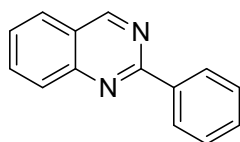


General Methods

NMR spectra were recorded on Bruker Avance 300 and Bruker ARX 400 spectrometers. Chemical shifts (ppm) are given relative to solvent: references for CDCl_3 were 7.26 ppm (^1H NMR) and 77.00 ppm (^{13}C NMR). Multiplets were assigned as s (singlet), d (doublet), t (triplet), dd (doublet of doublet), m (multiplet) and br. s (broad singlet). All measurements were carried out at room temperature unless otherwise stated. Electron impact (EI) mass spectra were recorded on AMD 402 mass spectrometer (70 eV). High resolution mass spectra (HRMS) were recorded on Agilent 6210. The data are given as mass units per charge (m/z). Gas chromatography analysis was performed on an Agilent HP-5890 instrument with a FID detector and HP-5 capillary column (polydimethylsiloxane with 5% phenyl groups, 30 m, 0.32 mm i.d., 0.25 μm film thickness) using argon as carrier gas.

General Procedure:

The reaction was carried out in a Parr Instruments 4560 series 300 mL autoclave containing an alloy plate with wells for 5 10 mL Wheaton vials. $\text{Pd}(\text{OAc})_2$ (5.56 mg, 0.05 mmol, 5.0 mol%), BuPAd_2 (17.9 mg, 0.1 mmol, 10 mol%), DBU (228 μL , 3 equiv.), 2-aminobenzylamine (0.5 mmol, 61 mg), substituted bromobenzene (0.5 mmol) and a magnetic stir bar were placed in each vials, which were then capped with a septum equipped with an inlet needle and flushed with argon. Then DMSO (2 mL) were added to the vial *via* syringe. The vials were placed in an autoclave, which was then purged with 10 bar of CO at room temperature and the reaction is heated for 36 h at 140 $^\circ\text{C}$. After the reaction the autoclave was vented to discharge CO. The product was extracted with ethyl acetate (5 $\times$ 3 mL). The organic layers were washed with brine, dried over Na_2SO_4 , and evaporated to yield the crude reaction mixture. The purification occurred by combi flash (eluent: heptane/EtOAc 60:40).

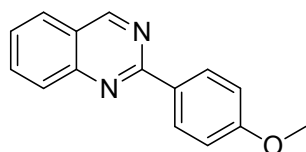


2-Phenylquinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.47 (s, 1H), 8.68 – 8.54 (m, 2H), 8.10 (dq, J = 8.3, 1.0 Hz, 1H), 7.97 – 7.84 (m, 2H), 7.68 – 7.45 (m, 4H).

¹³C NMR (75 MHz, CDCl₃) 161.10, 160.53, 150.81, 138.06, 134.14, 130.63, 128.67, 127.30, 127.15, 123.64.

MS (EI, 70 eV): m/z (%) = 206 ([M]⁺, 81), 179 (30), 152 (4).

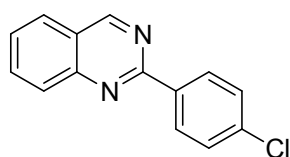


2-(4-Methoxyphenyl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.42 (s, 1H), 8.64 – 8.47 (m, 2H), 8.04 (dq, J = 8.2, 1.0 Hz, 1H), 7.94 – 7.83 (m, 2H), 7.63 – 7.51 (m, 1H), 7.09 – 6.97 (m, 2H), 3.90 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ 162.1, 161.1, 160.6, 151.0, 134.05, 130.23, 130.4, 128.6, 127.3, 126.9, 123.5, 114.2, 55.43

MS (EI, 70 eV): m/z (%) = 236 ([M]⁺, 100), 221 (10), 209 (7), 193 (8), 166 (6).

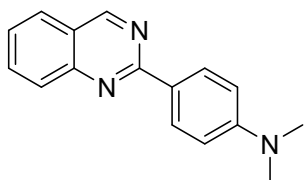


2-(4-Chlorophenyl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.45 (s, 1H), 8.63 – 8.50 (m, 2H), 8.08 (dt, J = 8.7, 0.8 Hz, 1H), 7.98 – 7.87 (m, 2H), 7.69 – 7.57 (m, 1H), 7.55 – 7.44 (m, 2H).

¹³C NMR (75 MHz, CDCl₃) δ 160.56, 160.09, 150.73, 136.87, 136.55, 134.29, 129.93, 128.85, 128.63, 127.49, 127.18, 123.66.

MS (EI, 70 eV): m/z (%) = 240 ([M]⁺, 100), 221 (10), 213 (14), 178 (10), 102 (5).

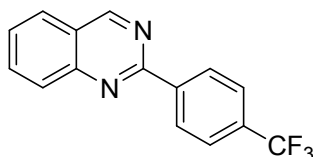


***N,N*-Dimethyl-4-(quinazolin-2-yl)aniline**

¹H NMR (300 MHz, Chloroform-*d*) δ 9.37 (s, 1H), 8.55 – 8.43 (m, 2H), 7.99 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.90 – 7.78 (m, 2H), 7.55 – 7.46 (m, 1H), 6.87 – 6.77 (m, 2H), 3.07 (s, 6H).

¹³C NMR (75 MHz, CDCl₃) δ 161.50, 160.25, 152.16, 150.02, 133.84, 129.90, 128.22, 127.15, 126.12, 124.98, 111.79, 40.30.

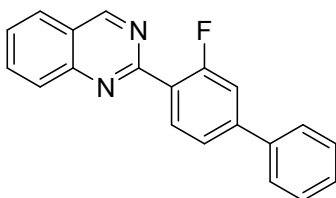
MS (EI, 70 eV): *m/z* (%) = 249 ([*M*]⁺, 100), 233 (04), 145 (08).



2-(4-(Trifluoromethyl)phenyl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.50 (s, 1H), 8.75 (dq, *J* = 8.8, 0.9 Hz, 2H), 8.12 (dq, *J* = 8.2, 1.0 Hz, 1H), 8.02 – 7.90 (m, 2H), 7.83 – 7.76 (m, 2H), 7.69-7.65 (m, 1H).

¹³C NMR (75 MHz, CDCl₃) δ 161.6, 158.4, 149.7, 141.2, 135.1, 130.7, 150.5, 128.7, 128.4, 128.0, 127.9, 125.8, 125.7, 125.3, 123.6, 123.1.

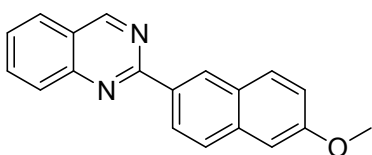


2-(3-Fluoro-[1,1'-biphenyl]-4-yl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.41 (s, 1H), 8.46 – 8.30 (m, 2H), 8.04 (dq, *J* = 8.2, 1.0 Hz, 1H), 7.92 – 7.81 (m, 2H), 7.64 – 7.51 (m, 4H), 7.47 – 7.29 (m, 3H).

¹⁹F NMR (282 MHz, Chloroform-*d*) δ -116.50 .

MS (EI, 70 eV): *m/z* (%) = 300 ([*M*]⁺, 100), 272 (05), 197 (05), 170 (03), 150 (02).

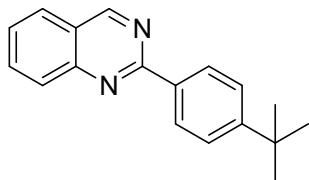


2-(6-Methoxynaphthalen-2-yl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.42 (s, 1H), 9.01 (s, 1H), 8.62 (dd, *J* = 8.6, 1.8 Hz, 1H), 8.04 (dq, *J* = 8.2, 1.0 Hz, 1H), 7.91 – 7.76 (m, 3H), 7.61 – 7.28 (m, 2H), 7.16 – 7.07 (m, 2H), 3.89 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) 161.22, 160.51, 158.76, 150.91, 136.12, 134.17, 133.33, 130.85, 128.90, 128.81, 128.58, 127.21, 127.15, 127.12, 126.05, 123.58, 119.14, 105.77, 55.39.

MS (EI, 70 eV): m/z (%) = 286 ([M]⁺, 100), 243 (40), 140 (10).

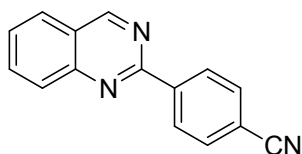


2-(4-(*tert*-Butyl)phenyl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.35 (s, 1H), 8.35 (d, *J* = 8.4 Hz, 2H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.68 – 7.56 (m, 2H), 7.53 – 7.39 (m, 3H), 1.21 (s, 9H).

¹³C NMR (75 MHz, CDCl₃) 161.20, 159.48, 152.99, 150.84, 135.39, 134.02, 128.67, 128.38, 127.26, 127.03, 125.58, 123.42, 34.93, 31.33.

MS (EI, 70 eV): m/z (%) = 262 ([M]⁺, 20), 247 (100), 231 (05), 193 (08), 166 (06).

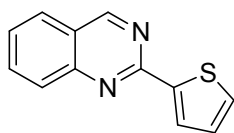


4-(Quinazolin-2-yl)benzonitrile

¹H NMR (400 MHz, Chloroform-*d*) δ 9.50 (s, 1H), 8.81 – 8.69 (m, 2H), 8.12 (dq, *J* = 8.3, 1.0 Hz, 1H), 8.01 – 7.92 (m, 2H), 7.86 – 7.78 (m, 2H), 7.72–7.68 (m, 1H).

¹³C NMR (75 MHz, CDCl₃) 160.72, 150.4, 142.16, 134.57, 132.43, 129.05, 128.84, 128.20, 127.24, 123.91, 118.92, 113.84.

MS (EI, 70 eV): m/z (%) = 231 ([M]⁺, 100), 204 (40), 177 (03), 102 (04), 76 (10), 50 (05).

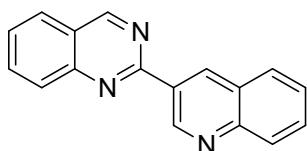


2-(Thiophen-2-yl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.45 (s, 1H), 8.14–8.16 (m, 1H), 8.01 (d, *J* = 8.7 Hz, 1H), 7.85–7.90 (m, 2H), 7.51–7.59 (m, 2H), 7.18–7.21 (m, 1H);

¹³C NMR (75 MHz, CDCl₃) δ 160.5, 158.9, 151.7, 143.9, 134.3, 129.9, 129.2, 128.3, 128.3, 127.2, 127.6, 123.4.

MS (EI, 70 eV): m/z (%) = 212 ([M]⁺, 100), 185 (13).

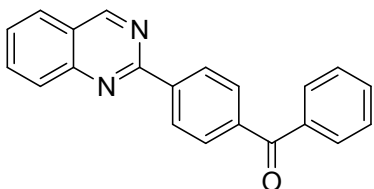


2-(Quinolin-3-yl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 10.13 (s, 1H), 9.53 (s, 1H), 9.38 (s, 1H), 8.23 – 8.13 (m, 2H), 8.07 – 7.91 (m, 3H), 7.81-7.97 (m, 1H), 7.64 (m, 2H).

¹³C NMR (75 MHz, CDCl₃) 160.75, 159.30, 150.74, 150.70, 149.02, 136.26, 134.52, 130.67, 130.56, 129.38, 129.00, 128.73, 127.84, 127.80, 127.30, 127.00, 123.87.

MS (EI, 70 eV): *m/z* (%) = 257 ([M]⁺, 100), 229 (10), 128 (03).

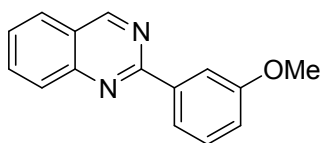


Phenyl(4-(quinazolin-2-yl)phenyl)methanone

¹H NMR (300 MHz, DMSO-*d*₆) δ 9.68 (s, 1H), 8.56 – 8.42 (m, 2H), 8.15 (dt, *J* = 8.1, 1.0 Hz, 1H), 8.07 – 7.97 (m, 2H), 7.74-7.70 (m, 1H), 7.58 (d, *J* = 8.3 Hz, 2H), 7.47 – 7.39 (m, 2H), 7.37 – 7.28 (m, 2H), 7.25 – 7.17 (m, 1H).

¹³C (75 MHz, DMSO-*d*₆) 202.11, 161.73, 150.31, 148.93, 145.82, 136.45, 135.27, 128.63, 128.46, 128.28, 127.32, 127.00, 126.81, 123.75.

MS (EI, 70 eV): *m/z* (%) = 310 ([M]⁺, 94), 233 (100), 205 (20), 105 (15), 77 (14).

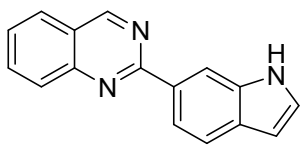


2-(3-Methoxyphenyl)quinazoline

¹H NMR (300 MHz, Chloroform-*d*) δ 9.40 (s, 1H), 8.19 – 8.08 (m, 2H), 8.03 (dq, *J* = 8.3, 0.8 Hz, 1H), 7.91 – 7.78 (m, 2H), 7.57-7.53 (m, 1H), 7.38 (dd, *J* = 8.3, 7.6 Hz, 1H), 7.03-6.98 (m, 1H), 3.89 (s, 3H).

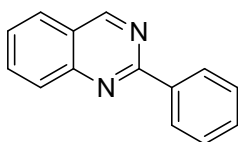
¹³C NMR (75 MHz, CDCl₃): δ 160.61, 160.38, 160.02, 150.12, 137.56, 133.15, 129.67, 128.70, 127.34, 127.18, 123.68, 121.19, 117.19, 113.04, 55.29.

MS (EI, 70 eV): *m/z* (%) = 236 ([M]⁺, 100), 206 (15), 192 (04), 179 (06), 103 (02).

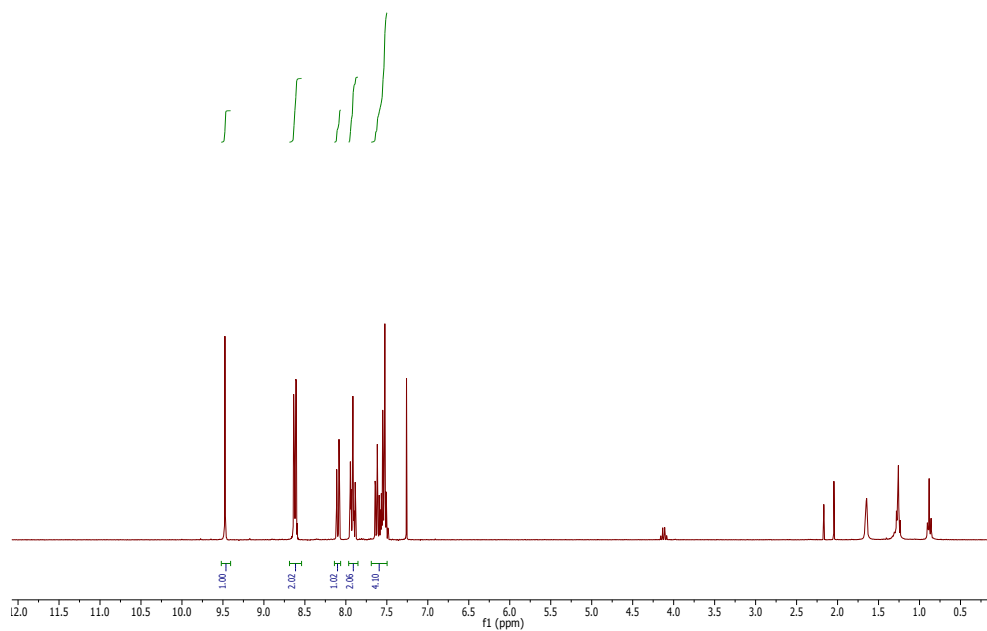


¹H NMR (300 MHz, DMSO-*d*₆) δ 9.65 (s, 1H), 8.87 – 8.83 (s, 1H), 8.36 (d, *J* = 1.6 Hz, 1H), 8.04 – 7.96 (m, 1H), 7.75 (dd, *J* = 8.6, 1.7 Hz, 1H), 7.54 (t, *J* = 0.8 Hz, 2H), 7.47 (d, *J* = 0.7 Hz, 1H), 7.45 – 7.40 (m, 1H), 6.61 (d, *J* = 1.0 Hz, 1H).

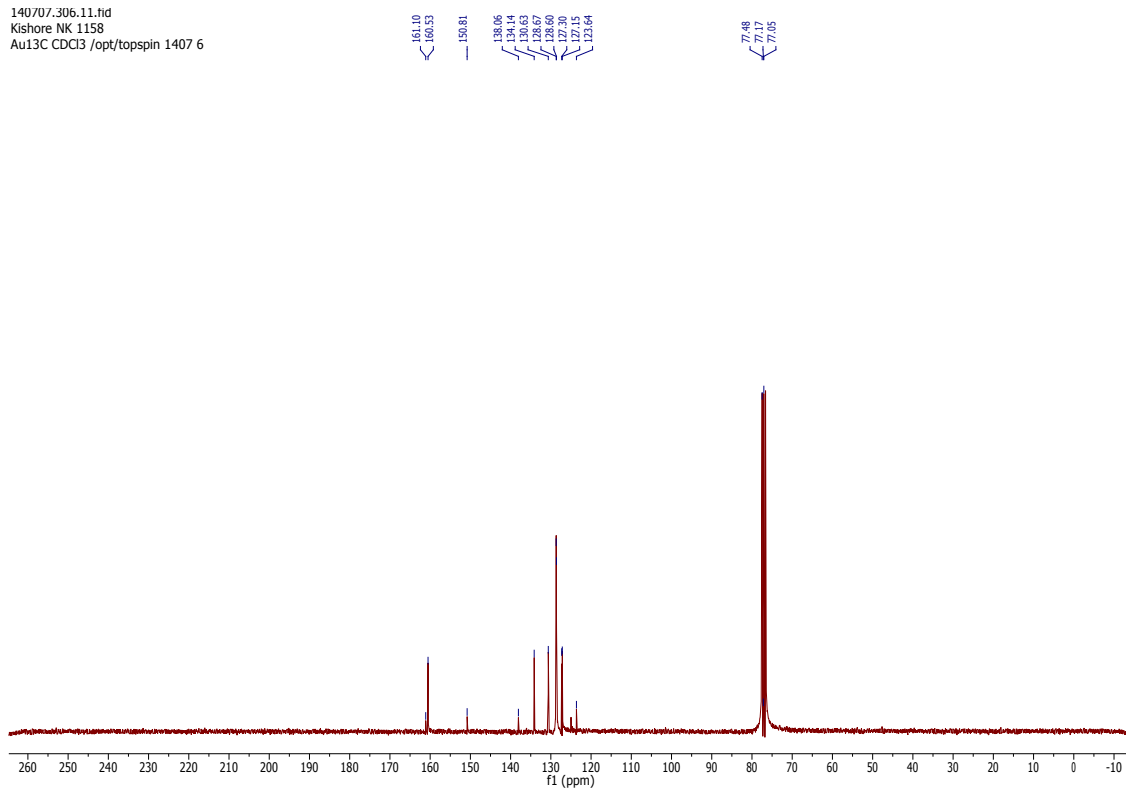
MS (EI, 70 eV): *m/z* (%) = 245 ([M]⁺, 100), 218 (15), 209 (07), 207 (04), 190 (03), 142 (08), 122 (05).

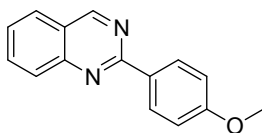


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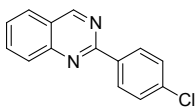
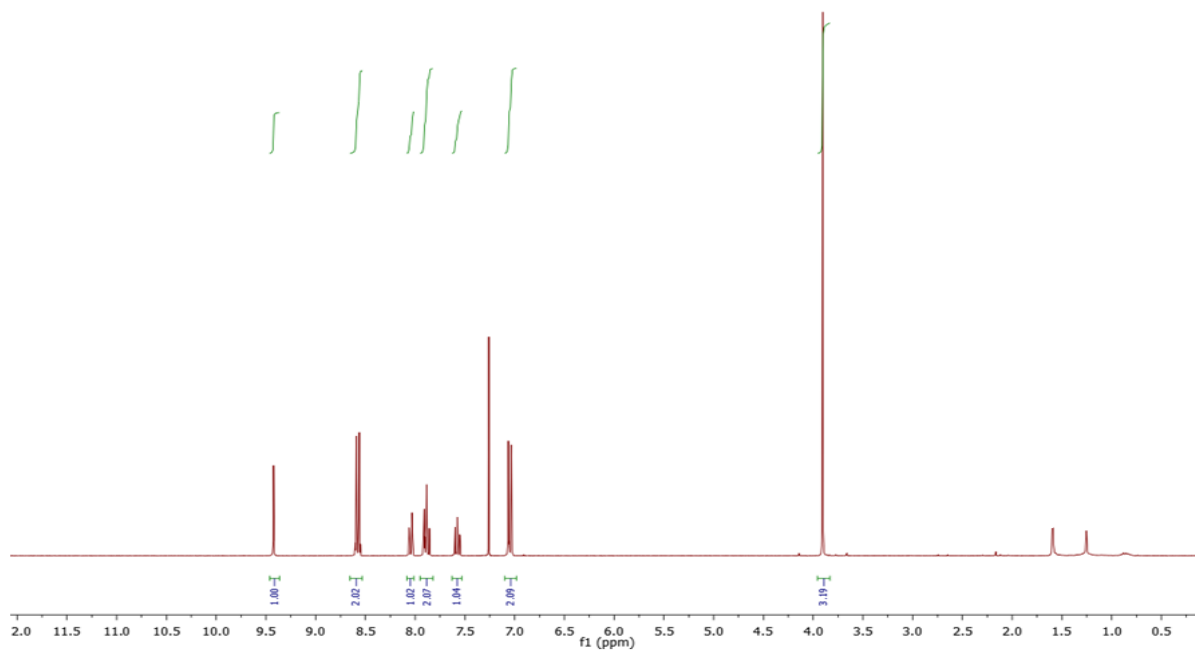


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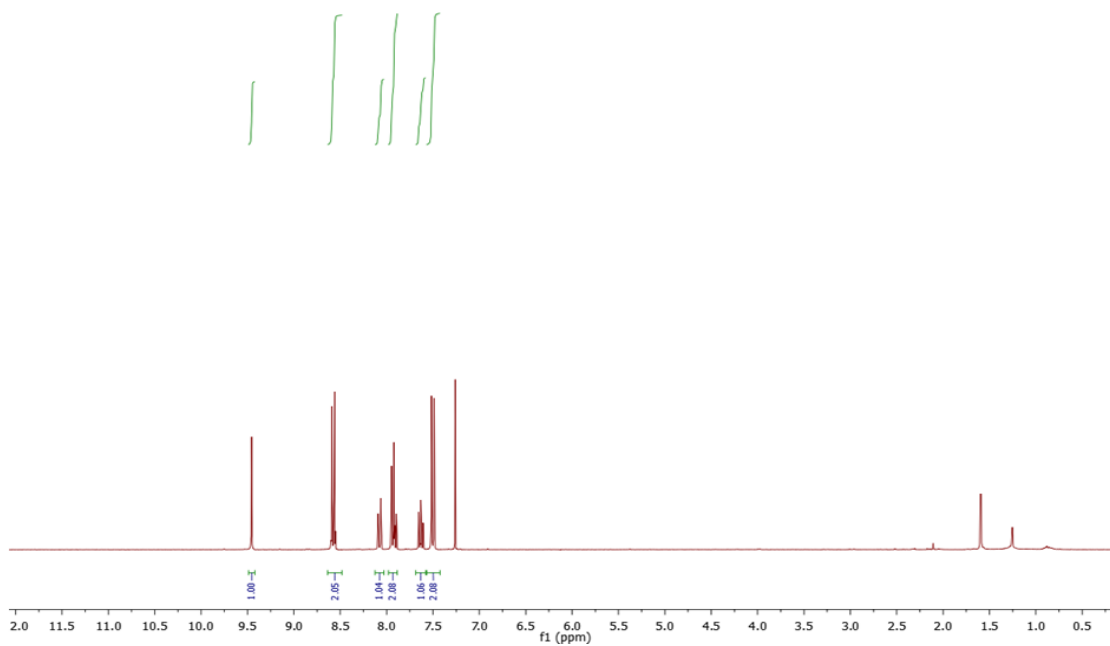




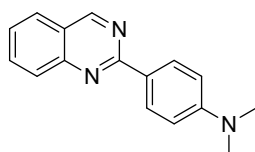
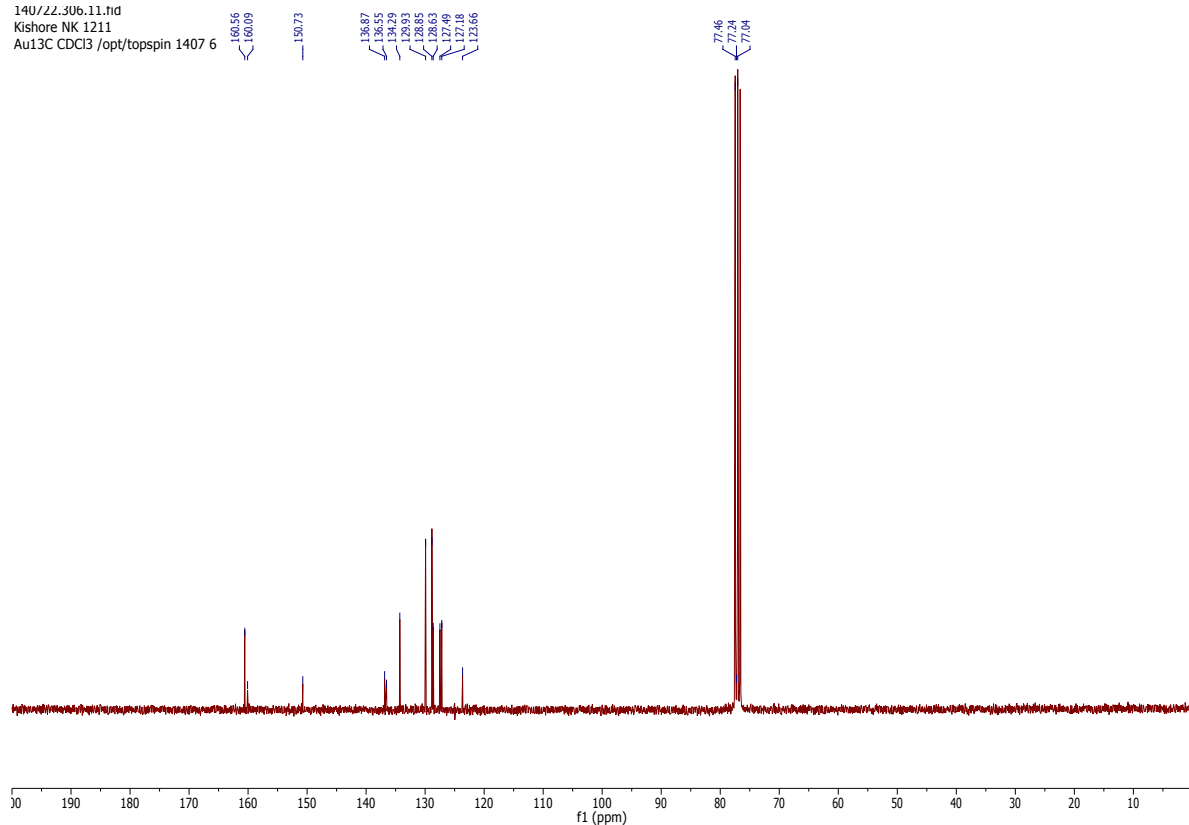
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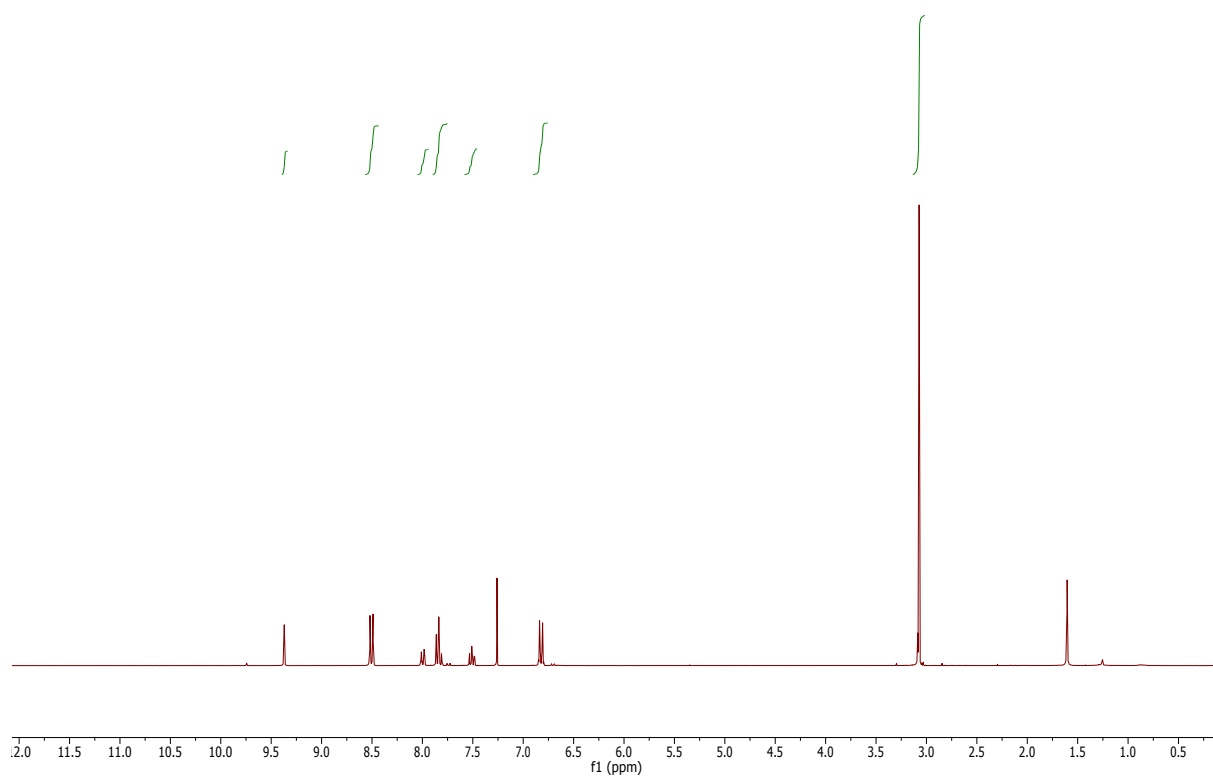
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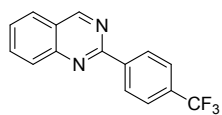


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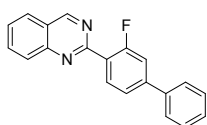
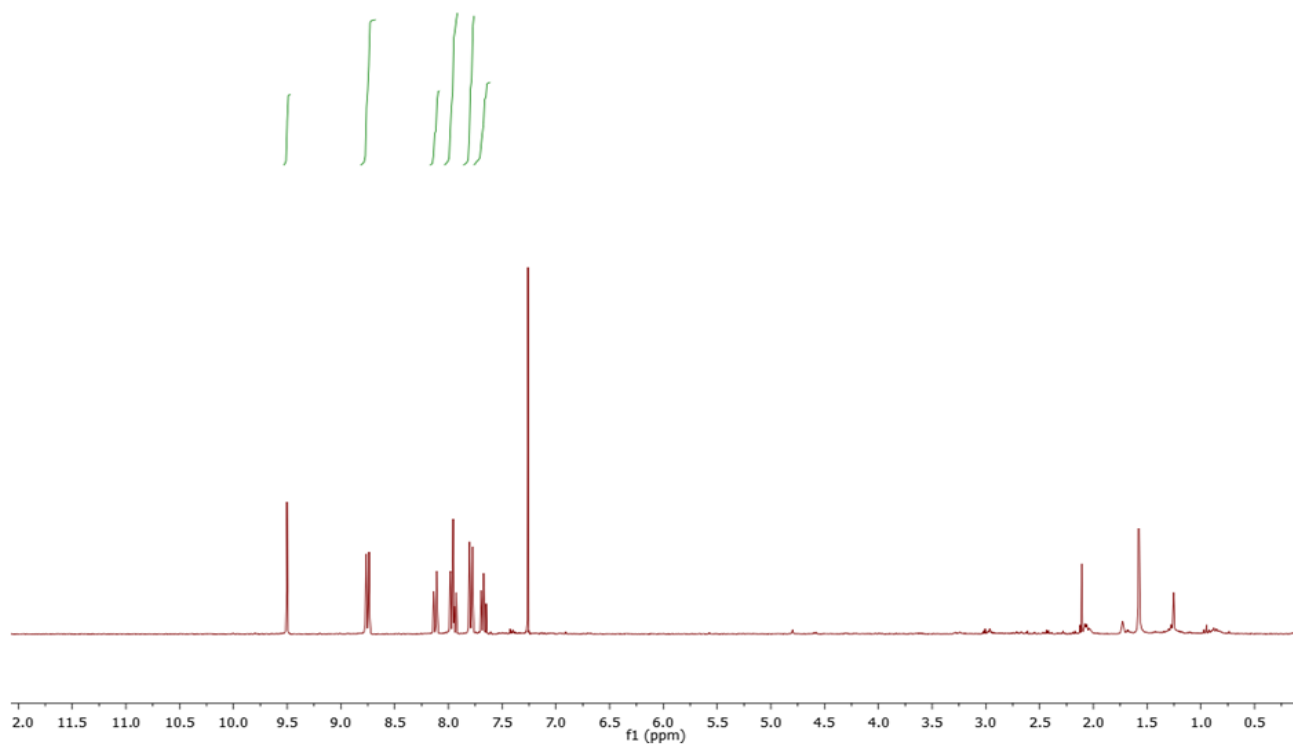


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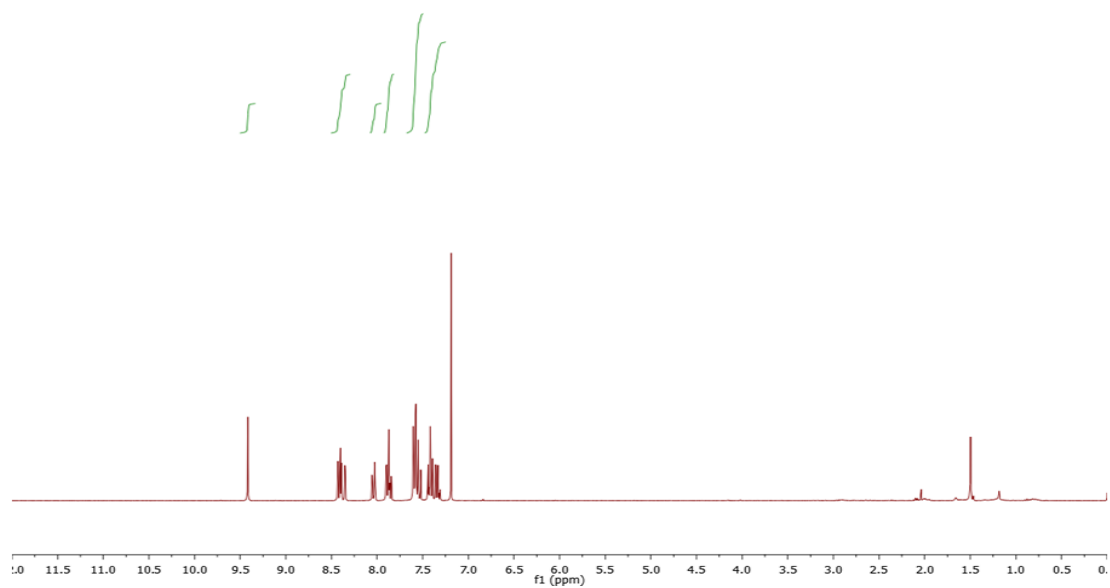


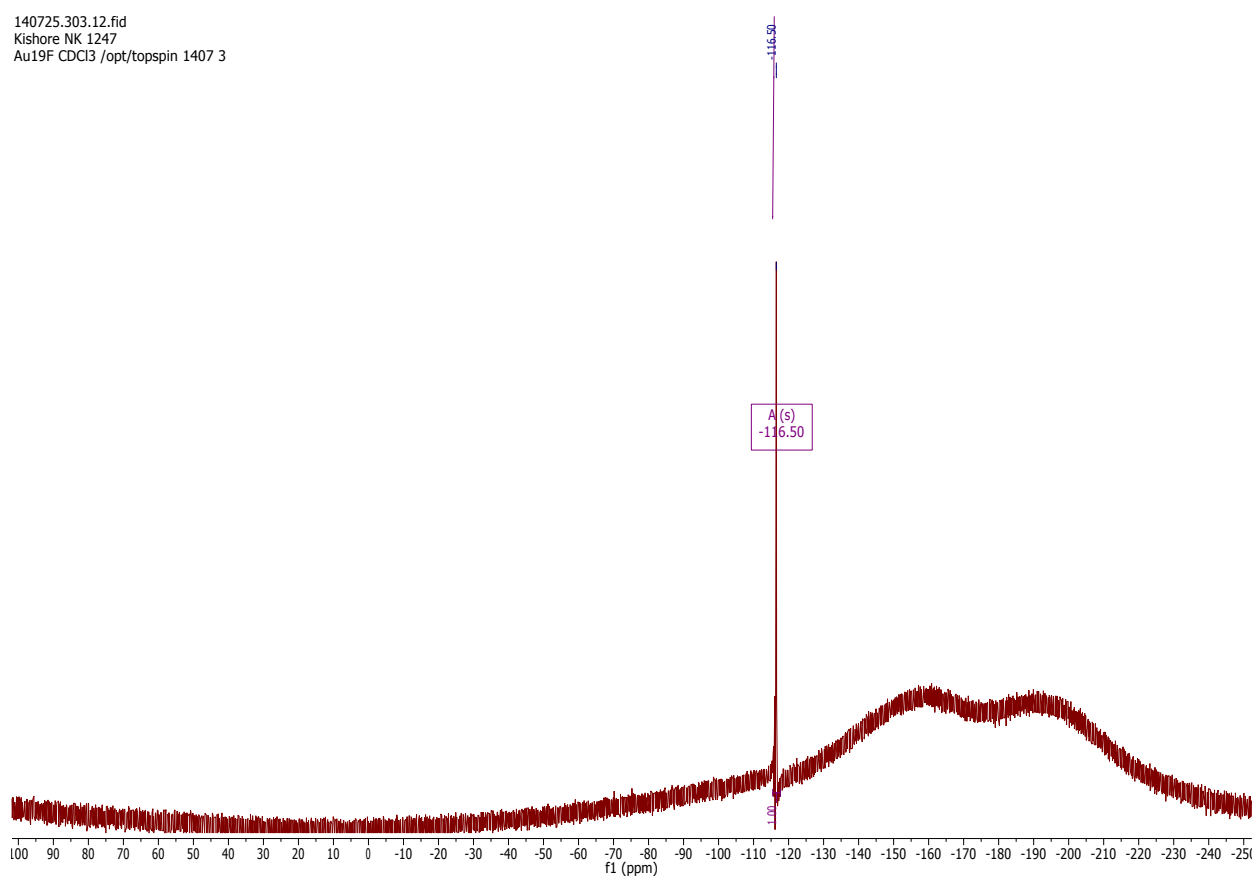
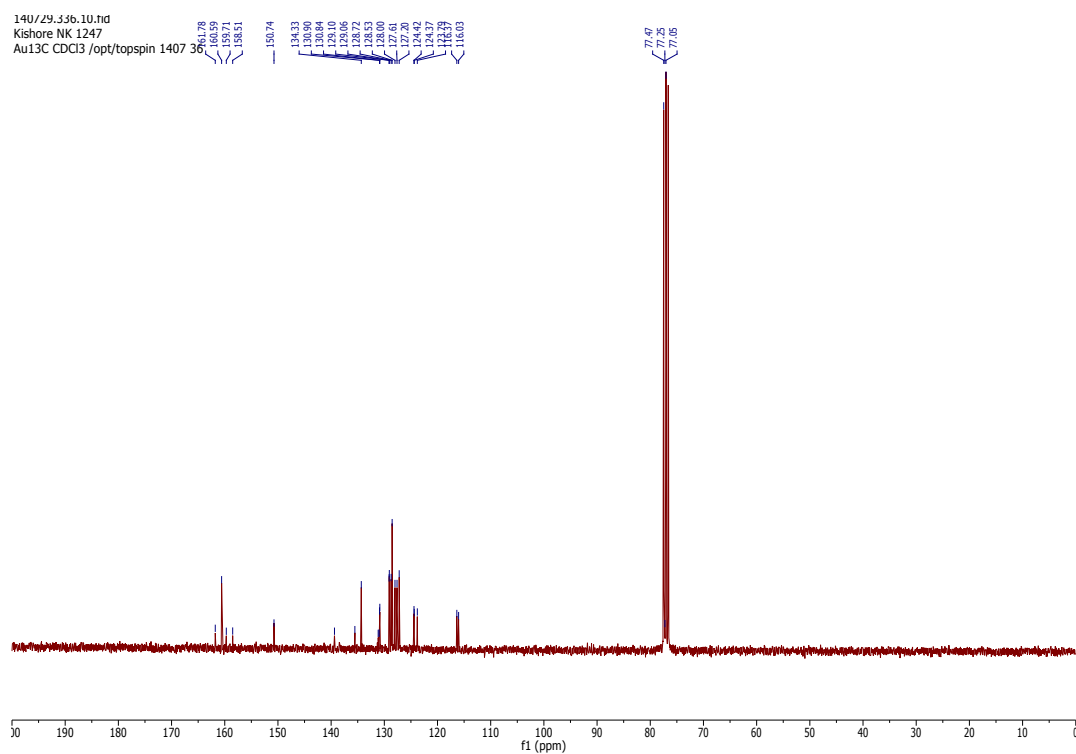


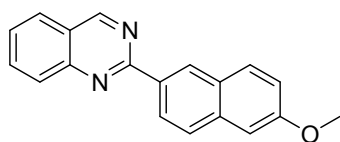
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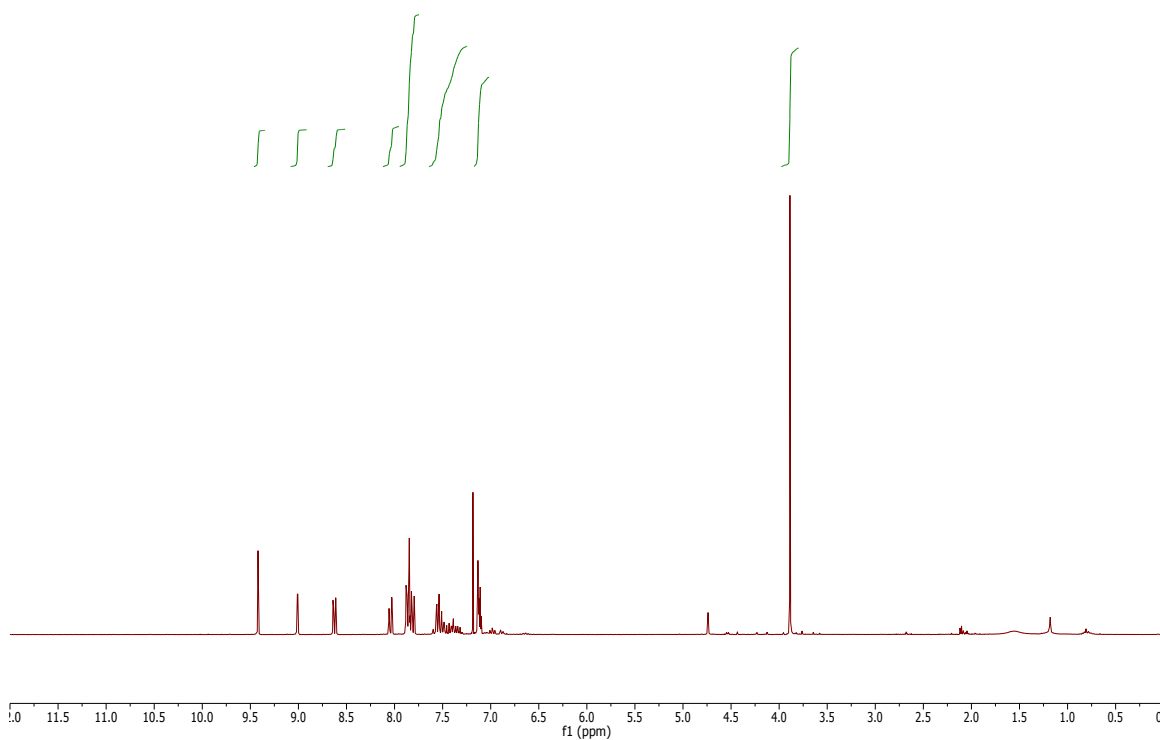
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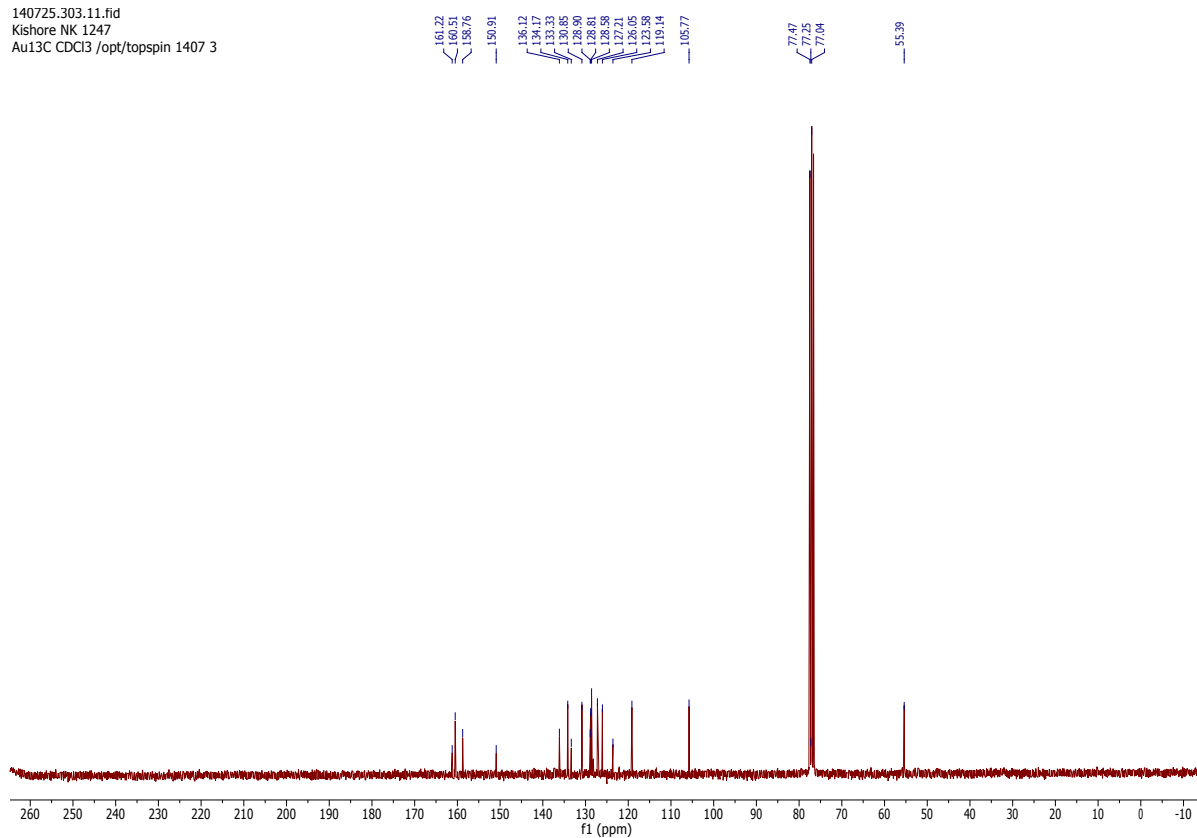


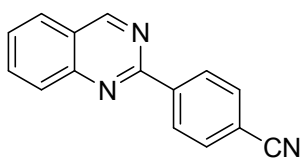


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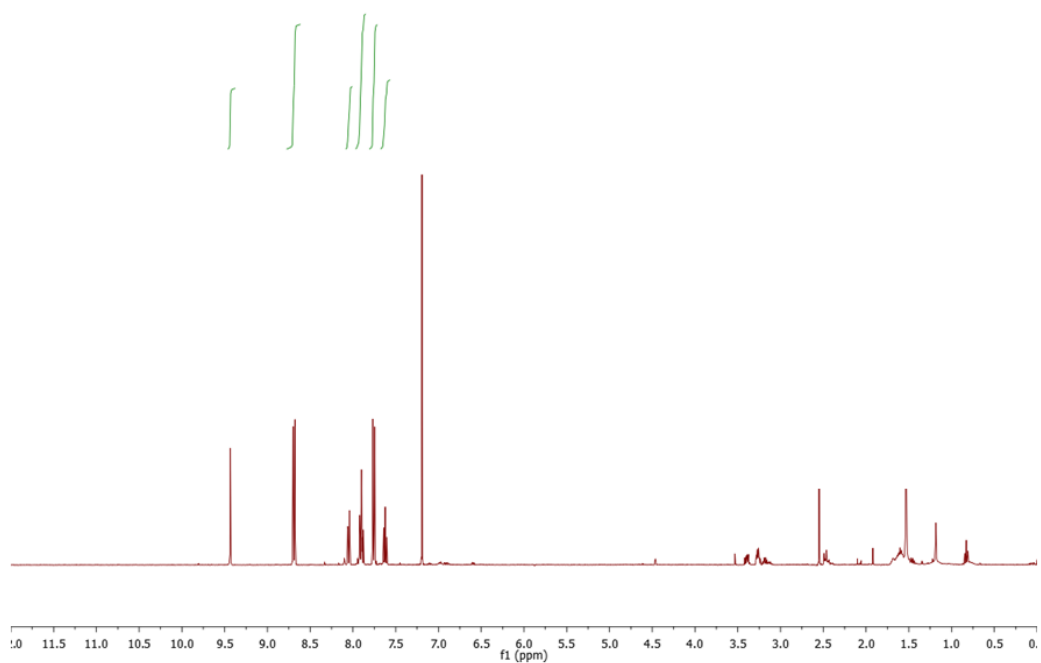


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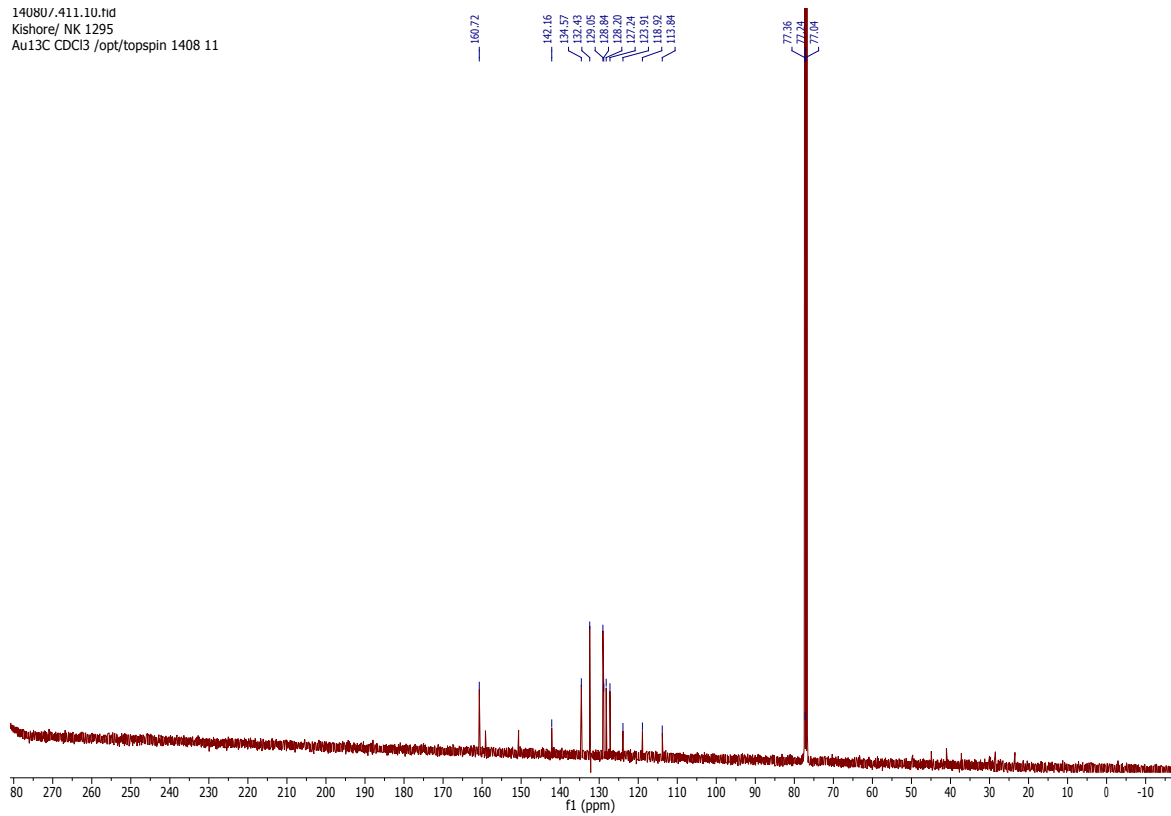


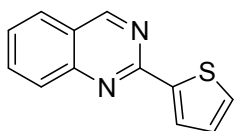


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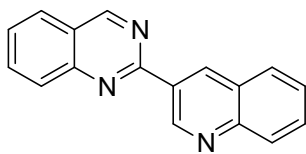
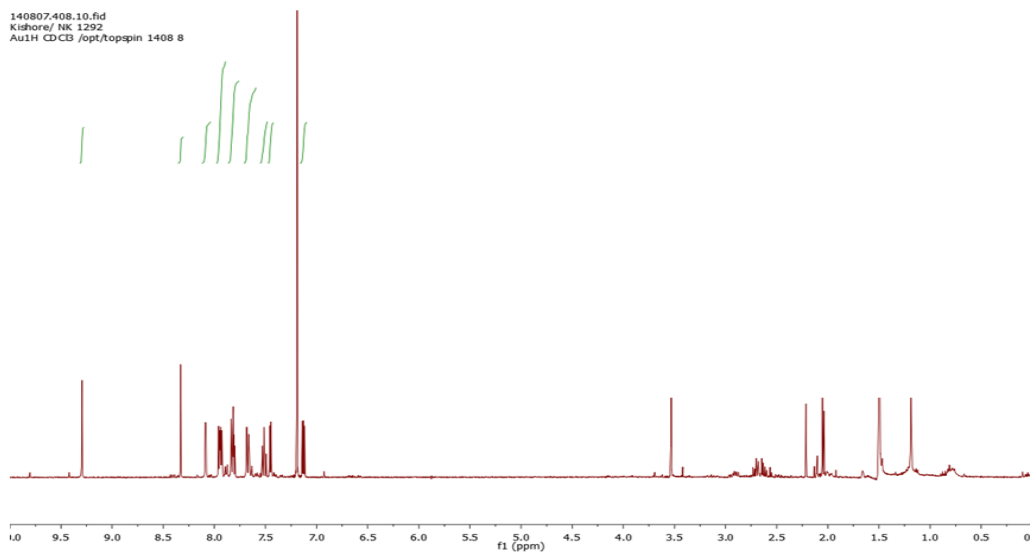


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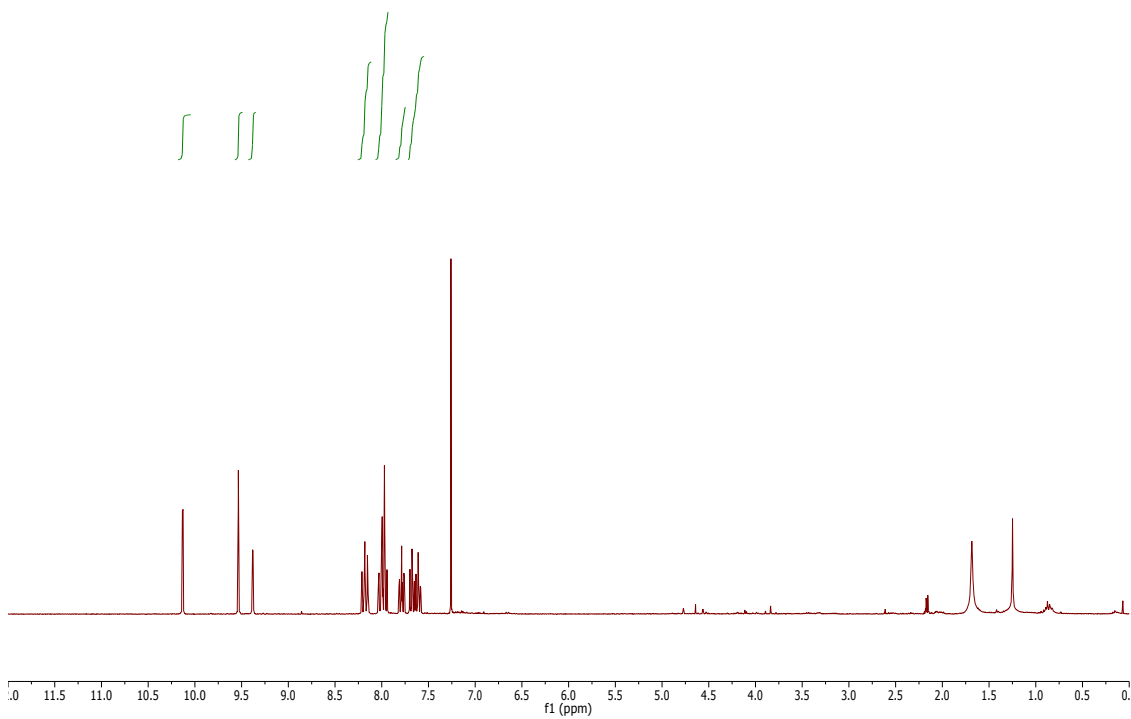




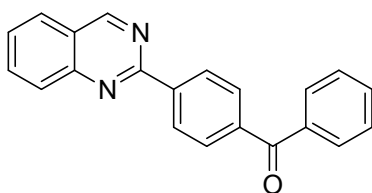
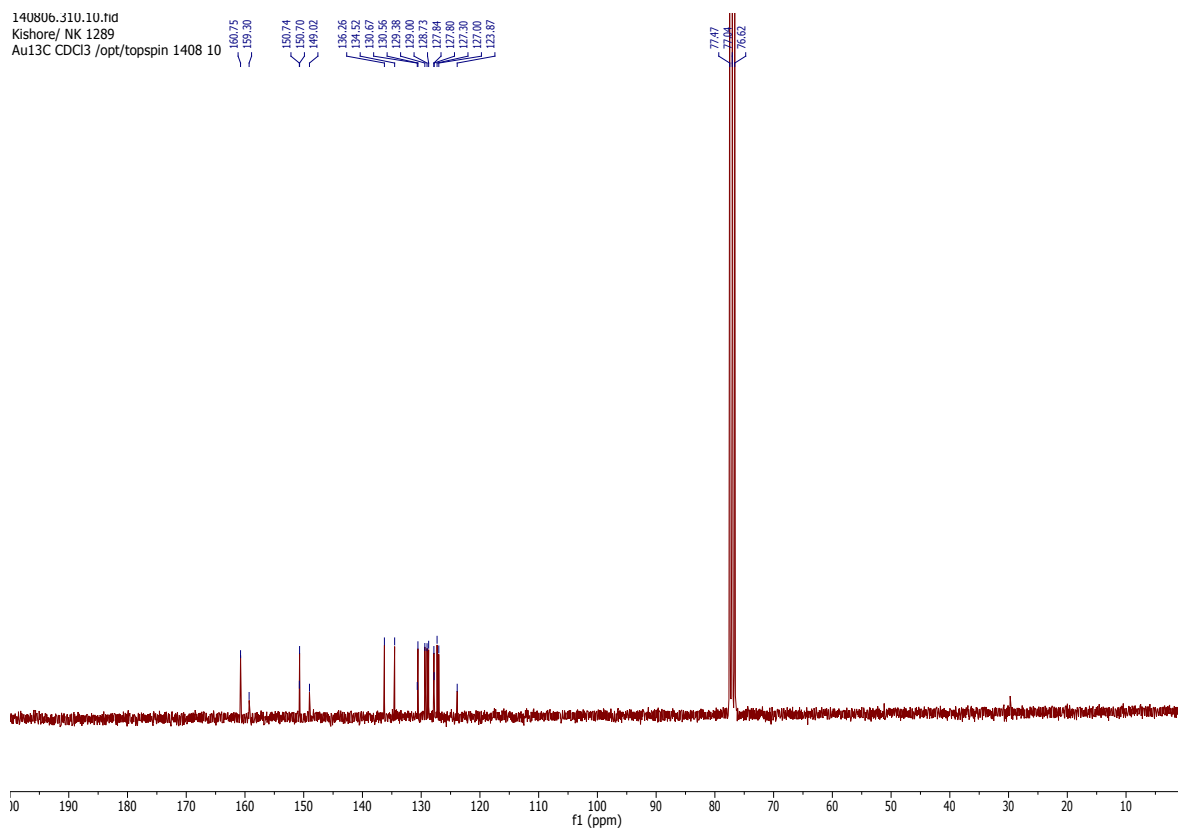
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