Electronic Supplementary Material (ESI) for RSC Advances.

Metal-Free Visible-Induced C(sp^2)-C(sp^2) Coupling of Quinoxalin-2(*H*)-ones via Oxidative Cleavage of C-N Bond

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Supporting information

1. General information

All reagents were purchased from commercial sources and used without further purification. All solvents were dried in a standard manner. Reactions were monitored by TLC on silica gel plates. Column chromatography was performed over silica gel (200-300 mesh) and petroleum ether/ethyl acetate. All products were characterized by NMR. ^{1}H NMR spectra were recorded at 400 MHz and ^{13}C NMR spectra were recorded at 101 MHz (Bruker DPX) with DMSO-d_6 as solvent. Chemical shifts are reported in ppm using TMS as internal standard. HPLC were recorded on an SHIMDZU LC-20A instrument with a HP5-MS 30 m x 0.25 mm capillary apolar columns.

2. General procedure for the catalytic reactions

In a round bottom flask equipped with a stir bar was added 1a (0.5 mmol), 2a (1.0 mmol), eosin Y (10.0 mol%), K_2CO_3 (1.0 mmol). The mixture was stirred at room temperature for 15 h, blue LED (12 W) in MeOH/H_2O (1/1) = 4 mL solvent. The reaction mixture was extracted with ethyl acetate. The combined organic layer was washed with brine (10 mL), dried over Na_2SO_4. After the reaction was completed the solution of the crude product was concentrated in vacuo, and the residue was purified by column chromatography on a silica gel (petroleum ether/ethyl acetate=10/1) to afford the target product 3a as a yellow solid.

3. General procedure for the gram scale experiment

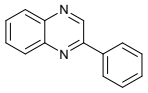
In a 100 ml round bottom flask equipped with a stir bar was added 1a (10.0 mmol), 2a (20.0 mmol), eosin Y (10.0 mol%), K_2CO_3 (20.0 mmol). The mixture was stirred at room temperature for 36 h, blue light LED (12 W) in MeOH/H_2O (1/1) = 45 mL solvent. After the reaction was completed the solution of the crude product was concentrated in vacuo, and the residue was purified by column chromatography on a silica gel (petroleum ether/ethyl acetate=10/1) to afford the target product 3a in 69% (1421.4 mg) as a yellow solid.

4. Cyclic voltammetry experiment

Cyclic voltammograms were measured using Shanghai chenhua CHI600E electrochemical workstation with electrochemical analysis software, using a conventional three-electrode cell. The working electrode was a platinum plate working electrode, the counter and reference electrodes consisted of a Pt wire and an Ag/AgCl, espectively. The platinum plate working electrode was polished with a polishing cloth before each measurement. The concentration of all tested compounds was 1 mmol L^{-1}. The scan rate was 0.1 V/s.

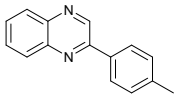
5. Characterization data

(3a) 2-phenylquinoxaline[1]



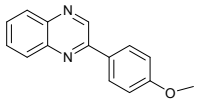
Yellow solid (89.6 mg, 87%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.55 (s, 1H), 8.35 – 8.28 (m, 2H), 8.10 (ddd, J = 8.4, 7.0, 1.9 Hz, 2H), 7.83 (td, J = 7.9, 1.7 Hz, 2H), 7.63 – 7.51 (m, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.40, 144.16, 141.87, 141.53, 136.49, 131.02, 130.85, 130.30, 129.67, 129.55, 129.30, 127.91. **MS** [EI, m/z]: 207.10 $[M+H]^+$.

(**3b**) **2-(p-tolyl)quinoxaline**[1]



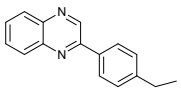
White solid (100.1 mg, 91%), ^{1}H NMR (400 MHz, DMSO) δ 9.56 (s, 1H), 8.28 – 8.21 (m, 2H), 8.16 – 8.06 (m, 2H), 7.91 – 7.78 (m, 2H), 7.45 – 7.37 (m, 2H), 2.41 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.40, 144.08, 141.91, 141.42, 140.80, 133.74, 131.03, 130.22, 130.13, 129.59, 129.30, 127.82, 21.44. **MS** [EI, m/z]: 221.10 $[M+H]^+$.

(**3c**) **2-(4-methoxyphenyl)quinoxaline**[1]



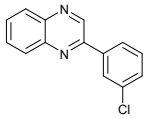
White solid (109.7 mg, 93%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.52 (s, 1H), 8.34 – 8.26 (m, 2H), 8.07 (dt, J = 8.1, 1.8 Hz, 2H), 7.81 (dddd, J = 21.1, 8.4, 6.9, 1.5 Hz, 2H), 7.15 – 7.08 (m, 2H), 3.85 (s, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.70, 151.10, 143.88, 141.90, 141.14, 130.92, 129.75, 129.44, 129.26, 128.86, 115.00, 55.83. **MS** [EI, m/z]: 237.11 $[M+H]^+$.

(**3d**) **2-(4-ethylphenyl)quinoxaline**[3]



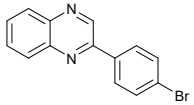
White solid (37.8 mg, 90%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.53 (s, 1H), 8.29 – 8.20 (m, 2H), 8.10 (ddd, J = 7.2, 5.0, 1.7 Hz, 2H), 7.89 – 7.76 (m, 2H), 7.45 – 7.36 (m, 2H), 2.68 (q, J = 7.6 Hz, 2H), 1.22 (t, J = 7.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.43, 146.90, 144.05, 141.94, 141.44, 134.02, 130.94, 130.05, 129.58, 129.28, 128.96, 127.90, 28.49, 15.77. **MS** [EI, m/z]: 257.12 $[M+Na]^+$.

(**3e**) **2-(3-chlorophenyl)quinoxaline**[1]



White solid (91.2 mg, 76%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.60 (s, 1H), 8.37 (td, J = 1.6, 0.9 Hz, 1H), 8.32 – 8.28 (m, 1H), 8.17 – 8.10 (m, 2H), 7.88 (ddt, J = 8.0, 6.9, 5.1 Hz, 2H), 7.64 – 7.61 (m, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.93, 144.15, 141.78, 141.73, 138.57, 134.53, 131.46, 131.26, 130.79, 130.64, 129.77, 129.32, 127.50, 126.53. **MS** [EI, m/z]: 263.70 $[M+Na]^+$

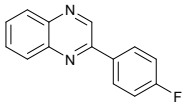
(**3f**) **2-(4-bromophenyl)quinoxaline**[2]



White solid (99.4 mg, 70%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.58 (s, 1H), 8.29 (d, J = 2.0 Hz,

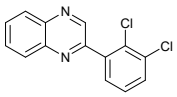
1H), 8.28 (d, *J* = 2.0 Hz, 1H), 8.15 – 8.10 (m, 2H), 7.87 (ddd, *J* = 7.4, 6.3, 1.8 Hz, 2H), 7.80 (d, *J* = 2.0 Hz, 1H), 7.79 (d, *J* = 1.9 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 150.37, 143.97, 141.77, 141.63, 135.66, 132.56, 131.23, 130.61, 129.90, 129.68, 129.34, 124.79. **MS** [EI, m/z]: 306.98 $[M+Na]^+$

(**3g**) **2-(4-fluorophenyl)quinoxaline**[2]



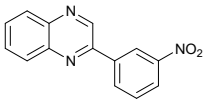
White solid (71.68 mg, 64%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.20 (s, 1H), 8.15 – 8.08 (m, 1H), 8.04 (ddd, *J* = 7.9, 6.0, 1.8 Hz, 1H), 7.68 (ddd, *J* = 9.6, 7.8, 1.6 Hz, 1H), 7.21 – 7.11 (m, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.28 (d, *J* = 251.0 Hz), 150.77, 142.88, 142.21, 141.42, 132.91 (d, *J* = 3.1 Hz), 130.46, 129.65, 129.57, 129.54, 129.48, 129.11, 116.36, 116.15. **MS** [EI, m/z]: 225.08 $[M+H]^+$

(**3h**) **2-(2, 3-dichlorophenyl)quinoxaline** [4]



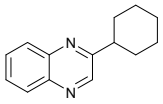
Yellow solid (94.89 mg, 69%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.21 (s, 1H), 8.27 (d, *J* = 2.1 Hz, 1H), 8.12 – 8.00 (m, 2H), 7.96 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.78 – 7.65 (m, 2H), 7.56 (d, *J* = 8.4 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 148.25, 141.49, 141.10, 140.83, 135.59, 133.62, 132.63, 130.07, 129.66, 129.13, 128.62, 128.33, 128.18, 125.38. **MS** [EI, m/z]: 275.10 $[M+H]^+$.

(**3i**) **2-(3-nitrophenyl)quinoxaline**[1]



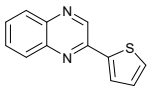
White solid (65.26 mg, 52%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.72 (s, 1H), 9.16 – 9.05 (m, 1H), 8.80 (d, *J* = 7.9 Hz, 1H), 8.41 (dd, *J* = 8.2, 2.4 Hz, 1H), 8.26 – 8.20 (m, 1H), 8.16 (d, *J* = 2.3 Hz, 1H), 7.97 – 7.86 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 149.26, 149.03, 144.20, 141.97, 141.68, 138.14, 134.17, 131.47, 131.25, 131.15, 129.85, 129.39, 125.31, 122.35. **MS** [EI, m/z]: 252.07 $[M+H]^+$.

(**3j**) **2-cyclohexylquinoxaline**[5]



White solid (78.4 mg, 74%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.90 (s, 1H), 8.10 – 7.96 (m, 2H), 7.84 – 7.71 (m, 2H), 2.96 (tt, *J* = 11.8, 3.4 Hz, 1H), 1.93 (dtt, *J* = 10.7, 3.4, 1.6 Hz, 2H), 1.86 – 1.77 (m, 2H), 1.74 – 1.65 (m, 1H), 1.61 (td, *J* = 12.4, 3.2 Hz, 2H), 1.40 (qt, *J* = 12.6, 3.3 Hz, 2H), 1.32 – 1.19 (m, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 161.41, 146.12, 141.86, 141.29, 130.43, 129.51, 129.27, 129.15, 44.15, 32.09, 26.29, 25.92. **MS** [EI, m/z]: 213.14 $[M+H]^+$

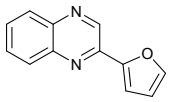
(**3k**) **2-(thiophen-2-yl)quinoxaline**[1]



White solid (67.8 mg, 64%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.57 (s, 1H), 8.24 (d, *J* = 1.1 Hz, 1H), 8.11 – 7.98 (m, 2H), 7.88 – 7.76 (m, 3H), 7.30 (dd, *J* = 5.0, 3.7 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 147.66, 143.25, 142.22, 141.68, 141.24, 131.50, 131.26, 129.92, 129.41 (d, *J* = 3.8 Hz),

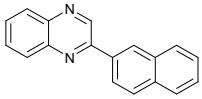
129.17, 129.00. **MS** [EI, m/z]: 213.04 $[M+H]^+$

(**3l**) **2-(furan-2-yl)quinoxaline**[1]



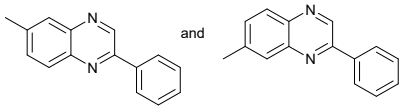
White solid (67.6 mg, 69%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.33 (s, 1H), 8.02 (dd, J = 8.3, 1.7 Hz, 3H), 7.78 (dddd, J = 21.6, 8.3, 6.9, 1.6 Hz, 2H), 7.54 (dd, J = 3.5, 0.8 Hz, 1H), 6.77 (dd, J = 3.5, 1.7 Hz, 1H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.39, 146.57, 143.89, 142.88, 141.74, 141.05, 131.16, 129.96, 129.36, 129.21, 113.26. **MS** [EI, m/z]: 197.97 $[M+H]^+$

(**3m**) **2-(naphthalen-2-yl)quinoxaline**[1]



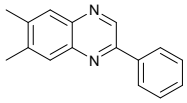
White solid (88.3 mg, 69%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.76 (s, 1H), 8.97 (d, J = 1.8 Hz, 1H), 8.49 (dd, J = 8.7, 1.8 Hz, 1H), 8.19 (dd, J = 8.3, 1.6 Hz, 1H), 8.14 (t, J = 8.9 Hz, 3H), 8.01 (dd, J = 6.0, 3.4 Hz, 1H), 7.92 – 7.83 (m, 2H), 7.63 (dt, J = 6.3, 3.5 Hz, 2H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.32, 144.46, 141.95, 141.55, 134.22, 133.85, 133.45, 131.15, 130.40, 129.70, 129.37, 129.23, 128.17, 128.01 (d, J = 3.4 Hz), 127.29, 124.78. **MS** [EI, m/z]: 257.10 $[M+H]^+$

(**3n**) **6-methyl-2-phenylquinoxaline** and **7-methyl-2-phenylquinoxaline**[1]



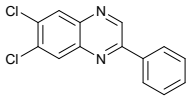
White solid (100.1 mg, 91%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.47 (d, J = 9.8 Hz, 1H), 8.28 (dt, J = 8.0, 2.3 Hz, 2H), 7.67–7.51 (m, 4H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 151.25, 150.55, 143.92, 143.13, 141.92 (d, J = 1.3 Hz), 141.57, 141.15, 140.47, 140.30, 140.02, 136.63, 133.12, 132.41, 130.73, 130.62, 129.52, 129.20, 128.82, 128.39, 128.05, 127.81, 127.71, 21.73 (d, J = 3.5 Hz). **MS** [EI, m/z]: 221.10 $[M+H]^+$, 243.10$[M+Na]^+$.

(**3o**) **6,7-dimethyl-2-phenylquinoxaline**[2]



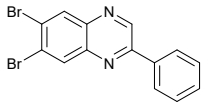
White solid (102.96 mg, 88%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.41 (s, 1H), 8.27 (d, J = 7.3 Hz, 2H), 7.83 (d, J = 8.6 Hz, 2H), 7.55 (dd, J = 10.0, 7.1 Hz, 3H), 2.43 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 150.43, 143.01 (d, J = 9.4 Hz), 141.33 (d, J = 11.1 Hz), 140.77, 140.55 (d, J = 10.8 Hz), 136.79, 130.55, 129.53 (d, J = 4.1 Hz), 128.54, 128.16, 127.66, 20.27 (d, J = 4.6 Hz). **MS** [EI, m/z]: 235.12 $[M+H]^+$.

(**3p**) **6,7-dichloro-2-phenylquinoxaline**[1]



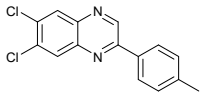
White solid (83.5 mg, 61%), ^{1}H NMR (400 MHz, DMSO-d_6+$CDCl_3$) δ 9.25 (d, J = 3.8 Hz, 1H), 8.19 (d, J = 3.8 Hz, 1H), 8.15 (d, J = 3.9 Hz, 1H), 8.12 (ddd, J = 7.7, 4.0, 2.0 Hz, 2H), 7.52 (dtd, J = 7.4, 4.9, 2.6 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6+$CDCl_3$) δ 152.55, 144.23, 141.01, 140.18, 135.86, 134.79, 133.87, 130.76, 130.12, 129.72, 129.23, 127.52. **MS** [EI, m/z]: 275.01 $[M+H]^+$.

(**3q**) **6,7-dibromo-2-phenylquinoxaline**[1]



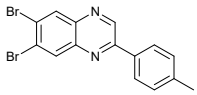
White solid (93.86 mg, 52%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.32 (s, 1H), 8.46 (s, 1H), 8.41 (s, 1H), 8.21 – 8.15 (m, 2H), 7.61 – 7.54 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 152.66, 144.37, 141.55, 140.75, 135.95, 133.62, 133.19, 130.82, 129.29, 127.59, 126.99, 125.99. **MS** [EI, m/z]: 364.90 $[M+H]^+$.

(**3r**) **6,7-dichloro-2-(p-tolyl)quinoxaline** [2], [7]



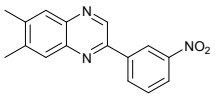
Yellow solid (97.15 mg, 67%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (d, J = 1.2 Hz, 1H), 8.14 (d, J = 1.5 Hz, 1H), 8.10 (d, J = 1.4 Hz, 1H), 7.99 (d, J = 1.5 Hz, 1H), 7.97 (s, 1H), 7.29 (s, 1H), 7.27 (s, 1H), 2.37 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.52, 143.13, 140.21, 140.06, 139.05, 133.74, 132.63, 132.11, 129.04, 128.97, 128.68, 126.40, 20.45. **MS** [EI, m/z]: 290.02 $[M+H]^+$.

(**3s**) **6,7-dibromo-2-(p-tolyl)quinoxaline**[2], [7]



White solid (107.98 mg, 57%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.32 (s, 1H), 8.28 (s, 1H), 7.97 (d, J = 1.9 Hz, 1H), 7.96 (d, J = 1.9 Hz, 1H), 7.27 (s, 1H), 7.25 (s, 1H), 2.36 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.51, 143.21, 140.51, 140.23, 139.54, 132.46, 132.08, 128.96, 126.39, 125.77, 124.57, 20.47. **MS** [EI, m/z]: 378.90 $[M+H]^+$.

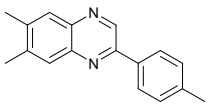
(**3t**) **6,7-dimethyl-2-(3-nitrophenyl)quinoxaline** [2], [8]



White solid (81.20 mg, 58%), ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.18 (s, 1H), 8.98 (t, J = 2.0 Hz, 1H), 8.43 (dt, J = 7.9, 1.4 Hz, 1H), 8.26 (ddd, J = 8.2, 2.3, 1.1 Hz, 1H), 7.84 (s, 1H), 7.81 (s, 1H), 7.65 (t, J = 8.0 Hz, 1H), 2.45 (d, J = 1.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.93, 147.19, 140.63, 140.41, 140.32, 140.13, 139.85, 137.75, 131.84, 129.04, 127.66, 127.06, 123.29, 121.22, 19.43 (d, J = 2.1 Hz).

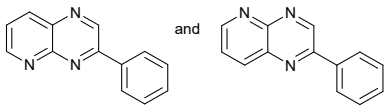
MS [EI, m/z]: 279.99 $[M+H]^+$.

(**3u**) **6,7-dimethyl-2-(p-tolyl)quinoxaline** [2], [8]



White solid (103.38 mg, 83%),^{1}H NMR (400 MHz, $CDCl_3$) δ 9.07 (s, 1H), 8.04 (d, J = 2.1 Hz, 1H), 8.02 (d, J = 2.1 Hz, 1H), 7.75 (s, 1H), 7.72 (s, 1H), 6.97 (d, J = 2.1 Hz, 1H), 6.95 (d, J = 2.1 Hz, 1H), 3.78 (s, 3H), 2.38 (t, J = 1.2 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 161.20, 150.59, 142.04, 141.19, 140.66, 140.11, 139.57, 129.62, 128.75, 128.45, 128.09, 114.50, 55.41, 20.34 (d, J = 7.1 Hz). **MS** [EI, m/z]: 249.13 $[M+H]^+$.

(**3v**) **3-phenylpyrido[2,3-b]pyrazine** and **2-phenylpyrido[2,3-b]pyrazine**[6]



White solid (69.3 mg, 67%), ^{1}H NMR (400 MHz, DMSO-d_6) δ 9.69 (d, J = 26.8 Hz, 1H), 9.14 (ddd, J = 15.6, 4.2, 1.9 Hz, 1H), 8.52 (ddd, J = 8.3, 4.3, 1.9 Hz, 1H), 8.40 – 8.25 (m, 2H), 7.91 – 7.77 (m, 1H), 7.58 (dddd, J = 10.8, 7.8, 5.3, 3.4 Hz, 3H). ^{13}C NMR (101 MHz, DMSO-d_6) δ 155.09, 154.14, 154.05, 152.28, 150.47, 150.32, 146.96, 145.20, 138.72, 138.36, 137.19, 136.82, 135.99, 135.81, 131.42, 131.19, 129.63, 129.59, 128.31, 128.09, 126.61, 125.79. **MS** [EI, m/z]: 208.08 $[M+H]^+$.

6. References

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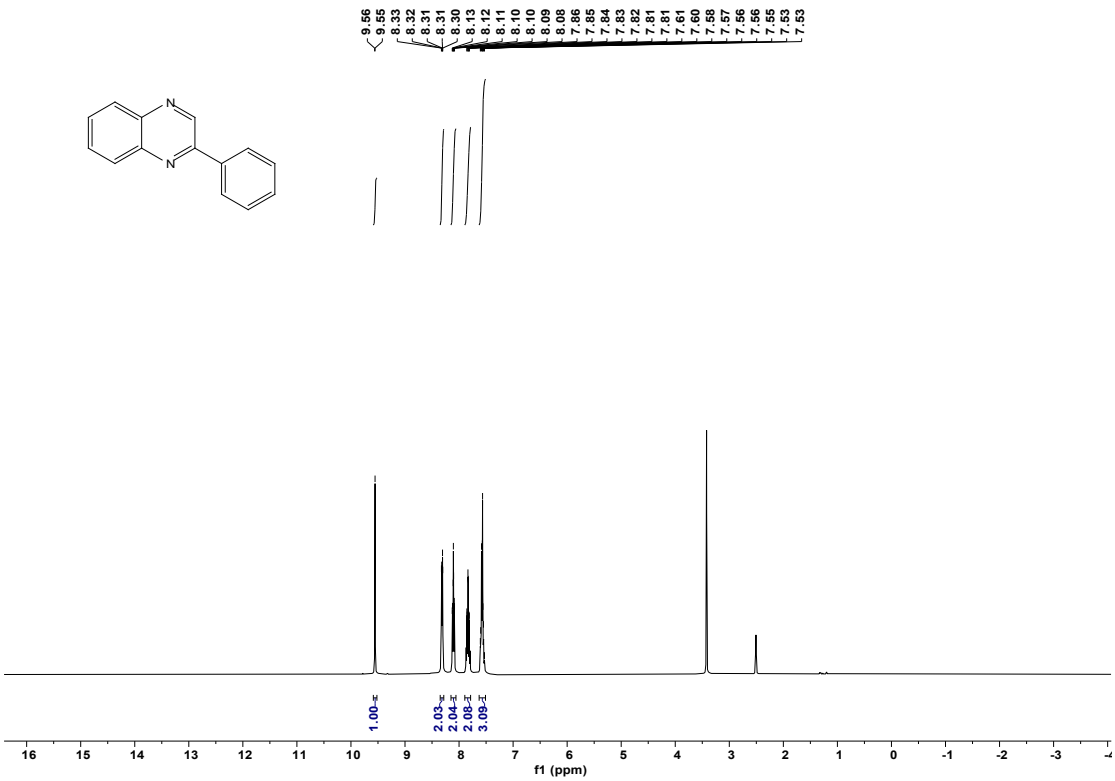
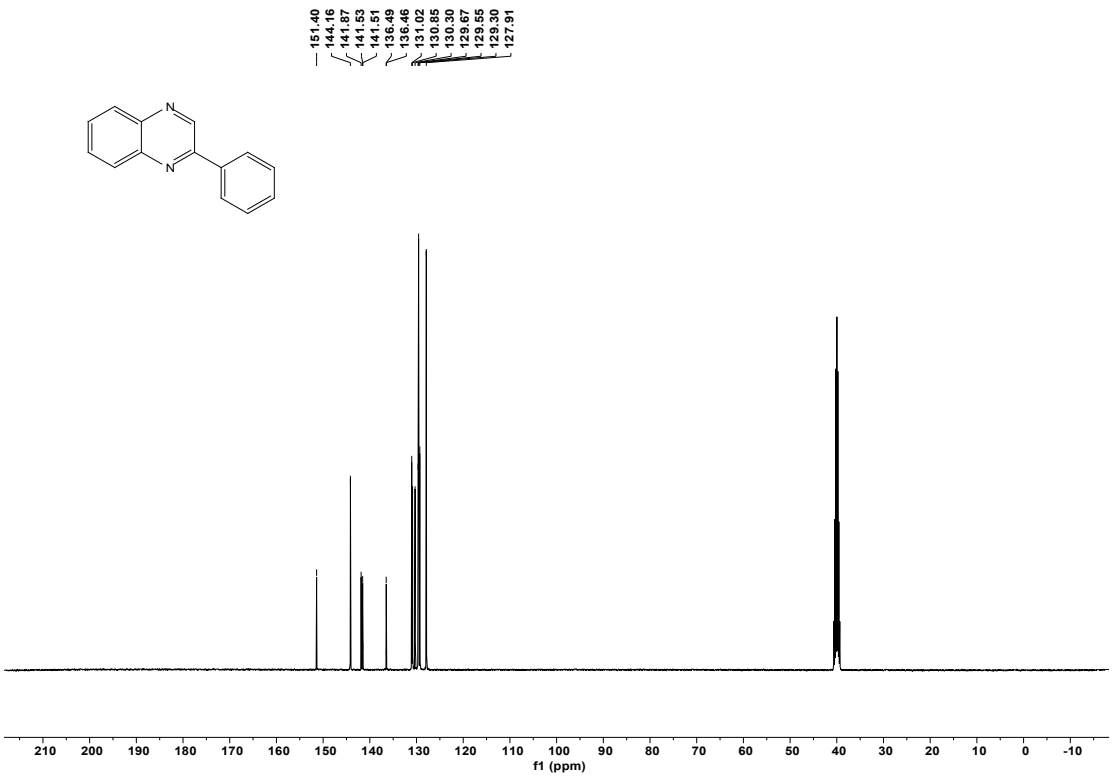
8. X.-T. Wang, J.-L. Song, M. Zhong, H.-J. Kang, H. X., T. Che, B. Shu, D. Peng, L. Zhang, S.-S. Zhang, Eur. J. Org. Chem., 2020, 2020, 3635-3639.

7. ^{1}H NMR and ^{13}C NMR spectra for the products

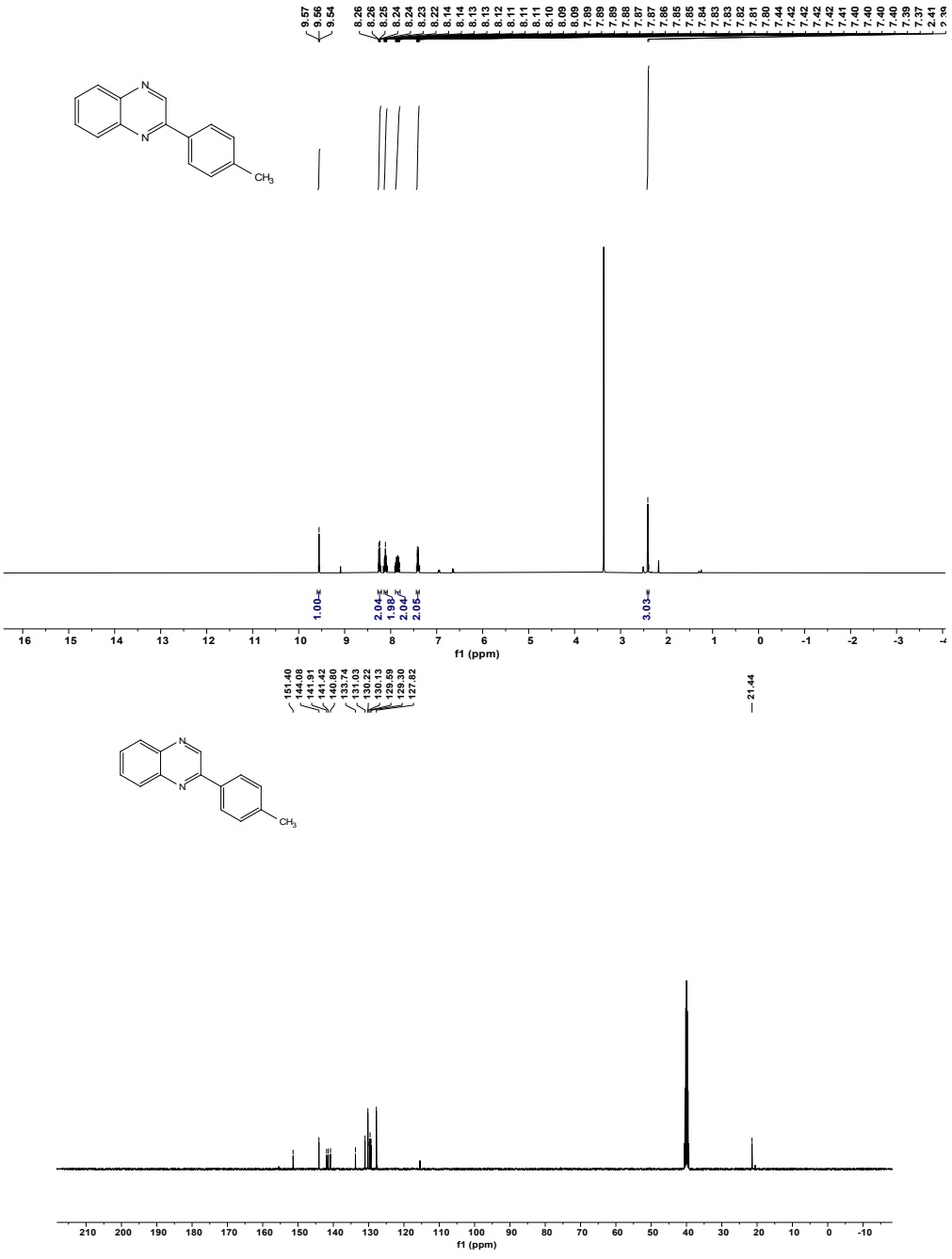
3a



z



3b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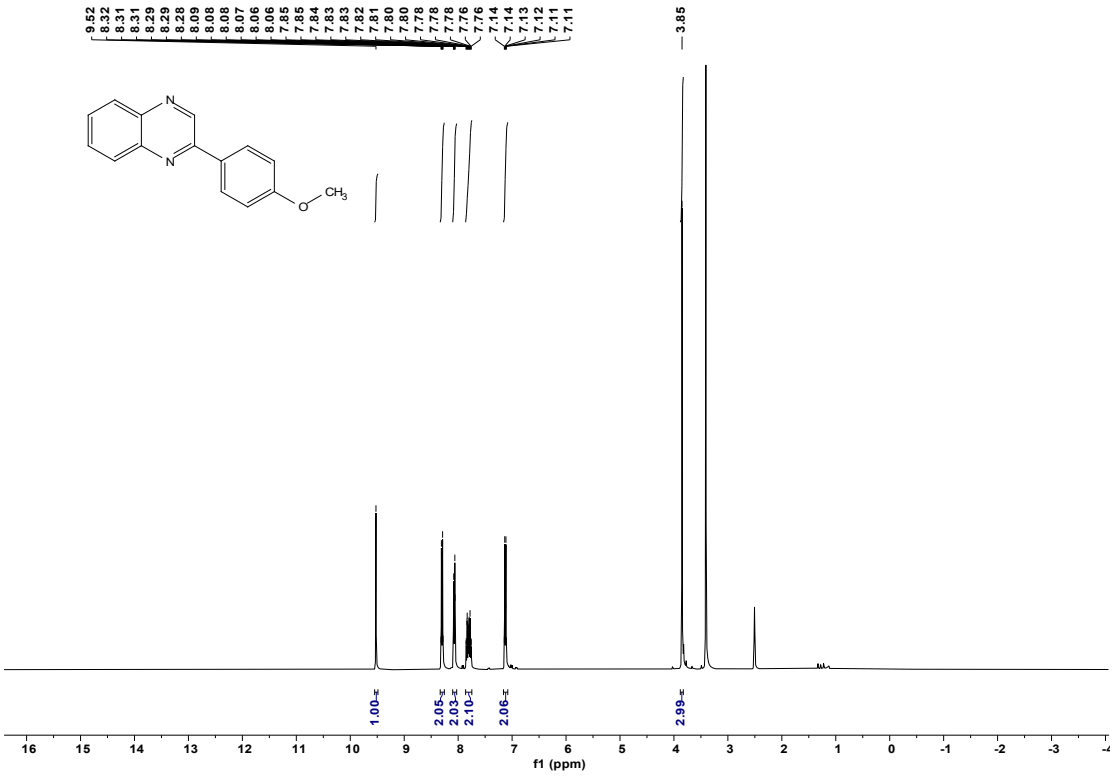
8.14
8.14
8.13
8.13
8.12
8.11
8.11
8.11
8.10
8.09
8.09
7.89
7.89
7.88
7.87
7.87
7.86
7.85
7.84
7.83
7.82
7.81
7.80
7.44
7.42
7.42
7.42
7.41
7.40
7.40
7.40
7.40
7.39
7.37
2.41
N
N
CH3
1.00
2.04
1.98
2.04
2.05
3.03
f1 (ppm)
151.40
144.08
141.91
141.42
140.60
133.74
131.03
130.22
130.13
129.89
129.30
127.82
21.44
N
N
CH3
f1 (ppm)

3c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7.84
7.83
7.83
7.82
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7.78
7.78
7.76
7.76
7.14
7.14
7.13
7.12
7.11
7.11
3.85
N
N
O
CH3
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2.05
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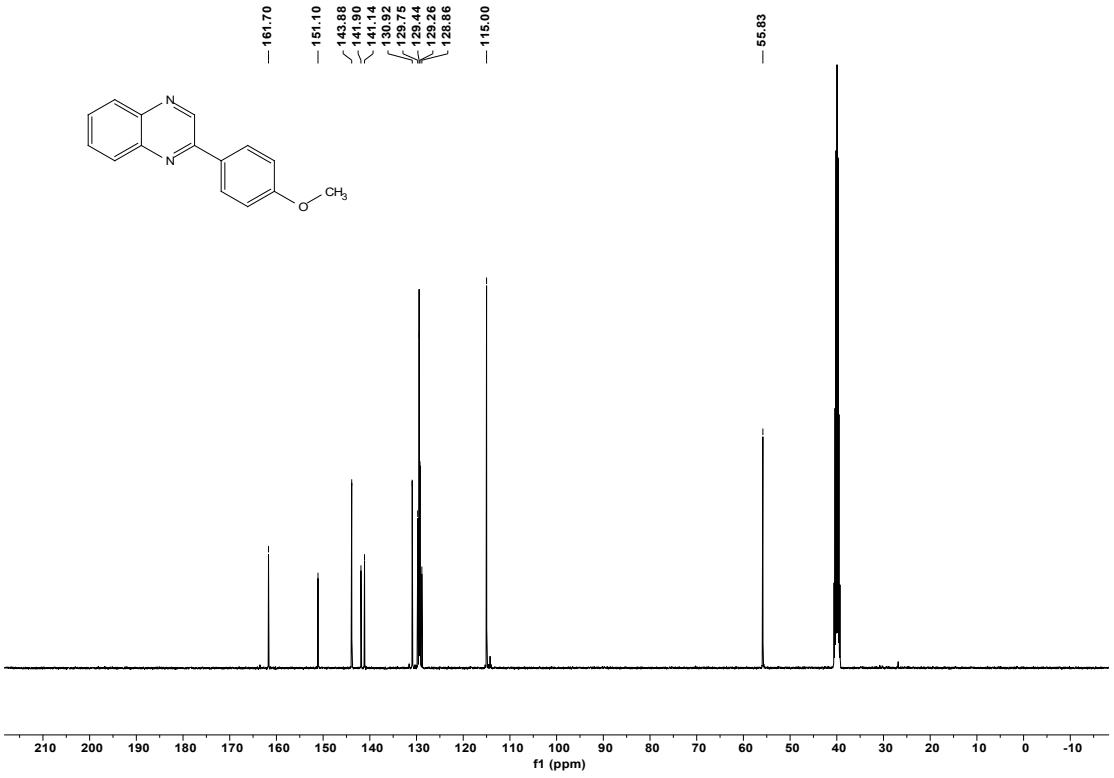
2.10
2.06
2.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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129.44
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128.86
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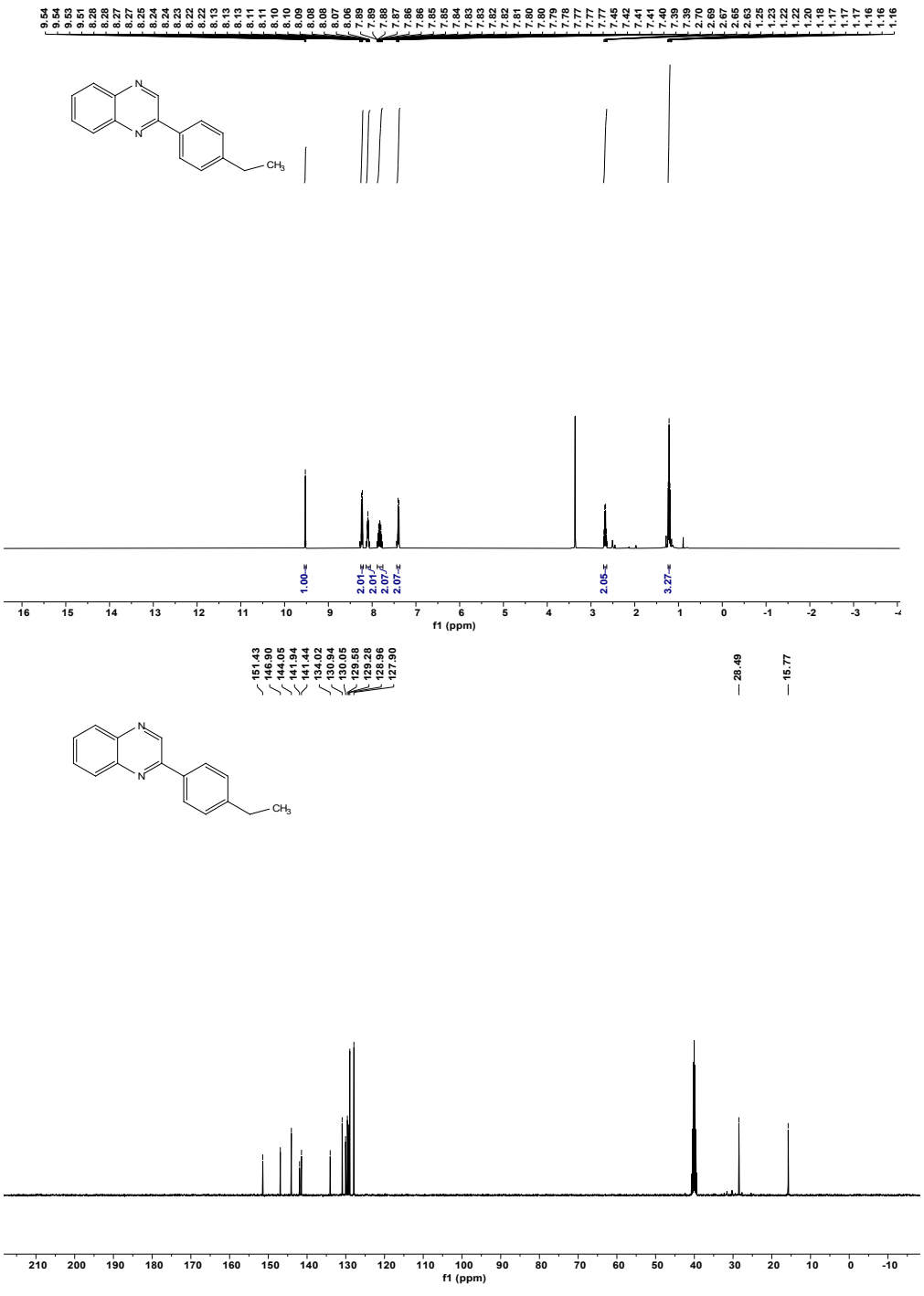
N
O
CH3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3d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8.23
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8.22
8.13
8.13
8.13
8.11
8.11
8.10
8.10
8.09
8.08
8.08
8.07
8.06
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7.40
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1.16
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1.16
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2.01
2.07
2.07
2.05
3.27
f1 (ppm)
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146.90
144.05
141.94
141.44
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128.96
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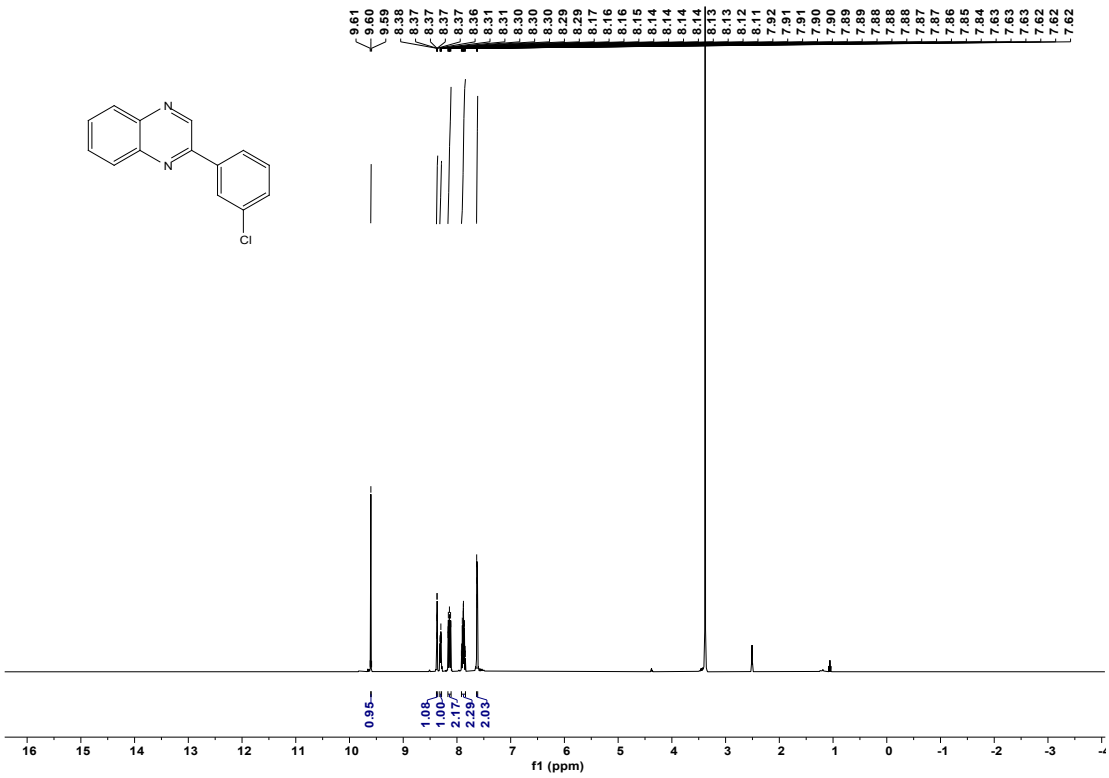
CH3
f1 (ppm)

3e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8.30
8.29
8.29
8.17
8.16
8.16
8.15
8.14
8.14
8.14
8.14
8.13
8.13
8.12
8.11
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7.87
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7.86
7.85
7.84
7.63
7.63
7.62
7.62
7.62
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Cl
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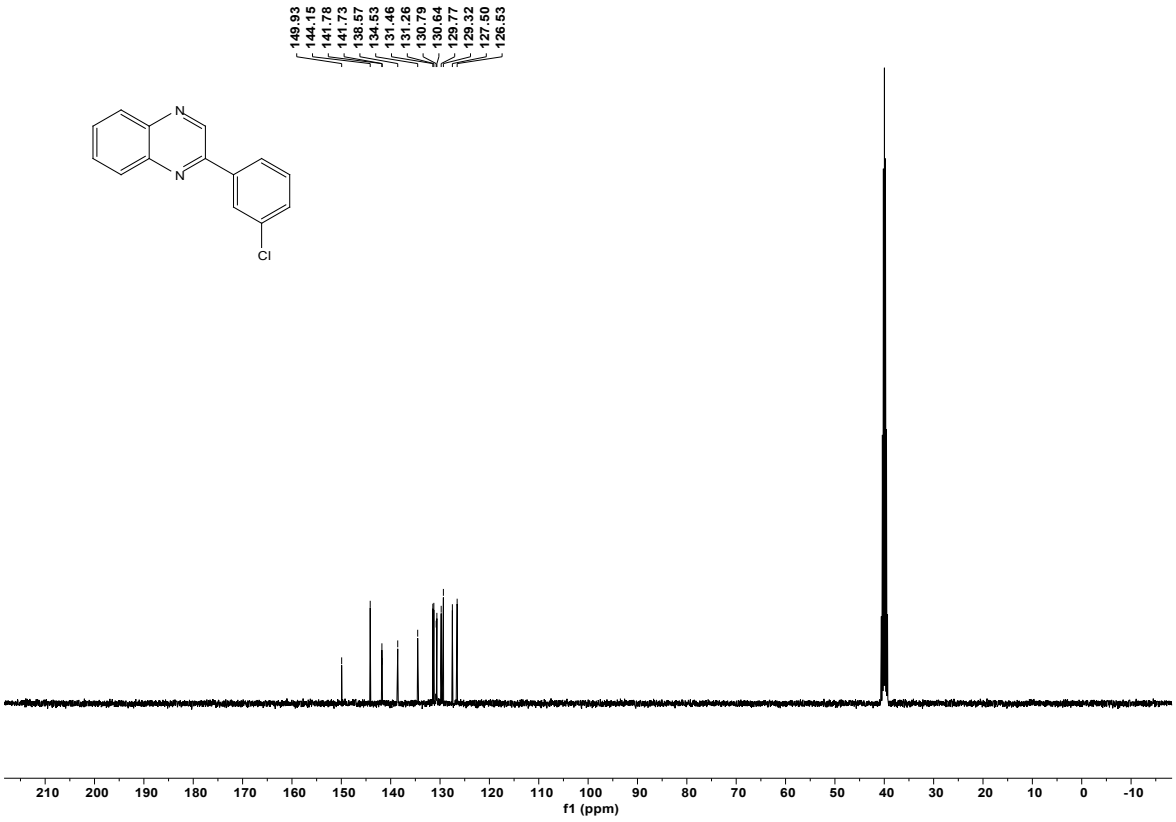
f1 (ppm)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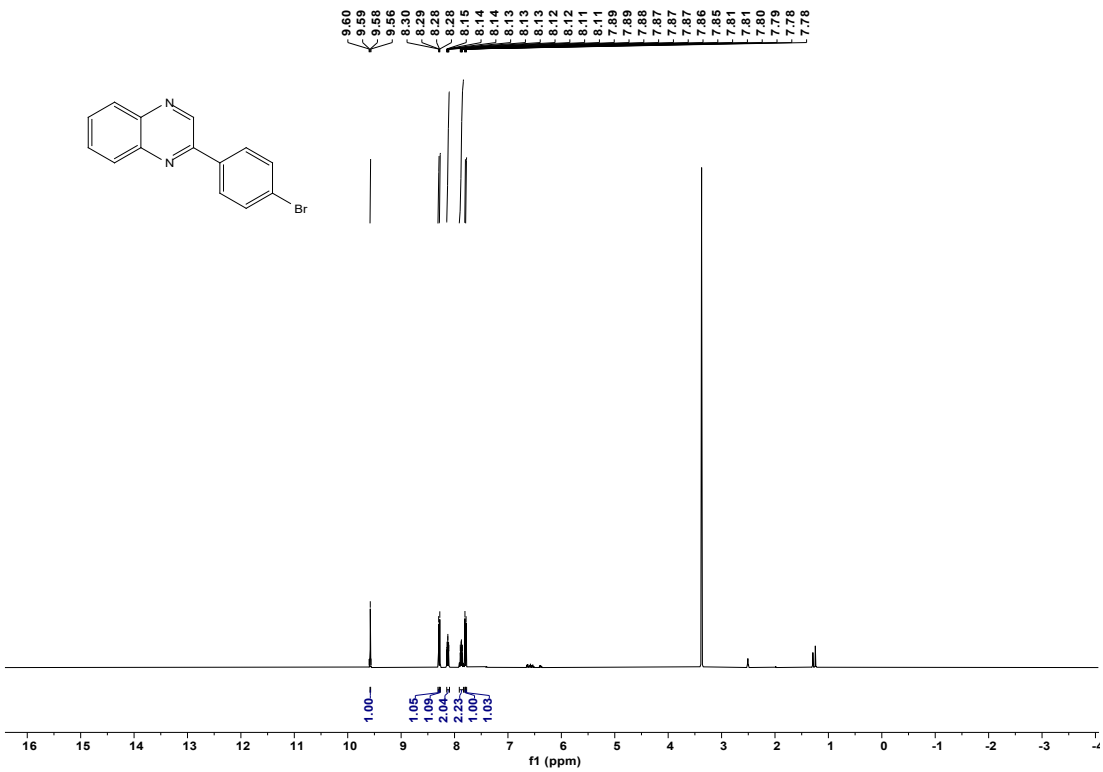
N
Cl
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3f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8.13
8.13
8.12
8.12
8.12
8.11
8.11
7.89
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7.88
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7.87
7.87
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7.85
7.81
7.81
7.80
7.79
7.78
7.78
N
N
Br
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2.23
1.00
1.03
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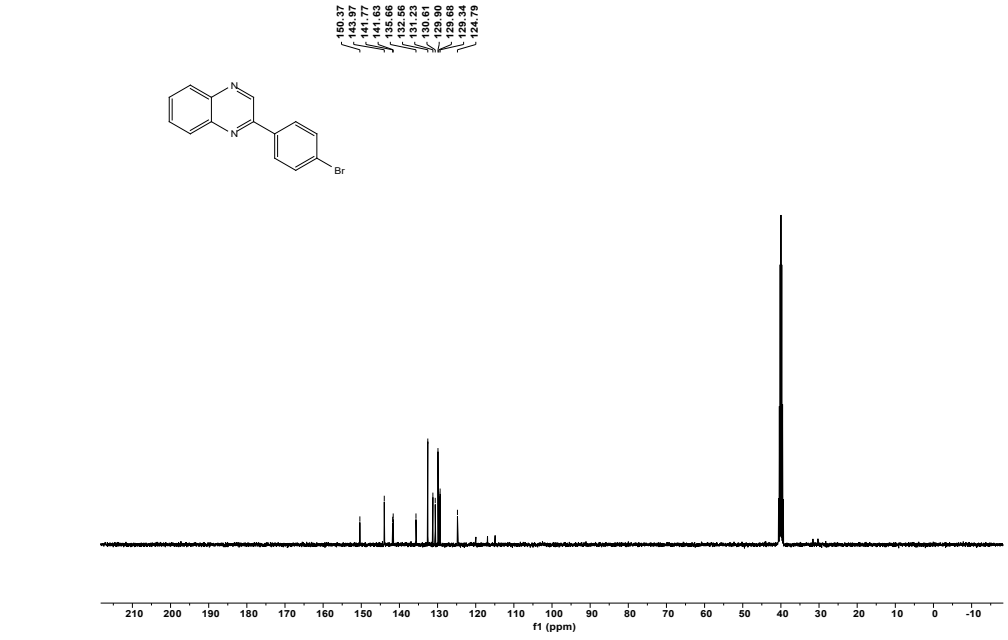
f1 (ppm)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130.61
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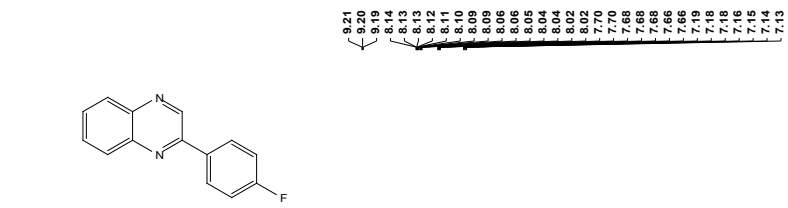
N
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3g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7.68
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7.13
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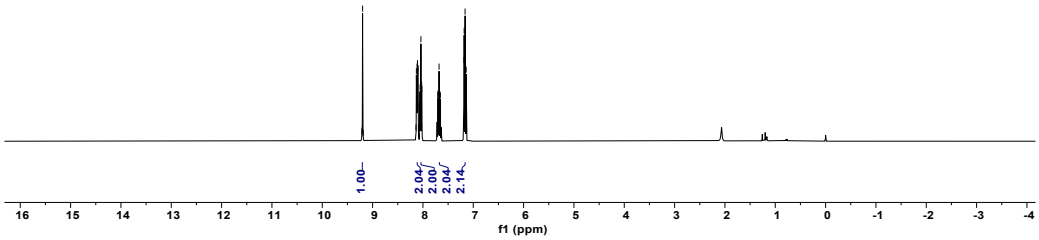
N
F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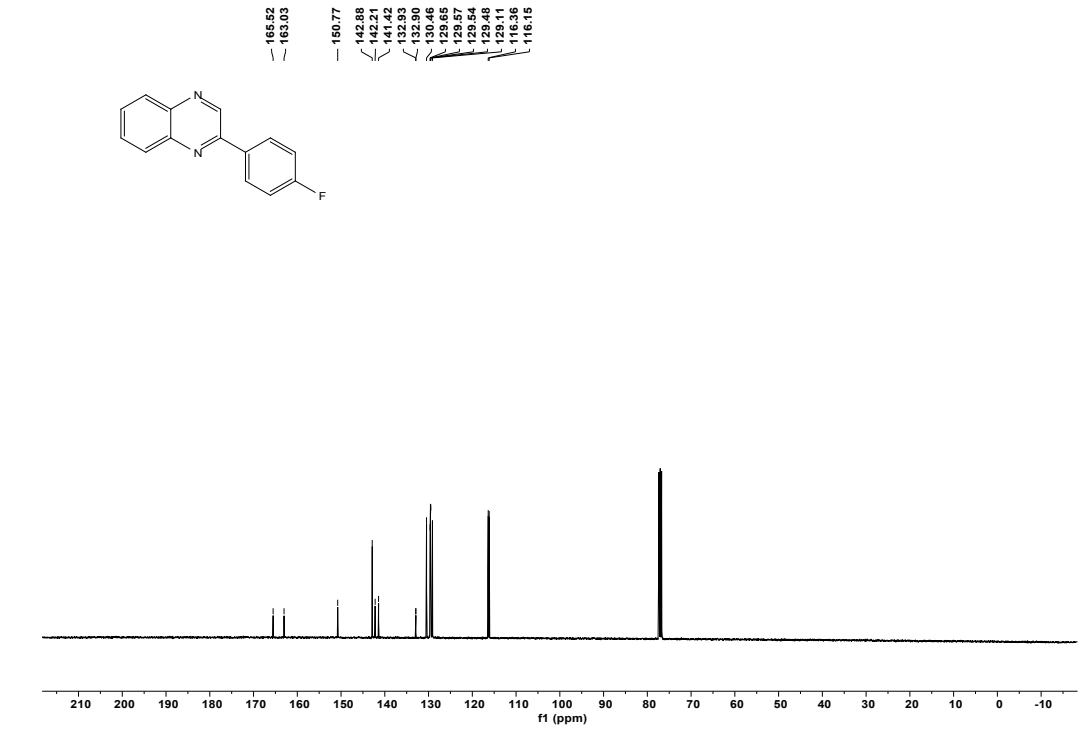
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N
F
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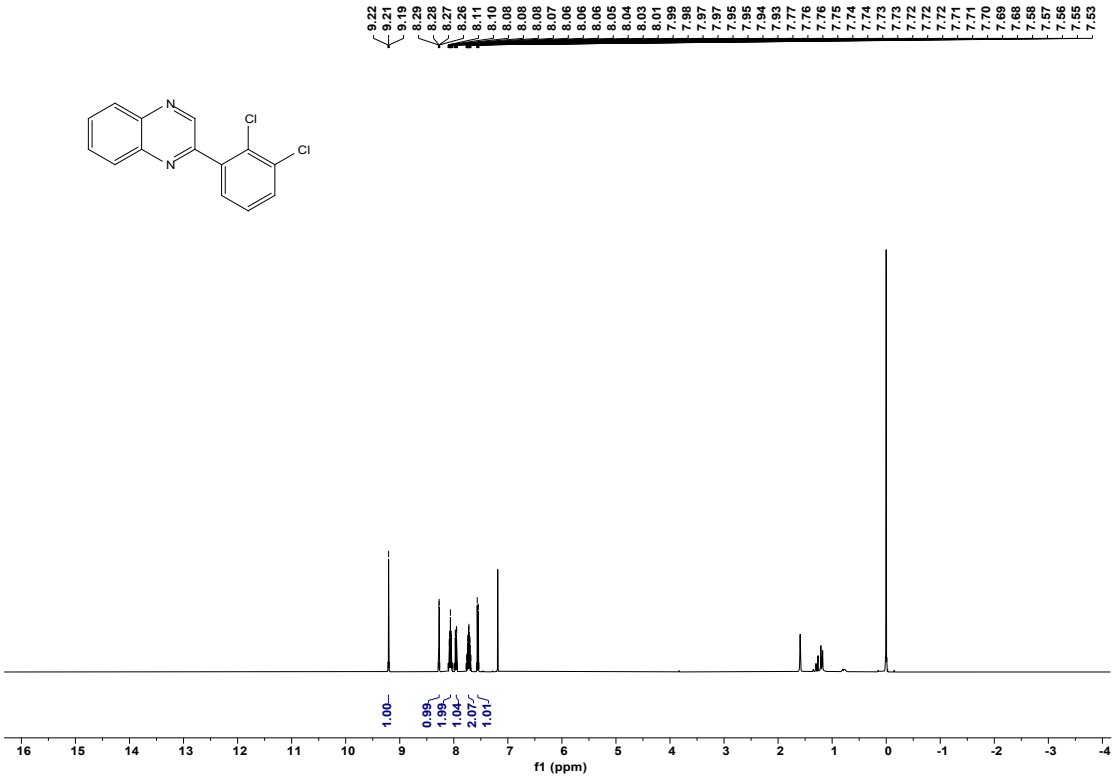
f1 (ppm)

3h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7.56
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Cl
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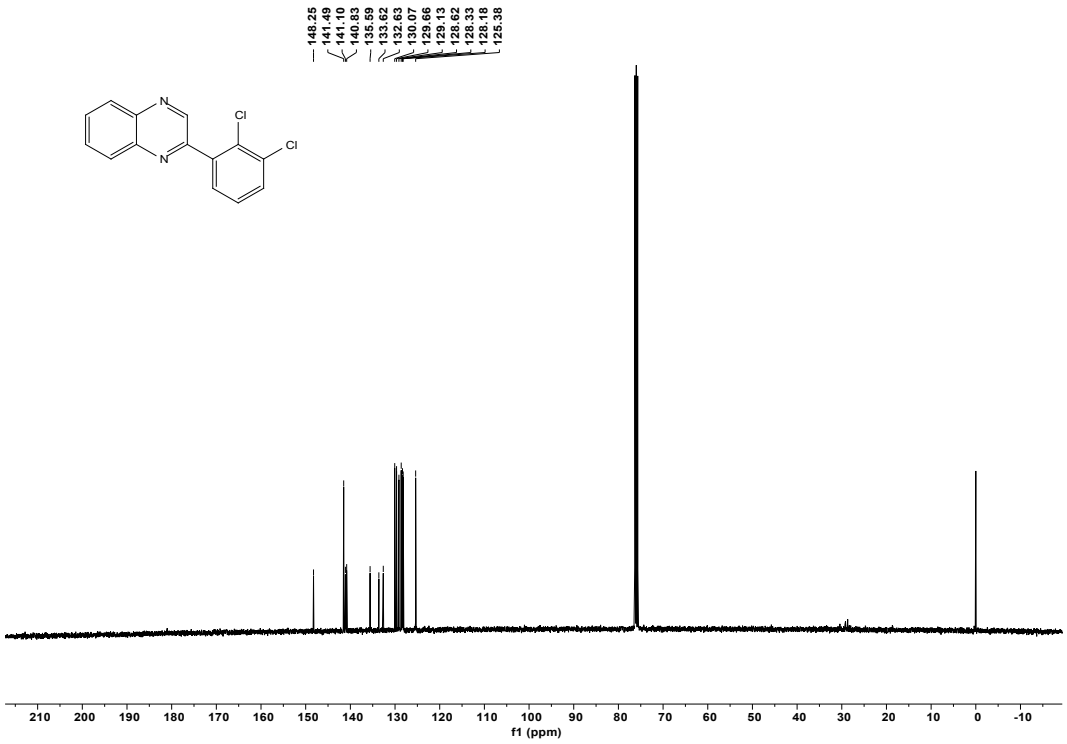
f1 (ppm)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Cl
Cl
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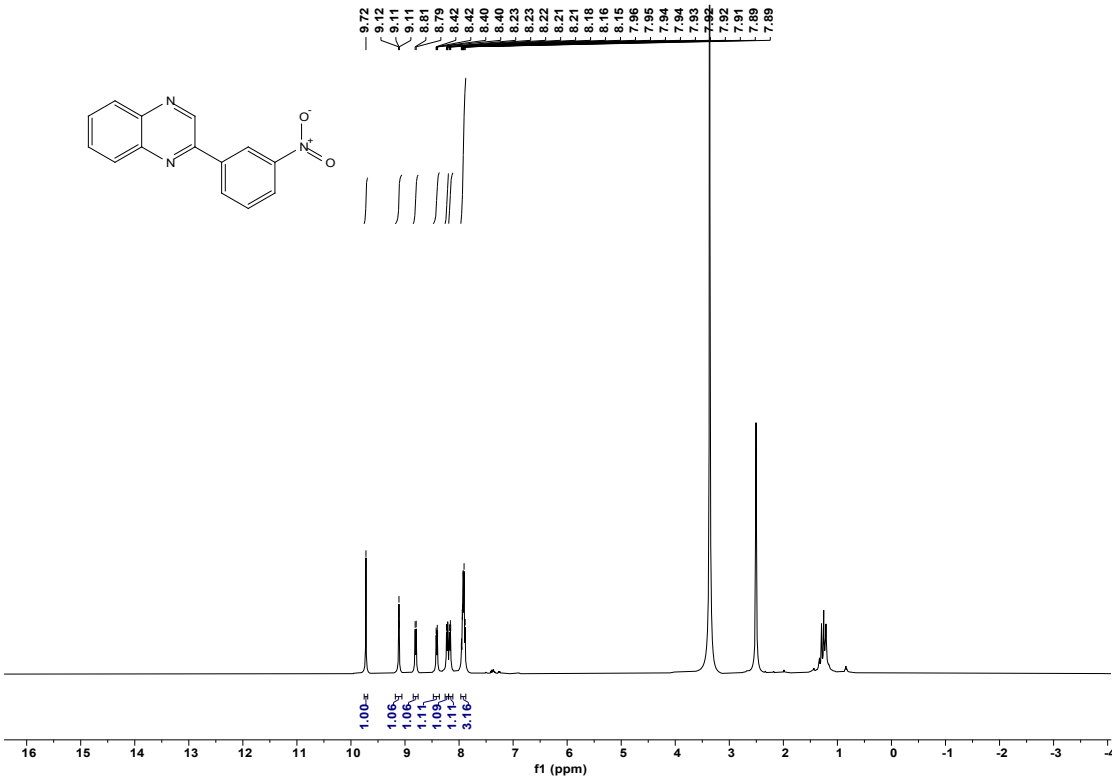
f1 (ppm)

3i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8.21
8.21
8.18
8.16
8.15
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7.93
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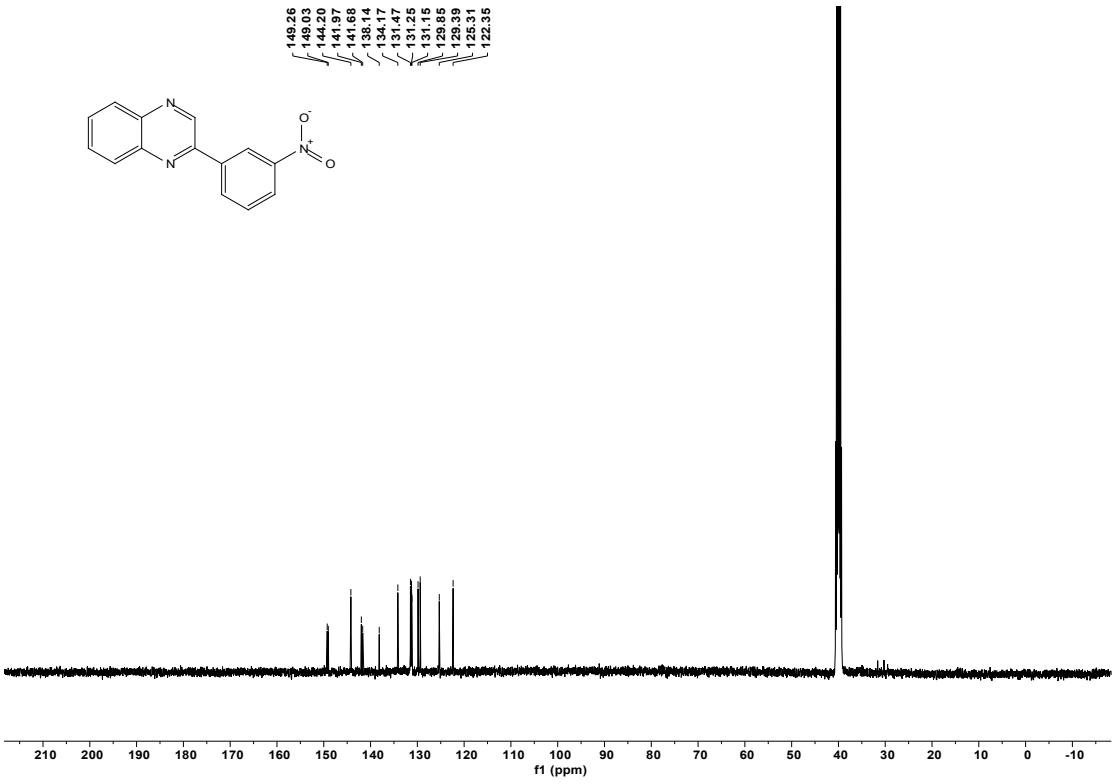
3.16
f1 (ppm)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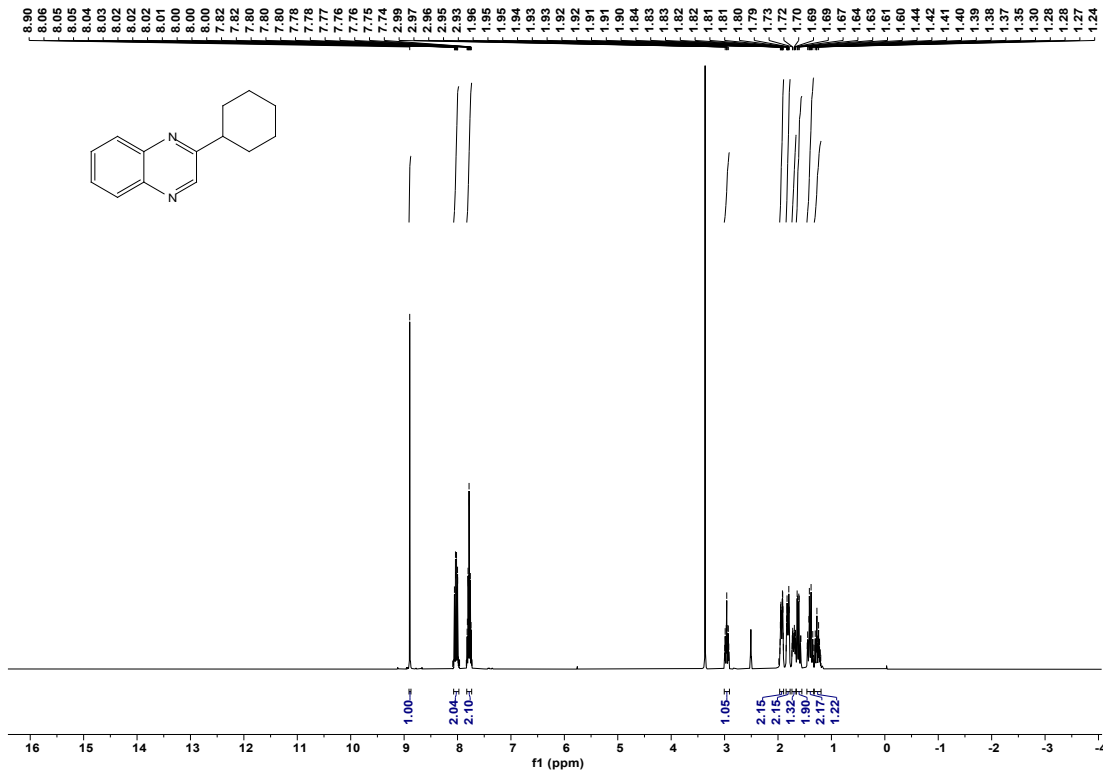
f1 (ppm)

3j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N
N
1.00
2.04
2.10
1.05
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1.90
2.17
1.22
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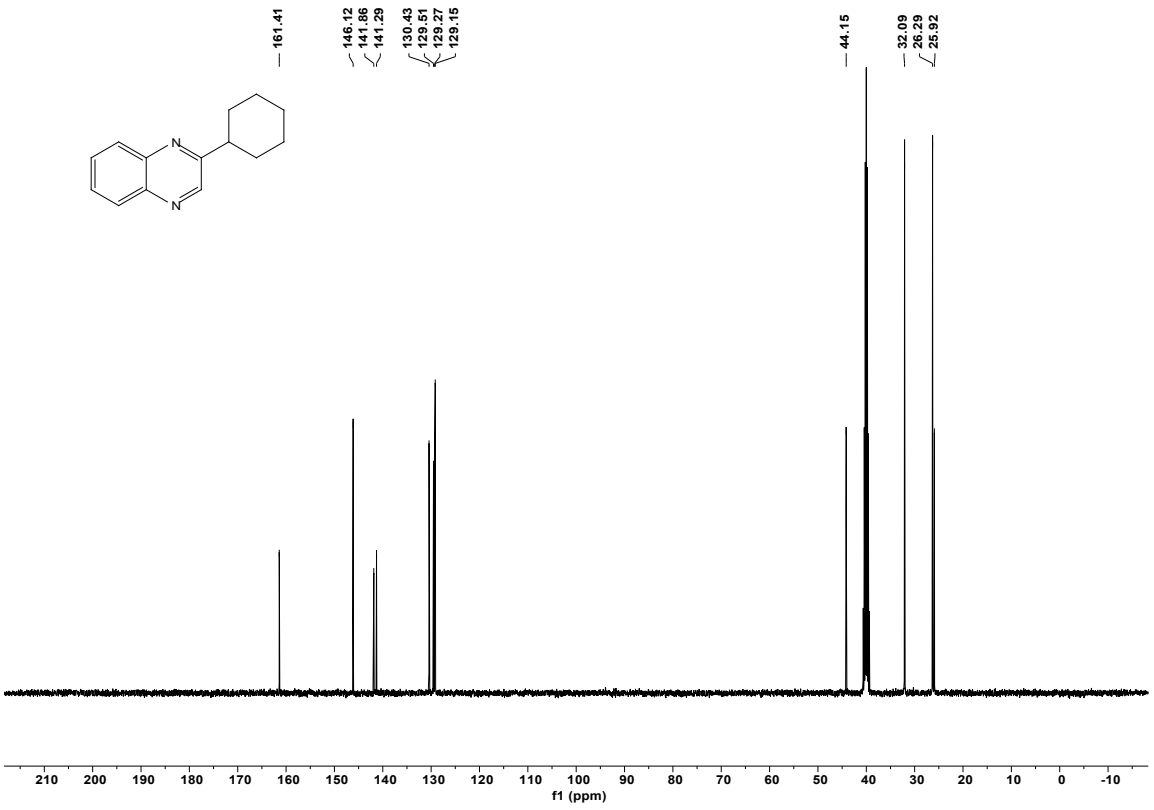
f1 (ppm)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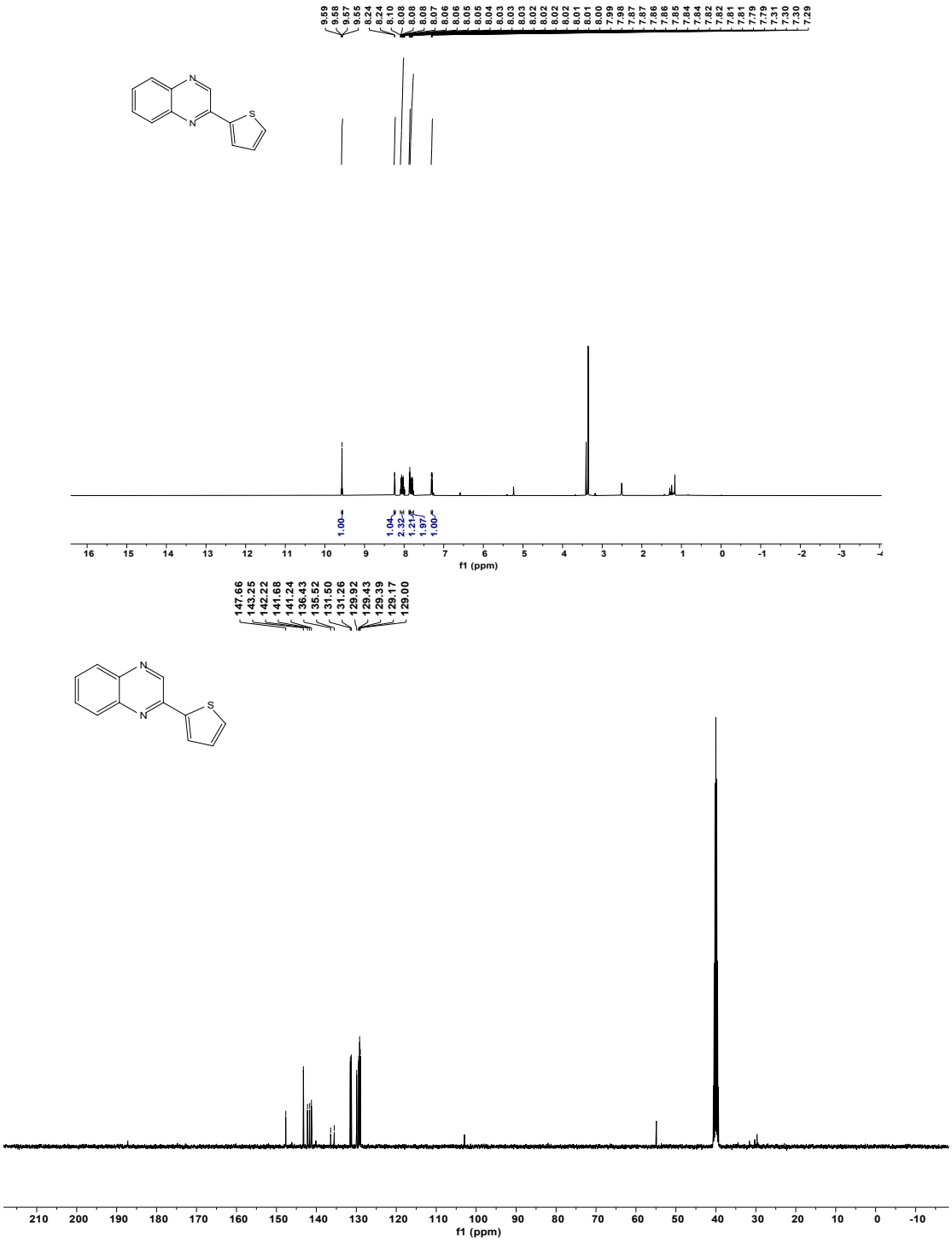
f1 (ppm)

3k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142.22
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131.50
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129.39
129.17
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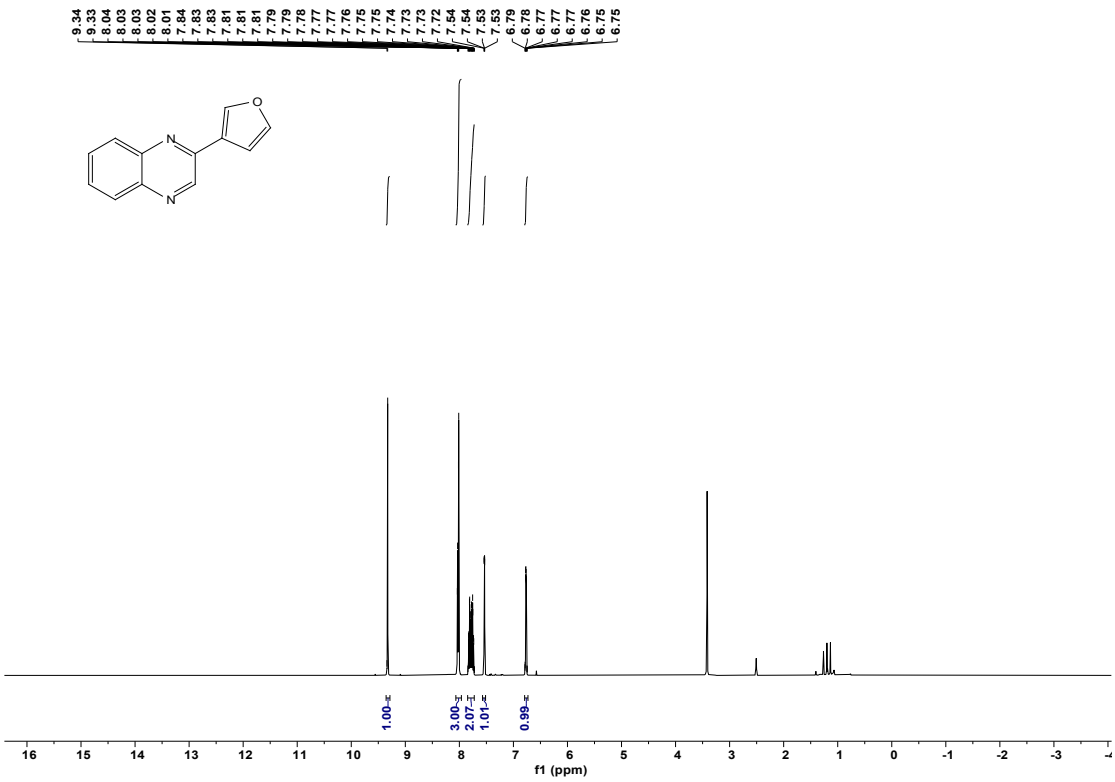
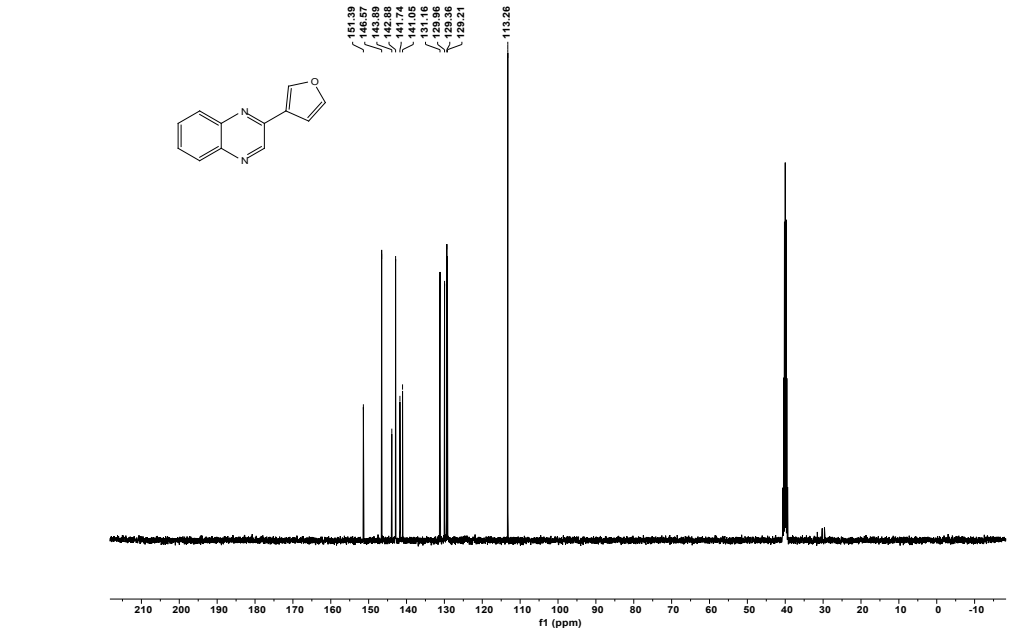
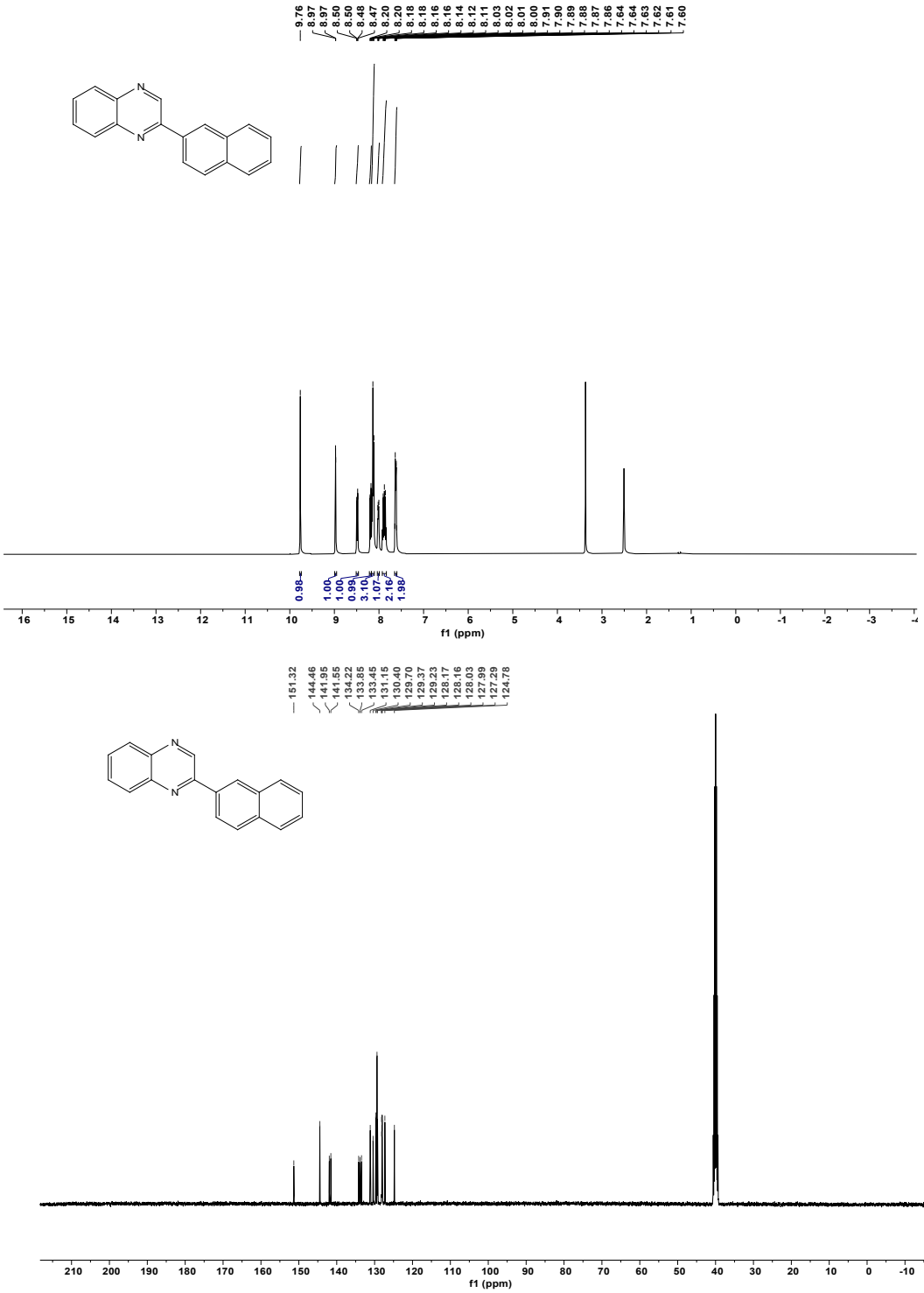
N
S
f1 (ppm)

3l

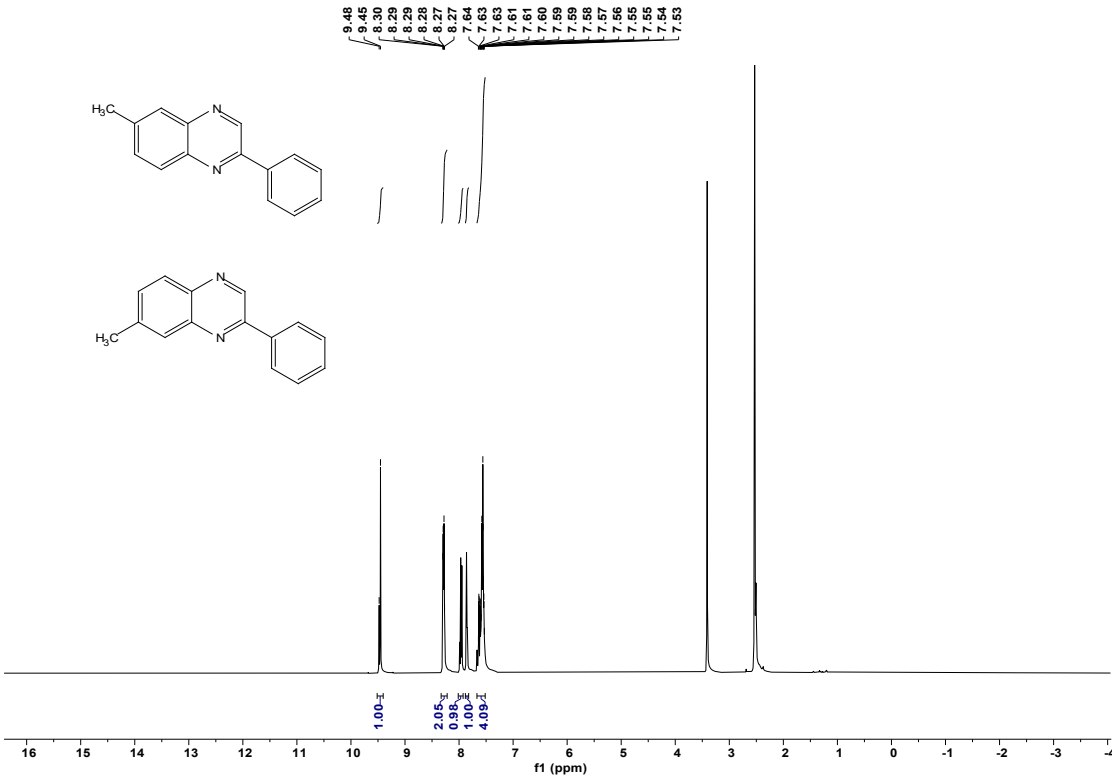

9.34
9.33
8.04
8.03
8.03
8.02
8.01
7.84
7.83
7.83
7.81
7.81
7.81
7.79
7.79
7.78
7.77
7.77
7.76
7.75
7.75
7.74
7.73
7.73
7.72
7.54
7.54
7.53
7.53
6.79
6.78
6.77
6.77
6.77
6.76
6.75
6.75
O
N
N
1.00
3.00
2.07
1.01
0.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

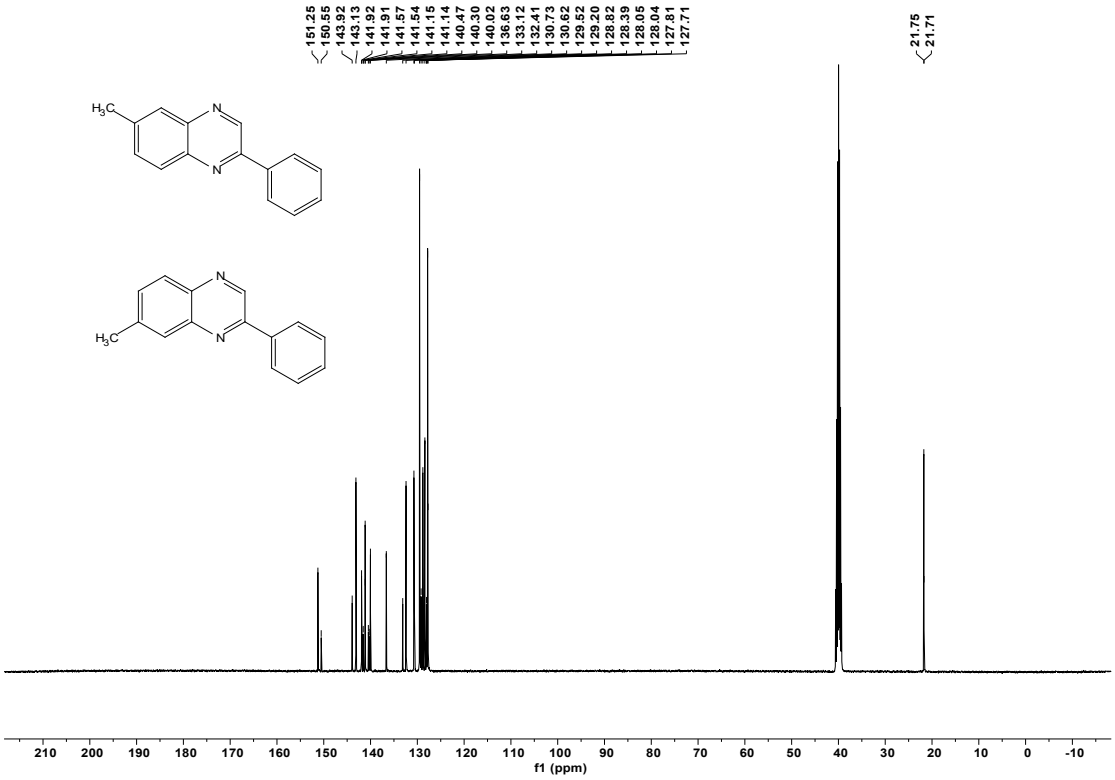

151.39
146.57
143.89
142.88
141.74
141.05
131.16
130.66
129.36
129.21
113.26
O
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3m

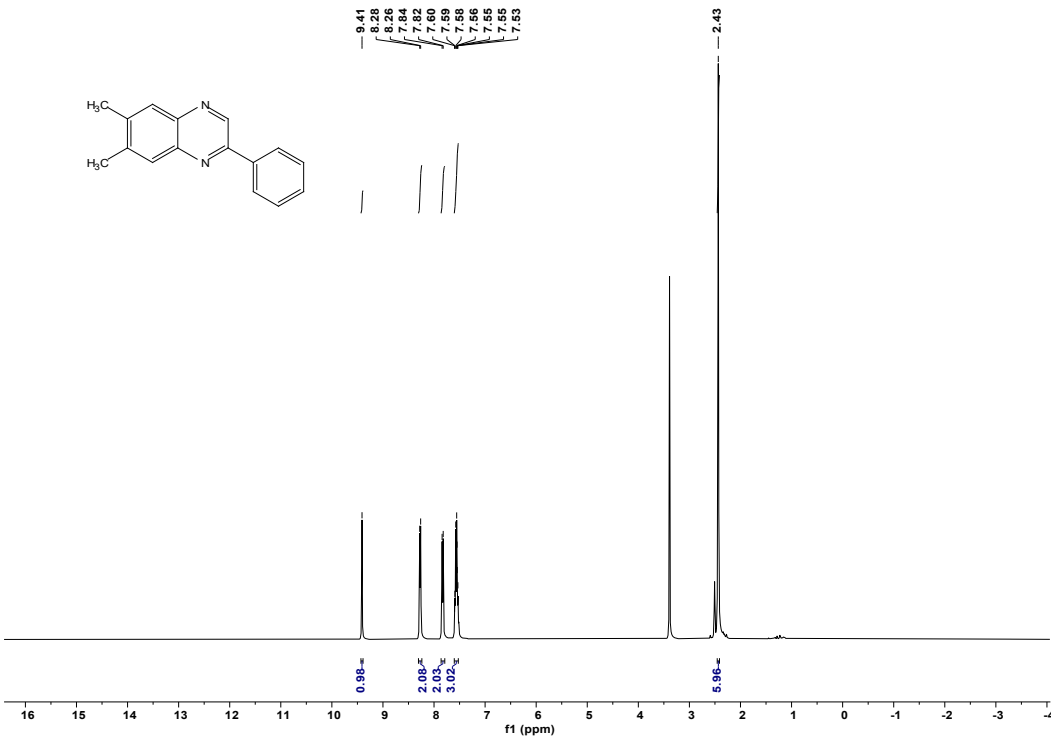

9.76
8.97
8.97
8.50
8.50
8.48
8.47
8.20
8.20
8.18
8.18
8.16
8.16
8.14
8.12
8.11
8.03
8.02
8.01
8.00
7.91
7.90
7.89
7.88
7.87
7.86
7.64
7.64
7.63
7.62
7.61
7.60
0.98
1.00
1.00
0.99
3.10
1.07
2.16
1.98
f1 (ppm)
151.32
144.46
141.95
141.55
134.22
133.85
133.45
131.15
130.40
129.70
129.37
129.23
128.17
128.16
128.03
127.99
127.29
124.78
f1 (ppm)

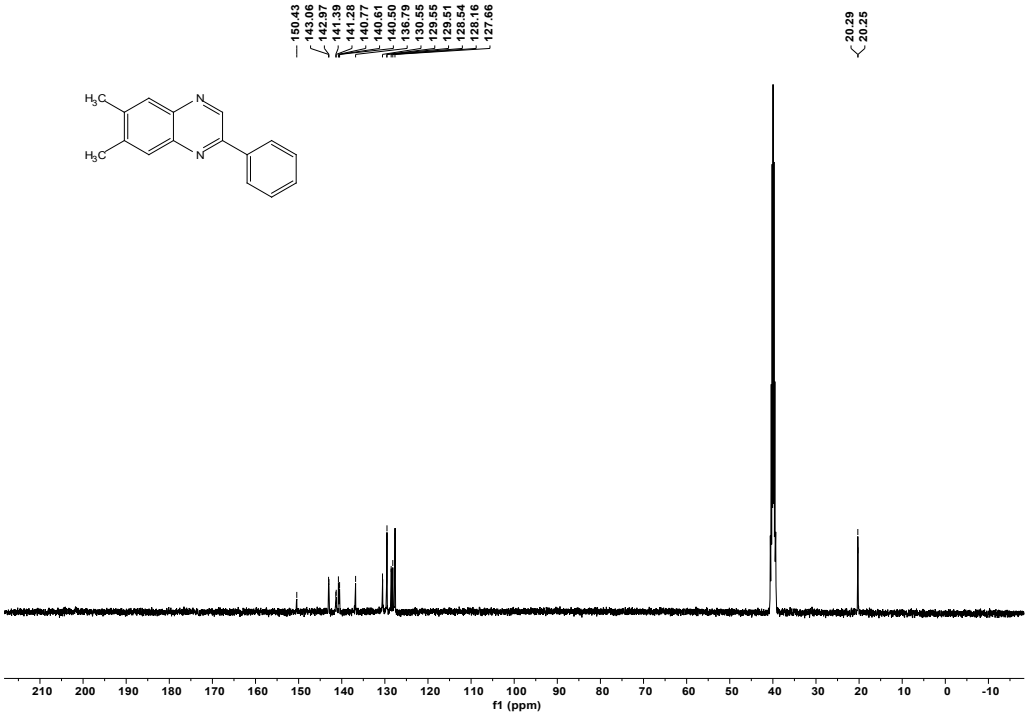
3n


9.48
9.45
8.30
8.29
8.29
8.28
8.27
8.27
7.64
7.63
7.63
7.61
7.61
7.60
7.59
7.59
7.58
7.57
7.56
7.55
7.55
7.54
7.53
1.00
2.05
0.98
1.00
4.09
f1 (ppm)

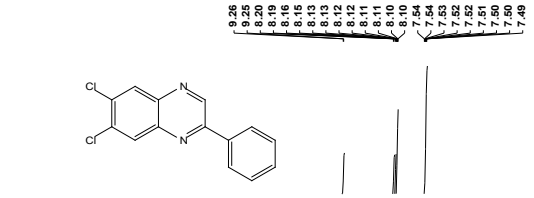

151.25
150.55
143.92
143.13
141.92
141.91
141.57
141.54
141.15
141.14
140.47
140.30
140.02
136.63
133.12
132.41
130.73
130.62
129.52
129.20
128.82
128.39
128.05
128.04
127.81
127.71
21.75
21.71
f1 (ppm)

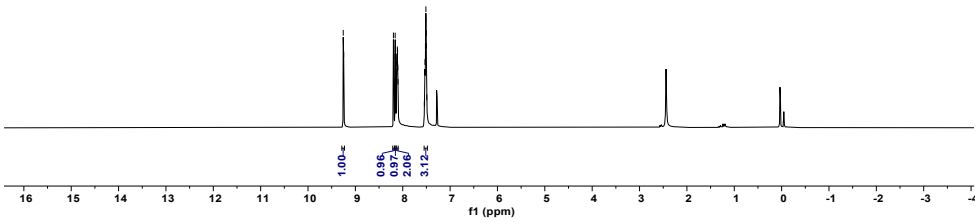
3o

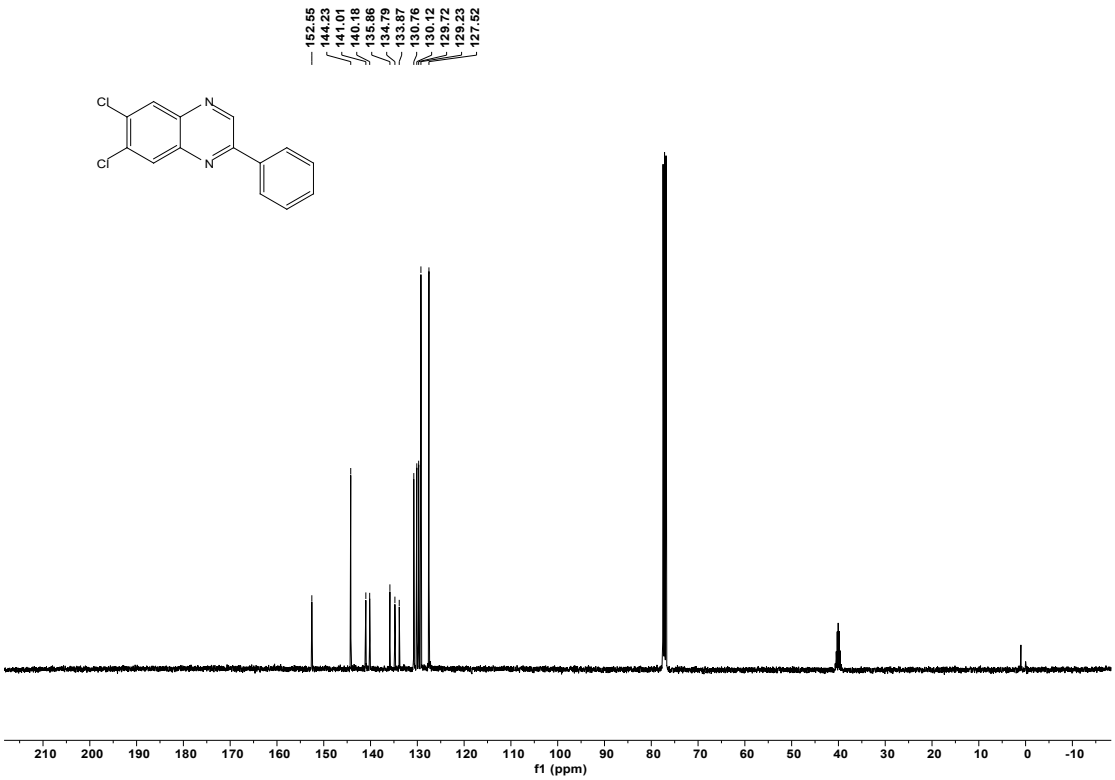

9.41
8.28
8.26
7.84
7.82
7.60
7.59
7.58
7.56
7.55
7.55
7.53
2.43
0.98
2.08
2.03
3.02
5.96
f1 (ppm)


150.43
143.06
142.97
141.39
141.28
140.77
140.61
140.50
136.79
130.55
129.55
129.51
128.54
128.16
127.66
20.29
20.25
f1 (ppm)

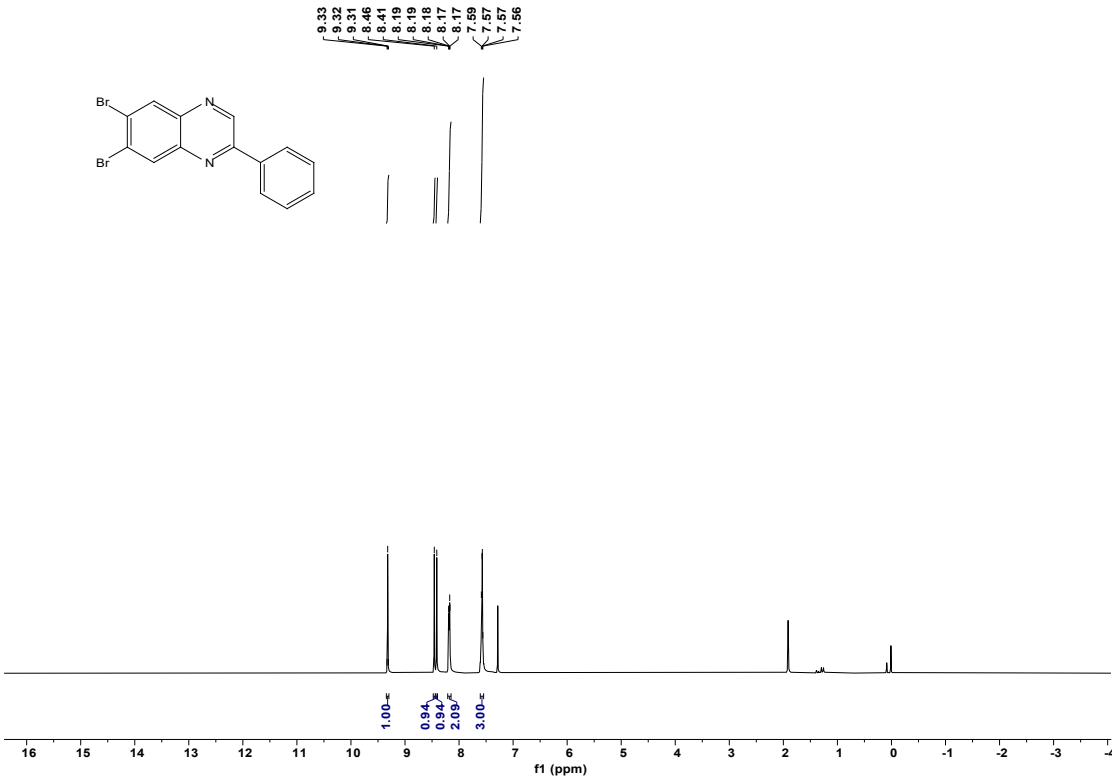
3p

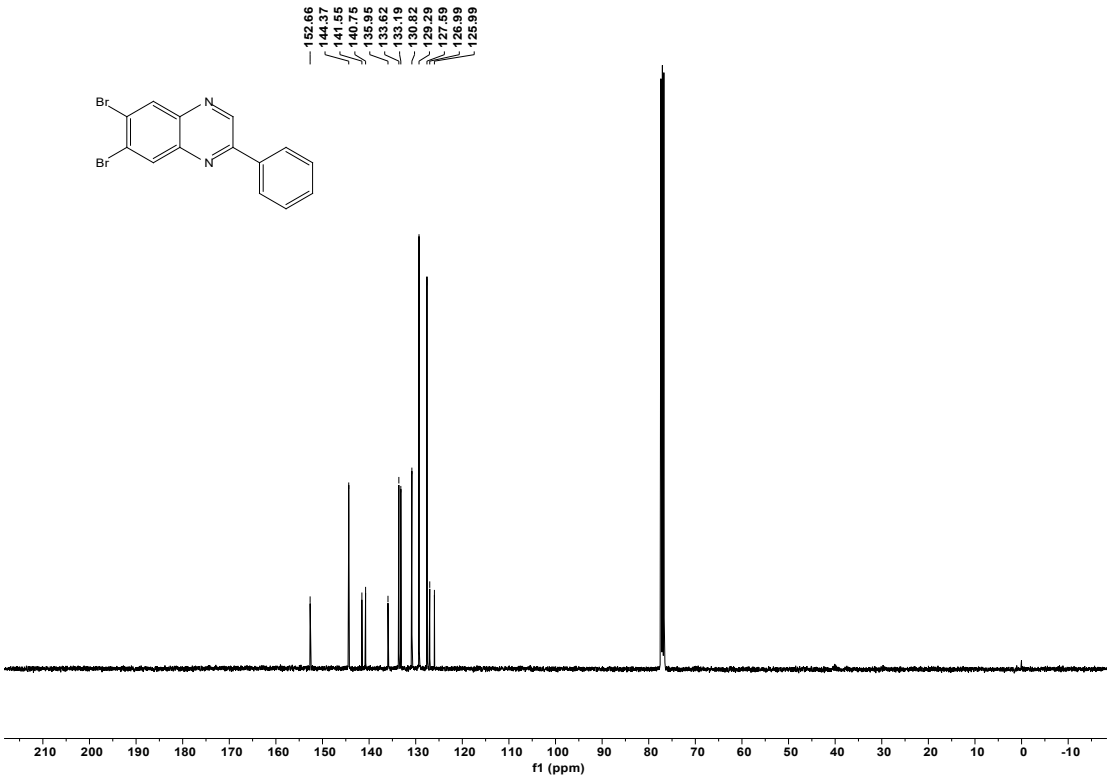

9.26
9.25
8.20
8.19
8.16
8.15
8.13
8.13
8.12
8.12
8.11
8.11
8.10
8.10
7.54
7.54
7.53
7.52
7.52
7.51
7.50
7.50
7.49
Cl
Cl
N
N


1.00
0.96
0.97
2.08
3.12
f1 (ppm)

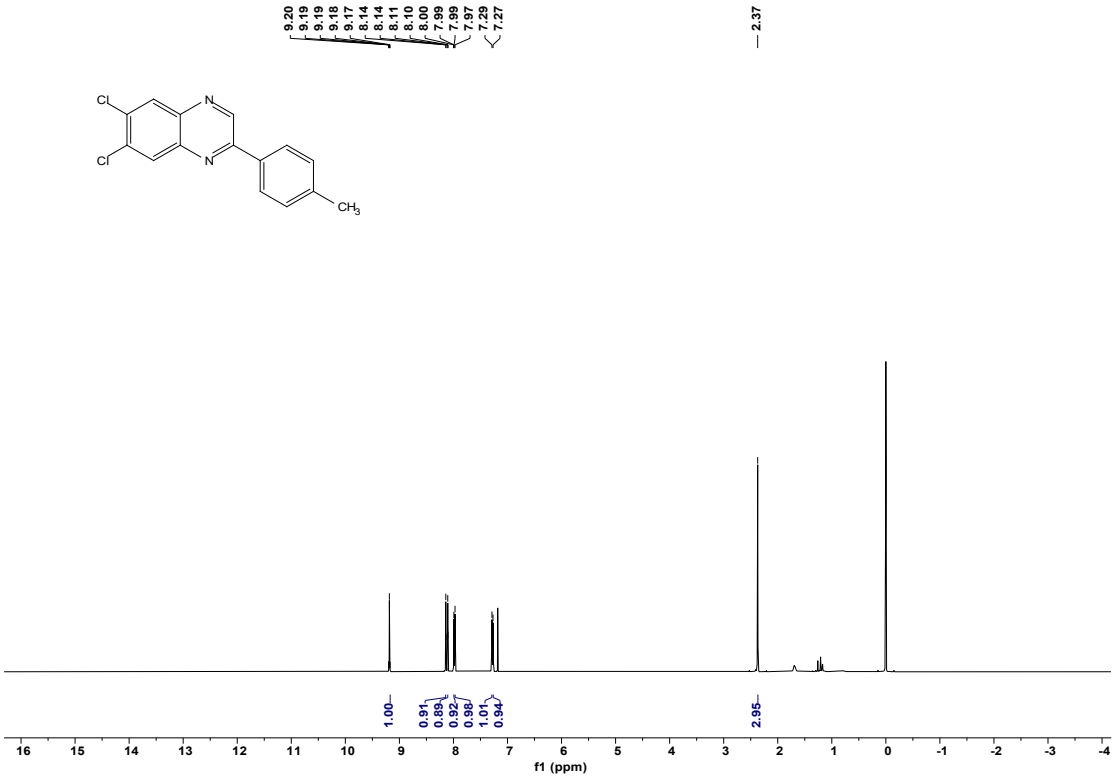

152.55
144.23
141.01
140.18
135.86
134.79
133.87
130.76
130.12
129.72
129.23
127.52
Cl
Cl
N
N
f1 (ppm)

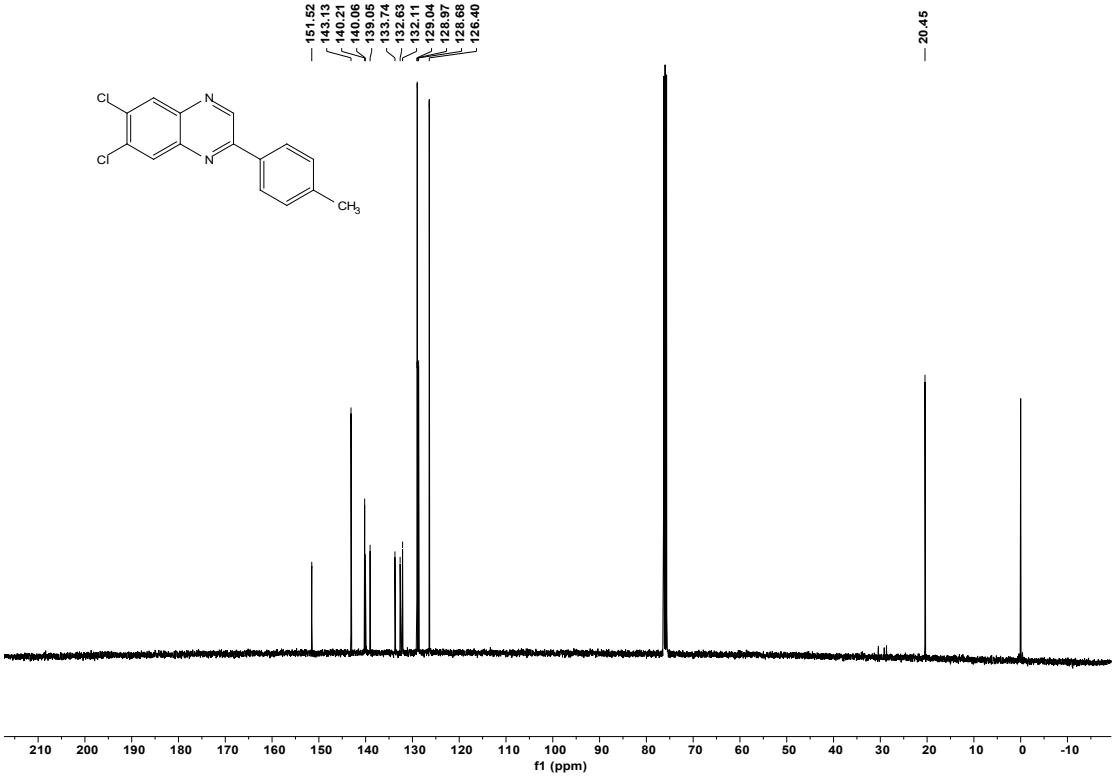
3q


9.33
9.32
9.31
8.46
8.41
8.19
8.19
8.18
8.17
8.17
7.59
7.57
7.57
7.56
Br
Br
N
N
1.00
0.94
0.94
2.09
3.00
f1 (ppm)

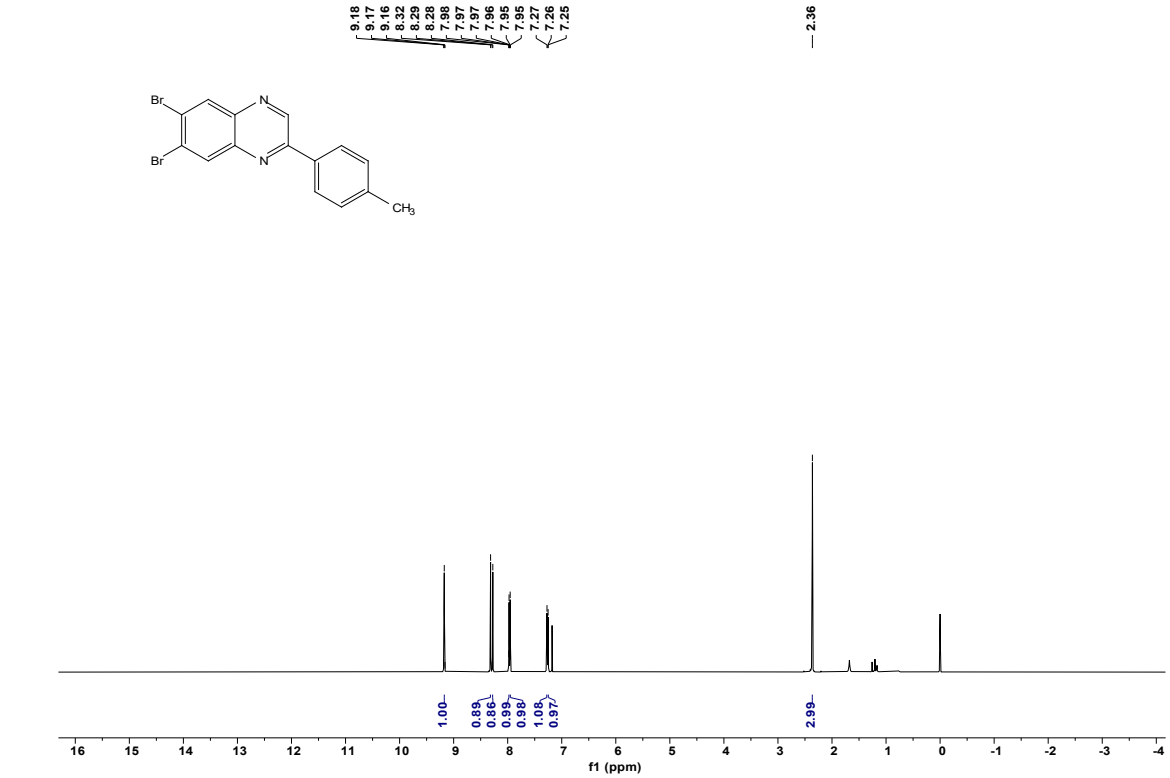

152.66
144.37
141.55
140.75
135.95
133.62
133.19
130.82
129.29
127.59
126.99
125.99
Br
Br
N
N
f1 (ppm)

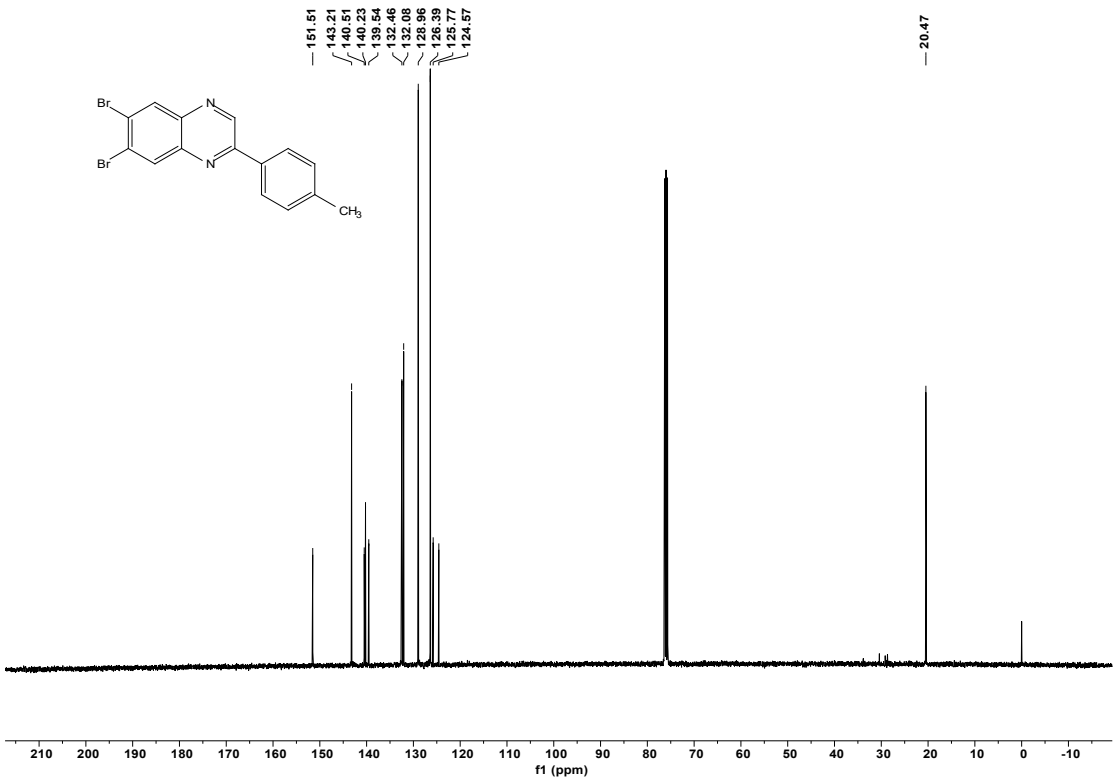
3r


9.20
9.19
9.19
9.18
9.17
8.14
8.14
8.11
8.10
8.00
7.99
7.99
7.97
7.29
7.27
2.37
Cl
Cl
N
N
CH3
1.00
0.91
0.89
0.92
0.98
1.01
0.94
2.95
f1 (ppm)

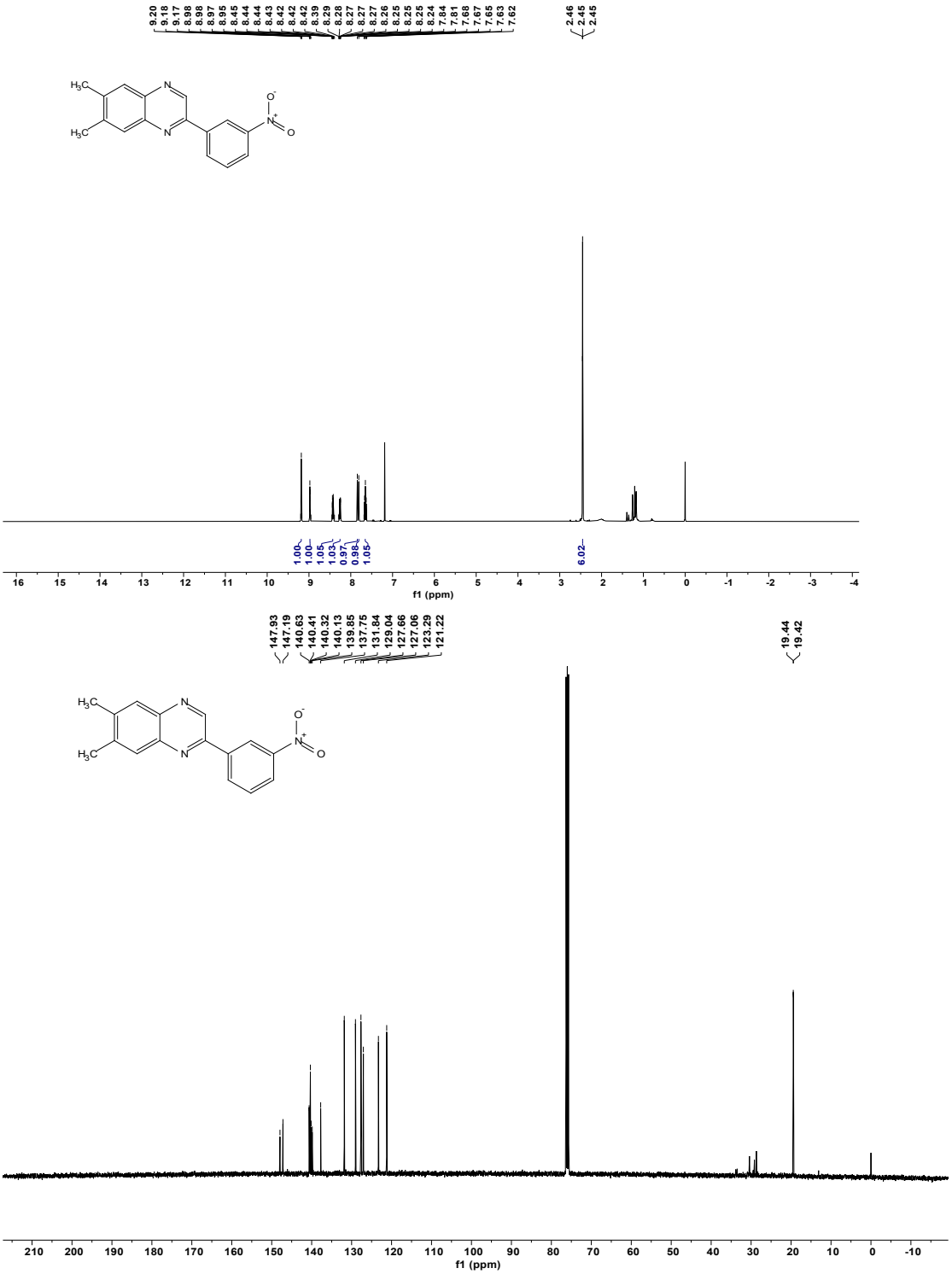

151.52
143.13
140.21
140.06
139.05
133.74
132.63
132.11
129.04
128.97
128.68
126.40
20.45
Cl
Cl
N
N
CH3
f1 (ppm)

3s

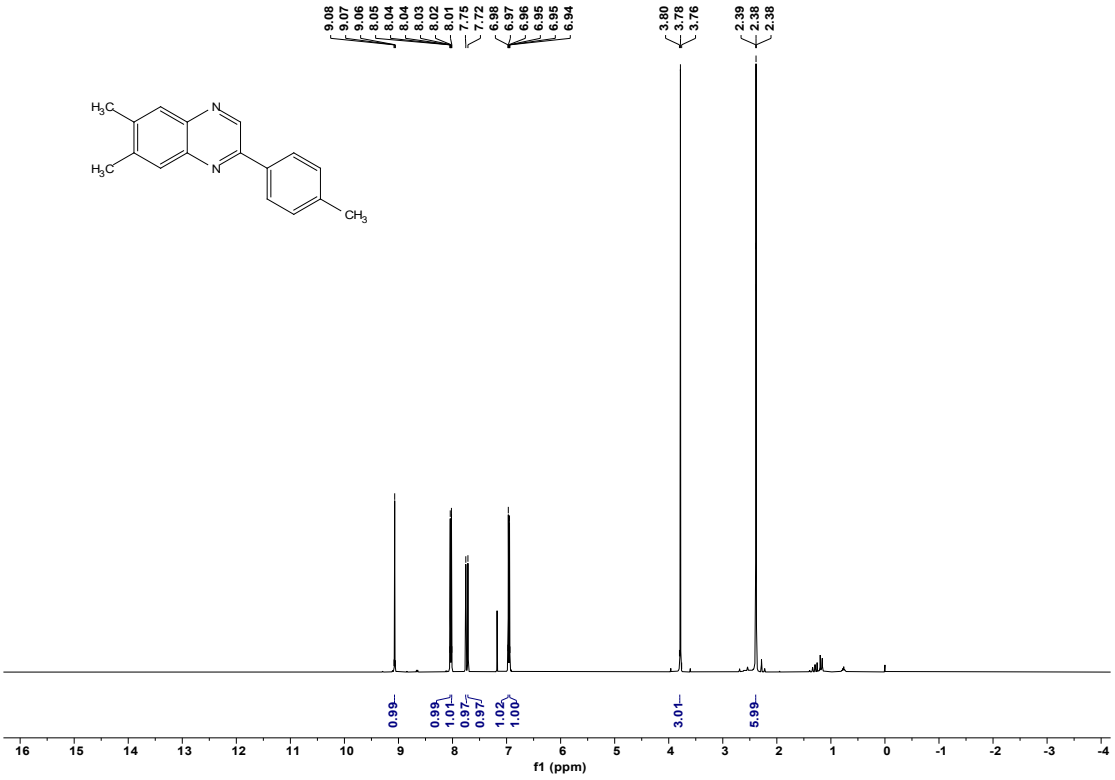

9.18
9.17
9.16
8.32
8.29
8.28
7.98
7.97
7.97
7.96
7.95
7.95
7.27
7.26
7.25
2.36
Br
Br
N
N
CH3
1.00
0.89
0.86
0.99
0.98
1.08
0.97
2.99
f1 (ppm)

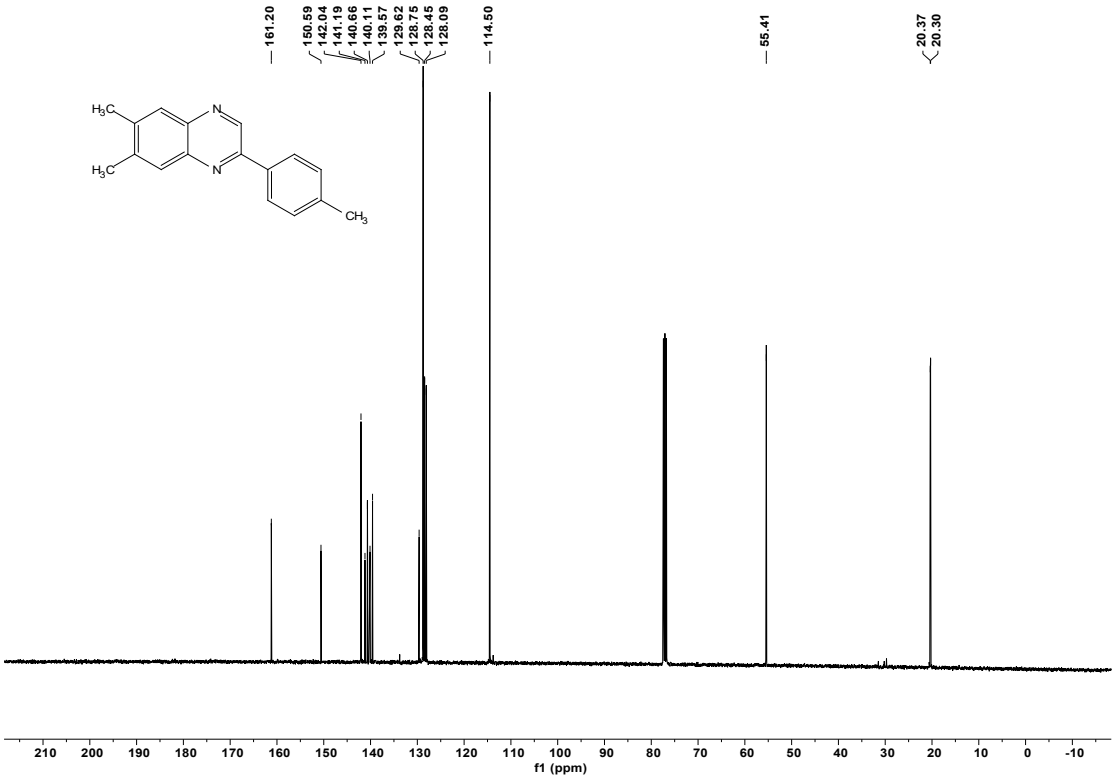

151.51
143.21
140.51
140.23
139.54
132.46
132.08
128.96
126.39
125.77
124.57
20.47
Br
Br
N
N
CH3
f1 (ppm)

3t

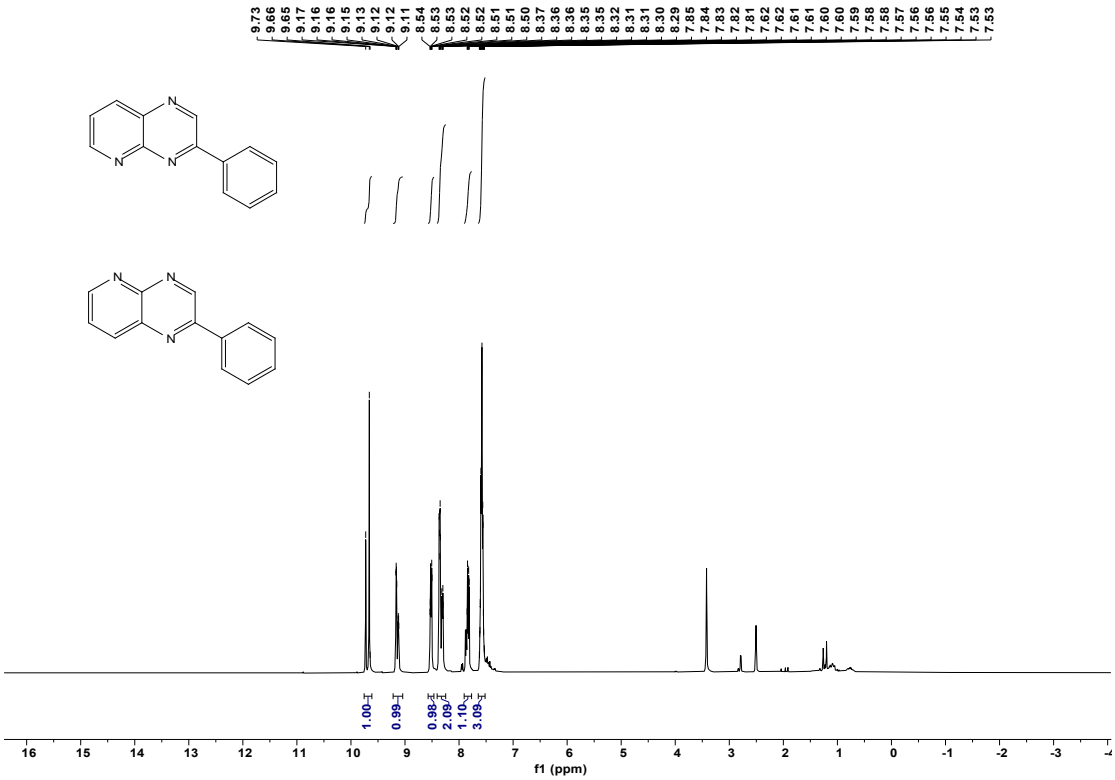

9.20
9.18
9.17
8.98
8.98
8.97
8.95
8.45
8.44
8.44
8.43
8.42
8.42
8.42
8.39
8.29
8.28
8.27
8.27
8.27
8.26
8.25
8.25
8.25
8.24
7.84
7.81
7.68
7.67
7.65
7.63
7.62
2.46
2.45
2.45
1.00
1.00
1.05
1.03
0.97
0.98
1.05
6.02
f1 (ppm)
147.93
147.19
140.63
140.41
140.32
140.13
139.85
137.75
131.84
129.04
127.66
127.06
123.29
121.22
19.44
19.42
f1 (ppm)

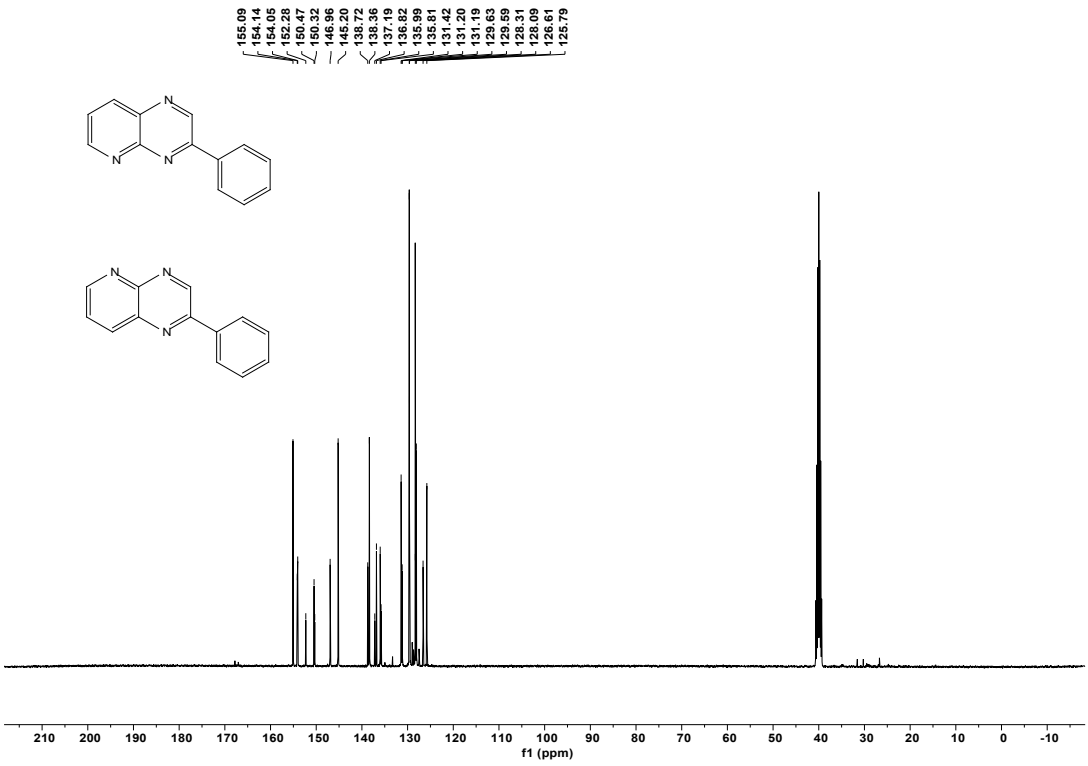
3u


9.08
9.07
9.06
8.05
8.04
8.04
8.03
8.02
8.01
7.75
7.72
6.98
6.97
6.96
6.95
6.94
3.80
3.78
3.76
2.39
2.38
2.38
H3C
H3C
N
N
CH3
0.99
0.99
1.01
0.97
0.97
1.02
1.00
3.01
5.99
f1 (ppm)

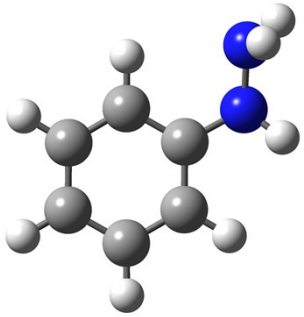

161.20
150.59
142.04
141.19
140.66
140.11
139.57
129.62
128.75
128.45
128.09
114.50
55.41
20.37
20.30
H3C
H3C
N
N
CH3
f1 (ppm)

3v


9.73 9.66 9.65 9.17 9.16 9.16 9.15 9.13 9.12 9.12 9.11 8.54 8.53 8.53 8.52 8.52 8.51 8.51 8.50 8.37 8.36 8.36 8.35 8.35 8.32 8.31 8.31 8.30 8.29 7.85 7.84 7.83 7.82 7.81 7.62 7.62 7.61 7.61 7.60 7.60 7.59 7.58 7.58 7.57 7.56 7.56 7.55 7.54 7.53 7.53
1.00 0.99 0.98 2.09 1.10 3.09
f1 (ppm)

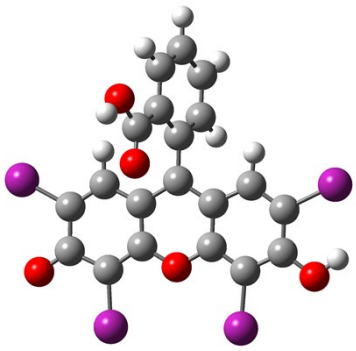

155.09 154.14 154.05 152.28 150.47 150.32 146.96 145.20 138.72 138.36 137.19 136.82 135.99 135.81 131.42 131.20 131.19 129.63 129.59 128.31 128.09 126.61 125.79
f1 (ppm)

8. Optimized Structures and Cartesian Coordinates



2a '

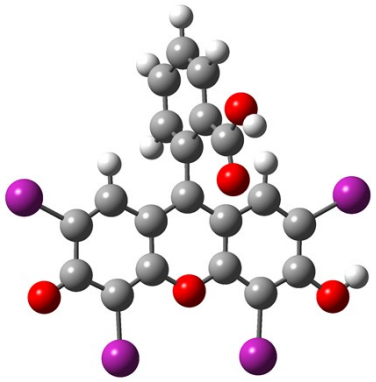
C	-0.45018300	-0.24612200	0.08316800
C	0.48592000	-1.29121800	0.00260200
C	1.84900500	-1.01365200	-0.06178600
C	2.30668300	0.30597300	-0.05546600
C	1.37463000	1.34305200	0.01856700
C	0.00711500	1.08022900	0.08700600
H	0.13960100	-2.32353400	-0.00320500
H	2.55650500	-1.83696300	-0.12331700
H	3.36999200	0.52100700	-0.10994500
H	1.71319900	2.37648700	0.02182700
H	-0.71773600	1.88376400	0.14229100
N	-1.81355100	-0.56420600	0.21257400
H	-2.03082800	-1.49568000	-0.13441500
N	-2.74071200	0.43832400	-0.14825300
H	-3.02549200	0.35065200	-1.12583800
H	-3.56442600	0.33586900	0.43781200



EY*

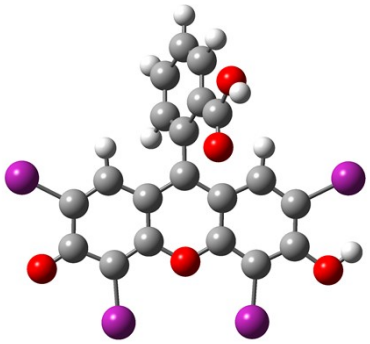
C	-0.02619300	1.17292200	-0.24840600
C	-1.06802300	-1.06128500	-0.09549300
C	-1.22597500	0.33351300	-0.21403200
C	-2.53737000	0.85118300	-0.32436600

H	-2.67206200	1.92002500	-0.43447500
C	-3.64076800	0.02925500	-0.29650600
C	-3.53396000	-1.41449400	-0.15910900
C	-2.16414700	-1.91947400	-0.06360500
C	-0.13289600	2.64508000	-0.41377800
C	-0.58641100	3.52341800	0.60334700
C	0.22092000	3.19972100	-1.65484800
C	-0.69146400	4.89904000	0.34471000
C	0.11851900	4.56856700	-1.89882100
H	0.56533300	2.53529600	-2.44206600
C	-0.34533800	5.42223100	-0.89747400
H	-1.04057300	5.55456800	1.13379700
H	0.39241000	4.96376100	-2.87313500
H	-0.43429900	6.48890800	-1.08071700
C	-0.90615300	3.00128800	1.96159200
O	-0.81318800	1.84266800	2.31599300
O	-1.31981600	3.97326900	2.81454800
H	-1.49526200	3.52160300	3.66088500
Br	-5.37678600	0.76277600	-0.44229300
O	-4.52174200	-2.17886800	-0.12895800
O	0.16516300	-1.64355700	-0.01562700
Br	-1.91665600	-3.76740800	0.09803800
C	3.72264000	-0.88054900	-0.04578300
C	3.66770700	0.52557700	-0.14799000
C	2.47795900	1.21827300	-0.21559900
C	1.23418400	0.53024900	-0.19352800
C	1.29659500	-0.89165200	-0.07463900
C	2.50298600	-1.57892200	-0.00655000
H	2.48792600	2.29837900	-0.28164100
Br	5.32948500	1.47815900	-0.18336700
Br	2.51306800	-3.46516600	0.14284700
O	4.87249700	-1.57742000	0.01931200
H	5.61745200	-0.94753800	-0.01242700



EY

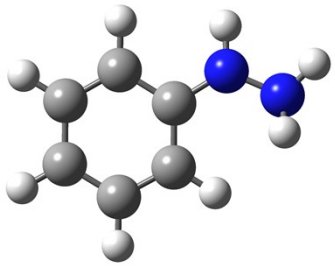
C	-0.06987900	1.13250500	-0.25508000
C	-1.21967900	-1.01824900	-0.08523100
C	-1.25288100	0.42573400	-0.20792000
C	-2.55318800	1.04776200	-0.25579200
H	-2.60827300	2.12618800	-0.34039400
C	-3.68491800	0.31025500	-0.19717300
C	-3.69333000	-1.17305100	-0.07971300
C	-2.35399200	-1.77223400	-0.02697300
C	-0.06296200	2.61709500	-0.44533300
C	0.05465800	3.54312600	0.61642100
C	-0.17853900	3.10463100	-1.75366400
C	0.05002100	4.91896400	0.34153100
C	-0.17776000	4.47506400	-2.01550800
H	-0.27348100	2.39683200	-2.57187800
C	-0.06260900	5.38536500	-0.96528800
H	0.13355100	5.61740400	1.16579800
H	-0.27061900	4.82667600	-3.03905000
H	-0.06400100	6.45343600	-1.16105200
C	0.17474400	3.06122700	2.02236500
O	0.25532700	1.89791700	2.36087200
O	0.19070100	4.07368000	2.92371300
H	0.27000200	3.64916200	3.79827300
Br	-5.38433500	1.14692700	-0.26355100
O	-4.72924400	-1.82456500	-0.03243300
O	-0.01652500	-1.66205200	-0.02758300
Br	-2.25753200	-3.65314500	0.12684000
C	3.57142000	-1.11531900	-0.11606300
C	3.59846700	0.29106300	-0.24088700
C	2.44287500	1.04295000	-0.29081700
C	1.18495000	0.41749100	-0.21640600
C	1.15302800	-0.98804100	-0.09552200
C	2.32385300	-1.74885000	-0.04540200
H	2.50494400	2.11970900	-0.38702100
Br	5.30822300	1.14664400	-0.34241400
Br	2.22870800	-3.62819000	0.11533700
O	4.68159900	-1.86985100	-0.06617700
H	5.46008900	-1.28361400	-0.12451800



EY•□

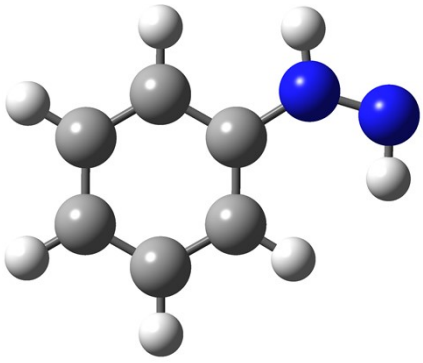
C	-0.03358300	1.17754300	-0.16664100
C	-1.37323600	-0.89796600	-0.04498800
C	-1.30300000	0.52711300	-0.11208900
C	-2.55442700	1.20449600	-0.06675100
H	-2.56434900	2.28749400	-0.05841500
C	-3.74328500	0.52457400	-0.02073400
C	-3.87193200	-0.92889100	0.00479900
C	-2.56593200	-1.58163000	0.00295300
C	0.04874900	2.62797000	-0.41982700
C	0.73226200	3.58536000	0.39266000
C	-0.57321200	3.11474000	-1.59290800
C	0.82013900	4.92989900	-0.03030500
C	-0.48636300	4.44158000	-1.98807300
H	-1.10323400	2.40255100	-2.21750800
C	0.22903100	5.36080500	-1.20628800
H	1.35370100	5.63413100	0.59734000
H	-0.95784900	4.75881500	-2.91516400
H	0.31479400	6.40005300	-1.51277900
C	1.25671000	3.23089600	1.72841300
O	1.21865900	2.14207500	2.27011600
O	1.81824400	4.30120700	2.38668500
H	2.09554700	3.92510900	3.24138300
Br	-5.38555900	1.51925400	0.03339900
O	-4.95449400	-1.53629800	0.03720400
O	-0.21791500	-1.64917300	-0.02314700
Br	-2.56485600	-3.48797900	0.07542400
C	3.41172500	-1.41892200	-0.13075100
C	3.55180000	-0.02963200	-0.22503500
C	2.47134300	0.83653400	-0.22777300
C	1.15068800	0.35216500	-0.13061300
C	1.00178600	-1.05797800	-0.06229300
C	2.10241700	-1.91707100	-0.05629800
H	2.64787100	1.90012700	-0.31729800
Br	5.34181400	0.68359000	-0.35092100

Br	1.82912800	-3.79551700	0.04297800
O	4.45944000	-2.28556000	-0.11560600
H	5.27350100	-1.75294800	-0.17512000



A

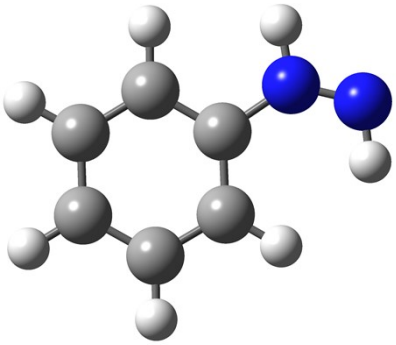
C	1.83445700	1.04107000	-0.02746100
C	0.47706700	1.30827200	-0.00072800
C	-0.44158200	0.22775600	0.02513300
C	0.01314300	-1.11260000	0.04147500
C	1.37630500	-1.35321100	0.01449000
C	2.29053800	-0.28615700	-0.02487300
H	2.54346400	1.86183000	-0.05086300
H	0.11365400	2.33267400	-0.01239700
H	-0.68227300	-1.94145900	0.11928900
H	1.73855100	-2.37568000	0.03894900
H	3.35611500	-0.49099200	-0.04305000
N	-1.77755000	0.54055100	0.01396100
H	-2.05447000	1.50319600	0.18889800
N	-2.79261400	-0.36107400	0.02802600
H	-3.69828100	0.07027400	-0.13331300
H	-2.62518800	-1.16696700	-0.56963500



B

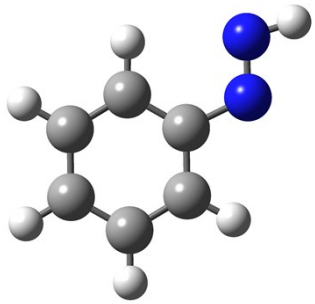
C	-1.76637800	-1.04967300	-0.00000100
C	-0.39716300	-1.28588200	-0.00000300
C	0.51067800	-0.20866100	0.00000300
C	0.01296900	1.10660800	-0.00000600

C	-1.36257000	1.32589600	0.00000000
C	-2.26260500	0.25814800	0.00000600
H	-2.45138600	-1.89329700	-0.00000600
H	-0.01765100	-2.30572700	-0.00000500
H	0.68838300	1.95642400	-0.00003700
H	-1.73274500	2.34771000	-0.00000500
H	-3.33284600	0.44068500	0.00001200
N	1.87629500	-0.49287100	0.00000700
H	2.12990500	-1.47368700	-0.00002200
N	2.94238000	0.31756100	-0.00000400
H	2.57603200	1.27643800	0.00004900



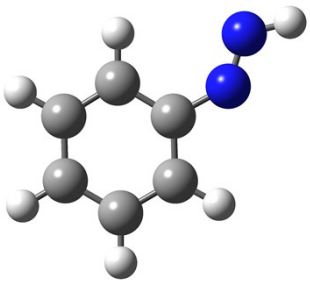
C

C	-1.73521400	-1.08279900	0.00000100
C	-0.36252700	-1.29086100	0.00000900
C	0.49390700	-0.17354800	0.00000800
C	0.00094900	1.14489000	0.00001800
C	-1.37184300	1.33077600	-0.00000200
C	-2.23745700	0.22328400	-0.00001800
H	-2.41096700	-1.93117700	0.00000300
H	0.04327100	-2.29988700	0.00002200
H	0.66044300	2.00773100	0.00008200
H	-1.77749100	2.33685400	0.00000300
H	-3.31091100	0.38557600	-0.00004500
N	1.87481700	-0.45349700	-0.00000700
H	2.10935800	-1.45470500	0.00003600
N	2.88968200	0.27847400	-0.00001900
H	2.60791300	1.27031900	-0.00001800



D

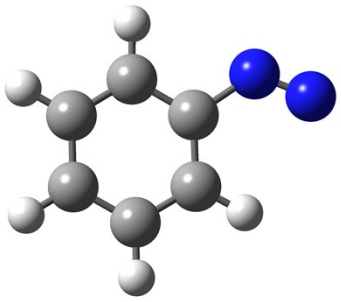
C	1.30524300	1.32921700	0.00000000
C	-0.06649500	1.10305300	0.00000000
C	-0.54741800	-0.21519100	0.00000000
C	0.34497000	-1.29193500	0.00000000
C	1.72054900	-1.05896500	0.00000000
C	2.20051500	0.25128300	0.00000000
H	1.68473700	2.34764900	0.00000000
H	-0.77811200	1.92160400	0.00000000
H	-0.06159800	-2.29872300	0.00000000
H	2.41386800	-1.89540600	0.00000000
H	3.27127800	0.43735300	0.00000000
N	-1.93330400	-0.57265200	0.00000000
N	-2.72373400	0.39996100	0.00000000
H	-3.67508700	-0.00841300	0.00000000



E

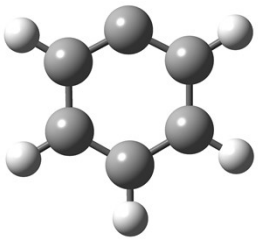
C	1.35840600	1.32255300	0.00000000
C	-0.01332000	1.15807800	0.00000000
C	-0.52144600	-0.16773400	0.00000000
C	0.32121500	-1.30283400	0.00000000
C	1.69327800	-1.10440200	0.00000000
C	2.20700300	0.19938800	0.00000000
H	1.78045500	2.32234800	0.00000000
H	-0.69511000	2.00226000	0.00000100
H	-0.11285200	-2.29706200	0.00000000
H	2.36424600	-1.95651600	-0.00000100
H	3.28263700	0.34860800	-0.00000100
N	-1.87068500	-0.40329000	0.00000100

N	-2.85696200	0.27505300	-0.00000200
H	-3.79665900	-0.15228100	0.00000200



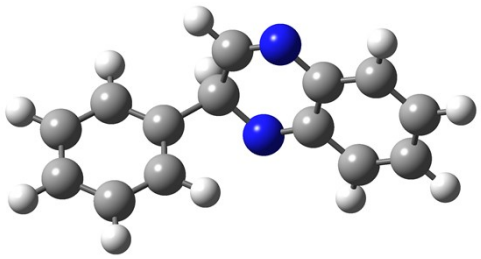
F

C	-1.27829700	1.31975900	0.00000000
C	0.09853200	1.11634900	0.00000000
C	0.59001000	-0.19317800	0.00000000
C	-0.27046400	-1.28967500	0.00000000
C	-1.64919100	-1.07593100	0.00000000
C	-2.15224400	0.22645300	0.00000000
H	-1.67329200	2.33203100	0.00000000
H	0.79657000	1.94785900	0.00000000
H	0.15029300	-2.29051000	0.00000000
H	-2.32779700	-1.92408400	0.00000000
H	-3.22589300	0.39290500	0.00000000
N	2.01634700	-0.48555500	0.00000000
N	2.87651700	0.33114600	0.00000000



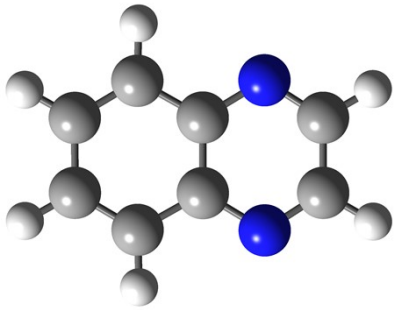
G

C	-1.21419800	0.63260900	-0.00000600
C	-1.22640100	-0.77179400	0.00002200
C	-0.00001200	-1.40013100	-0.00001000
C	1.22640400	-0.77178500	-0.00000800
C	1.21421200	0.63258300	0.00001800
C	-0.00000300	1.32471600	-0.00000500
H	-2.15467600	1.17909500	-0.00002800
H	-2.16291000	-1.32331500	-0.00000900
H	2.16288300	-1.32336000	-0.00002600
H	2.15466800	1.17910700	0.00001100
H	0.00002700	2.41128500	-0.00002200



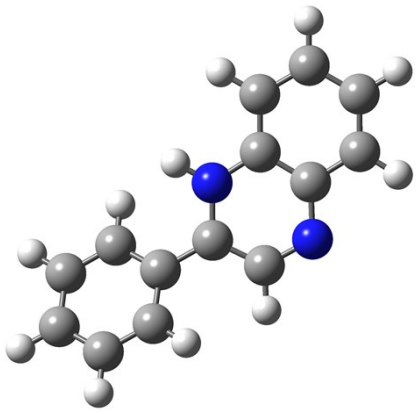
H

C	3.86317500	-1.33488400	-0.23016200
C	2.59609000	-1.38949000	-0.77480100
C	1.64682900	-0.34715200	-0.52678600
C	2.05345600	0.75240500	0.31528200
C	3.33741800	0.77959700	0.85570600
C	4.24194000	-0.24974400	0.58768200
H	4.57495800	-2.13090900	-0.43087800
H	2.27717600	-2.21162000	-1.40823600
H	3.60823500	1.62020300	1.48764300
H	5.24079800	-0.21584000	1.01300500
C	0.00417900	1.73763000	0.08560100
C	-0.49712100	0.63962600	-0.83379200
H	-0.69564100	2.54603700	0.31090400
N	1.17098800	1.79702900	0.61548900
N	0.43265400	-0.44858400	-1.07604800
C	-1.85186000	0.12282500	-0.33764500
C	-3.03555600	0.75519200	-0.73342700
C	-1.91960900	-0.95209800	0.55543200
C	-4.26887800	0.32425700	-0.24278000
H	-2.99471500	1.58513600	-1.43616400
C	-3.15252100	-1.38754400	1.04177000
H	-1.00551800	-1.45607900	0.85445200
C	-4.33006900	-0.74945200	0.64696600
H	-5.18068000	0.82200500	-0.56223100
H	-3.19297500	-2.22757100	1.73025500
H	-5.28971300	-1.08987900	1.02650600
H	-0.69226400	1.11239800	-1.81561100



1a

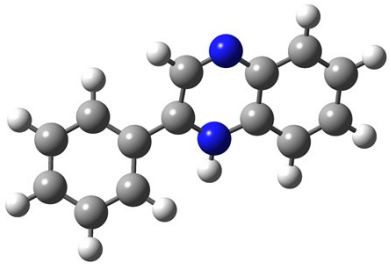
C	2.37779100	-0.70941500	-0.00000500
C	1.19317100	-1.41147100	-0.00000600
C	-0.04249600	-0.71529600	0.00000900
C	-0.04249000	0.71528700	0.00001300
C	1.19316900	1.41146400	0.00000600
C	2.37779200	0.70941600	0.00000100
H	3.32461700	-1.24218300	-0.00000800
H	1.16577800	-2.49671600	-0.00001100
H	1.16577900	2.49671000	0.00000200
H	3.32461400	1.24219200	-0.00000200
C	-2.31943800	0.71094300	-0.00003300
C	-2.31944500	-0.71093900	0.00001000
H	-3.26312900	1.25520600	0.00003400
H	-3.26312700	-1.25521300	0.00004500
N	-1.21162900	1.42121800	-0.00000200
N	-1.21163600	-1.42120900	-0.00000300



I

C	-4.02440000	1.36127800	-0.21961200
C	-2.64989100	1.59615900	-0.24474500
C	-1.76197600	0.53002900	-0.07753400
C	-2.24049300	-0.79686800	0.11520700
C	-3.63252700	-0.99837100	0.13988100
C	-4.51498100	0.06442100	-0.02541300

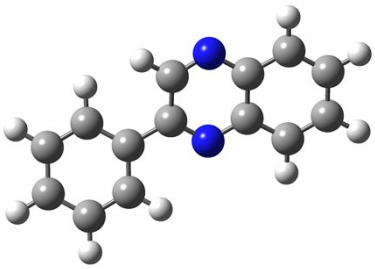
H	-4.71148500	2.19223200	-0.35107200
H	-2.26295600	2.60232100	-0.39311700
H	-3.98635100	-2.01387900	0.28795400
H	-5.58646800	-0.11279800	-0.00554600
C	-0.08286700	-1.61453000	0.22721500
C	0.49524800	-0.35684200	0.03324700
H	0.57857500	-2.46309200	0.38640800
N	-1.38888500	-1.87396400	0.27292600
N	-0.38471600	0.71209200	-0.09481900
C	1.93032200	-0.08804500	0.01573000
C	2.85000800	-1.07788300	-0.39288900
C	2.44325700	1.17122800	0.39422500
C	4.21621600	-0.82031400	-0.41004500
H	2.48376900	-2.04393600	-0.72628400
C	3.81247700	1.42655800	0.36556300
H	1.77117100	1.94259200	0.76176200
C	4.70824800	0.43424700	-0.03556600
H	4.90206400	-1.59874400	-0.73373300
H	4.18086700	2.40234500	0.67128000
H	5.77567000	0.63422300	-0.05780300
H	-0.02150200	1.60543900	-0.39819600



J

C	-3.98740400	1.36301900	-0.24030000
C	-2.62703000	1.61009800	-0.28131300
C	-1.74996300	0.52997500	-0.09678800
C	-2.23687500	-0.79336400	0.12328200
C	-3.63515000	-1.00662800	0.16032300
C	-4.49266300	0.05825900	-0.01960200
H	-4.68103100	2.18615400	-0.37983800
H	-2.24336600	2.61247000	-0.45100400
H	-3.99159000	-2.01662100	0.33123600
H	-5.56608400	-0.09777400	0.00659500
C	-0.08867400	-1.61905600	0.25905100
C	0.49183100	-0.33051400	0.04299800
H	0.56738300	-2.46617000	0.43283900

N	-1.38103200	-1.83794100	0.29484100
N	-0.38078300	0.67824600	-0.13108500
C	1.92687100	-0.07144100	0.02400800
C	2.81311200	-1.07106300	-0.42688000
C	2.44459200	1.17107700	0.44720000
C	4.18097400	-0.82285700	-0.46787500
H	2.43174200	-2.02303600	-0.78211200
C	3.81372200	1.40658300	0.41133900
H	1.78958600	1.93372400	0.86231900
C	4.68315600	0.41249200	-0.04992900
H	4.85555400	-1.59174300	-0.83049200
H	4.20627900	2.35762300	0.75668300
H	5.75226000	0.59949300	-0.07634600
H	-0.00701900	1.60426800	-0.32926400



3a

C	3.95452500	-1.40100300	-0.16922700
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C	1.70069900	-0.52372300	-0.05736900
C	2.22951000	0.79639200	0.08082500
C	3.63246100	0.99223800	0.08817700
C	4.47724700	-0.08910700	-0.03571000
H	4.63858200	-2.23983400	-0.26447500
H	2.17155100	-2.61346100	-0.28365300
H	4.00539600	2.00630200	0.19476900
H	5.55360600	0.05849600	-0.03071800
C	0.10578100	1.61810600	0.19652000
C	-0.44237000	0.30279300	0.03102900
H	-0.55391400	2.47137000	0.33727100
N	1.39405600	1.86778600	0.21820300
N	0.35876100	-0.74576300	-0.08078400
C	-1.90730800	0.06807400	0.00506700
C	-2.81897300	1.09373000	-0.29609700
C	-2.40756500	-1.21627600	0.27985700
C	-4.19071000	0.84394400	-0.31171600
H	-2.46297200	2.08836000	-0.54640400

C	-3.77720400	-1.46265900	0.26701600
H	-1.70239300	-2.00968300	0.50230200
C	-4.67546800	-0.43305700	-0.02643700
H	-4.88013100	1.64825000	-0.55369100
H	-4.14657000	-2.46054100	0.48818200
H	-5.74481400	-0.62608700	-0.03630900