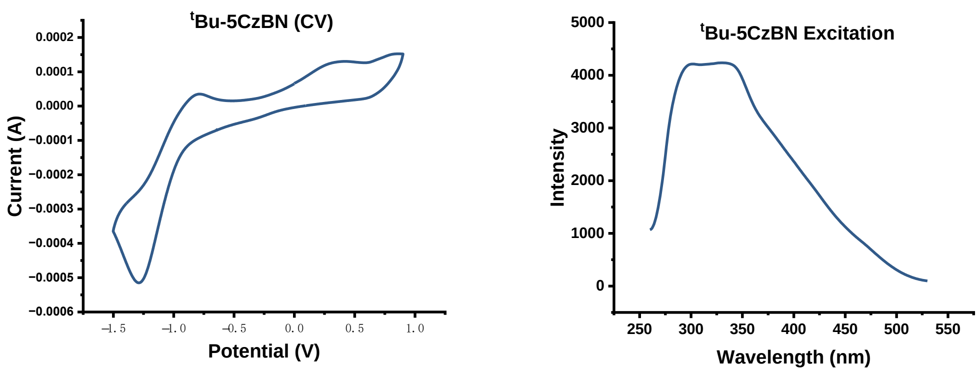


Figure S11 Cyclic voltammogram of ^{t}Bu-5CzBN (1 M) in DMF. **E (PC$^{\cdot+}$/PC) = 0.83 eV vs SCE** and optimal excitation wavelength.

The zero-zero vibrational state excitation energy $E_{0,0}$ of ^{t}Bu-5CzBN was estimated by the corresponding energy of the wavelength at optimal excitation (**338 nm**). Excited state oxidation and reduction potentials were calculated by the following approximating formulas:

E(PC$^{\cdot+}$/PC*) = E(PC$^{\cdot+}$/PC) – $E_{0,0}$

The excited state oxidation potentials for Br-5CzBN were thus calculated:

E (PC$^{\cdot+}$/PC*) = E (PC$^{\cdot+}$/PC) - $E_{0,0}$ = 0.83 V – 3.66 V

E (PC$^{\cdot+}$/PC*) = –2.83 V vs SCE

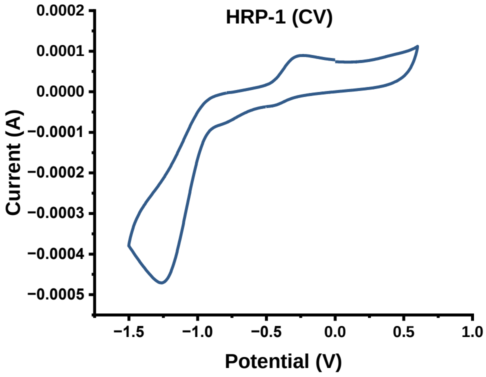


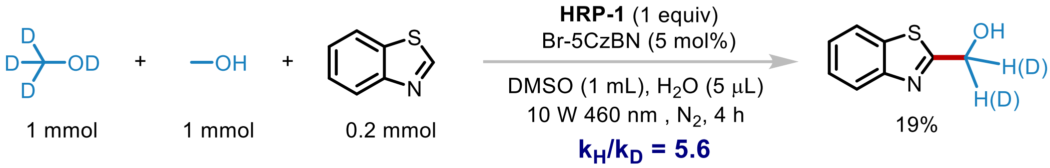
Figure S12 Cyclic voltammogram of HRP-1 (1 M) in DMF. **$E_{Red.}$ = -1.35 V vs SCE**.

Results and Discussion

Comparing the redox potentials of **HRP-1** and Br-5-CzBN clearly indicates that the Br-5-CzBN* can facilitate the reduction cleavage of the N-O bond in **HRP-1**, resulting in the formation of nitrogen-centered radicals and oxygen anions. However, considering comprehensive factors during the reaction, such as the solubility of photoredox-catalysts within the system, the optimal concentration of photoredox-catalysts is ultimately determined by the yield of the desired target product.

6.5 Kinetic Isotope Effect experiments

In a 10 mL Schlenk tube, methanol (1.0 mmol) and methanol-*d*$_4$ (1.0 mmol), benzothiazole (1.0 equiv., 0.2 mmol), **HRP-1** (1.0 equiv., 0.2 mmol), Br-5CzBN (5 mol%) were dissolved in DMSO (2.0 mL) and H_2O (10.0 μL), and then charging with nitrogen more than three times. The tube was stirred for 4 h with the irradiation of 10 W blue LED (λ = 460 nm), at 40 ^{o}C. After the reaction, the mixture was extracted with saturated sodium bicarbonate solution and ethyl acetate, and the organic layer was washed with saturated brine and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo, and the residue was purified by column chromatography on silica gel to afford the desired product (19% yield). Following this, we carried out NMR analysis, which yielded a k_H/k_D value of 5.6. This result not only confirmed the validity of our HAT process but also suggested that the HAT process is the rate-determining step within our catalytic system.



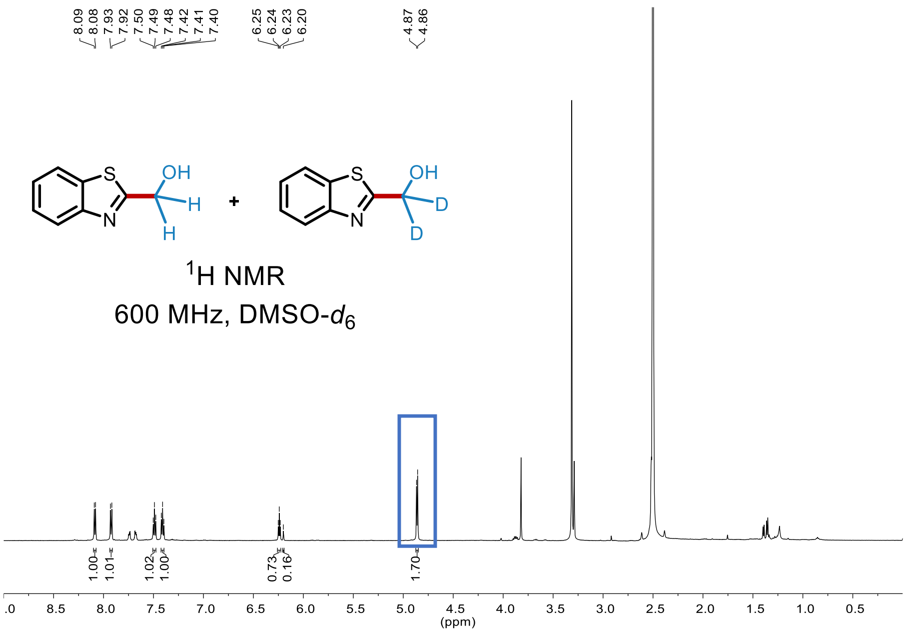


Figure S13 ^{1}H NMR of mixture product from methanol and methanol-$d4$

7. Other information

7.1 Substrate Propylene Glycol Site Selectivity

The synthesis of product 26 was conducted with particular attention to potential byproduct formation at the α-position relative to the primary alcohol functionality. Through comprehensive analytical characterization, no evidence of primary-alcohol-heteroarylated product formation was detected. This observation can be rationalized by considering the stability of the radical intermediate, which appears to effectively suppress the formation of such byproducts (Figure S14).

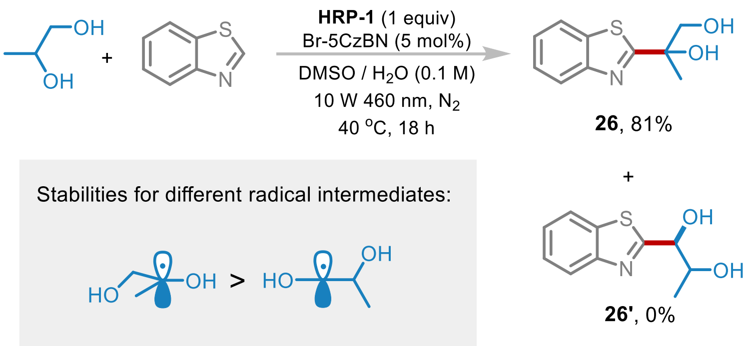


Figure S14 Stability for de radical generated during the HAT process

7.2 Unsuccessful substrates

CF_3CH_2OH and 4-methylbenzonitrile

CF_3CH_2OH exhibited poor reactivity in our initial experiments. Our analysis suggests that this is primarily due to the high polarity of the CF_3CH_2OH radical (ω = 1.21 eV), which is significantly higher than that of the ethanol radical (ω =0.6 eV) and approaches the critical polarity value of 2.0 eV.[2] This high polarity may hinder the desired reaction pathway, as similar trends have been reported in the literature.[3] The poor reactivity of 4-methylbenzonitrile may be due to reasons similar to those observed with CF_3CH_2OH (Figure S15). We attempted to enhance the reactivity by increasing the substrate equivalents and modifying the reaction conditions, such as extending reaction times and elevating temperatures. However, these adjustments did not yield the desired improvements.

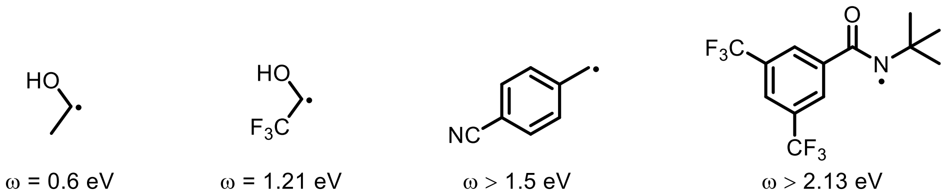
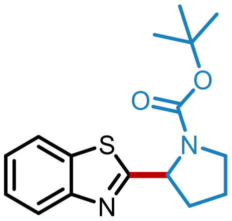


Figure S15 The polarity of corresponding radicals during HAT process

8. Characterization data for photoredox-catalysts, HRPs, and products

tert-butyl 2-(benzo[d]thiazol-2-yl)pyrrolidine-1-carboxylate (3)[4]

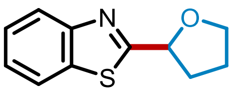


Follow the general procedure A. **3** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (51.7 mg, 85%),

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 – 7.94 (m, 1H), 7.90 – 7.82 (m, 1H), 7.50 – 7.40 (m, 1H), 7.40 – 7.33 (m, 1H), 5.36 – 5.19 (m, 1H), 3.71 – 3.45 (m, 2H), 2.51 – 2.22 (m, 2H), 2.07 – 1.93 (m, 2H), 1.40 (br s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 177.5, 176.8, 154.2, 154.1, 152.4, 136.4, 129.5, 129.3, 124.3, 123.9, 118.4, 59.9, 59.5, 47.1, 46.8, 34.1, 32.8, 28.4, 28.2, 24.2, 23.4

2-(tetrahydrofuran-2-yl)benzo[d]thiazole (4)[5]

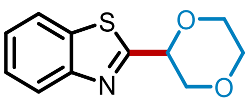


Follow the general procedure A. **4** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (34.0 mg, 83%),

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.96 (m, 1H), 7.92 – 7.85 (m, 1H), 7.49 – 7.44 (m, 1H), 7.39 – 7.34 (m, 1H), 5.38 – 5.33 (m, 1H), 4.19 – 4.13 (m, 1H), 4.04 – 3.98 (m, 1H), 2.56 – 2.49 (m, 1H), 2.31 – 2.24 (m, 1H), 2.08 – 2.01 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-d) δ 176.3, 153.7, 134.8, 125.9, 124.8, 122.8, 121.8, 78.8, 69.5, 33.4, 25.7.

2-(1,4-dioxan-2-yl)benzo[d]thiazole (5)[6]

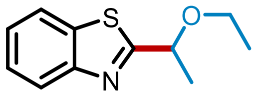


Follow the general procedure A. **5** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (34.9 mg, 79%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 – 7.99 (m, 1H), 7.94 – 7.90 (m, 1H), 7.51 – 7.46 (m, 1H), 7.42 – 7.37 (m, 1H), 5.09 – 5.03 (m, 1H), 4.33 – 4.27 (m, 1H), 4.05 – 3.95 (m, 2H), 3.88 – 3.81 (m, 1H), 3.81 – 3.75 (m, 1H), 3.75 – 3.67 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.0, 153.0, 134.6, 126.1, 125.1, 123.1, 121.8, 75.5, 70.5, 67.0, 66.4.

2-(1-ethoxyethyl)benzo[d]thiazole (6)[6]

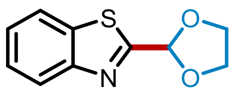


Follow the general procedure A. **6** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (33.5 mg, 81%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 – 7.97 (m, 1H), 7.92 – 7.88 (m, 1H), 7.49 – 7.45 (m, 1H), 7.40 – 7.36 (m, 1H), 4.89 – 4.83 (m, 1H), 3.65 – 3.60 (m, 2H), 1.65 – 1.64 (m, 3H), 1.28 – 1.26 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 176.7, 153.2, 134.9, 125.9, 125.0, 122.9, 121.9, 76.1, 65.5, 22.7, 15.3.

2-(1,3-dioxolan-2-yl)benzo[d]thiazole (7)[7]

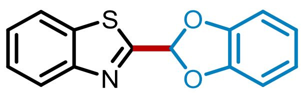


Follow the general procedure A. **7** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (33.1 mg, 80%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.10 – 8.06 (m, 1H), 7.94 – 7.90 (m, 1H), 7.53 – 7.49 (m, 1H), 7.45 – 7.41 (m, 1H), 6.25 (s, 1H), 4.24 – 4.18 (m, 2H), 4.17 – 4.11 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 169.2, 153.3, 135.0, 126.2, 125.7, 123.8, 121.9, 100.6, 65.7.

2-(benzo[d][1,3]dioxol-2-yl)benzo[d]thiazole (8)[6]

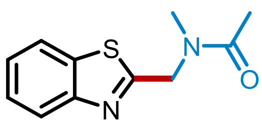


Follow the general procedure A. **8** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (33.2 mg, 65%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.15 – 8.11 (m, 1H), 7.93 – 7.89 (m, 1H), 7.56 – 7.51 (m, 1H), 7.48 – 7.43 (m, 1H), 7.31 (s, 1H), 6.98 – 6.89 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 166.0, 153.0, 146.5, 134.9, 126.6, 126.3, 124.1, 122.5, 122.0, 109.2, 105.7.

N-(benzo[d]thiazol-2-ylmethyl)-N-methylacetamide (9)[8]



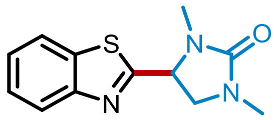
Follow the general procedure A. **9** was purified by flash chromatography (silica gel,

petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (32.1 mg, 73%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.03 – 7.98 (m, 1H), 7.91 – 7.84 (m, 1H), 7.54 – 7.45 (m, 1H), 7.44 – 7.36 (m, 1H), 4.99 – 4.88 (m, 2H), 3.15 – 3.09 (m, 3H), 2.25 – 2.17 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 170.93, 170.88, 168.1, 167.8, 153.3, 152.8, 135.7, 134.8, 126.5, 126.1, 125.5, 125.2, 123.2, 123.0, 121.9, 121.8, 53.1, 49.4, 36.4, 34.4, 21.6, 21.5.

4-(benzo[d]thiazol-2-yl)-1,3-dimethylimidazolidin-2-one (10)[9]

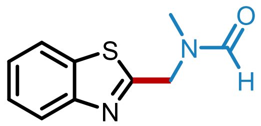


Follow the general procedure A. **10** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (38.0 mg, 77%),

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.04 – 7.99 (m, 1H), 7.94 – 7.89 (m, 1H), 7.54 – 7.48 (m, 1H), 7.45 – 7.40 (m, 1H), 4.96 – 4.88 (m, 1H), 3.89 – 3.79 (m, 1H), 3.42 – 3.34 (m, 1H), 2.89 – 2.83 (m, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.6, 160.8, 153.1, 135.1, 126.3, 125.6, 123.3, 122.0, 58.9, 52.1, 31.1, 30.6.

N-(benzo[d]thiazol-2-ylmethyl)-N-methylformamide (11)[8]

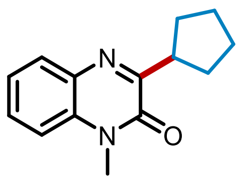


Follow the general procedure A. **11** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (33.0 mg, 80%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.38 – 8.18 (m, 1H), 8.08 – 7.98 (m, 1H), 7.95 – 7.83 (m, 1H), 7.59 – 7.38 (m, 2H), 4.98 – 4.81 (m, 2H), 3.12 – 2.97 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 166.2, 162.6, 162.4, 135.7, 126.4, 126.1, 125.6, 125.3, 123.3, 123.1, 121.8, 121.7, 51.6, 46.2, 34.5, 30.3.

3-cyclopentyl-1-methylquinoxalin-2(1H)-one (12)[10]



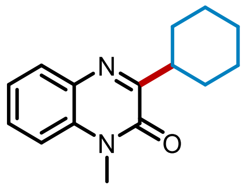
Follow the general procedure A. **12** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (31.0 mg, 68%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.84 – 7.81 (m, 1H), 7.53 – 7.48 (m, 1H), 7.35 – 7.30

(m, 1H), 7.30 – 7.27 (m, 1H), 3.75 – 3.68 (m, 4H), 2.10 – 2.03 (m, 2H), 1.96 – 1.89 (m, 2H), 1.86 – 1.78 (m, 2H), 1.75 – 1.67 (m, 2H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.7, 155.0, 133.0, 132.7, 129.8, 129.3, 123.4, 113.4, 42.7, 30.8, 29.0, 25.9.

3-cyclohexyl-1-methylquinoxalin-2(1H)-one (13)[10]

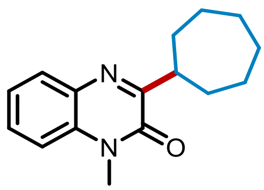


Follow the general procedure A. **13** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (36.3 mg, 75%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.85 – 7.82 (m, 1H), 7.53 – 7.49 (m, 1H), 7.35 – 7.30 (m, 1H), 7.30 – 7.27 (m, 1H), 3.70 (s, 3H), 3.38 – 3.31 (m, 1H), 1.99 – 1.93 (m, 2H), 1.90 – 1.84 (m, 2H), 1.80 – 1.74 (m, 1H), 1.59 – 1.53 (m, 2H), 1.51 – 1.43 (m, 2H), 1.35 – 1.29 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.3, 154.6, 132.91, 132.88, 129.8, 129.4, 123.4, 113.4, 40.8, 30.5, 29.1, 26.3, 26.2.

3-cycloheptyl-1-methylquinoxalin-2(1H)-one (14)[11]

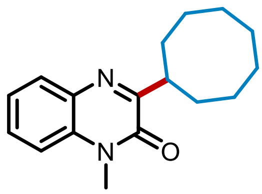


Follow the general procedure A. **14** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (36.3 mg, 71%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.84 – 7.81 (m, 1H), 7.52 – 7.48 (m, 1H), 7.34 – 7.30 (m, 1H), 7.29 – 7.27 (m, 1H), 3.70 (s, 3H), 3.52 – 3.45 (m, 1H), 2.01 – 1.94 (m, 2H), 1.88 – 1.76 (m, 4H), 1.75 – 1.67 (m, 2H), 1.66 – 1.59 (m, 4H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 165.4, 154.5, 132.9, 132.8, 129.7, 129.3, 123.4, 113.4, 42.5, 32.3, 29.1, 28.2, 27.1.

3-cyclooctyl-1-methylquinoxalin-2(1H)-one (15)[11]



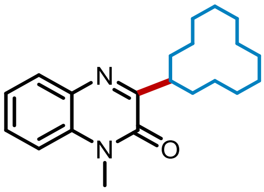
Follow the general procedure A. **15** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless

oil (32.4 mg, 60%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.85 – 7.82 (m, 1H), 7.53 – 7.49 (m, 1H), 7.35 – 7.31 (m, 1H), 7.30 – 7.27 (m, 1H), 3.70 (s, 3H), 3.60 – 3.53 (m, 1H), 1.91 – 1.87 (m, 4H), 1.84 – 1.79 (m, 2H), 1.72 – 1.61 (m, 8H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 165.8, 154.5, 132.9, 132.8, 129.7, 129.3, 123.4, 113.4, 40.5, 30.6, 29.1, 26.7, 26.6, 25.9.

3-cyclododecyl-1-methylquinoxalin-2(1H)-one (16)[12]

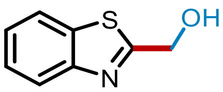


Follow the general procedure A. **16** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (35.9 mg, 55 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.84 (m, 1H), 7.53 – 7.49 (m, 1H), 7.35 – 7.31 (m, 1H), 7.30 – 7.27 (m, 1H), 3.71 (s, 4H), 1.82 – 1.73 (m, 4H), 1.66 – 1.59 (m, 2H), 1.51 – 1.41 (m, 7H), 1.41 – 1.26 (m, 10H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 164.5, 154.9, 132.88, 132.85, 129.8, 129.3, 123.3, 113.4, 36.2, 29.1, 28.1, 24.0, 23.9, 23.6, 23.3, 23.1.

benzo[d]thiazol-2-ylmethanol (17)[6]

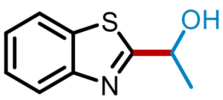


Follow the general procedure B. **17** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: white solid (24.8 mg, 75%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.02 – 7.98 (m, 1H), 7.92 – 7.88 (m, 1H), 7.51 – 7.47 (m, 1H), 7.42 – 7.38 (m, 1H), 5.09 (s, 2H), 3.06 (s, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 152.8, 134.8, 126.2, 125.1, 122.9, 121.9, 62.8.

1-(benzo[d]thiazol-2-yl)ethan-1-ol (18)[6]

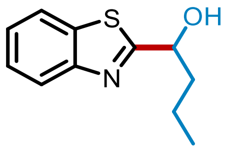


Follow the general procedure B. **18** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (31.2 mg, 87%),

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.97 (m, 1H), 7.90 – 7.88 (m, 1H), 7.50 – 7.46 (m, 1H), 7.40 – 7.37 (m, 1H), 5.28 – 5.24 (m, 1H), 3.34 (s, 1H), 1.73 – 1.71 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 176.7, 152.8, 134.9, 126.1, 125.1, 122.9, 121.9, 68.6, 24.1.

1-(benzo[d]thiazol-2-yl)butan-1-ol(19)[6]

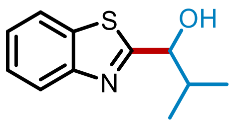


Follow the general procedure B. **19** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (31.1 mg, 75 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.96 (m, 1H), 7.90 – 7.87 (m, 1H), 7.49 – 7.45 (m, 1H), 7.40 – 7.36 (m, 1H), 5.13 – 5.09 (m, 1H), 3.26 (s, 1H), 2.05 – 1.98 (m, 1H), 1.95 – 1.88 (m, 1H), 1.62 – 1.48 (m, 2H), 1.01 – 0.96 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 176.3, 152.8, 134.8, 126.1, 125.0, 122.9, 121.8, 72.2, 40.2, 18.4, 13.8.

1-(benzo[d]thiazol-2-yl)-2-methylpropan-1-ol (20)[13]

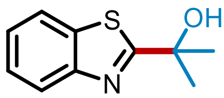


Follow the general procedure B. **20** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (30.6 mg, 74 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 – 7.98 (m, 1H), 7.90 – 7.87 (m, 1H), 7.50 – 7.46 (m, 1H), 7.40 – 7.36 (m, 1H), 4.94 – 4.89 (m, 1H), 3.22 – 3.14 (m, 1H), 2.33 – 2.24 (m, 1H), 1.10 – 1.07 (m, 3H), 0.99 – 0.97 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 175.2, 152.6, 134.9, 126.0, 125.0, 122.9, 121.8, 35.2, 19.0, 16.3.

2-(benzo[d]thiazol-2-yl)propan-2-ol (21)[14]

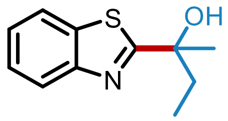


Follow the general procedure B. **21** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (34.8 mg, 90 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.96 (m, 1H), 7.90 – 7.86 (m, 1H), 7.49 – 7.44 (m, 1H), 7.39 – 7.34 (m, 1H), 3.27 (s, 1H), 1.75 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 180.0, 153.0, 135.4, 126.0, 124.9, 122.9, 121.8, 73.6, 30.8.

2-(benzo[d]thiazol-2-yl)butan-2-ol (22)[13]

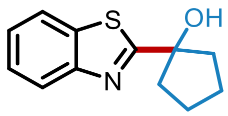


Follow the general procedure B. **22** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (35.2 mg, 85 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.02 – 7.98 (m, 1H), 7.91 – 7.87 (m, 1H), 7.50 – 7.46 (m, 1H), 7.41 – 7.36 (m, 1H), 3.35 (s, 1H), 2.10 – 1.98 (m, 2H), 1.72 (s, 3H), 0.95 – 0.91 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 135.4, 126.1, 125.0, 122.8, 121.8, 36.4, 29.2, 8.0.

1-(benzo[d]thiazol-2-yl)cyclopentan-1-ol (23)[13]

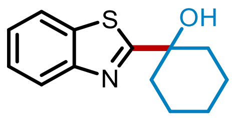


Follow the general procedure B. **23** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (35.1 mg, 80 %).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.95 (m, 1H), 7.91 – 7.85 (m, 1H), 7.50 – 7.43 (m, 1H), 7.41 – 7.33 (m, 1H), 3.07 (s, 1H), 2.39 – 2.25 (m, 2H), 2.16 – 2.06 (m, 2H), 2.06 – 1.89 (m, 4H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 179.0, 153.1, 135.5, 125.9, 124.8, 122.8, 121.6, 83.9, 42.8, 24.3.

1-(benzo[d]thiazol-2-yl)cyclohexan-1-ol (24)[15]

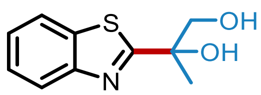


Follow the general procedure B. **24** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (41.0 mg, 88%),

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.97 (m, 1H), 7.90 – 7.86 (m, 1H), 7.49 – 7.44 (m, 1H), 7.38 – 7.34 (m, 1H), 2.92 (s, 1H), 2.12 – 2.04 (m, 2H), 1.99 – 1.93 (m, 2H), 1.83 – 1.71 (m, 5H), 1.46 – 1.37 (m, 1H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 180.7, 153.2, 135.2, 125.9, 124.8, 122.9, 121.8, 74.8, 38.5, 25.1, 21.7.

2-(benzo[d]thiazol-2-yl)butane-1,2-diol (25)[13]



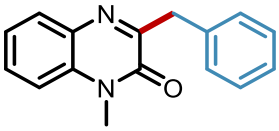
Follow the general procedure B. **25** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless

oil (33.7 mg, 81%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.01 – 7.94 (m, 1H), 7.92 – 7.85 (m, 1H), 7.51 – 7.44 (m, 1H), 7.42 – 7.36 (m, 1H), 4.22 – 4.15 (m, 1H), 3.84 – 3.77 (m, 1H), 1.65 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 177.8, 152.7, 135.2, 126.1, 125.2, 122.9, 121.8, 75.7, 70.0, 25.6.

3-benzyl-1-methylquinoxalin-2(1H)-one (27)[16]

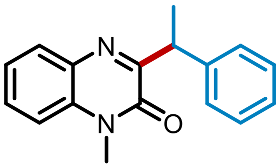


Follow the general procedure C. **27** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 10:1, v/v) to give the desired product: colorless oil (35.5 mg, 71%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.84 (m, 1H), 7.54 – 7.49 (m, 1H), 7.49 – 7.45 (m, 2H), 7.35 – 7.31 (m, 1H), 7.31 – 7.25 (m, 3H), 7.23 – 7.18 (m, 1H), 4.27 (s, 2H), 3.66 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 159.3, 154.7, 137.1, 133.4, 132.8, 130.0, 129.9, 129.5, 128.4, 126.6, 123.6, 113.5, 40.8, 29.1.

1-methyl-3-(1-phenylethyl)quinoxalin-2(1H)-one (28)[17]

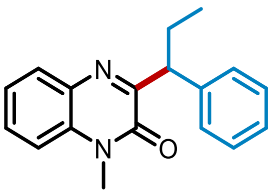


Follow the general procedure C. **28** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 10:1, v/v) to give the desired product: colorless oil (42.3 mg, 80%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 – 7.91 (m, 1H), 7.53 – 7.49 (m, 1H), 7.46 – 7.42 (m, 2H), 7.37 – 7.32 (m, 1H), 7.29 – 7.24 (m, 3H), 7.20 – 7.15 (m, 1H), 4.87 – 4.78 (m, 1H), 3.62 (s, 3H), 1.70 – 1.67 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 161.9, 154.4, 143.1, 133.1, 132.7, 130.1, 129.7, 128.4, 128.1, 126.5, 123.4, 113.5, 41.9, 29.1, 19.7.

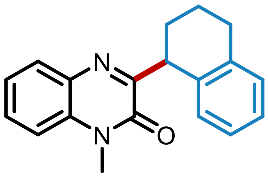
1-methyl-3-(1-phenylpropyl)quinoxalin-2(1H)-one (29)[18]



Follow the general procedure C. **29** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 10:1, v/v) to give the desired product: colorless oil (42.8 mg, 77%).

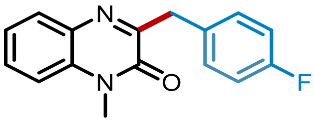
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 – 7.91 (m, 1H), 7.53 – 7.49 (m, 1H), 7.47 – 7.43 (m, 2H), 7.36 – 7.32 (m, 1H), 7.28 – 7.25 (m, 3H), 7.19 – 7.15 (m, 1H), 4.60 – 4.56 (m, 1H), 3.62 (s, 3H), 2.36 – 2.27 (m, 1H), 2.09 (dt, *J* = 13.5, 7.5 Hz, 1H), 0.94 – 0.89 (m, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 161.4, 154.6, 141.6, 133.0, 132.8, 130.1, 129.6, 128.7, 128.3, 126.5, 123.4, 113.5, 49.2, 29.1, 27.1, 12.5.

1-methyl-3-(1,2,3,4-tetrahydronaphthalen-1-yl)quinoxalin-2(1H)-one (30)



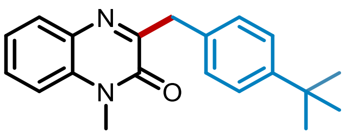
Follow the general procedure C. **30** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 50:1 to 10:1, v/v) to give the desired product: colorless oil (40.6 mg, 70%).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.79 – 7.76 (m, 1H), 7.54 – 7.50 (m, 1H), 7.32 – 7.28 (m, 2H), 7.18 – 7.10 (m, 2H), 7.05 – 7.01 (m, 1H), 6.92 – 6.89 (m, 1H), 4.90 – 4.86 (m, 1H), 3.72 (s, 3H), 3.03 – 2.96 (m, 1H), 2.89 – 2.81 (m, 1H), 2.21 – 2.16 (m, 2H), 2.10 – 2.03 (m, 1H), 1.86 – 1.77 (m, 1H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 163.9, 154.5, 137.8, 137.1, 133.2, 132.7, 130.1, 129.8, 129.2, 128.8, 125.9, 125.6, 123.4, 113.4, 43.1, 29.7, 29.2, 28.0, 21.3.
HRMS (ESI-TOF): m/z: $[M + K]^+$ Calcd for $C_{19}H_{18}N_2OK^+$ 329.1051; Found 329.1049.

3-(4-fluorobenzyl)-1-methylquinoxalin-2(1H)-one (31)[19]



Follow the general procedure C. **31** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 10:1, v/v) to give the desired product: colorless oil (32.2 mg, 50%).
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.86 – 7.84 (m, 1H), 7.56 – 7.51 (m, 1H), 7.45 – 7.40 (m, 2H), 7.37 – 7.33 (m, 1H), 7.29 – 7.27 (m, 1H), 6.99 – 6.95 (m, 2H), 4.23 (s, 2H), 3.67 (s, 3H).
^{13}C NMR (151 MHz, Chloroform-*d*) δ 162.6, 161.0, 159.1, 154.7, 133.3, 132.7, 132.6, 132.6, 131.02, 130.97, 129.98, 129.97, 123.6, 115.2, 115.1, 113.6, 39.9, 29.1.
^{19}F NMR (565 MHz, Chloroform-*d*) δ -116.65.

3-(4-(tert-butyl)benzyl)-1-methylquinoxalin-2(1H)-one (32)[19]



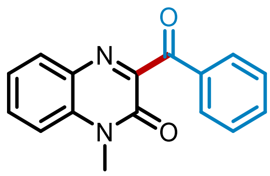
Follow the general procedure C. **32** was purified by flash chromatography (silica gel,

petroleum ether/ethyl acetate from 20:1 to 10:1, v/v) to give the desired product: colorless oil (42.7 mg, 70%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.84 (m, 1H), 7.53 – 7.49 (m, 1H), 7.43 – 7.39 (m, 2H), 7.35 – 7.31 (m, 2H), 7.26 – 7.24 (m, 1H), 4.23 (s, 2H), 3.66 (s, 3H), 1.28 (s, 9H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 159.5, 154.8, 149.3, 133.9, 133.4, 132.8, 129.9, 129.8, 129.2, 125.3, 123.5, 113.5, 40.3, 34.4, 31.4, 29.1.

3-benzoyl-1-methylquinoxalin-2(1H)-one (34)[16]

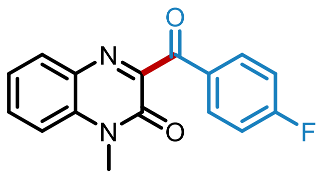


Follow the general procedure D. **34** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 5:1 to 2:1, v/v) to give the desired product: colorless oil (40.1 mg, 76%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 – 7.98 (m, 2H), 7.96 – 7.92 (m, 1H), 7.71 – 7.67 (m, 1H), 7.65 – 7.60 (m, 1H), 7.51 – 7.47 (m, 2H), 7.44 – 7.40 (m, 2H), 3.76 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.7, 134.9, 134.2, 133.9, 132.0, 131.1, 130.0, 128.7, 124.2, 114.0, 29.1.

3-(4-fluorobenzoyl)-1-methylquinoxalin-2(1H)-one (35)[20]



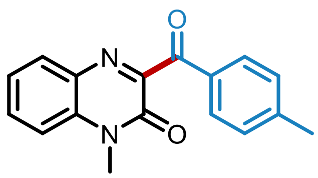
Follow the general procedure C. **35** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 5:1 to 2:1, v/v) to give the desired product: colorless oil (33.9 mg, 60%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.06 – 8.00 (m, 2H), 7.95 – 7.90 (m, 1H), 7.72 – 7.66 (m, 1H), 7.45 – 7.39 (m, 2H), 7.20 – 7.12 (m, 2H), 3.75 (s, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 189.9, 166.4 (d, *J* = 256.8 Hz), 154.4, 153.3, 134.0, 132.7 (d, *J* = 9.6 Hz), 132.2, 132.0, 131.6 (d, J = 2.0 Hz), 131.1, 124.1, 115.9 (d, *J* = 22.4 Hz), 113.9, 29.0.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -102.84.

1-methyl-3-(4-methylbenzoyl)quinoxalin-2(1H)-one (36)[20]



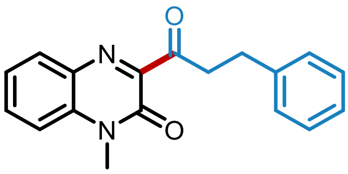
Follow the general procedure C. **36** was purified by flash chromatography (silica gel,

petroleum ether/ethyl acetate from 5:1 to 2:1, v/v) to give the desired product: colorless oil (41.2 mg, 74%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.94 – 7.92 (m, 1H), 7.90 – 7.87 (m, 2H), 7.70 – 7.65 (m, 1H), 7.43 – 7.39 (m, 2H), 7.30 – 7.26 (m, 2H), 3.75 (s, 3H), 2.43 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 191.4, 154.9, 153.4, 145.4, 133.9, 132.4, 132.2, 131.9, 131.0, 130.1, 129.4, 124.2, 113.9, 29.1, 21.9.

1-methyl-3-(3-phenylpropanoyl)quinoxalin-2(1H)-one (37)[21]

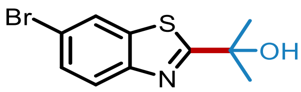


Follow the general procedure C. **37** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 5:1 to 2:1, v/v) to give the desired product: colorless oil (47.3 mg, 81%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.94 – 7.90 (m, 1H), 7.69 – 7.64 (m, 1H), 7.42 – 7.35 (m, 2H), 7.29 – 7.25 (m, 4H), 7.19 – 7.17 (m, 1H), 3.71 (s, 3H), 3.46 – 3.40 (m, 2H), 3.13 – 3.06 (m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 199.4, 140.9, 134.4, 132.5, 132.1, 131.4, 128.4, 128.2, 126.0, 124.0, 113.7, 42.3, 29.6, 28.9.

2-(6-bromobenzo[d]thiazol-2-yl)propan-2-ol (38)[15]

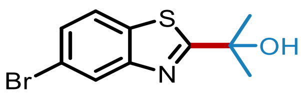


Follow the general procedure B. **38** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (49.9 mg, 92%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.01 – 7.98 (m, 1H), 7.81 (d, *J* = 8.7 Hz, 1H), 7.58 – 7.54 (m, 1H), 3.19 (s, 1H), 1.74 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 180.8, 152.1, 137.0, 129.5, 124.3, 124.0, 118.4, 73.7, 30.7.

2-(5-bromobenzo[d]thiazol-2-yl)propan-2-ol (39)[15]

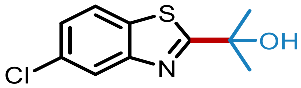


Follow the general procedure B. **39** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (50.9 mg, 94%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.06 – 8.04 (m, 1H), 7.66 – 7.63 (m, 1H), 7.41 – 7.38 (m, 1H), 3.05 (s, 1H), 1.67 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 181.9, 154.4, 134.2, 128.0, 125.9, 122.8, 119.6, 73.7, 30.7.

2-(5-chlorobenzo[d]thiazol-2-yl)propan-2-ol (40)[15]

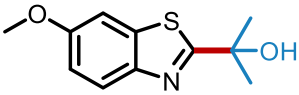


Follow the general procedure B. **40** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (38.6 mg, 85%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.98 – 7.96 (m, 1H), 7.80 – 7.78 (m, 1H), 7.36 – 7.34 (m, 1H), 2.95 (s, 1H), 1.74 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 182.0, 154.1, 133.7, 132.0, 125.4, 122.8, 122.5, 73.7, 30.7.

2-(6-methoxybenzo[d]thiazol-2-yl)propan-2-ol (41)[15]

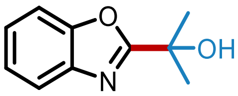


Follow the general procedure B. **41** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (40.6 mg, 91%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.87 – 7.83 (m, 1H), 7.34 – 7.31 (m, 1H), 7.08 – 7.04 (m, 1H), 3.87 (s, 3H), 3.21 (s, 1H), 1.73 (s, 6H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 177.3, 157.5, 147.5, 136.7, 123.3, 115.3, 104.3, 73.4, 55.8, 30.8.

2-(benzo[d]oxazol-2-yl)propan-2-ol (42)[22]

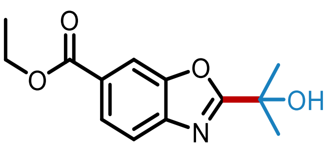


Follow the general procedure B. **42** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (28.7 mg, 81%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.73 (m, 1H), 7.55 – 7.50 (m, 1H), 7.38 – 7.32 (m, 2H), 3.38 (s, 1H), 1.75 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 170.8, 151.1, 140.6, 125.1, 124.5, 120.1, 110.7, 69.8, 28.6.

Ethyl-(2-hydroxypropan-2-yl)benzo[d]oxazole-6-arboxylate (43)



Follow the general procedure B. **43** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless

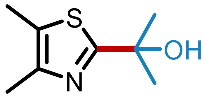
oil (40.4 mg, 81%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.43 – 8.37 (m, 1H), 8.11 – 8.04 (m, 1H), 7.57 – 7.49 (m, 1H), 4.44 – 4.35 (m, 2H), 3.55 (s, 1H), 1.75 (s, 6H), 1.44 – 1.37 (m, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 171.9, 166.0, 153.8, 140.8, 127.5, 127.0, 122.1, 110.4, 69.8, 61.1, 28.5, 14.2.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{13}H_{16}NO_4^+$ 250.1074; Found 250.1075.

2-(4,5-dimethylthiazol-2-yl)propan-2-ol (44)



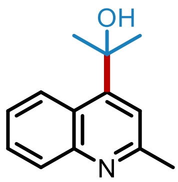
Follow the general procedure B. **44** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (31.5 mg, 92%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 3.33 (s, 1H), 2.29 (d, *J* = 11.5 Hz, 6H), 1.61 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 147.2, 125.9, 72.6, 31.0, 14.5, 11.1.

HRMS (ESI-TOF): m/z: [M + K]$^+$ Calcd for $C_8H_{13}NOSK^+$ 210.0349; Found 210.0360.

2-(2-methylquinolin-4-yl)propan-2-ol (45)



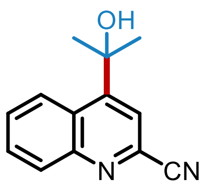
Follow the general procedure B, the isopropanol was mixed with the DMSO for the ratio of 1:1, and the TFA was employed for 0.3 mmol. **45** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product: colorless oil (26.1 mg, 65%).

^{1}H NMR (600 MHz, DMSO-*d*$_6$) δ 8.08 – 8.03 (m, 1H), 7.83 – 7.80 (m, 1H), 7.69 – 7.65 (m, 1H), 7.48 – 7.43 (m, 1H), 6.94 (s, 1H), 4.97 – 4.92 (m, 1H), 2.59 (s, 3H), 1.41 (d, *J* = 6.0 Hz, 6H).

^{13}C NMR (151 MHz, DMSO-*d*$_6$) δ 160.3, 160.1, 130.0, 128.3, 125.0, 122.0, 120.3, 102.7, 70.8, 25.8, 22.0.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{13}H_{16}NO^+$ 202.1226; Found 202.1236.

4-(2-hydroxypropan-2-yl)quinoline-2-carbonitrile (46)



Follow the general procedure B, the isopropanol was mixed with the DMSO for the ratio of 1:1, and the TFA was employed for 0.3 mmol. **46** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product:

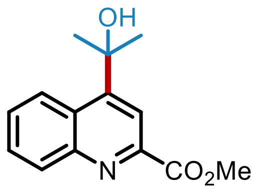
colorless oil (32.6 mg, 77%).

^{1}H NMR (600 MHz, Methanol-d_4) δ 8.28 – 8.24 (m, 1H), 8.02 – 7.97 (m, 1H), 7.86 – 7.82 (m, 1H), 7.69 – 7.66 (m, 1H), 7.39 (s, 1H), 5.07 – 5.01 (m, 1H), 1.51 (d, J = 6.1 Hz, 6H).

^{13}C NMR (151 MHz, Methanol-d_4) δ 162.0, 148.8, 134.4, 131.2, 128.3, 128.0, 122.4, 121.9, 117.2, 104.3, 72.4, 20.4.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{13}H_{13}N_2O^+$ 213.1022; Found 213.1027.

Methyl 4-(2-hydroxypropan-2-yl)quinoline-2-carboxylate (47)



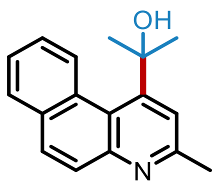
Follow the general procedure B. the isopropanol was mixed with the DMSO for the ratio of 1:1, and the TFA was employed for 0.3 mmol. **47** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product: colorless oil (32.8 mg, 67%).

^{1}H NMR (600 MHz, DMSO-d_6) δ 8.21 – 8.18 (m, 1H), 8.10 – 8.06 (m, 1H), 7.86 – 7.83 (m, 1H), 7.70 – 7.67 (m, 1H), 7.54 (s, 1H), 5.10 – 5.05 (m, 1H), 3.96 (s, 3H), 1.45 (d, J = 6.0 Hz, 6H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 166.1, 161.3, 149.4, 148.5, 131.2, 130.0, 128.1, 122.5, 122.2, 101.7, 71.7, 53.1, 21.9.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{14}H_{16}NO_3^+$ 246.1125; Found 246.1135.

2-(3-methylbenzo[f]quinolin-1-yl)propan-2-ol (48)



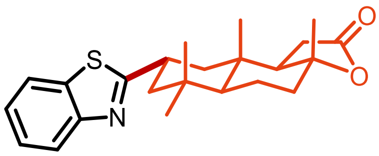
Follow the general procedure B. the isopropanol was mixed with the DMSO for the ratio of 1:1, and the TFA was employed for 0.3 mmol. **48** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product: colorless oil (35.6 mg, 71%).

^{1}H NMR (600 MHz, DMSO-d_6) δ 9.56 – 9.52 (m, 1H), 8.04 – 8.00 (m, 2H), 7.80 – 7.77 (m, 1H), 7.70 – 7.67 (m, 1H), 7.65 – 7.61 (m, 1H), 7.23 (s, 1H), 5.15 – 5.10 (m, 1H), 2.64 (s, 3H), 1.54 (d, J = 6.0 Hz, 6H).

^{13}C NMR (151 MHz, DMSO-d_6) δ 163.1, 159.1, 150.3, 131.8, 131.6, 129.7, 128.9, 128.4, 128.2, 127.5, 126.5, 114.7, 105.6, 71.6, 25.1, 22.3.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{17}H_{18}NO^+$ 252.1383; Found 252.1399.

(3aR,5aS,8S,9aS,9bR)-8-(benzo[d]thiazol-2-yl)-3a,6,6,9a-tetramethyldecahydronaphtho[2,1-b]furan-2(1H)-one (49) [23]

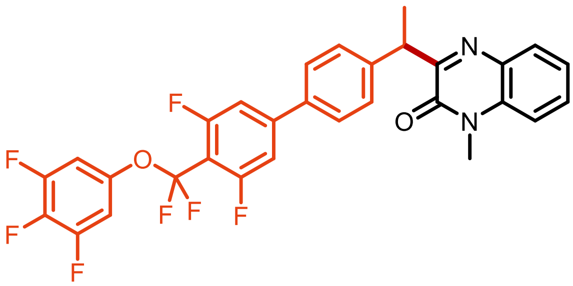


Follow the general procedure A. **49** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (46.0 mg, 60 %).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.00 – 7.96 (m, 1H), 7.88 – 7.85 (m, 1H), 7.49 – 7.44 (m, 1H), 7.39 – 7.34 (m, 1H), 3.61 – 3.54 (m, 1H), 2.45 (dd, *J* = 16.3, 14.7 Hz, 1H), 2.29 (dd, *J* = 16.2, 6.5 Hz, 1H), 2.14 (dt, *J* = 12.0, 3.3 Hz, 1H), 2.08 (dd, *J* = 14.7, 6.5 Hz, 1H), 2.01 – 1.94 (m, 3H), 1.75 (td, *J* = 12.5, 4.2 Hz, 1H), 1.64 (d, *J* = 12.9 Hz, 1H), 1.50 – 1.44 (m, 2H), 1.38 (s, 3H), 1.28 – 1.25 (m, 2H), 1.08 (s, 3H), 1.02 (s, 3H), 1.00 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 176.4, 176.3, 153.0, 134.3, 126.1, 124.8, 122.6, 121.6, 86.0, 58.8, 56.2, 48.6, 46.0, 38.6, 36.9, 35.7, 34.1, 33.0, 28.7, 21.7, 21.4, 20.4, 15.8.

3-(1-(4'-(difluoro(3,4,5-trifluorophenoxy)methyl)-3',5'-difluoro-[1,1'-biphenyl]-4-yl)ethyl)-1-methylquinoxalin-2(1H)-one (50)



Follow the general procedure C. **50** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 10:1 to 5:1, v/v) to give the desired product: light yellow oil (83.5 mg, 73%).

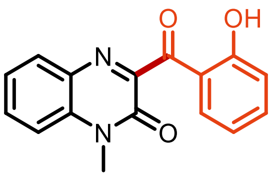
^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.96 – 7.93 (m, 1H), 7.57 – 7.52 (m, 3H), 7.49 – 7.46 (m, 2H), 7.40 – 7.35 (m, 1H), 7.31 – 7.27 (m, 1H), 7.19 – 7.14 (m, 2H), 7.00 – 6.95 (m, 2H), 4.90 – 4.84 (m, 1H), 3.65 (s, 3H), 1.74 – 1.70 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 161.3, 161.1 – 160.9 (m), 159.6 – 159.1 (m), 154.4, 151.8 (dd, *J* = 10.4, 5.4 Hz), 150.2 (dd, *J* = 10.4, 4.8 Hz), 146.9 (t, *J* = 10.3 Hz), 144.8, 135.6, 132.9 (d, *J* = 58.1 Hz), 130.1 (d, *J* = 36.8 Hz), 129.0, 127.0, 123.6, 113.6, 110.8 (dd, *J* = 23.1, 3.5 Hz), 110.77 (q, *J* = 23.1, 3.5 Hz), 41.7, 29.1, 19.6.

^{19}F NMR (565 MHz, Chloroform-*d*) δ -61.65, -110.60, -132.56, -163.28.

HRMS (ESI-TOF): m/z: [M + H]$^+$ Calcd for $C_{30}H_{20}F_7N_2O_2^+$ 573.4108; Found 573.1410.

3-(2-hydroxybenzoyl)-1-methylquinoxalin-2(1H)-one (51)



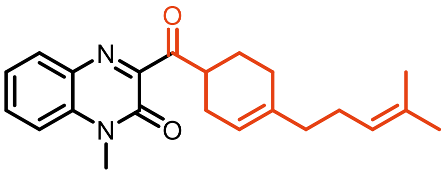
Follow the general procedure C. **51** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 5:1 to 2:1, v/v) to give the desired product: colorless oil (39.2 mg, 70%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 11.68 (s, 1H), 7.96 – 7.93 (m, 1H), 7.73 – 7.69 (m, 1H), 7.57 – 7.52 (m, 1H), 7.52 – 7.48 (m, 1H), 7.46 – 7.41 (m, 2H), 7.09 – 7.06 (m, 1H), 6.89 – 6.84 (m, 1H), 3.78 (s, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 196.5, 163.6, 153.1, 153.0, 137.6, 133.9, 132.7, 132.4, 132.1, 131.1, 124.4, 119.2, 118.6, 118.5, 114.0, 29.2.

HRMS (ESI-TOF): m/z: $[M + Na]^+$ Calcd for $C_{16}H_{12}N_2O_3Na^+$ 303.0740; Found 303.0743.

1-methyl-3-(4-(4-methylpent-3-en-1-yl)cyclohex-3-ene-1-carbonyl)quinoxalin-2(1H)-one (52)

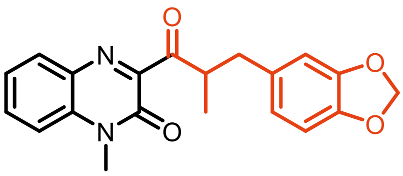


Follow the general procedure D. **52** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product: colorless oil (46.2 mg, 66%).

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.95 – 7.92 (m, 1H), 7.66 (dt, *J* = 8.7, 4.6 Hz, 1H), 7.43 – 7.39 (m, 1H), 7.38 – 7.35 (m, 1H), 5.46 – 5.43 (m, 1H), 5.12 – 5.08 (m, 1H), 3.73 (s, 3H), 3.62 – 3.52 (m, 1H), 2.46 – 2.23 (m, 2H), 2.16 – 2.04 (m, 5H), 2.00 – 1.95 (m, 2H), 1.69 – 1.67 (m, 3H), 1.66 – 1.61 (m, 1H), 1.61 – 1.59 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-*d*) δ 203.64, 153.83, 153.03, 137.51, 136.19, 134.11, 132.24, 132.11, 131.50, 131.24, 124.24, 124.21, 124.11, 120.30, 118.92, 113.86, 44.63, 44.23, 37.78, 37.58, 29.43, 29.01, 27.86, 26.58, 26.43, 25.72, 24.76, 24.52, 24.25, 17.71.

3-(3-(benzo[d][1,3]dioxol-5-yl)-2-methylpropanoyl)-1-methylquinoxalin-2(1H)-one (53)

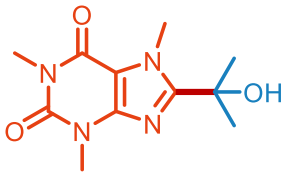


Follow the general procedure D. **53** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 1:1, v/v) to give the desired product: colorless oil (51.1 mg, 73%).

^{1}H NMR (600 MHz, Chloroform-d) δ 7.93 – 7.90 (m, 1H), 7.68 – 7.64 (m, 1H), 7.42 – 7.38 (m, 1H), 7.35 – 7.32 (m, 1H), 6.72 (s, 1H), 6.66 (s, 2H), 5.88 – 5.80 (m, 2H), 3.90 – 3.83 (m, 1H), 3.70 (s, 3H), 3.12 – 3.07 (m, 1H), 2.67 – 2.62 (m, 1H), 1.23 – 1.17 (m, 3H).

^{13}C NMR (151 MHz, Chloroform-d) δ 203.29, 152.97, 152.90, 147.45, 145.82, 134.21, 133.23, 132.37, 132.00, 131.31, 124.05, 122.24, 113.78, 109.58, 107.94, 100.73, 45.31, 38.25, 28.98, 15.22.

8-(2-hydroxypropan-2-yl)-1,3,7-trimethyl-3,7-dihydro-1H-purine-2,6-dione (54)[24]

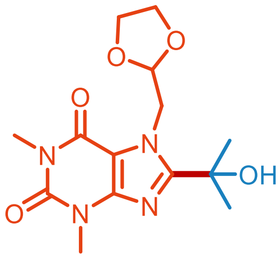


Follow the general procedure B. **54** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 10:1 to 1:2, v/v) to give the desired product: colorless oil (35.8 mg, 71%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.16 (s, 3H), 3.51 (s, 3H), 3.37 (s, 3H), 2.97 (s, 1H), 1.69 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 156.9, 155.5, 151.7, 146.7, 108.5, 70.8, 33.9, 29.5, 29.4, 27.8.

7-((1,3-dioxolan-2-yl)methyl)-8-(2-hydroxypropan-2-yl)-1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione (55)



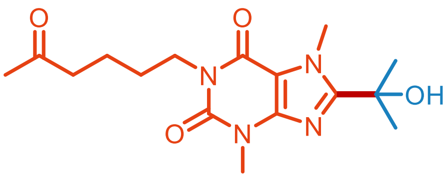
Follow the general procedure B. **55** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 10:1 to 1:2, v/v) to give the desired product: colorless oil (51.7 mg, 80%).

^{1}H NMR (400 MHz, Chloroform-*d*) δ 5.29 – 5.24 (m, 1H), 5.09 – 5.03 (m, 2H), 3.91 (t, *J* = 1.0 Hz, 4H), 3.56 (s, 3H), 3.40 (s, 3H), 1.67 (s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 208.4, 157.0, 155.3, 151.4, 146.8, 108.5, 70.8, 43.1, 40.7, 33.9, 33.8, 29.7, 29.4, 27.5, 21.0.

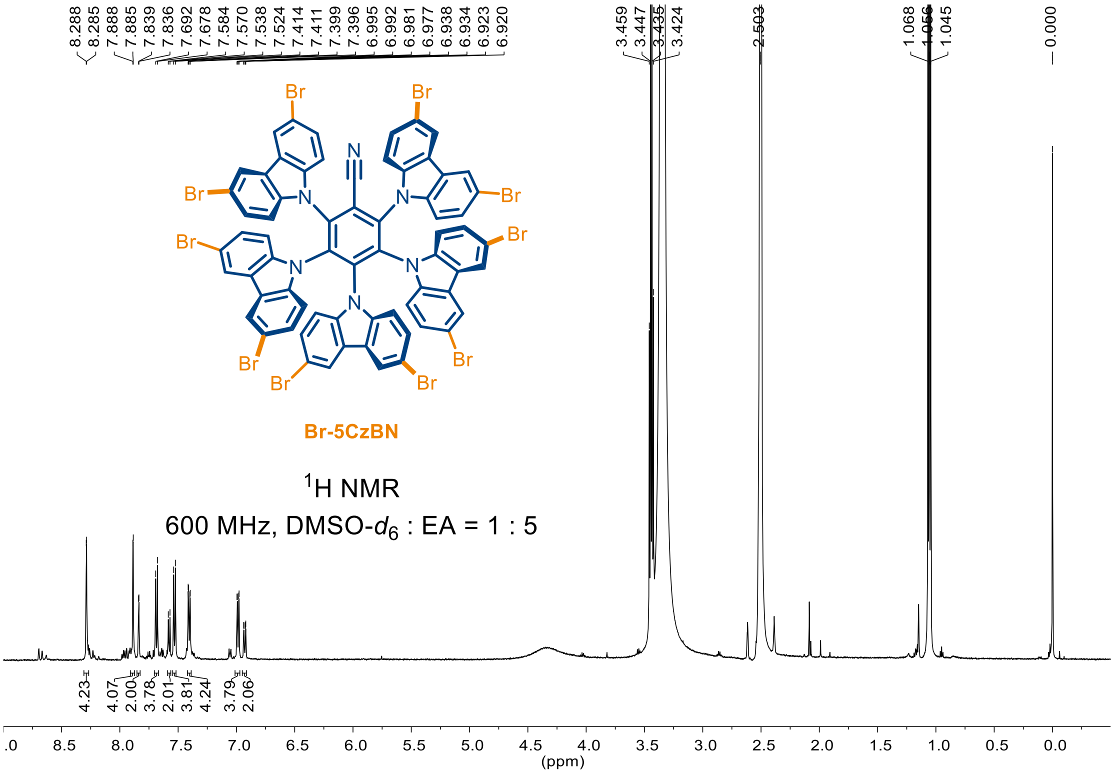
HRMS (ESI-TOF): m/z: $[M + K]^+$ Calcd for $C_{14}H_{20}N_4O_5K^+$ 363.1065; Found 363.1067.

8-(2-hydroxypropan-2-yl)-3,7-dimethyl-1-(5-oxohexyl)-3,7-dihydro-1H-purine-2,6-dione (56)[24]

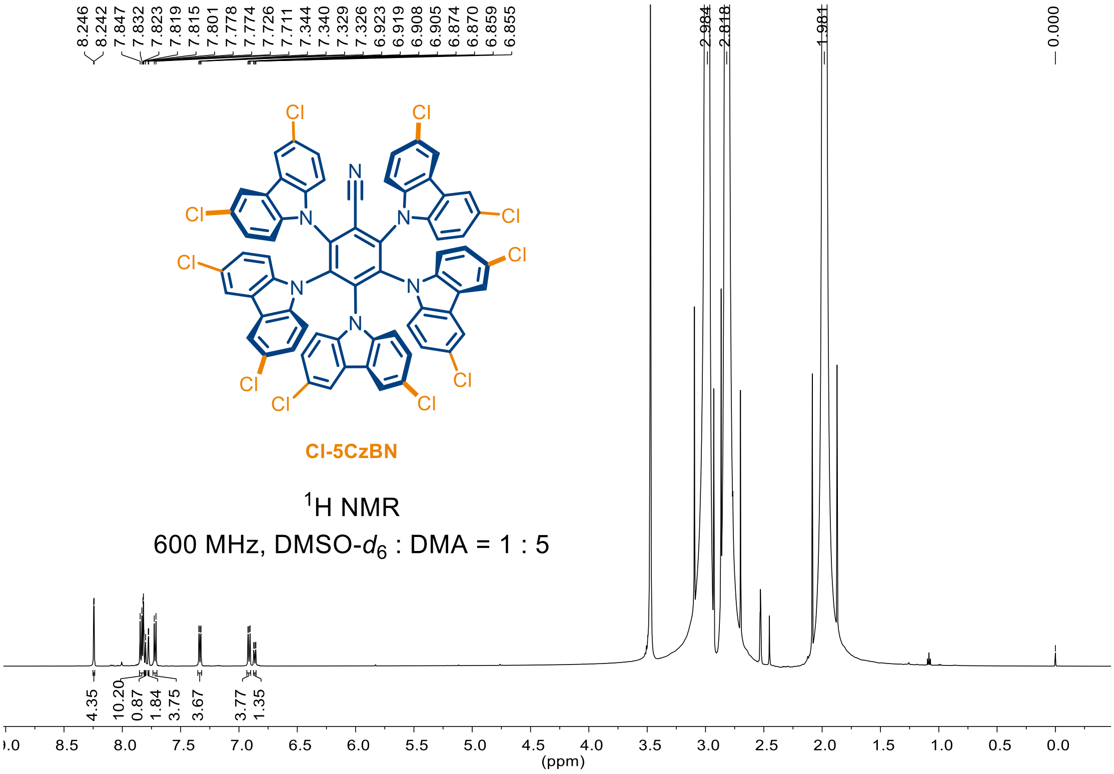


Follow the general procedure B. **56** was purified by flash chromatography (silica gel, petroleum ether/ethyl acetate from 20:1 to 5:1, v/v) to give the desired product: colorless oil (51.8 mg, 77%).

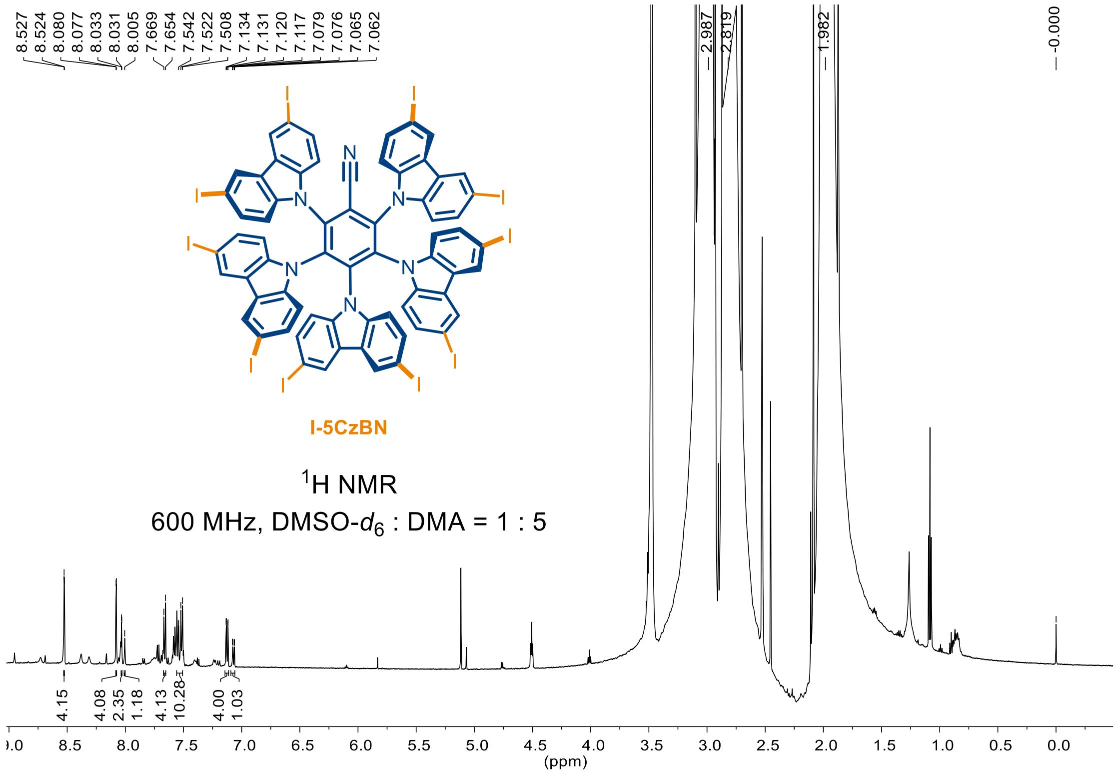
^{1}H NMR (400 MHz, Chloroform-*d*) δ 4.13 (s, 3H), 3.99 – 3.92 (m, 2H), 3.48 (s, 3H), 3.13 (s, 1H), 2.46 (t, *J* = 6.9 Hz, 2H), 2.11 (s, 3H), 1.66 (s, 6H), 1.64 – 1.57 (m, 4H).
^{13}C NMR (101 MHz, Chloroform-*d*) δ 158.3, 155.3, 151.7, 147.4, 107.7, 102.0, 72.4, 65.1, 47.9, 31.1, 29.5, 27.8.



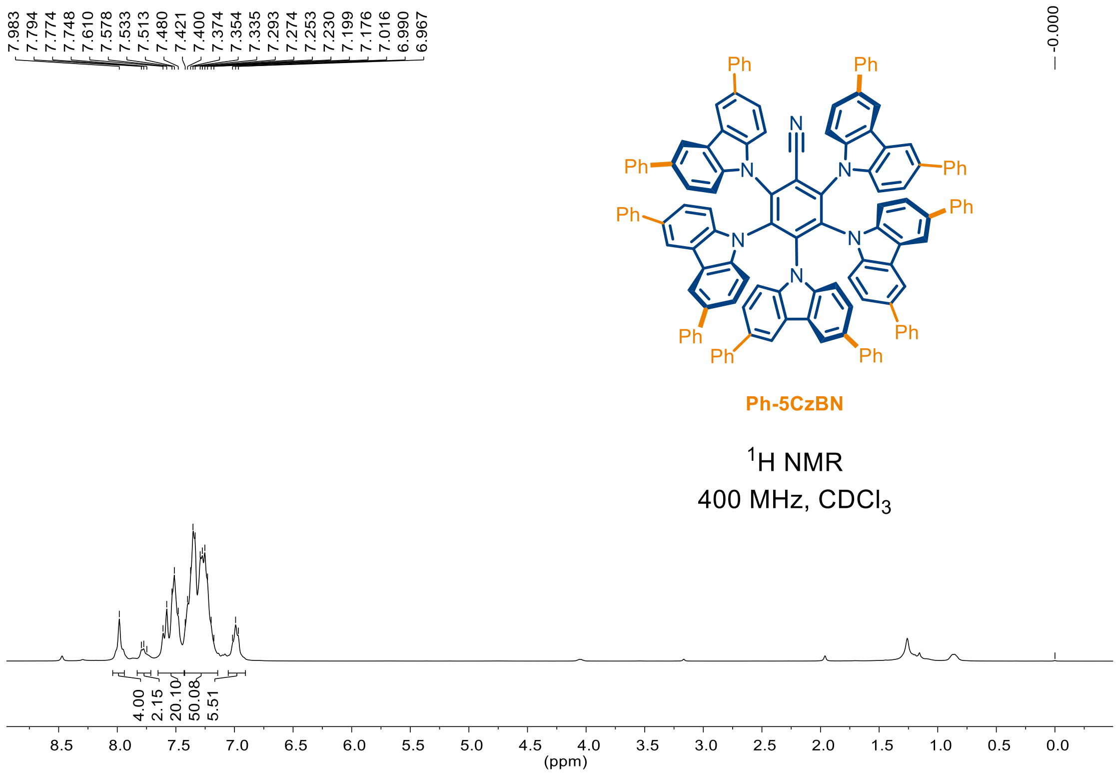
Br-5CzBN
^{1}H NMR
600 MHz, DMSO-d_6 : EA = 1 : 5
(ppm)

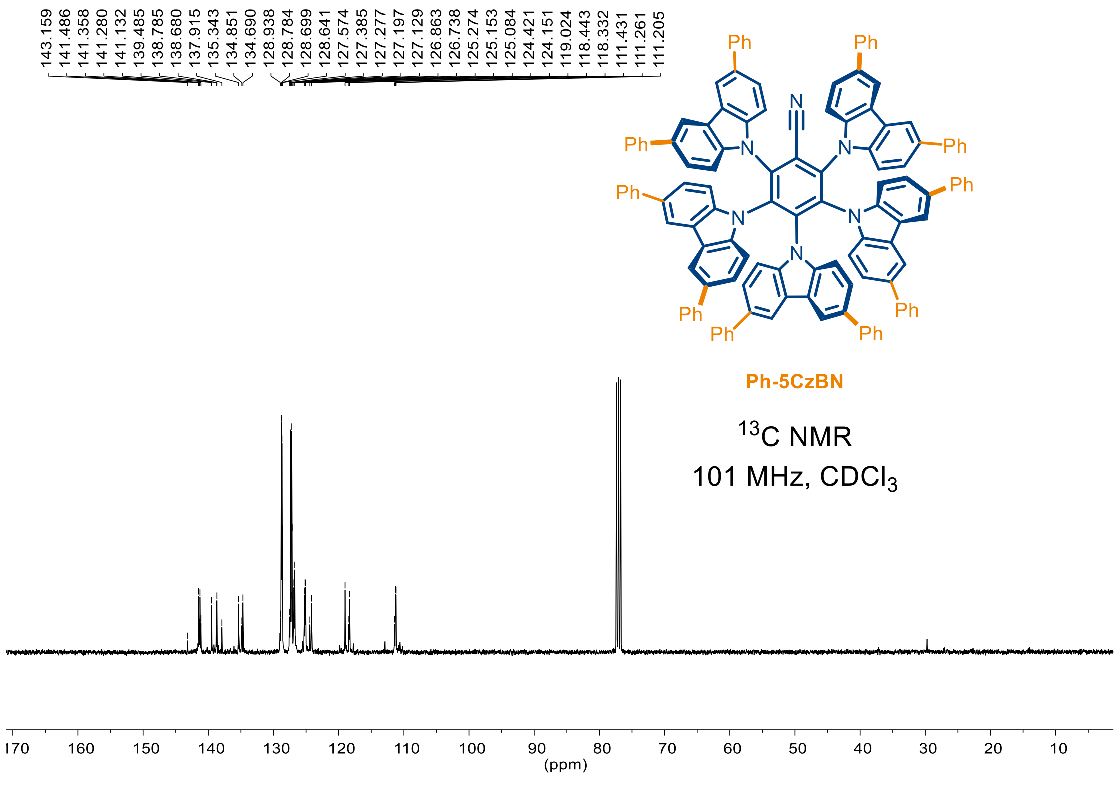


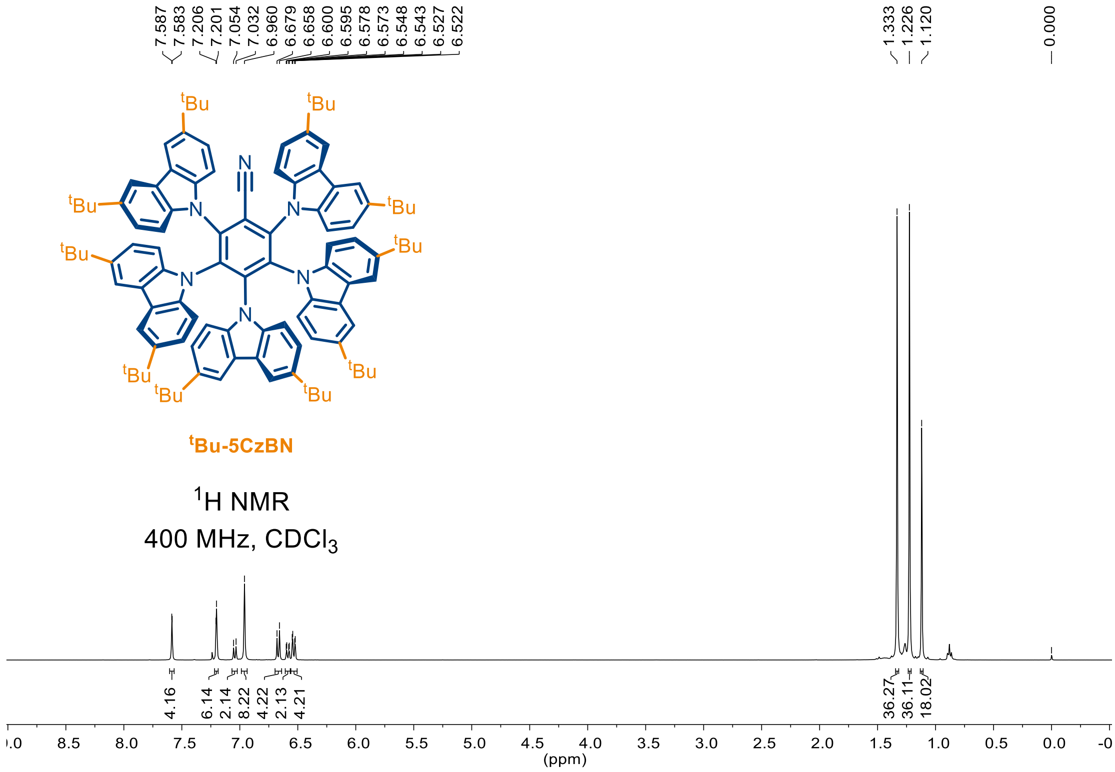
Cl-5CzBN
^{1}H NMR
600 MHz, DMSO-d_6 : DMA = 1 : 5
(ppm)

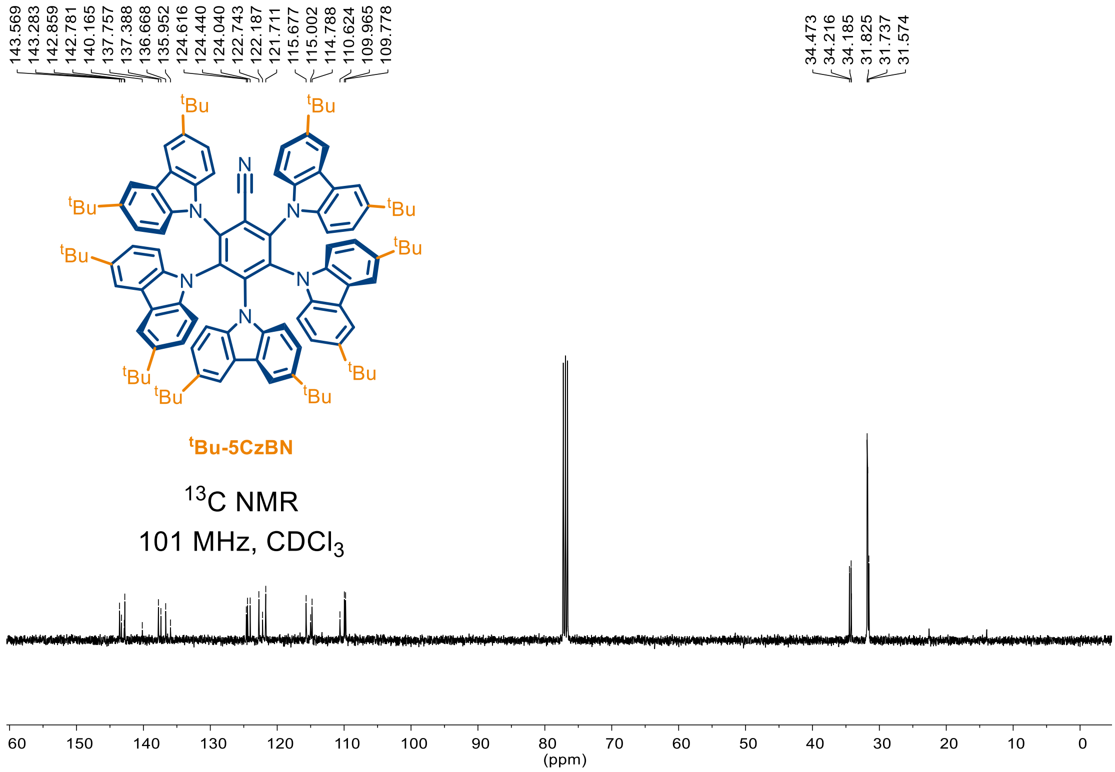


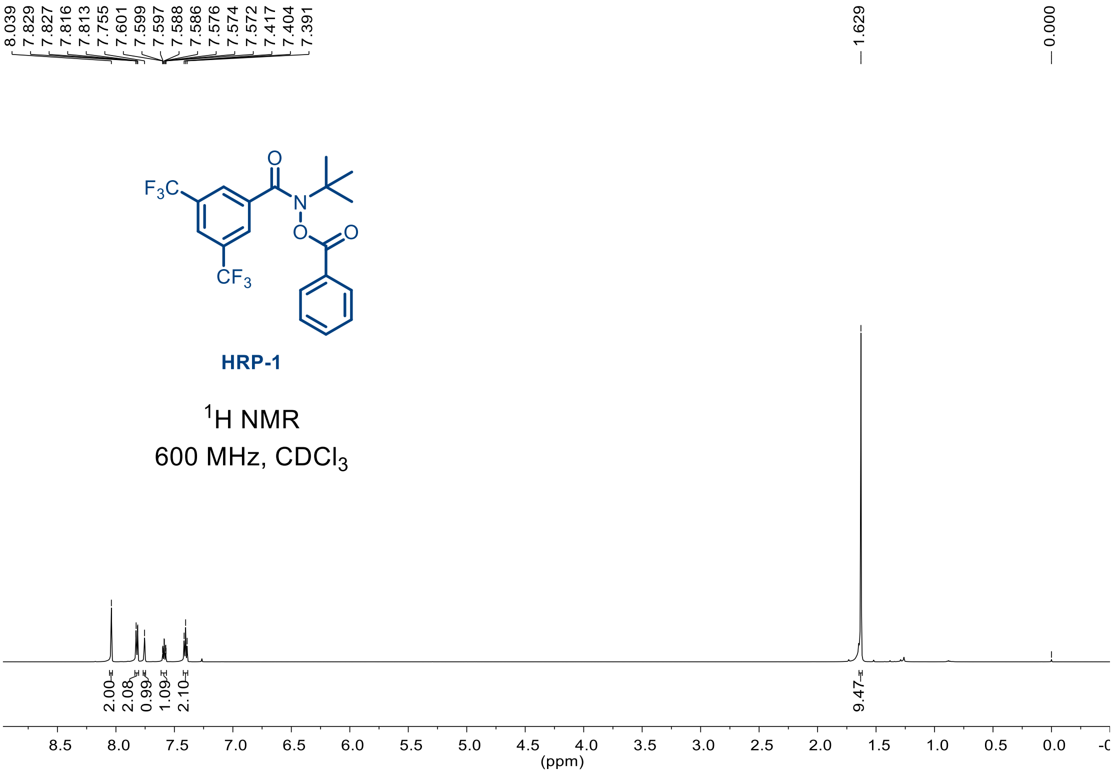
8.527
8.524
8.080
8.077
8.033
8.031
8.005
7.669
7.654
7.542
7.522
7.508
7.134
7.131
7.120
7.117
7.079
7.076
7.065
7.062
2.987
2.819
1.982
-0.000
I-5CzBN
^{1}H NMR
600 MHz, DMSO-d_6 : DMA = 1 : 5
4.15
4.08
2.35
1.18
4.13
10.28
4.00
1.03
(ppm)

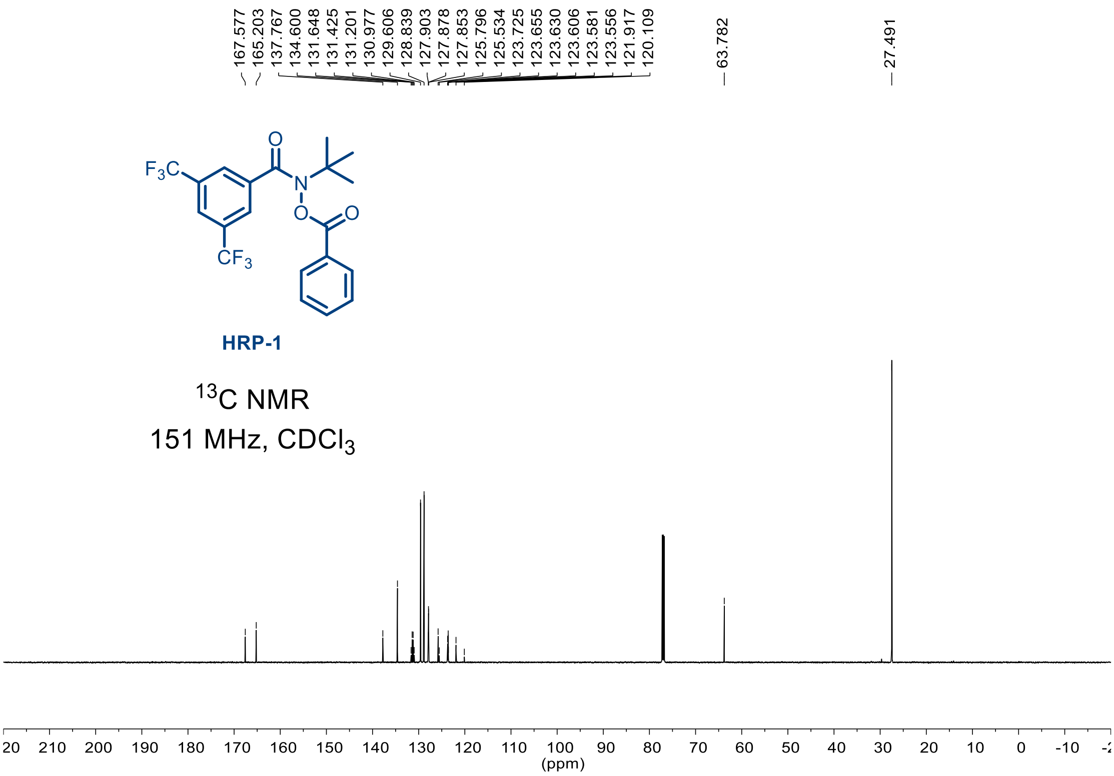

7.983 7.794 7.774 7.748 7.610 7.578 7.533 7.513 7.480 7.421 7.400 7.374 7.354 7.335 7.293 7.274 7.253 7.230 7.199 7.176 7.016 6.990 6.967
-0.000
Ph
N
N
Ph-5CzBN
^{1}H NMR
400 MHz, $CDCl_3$
4.00
2.15
20.10
50.08
5.51
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

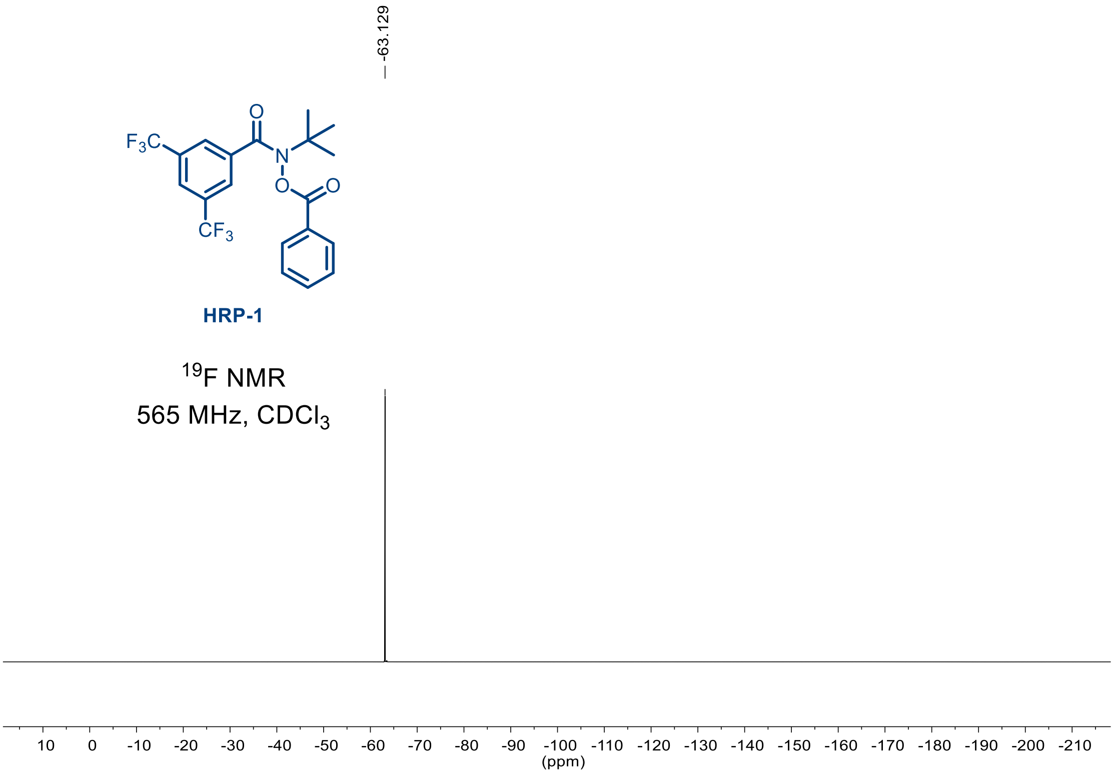

143.159 141.486 141.358 141.280 141.132 139.485 138.785 138.680 137.915 135.343 134.851 134.690 128.938 128.784 128.699 128.641 127.574 127.385 127.277 127.197 127.129 126.863 126.738 125.274 125.153 125.084 124.421 124.151 119.024 118.443 118.332 111.431 111.261 111.205
Ph
N
N
Ph-5CzBN
^{13}C NMR
101 MHz, $CDCl_3$
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
(ppm)

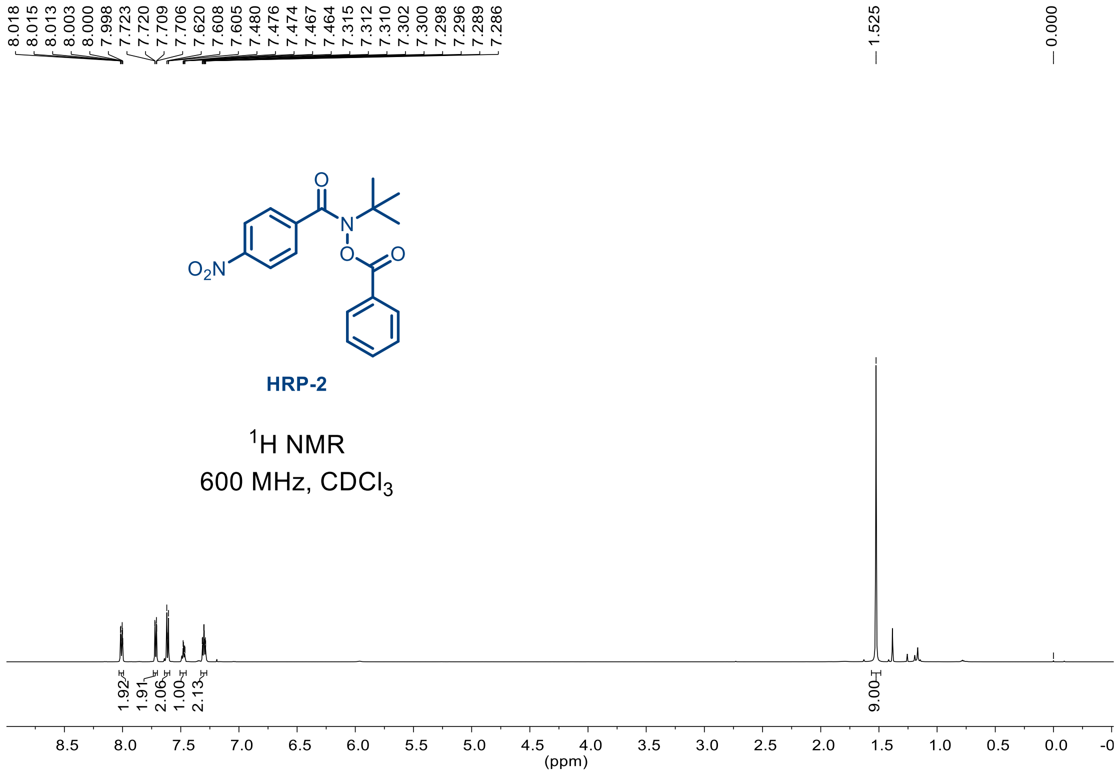

7.587
7.583
7.206
7.201
7.054
7.032
6.960
6.679
6.658
6.600
6.595
6.578
6.573
6.548
6.543
6.527
6.522
1.333
1.226
1.120
0.000
tBu-5CzBN
1H NMR
400 MHz, CDCl3
4.16
6.14
2.14
8.22
4.22
2.13
4.21
36.27
36.11
18.02
(ppm)


143.569
143.283
142.859
142.781
140.165
137.757
137.388
136.668
135.952
124.616
124.440
124.040
122.743
122.187
121.711
115.677
115.002
114.788
110.624
109.965
109.778
34.473
34.216
34.185
31.825
31.737
31.574
tBu-5CzBN
13C NMR
101 MHz, CDCl3
(ppm)


8.039
7.829
7.827
7.816
7.813
7.755
7.601
7.599
7.597
7.588
7.586
7.576
7.574
7.572
7.417
7.404
7.391
1.629
0.000
F3C
O
N
O
O
CF3
HRP-1
1H NMR
600 MHz, CDCl3
2.00
2.08
0.99
1.09
2.10
9.47
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

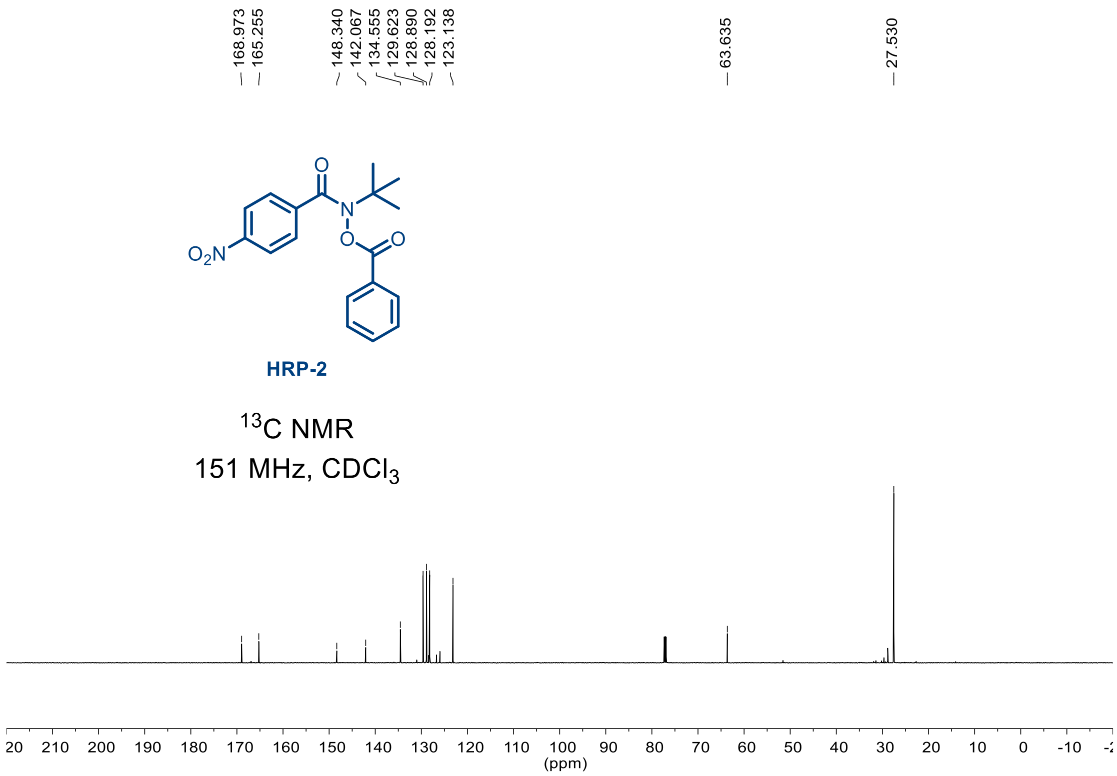

167.577
165.203
137.767
134.600
131.648
131.425
131.201
130.977
129.606
128.839
127.903
127.878
127.853
125.796
125.534
123.725
123.655
123.630
123.606
123.581
123.556
121.917
120.109
63.782
27.491
F3C
O
N
O
O
CF3
HRP-1
13C NMR
151 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


-63.129
HRP-1
19F NMR
565 MHz, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)



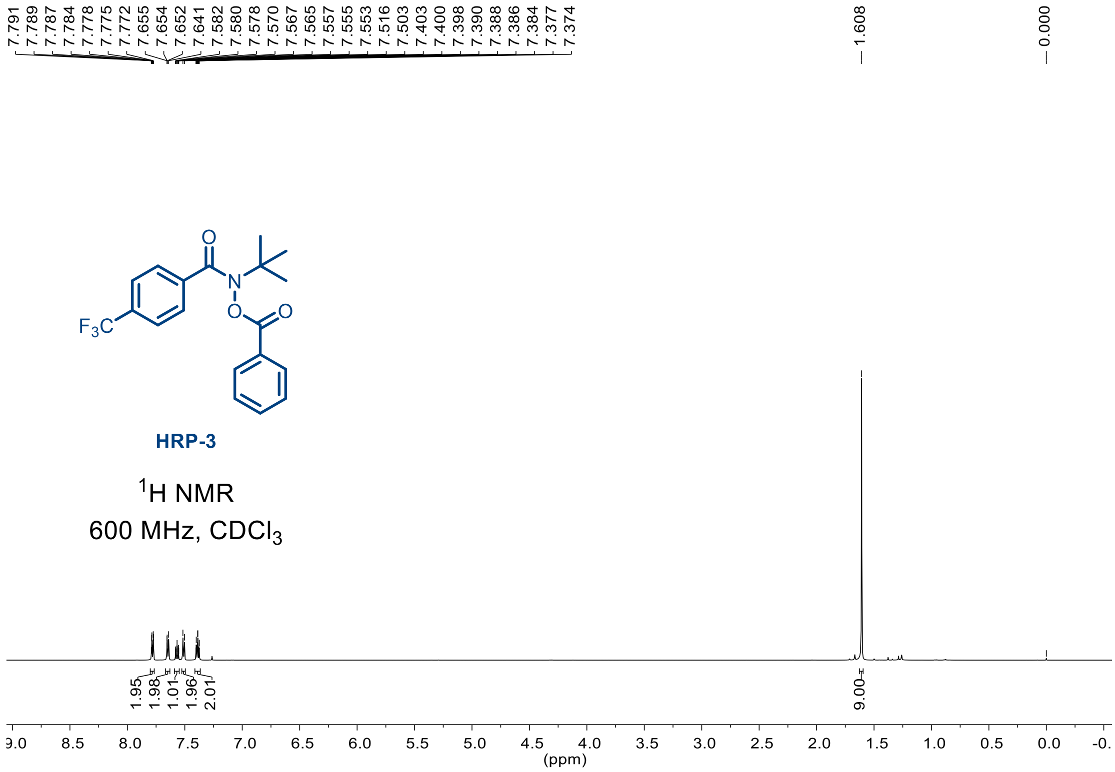
HRP-2

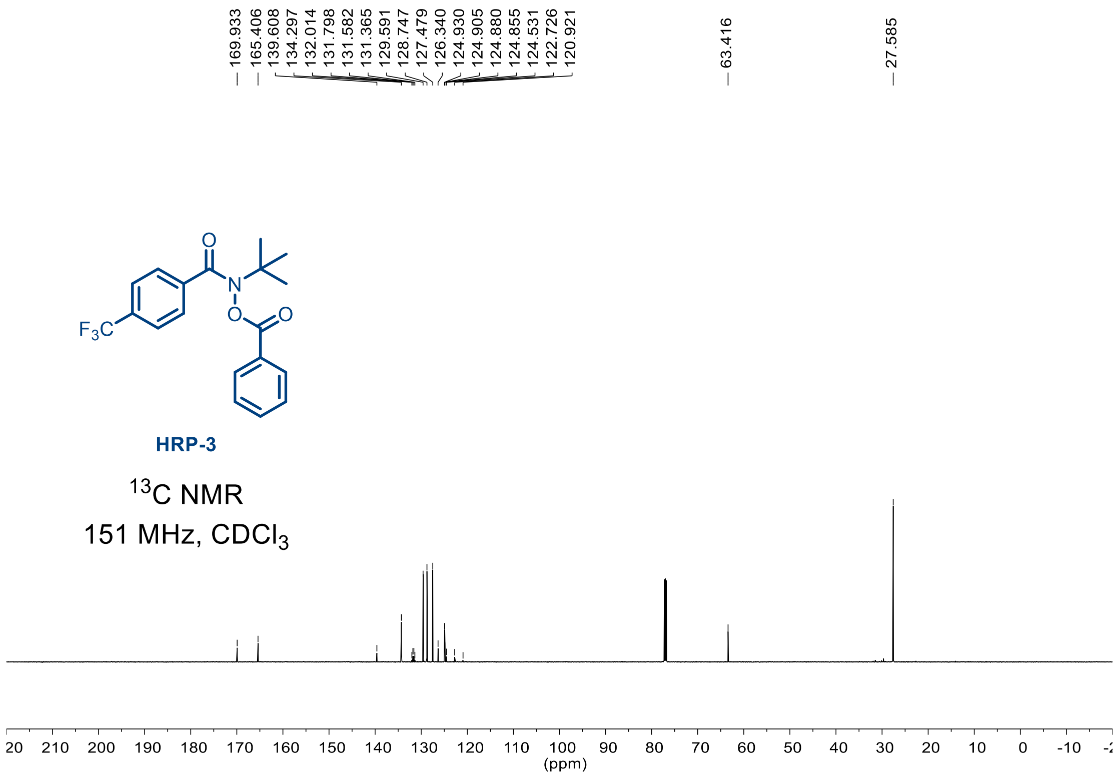
^{1}H NMR
600 MHz, $CDCl_3$

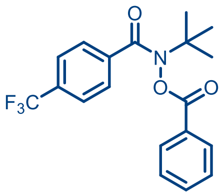


HRP-2

^{13}C NMR
151 MHz, $CDCl_3$

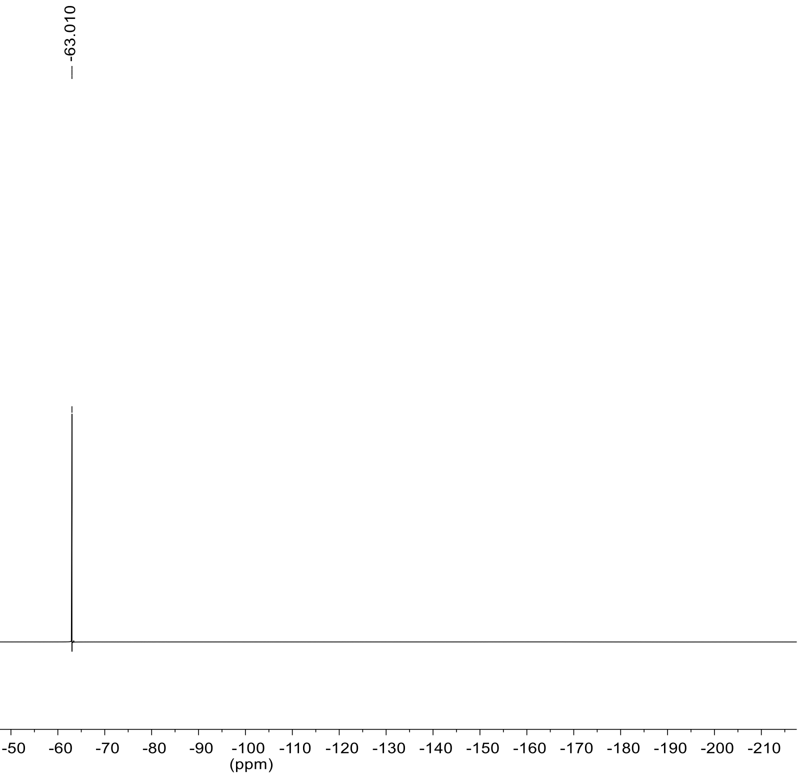

7.791
7.789
7.787
7.784
7.778
7.775
7.772
7.655
7.654
7.652
7.641
7.582
7.580
7.578
7.570
7.567
7.565
7.557
7.555
7.553
7.516
7.503
7.403
7.400
7.398
7.390
7.388
7.386
7.384
7.377
7.374
1.608
0.000
HRP-3
1H NMR
600 MHz, CDCl3
1.95
1.98
1.01
1.96
2.01
9.00
(ppm)

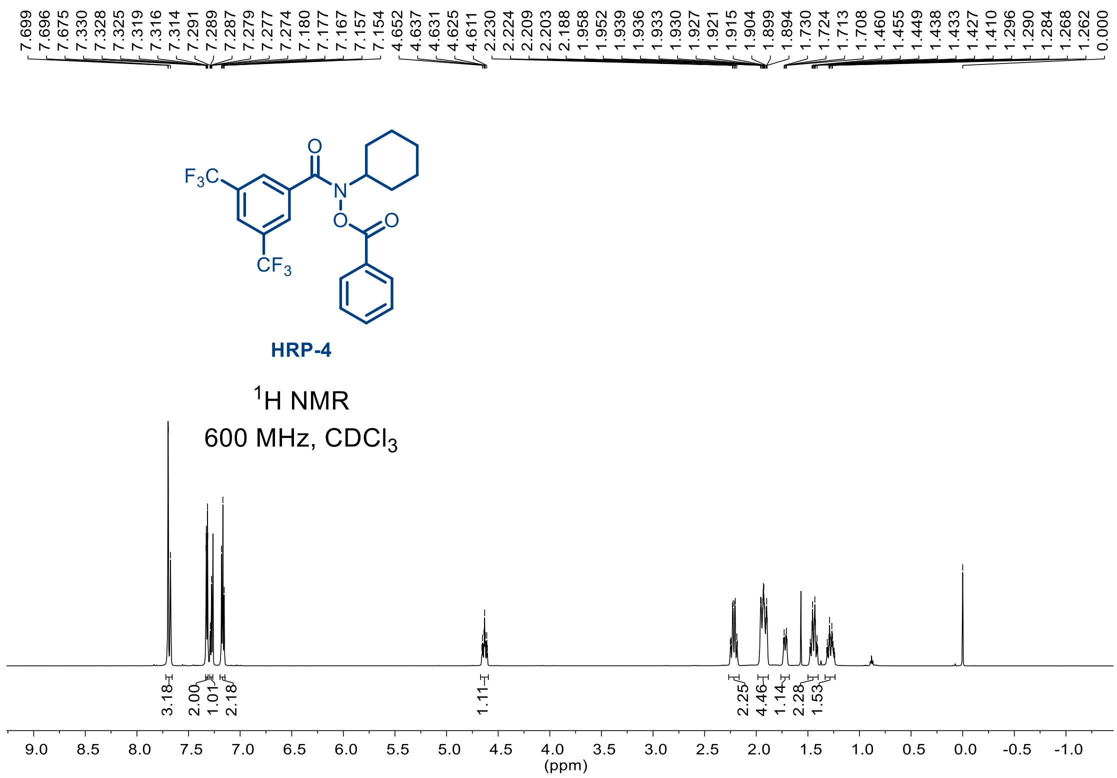

169.933
165.406
139.608
134.297
132.014
131.798
131.582
131.365
129.591
128.747
127.479
126.340
124.930
124.905
124.880
124.855
124.531
122.726
120.921
63.416
27.585
HRP-3
13C NMR
151 MHz, CDCl3
(ppm)

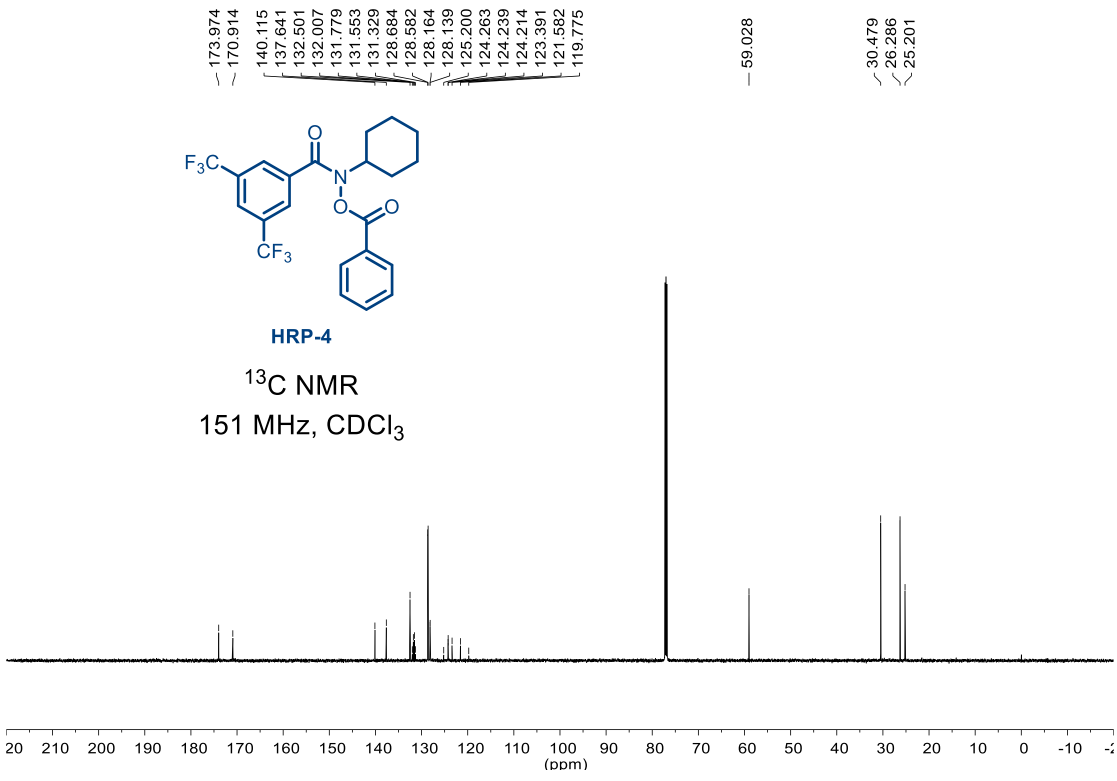


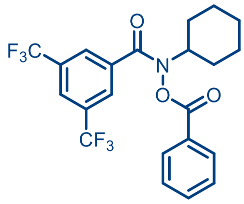
HRP-3

^{19}F NMR
565 MHz, $CDCl_3$



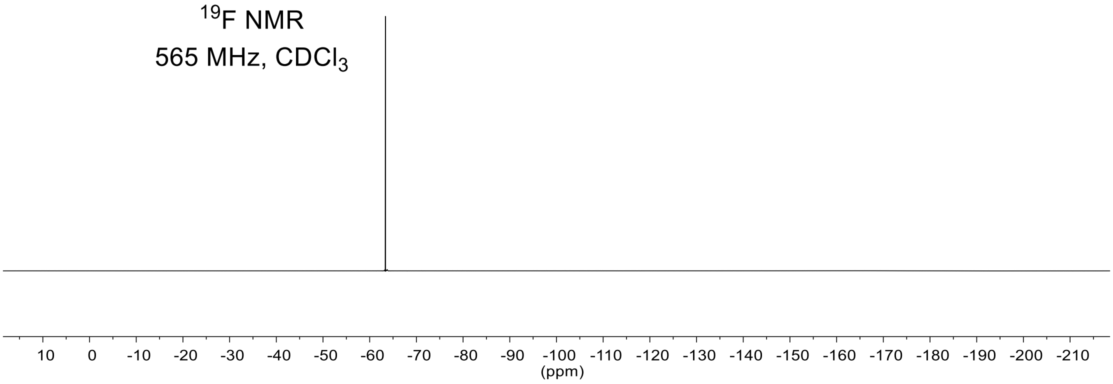

HRP-4
^{1}H NMR
600 MHz, $CDCl_3$

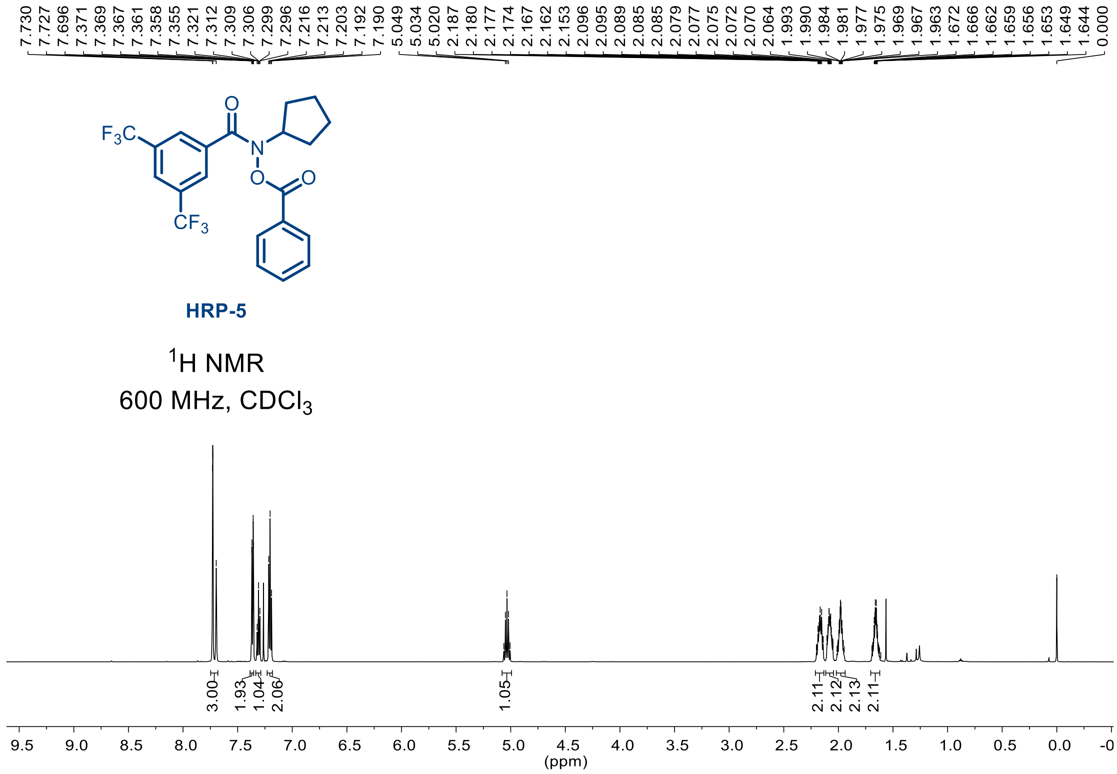

HRP-4
^{13}C NMR
151 MHz, $CDCl_3$

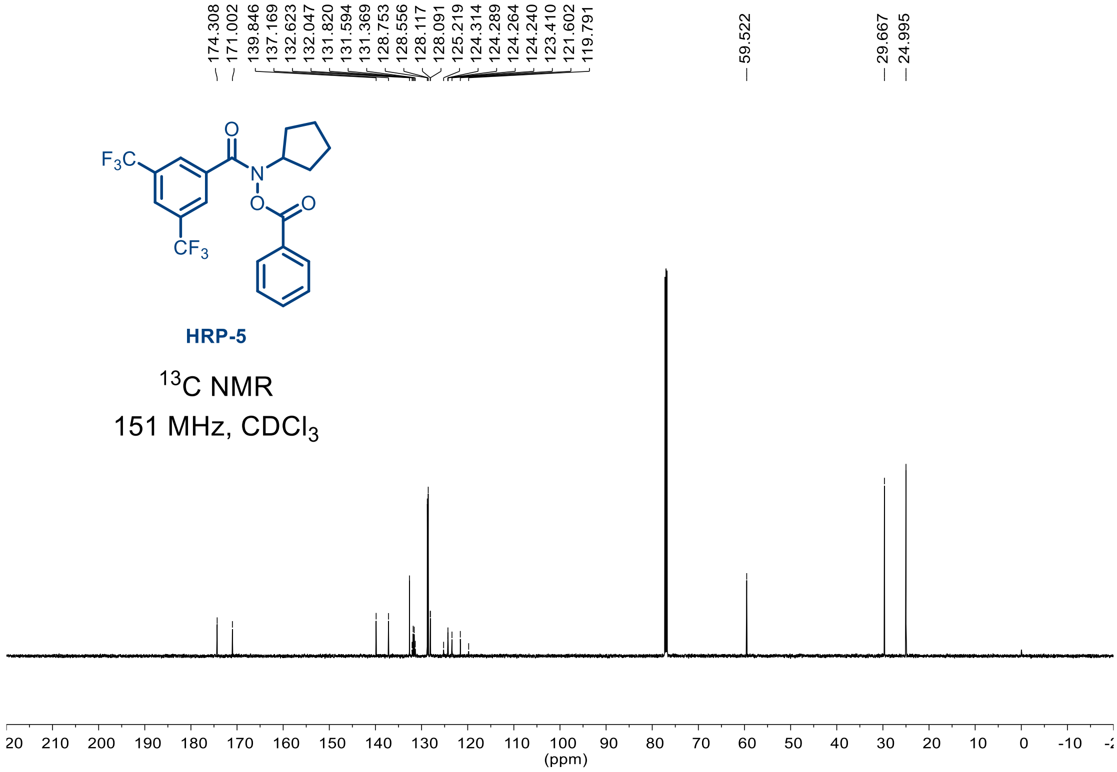


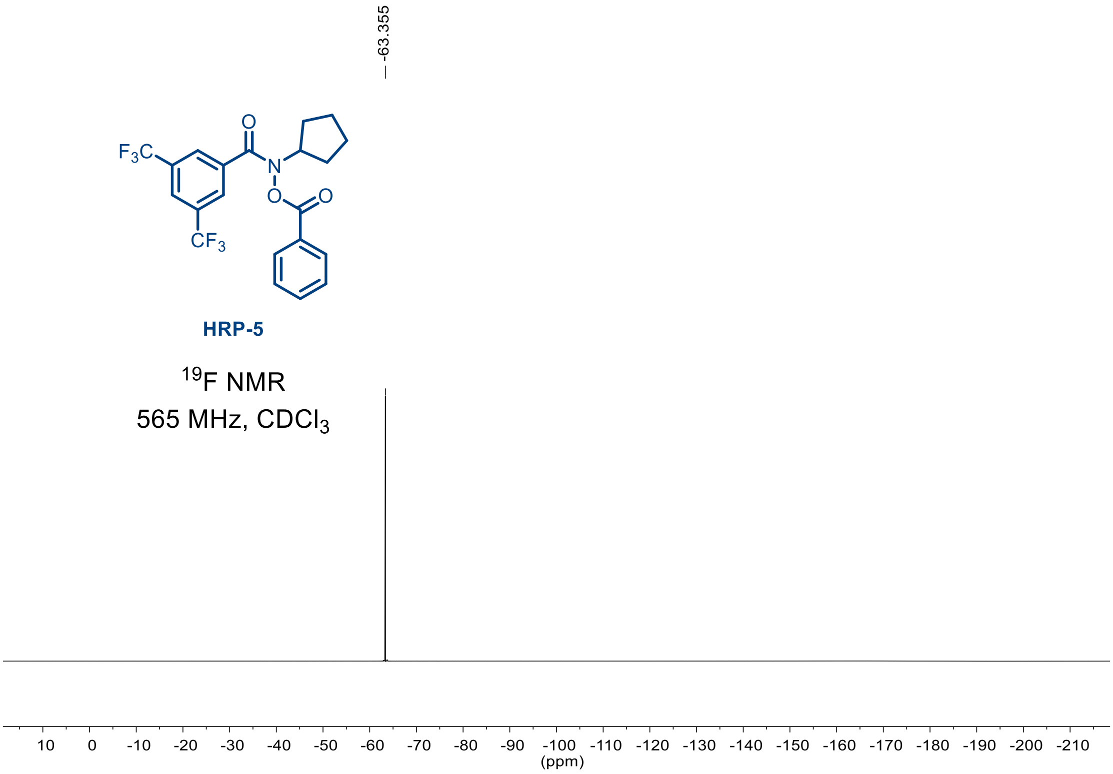
HRP-4

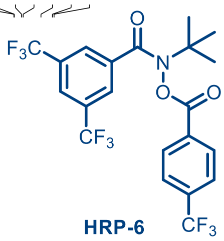
^{19}F NMR
565 MHz, $CDCl_3$




7.730 7.727 7.696 7.371 7.369 7.367 7.361 7.358 7.355 7.321 7.312 7.309 7.306 7.299 7.296 7.216 7.213 7.203 7.192 7.190 5.049 5.034 5.020 2.187 2.180 2.177 2.174 2.167 2.162 2.153 2.096 2.095 2.089 2.085 2.079 2.077 2.075 2.072 2.070 2.064 1.993 1.990 1.984 1.981 1.977 1.975 1.969 1.967 1.963 1.672 1.666 1.662 1.659 1.656 1.653 1.649 1.644 0.000
HRP-5
1H NMR
600 MHz, CDCl3
3.00 1.93 1.04 2.06 1.05 2.11 2.12 2.13 2.11
(ppm)

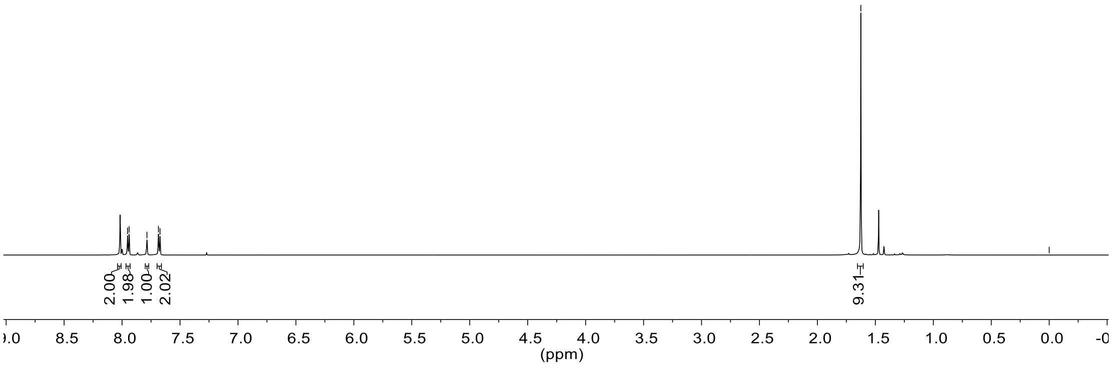

174.308 171.002 139.846 137.169 132.623 132.047 131.820 131.594 131.369 128.753 128.556 128.117 128.091 125.219 124.314 124.289 124.264 124.240 123.410 121.602 119.791 59.522 29.667 24.995
HRP-5
13C NMR
151 MHz, CDCl3
(ppm)

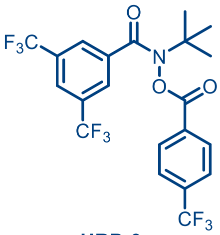

-63.355
F3C
O
N
O
O
CF3
HRP-5
19F NMR
565 MHz, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
(ppm)



HRP-6

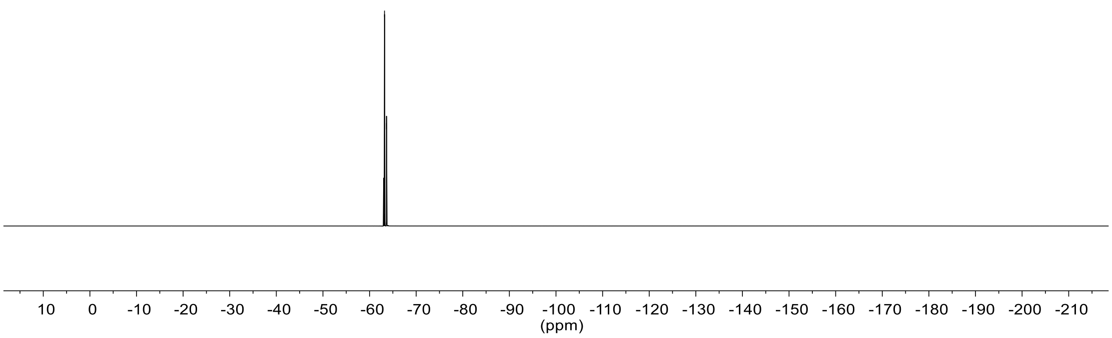
^{1}H NMR
600 MHz, $CDCl_3$

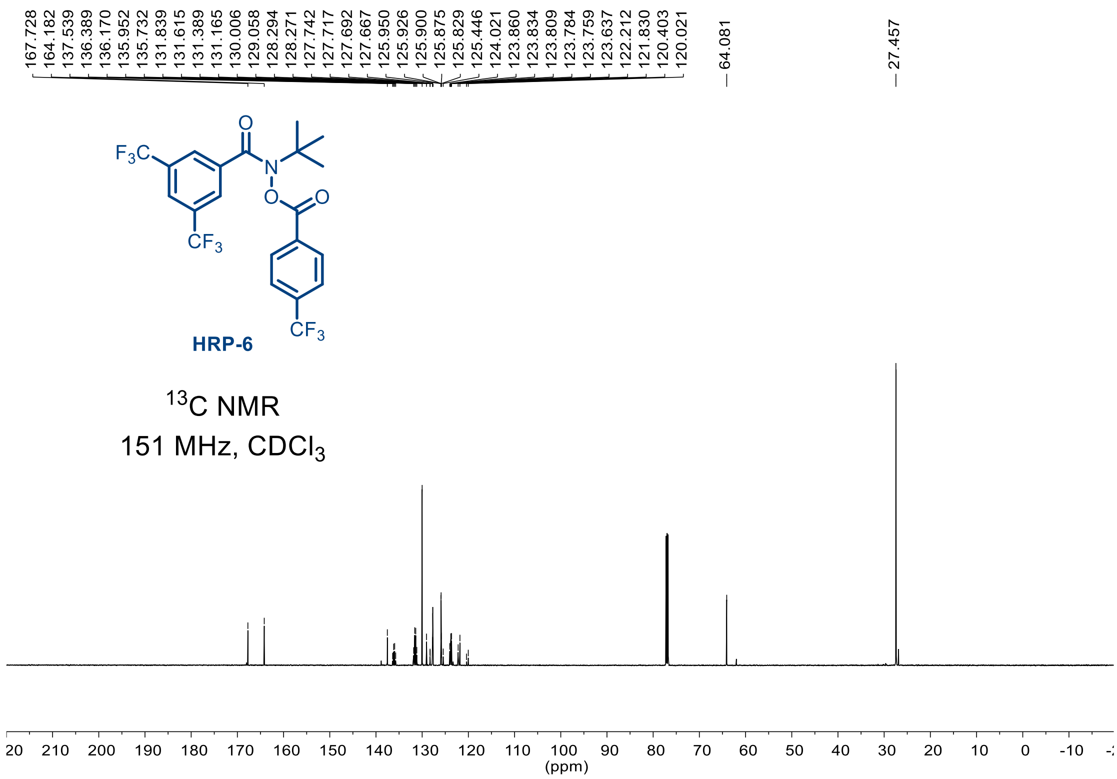




HRP-6

^{19}F NMR
565 MHz, $CDCl_3$




167.728
164.182
137.539
136.389
136.170
135.952
135.732
131.839
131.615
131.389
131.165
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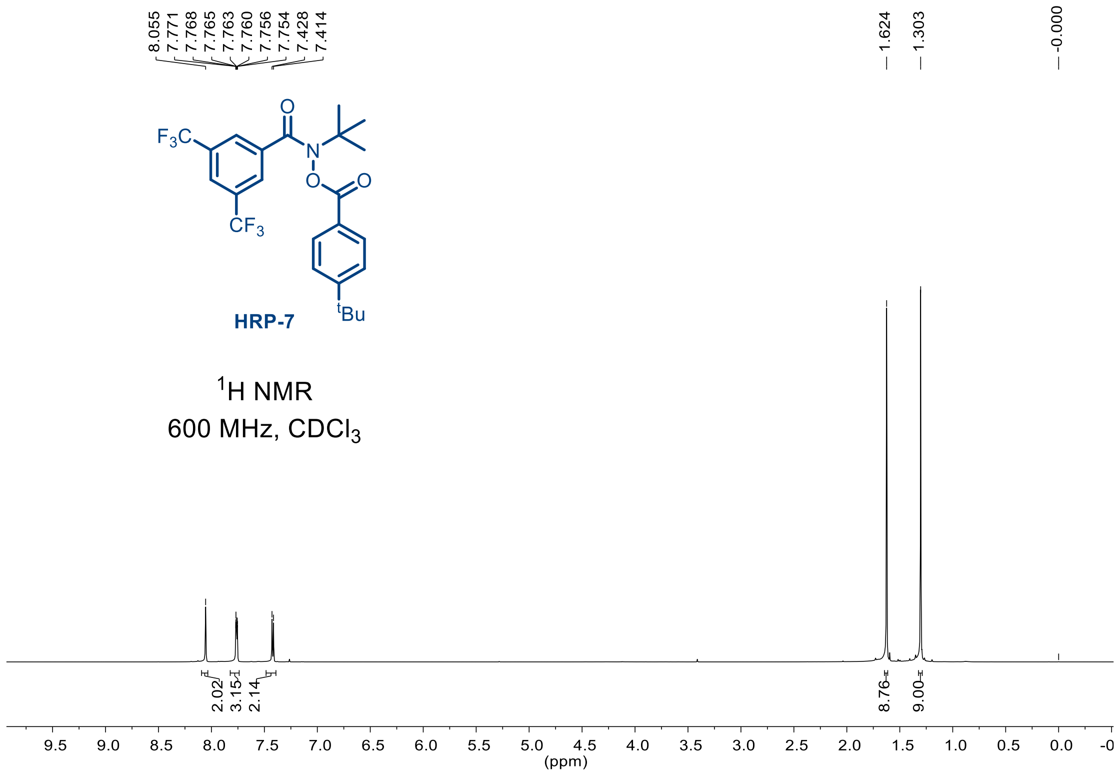
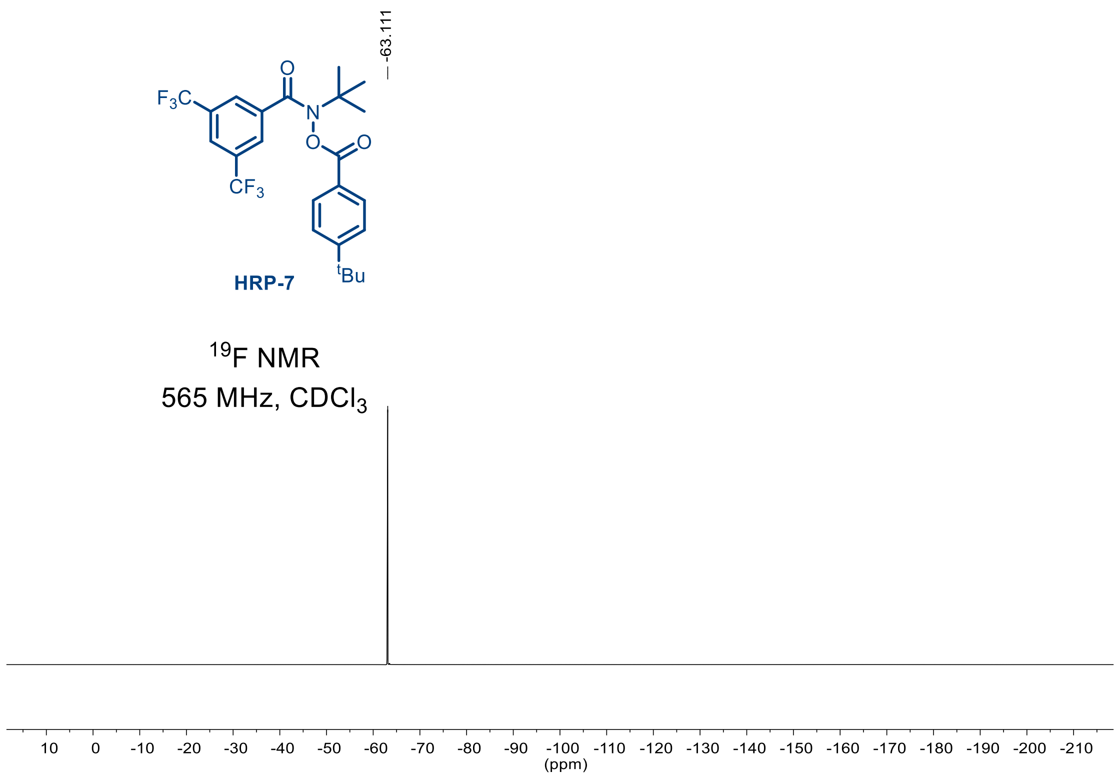
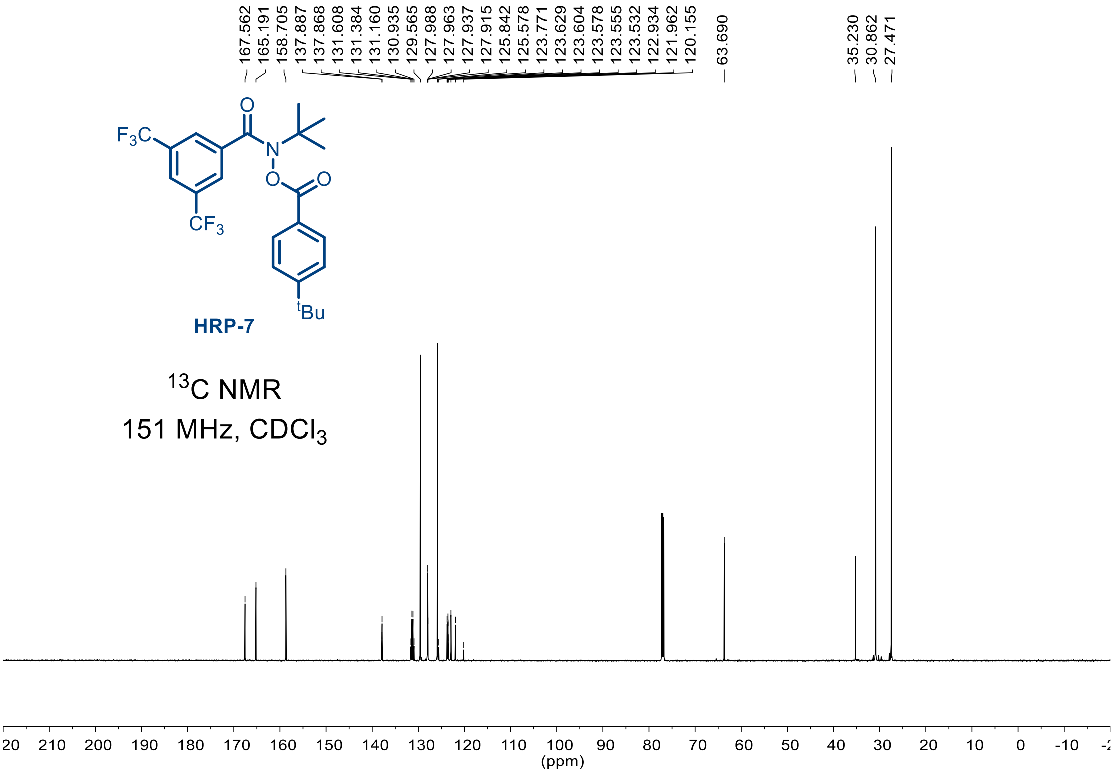
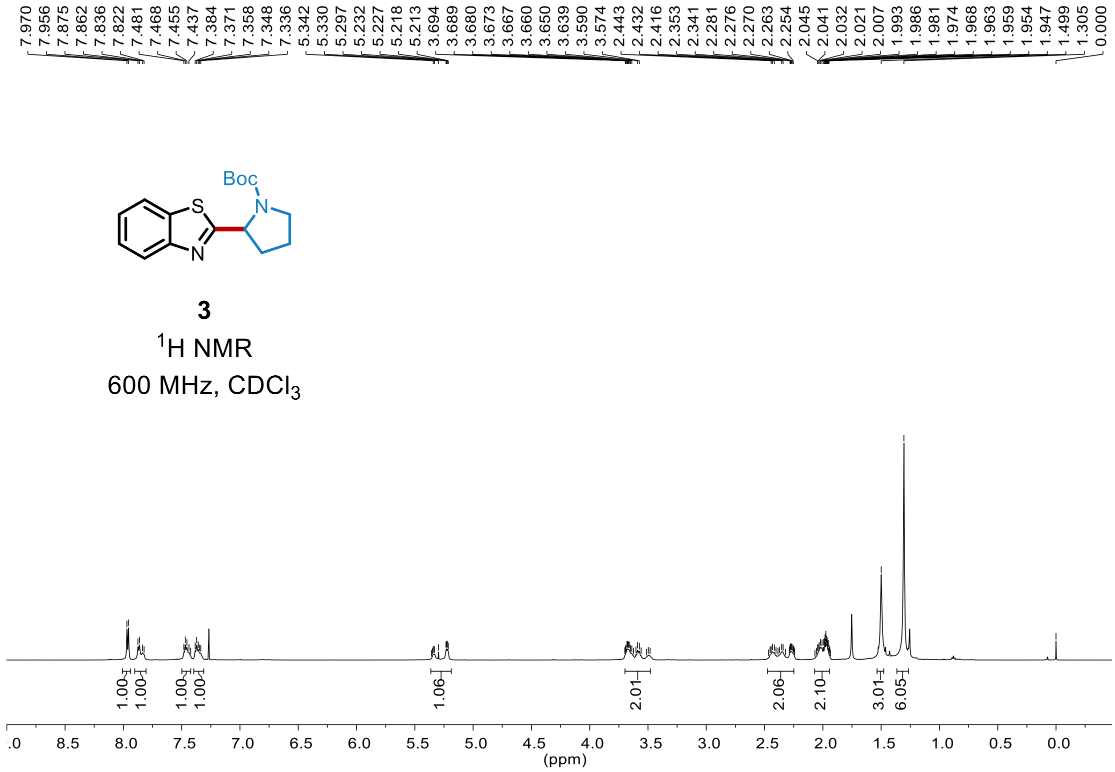
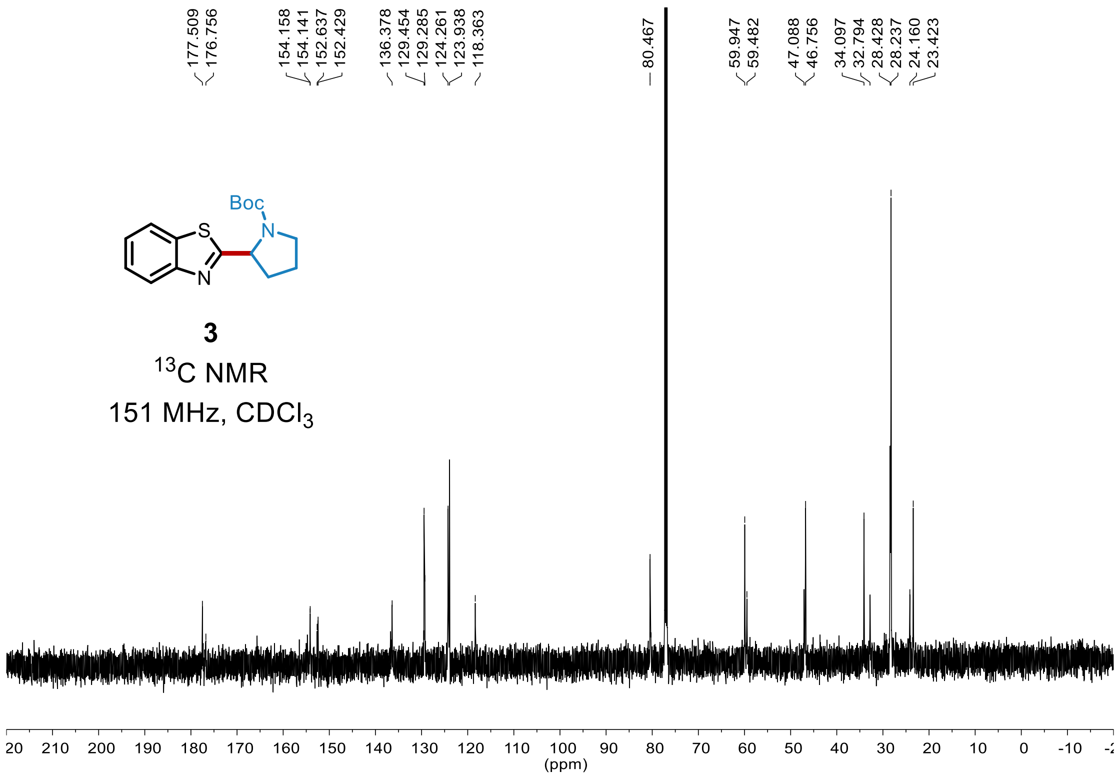
129.058
128.294
128.271
127.742
127.717
127.692
127.667
125.950
125.926
125.900
125.875
125.829
125.446
124.021
123.860
123.834
123.809
123.784
123.759
123.637
122.212
121.830
120.403
120.021
64.081
27.457
HRP-6
13C NMR
151 MHz, CDCl3
(ppm)

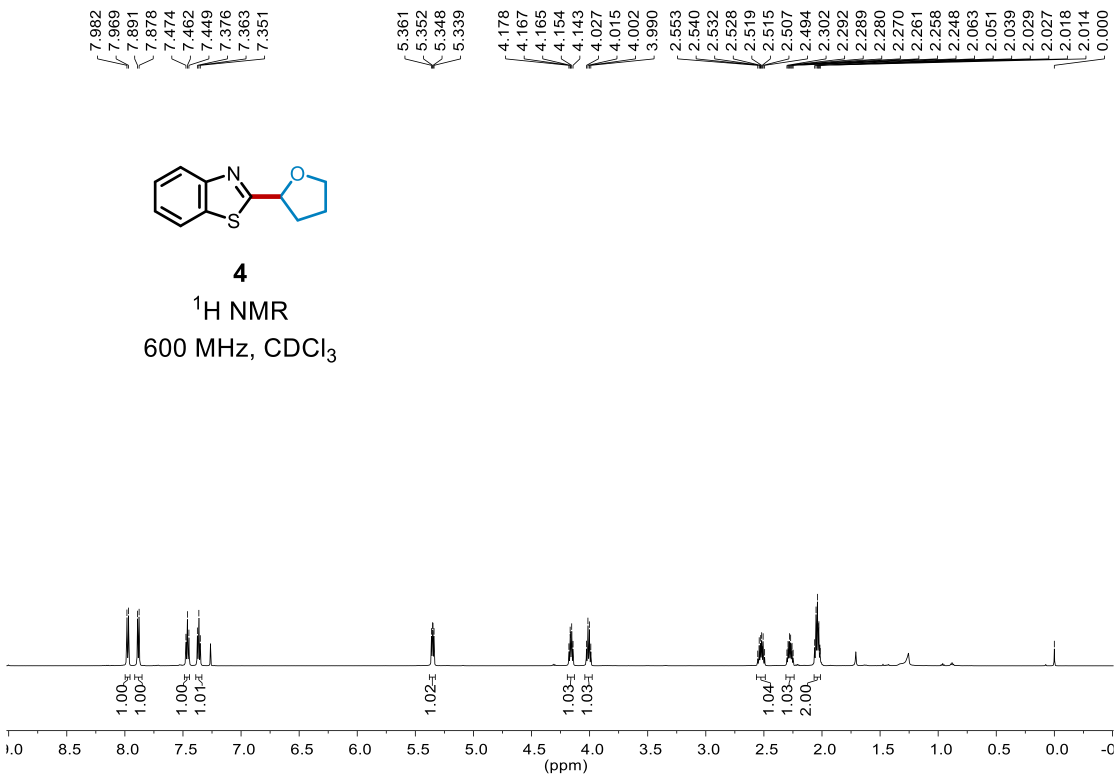

8.055
7.771
7.768
7.765
7.763
7.760
7.756
7.754
7.428
7.414
1.624
1.303
-0.000
F3C
O
N
O
O
CF3
tBu
HRP-7
1H NMR
600 MHz, CDCl3
2.02
3.15
2.14
8.76
9.00
(ppm)


-63.111
F3C
O
N
O
O
CF3
tBu
HRP-7
19F NMR
565 MHz, CDCl3
(ppm)


167.562
165.191
158.705
137.887
137.868
131.608
131.384
131.160
130.935
129.565
127.988
127.963
127.937
127.915
125.842
125.578
123.771
123.629
123.604
123.578
123.555
123.532
122.934
121.962
120.155
63.690
35.230
30.862
27.471
HRP-7
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)


7.970
7.956
7.875
7.862
7.836
7.822
7.481
7.468
7.455
7.437
7.384
7.371
7.358
7.348
7.336
5.342
5.330
5.297
5.232
5.227
5.218
5.213
3.694
3.689
3.680
3.673
3.667
3.660
3.650
3.639
3.590
3.574
2.443
2.432
2.416
2.353
2.341
2.281
2.276
2.270
2.263
2.254
2.045
2.041
2.032
2.021
2.007
1.993
1.986
1.981
1.974
1.968
1.963
1.959
1.954
1.947
1.499
1.305
0.000
Boc
S
N
N
3
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.00
1.00
1.00
1.06
2.01
2.06
2.10
3.01
6.05
(ppm)

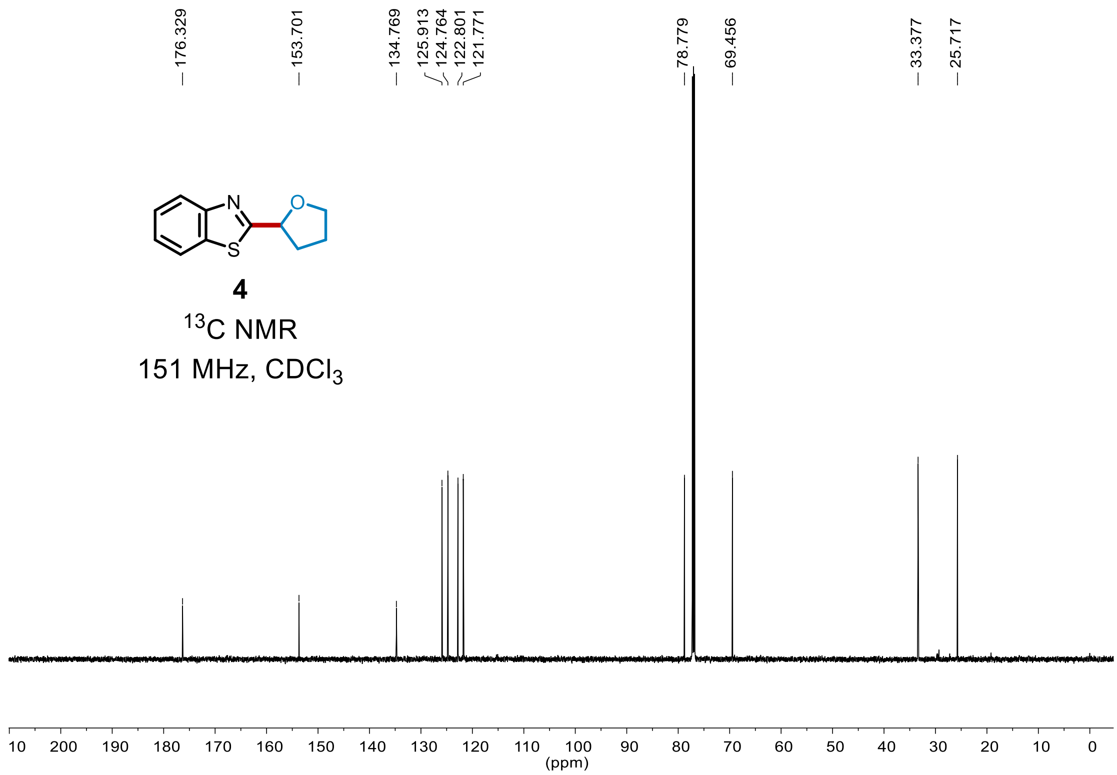

177.509
176.756
154.158
154.141
152.637
152.429
136.378
129.454
129.285
124.261
123.938
118.363
80.467
59.947
59.482
47.088
46.756
34.097
32.794
28.428
28.237
24.160
23.423
Boc
S
N
N
3
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)



4

^{1}H NMR

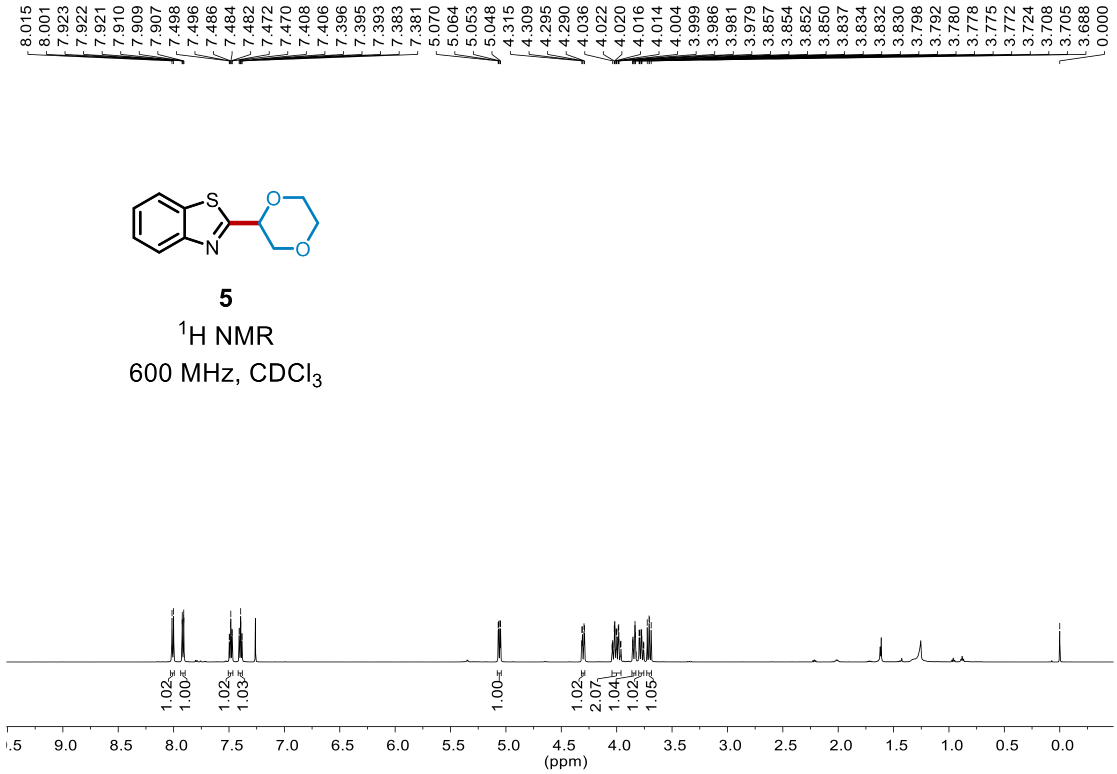
600 MHz, $CDCl_3$

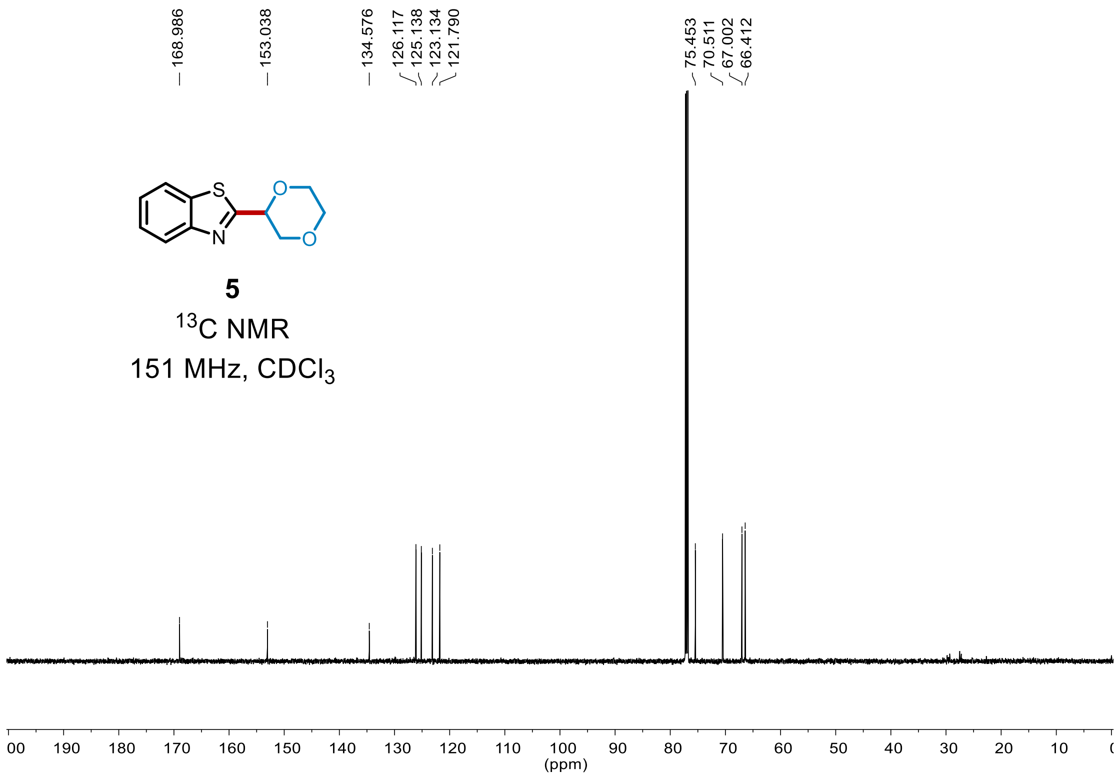


4

^{13}C NMR

151 MHz, $CDCl_3$

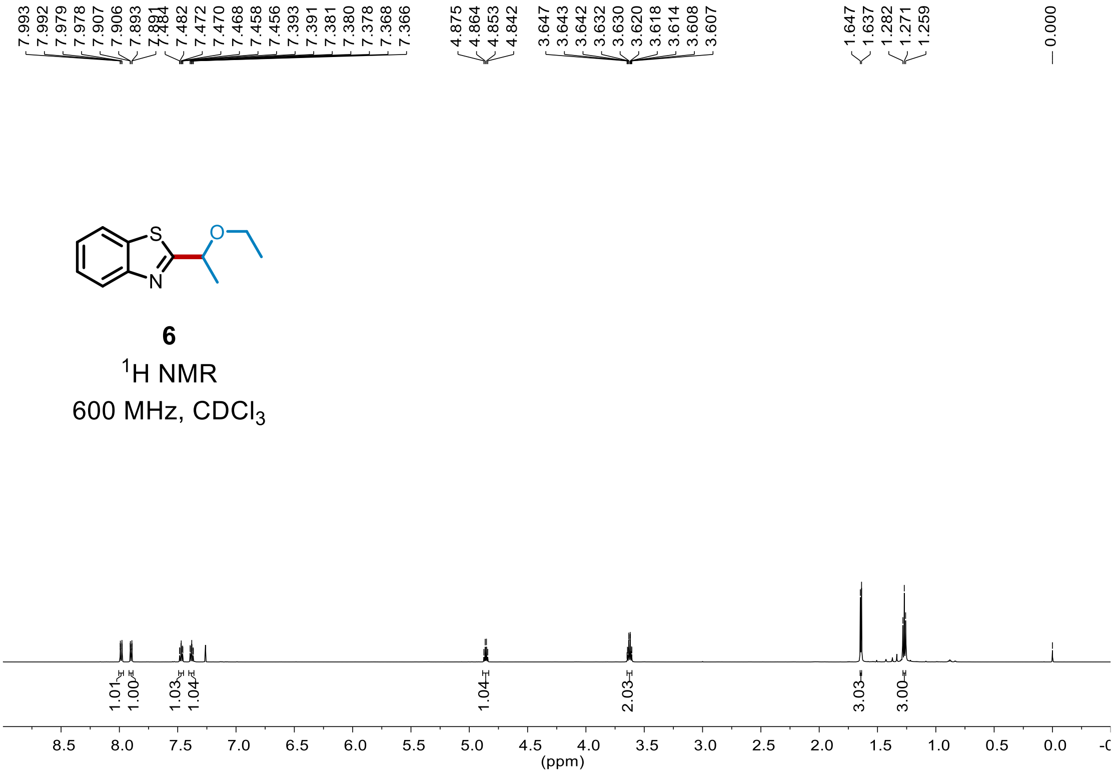

8.015
8.001
7.923
7.922
7.921
7.910
7.909
7.907
7.498
7.496
7.486
7.484
7.482
7.472
7.470
7.408
7.406
7.396
7.395
7.393
7.383
7.381
5.070
5.064
5.053
5.048
4.315
4.309
4.295
4.290
4.036
4.022
4.020
4.016
4.014
4.004
3.999
3.986
3.981
3.979
3.857
3.854
3.852
3.850
3.837
3.834
3.832
3.830
3.798
3.792
3.780
3.778
3.775
3.772
3.724
3.708
3.705
3.688
0.000
S
N
O
O
5
1H NMR
600 MHz, CDCl3
1.02
1.00
1.02
1.03
1.00
1.02
2.07
1.04
1.02
1.05
(ppm)


168.986
153.038
134.576
126.117
125.138
123.134
121.790
75.453
70.511
67.002
66.412
S
N
O
O
5
13C NMR
151 MHz, CDCl3
(ppm)

6

^{1}H NMR

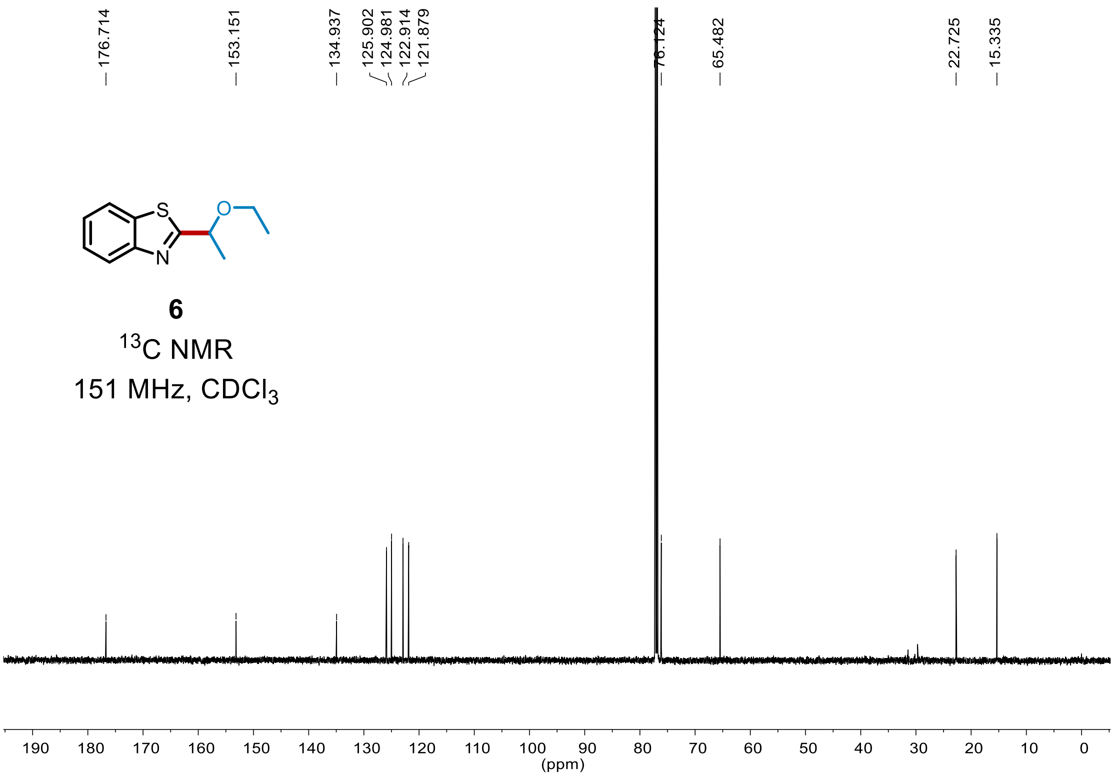
600 MHz, $CDCl_3$

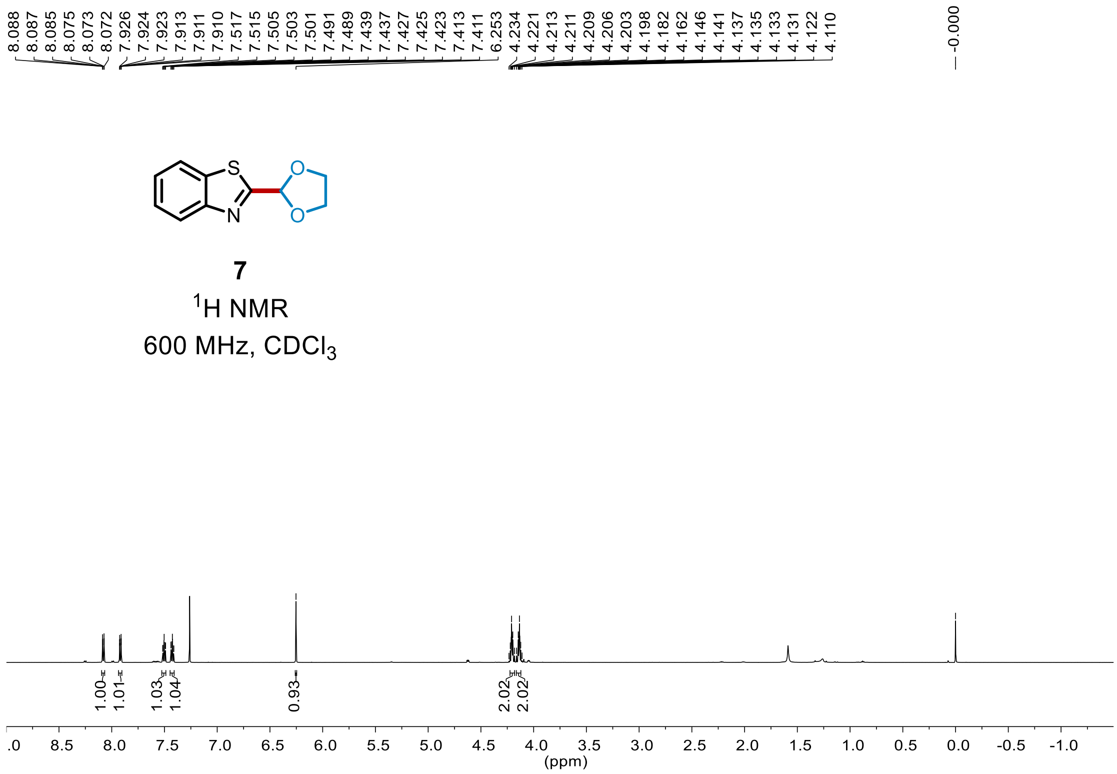


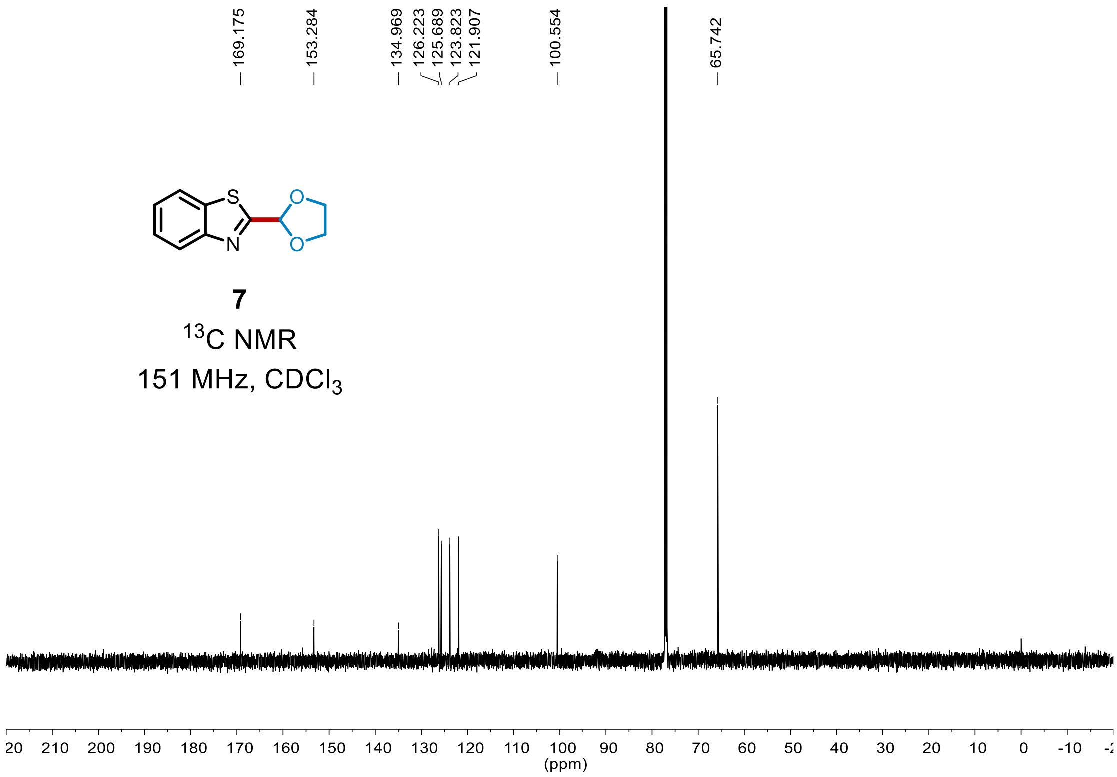
6

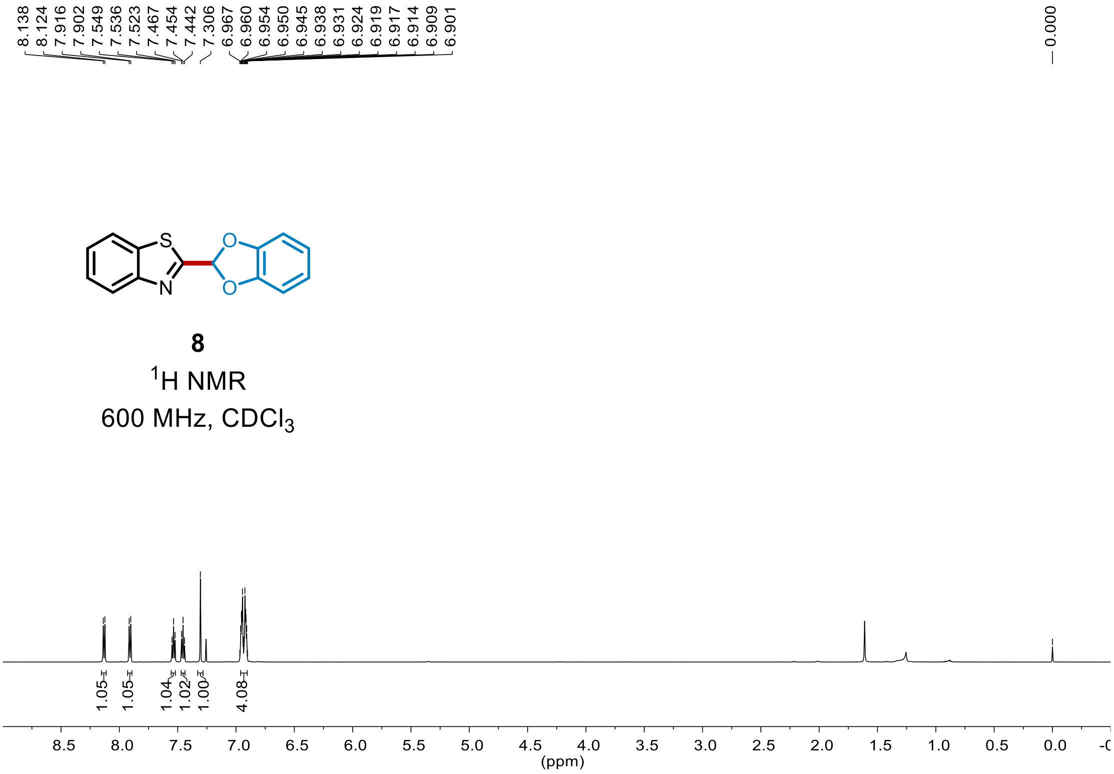
^{13}C NMR

151 MHz, $CDCl_3$

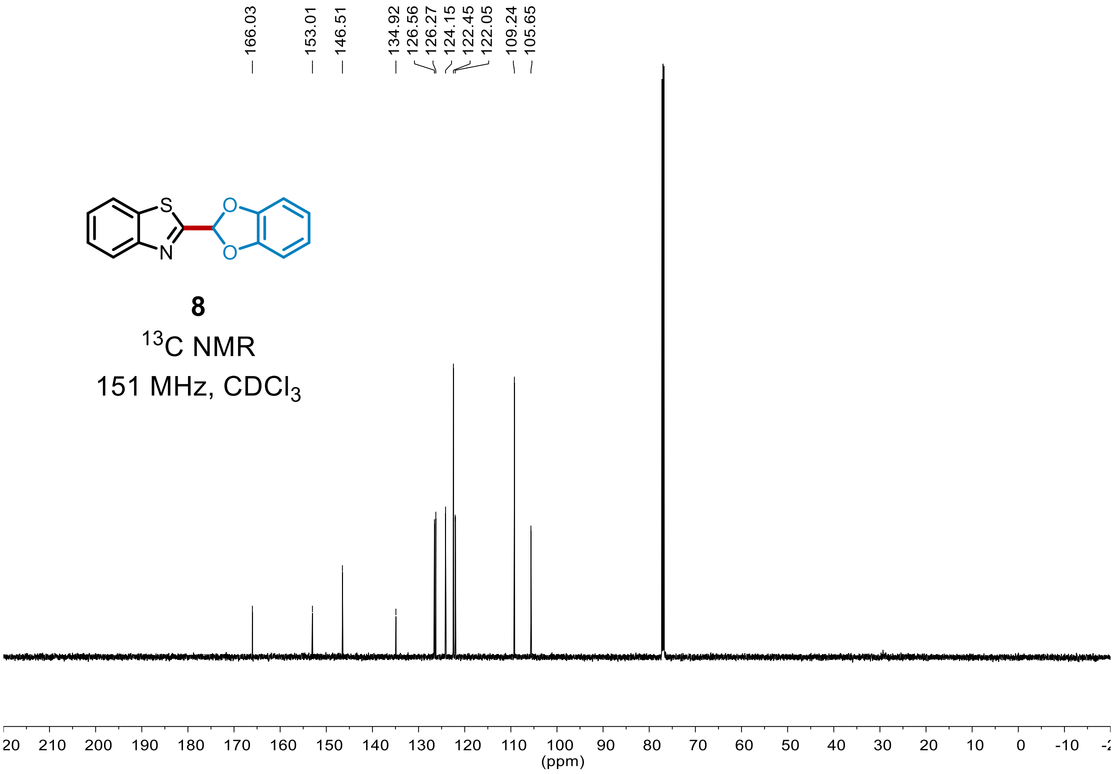



8.088 8.087 8.085 8.075 8.073 8.072 7.926 7.924 7.923 7.913 7.911 7.910 7.517 7.515 7.505 7.503 7.501 7.491 7.489 7.439 7.437 7.427 7.425 7.423 7.413 7.411 6.253 4.234 4.221 4.213 4.211 4.209 4.206 4.203 4.198 4.182 4.162 4.146 4.141 4.137 4.135 4.133 4.131 4.122 4.110
-0.000
S
N
O
O
7
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.01
1.03
1.04
0.93
2.02
2.02
(ppm)

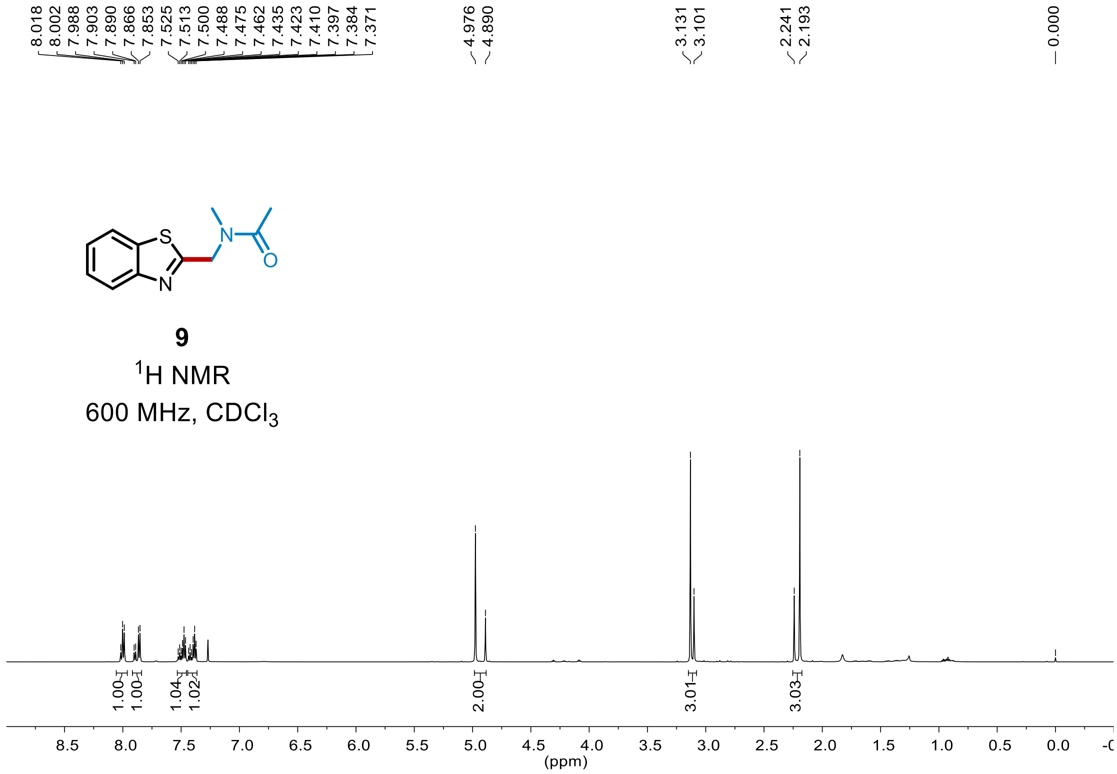

169.175
153.284
134.969
126.223
125.689
123.823
121.907
100.554
65.742
S
N
O
O
7
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)

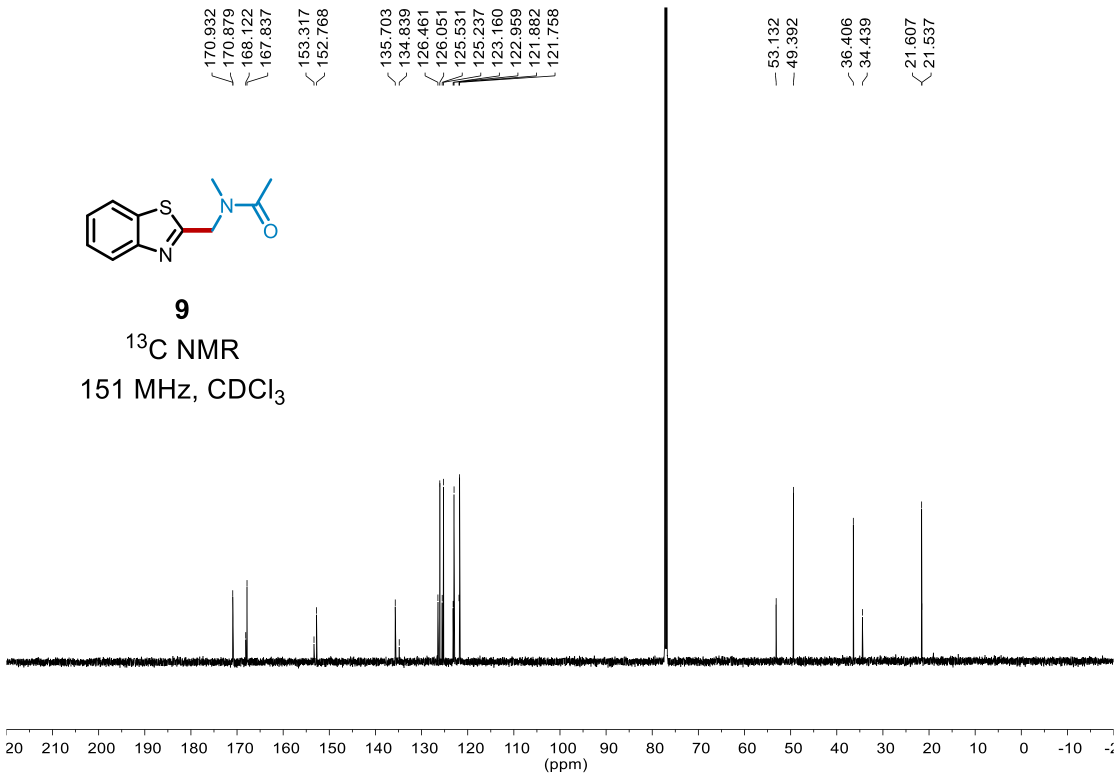


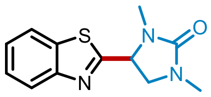
8.138
8.124
7.916
7.902
7.549
7.536
7.523
7.467
7.454
7.442
7.306
6.967
6.960
6.954
6.950
6.945
6.938
6.931
6.924
6.919
6.917
6.914
6.909
6.901
0.000
8
^{1}H NMR
600 MHz, $CDCl_3$
1.05
1.05
1.04
1.02
1.00
4.08
(ppm)



166.03
153.01
146.51
134.92
126.56
126.27
124.15
122.45
122.05
109.24
105.65
8
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)


8.018
8.002
7.988
7.903
7.890
7.866
7.853
7.525
7.513
7.500
7.488
7.475
7.462
7.435
7.423
7.410
7.397
7.384
7.371
4.976
4.890
3.131
3.101
2.241
2.193
0.000
9
1H NMR
600 MHz, CDCl3
1.00
1.00
1.04
1.02
2.00
3.01
3.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

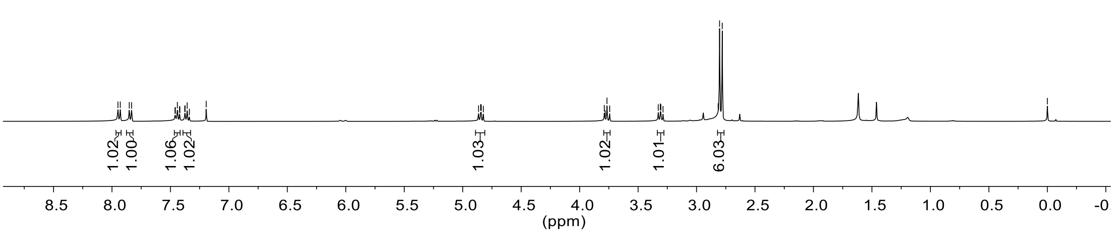

170.932
170.879
168.122
167.837
153.317
152.768
135.703
134.839
126.461
126.051
125.531
125.237
123.160
122.959
121.882
121.758
53.132
49.392
36.406
34.439
21.607
21.537
9
13C NMR
151 MHz, CDCl3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

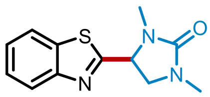


10

^{1}H NMR

400 MHz, $CDCl_3$

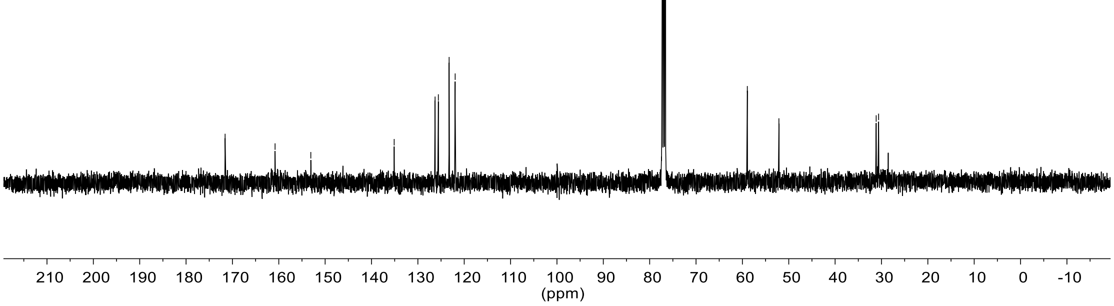


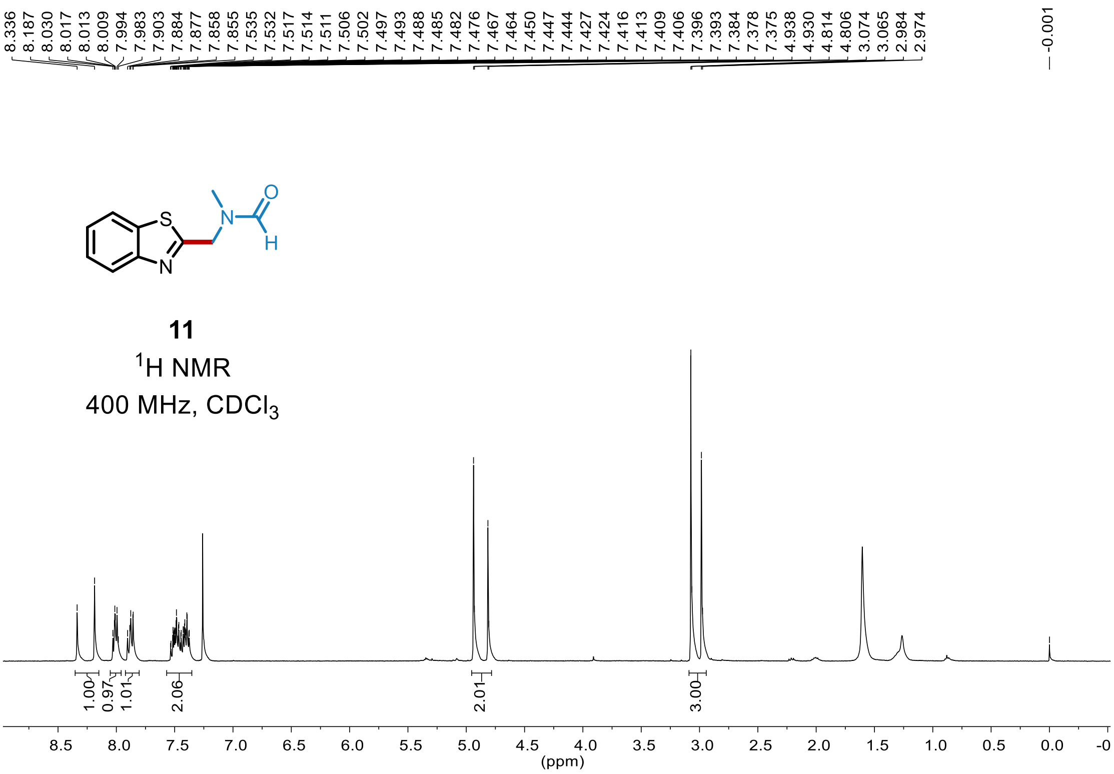


10

^{13}C NMR

101 MHz, $CDCl_3$

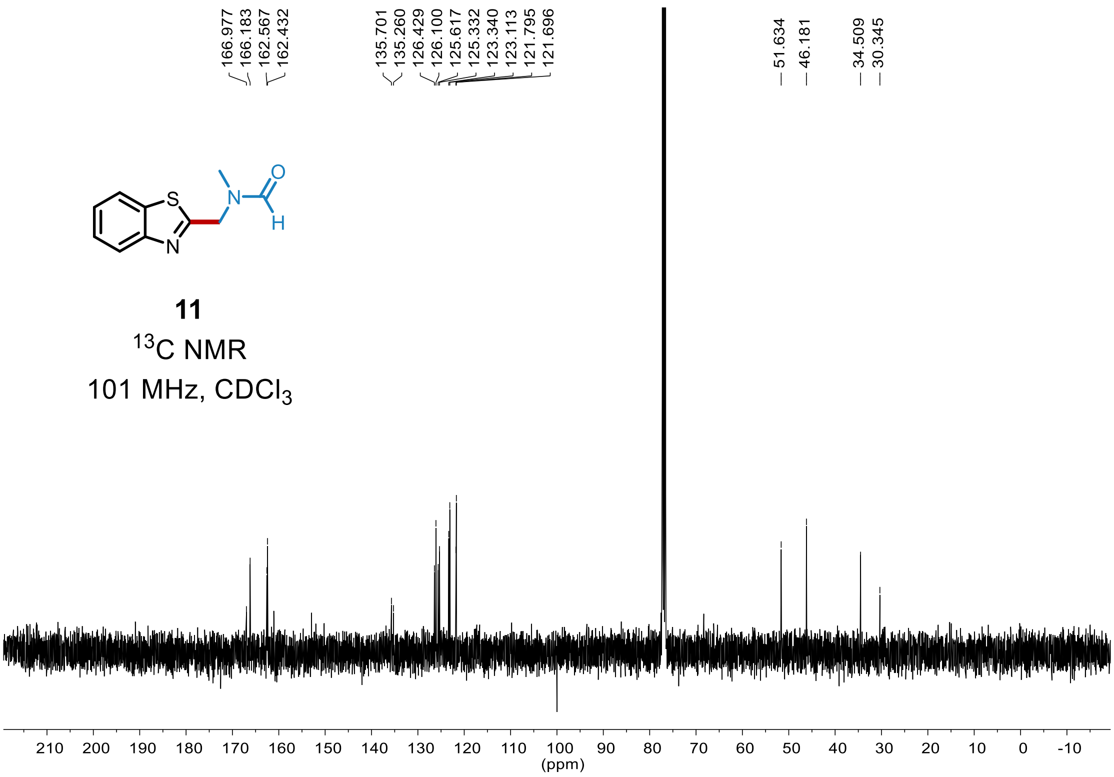




11

^{1}H NMR

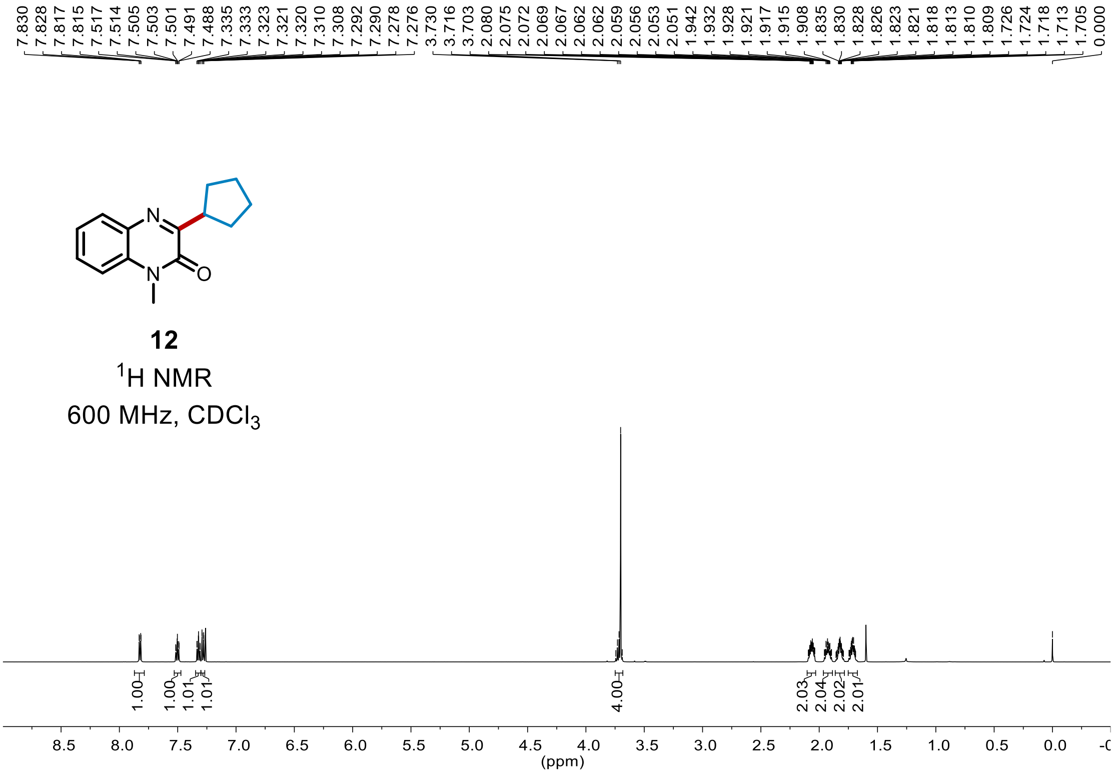
400 MHz, $CDCl_3$

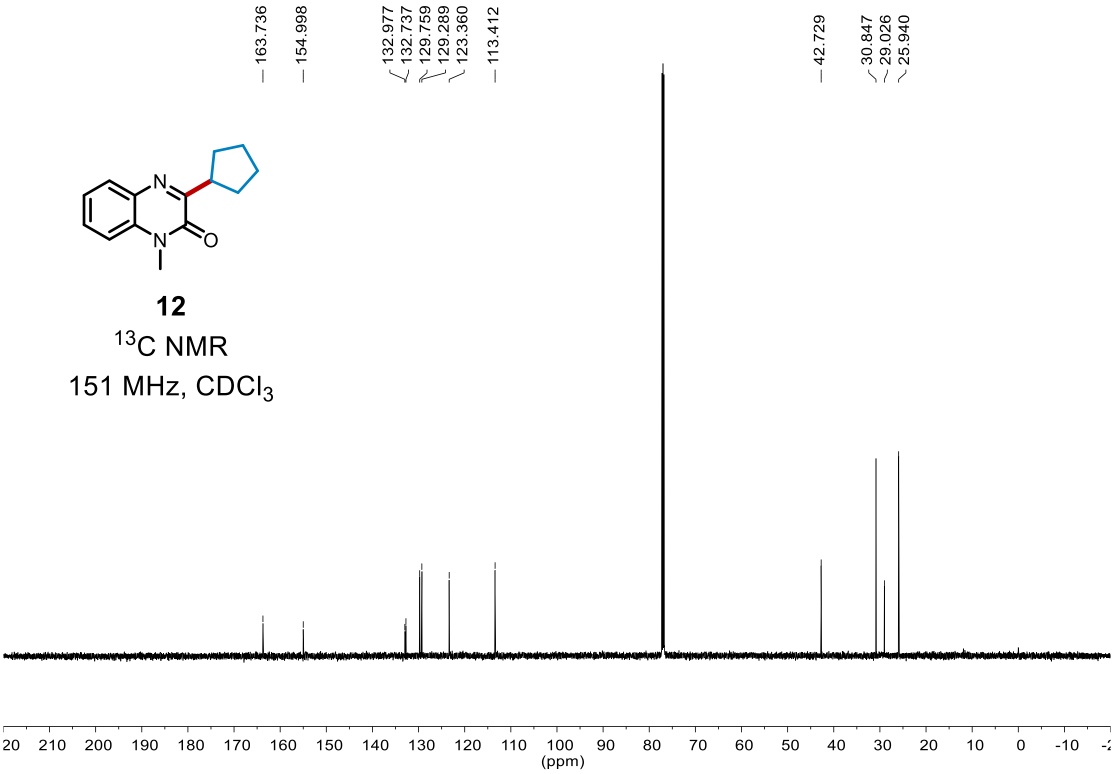


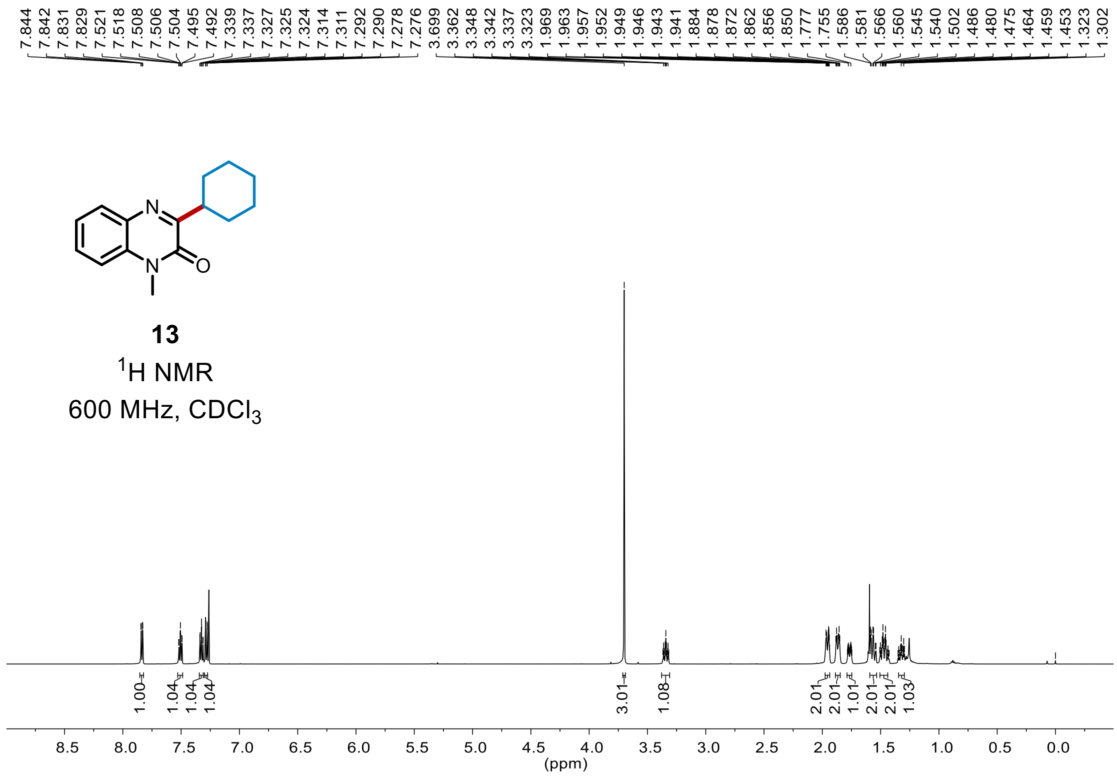
11

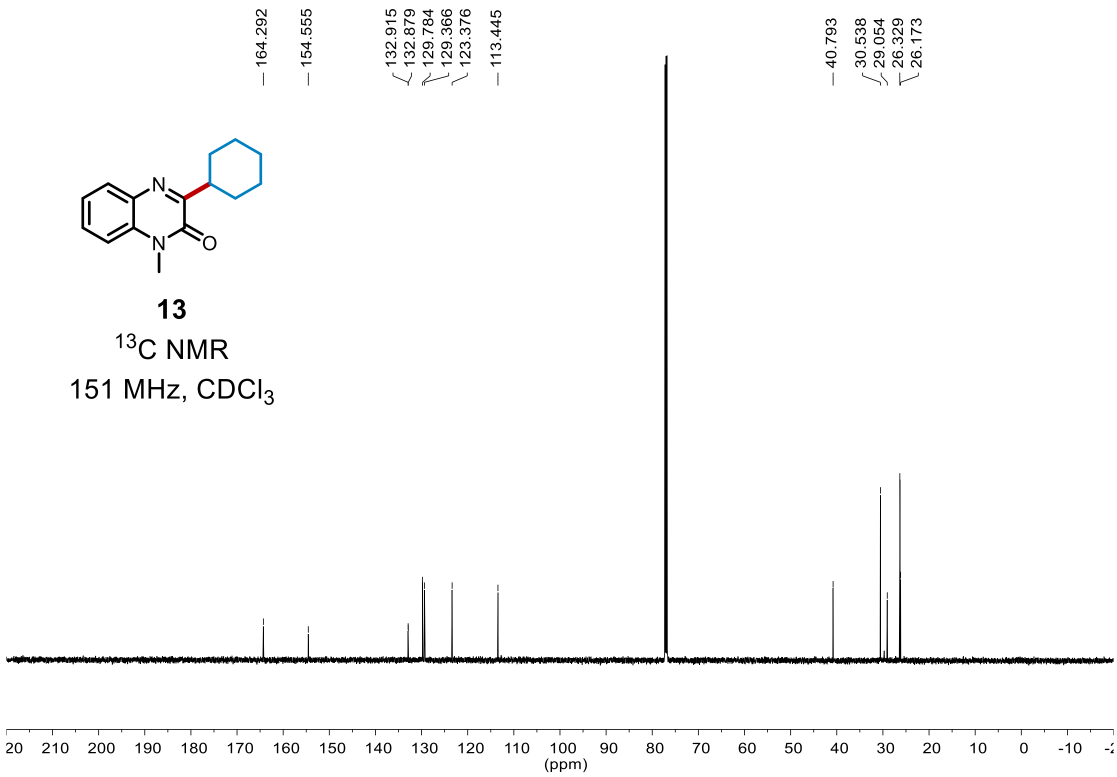
^{13}C NMR

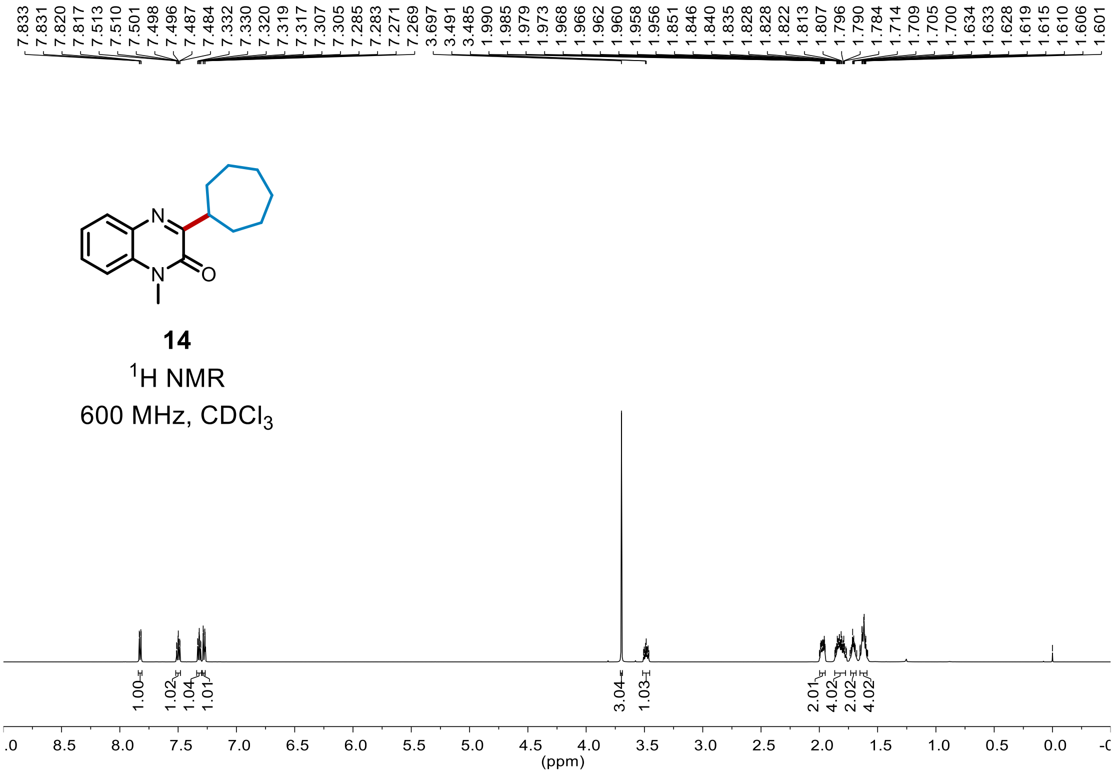
101 MHz, $CDCl_3$

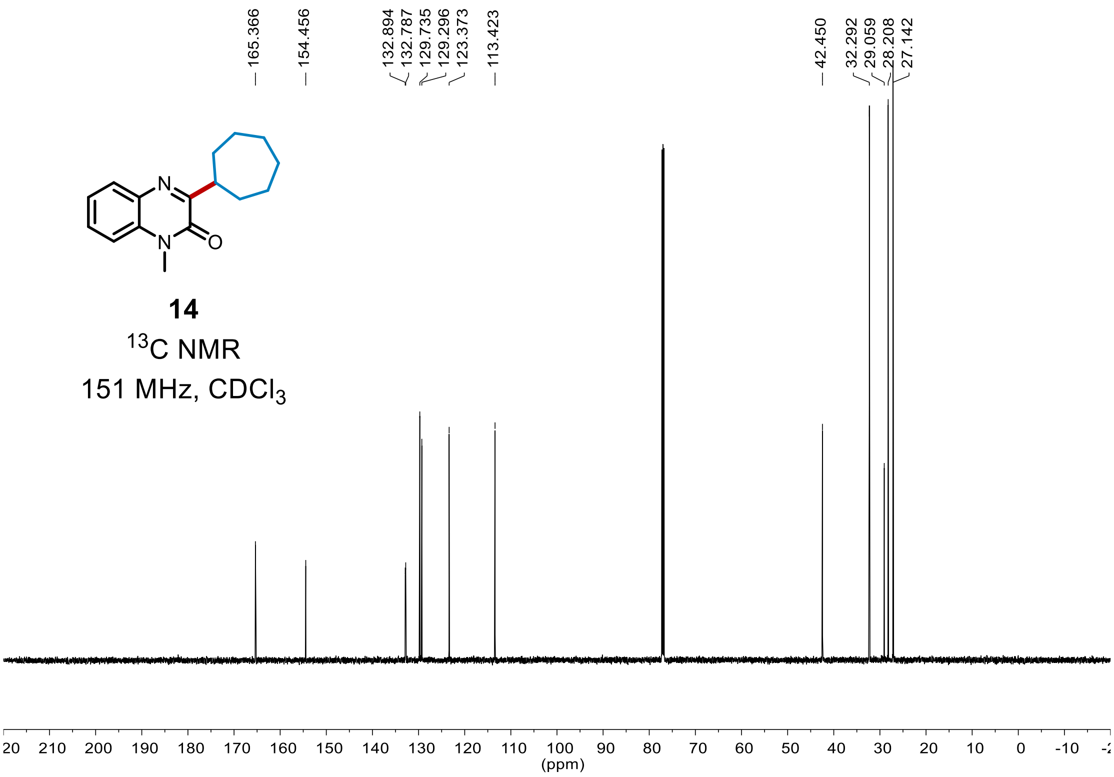

7.830 7.828 7.817 7.815 7.517 7.514 7.505 7.503 7.501 7.491 7.488 7.335 7.333 7.323 7.321 7.320 7.310 7.308 7.292 7.290 7.278 7.276 3.730 3.716 3.703 2.080 2.075 2.072 2.069 2.067 2.062 2.062 2.059 2.056 2.053 2.051 1.942 1.932 1.928 1.921 1.917 1.915 1.908 1.835 1.830 1.828 1.826 1.823 1.821 1.818 1.813 1.810 1.809 1.726 1.724 1.718 1.713 1.705 0.000
N
N
O
12
1H NMR
600 MHz, CDCl3
1.00 1.00 1.01 1.01
4.00
2.03 2.04 2.02 2.01
(ppm)

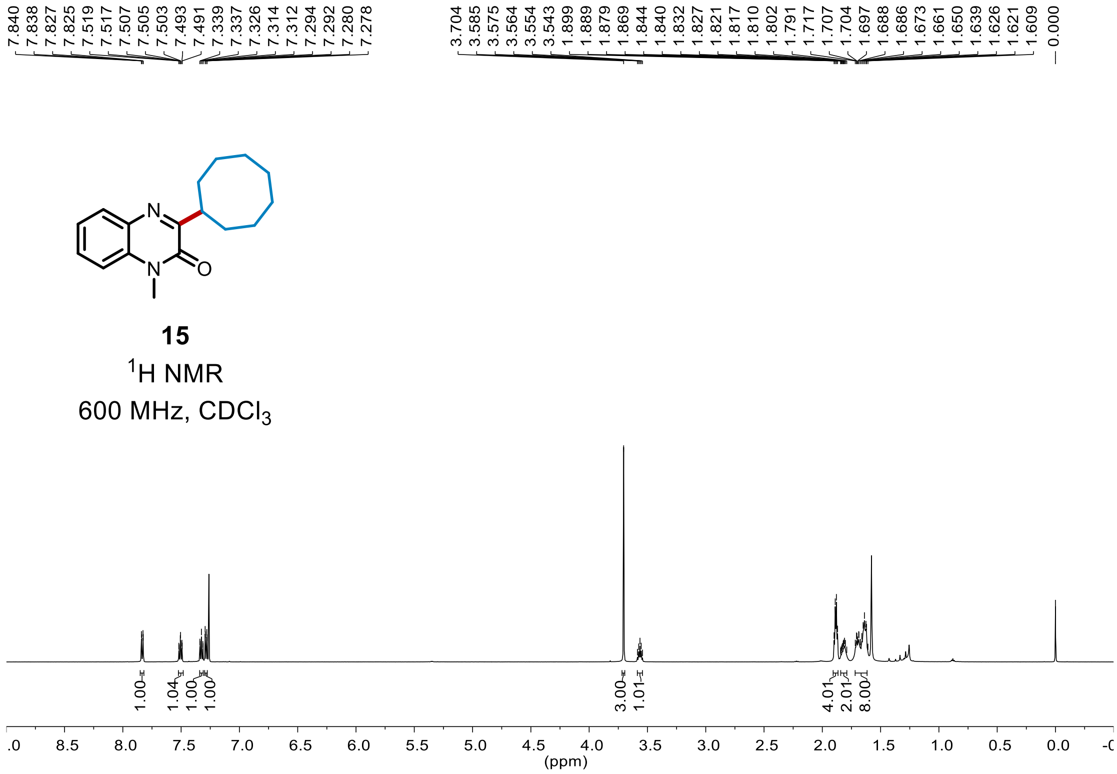

163.736 154.998 132.977 132.737 129.759 129.289 123.360 113.412 42.729 30.847 29.026 25.940
N
N
O
12
13C NMR
151 MHz, CDCl3
(ppm)

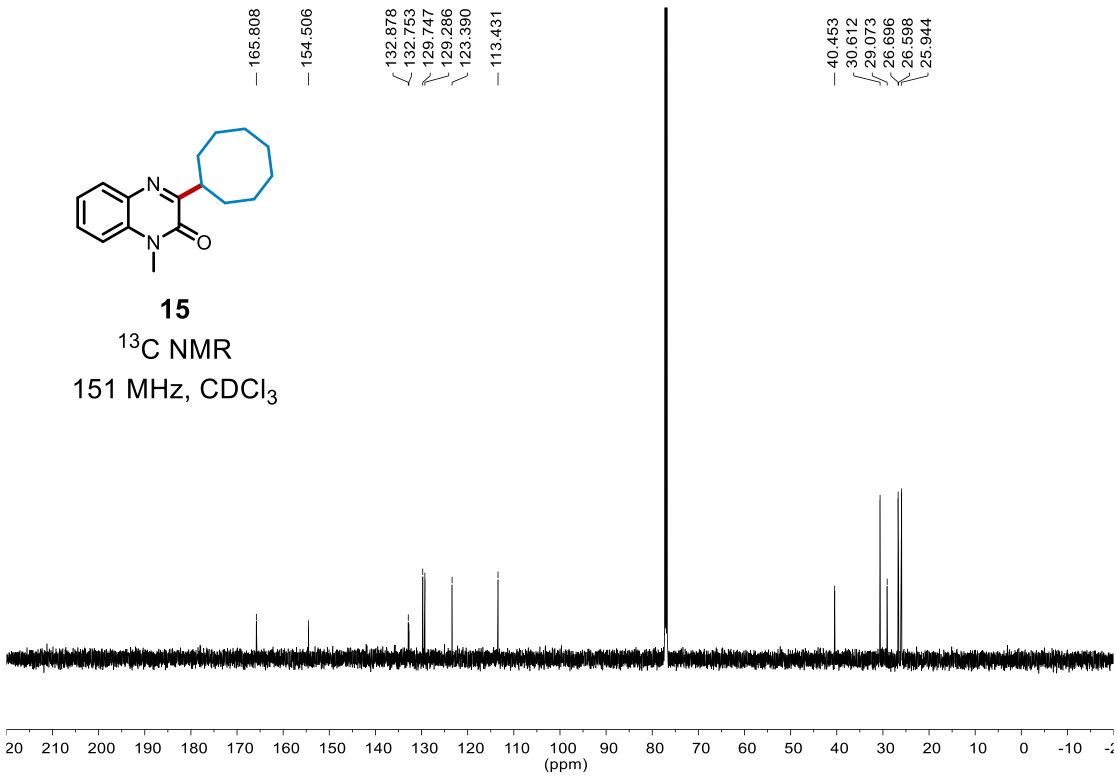

7.844 7.842 7.831 7.829 7.521 7.518 7.508 7.506 7.504 7.495 7.492 7.339 7.337 7.327 7.325 7.324 7.314 7.311 7.292 7.290 7.278 7.276 3.699 3.362 3.348 3.342 3.337 3.323 1.969 1.963 1.957 1.952 1.949 1.946 1.943 1.941 1.884 1.878 1.872 1.862 1.856 1.850 1.777 1.755 1.586 1.581 1.566 1.560 1.545 1.540 1.502 1.486 1.480 1.475 1.464 1.459 1.453 1.323 1.302
N
N
O
13
^{1}H NMR
600 MHz, CDCl$_3$
1.00 1.04 1.04 1.04 3.01 1.08 2.01 2.01 1.01 2.01 2.01 1.03
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

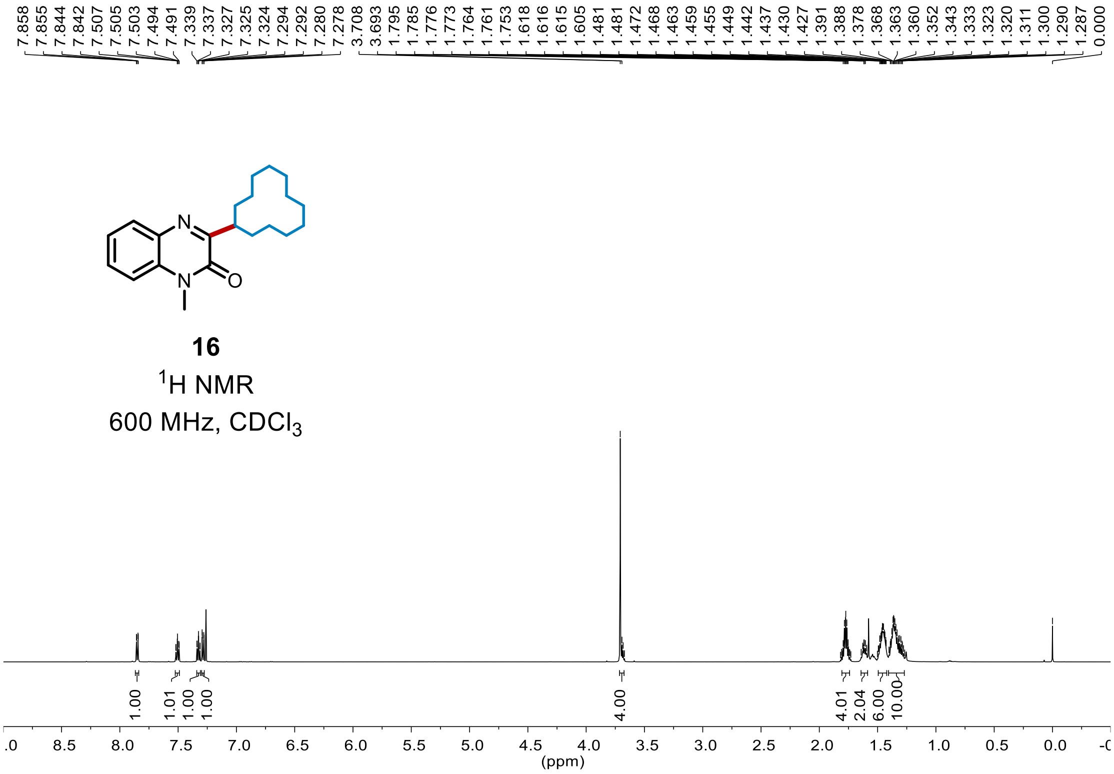

164.292
154.555
132.915 132.879 129.784 129.366 123.376
113.445
40.793
30.538 29.054 26.329 26.173
N
N
O
13
^{13}C NMR
151 MHz, CDCl$_3$
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

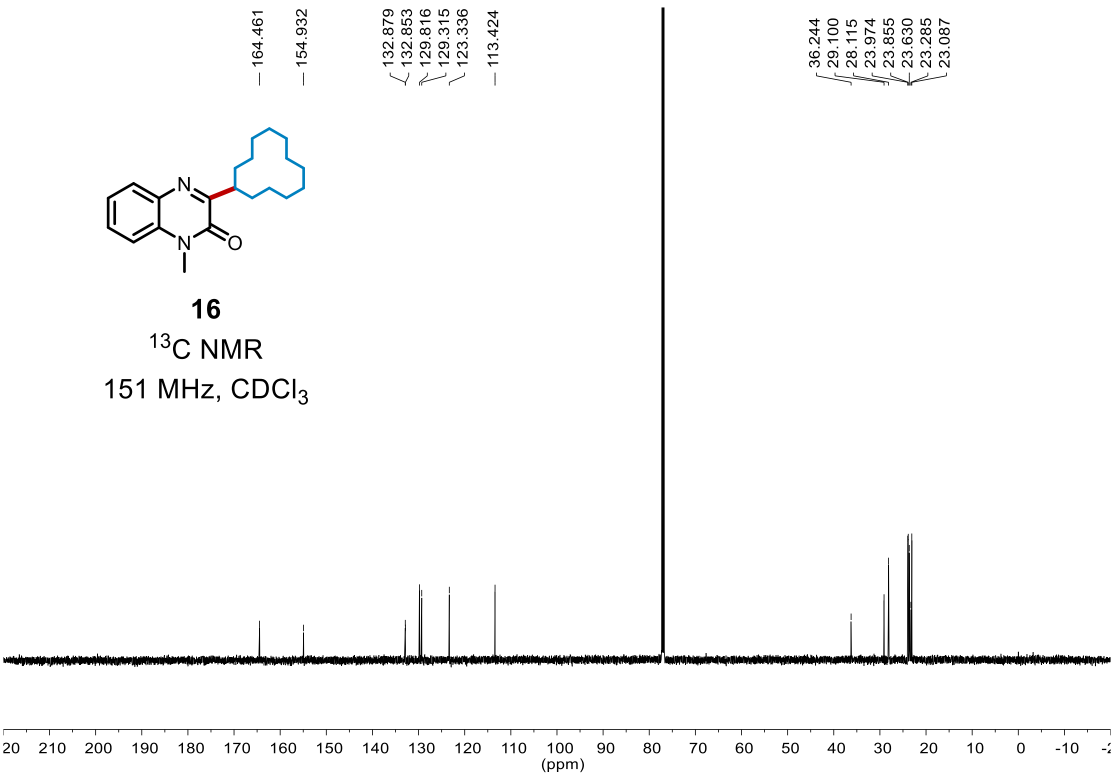

14
^{1}H NMR
600 MHz, $CDCl_3$
(ppm)

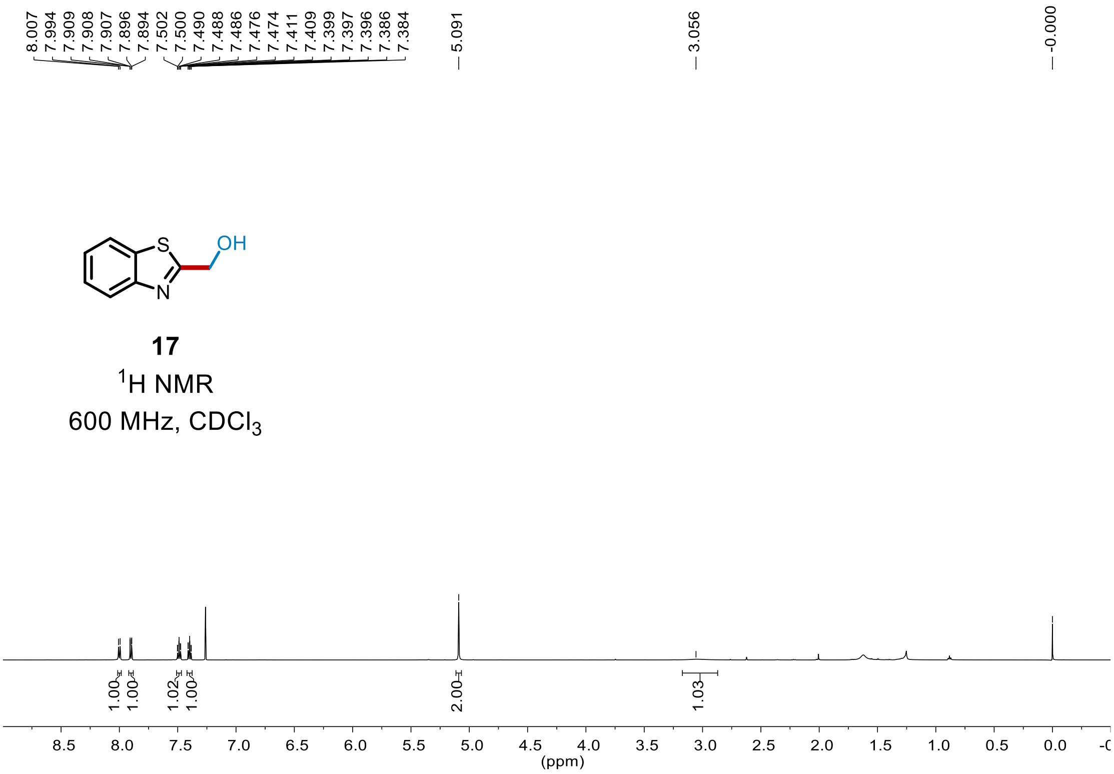

165.366
154.456
132.894
132.787
129.735
129.296
123.373
113.423
42.450
32.292
29.059
28.208
27.142
14
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)


7.840
7.838
7.827
7.825
7.519
7.517
7.507
7.505
7.503
7.493
7.491
7.339
7.337
7.326
7.314
7.312
7.294
7.292
7.280
7.278
3.704
3.585
3.575
3.564
3.554
3.543
1.899
1.889
1.879
1.869
1.844
1.840
1.832
1.827
1.821
1.817
1.810
1.802
1.791
1.717
1.707
1.704
1.697
1.688
1.686
1.673
1.661
1.650
1.639
1.626
1.621
1.609
0.000
N
N
O
15
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.04
1.00
1.00
3.00
1.01
4.01
2.01
8.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
(ppm)

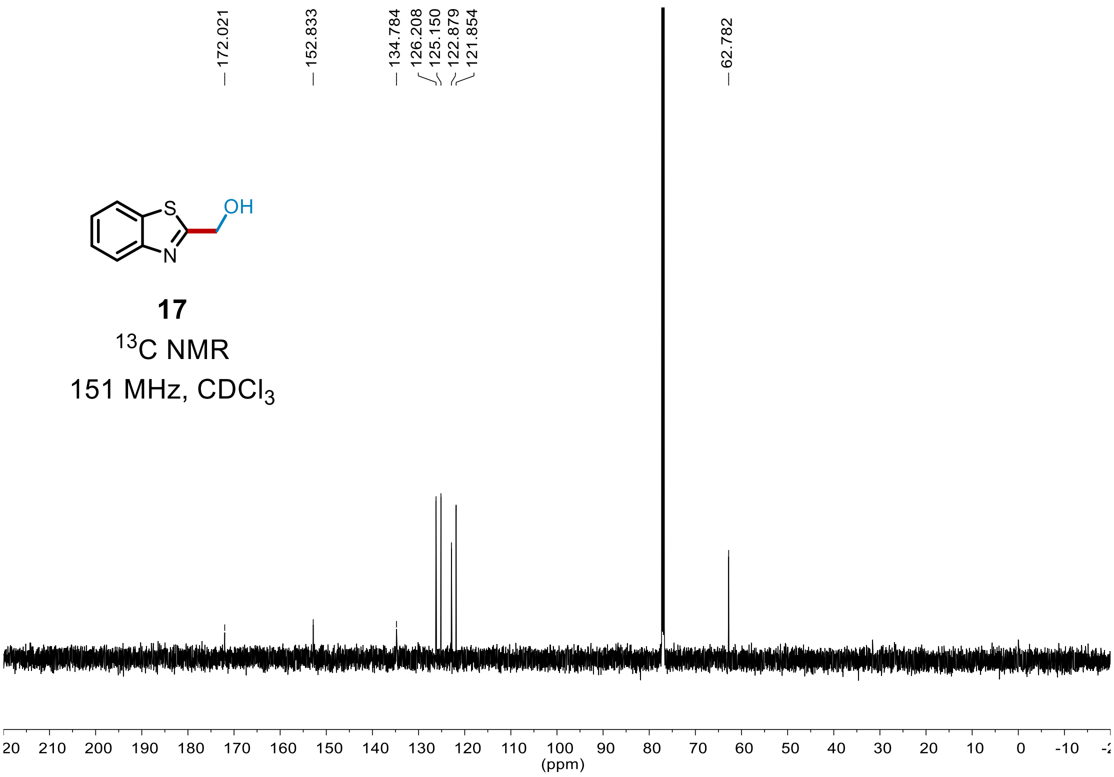

165.808
154.506
132.878
132.753
129.747
129.286
123.390
113.431
40.453
30.612
29.073
26.696
26.598
25.944
N
N
O
15
^{13}C NMR
151 MHz, $CDCl_3$
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
(ppm)


7.858
7.855
7.844
7.842
7.507
7.505
7.503
7.494
7.491
7.339
7.337
7.327
7.325
7.324
7.294
7.292
7.280
7.278
3.708
3.693
1.795
1.785
1.776
1.773
1.764
1.761
1.753
1.618
1.616
1.615
1.605
1.481
1.481
1.472
1.468
1.463
1.459
1.455
1.449
1.442
1.437
1.430
1.427
1.391
1.388
1.378
1.368
1.363
1.360
1.352
1.343
1.333
1.323
1.320
1.311
1.300
1.290
1.287
0.000
N
N
O
16
1H NMR
600 MHz, CDCl3
1.00
1.01
1.00
1.00
4.00
4.01
2.04
6.00
10.00
(ppm)

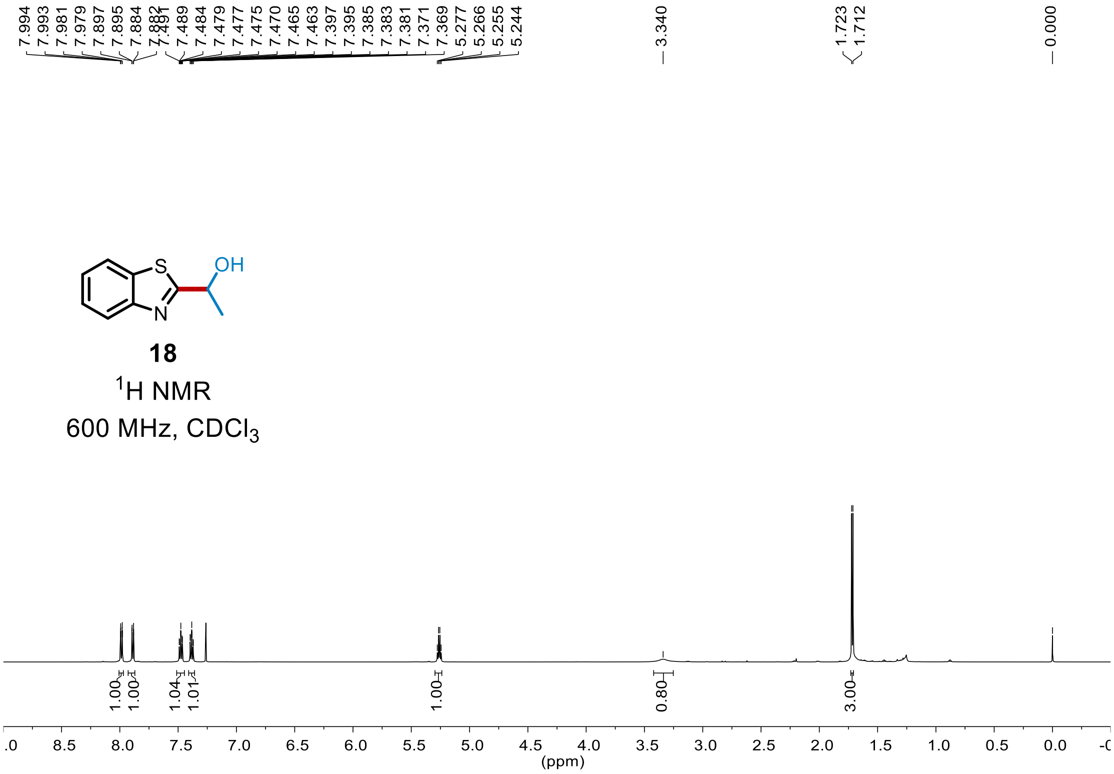

164.461
154.932
132.879
132.853
129.816
129.315
123.336
113.424
36.244
29.100
28.115
23.974
23.855
23.630
23.285
23.087
N
N
O
16
13C NMR
151 MHz, CDCl3
(ppm)



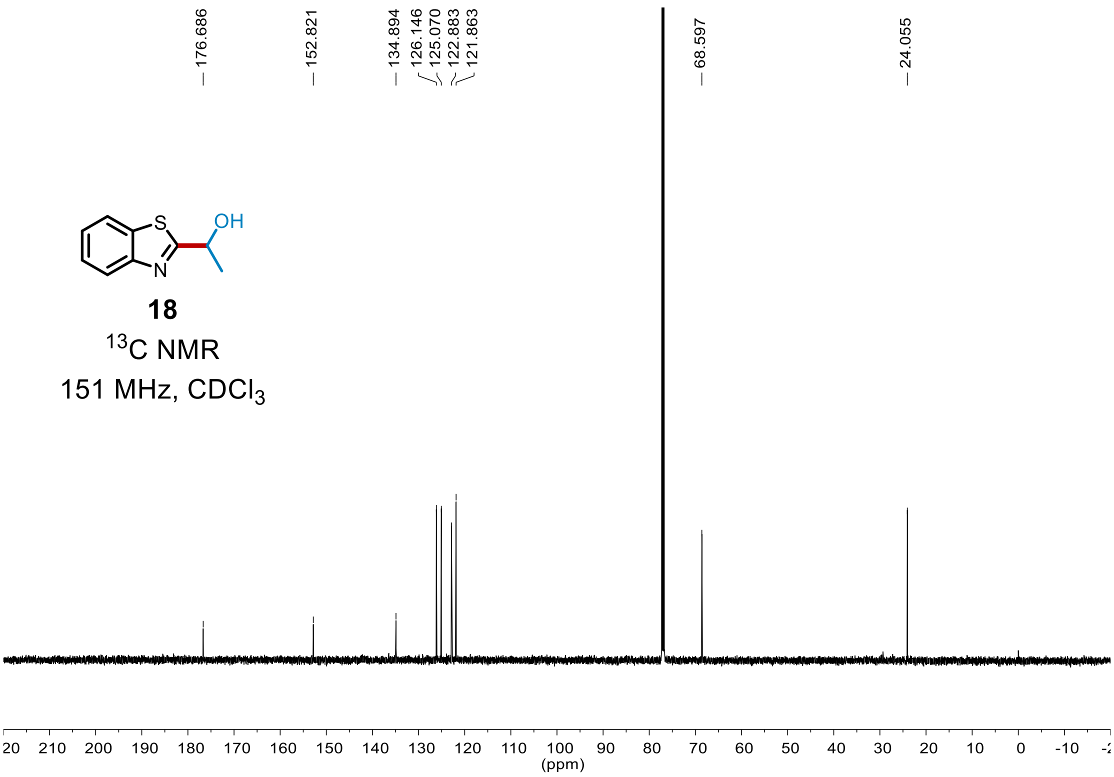
17
^{1}H NMR
600 MHz, $CDCl_3$



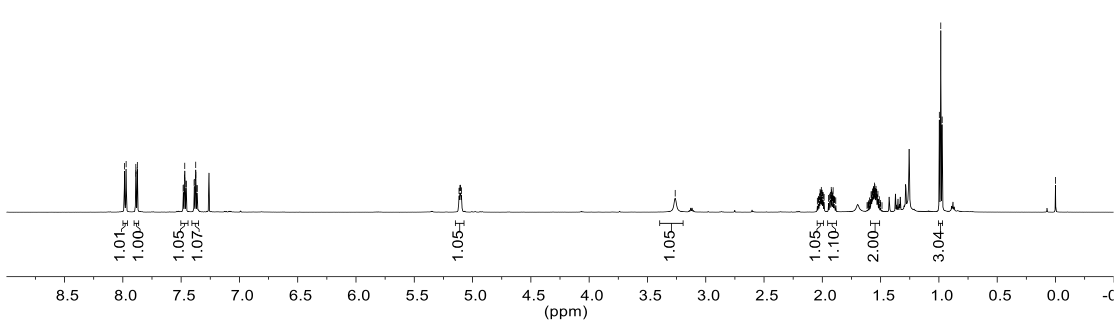
17
^{13}C NMR
151 MHz, $CDCl_3$

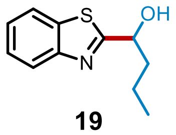


18
1H NMR
600 MHz, CDCl3
7.994
7.993
7.981
7.979
7.897
7.895
7.884
7.882
7.491
7.489
7.484
7.479
7.477
7.475
7.470
7.465
7.463
7.397
7.395
7.385
7.383
7.381
7.371
7.369
5.277
5.266
5.255
5.244
3.340
1.723
1.712
0.000
1.00
1.00
1.04
1.01
1.00
0.80
3.00
(ppm)



18
13C NMR
151 MHz, CDCl3
176.686
152.821
134.894
126.146
125.070
122.883
121.863
68.597
24.055
(ppm)

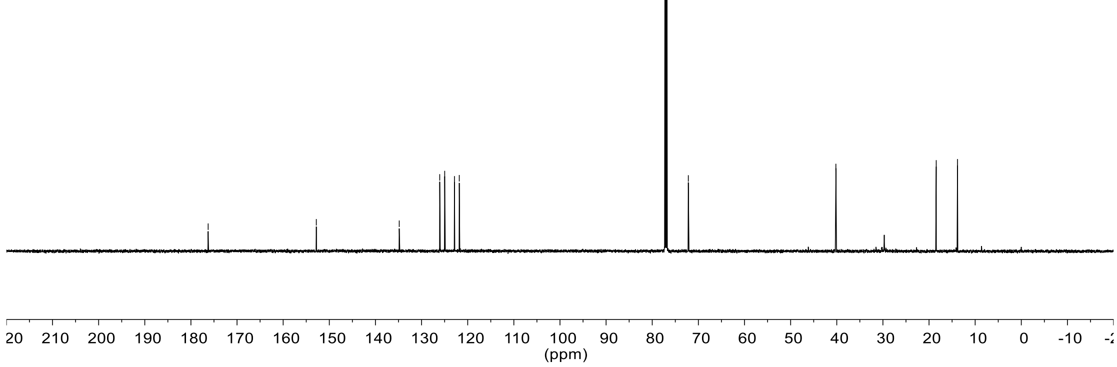


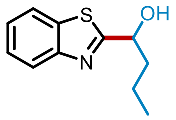


19

^{1}H NMR

600 MHz, $CDCl_3$

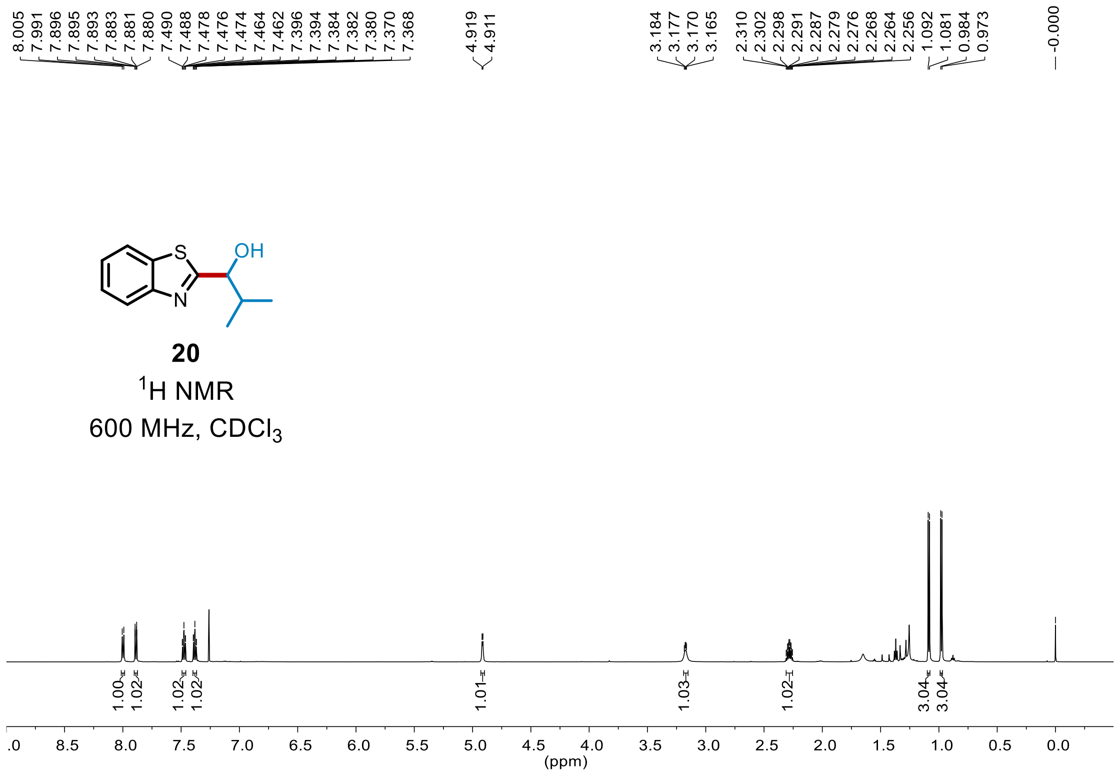


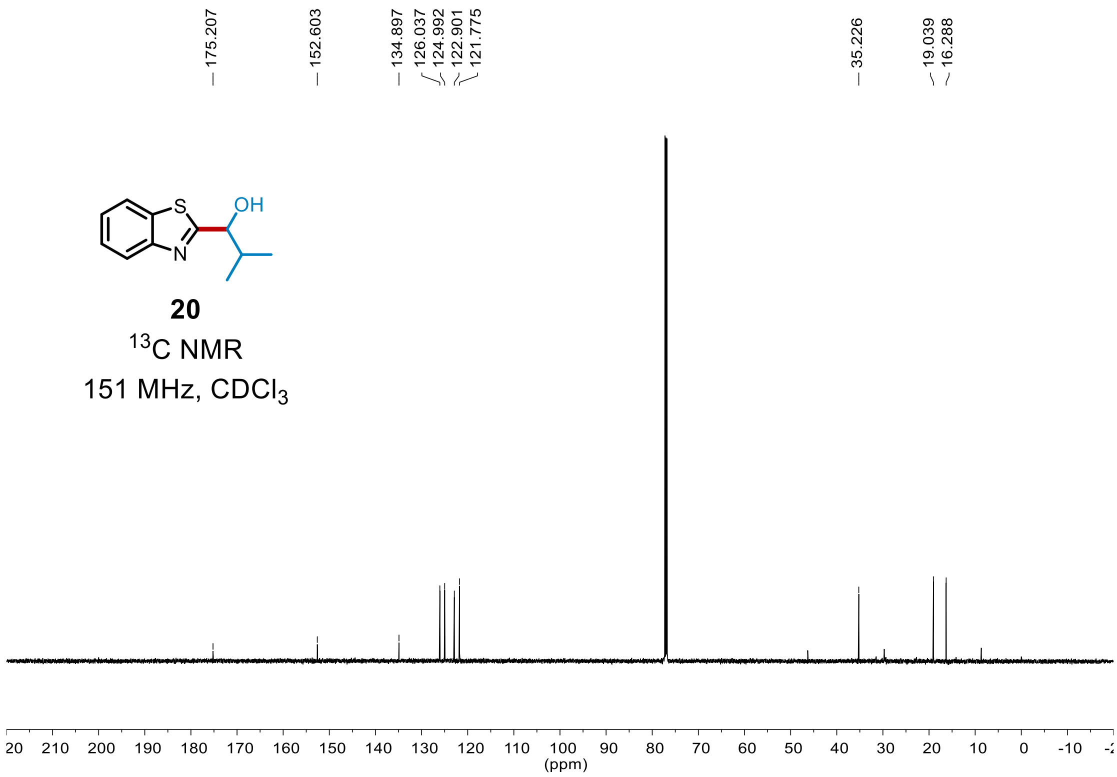


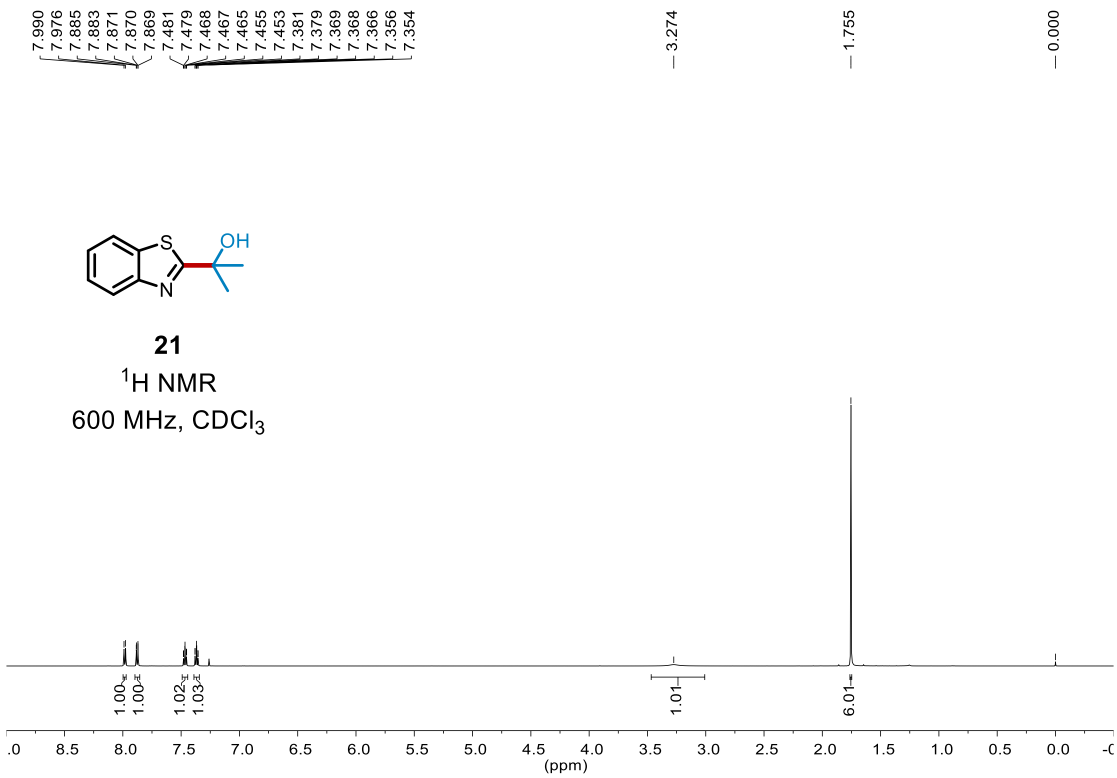
19

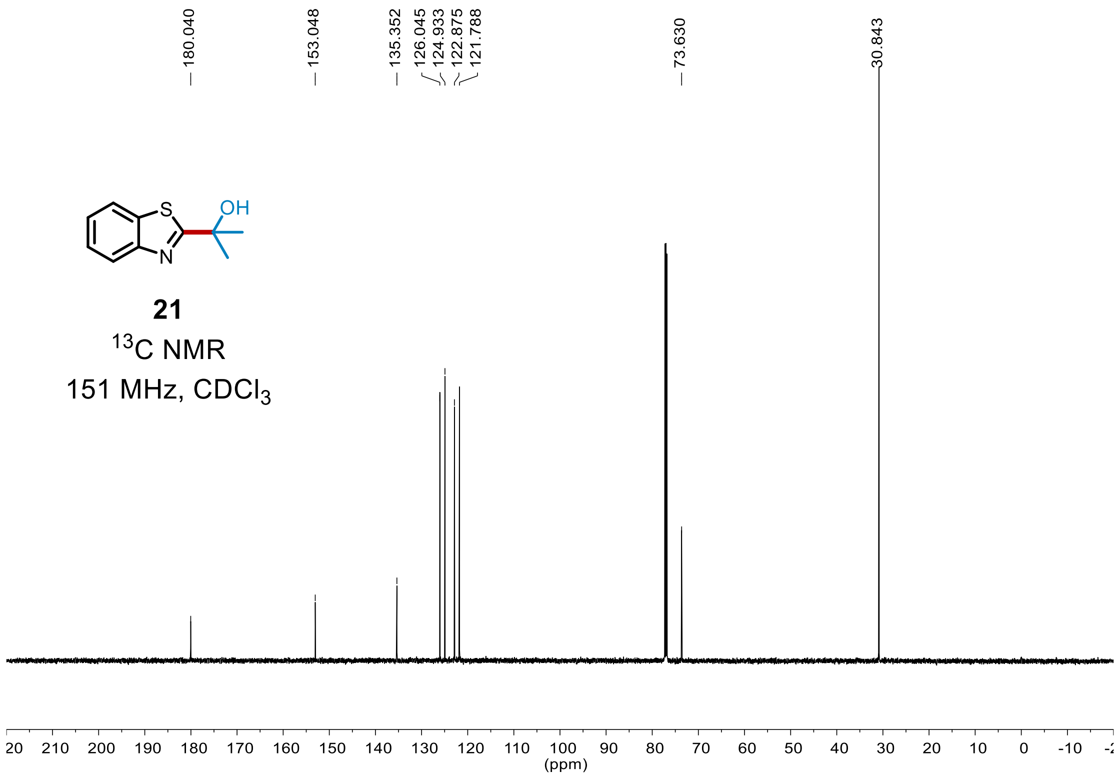
^{13}C NMR

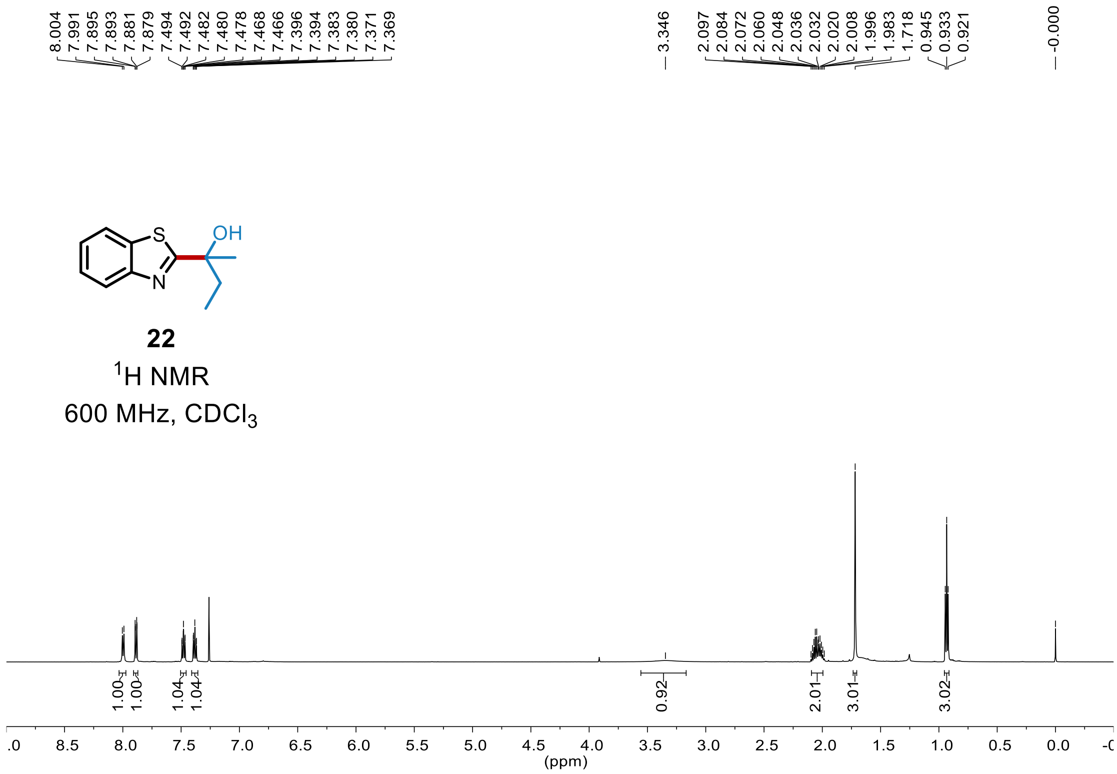
151 MHz, $CDCl_3$

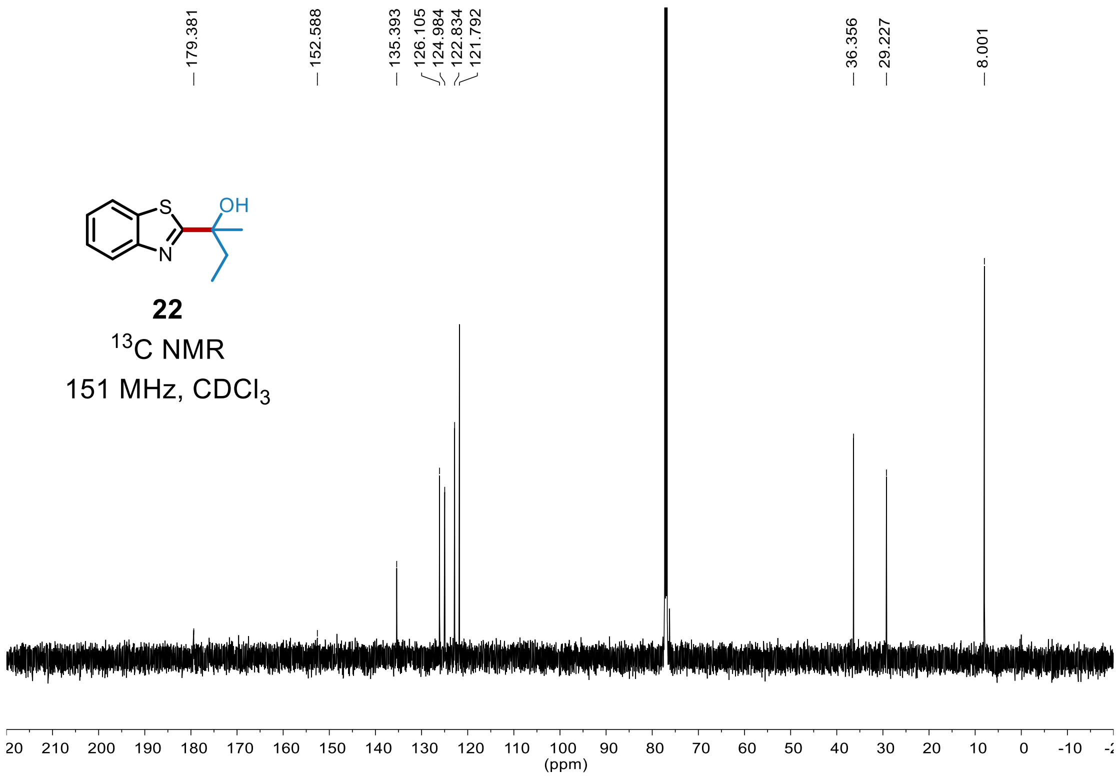

8.005 7.991 7.896 7.895 7.893 7.883 7.881 7.880 7.490 7.488 7.476 7.474 7.464 7.462 7.396 7.394 7.384 7.382 7.380 7.370 7.368
4.919 4.911
3.184 3.177 3.170 3.165
2.310 2.302 2.298 2.291 2.287 2.279 2.276 2.268 2.264 2.256 1.092 1.081 0.984 0.973
-0.000
OH
S
N
20
1H NMR
600 MHz, CDCl3
1.00 1.02 1.02 1.02 1.01 1.03 1.02 3.04 3.04
(ppm)

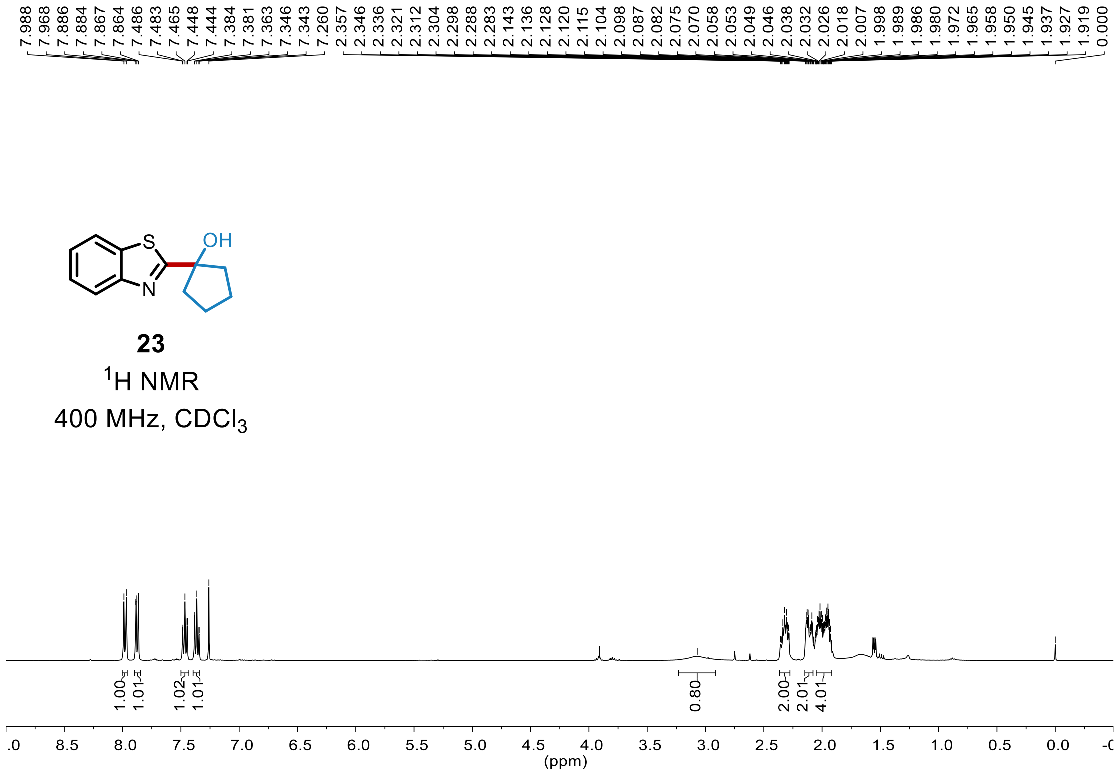

175.207
152.603
134.897 126.037 124.992 122.901 121.775
35.226
19.039 16.288
OH
S
N
20
13C NMR
151 MHz, CDCl3
(ppm)

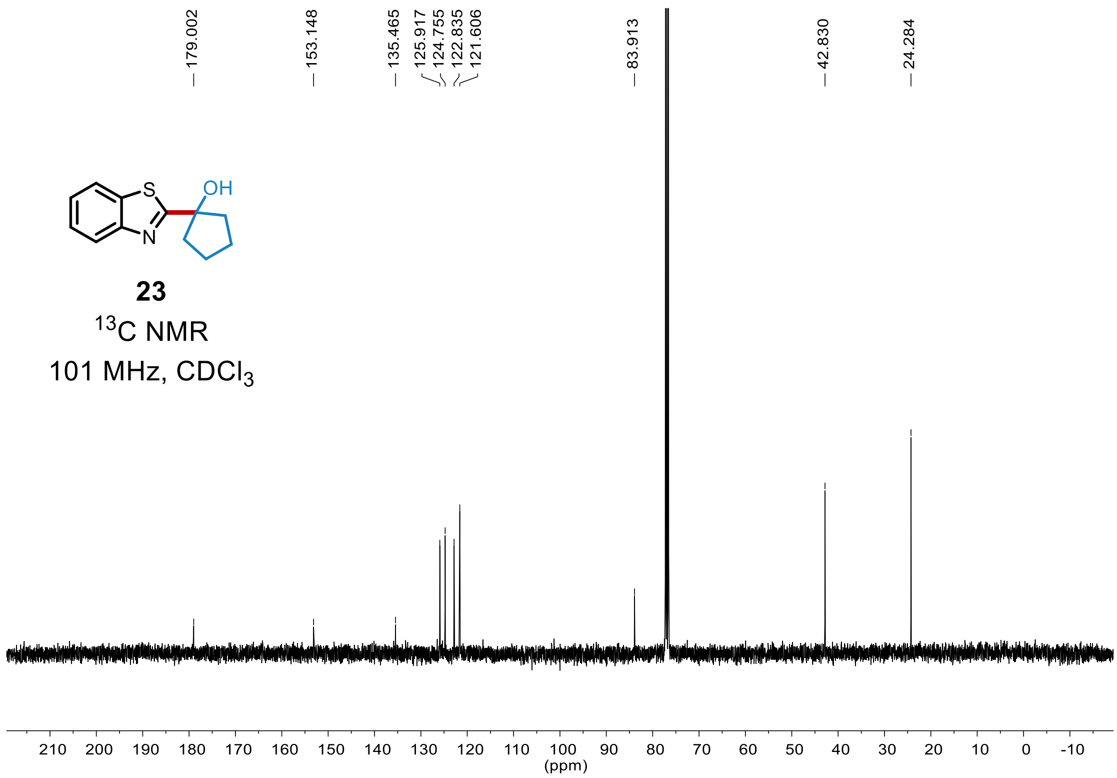

7.990
7.976
7.885
7.883
7.871
7.870
7.869
7.481
7.479
7.468
7.467
7.465
7.455
7.453
7.381
7.379
7.369
7.368
7.366
7.356
7.354
3.274
1.755
0.000
S
N
OH
21
1H NMR
600 MHz, CDCl3
1.00
1.00
1.02
1.03
1.01
6.01
(ppm)

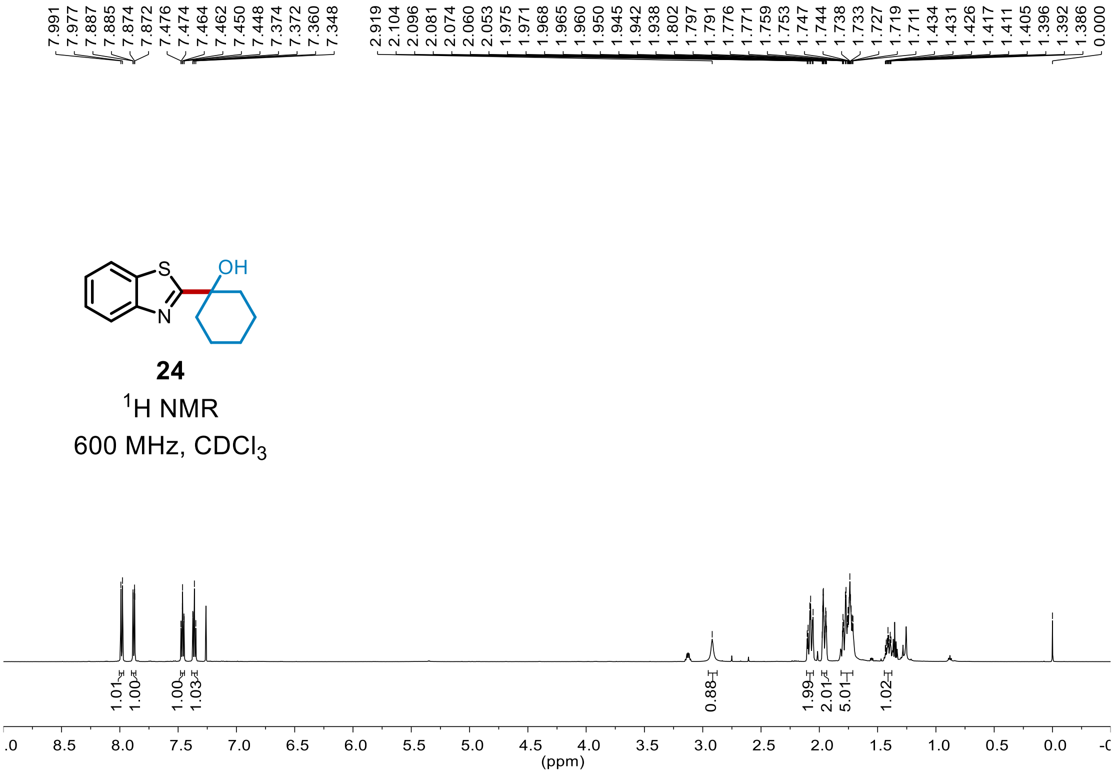

180.040
153.048
135.352
126.045
124.933
122.875
121.788
73.630
30.843
S
N
OH
21
13C NMR
151 MHz, CDCl3
(ppm)

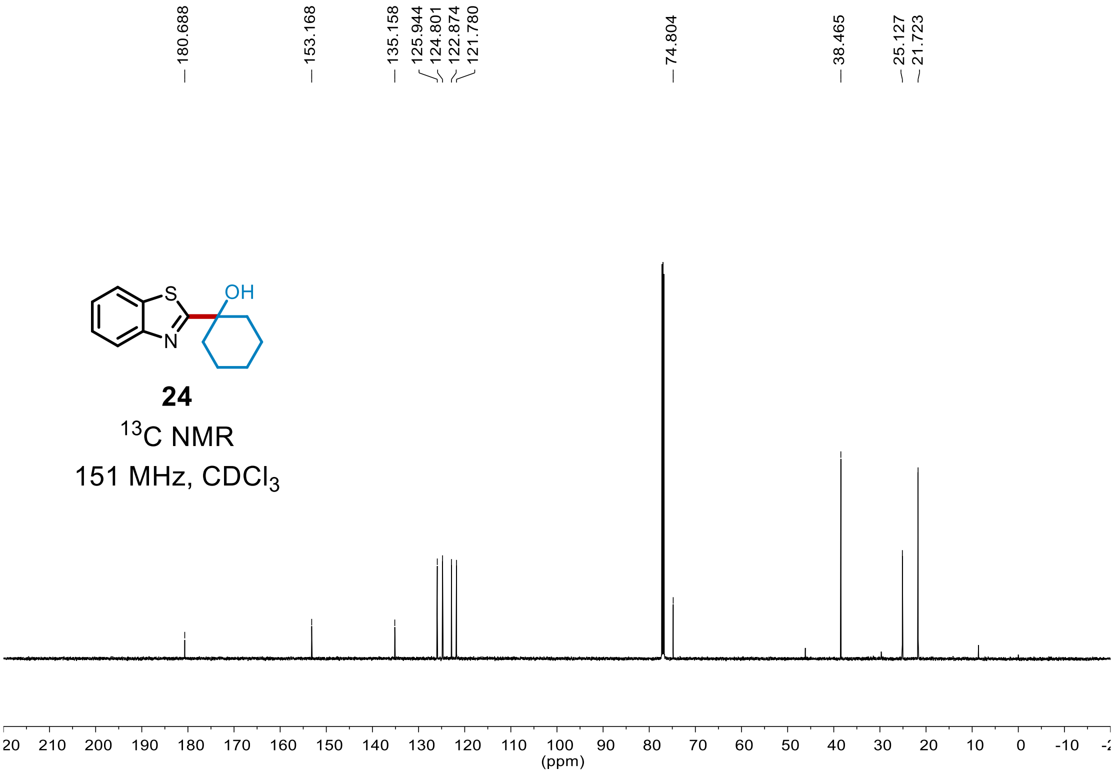

8.004
7.991
7.895
7.893
7.881
7.879
7.494
7.492
7.482
7.480
7.478
7.468
7.466
7.396
7.394
7.383
7.380
7.371
7.369
3.346
2.097
2.084
2.072
2.060
2.048
2.036
2.032
2.020
2.008
1.996
1.983
1.718
0.945
0.933
0.921
-0.000
OH
S
N
22
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.00
1.04
1.04
0.92
2.01
3.01
3.02
(ppm)

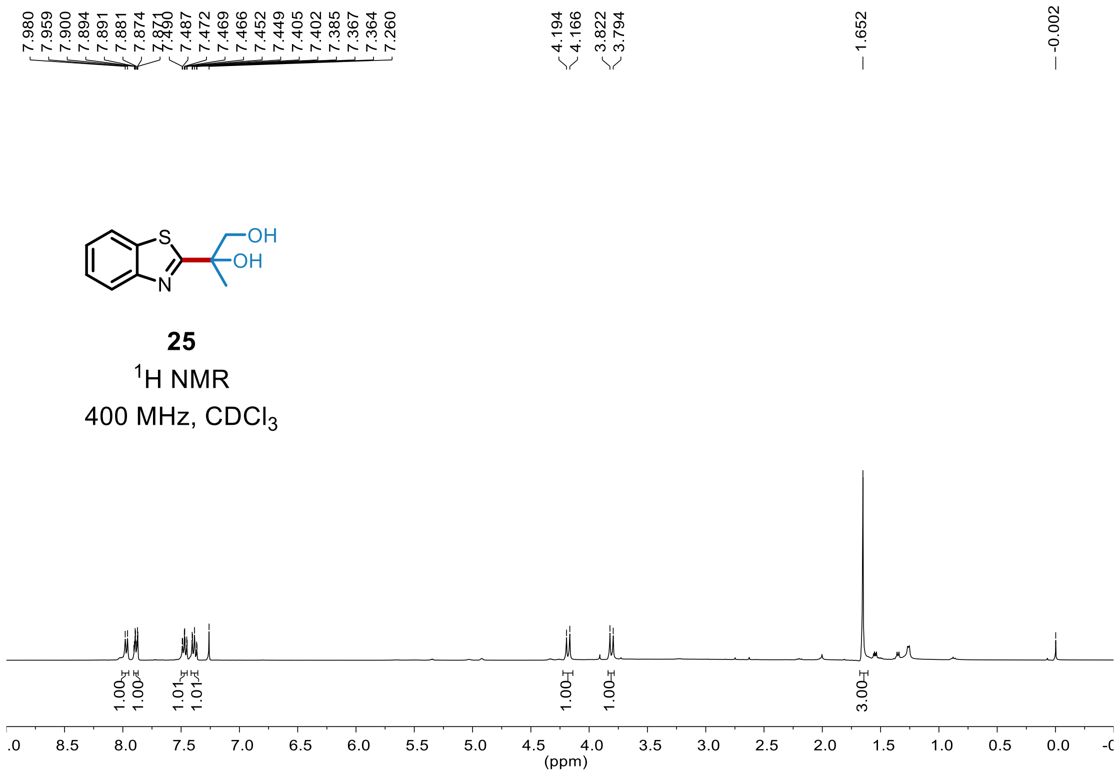

179.381
152.588
135.393
126.105
124.984
122.834
121.792
36.356
29.227
8.001
OH
S
N
22
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)

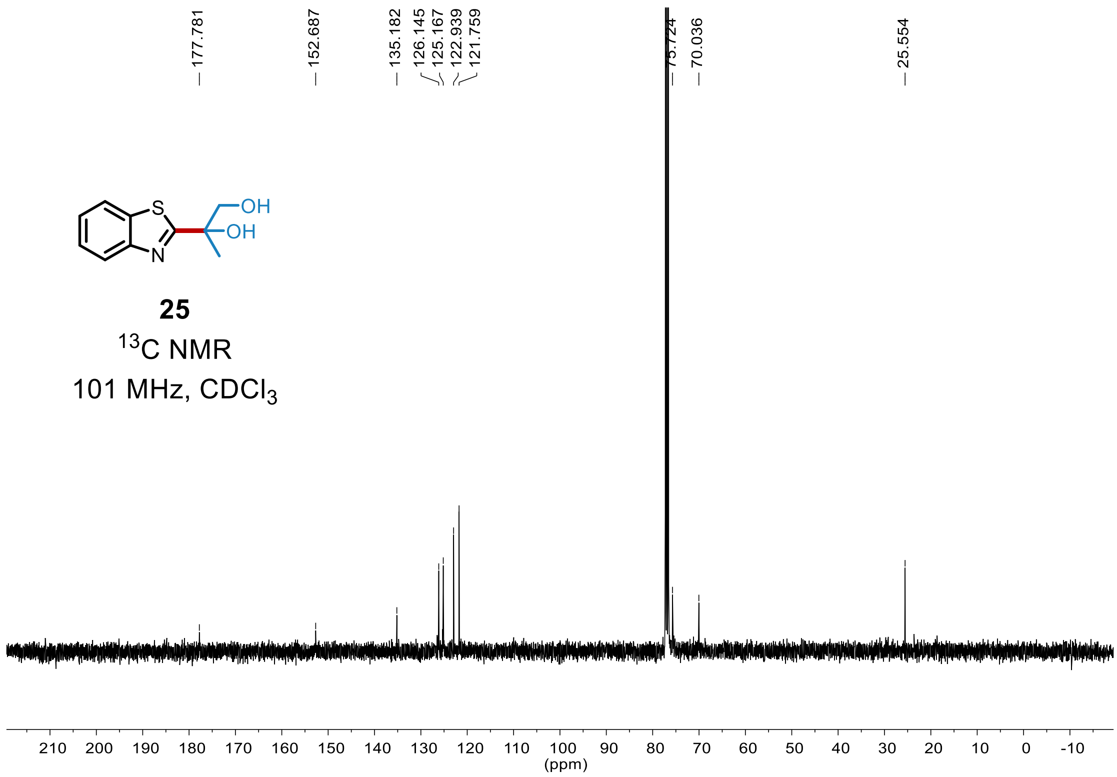

7.988 7.968 7.886 7.884 7.867 7.864 7.486 7.483 7.465 7.448 7.444 7.384 7.381 7.363 7.346 7.343 7.260 2.357 2.346 2.336 2.321 2.312 2.304 2.298 2.288 2.283 2.143 2.136 2.128 2.120 2.115 2.104 2.098 2.087 2.082 2.075 2.070 2.058 2.053 2.049 2.046 2.038 2.032 2.026 2.018 2.007 1.998 1.989 1.986 1.980 1.972 1.965 1.958 1.950 1.945 1.937 1.927 1.919 0.000
S
OH
N
23
^{1}H NMR
400 MHz, $CDCl_3$
1.00
1.01
1.02
1.01
0.80
2.00
2.01
4.01
(ppm)

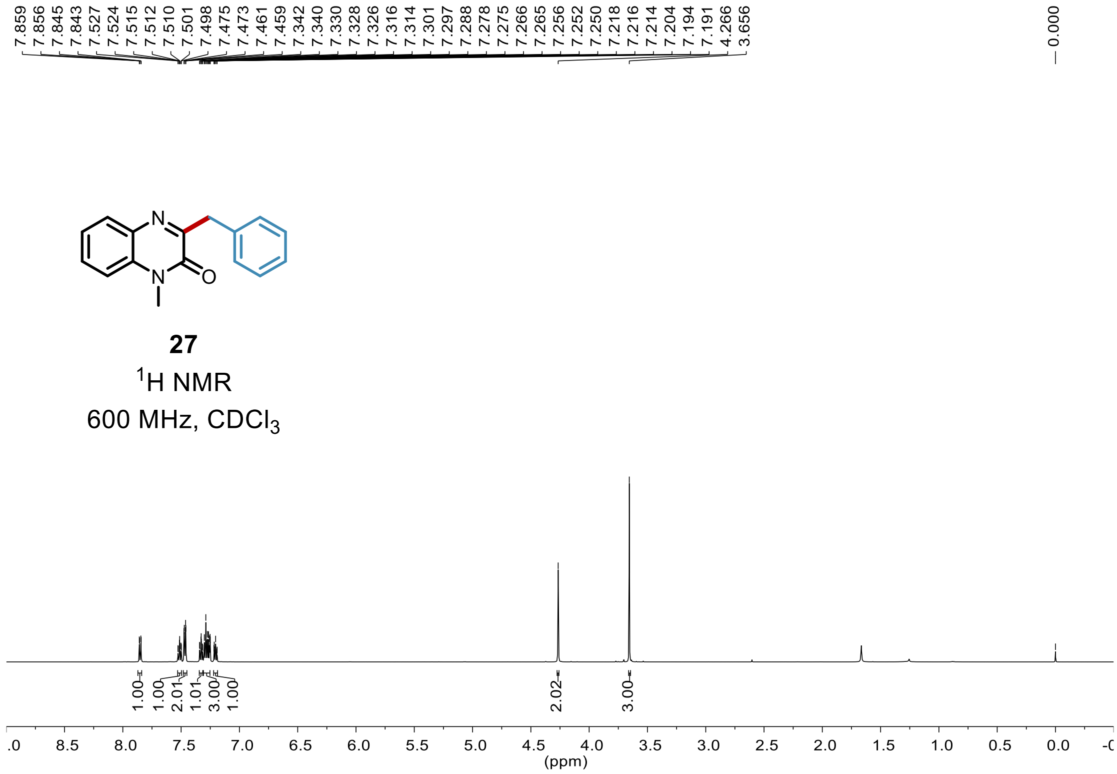

179.002
153.148
135.465
125.917
124.755
122.835
121.606
83.913
42.830
24.284
S
OH
N
23
^{13}C NMR
101 MHz, $CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)

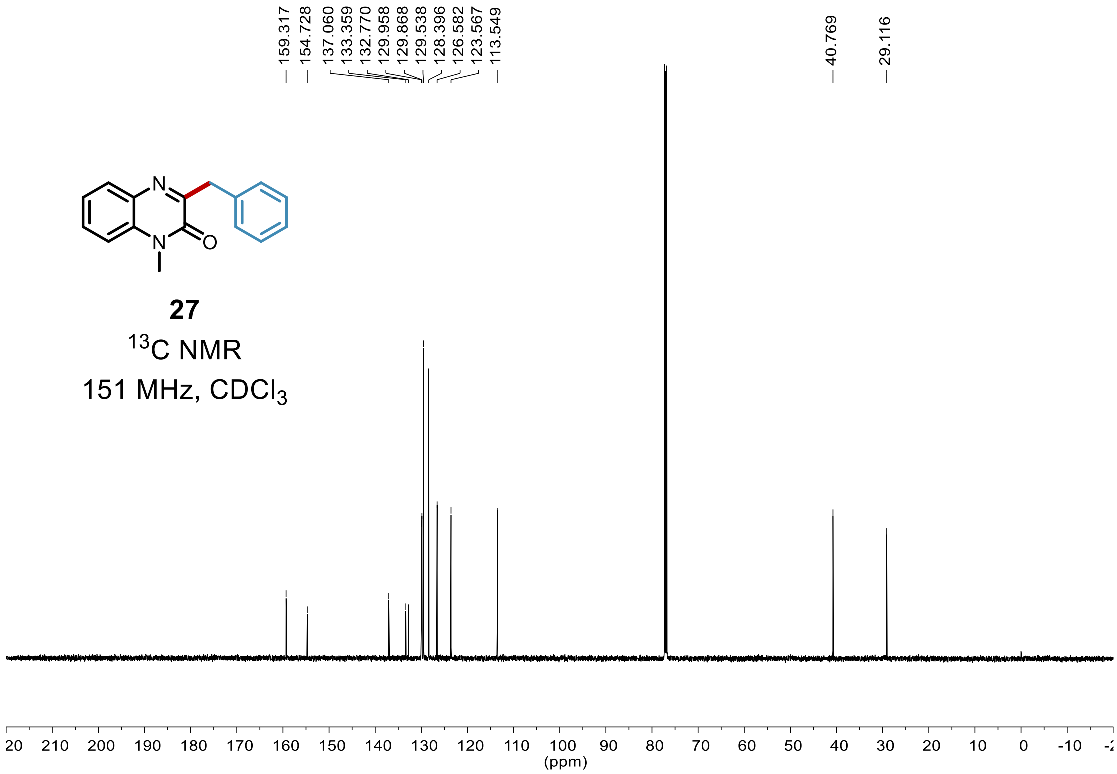

7.991 7.977 7.887 7.885 7.874 7.872 7.476 7.474 7.464 7.462 7.450 7.448 7.374 7.372 7.360 7.348
2.919 2.104 2.096 2.081 2.074 2.060 2.053 1.975 1.971 1.968 1.965 1.960 1.950 1.945 1.942 1.938 1.802 1.797 1.791 1.776 1.771 1.759 1.753 1.747 1.744 1.738 1.733 1.727 1.719 1.711 1.434 1.431 1.426 1.417 1.411 1.405 1.396 1.392 1.386 0.000
S
N
OH
24
^{1}H NMR
600 MHz, $CDCl_3$
1.01 1.00 1.00 1.03 0.88 1.99 2.01 5.01 1.02
(ppm)

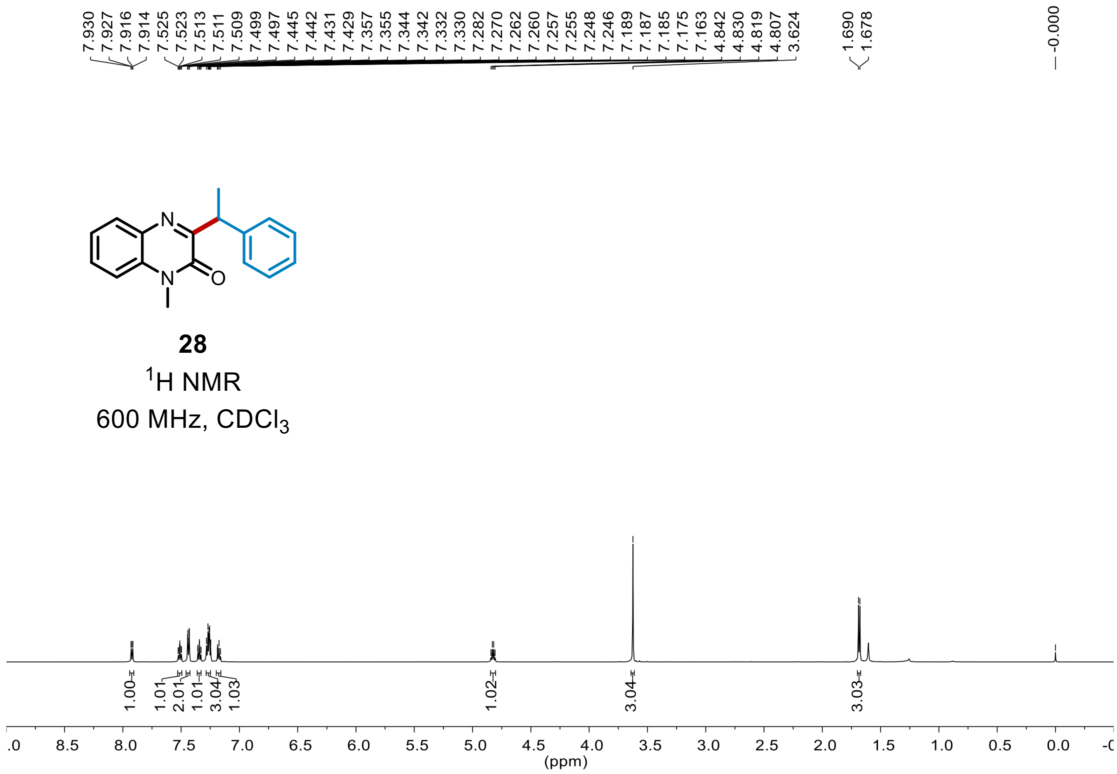

180.688
153.168
135.158 125.944 124.801 122.874 121.780
74.804
38.465
25.127 21.723
S
N
OH
24
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)

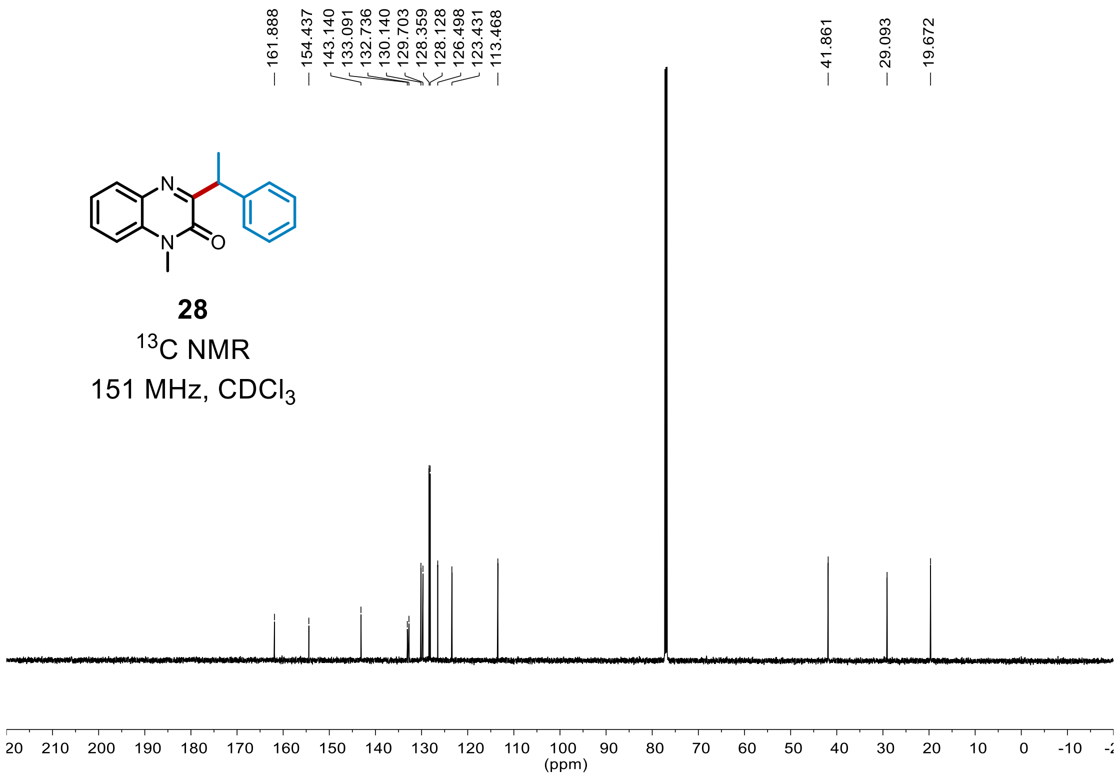

7.980 7.959 7.900 7.894 7.891 7.881 7.874 7.871 7.490 7.487 7.472 7.469 7.466 7.452 7.449 7.405 7.402 7.385 7.367 7.364 7.260
4.194 4.166 3.822 3.794
1.652
-0.002
S
N
OH
OH
25
^{1}H NMR
400 MHz, $CDCl_3$
1.00 1.00 1.01 1.01 1.00 1.00 3.00
(ppm)

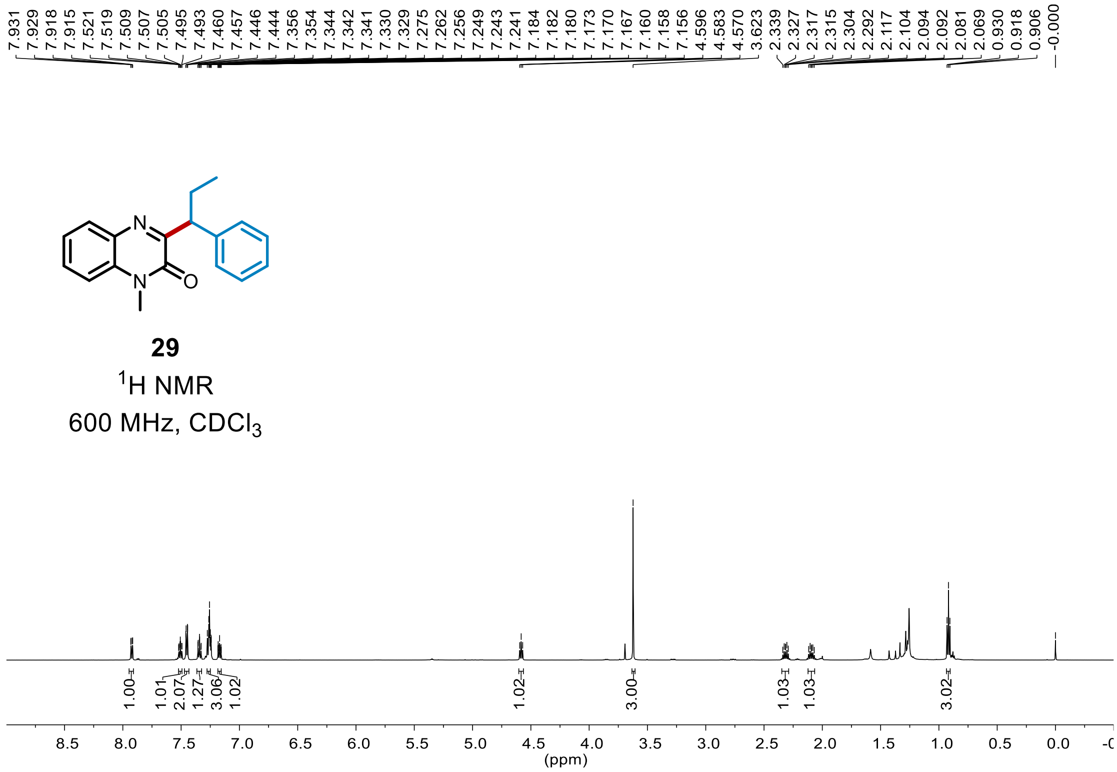

177.781
152.687
135.182 126.145 125.167 122.939 121.759
70.036
25.554
S
N
OH
OH
25
^{13}C NMR
101 MHz, $CDCl_3$
(ppm)

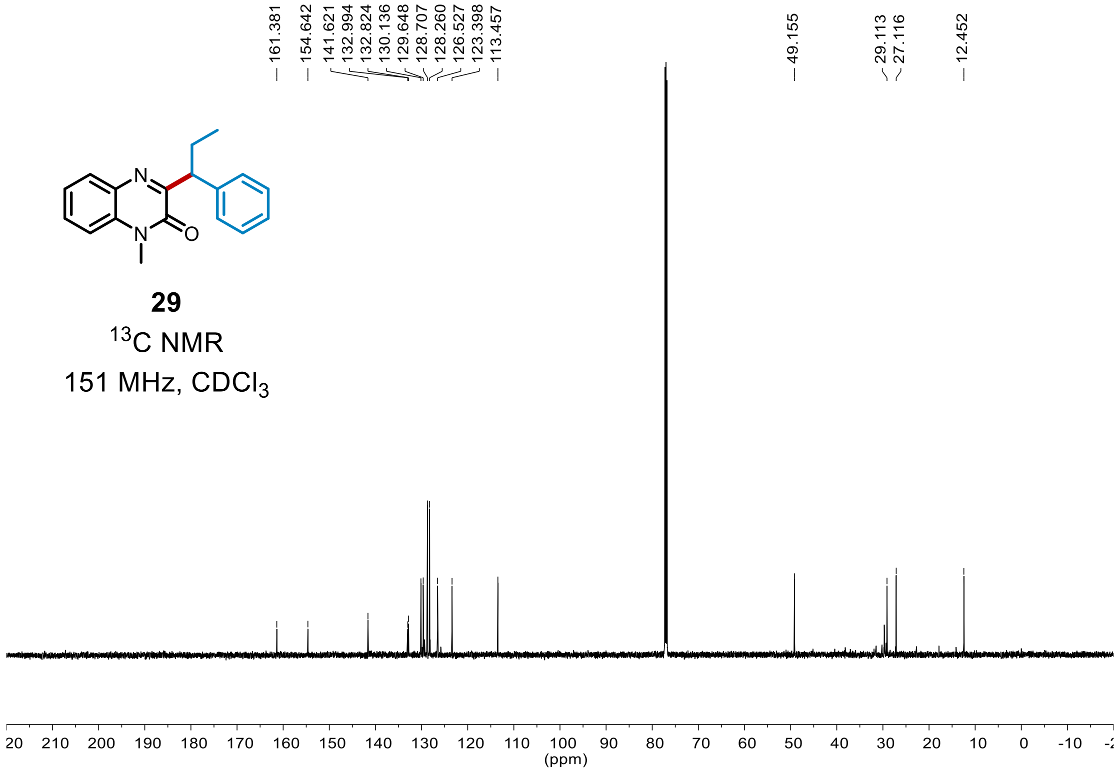

7.859
7.856
7.845
7.843
7.527
7.524
7.515
7.512
7.510
7.501
7.498
7.475
7.473
7.461
7.459
7.342
7.340
7.330
7.328
7.326
7.316
7.314
7.301
7.297
7.288
7.278
7.275
7.266
7.265
7.256
7.252
7.250
7.218
7.216
7.214
7.204
7.194
7.191
4.266
3.656
0.000
N
N
O
27
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.00
2.01
1.01
3.00
1.00
2.02
3.00
(ppm)

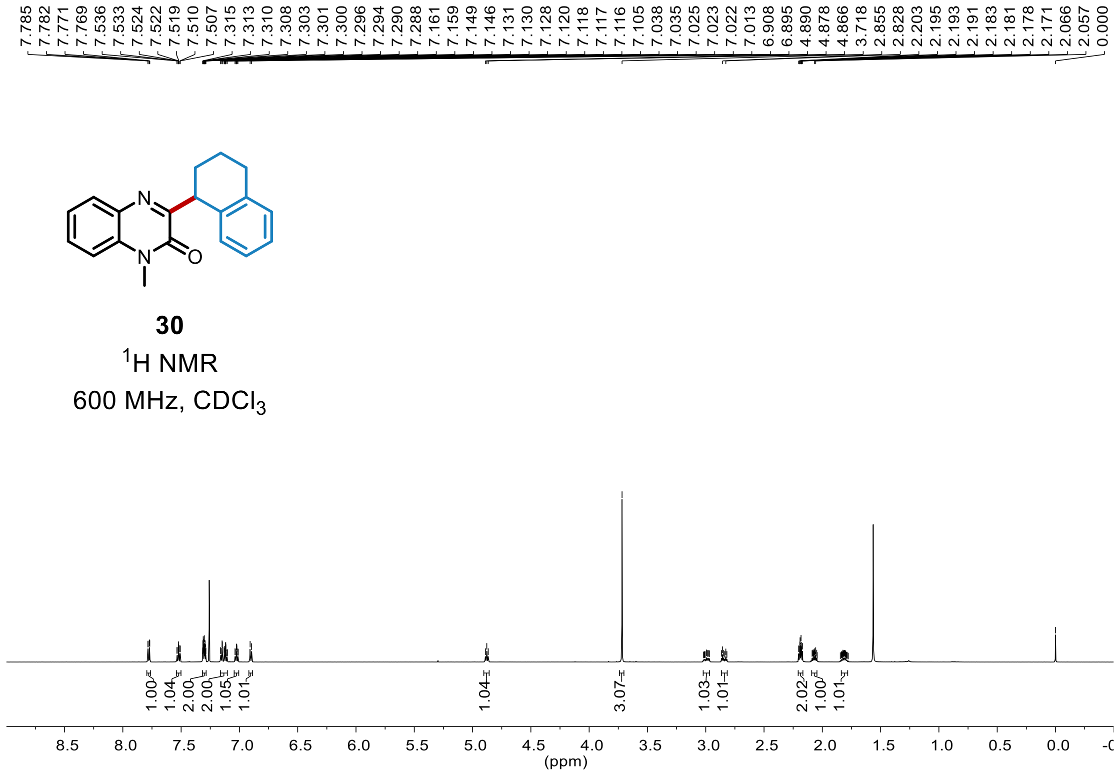

159.317
154.728
137.060
133.359
132.770
129.958
129.868
129.538
128.396
126.582
123.567
113.549
40.769
29.116
N
N
O
27
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)

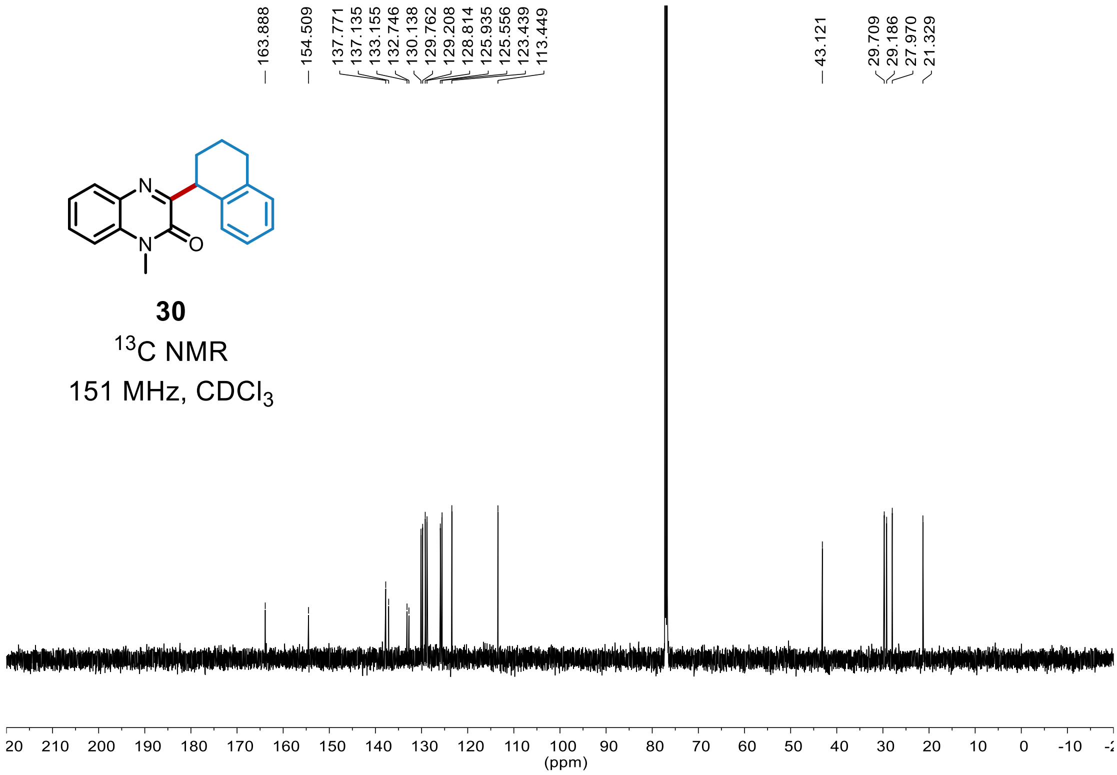

28
^{1}H NMR
600 MHz, $CDCl_3$
7.930
7.927
7.916
7.914
7.525
7.523
7.513
7.511
7.509
7.499
7.497
7.445
7.442
7.431
7.429
7.357
7.355
7.344
7.342
7.332
7.330
7.282
7.270
7.262
7.260
7.257
7.255
7.248
7.246
7.189
7.187
7.185
7.175
7.163
4.842
4.830
4.819
4.807
3.624
1.690
1.678
-0.000
1.00
1.01
2.01
1.01
3.04
1.03
1.02
3.04
3.03
(ppm)

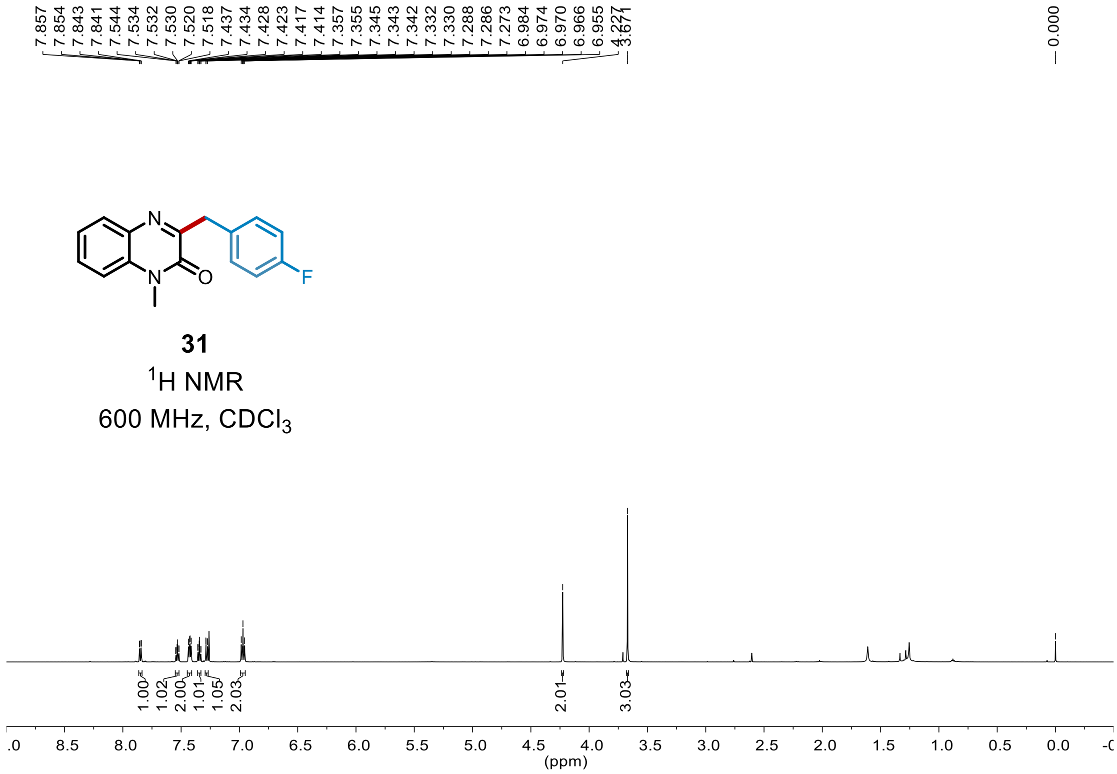

28
^{13}C NMR
151 MHz, $CDCl_3$
161.888
154.437
143.140
133.091
132.736
130.140
129.703
128.359
128.128
126.498
123.431
113.468
41.861
29.093
19.672
(ppm)

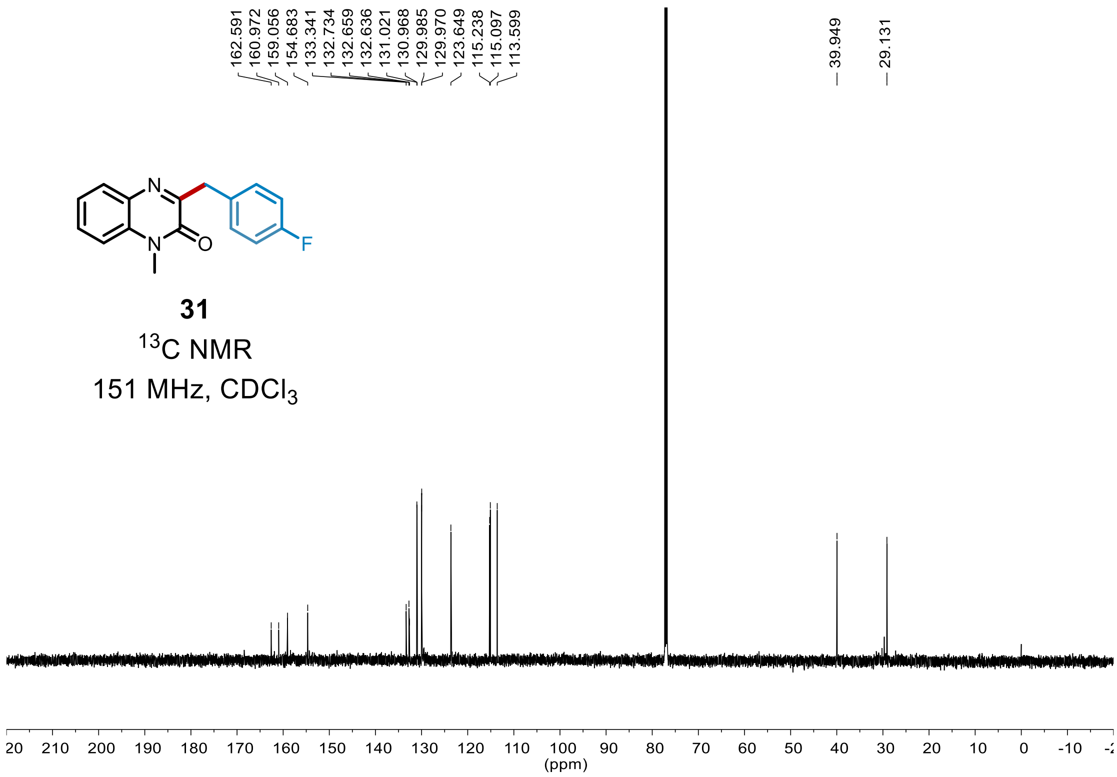

7.931 7.929 7.918 7.915 7.521 7.519 7.509 7.507 7.505 7.495 7.493 7.460 7.457 7.446 7.444 7.356 7.354 7.344 7.342 7.341 7.330 7.329 7.275 7.262 7.256 7.249 7.243 7.241 7.184 7.182 7.180 7.173 7.170 7.167 7.160 7.158 7.156 4.596 4.583 4.570 3.623 2.339 2.327 2.317 2.315 2.304 2.292 2.117 2.104 2.094 2.092 2.081 2.069 0.930 0.918 0.906 -0.000
N
N
O
29
^{1}H NMR
600 MHz, $CDCl_3$
1.00 1.01 2.07 1.27 3.06 1.02 1.02 3.00 1.03 1.03 3.02
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

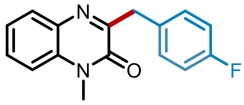

161.381 154.642 141.621 132.994 132.824 130.136 129.648 128.707 128.260 126.527 123.398 113.457 49.155 29.113 27.116 12.452
N
N
O
29
^{13}C NMR
151 MHz, $CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


7.785 7.782 7.771 7.769 7.536 7.533 7.524 7.522 7.519 7.510 7.507 7.315 7.313 7.310 7.308 7.303 7.301 7.300 7.296 7.294 7.290 7.288 7.161 7.159 7.149 7.146 7.131 7.130 7.128 7.120 7.118 7.117 7.116 7.105 7.038 7.035 7.025 7.023 7.022 7.013 6.908 6.895 4.890 4.878 4.866 3.718 2.855 2.828 2.203 2.195 2.193 2.191 2.183 2.181 2.178 2.171 2.066 2.057 0.000
N
N
O
30
^{1}H NMR
600 MHz, $CDCl_3$
1.00 1.04 2.00 2.00 1.05 1.01 1.04 3.07 1.03 1.01 2.02 1.00 1.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)


163.888
154.509
137.771 137.135 133.155 132.746 130.138 129.762 129.208 128.814 125.935 125.556 123.439 113.449
43.121
29.709 29.186 27.970 21.329
N
N
O
30
^{13}C NMR
151 MHz, $CDCl_3$
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
(ppm)


7.857 7.854 7.843 7.841 7.544 7.534 7.532 7.530 7.520 7.518 7.437 7.434 7.428 7.423 7.417 7.414 7.357 7.355 7.345 7.343 7.342 7.332 7.330 7.288 7.286 7.273 6.984 6.974 6.970 6.966 6.955 4.227 3.671
0.000
N
N
O
F
31
^{1}H NMR
600 MHz, $CDCl_3$
1.00 1.02 2.00 1.01 1.05 2.03
2.01
3.03
(ppm)

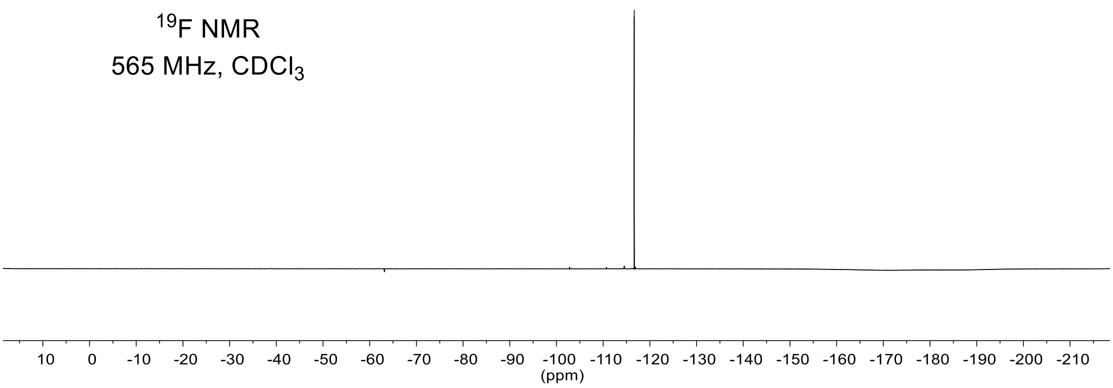

162.591 160.972 159.056 154.683 133.341 132.734 132.659 132.636 131.021 130.968 129.985 129.970 123.649 115.238 115.097 113.599
39.949
29.131
N
N
O
F
31
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)

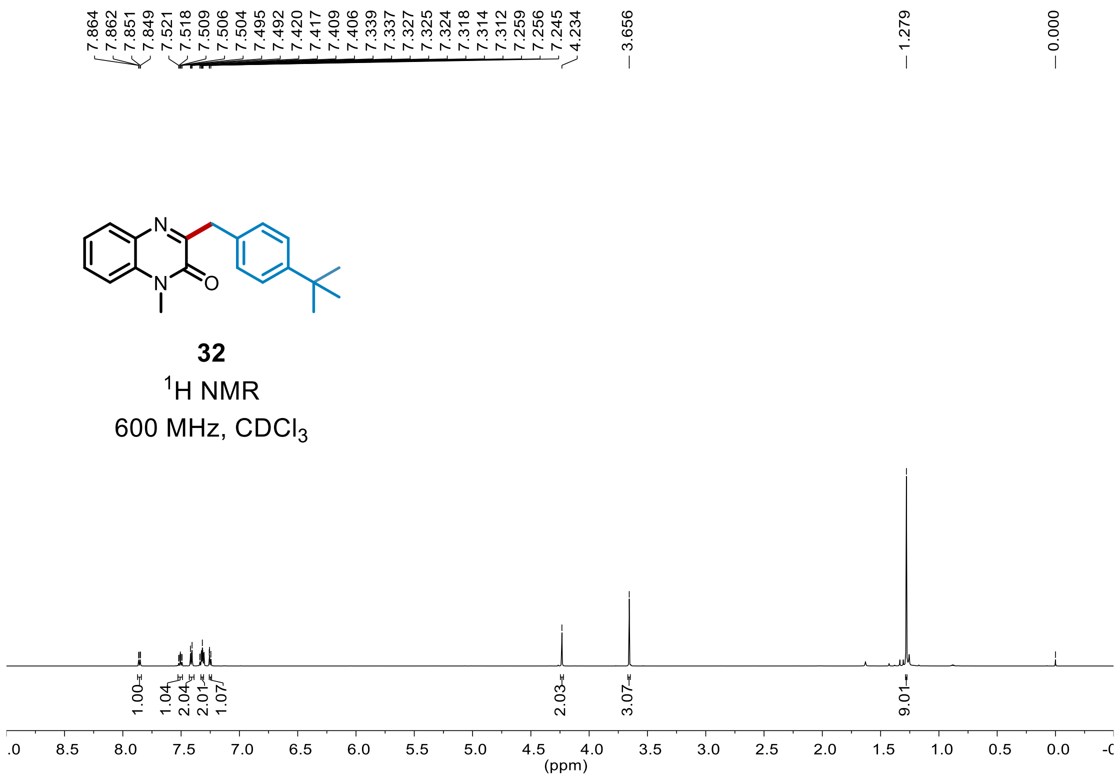


31

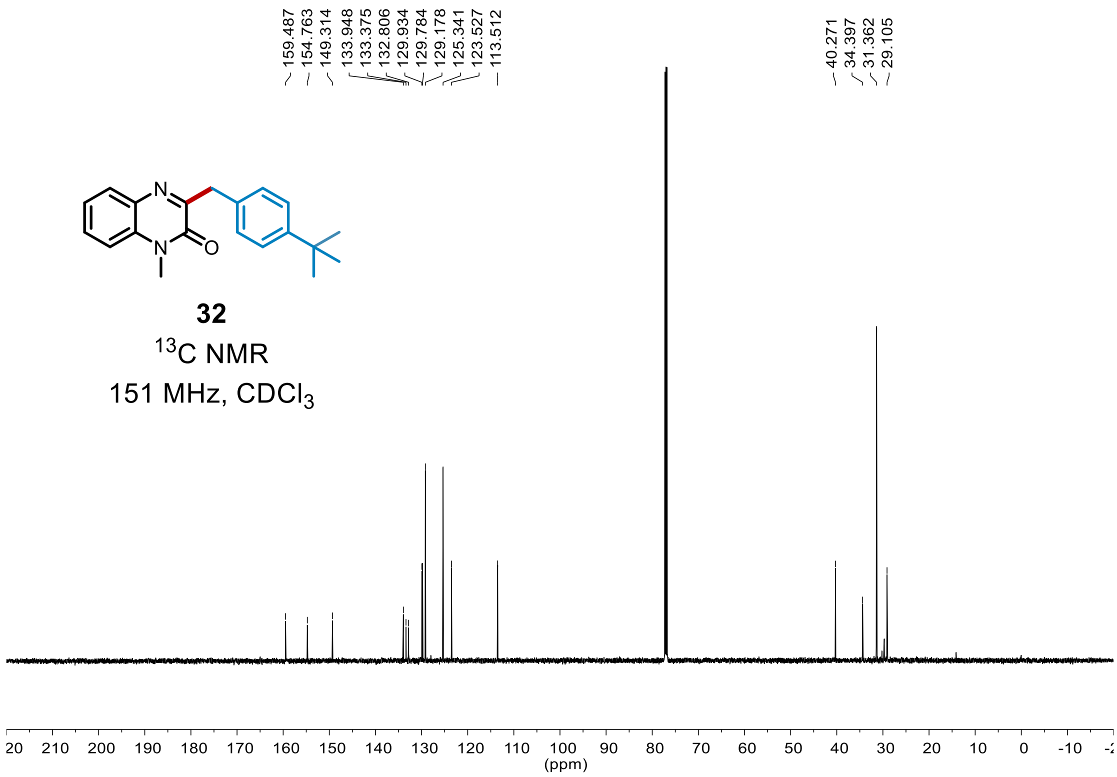
^{19}F NMR

565 MHz, $CDCl_3$

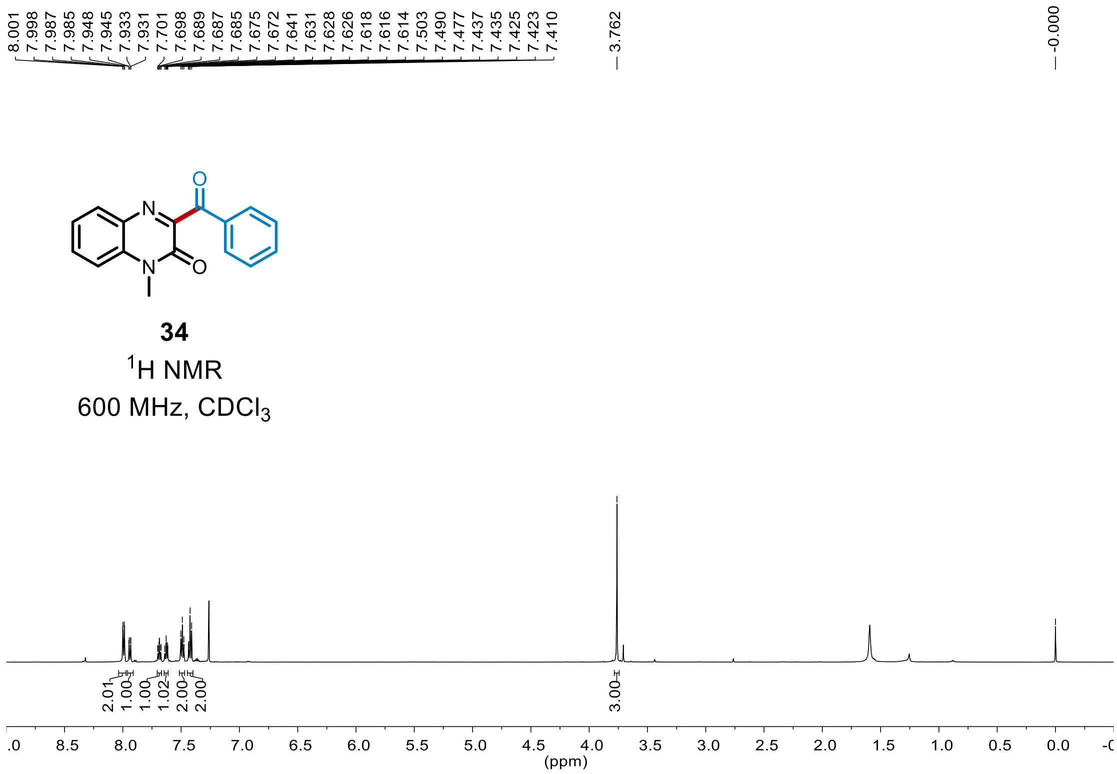




32
^1H NMR
600 MHz, $CDCl_3$



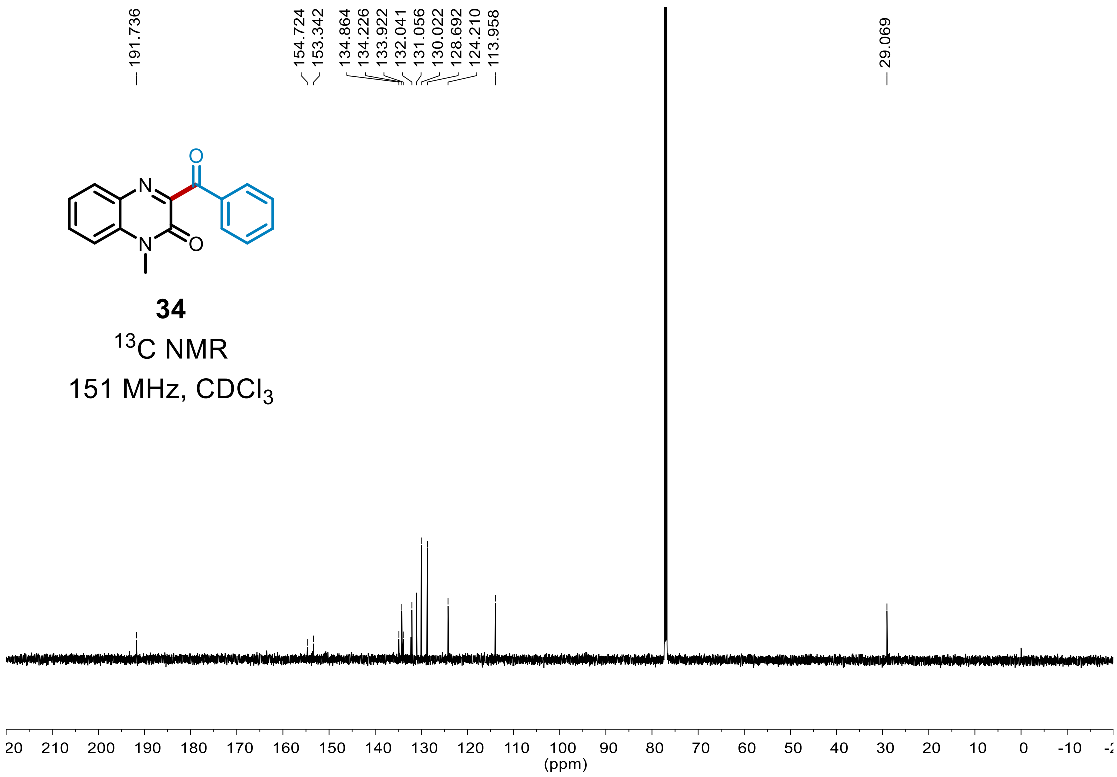
32
^{13}C NMR
151 MHz, $CDCl_3$



34

^{1}H NMR

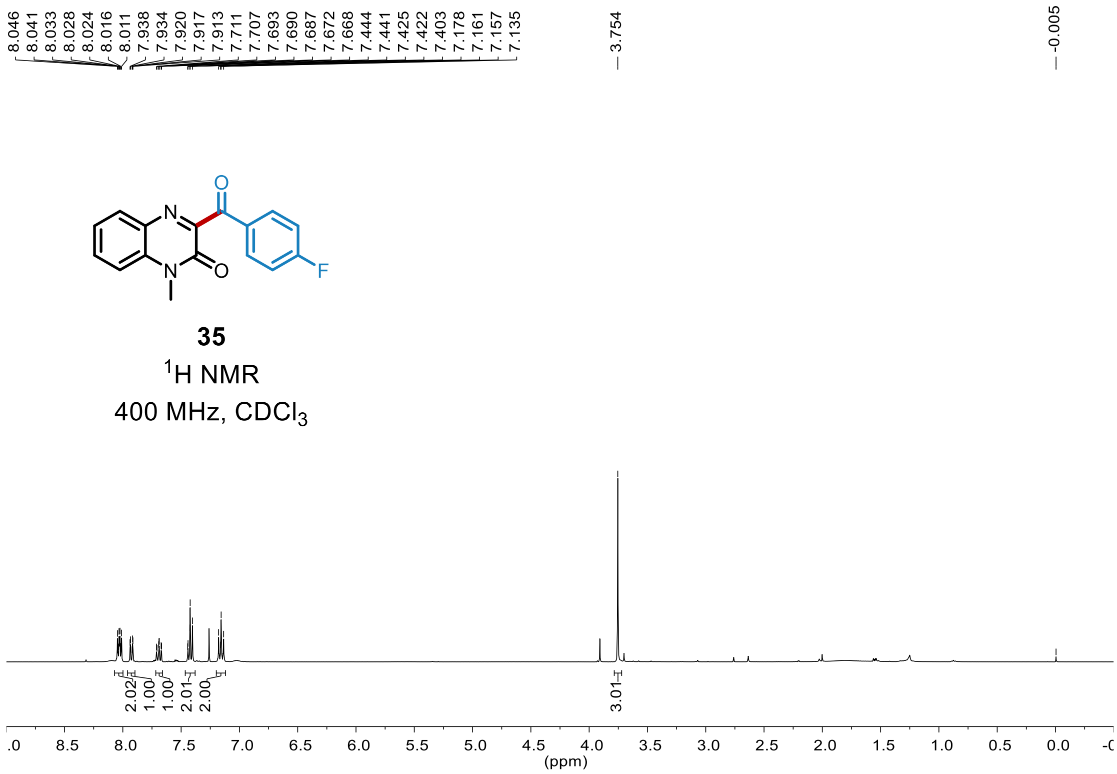
600 MHz, $CDCl_3$

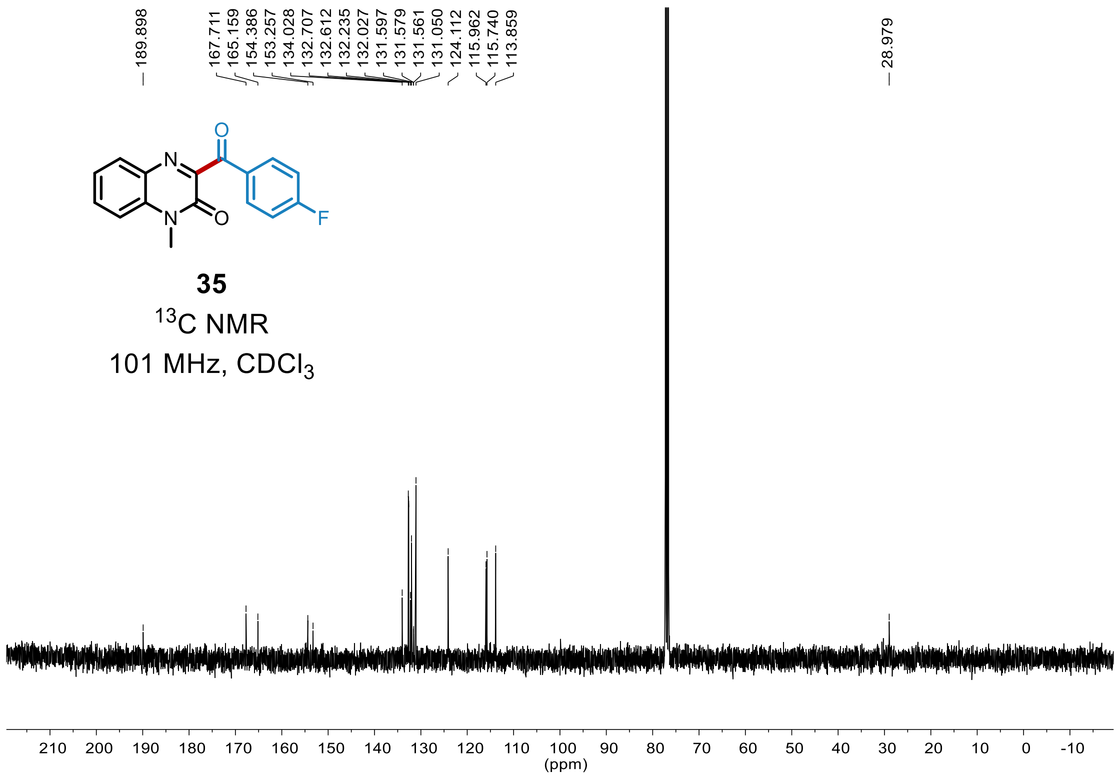


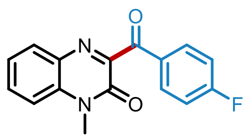
34

^{13}C NMR

151 MHz, $CDCl_3$


8.046 8.041 8.033 8.028 8.024 8.016 8.011 7.938 7.934 7.920 7.917 7.913 7.711 7.707 7.693 7.690 7.687 7.672 7.668 7.444 7.441 7.425 7.422 7.403 7.178 7.161 7.157 7.135
3.754
-0.005
N
O
N
O
F
35
^{1}H NMR
400 MHz, $CDCl_3$
2.02 1.00 1.00 2.01 2.00
3.01
(ppm)

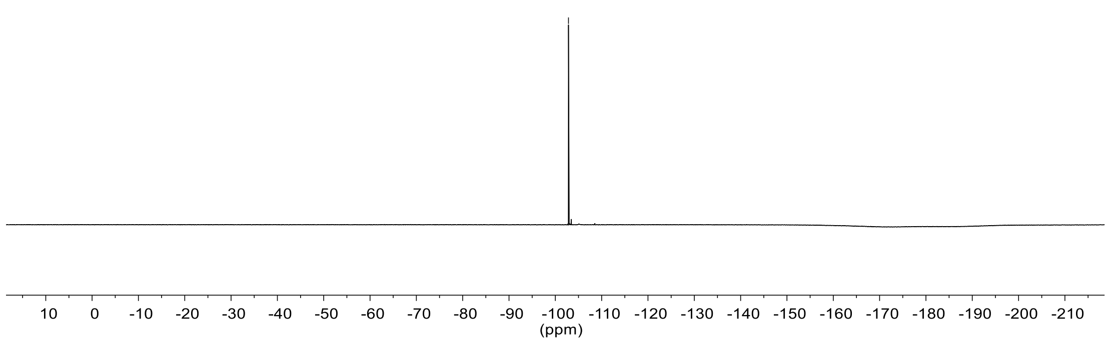

189.898
167.711 165.159 154.386 153.257 134.028 132.707 132.612 132.235 132.027 131.597 131.579 131.561 131.050 124.112 115.962 115.740 113.859
28.979
N
O
N
O
F
35
^{13}C NMR
101 MHz, $CDCl_3$
(ppm)

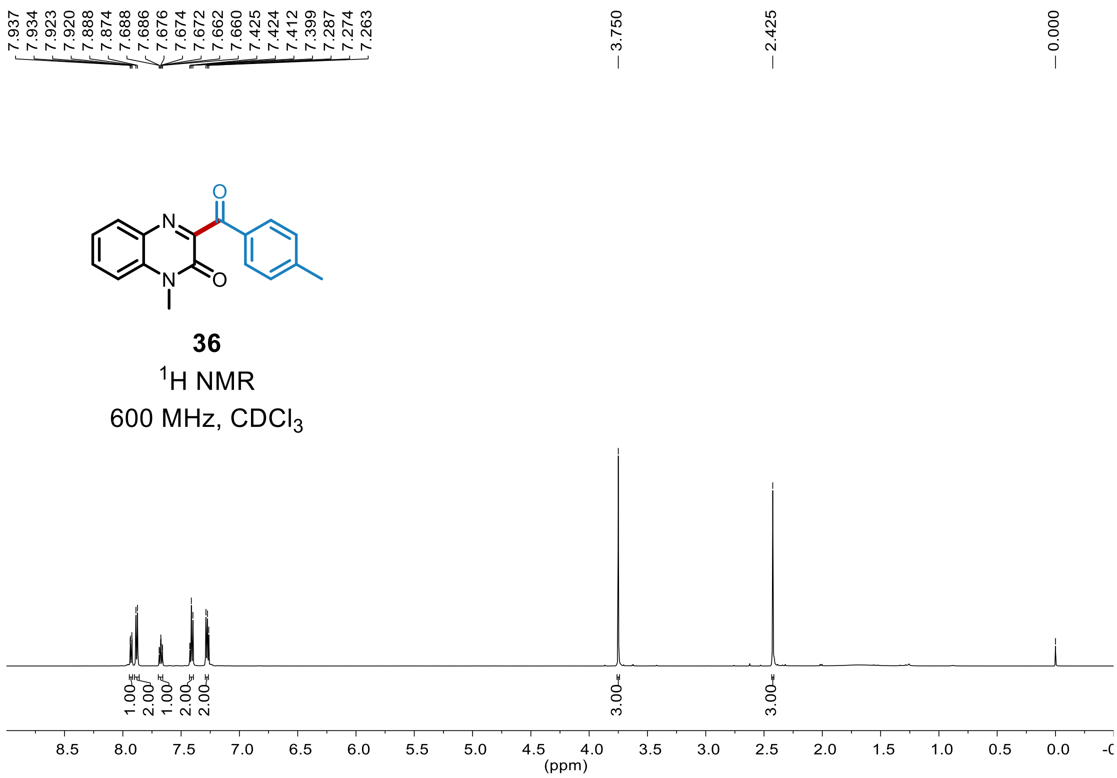


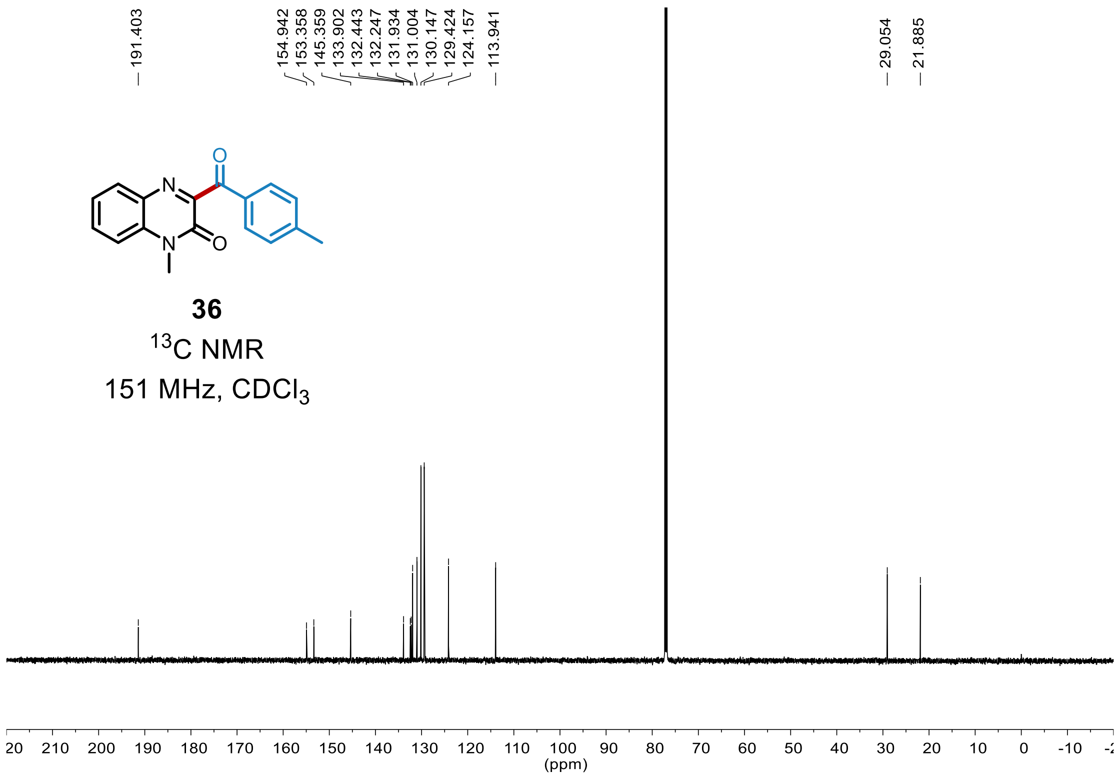
35

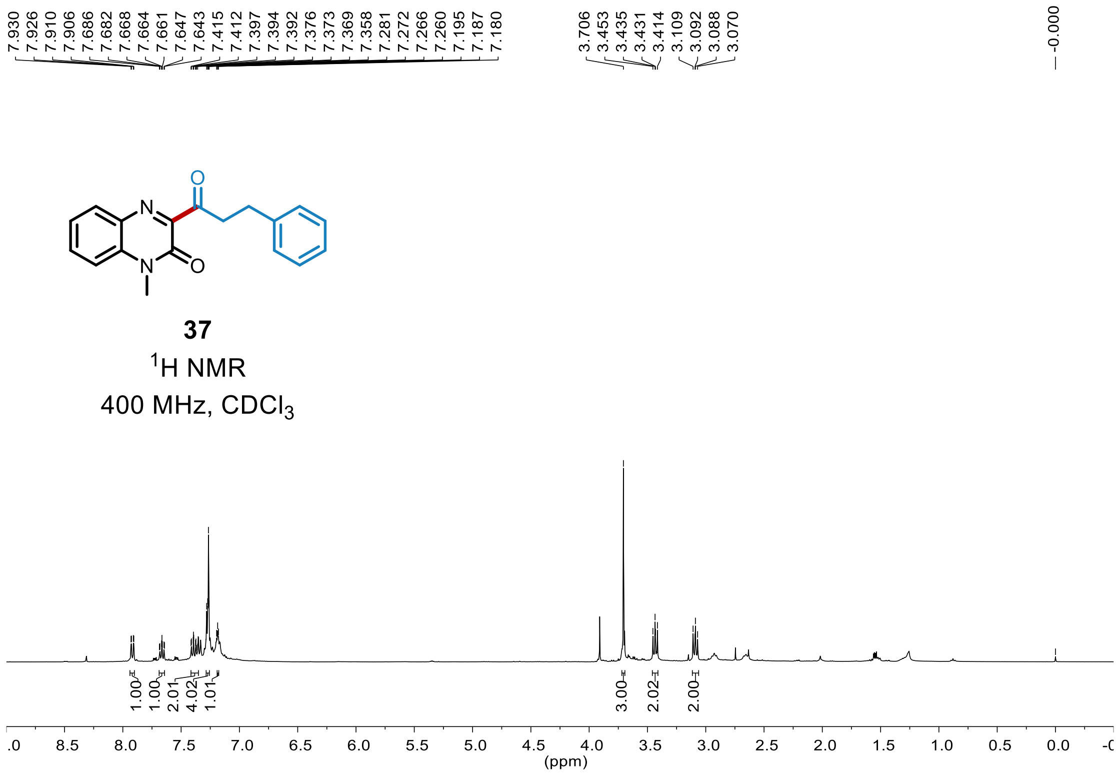
^{19}F NMR

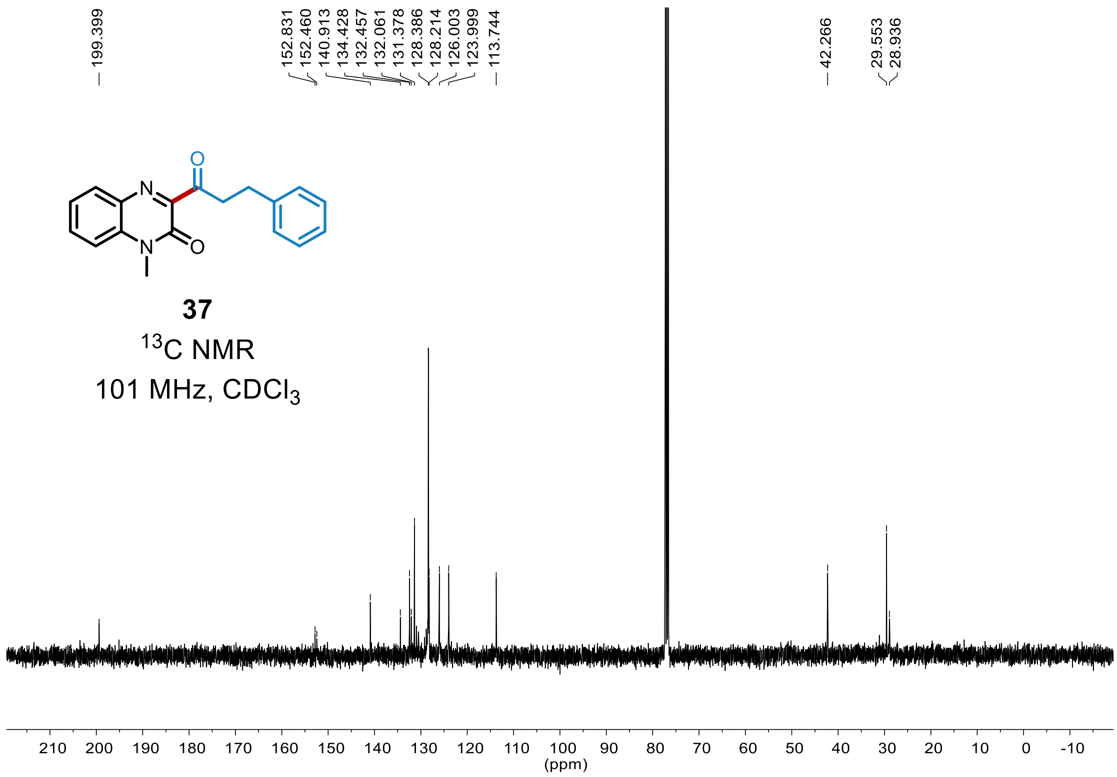
565 MHz, $CDCl_3$

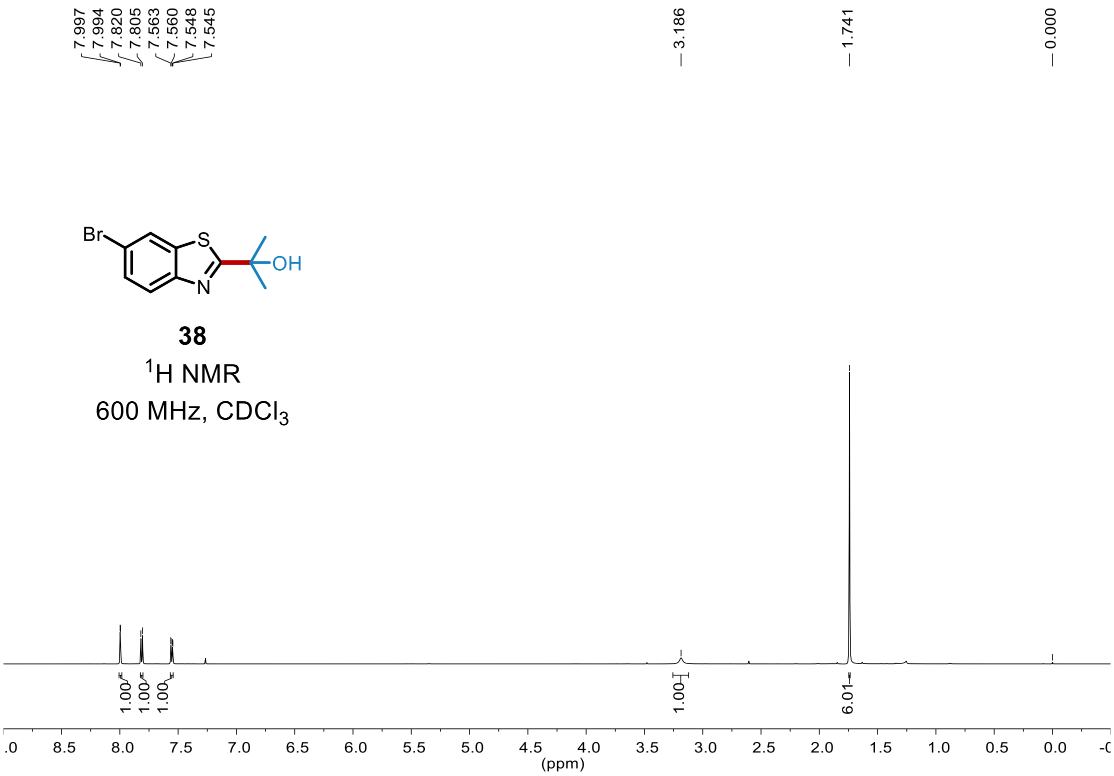


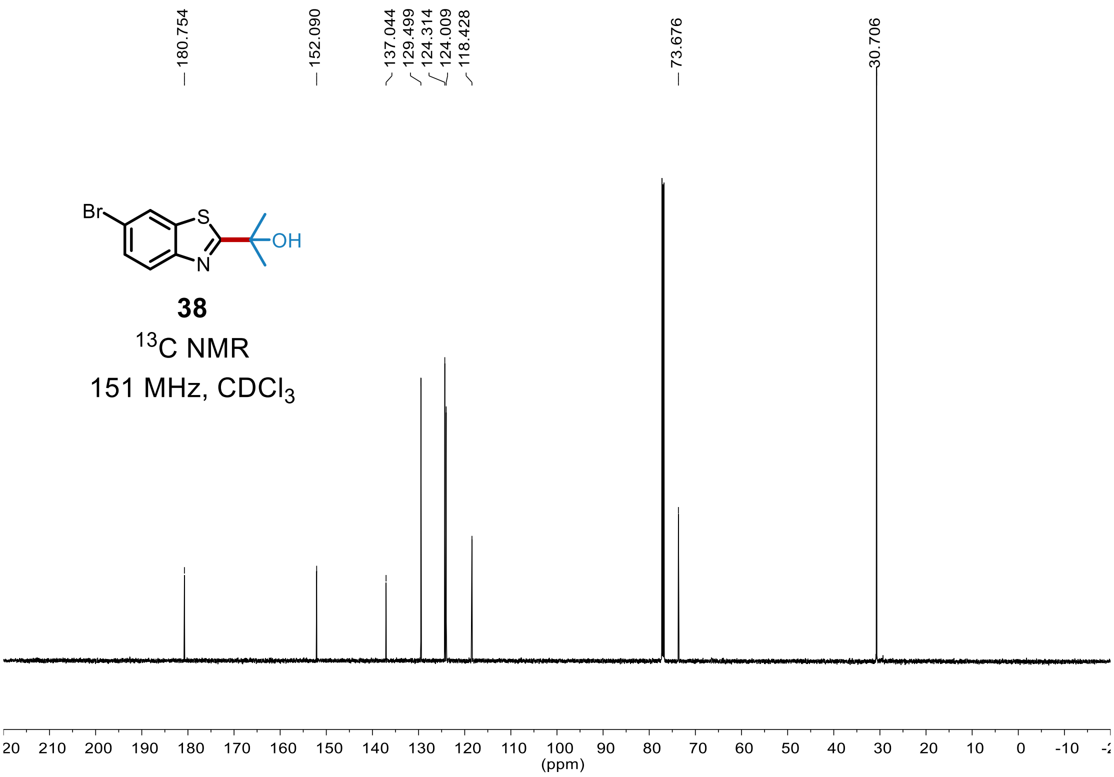

7.937
7.934
7.923
7.920
7.888
7.874
7.688
7.686
7.676
7.674
7.672
7.662
7.660
7.425
7.424
7.412
7.399
7.287
7.274
7.263
3.750
2.425
0.000
36
^{1}H NMR
600 MHz, $CDCl_3$
1.00
2.00
1.00
2.00
2.00
3.00
3.00
(ppm)

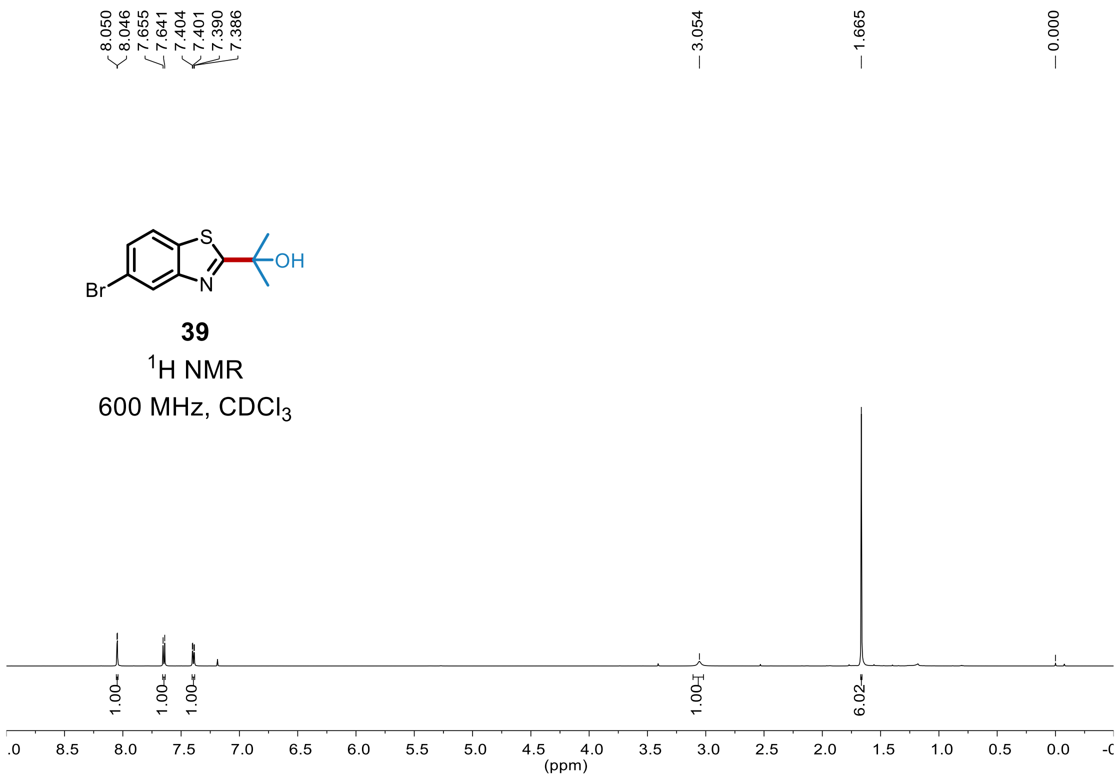

191.403
154.942
153.358
145.359
133.902
132.443
132.247
131.934
131.004
130.147
129.424
124.157
113.941
29.054
21.885
36
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)


7.930 7.926 7.910 7.906 7.686 7.682 7.668 7.664 7.661 7.647 7.643 7.415 7.412 7.397 7.394 7.392 7.376 7.373 7.369 7.358 7.281 7.272 7.266 7.260 7.195 7.187 7.180
3.706 3.453 3.435 3.431 3.414 3.109 3.092 3.088 3.070
-0.000
37
1H NMR
400 MHz, CDCl3
1.00 1.00 2.01 4.02 1.01
3.00 2.02 2.00
(ppm)

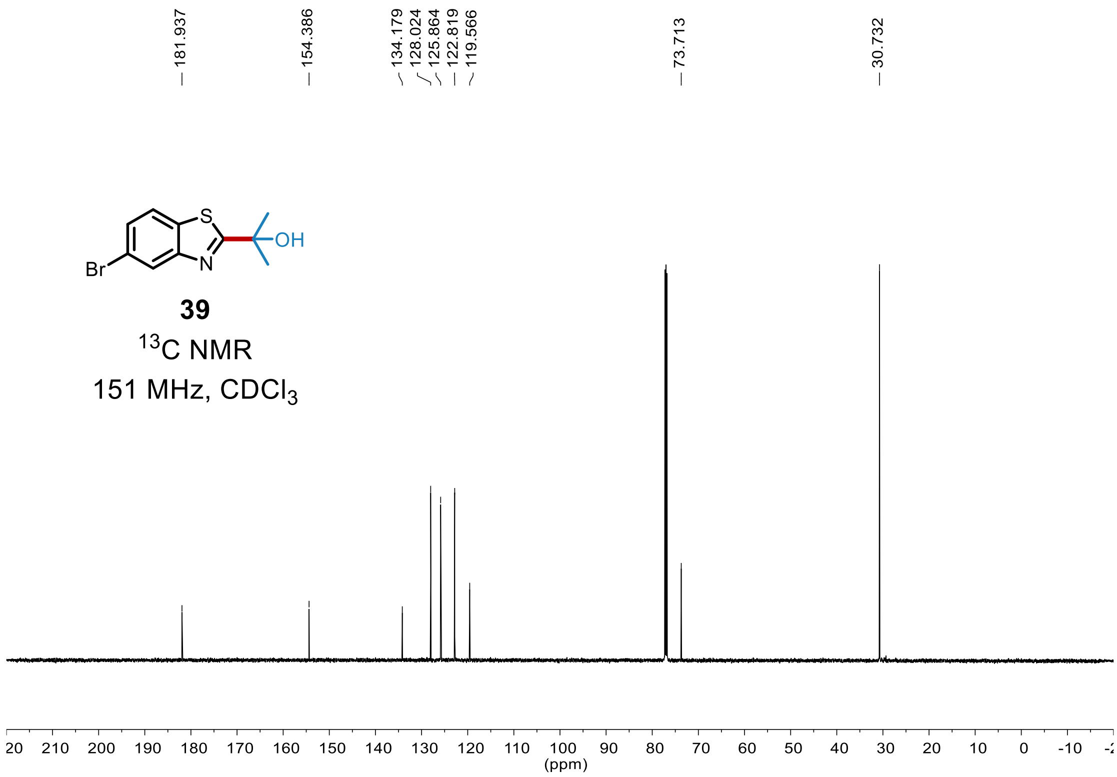

199.399
152.831 152.460 140.913 134.428 132.457 132.061 131.378 128.386 128.214 126.003 123.999 113.744
42.266
29.553 28.936
37
13C NMR
101 MHz, CDCl3
(ppm)


7.997
7.994
7.820
7.805
7.563
7.560
7.548
7.545
3.186
1.741
0.000
Br
S
N
OH
38
^{1}H NMR
600 MHz, CDCl$_3$
1.00
1.00
1.00
1.00
6.01
(ppm)

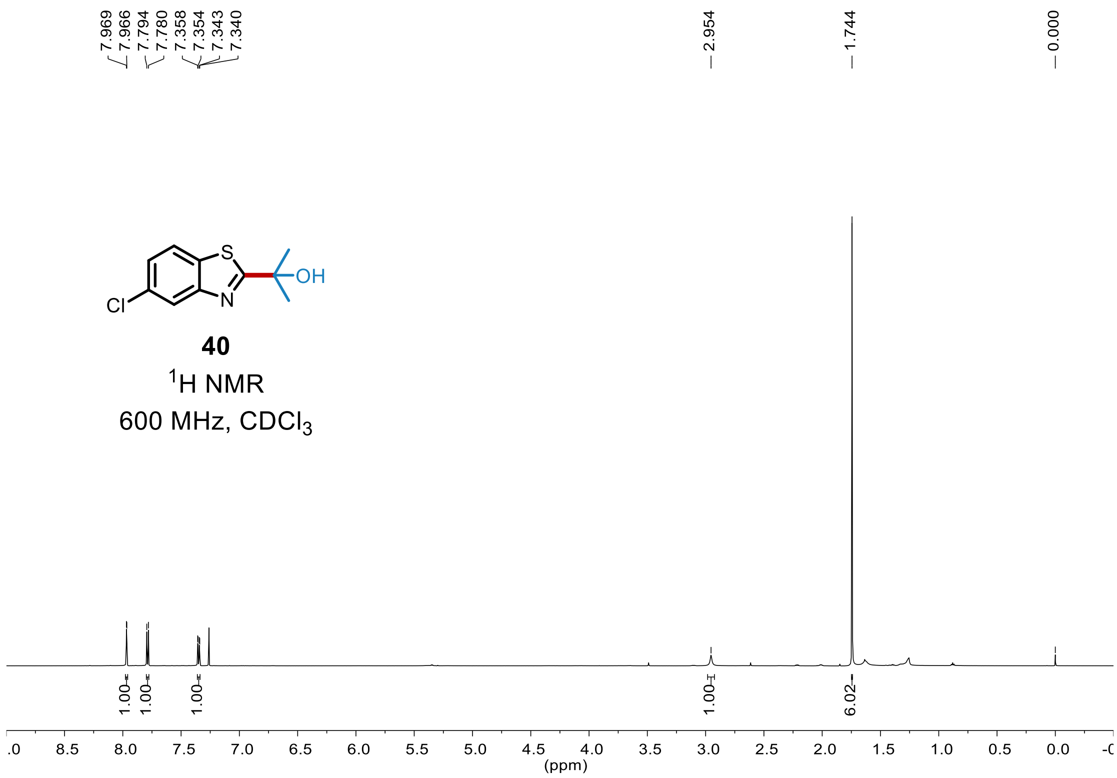

180.754
152.090
137.044
129.499
124.314
124.009
118.428
73.676
30.706
Br
S
N
OH
38
^{13}C NMR
151 MHz, CDCl$_3$
(ppm)

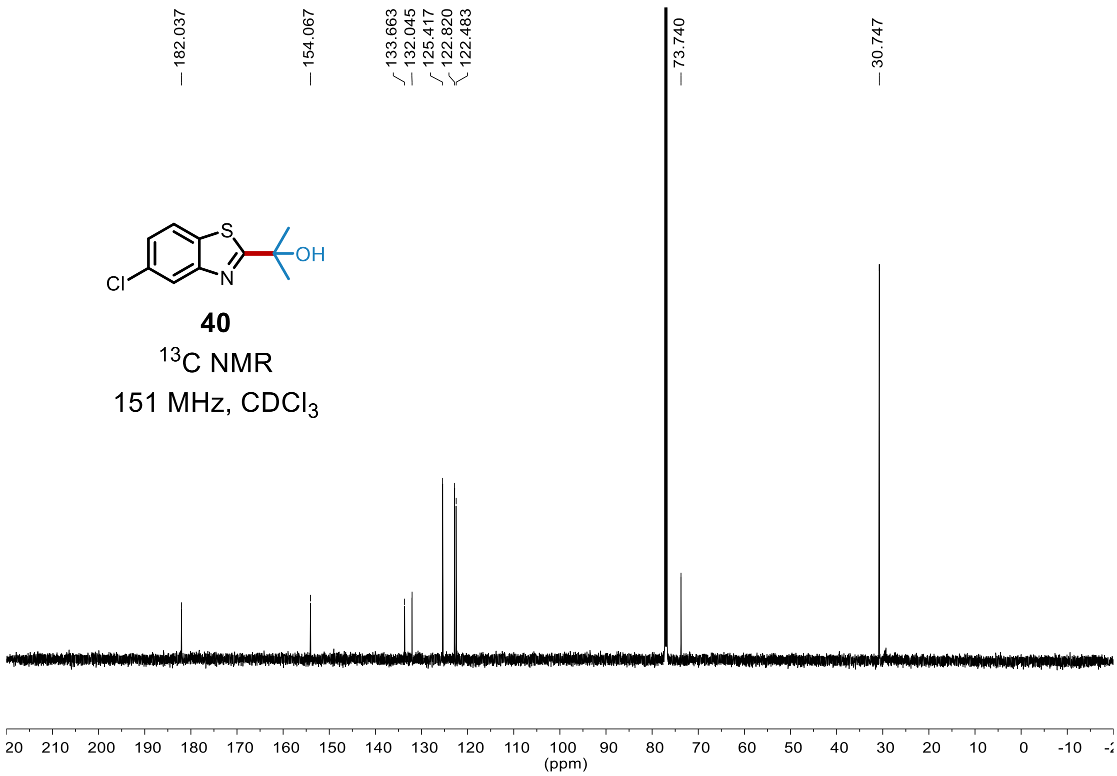


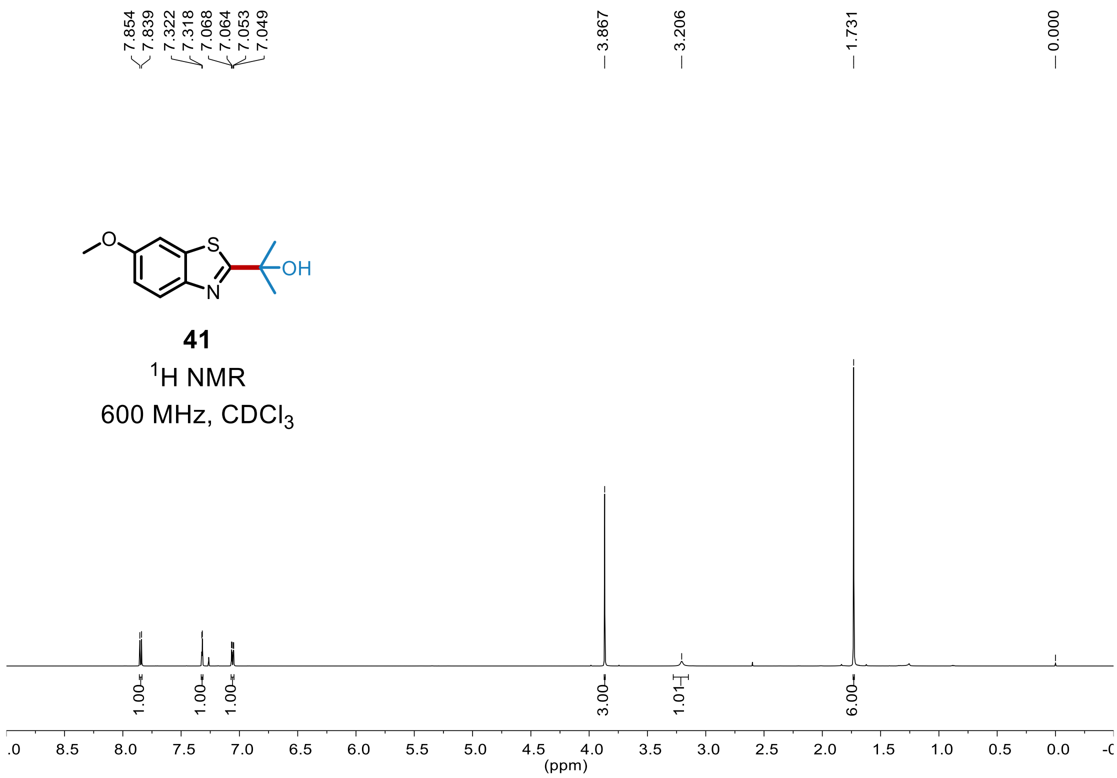
39
^{1}H NMR
600 MHz, $CDCl_3$

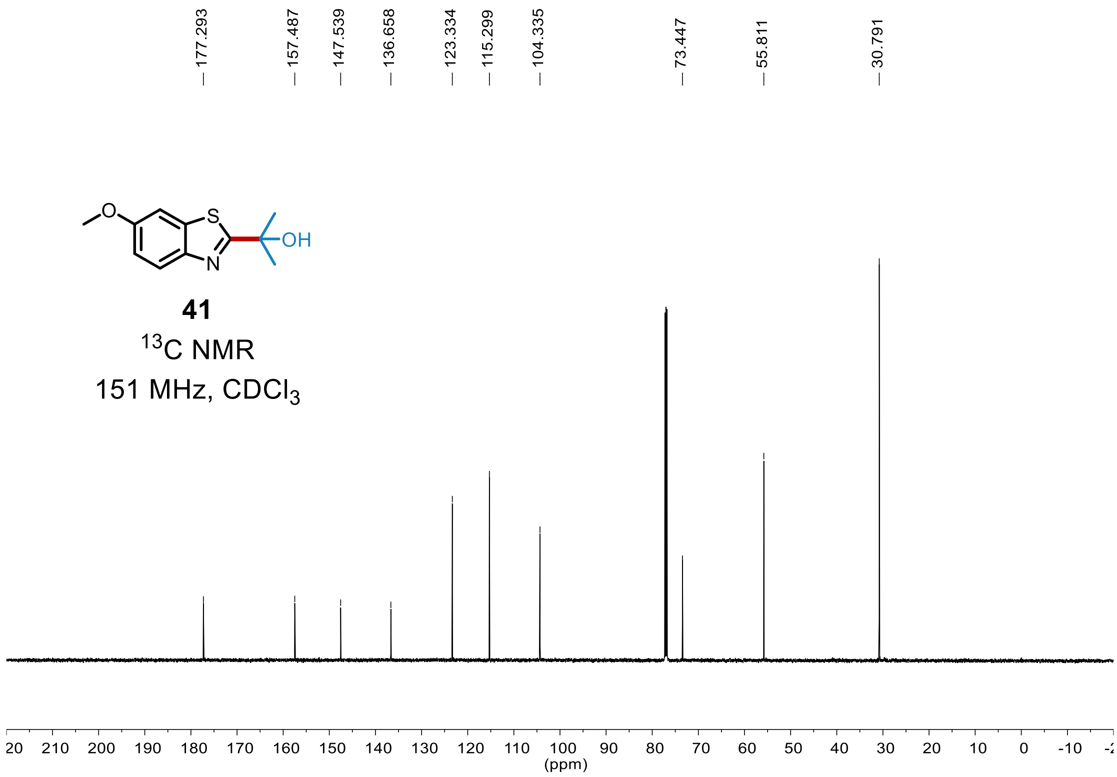


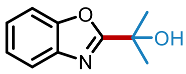
39
^{13}C NMR
151 MHz, $CDCl_3$


7.969
7.966
7.794
7.780
7.358
7.354
7.343
7.340
2.954
1.744
0.000
S
OH
Cl
N
40
^{1}H NMR
600 MHz, CDCl$_3$
1.00
1.00
1.00
1.00
6.02
(ppm)


182.037
154.067
133.663
132.045
125.417
122.820
122.483
73.740
30.747
S
OH
Cl
N
40
^{13}C NMR
151 MHz, CDCl$_3$
(ppm)


7.854
7.839
7.322
7.318
7.068
7.064
7.053
7.049
3.867
3.206
1.731
0.000
41
^{1}H NMR
600 MHz, CDCl$_3$
OH
1.00
1.00
1.00
3.00
1.01
6.00
(ppm)

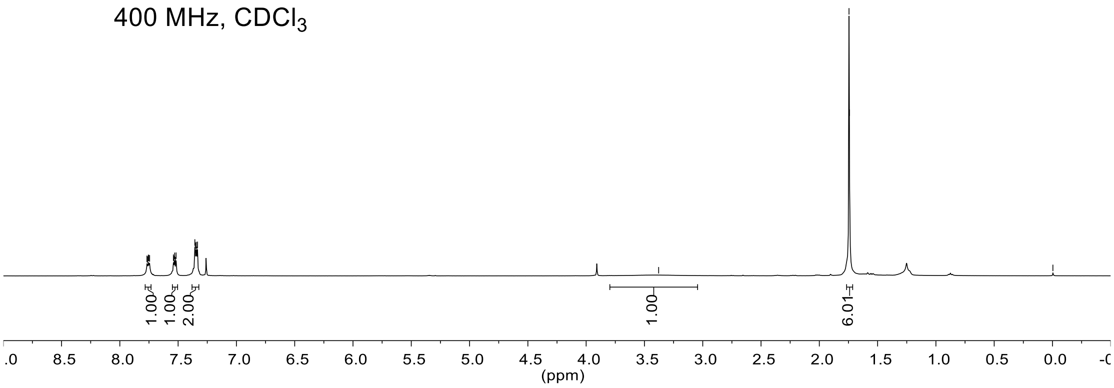

177.293
157.487
147.539
136.658
123.334
115.299
104.335
73.447
55.811
30.791
41
^{13}C NMR
151 MHz, CDCl$_3$
OH
(ppm)

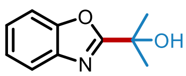


42

^{1}H NMR

400 MHz, $CDCl_3$

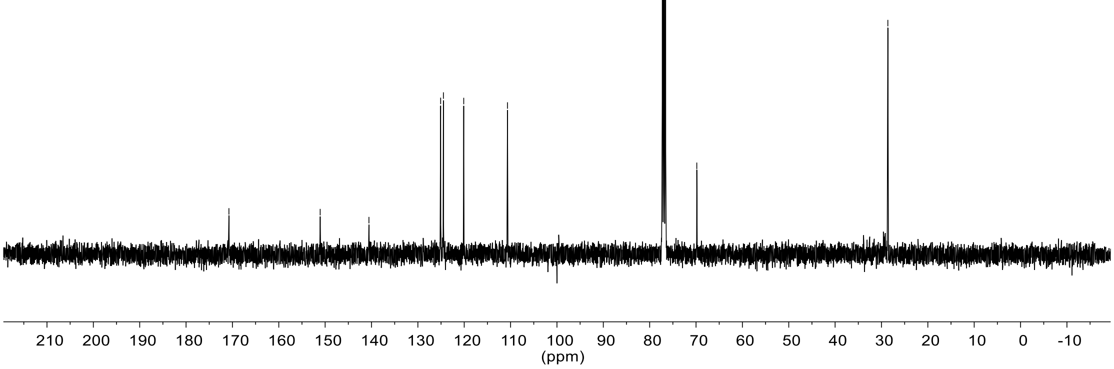


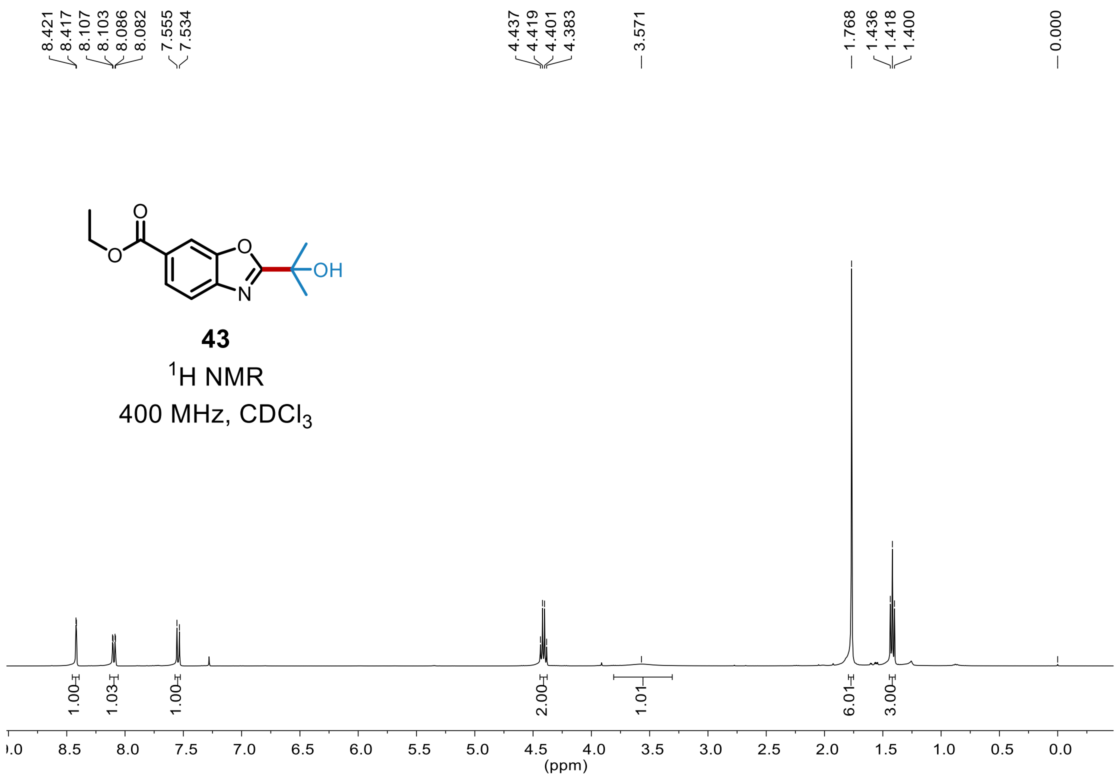


42

^{13}C NMR

101 MHz, $CDCl_3$

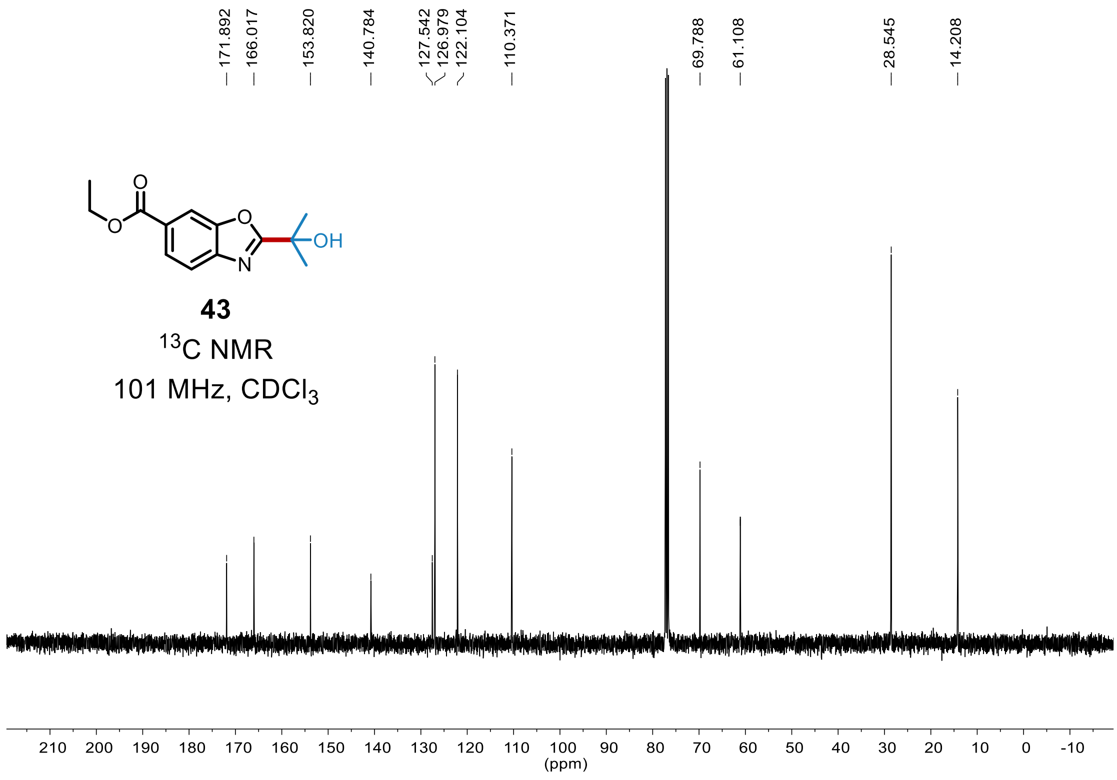




43

^{1}H NMR

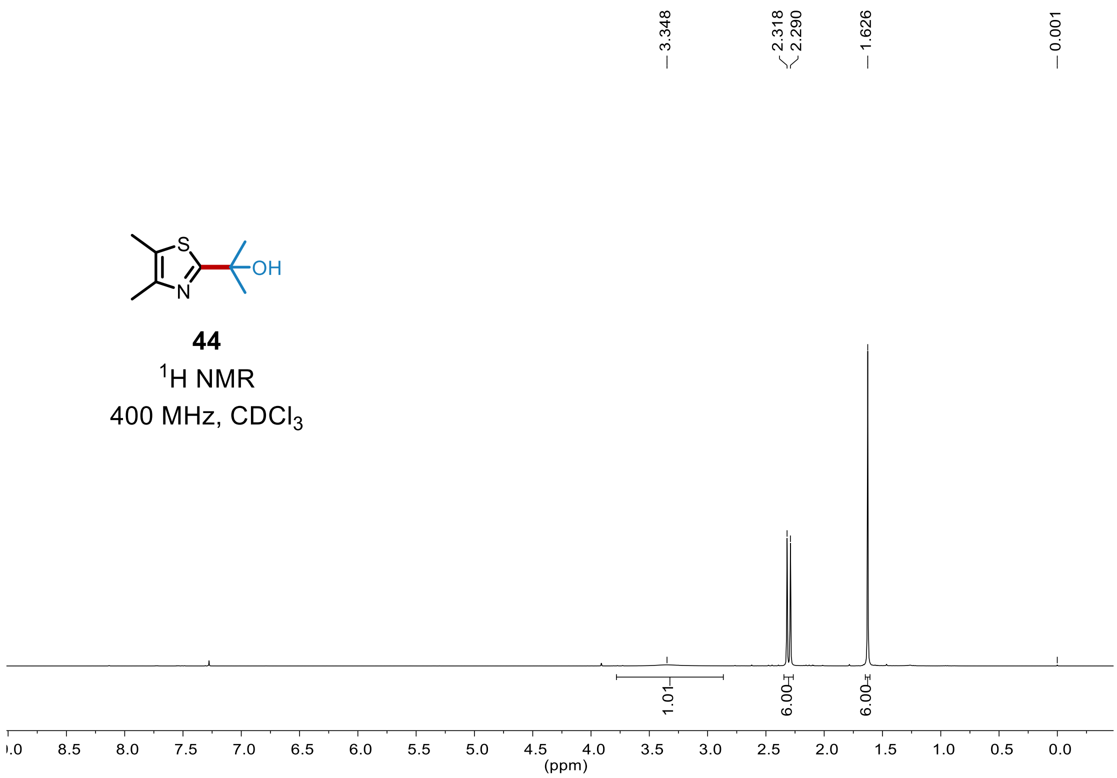
400 MHz, $CDCl_3$

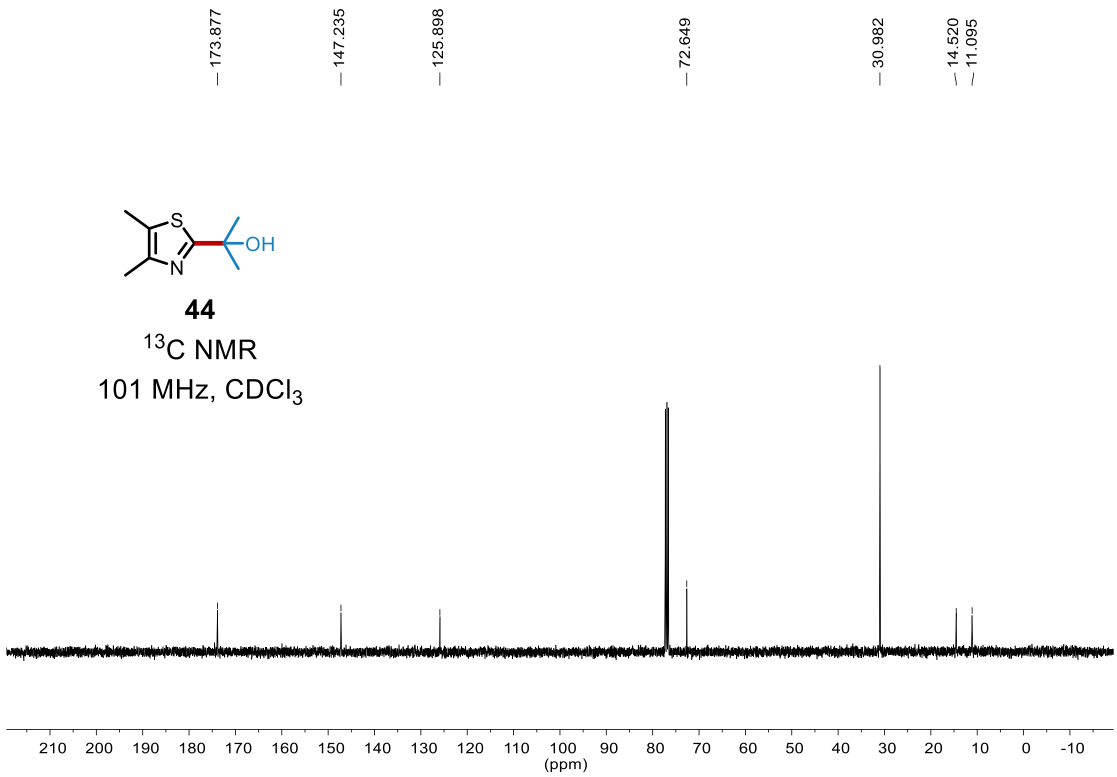


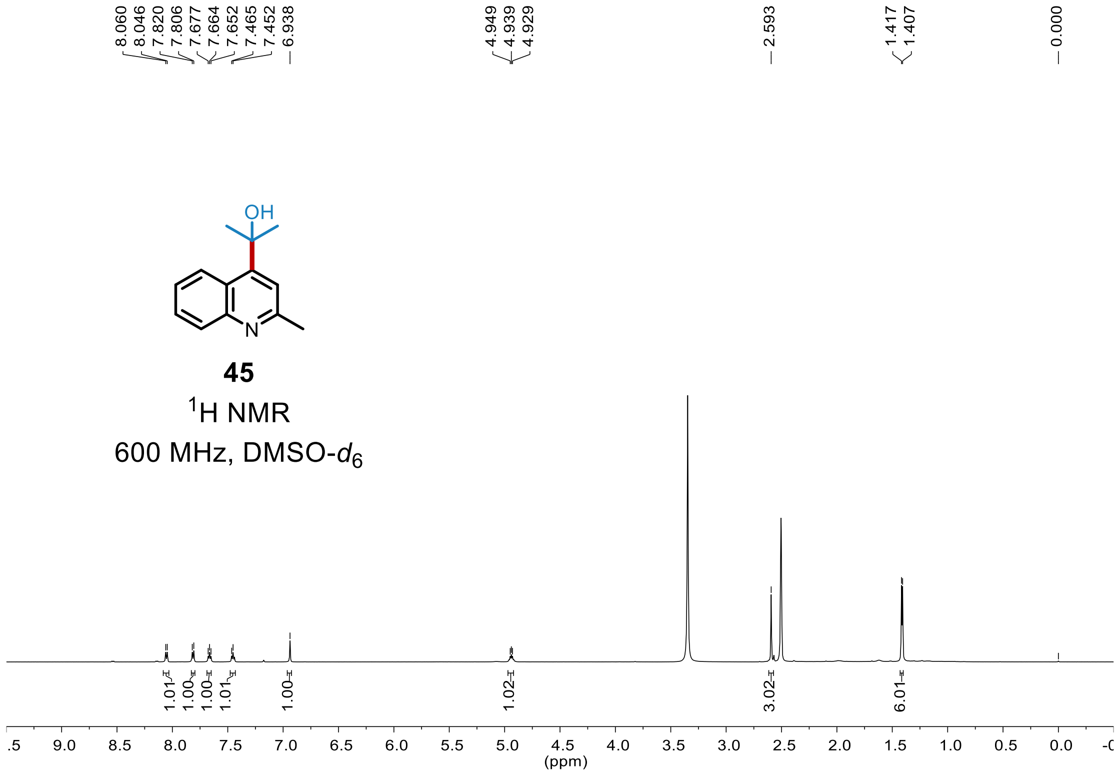
43

^{13}C NMR

101 MHz, $CDCl_3$


3.348
2.318
2.290
1.626
0.001
S
N
OH
44
^{1}H NMR
400 MHz, $CDCl_3$
1.01
6.00
6.00
(ppm)

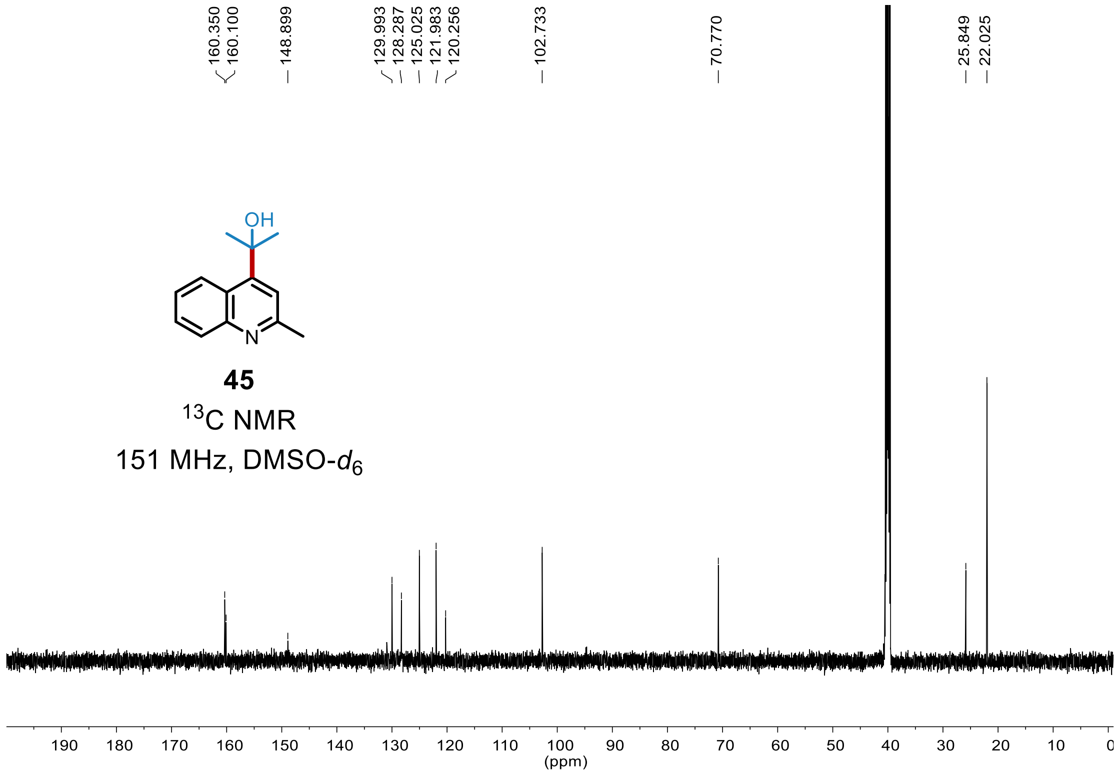

173.877
147.235
125.898
72.649
30.982
14.520
11.095
S
N
OH
44
^{13}C NMR
101 MHz, $CDCl_3$
(ppm)



45

^{1}H NMR

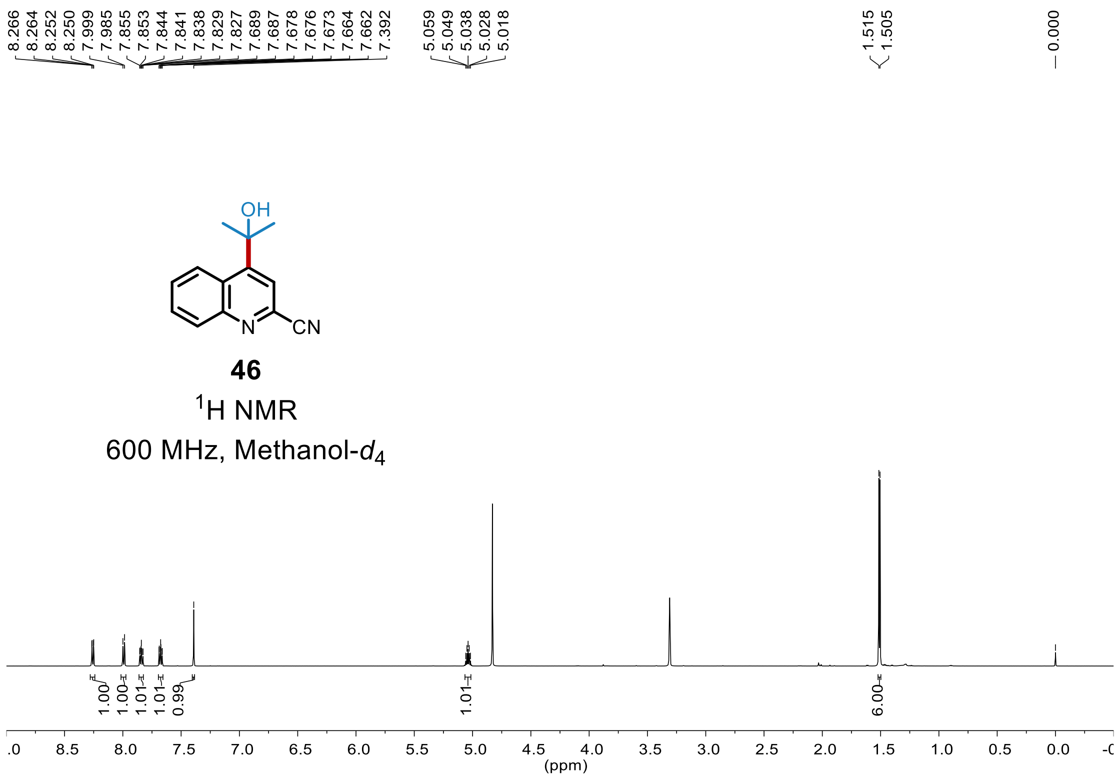
600 MHz, DMSO-d_6

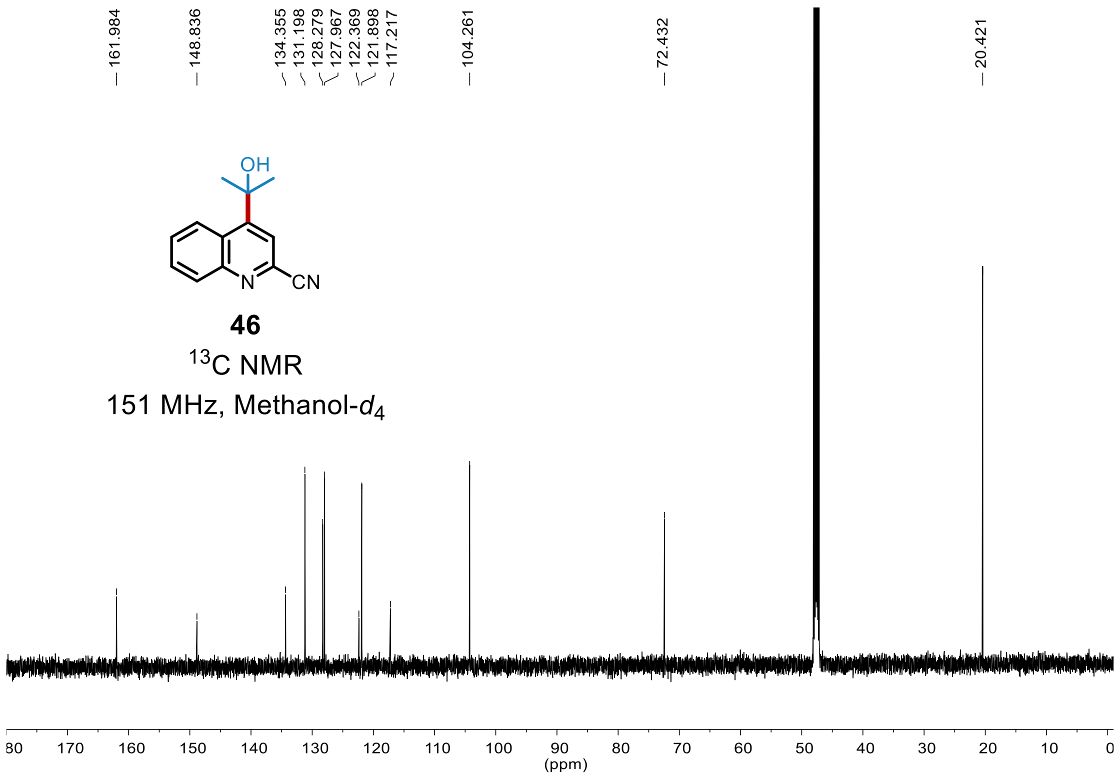


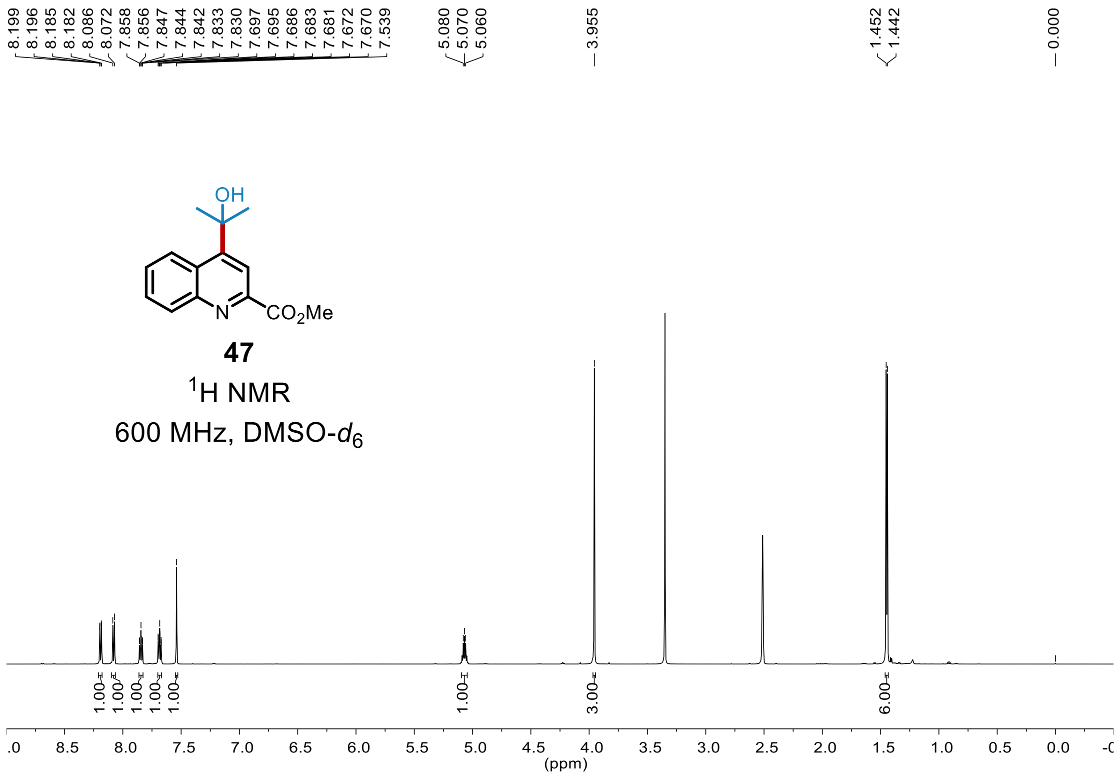
45

^{13}C NMR

151 MHz, DMSO-d_6


8.266
8.264
8.252
8.250
7.999
7.985
7.855
7.853
7.844
7.841
7.838
7.829
7.827
7.689
7.687
7.678
7.676
7.673
7.664
7.662
7.392
5.059
5.049
5.038
5.028
5.018
1.515
1.505
0.000
OH
N
CN
46
^{1}H NMR
600 MHz, Methanol-d_4
1.00
1.00
1.01
1.01
0.99
1.01
6.00
(ppm)

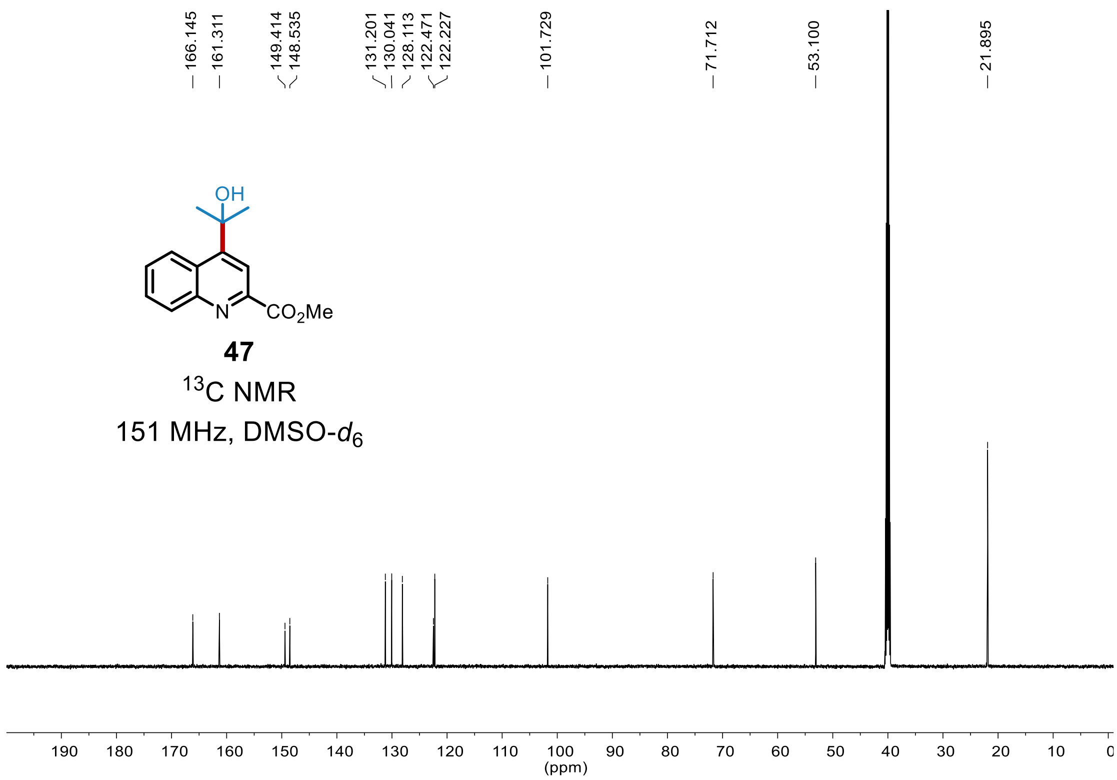

161.984
148.836
134.355
131.198
128.279
127.967
122.369
121.898
117.217
104.261
72.432
20.421
OH
N
CN
46
^{13}C NMR
151 MHz, Methanol-d_4
(ppm)



47

^1H NMR

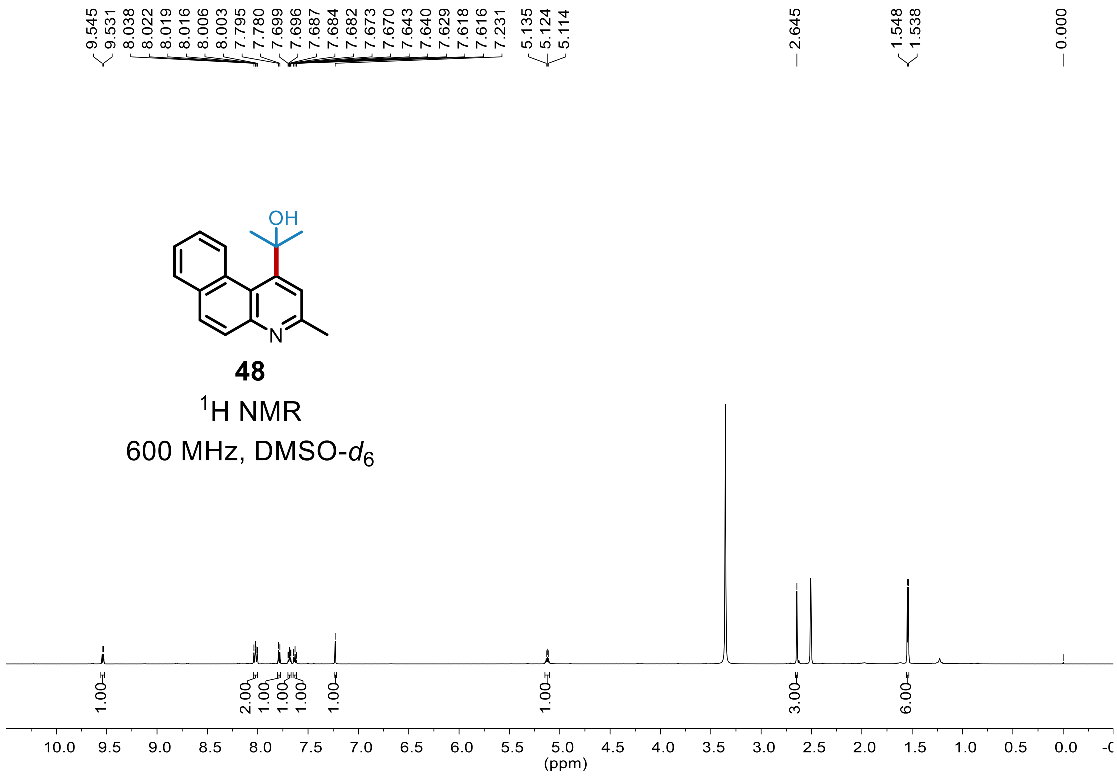
600 MHz, DMSO-d_6

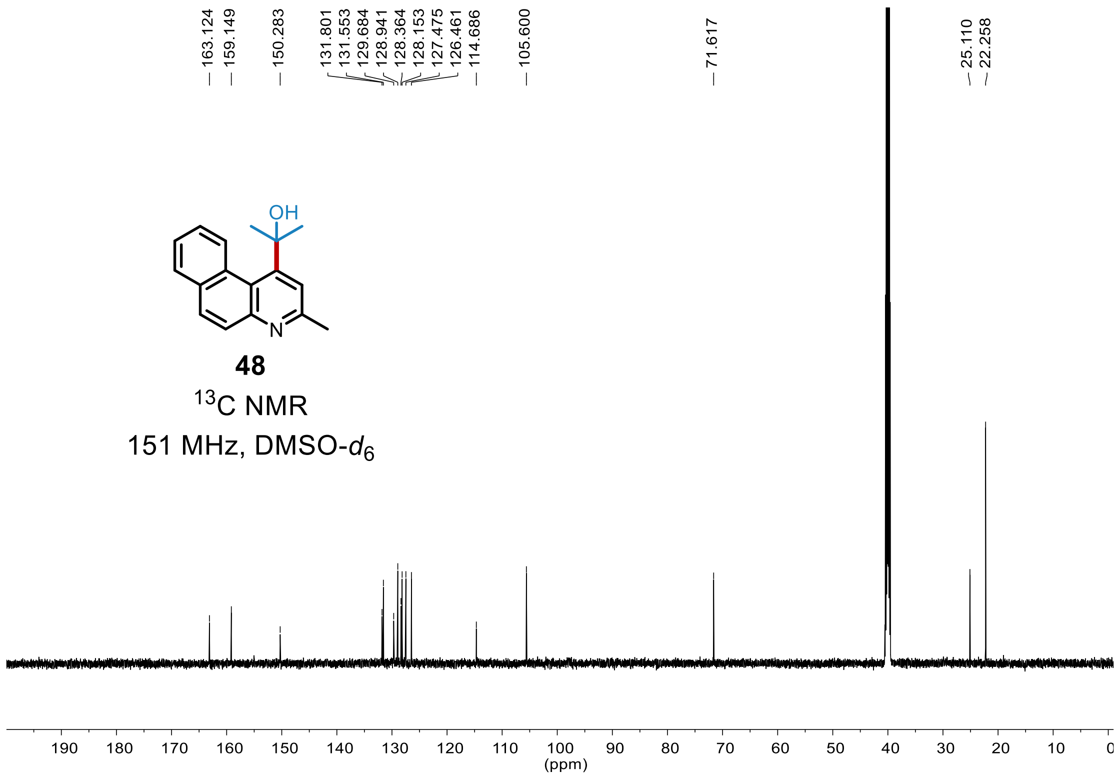


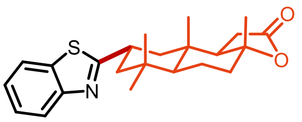
47

^{13}C NMR

151 MHz, DMSO-d_6


9.545
9.531
8.038
8.022
8.019
8.016
8.006
8.003
7.795
7.780
7.699
7.696
7.687
7.684
7.682
7.673
7.670
7.643
7.640
7.629
7.618
7.616
7.231
5.135
5.124
5.114
2.645
1.548
1.538
0.000
OH
N
48
^{1}H NMR
600 MHz, DMSO-d_6
1.00
2.00
1.00
1.00
1.00
1.00
1.00
3.00
6.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
(ppm)

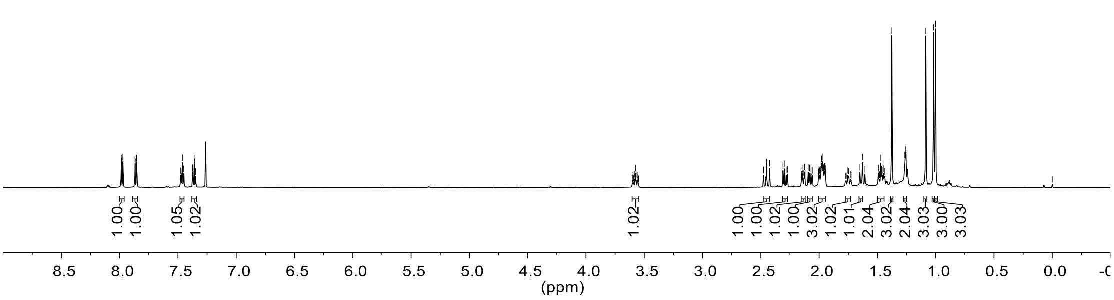

163.124
159.149
150.283
131.801
131.553
129.684
128.941
128.364
128.153
127.475
126.461
114.686
105.600
71.617
25.110
22.258
OH
N
48
^{13}C NMR
151 MHz, DMSO-d_6
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
(ppm)

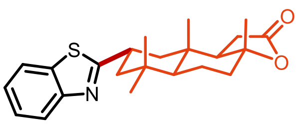


49

^{1}H NMR

600 MHz, $CDCl_3$

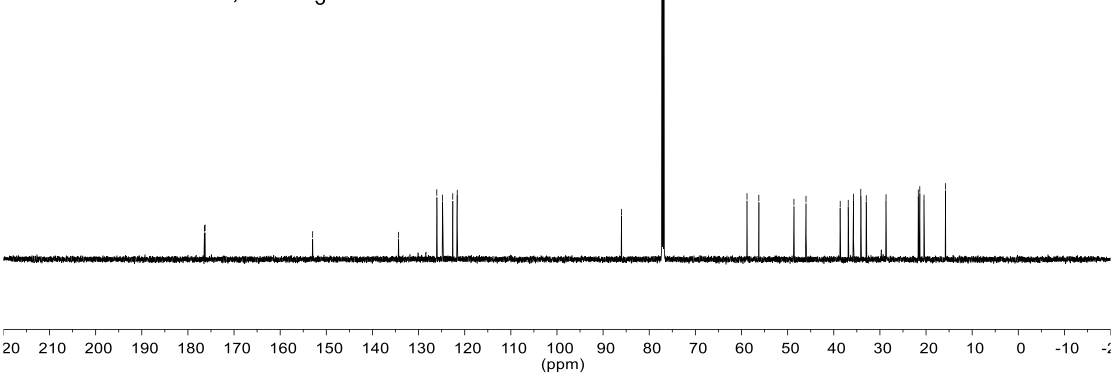


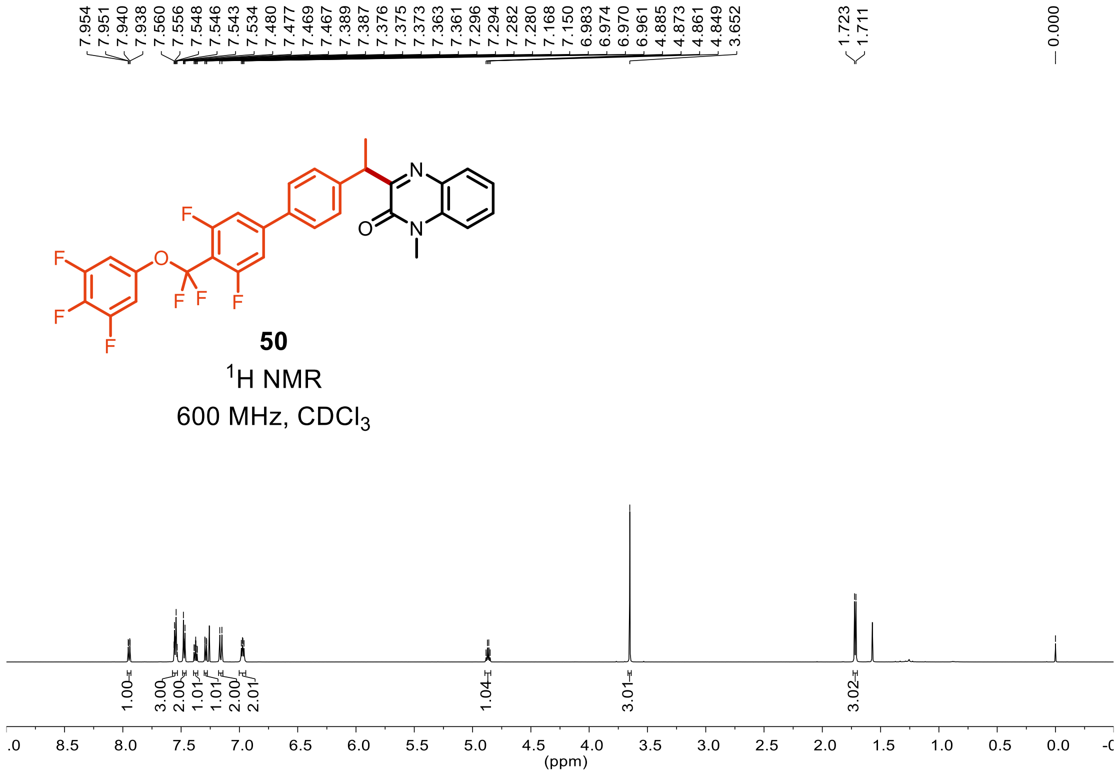


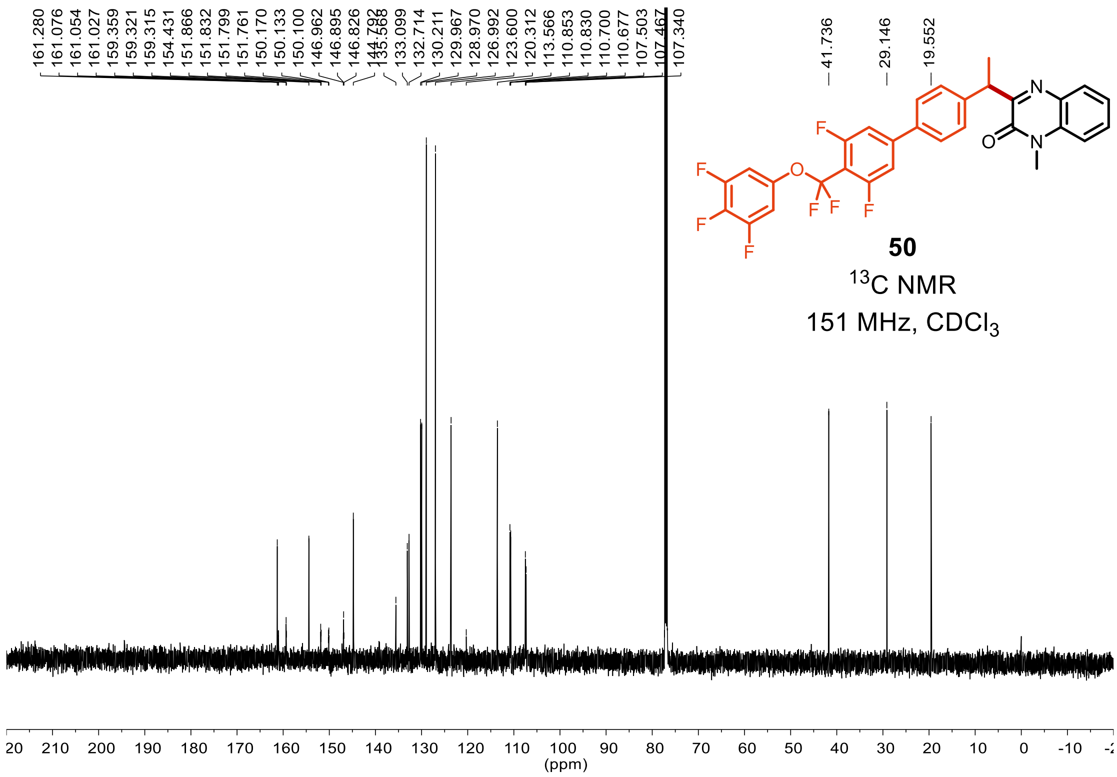
49

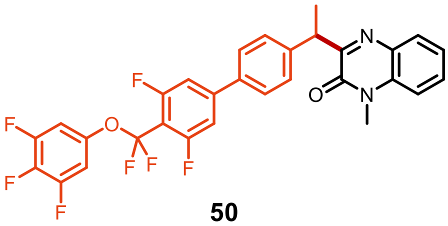
^{13}C NMR

151 MHz, $CDCl_3$




7.954
7.951
7.940
7.938
7.560
7.556
7.548
7.546
7.543
7.534
7.480
7.477
7.469
7.467
7.389
7.387
7.376
7.375
7.373
7.363
7.361
7.296
7.294
7.282
7.280
7.168
7.150
6.983
6.974
6.970
6.961
4.885
4.873
4.861
4.849
3.652
1.723
1.711
0.000
50
1H NMR
600 MHz, CDCl3
1.00
3.00
2.00
1.01
1.01
2.00
2.01
1.04
3.01
3.02
(ppm)

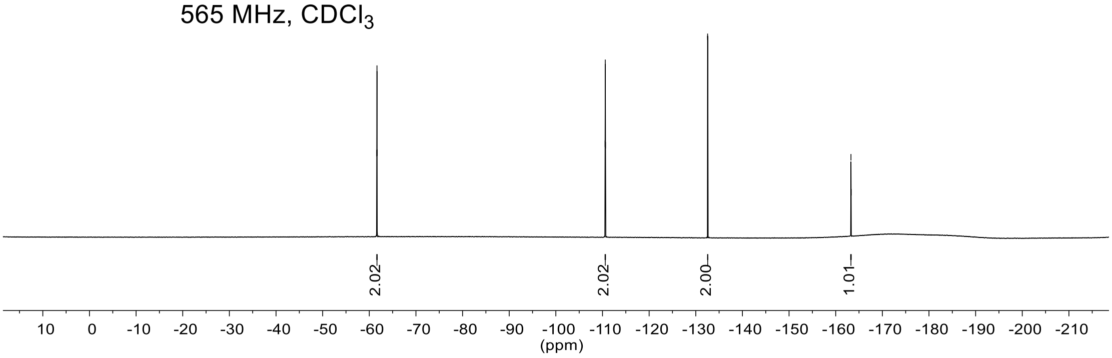

161.280
161.076
161.054
161.027
159.359
159.321
159.315
154.431
151.866
151.832
151.799
151.761
150.170
150.133
150.100
146.962
146.895
146.826
144.792
135.568
133.099
132.714
130.211
129.967
128.970
126.992
123.600
120.312
113.566
110.853
110.830
110.700
110.677
107.503
107.467
107.340
41.736
29.146
19.552
50
13C NMR
151 MHz, CDCl3
(ppm)

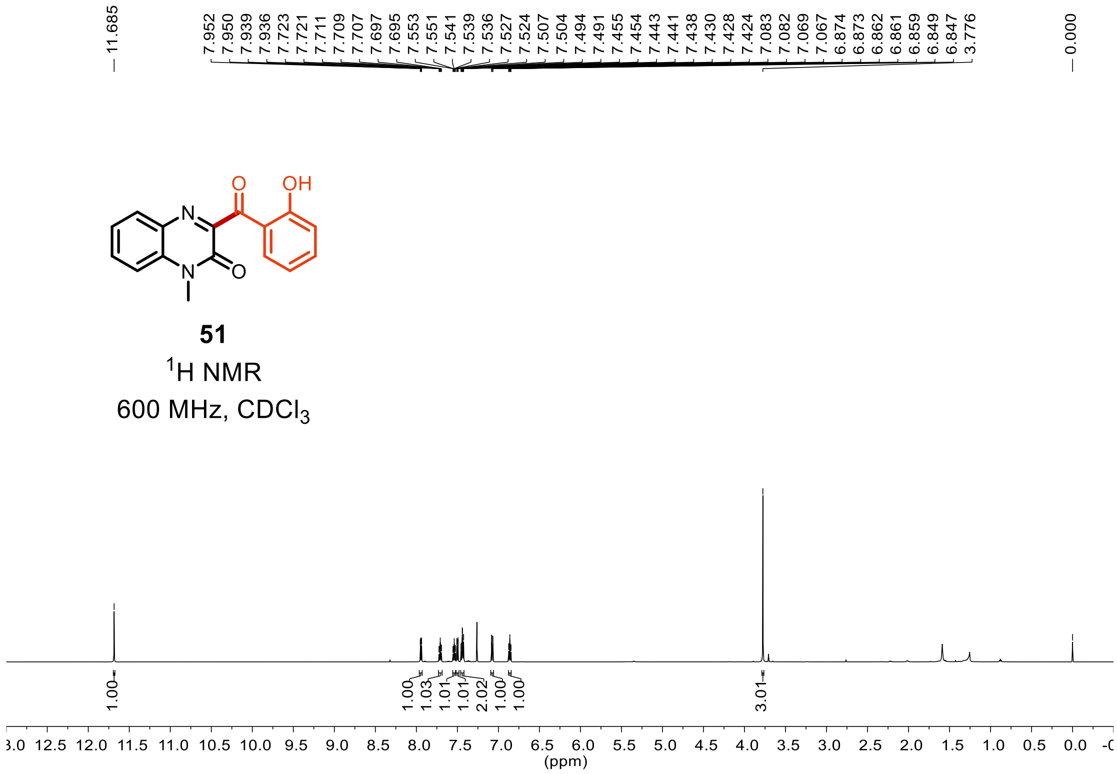


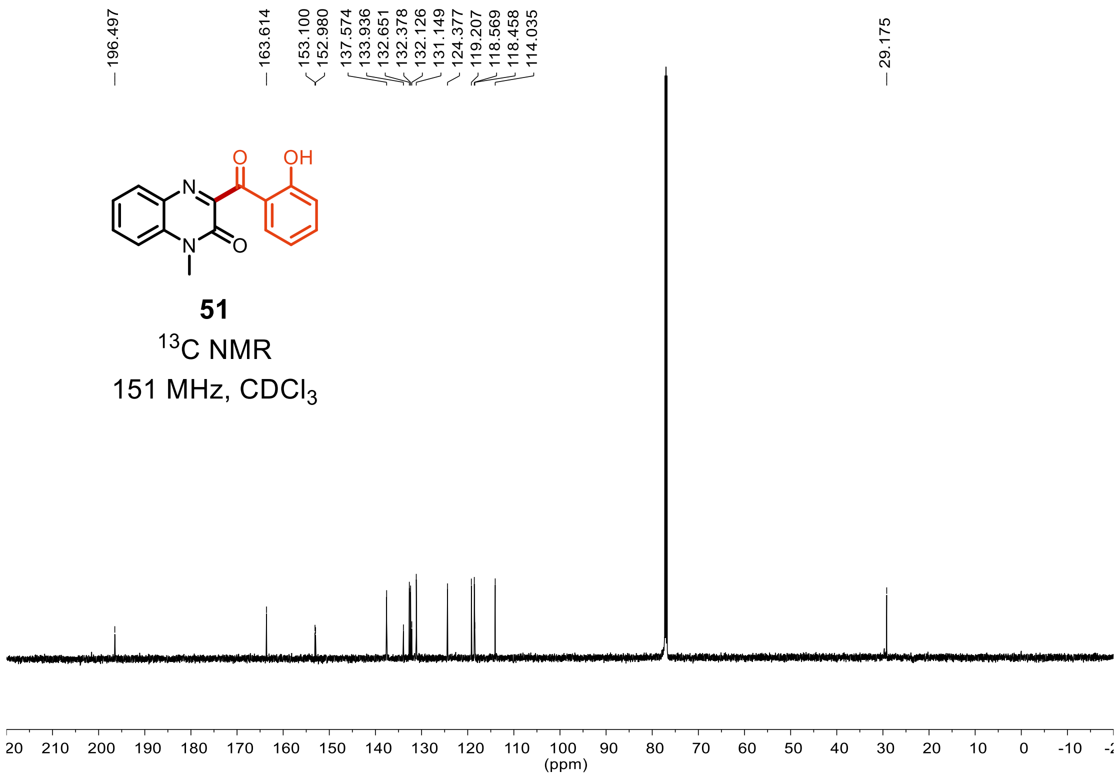
50

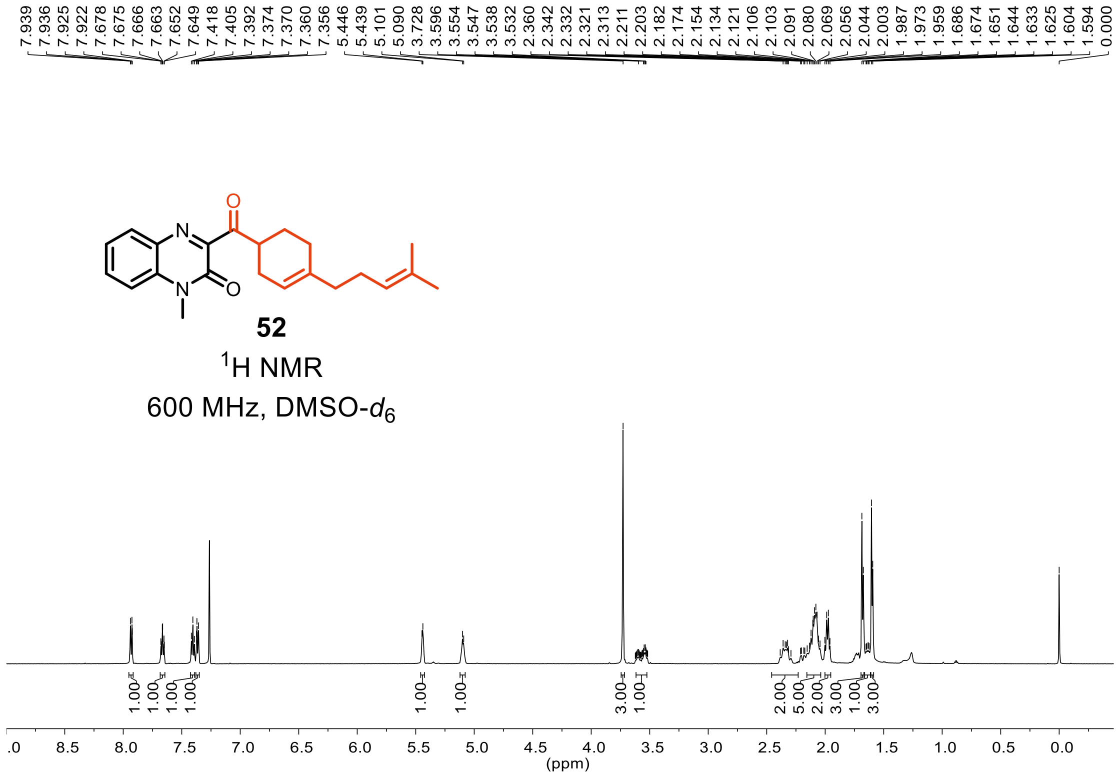
^{19}F NMR

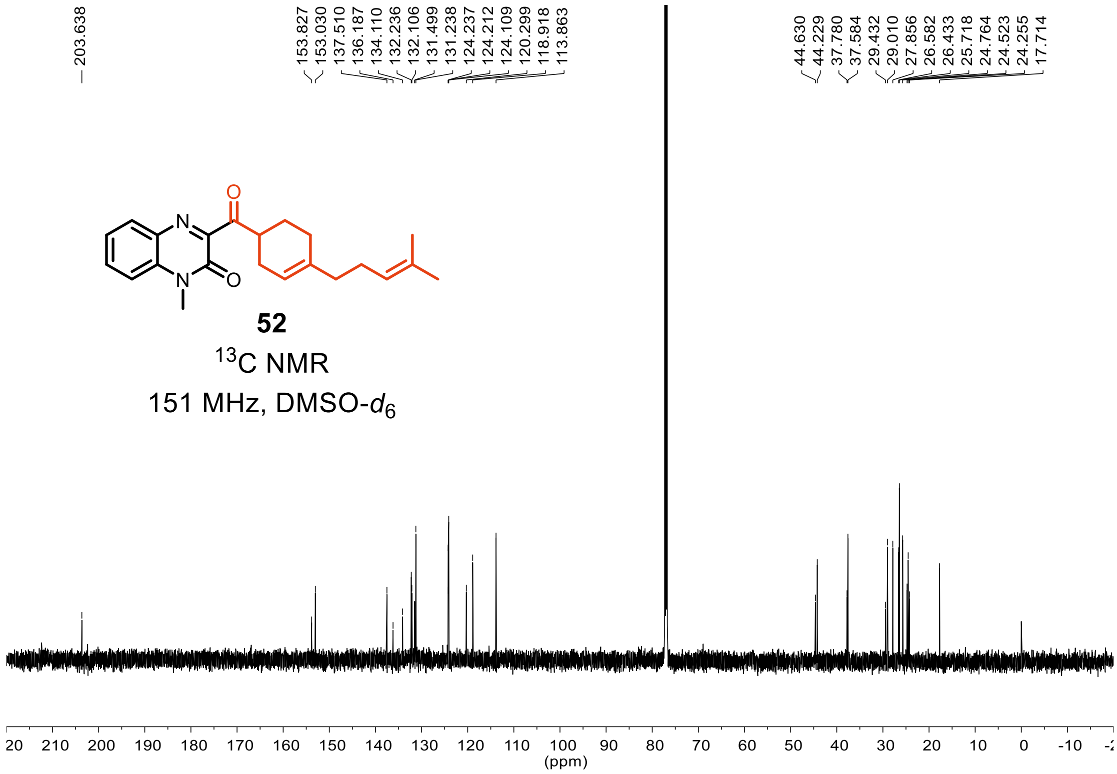
565 MHz, $CDCl_3$

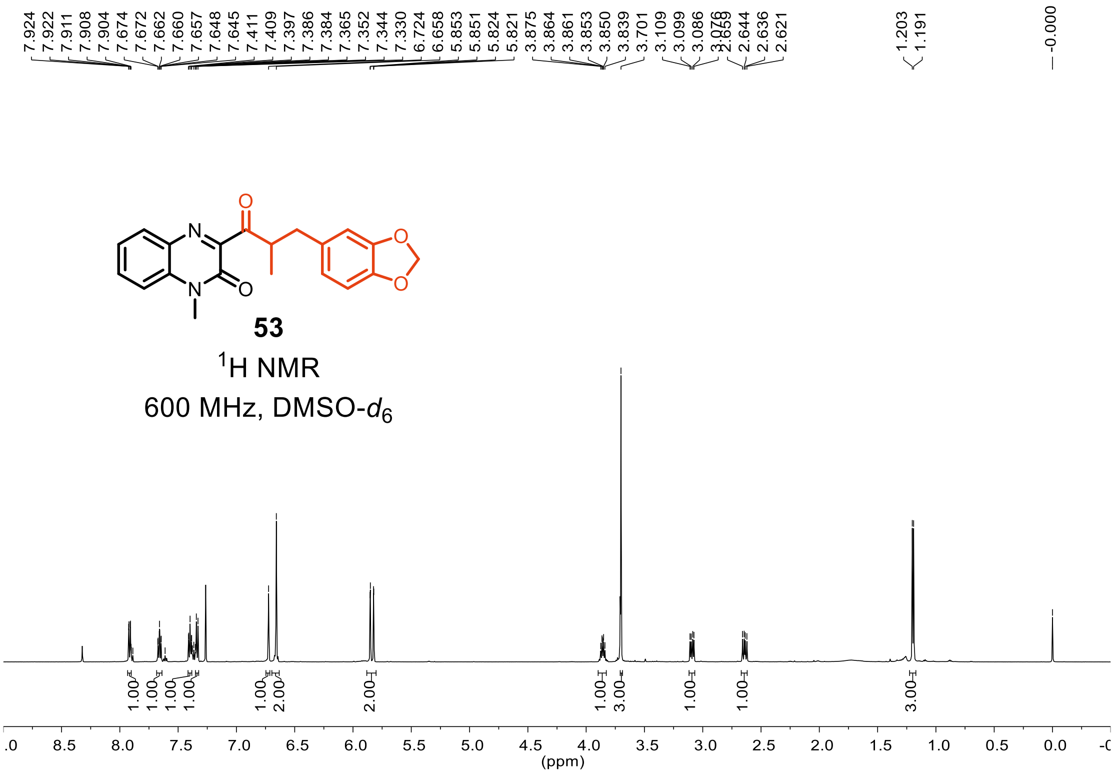



11.685
7.952
7.950
7.939
7.936
7.723
7.721
7.711
7.709
7.707
7.697
7.695
7.553
7.551
7.541
7.539
7.536
7.527
7.524
7.507
7.504
7.494
7.491
7.455
7.454
7.443
7.441
7.438
7.430
7.428
7.424
7.083
7.082
7.069
7.067
6.874
6.873
6.862
6.861
6.859
6.849
6.847
3.776
0.000
O
OH
N
N
O
51
^{1}H NMR
600 MHz, $CDCl_3$
1.00
1.00
1.03
1.01
1.01
2.02
1.00
1.00
3.01
(ppm)


196.497
163.614
153.100
152.980
137.574
133.936
132.651
132.378
132.126
131.149
124.377
119.207
118.569
118.458
114.035
29.175
O
OH
N
N
O
51
^{13}C NMR
151 MHz, $CDCl_3$
(ppm)


7.939 7.936 7.925 7.922 7.678 7.675 7.666 7.663 7.652 7.649 7.418 7.405 7.392 7.374 7.370 7.360 7.356 5.446 5.439 5.101 5.090 3.728 3.596 3.554 3.547 3.538 3.532 2.360 2.342 2.332 2.321 2.313 2.211 2.203 2.182 2.174 2.154 2.134 2.121 2.106 2.103 2.091 2.080 2.069 2.056 2.044 2.003 1.987 1.973 1.959 1.686 1.674 1.651 1.644 1.633 1.625 1.604 1.594 0.000
N
O
O
N
52
^{1}H NMR
600 MHz, DMSO-d_6
1.00 1.00 1.00 1.00 1.00 1.00 3.00 1.00 2.00 5.00 2.00 3.00 1.00 3.00
(ppm)

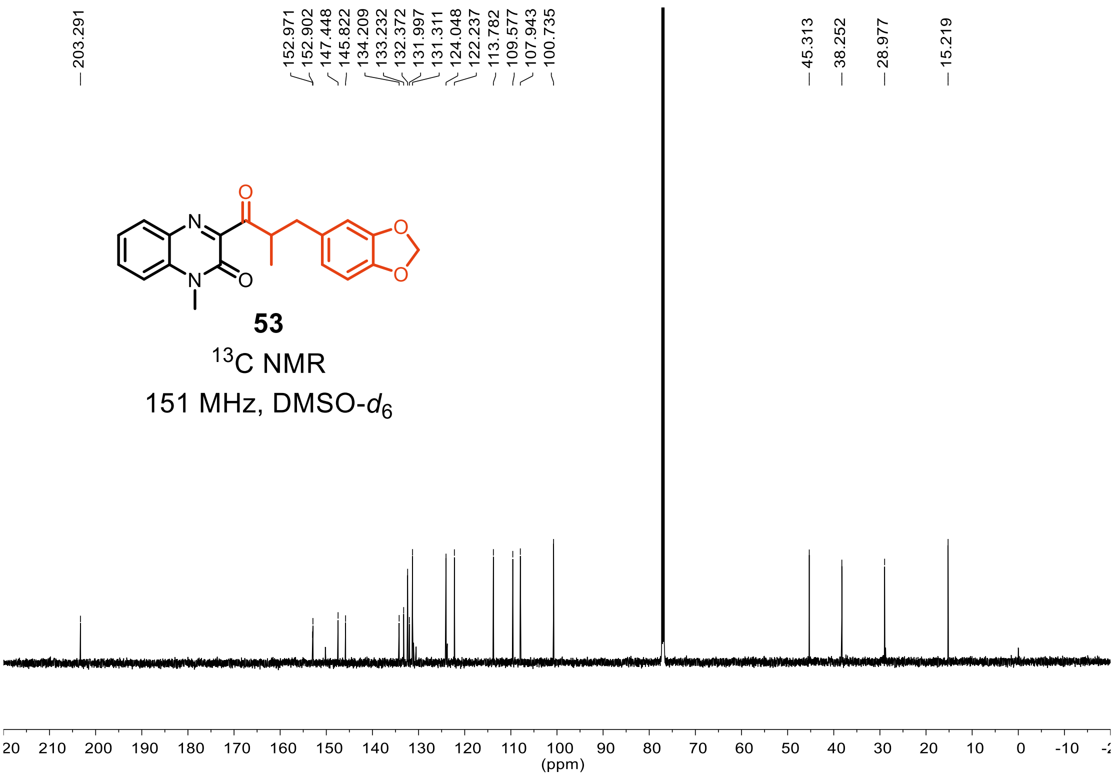

203.638
153.827 153.030 137.510 136.187 134.110 132.236 132.106 131.499 131.238 124.237 124.212 124.109 120.299 118.918 113.863
44.630 44.229 37.780 37.584 29.432 29.010 27.856 26.582 26.433 25.718 24.764 24.523 24.255 17.714
N
O
O
N
52
^{13}C NMR
151 MHz, DMSO-d_6
(ppm)



53

^{1}H NMR

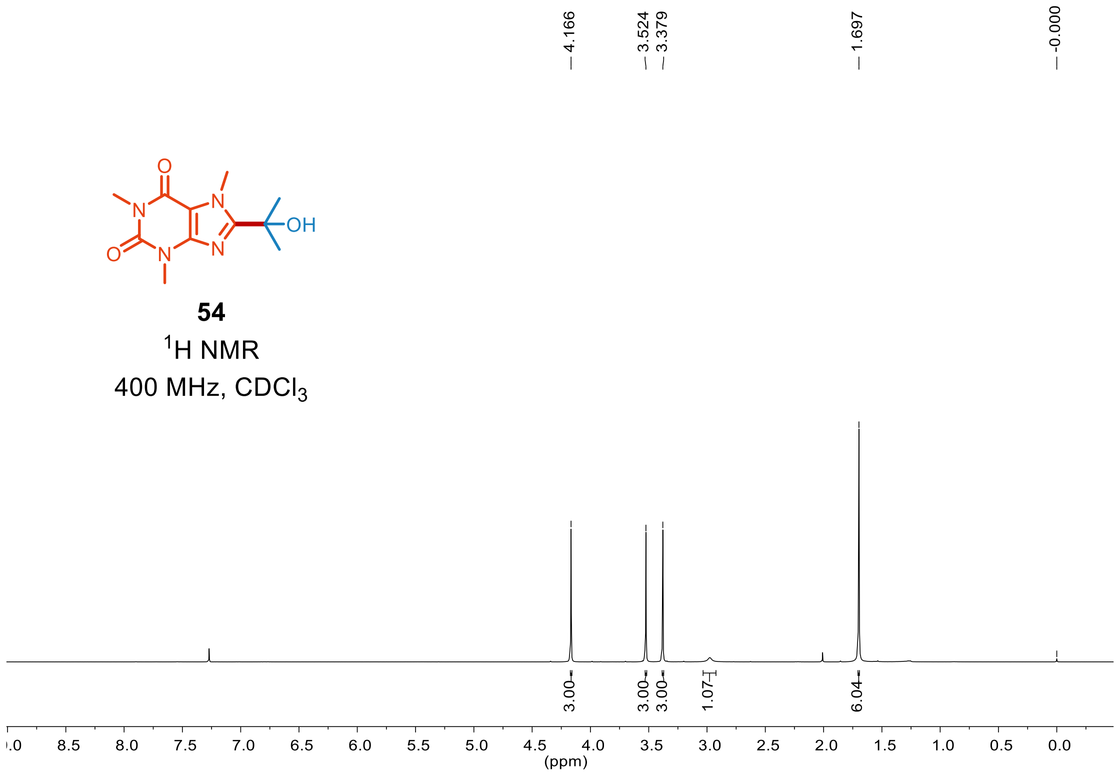
600 MHz, DMSO-d_6



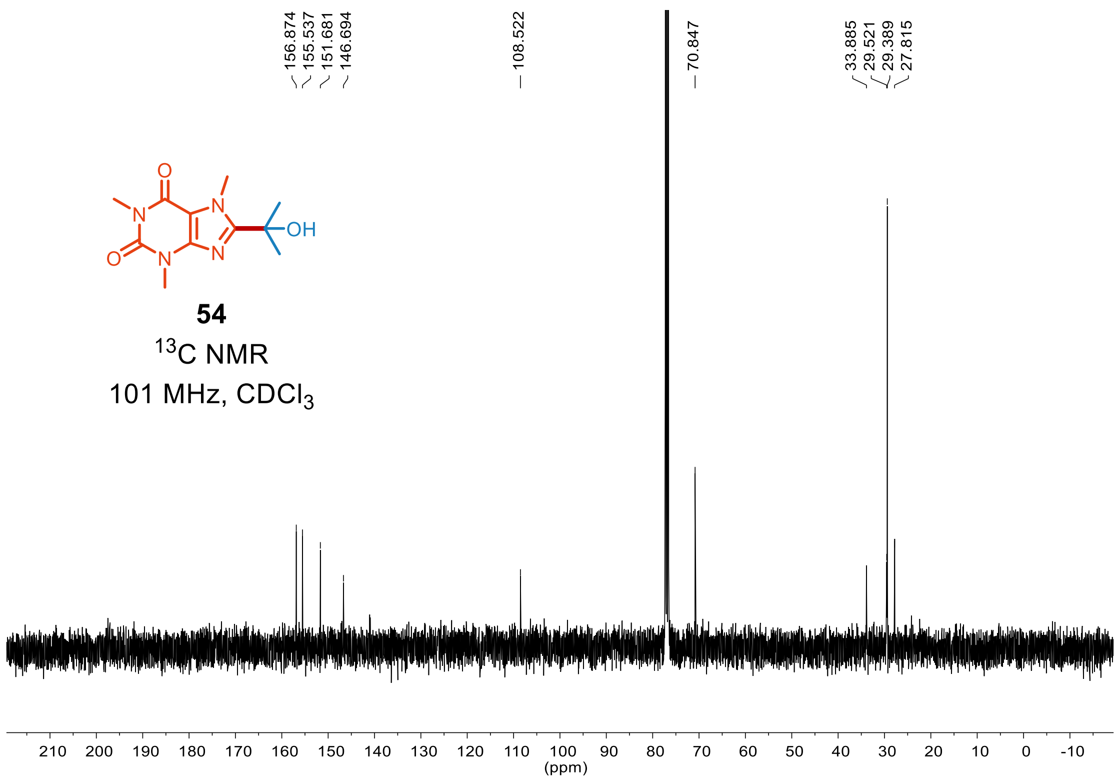
53

^{13}C NMR

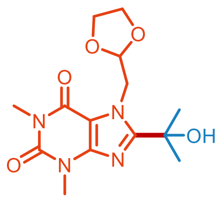
151 MHz, DMSO-d_6



54
^{1}H NMR
400 MHz, $CDCl_3$
4.166
3.524
3.379
1.697
-0.000
3.00
3.00
3.00
1.07
6.04
(ppm)



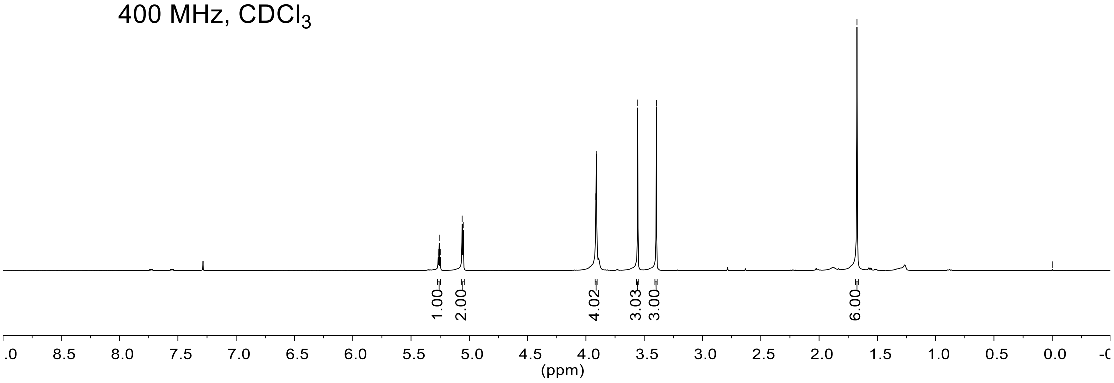
54
^{13}C NMR
101 MHz, $CDCl_3$
156.874
155.537
151.681
146.694
108.522
70.847
33.885
29.521
29.389
27.815
(ppm)

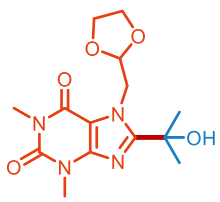


55

^{1}H NMR

400 MHz, $CDCl_3$

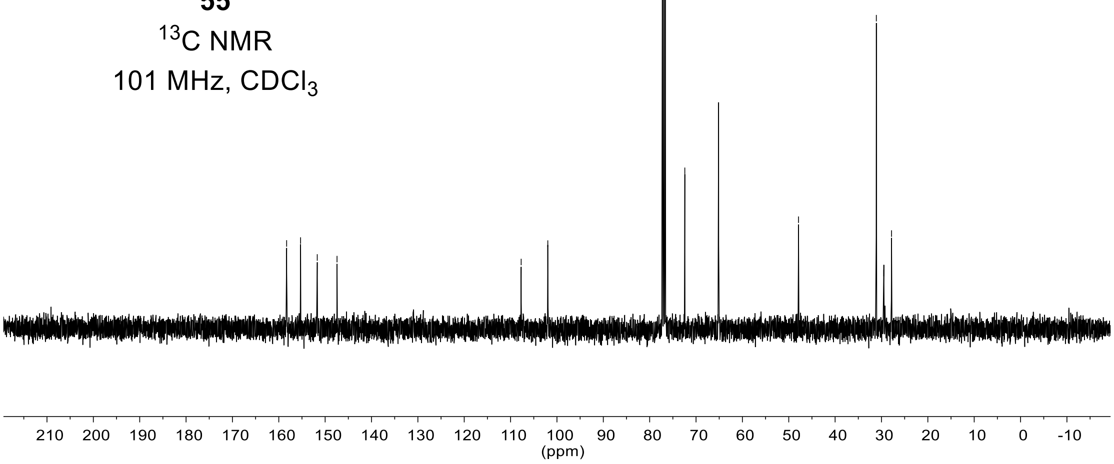


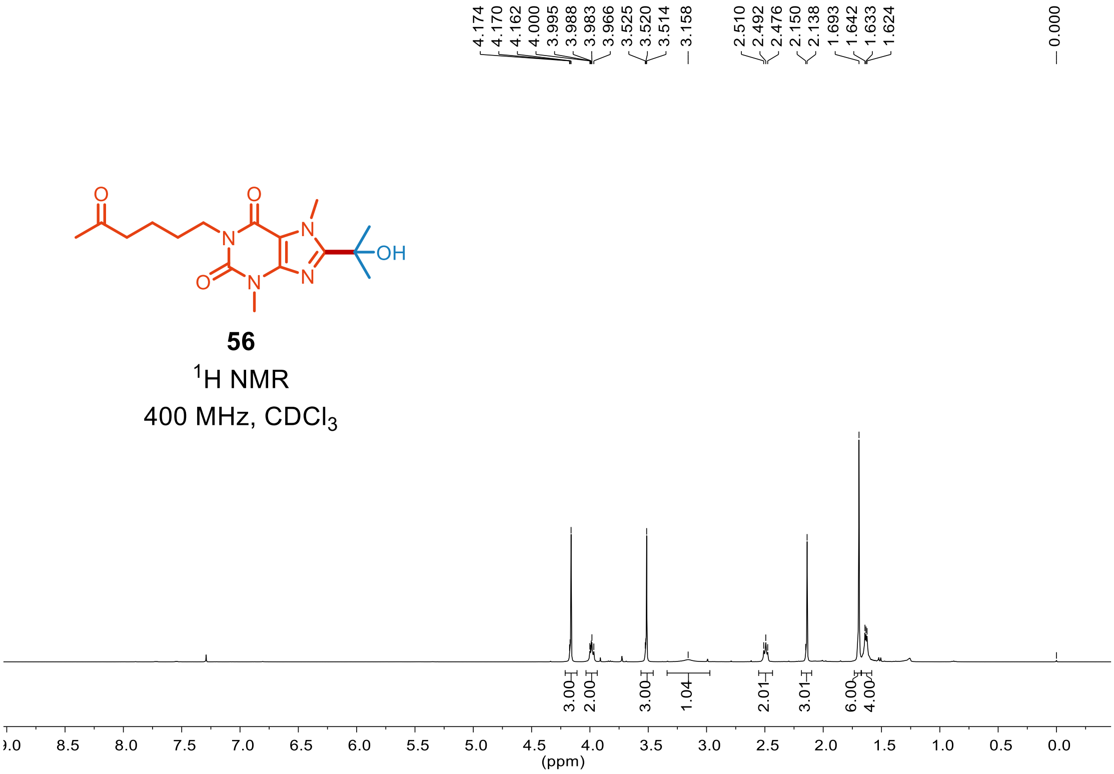


55

^{13}C NMR

101 MHz, $CDCl_3$

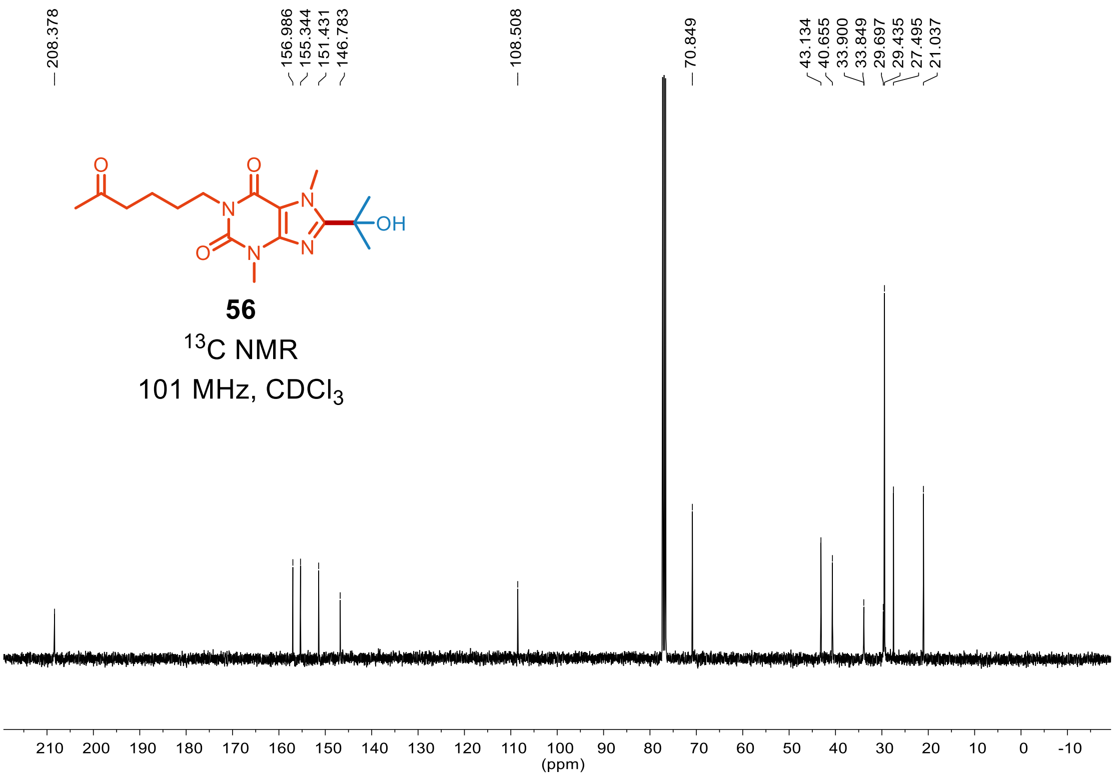




56

^{1}H NMR

400 MHz, $CDCl_3$



56

^{13}C NMR

101 MHz, $CDCl_3$

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