Experimental section

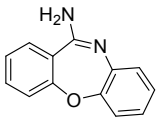
General comments

All reactions were carried out under air. Reactions were monitored by TLC analysis (pre-coated silica gel plates with fluorescent indicator UV254, 0.2 mm) and visualized with 254 nm UV light. Chemicals were purchased from Aldrich, Alfa-Asar, TCI and unless otherwise noted were used without further purification. All compounds were characterized by ^{1}H NMR and ^{13}C NMR spectroscopy and recorded on Bruker AV 300 and AV 400spectrometers. GC was performed on Agilent 6890 chromatograph with a 30 m HP5 column.

General procedure for the synthesis of dibenzo[*b,f*][1,4]oxazepin-11-amine

In a 25 mL pressure tube equipped with a stirring bar, 2-fluorobenzonitrile (1 mmol), 2-aminophenol (1.5 mmol), K_3PO_4 (2 equiv.) and DMF (2 mL) were added. Then close the tube and heat it up to 100 ℃ for 6 h., Cool the reaction mixture to room temperature when the reaction completed. The reaction solution was quenched with distilled water and extracted with ethyl acetate three times. The combined organic phases were washed with saturated NaCl solution and dried over Na_2SO_4. The crude product was purified by column chromatography (ethyl acetate/pentane = 1:6) to give the pure product.

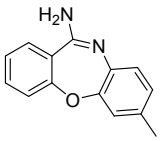
Dibenzo[*b,f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.62 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.42 (ddd, *J* = 8.9, 7.5, 1.7 Hz, 1H), 7.07 (dtd, *J* = 11.8, 7.5, 1.2 Hz, 2H), 6.88 (ddd, *J* = 19.0, 8.0, 1.5 Hz, 2H), 6.82 – 6.68 (m, 2H), 3.83 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.71, 141.17, 139.10, 134.54, 133.83, 126.56, 122.62, 121.24, 118.95, 117.12, 116.26, 115.50, 102.59.

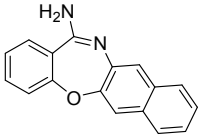
7-Methyldibenzo[*b,f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.62 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.43 (ddd, *J* = 8.5, 7.5, 1.7 Hz, 1H), 7.08 (td, *J* = 7.6, 1.0 Hz, 1H), 6.86 (ddd, *J* = 8.2, 2.0, 0.8 Hz, 1H), 6.82 – 6.69 (m, 3H), 3.68 (s, 2H), 2.22 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.77, 141.06, 136.35, 134.46, 133.72, 128.73, 127.04, 122.44, 121.66, 117.11, 116.22, 115.47, 102.47, 20.46 (d, *J* = 2.4 Hz).

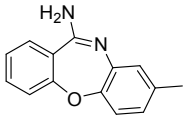
Benzo[*f*]naphtho[2,3-*b*][1,4]oxazepin-13-amine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.76 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.72 – 7.62 (m, 2H), 7.54 (ddd, *J* = 9.0, 7.6, 1.7 Hz, 1H), 7.45 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.38 (s, 1H), 7.33 (ddd, *J* = 8.2, 6.9, 1.2 Hz, 1H), 7.28 – 7.19 (m, 2H), 7.00 (dd, *J* = 8.5, 1.0 Hz, 1H), 4.28 – 4.07 (m, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.27, 143.70, 137.67, 134.53, 133.91, 132.48, 127.89, 127.17, 126.01, 123.91 – 122.75 (m), 125.69, 123.35, 123.29, 117.09, 116.80, 115.99, 111.18, 103.53.

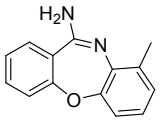
8-Methyldibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.63 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.43 (ddd, *J* = 8.7, 7.5, 1.7 Hz, 1H), 7.07 (td, *J* = 7.6, 1.0 Hz, 1H), 6.85 – 6.75 (m, 2H), 6.68 (dd, *J* = 2.1, 1.0 Hz, 1H), 6.57 (ddd, *J* = 8.2, 1.9, 0.9 Hz, 1H), 3.71 (s, 2H), 2.28 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.95, 139.04, 138.37, 136.37, 134.37, 133.72, 122.30, 121.13, 119.83, 117.68, 116.19, 115.19, 102.41, 21.07 (d, *J* = 2.7 Hz).

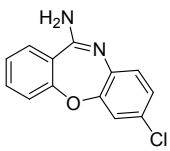
9-Methyldibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.62 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.42 (ddd, *J* = 8.6, 7.5, 1.7 Hz, 1H), 7.08 (td, *J* = 7.6, 1.0 Hz, 1H), 6.95 (ddd, *J* = 7.5, 1.5, 0.8 Hz, 1H), 6.81 – 6.76 (m, 2H), 6.70 – 6.63 (m, 1H), 3.77 (s, 2H), 2.22 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.78, 140.95, 137.31, 134.46, 133.75, 127.46, 124.67, 122.52, 118.58, 117.96, 116.22, 102.59, 17.40 (d, *J* = 3.0 Hz).

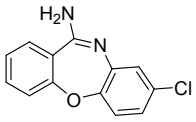
7-Chlorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.67 – 7.56 (m, 1H), 7.46 (ddd, *J* = 8.5, 7.5, 1.7 Hz, 1H), 7.13 (td, *J* = 7.6, 1.0 Hz, 1H), 6.98 (dd, *J* = 8.5, 2.3 Hz, 1H), 6.87 (d, *J* = 2.3 Hz, 1H), 6.85 – 6.74 (m, 2H), 3.88 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.86, 141.48, 137.76, 134.64, 133.90, 126.26, 123.25, 122.56, 120.83, 117.57, 115.93, 102.96.

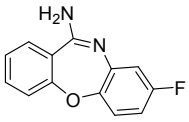
8-Chlorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.65 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.47 (ddd, *J* = 9.0, 7.6, 1.7 Hz, 1H), 7.13 (td, *J* = 7.6, 1.0 Hz, 1H), 6.89 – 6.77 (m, 3H), 6.71 (dt, *J* = 8.7, 2.2 Hz, 1H), 3.89 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.21, 139.90, 139.78, 134.50, 133.88, 131.40, 122.94, 121.99, 118.64, 116.56, 115.93, 115.48, 102.83.

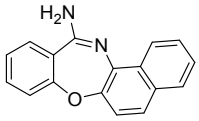
8-Fluorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.64 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.46 (ddd, *J* = 8.6, 7.5, 1.7 Hz, 1H), 7.11 (td, *J* = 7.6, 1.0 Hz, 1H), 6.88 (dd, *J* = 8.8, 5.3 Hz, 1H), 6.83 – 6.74 (m, 1H), 6.57 (dd, *J* = 9.8, 2.9 Hz, 1H), 6.44 (ddd, *J* = 8.9, 8.0, 2.9 Hz, 1H), 3.90 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 162.42 , 159.43 (d, *J* = 32.5 Hz), 140.22 (d, *J* = 11.6 Hz), 137.02 (d, *J* = 2.6 Hz), 134.48, 133.84, 122.67, 122.30 (d, *J* = 10.5 Hz), 116.02, 115.05, 105.15 (d, *J* = 24.0 Hz), 103.54 (d, *J* = 26.6 Hz), 102.52.

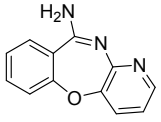
Benzo[*f*]naphtho[2,1-*b*][1,4]oxazepin-12-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.84 (dddd, *J* = 6.0, 4.5, 2.6, 1.5 Hz, 2H), 7.71 – 7.64 (m, 1H), 7.54 – 7.46 (m, 2H), 7.44 – 7.28 (m, 2H), 7.17 – 7.03 (m, 2H), 6.77 – 6.70 (m, 1H), 4.24 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.95, 135.91, 134.48, 133.87, 133.58, 132.16, 128.67, 125.76, 125.62, 124.55, 122.50, 120.99, 120.65, 119.22, 116.33, 115.22, 102.49.

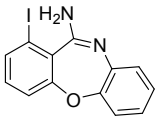
Benzo[*f*]pyrido[3,2-*b*][1,4]oxazepin-10-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.96 (dd, *J* = 5.0, 1.5 Hz, 1H), 7.67 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.50 (ddd, *J* = 8.5, 7.5, 1.7 Hz, 1H), 7.23 – 7.10 (m, 2H), 6.89 – 6.80 (m, 1H), 6.68 (dd, *J* = 7.8, 5.0 Hz, 1H), 4.82 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.48, 151.83, 144.44, 136.92, 134.54, 134.03, 127.30, 123.47, 116.01, 115.65, 114.18, 103.47.

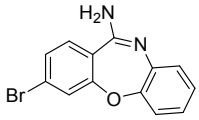
1-Iododibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.64 – 7.51 (m, 1H), 7.17 – 7.01 (m, 2H), 6.93 (dt, *J* = 8.1, 1.1 Hz, 1H), 6.86 (dt, *J* = 8.0, 1.3 Hz, 1H), 6.75 (dtd, *J* = 7.9, 3.7, 1.4 Hz, 2H), 3.75 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.15, 140.80, 138.90, 134.79, 132.85, 126.87, 121.31, 119.04, 117.22, 116.83, 114.56, 110.71, 99.48.

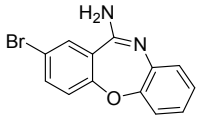
3-Bromodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.54 (dd, *J* = 8.7, 7.3 Hz, 1H), 7.12 (ddd, *J* = 7.9, 7.3, 1.5 Hz, 1H), 6.95 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.89 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.87 – 6.78 (m, 2H), 6.75 (dd, *J* = 10.5, 2.4 Hz, 1H), 3.84 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 160.04 , 140.54 , 138.66 , 134.42 , 128.98 , 127.04 , 126.02 , 121.34 , 119.31 , 118.75 , 117.36 , 115.44 , 101.51 .

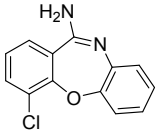
2-Bromodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.72 (d, *J* = 2.4 Hz, 1H), 7.51 (dd, *J* = 9.0, 2.4 Hz, 1H), 7.07 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H), 6.92 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.76 (ddd, *J* = 8.0, 7.3, 1.6 Hz, 1H), 6.68 (d, *J* = 9.0 Hz, 1H), 3.79 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.90, 140.81, 138.91, 137.40, 135.80 (d, *J* = 1.6 Hz), 126.88, 121.17, 119.07, 117.21, 117.07, 114.74, 114.18, 104.25.

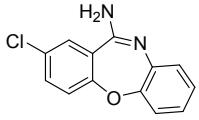
4-Chlorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (dd, *J* = 8.1, 1.6 Hz, 1H), 7.60 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.26 (t, *J* = 8.0 Hz, 1H), 6.94 (ddd, *J* = 7.9, 7.3, 1.3 Hz, 1H), 6.85 (dd, *J* = 7.9, 1.6 Hz, 1H), 6.62 (ddd, *J* = 8.1, 7.3, 1.6 Hz, 1H), 6.37 (dd, *J* = 8.1, 1.3 Hz, 1H), 4.09 (s, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 153.55, 144.82, 136.82, 135.71, 132.43, 129.25, 126.33, 124.29, 118.24, 116.65, 114.72, 114.10, 109.69.

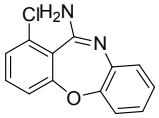
2-Chlorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 (d, *J* = 2.6 Hz, 1H), 7.40 (ddd, *J* = 9.1, 2.6, 0.5 Hz, 1H), 7.10 (tdd, *J* = 7.3, 1.4, 0.5 Hz, 1H), 6.92 (ddd, *J* = 21.6, 8.0, 1.5 Hz, 2H), 6.86 – 6.70 (m, 2H), 3.97 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.42, 140.89, 139.00, 134.56, 132.95, 127.38, 126.87, 121.17, 119.04, 117.21, 116.79, 114.92, 103.78.

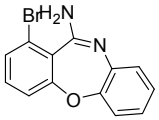
1-Chlorodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.35 (dd, *J* = 8.6, 8.1 Hz, 1H), 7.19 – 7.03 (m, 2H), 6.95 (dd, *J* = 8.1, 1.5 Hz, 1H), 6.87 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.78 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H), 6.69 (dd, *J* = 8.6, 0.9 Hz, 1H), 3.78 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.13, 140.87, 138.69, 138.01, 134.32, 126.93, 123.27, 121.40, 119.25, 117.32, 113.32, 113.26, 103.93.

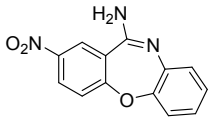
1-Bromodibenzo[*b*,*f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.40 – 7.27 (m, 2H), 7.08 (ddd, *J* = 8.0, 7.3, 1.5 Hz, 1H), 6.94 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.87 (dd, *J* = 8.0, 1.6 Hz, 1H), 6.81 – 6.70 (m, 2H), 3.83 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 161.36 , 140.71 , 139.00 , 134.69 , 126.97 , 126.42 , 126.27 , 121.36 , 119.01 , 117.24 , 114.65 , 113.81 , 106.12 .

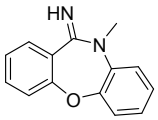
2-Nitrodibenzo[*b,f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, DMSO-*d*^{6}) δ 9.86 (s, 1H), 9.05 (s, 1H), 8.49 (d, *J* = 2.7 Hz, 1H), 8.16 (dd, *J* = 9.5, 2.7 Hz, 1H), 7.24 – 7.11 (m, 2H), 6.98 (dd, *J* = 8.0, 1.4 Hz, 1H), 6.87 (td, *J* = 7.6, 1.4 Hz, 1H), 6.54 (d, *J* = 9.5 Hz, 1H).

^{13}C NMR (75 MHz, DMSO-*d*^{6}) δ 153.23, 152.39, 136.72, 130.65, 129.16, 128.01, 127.58, 124.91, 119.52, 116.52, 115.96, 114.13, 94.78.

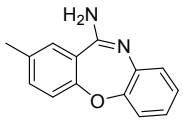
10-Methyldibenzo[*b,f*][1,4]oxazepin-11(10*H*)-imine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.63 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.42 (dddd, *J* = 8.3, 7.6, 1.7, 0.7 Hz, 1H), 7.22 – 7.02 (m, 2H), 6.98 – 6.88 (m, 1H), 6.77 (ddd, *J* = 8.1, 5.0, 1.2 Hz, 2H), 6.74 – 6.63 (m, 1H), 4.15 (s, 1H), 2.83 (d, *J* = 0.7 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.86, 141.79, 140.90, 134.48, 133.77, 126.75, 122.54, 120.45, 116.73, 116.23, 115.43, 111.57, 102.61, 30.28.

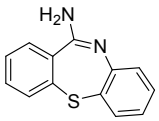
2-Methyldibenzo[*b,f*][1,4]oxazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.40 (dd, *J* = 2.2, 0.8 Hz, 1H), 7.22 (ddd, *J* = 8.6, 2.2, 0.8 Hz, 1H), 7.02 (td, *J* = 7.6, 1.5 Hz, 1H), 6.86 (ddd, *J* = 13.1, 8.0, 1.5 Hz, 2H), 6.77 – 6.64 (m, 2H), 3.82 (s, 2H), 2.30 (s, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 157.55, 141.66, 139.01, 135.23, 133.69, 132.48, 126.21, 120.84, 118.82, 116.99, 116.37, 115.73, 102.40, 20.32.

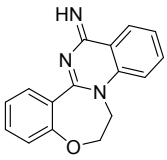
Dibenzo[*b,f*][1,4]thiazepin-11-amine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.62 (dd, *J* = 7.7, 1.5 Hz, 1H), 7.48 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.42 – 7.28 (m, 2H), 7.21 (td, *J* = 7.6, 1.1 Hz, 1H), 6.96 – 6.73 (m, 3H), 4.38 (s, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 149.39 , 142.47 , 137.84 , 133.52 , 133.18 , 132.29 , 126.38 , 125.49 , 119.05 , 117.11 , 115.80 , 111.28 , 110.22 .

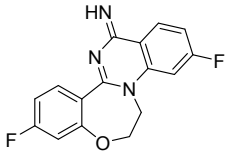
1, 2-Dihydro-9*H*-benzo[6,7][1,4]oxazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.64 – 7.48 (m, 2H), 7.48 – 7.35 (m, 2H), 7.04 (td, J = 7.6, 0.9 Hz, 1H), 7.00 – 6.94 (m, 1H), 6.88 (d, J = 8.5 Hz, 1H), 6.73 (td, J = 7.6, 0.9 Hz, 1H), 4.90 (s, 1H), 4.27 (t, J = 5.5 Hz, 2H), 3.76 (t, J = 5.5 Hz, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 160.01, 149.78, 134.50, 134.37, 133.95, 132.88, 121.47, 117.69, 117.33, 116.18, 112.30, 111.12, 102.38, 96.40, 67.80, 42.48.

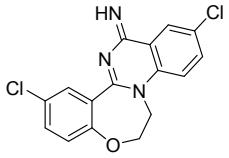
5,12-Difluoro-1,2-dihydro-9*H*-benzo[6,7][1,4]oxazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.54 (dd, J = 8.7, 7.5 Hz, 1H), 7.45 – 7.33 (m, 1H), 6.93 – 6.61 (m, 2H), 6.56 – 6.35 (m, 2H), 5.07 (s, 1H), 4.22 (t, J = 5.2 Hz, 2H), 3.76 – 3.53 (m, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 166.86(d, J = 254,2 Hz), 164.55 (d, J = 258,8 Hz), 163.28 (d, J = 10.9 Hz), 151.85 (d, J = 12.0 Hz), 135.20 (d, J = 11.7 Hz), 134.46 (d, J = 2.3 Hz), 117.05 , 114.16 , 111.67 (d, J = 2.9 Hz), 105.29 (d, J = 23.6 Hz), 102.96 (d, J = 23.0 Hz), 98.13 (d, J = 27.2 Hz), 93.97 (d, J = 15.6 Hz), 92.76, 66.89, 42.35.

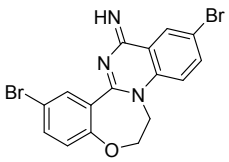
6,11-Dichloro-1,2-dihydro-9*H*-benzo[6,7][1,4]oxazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.59 – 7.45 (m, 2H), 7.44 – 7.32 (m, 2H), 6.89 (dd, J = 14.2, 8.9 Hz, 2H), 4.97 (s, 1H), 4.25 (t, J = 5.3 Hz, 2H), 3.74 (t, J = 5.2 Hz, 2H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.63, 148.51, 134.78, 134.44, 133.23, 131.81, 126.57, 121.89, 116.48, 114.88, 113.61, 112.67, 103.68, 97.34, 68.50, 42.65.

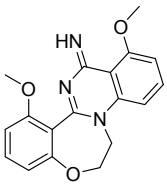
6,11-Dibromo-1,2-dihydro-9*H*-benzo[6,7][1,4]oxazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 – 7.57 (m, 1H), 7.57 – 7.41 (m, 1H), 6.83 (dd, J = 15.9, 9.0 Hz, 1H), 4.97 (s, 1H), 4.24 (t, J = 5.3 Hz, 1H), 3.75 (dd, J = 6.2, 3.3 Hz, 1H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 159.09, 148.82, 137.48, 137.29, 136.09, 134.67, 116.32, 114.71, 113.99, 113.30, 112.99, 108.31, 104.24, 98.00, 68.44, 42.60.

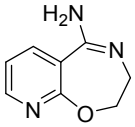
7,10-Dimethoxy-1,2-dihydro-9*H*-benzo[6,7][1,4]oxazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 (t, J = 8.5 Hz, 1H), 7.33 (t, J = 8.4 Hz, 1H), 6.57 (d, J = 8.5 Hz, 1H), 6.55 – 6.50 (m, 1H), 6.46 (d, J = 8.2 Hz, 1H), 6.24 (dd, J = 8.3, 0.7 Hz, 1H), 4.88 (s, 1H), 4.23 (d, J = 5.7 Hz, 2H), 3.90 (s, 3H), 3.86 (s, 3H), 3.72 (t, J = 5.7 Hz, 2H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 162.78, 162.36, 161.47, 151.24, 135.09, 134.72, 115.64, 113.76, 104.41, 104.08, 103.65, 99.43, 92.00, 86.38, 68.02, 56.29, 55.95, 42.61.

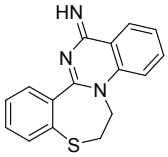
3, 4-Dihydropyrido[3,2-*f*][1,4]oxazepin-5(2*H*)-imine



^{1}H NMR (300 MHz, Chloroform-*d*) δ 8.23 (dd, J = 5.0, 1.9 Hz, 1H), 7.67 (ddd, J = 7.6, 1.9, 0.5 Hz, 1H), 6.80 – 6.43 (m, 1H), 5.70 (s, 1H), 3.83 (dd, J = 5.5, 4.0 Hz, 2H), 3.68 (td, J = 5.4, 3.9 Hz, 2H), 3.61 – 3.30 (m, 1H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 158.76, 152.14, 141.87, 116.53, 112.39, 92.20, 63.04, 44.74.

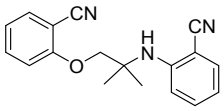
1, 2-Dihydro-9*H*-benzo[6,7][1,4]thiazepino[4,5-*a*]quinazolin-9-imine



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.65 (dd, J = 7.9, 1.2 Hz, 1H), 7.59 – 7.47 (m, 3H), 7.44 – 7.29 (m, 4H), 6.70 (td, J = 7.5, 1.0 Hz, 1H), 6.66 – 6.58 (m, 1H), 4.88 (s, 1H), 3.51 (t, J = 6.7 Hz, 3H), 3.28 (dd, J = 7.3, 6.2 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 149.29, 139.41, 134.36, 134.02, 133.12, 133.00, 131.25, 133.31 – 132.81 (m), 127.35, 117.62, 117.25, 117.11, 115.32, 110.54, 96.37, 42.40, 33.34.

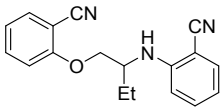
2-((1-(2-Cyanophenoxy)-2-methylpropan-2-yl)amino)benzonitrile



^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (dd, J = 7.7, 1.8 Hz, 1H), 7.51 (ddd, J = 8.5, 7.5, 1.7 Hz, 1H), 7.46 – 7.33 (m, 2H), 7.09 (dt, J = 8.6, 0.7 Hz, 1H), 7.04 (td, J = 7.6, 0.9 Hz, 1H), 6.94 (dd, J = 8.4, 0.9 Hz, 1H), 6.73 (td, J = 7.5, 0.9 Hz, 1H), 4.71 (s, 1H), 4.10 (s, 2H), 1.61(s, 6H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.15, 148.51, 134.33, 133.88, 133.72, 133.26, 132.18, 121.49, 117.81, 117.61, 116.11, 114.66, 112.60, 102.57, 98.90, 75.39, 54.59, 25.26.

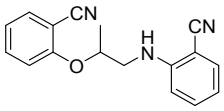
2-((1-(2-Cyanophenoxy)butan-2-yl)amino)benzonitrile



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.57 – 7.46 (m, 2H), 7.44 – 7.34 (m, 2H), 7.01 (td, J = 7.6, 0.9 Hz, 1H), 6.96 – 6.91 (m, 1H), 6.86 (dd, J = 8.5, 0.9 Hz, 1H), 6.68 (ddd, J = 7.8, 7.3, 0.9 Hz, 1H), 4.54 (d, J = 8.5 Hz, 1H), 4.14 (dd, J = 9.2, 4.8 Hz, 1H), 4.04 (dd, J = 9.2, 5.5 Hz, 1H), 3.95 – 3.81 (m, 1H), 2.00 (ddd, J = 14.2, 7.5, 5.3 Hz, 1H), 1.83 – 1.64 (m, 1H), 1.07 (t, J = 7.4 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 160.17, 149.59, 134.56, 134.43, 133.86, 132.94, 121.38, 117.79, 117.09, 116.22, 112.37, 111.56, 102.28, 96.20, 70.59, 53.86, 25.35, 10.49.

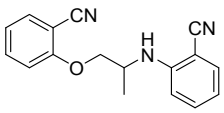
2-((2-(2-Cyanophenoxy)propyl)amino)benzonitrile



^{1}H NMR (300 MHz, Chloroform-*d*) δ 7.56 – 7.44 (m, 2H), 7.41 (ddd, J = 8.7, 7.3, 1.6 Hz, 1H), 7.35 (dd, J = 7.8, 1.5 Hz, 1H), 7.05 – 6.94 (m, 2H), 6.86 – 6.80 (m, 1H), 6.69 (td, J = 7.5, 1.0 Hz, 1H), 4.94 – 4.43 (m, 1H), 3.71 – 3.30 (m, 2H), 1.42 (dd, J = 6.2, 1.2 Hz, 3H).

^{13}C NMR (75 MHz, Chloroform-*d*) δ 159.40, 149.90, 134.48, 134.31, 134.03, 132.87, 121.49, 117.73, 117.20, 116.47, 114.06, 111.21, 103.42, 96.25, 74.78, 48.49, 17.47.

2-((1-(2-Cyanophenoxy)propan-2-yl)amino)benzonitrile

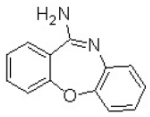


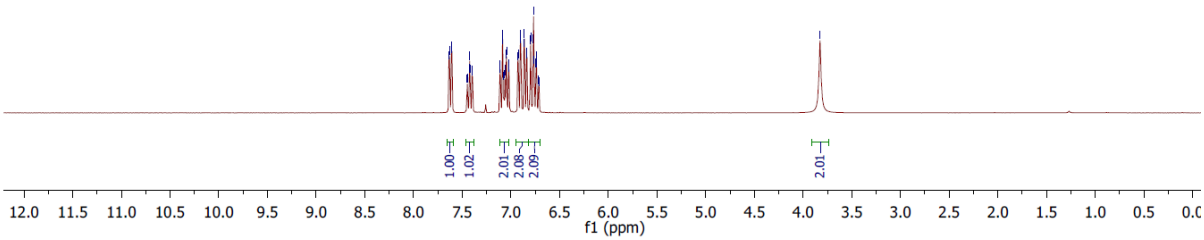
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.46 (m, 2H), 7.46 – 7.33 (m, 2H), 7.01 (td, J = 7.6, 0.9 Hz, 1H), 6.93 (dd, J = 8.6, 0.8 Hz, 1H), 6.89 – 6.79 (m, 1H), 6.69 (td, J = 7.5, 0.9 Hz, 1H), 4.58 (d, J = 7.9 Hz, 1H), 4.25 – 4.04 (m, 2H), 3.99 (dd, J = 8.5, 5.5 Hz, 1H), 1.48 (d, J = 6.3 Hz, 3H).

^{13}C NMR (101 MHz, Chloroform-*d*) δ 160.12, 149.08, 134.55, 134.44, 133.85, 134.75 – 134.22 (m), 132.98, 121.42, 117.75, 117.17, 116.20, 112.42, 111.50, 102.30, 96.30, 71.94, 47.93, 18.28.

150309.f337.10.fid
Feng FII b
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 5

7.64 7.63 7.61 7.61 7.45 7.45 7.43 7.42 7.42 7.40 7.39 7.11 7.09 7.08 7.08 7.07 7.06 7.06 7.05 7.04 7.02 7.02 6.93 6.92 6.90 6.90 6.87 6.86 6.84 6.83 6.80 6.80 6.77 6.77 6.76 6.74 6.74 6.74 6.73 6.72 6.71 3.83





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Feng FII b
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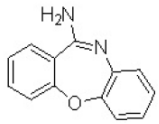
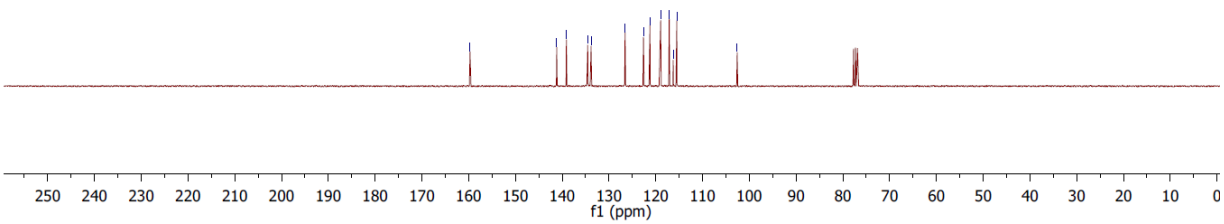
159.71 141.17 139.10 134.54 133.83 126.56 122.62 121.24 118.95 117.12 116.26 115.50 102.59





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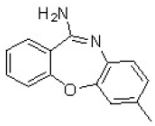

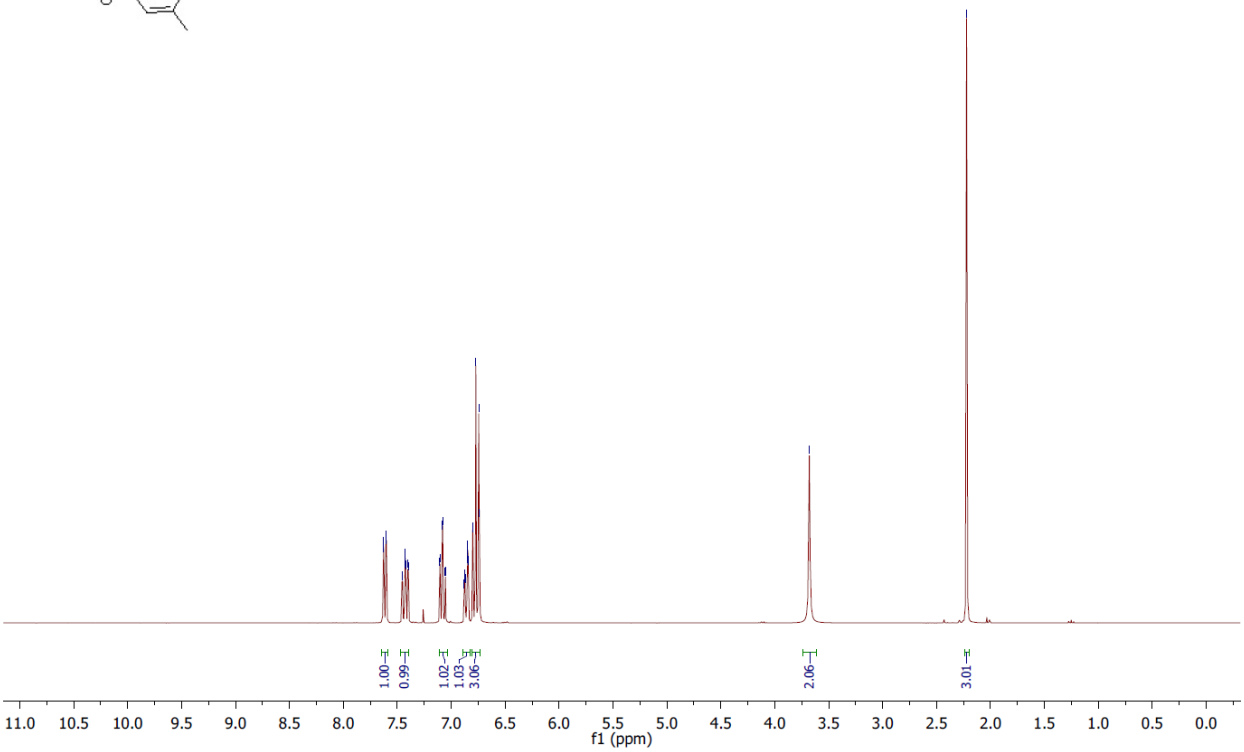

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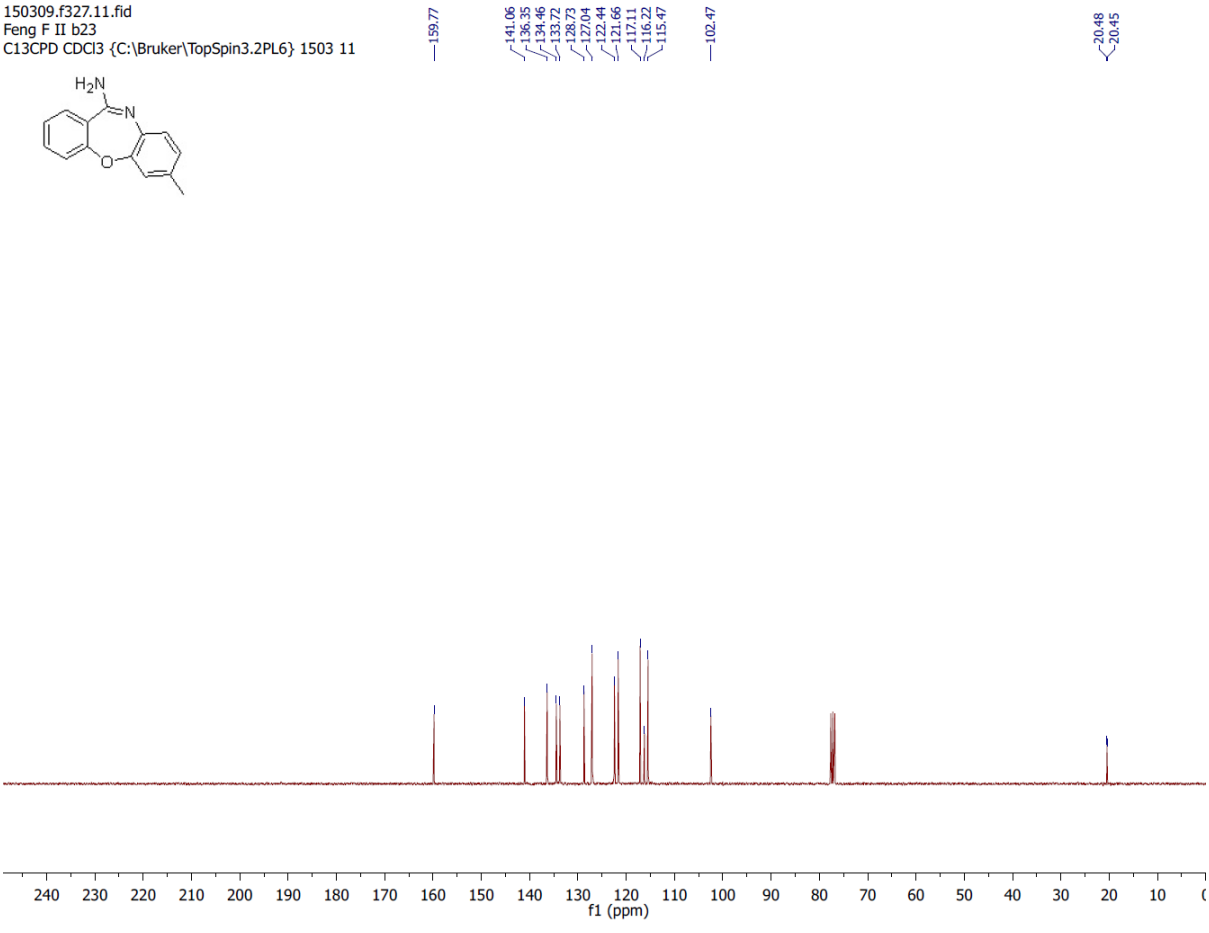

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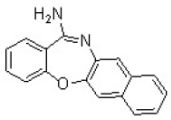

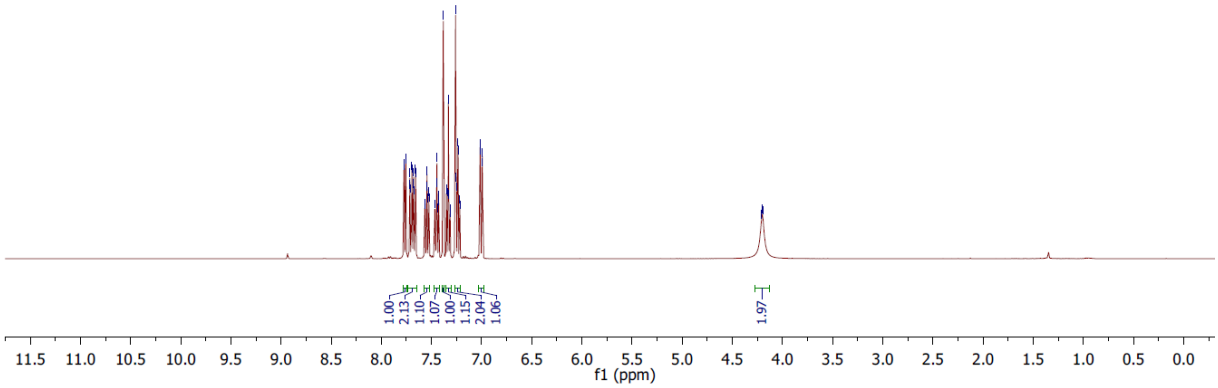

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Feng F11b24
Au13C CDCl3 /opt/topspin 1503 15

159.27
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133.91
127.17
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123.35
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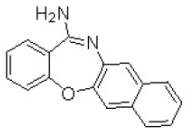
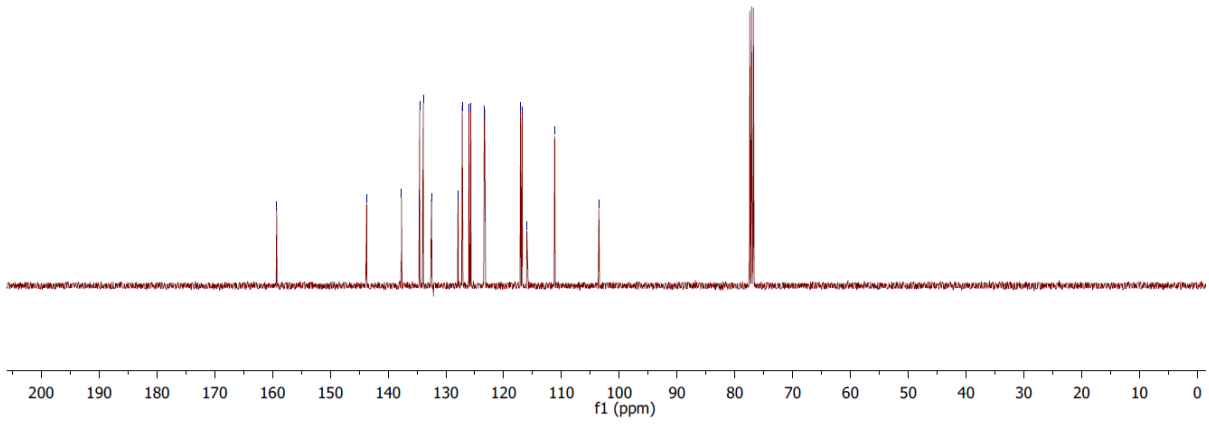
111.18
103.53





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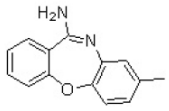

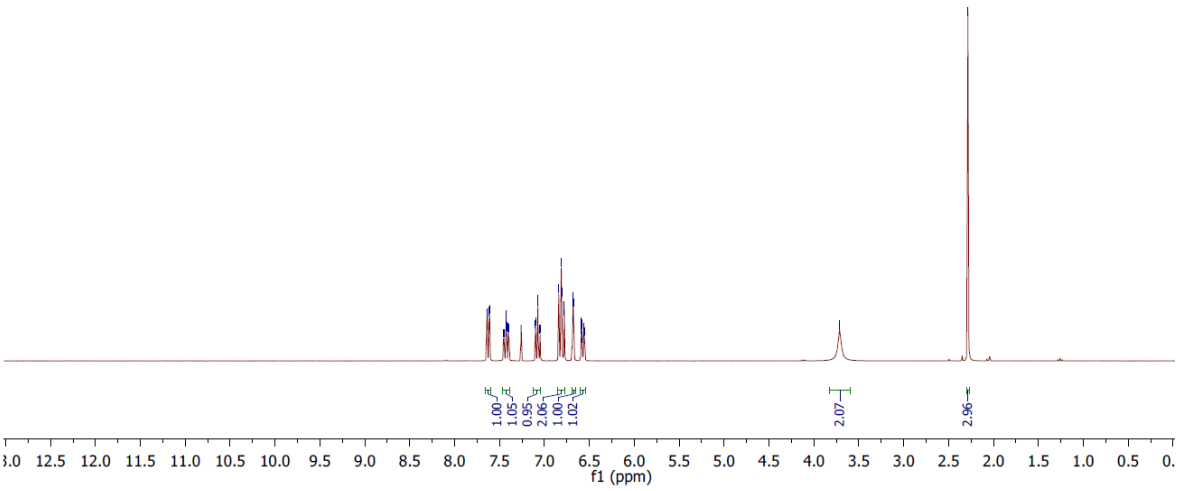

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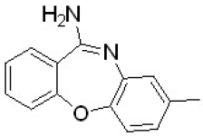

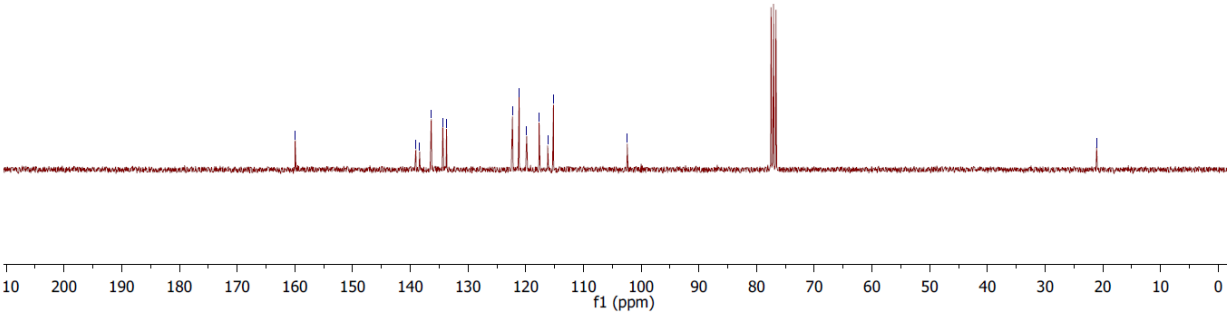

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Feng FII b26
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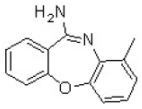

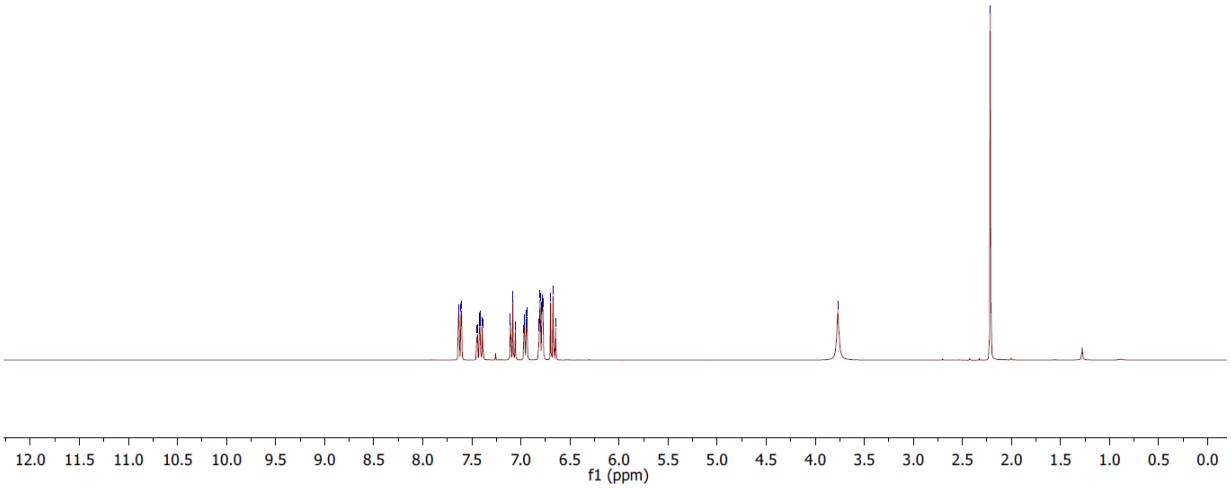

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Feng FII b26
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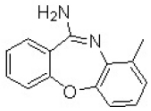
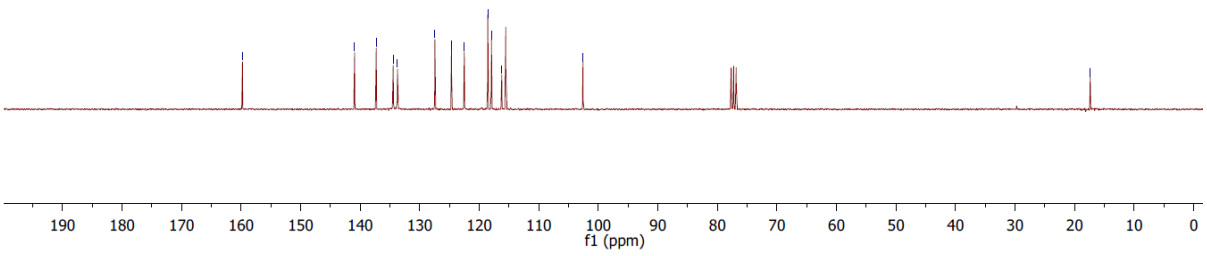
159.78 140.95 137.31 134.46 133.75 127.46 124.67 122.52 118.58 117.96 116.22 102.59 17.42 17.38





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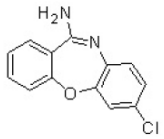
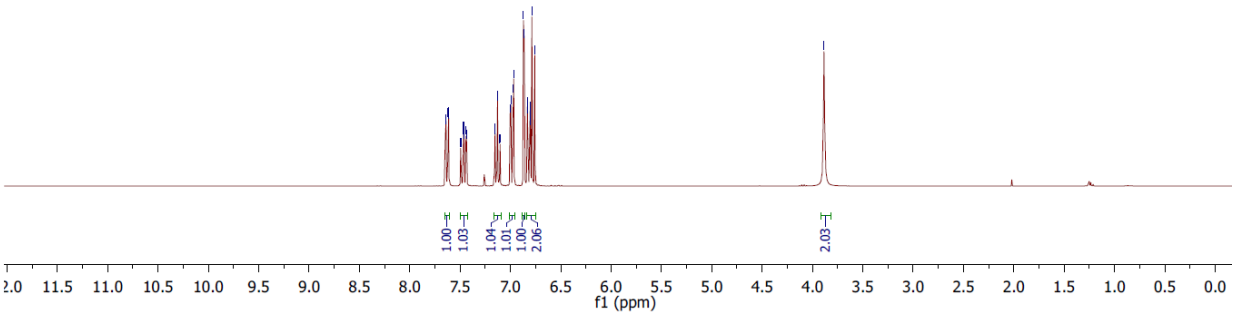
Feng FII b27
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 14

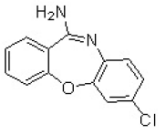
7.64 7.64 7.64 7.62 7.61 7.61 7.49 7.49 7.47 7.47 7.47 7.46 7.46 7.44 7.44 7.16 7.15 7.13 7.13 7.11 7.10 7.00 7.00 6.97 6.97 6.87 6.86 6.83 6.83 6.83 6.81 6.80 6.80 6.80 6.79 6.76 3.88

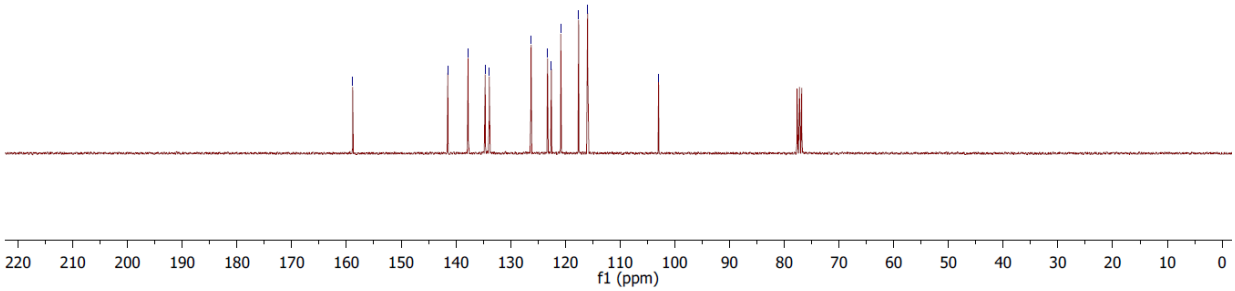




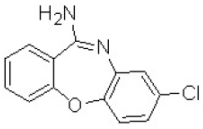
150309.f330.11.fid
Feng FII b27
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 14

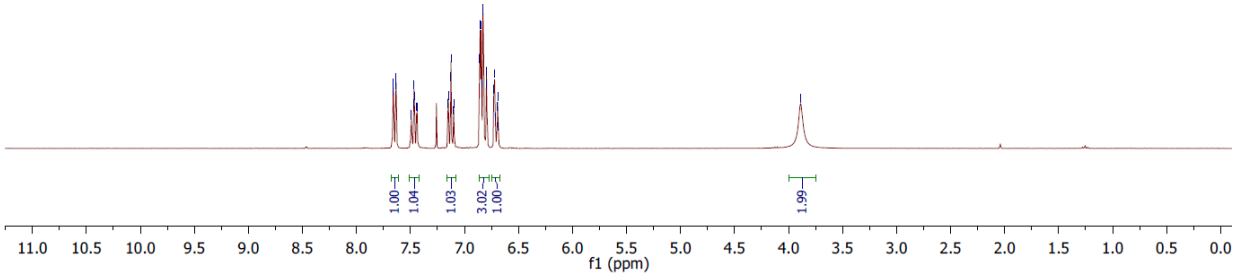
158.86 141.48 137.76 134.64 133.90 126.26 123.25 122.56 120.83 117.57 115.93 102.96



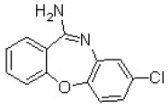


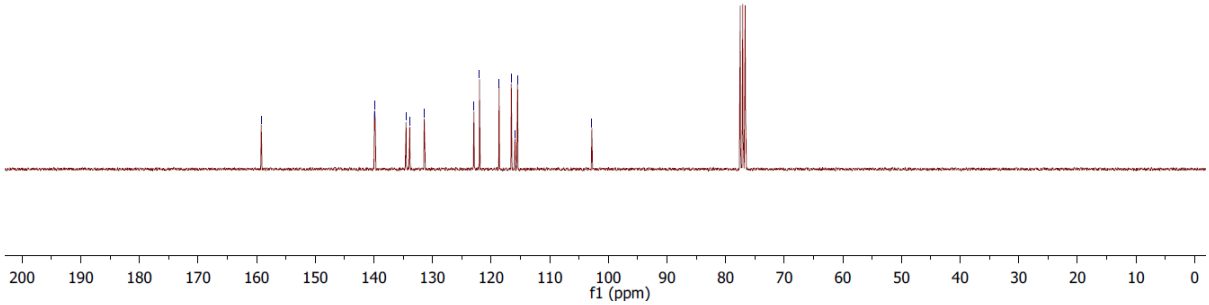
150309.f333.10.fid
Feng FII b28
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 1





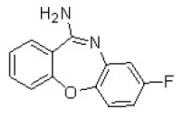
150311.f329.10.fid
Feng F11b28
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 13

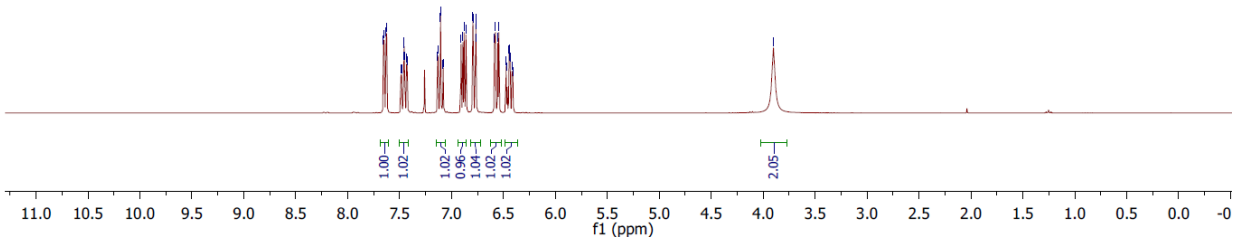




150309.f332.10.fid
Feng FII b29
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 16

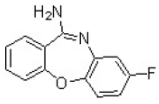
7.66 7.65 7.63 7.62 7.49 7.48 7.46 7.46 7.46 7.45 7.43 7.43 7.13 7.13 7.11 7.11 6.91 6.89 6.88 6.86 6.80 6.79 6.77 6.77 6.76 6.59 6.58 6.55 6.54 6.47 6.45 6.45 6.44 6.44 3.90

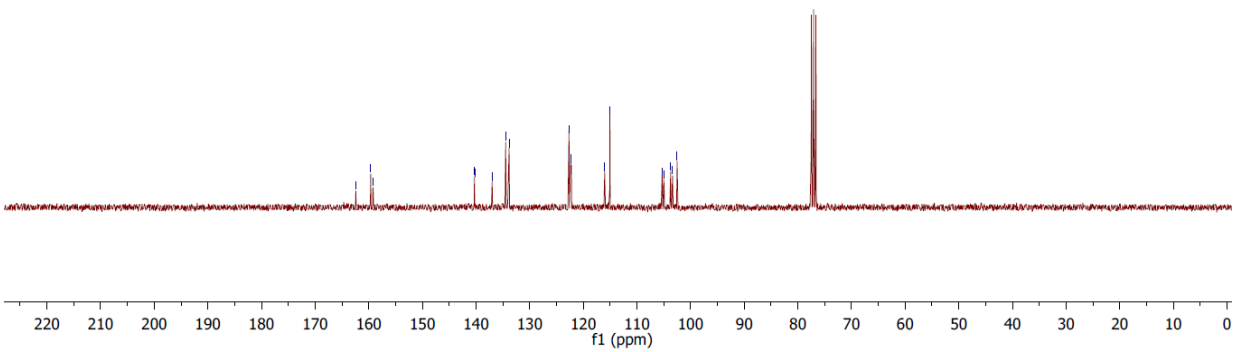




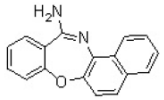
150309.f332.11.fid
Feng FII b29
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 16

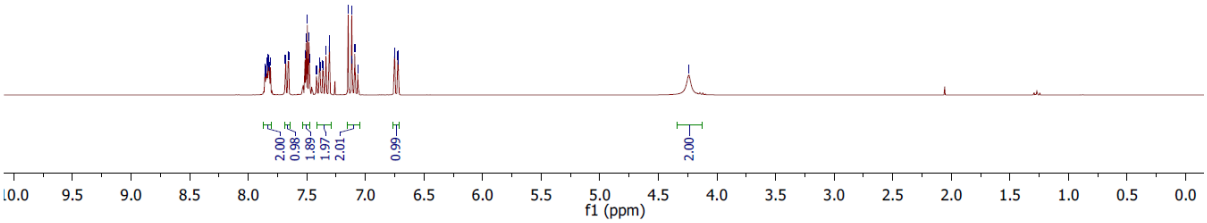
162.42 159.64 159.21 140.30 140.14 137.03 137.00 134.48 133.84 122.67 122.36 122.23 116.02 115.05 105.31 104.99 103.72 103.37 102.52



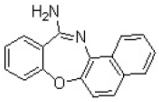


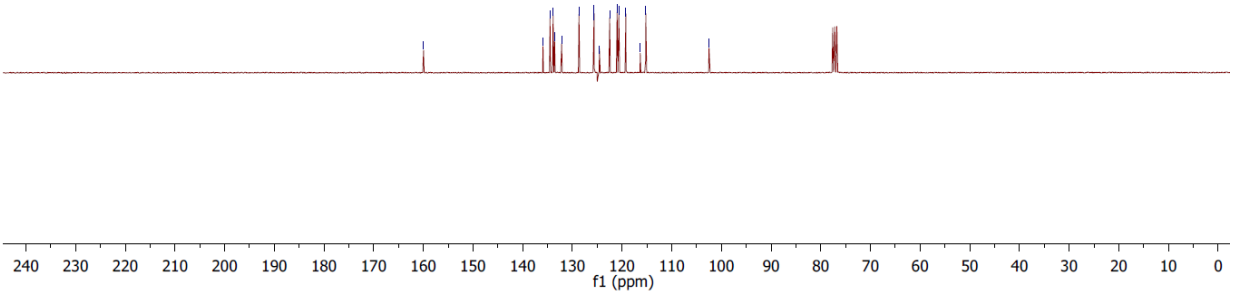
150320.338.10.fid
Feng F11b30
Au1H CDCl3 /opt/topspin 1503 38



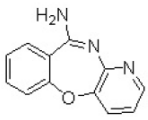


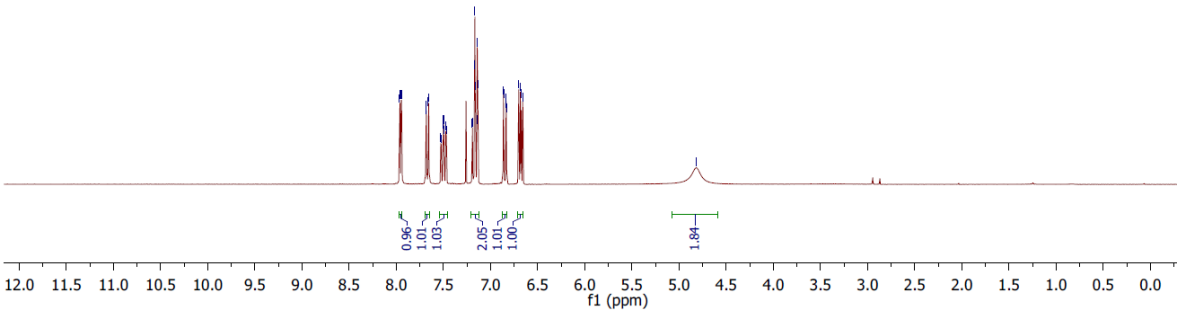
150320.338.11.fid
Feng F11b30
Au13C CDCl3 /opt/topspin 1503 38



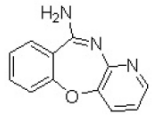


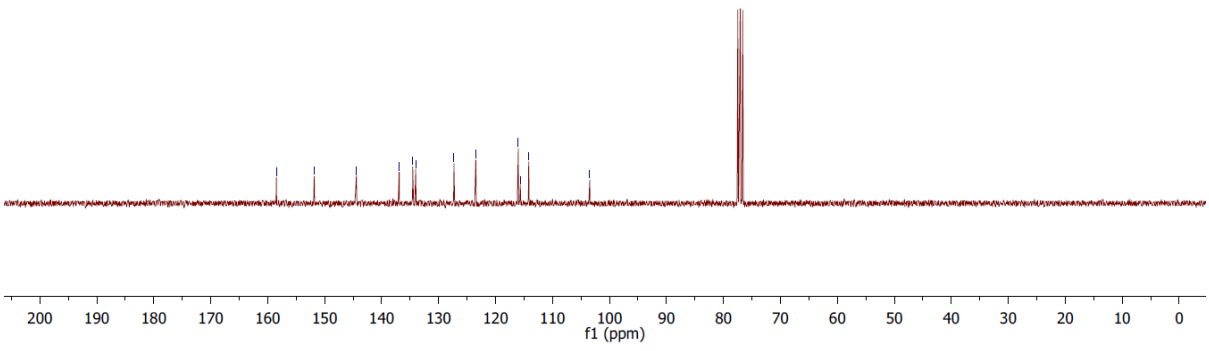
150309.f331.10.fid
Feng FII b31
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 15



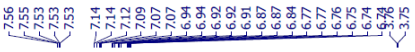


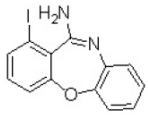
150309.f331.11.fid
Feng FII b31
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 15

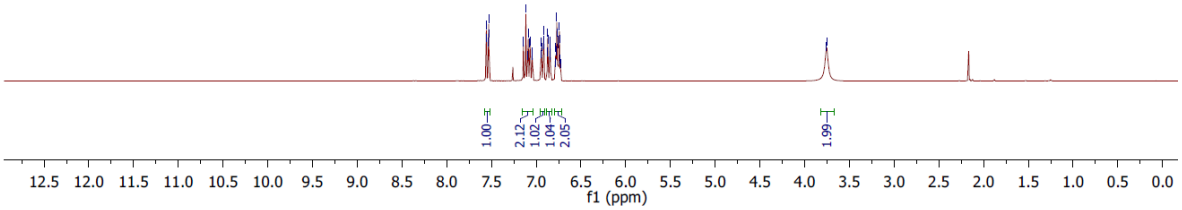




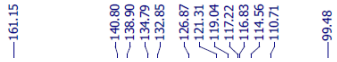
150325.322.10.fid
Feng F11b32
Au1H CDCl3 /opt/topspin 1503 22

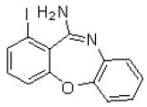


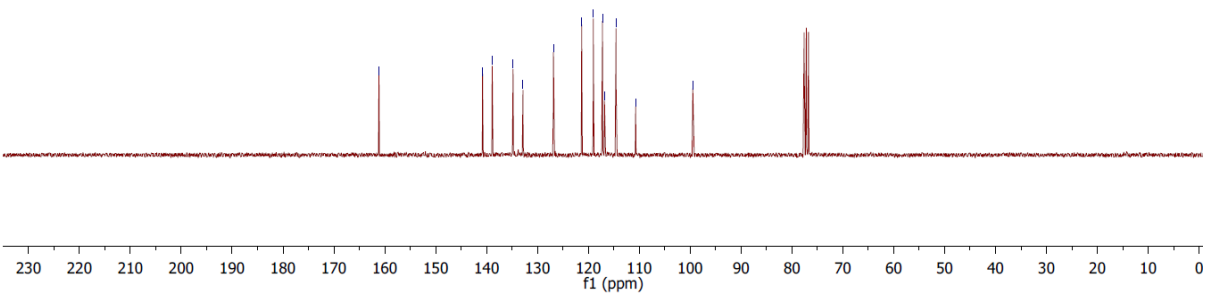




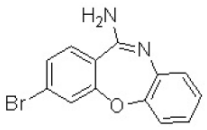
150309.f328.11.fid
Feng FII b32
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 12

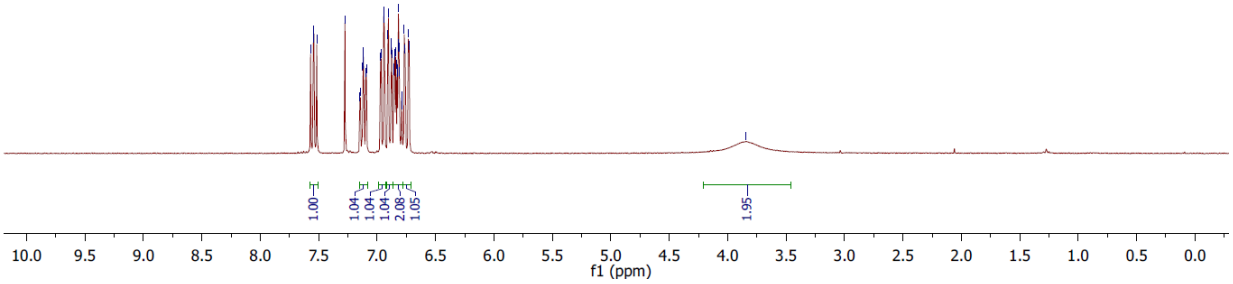




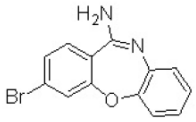


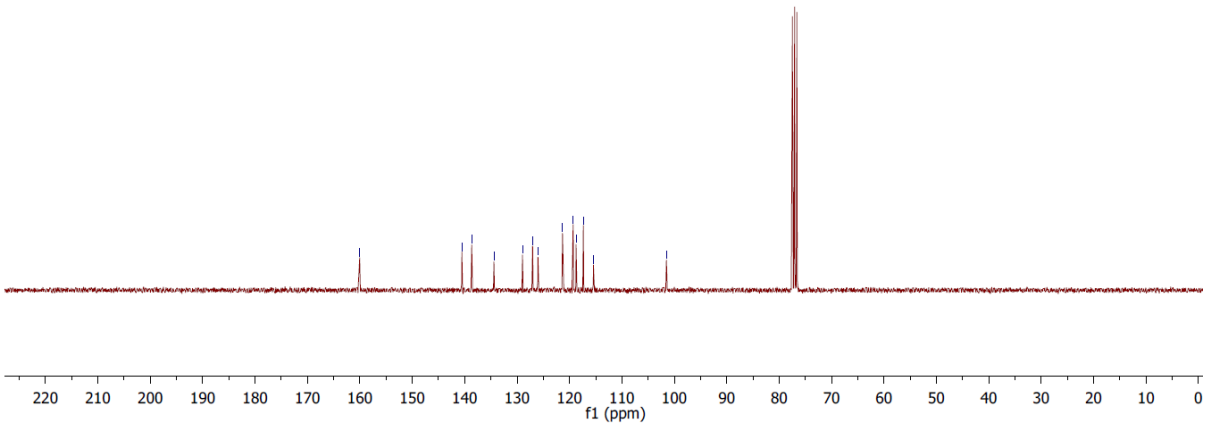
150316.f304.10.fid
Feng / F11b34
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 4



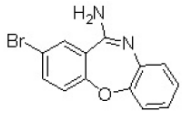


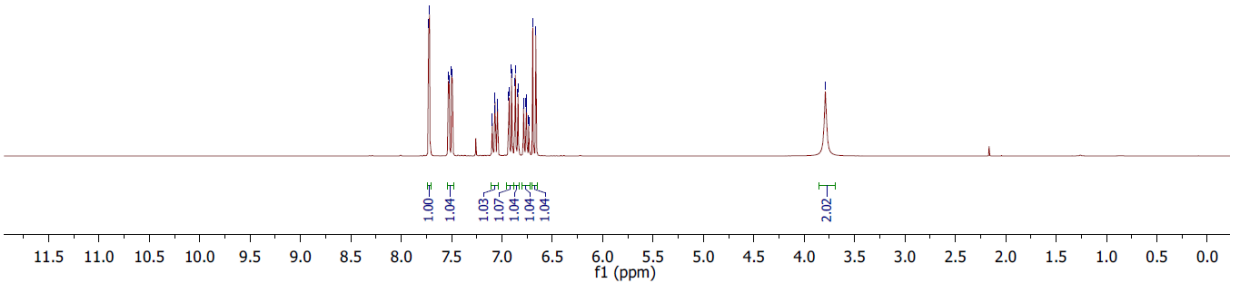
150330.f315.11.fid
Feng/ F 11 b34
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 15





150318.f302.10.fid
Feng F11b35
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 2





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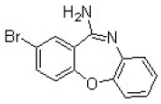
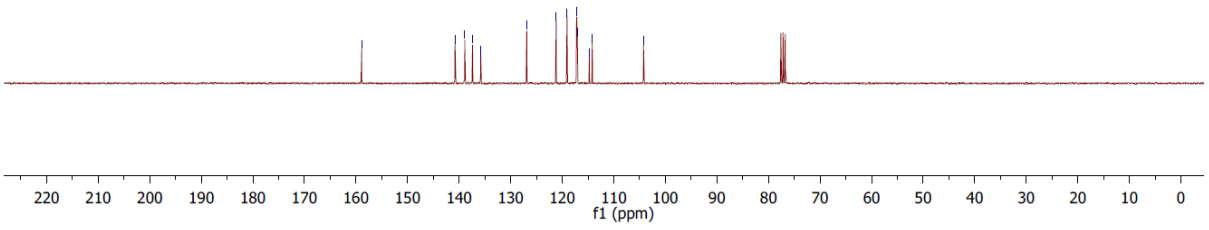
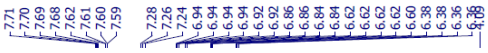
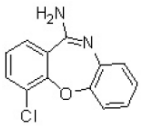
Feng 11b35
C13CPD CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 7

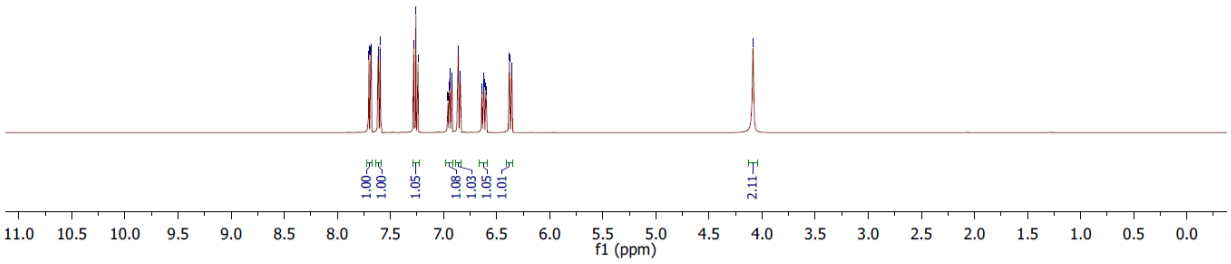




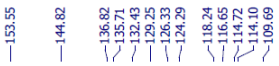
150318.410.10.fid
Feng F11b37
Au1H CDCl3 /opt/topspin 1503 10

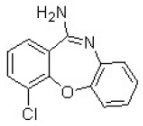


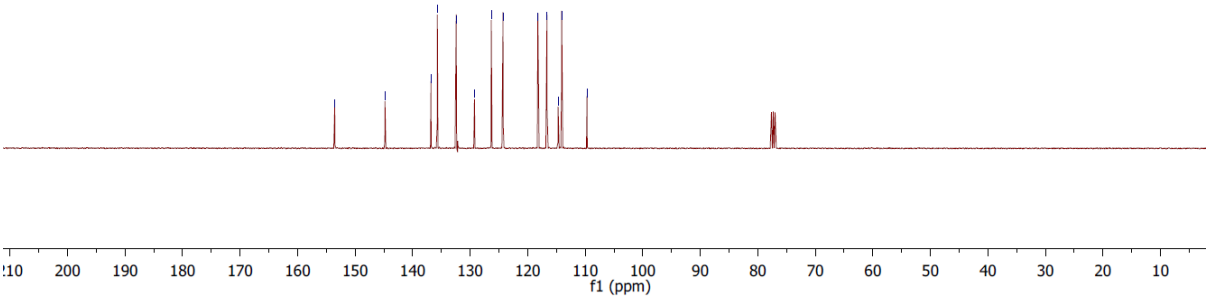




150318.410.11.fid
Feng F11b37
Au13C CDCl3 /opt/topspin 1503 10

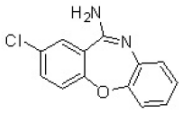


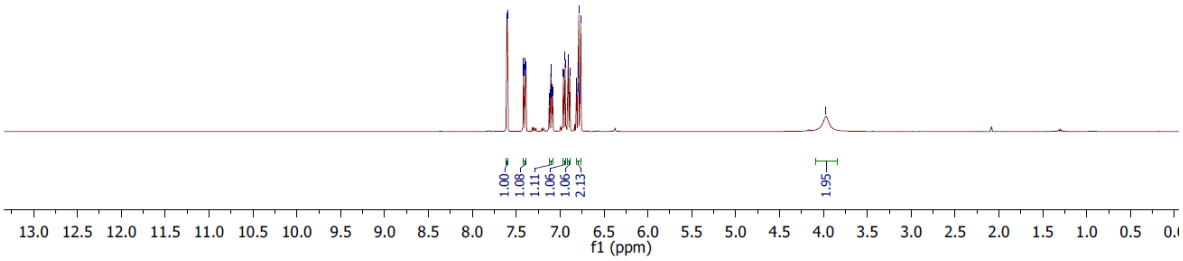




150318.411.10.fid
Feng F11b38
Au1H CDCl3 /opt/topspin 1503 11

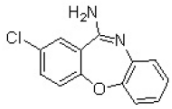
7.61 7.60 7.42 7.42 7.41 7.41 7.40 7.40 7.39 7.39 7.13 7.12 7.12 7.12 7.11 7.11 7.10 7.10 7.09 7.09 7.08 7.08 6.96 6.96 6.94 6.94 6.91 6.91 6.89 6.89 6.81 6.81 6.81 6.81 6.80 6.79 6.79 6.79 6.77 6.77 6.76 3.97

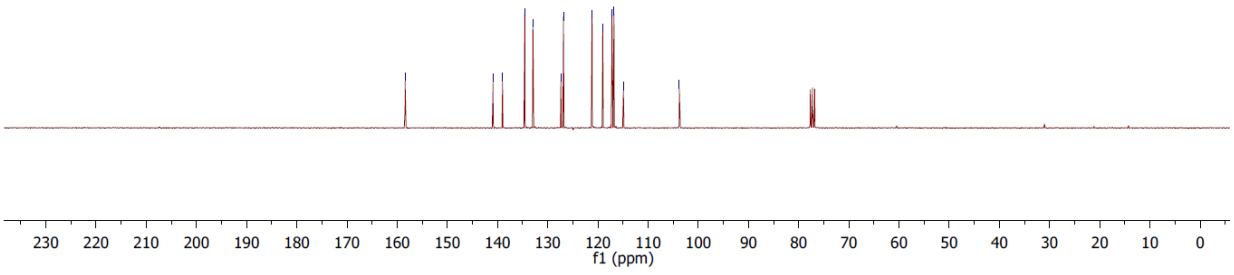




150320.323.10.fid
Feng F11b38
Au13C CDCl3 /opt/topspin 1503 23

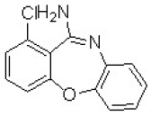
158.42 140.89 139.00 134.56 132.95 127.38 126.87 121.17 119.04 117.21 116.79 114.92 103.78

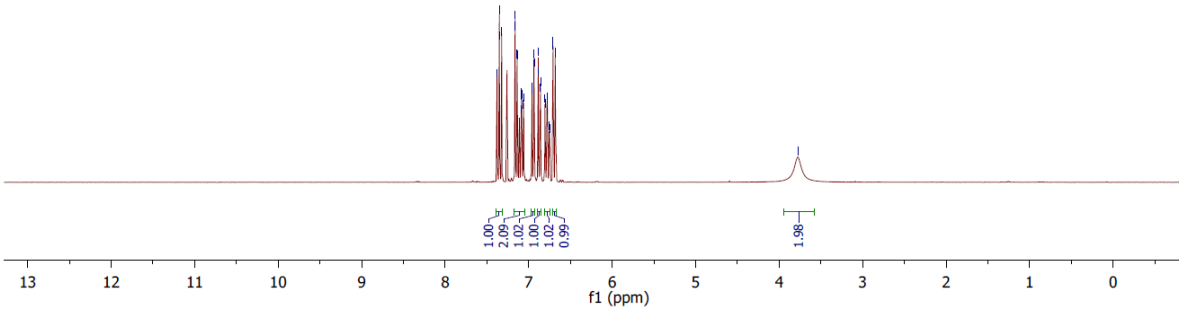




150319.f337.10.fid
Feng F11b39-3
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 5

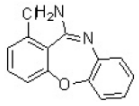
7.38 7.35 7.35 7.32 7.17 7.16 7.14 7.14 7.11 7.11 7.09 7.09 7.09 7.08 7.06 7.06 6.96 6.96 6.94 6.93 6.89 6.88 6.86 6.86 6.81 6.80 6.78 6.78 6.78 6.77 6.75 6.75 6.71 6.71 6.68 6.68 3.78

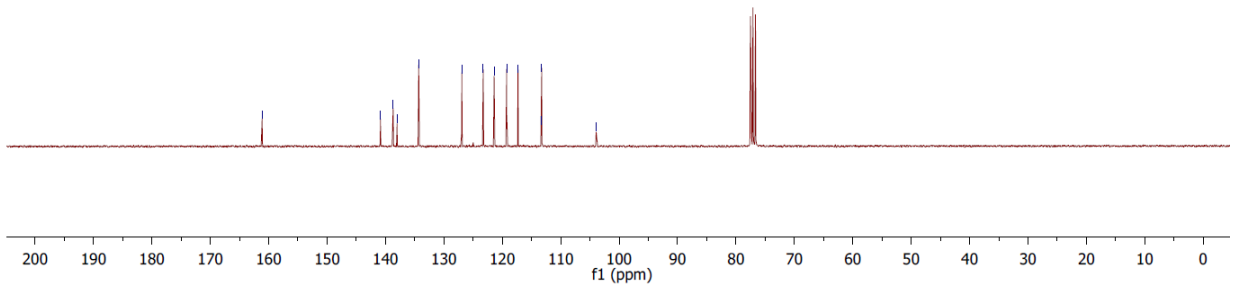




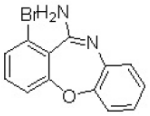
150320.322.10.fid
Feng F11b39-3
Au13C CDCl3 /opt/topspin 1503 22

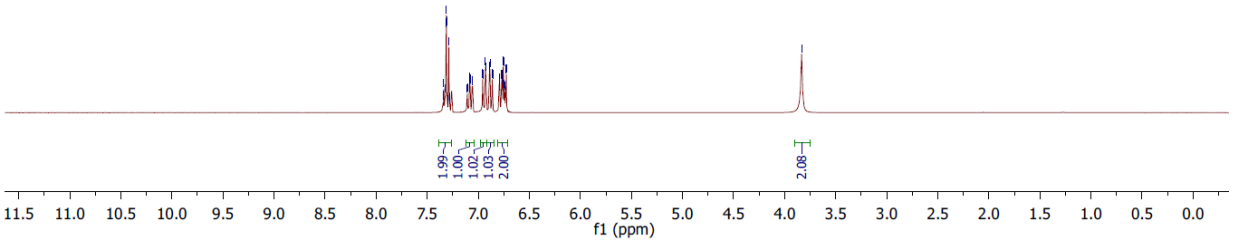
161.13 140.87 138.69 138.01 134.32 126.93 123.27 121.40 119.25 117.32 113.32 113.26 103.93



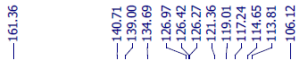


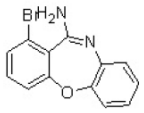
150325.318.10.fid
Feng F11b41
Au1H CDCl3 /opt/topspin 1503 18

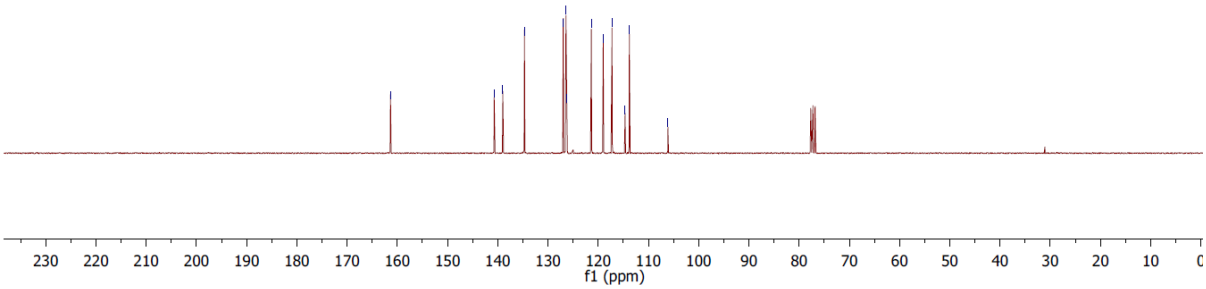




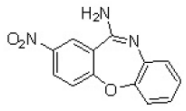
150320.327.11.fid
Feng F11b41-2
Au13C CDCl3 /opt/topspin 1503 27

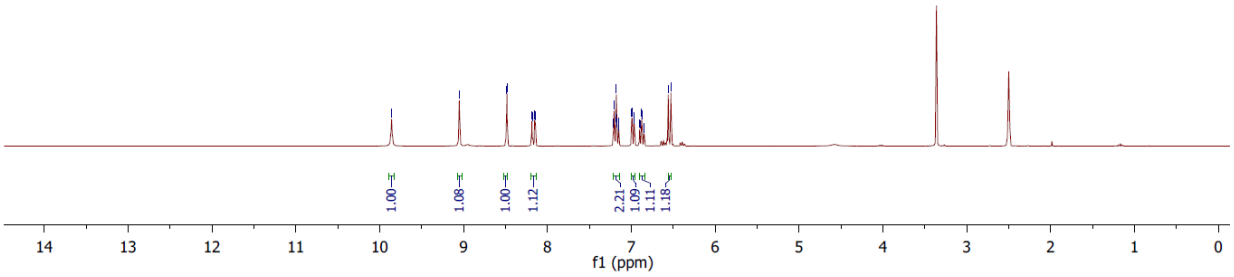






150327.342.10.fid
Feng F11b44
Au1H DMSO /opt/topspin 1503 42





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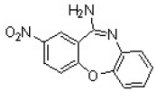
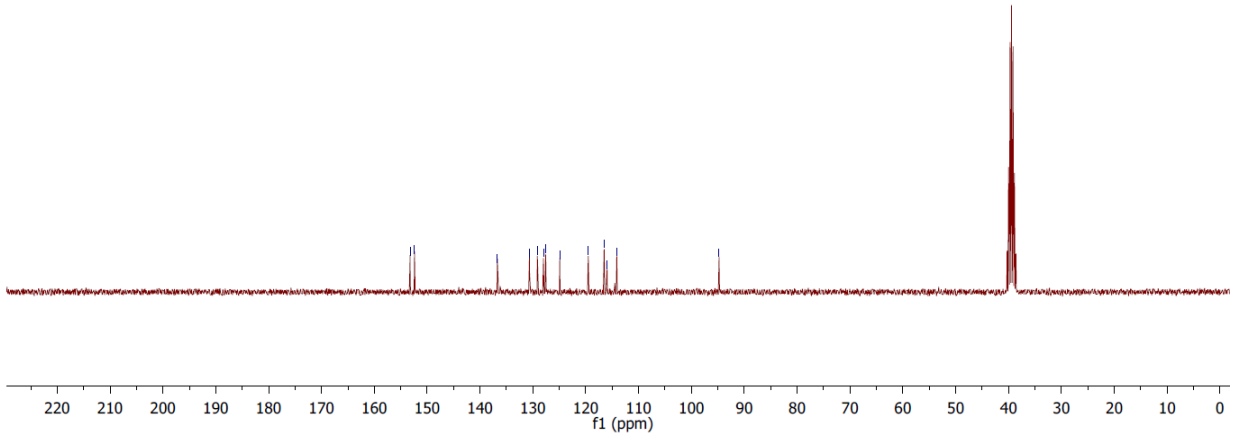
Feng F11b44
Au13C DMSO /opt/topspin 1503 42





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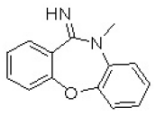
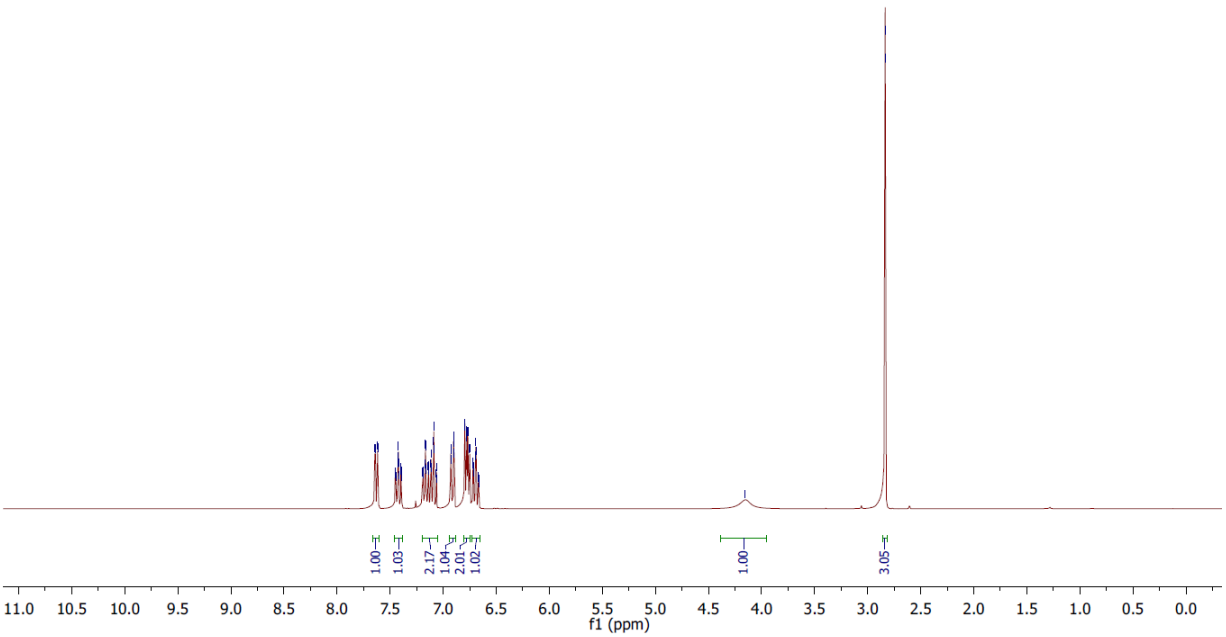
Feng F11b46
Au1H CDCl3 /opt/topspin 1503 50





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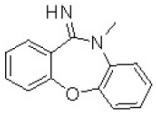
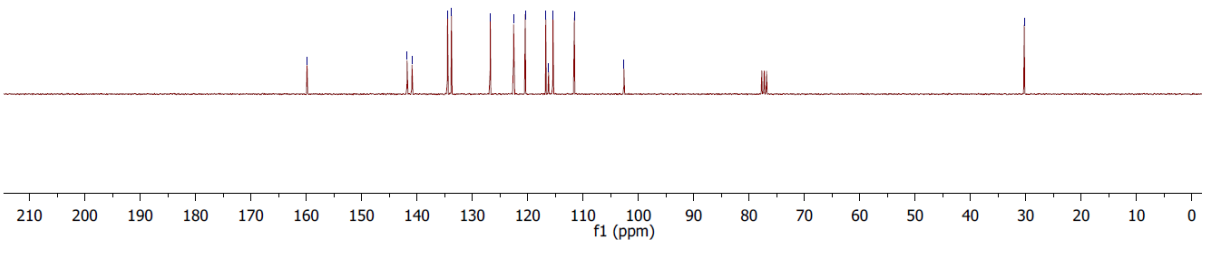
Feng F11b46
Au13C CDCl3 /opt/topspin 1503 50





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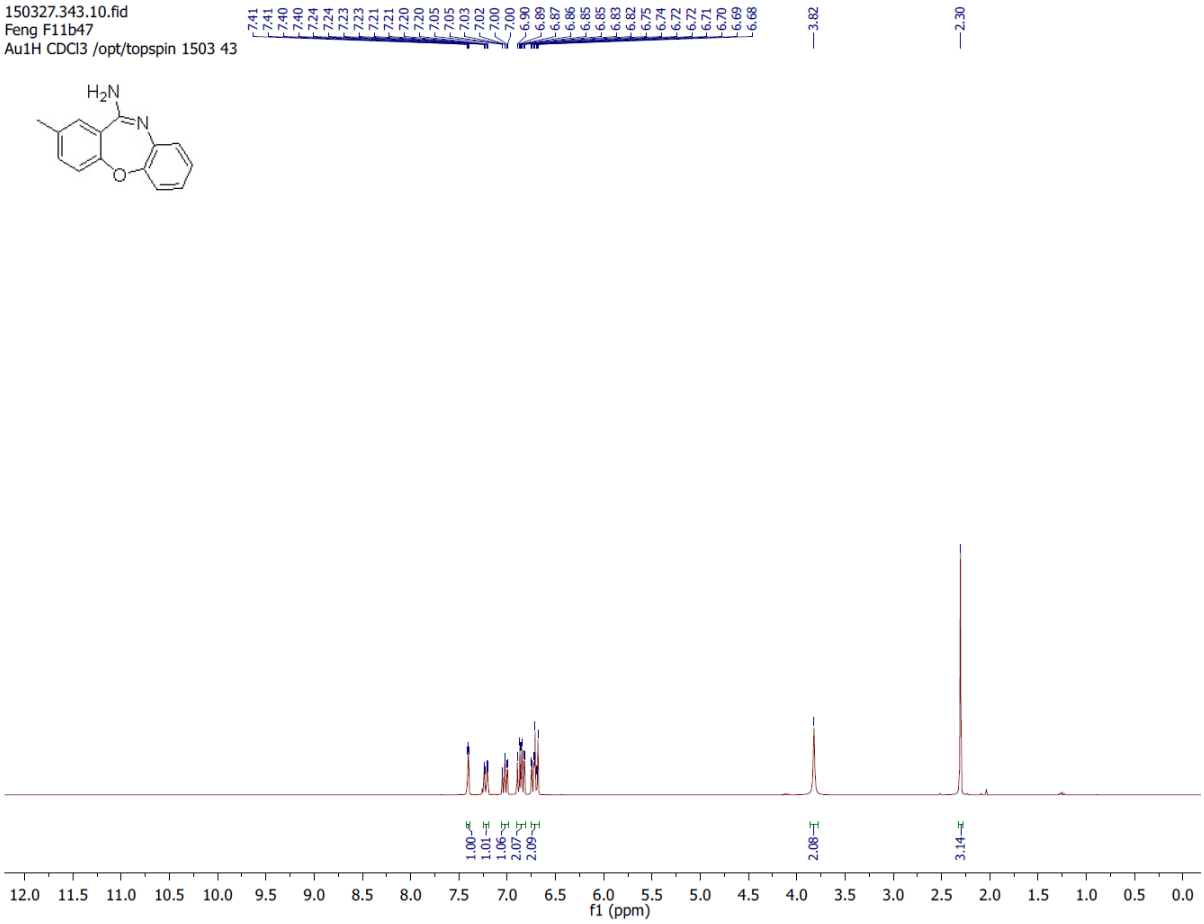
Feng F11b47
Au1H CDCl3 /opt/topspin 1503 43



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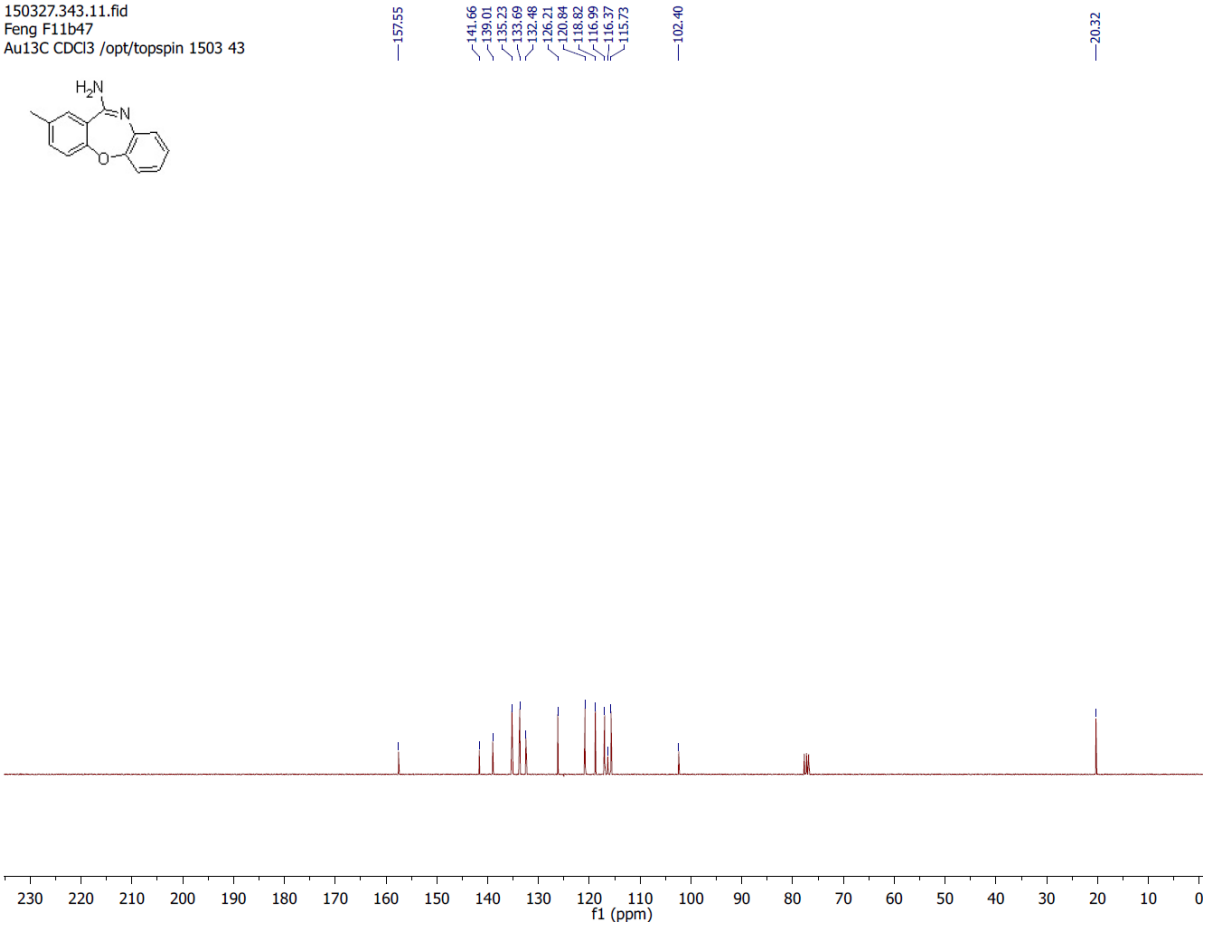
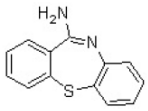
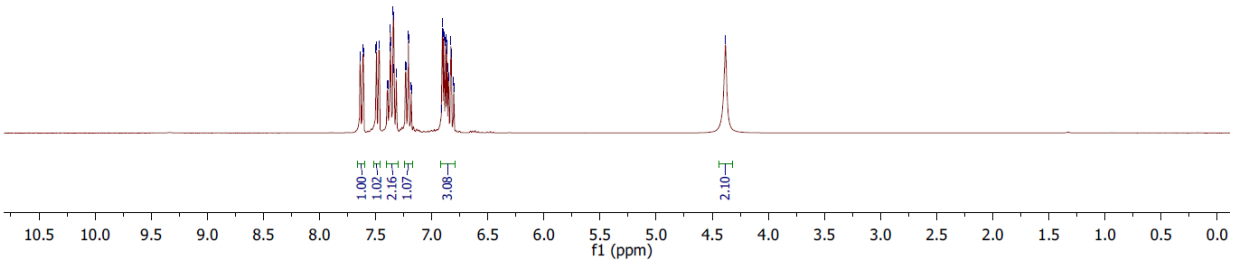


150401.307.10.fid
Feng/ FIIb49
Au1H CDCl3 /opt/topspin 1504 7

7.63 7.63 7.61 7.61 7.50 7.49 7.47 7.47 7.40 7.39 7.37 7.37 7.36 7.34 7.34 7.34 7.32 7.31 7.23 7.23 7.21 7.20 7.18 7.18 6.91 6.91 6.90 6.89 6.89 6.88 6.87 6.87 6.86 6.85 6.85 6.83 6.82 6.80 6.80 4.38





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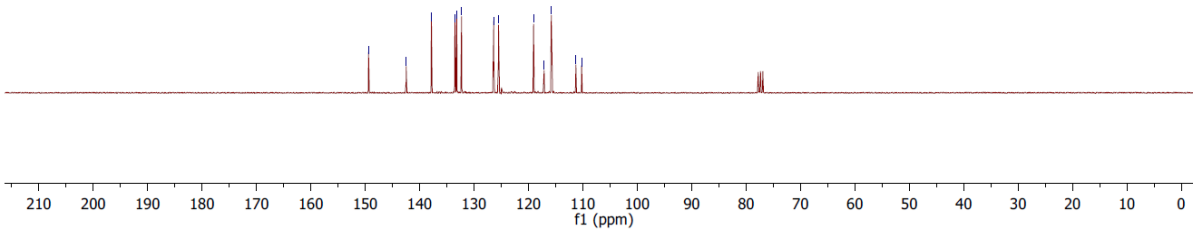
Feng/ FIIb49
Au13C CDCl3 /opt/topspin 1504 7

149.39 142.47 137.84 133.52 133.18 132.29 126.38 125.49 119.05 117.11 115.80 111.28 110.22



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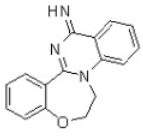
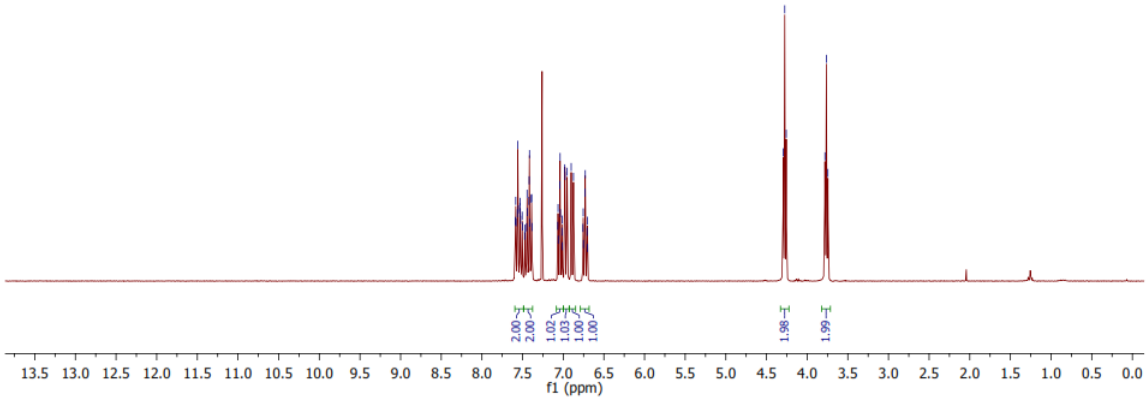
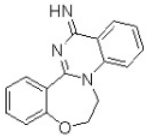
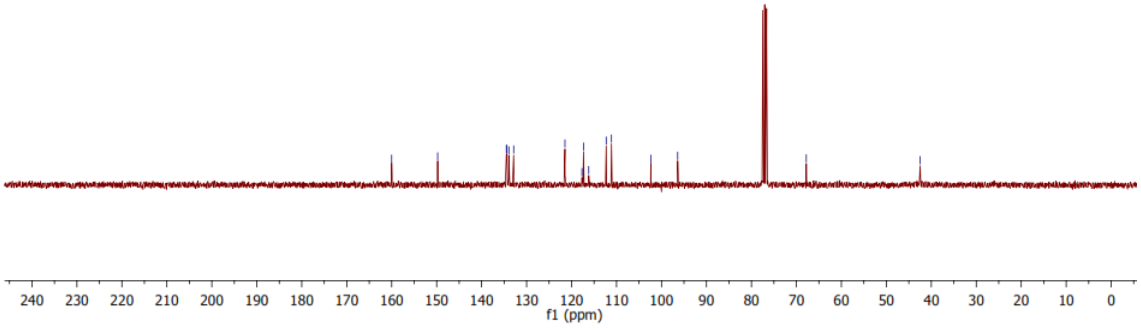
Feng f11d-1
PROTON CDCl3 {C:\Bruker\TopSpin3.2PL6} 1503 4









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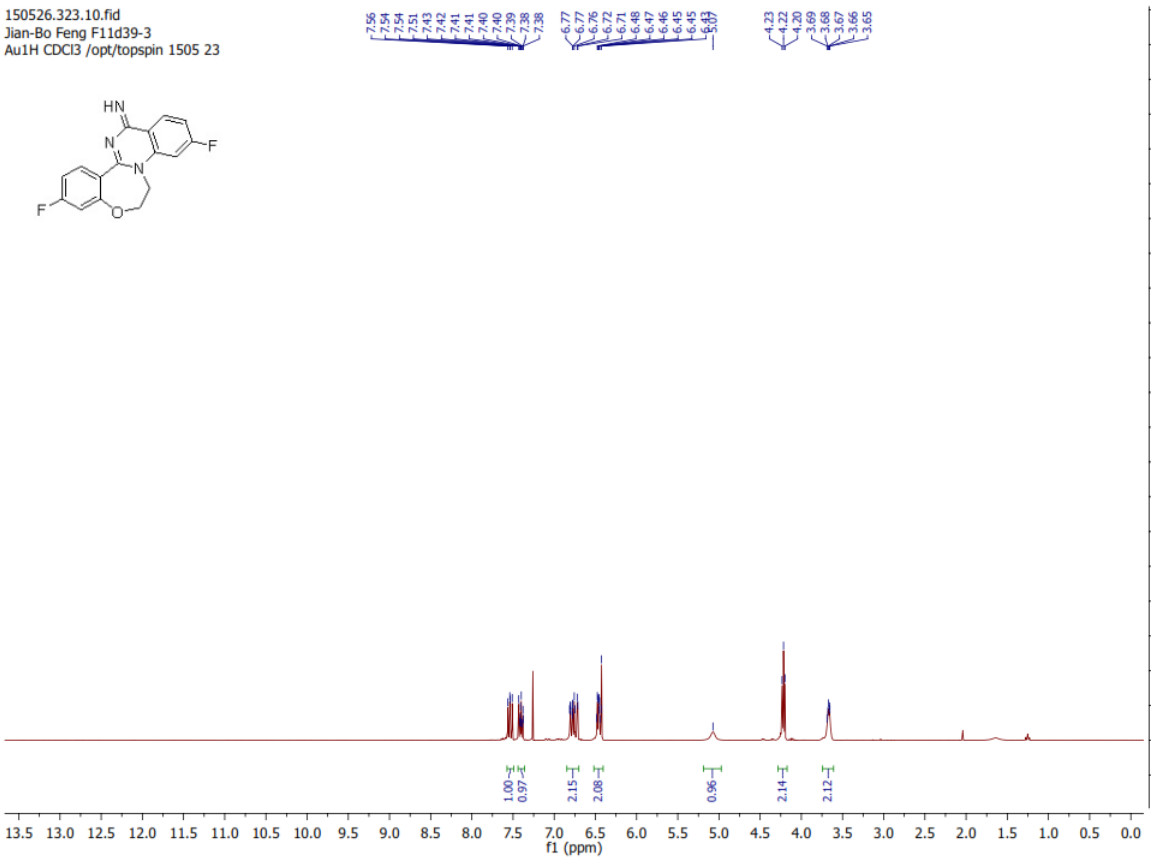
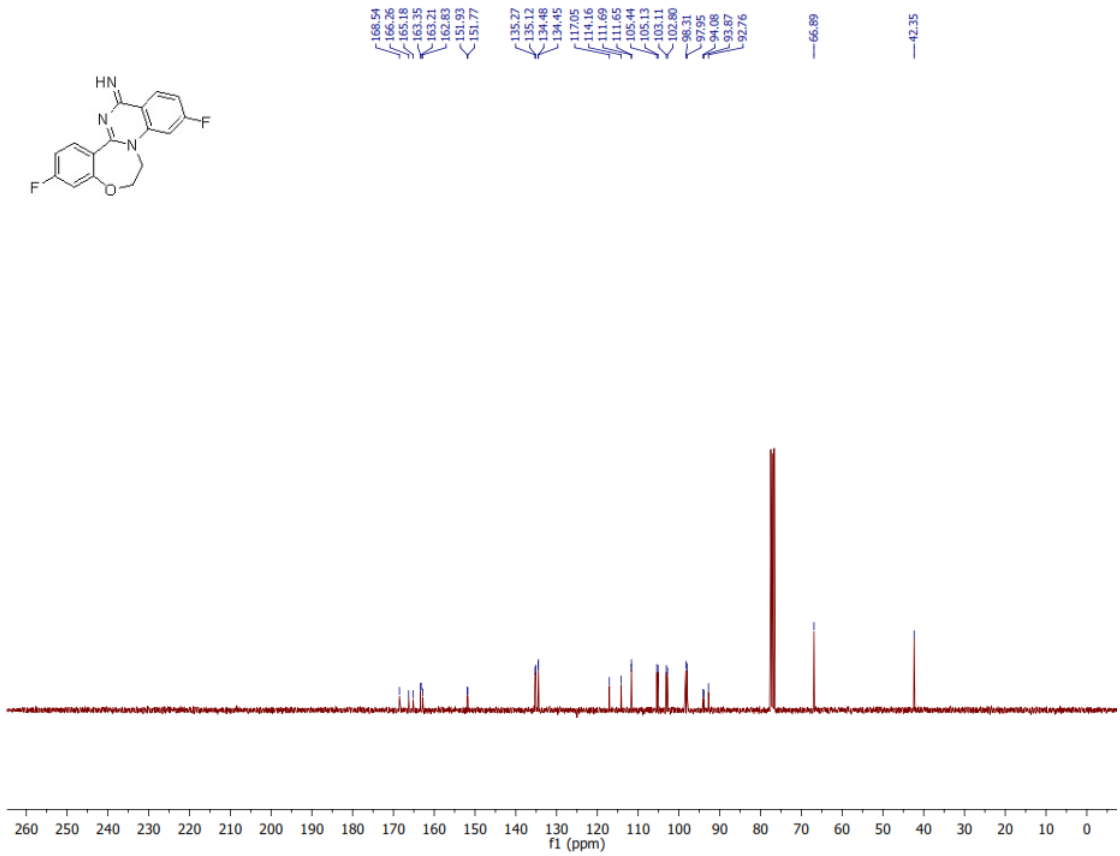
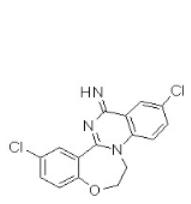
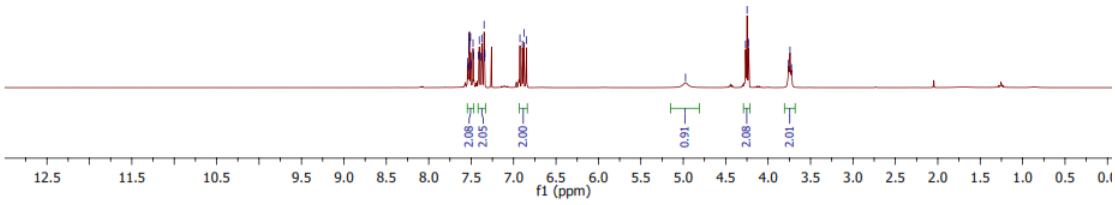
Jian-Bo Feng F11d39-3
Au1H CDCl3 /opt/topspin 1505 23

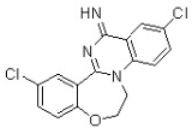




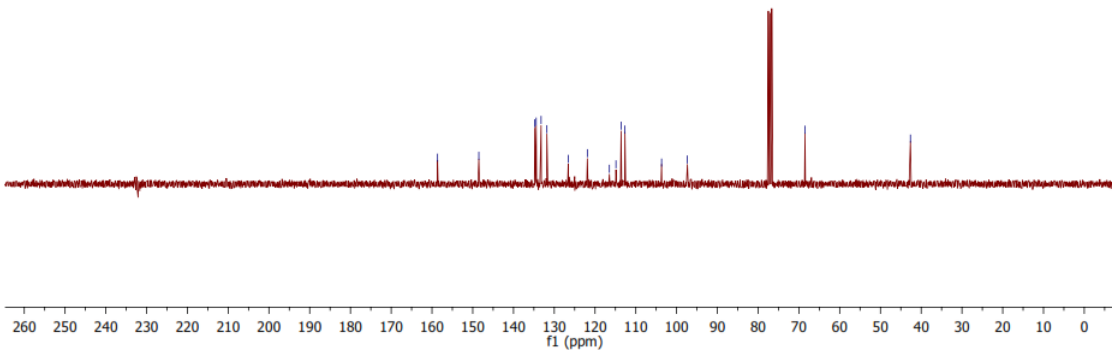

HN
Cl
N
N
Cl
O

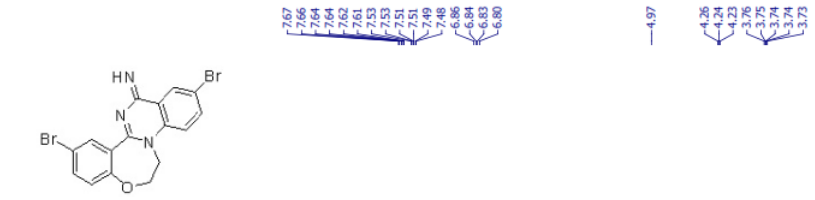

7.54
7.53
7.53
7.52
7.52
7.51
7.50
7.48
7.47
7.41
7.40
7.38
7.37
7.35
7.34
7.34
6.93
6.90
6.88
6.85
4.97
4.27
4.25
4.23
3.76
3.74
3.72


2.08
2.05
2.00
0.91
2.08
2.01
12.5
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
f1 (ppm)

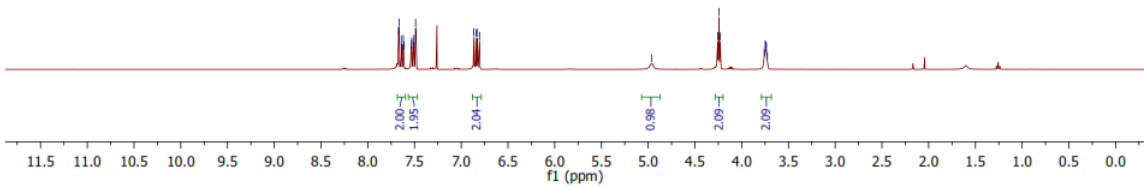

HN
Cl
N
N
Cl
O

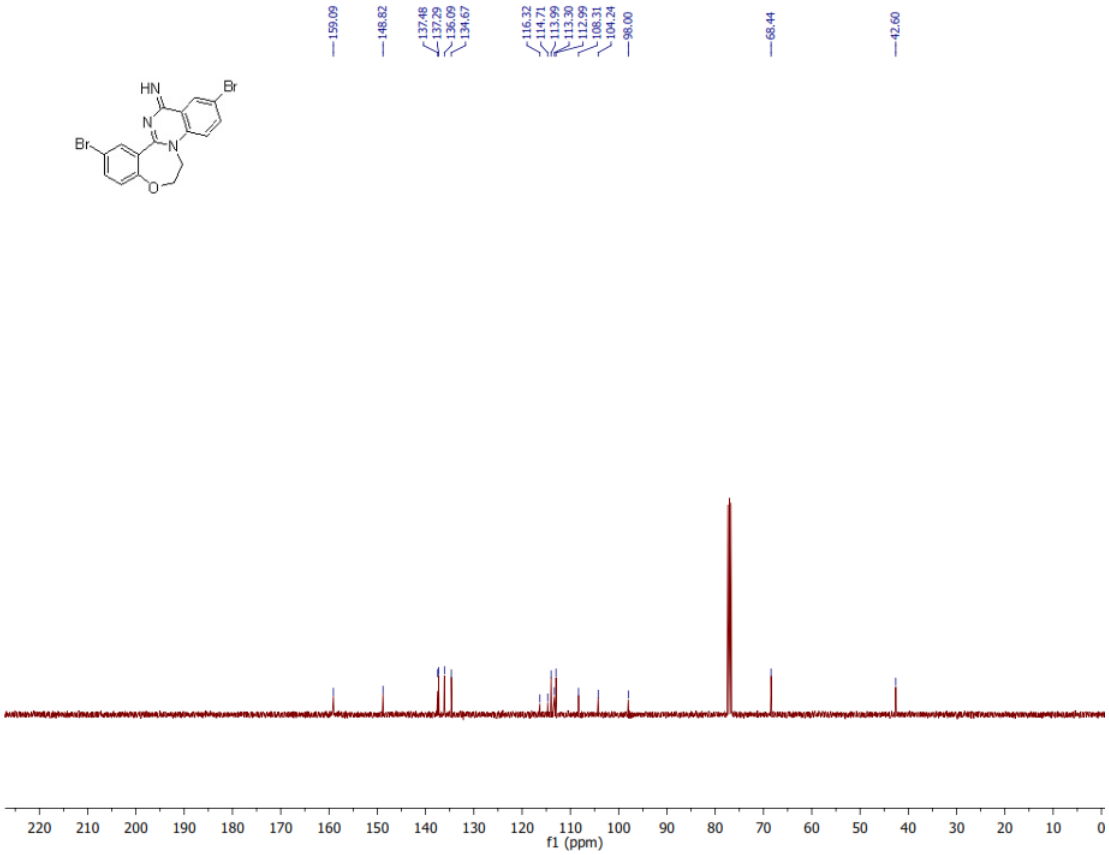

158.63
148.51
134.78
134.44
133.23
131.81
126.57
121.89
116.48
114.88
113.61
112.67
103.68
97.34
68.50
42.65


260
250
240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

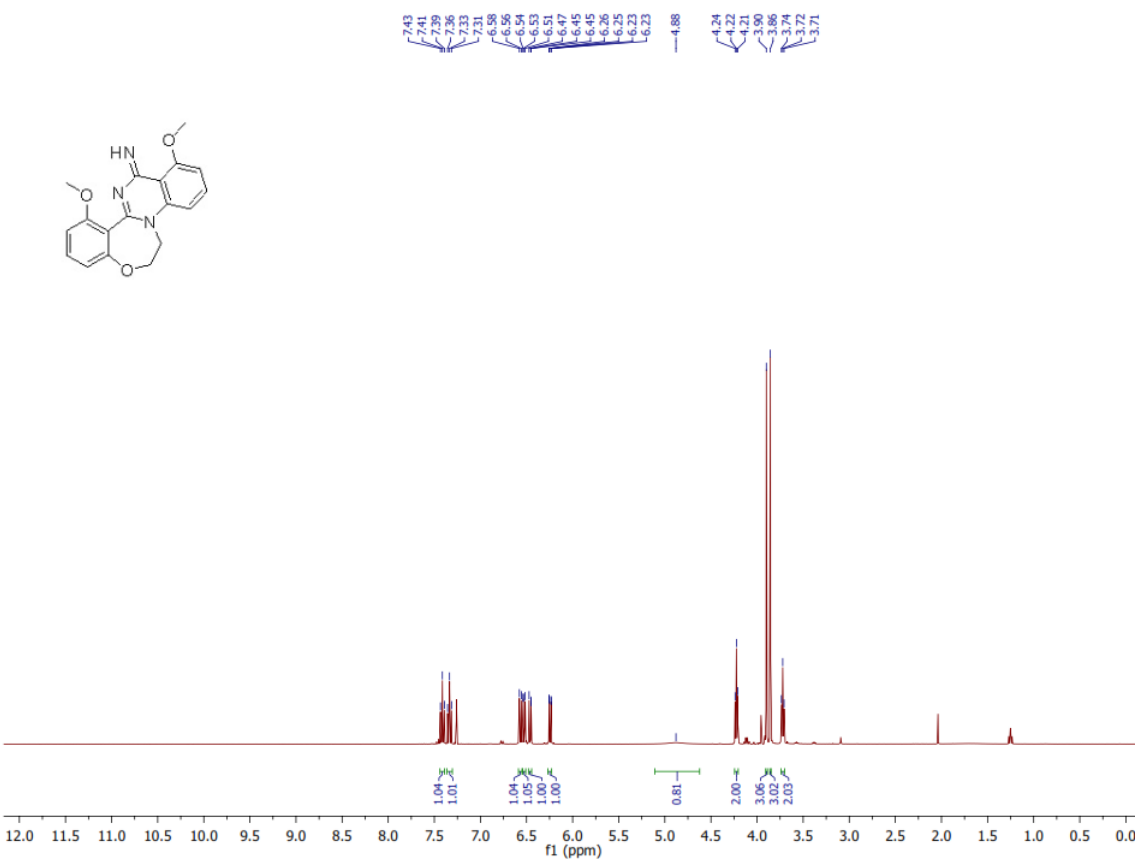

7.67
7.66
7.64
7.64
7.62
7.61
7.53
7.53
7.51
7.51
7.49
7.48
6.86
6.84
6.83
6.80
4.97
4.26
4.24
4.23
3.76
3.75
3.74
3.74
3.73

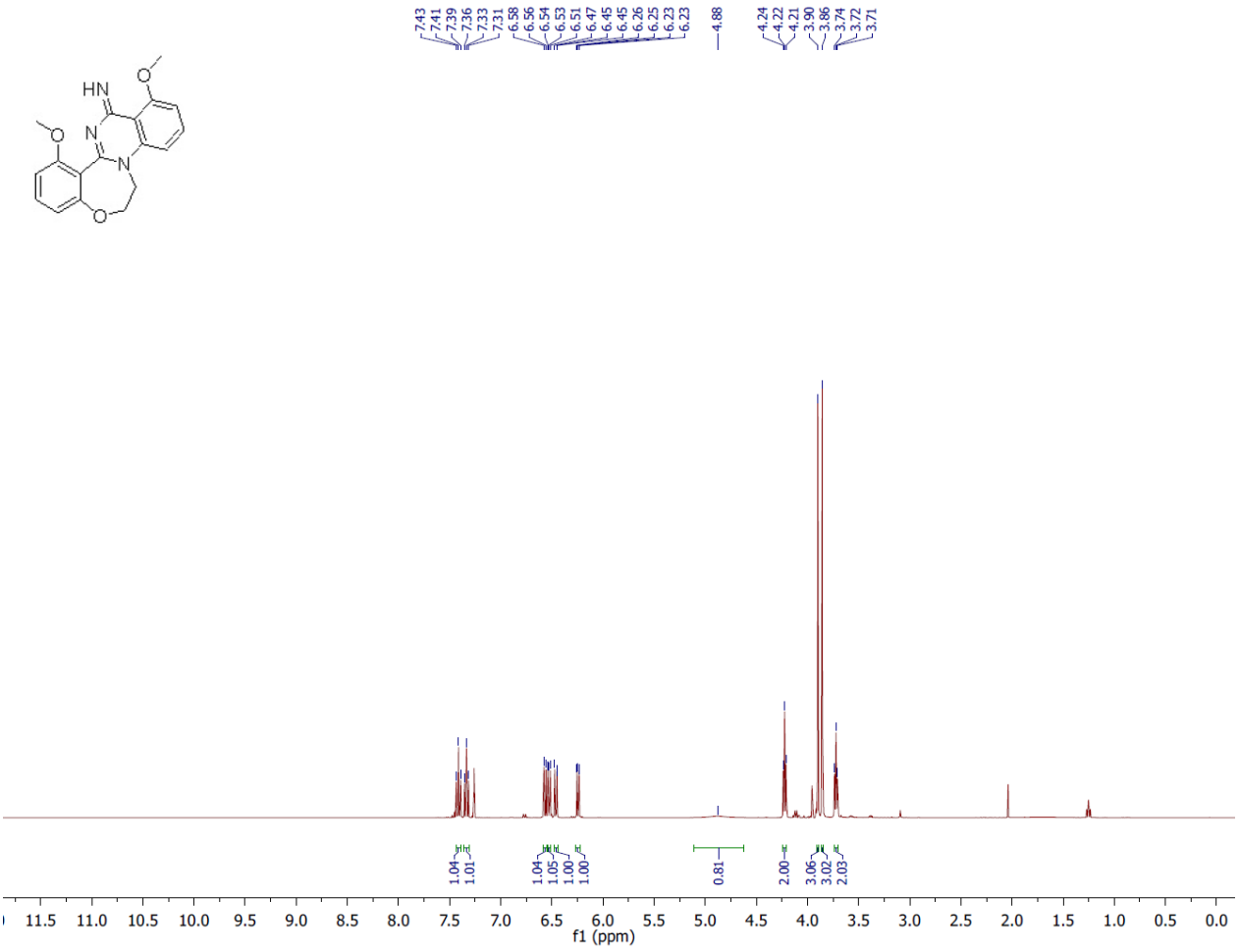
HN
Br
N
N
Br
O


2.00
1.95
2.04
0.98
2.09
2.09
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

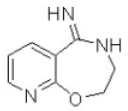

159.09
148.82
137.48
137.29
136.09
134.67
116.32
114.71
113.99
113.30
112.99
108.31
104.24
98.00
68.44
42.60
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

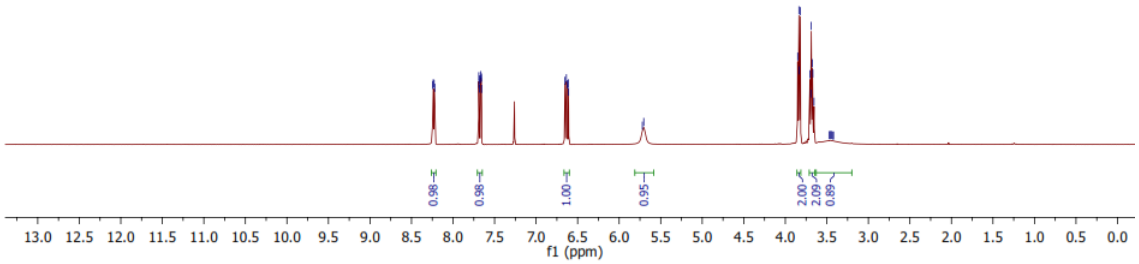
HN
Br
N
N
Br
O


7.43
7.41
7.39
7.36
7.33
7.31
6.58
6.56
6.54
6.53
6.51
6.47
6.45
6.45
6.26
6.25
6.23
6.23
4.88
4.24
4.22
4.21
3.90
3.86
3.74
3.72
3.71
HN
O
N
N
O
O
1.04
1.01
1.04
1.05
1.00
1.00
0.81
2.00
3.06
3.02
2.03
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

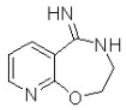

7.43
7.41
7.39
7.36
7.33
7.31
6.58
6.56
6.54
6.53
6.51
6.47
6.45
6.45
6.26
6.25
6.23
6.23
4.88
4.24
4.22
4.21
3.90
3.86
3.74
3.72
3.71
HN
O
N
N
O
O
1.04
1.01
1.04
1.05
1.00
1.00
0.81
2.00
3.06
3.02
2.03
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

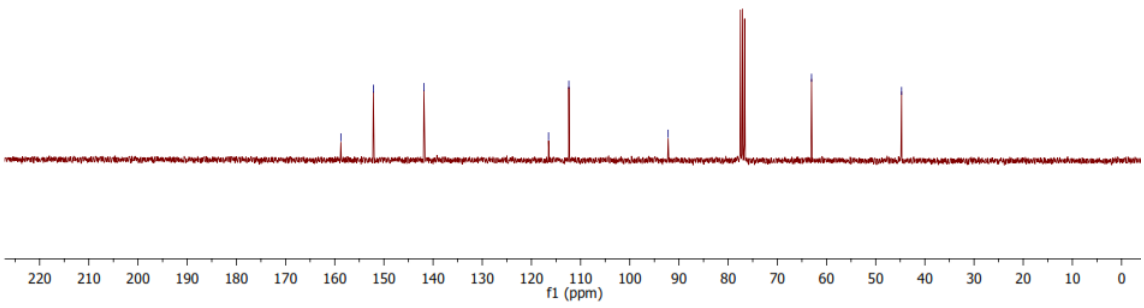

8.24
8.24
8.23
8.22
7.69
7.68
7.66
7.66
7.66
6.64
6.63
6.61
6.61
5.72
5.70
3.85
3.84
3.83
3.82
3.70
3.69
3.69
3.67
3.67
3.65
3.47
3.46
3.44
3.42
3.42

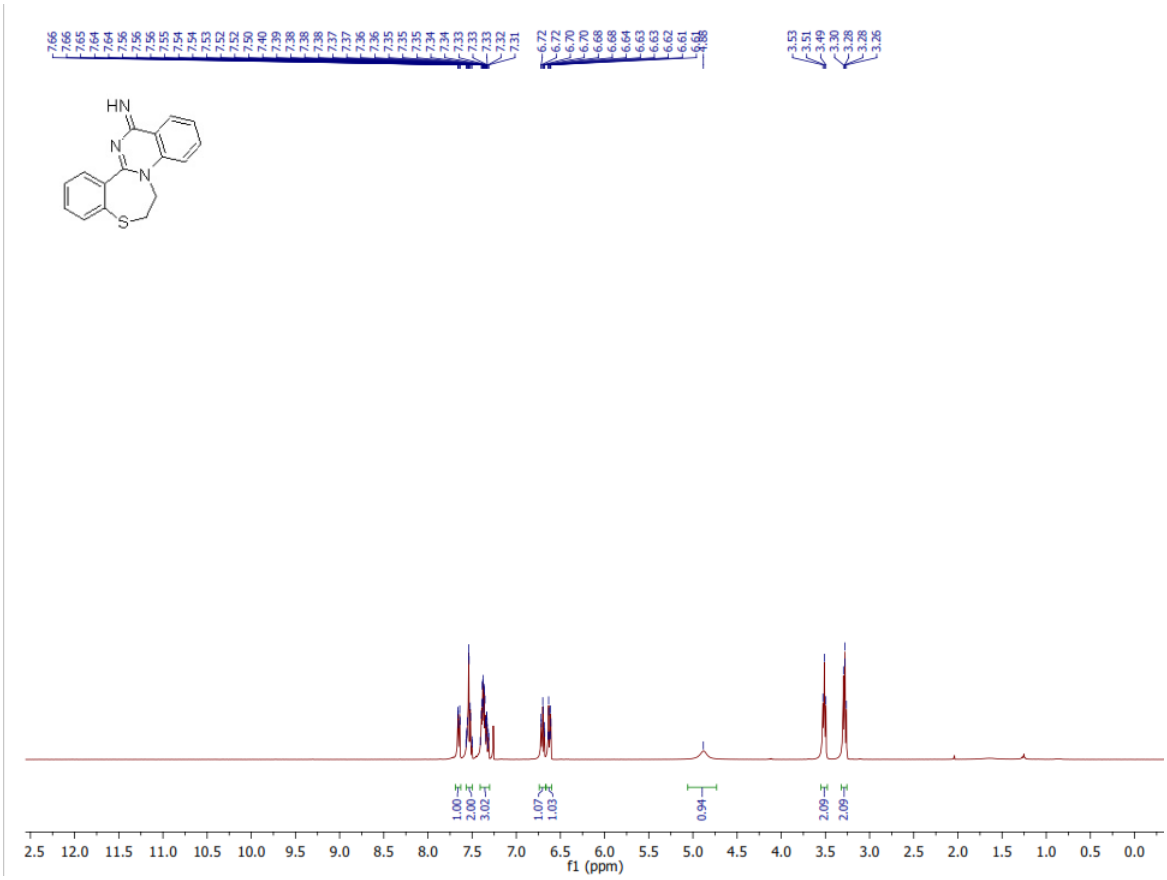

HN
NH
N
O


0.98
0.98
1.00
0.95
2.00
2.09
0.89
13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

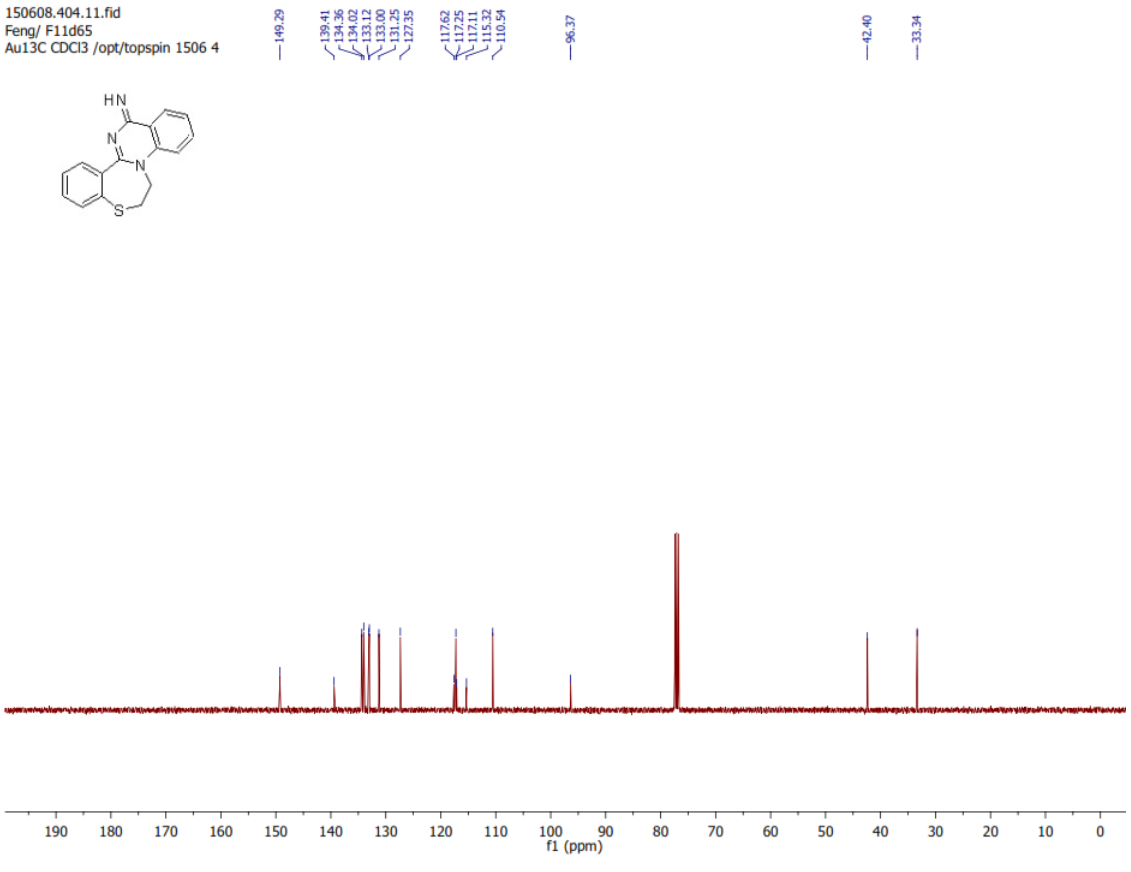

158.76
152.14
141.87
116.53
112.39
92.20
63.04
44.74

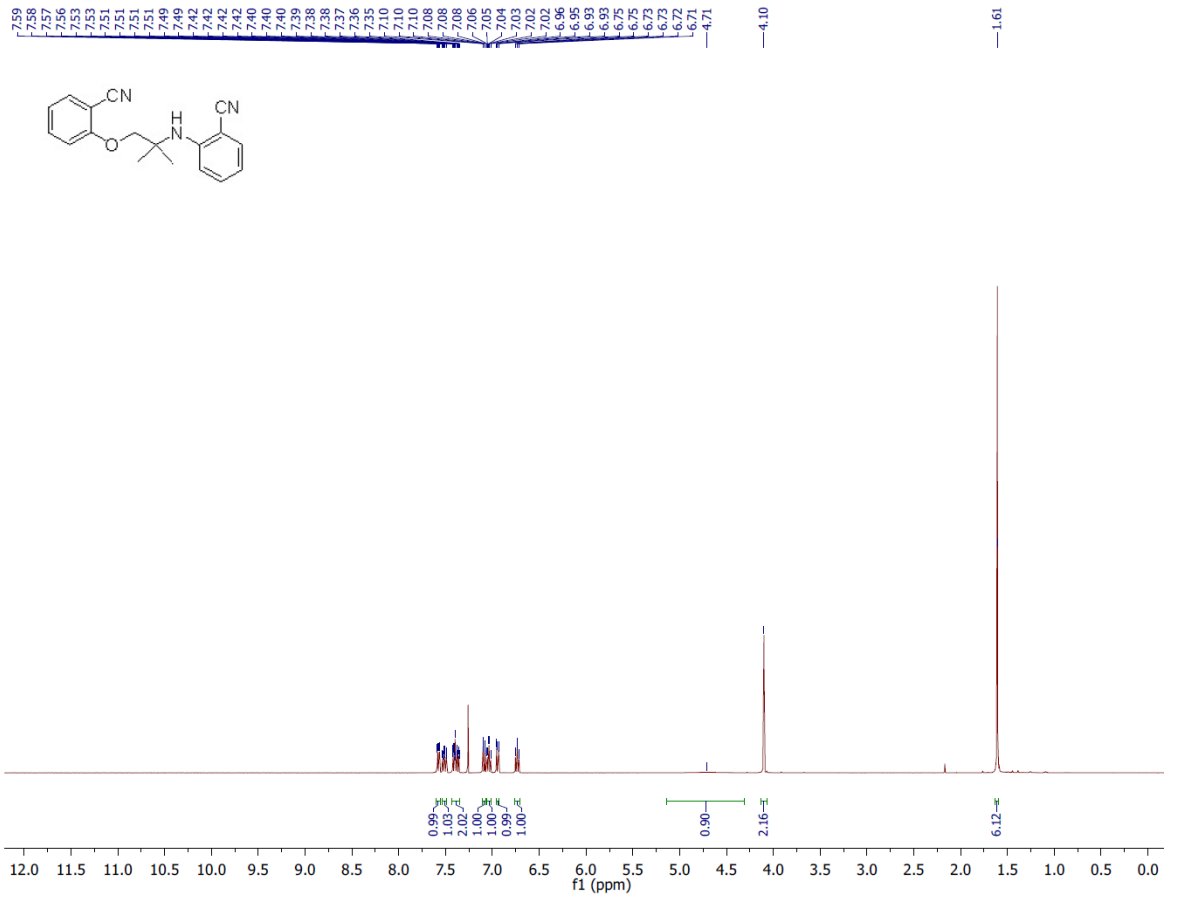

HN
NH
N
O

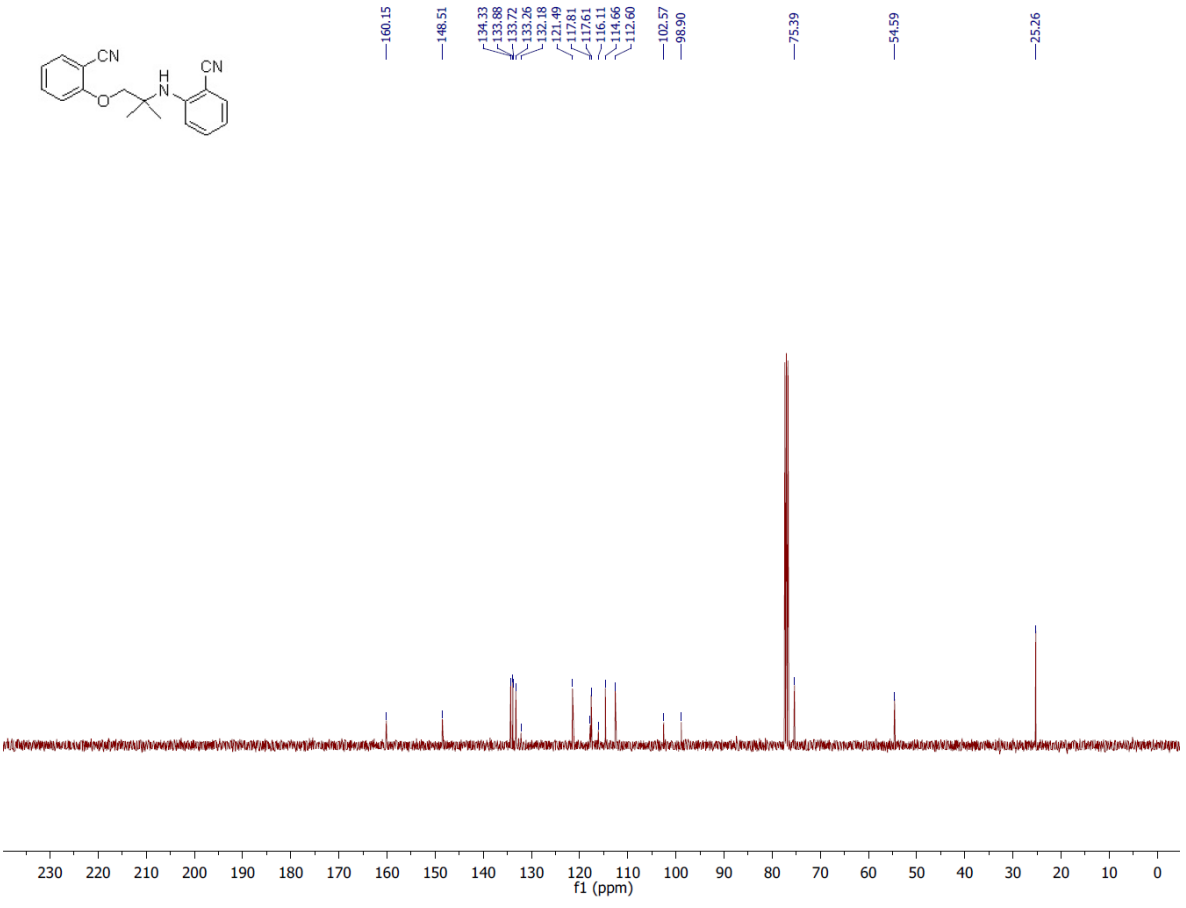

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

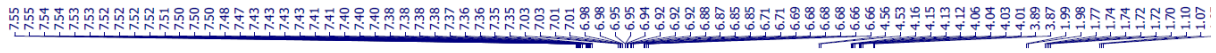


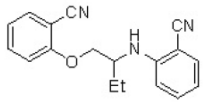
150608.404.11.fid
Feng/ F11d65
Au13C CDCl3 /opt/topspin 1506 4

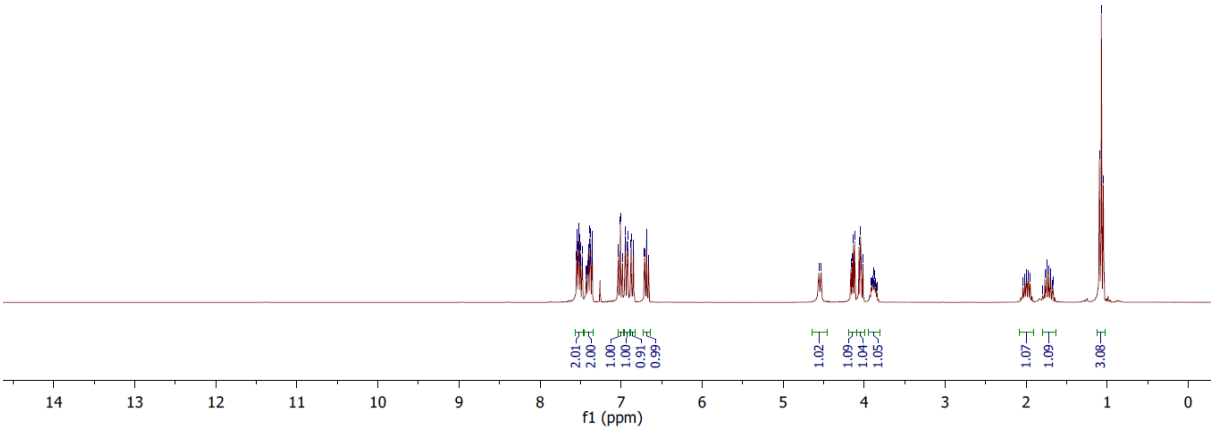



7.59 7.58 7.57 7.56 7.53 7.53 7.51 7.51 7.51 7.51 7.49 7.49 7.42 7.42 7.42 7.42 7.40 7.40 7.40 7.40 7.39 7.38 7.38 7.37 7.36 7.35 7.10 7.10 7.10 7.08 7.08 7.08 7.08 7.06 7.05 7.04 7.03 7.02 7.02 6.96 6.95 6.93 6.93 6.75 6.75 6.73 6.73 6.72 6.71 6.71 4.10 1.61
CN
CN
H
N
O
0.99 1.03 2.02 1.00 1.00 0.99 1.00 0.90 2.16 6.12
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

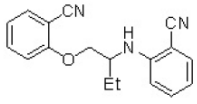

160.15 148.51 134.33 133.88 133.72 133.26 132.18 121.49 117.81 117.61 116.11 114.66 112.60 102.57 98.90 75.39 54.59 25.26
CN
CN
H
N
O
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

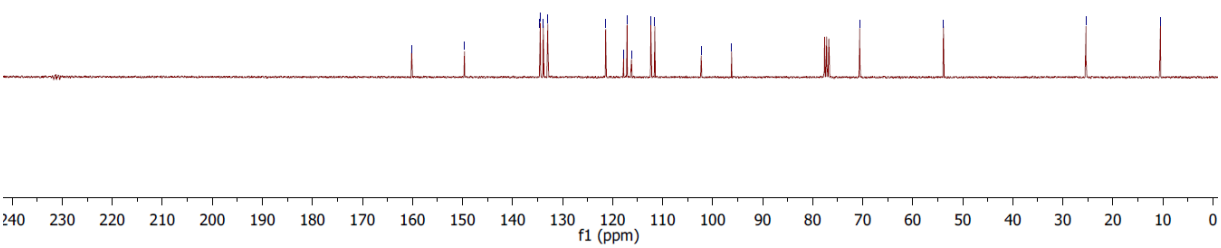


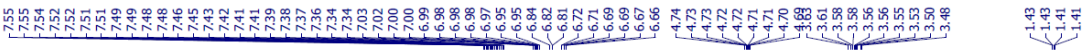

CN
O
H
N
CN
Et

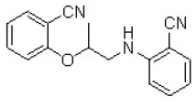

2.01
2.00
1.00
1.00
0.91
0.99
1.02
1.09
1.04
1.05
1.07
1.09
3.08
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

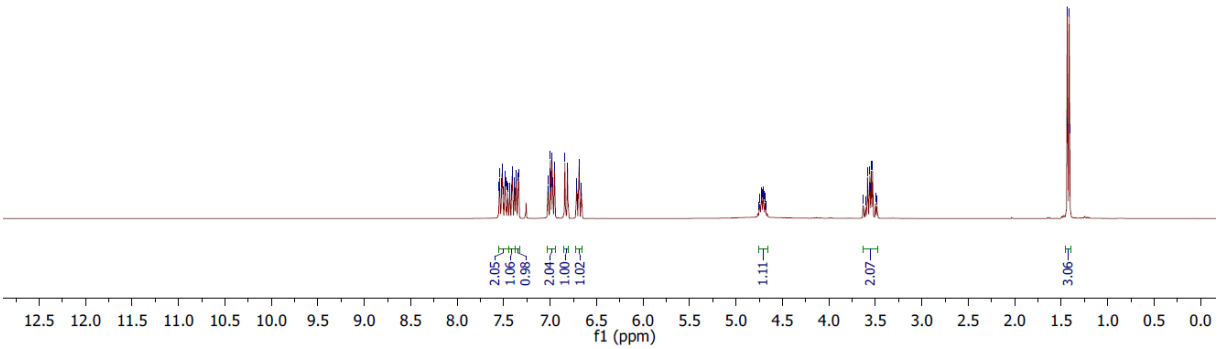

160.17
149.59
134.56
134.43
133.86
132.94
121.38
117.79
117.09
116.22
112.37
111.56
102.28
96.20
70.59
53.86
25.35
10.49


CN
O
H
N
CN
Et

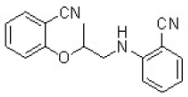

240
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

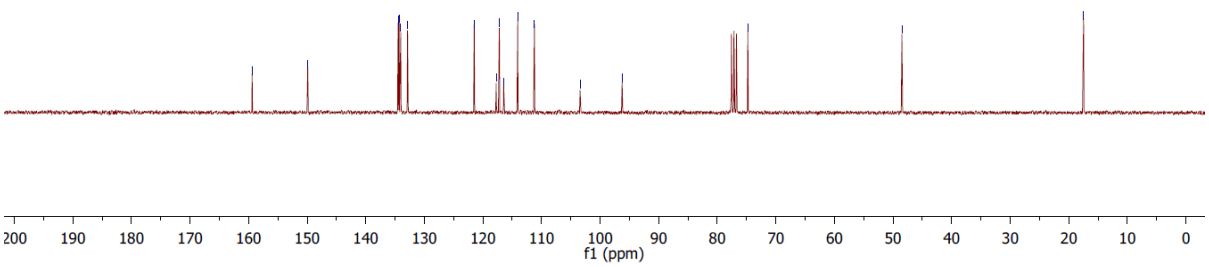

7.55
7.55
7.54
7.52
7.52
7.51
7.51
7.49
7.49
7.48
7.48
7.46
7.45
7.43
7.42
7.41
7.41
7.39
7.38
7.37
7.36
7.34
7.34
7.03
7.02
7.00
7.00
6.99
6.98
6.98
6.98
6.97
6.95
6.95
6.84
6.82
6.81
6.72
6.71
6.69
6.69
6.67
6.66
4.74
4.73
4.73
4.72
4.72
4.71
4.71
4.70
3.61
3.58
3.58
3.56
3.56
3.55
3.53
3.50
3.48
1.43
1.43
1.41
1.41

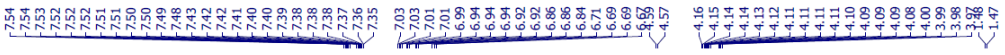

CN
CN
H
N
O

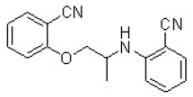

2.05
1.06
0.98
2.04
1.00
1.02
1.11
2.07
3.06
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

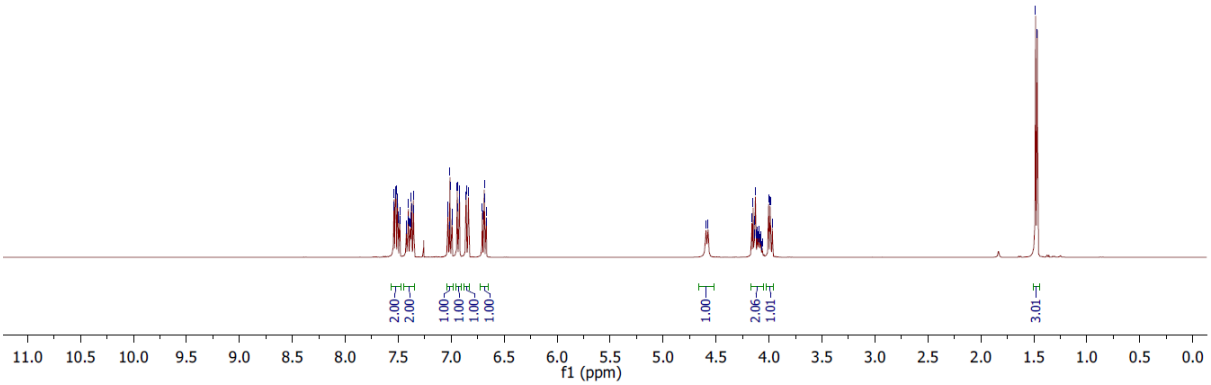

159.40
149.90
134.48
134.31
134.03
132.87
121.49
117.73
117.20
116.47
114.06
111.21
103.42
96.25
74.78
48.49
17.47


CN
CN
H
N
O

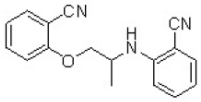

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

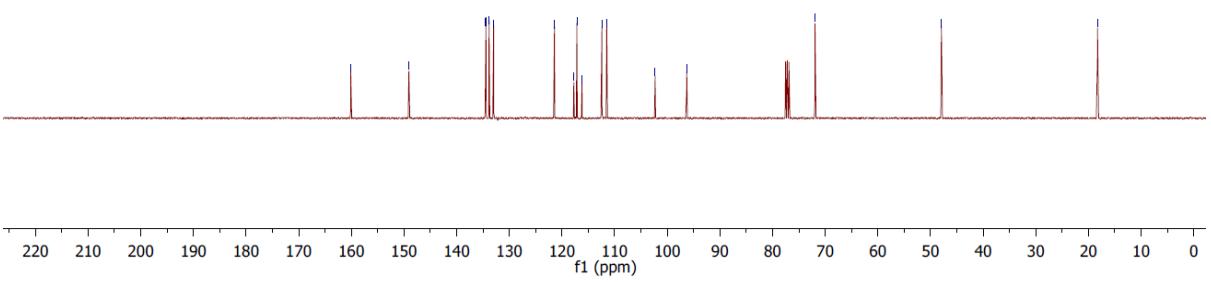



CN
O
H
N
CN


2.00
2.00
1.00
1.00
1.00
1.00
1.00
2.06
1.01
3.01
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


160.12
149.08
134.55
134.44
133.85
132.98
121.42
117.75
117.17
116.20
112.42
111.50
102.30
96.30
71.94
47.93
18.28


CN
O
H
N
CN


220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)