Electronic Supplementary Material (ESI) for Green Chemistry.

Cooperative Iridium Complex Catalyzed Synthesis of Quinoxalines, Benzimidazoles and Quinazolines in Water

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Contents

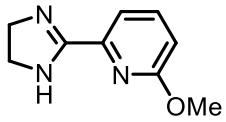
1. General procedure and materials.

All the reactions were carried out under air or argon atmosphere by using standard schlenk line technique. Glasswares were oven dried prior to use. All the commercial reagents and metal precursors were purchased from Sigma-aldrich, Alfa-acear, Spectrochem, Avra, SD-fine chemical and arora matthey India. ^{1}H, ^{13}C, ^{31}P NMR spectra were recorded with $CDCl_3$, D_2O, CD_3OD and DMSO-d_6 in JEOL 500 MHz and 400 MHz Spectrometers. ESI-MS were recorded on a Waters Micromass Quattro Micro triple-quadrupole mass spectrometer. FT-IR were recorded on a Perkin Elmer IR spectrometer. All the GC analysis were performed using Perkein Elmer Clarus 600 and Agilent 7890 B Gas Chromatograph, where as GC-MS were measured using Agilent 7890 A Gas Chromatograph equipped with Agilent 5890 triple-quadrupole mass system.

2. Synthesis of ligands and metal complexes.

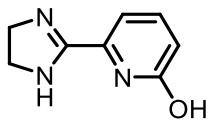
Ligands L1-L5 were synthesised according to the literature procedure.[1, 2] Metal complexes 1a, 1c, 1d and 1e were synthesised following known literature procedure.[2]

2-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxypyridine (L1)



In a two-neck round bottom flask, a solution of ethylenediamine (133 mg, 2.20 mmol) in *tert*-butyl alcohol (20 mL) was added over 6-methoxypyridine-2-carboxaldehyde (250 mg, 1.83 mmol). Then, the mixture was stirred at room temperature under an argon atmosphere for 30 min. After that, K_2CO_3 (760 mg, 5.50 mmol) and solid I_2 (606 mg, 2.38 mmol) were added to the reaction mixture and stirred at 70 °C for 12 h. The mixture was quenched with sat. aq. Na_2SO_3 until the iodine colour almost disappeared and was extracted with $CHCl_3$. The organic layer was washed with sat. aq. $NaHCO_3$ solution and dried over anhydrous Na_2SO_4. After filtration, the mixture was evaporated under reduced pressure to provide crude product as a dark brown oil. It was then purified by column chromatography on alumina using EtOAc/MeOH (95:5) as eluent to give the desire product (271 mg, yield: 84%) as a yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.72 (dd, *J* = 9.3, 0.9 Hz, 1H), 7.62 (t, *J* = 10.1 Hz, 1H), 6.79 (d, *J* = 10.5 Hz, 1H), 3.93 (s, 3H), 3.81 (brs, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 164.40, 163.38, 145.98, 139.34, 115.34, 112.71, 53.63, 49.71. **GC-MS** (M^+) = 177.1.

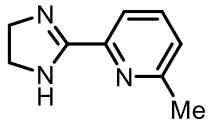
6-(4,5-dihydro-1H-imidazol-2-yl)pyridin-2-ol (L2)



In a two neck round bottom flask, a mixture of 2-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxypyridine (250 mg, 1.4 mmol) and 15 mL of aq. HBr (47 %) was stirred at 95 °C for 24 h. After that, the solvent was removed under reduced pressure. To the residue, 3 mL water was added. Then, the solution pH was adjusted to 6-7 with 0.5 M NaOH. The mixture was evaporated in vacuum, then 2 mL ethanol was added to remove the insoluble solid. The solution was concentrated to obtain the crude product. It was then purified by column chromatography

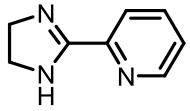
on neutral alumina using MeOH/H_2O (7:1) as eluent to give the product (132.5 mg, yield: 58%) as a white solid. **^{1}H NMR** (500 MHz, D_2O): δ = 7.64 (t, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 7.0 Hz, 1H), 6.78 (d, *J* = 8.7 Hz, 1H), 3.96 (brs, 4H). **^{13}C NMR** (125 MHz, D_2O): δ = 165.73, 163.14, 141.14, 135.02, 120.59, 114.21, 44.96. **HRMS (ESI)**: Calcd. for $C_8H_9N_3O$ $[M+H]^+$: 164.0824; found: 164.0829.

2-(4,5-dihydro-1H-imidazol-2-yl)-6-methylpyridine (L3)



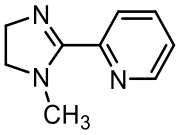
In a two-neck round bottom flask, ethylenediamine (150 mg, 2.49 mmol) was added over 6-methylpyridine-2-carboxaldehyde (250 mg, 2.08 mmol) in *tert*-butyl alcohol (20 mL). Then, the mixture was stirred at room temperature under an argon atmosphere for 30 min. After that, K_2CO_3 (862 mg, 6.24 mmol) and solid I_2 (686 mg, 2.70 mmol) were added to the reaction mixture and stirred at 70 °C for 12 h. The mixture was quenched with sat. aq. Na_2SO_3 until the iodine colour almost disappeared, and was extracted with $CHCl_3$. The organic layer was washed with sat. aq. $NaHCO_3$ solution and dried over anhydrous Na_2SO_4. After filtration, the mixture was evaporated under reduced pressure to provide crude product as a yellow oil. It was then purified by column chromatography on alumina using ethyl acetate and hexane as eluent to give the desire product (242 mg, yield: 73%) as a yellow oil. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 7.92 (d, *J* = 7.8 Hz, 1H), 7.63 (t, *J* = 7.7 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 3.82 (brs, 4H), 2.54 (s, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ = 164.64, 157.64, 147.89, 136.82, 124.72, 119.32, 24.39. **GC-MS** (M^+) = 161.1.

2-(4,5-dihydro-1H-imidazol-2-yl)pyridine (L4)



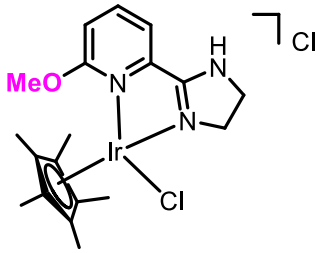
In a two-neck round bottom flask, ethylenediamine (168 mg, 2.80 mmol) was added over pyridine-2-carboxaldehyde (250 mg, 2.33 mmol) in *tert*-butyl alcohol (20 mL). Then, the mixture was stirred at room temperature under an argon atmosphere for 30 min. After that, K_2CO_3 (967 mg, 7.00 mmol) and solid I_2 (770 mg, 3.03 mmol) were added to the reaction mixture and stirred at 70 °C for 12 h. The mixture was quenched with sat. aq. Na_2SO_3 until the iodine colour almost disappeared, and was extracted with $CHCl_3$. The organic layer was washed with sat. aq. $NaHCO_3$ solution and dried over anhydrous Na_2SO_4. After filtration, the mixture was evaporated under reduced pressure to provide crude product as a yellow oil. It was then purified by column chromatography on alumina using ethyl acetate and hexane as eluent to give the desire product (242 mg, yield: 73%) as a yellow solid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.46 (d, *J* = 4.5 Hz, 1H), 8.05 (d, *J* = 7.9 Hz, 1H), 7.65 (t, *J* = 8.8 Hz, 1H), 7.24 (t, *J* = 8.7 Hz, 1H), 5.37 (brs, 1H), 3.73 (brs, 4H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 164.33, 148.60, 136.56, 125.05, 122.28, 50.52. **GC-MS** (M^+) = 146.1.

2-(1-methyl-1H-imidazol-2-yl)pyridine (L5)



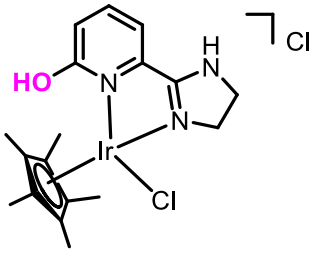
In a two-neck round bottom flask, a solution of pyridine-2-carboxaldehyde (107 mg, 1 mmol) in dichloromethane (10 mL) was dropwise added to *N*-methylethylenediamine (78 mg, 1.05 mmol) in 5 mL of DCM. The mixture was stirred for 1 h, and was then cooled to 0 °C. *N*-Bromosuccinimide (196 mg, 1.1 mmol) was added to the mixture and it was stirred overnight at room temperature. The reaction mixture was washed with 5% NaOH solution (10 mL) and then saturated $Na_2S_2O_3$ solution (10 mL), drying with Na_2SO_4 and removal of the dichloromethane under vacuum directly gave the desired crude product (142 mg, Yield: 90%) as yellow liquid. **^{1}H NMR** (400 MHz, $CDCl_3$): δ = 8.60 (d, *J* = 4.0 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.72 (td, *J* = 7.8, 1.7 Hz, 1H), 7.31-7.28 (m, 1H), 3.86 (t, *J* = 10.1, 2H), 3.47 (t, *J* = 10.0, 2H), 3.02 (s, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$): δ = 165.80, 150.71, 148.64, 136.67, 124.42, 124.26, 54.49, 53.07, 36.06. **GC-MS** (M^+) = 161.1.

Synthesis of complex 1a



In a Schlenk flask a mixture of **L1** (50 mg, 0.28 mmol) and $[Cp^*IrCl_2]_2$ (111.5 mg, 0.14 mmol) was stirred in dry DCM (20 mL) at room temperature for 24 h under an argon atmosphere. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure compound (121.7 mg, Yield: 75%) as a yellow solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 10.58 (s, 1H), 8.84 (d, *J* = 7.5 Hz, 1H), 8.06 (t, *J* = 7.7 Hz, 1H), 7.15 (d, *J* = 8.6 Hz, 1H), 4.14 (s, 6H), 3.96-3.87 (m, 1H), 1.72 (s, 15H). **^{13}C NMR** (125 MHz, $CDCl_3$): δ = 170.17, 163.95, 145.65, 143.72, 121.24, 110.67, 87.79, 57.98, 52.43, 46.06, 9.99. **HRMS (ESI)**: Calcd. for $C_{19}H_{26}ClIrN_3O$ $[M\text{-}Cl]^+$: 540.1394; found: 540.1395. Anal. Calculated ($C_{19}H_{26}Cl_2IrN_3O$): C, 39.65; H, 4.55; N, 7.30; Found: C, 39.43; H, 4.33; N, 7.17.

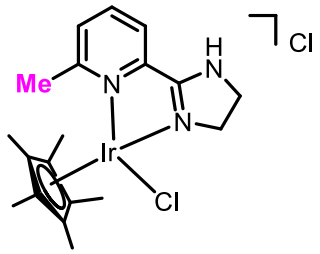
Synthesis of complex 1b



In a round bottom flask a mixture of **L2** (50 mg, 0.3 mmol) and $[Cp^*IrCl_2]_2$ (119.5 mg, 0.15 mmol) was taken. Then, dry MeOH (20 mL) was added to it and reflux for 24 h under argon atmosphere. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure

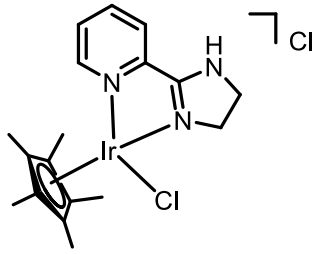
compound (Yield: 121.03 mg, 65%) as a yellowish orange solid. **^{1}H NMR** (500 MHz, DMSO-d_6): δ = 9.28 (s, 1H), 7.93 (t, *J* = 7.8 Hz, 1H), 7.68 (d, *J* = 7.1 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 4.35-4.29 (m, 1H), 3.92-3.86 (m, 2H), 3.75-3.68 (m, 1H), 1.59 (s, 15H). **^{13}C NMR** (125 MHz, CD_3OD): 168.02, 154.08, 142.87, 118.79, 117.59, 92.30, 87.31, 52.17, 45.34, 8.64. **HRMS (ESI)**: Calcd. for $C_{18}H_{24}ClIrN_3O$ $[M\text{-}Cl]^+$: 526.1237; found: 526.1238. Anal. Calculated ($C_{18}H_{24}Cl_2IrN_3O$): C, 38.50; H, 4.31; N, 7.48; Found: C, 38.37; H, 4.19; N, 7.34.

Synthesis of complex 1c

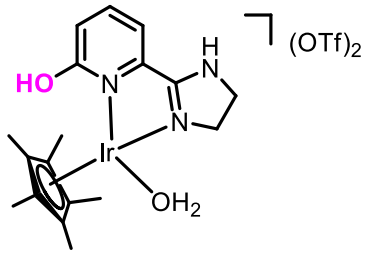


A mixture of **L3** (50 mg, 0.31 mmol) and $[Cp^*IrCl_2]_2$ (123.4 mg, 0.155 mmol) was stirred in dry DCM (20 mL) at room temperature for 24 h under argon atmosphere. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure compound (124.9 mg, yield: 72%) as a yellow solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 10.55 (s, 1H), 8.98 (d, *J* = 7.5 Hz, 1H), 7.88 (t, *J* = 7.7 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 4.17-4.06 (m, 3H), 3.88-3.82 (m, 1H), 2.90 (s, 3H), 1.61 (s, 15H). **^{13}C NMR** (125 MHz, $CDCl_3$): 169.60, 161.97, 146.63, 139.96, 128.96, 125.16, 87.81, 52.03, 45.71, 28.84, 9.88. **HRMS (ESI)**: Calcd. for $C_{19}H_{26}ClIrN_3$ $[M\text{-}Cl]^+$: 524.1444; found: 524.1441. Anal. Calculated ($C_{19}H_{26}Cl_2IrN_3$): C, 40.78; H, 4.68; N, 7.51; Found: C, 40.43; H, 4.29; N, 7.39.

Synthesis of complex 1d



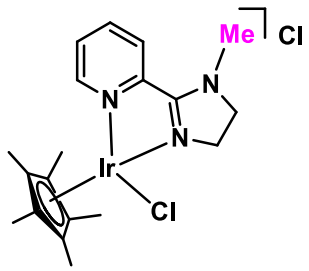
A mixture of **L4** (50 mg, 0.34 mmol) and $[Cp^*IrCl_2]_2$ (135 mg, 0.17 mmol) was stirred in dry DCM (20 mL) at room temperature for 24 h under argon atmosphere. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure compound (168 mg, yield: 82%) as a yellow solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 10.58 (s, 1H), 9.15 (d, *J* = 7.8 Hz, 1H), 8.71 (d, *J* = 5.5 Hz, 1H), 8.01 (t, *J* = 7.7 Hz, 1H), 7.65 (t, *J* = 6.1 Hz, 1H), 4.15-4.07 (m, 3H), 3.88-3.83 (m, 1H), 1.67 (s, 15H). **^{13}C NMR** (125 MHz, $CDCl_3$): 169.40, 151.15, 147.12, 140.19, 129.31, 128.00, 87.77, 52.02, 46.28, 9.26. **HRMS (ESI)**: Calcd. for $C_{18}H_{24}ClIrN_3$ $[M\text{-}Cl]^+$: 510.1288; found: 510.1276. Anal. Calculated ($C_{19}H_{24}Cl_2IrN_3$): C, 39.63; H, 4.43; N, 7.70; Found: C, 39.42; H, 4.27; N, 7.49.



Synthesis of complex 2

In a round bottom flask a mixture of **L2** (40 mg, 0.24 mmol) and $[Cp^*Ir(H_2O)_3](OTf)_2$ (158.7 mg, 0.24 mmol) was taken under argon atmosphere. Then, H_2O (20 mL) was added to it and stirred at room temperature for 18 h. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure compound (Yield: 134 mg, 68%) as a yellowish-orange solid. **^{1}H NMR** (500 MHz, CD_3OD): δ = 7.88 (t, *J* = 8.3 Hz, 1H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 3.98 (t, *J* = 9.7 Hz, 2H), 3.29-3.28 (m, 2H), 1.74 (s, 15H). **^{13}C NMR** (125 MHz, CD_3OD): 170.24, 165.10, 143.98, 141.30, 121.70, 119.17, 115.46, 88.08, 52.44, 45.49, 8.56. **HRMS (ESI)**: Calcd. for $C_{18}H_{25}IrN_3O_2$ $[M-H_2O-2OTf-H]^+$: 490.1470; found: 490.1521. Anal. Calculated ($C_{20}H_{26}F_6IrN_3O_8S_2$): C, 29.77; H, 3.25; N, 5.21; Found: C, 29.43; H, 3.13; N, 5.09.

Synthesis of complex 1e



A mixture of **L5** (35 mg, 0.21 mmol) and $[Cp^*IrCl_2]_2$ (86.5 mg, 0.108 mmol) was stirred in dry DCM (16 mL) at room temperature for 24 h under argon atmosphere. The resulting solution was filtered and insoluble part was removed. The filtrate was evaporated to dryness under reduced pressure and washed with diethyl ether to give pure compound (97.2 mg, yield: 75%) as a yellow solid. **^{1}H NMR** (500 MHz, $CDCl_3$): δ = 8.90 (d, *J* = 4.9 Hz, 1H), 8.52 (d, *J* = 7.8 Hz, 1H), 8.24 (t, *J* = 7.6 Hz, 1H), 7.85 (t, *J* = 5.2 Hz, 1H), 4.20-4.13 (m, 2H), 4.06-3.99 (m, 1H), 3.83-3.76 (m, 1H), 3.49 (s, 3H), 1.66 (s, 15H). **^{13}C NMR** (125 MHz, $CDCl_3$): 167.20, 153.12, 145.95, 140.70, 130.08, 127.28, 88.33, 55.86, 50.67, 36.02, 9.28. **HRMS (ESI)**: Calcd. for $C_{19}H_{26}ClIrN_3$ $[M-Cl]^+$: 524.1444; found: 524.1453. Anal. Calculated ($C_{19}H_{26}Cl_2IrN_3$): C, 40.78; H, 4.68; N, 7.51; Found: C, 40.47; H, 4.33; N, 7.43.

3. X-ray crystallographic studies.

Single crystal of complex **1b** was obtained from DCM-methanol-hexane mixture under slow evaporation. Single-crystal X-ray data of complex **1b** was collected at 100 K by using a Bruker SMART APEX II CCD diffractometer and Bruker D8 Quest Single Crystal diffractometer with graphite monochromatic MoK_α radiation (λ =0.71073 Å). The frames were indexed, integrated and scaled using SMART and SAINT software package and the data were corrected for absorption using the SADABS program. The structure was solved and refined using WINGX

and SHELX programs. The crystallographic figure has been generated using Diamond 3 software10 (30% probability thermal ellipsoids). The CCDC number of complex **1b** is CCDC 1878158. One molecule dichloromethane was co-crystallized in this method.

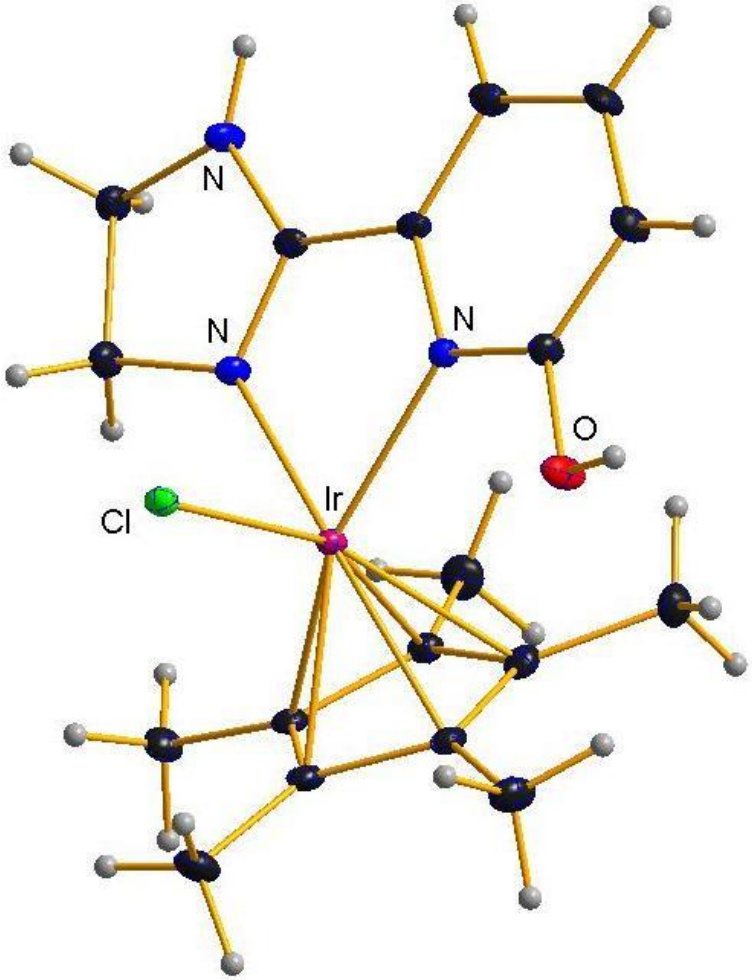


Fig. S1 Solid state structure of complex **1b** (30% thermal ellipsoids, Cl counter anion was omitted for clarity).

Crystal data and structure refinement for 1b.

Identification code	1b
Empirical formula	$C_{19}H_{26}Cl_4IrN_3O$
Formula weight	646.43
Temperature/K	100(2)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.768(3)
b/Å	14.165(3)
c/Å	13.588(3)
α/°	90
β/°	111.994(6)
γ/°	90
Volume/Å^3	2278.6(10)

Z	4
ρ_{calc}g/cm^3	1.884
μ/mm^{-1}	6.344
F(000)	1256.0
Crystal size/mm^3	0.010 × 0.010 × 0.010
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.534 to 56.568
Index ranges	$-17 \leq h \leq 17$, $-18 \leq k \leq 18$, $-18 \leq l \leq 18$
Reflections collected	35066
Independent reflections	5634 [R_{int} = 0.0556, R_{sigma} = 0.0324]
Data/restraints/parameters	5634/0/259
Goodness-of-fit on F^2	1.069
Final R indexes [I>=2σ (I)]	R_1 = 0.0228, wR_2 = 0.0573
Final R indexes [all data]	R_1 = 0.0257, wR_2 = 0.0591
Largest diff. peak/hole / e Å^{-3}	1.67/-1.05

4: Synthesis of quinoxaline derivatives

4A. General procedure for quinoxaline synthesis from di-amine derivatives: In a Schlenk tube 1,2-diamine derivatives (0.5 mmol), diol (2.5 mmol), Cat. **1b** (2.5 mol %), KOH (0.75 mmol) and H_2O (3.0 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the quinoxaline derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

4B. General procedure for quinoxaline synthesis from nitroamine derivatives: In a Schlenk tube 1,2-nitroamine derivatives (0.5 mmol), diol (2.5 mmol), Cat. **1b** (2.5 mol %), KOH (0.75 mmol) and H_2O (3.0 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the quinoxaline derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

5. Synthesis of benzimidazole derivatives

5A. General procedure for benzimidazole synthesis from di-amine derivatives: In a Schlenk tube 1,2-diamine derivatives (0.3 mmol), primary alcohol (0.45 mmol), Cat. **2** (2.5 mol %) and H_2O (2.0 mL) were taken under argon atmosphere. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the benzimidazole derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

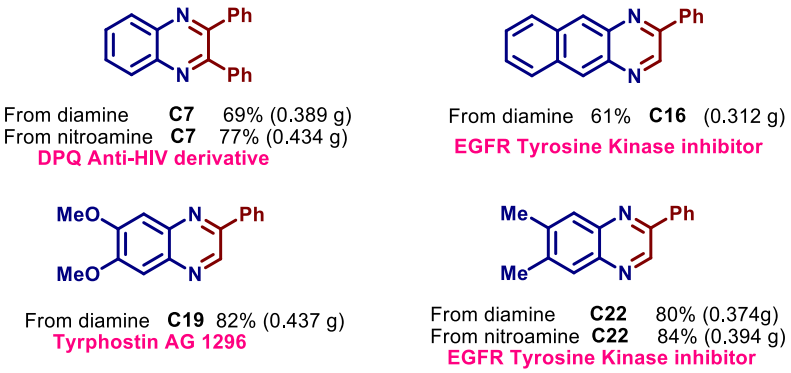
6. Synthesis of quinazolines derivatives

6A. General procedure for quinazolines synthesis from di-amine derivatives: In a Schlenk tube 2-aminobenzyl amine (0.3 mmol), primary alcohol (0.45 mmol), Cat. **2** (2.0 mol %) and H_2O (2.0 mL) were taken under argon atmosphere. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with

ethyl acetate. Finally, the quinazolines were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

7. Procedure for synthesis of pharmaceutically active quinoxaline derivatives

In a Schlenk flask 1,2-diamine/nitroamine derivatives (2 mmol), diol (10 mmol), Cat. **1b** (2.5 mol %), KOH (3 mmol) and H_2O (15 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the quinoxalines were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.



Scheme S1 synthesis of pharmaceutically active quinoxaline derivatives.

8. Procedure for preparative scale reaction

8A. Quinoxaline derivatives synthesis

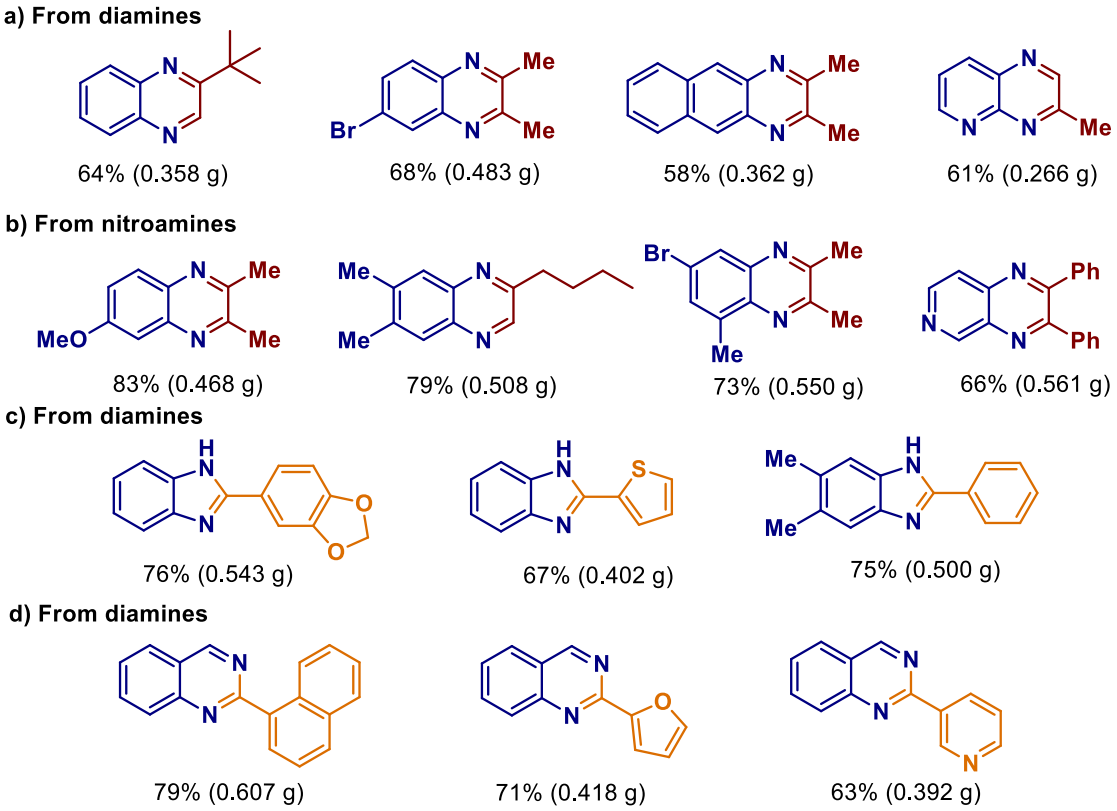
In a Schlenk flask 1,2-diamine/nitroamine derivatives (3 mmol), diol (15 mmol), Cat. **1b** (2.5 mol %), KOH (4.5 mmol) and H_2O (20 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the quinoxaline derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

8B. Benzimidazole derivatives synthesis

In a Schlenk flask 1,2-diamine derivatives (3 mmol), primary alcohol (4.5 mmol), Cat. **2** (2.5 mol %) and H_2O (25 mL) were taken under argon atmosphere. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the benzimidazole derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.

8C. Quinazoline derivatives synthesis

In a Schlenk flask 2-aminobenzyl amine (3 mmol), primary alcohol (4.5 mmol), Cat. **2** (2.0 mol %) and H_2O (25 mL) were taken under argon atmosphere. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally, the quinazolines derivatives were purified by column chromatography using hexane/ethyl acetate as eluent to afford the corresponding pure product.



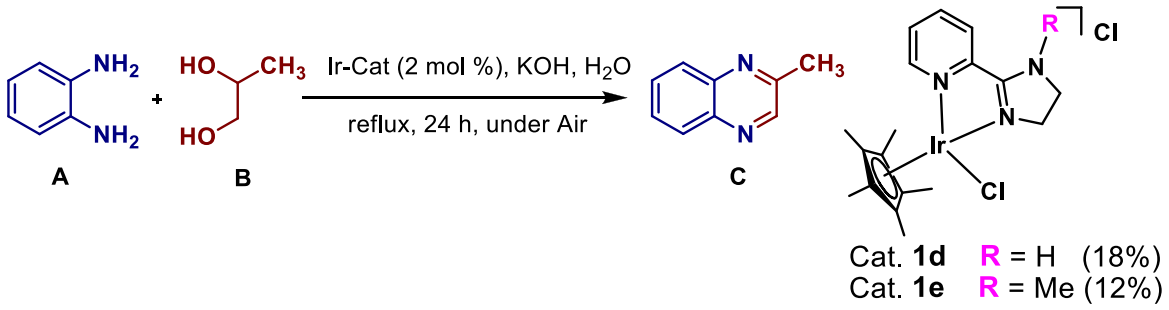
Scheme S2 Preparative scale reaction.

9. Control experiments and reusability

9A. Procedure for control experiments

In a Schlenk tube 1,2-diamine/nitroamine derivatives (0.5 mmol), diol (2.5 mmol), Cat. **1b** (2.5 mol %), KOH (0.75 mmol) and H_2O (3.0 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for different time interval. Then, it was cooled to room temperature and extracted with ethyl acetate. Finally the yield of quinoxaline derivatives were confirmed by Gas chromatography using mesitylene as internal standard.

9B. Effect of proton responsive N-H functionality



Scheme S3 Effect of proton responsive N-H functionality.

9C. Synthesis of Ir-H species of Complex 1b

In a J-Young NMR tube, complex **1b** (0.02 mmol), KO*t*Bu (0.06 mmol) and *i*PrOH (0.5 mL) were taken and heated at 82 °C for 30 minutes. After that, solvent was removed in vacuum and ^{1}H NMR spectrum was recorded in DMSO-d6.

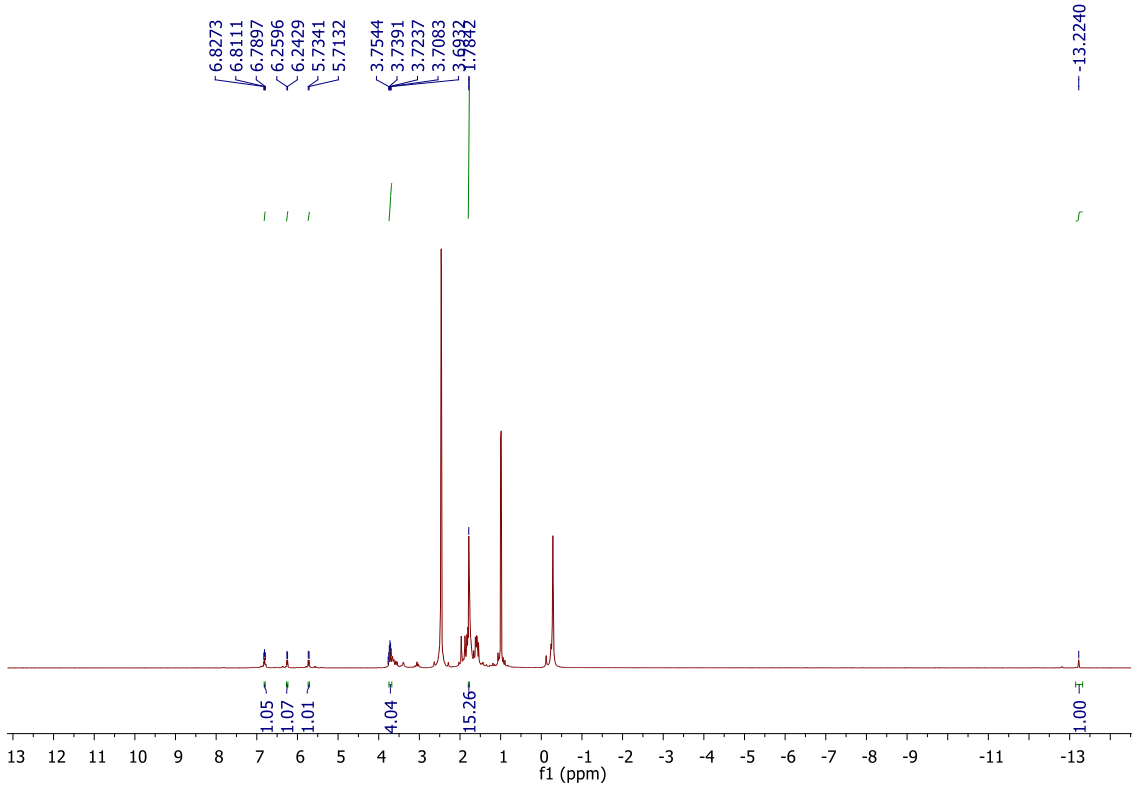
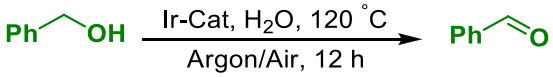


Fig. S2 ^{1}H NMR spectrum of Ir-H for complex **1b**.

9D. Activity difference of cat 1b and 2 in aerobic and argon condition

Table S1. Catalytic activity difference of cat 1b and 2



Entry	Catalyst	Base	Condition	Conversion
1	1b	KOH (1.5 equiv.)	Aerobic	24
2	1b	KOH (1.5 equiv.)	Argon	4
3	2	-	Argon	55
4	2	-	Aerobic	23

Reaction Conditions: Benzyl alcohol (0.15 mmol), Ir cat. (2 mol %), H_2O (1.0 mL), 120 °C (oil bath temperature), 12 h. Yield determined by GC analysis.

9E. Procedure for reusability

In a Schlenk tube benzene-1,2-diamine (0.5 mmol), propane-1,2-diol (2.5 mmol), Cat. **1b** (2.5 mol %), KOH (0.75 mmol) and H_2O (3.0 mL) were taken under air. The reaction mixture was heated at 120 °C in a preheated oil bath for 24 h. Then, it was cooled to room temperature and extracted with diethylether and the aqueous layer containing the catalyst was used for the next run. In the successive runs, benzene-1,2-diamine (0.5 mmol), propane-1,2-diol (2.5 mmol) and

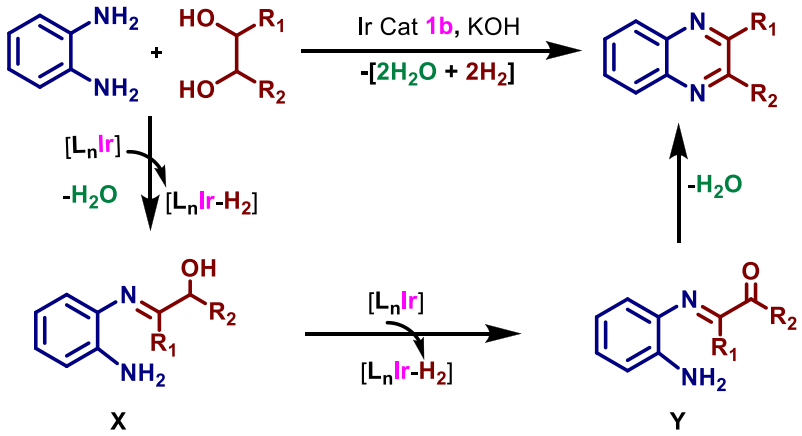
KOH (0.75 mmol) were added to the aqueous layer. The yield of product **C1** was determined by GC analysis using mesitylene as an internal standard.

Table S2. Reusability of catalytic system for synthesis of 2-methylquinoxaline

Run	1	2	3
Yield (%)	92	57	23

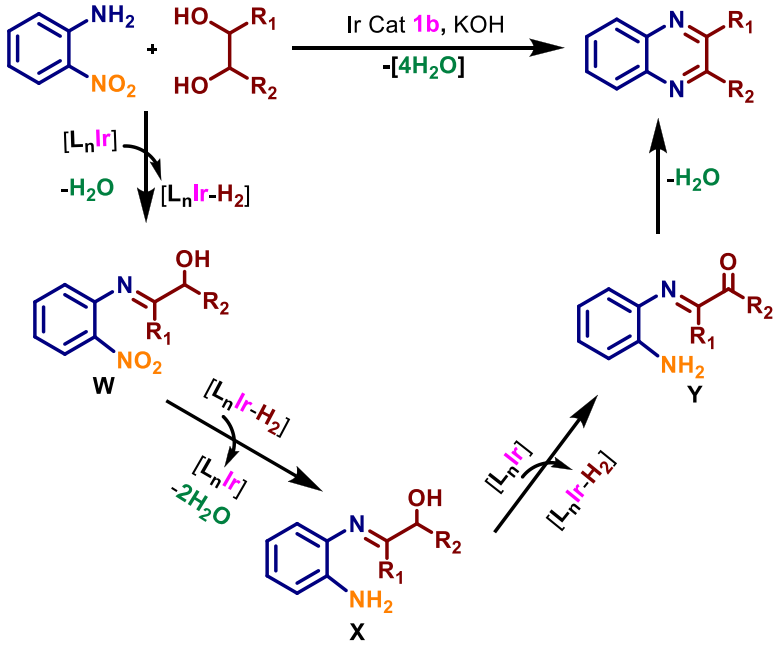
10. Proposed pathways of the reactions

10A. Stepwise mechanism of quinoxaline synthesis from diamine



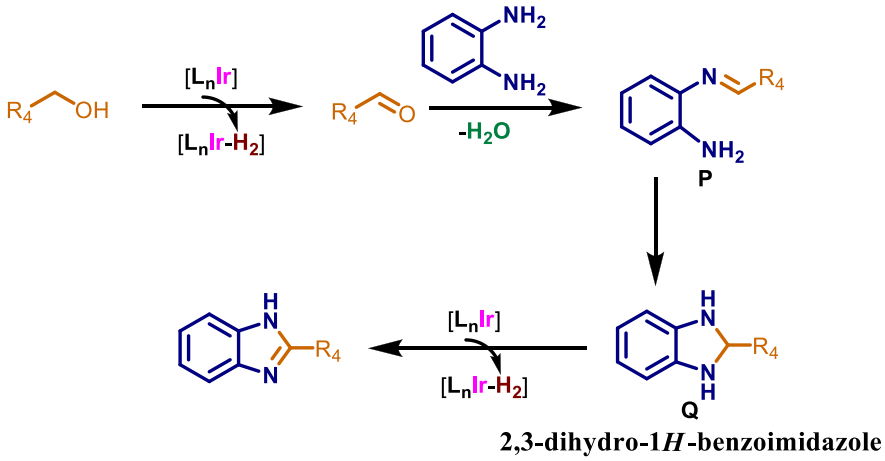
Scheme S4 Stepwise mechanism of quinoxaline synthesis from diamine.

10B. Stepwise mechanism of quinoxaline synthesis from nitroamine



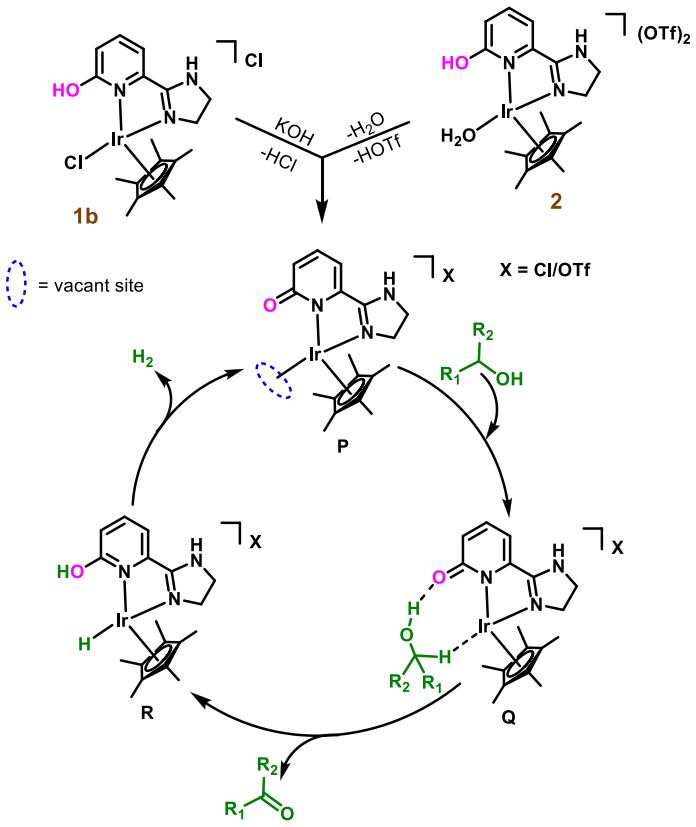
Scheme S5 Stepwise mechanism of quinoxaline synthesis from nitroamine.

10C. Stepwise mechanism of benzimidazole synthesis from diamine



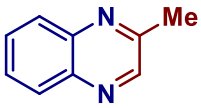
Scheme S6 Stepwise mechanism of benzimidazole synthesis from diamine.

10D. Proposed mechanism of alcohol dehydrogenation by cat. 1b or 2



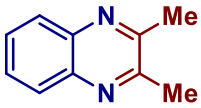
Scheme S7 Proposed mechanism of alcohol dehydrogenation by cat. **1b** or **2.**

11. Characterization of the products



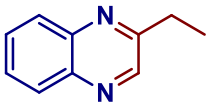
2-methylquinoxaline (**C1**)[3]

62 mg; 86% isolated yield from diamine and 63 mg; 87% isolated yield from nitroamine; yellow liquid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.71 (s, 1H), 8.04 (dd, *J* = 8.6 Hz, 1.6 Hz, 1H), 7.98 (dd, *J* = 7.6 Hz, 1.6 Hz, 1H), 7.73-7.65 (m, 2H), 2.74 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.87, 146.10, 142.15, 141.04, 130.10, 129.26, 129.01, 128.74, 22.68. **GC-MS** (M^+) = 144.1.



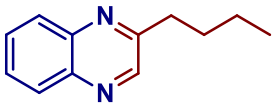
2,3-dimethylquinoxaline (**C2**)[4]

70 mg; 89% isolated yield from diamine and 72 mg; 90% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 7.96 (dd, *J* = 6.3 Hz, 3.6 Hz, 2H), 7.65 (dd, *J* = 6.4 Hz, 3.5 Hz, 2H), 2.71 (s, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.58, 141.15, 128.94, 128.38, 23.29. **GC-MS** (M^+) = 158.1.



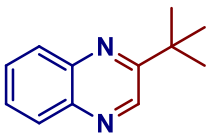
2-ethylquinoxaline (**C3**)[5]

56 mg; 70% isolated yield from diamine; yellow oil. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 8.69 (s, 1H), 8.02-7.97 (m, 2H), 7.68-7.62 (m, 2H), 2.98 (q, *J* = 7.6 Hz, 2H), 1.37 (t, *J* = 7.7 Hz, 3H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 158.49, 145.61, 142.19, 141.26, 129.94, 129.21, 128.93, 128.90, 29.67, 13.46. **GC-MS** (M^+) = 158.0.



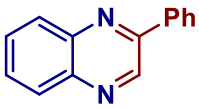
2-butylquinoxaline (**C4**)[5]

68 mg; 73% isolated yield from diamine and 72 mg; 77% isolated yield from nitroamine; yellow oil. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.72 (s, 1H), 8.06-8.00 (m, 2H), 7.74-7.66 (m, 2H), 3.00 (t, *J* = 7.9 Hz, 2H), 1.85-1.77 (m, 2H), 1.49-1.39 (m, 2H), 0.95 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ =157.79, 145.93, 142.27, 141.27, 130.00, 129.24, 128.99, 128.93, 36.35, 31.75, 22.67, 13.99. **GC-MS** (M^+) = 186.1.



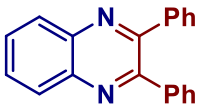
2-tert-butylquinoxaline (**C5**)[6]

63 mg; 68% isolated yield from diamine and 75 mg; 80% isolated yield from nitroamine; yellow oil. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 8.97 (s, 1H), 8.06-8.03 (m, 2H), 7.73-7.66 (m, 2H), 1.50 (s, 9H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 163.77, 143.50, 141.70, 140.87, 129.71, 129.37, 128.98, 128.94, 37.33, 29.83. **GC-MS** (M^+) = 186.0.



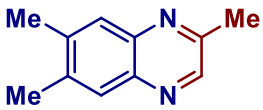
2-phenylquinoxaline (**C6**)[7]

88 mg; 85% isolated yield from diamine and 95 mg; 92% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.31 (s, 1H), 8.19-8.09 (m, 4H), 7.79-7.70 (m, 2H), 7.57-7.50 (m, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 151.96, 143.47, 142.40, 141.68, 136.88, 130.38, 130.28, 129.72, 129.64, 129.25, 127.65. **GC-MS** (M^+) = 206.1.



2,3-diphenylquinoxaline (**C7**)[7]

109 mg; 77% isolated yield from diamine and 116 mg; 83% isolated yield from nitroamine; cream yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.17 (dd, *J* = 6.5 Hz, 3.7 Hz, 2H), 7.76 (dd, *J* = 6.5 Hz, 3.4 Hz, 2H), 7.52-7.50 (m, 4H), 7.35-7.30 (m, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.56, 141.33, 139.18, 130.03, 129.93, 129.30, 128.88, 128.35. **GC-MS** (M^+) = 282.1.

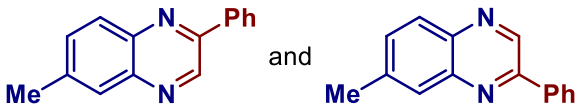


2,6,7-trimethylquinoxaline (**C8**)[8]

62 mg; 72% isolated yield from diamine and 72 mg; 83% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 8.61 (s, 1H), 7.77 (s, 1H), 7.73 (s, 1H), 2.71 (s, 3H), 2.45 (s, 6H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 152.77, 145.09, 141.09, 140.53, 139.99, 139.32, 128.27, 127.84, 22.52, 20.44, 20.28. **GC-MS** (M^+) = 172.1.

2,6-dimethylquinoxaline (**C9a**) and 2,7-dimethylquinoxaline (**C9b**)[9]

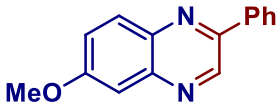
This two regio-isomers were inseparable in column chromatography. The mixture yield is 60 mg; 76% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.68-8.65 (s, 1H), 7.94-7.87 (m, 1H), 7.81-7.76 (s, 1H), 7.56-7.50 (m, 1H), 2.74 (s, 3H), 2.56 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.75, 152.88, 145.98, 145.18, 142.26, 141.13, 140.62, 139.54, 139.41, 132.37, 131.27, 128.76, 128.26, 128.13, 127.67, 22.64, 22.54, 21.94, 21.78. **GC-MS** (M^+) = 158.0.



6-methyl-2-phenylquinoxaline (**C10a**) and 7-methyl-2-phenylquinoxaline (**C10b**)[10]

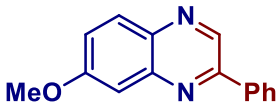
This two regio-isomers were inseparable in column chromatography. The mixture yield is 90 mg; 82% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.26-9.24 (s, 1H), 8.18-8.15 (m, 2H), 8.03-7.97 (d, *J* = 8.6 Hz, 1H), 7.91-7.87 (s, 1H), 7.67-7.49 (m, 4H), 2.59 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 151.86, 151.15, 143.33, 142.54, 142.46, 141.72, 140.90, 140.85, 140.20, 140.16, 137.04, 132.69, 131.95, 130.14, 130.04, 129.20, 128.69, 128.55, 128.05, 127.57, 127.50, 21.96, 21.93. **GC-MS** (M^+) = 220.1.

This two regio-isomers (**C11a** and **C11b**) were separated by column chromatography. The total (**C11a** + **C11b**) yield is 102 mg; 86% isolated yield from diamine with selectivity **C11a**:**C11b** = 3.4:1; the total (**C11a** + **C11b**) yield is 107 mg; 90% isolated yield from nitroamine with selectivity **C11a**:**C11b** = 4.1:1; cream yellow solid.



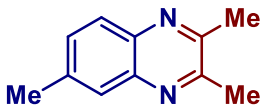
6-methoxy-2-phenylquinoxaline (**C11a**) [3]

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.23 (s, 1H), 8.15-8.13 (m, 2H), 8.02 (d, *J* = 9.1 Hz, 1H), 7.56-7.47 (m, 3H), 7.44-7.38 (m, 2H), 3.98 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.64, 149.73, 143.31, 138.50, 137.09, 130.66, 129.80, 129.19, 127.29, 123.66, 106.60, 55.92. **GC-MS** (M^+) = 236.1.



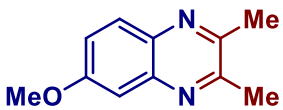
7-methoxy-2-phenylquinoxaline (**C11b**)[3]

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.14 (s, 1H), 8.15-8.13 (m, 2H), 7.96 (d, *J* = 9.1 Hz, 1H), 7.55-7.48 (m, 3H), 7.41-7.35 (m, 2H), 3.96 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 161.12, 152.00, 144.03, 140.82, 137.84, 137.06, 130.12, 129.20, 127.59, 122.98, 106.93, 55.91. **GC-MS** (M^+) = 236.1.



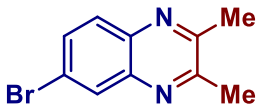
2,3,6-trimethylquinoxaline (**C12**)[11]

66 mg; 77% isolated yield from diamine; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 7.83 (d, *J* = 8.5 Hz, 1H), 7.72 (s, 1H), 7.47 (d, *J* = 8.5 Hz, 1H), 2.68 (s, 6H), 2.53 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.38, 152.52, 141.18, 139.54, 139.23, 131.12, 127.88, 127.36, 23.25, 23.15, 21.83. **GC-MS** (M^+) = 172.0.



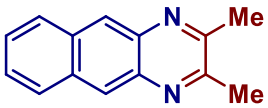
6-methoxy-2,3-dimethylquinoxaline (**C13**)[3]

79 mg; 84% isolated yield from diamine and 84 mg; 89% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 7.82 (d, *J* = 8.9 Hz, 1H), 7.29-7.25 (m, 2H), 3.90 (s, 3H), 2.67 (s, 3H), 2.65 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.01, 153.42, 150.69, 142.51, 137.06, 129.31, 121.73, 106.22, 55.73, 23.18, 22.87. **GC-MS** (M^+) = 188.0.



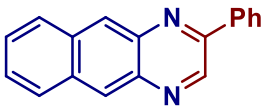
6-bromo-2,3-dimethylquinoxaline (**C14**)[12]

87 mg; 73% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 8.14 (d, *J* = 1.9 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.72 (dd, *J* = 8.9 Hz, 2 Hz, 1H) 2.71 (s, 3H), 2.69 (s, 3H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 154.60, 154.00, 141.82, 139.92, 132.40, 130.86, 130.81, 129.79, 122.56, 23.26. **GC-MS** (M^+) = 237.0.



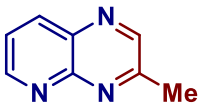
2,3-dimethylbenzo[g]quinoxaline (**C15**)[13]

65 mg; 62% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.51 (s, 2H), 8.05 (dd, *J* = 6.4 Hz, 3.2 Hz, 2H), 7.51 (dd, *J* = 6.4 Hz, 3.0Hz, 2H), 2.76 (s, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 154.54, 138.15, 133.36, 128.46, 126.51, 126.40, 23.75. **GC-MS** (M^+) = 208.1.



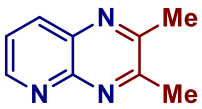
2-phenylbenzo[g]quinoxaline (**C16**)[14]

89 mg; 69% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.38 (s, 2H), 8.71 (s, 1H), 8.67 (s, 1H), 8.26 (d, *J* = 7.1 Hz, 2H), 8.12-8.09 (m, 2H), 7.60-7.54 (m, 5H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 151.92, 144.68, 138.86, 138.25, 136.89, 134.31, 133.74, 130.55, 129.31, 128.64, 128.56, 128.06, 127.75, 127.67, 127.02, 126.85. **GC-MS** (M^+) = 256.0.



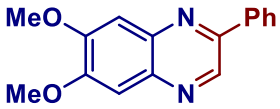
3-methylpyrido[2,3-b]pyrazine (**C17**)[15]

47 mg; 65% isolated yield from diamine; cream yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 9.11 (t, *J* = 1.7 Hz, 1H), 8.81 (s, 1H), 8.41 (dd, *J* = 8.3 Hz, 1.8 Hz, 1H), 7.65 (dd, *J* = 8.3 Hz, 4.2 Hz, 1H), 2.84 (s, 3H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 157.76, 154.02, 150.86, 147.22, 138.26, 136.06, 124.51, 22.91. **GC-MS** (M^+) = 144.9.



2,3-dimethylpyrido[2,3-b]pyrazine (**C18**)[16]

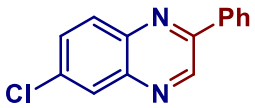
56 mg; 70% isolated yield from diamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 9.03 (s, 1H), 8.32 (d, *J* = 7.8 H, 1H), 7.60 (dd, *J* = 7.9 Hz, 3.8 Hz, 1H), 2.79 (s, 3H), 2.75 (s, 3H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 157.44, 155.12, 152.81, 150.30, 137.43, 135.98, 124.41, 23.58, 23.10. **GC-MS** (M^+) = 159.1.



6,7-dimethoxy-2-phenylquinoxaline (**C19**)[17]

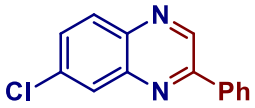
117 mg; 88% isolated yield from diamine; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.09 (s, 1H), 8.11 (d, *J* = 7.3 Hz, 2H), 7.54-7.44 (m, 3H), 7.40 (s, 1H), 7.35 (s, 1H), 4.50 (s, 3H), 4.04 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 153.11, 152.64, 149.93, 140.76, 139.58, 138.83, 137.30, 129.67, 129.15, 128.60, 127.24, 126.15, 107.11, 106.67, 56.47, 56.44. **GC-MS** (M^+) = 266.1.

This two regio-isomers (**C20a** and **C20b**) were separated by column chromatography. The total (**C20a** + **C20b**) yield is 105 mg; 87% isolated yield from nitroamine with selectivity **C11a**:**C11b** = 1:1.7; cream yellow solid.



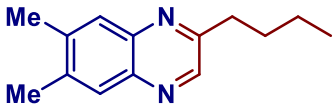
6-chloro-2-phenylquinoxaline (**C20a**)[3]

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.31 (s, 1H), 8.18-8.15 (m, 2H), 8.10-8.06 (m, 2H), 7.71 (dd, *J* = 9.1 Hz, 2.3 Hz, 1H), 7.58-7.50 (m, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 152.04, 144.23, 141.87, 140.92, 136.43, 135.35, 131.43, 130.92, 130.54, 129.31, 128.15, 127.60. **GC-MS** (M^+) = 240.0.



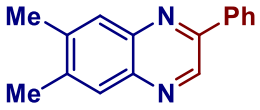
7-chloro-2-phenylquinoxaline (**C20b**)[3]

^{1}H NMR ($CDCl_3$, 400 MHz): δ = 9.36 (s, 1H), 8.25-8.20 (m, 3H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.73 (dd, *J* = 9.0 Hz, 2.3 Hz, 1H), 7.65-7.57 (m, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 152.63, 143.49, 142.74, 140.17, 136.38, 136.19, 130.64, 130.60, 130.43, 129.30, 128.58, 127.69. **GC-MS** (M^+) = 240.0.



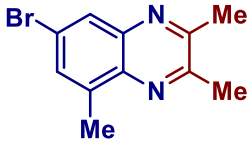
2-butyl-6,7-dimethylquinoxaline (**C21**)[18]

90 mg; 84% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.60 (s, 1H), 7.77 (s, 1H), 7.75 (s, 1H), 2.94 (t, *J* = 8.0 Hz, 2H), 2.45 (s, 6H), 1.82-1.74 (m, 2H), 1.46-1.37 (m, 2H), 0.94 (t, *J* = 7.5 Hz, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 156.73, 144.91, 140.42, 140.19, 139.31, 128.24, 128.01, 36.24, 31.84, 22.65, 20.45, 20.31, 13.99. **GC-MS** (M^+) = 214.0.



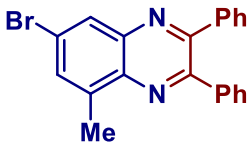
6,7-dimethyl-2-phenylquinoxaline (**C22**)[10]

106 mg; 90% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.19 (s, 1H), 8.15-8.13 (m, 2H), 7.87 (s, 1H), 7.82 (s, 1H), 7.55-7.45 (m, 3H), 2.84 (s, 6H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 151.06, 142.47, 141.30, 140.87, 140.62, 140.19, 137.20, 129.91, 129.15, 128.73, 128.21, 127.46, 20.48, 20.45. **GC-MS** (M^+) = 234.0.



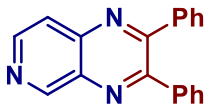
7-bromo-2,3,5-trimethylquinoxaline (**C23**)[11]

98 mg; 78% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 7.96 (d, *J* = 1.9 Hz, 1H), 7.57 (d, *J* = 1.0 Hz, 1H), 2.72 (s, 3H), 2.69 (s, 6H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 153.98, 152.63, 141.83, 139.18, 138.78, 132.11, 128.53, 122.16, 23.39, 23.12, 16.93. **GC-MS** (M^+) = 250.9.



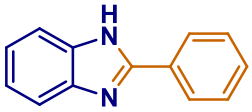
7-bromo-5-methyl-2,3-diphenylquinoxaline (**C24**)

137 mg; 73% isolated yield from nitroamine; yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 8.17 (s, 1H), 7.68 (s, 1H), 7.56-7.49 (m, 4H), 7.38-7.30 (m, 6H), 2.81 (s, 3H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 153.75, 152.14, 141.83, 139.61, 139.25, 139.13, 139.04, 133.15, 130.13, 129.88, 129.25, 129.05, 128.97, 128.38, 128.23, 123.63, 16.94. **GC-MS** (M^+) = 374.9. **HRMS (ESI)**: Calcd. for $C_{21}H_{15}BrN_2$ $[M]^+$: 374.0419; found: 374.0417.



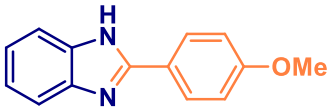
2,3-diphenylpyrido[3,4-b]pyrazine (**C25**)[19]

99 mg; 70% isolated yield from nitroamine; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 9.60 (s, 1H), 8.82 (d, *J* = 6.0 Hz, 1H), 7.99 (d, *J* = 5.8 Hz, 1H), 7.54-7.52 (m, 4H), 7.41-7.38 (m, 2H), 7.37-7.34 (m, 4H). **^{13}C NMR** ($CDCl_3$, 125 MHz): δ = 158.05, 155.48, 154.54, 147.39, 143.68, 138.37, 136.41, 129.95, 129.86, 129.77, 129.50, 128.50, 121.45. **GC-MS** (M^+) = 283.1.



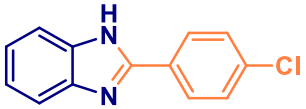
2-phenyl-1H-benzimidazole (**E1**)[20]

51 mg; 87% isolated yield; white solid. **^{1}H NMR** (DMSO-D_6, 500 MHz): δ = 12.89 (brs, 1H), 8.14 (d, *J* = 7.4 Hz, 2H), 7.62-7.43 (m, 5H), 7.17 (d, *J* = 4.6 Hz, 2H). **^{13}C NMR** (DMSO-D_6, 125 MHz): δ = 151.76, 144.28, 135.47, 130.64, 130.40, 129.49, 126.96, 123.10, 122.23, 119.35, 111.87. **GC-MS** (M^+) = 194.0.



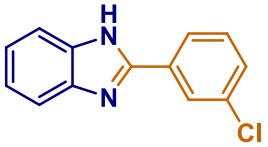
2-(4-methoxyphenyl)-1H-benzimidazole (**E2**)[21]

57 mg; 84% isolated yield; cream white solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.73 (brs, 1H), 8.09 (d, *J* = 7.7 Hz, 2H), 7.65-7.39 (m, 2H), 7.13-7.06 (m, 4H), 3.79 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 161.12, 151.58, 144.32, 135.37, 131.04, 128.54, 127.93, 123.20, 122.26, 118.92, 114.88, 55.83. **GC-MS** (M^+) = 224.1.



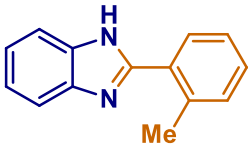
2-(4-chlorophenyl)-1H-benzimidazole (**E3**)[22]

52 mg; 75% isolated yield; white solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.95 (brs, 1H), 8.15 (d, *J* = 8.6 Hz, 2H), 7.70-7.49 (m, 4H), 7.22-7.10 (m, 2H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 150.68, 144.26, 135.54, 135.02, 129.59, 128.66, 123.30, 122.37, 119.49, 111.95. **GC-MS** (M^+) = 228.2.



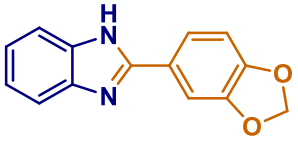
2-(3-chlorophenyl)-1H-benzimidazole (**E4**)[23]

54 mg; 78% isolated yield; white solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 13.02 (brs, 1H), 8.18 (s, 1H), 8.10 (d, *J* = 7.1 Hz, 1H), 7.56-7.50 (m, 4H), 7.24-7.18 (m, 2H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 150.26, 147.89, 134.31, 132.70, 131.48, 130.09, 126.54, 125.54, 123.47, 122.53, 119.60, 112.07. **GC-MS** (M^+) = 228.0.



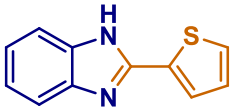
2-o-tolyl-1H-benzimidazole (**E5**)[24]

35 mg; 56% isolated yield; cream white solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.58 (brs, 1H), 7.70 (d, *J* = 7.1 Hz, 1H), 7.64 (d, *J* = 7.5 Hz, 1H), 7.49 (d, *J* = 7.4 Hz, 1H), 7.36-7.30 (m, 3H), 7.20-7.13 (m, 2H), 2.57 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 152.47, 144.24, 137.54, 134.95, 131.78, 130.62, 129.97, 129.83, 126.48, 122.88, 121.92, 119.45, 111.78, 21.55. **GC-MS** (M^+) = 208.1.



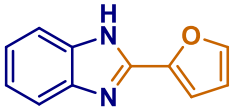
2-(benzo[d][1,3]dioxol-5-yl)-1H-benzimidazole (**E6**)[22]

57 mg; 80% isolated yield; cream white solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.71 (brs, 1H), 7.69 (dd, *J* = 8.0 Hz, 1.7 Hz, 1H), 7.65 (d, *J* = 1.4 Hz, 1H), 7.58 (brs, 1H), 7.46 (brs, 1H), 7.14 (d, *J* = 5.0 Hz, 2H), 7.05 (d, *J* = 8.0 Hz, 1H), 6.08 (s, 2H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 151.68, 149.26, 148.40, 144.21, 135.43, 124.78, 122.79, 122.11, 121.42, 119.10, 111.61, 109.26, 107.02, 102.10. **GC-MS** (M^+) = 238.1.



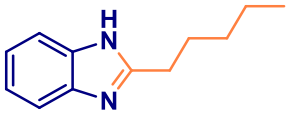
2-(thiophen-2-yl)-1H-benzimidazole (**E7**)[25]

43 mg; 72% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.92 (brs, 1H), 7.79 (dd, *J* = 3.6 Hz, 1.0 Hz, 1H), 7.68 (dd, *J* = 4.9 Hz, 0.72 Hz, 1H), 7.57 (d, *J* = 6.4 Hz, 1H), 7.46 (d, *J* = 6.0 Hz, 1H), 7.20-7.15 (m, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 147.57, 144.13, 135.21, 134.22, 129.27, 128.81, 127.22, 123.17, 122.30, 119.06, 111.63. **GC-MS** (M^+) = 200.0.



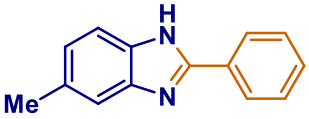
2-(furan-2-yl)-1H-benzimidazole (**E8**)[10]

36 mg; 64% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.89 (brs, 1H), 7.89 (s, 1H), 7.59 (d, *J* = 6.9 Hz, 1H), 7.45 (d, *J* = 6.8 Hz, 1H), 7.16 (d, *J* = 3.5 Hz, 3H), 6.69-6.67 (m, 1H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 146.10, 145.14, 144.17, 134.76, 123.16, 122.33, 119.29, 112.85, 111.87, 111.00. **GC-MS** (M^+) = 184.1.



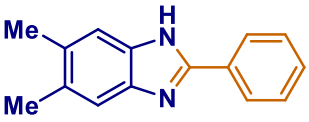
2-pentyl-1H-benzimidazole (**E9**)[26]

23 mg; 41% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 7.41 (dd, *J* = 5.9 Hz, 3.2 Hz, 2H), 7.05 (dd, *J* = 6.0 Hz, 3.1 Hz, 2H), 2.75 (t, *J* = 7.6 Hz, 2H), 1.75-1.68 (m, 2H), 1.27-1.24 (m, 4H), 0.81 (t, *J* = 6.9 Hz, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 155.68, 139.31, 121.55, 114.85, 31.41, 29.01, 27.81, 22.37, 14.37. **GC-MS** (M^+) = 188.0.



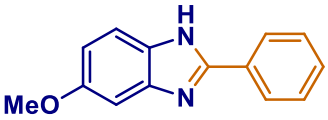
5-methyl-2-phenyl-1H-benzimidazole (**E10**)[27]

51 mg; 81% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.72 (brs, 1H), 8.12 (d, *J* = 7.2 Hz, 2H), 7.51-7.41 (m, 4H), 7.38-7.27 (m, 1H), 7.01-6.69 (m, 1H), 2.39 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 151.25, 142.46, 135.78, 132.40, 130.82, 130.17, 129.44, 126.82, 124.51, 123.79, 118.97, 111.57, 21.89. **GC-MS** (M^+) = 208.0.



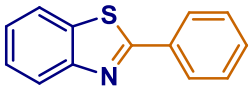
5,6-dimethyl-2-phenyl-1H-benzimidazole (**E11**)[28]

53 mg; 80% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.60 (brs, 1H), 8.10 (d, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.7 Hz, 2H), 7.41 (t, *J* = 7.1 Hz, 2H), 7.28-7.25 (m, 1H), 2.28 (s, 3H), 2.27 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 150.85, 143.03, 134.05, 131.69, 130.97, 130.44, 129.98, 129.38, 126.72, 119.45, 111.85, 20.56. **GC-MS** (M^+) = 222.0.



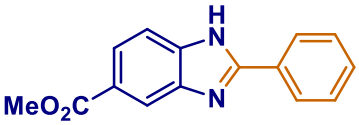
5-methoxy-2-phenyl-1H-benzimidazole (**E12**)[29]

55 mg; 82% isolated yield; pale yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 12.72 (brs, 1H), 8.09 (d, *J* = 7.6 Hz, 2H), 7.51-7.40 (m, 4H), 7.00 (brs, 1H), 6.79 (dd, *J* = 8.7 Hz, 2.0 Hz, 1H), 3.76 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 156.33, 154.18, 151.16, 139.37, 130.85, 130.02, 129.43, 126.64, 119.09, 111.81, 101.75, 55.96. **GC-MS** (M^+) = 224.1.



2-phenylbenzothiazole (**E13**)[30]

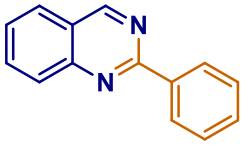
33 mg; 52% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 8.10-8.08 (m, 3H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.50-7.47 (m, 4H), 7.37 (t, *J* = 7.8 Hz, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 168.15, 154.25, 135.17, 133.73, 131.06, 129.11, 127.66, 126.41, 125.28, 123.34, 121.71. **GC-MS** (M^+) = 211.1.



methyl 2-phenyl-1H-benzimidazole-5-carboxylate

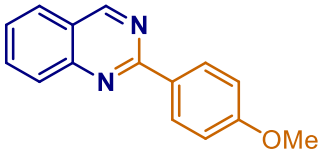
48 mg; 64% isolated yield; yellow solid. **^{1}H NMR** (DMSO-D_6, 400 MHz): δ = 13.22 (brs, 1H), 8.23-8.09 (m, 3H), 7.80 (brs, 1H), 7.55-7.46 (m, 4H), 3.82 (s, 3H). **^{13}C NMR** (DMSO-D_6, 100 MHz): δ = 167.28, 154.79, 143.95, 139.06, 135.25, 130.98, 130.06, 129.57, 127.29, 124.25,

121.02, 113.53, 111.92, 52.51. $\nu_{C=O}$: 1715 cm^{-1}. **HRMS (ESI)**: Calcd. for $C_{15}H_{12}N_2O_2$ $[M+H]^+$: 253.0977; found: 253.0977.



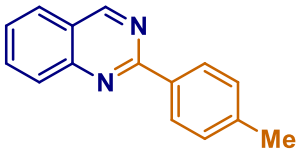
2-phenylquinazoline (**G1**)[31]

58 mg; 94% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.45 (s, 1H), 8.61 (d, *J* = 7.4 Hz, 2H), 8.08 (d, *J* = 8.4 Hz, 1H), 7.91-7.86 (m, 2H), 7.59 (t, *J* = 7.9 Hz, 1H), 7.55-7.49 (m, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 161.16, 160.57, 150.87, 138.14, 134.18, 130.69, 128.72, 128.67, 127.34, 127.20, 123.70. **GC-MS** (M^+) = 206.1.



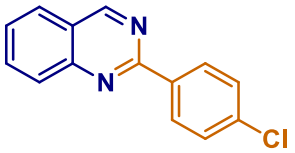
2-(4-methoxyphenyl)quinazoline (**G2**)[32]

64 mg; 90% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.39 (s, 1H), 8.56 (d, *J* = 8.8 Hz, 2H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.87-7.83 (m, 2H), 7.54 (t, *J* = 7.4 Hz, 1H), 7.02 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 161.92, 160.95, 160.46, 150.93, 134.08, 130.82, 130.29, 128.50, 127.20, 126.85, 123.40, 114.05, 55.46. **GC-MS** (M^+) = 236.0.



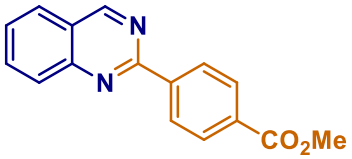
2-p-tolylquinazoline (**G3**)[32]

58 mg; 88% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.43 (s, 1H), 8.50 (d, *J* = 8.1 Hz, 2H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.90-7.85 (m, 2H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 2.43 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 161.24, 160.51, 150.89, 140.94, 135.41, 134.11, 129.50, 128.62, 127.19, 127.10, 123.60, 21.60. **GC-MS** (M^+) = 220.1.



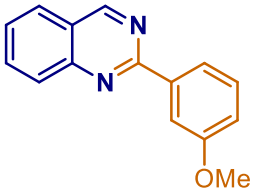
2-(4-chlorophenyl)quinazoline (**G4**)[31]

61 mg; 85% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.41 (s, 1H), 8.56-8.54 (m, 2H), 8.04 (d, *J* = 8.8 Hz, 1H), 7.89 (d, *J* = 7.6 Hz, 2H), 7.59 (t, *J* = 7.6 Hz, 1H), 7.47 (d, *J* = 8.6 Hz, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.60, 160.10, 150.76, 136.91, 136.60, 134.34, 129.98, 128.90, 128.68, 127.54, 127.23, 123.69. **GC-MS** (M^+) = 240.1.



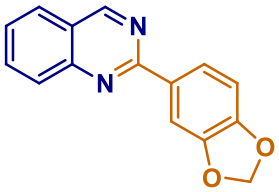
methyl 4-(quinazolin-2-yl)benzoate (**G5**)

47 mg; 60% isolated yield; yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.48 (s, 1H), 8.68 (d, *J* = 8.6 Hz, 2H), 8.18 (d, *J* = 8.6 Hz, 2H), 8.10 (d, *J* = 8.0 Hz, 1H) 7.95-7.92 (m, 2H), 7.64 (t, *J* = 7.3 Hz, 1H), 3.95 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 167.06, 160.08, 160.11, 150.77, 142.21, 134.45, 131.78, 129.95, 128.86, 128.57, 127.91, 127.26, 123.85, 52.33. **$\nu_{C=O}$**: 1720 cm^{-1}. **HRMS (ESI)**: Calcd. for $C_{16}H_{12}N_2O_2$ $[M+H]^+$: 265.0977; found: 265.0975.



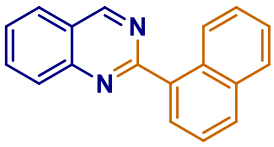
2-(3-methoxyphenyl)quinazoline (**G6**)[33]

63 mg; 88% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.43 (s, 1H), 8.22 (d, *J* = 7.8 Hz, 1H), 8.18-8.17 (m, 1H), 8.07 (d, *J* = 8.6 Hz, 1H), 7.90-7.85 (m, 2H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 8.0 Hz, 1H), 7.05 (dd, *J* = 8.2, 2.6 Hz, 1H), 3.93 (s, 3H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.92, 160.51, 160.11, 150.81, 139.58, 134.18, 129.72, 128.75, 127.38, 127.19, 123.74, 121.25, 117.33, 113.12, 55.53. **GC-MS** (M^+) = 236.1.



2-(benzo[d][1,3]dioxol-5-yl)quinazoline (**G7**)[34]

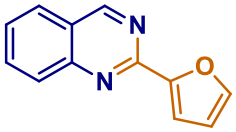
65 mg; 87% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.37 (s, 1H), 8.21 (dd, *J* = 8.3, 1.7 Hz, 1H), 8.10 (d, *J* = 1.6 Hz, 1H), 8.00 (d, *J* = 9.1 Hz, 1H), 7.87-7.82 (m, 2H), 7.54 (td, *J* = 7.0, 0.8 Hz, 1H), 6.93 (d, *J* = 8.3 Hz, 1H), 6.02 (s, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.61, 160.40, 150.83, 149.97, 148.27, 134.13, 132.60, 128.52, 127.18, 126.99, 123.60, 123.47, 108.80, 108.40, 101.51. **GC-MS** (M^+) = 250.0.



2-(naphthalen-1-yl)quinazoline (**G8**)[35]

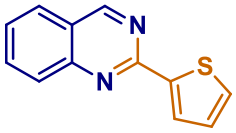
64 mg; 83% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.58 (s, 1H), 8.69 (d, *J* = 9.3 Hz, 1H), 8.18-8.15 (m, 2H), 8.02-7.91 (m, 4H), 7.69 (t, *J* = 7.8 Hz, 1H), 7.62 (t, *J* = 7.6 Hz, 1H), 7.55-7.51 (m, 2H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.52, 158.41,

157.69, 150.68, 150.06, 134.43, 134.27, 129.72, 128.78, 128.58, 127.85, 127.25, 126.96, 125.99, 125.48, 123.24. **GC-MS** (M^+) = 256.2.



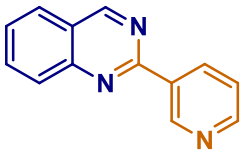
2-(furan-2-yl)quinazoline (**G9**)[36]

44 mg; 74% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 9.35 (s, 1H), 8.07 (d, *J* = 6.6 Hz, 1H), 7.88-7.85 (m, 2H), 7.67 (d, *J* = 1.0, 1H), 7.56 (t, *J* = 5.8 Hz, 1H), 7.43 (t, *J* = 3.1 Hz, 1H), 6.60-6.58 (m, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.83, 154.18, 152.58, 150.51, 145.44, 134.62, 128.48, 127.37, 123.46, 114.19, 112.42. **GC-MS** (M^+) = 195.9.



2-(thiophen-2-yl)quinazoline (**G10**)[37]

50 mg; 78% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 400 MHz): δ = 9.32 (s, 1H), 8.13 (d, *J* = 3.7 Hz, 1H), 7.98 (d, *J* = 8.9 Hz, 1H), 7.87-7.83 (m, 2H), 7.56-7.49 (m, 2H), 7.18-7.16 (m, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.60, 157.95, 150.71, 143.94, 134.43, 130.03, 129.32, 128.46, 128.27, 127.35, 127.07, 123.46. **GC-MS** (M^+) = 212.1.



2-(pyridin-3-yl)quinazoline (**G11**)[38]

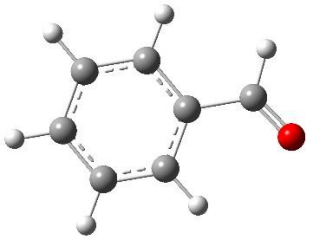
43 mg; 68% isolated yield; pale yellow solid. **^{1}H NMR** ($CDCl_3$, 500 MHz): δ = 9.81 (s, 1H), 9.48 (s, 1H), 8.86 (dt, *J* = 7.9, 1.7 Hz, 1H), 8.73 (d, *J* = 3.5 Hz, 1H), 8.10 (d, *J* = 8.4 Hz, 1H) 7.96-7.92 (m, 2H), 7.65 (t, *J* = 7.9 Hz, 1H), 7.46-7.44 (m, 1H). **^{13}C NMR** ($CDCl_3$, 100 MHz): δ = 160.75, 159.29, 151.25, 150.74, 150.32, 135.91, 134.49, 133.66, 128.76, 127.88, 127.29, 123.93, 123.51. **GC-MS** (M^+) = 207.1.

12. Computational studies

All the calculations were performed using the Gaussian 09 package.[39] Full geometry optimization followed by frequency calculations on the stationary points were carried out to ascertain the nature of the stationary points as minima or first order saddle point. Hybrid functional, M062X was used with the LANL2DZ basis set[40] for Ir and 6-31G** basis set[41] for non-metal elements. The transition states (TS) were further confirmed by performing intrinsic reaction coordinate (IRC) calculation using the same method. Solvent effect was incorporated using the conductor-like polarizable continuum model (CPCM) with water as solvent.[42]

13. Cartesian coordinates and statistical thermodynamic analysis

Benzaldehyde



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Thermal correction to Gibbs Free Energy=         0.080631
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SCF done (for solvent)                        -345.42966126
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C	-0.36149800	1.29085300	0.00000100
C	0.05113800	-1.09565300	0.00000200
C	-1.73300900	1.05561500	-0.00000100
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H	-2.42937400	1.88750400	-0.00000300
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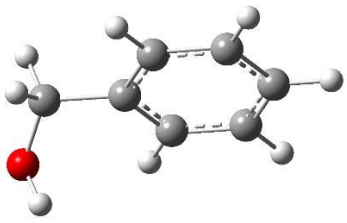
Benzyl alcohol



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Thermal correction to Gibbs Free Energy=         0.104027
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SCF done (for solvent)                        -346.63115488
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H	-1.69723900	-2.37261000	0.08064500
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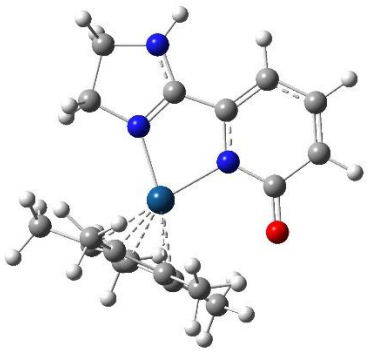
H	2.50137400	-0.62673900	-1.15954800

I1



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SCF done (for solvent) -1043.35927815

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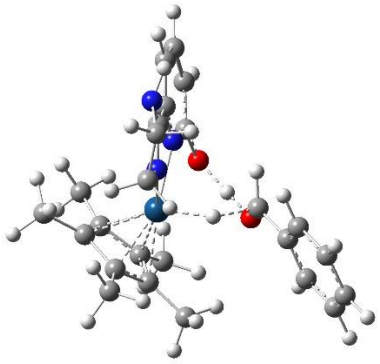
$TS1_{outer}$



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SCF done (for solvent) -1389.97607277

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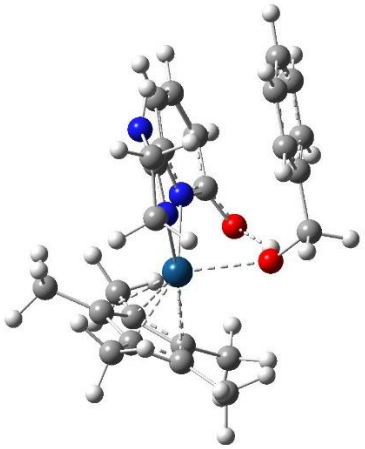
C	0.35282800	-2.76508500	-2.12326000
C	-1.52124600	-2.13904300	1.09981300
C	-2.73790700	-2.02271100	1.96146000
C	-1.48950400	-2.29181500	-0.31977300
C	-2.65741400	-2.29224200	-1.25204500
Ir	-0.34979600	-0.46322500	0.23243200
N	-2.10899200	2.94813400	1.91020400
N	-0.86631600	1.13851800	1.49405700
N	-1.33127900	0.96289100	-1.04520100
O	-0.64861300	0.03357100	-3.02297500
H	-2.41448500	3.86054700	1.60402200
H	2.63277800	-1.94171400	1.30684700
H	1.27728900	-1.65251600	3.10591700
H	2.61877400	-2.01373700	-0.45935800
H	-0.41194600	-1.56687800	3.62605700
H	2.50154200	-3.50957600	0.48493100
H	-3.41976700	3.57566600	-0.50299100
H	0.36023100	-3.13720300	3.40211500
H	1.37059000	-2.41280800	-2.29672600
H	-3.77474800	3.25039800	-2.97457600
H	-2.53982000	-1.41058800	2.84445400
H	-2.43528400	1.51489700	-4.16571700
H	0.33936900	-3.85324400	-2.24390900
H	0.62958200	-0.00219100	-2.66700800
H	-0.28911800	-2.31763200	-2.88296500
H	-3.05562500	-3.01136300	2.30779500
H	-3.56896800	-1.57155500	1.41621900
H	-2.39044400	-1.79979600	-2.19044100
H	-3.51881200	-1.78096600	-0.81851900
H	-2.94936500	-3.32244500	-1.47989300
C	1.80151600	0.86487800	-1.35595300
H	1.05650300	0.33781400	-0.10664300
H	1.14967600	1.74564600	-1.34809000
C	3.12080900	1.01368400	-0.71587900
C	3.29953700	1.99052000	0.26924300
C	4.18852400	0.20270000	-1.10878500
C	4.54129900	2.15185600	0.86616400
H	2.45760100	2.61342700	0.56428400
C	5.43241800	0.36955100	-0.50911700
C	5.60739800	1.33835200	0.47703200
H	4.68639800	2.91071900	1.62719700
H	6.26877600	-0.24882300	-0.81634200
H	6.58017300	1.46735300	0.93995300
O	1.67259600	0.01573900	-2.31304400
H	4.03751600	-0.52895600	-1.89586400
H	0.32759400	1.28302200	3.23683600
H	-1.31161700	0.64474100	3.48304800
H	-0.47935100	3.55840800	3.12288600
H	-1.87522600	2.91398800	4.02335100

I2



Zero-point correction=	0.524781
Thermal correction to Gibbs Free Energy=	0.465679
SCF done	-1389.95651117
SCF done (for solvent)	-1390.01716087

C	1.84200300	3.42955000	-0.85083000
C	0.45167200	3.04754400	-0.29244400
C	1.40938500	1.21671800	-1.16989400
C	-3.05417600	2.63342400	-0.18986900
C	-2.49783700	0.71388700	-2.70917000
C	1.57968900	-0.21586900	-1.43526100
C	2.59212000	-0.78277800	-2.16120700
C	-2.86358500	1.15134900	-0.13764100
C	-2.57557300	0.28819400	-1.27810400
C	2.67127600	-2.19896100	-2.15041200
C	0.83961600	-2.28383000	-0.52985200
C	1.83281300	-2.93083400	-1.35768100
C	-2.92156900	0.33986500	1.02723000
C	-3.12772100	0.79486100	2.43553500
C	-2.57223200	-1.08460500	-0.78761100
C	-2.34854600	-2.30645900	-1.61624600
C	-2.74027000	-1.05431800	0.62696400
C	-2.75381900	-2.22830700	1.55098600
Ir	-0.97263300	0.09083100	0.07458100
N	2.18656800	2.22574100	-1.62189600
N	0.42993000	1.58622700	-0.39703600
N	0.65815800	-0.94245400	-0.75123500
O	0.17846700	-2.86010100	0.36433500
H	3.15076300	2.03742300	-1.86007700
H	-2.64880200	3.05136300	-1.11282000
H	-2.03275700	1.69793400	-2.80014600
H	-2.57635800	3.12991900	0.65752200
H	-1.90282700	0.00817800	-3.29186900
H	-4.12294300	2.86679700	-0.16223200
H	3.30996600	-0.17995000	-2.70405200
H	-3.49819300	0.76480900	-3.14991600

H	-2.98950300	1.87332300	2.52817000
H	3.42998800	-2.69783600	-2.74500800
H	-1.72102900	-2.08325900	-2.48174600
H	1.90590800	-4.00973100	-1.28363400
H	-4.14242700	0.54968100	2.76389700
H	0.21465300	-1.57143300	1.67160500
H	-2.42291200	0.29623300	3.10528800
H	-3.30996900	-2.68312000	-1.97871800
H	-1.85855900	-3.08367500	-1.02757700
H	-2.39513800	-1.93970000	2.54127400
H	-2.10397100	-3.01979100	1.17497000
H	-3.77306900	-2.61299300	1.65461600
O	0.05849900	-0.64419400	1.97807400
C	1.16129000	-0.10641100	2.71660300
H	0.83954400	0.88455600	3.04708000
H	1.30411100	-0.73207600	3.60505500
C	2.44356400	-0.00962300	1.92830900
C	3.03231300	1.22925600	1.67761900
C	3.07095000	-1.16876700	1.46197800
C	4.22458000	1.31568700	0.95866900
C	4.25460100	-1.08575800	0.73691000
H	2.62717900	-2.14260000	1.66239600
C	4.83396000	0.15781900	0.48279300
H	4.68965000	2.28396300	0.79359600
H	4.72872600	-1.99221600	0.37463000
H	5.76851000	0.21942200	-0.06580600
H	2.56932200	3.58422400	-0.04686900
H	1.81441900	4.31374200	-1.48763100
H	0.30376600	3.36644200	0.74194400
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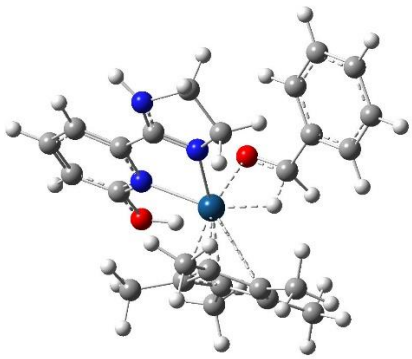
H	2.56274500	2.13202000	2.06396500

$TS1_{inner}$



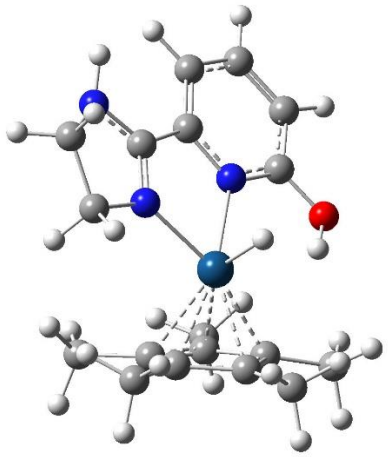
Zero-point correction= 0.518191
Thermal correction to Gibbs Free Energy= 0.457493
SCF done -1389.85172227
SCF done (for solvent) -1389.91274507

C	-1.67607900	-3.18426900	1.76878400
C	-1.74260900	-1.66650000	1.51815000
C	0.26168300	-2.41528000	0.87054800

C	-1.59752200	3.01760200	2.09982900
C	0.47506500	0.88700400	3.06547300
C	1.59878200	-2.34980000	0.26036300
C	2.50163600	-3.38812300	0.23985900
C	-0.35104800	2.69922500	1.34351000
C	0.53414300	1.53878800	1.71510200
C	3.68863500	-3.22311900	-0.49232400
C	2.90836500	-1.05857100	-1.15129400
C	3.88710200	-2.06810100	-1.21234000
C	0.10749600	3.20900100	0.17988300
C	-0.47593800	4.28420300	-0.67682700
C	1.69558400	1.61578300	0.89021800
C	3.06900200	1.12880900	1.23785800
C	1.29557900	2.39993500	-0.25292100
C	2.22458400	2.94975700	-1.30416700
Ir	0.33425200	0.32791600	-0.14214300
N	-0.22833300	-3.42884300	1.63197000
N	-0.53930200	-1.41390800	0.71075900
N	1.83949500	-1.16097700	-0.36155900
O	3.06358400	0.02387800	-1.89689800
H	0.11188500	-4.37210600	1.51210400
H	-2.30124200	2.17438100	2.05323000
H	-0.55928500	0.69012500	3.36005900
H	-2.10074600	3.89723200	1.69502200
H	1.02398800	-0.05844700	3.08449700
H	-1.39191200	3.20562500	3.15858400
H	2.29772600	-4.31277100	0.76603900
H	0.90724300	1.54809700	3.82541200
H	-1.35491500	4.73751400	-0.21572800
H	4.42647900	-4.01735700	-0.52072600
H	3.03787500	0.19448200	1.80457100
H	4.75373200	-1.90685600	-1.84150600
H	0.25203400	5.08065700	-0.86392600
H	2.23549400	0.54169200	-1.90067000
H	-0.77010400	3.89305700	-1.65855200
H	3.55821600	1.88387400	1.86185700
H	3.68914100	0.98377100	0.35089800
H	1.74415300	2.99206700	-2.28667600
H	3.15036700	2.37832200	-1.39290800
H	2.50578800	3.97546500	-1.04113300
O	-0.55383900	-0.19669200	-1.99819800
C	-1.53345700	0.59228200	-1.62185700
H	-1.20986300	1.09723600	-0.38034500
H	-1.59984500	1.58120000	-2.10257700
C	-2.85154100	-0.04549600	-1.28945800
C	-3.87346000	0.69405500	-0.69303000
C	-3.03503700	-1.39757100	-1.57591500
C	-5.07227900	0.07432700	-0.35775000
C	-4.24217200	-2.01269400	-1.25148700
H	-2.22623300	-1.94152400	-2.05239000
C	-5.25539700	-1.28123900	-0.63453600
H	-5.86615500	0.64485000	0.11248500
H	-4.39732900	-3.06087000	-1.48693300
H	-6.19445200	-1.76209500	-0.38106900
H	-2.23217500	-3.73222200	0.99871300
H	-2.03396300	-3.47306100	2.75648200

H	-2.64742500	-1.35319600	0.99646800
H	-1.64993200	-1.10139200	2.45324200
H	-3.72365700	1.75126000	-0.48093400

I3

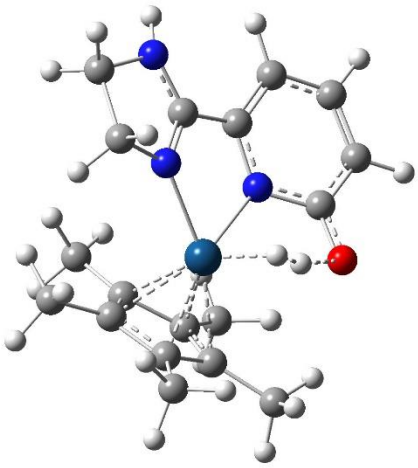


Zero-point correction=	0.407485
Thermal correction to Gibbs Free Energy=	0.355433
SCF done	-1044.49636216
SCF done (for solvent)	-1044.55570476

C	-2.38690100	3.54563200	-0.30136700
C	-0.92056300	3.06949000	-0.17708400
C	-2.26863400	1.29062100	-0.01018900
C	3.19353400	0.08179500	-2.01258600
C	2.59017700	2.48277900	0.01724200
C	-2.60796100	-0.13466100	0.04071700
C	-3.86806300	-0.64690300	0.26021600
C	2.53392100	-0.03174900	-0.67454800
C	2.24518900	1.04142900	0.23009000
C	-4.02449800	-2.04015800	0.23561500
C	-1.68977400	-2.23779200	-0.25657500
C	-2.93831800	-2.84353100	-0.03402400
C	2.12051900	-1.25580300	-0.04030700
C	2.44857600	-2.63676100	-0.53339800
C	1.79016500	0.46297000	1.49736400
C	1.48302200	1.24954800	2.73314200
C	1.70507600	-0.92732600	1.32353400
C	1.24311700	-1.94548800	2.31830100
Ir	0.39178600	0.07087700	-0.33778000
N	-3.12532100	2.33858400	0.11271500
N	-1.02859200	1.60744300	-0.17961400
N	-1.52069500	-0.91788400	-0.18019400
O	-0.64452600	-2.99804500	-0.55336000
H	-4.09311400	2.23316800	-0.15683800
H	3.00626100	1.05625200	-2.46608600
H	2.51862100	2.75561800	-1.03751400
H	2.82999500	-0.68464000	-2.69883800

H	1.92953400	3.13977900	0.58756700
H	4.27553600	-0.04169600	-1.90001800
H	-4.70756900	0.00869000	0.45838300
H	3.61489700	2.67685000	0.35017100
H	2.31756500	-2.72344100	-1.61518800
H	-4.99835600	-2.48308200	0.41225000
H	0.96264400	2.18113900	2.49757400
H	-3.00723300	-3.92251300	-0.09299200
H	3.49468600	-2.86768800	-0.30869100
H	0.08593300	-2.41338100	-0.83567700
H	1.83760000	-3.40138800	-0.04745300
H	2.40889000	1.51472600	3.25389300
H	0.85920800	0.68160000	3.42492200
H	0.61878500	-2.70461900	1.83877400
H	0.66958800	-1.48880100	3.12619600
H	2.10392300	-2.45715700	2.76098000
H	0.09840000	0.12718500	-1.87471200
H	-0.28352900	3.40768200	-0.99633500
H	-0.47248500	3.39101300	0.77008000
H	-2.63636000	3.81208900	-1.33366300
H	-2.61397000	4.38789400	0.35198400

TS2



Zero-point correction= 0.400392
Thermal correction to Gibbs Free Energy= 0.348665
SCF done -1044.43918354
SCF done (for solvent) -1044.50159852

C	-2.25932200	3.56089200	-0.22542200
C	-0.96720800	2.99018400	-0.85364800
C	-2.19353300	1.28653500	-0.06090200
C	3.48806800	0.51369600	-1.56161800
C	2.31808900	2.60376400	0.54368300
C	-2.51730100	-0.12943200	0.15779000
C	-3.76217600	-0.67451000	0.32928700
C	2.63284500	0.19610200	-0.37647000
C	2.11145000	1.12415200	0.56655900
C	-3.86800900	-2.08416600	0.21774500

C	-1.52760700	-2.20968000	-0.42084800
C	-2.79249400	-2.83976400	-0.16686000
C	2.25279300	-1.14395300	0.06057200
C	2.63858200	-2.42750300	-0.60285100
C	1.36438600	0.39477200	1.57899700
C	0.71670800	0.98646500	2.79036100
C	1.50718000	-1.01838900	1.27532400
C	0.91556200	-2.15543000	2.04266000
Ir	0.43486500	-0.00079600	-0.31797000
N	-3.04448700	2.33374300	-0.03355800
N	-0.99247400	1.57116800	-0.47554200
N	-1.41989800	-0.89664200	-0.06444800
O	-0.53028800	-2.74281900	-0.98344100
H	-3.89338000	2.31925000	0.51131800
H	3.30611700	1.52702900	-1.92275400
H	2.34827900	2.99046100	-0.47699700
H	3.29559200	-0.17744000	-2.38340200
H	1.53552700	3.12465100	1.09853800
H	4.54502400	0.43178600	-1.28920800
H	-4.63825500	-0.05629600	0.48317500
H	3.27434500	2.84010400	1.02140100
H	2.84391300	-2.27321500	-1.66367400
H	-4.83026000	-2.55940300	0.37680300
H	0.24520900	1.94345500	2.55393600
H	-2.87045700	-3.90547000	-0.34413800
H	3.54392200	-2.82772400	-0.13642000
H	1.83690800	-3.16295100	-0.51935500
H	1.45622000	1.15546300	3.57899900
H	-0.05343300	0.32088100	3.18478700
H	0.61613900	-2.95446400	1.36073200
H	0.03761200	-1.83683200	2.60754200
H	1.65276400	-2.55295300	2.74661300
H	0.05110900	-1.46107600	-1.60874800
H	0.19394600	-0.63793300	-1.99659800
H	-2.77360100	4.26102700	-0.88380400
H	-2.06516000	4.04777600	0.73725300
H	-0.98292700	3.06082500	-1.94652300
H	-0.06755500	3.48659900	-0.48957800

14. References

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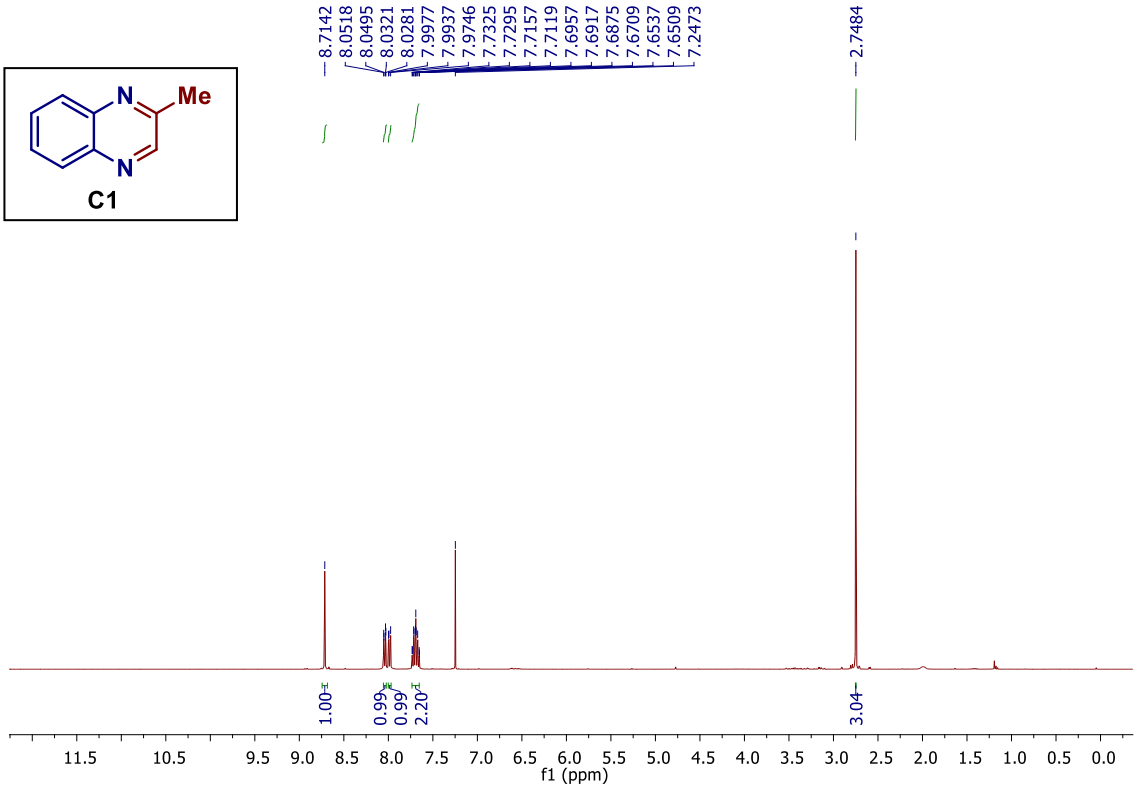
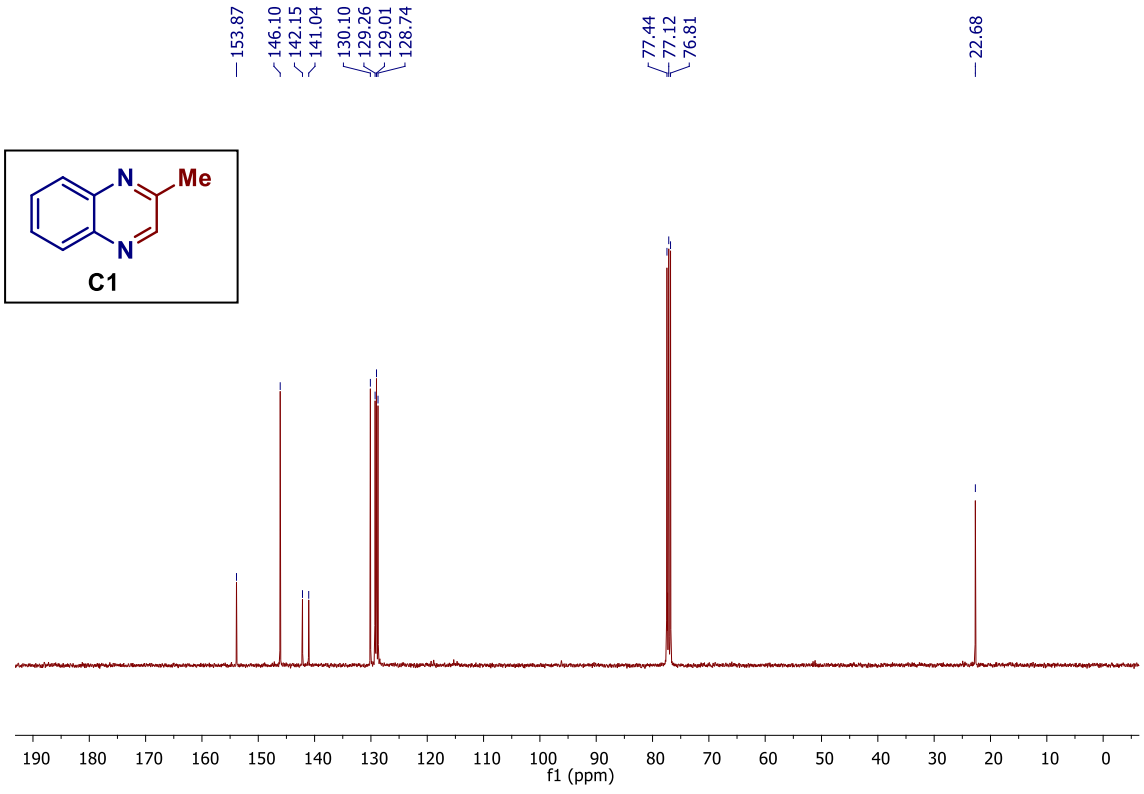
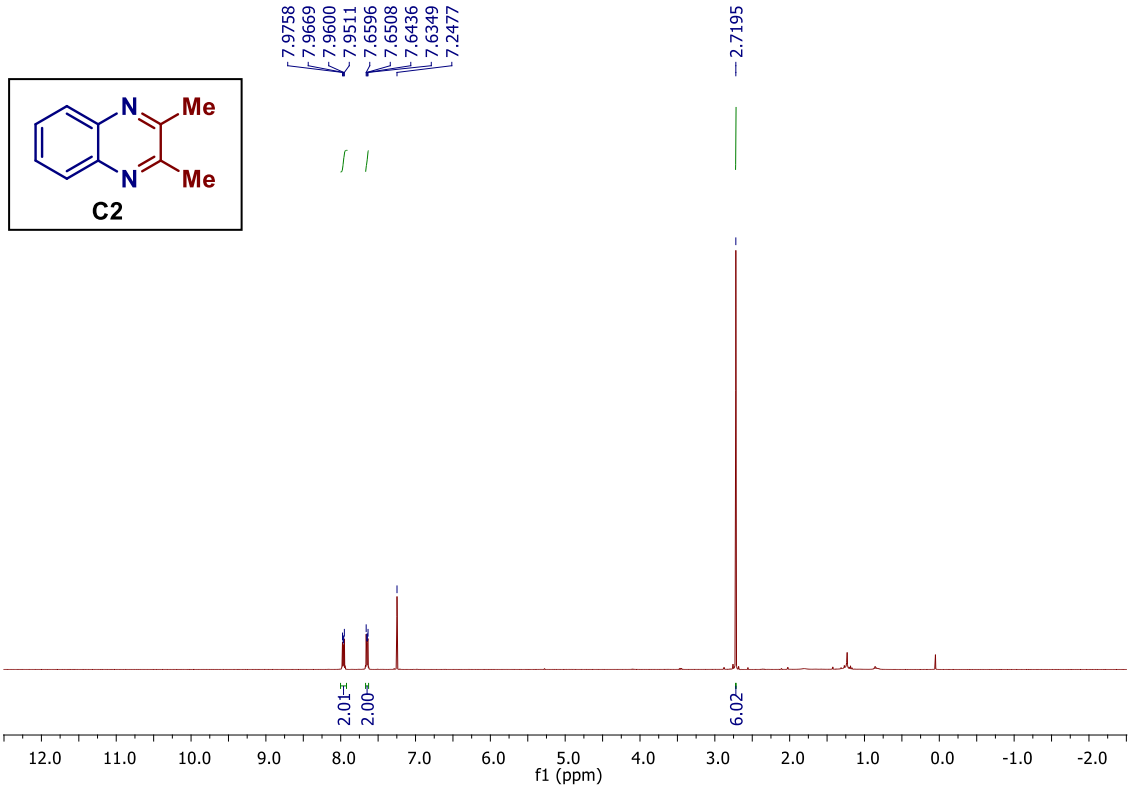
15. Copies of ^{1}H and ^{13}C NMR spectra of the products



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N
Me
N
Me
C2
2.01
2.00
6.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
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0.0
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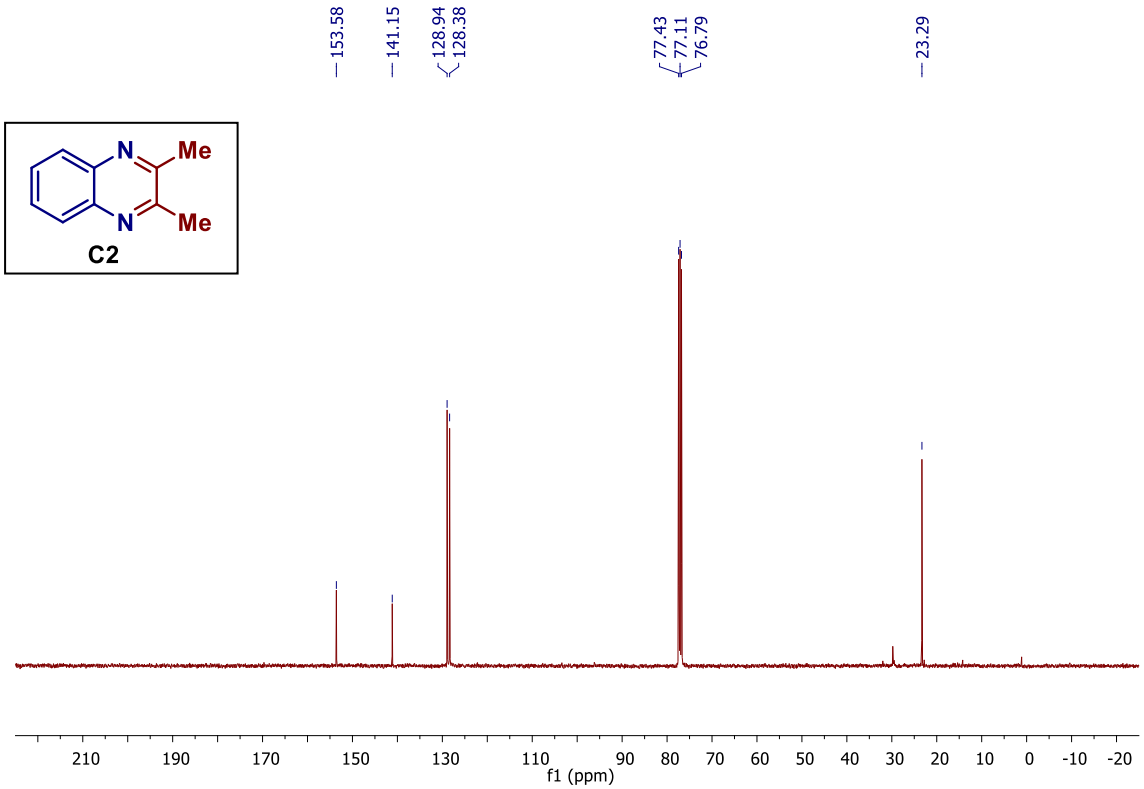
-2.0
f1 (ppm)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77.43
77.11
76.79
23.29
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Me
N
Me
C2
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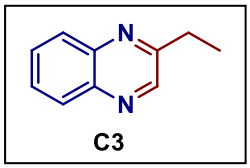
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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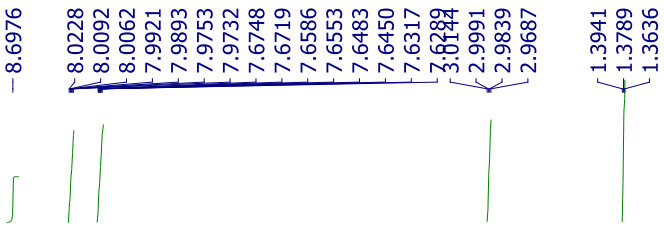
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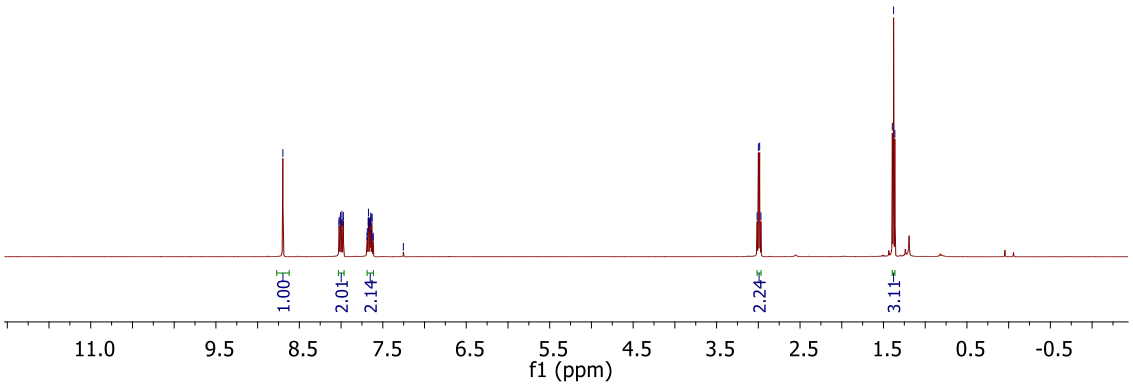
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3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


158.49
145.61
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128.90
77.43
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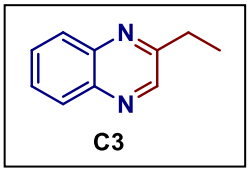
76.92
29.67
13.46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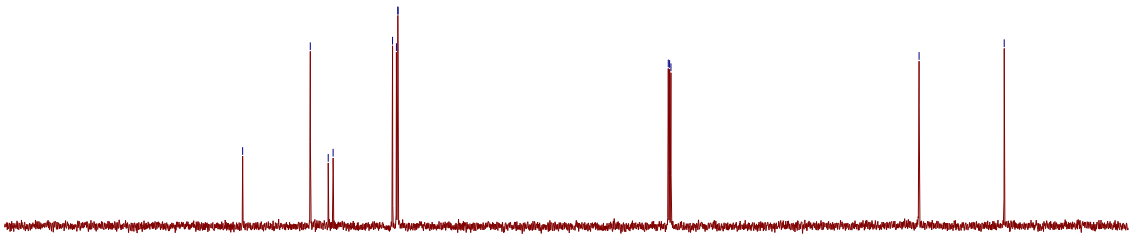

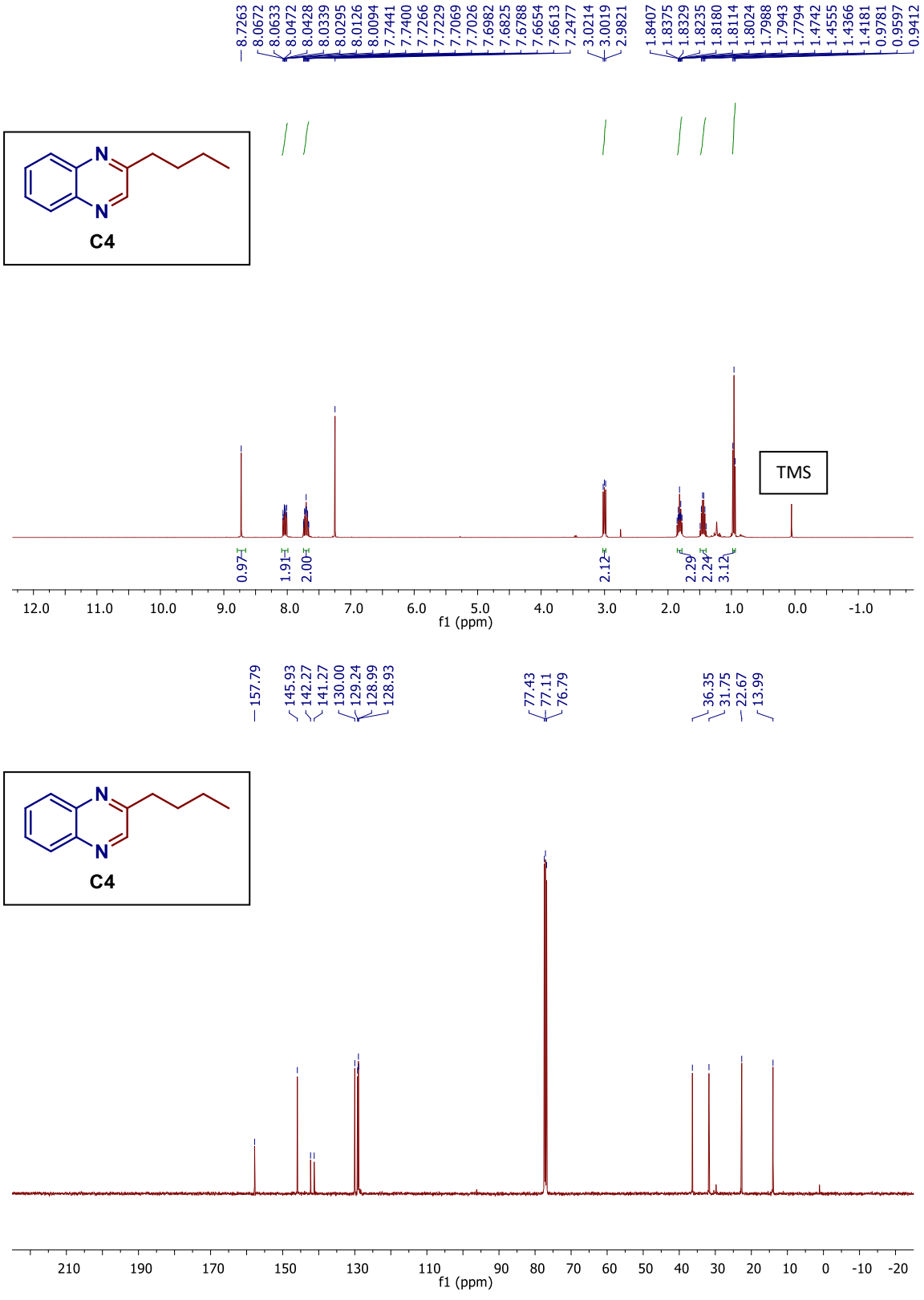
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0.9412
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C4
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2.00
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2.29
2.24
3.12
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)
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142.27
141.27
130.00
129.24
128.99
128.93
77.43
77.11
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22.67
13.99
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N
C4
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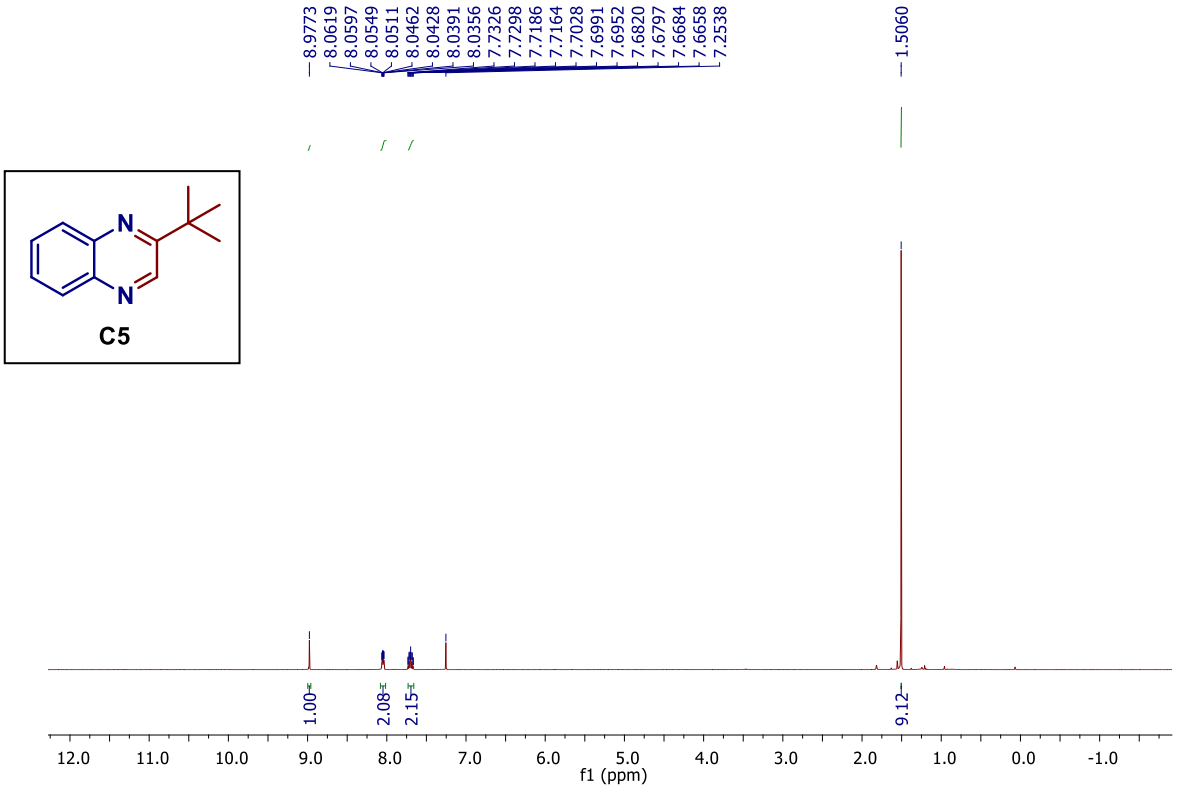
f1 (ppm)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7.7164
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7.6684
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7.2538
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C5
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2.15
9.12
12.0
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10.0
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4.0
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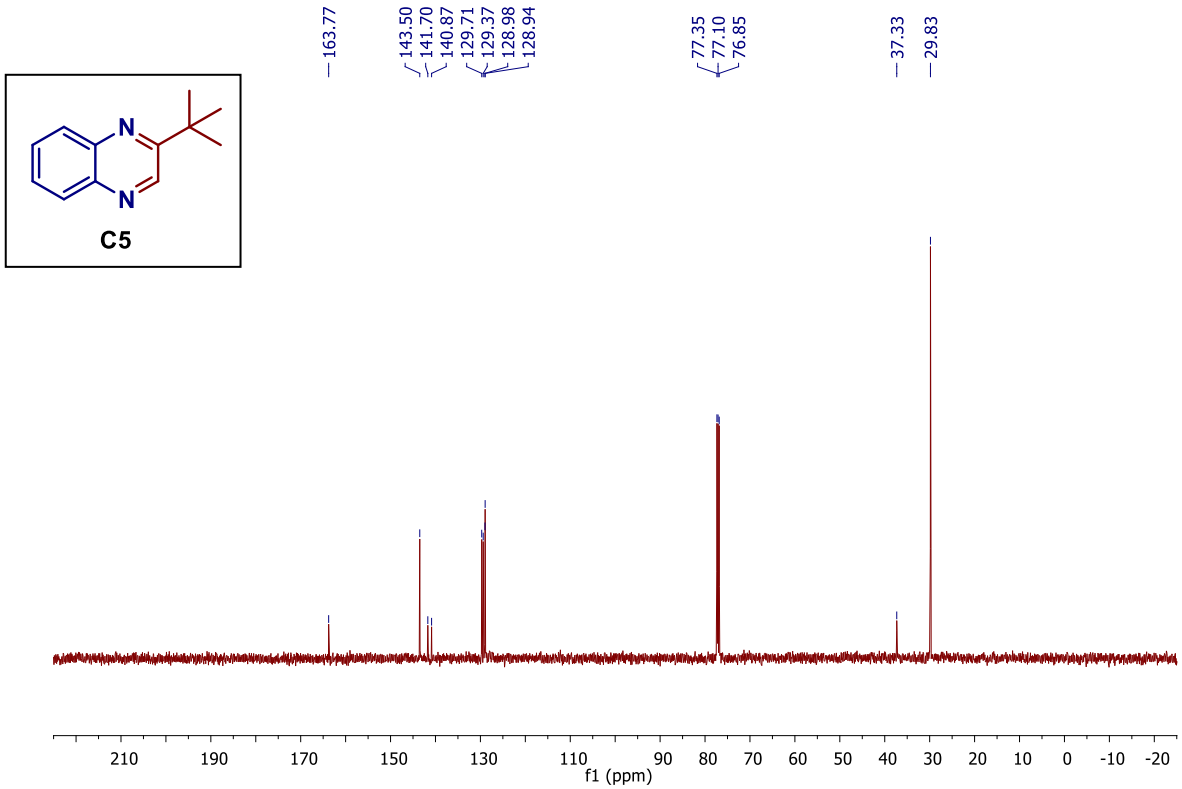
f1 (ppm)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29.83
N
N
C5
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130
110
90
80
70
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40
30
20
10
0
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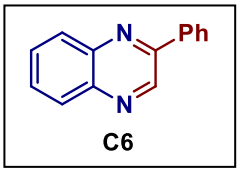
-20
f1 (ppm)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Ph
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C6


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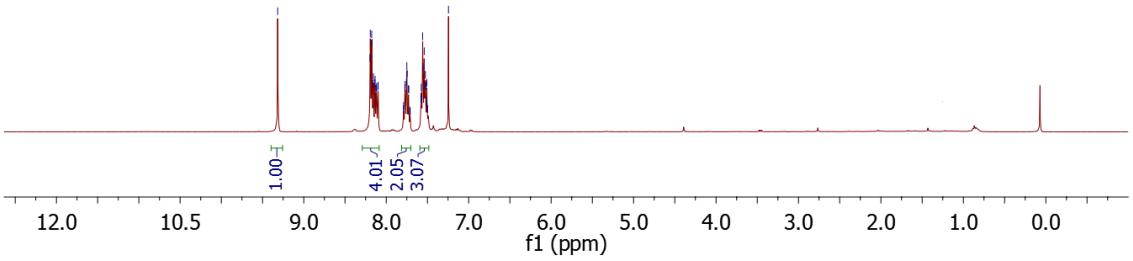
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2.0
1.0
0.0
f1 (ppm)


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129.22
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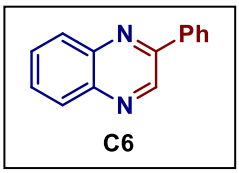
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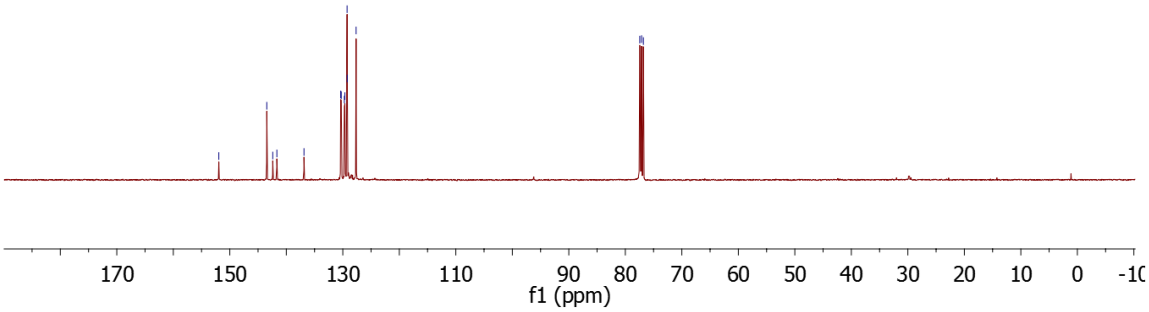
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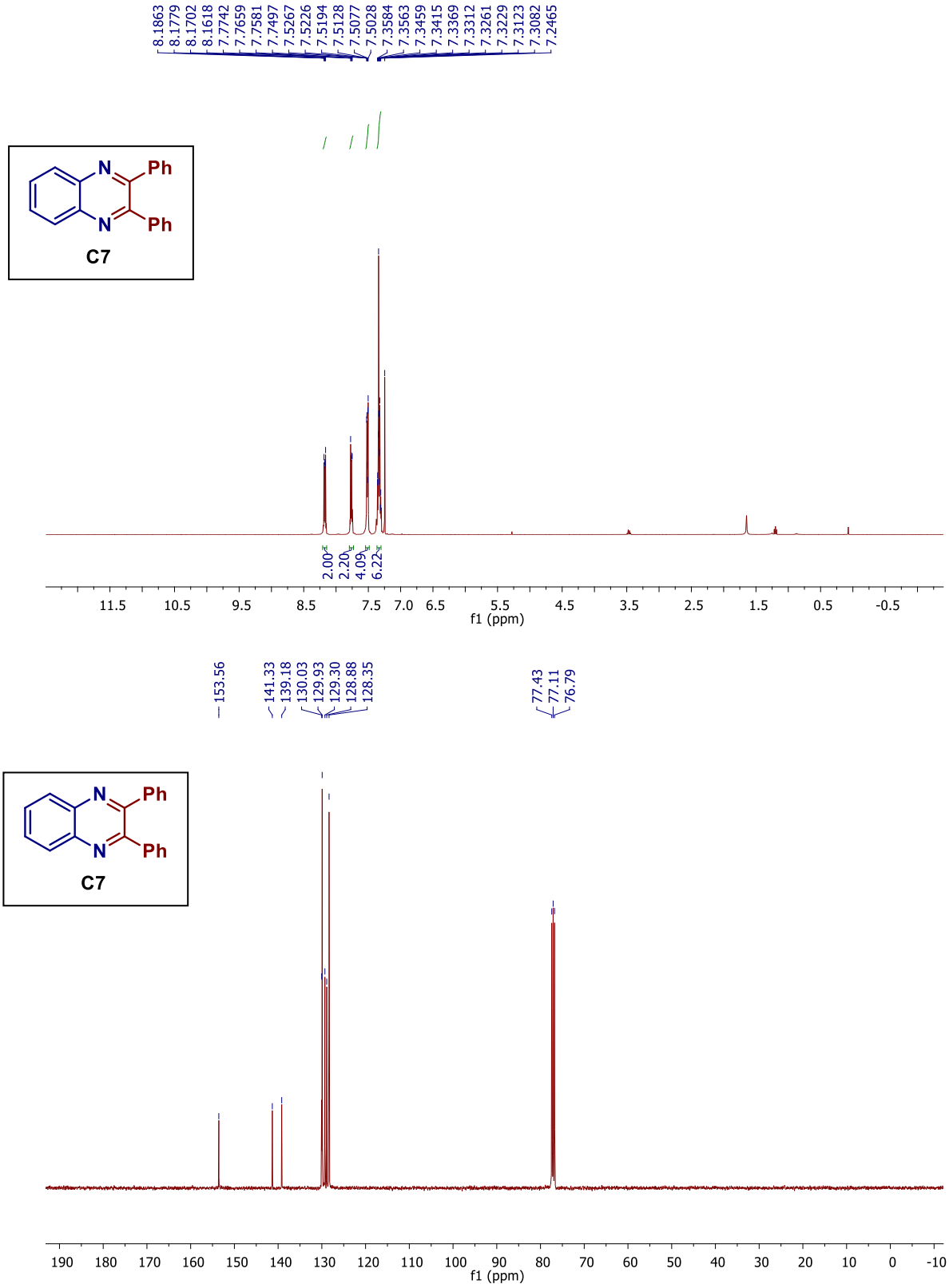
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7.3082
7.2465
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Ph
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Ph
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10.5
9.5
8.5
7.5
7.0
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)
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130.03
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129.30
128.88
128.35
77.43
77.11
76.79
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Ph
C7
190
180
170
160
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100
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80
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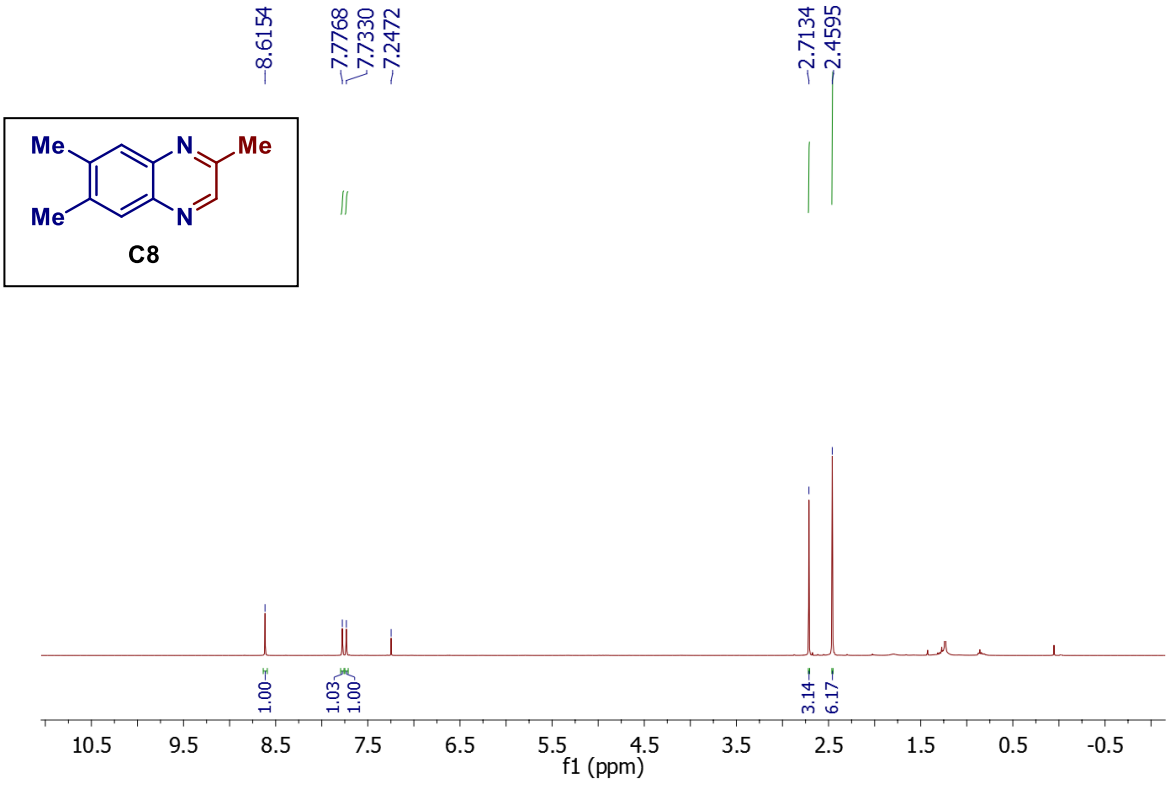
f1 (ppm)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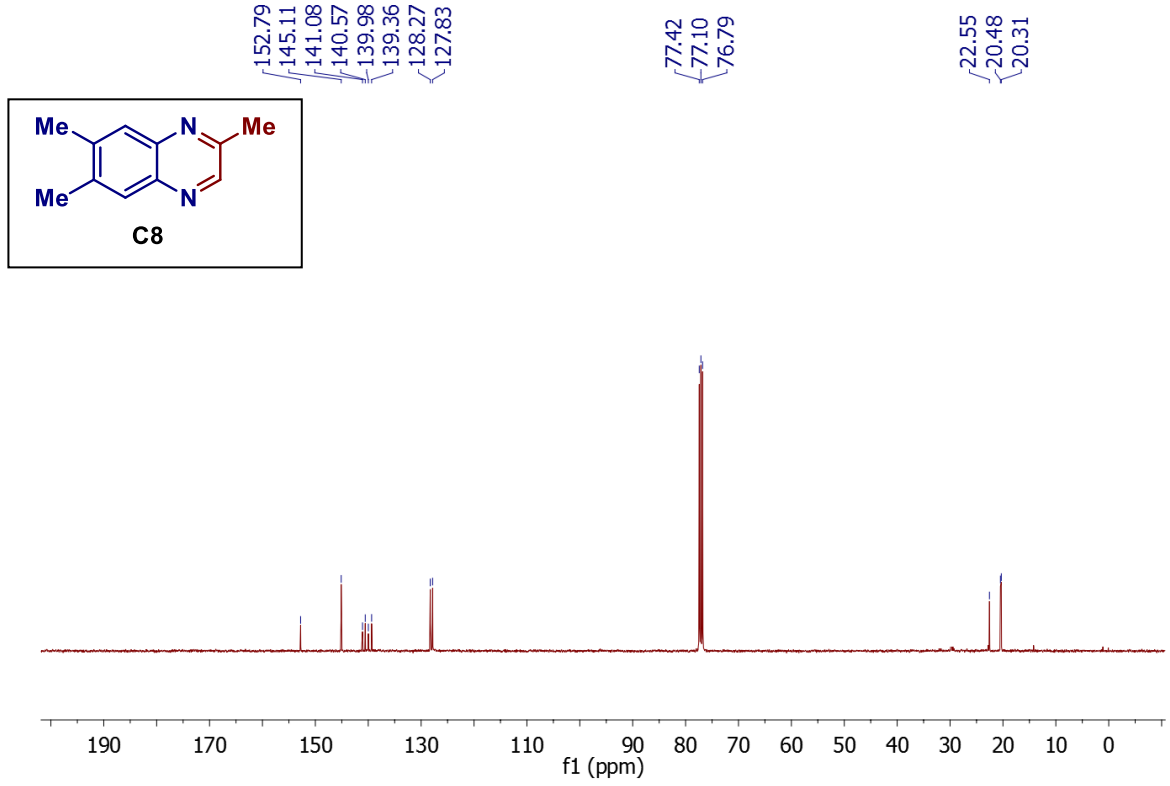
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Me
N
Me
Me
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150
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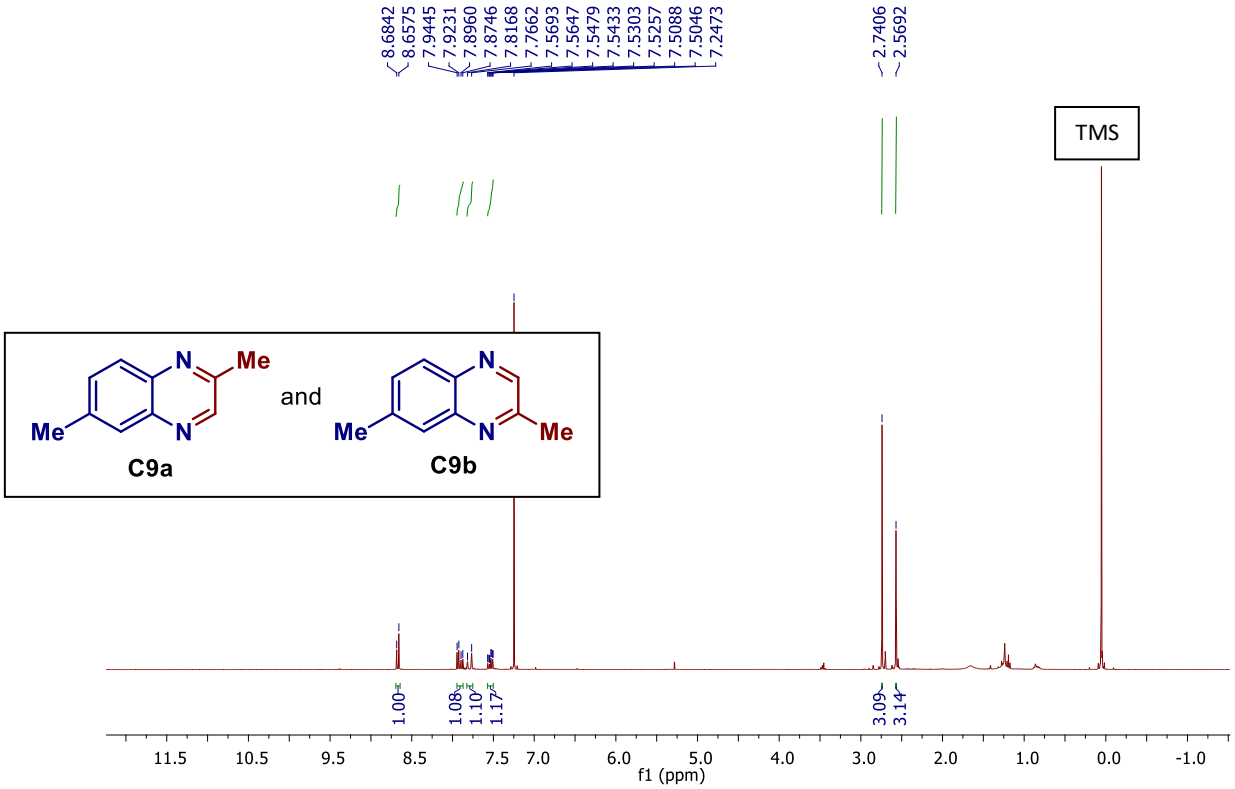
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7.5257
7.5088
7.5046
7.2473
2.7406
2.5692
TMS
Me
N
Me
N
C9a
and
Me
N
Me
N
Me
C9b
1.00
1.08
1.10
1.17
3.09
3.14
11.5
10.5
9.5
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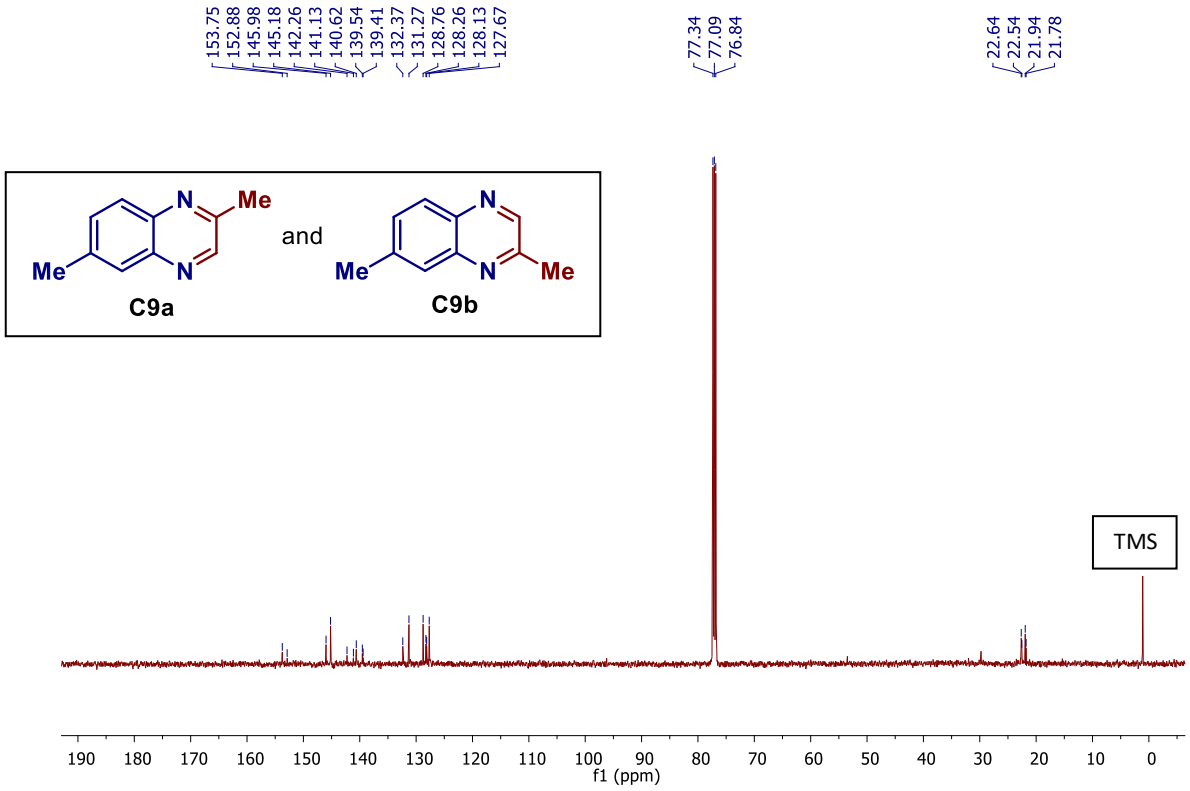
f1 (ppm)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128.13
127.67
77.34
77.09
76.84
22.64
22.54
21.94
21.78
Me
N
Me
N
C9a
and
Me
N
Me
N
Me
C9b
TMS
190
180
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90
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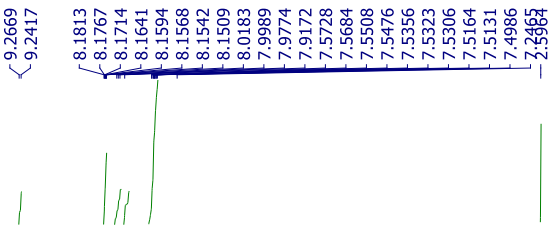
f1 (ppm)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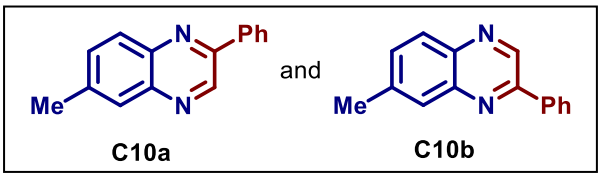
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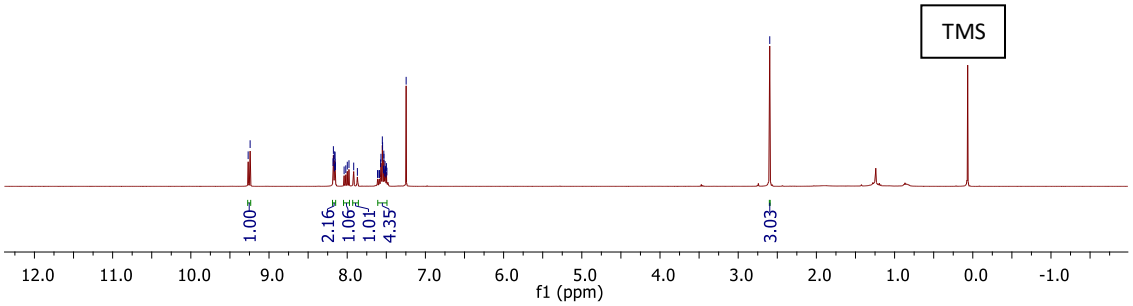
Ph
N
and
Me
N
Ph
N
C10a
C10b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6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)


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142.54
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140.85
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137.04
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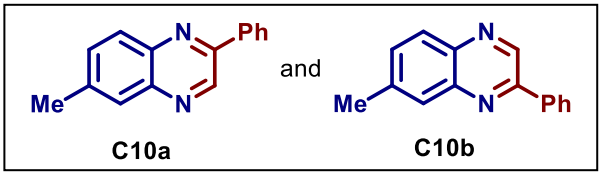
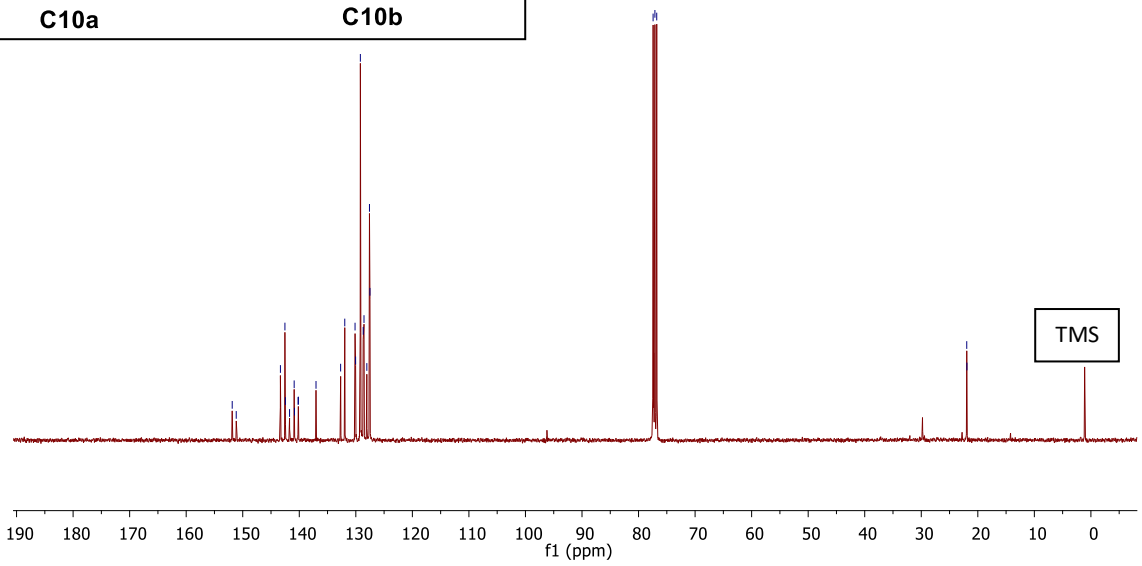
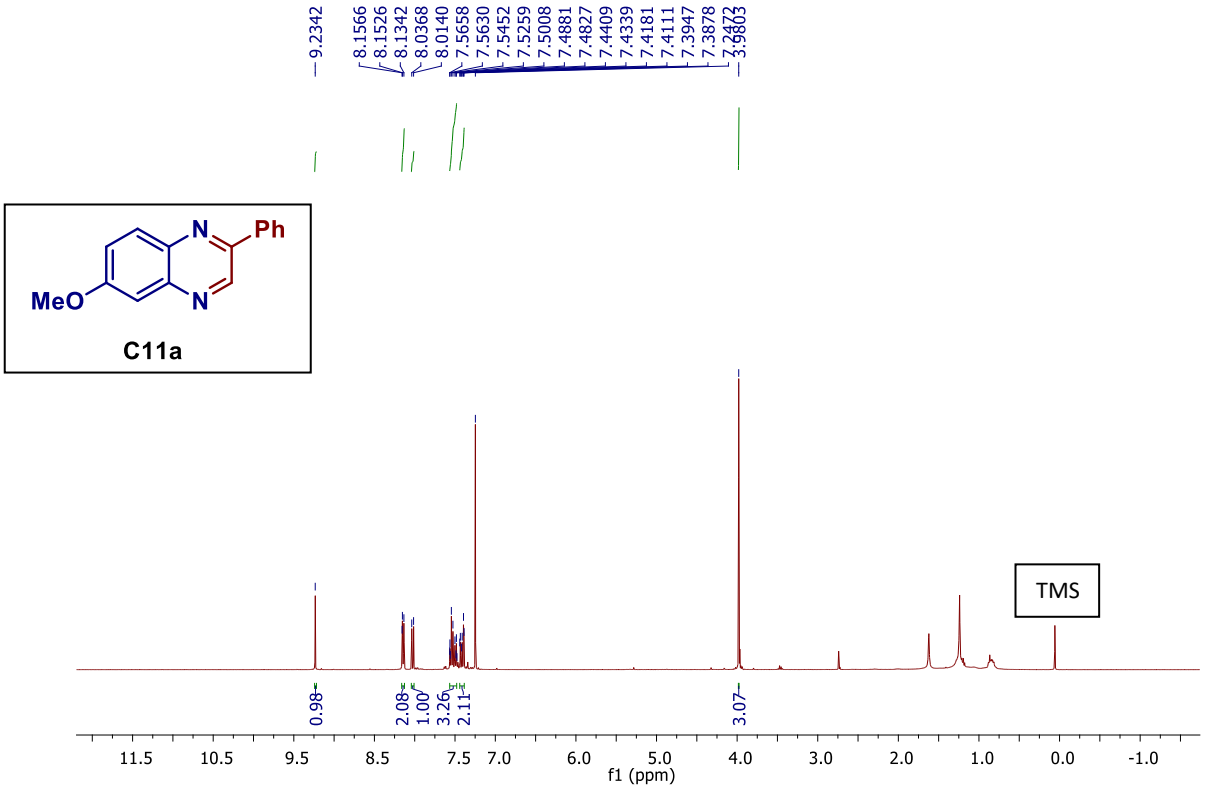
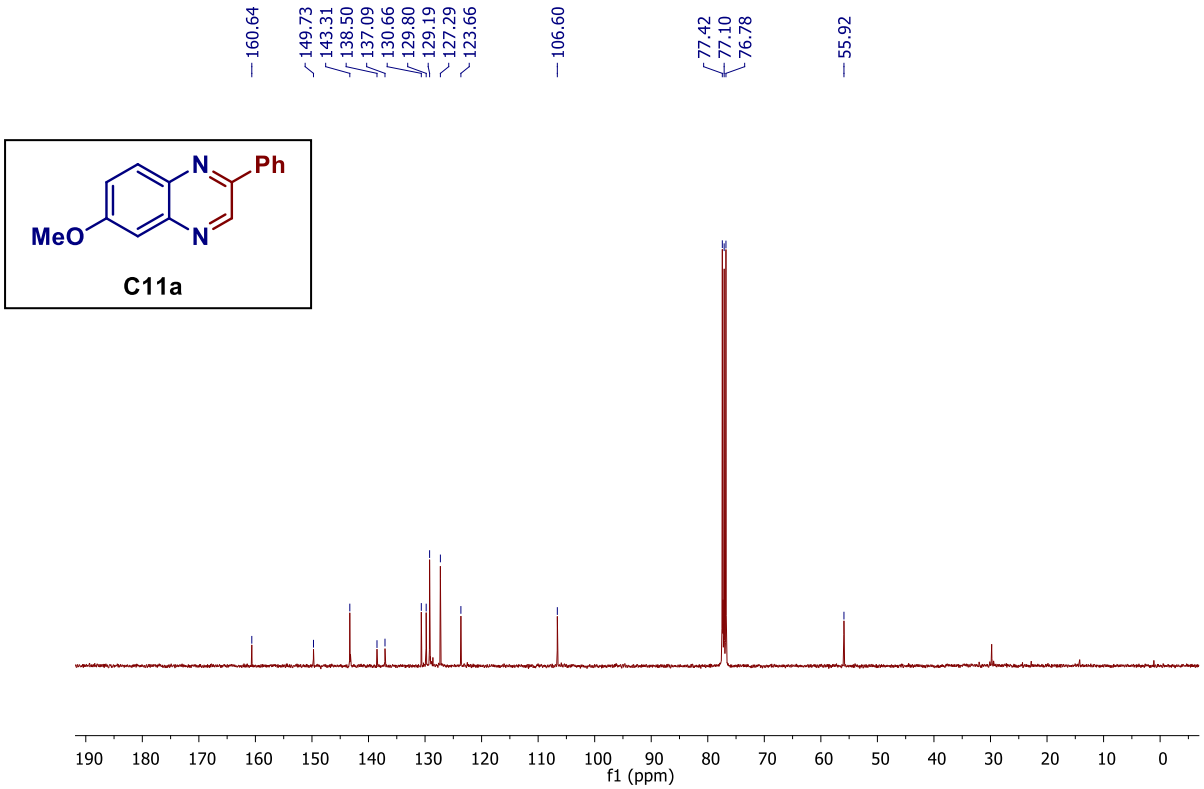
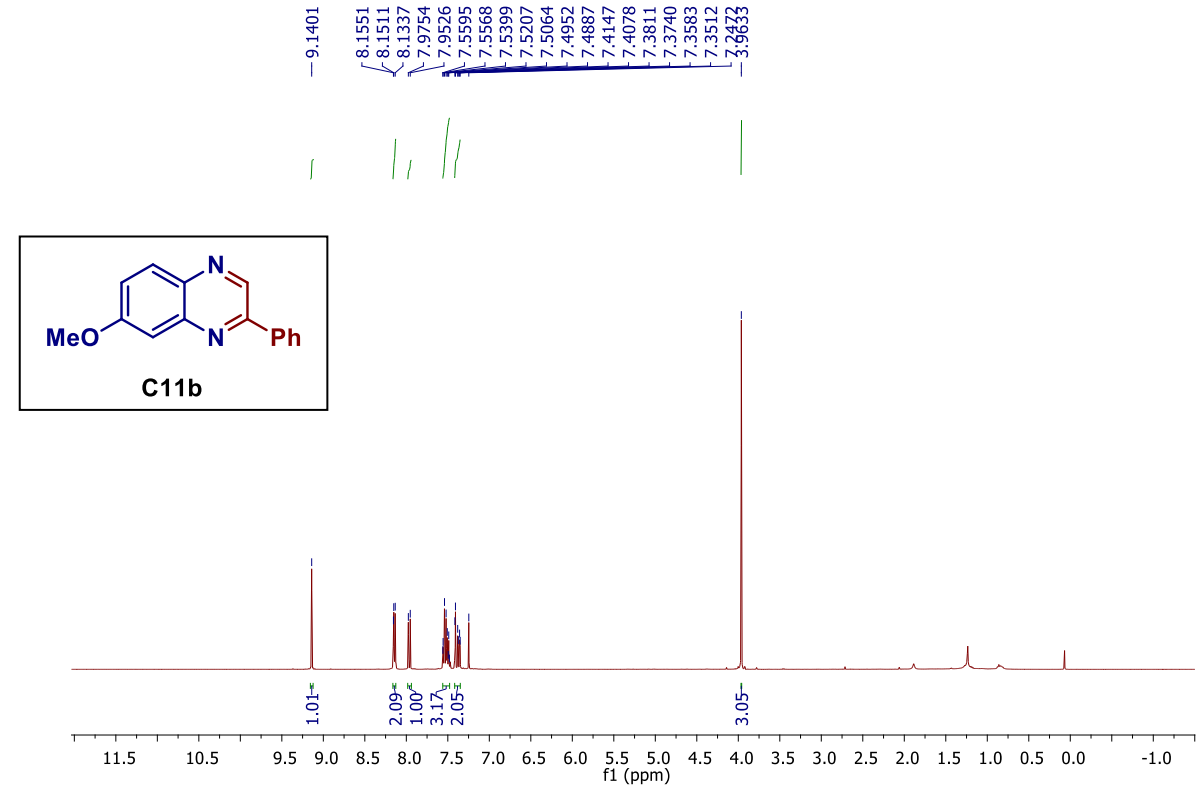
128.55
128.05
127.59
77.11
76.78
21.96
21.93

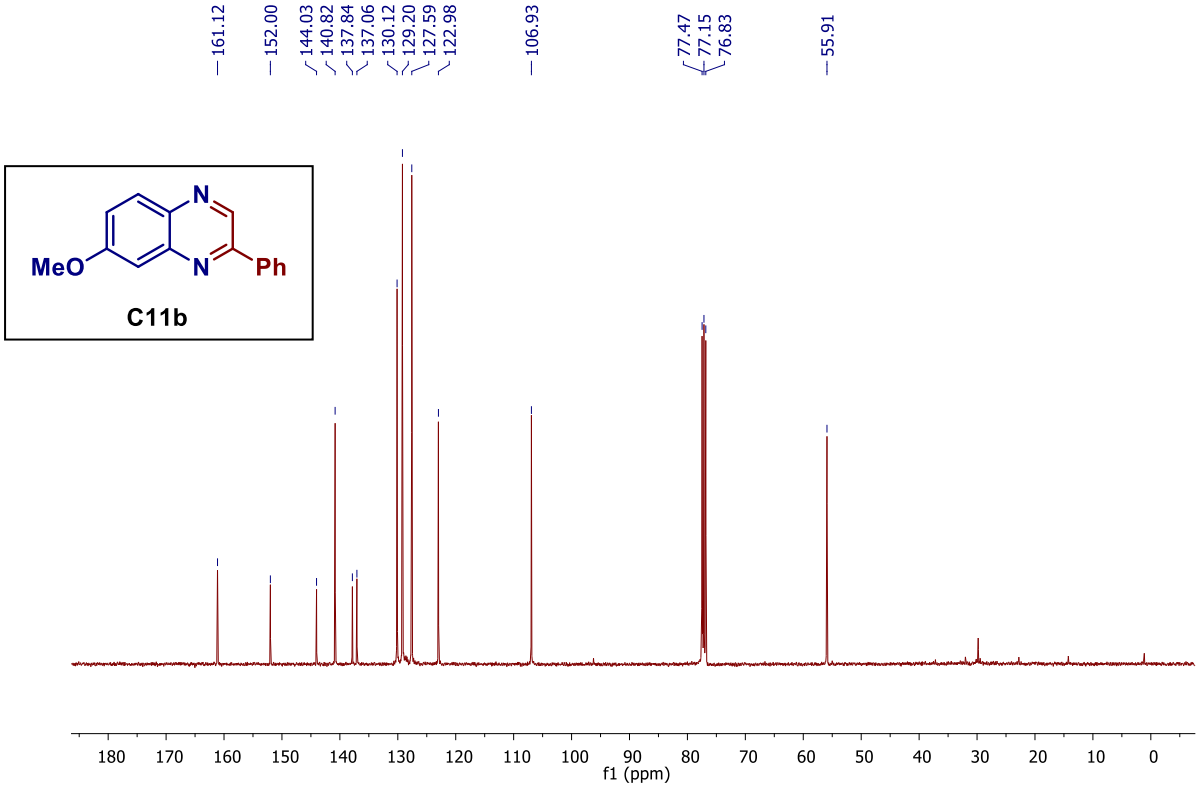

Me
N
Ph
N
and
Me
N
Ph
N
C10a
C10b

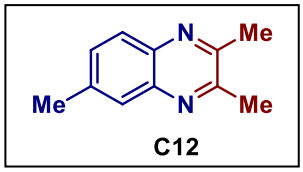

TMS
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.2342
8.1566
8.1526
8.1342
8.0368
8.0140
7.5658
7.5630
7.5452
7.5259
7.5008
7.4881
7.4827
7.4409
7.4339
7.4181
7.4111
7.3947
7.3878
7.2473
3.9803
N
Ph
MeO
N
C11a
TMS
0.98
2.08
1.00
3.26
2.11
3.07
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

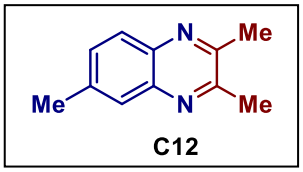

160.64
149.73
143.31
138.50
137.09
130.66
129.80
129.19
127.29
123.66
106.60
77.42
77.10
76.78
55.92
N
Ph
MeO
N
C11a
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.1401
8.1551
8.1511
8.1337
7.9754
7.9526
7.5595
7.5568
7.5399
7.5207
7.5064
7.4952
7.4887
7.4147
7.4078
7.3811
7.3740
7.3583
7.3512
7.2472
3.9633
MeO
N
N
Ph
C11b
1.01
2.09
1.00
3.17
2.05
3.05
11.5
10.5
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
-1.0
f1 (ppm)

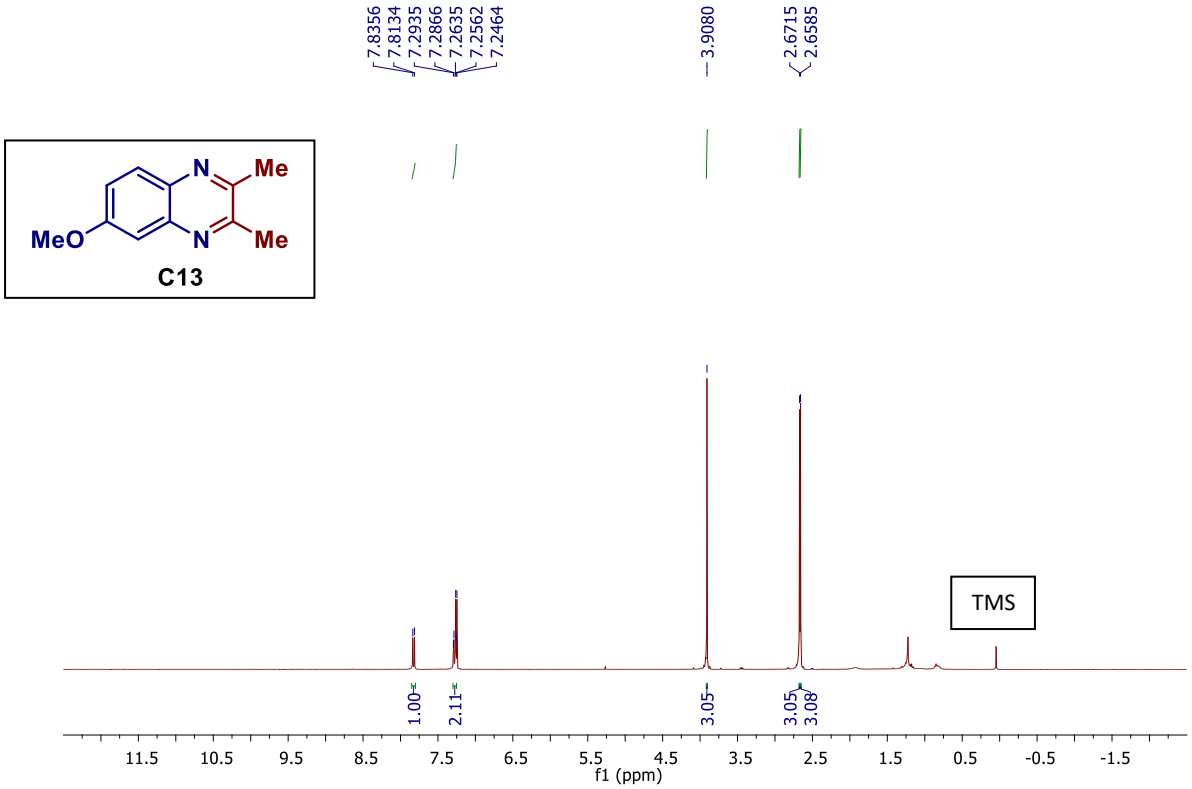

161.12
152.00
144.03
140.82
137.84
137.06
130.12
129.20
127.59
122.98
106.93
77.47
77.15
76.83
55.91
MeO
N
N
Ph
C11b
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

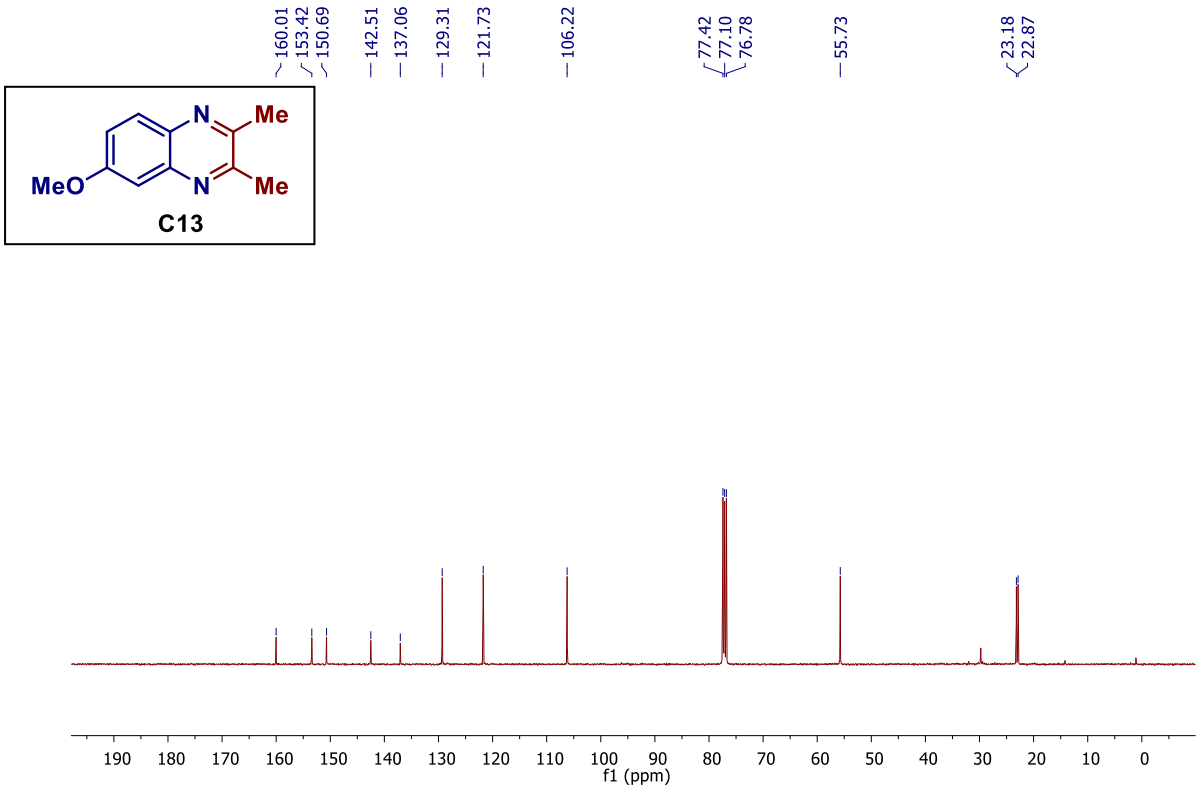

N
Me
Me
N
Me
C12

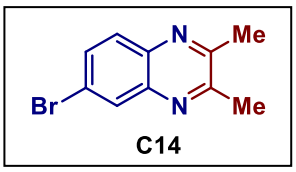
8.6139
7.7758
7.7322
7.2546
2.7122
2.4573
TMS
1.00
1.06
1.03
3.09
6.13
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)


N
Me
Me
N
Me
C12

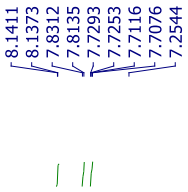
152.77
145.09
141.09
140.53
139.99
139.32
128.27
127.84
77.36
77.11
76.86
22.52
20.44
20.28
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


7.8356
7.8134
7.2935
7.2866
7.2635
7.2562
7.2464
3.9080
2.6715
2.6585
N
Me
MeO
N
Me
C13
TMS
1.00
2.11
3.05
3.05
3.08
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

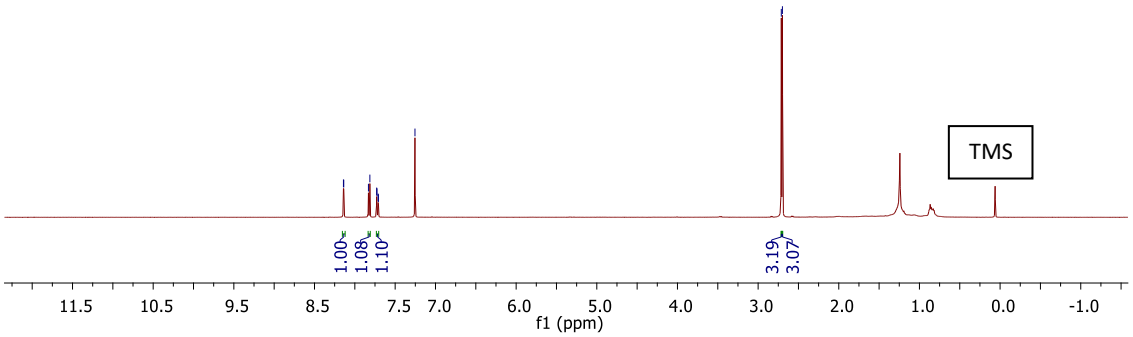

160.01
153.42
150.69
142.51
137.06
129.31
121.73
106.22
77.42
77.10
76.78
55.73
23.18
22.87
N
Me
MeO
N
Me
C13
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Br
N
Me
N
Me

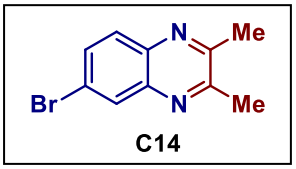
C14


8.1411
8.1373
7.8312
7.8135
7.7293
7.7253
7.7116
7.7076
7.2544

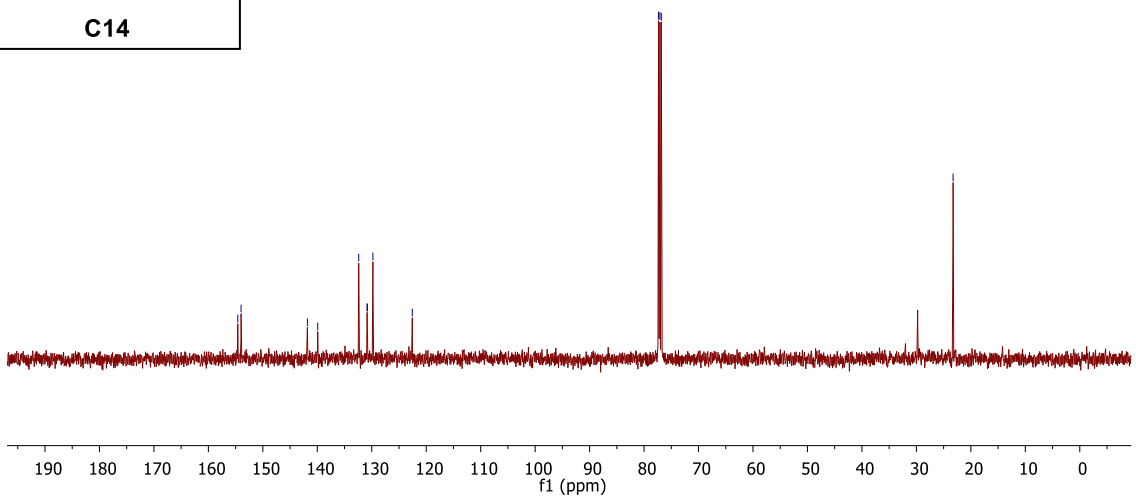

2.7126
2.6986

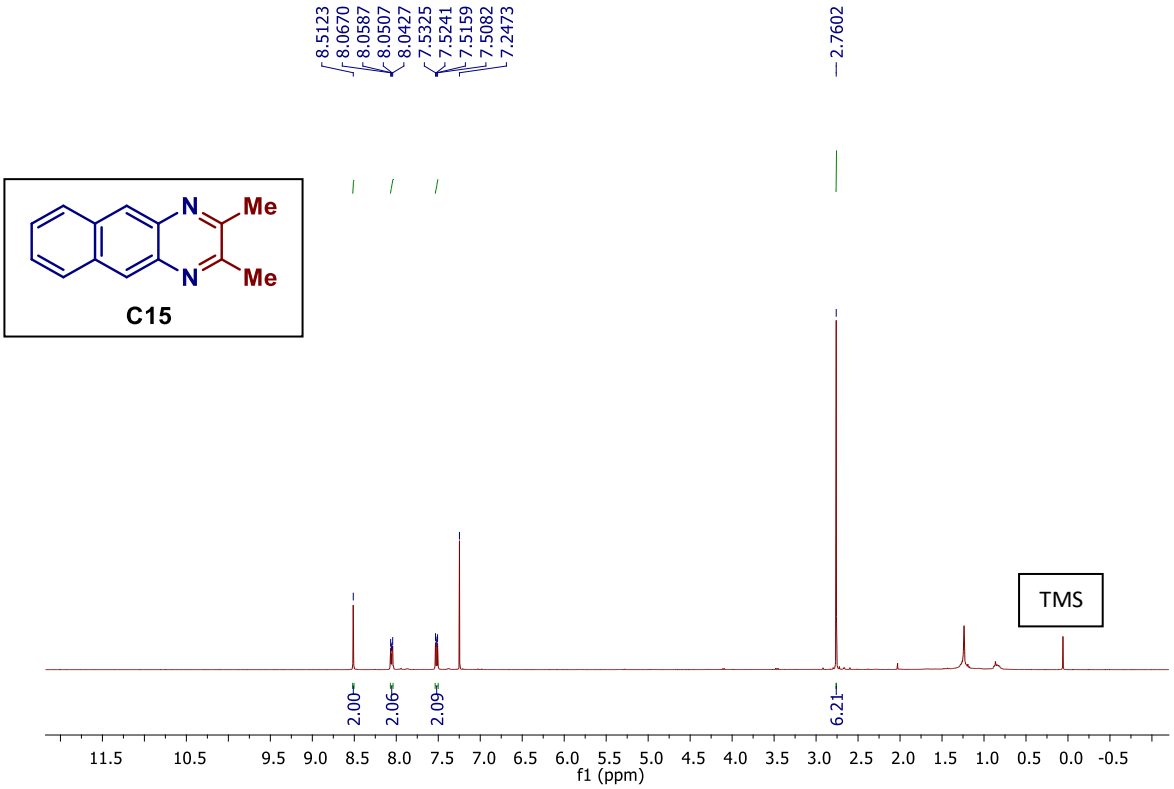

TMS
1.00
1.08
1.10
3.19
3.07
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

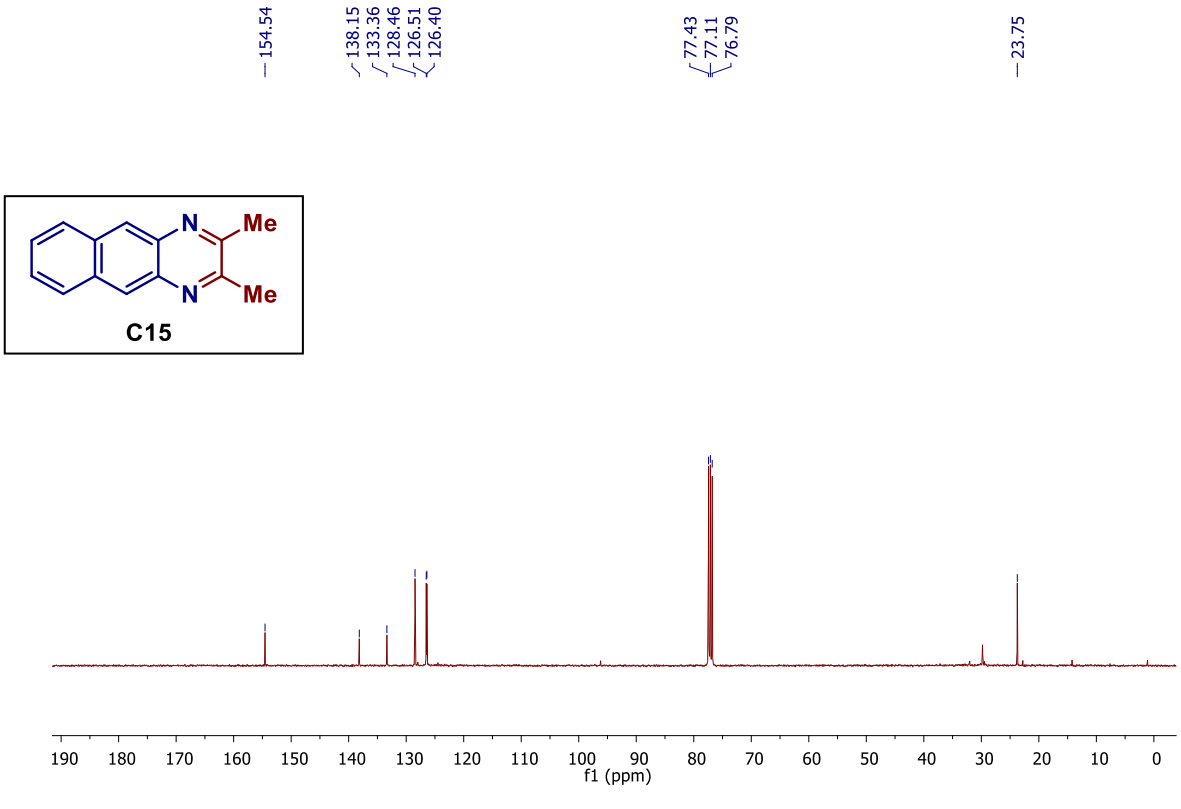

154.60
154.00
141.82
139.92
132.40
130.86
130.81
129.79
122.56
77.34
77.09
76.84
23.26

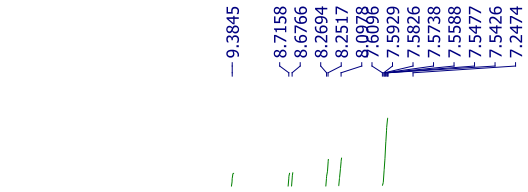

Br
N
Me
N
Me

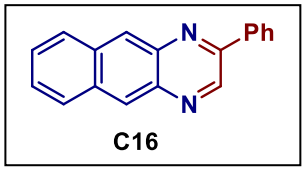
C14

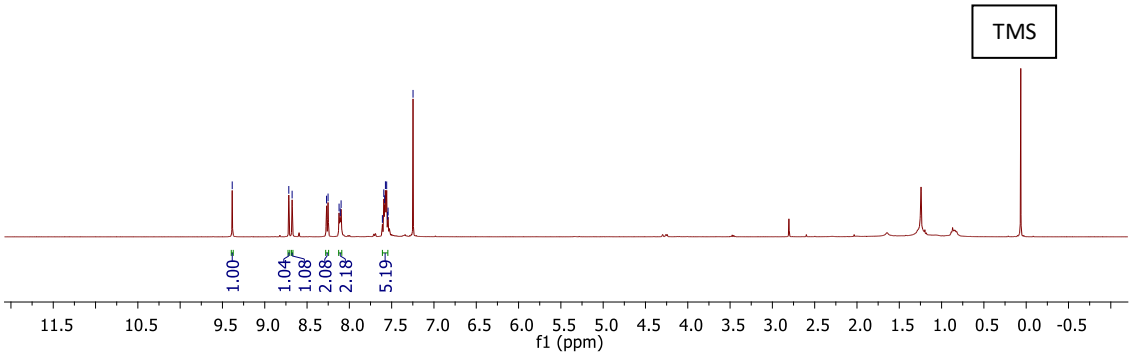

190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.5123
8.0670
8.0587
8.0507
8.0427
7.5325
7.5241
7.5159
7.5082
7.2473
2.7602
N
Me
N
Me
C15
TMS
2.00
2.06
2.09
6.21
11.5
10.5
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
-0.5
f1 (ppm)

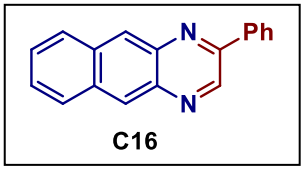

154.54
138.15
133.36
128.46
126.51
126.40
77.43
77.11
76.79
23.75
N
Me
N
Me
C15
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

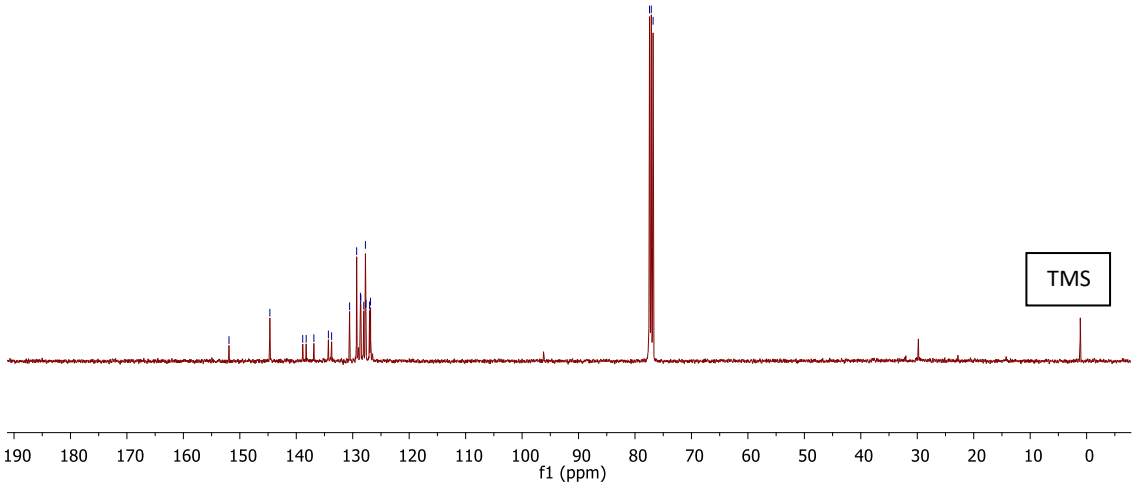

9.3845
8.7158
8.6766
8.2694
8.2517
8.0978
8.0808
7.5929
7.5826
7.5738
7.5588
7.5477
7.5426
7.2474

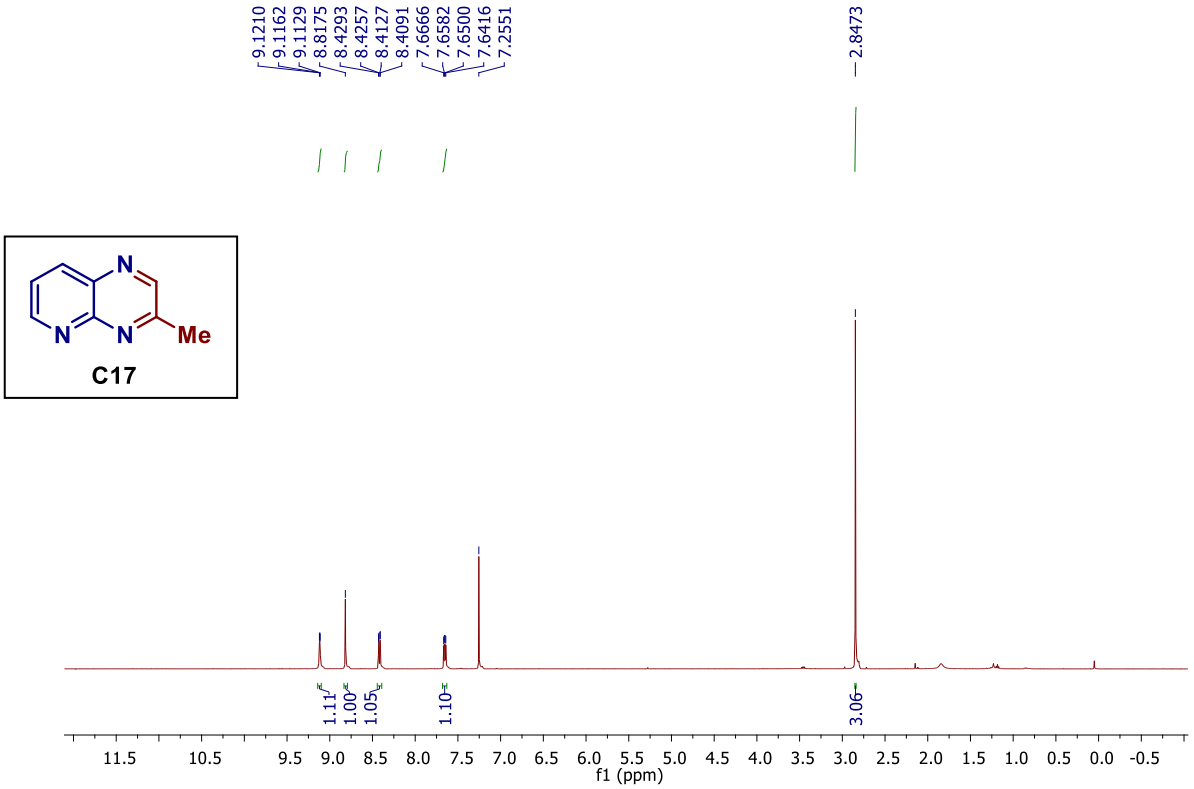

N
Ph
N
C16

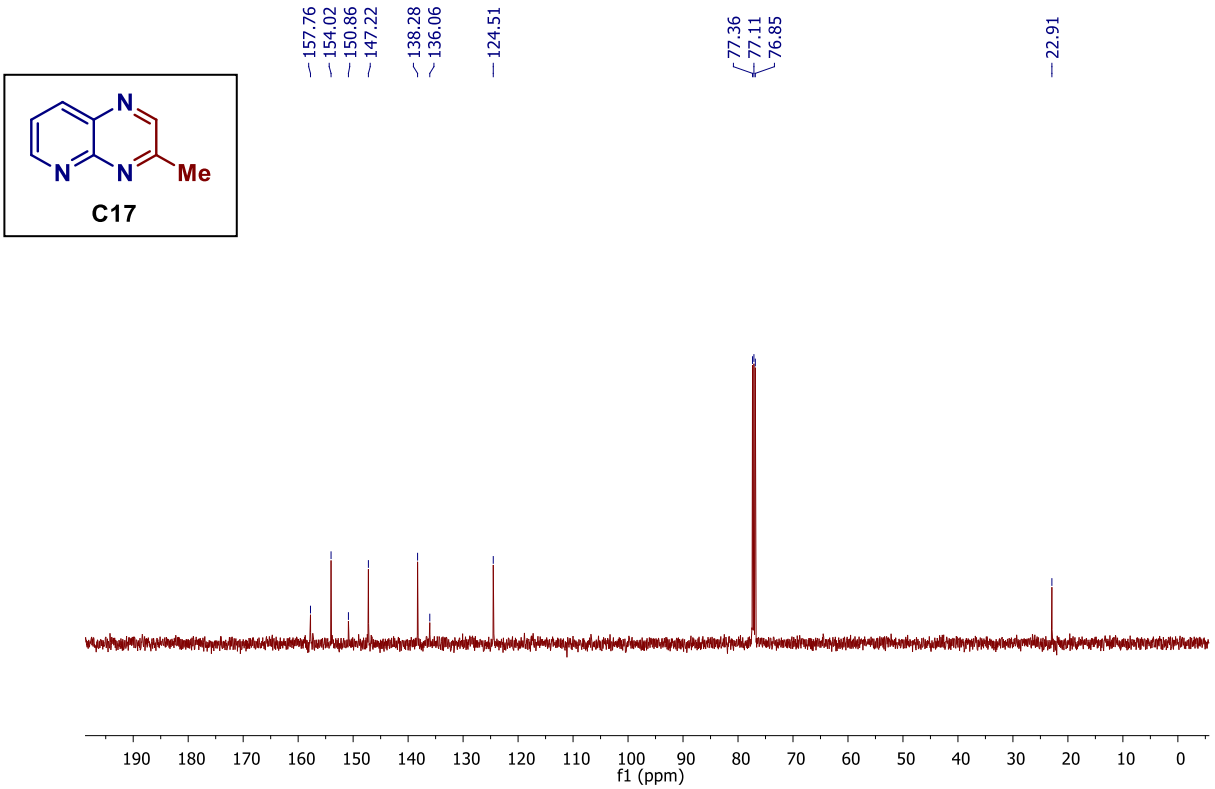

TMS
1.00
1.04
1.08
2.08
2.18
5.19
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

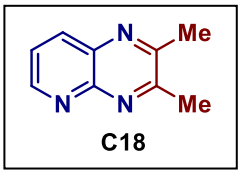

151.92
144.68
138.86
138.25
136.89
134.31
133.74
130.55
129.31
128.64
128.56
128.05
127.75
127.67
127.02
126.85
77.43
77.11
76.79


N
Ph
N
C16


TMS
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

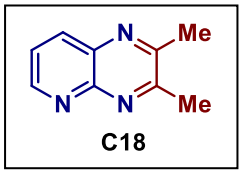

9.1210
9.1162
9.1129
8.8175
8.4293
8.4257
8.4127
8.4091
7.6666
7.6582
7.6500
7.6416
7.2551
2.8473
N
N
N
Me
C17
1.11
1.00
1.05
1.10
3.06
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


157.76
154.02
150.86
147.22
138.28
136.06
124.51
77.36
77.11
76.85
22.91
N
N
N
Me
C17
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


N
Me
N
N
Me

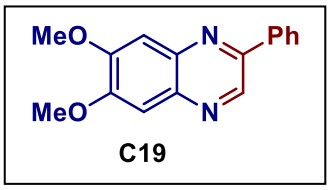
C18

9.0379
8.3295
8.3139
7.6191
7.6115
7.6033
7.5958
7.2544
2.7963
2.7562
1.00
1.04
1.06
3.10
3.07
11.5
10.5
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
f1 (ppm)

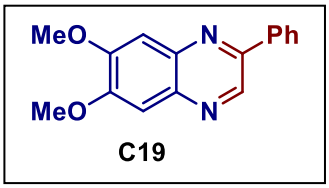

N
Me
N
N
Me

C18

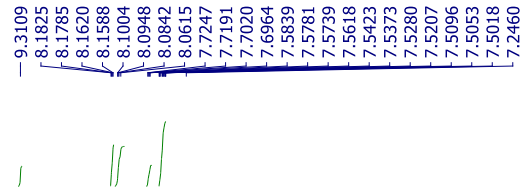
157.44
155.12
152.81
150.30
137.43
135.98
124.41
77.36
77.11
76.85
23.58
23.10
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

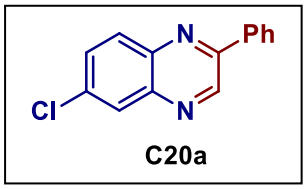

MeO
MeO
N
N
Ph
C19

9.0945
8.1191
8.1008
7.5462
7.5284
7.5090
7.4831
7.4705
7.4652
7.4585
7.4469
7.4030
7.3544
7.2470
4.0564
4.0488
TMS
0.98
2.00
3.08
0.99
1.03
3.02
3.04
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)

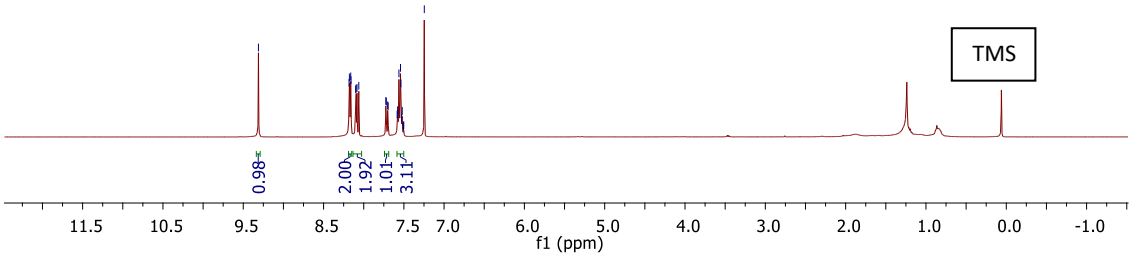

MeO
MeO
N
N
Ph
C19

153.11
152.64
149.93
140.76
139.58
138.83
137.30
129.67
129.15
127.24
107.11
106.67
77.44
77.12
76.80
56.47
56.44
TMS
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

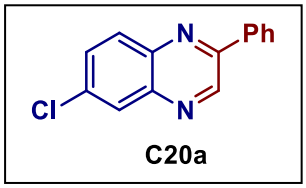

9.3109
8.1825
8.1785
8.1620
8.1588
8.1004
8.0948
8.0842
8.0615
7.7247
7.7191
7.7020
7.6964
7.5839
7.5781
7.5739
7.5618
7.5423
7.5373
7.5280
7.5207
7.5096
7.5053
7.5018
7.2460


N
Ph
Cl
N

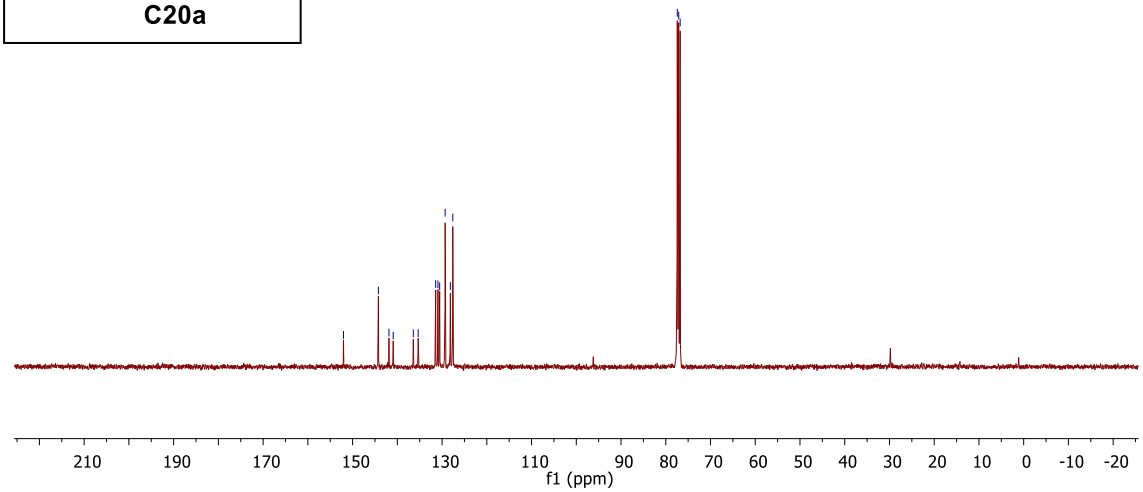
C20a

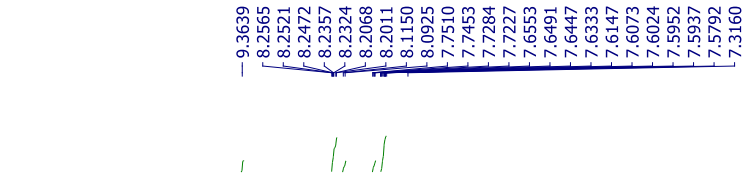

TMS
0.98
2.00
1.92
1.01
3.11
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

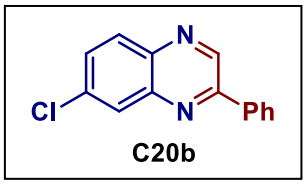

152.04
144.23
141.87
140.92
136.43
135.35
131.43
130.92
130.54
129.31
128.15
127.60
77.43
77.11
76.78


N
Ph
Cl
N

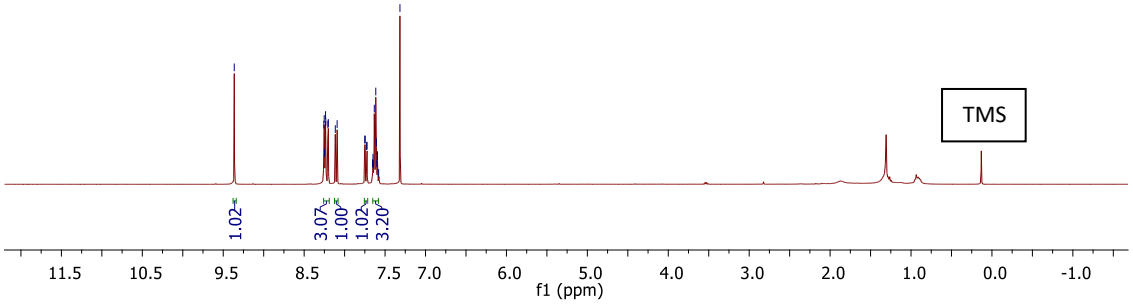
C20a

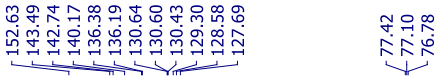

210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

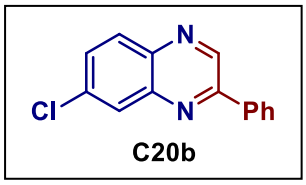

9.3639
8.2565
8.2521
8.2472
8.2357
8.2324
8.2068
8.2011
8.1150
8.0925
7.7510
7.7453
7.7284
7.7227
7.6553
7.6491
7.6447
7.6333
7.6147
7.6073
7.6024
7.5952
7.5937
7.5792
7.3160


N
Cl
N
Ph

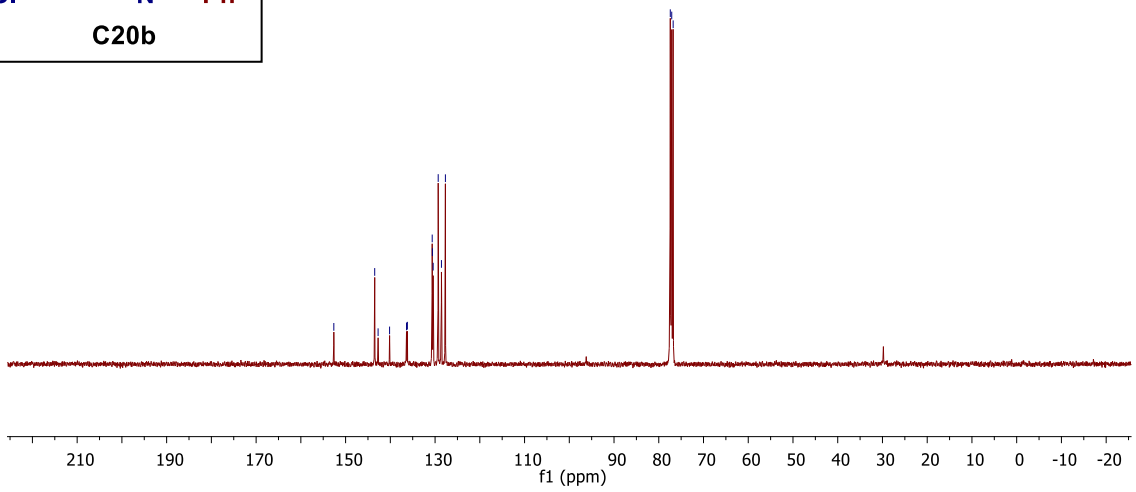
C20b

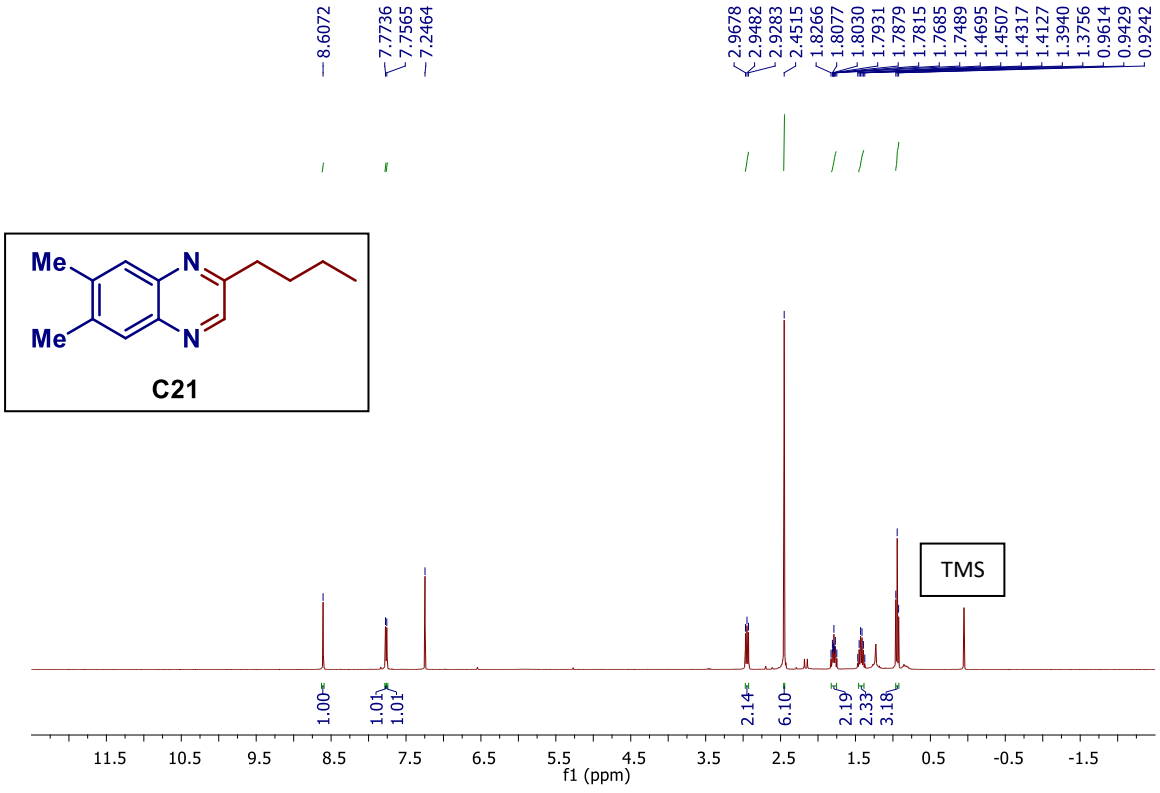

TMS
1.02
3.07
1.00
1.02
3.20
11.5
10.5
9.5
8.5
7.5
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

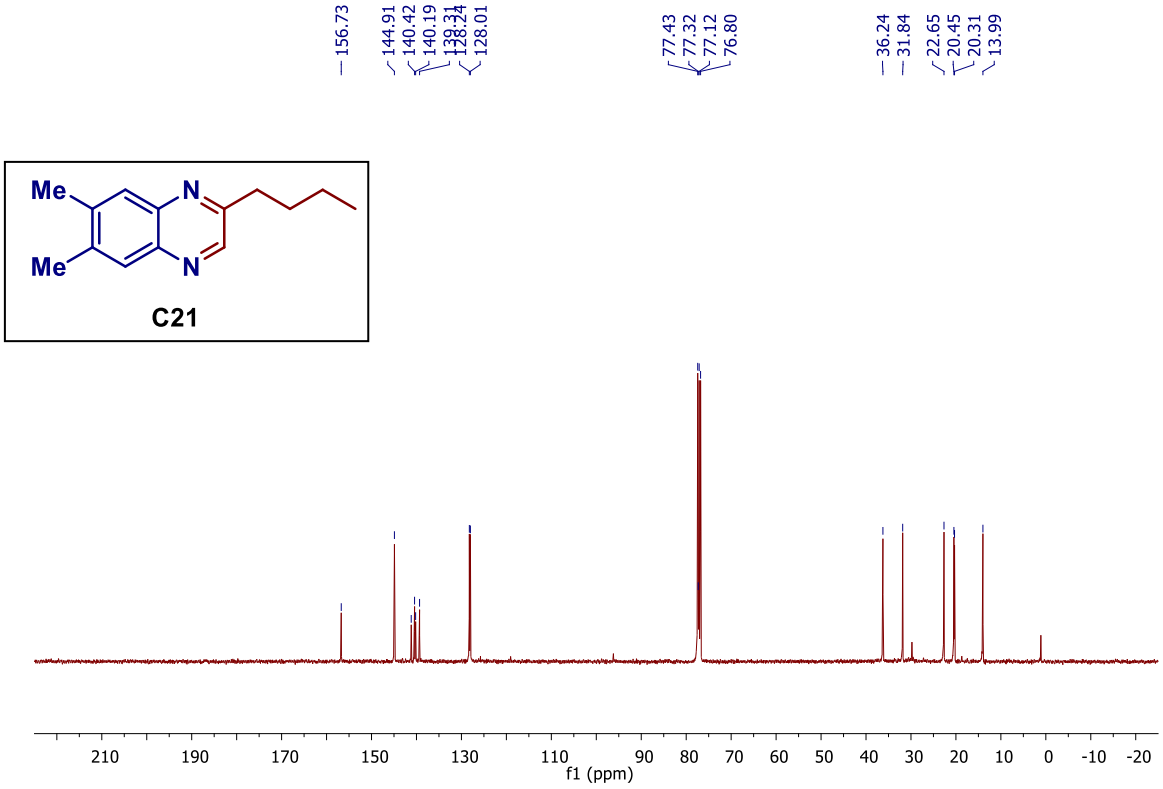

152.63
143.49
142.74
140.17
136.38
136.19
130.64
130.60
130.43
129.30
128.58
127.69
77.42
77.10
76.78

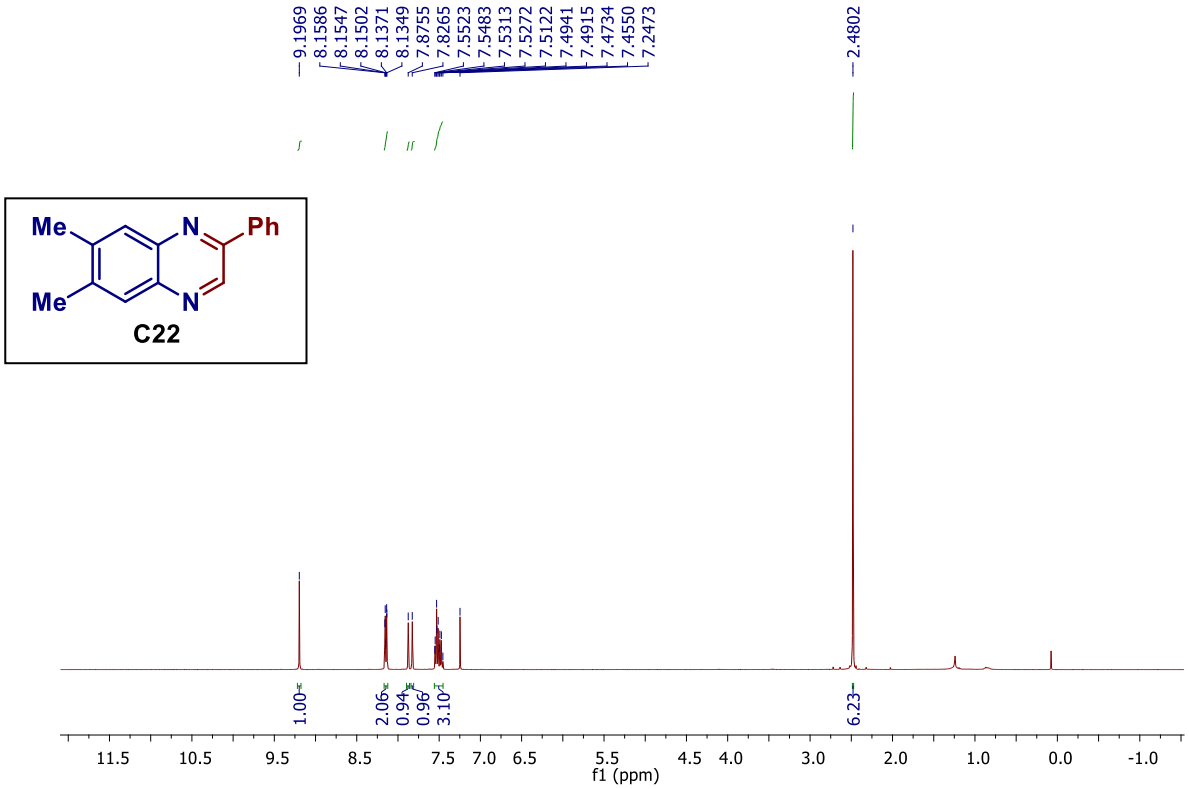

N
Cl
N
Ph

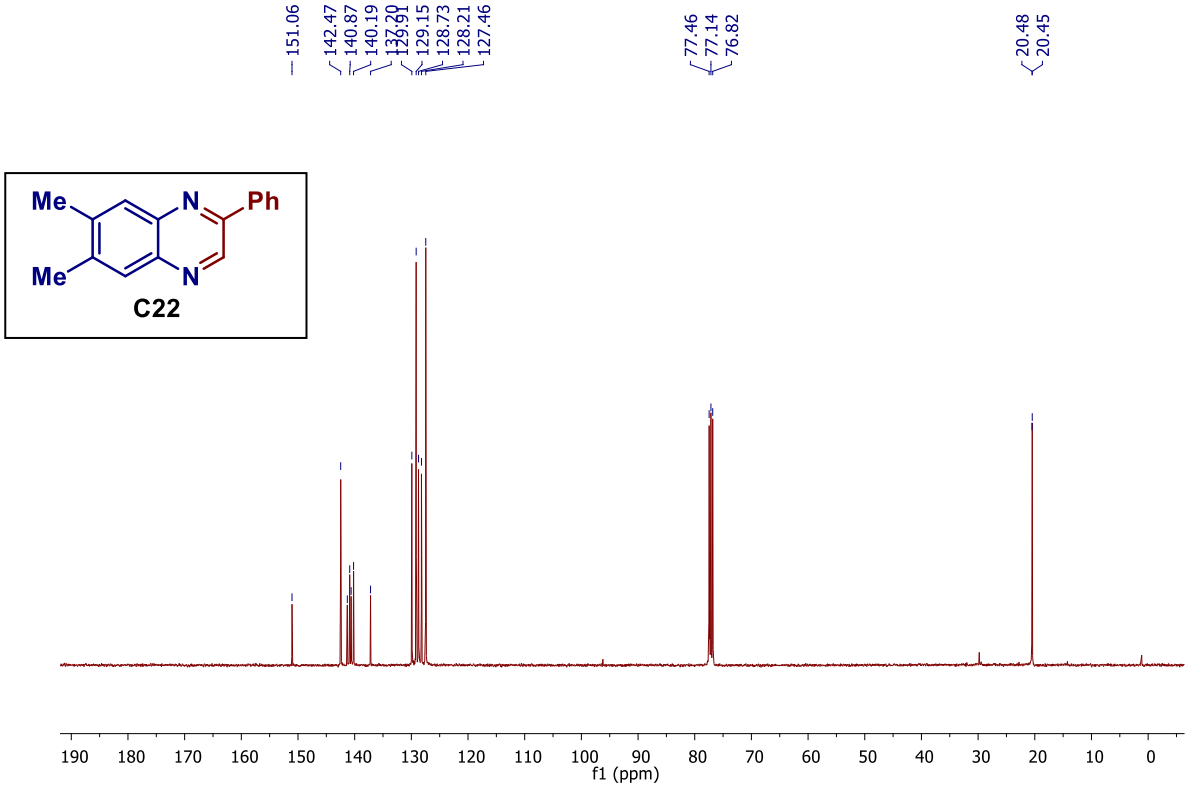
C20b

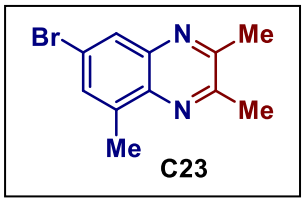

210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


8.6072
7.7736
7.7565
7.2464
2.9678
2.9482
2.9283
2.4515
1.8266
1.8077
1.8030
1.7931
1.7879
1.7815
1.7685
1.7489
1.4695
1.4507
1.4317
1.4127
1.3940
1.3756
0.9614
0.9429
0.9242
Me
N
Me
N
C21
TMS
1.00
1.01
1.01
2.14
6.10
2.19
2.33
3.18
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
-1.5
f1 (ppm)

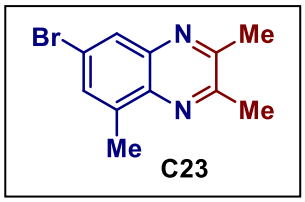

156.73
144.91
140.42
140.19
128.24
128.01
77.43
77.32
77.12
76.80
36.24
31.84
22.65
20.45
20.31
13.99
Me
N
Me
N
C21
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


9.1969
8.1586
8.1547
8.1502
8.1371
8.1349
7.8755
7.8265
7.5523
7.5483
7.5313
7.5272
7.5122
7.4941
7.4915
7.4734
7.4550
7.2473
2.4802
Me
N
Ph
Me
N
C22
1.00
2.06
0.94
0.96
3.10
6.23
11.5
10.5
9.5
8.5
7.5
7.0
6.5
5.5
4.5
4.0
3.0
2.0
1.0
0.0
-1.0
f1 (ppm)

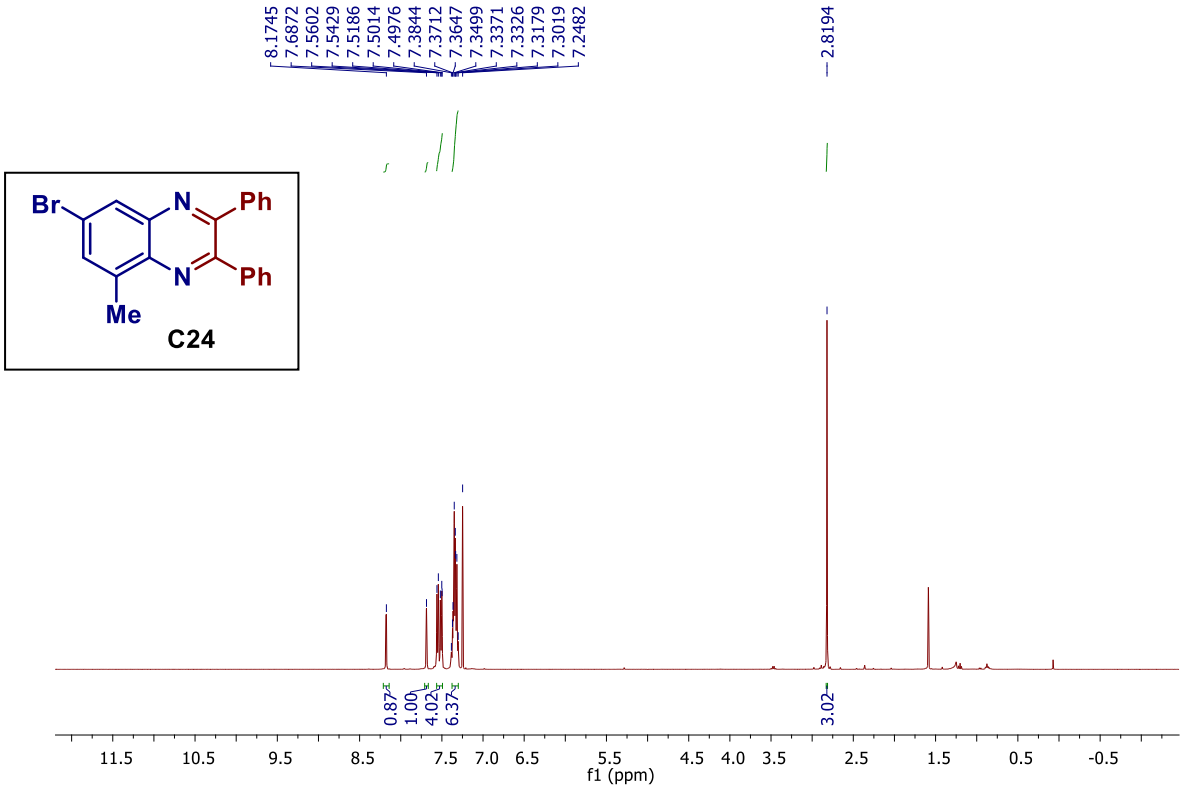

151.06
142.47
140.87
140.19
137.20
129.61
129.15
128.73
128.21
127.46
77.46
77.14
76.82
20.48
20.45
Me
N
Ph
Me
N
C22
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

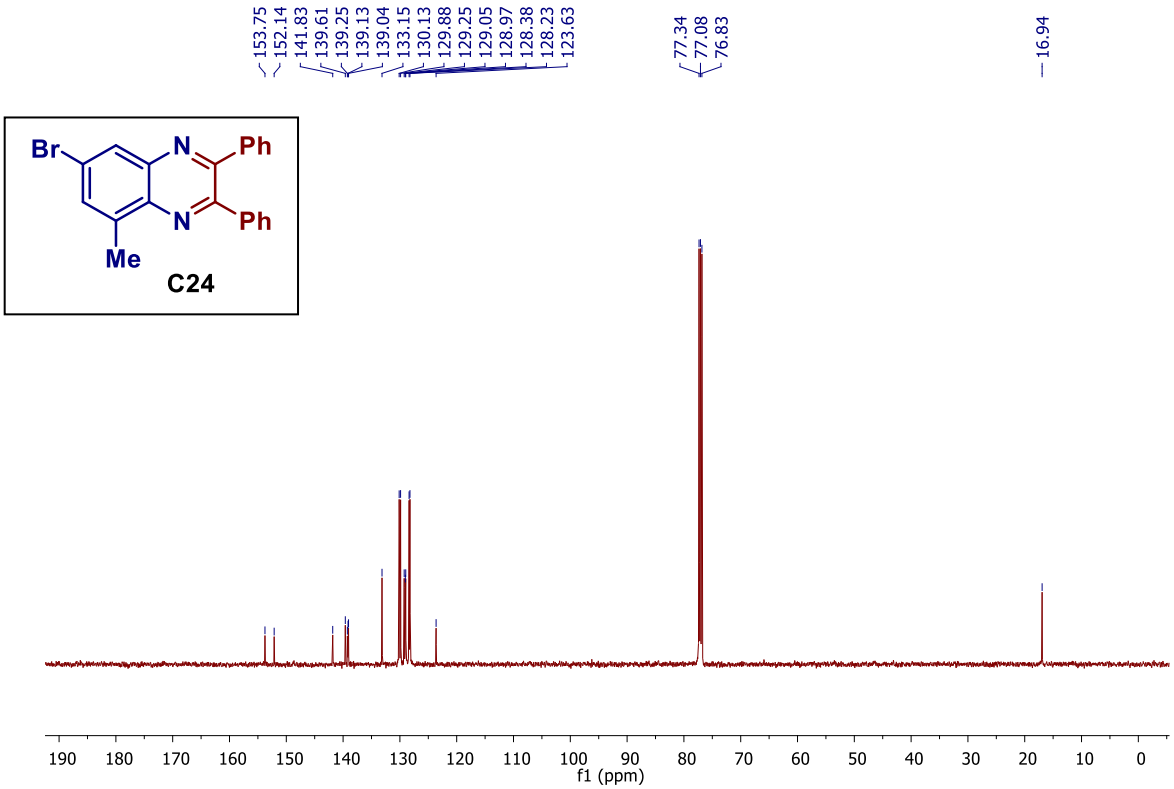

Br
N
Me
N
Me
Me
C23

7.9696
7.9659
7.5745
7.5726
7.2546
2.7202
2.6978
1.00
1.00
3.07
6.02
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

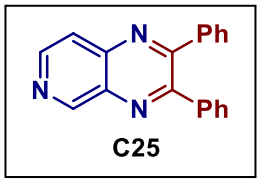

Br
N
Me
N
Me
Me
C23

153.98
152.63
141.83
139.18
138.78
132.11
128.53
122.16
77.34
77.09
76.84
23.39
23.12
16.93
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

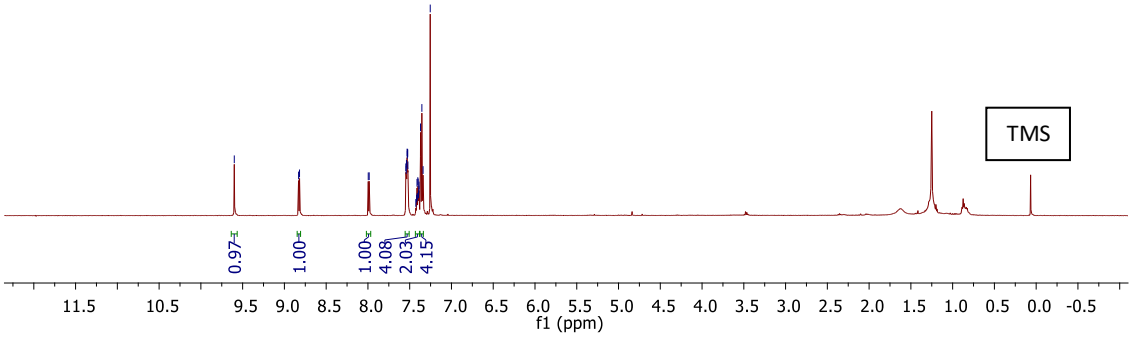

8.1745
7.6872
7.5602
7.5429
7.5186
7.5014
7.4976
7.3844
7.3712
7.3647
7.3499
7.3371
7.3326
7.3179
7.3019
7.2482
2.8194
Br
N
Ph
N
Ph
Me
C24
0.87
1.00
4.02
6.37
3.02
11.5
10.5
9.5
8.5
7.5
7.0
6.5
5.5
4.5
4.0
3.5
2.5
1.5
0.5
-0.5
f1 (ppm)


153.75
152.14
141.83
139.61
139.25
139.13
139.04
133.15
130.13
129.88
129.25
129.05
128.97
128.38
128.23
123.63
77.34
77.08
76.83
16.94
Br
N
Ph
N
Ph
Me
C24
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

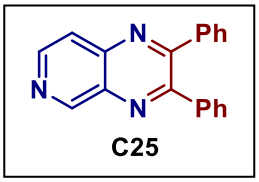

9.6001
8.8303
8.8188
7.9963
7.9848
7.5461
7.5415
7.5388
7.5313
7.5284
7.5252
7.5245
7.5214
7.4266
7.4173
7.4123
7.4087
7.4029
7.3981
7.3944
7.3906
7.3884
7.3701
7.3543
7.3400
7.2541


N
Ph
N
N
Ph

C25

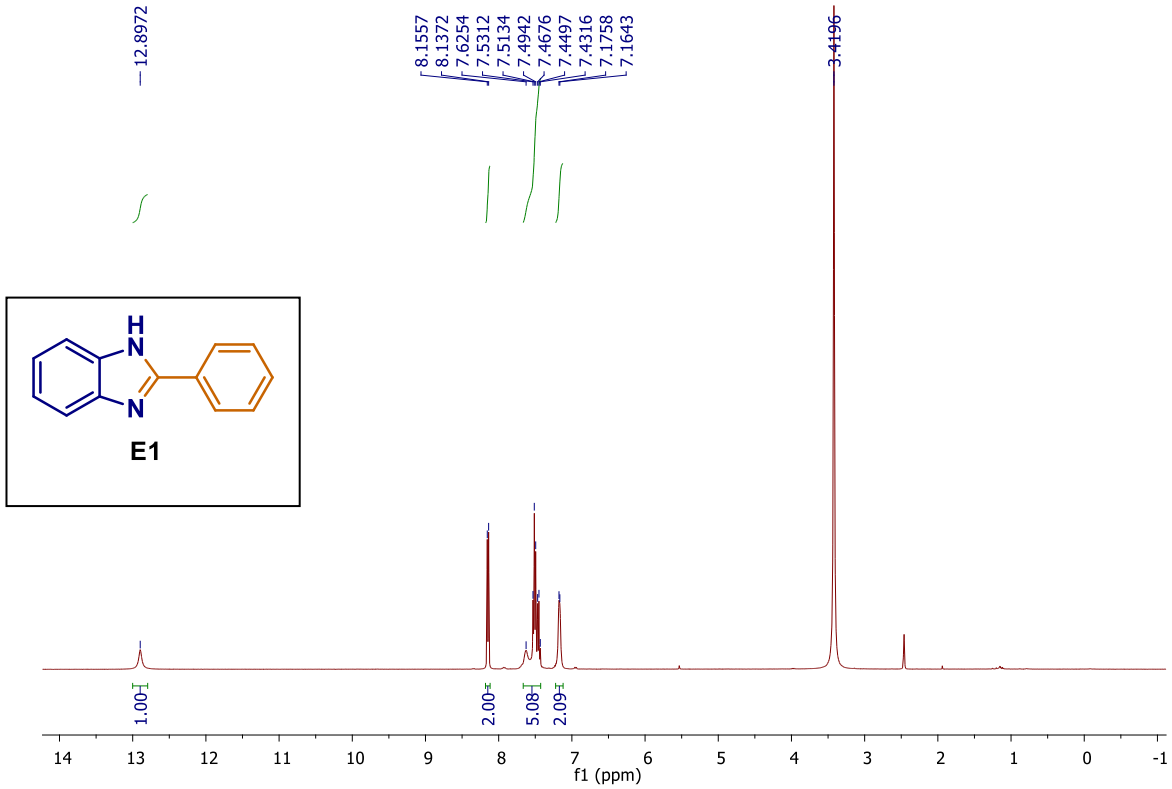

TMS
0.97
1.00
1.00
4.08
2.03
4.15
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

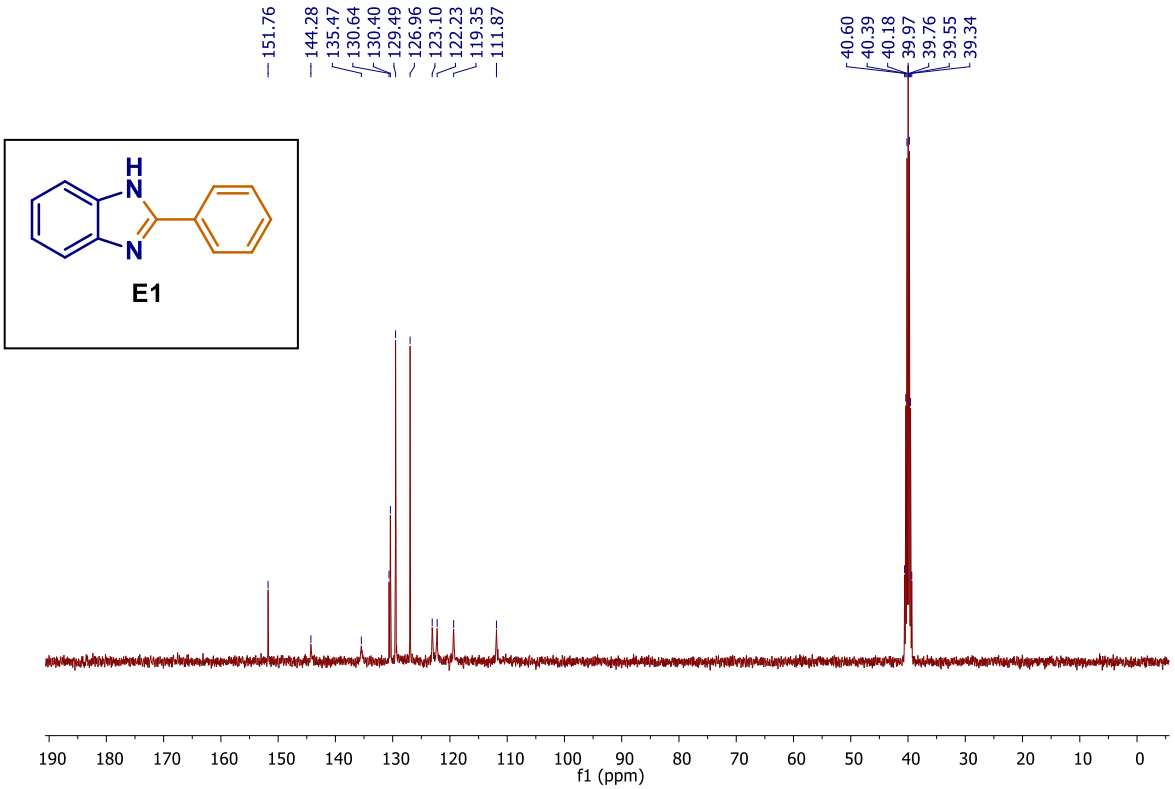

158.05
155.48
154.54
147.39
143.68
138.37
136.41
129.95
129.88
129.77
129.50
128.50
121.45
77.34
77.08
76.83

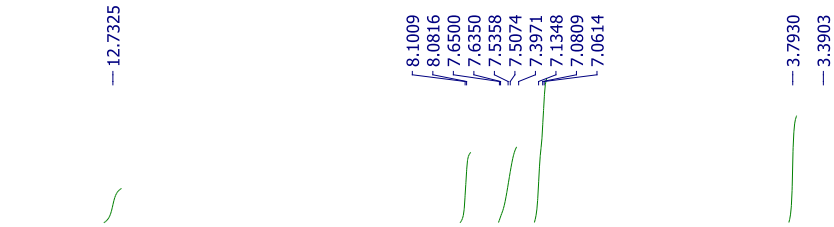

N
Ph
N
N
Ph

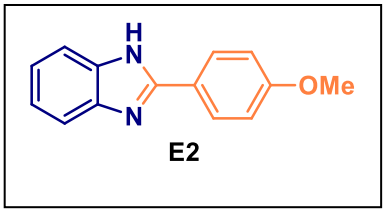
C25

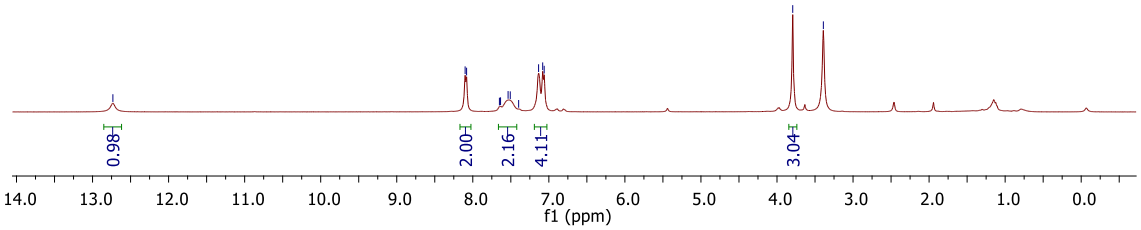
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.8972
8.1557
8.1372
7.6254
7.5312
7.5134
7.4942
7.4676
7.4497
7.4316
7.1758
7.1643
3.4196
E1
1.00
2.00
5.08
2.09
f1 (ppm)

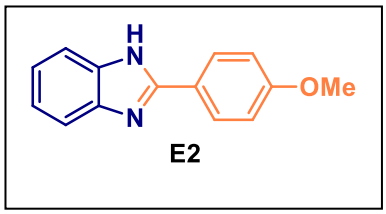

151.76
144.28
135.47
130.64
130.40
129.49
126.96
123.10
122.23
119.35
111.87
40.60
40.39
40.18
39.97
39.76
39.55
39.34
E1
f1 (ppm)


12.7325
8.1009
8.0816
7.6500
7.6350
7.5358
7.5074
7.3971
7.1348
7.0809
7.0614
3.7930
3.3903

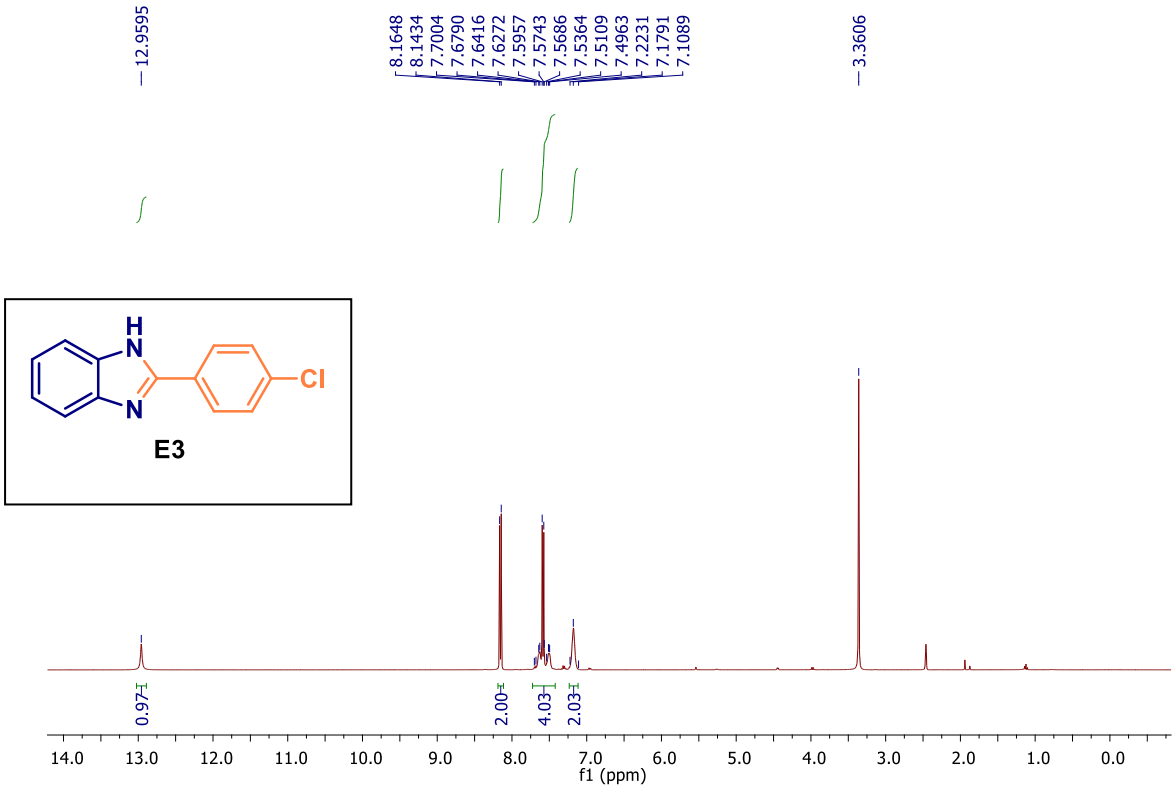

H
N
N
OMe
E2

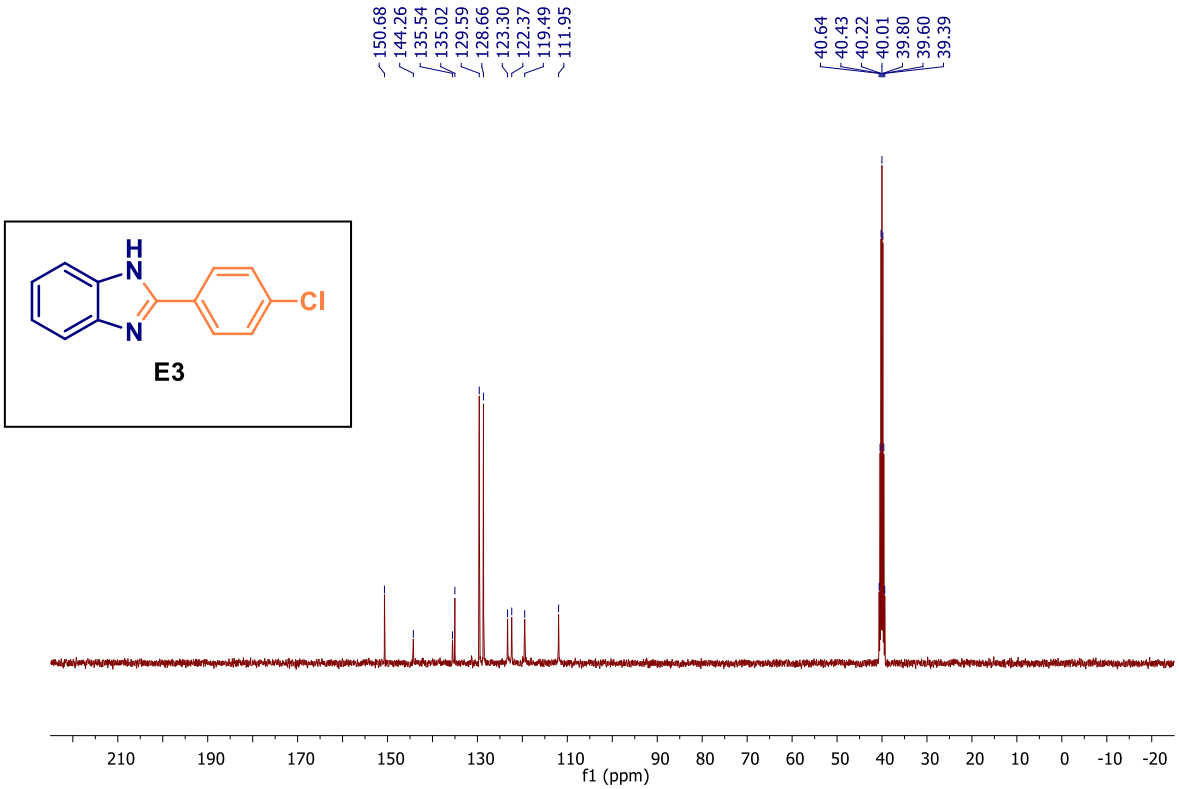

0.98
2.00
2.16
4.11
3.04
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

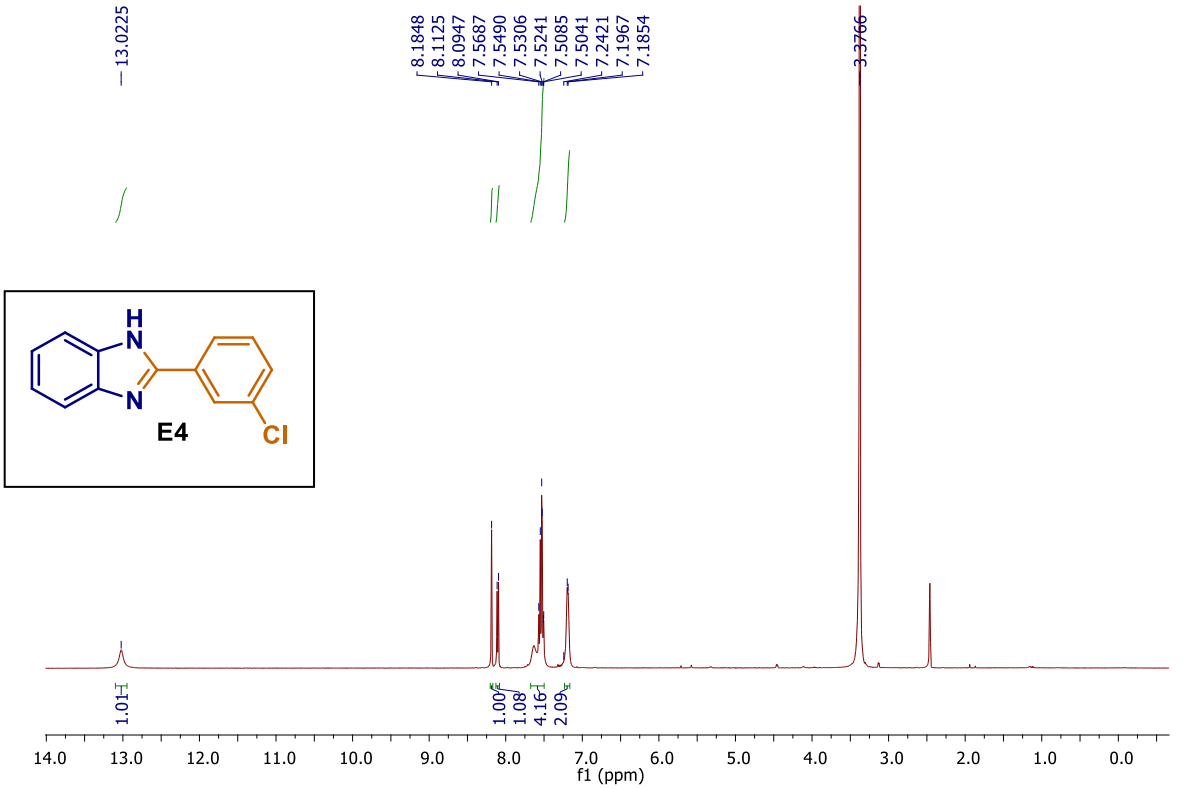

161.12
151.88
144.32
135.37
131.04
128.54
127.93
123.20
122.26
118.92
114.88
55.83
40.61
40.41
40.20
39.99
39.78
39.57
39.36

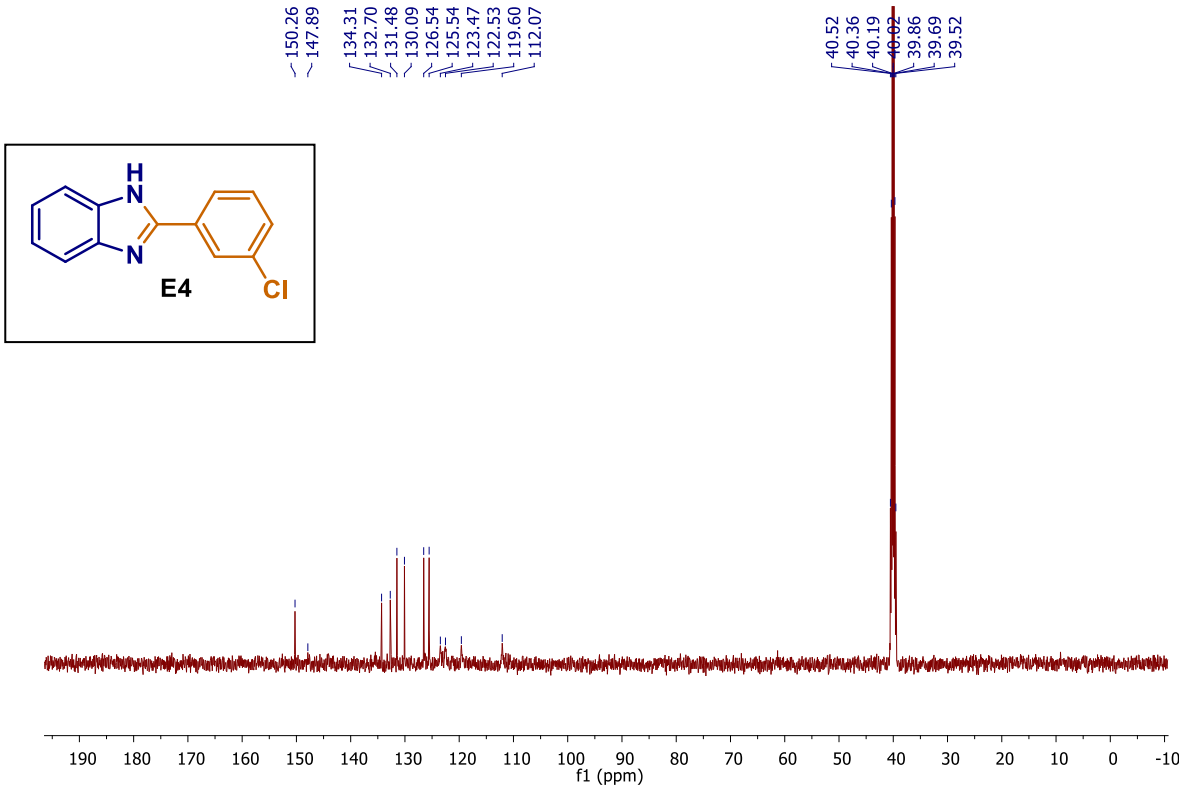

H
N
N
OMe
E2

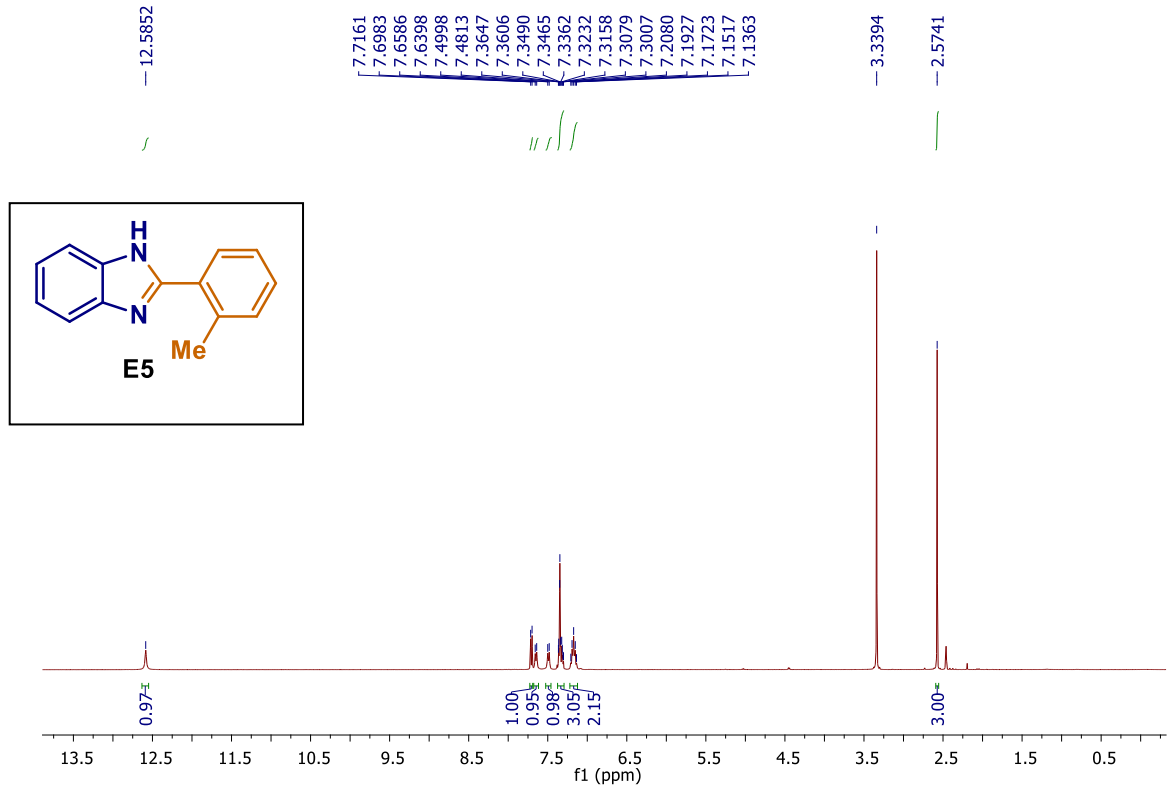
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

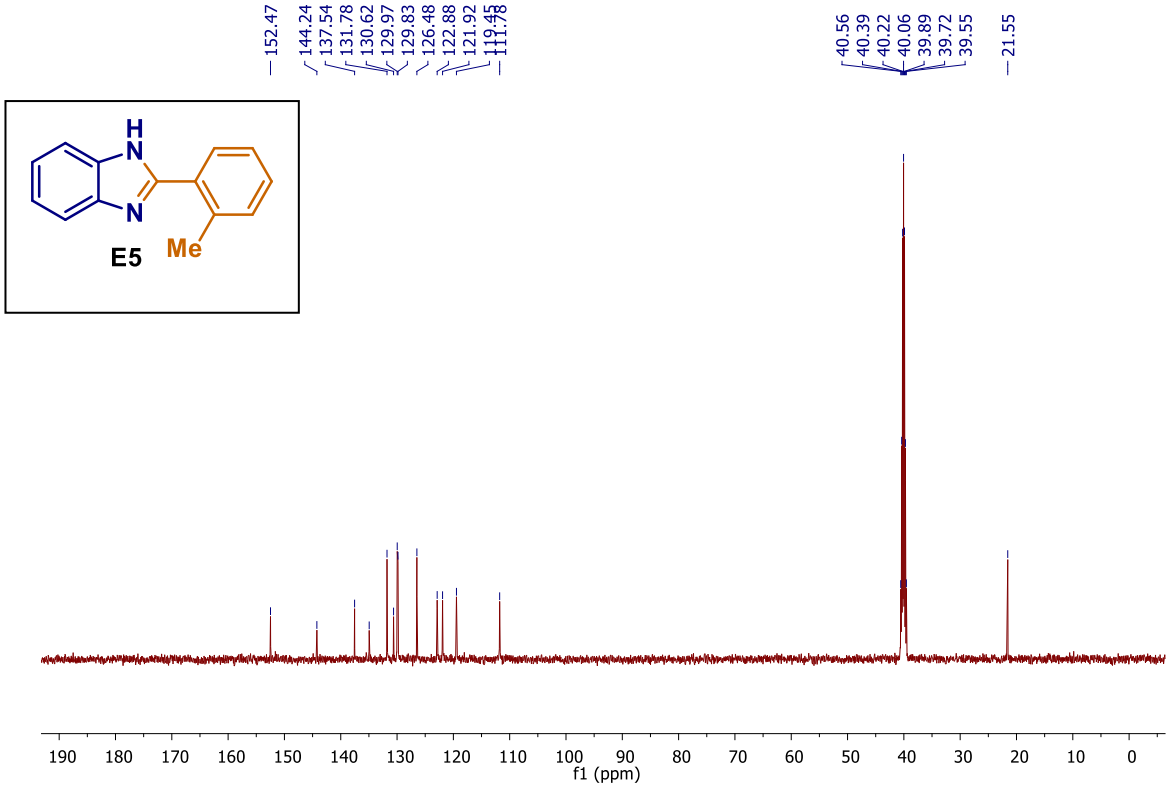

12.9595
8.1648
8.1434
7.7004
7.6790
7.6416
7.6272
7.5957
7.5743
7.5686
7.5364
7.5109
7.4963
7.2231
7.1791
7.1089
3.3606
E3
0.97
2.00
4.03
2.03
f1 (ppm)


150.68
144.26
135.54
135.02
129.59
128.66
123.30
122.37
119.49
111.95
40.64
40.43
40.22
40.01
39.80
39.60
39.39
E3
f1 (ppm)


13.0225
8.1848
8.1125
8.0947
7.5687
7.5490
7.5306
7.5241
7.5085
7.5041
7.2421
7.1967
7.1854
3.3766
E4
Cl
1.01
1.00
1.08
4.16
2.09
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)


150.26
147.89
134.31
132.70
131.48
130.09
126.54
125.54
123.47
122.53
119.60
112.07
40.52
40.36
40.19
40.02
39.86
39.69
39.52
E4
Cl
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


12.5852
7.7161
7.6983
7.6586
7.6398
7.4998
7.4813
7.3647
7.3606
7.3490
7.3465
7.3362
7.3232
7.3158
7.3079
7.3007
7.2080
7.1927
7.1723
7.1517
7.1363
3.3394
2.5741
H
N
N
Me
E5
0.97
1.00
0.95
0.98
3.05
2.15
3.00
13.5
12.5
11.5
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)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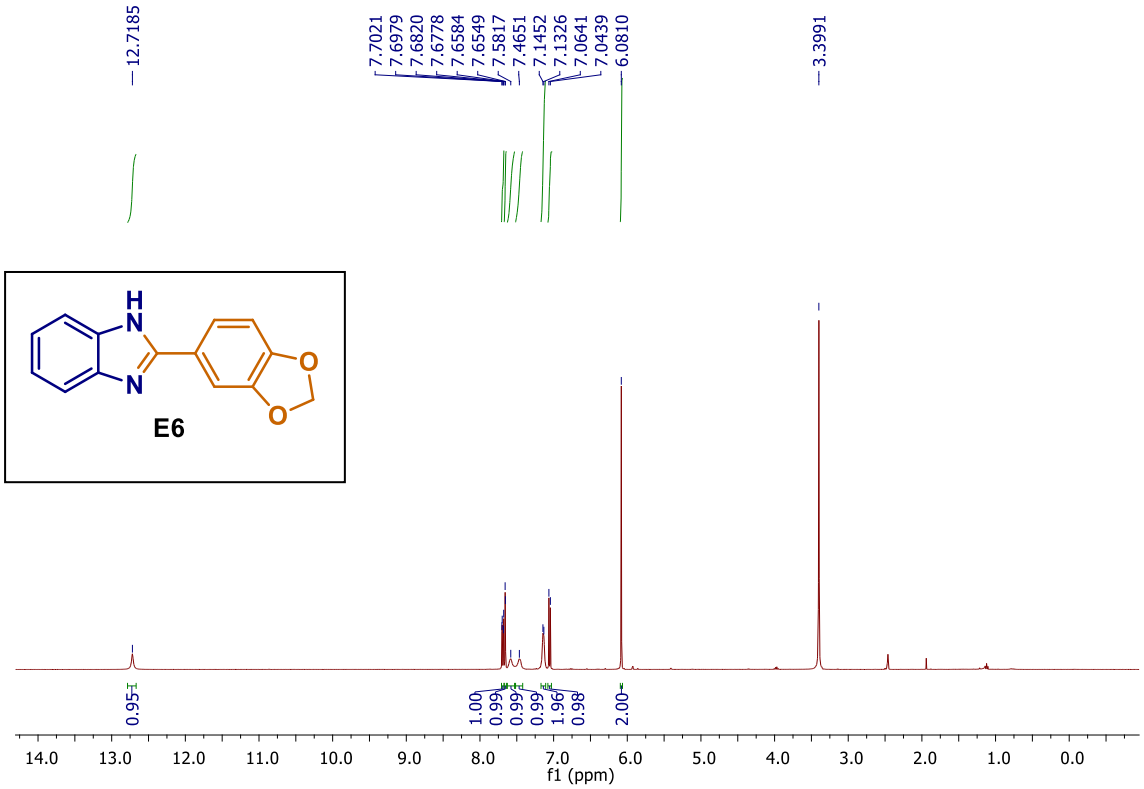
144.24
137.54
131.78
130.62
129.97
129.83
126.48
122.88
121.92
119.45
111.78
40.56
40.39
40.22
40.06
39.89
39.72
39.55
21.55
H
N
N
Me
E5
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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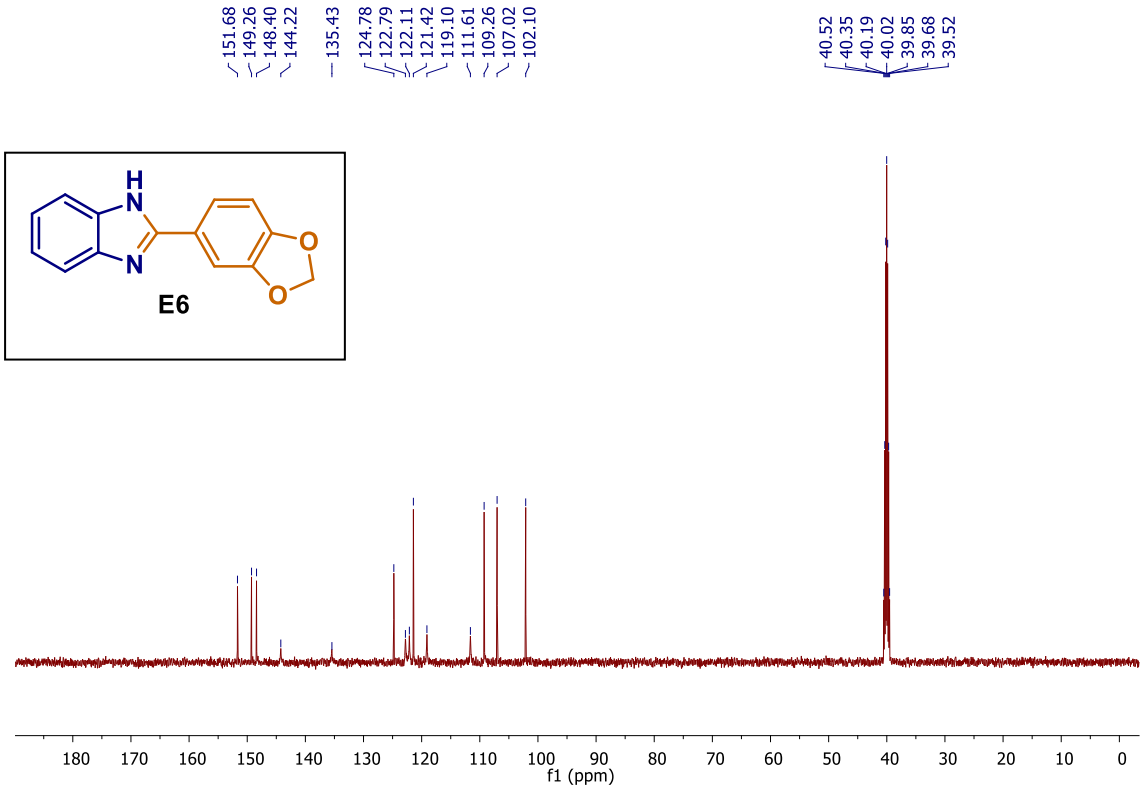
7.6979
7.6820
7.6778
7.6584
7.6549
7.5817
7.4651
7.1452
7.1326
7.0641
7.0439
6.0810
3.3991
E6
0.95
1.00
0.99
0.99
0.99
1.96
0.98
2.00
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)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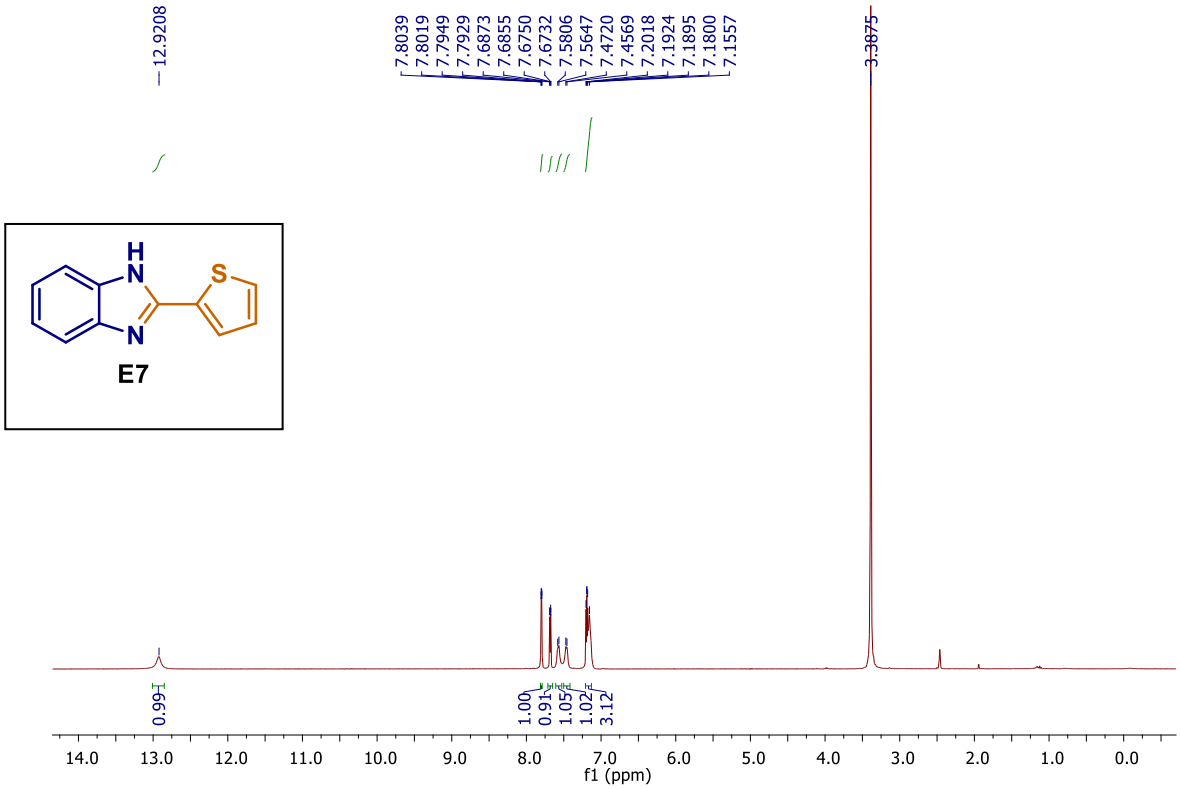
149.26
148.40
144.22
135.43
124.78
122.79
122.11
121.42
119.10
111.61
109.26
107.02
102.10
40.52
40.35
40.19
40.02
39.85
39.68
39.52
E6
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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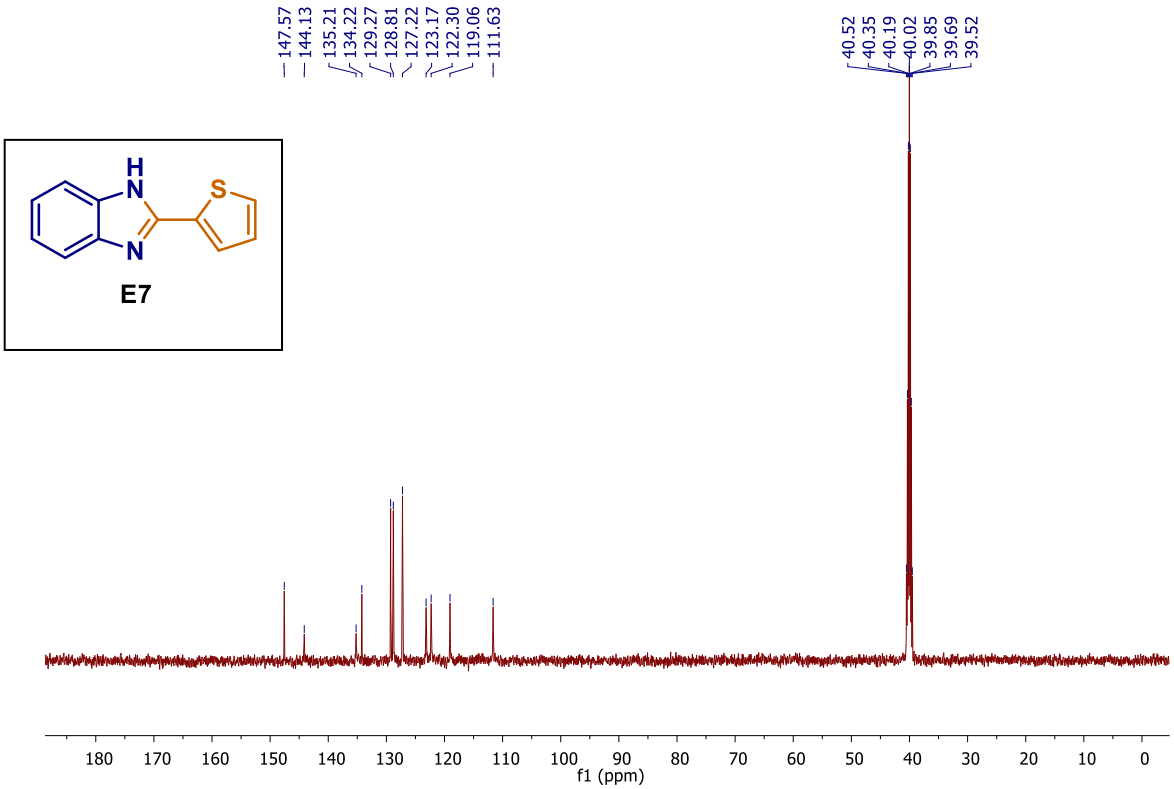
7.8019
7.7949
7.7929
7.6873
7.6855
7.6750
7.6732
7.5806
7.5647
7.4720
7.4569
7.2018
7.1924
7.1895
7.1800
7.1557
3.3875
E7
0.99
1.00
0.91
1.05
1.02
3.12
f1 (ppm)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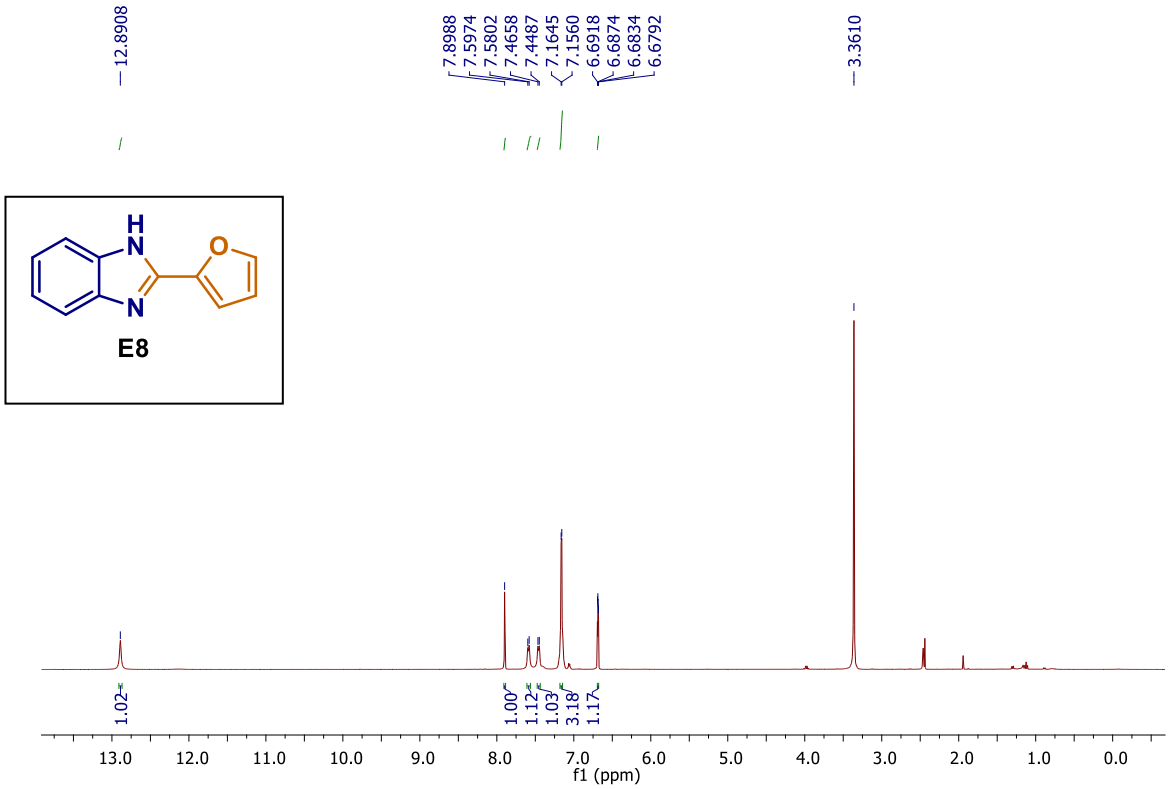
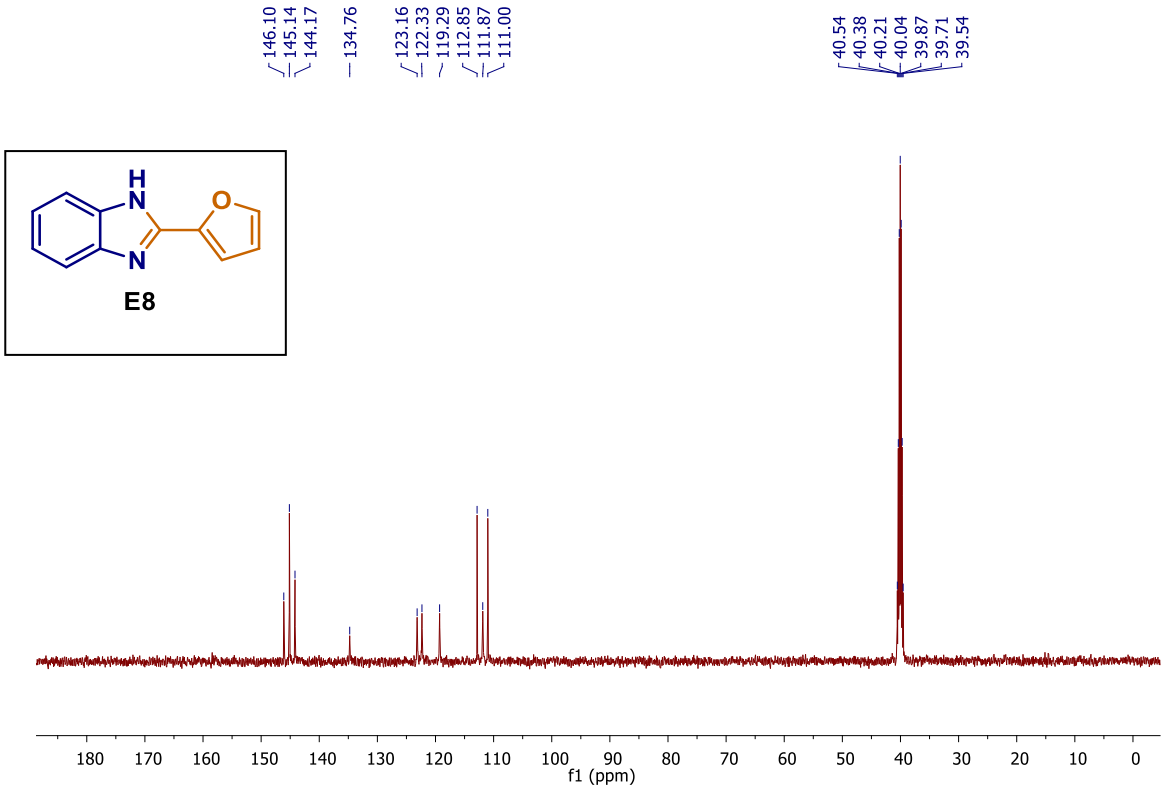
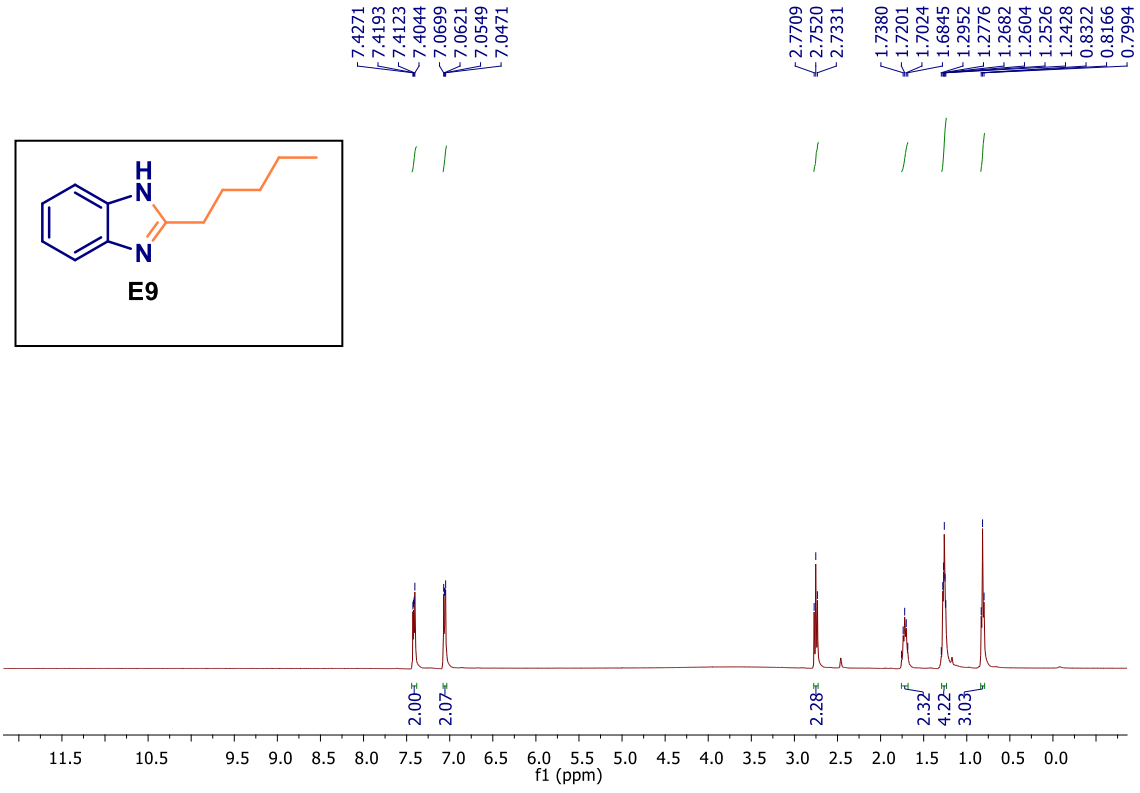
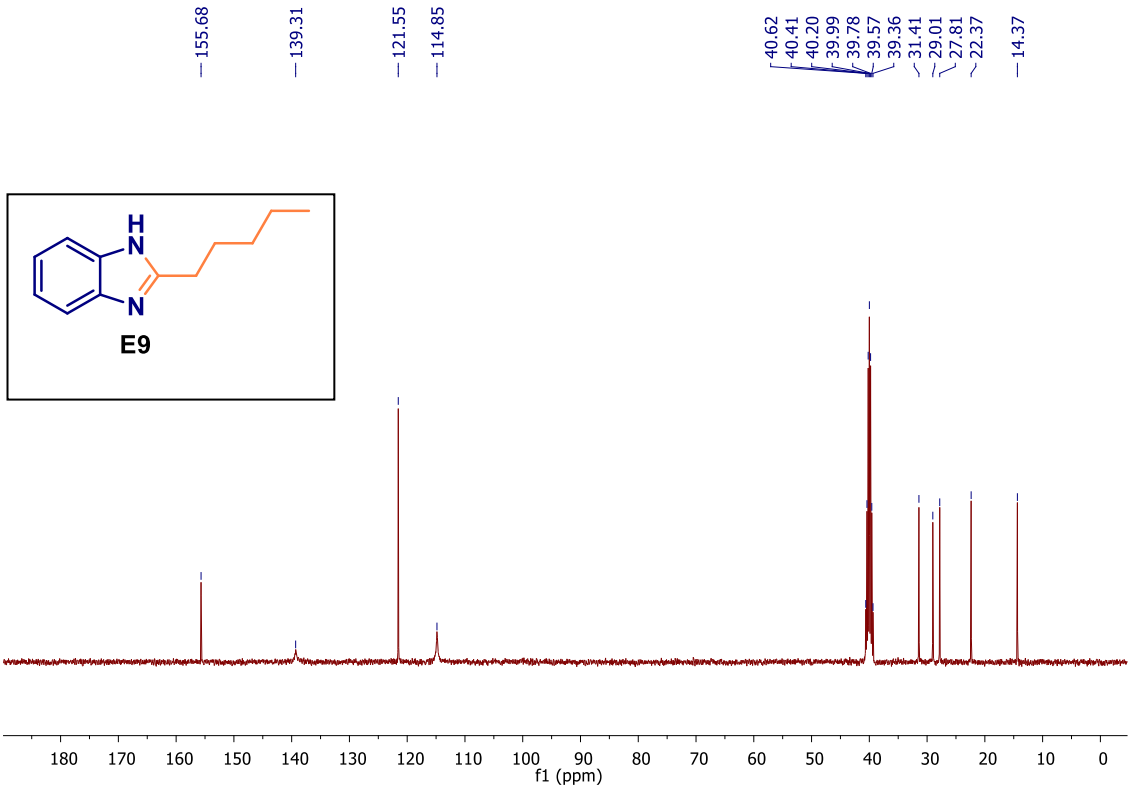
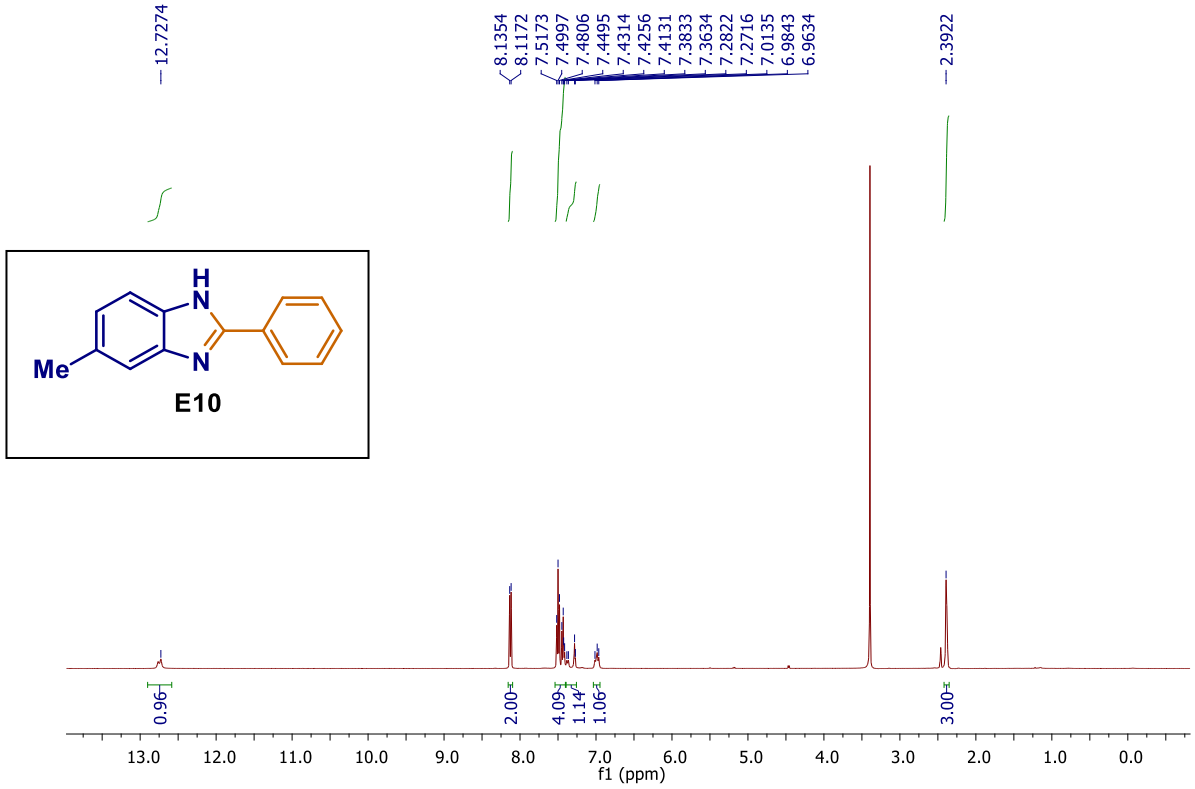
144.13
135.21
134.22
129.27
128.81
127.22
123.17
122.30
119.06
111.63
40.52
40.35
40.19
40.02
39.85
39.69
39.52
E7
f1 (ppm)

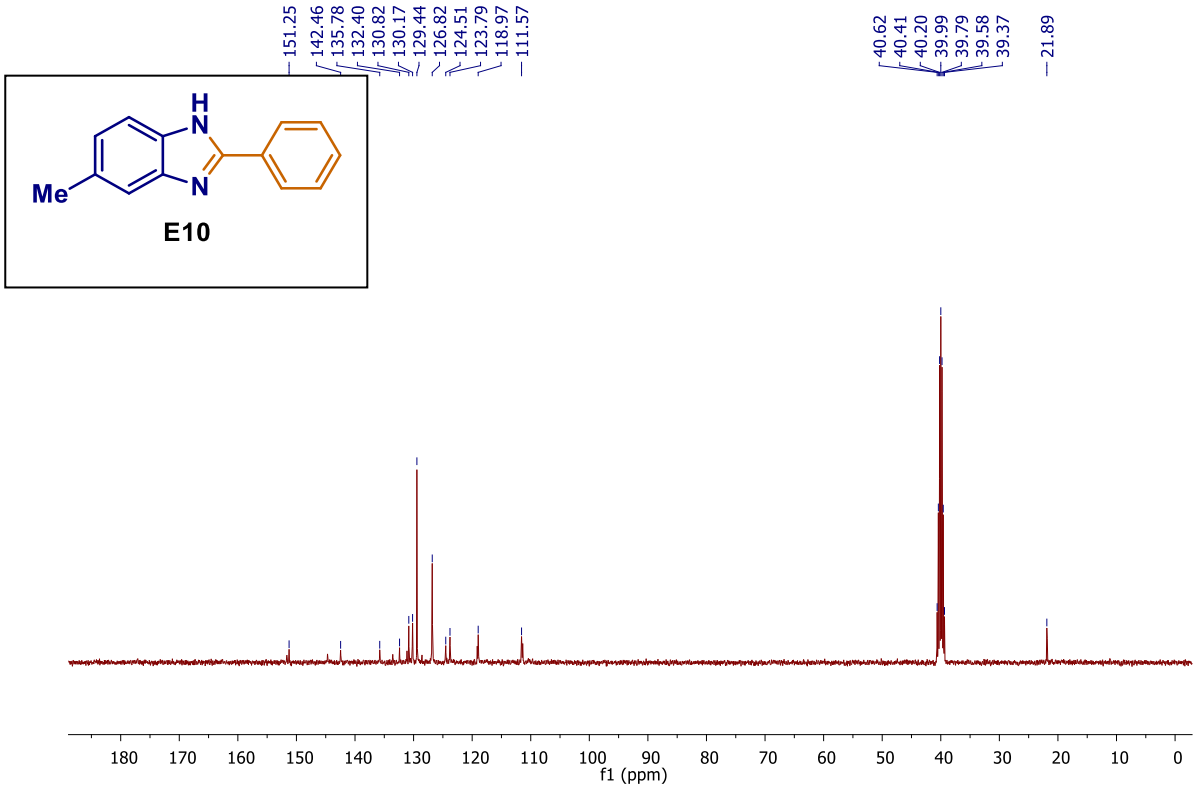

12.8908
7.8988
7.5974
7.5802
7.4658
7.4487
7.1645
7.1560
6.6918
6.6874
6.6834
6.6792
3.3610
E8
1.02
1.00
1.12
1.03
3.18
1.17
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

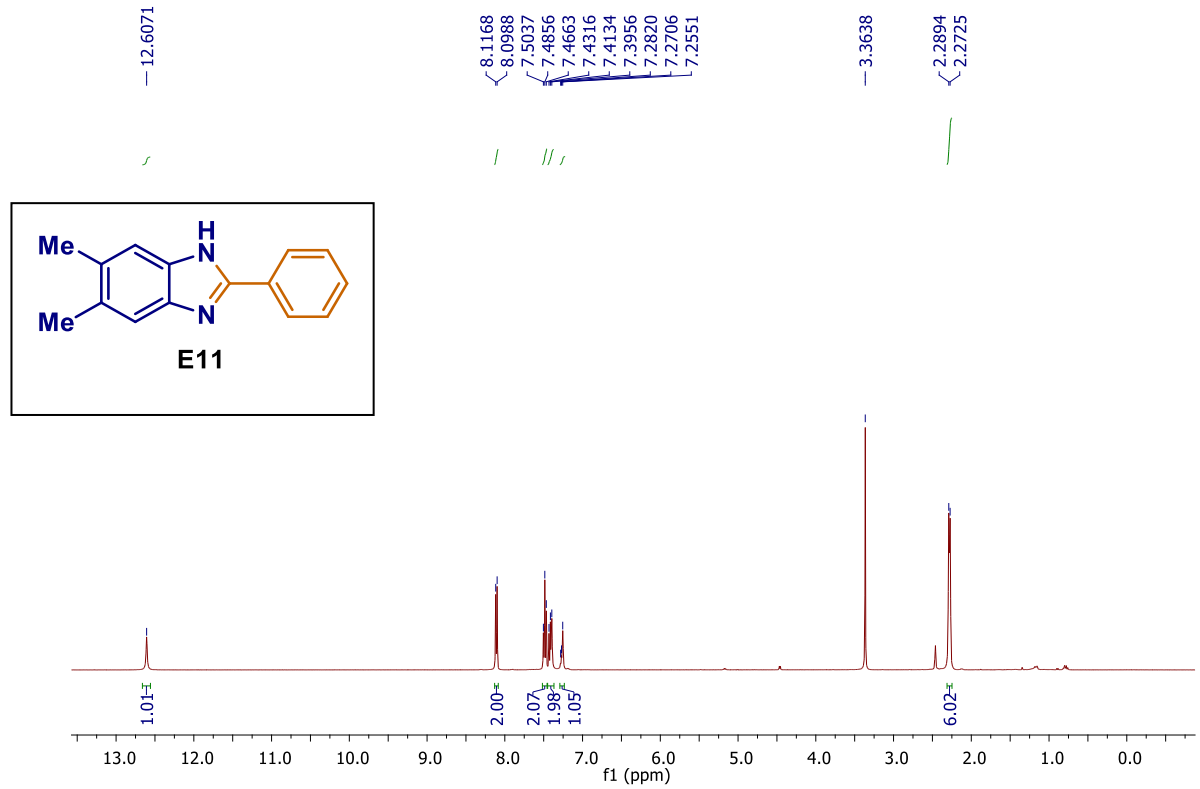

146.10
145.14
144.17
134.76
123.16
122.33
119.29
112.85
111.87
111.00
40.54
40.38
40.21
40.04
39.87
39.71
39.54
E8
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

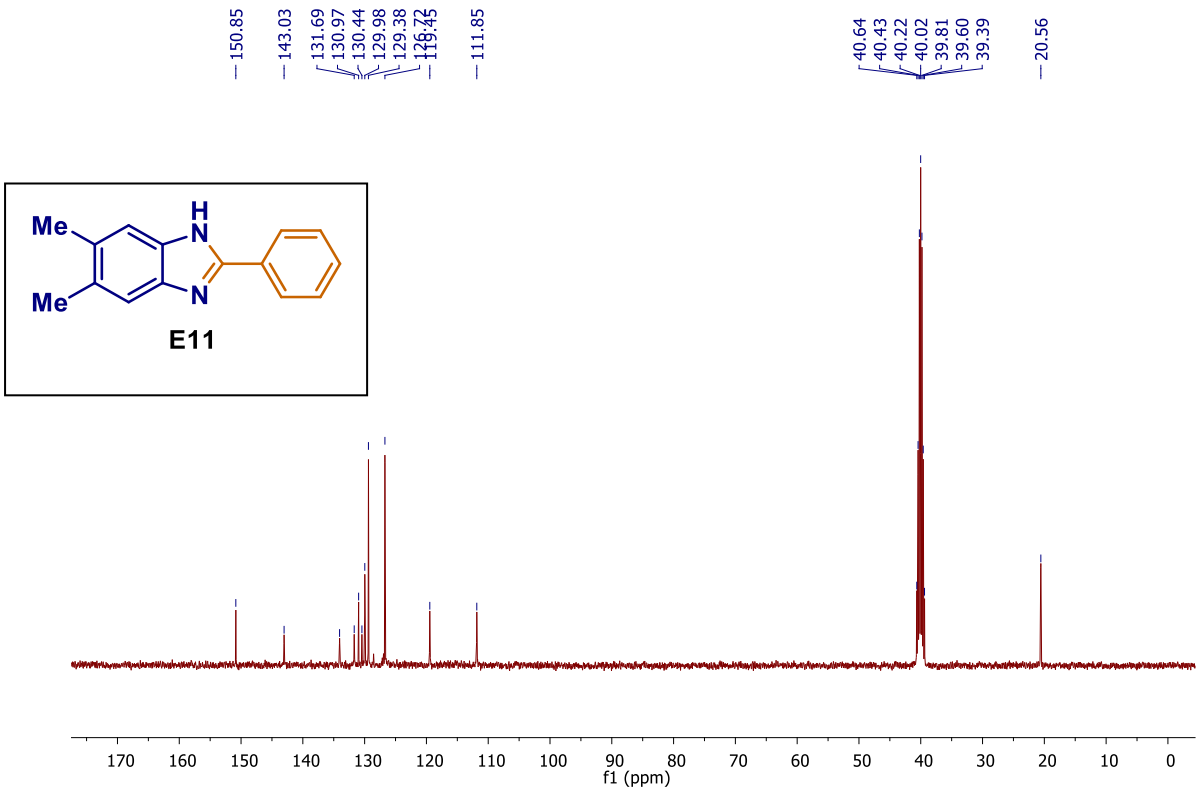

7.4271
7.4193
7.4123
7.4044
7.0699
7.0621
7.0549
7.0471
2.7709
2.7520
2.7331
1.7380
1.7201
1.7024
1.6845
1.2952
1.2776
1.2682
1.2604
1.2526
1.2428
0.8322
0.8166
0.7994
H
N
N
E9
2.00
2.07
2.28
2.32
4.22
3.03
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

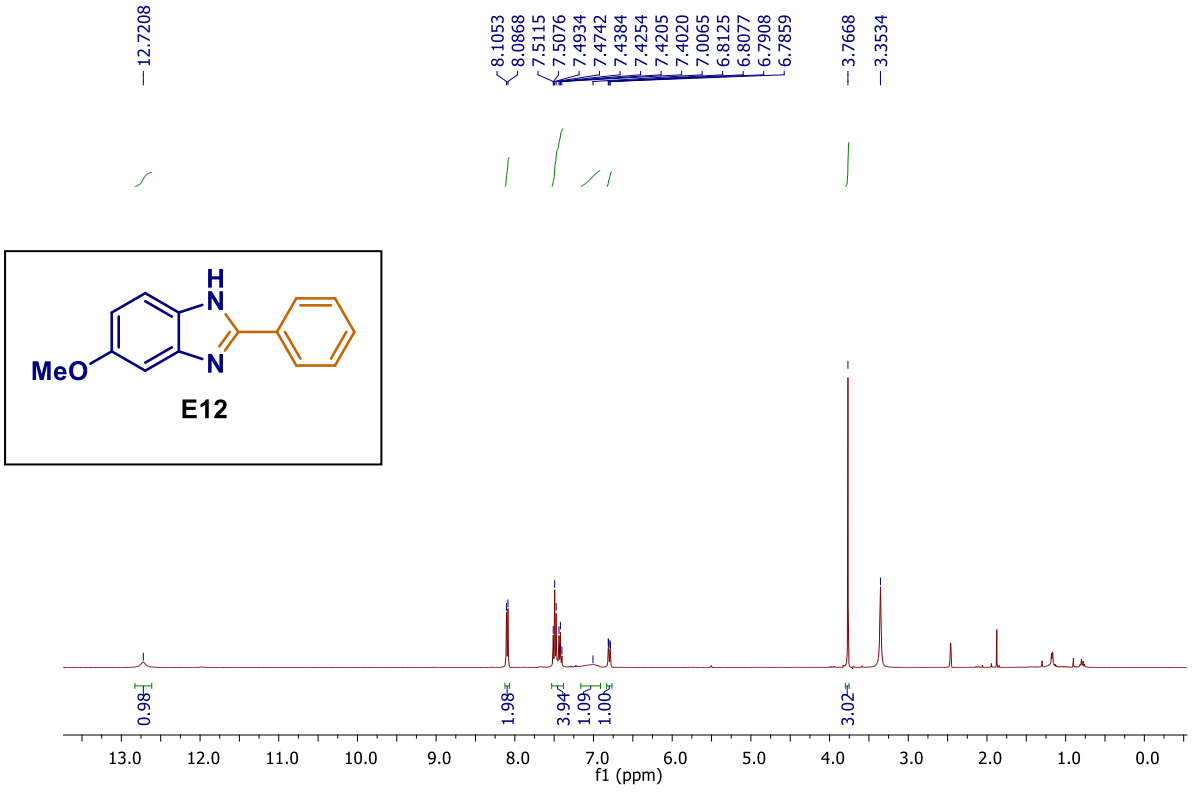

155.68
139.31
121.55
114.85
40.62
40.41
40.20
39.99
39.78
39.57
39.36
31.41
29.01
27.81
22.37
14.37
H
N
N
E9
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

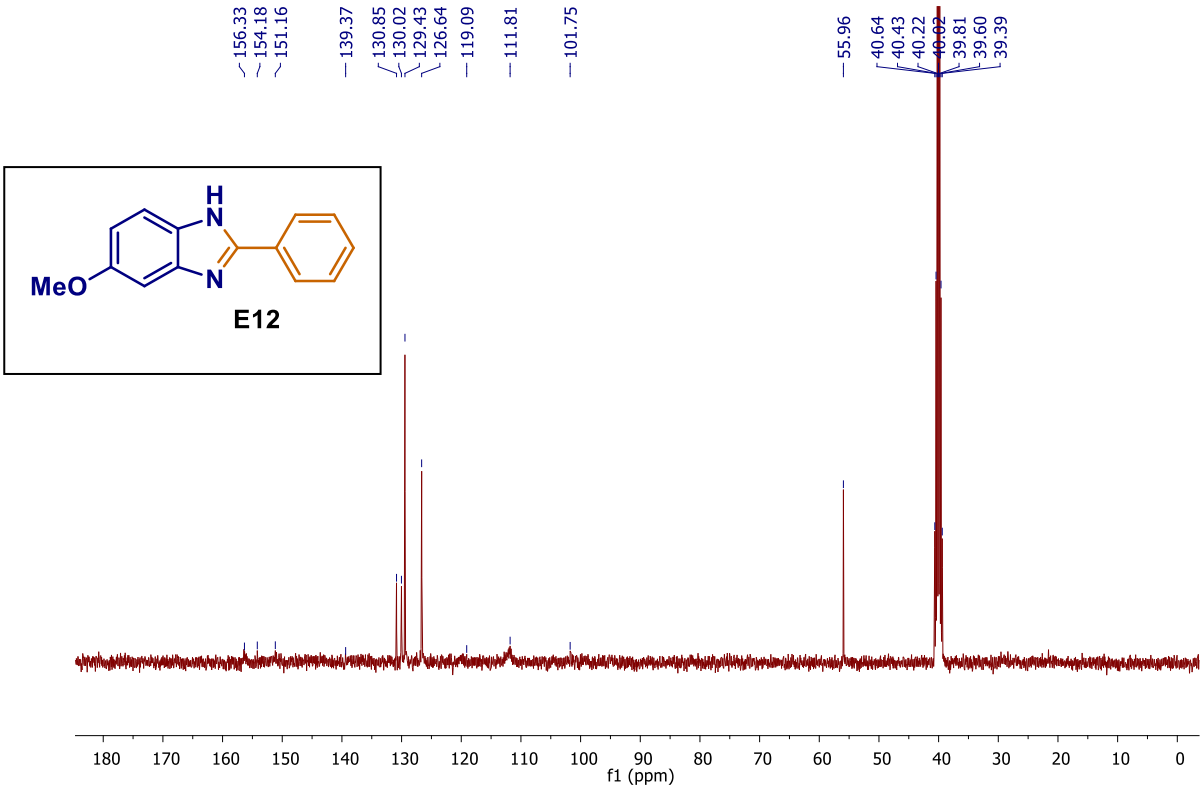

12.7274
8.1354
8.1172
7.5173
7.4997
7.4806
7.4495
7.4314
7.4256
7.4131
7.3833
7.3634
7.2822
7.2716
7.0135
6.9843
6.9634
2.3922
H
N
N
Me
E10
0.96
2.00
4.09
1.14
1.06
3.00
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

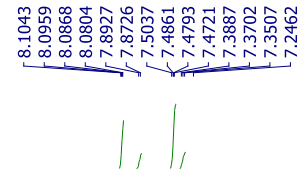

151.25
142.46
135.78
132.40
130.82
130.17
129.44
126.82
124.51
123.79
118.97
111.57
40.62
40.41
40.20
39.99
39.79
39.58
39.37
21.89
H
N
N
Me
E10
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

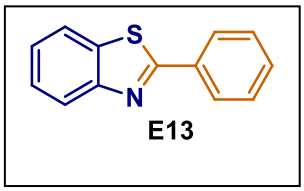

12.6071
8.1168
8.0988
7.5037
7.4856
7.4663
7.4316
7.4134
7.3956
7.2820
7.2706
7.2551
3.3638
2.2894
2.2725
Me
Me
H
N
N
E11
1.01
2.00
2.07
1.98
1.05
6.02
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

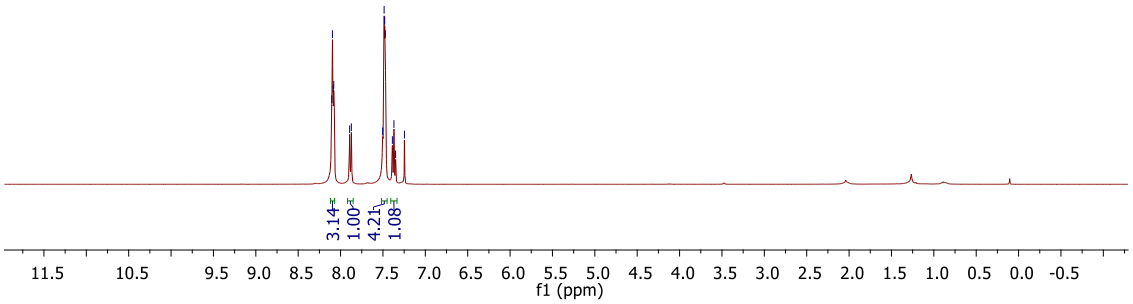

150.85
143.03
131.69
130.97
130.44
129.98
129.38
111.85
40.64
40.43
40.22
40.02
39.81
39.60
39.39
20.56
Me
Me
H
N
N
E11
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


12.7208
8.1053
8.0868
7.5115
7.5076
7.4934
7.4742
7.4384
7.4254
7.4205
7.4020
7.0065
6.8125
6.8077
6.7908
6.7859
3.7668
3.3534
MeO
E12
0.98
1.98
3.94
1.09
1.00
3.02
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

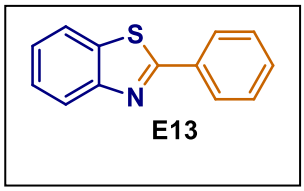

156.33
154.18
151.16
139.37
130.85
130.02
129.43
126.64
119.09
111.81
101.75
55.96
40.64
40.43
40.22
40.02
39.81
39.60
39.39
MeO
E12
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

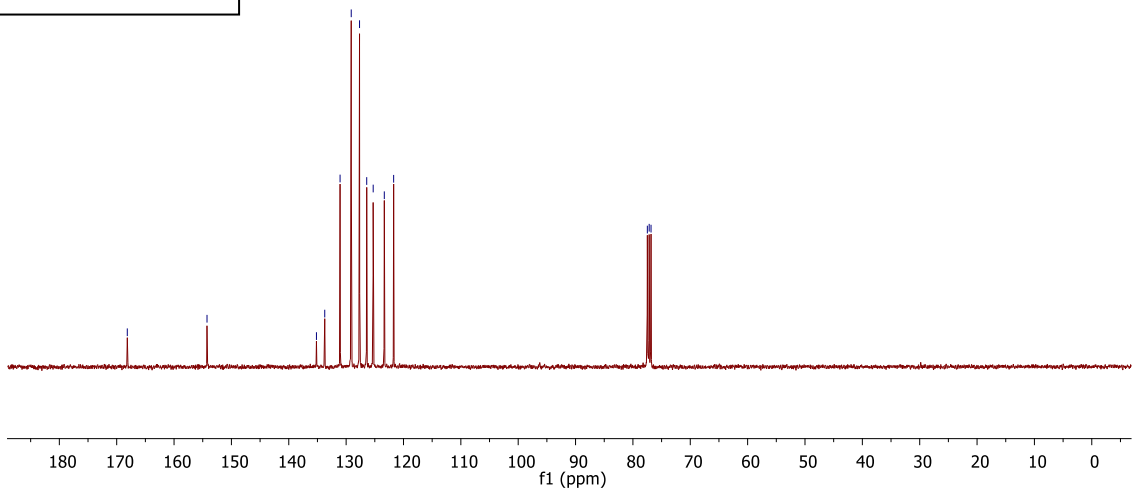

8.1043
8.0959
8.0868
8.0804
7.8927
7.8726
7.5037
7.4861
7.4793
7.4721
7.3887
7.3702
7.3507
7.2462

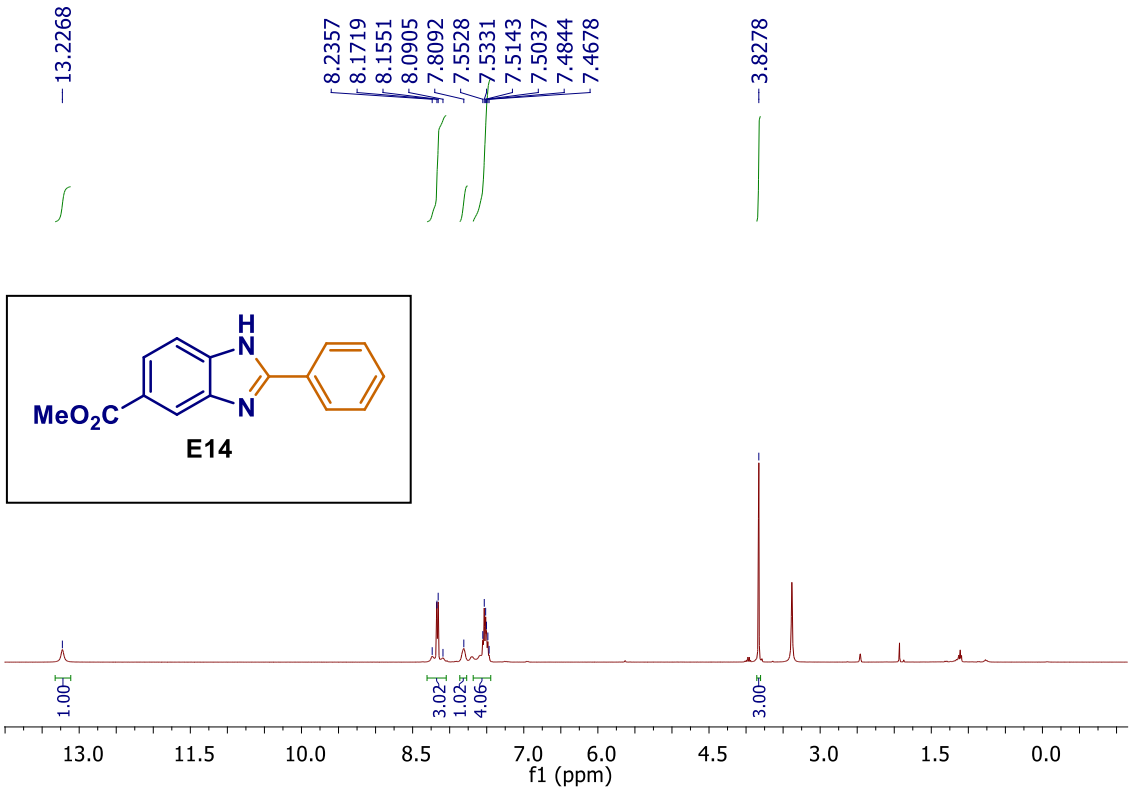

S
N
E13

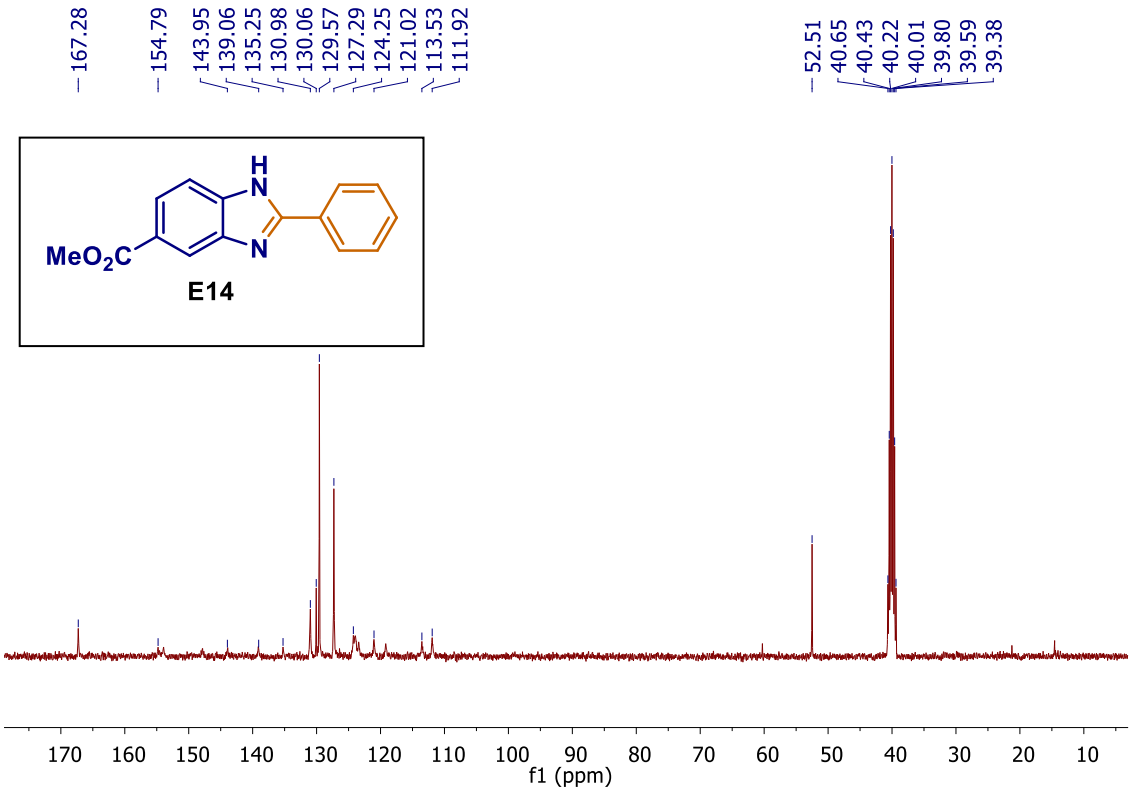

3.14
1.00
4.21
1.08
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

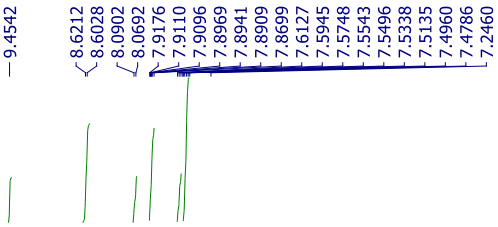

168.15
154.25
135.17
133.73
131.06
129.11
127.66
126.41
125.28
123.34
121.71
77.48
77.16
76.84

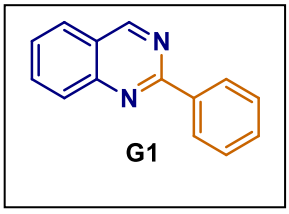

S
N
E13

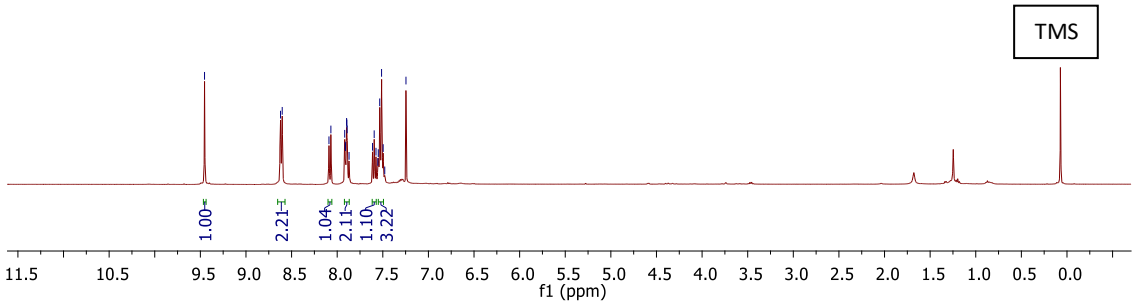

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


13.2268
8.2357
8.1719
8.1551
8.0905
7.8092
7.5528
7.5331
7.5143
7.5037
7.4844
7.4678
3.8278
MeO2C
E14
1.00
3.02
1.02
4.06
3.00
13.0
11.5
10.0
8.5
7.0
6.0
4.5
3.0
1.5
0.0
f1 (ppm)

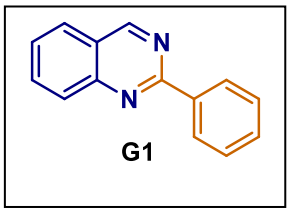

167.28
154.79
143.95
139.06
135.25
130.98
130.06
129.57
127.29
124.25
121.02
113.53
111.92
52.51
40.65
40.43
40.22
40.01
39.80
39.59
39.38
MeO2C
E14
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

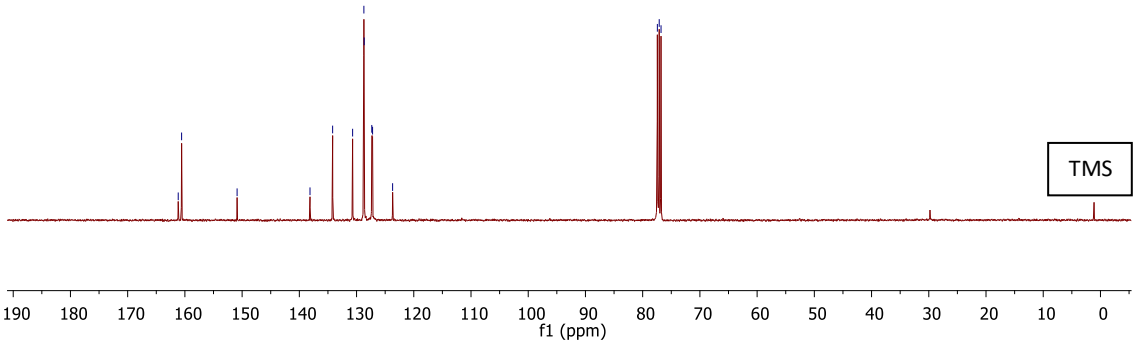

9.4542
8.6212
8.6028
8.0902
8.0692
7.9176
7.9110
7.9096
7.8969
7.8941
7.8909
7.8699
7.6127
7.5945
7.5748
7.5543
7.5496
7.5338
7.5135
7.4960
7.4786
7.2460

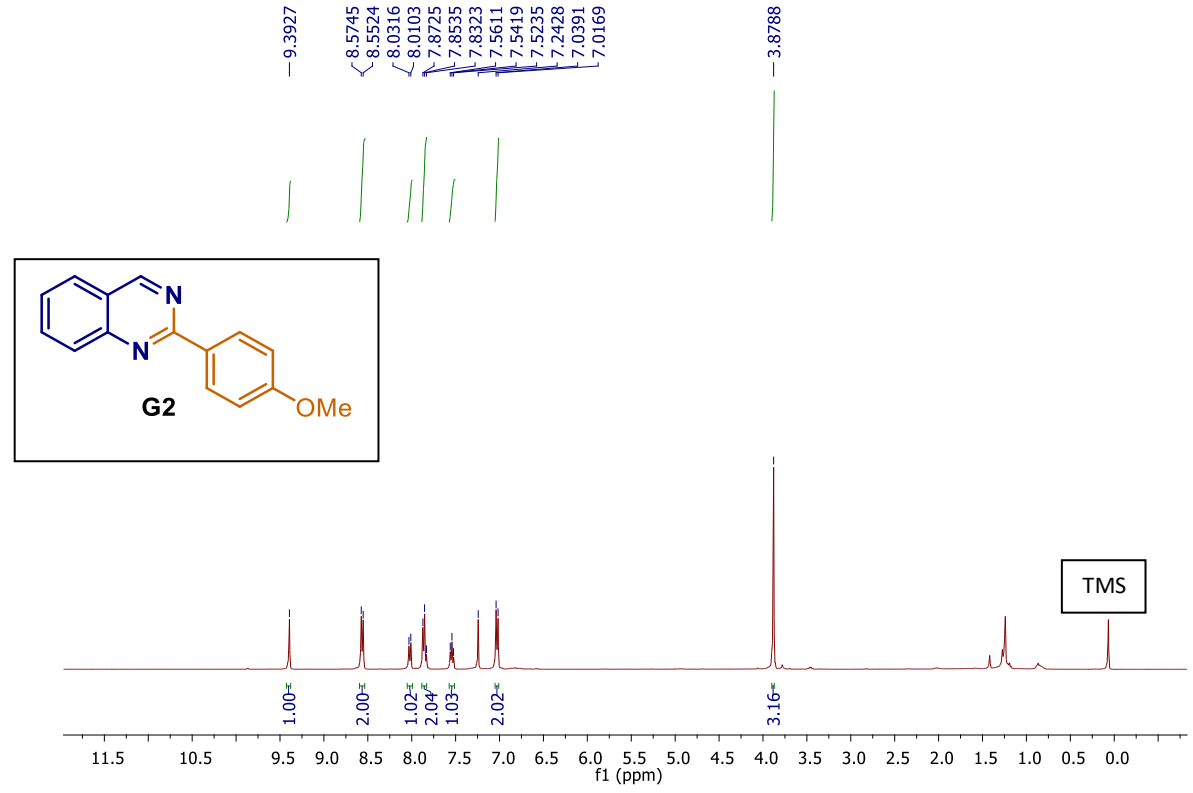

N
N
G1

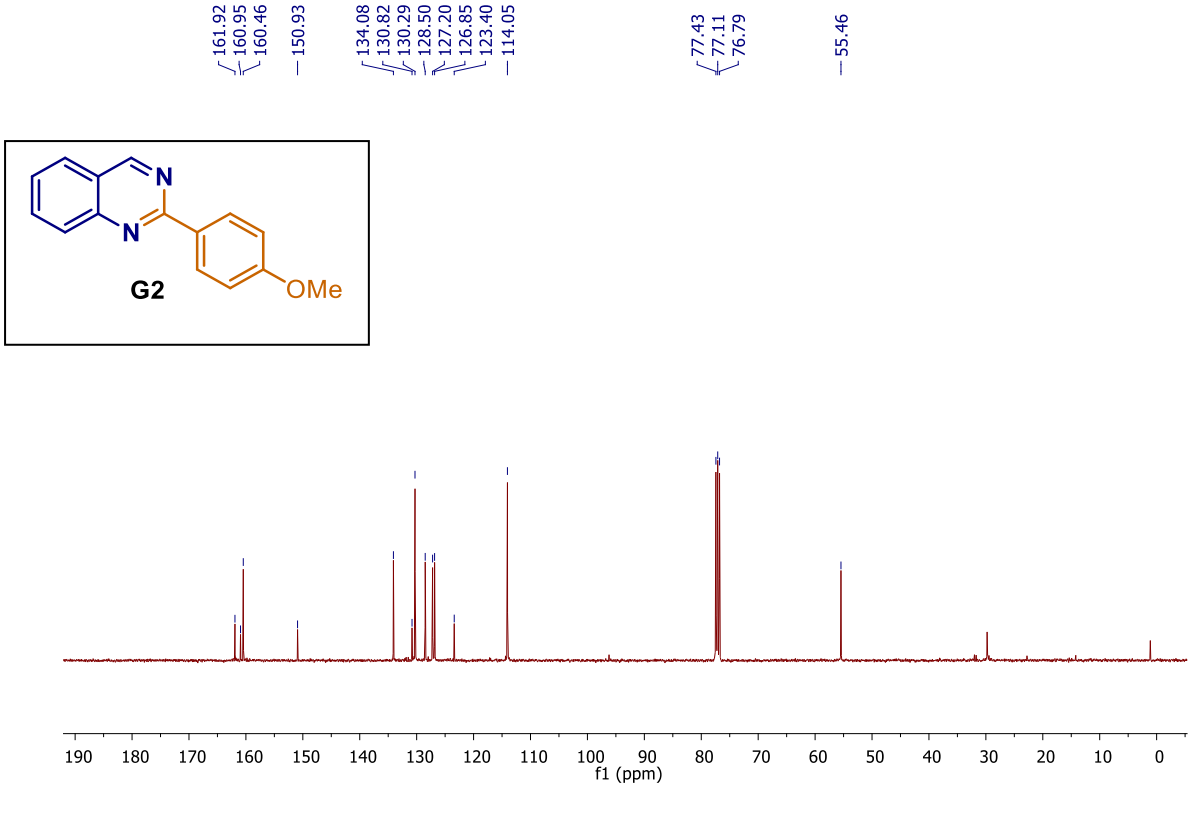

TMS
1.00
2.21
1.04
2.11
1.10
3.22
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.16
160.57
150.87
138.14
134.18
130.69
128.72
128.67
127.34
127.20
123.70
77.43
77.11
76.79


N
N
G1


TMS
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.3927
8.5745
8.5524
8.0316
8.0103
7.8725
7.8535
7.8323
7.5611
7.5419
7.5235
7.2428
7.0391
7.0169
3.8788
N
N
G2
OMe
TMS
1.00
2.00
1.02
2.04
1.03
2.02
3.16
11.5
10.5
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
f1 (ppm)


161.92
160.95
160.46
150.93
134.08
130.82
130.29
128.50
127.20
126.85
123.40
114.05
77.43
77.11
76.79
55.46
N
N
G2
OMe
190
180
170
160
150
140
130
120
110
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90
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70
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50
40
30
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10
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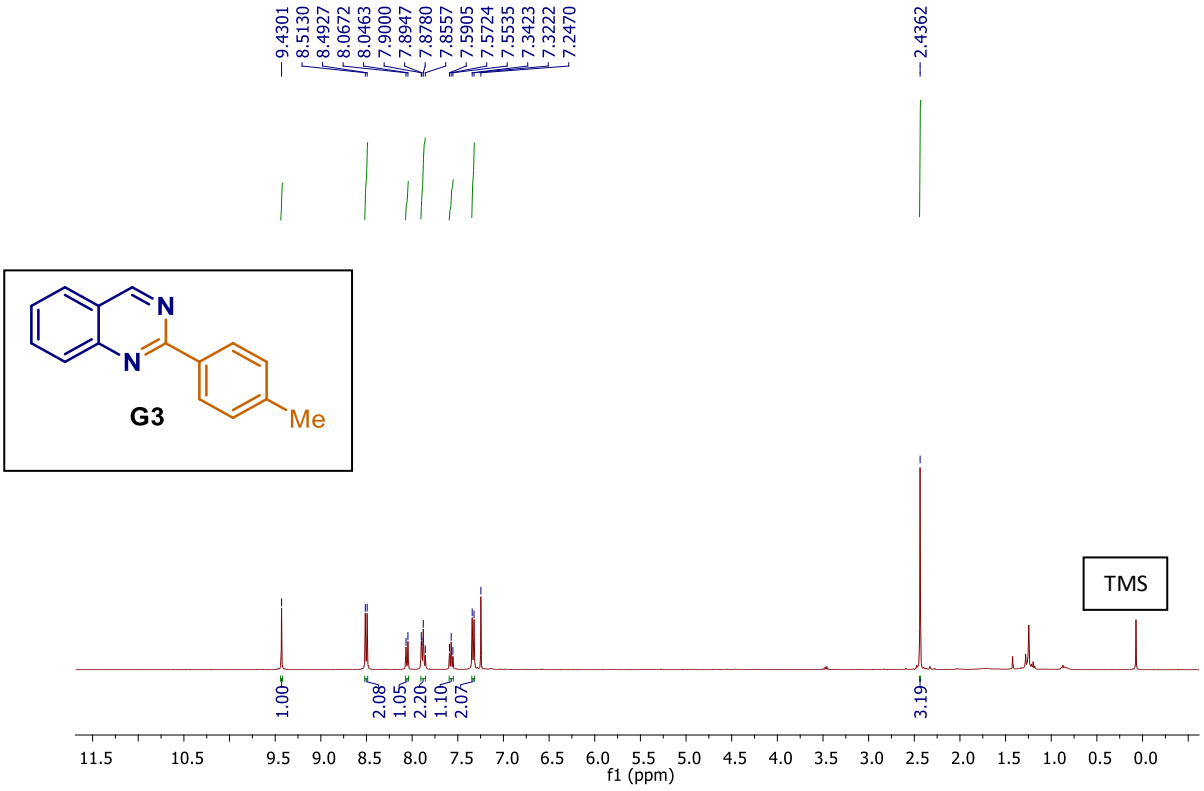
f1 (ppm)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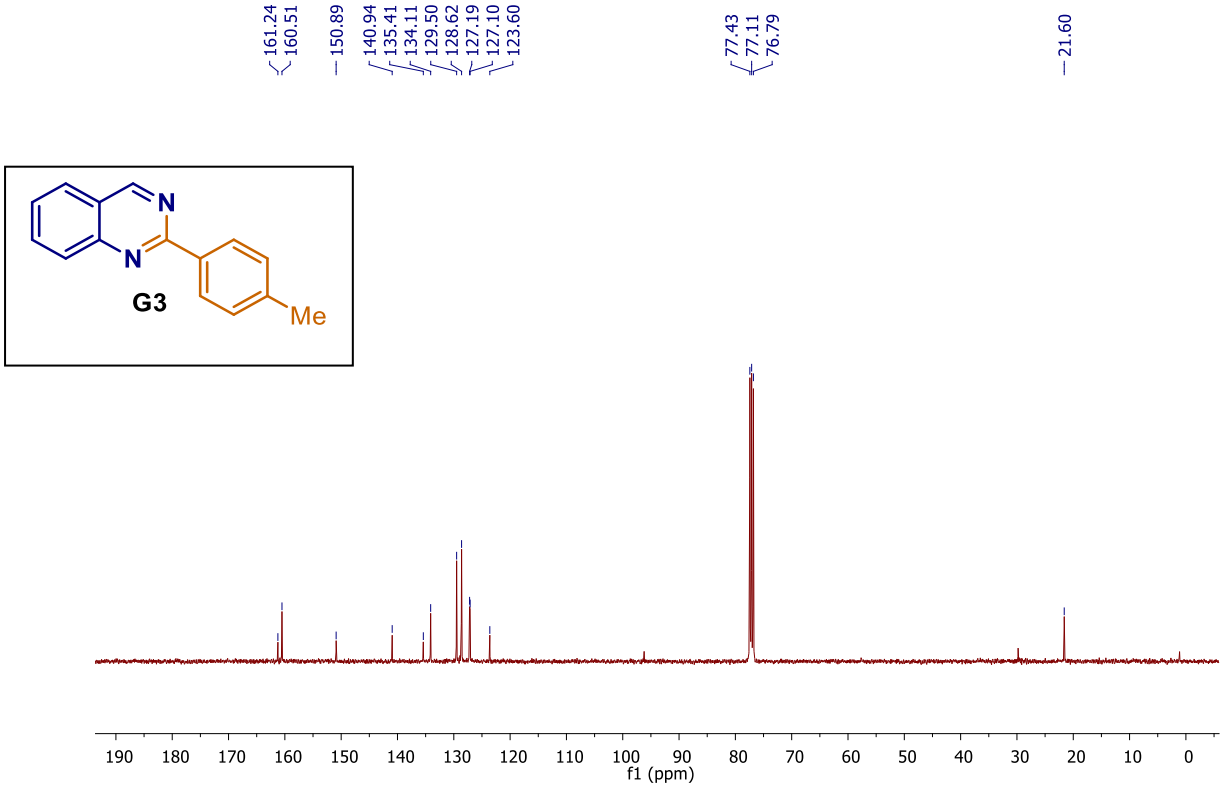
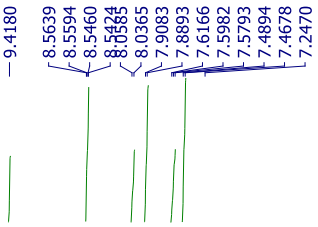
8.4927
8.0672
8.0463
7.9000
7.8947
7.8780
7.8557
7.5905
7.5724
7.5535
7.3423
7.3222
7.2470
2.4362
N
N
G3
Me
TMS
1.00
2.08
1.05
2.20
1.10
2.07
3.19
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


161.24
160.51
150.89
140.94
135.41
134.11
129.50
128.62
127.19
127.10
123.60
77.43
77.11
76.79
21.60
N
N
G3
Me
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.5594
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8.0365
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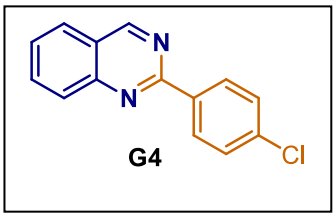
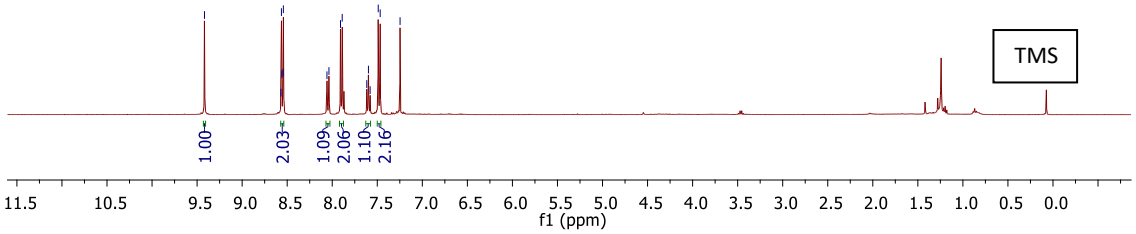
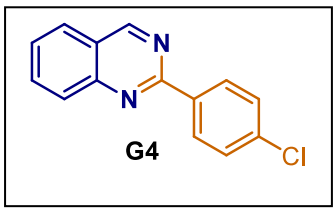
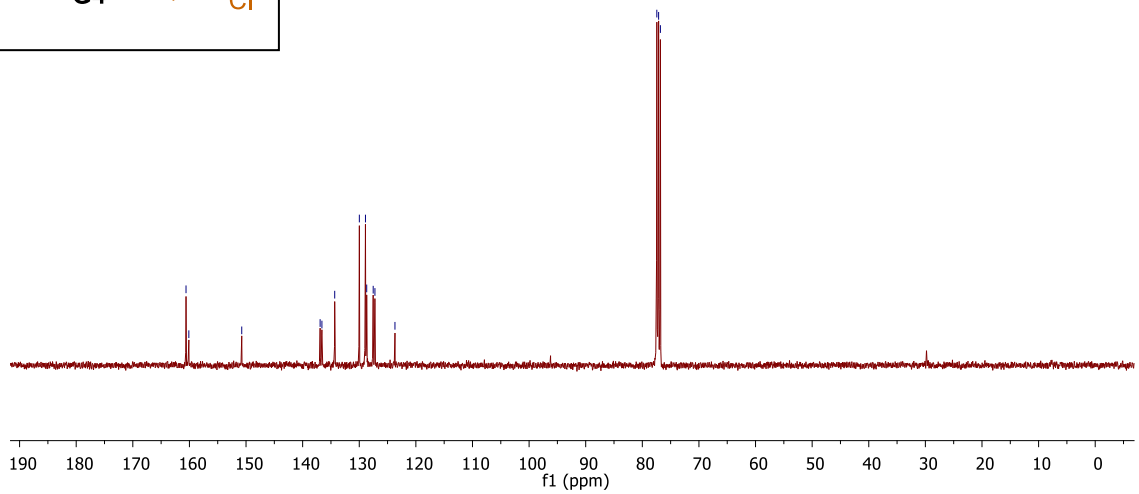
7.8893
7.6166
7.5982
7.5793
7.4894
7.4678
7.2470

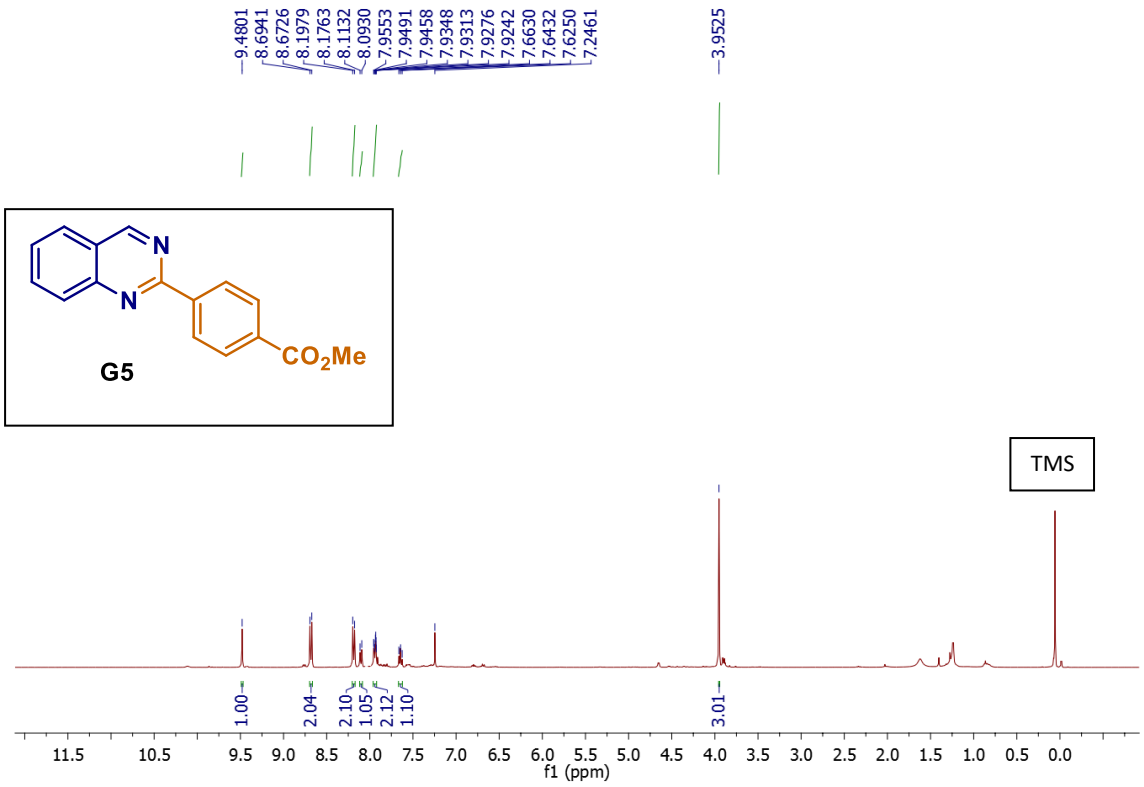

N
N
Cl
G4


TMS
1.00
2.03
1.09
2.06
1.10
2.16
11.5
10.5
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
f1 (ppm)


160.60
160.10
150.76
136.91
136.60
134.34
129.98
128.90
128.68
127.54
127.23
123.69
77.44
77.12
76.80


N
N
Cl
G4


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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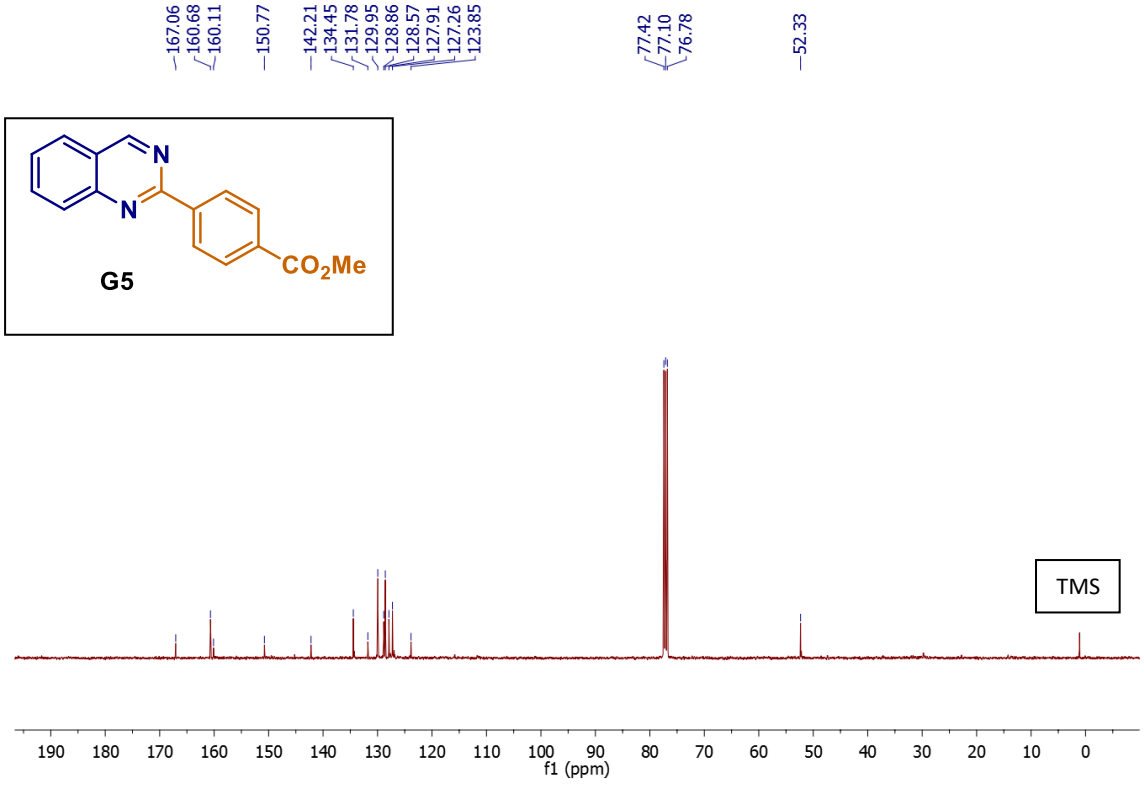
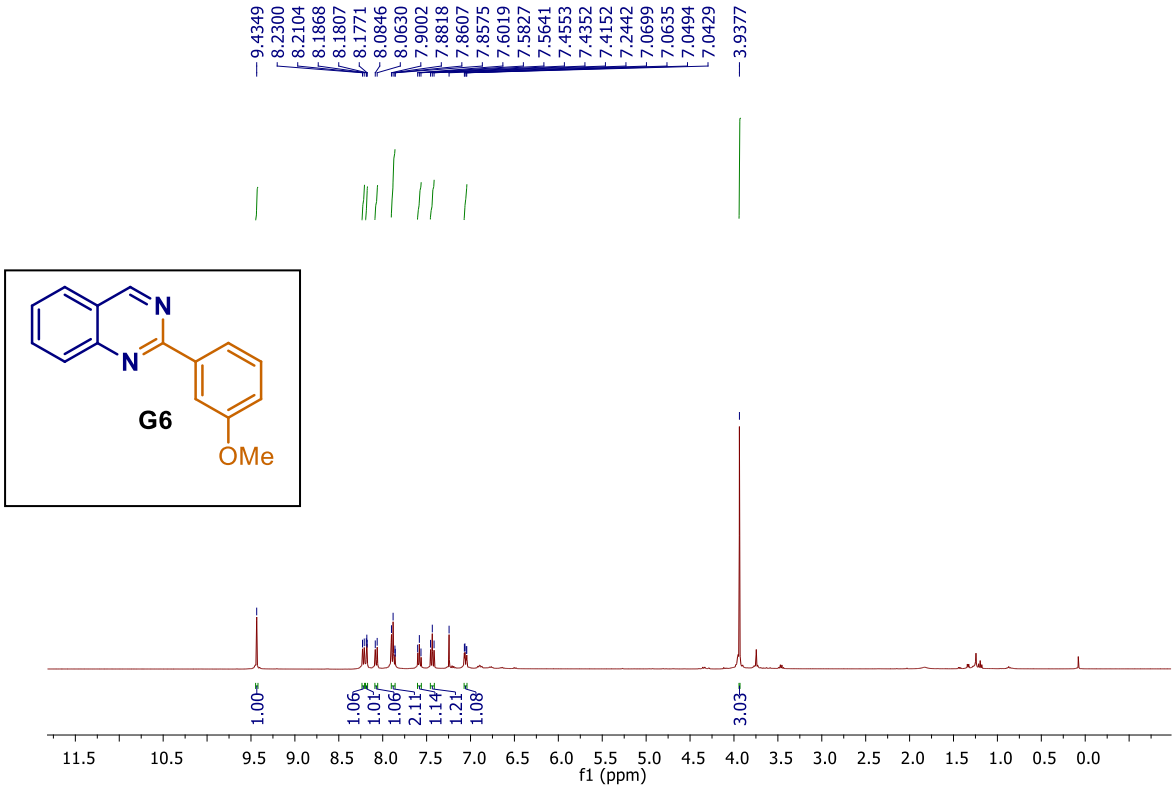
8.6941
8.6726
8.1979
8.1763
8.1132
8.0930
7.9553
7.9491
7.9458
7.9348
7.9313
7.9276
7.9242
7.6630
7.6432
7.6250
7.2461
3.9525
N
N
CO2Me
G5
TMS
1.00
2.04
2.10
1.05
2.12
1.10
3.01
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


167.06
160.68
160.11
150.77
142.21
134.45
131.78
129.95
128.86
128.57
127.91
127.26
123.85
77.42
77.10
76.78
52.33
N
N
CO2Me
G5
TMS
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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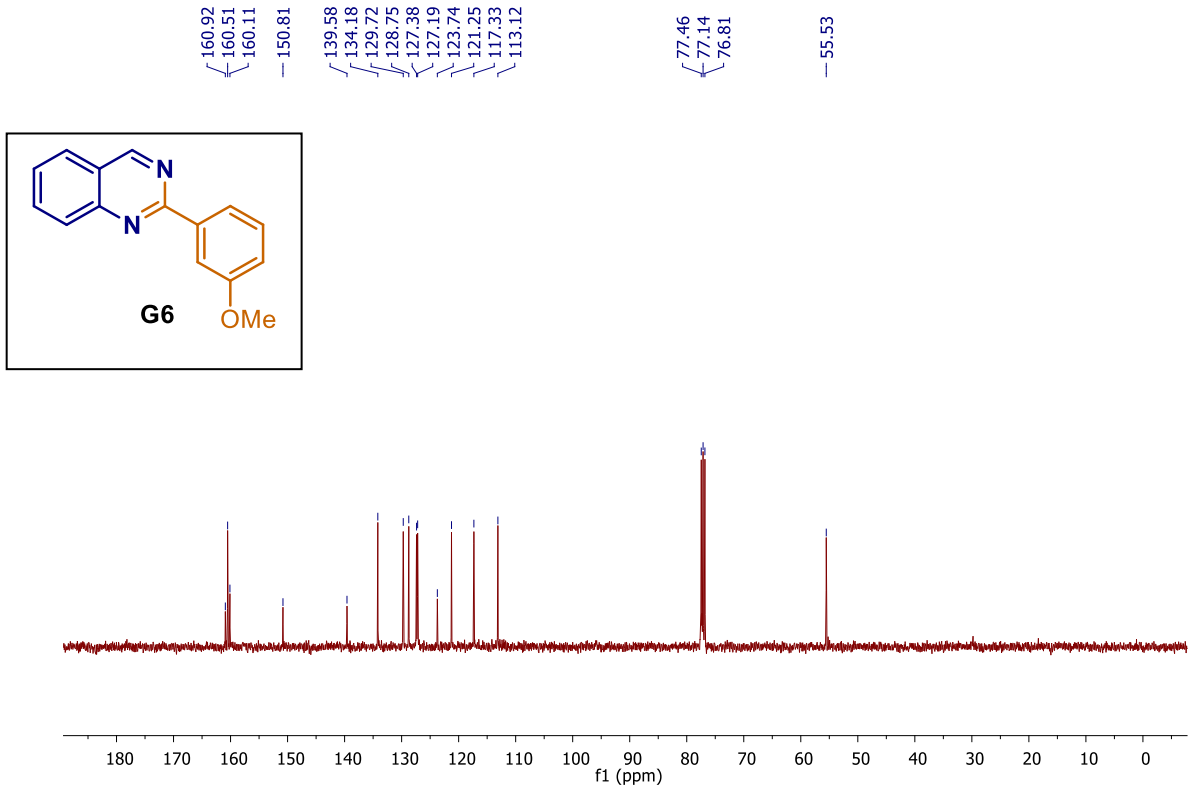
8.2104
8.1868
8.1807
8.1771
8.0846
8.0630
7.9002
7.8818
7.8607
7.8575
7.6019
7.5827
7.5641
7.4553
7.4352
7.4152
7.2442
7.0699
7.0635
7.0494
7.0429
3.9377
N
N
G6
OMe
1.00
1.06
1.01
1.06
2.11
1.14
1.21
1.08
3.03
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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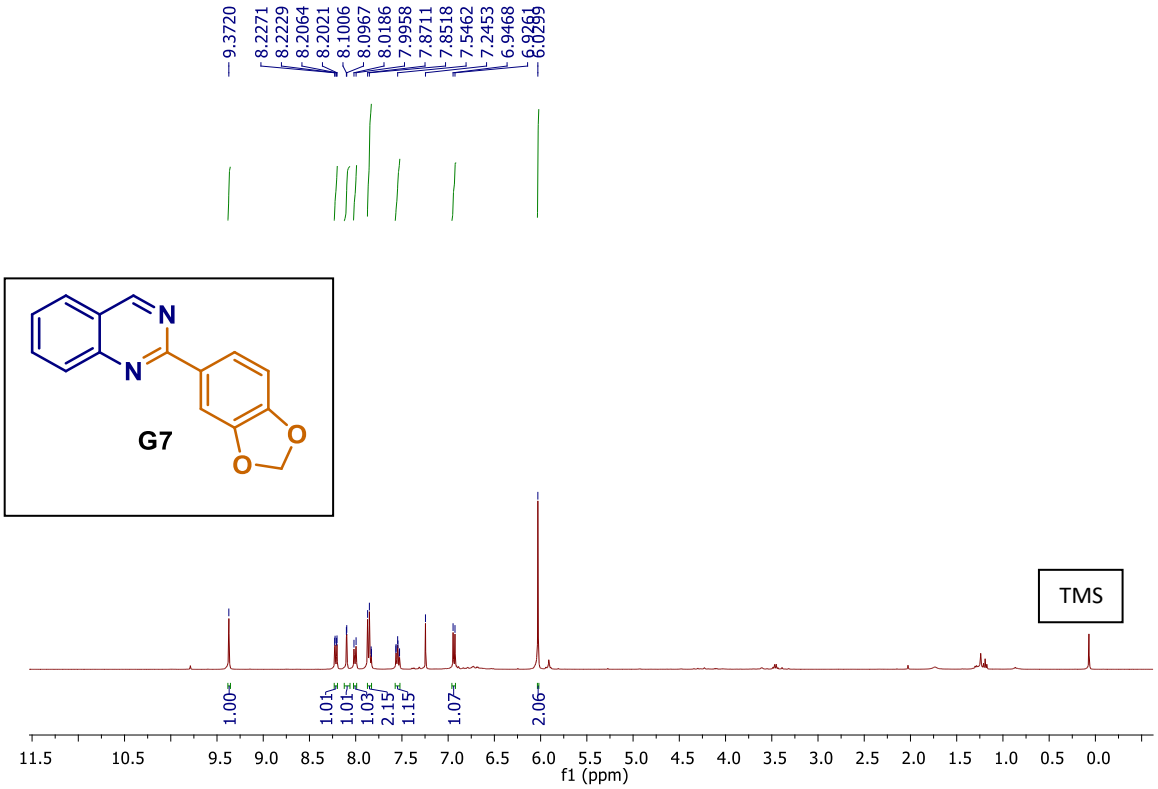
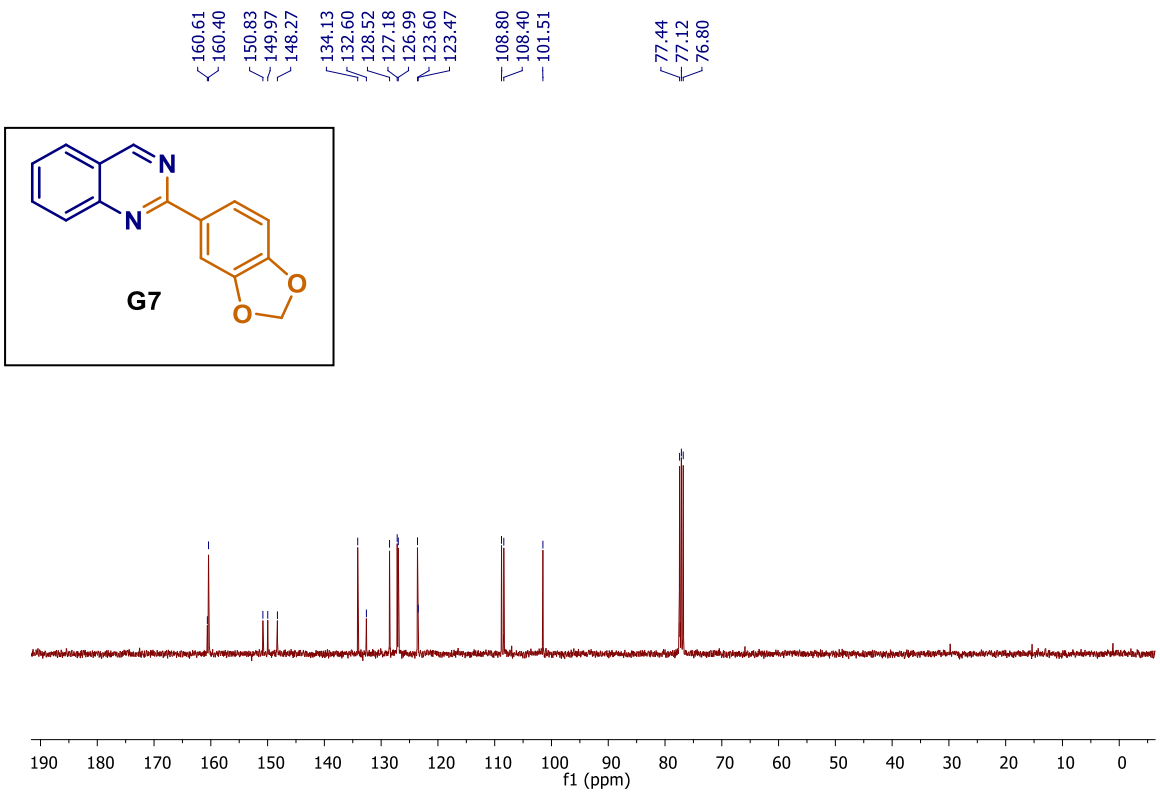
160.51
160.11
150.81
139.58
134.18
129.72
128.75
127.38
127.19
123.74
121.25
117.33
113.12
77.46
77.14
76.81
55.53
N
N
G6
OMe
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


9.3720
8.2271
8.2229
8.2064
8.2021
8.1006
8.0967
8.0186
7.9958
7.8711
7.8518
7.5462
7.2453
6.9468
6.9261
6.9259
N
N
O
O
G7
TMS
1.00
1.01
1.01
1.03
2.15
1.15
1.07
2.06
11.5
10.5
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
f1 (ppm)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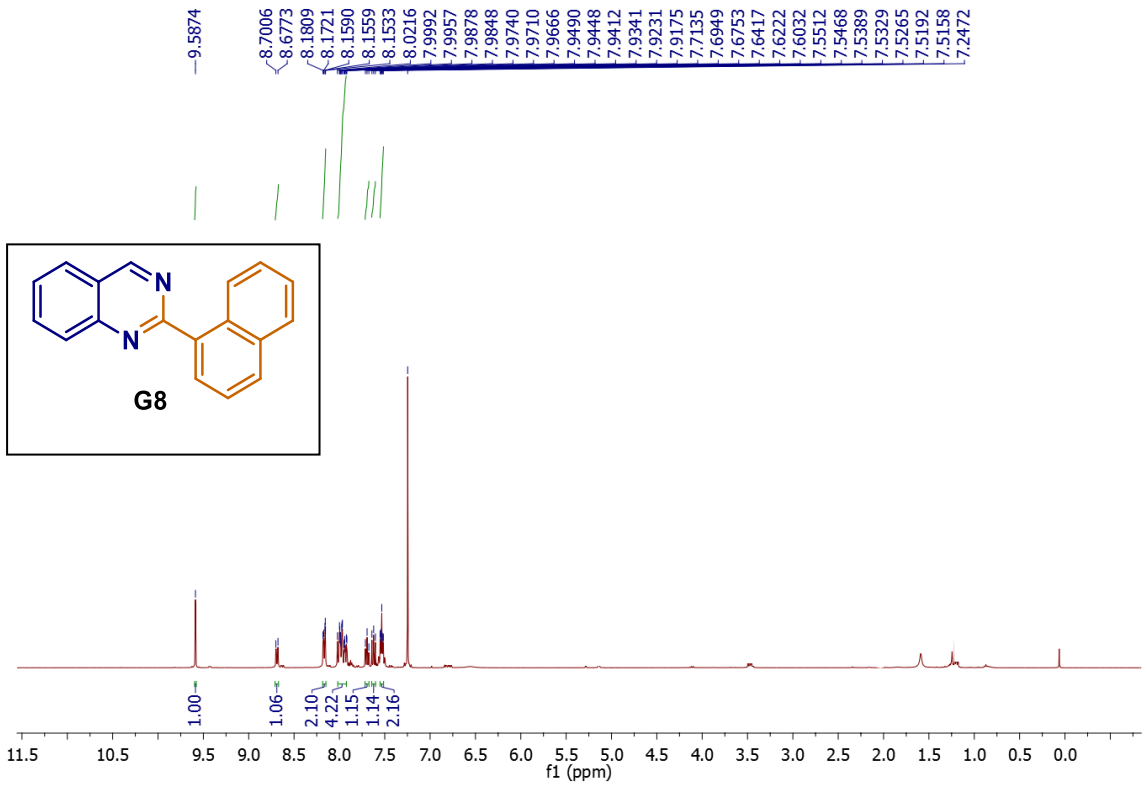
160.40
150.83
149.97
148.27
134.13
132.60
128.52
127.18
126.99
123.60
123.47
108.80
108.40
101.51
77.44
77.12
76.80
N
N
O
O
G7
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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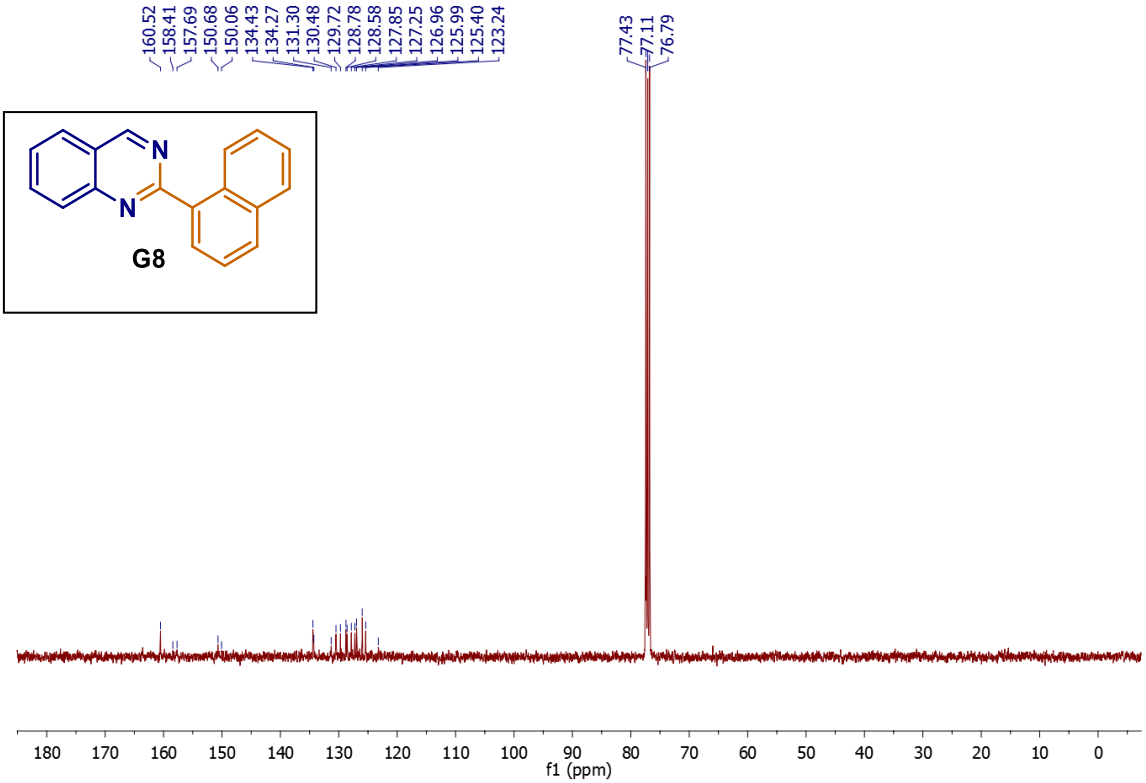
8.6773
8.1809
8.1721
8.1590
8.1559
8.1533
8.0216
7.9992
7.9957
7.9878
7.9848
7.9740
7.9710
7.9666
7.9490
7.9448
7.9412
7.9341
7.9231
7.9175
7.7135
7.6949
7.6753
7.6417
7.6222
7.6032
7.5512
7.5468
7.5389
7.5329
7.5265
7.5192
7.5158
7.2472
N
N
G8
1.00
1.06
2.10
4.22
1.15
1.14
2.16
11.5
10.5
9.5
9.0
8.5
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
f1 (ppm)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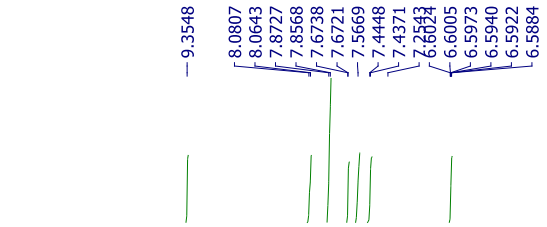
157.69
150.68
150.06
134.43
134.27
131.30
130.48
129.72
128.78
128.58
127.85
127.25
126.96
125.99
125.40
123.24
77.43
77.11
76.79
N
N
G8
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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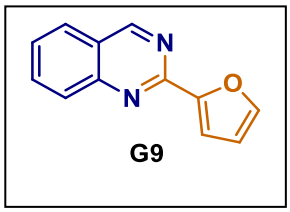
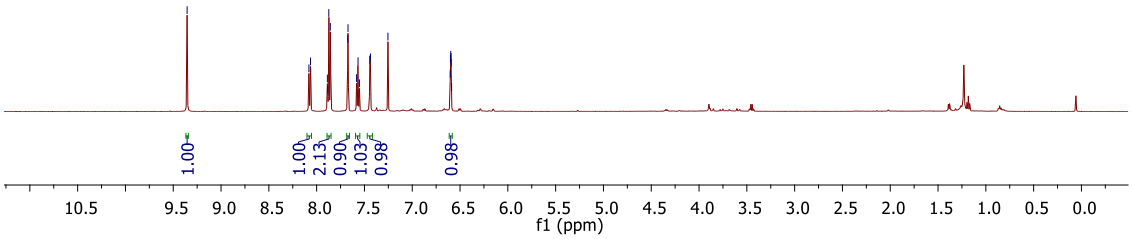
8.0643
7.8727
7.8568
7.6738
7.6721
7.5669
7.4448
7.4371
7.2543
6.6024
6.6005
6.5973
6.5940
6.5922
6.5884


N
N
O
G9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1.00
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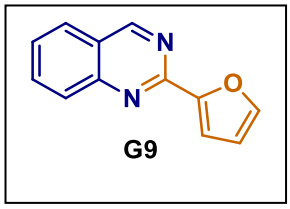
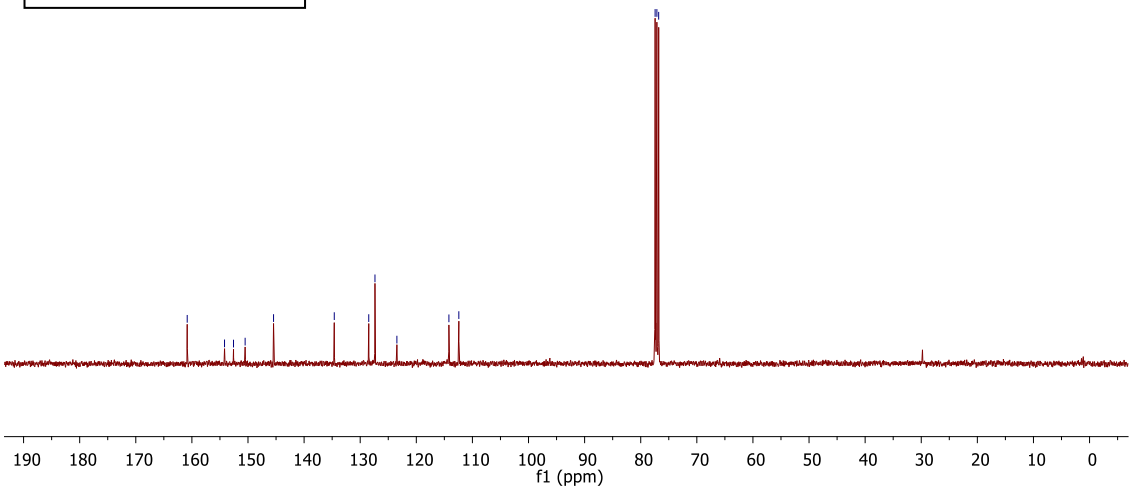
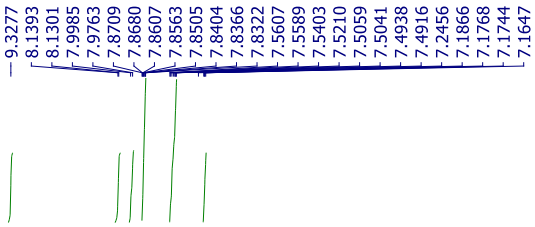
1.03
0.98
0.98
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.83
154.18
152.58
150.51
145.44
134.62
128.48
127.37
123.46
114.19
112.42
77.44
77.12
76.80


N
N
O
G9


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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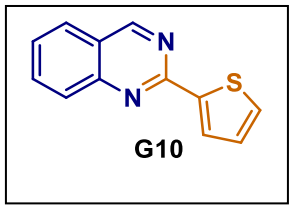
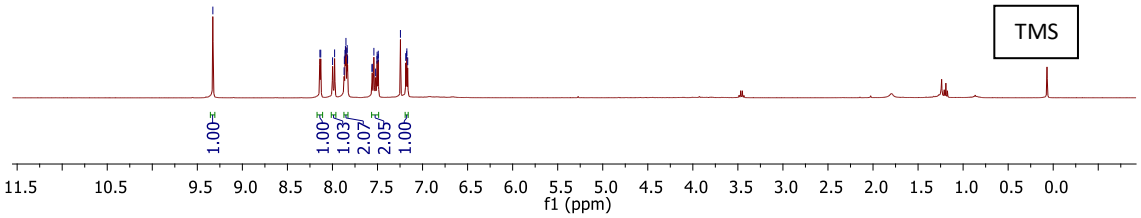
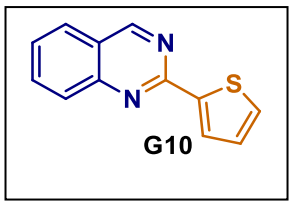
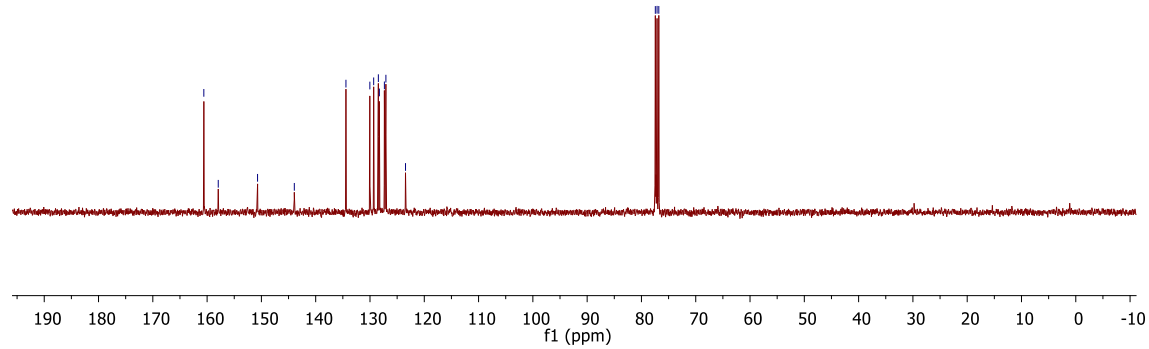
8.1393
8.1301
7.9985
7.9763
7.8709
7.8680
7.8607
7.8563
7.8505
7.8404
7.8366
7.8322
7.5607
7.5589
7.5403
7.5210
7.5059
7.5041
7.4938
7.4916
7.2456
7.1866
7.1768
7.1744
7.1647

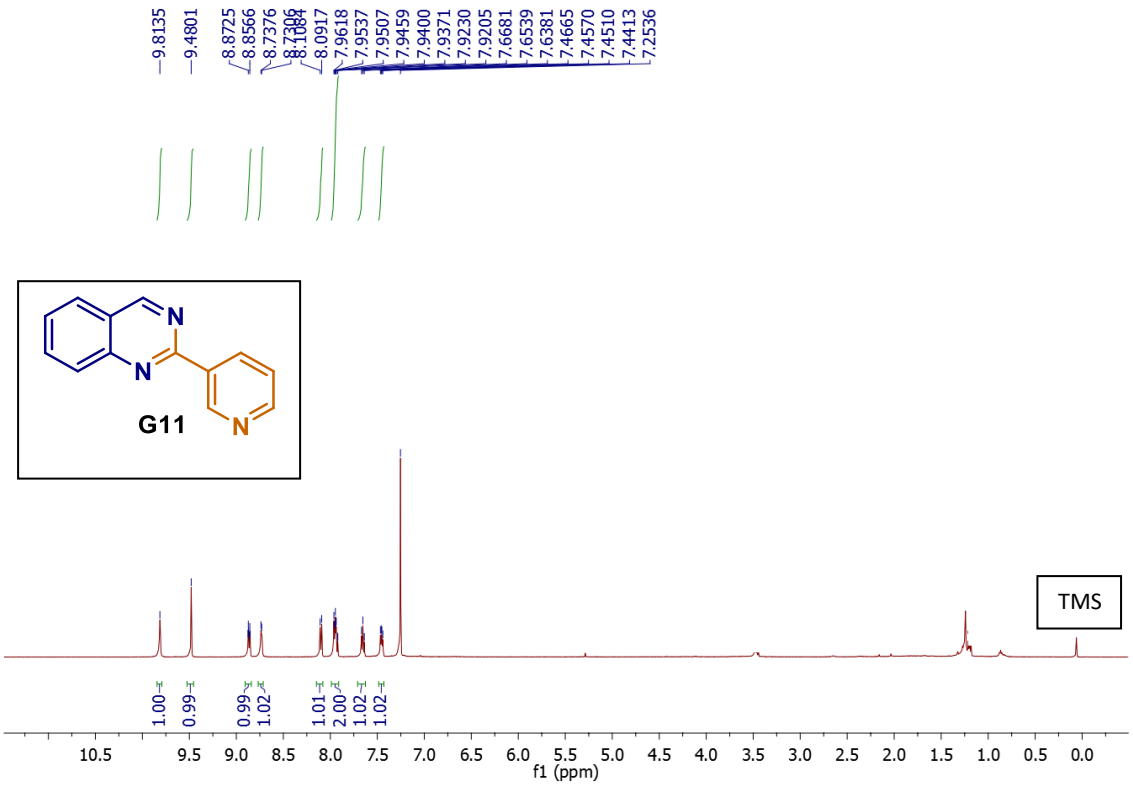

N
N
S
G10

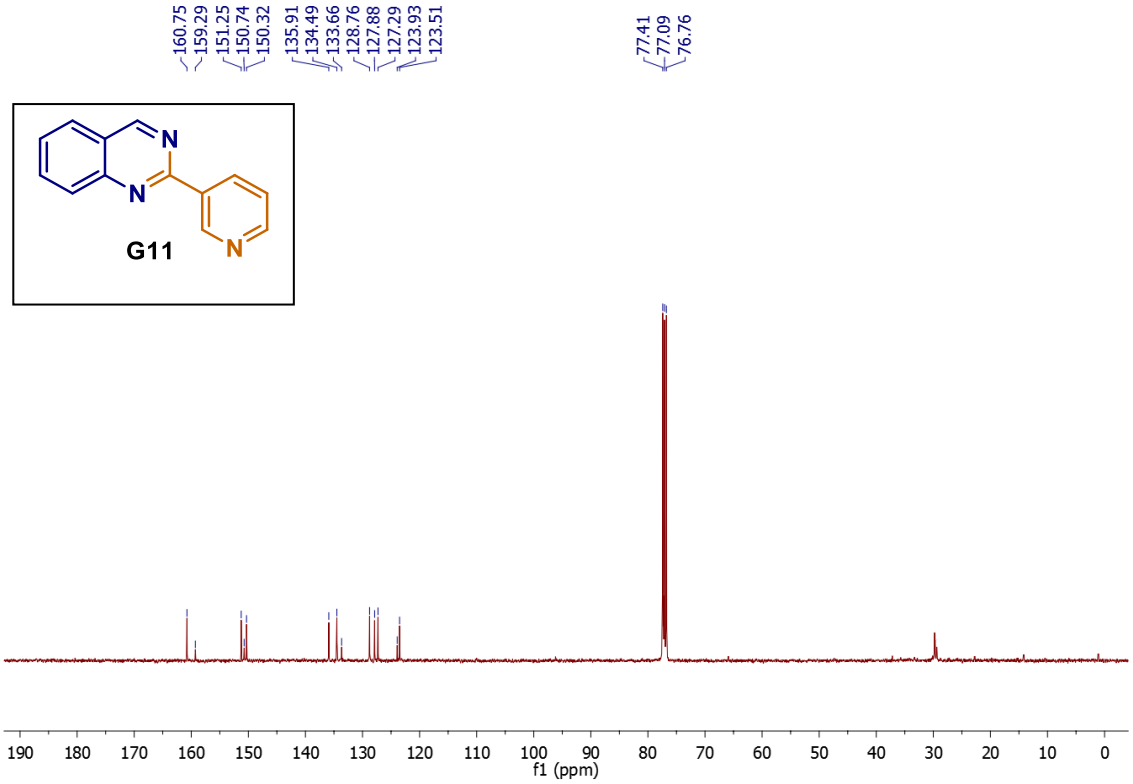

TMS
1.00
1.00
1.03
2.07
2.05
1.00
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


160.60
157.95
150.71
143.94
134.43
130.03
129.32
128.46
128.27
127.35
127.07
123.46
77.44
77.12
76.80


N
N
S
G10


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


9.8135
9.4801
8.8725
8.8566
8.7376
8.7306
8.1084
8.0917
7.9618
7.9537
7.9507
7.9459
7.9400
7.9371
7.9230
7.9205
7.6681
7.6539
7.6381
7.4665
7.4570
7.4510
7.4413
7.2536
G11
TMS
1.00
0.99
0.99
1.02
1.01
2.00
1.02
1.02
10.5
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
f1 (ppm)


160.75
159.29
151.25
150.74
150.32
135.91
134.49
133.66
128.76
127.88
127.29
123.93
123.51
77.41
77.09
76.76
G11
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)