Supporting Information

Synthesis of Fused Polycyclic Compounds via Intramolecular Oxidative Cyclization/Aromatization of β-Tetralone or β-Tetralone Oximes

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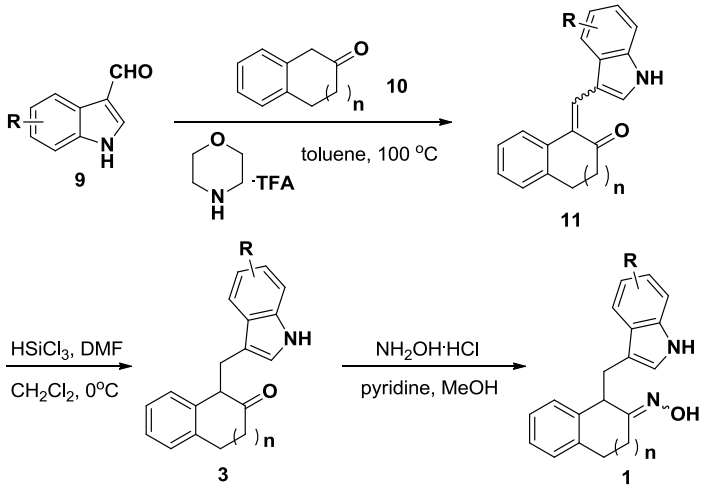
General

All starting materials were of the highest commercially available grade and used without further purification. All solvents used in the reactions were distilled from appropriate drying agents prior to use. Reactions were monitored by thin layer chromatography using silica gel HSGF254 plates. Flash chromatography (FC) was performed using silica gel HG/T2354-2010. Melting points were measured on a melt-Temp apparatus and uncorrected. ^{1}H and ^{13}C NMR (300 and 75 MHz, 600 and 151 MHz respectively) spectra were recorded in DMSO-d_6 and $CDCl_3$. ^{1}H NMR chemical shifts are reported in ppm ($\boldsymbol{\delta}$) relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$, $\boldsymbol{\delta}$ = 7.26 ppm; DMSO-d_6, $\boldsymbol{\delta}$ = 2.50 ppm). Data are reported as follows: chemical shift, multiplicity (s = singlet, br s = broad singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constants (Hz) and integration. ^{13}C NMR chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$, $\boldsymbol{\delta}$ = 77.16 ppm; DMSO-d_6, $\boldsymbol{\delta}$ = 39.52 ppm). ESI HRMS spectra were recorded on BioTOF Q.

General procedure for preparation of the substrates [1, 2, 3, 4, 5]



*I*ndole-3-carbaldehyde **9** (4 mmol, 1 eq), morpholinetrifluoroacetate (80 mg, 0.4 mmol, 0.1 eq) and 3,4-dihydronaphthalen-2(1H)-one **10** (4 mmol, 1 eq) were reacted in toluene at 100℃ for 5-12 h. The resulting mixture was cooled to room temperature, evaporated the solvent. Purification by recrystallization or column chromatography (silica gel, hexane/EtOAc = 5/1 to 3/1) to afforded pure **11**.

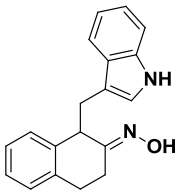
*T*richlorosilane (2 eq) was added to a stirred solution of **11** (1 eq) and DMF (5 eq) in anhydrous CH_2Cl_2 at 0°C. The mixture was allowed to stir at the same temperature until the reaction finished. The reaction was quenched with a saturated aqueous solution of $NaHCO_3$ and was extracted with CH_2Cl_2. The combined extracts were washed with brine and dried over anhydrous Na_2SO_4 and the

solvents were evaporated. Purification by recrystallization or column chromatography (silica gel, hexane/EtOAc = 3/1) to afforded pure **3**.

*T*he solution of compound **3** (1 eq), hydroxylammonium chloride (1.2 eq), pyridine (2.2 eq) in methanol was stirred at room temperature for 2 h. Then, the resulting mixture was poured into water, and extracted with EtOAc for three times, the combined extracts were washed with brine, dried with anhydrous Na_2SO_4, filtered and evaporated. The residue was purified by carefully column chromatography to receive a higher *E*/*Z* ratio of oxime **1**.

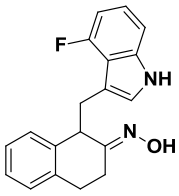
Experiment data for substrate 1

(E)-1-((1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1a)



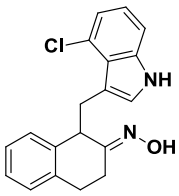
^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.72 (s, 1H), 10.41 (s, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.12 (td, *J* = 7.4, 1.2 Hz, 1H), 7.04 (dt, *J* = 15.2, 3.9 Hz, 2H), 6.91-6.97 (m, 3H), 3.82 (t, *J* = 7.4 Hz, 1H), 3.14 (dd, *J* = 14.5, 7.3 Hz, 1H), 3.04 (dd, *J* = 14.5, 7.5 Hz, 1H), 2.90-2.99 (m, 1H), 2.79 (ddd, *J* = 15.5, 7.0, 4.2 Hz, 1H), 2.69 (ddd, *J* = 17.9, 6.9, 4.1 Hz, 1H), 2.53-2.61 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 158.05, 139.08, 137.21, 136.13, 127.99, 127.73, 127.35, 126.25, 126.08, 123.45, 120.70, 118.24, 118.18, 111.68, 111.29, 46.09, 30.89, 26.30, 22.37. ESI HRMS exact mass calcd. for $(C_{19}H_{18}N_2O + Na)^+$ requires m/z 313.1311, found m/z 313.1307.

(E)-1-((4-fluoro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1b)



^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 11.01 (s, 1H), 10.36 (s, 1H), 7.18 (d, *J* = 7.4 Hz, 1H), 7.10-7.16 (m, 2H), 7.07 (t, *J* = 7.3 Hz, 1H), 7.00 (td, *J* = 7.9, 5.2 Hz, 1H), 6.93 (dd, *J* = 14.7, 4.7 Hz, 2H), 6.71 (dd, *J* = 11.5, 7.7 Hz, 1H), 3.81 (t, *J* = 7.8 Hz, 1H), 3.18 (dd, *J* = 14.3, 8.6 Hz, 1H), 3.03-3.13 (m, 2H), 2.84 (dd, *J* = 10.0, 5.7 Hz, 1H), 2.70 (dd, *J* = 7.1, 4.2 Hz, 1H), 2.57-2.66 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 157.42, 156.62 (d, *J* = 242.8 Hz), 139.26 (d, *J* = 12.1 Hz), 139.12, 137.17, 127.84, 127.76, 126.32, 126.17, 124.18, 121.23 (d, *J* = 7.7 Hz), 115.60 (d, *J* = 19.4 Hz), 110.38, 107.98 (d, *J* = 2.8 Hz), 103.26 (d, *J* = 19.2 Hz), 47.05, 31.48, 26.35, 22.20. ESI HRMS exact mass calcd. for $(C_{19}H_{17}FN_2O + H)^+$ requires m/z 309.1398, found m/z 309.1398.

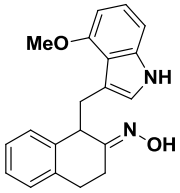
(E)-1-((4-chloro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1c)



^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 11.10 (d, *J* = 1.6 Hz, 1H), 10.35 (s, 1H), 7.30 (dd, *J* = 7.5, 1.4 Hz, 1H), 7.19 (d, *J* = 7.4 Hz, 1H), 7.13 (td, *J* = 7.4, 1.2 Hz, 1H), 7.07 (t, *J* = 7.1 Hz, 1H), 6.99-7.04 (m, 2H), 6.97 (d, *J* = 2.4 Hz, 1H), 6.92 (d, *J* = 7.0 Hz, 1H), 3.91 (t, *J* = 7.9 Hz, 1H), 3.27 (qd, *J* = 14.4, 7.9 Hz, 2H), 3.07-3.18 (m, 1H), 2.85 (ddd, *J* = 15.6, 7.2, 4.2 Hz, 1H), 2.73 (ddd, *J* = 17.9, 7.2, 4.1 Hz, 1H), 2.58-2.68 (m,

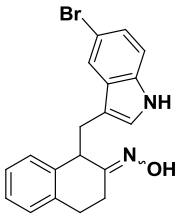
1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 157.40, 139.15, 137.92, 137.19, 127.89, 127.75, 126.32, 126.16, 126.00, 124.59, 123.61, 121.47, 119.18, 111.74, 110.76, 47.49, 30.91, 26.34, 22.28. ESI HRMS exact mass calcd. for $(C_{19}H_{17}ClN_2O + H)^+$ requires m/z 325.1102, found m/z 325.1108.

(E)-1-((4-methoxy-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1d)



^{1}H NMR (300 MHz, $CDCl_3$): ***δ*** 8.44 (br s, 1H), 7.81 (s, 1H), 7.16-7.13 (m, 2H), 7.09-7.03 (m, 2H), 6.89 (dd, *J* = 8.2, 0.4 Hz, 2H), 6.52 (d, *J* = 1.9 Hz, 1H), 6.48 (d, *J* = 7.7 Hz, 1H), 3.97-3.92 (m, 4H), 3.38-3.31 (m, 1H), 3.26-3.21 (m, 1H), 3.17-3.12 (m, 1H), 2.92-2.90 (m, 1H), 2.87-2.75 (m, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): ***δ*** 160.92, 154.78, 138.89, 137.88, 136.92, 128.69, 127.64, 126.26, 126.13, 122.55, 121.51, 117.37, 113.60, 104.41, 99.26, 54.97, 47.81, 32.47, 26.84, 22.62. ESI HRMS exact mass calcd. for $(C_{20}H_{20}N_2O_2 + Na)^+$ requires m/z 343.1417, found m/z 343.1406.

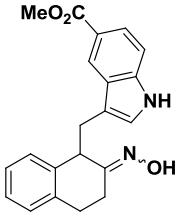
1-((5-bromo-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1e)



E/Z = 1.3/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.96 (s, 1H), 10.91 (s, 0.75H), 10.67 (s, 0.75H), 10.43 (s, 1H), 7.50 (s, 0.75H), 7.47 (s, 1H), 7.27 (dd, *J* = 8.5, 5.1 Hz, 1.78H), 7.09-7.18 (m, 4.53H), 6.99-7.09 (m, 3.56H), 6.96 (d, *J* = 7.4 Hz, 1H), 6.79 (d, *J* = 7.5 Hz, 0.75H), 6.72 (d, *J* = 1.4 Hz, 0.75H), 4.45 (dd, *J* = 7.1, 5.0 Hz, 0.75H), 3.78 (t, *J* = 7.4 Hz, 1H), 3.20 (dd, *J* = 14.0, 4.7 Hz, 0.80H), 3.10 (m, 1.82H), 3.03 (dd, *J* = 14.5, 7.7 Hz, 1H), 2.88-2.99 (m, 1H), 2.76-2.80 (m, 1H), 2.62-2.75 (m, 2.62H), 2.51-2.61 (m, 1H), 2.31 (dt, *J* = 13.5, 6.5 Hz, 0.78H), 2.20-2.29 (m, 0.80H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 158.20, 157.96, 138.83, 137.73, 137.20, 136.89, 134.76, 134.69, 129.35, 129.22, 128.86, 128.11, 127.98, 127.74, 126.32, 126.06, 125.78, 125.23, 123.19, 123.14, 120.96, 120.62, 113.24, 113.21, 111.65, 111.42, 110.95, 110.93, 46.06, 30.87, 30.05, 28.21, 27.61, 26.22, 22.33. ESI HRMS exact mass calcd. for $(C_{19}H_{17}BrN_2O + Na)^+$ requires m/z 391.0416, found m/z 391.0406.

methyl

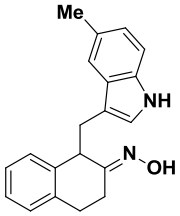
3-((2-(hydroxyimino)-1,2,3,4-tetrahydronaphthalen-1-yl)methyl)-1H-indole-5-carboxylate



(1f): E/Z = 4/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 11.16 (s, 1H), 10.45 (s, 1H), 8.08-8.11 (m, 1H), 7.68 (dd, *J* = 13.3, 8.5 Hz, 1H), 7.39 (d, *J* = 11.8 Hz, 1H), 7.17 (d, *J* = 7.4 Hz, 1H), 7.11 (td, *J* = 7.4, 1.2 Hz, 1H), 7.02-7.07 (m, 2H), 6.87 (d, *J* = 7.3 Hz, 1H), 3.84 (s, 3H), 3.79-3.83 (m, 1H), 3.15-3.18 (m, 1H), 3.09 (dd, *J* = 14.5, 7.9 Hz, 1H), 2.94-2.98 (m, 1H), 2.81 (ddd, *J* = 15.5, 7.0, 3.9 Hz, 1H), 2.67-2.77 (m, 1H), 2.51-2.60 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 167.35, 157.98, 138.74, 138.68, 137.24, 127.99, 127.79, 126.94, 126.36, 126.07, 125.39, 121.83, 120.96, 119.81, 113.35, 111.29, 51.61, 46.15, 30.64, 26.23, 22.45. ESI

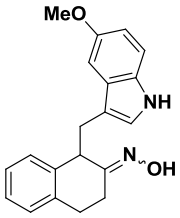
HRMS exact mass calcd. for $(C_{21}H_{20}N_2O_3 + H)^+$ requires m/z 349.1547, found m/z 349.1546.

(E)-1-((5-methyl-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1g)



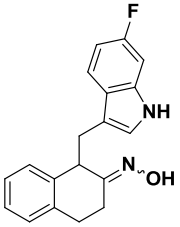
^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.56 (s, 1H), 10.41 (s, 1H), 7.15-7.19 (m, 3H), 7.12 (td, *J* = 7.4, 1.2 Hz, 1H), 7.05 (dd, *J* = 10.6, 4.0 Hz, 1H), 6.91 (d, *J* = 7.3 Hz, 1H), 6.86 (dd, *J* = 8.2, 1.3 Hz, 1H), 6.83 (d, *J* = 2.2 Hz, 1H), 3.81 (t, *J* = 7.4 Hz, 1H), 3.09 (dd, *J* = 14.4, 7.1 Hz, 1H), 3.00 (dd, *J* = 14.4, 7.7 Hz, 1H), 2.89-2.97 (m, 1H), 2.78 (ddd, *J* = 15.5, 7.0, 4.1 Hz, 1H), 2.69 (ddd, *J* = 17.9, 6.9, 4.1 Hz, 1H), 2.52-2.60 (m, 1H), 2.35 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 158.15, 139.06, 137.22, 134.53, 128.06, 127.70, 127.55, 126.48, 126.21, 126.02, 123.52, 122.31, 117.92, 111.09, 110.96, 46.00, 31.06, 26.27, 22.38, 21.31. ESI HRMS exact mass calcd. for $(C_{20}H_{20}N_2O + H)^+$ requires m/z 305.1648, found m/z 305.1646.

1-((5-methoxy-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1h)



E/Z = 2.5/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 10.56 (d, *J* = 1.4 Hz, 1H), 10.44 (s, 1H), 7.18 (d, *J* = 8.7 Hz, 1H), 7.12-7.14 (m, 1H), 7.02-7.09 (m, 2H), 6.97 (d, *J* = 7.3 Hz, 1H), 6.86 (d, *J* = 2.3 Hz, 1H), 6.79 (d, *J* = 2.3 Hz, 1H), 6.67 (dd, *J* = 8.6, 2.5 Hz, 1H), 3.81 (t, *J* = 7.2 Hz, 1H), 3.71 (s, 3H), 3.07-3.14 (m, 1H), 3.03 (dd, *J* = 14.4, 7.5 Hz, 1H), 2.82-2.84 (m, 1H), 2.72-2.79 (m, 1H), 2.63-2.68 (m, 1H), 2.51-2.59 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 158.23, 152.87, 139.05, 137.31, 131.22, 128.91, 128.15, 127.70, 126.24, 126.08, 124.14, 111.86, 111.44, 110.88, 100.04, 55.21, 46.01, 31.29, 26.24, 22.46. ESI HRMS exact mass calcd. for $(C_{20}H_{20}N_2O_2 + Na)^+$ requires m/z 343.1417, found m/z 343.1419.

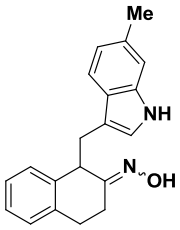
1-((6-fluoro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1i)



E/Z = 1.5/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.81 (s, 1H), 10.76 (s, 0.67H), 10.63 (s, 0.66H), 10.41 (s, 1H), 7.38 (ddd, *J* = 14.4, 8.6, 5.5 Hz, 1.77H), 7.15 (d, *J* = 7.2 Hz, 1H), 7.12 (td, *J* = 7.3, 1.1 Hz, 1.2H), 7.105-7.10 (m, 3.73H), 7.03 (ddd, *J* = 8.7, 5.0, 1.5 Hz, 1H), 6.96 (d, *J* = 7.3 Hz, 1H), 6.94 (d, *J* = 2.2 Hz, 1H), 6.76-6.79 (m, 2.41H), 6.65 (d, *J* = 2.2 Hz, 0.68H), 4.49 (dd, *J* = 7.5, 5.0 Hz, 0.70H), 3.80 (t, *J* = 7.4 Hz, 1H), 3.22 (dd, *J* = 14.1, 4.8 Hz, 0.72H), 3.11 (ddd, *J* = 13.9, 7.5, 3.3 Hz, 1.78H), 3.02 (dd, *J* = 14.5, 7.5 Hz, 1H), 2.92 (dd, *J* = 9.3, 6.9 Hz, 1H), 2.78 (ddd, *J* = 15.6, 7.0, 4.1 Hz, 1H), 2.71 (dd, *J* = 7.0, 4.1 Hz, 0.51H), 2.67 (t, *J* = 6.3 Hz, 1.95H), 2.52-2.62 (m, 1.11H), 2.29-2.39 (m, 0.72H), 2.24 (dd, *J* = 14.1, 7.3 Hz, 0.72H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 159.49, 158.30, 157.97, 157.94, 138.99, 137.83, 137.22, 136.83, 135.94, 135.86, 128.86, 128.01, 127.75, 126.29, 126.11, 126.00, 125.78, 124.39, 124.26, 124.03 (d, *J* = 3.2 Hz), 119.48 (d, *J* = 10.0 Hz), 119.20 (d, *J* = 10.0 Hz), 112.01, 111.73, 106.67, 106.51, 97.21 (d, *J* = 25.2 Hz), 97.17 (d,

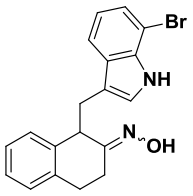
J = 25.3 Hz), 46.11, 30.81, 30.18, 28.30, 27.54, 26.27, 22.35. ESI HRMS exact mass calcd. for $(C_{19}H_{17}FN_2O + Na)^+$ requires m/z 331.1217, found m/z 331.1214.

1-((6-methyl-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1j)



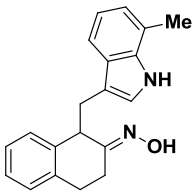
E/Z = 4/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.60 (s, 0.25H), 10.54 (s, 1H), 10.49 (s, 0.25H), 10.40 (s, 1H), 7.32 (d, *J* = 8.0 Hz, 0.27H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.15 (d, *J* = 7.3 Hz, 1H), 7.11 (dd, *J* = 7.8, 7.1 Hz, 1H), 7.09 (s, 1H), 7.00-7.08 (m, 2H), 6.91 (d, *J* = 7.4 Hz, 1H), 6.80 (d, *J* = 2.0 Hz, 1H), 6.77 (d, *J* = 8.0 Hz, 1H), 6.72-6.76 (m, 0.55H), 6.53 (d, *J* = 2.0 Hz, 0.25H), 4.50 (dd, *J* = 7.5, 4.9 Hz, 0.26H), 3.81 (t, *J* = 7.4 Hz, 1H), 3.21 (dd, *J* = 14.0, 4.7 Hz, 0.25H), 3.10 (dd, *J* = 14.4, 7.1 Hz, 1.31H), 3.00 (dd, *J* = 14.4, 7.7 Hz, 1H), 2.88-2.96 (m, 1H), 2.77 (ddd, *J* = 15.5, 7.0, 4.1 Hz, 1H), 2.66-2.70 (m, 1.57H), 2.51-2.59 (m, 1H), 2.37 (s, 3H), 2.36 (s, 0.85H), 2.30 (dt, *J* = 14.0, 6.9 Hz, 0.28H), 2.19-2.27 (m, 0.29H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 158.15, 139.06, 137.21, 136.60, 129.63, 128.01, 127.71, 126.23, 126.05, 125.34, 122.71, 119.97, 117.99, 111.51, 111.16, 46.11, 31.09, 26.30, 22.39, 21.39. ESI HRMS exact mass calcd. for $(C_{20}H_{20}N_2O + H)^+$ requires m/z 305.1648, found m/z 305.1648.

1-((7-bromo-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1k)



E/Z = 2.5/1; ^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 10.98 (s, 1H), 10.40 (s, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.25 (t, *J* = 7.1 Hz, 1H), 7.17 (d, *J* = 7.3 Hz, 1H), 7.13 (td, *J* = 7.3, 1.2 Hz, 1H), 7.05-7.11 (m, 1H), 7.02 (d, *J* = 2.4 Hz, 1H), 6.99 (d, *J* = 7.2 Hz, 1H), 6.90 (t, *J* = 7.3 Hz, 1H), 3.81 (t, *J* = 7.5 Hz, 1H), 3.12 (dd, *J* = 14.3, 7.8 Hz, 1H), 3.04 (dd, *J* = 14.5, 7.3 Hz, 1H), 2.91-3.00 (m, 1H), 2.80 (ddd, *J* = 15.5, 7.0, 4.2 Hz, 1H), 2.64-2.73 (m, 1H), 2.58 (dd, *J* = 9.8, 7.3 Hz, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** (major *E* isomer) 157.78, 138.92, 137.23, 134.33, 129.17, 127.99, 127.79, 126.33, 126.17, 124.88, 123.29, 119.70, 117.92, 113.28, 104.09, 46.02, 30.73, 26.27, 22.31. ESI HRMS exact mass calcd. for $(C_{19}H_{17}BrN_2O + H)^+$ requires m/z 369.0597, found m/z 369.0602.

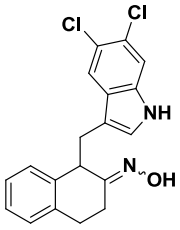
(E)-1-((7-methyl-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1l)



^{1}H NMR (600 MHz, DMSO-d_6): ***δ*** 10.68 (s, 1H), 10.40 (s, 1H), 7.27 (d, *J* = 7.4 Hz, 1H), 7.16 (d, *J* = 7.3 Hz, 1H), 7.12 (td, *J* = 7.4, 1.1 Hz, 1H), 7.06 (t, *J* = 7.4 Hz, 1H), 6.95 (d, *J* = 7.3 Hz, 1H), 6.90 (d, *J* = 2.3 Hz, 1H), 6.86 (dd, *J* = 13.2, 5.8 Hz, 2H), 3.82 (t, *J* = 7.4 Hz, 1H), 3.13 (dd, *J* = 14.5, 7.4 Hz, 1H), 3.02 (dd, *J* = 14.5, 7.5 Hz, 1H), 2.91-3.00 (m, 1H), 2.79 (ddd, *J* = 15.5, 7.0, 4.2 Hz, 1H), 2.69 (ddd, *J* = 17.9, 6.9, 4.2 Hz, 1H), 2.53-2.63 (m, 1H), 2.42 (s, 3H). ^{13}C NMR (151 MHz, DMSO-d_6): ***δ*** 158.08, 139.14, 137.23, 135.67, 127.99, 127.75, 127.04, 126.25, 126.10, 123.19, 121.28, 120.28, 118.44, 115.89, 112.11, 46.11, 31.00, 26.33, 22.36, 16.77. ESI HRMS exact mass calcd. for

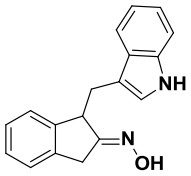
$(C_{20}H_{20}N_2O + H)^+$ requires m/z 305.1648, found m/z 305.1644.

1-((5,6-dichloro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one oxime (1m)



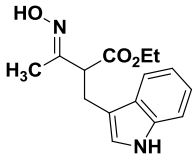
E/Z = 1.6/1; ^{1}H NMR (600 MHz, DMSO-d_6): $\boldsymbol{\delta}$ (major *E* isomer) 11.05 (d, *J* = 1.4 Hz, 1H), 10.43 (s, 1H), 7.54 (s, 1H), 7.47 (s, 1H), 7.10 (ddd, *J* = 8.4, 6.8, 1.2 Hz, 2H), 7.03-7.09 (m, 2H), 6.99 (d, *J* = 7.2 Hz, 1H), 3.78 (t, *J* = 7.5 Hz, 1H), 2.99-3.11 (m, 2H), 2.87-2.97 (m, 1H), 2.77 (ddd, *J* = 15.6, 7.0, 4.0 Hz, 1H), 2.66-2.73 (m, 1H), 2.551-2.58 (m, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): $\boldsymbol{\delta}$ (major *E* isomer) 157.86, 138.76, 137.23, 134.92, 128.17, 127.76, 127.45, 126.42, 126.37, 126.11, 122.93, 120.84, 119.57, 112.74, 112.04, 46.07, 30.74, 26.20, 22.32. ESI HRMS exact mass calcd. for $(C_{19}H_{16}Cl_2N_2O + H)^+$ requires m/z 359.0712, found m/z 359.0714.

(E)-1-((1H-indol-3-yl)methyl)-1H-inden-2(3H)-one oxime (1n)



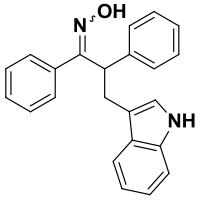
^{1}H NMR (600 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 10.75 (s, 1H), 10.73 (s, 1H), 7.49 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.20 (d, *J* = 7.4 Hz, 1H), 7.14 (t, *J* = 7.3 Hz, 1H), 7.09 (t, *J* = 7.1 Hz, 1H), 7.01-7.05 (m, 1H), 6.99 (d, *J* = 7.5 Hz, 1H), 6.91-6.95 (m, 1H), 6.85 (d, *J* = 2.2 Hz, 1H), 4.21 (t, *J* = 6.1 Hz, 1H), 3.63 (d, *J* = 22.3 Hz, 1H), 3.45 (d, *J* = 22.3 Hz, 1H), 3.31 (dd, *J* = 14.4, 5.0 Hz, 1H), 3.11 (dd, *J* = 14.6, 7.3 Hz, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 162.60, 143.82, 138.80, 135.98, 127.45, 126.92, 126.40, 124.79, 124.54, 123.45, 120.76, 118.49, 118.19, 111.39, 111.25, 46.94, 33.11, 30.66. ESI HRMS exact mass calcd. for $(C_{18}H_{16}N_2O + H)^+$ requires m/z 277.1335, found m/z 277.1335.

(E)-ethyl 2-((1H-indol-3-yl)methyl)-3-(hydroxyimino)butanoate (1o)



^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 8.00 (s, 2H), 7.59 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.16-7.22 (m, 1H), 7.12 (td, *J* = 7.5, 0.9 Hz, 1H), 6.99 (d, *J* = 2.3 Hz, 1H), 4.12 (qd, *J* = 7.1, 3.3 Hz, 2H), 3.70 (t, *J* = 7.7 Hz, 1H), 3.39 (ddd, *J* = 14.9, 8.0, 0.6 Hz, 1H), 3.15 (ddd, *J* = 14.9, 7.4, 0.6 Hz, 1H), 1.94 (s, 3H), 1.18 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 171.89, 156.24, 136.23, 127.40, 122.56, 122.19, 119.56, 118.72, 112.65, 111.27, 61.25, 52.29, 25.09, 14.20, 12.09. ESI HRMS exact mass calcd. for $(C_{15}H_{18}N_2O_3 + H)^+$ requires m/z 275.1390, found m/z 275.1394.

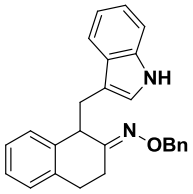
3-(1H-indol-3-yl)-1,2-diphenylpropan-1-one oxime (1p)



E/Z = 1/1.5; ^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 8.39 (s, 1.4H), 7.84-7.86 (m, 3.1H), 7.56 (t, *J* = 8.7 Hz, 2.3H), 7.45 (d, *J* = 7.6 Hz, 3.0H), 7.32-7.34 (m, 5H), 7.22-7.29 (m, 10H), 7.14-7.21 (m, 5.5H), 7.07-7.13 (m, 2.4H), 7.04 (d, *J* = 7.4 Hz, 3.0H), 6.96-6.98 (m, 1.7H), 6.90 (d, *J* = 1.8 Hz, 1.5H), 6.81 (d, *J* = 2.0 Hz, 0.8H), 5.43-5.54 (m, 1.5H), 4.24 (t, *J* = 7.6 Hz, 1H), 3.60 (dd, *J* = 14.8, 7.7 Hz, 1H), 3.38-3.50 (m, 3H), 3.24 (dd, *J* = 14.8, 7.6 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 162.33,

160.79, 140.87, 140.32, 136.26, 136.16, 135.44, 133.89, 128.76, 128.60, 128.51, 128.29, 128.24, 128.10, 128.08, 127.74, 127.70, 127.00, 126.81, 122.62, 122.12, 122.04, 122.00, 119.40, 119.36, 119.07, 118.80, 114.09, 113.80, 111.19, 111.12, 52.41, 42.51, 29.22, 26.35. ESI HRMS exact mass calcd. for $(C_{23}H_{20}N_2O + Na)^+$ requires m/z 363.1468, found m/z 363.1458.

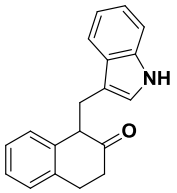
(E)-1-((1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one O-benzyl oxime (5)



^{1}H NMR (600 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 10.74 (s, 1H), 7.30-7.37 (m, 4H), 7.27 (t, *J* = 6.5 Hz, 3H), 7.12 (ddd, *J* = 10.5, 8.3, 4.0 Hz, 2H), 7.04 (t, *J* = 7.4 Hz, 2H), 6.90-6.95 (m, 2H), 6.89 (d, *J* = 2.1 Hz, 1H), 4.93-5.05 (m, 2H), 3.82 (t, *J* = 7.3 Hz, 1H), 3.13 (dd, *J* = 14.4, 6.9 Hz, 1H), 3.07 (dd, *J* = 14.4, 7.7 Hz, 1H), 2.83-2.93 (m, 1H), 2.77 (ddd, *J* = 14.4, 7.5, 3.5 Hz, 2H), 2.61 (dd, *J* = 18.3, 8.0 Hz, 1H). ^{13}C NMR (151 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 160.43, 138.39, 138.33, 137.02, 136.05, 128.21, 128.09, 127.73, 127.62, 127.44, 127.35, 126.39, 126.17, 123.52, 120.71, 118.20, 111.28, 74.61, 46.02, 30.83, 26.03, 23.25. ESI HRMS exact mass calcd. for $(C_{26}H_{24}N_2O + Na)^+$ requires m/z 403.1781, found m/z 403.1773.

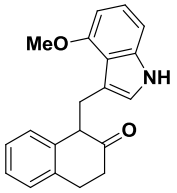
Experiment data for substrate 3

1-((1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3a)



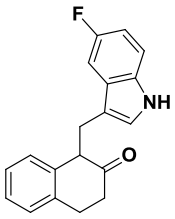
^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 7.91 (s, 1H), 7.35 (d, *J* = 7.9 Hz, 1H), 7.30 (d, *J* = 8.1 Hz, 1H), 7.13-7.21 (m, 3H), 7.10 (d, *J* = 7.3 Hz, 1H), 6.98-7.07 (m, 2H), 6.64 (d, *J* = 2.3 Hz, 1H), 3.81 (t, *J* = 6.2 Hz, 1H), 3.31-3.45 (m, 2H), 2.82 (dt, *J* = 15.5, 5.7 Hz, 1H), 2.65 (ddd, *J* = 15.5, 9.9, 5.7 Hz, 1H), 2.42-2.58 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 213.11, 137.43, 136.98, 136.09, 128.67, 127.77, 127.49, 126.81, 126.77, 122.99, 122.06, 119.55, 119.05, 112.63, 111.02, 54.24, 38.32, 28.99, 27.58. ESI HRMS exact mass calcd. for $(C_{19}H_{17}NO + H)^+$ requires m/z 276.1383, found m/z 276.1384.

1-((4-methoxy-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3b)



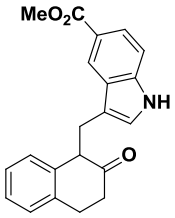
^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 7.91 (s, 1H), 7.12-7.22 (m, 2H), 7.03-7.11 (m, 2H), 6.92 (dd, *J* = 7.8, 4.7 Hz, 2H), 6.61 (d, *J* = 2.2 Hz, 1H), 6.46 (d, *J* = 7.7 Hz, 1H), 3.84-3.96 (m, 4H), 3.55 (dd, *J* = 14.2, 6.8 Hz, 1H), 3.33 (dd, *J* = 14.2, 7.5 Hz, 1H), 3.10-3.22 (m, 1H), 3.00 (dt, *J* = 15.6, 6.1 Hz, 1H), 2.68 (dt, *J* = 17.2, 5.8 Hz, 1H), 2.51 (ddd, *J* = 17.1, 9.1, 6.5 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 212.54, 154.87, 138.00, 137.79, 136.54, 128.70, 127.65, 126.57, 126.52, 122.91, 121.71, 117.41, 113.44, 104.56, 99.47, 56.13, 55.10, 37.61, 29.88, 28.16. ESI HRMS exact mass calcd. for $(C_{20}H_{19}NO_2 + H)^+$ requires m/z 306.1489, found m/z 306.1485.

1-((5-fluoro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3c)



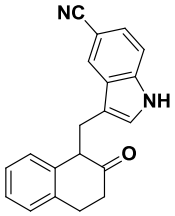
^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 7.95 (s, 1H), 7.13-7.24 (m, 3H), 7.07-7.12 (m, 1H), 7.00-7.06 (m, 1H), 6.88 (dd, *J* = 14.2, 5.9 Hz, 2H), 6.71 (d, *J* = 2.3 Hz, 1H), 3.72-3.84 (m, 1H), 3.37 (dd, *J* = 14.5, 6.8 Hz, 1H), 3.26-3.33 (m, 1H), 2.81 (dt, *J* = 15.4, 5.6 Hz, 1H), 2.59 (ddd, *J* = 15.5, 10.2, 5.5 Hz, 1H), 2.42-2.56 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 213.02, 157.88 (d, *J* = 234.3 Hz), 137.32, 136.98, 132.51, 128.64, 127.96 (d, *J* = 9.8 Hz), 127.85, 126.95, 126.88, 124.82, 112.88 (d, *J* = 4.6 Hz), 111.57 (d, *J* = 9.7 Hz), 110.45 (d, *J* = 26.4 Hz), 103.93 (d, *J* = 23.8 Hz), 54.09, 38.43, 29.12, 27.50. ESI HRMS exact mass calcd. for $(C_{19}H_{16}FNO + H)^+$ requires m/z 294.1289, found m/z 294.1297.

methyl 3-((2-oxo-1,2,3,4-tetrahydronaphthalen-1-yl)methyl)-1H-indole-5-carboxylate (3d)



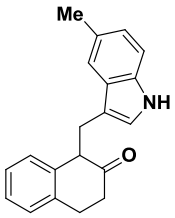
^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 8.25 (s, 1H), 8.02 (s, 1H), 7.84 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.30 (d, *J* = 8.5 Hz, 1H), 7.13-7.21 (m, 2H), 7.07-7.12 (m, 1H), 7.04 (dd, *J* = 5.0, 3.9 Hz, 1H), 6.77 (d, *J* = 2.1 Hz, 1H), 3.92 (s, 3H), 3.82 (t, *J* = 6.3 Hz, 1H), 3.41 (qd, *J* = 14.6, 6.2 Hz, 2H), 2.84 (dt, *J* = 15.5, 5.8 Hz, 1H), 2.66 (ddd, *J* = 15.5, 9.6, 5.8 Hz, 1H), 2.45-2.59 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 212.70, 168.27, 138.62, 137.14, 136.91, 128.55, 127.82, 127.18, 126.98, 126.90, 124.28, 123.52, 122.07, 121.66, 114.26, 110.78, 54.10, 51.91, 38.30, 28.43, 27.59. ESI HRMS exact mass calcd. for $(C_{21}H_{19}NO_3 + Na)^+$ requires m/z 356.1257, found m/z 356.1249.

3-((2-oxo-1,2,3,4-tetrahydronaphthalen-1-yl)methyl)-1H-indole-5-carbonitrile (3e)



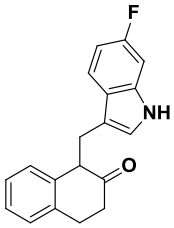
^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 8.40 (s, 1H), 7.29-7.39 (m, 3H), 7.19-7.25 (m, 2H), 7.03-7.13 (m, 2H), 6.87 (d, *J* = 2.2 Hz, 1H), 3.78 (t, *J* = 5.9 Hz, 1H), 3.47 (dd, *J* = 14.5, 6.6 Hz, 1H), 3.29 (dd, *J* = 14.5, 5.3 Hz, 1H), 2.74-2.83 (m, 1H), 2.40-2.54 (m, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 212.71, 137.57, 137.10, 136.98, 128.66, 128.03, 127.43, 127.27, 127.12, 125.20, 124.95, 124.93, 120.76, 113.80, 111.89, 102.63, 53.94, 38.61, 29.02, 27.38. ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2O + Na)^+$ requires m/z 323.1155, found m/z 323.1155.

1-((5-methyl-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3f)



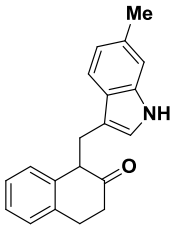
^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 7.81 (s, 1H), 7.16 (ddd, *J* = 10.2, 8.8, 4.6 Hz, 3H), 7.10 (d, *J* = 7.3 Hz, 1H), 7.06 (s, 1H), 6.93-7.02 (m, 2H), 6.60 (d, *J* = 2.2 Hz, 1H), 3.79 (t, *J* = 6.2 Hz, 1H), 3.34 (d, *J* = 6.2 Hz, 2H), 2.82 (dt, *J* = 15.5, 5.7 Hz, 1H), 2.66 (ddd, *J* = 15.5, 10.0, 5.6 Hz, 1H), 2.43-2.58 (m, 2H), 2.38 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 213.22, 137.51, 136.99, 134.45, 128.79, 128.70, 127.74, 126.77, 126.70, 123.66, 123.17, 118.73, 112.09, 110.63, 54.30, 38.32, 29.14, 27.57, 21.54. ESI HRMS exact mass calcd. for $(C_{20}H_{19}NO + H)^+$ requires m/z 290.1539, found m/z 290.1543.

1-((6-fluoro-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3g)



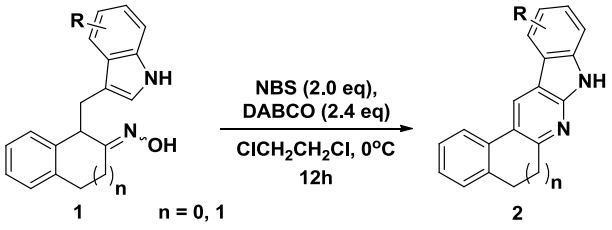
^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 7.93 (s, 1H), 7.15-7.18 (m, 3H), 7.06-7.12 (m, 1H), 6.99-7.04 (m, 1H), 6.96 (dd, *J* = 9.6, 2.3 Hz, 1H), 6.77 (ddd, *J* = 9.5, 8.9, 2.3 Hz, 1H), 6.61 (d, *J* = 2.3 Hz, 1H), 3.75-3.82 (m, 1H), 3.40 (dd, *J* = 14.5, 6.9 Hz, 1H), 3.30 (dd, *J* = 14.5, 5.3 Hz, 1H), 2.79 (dt, *J* = 15.3, 5.5 Hz, 1H), 2.57 (ddd, *J* = 15.4, 10.1, 5.6 Hz, 1H), 2.42-2.53 (m, 2H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 213.15, 160.01 (d, *J* = 237.6 Hz), 137.34, 136.99, 135.91 (d, *J* =12.5 Hz), 128.65, 127.84, 126.88, 126.83, 124.11, 123.22, 119.83 (d, *J* = 10.0 Hz), 112.74, 108.30 (d, *J* = 24.4 Hz), 97.29 (d, *J* = 26.2 Hz), 54.13, 38.45, 29.17, 27.48. ESI HRMS exact mass calcd. for ($C_{19}H_{16}FNO$ + H)$^+$ requires m/z 294.1289, found m/z 294.1291.

1-((6-methyl-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (3h)



^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 7.79 (s, 1H), 7.23 (d, *J* = 8.1 Hz, 1H), 7.12-7.19 (m, 2H), 7.10 (d, *J* = 7.3 Hz, 1H), 7.08 (s, 1H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.54 (d, *J* = 2.2 Hz, 1H), 3.79 (t, *J* = 6.2 Hz, 1H), 3.30-3.39 (m, 2H), 2.82 (dt, *J* = 15.5, 5.8 Hz, 1H), 2.66 (ddd, *J* = 15.5, 9.9, 5.7 Hz, 1H), 2.44-2.57 (m, 2H), 2.43 (s, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 213.21, 137.47, 136.95, 136.57, 131.82, 128.68, 127.74, 126.75, 126.72, 125.36, 122.34, 121.33, 118.71, 112.39, 110.99, 54.26, 38.31, 29.14, 27.60, 21.80. ESI HRMS exact mass calcd. for ($C_{20}H_{19}NO$ + H)$^+$ requires m/z 290.1539, found m/z 290.1539.

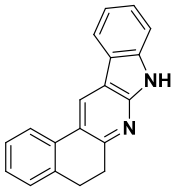
General procedure for the construction of benzo[f]indolo[2,3-b]quinolone 2



NBS (0.2 mmol, 35.6 mg) and DABCO (0.24 mmol, 27 mg) were added to the stirred solution of oxime 1 (0.1 mmol) in $ClCH_2CH_2Cl$ (3 mL) at 0^{o}C in sequence. The mixture was allowed to stir at the same temperature for 12 h. The resulting mixture was directly purified by column chromatography (silica gel, hexane/EtOAc = 3/1) to afforded pure benzo[f]indolo[2,3-b]quinolone **2**.

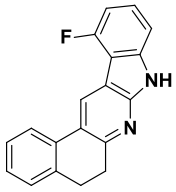
Experiment data for the benzo[f]indolo[2,3-b]quinolone 2

6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2a)



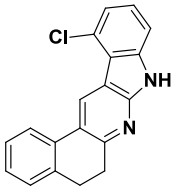
brown yellow solid, mp 264.5-266.2 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.72 (br s, 1H), 8.97 (s, 1H), 8.20 (d, J = 7.7 Hz, 1H), 7.98 (d, J = 7.7 Hz, 1H), 7.42- 7.50 (m, 2H), 7.29-7.40 (m, 2H), 7.20-7.25 (m, 2H), 3.06-3.11 (m, 2H), 2.95-2.99 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 155.00, 150.97, 138.95, 135.72, 134.03, 128.08, 127.05, 126.77, 126.17, 123.66, 123.34, 121.23, 121.03, 120.90, 119.41, 114.38, 111.27, 31.99, 28.33; ESI HRMS exact mass calcd. for $(C_{19}H_{14}N_2 + H)^+$ requires m/z 271.1230, found m/z 271.1222.

12-fluoro-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2b)



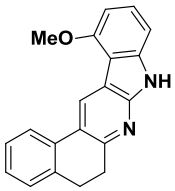
white solid, mp 306.9-308.5 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 12.07 (br s, 1H), 8.70 (s, 1H), 7.95 (d, J = 7.5 Hz, 1H), 7.42-7.45 (m, 1H), 7.34-7.40 (m, 3H), 7.30-7.32 (m, 1H), 6.99-7.06 (m, 1H), 3.07-3.12 (m, 2H), 2.95-3.00 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 157.73 (d, J = 245 Hz), 155.63, 150.43, 141.08 (d, J = 9.9 Hz), 135.82, 133.52, 128.07, 127.30, 127.19, 127.03, 124.58 (d, J = 2.5 Hz), 123.40, 121.91, 111.48, 108.85 (d, J = 20.4 Hz), 107.74 (d, J = 3.3 Hz), 105.10 (d, J = 18.2 Hz), 32.00, 28.17; ESI HRMS exact mass calcd. for $(C_{19}H_{13}FN_2 + H)^+$ requires m/z 289.1136, found m/z 289.1125.

12-chloro-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2c)



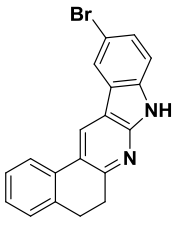
white solid, mp 351.8-353.6 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 12.13 (br s, 1H), 8.99 (s, 1H), 7.91 (d, J = 7.9 Hz, 1H), 7.23-7.50 (m, 6H), 3.09-3.11 (m, 2H), 2.98-3.00 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 156.09, 150.74, 140.11, 135.92, 133.56, 128.20, 127.59, 127.31, 127.14, 127.11, 124.59, 123.24, 121.70, 119.88, 117.97, 113.14, 110.34, 32.03, 28.19; ESI HRMS exact mass calcd. for $(C_{19}H_{13}ClN_2 + H)^+$ requires m/z 305.0840, found m/z 305.0833.

12-methoxy-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2d)



white solid, mp 289.3-291.5 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.75 (br s, 1H), 8.72 (s, 1H), 7.87 (d, J = 7.7 Hz, 1H), 7.30-7.40 (m, 3H), 7.20-7.25 (m, 1H), 7.09 (d, J = 7.7 Hz, 1H), 6.79 (d, J = 7.8 Hz, 1H), 4.07 (s, 3H), 3.06-3.10 (m, 2H), 2.95-2.99 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 155.84, 153.96, 150.32, 140.18, 135.76, 133.93, 128.11, 127.36, 127.15, 126.75, 124.36, 123.01, 121.18, 113.64, 109.69, 104.23, 100.86, 55.47, 31.90, 28.32; ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2O + H)^+$ requires m/z 301.1335, found m/z 301.1337.

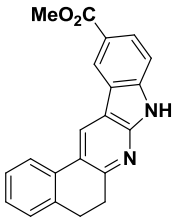
11-bromo-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2e)



white solid, mp 361.0-363.2 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.90 (br s, 1H), 9.06 (s, 1H), 8.45 (s, 1H), 7.95 (d, J = 7.7 Hz, 1H), 7.53-7.56 (m, 1H), 7.45

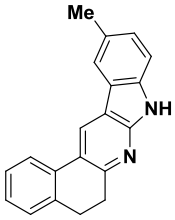
(d, *J* = 8.4 Hz, 1H), 7.21-7.39 (m, 3H), 3.07-3.11 (m, 2H), 2.95-3.00 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 156.07, 151.10, 137.64, 135.77, 133.83, 128.54, 128.14, 127.12, 126.98, 124.43, 123.64, 123.36, 122.89, 121.78, 113.51, 113.30, 111.46, 32.01, 28.22; ESI HRMS exact mass calcd. for $(C_{19}H_{13}BrN_2 + H)^+$ requires m/z 349.0335, found m/z 349.0327.

Methyl 6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline-11-carboxylate (2f)



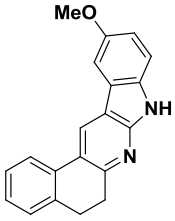
white solid, mp 295.4-297.2 ºC; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 12.15 (br s, 1H), 9.19 (s, 1H), 8.92 (s, 1H), 8.03-8.06 (m, 2H), 7.56 (d, *J* = 7.7 Hz, 1H), 7.27-7.38 (m, 2H), 7.22-7.24 (m, 1H), 3.90 (s, 3H), 3.08-3.12 (m, 2H), 2.96-3.01 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 166.83, 155.96, 151.53, 141.93, 135.81, 133.80, 128.11, 127.26, 127.13, 127.06, 124.62, 123.66, 123.31, 122.27, 120.85, 120.78, 114.50, 111.21, 51.85, 31.98, 28.23; ESI HRMS exact mass calcd. for $(C_{21}H_{16}N_2O_2 + H)^+$ requires m/z 329.1285, found m/z 329.1278.

11-methyl-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2g)



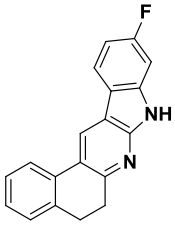
white solid, mp 300.3-301.9 ºC; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.58 (br s, 1H), 8.92 (s, 1H), 7.95-8.05 (m, 2H), 7.20-7.43 (m, 5H), 3.05-3.09 (m, 2H), 2.96-2.99 (m, 2H), 2.53 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 154.79, 151.17, 137.11, 135.68, 134.09, 128.10, 128.06, 127.42, 127.06, 126.69, 123.50, 123.25, 121.02, 120.83, 114.25, 110.99, 31.97, 28.35, 21.10; ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2 + H)^+$ requires m/z 285.1386, found m/z 285.1390.

11-methoxy-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2h)



white solid, mp 265.3-266.9 ºC; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.51 (br s, 1H), 8.97 (s, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.81 (s, 1H), 7.29-7.40 (m, 3H), 7.20-7.24 (m, 1H), 7.03-7.07 (m, 1H), 3.86 (s, 3H), 3.05-3.09 (m, 2H), 2.95-2.99 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 154.92, 153.52, 151.38, 135.67, 134.12, 133.54, 128.09, 127.03, 126.68, 123.75, 123.21, 121.33, 120.79, 115.25, 114.53, 112.01, 103.98, 55.54, 32.00, 28.35; ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2O + H)^+$ requires m/z 301.1335, found m/z 301.1344.

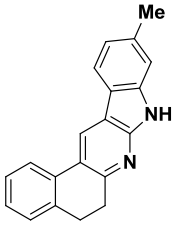
10-fluoro-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2i)



white solid, mp 284.4-286.3 ºC; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.85 (br s, 1H), 8.97 (s, 1H), 8.19-8.24 (m, 1H), 7.97 (d, *J* = 7.8 Hz, 1H), 7.30-7.38 (m, 2H), 7.21-7.25 (m, 2H), 7.04-7.10 (m, 1H), 3.05-3.10 (m, 2H), 2.95-3.00 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 161.30 (d, *J* = 238 Hz), 154.61, 151.45, 139.66 (d, *J* = 12.8 Hz), 135.78, 133.89, 128.11, 127.06, 126.91, 123.56, 123.39, 122.54 (d, *J* = 10.2 Hz), 121.67, 117.64, 114.10, 107.42 (d, *J* = 23.9 Hz), 97.86 (d, *J* = 26.1 Hz), 31.87, 28.29;

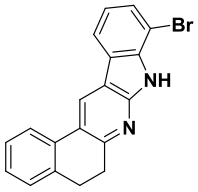
ESI HRMS exact mass calcd. for $(C_{19}H_{13}FN_2 + H)^+$ requires m/z 289.1136, found m/z 289.1135.

10-methyl-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2j)



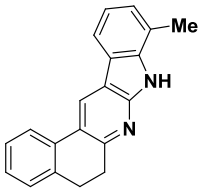
white solid, mp 323.0-324.8 °C; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.60 (br s, 1H), 8.88 (s, 1H), 8.06 (d, *J* = 7.9 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 7.22-7.37 (m, 4H), 7.05 (d, *J* = 7.9 Hz, 1H), 3.04-3.07 (m, 2H), 2.94-2.98 (m, 2H), 2.07 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 154.29, 151.06, 139.40, 135.82, 135.69, 134.09, 128.05, 127.02, 126.68, 123.26, 123.14, 121.07, 120.88, 120.73, 118.58, 114.53, 111.28, 31.92, 28.37, 21.71. ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2 + H)^+$ requires m/z 285.1386, found m/z 285.1389.

9-bromo-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2k)



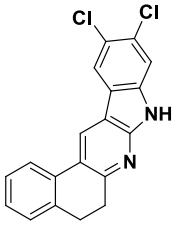
white solid, mp 216.7-218.2 °C; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 12.05 (br s, 1H), 9.03 (s, 1H), 8.24 (d, *J* = 7.7 Hz, 1H), 7.99 (d, *J* = 7.3 Hz, 1H), 7.64 (d, *J* = 7.7 Hz, 1H), 7.31-7.39 (m, 2H), 7.16-7.27 (m, 2H), 3.10-3.14 (m, 2H), 2.97-3.01 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 156.02, 151.03, 137.58, 135.82, 133.70, 128.70, 128.15, 127.10, 127.07, 124.41, 123.52, 122.77, 122.11, 120.91, 120.31, 114.63, 103.83, 31.97, 28.21; ESI HRMS exact mass calcd. for $(C_{19}H_{13}BrN_2 + H)^+$ requires m/z 349.0335, found m/z 349.0323.

9-methyl-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2l)



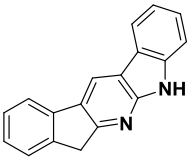
white solid, mp 328.5-330.3 °C; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.76 (br s, 1H), 8.94 (s, 1H), 7.97-8.04 (m, 2H), 7.30-7.38 (m, 2H), 7.22-7.25 (m, 2H), 7.11-7.7.16 (m, 1H), 3.08-3.12 (m, 2H), 2.96-3.01 (m, 2H), 2.54 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 154.75, 151.17, 138.23, 135.67, 134.03, 128.03, 127.00, 126.72, 123.59, 123.29, 121.16, 120.59, 120.49, 119.50, 118.34, 114.76, 31.97, 28.33, 16.89; ESI HRMS exact mass calcd. for $(C_{20}H_{16}N_2 + H)^+$ requires m/z 285.1386, found m/z 285.1388.

10,11-dichloro-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinoline (2m)



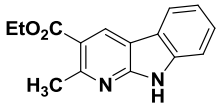
white solid, mp 334.4-336.2 °C; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 12.00 (br s, 1H), 9.05 (s, 1H), 8.50 (s, 1H), 7.92 (d, *J* = 7.7 Hz, 1H), 7.66 (s, 1H), 7.22-7.39 (m, 3H), 3.05-3.10 (m, 2H), 2.94-2.99 (m, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 156.50, 151.49, 137.94, 135.81, 133.63, 128.16, 128.06, 127.12, 124.59, 123.37, 122.57, 122.17, 121.76, 121.21, 113.23, 112.78, 32.00, 28.14; ESI HRMS exact mass calcd. for $(C_{19}H_{12}Cl_2N_2 + H)^+$ requires m/z 339.0450, found m/z 339.0455.

5,7-dihydroindeno[1',2':5,6]pyrido[2,3-b]indole (2n)



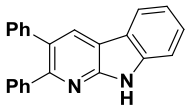
white solid, mp 336.1-337.5 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.77 (br s, 1H), 8.93 (s, 1H), 8.16 (d, J = 7.7 Hz, 1H), 7.92 (d, J = 7.7 Hz, 1H), 7.47-7.57 (m, 2H), 7.36-7.43 (m, 2H), 7.18-7.28 (m, 2H), 4.01 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 162.12, 151.71, 140.17, 140.09, 138.84, 126.94, 126.81, 126.08, 125.95, 125.04, 120.74, 119.75, 119.41, 119.37, 113.86, 111.33, 37.85; ESI HRMS exact mass calcd. for $(C_{18}H_{12}N_2 + H)^+$ requires m/z 257.1073, found m/z 257.1065.

ethyl 2-methyl-9H-pyrido[2,3-b]indole-3-carboxylate (2o)



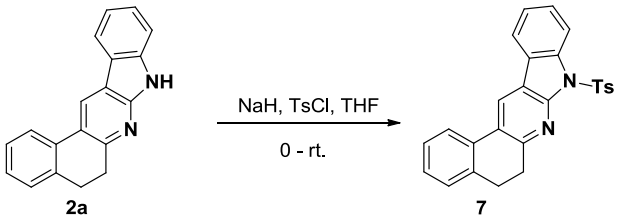
yellowish solid, mp 226.3-227.1 °C; ^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 11.10 (d, J = 24.8 Hz, 1H), 8.93 (s, 1H), 8.07 (d, J = 7.8 Hz, 1H), 7.56 (d, J = 8.1 Hz, 1H), 7.50 (t, J = 7.6 Hz, 1H), 7.31 (t, J = 7.5 Hz, 1H), 4.46 (q, J = 7.1 Hz, 2H), 3.09 (s, 3H), 1.49 (t, J = 7.1 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 167.32, 158.02, 153.17, 139.24, 131.96, 127.27, 121.40, 121.21, 120.96, 117.52, 114.33, 111.67, 61.09, 25.71, 14.61. ESI HRMS exact mass calcd. for $(C_{15}H_{14}N_2O_2 + H)^+$ requires m/z 255.1128, found m/z 255.1123.

2,3-diphenyl-9H-pyrido[2,3-b]indole (2p)



yellow solid, mp 273.5-274.8 °C; ^{1}H NMR (600 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 11.77 (br s, 1H), 8.39 (s, 1H), 8.00 (d, J = 7.0 Hz, 1H), 7.59 (d, J = 6.9 Hz, 2H), 7.27-7.39 (m, 8H), 7.14-7.22 (m, 2H), 6.19 (d, J = 11.2 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): $\boldsymbol{\delta}$ 153.74, 151.87, 141.27, 140.98, 139.77, 131.19, 130.70, 130.43, 128.53, 128.37, 128.34, 127.85, 126.75, 126.68, 120.83, 120.78, 119.96, 115.70, 111.67. ESI HRMS exact mass calcd. for $(C_{23}H_{16}N_2 + H)^+$ requires m/z 321.1386, found m/z 321.1390.

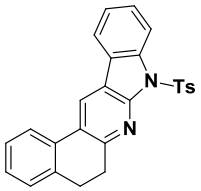
Tosyl protection of 2a



*T*o a stirred solution of **2a** (54 mg, 0.2 mmol) in THF (2 mL) was added NaH (1.2 mmol) at 0°C. The mixture was stirred for 10 min at 0°C, then, TsCl (190 mg, 1 mmol) was added in one portion. The resulting mixture was stirred at room temperature until the start material 2a consumed. NH_4Cl (aq) was added, and quenched with CH_2Cl_2 for three times. The combined extracts were washed with brine and dried over anhydrous Na_2SO_4 and the solvents were evaporated. Purification by

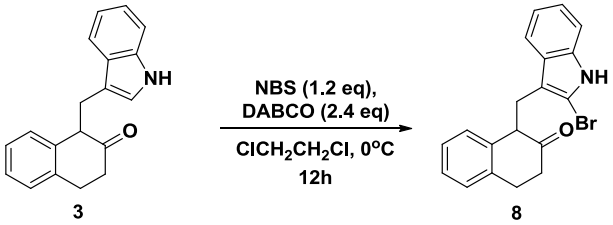
column chromatography (silica gel, hexane/EtOAc = 10/1) to afforded pure product **7** as a white solid (90% yield).

8-tosyl-6,8-dihydro-5H-benzo[f]indolo[2,3-b]quinolone (7)



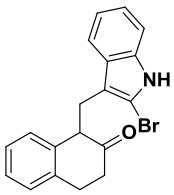
white solid, mp 214.3-215.3 ^{o}C; ^{1}H NMR (300 MHz, $CDCl_3$): ***δ*** 8.86 (s, 1H), 8.34 (d, *J* = 8.3 Hz, 1H), 8.17 (d, *J* = 7.4 Hz, 1H), 7.99 (d, *J* = 8.0 Hz, 2H), 7.91 (d, *J* = 7.5 Hz, 1H), 7.55 (t, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 1H), 7.22-7.29 (m, 5H), 3.11-3.16 (m, 2H), 2.96-2.98 (m, 2H), 2.27 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6 + $CDCl_3$): ***δ*** 155.64, 148.68, 144.99, 136.94, 135.94, 134.99, 132.48, 129.40, 127.94, 127.70, 127.21, 126.87, 125.58, 123.87, 123.79, 123.67, 122.85, 121.06, 116.96, 114.24, 31.68, 27.95, 20.98; ESI HRMS exact mass calcd. for $(C_{26}H_{20}N_2O_2S + H)^+$ requires m/z 425.1318, found m/z 425.1303.

The reaction of α-(indol-3-yl)methyl)-β-tetralone with NBS



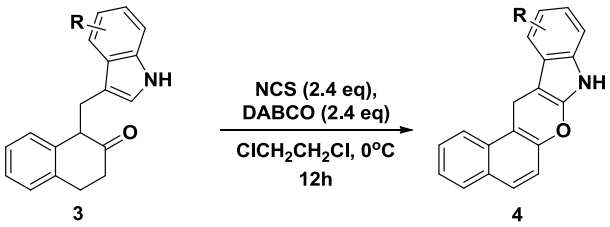
NBS (0.12 mmol, 21.4 mg) and DABCO (0.24 mmol, 27 mg) were added to the stirred solution of β-tetralone **3** (0.1 mmol, 27.5 mg) in $ClCH_2CH_2Cl$ (3 mL) at 0^{o}C in sequence. The mixture was allowed to stir at the same temperature for 12 h. The resulting mixture was directly purified by column chromatography (silica gel, hexane/EtOAc = 5/1) to afforded pure product **8**.

1-((2-bromo-1H-indol-3-yl)methyl)-3,4-dihydronaphthalen-2(1H)-one (8)



White solid, mp 108.5-110.3 ^{o}C; ^{1}H NMR (600 MHz, $CDCl_3$): ***δ*** 8.00 (s, 1H), 7.40 (d, *J* = 7.5 Hz, 1H), 7.26 (d, *J* = 2.2 Hz, 1H), 7.22 – 7.12 (m, 3H), 7.07 (td, *J* = 7.6, 1.0 Hz, 1H), 7.00-7.05 (m, 1H), 6.68 (d, *J* = 7.5 Hz, 1H), 3.78 (dd, *J* = 8.9, 5.8 Hz, 1H), 3.30 (dd, *J* = 14.2, 5.8 Hz, 1H), 3.16 (dd, *J* = 14.2, 8.9 Hz, 1H), 3.05-3.14 (m, 1H), 2.93 (ddd, *J* = 15.6, 6.5, 3.6 Hz, 1H), 2.75 (ddd, *J* = 17.6, 5.4, 3.6 Hz, 1H), 2.50 (ddd, *J* = 17.7, 11.6, 6.5 Hz, 1H). ^{13}C NMR (151 MHz, $CDCl_3$): ***δ*** 212.99, 136.65, 136.55, 136.08, 129.14, 127.88, 127.59, 127.04, 126.75, 122.2, 120.37, 118.41, 112.01, 110.52, 109.92, 54.36, 38.08, 29.27, 27.64. ESI HRMS exact mass calcd. for $(C_{19}H_{16}BrNO + H)^+$ requires m/z 354.0488, found m/z 354.0485.

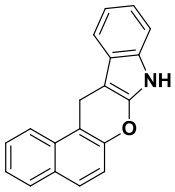
General procedure for the construction of benzo[5,6]chromeno[2,3-b]indole 4



NCS (0.24 mmol, 32 mg) was added to the stirred solution of **3** (0.1 mmol) and DABCO (0.24 mmol, 27 mg) in $ClCH_2CH_2Cl$ (3 mL) at 0°C. The mixture was allowed to stir at the same temperature for 12 h. The resulting mixture was directly purified by column chromatography (silica gel, hexane/EtOAc = 10/1) to afforded pure benzo[5,6]chromeno[2,3-b]indole **4**.

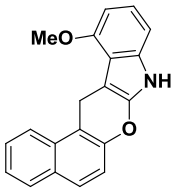
Experiment data for the benzo[5,6]chromeno[2,3-b]indole 4

8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4a)



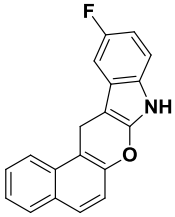
white solid, mp 204.8-206.3 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.49 (s, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.9 Hz, 1H), 7.64-7.67 (m, 1H), 7.50-7.53 (m, 2H), 7.41 (d, J = 8.9 Hz, 1H), 7.31-7.33 (m, 1H), 7.07-7.10 (m, 2H), 4.34 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 148.19, 144.50, 132.32, 131.12, 130.22, 128.43, 128.21, 127.03, 125.99, 124.74, 123.15, 120.05, 119.36, 117.93, 117.10, 112.78, 110.76, 84.73, 20.37; ESI HRMS exact mass calcd. for $(C_{19}H_{13}NO + H)^+$ requires m/z 272.1070, found m/z 272.1069.

12-methoxy-8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4b)



white solid, mp 197.2-199.2 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.40 (s, 1H), 7.94 (d, J = 8.0 Hz, 2H), 7.88 (d, J = 8.9 Hz, 1H), 7.64 (t, J = 7.2 Hz, 1H), 7.47-7.52 (m, 1H), 7.34 (d, J = 8.9 Hz, 1H), 6.85-6.95 (m, 2H), 6.54 (d, J = 7.5 Hz, 1H), 4.49 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 153.30, 148.06, 142.86, 132.22, 131.99, 130.17, 128.39, 128.22, 127.08, 124.67, 122.90, 120.72, 117.87, 115.61, 112.87, 104.50, 100.40, 84.21, 55.30, 22.16; ESI HRMS exact mass calcd. for $(C_{20}H_{15}NO_2 + H)^+$ requires m/z 302.1176, found m/z 302.1188.

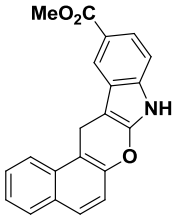
11-fluoro-8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4c)



white solid, mp 196.5-197.8 °C; ^{1}H NMR (300 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 11.56 (s, 1H), 7.88-8.02 (m, 3H), 7.64-7.67 (m, 1H), 7.50-7.51 (m, 1H), 7.38 (d, J = 8.9 Hz, 1H), 7.22-7.27 (m, 2H), 6.81-6.84 (m, 1H), 4.29 (s, 2H); ^{13}C NMR (75 MHz, DMSO-d_6): $\boldsymbol{\delta}$ 157.33 (d, J = 229.8 Hz), 148.03, 145.90, 132.23, 130.26, 128.52, 128.25, 127.58, 127.09, 126.50 (d, J = 10.5 Hz), 124.84, 123.13, 117.88, 112.71,

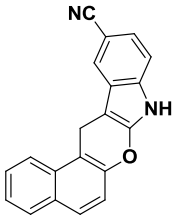
111.60 (d, *J* = 9.7 Hz), 107.37 (d, *J* = 25.2 Hz), 102.51 (d, *J* = 23.9 Hz), 85.52 (d, *J* = 4.1 Hz), 20.25; ESI HRMS exact mass calcd. for $(C_{19}H_{12}FNO + H)^+$ requires m/z 290.0976, found m/z 290.0966.

Methyl 8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole-11-carboxylate (4d)



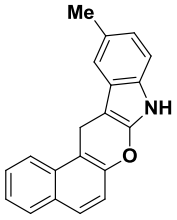
white solid, mp 287.1-288.5 ºC; ^{1}H NMR (300 MHz, DMSO-*d*$_6$): ***δ*** 11.98 (s, 1H), 8.22 (s, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.95-8.00 (m, 1H), 7.92 (s, 1H), 7.69-7.75 (m, 2H), 7.54-7.56 (m, 1H), 7.37-7.44 (m, 2H), 4.41 (s, 2H), 3.87 (s, 3H); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): ***δ*** 167.27, 148.00, 145.62, 134.06, 132.25, 130.33, 128.58, 128.22, 127.13, 125.63, 124.92, 123.34, 121.40, 120.80, 119.29, 117.87, 112.82, 110.65, 86.01, 51.67, 20.19; ESI HRMS exact mass calcd. for $(C_{21}H_{15}NO_3 + H)^+$ requires m/z 330.1125, found m/z 330.1131.

8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole-11-carbonitrile (4e)



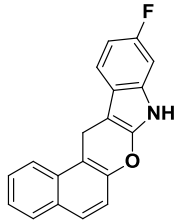
white solid, mp 329.9-331.2 ºC; ^{1}H NMR (300 MHz, DMSO-*d*$_6$): ***δ*** 12.15 (s, 1H), 7.88-8.00 (m, 4H), 7.63-7.68 (m, 1H), 7.49-7.54 (m, 1H), 7.37-7.44 (m, 3H), 4.32 (s, 2H); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): ***δ*** 147.85, 146.16, 133.24, 132.08, 130.32, 128.58, 128.22, 127.11, 125.93, 124.91, 123.17, 123.03, 121.92, 120.69, 117.74, 112.63, 111.75, 101.36, 85.81, 19.97; ESI HRMS exact mass calcd. for $(C_{20}H_{12}N_2O + H)^+$ requires m/z 297.1022, found m/z 297.1022.

11-methyl-8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4f)



white solid, mp 219.8-221.5 ºC; ^{1}H NMR (300 MHz, $CDCl_3$): ***δ*** 8.01 (d, *J* = 8.6 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.76-7.79 (m, 2H), 7.63-7.65 (m, 1H), 7.50-7.52 (m, 1H), 7.36 (s, 1H), 7.25-7.30 (m, 1H), 7.21 (d, *J* = 8.1 Hz, 1H), 7.00 (d, *J* = 8.1 Hz, 1H), 4.36 (s, 2H), 2.50 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): ***δ*** 148.65, 144.70, 132.84, 131.02, 130.60, 129.63, 129.13, 128.28, 128.22, 127.03, 126.80, 124.58, 123.08, 121.93, 121.70, 118.01, 117.42, 113.14, 110.21, 85.93, 21.59, 20.85; ESI HRMS exact mass calcd. for $(C_{20}H_{15}NO + H)^+$ requires m/z 286.1226, found m/z 286.1214.

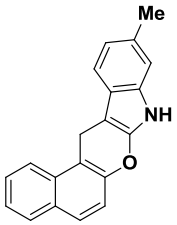
10-fluoro-8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4g)



white solid, mp 191.6-192.7 ºC; ^{1}H NMR (300 MHz, DMSO-*d*$_6$): ***δ*** 11.63 (s, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.99 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 9.0 Hz, 1H), 7.67-7.69 (m, 1H), 7.46-7.54 (m, 2H), 7.41 (d, *J* = 8.9 Hz, 1H), 7.08-7.12 (m, 1H), 6.92-6.94 (m, 1H), 4.34 (s, 2H); ^{13}C NMR (75 MHz, DMSO-*d*$_6$): ***δ*** 158.12 (d, *J* = 230.9 Hz), 148.00, 144.62 (d, *J* = 2.8 Hz), 132.26, 131.01 (d, *J* = 12.6 Hz), 130.23, 128.48, 128.22, 127.06, 124.80, 123.16, 122.67, 117.89, 117.78, 112.66, 107.17 (d, *J*

= 23.5 Hz), 97.51 (d, *J* = 26.1 Hz), 84.73, 20.29; ESI HRMS exact mass calcd. for ($C_{19}H_{12}FNO$ + H)$^+$ requires m/z 290.0976, found m/z 290.0964.

10-methyl-8,13-dihydrobenzo[5,6]chromeno[2,3-b]indole (4h)



white solid, mp 228.5-230.6 °C; ^{1}H NMR (300 MHz, DMSO-d_6): ***δ*** 11.31 (s, 1H), 8.05 (d, *J* = 8.6 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.67 (t, *J* = 7.9 Hz, 1H), 7.56 (t, *J* = 7.8 Hz, 1H), 7.37-7.41 (m, 2H), 7.09 (s, 1H), 6.90 (d, *J* = 8.2 Hz, 1H), 4.33 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (75 MHz, DMSO-d_6): ***δ*** 148.18, 143.98, 132.33, 131.45, 130.18, 128.95, 128.37, 128.19, 127.01, 124.70, 123.73, 123.14, 120.74, 117.94, 116.85, 112.73, 110.85, 84.41, 21.45, 20.42; ESI HRMS exact mass calcd. for ($C_{20}H_{15}NO$ + H)$^+$ requires m/z 286.1226, found m/z 286.1217.

X-ray crystal structure of substrate 1d and compound 7

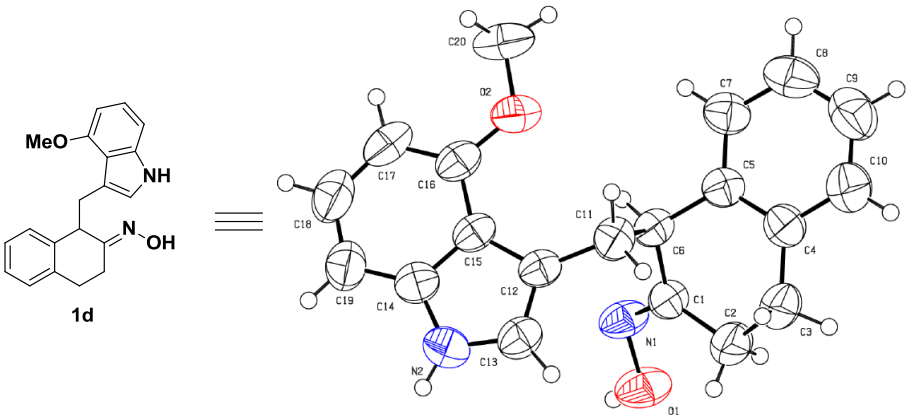
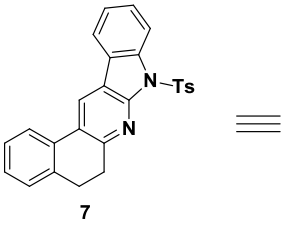


Table 1. Crystal data and structure refinement for **1d**.

Identification code	**1d**
Empirical formula	C_{20} H_{20} N_2 O_2
Formula weight	320.38
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 12.761(2) A alpha = 90 deg.
	b = 5.4290(10) A beta = 117.22(3) deg.
	c = 27.3250(10) A gamma = 90 deg.
Volume	1683.4(4) A^3
Z, Calculated density	4, 1.264 Mg/m^3
Absorption coefficient	0.082 mm^-1
F(000)	680
Crystal size	0.26 x 0.21 x 0.15 mm
Theta range for data collection	1.68 to 25.00 deg.
Limiting indices	-15<=h<=15, -6<=k<=6, -25<=l<=32

Reflections collected / unique	8071 / 2965 [R(int) = 0.0805]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9877 and 0.9789
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2965 / 0 / 217
Goodness-of-fit on F^2	1.079
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1170
R indices (all data)	R1 = 0.1317, wR2 = 0.1327
Largest diff. peak and hole	0.152 and -0.201 e.A^-3



7

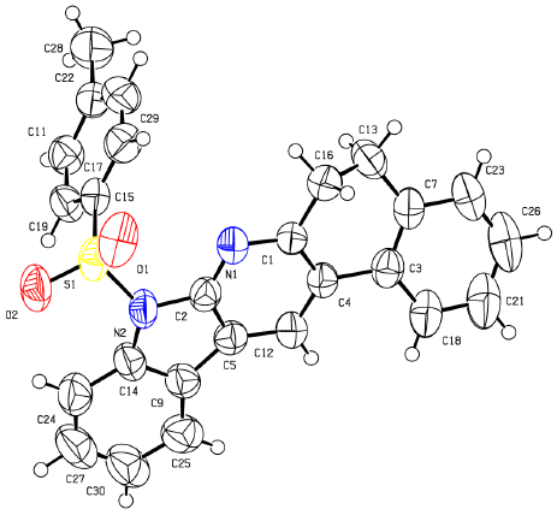


Table 2. Crystal data and structure refinement for 7.

Identification code	**7**
Empirical formula	C_{26} H_{20} N_2 O_2 S
Formula weight	424.50
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Orthorhombic, Pna2(1)
Unit cell dimensions	a = 7.979(3) A alpha = 90 deg.
	b = 19.9763(13) A beta = 90 deg.
	c = 13.149(4) A gamma = 90 deg.
Volume	2095.9(9) A^3
Z, Calculated density	4, 1.345 Mg/m^3
Absorption coefficient	0.181 mm^-1
F(000)	888
Crystal size	0.29 x 0.25 x 0.22 mm
Theta range for data collection	1.85 to 25.00 deg.
Limiting indices	-9<=h<=9, -23<=k<=23, -15<=l<=14
Reflections collected / unique	10090 / 3296 [R(int) = 0.0791]
Completeness to theta = 25.00	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9613 and 0.9494

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3296 / 1 / 280
Goodness-of-fit on F^2	0.967
Final R indices [I>2sigma(I)]	R1 = 0.0533, wR2 = 0.0967
R indices (all data)	R1 = 0.1220, wR2 = 0.1158
Absolute structure parameter	-0.14(12)
Largest diff. peak and hole	0.148 and -0.162 e.A^-3

Reference

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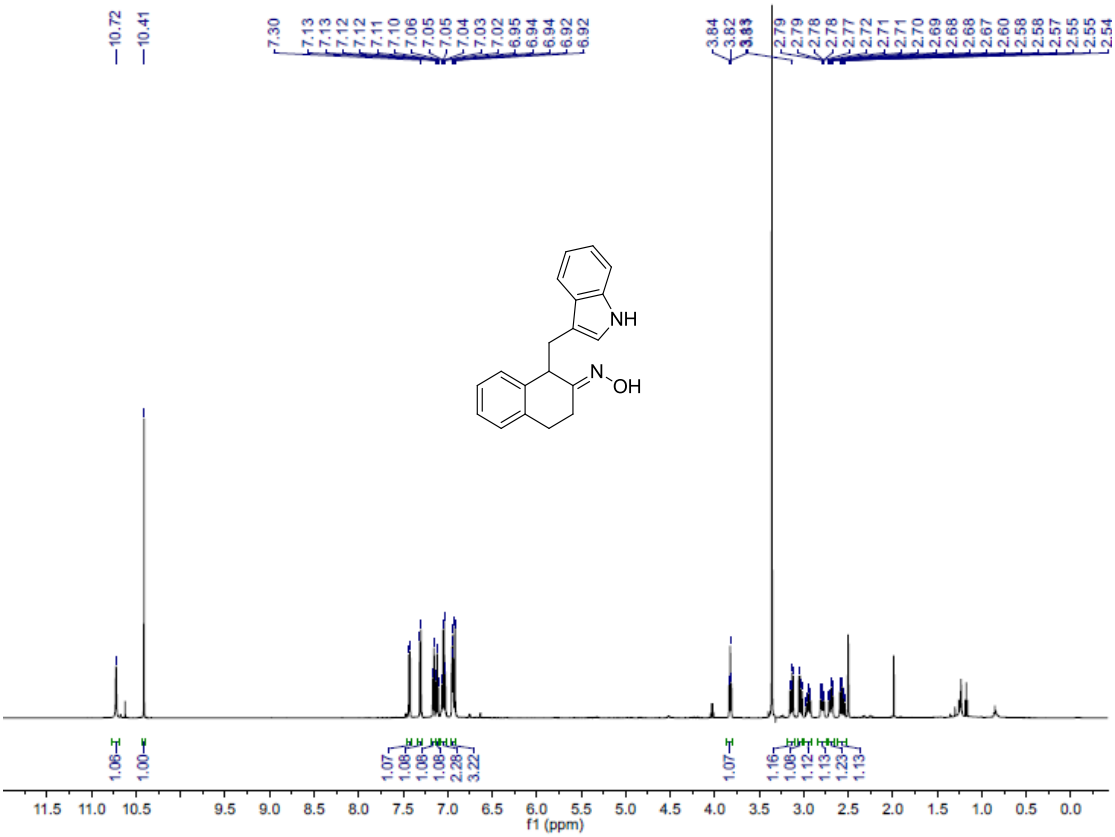
[2] F. R. Kinder Jr, C. P. Chen, K. W. Bair, *Synth. Commun.* **1997**, *27*, 871–881.

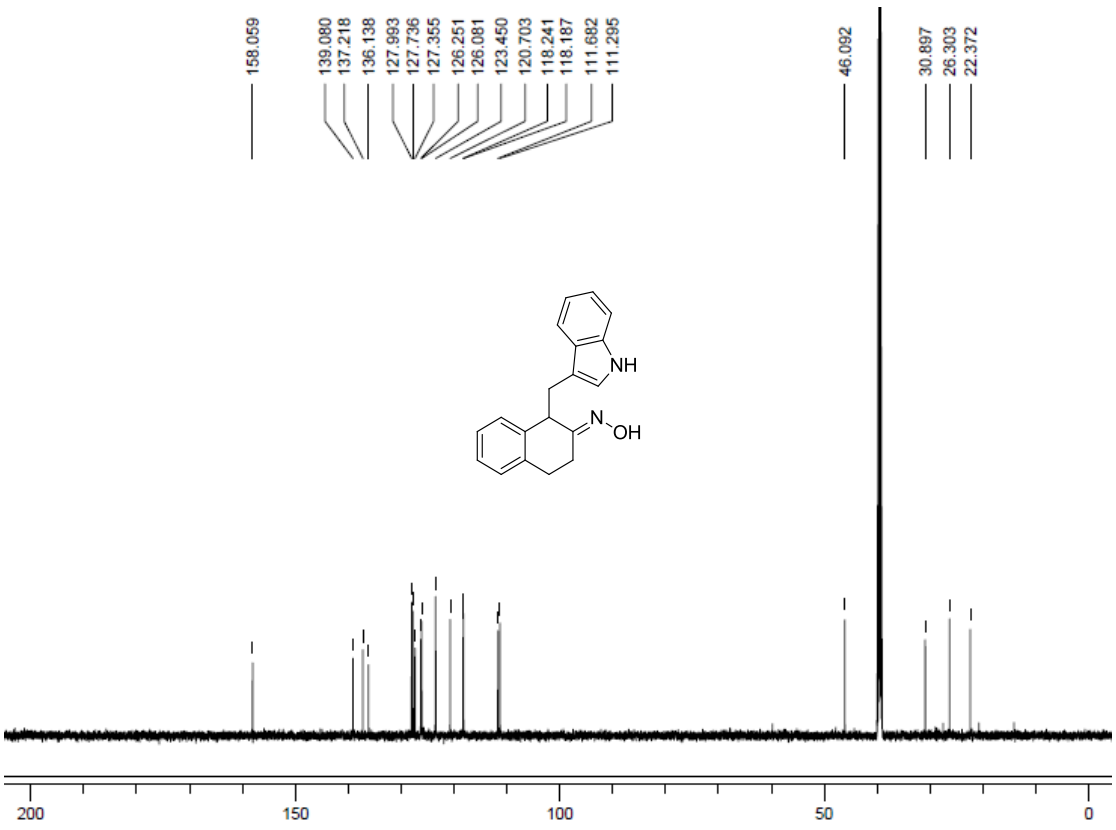
[3] J. R. Dimmock, M. P. Padmanilyam, G. A. Zello, *Eur. J. Med. Chem.* **2002**, *37*, 813–824.

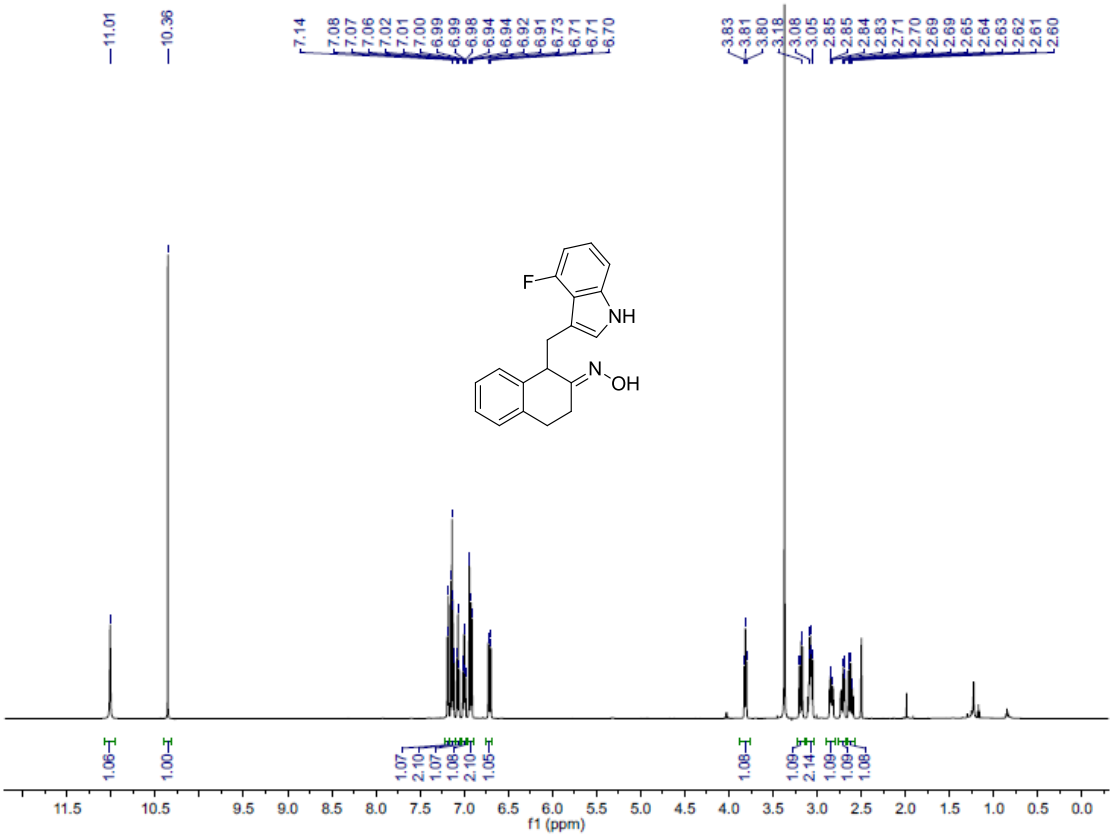
[4] W. E. Rosen, M. J. Green, *J. Org. Chem.* **1963**, *28*, 2797–2804.

[5] B. L. Jensen, D. P. Michaud, *J. Heterocycl. Chem.* **1978**, *15*, 321–324.

Copies of NMR spectra



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6.94
6.92
6.91
6.73
6.71
6.71
6.70
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3.81
3.80
3.18
3.08
3.05
2.85
2.85
2.84
2.83
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2.70
2.69
2.69
2.65
2.64
2.63
2.62
2.61
2.60
F
NH
N
OH
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1.07
2.10
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1.08
2.10
1.05
1.08
1.09
2.14
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1.08
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9.5
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7.5
7.0
6.5
6.0
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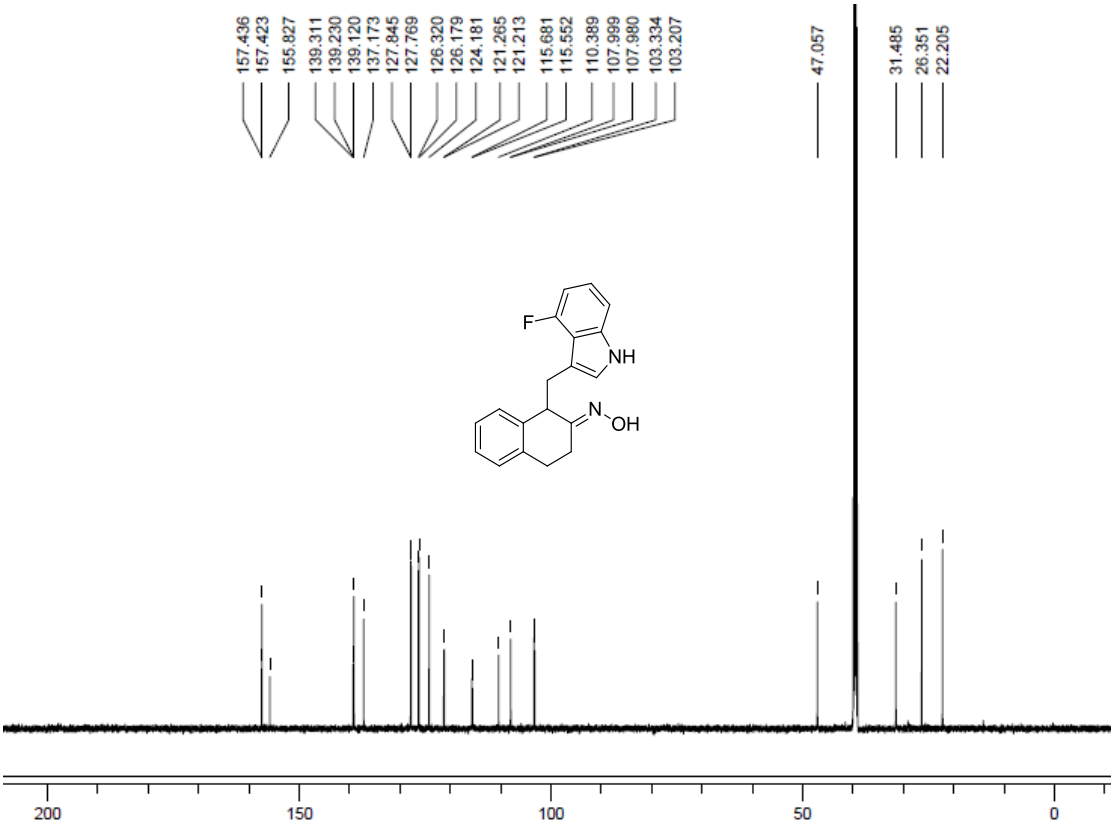
f1 (ppm)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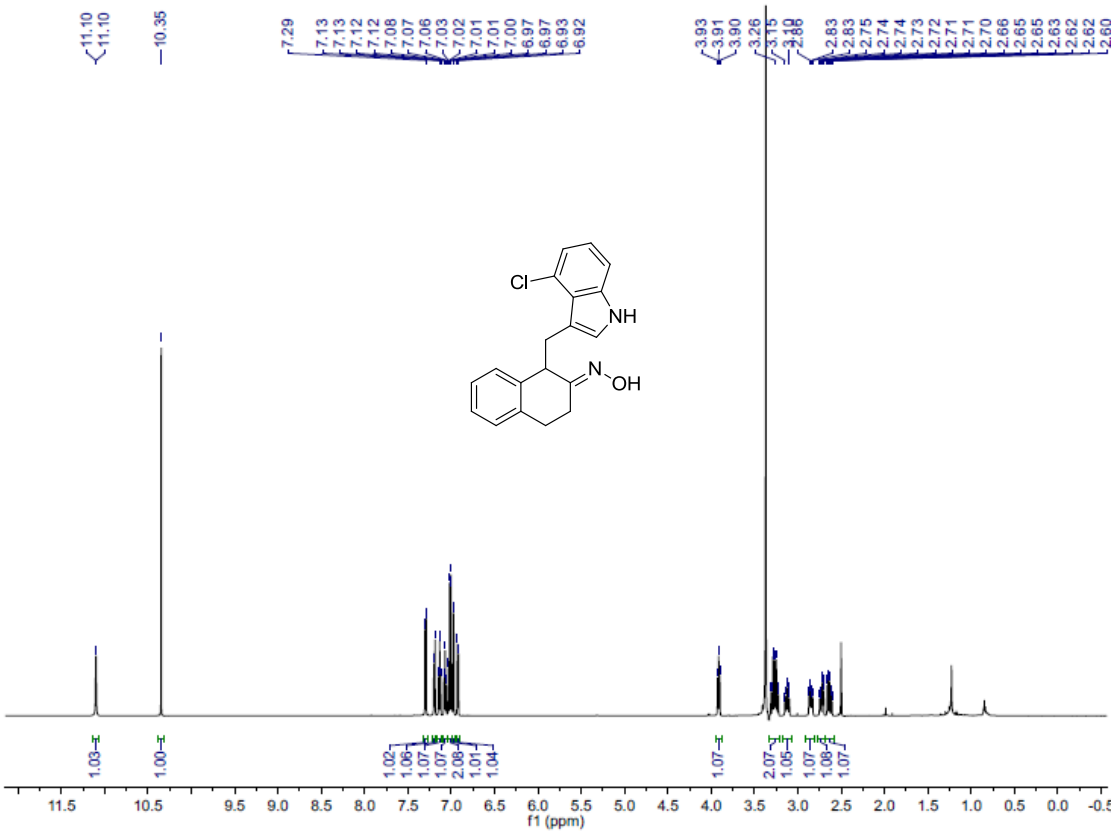
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7.01
7.01
7.00
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6.97
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2.72
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2.71
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2.65
2.65
2.63
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1.06
1.07
1.07
2.06
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1.04
1.07
2.07
1.05
1.07
1.06
1.07
11.5
10.5
9.5
9.0
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8.0
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7.0
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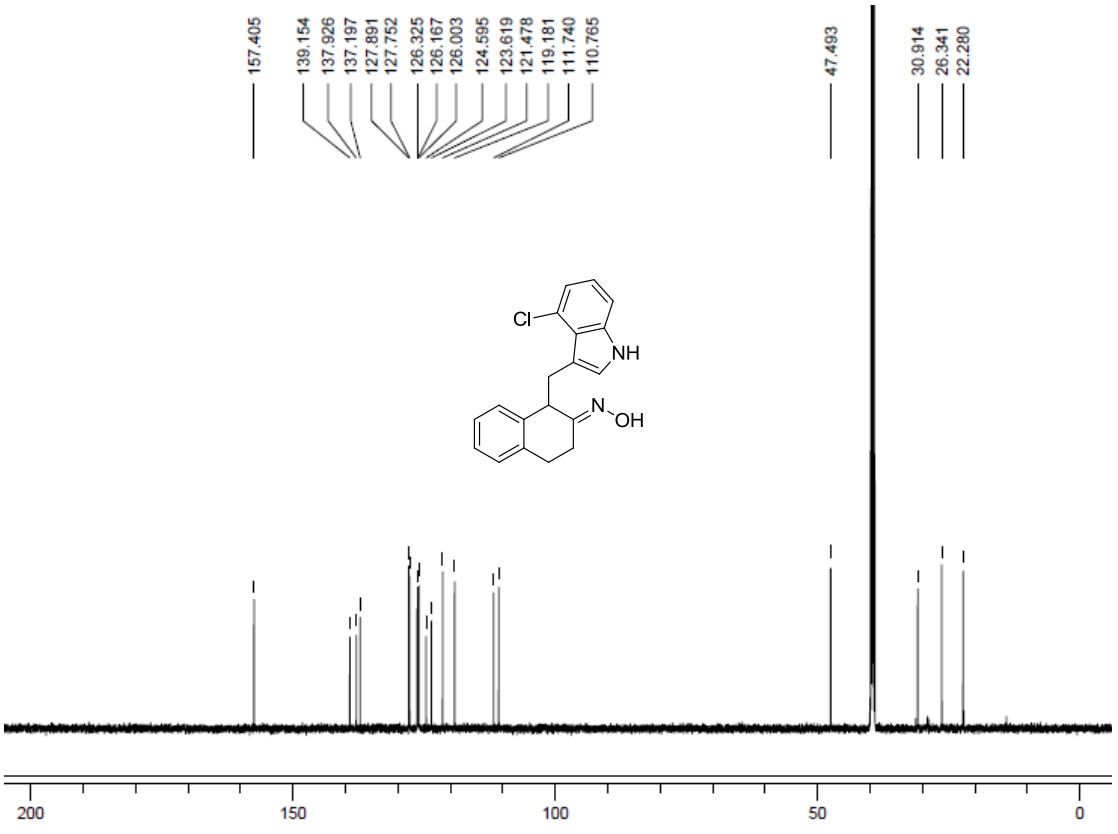
f1 (ppm)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150
100
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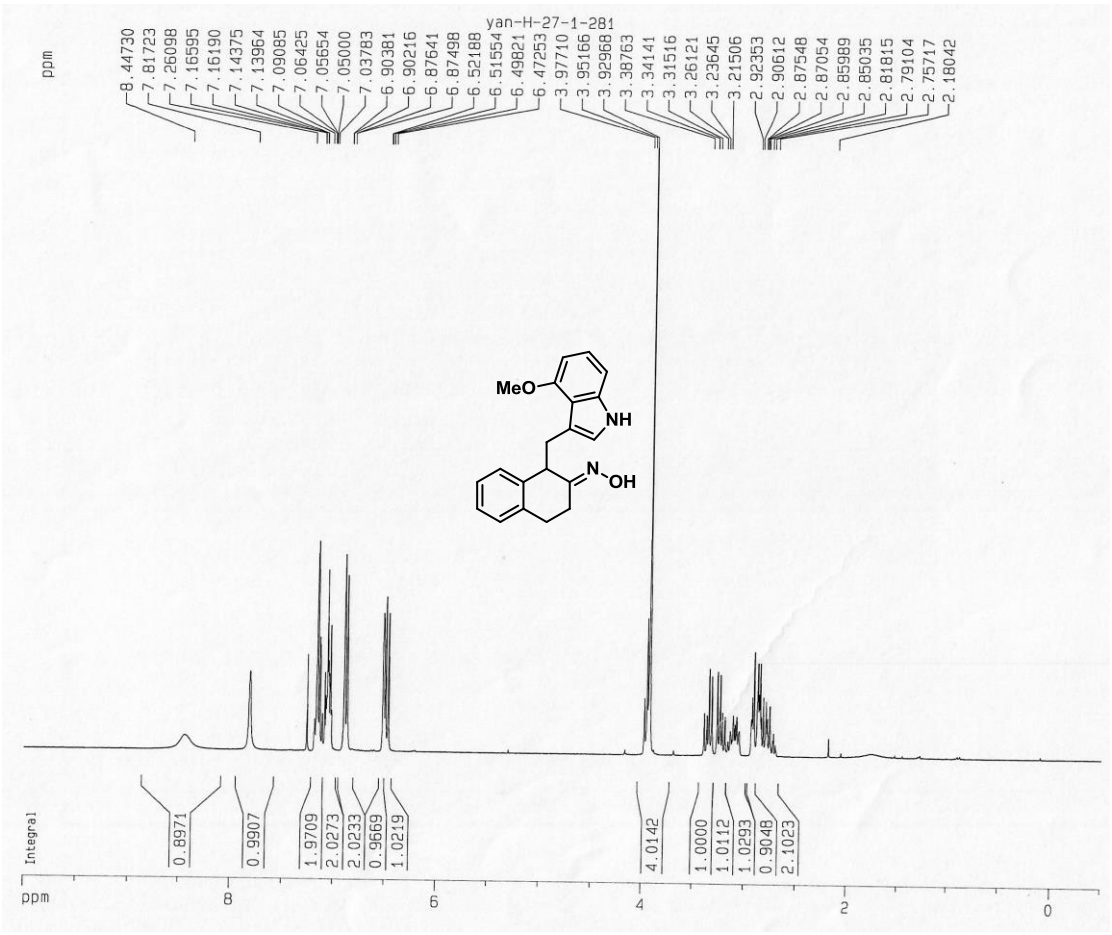
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7.03783
6.90381
6.90216
6.87641
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6.52188
6.51554
6.49821
6.47253
3.97710
3.95166
3.92968
3.38763
3.34141
3.31516
3.26121
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2
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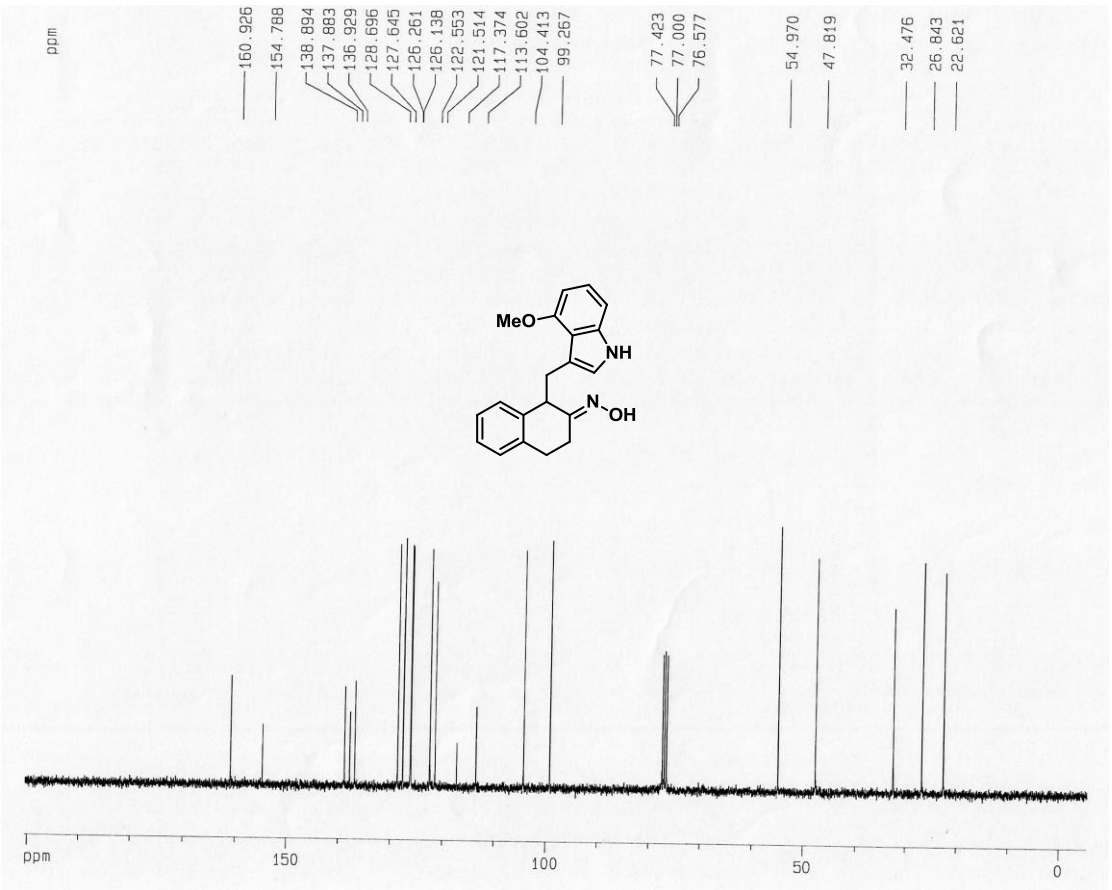
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NH
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OH
ppm
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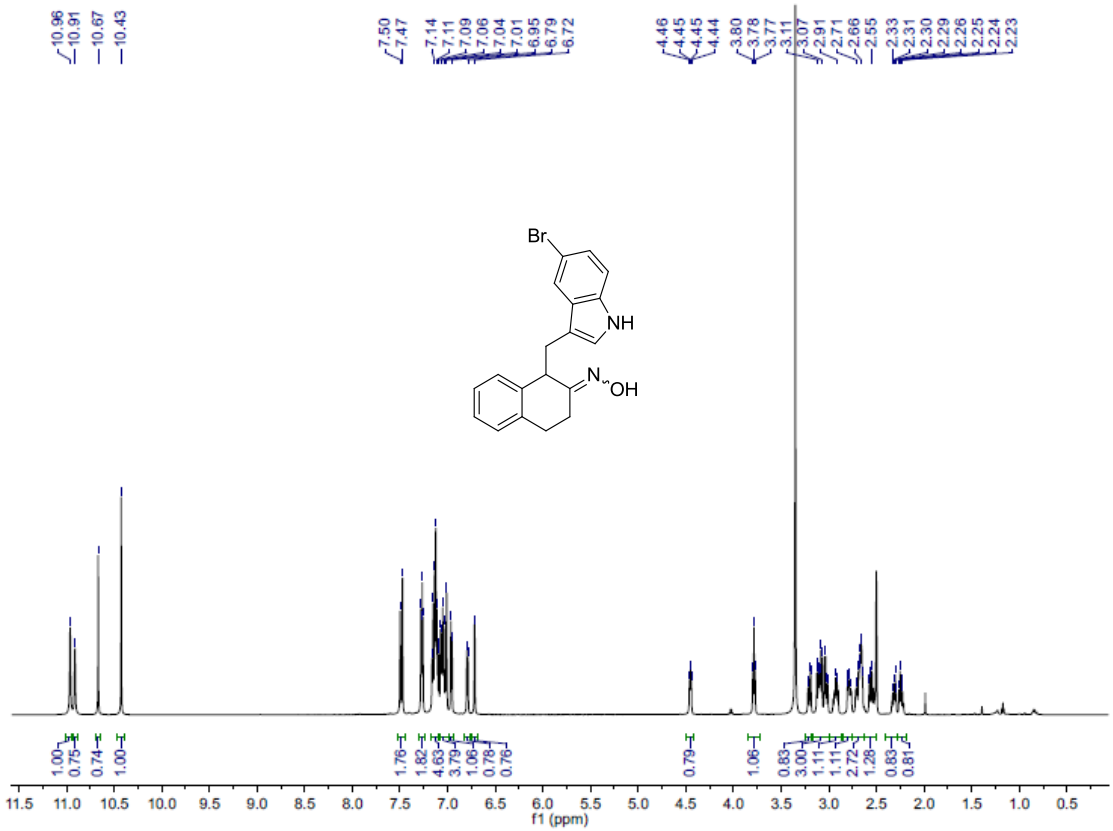
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4.45
4.45
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3.07
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2.24
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3.79
1.06
0.78
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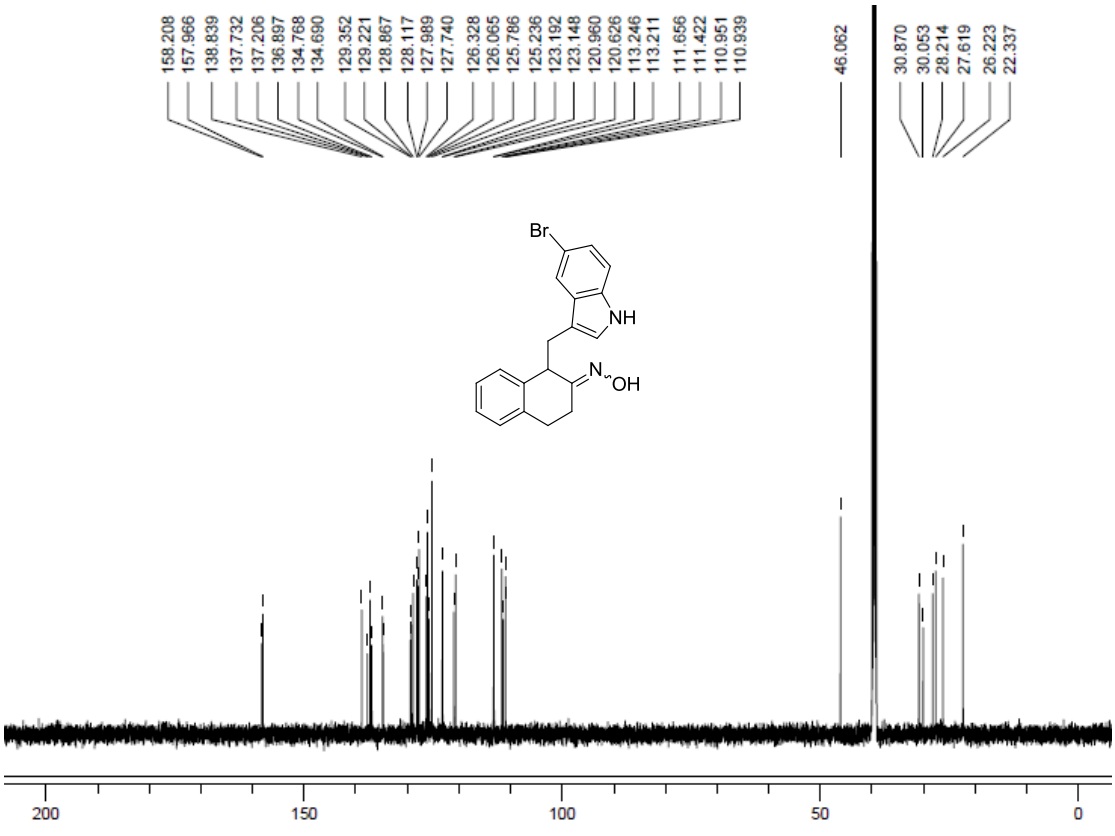
f1 (ppm)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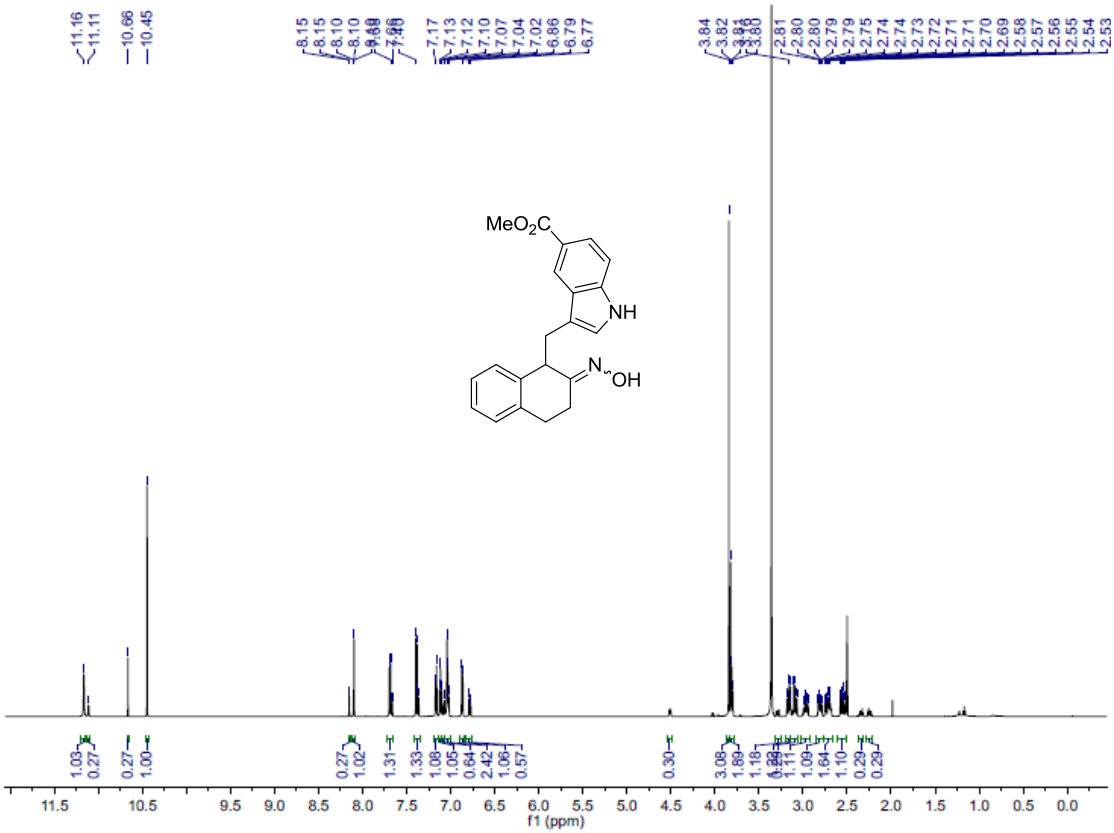
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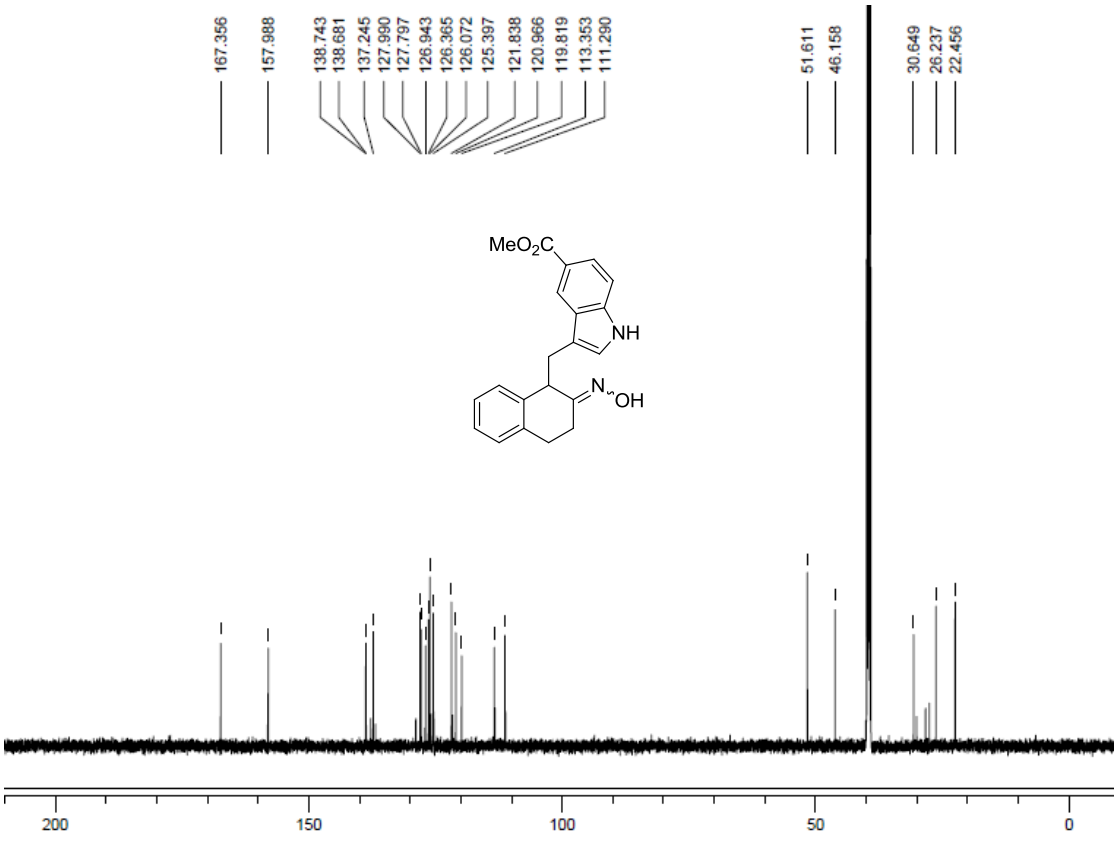
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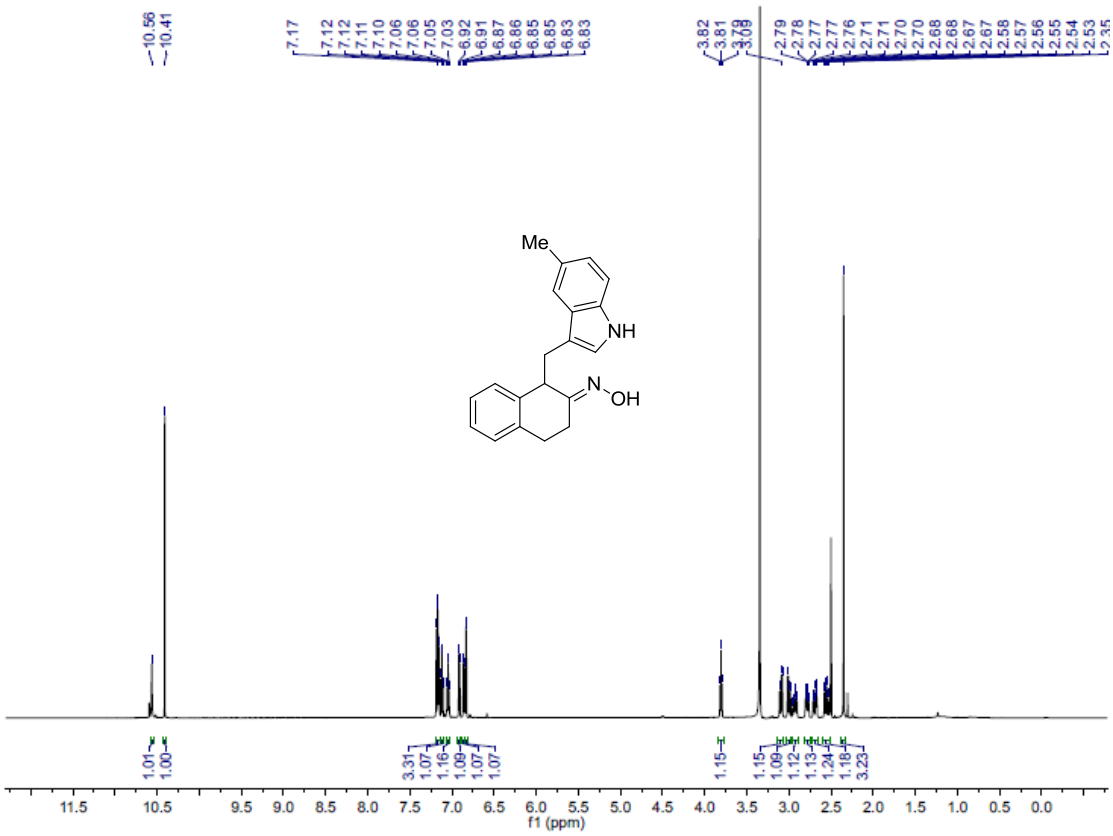
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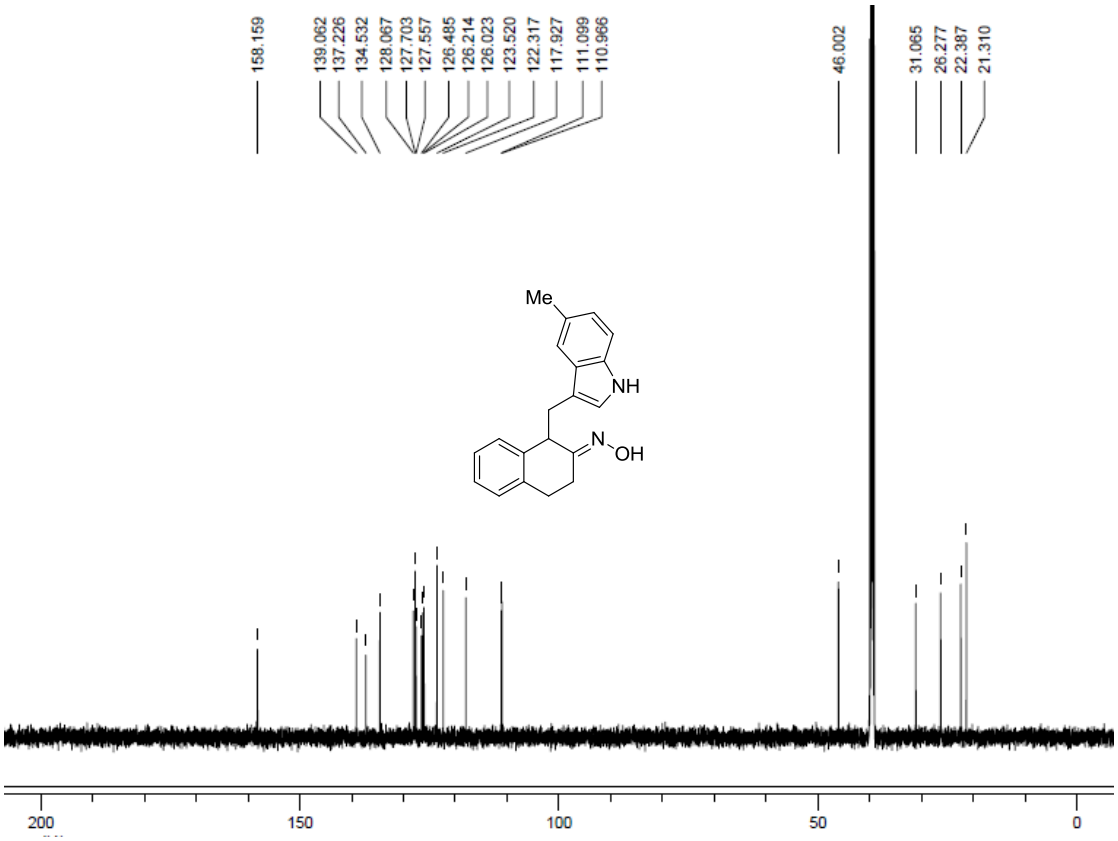
f1 (ppm)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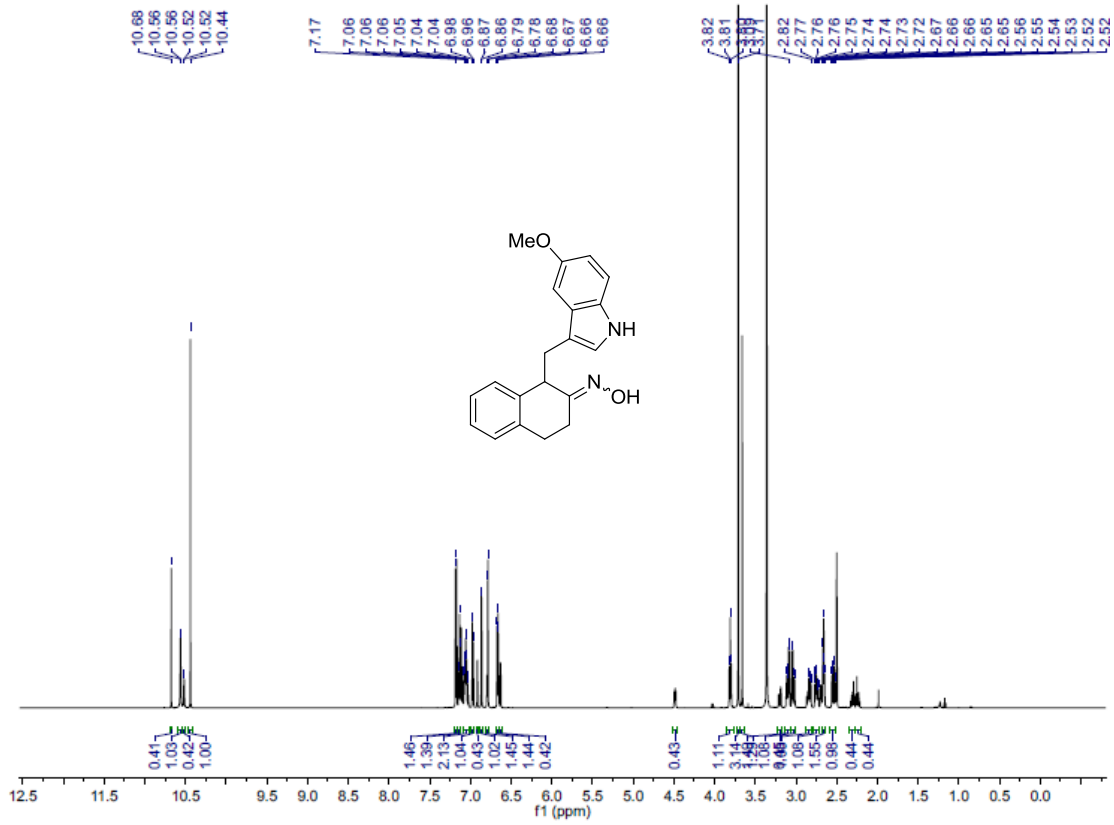
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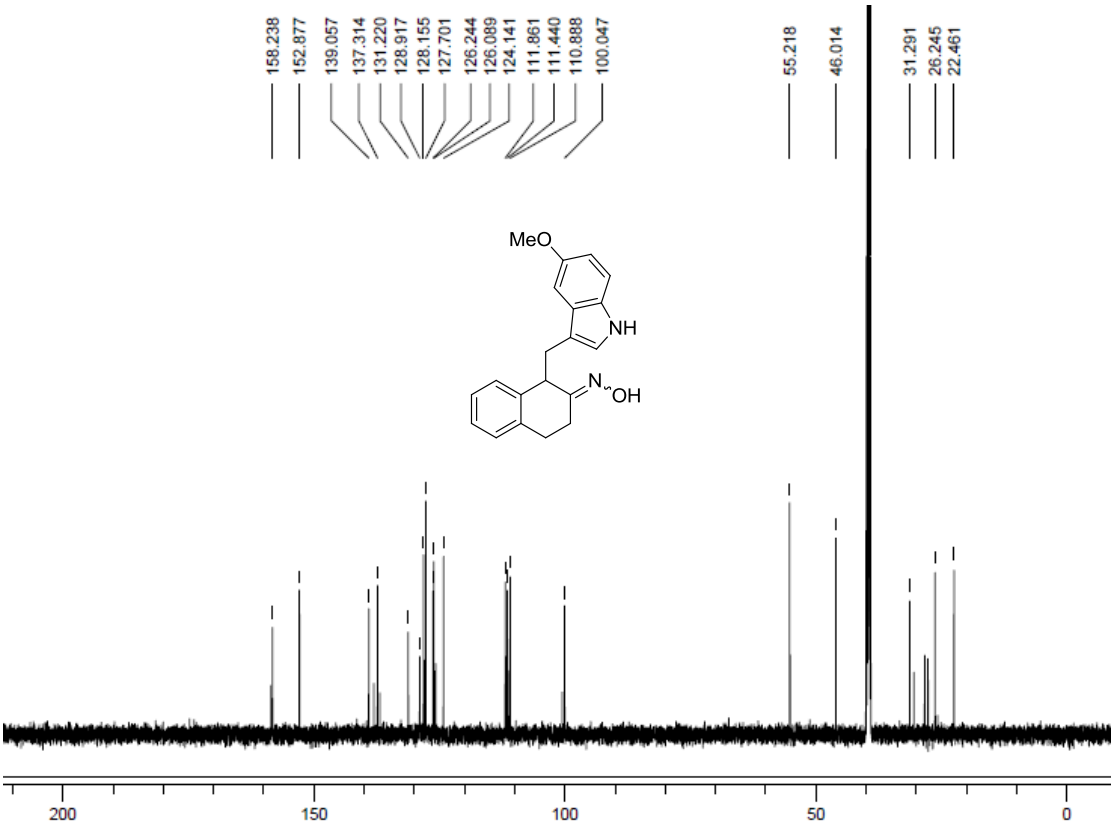
OH
f1 (ppm)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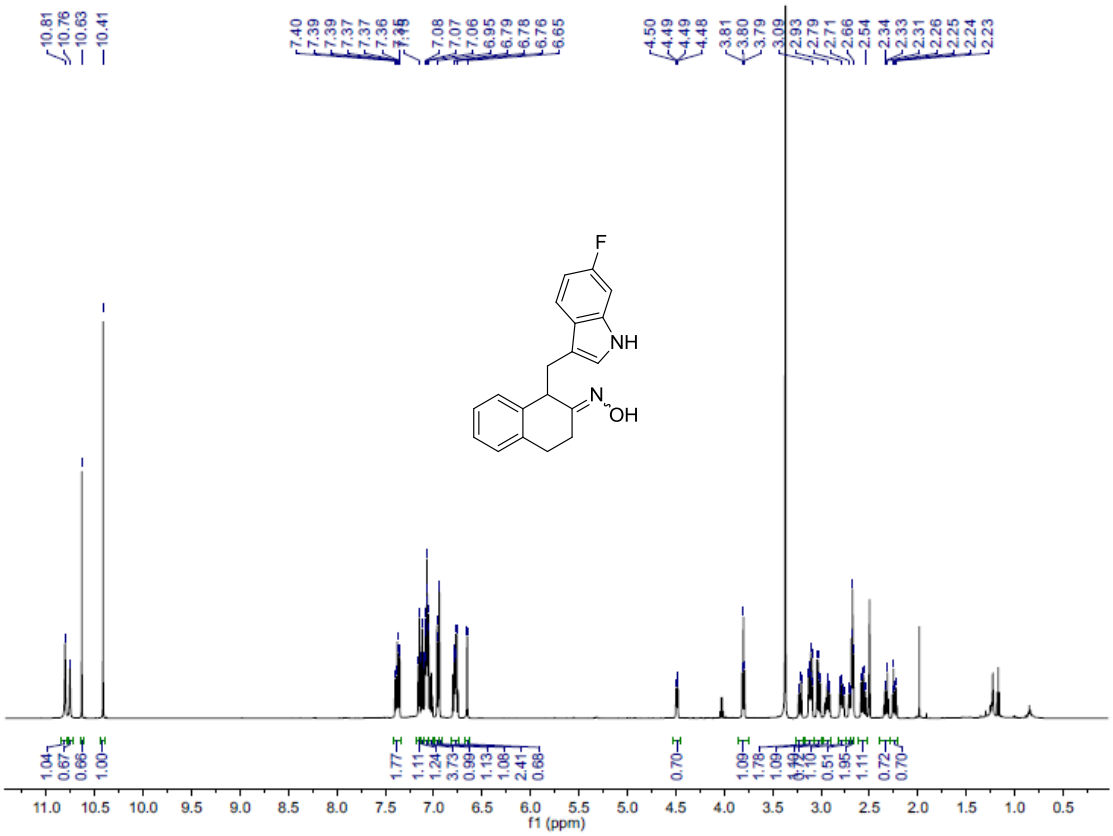
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2.23
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9.0
8.5
8.0
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7.0
6.5
6.0
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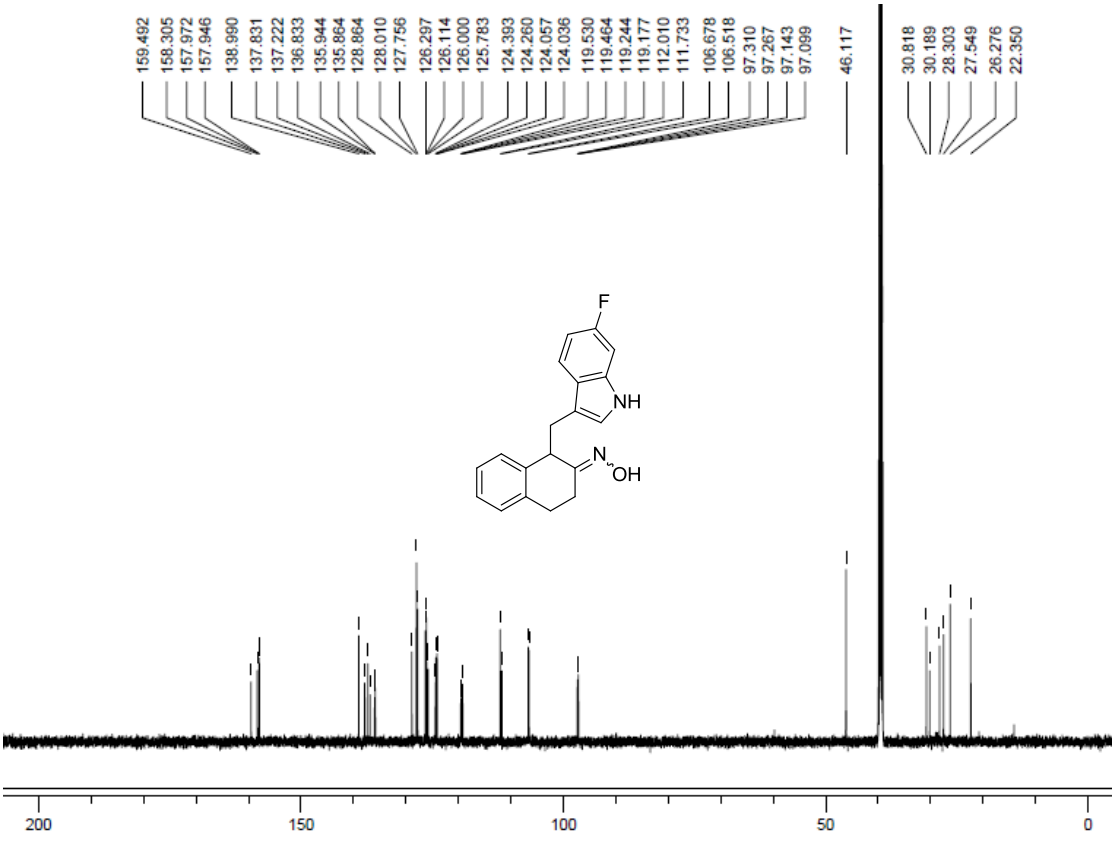
f1 (ppm)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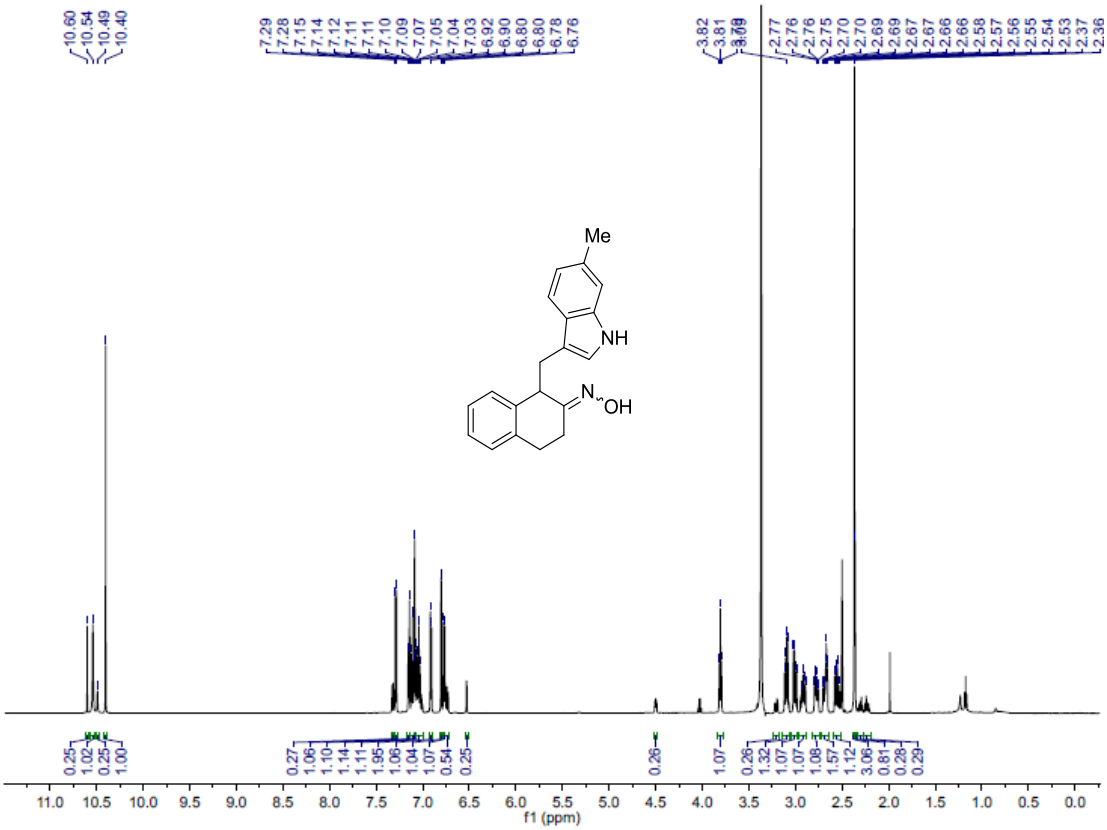
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7.07
7.05
7.04
7.03
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6.80
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6.76
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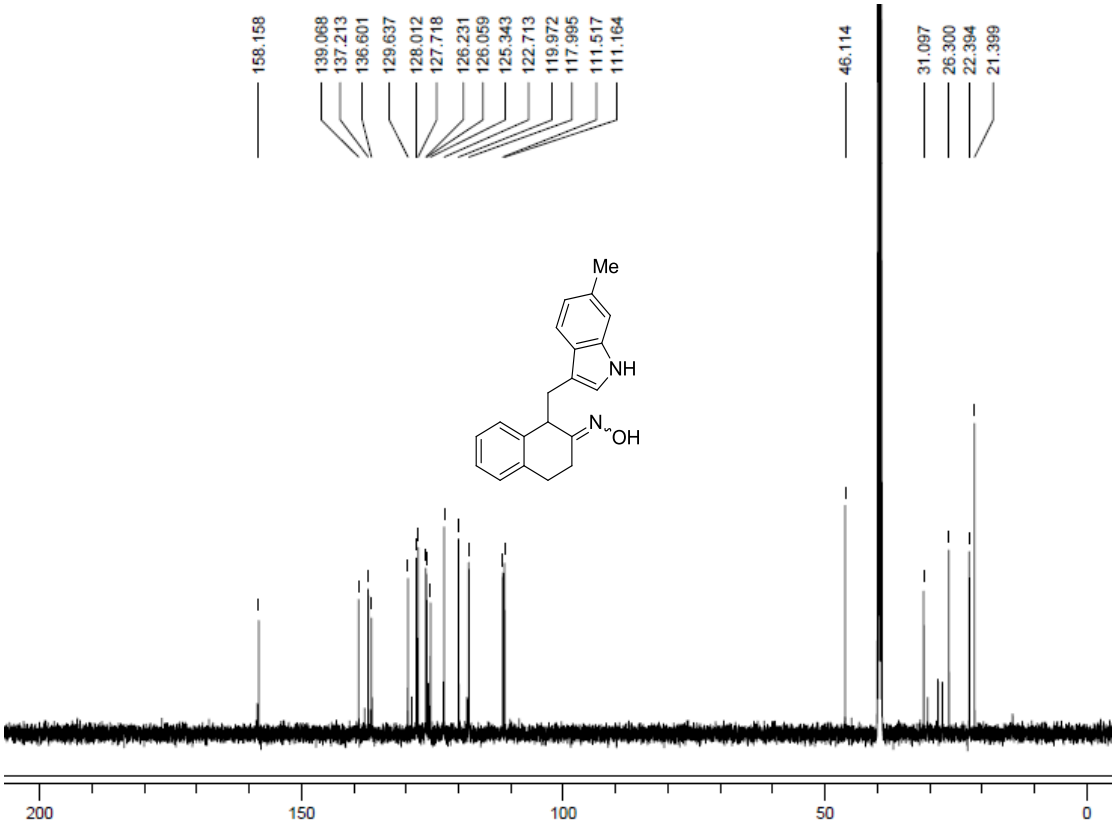
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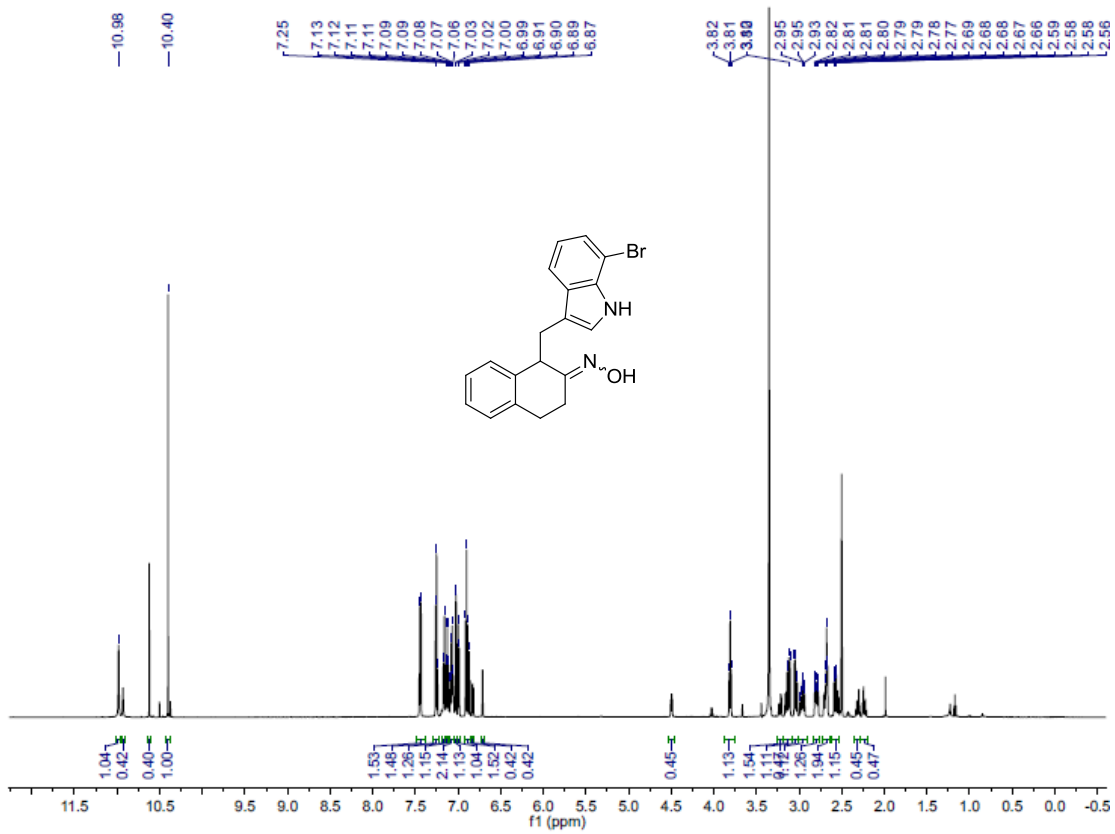
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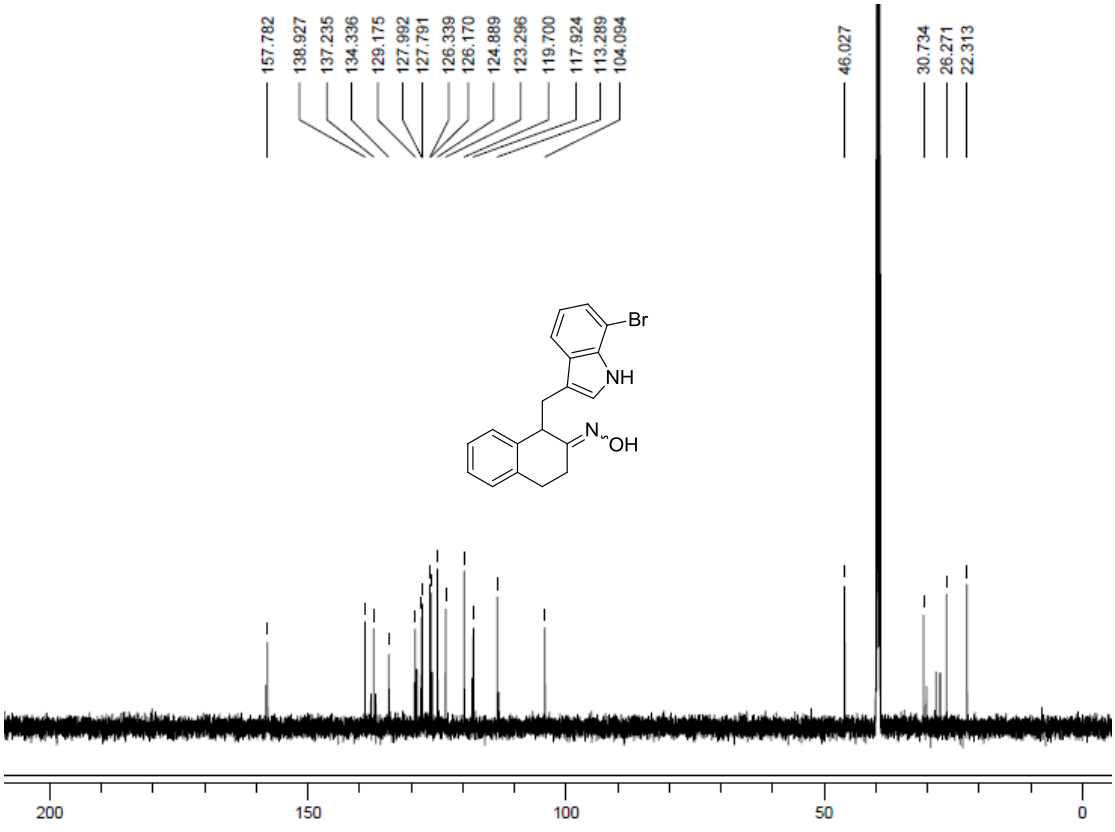
f1 (ppm)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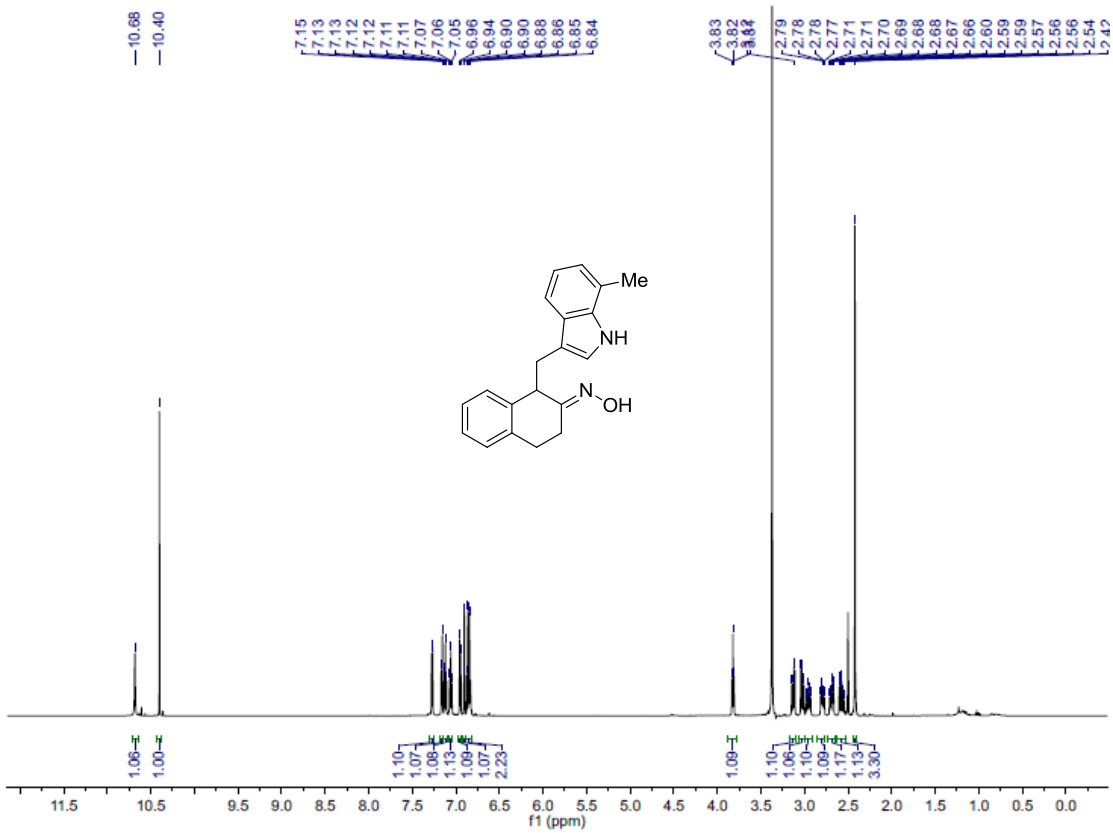
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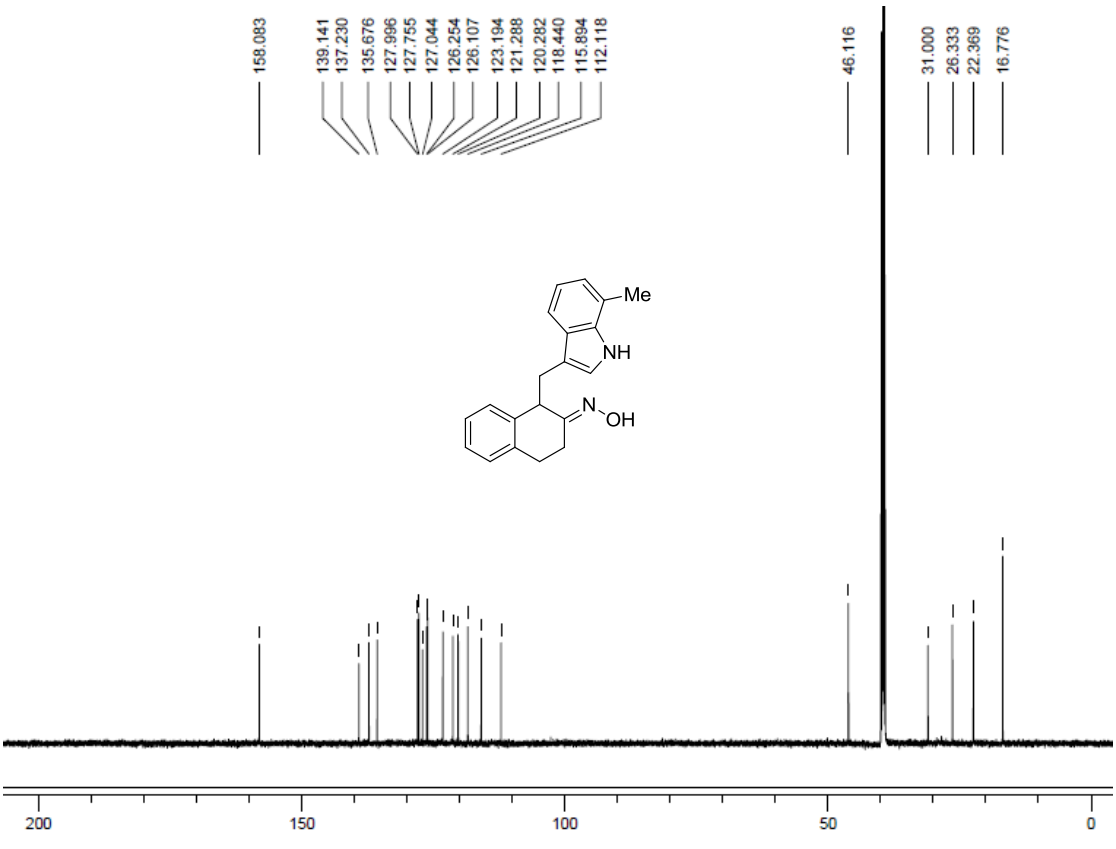
f1 (ppm)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46.116
31.000
26.333
22.369
16.776
Me
NH
N
OH
200
150
100
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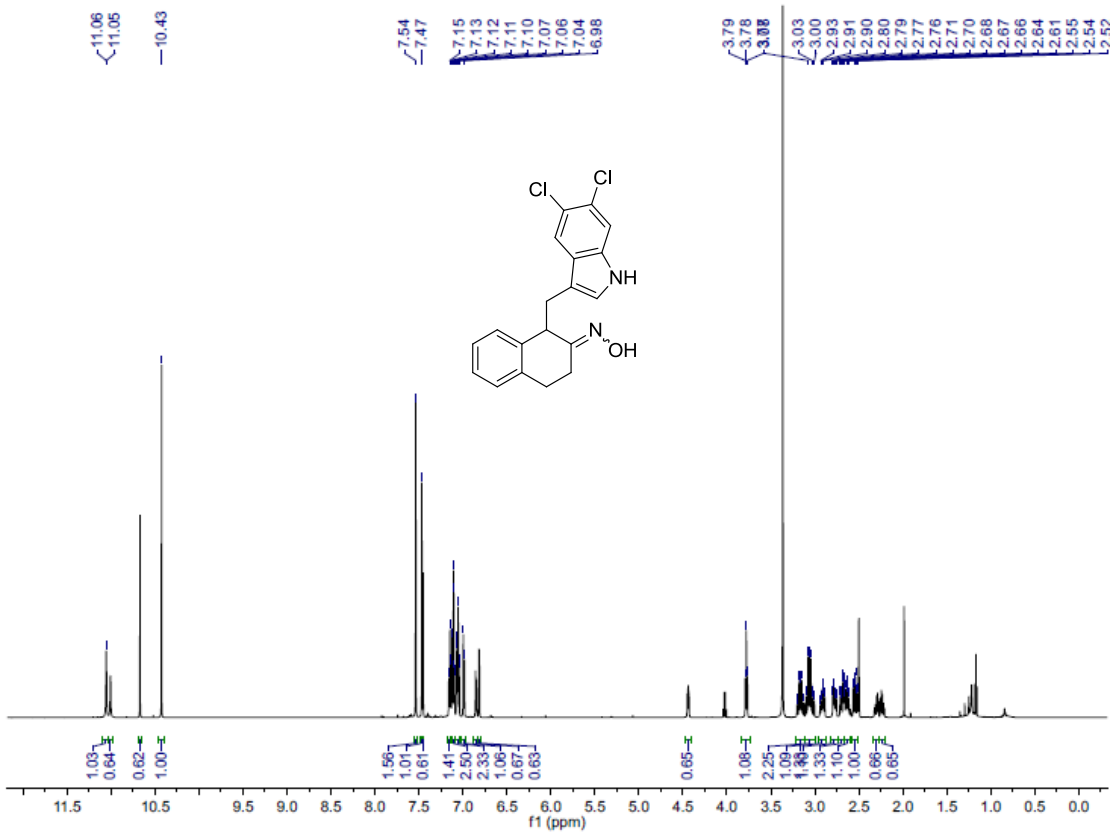
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7.06
7.04
6.98
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3.78
3.03
3.00
2.93
2.91
2.90
2.80
2.79
2.77
2.76
2.71
2.70
2.68
2.67
2.66
2.64
2.61
2.55
2.54
Cl
Cl
NH
N
OH
1.03
0.64
0.62
1.00
1.56
1.01
0.61
1.41
2.50
2.33
1.06
0.67
0.63
0.65
1.08
2.25
1.09
1.33
1.10
1.00
0.66
0.65
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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3.0
2.5
2.0
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1.0
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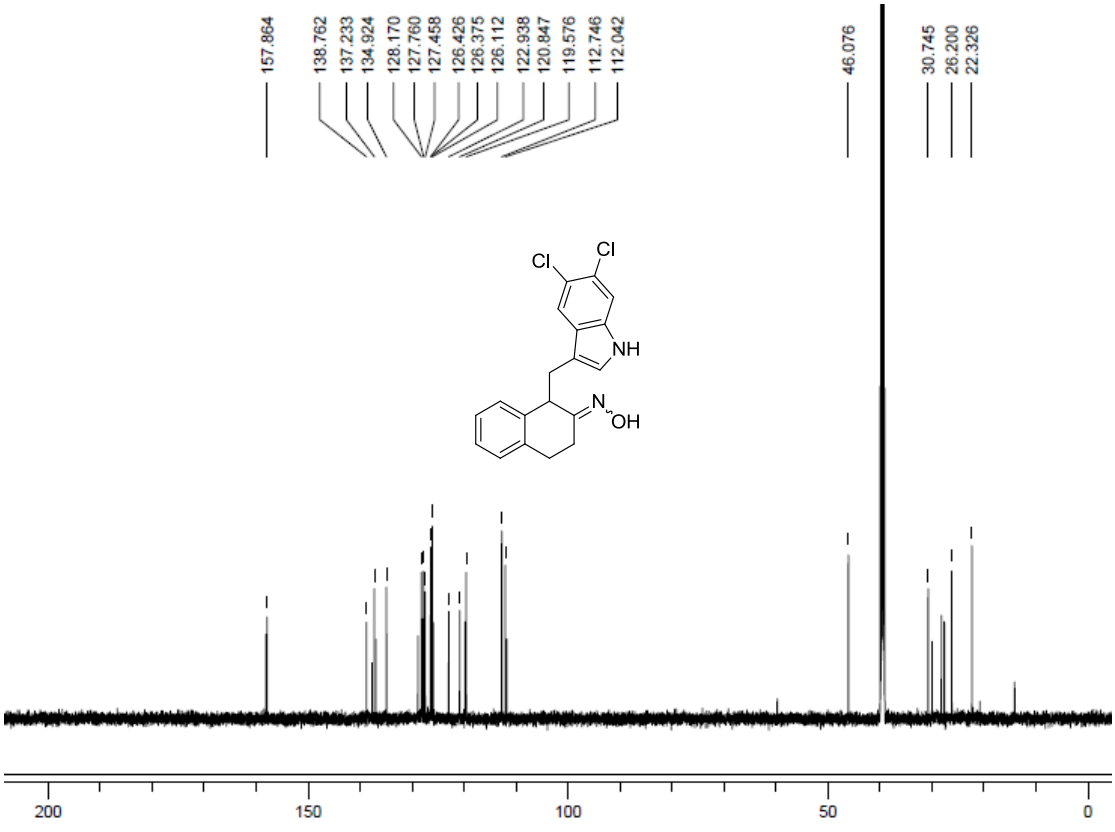
0.0
f1 (ppm)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119.576
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46.076
30.745
26.200
22.326
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Cl
NH
N
OH
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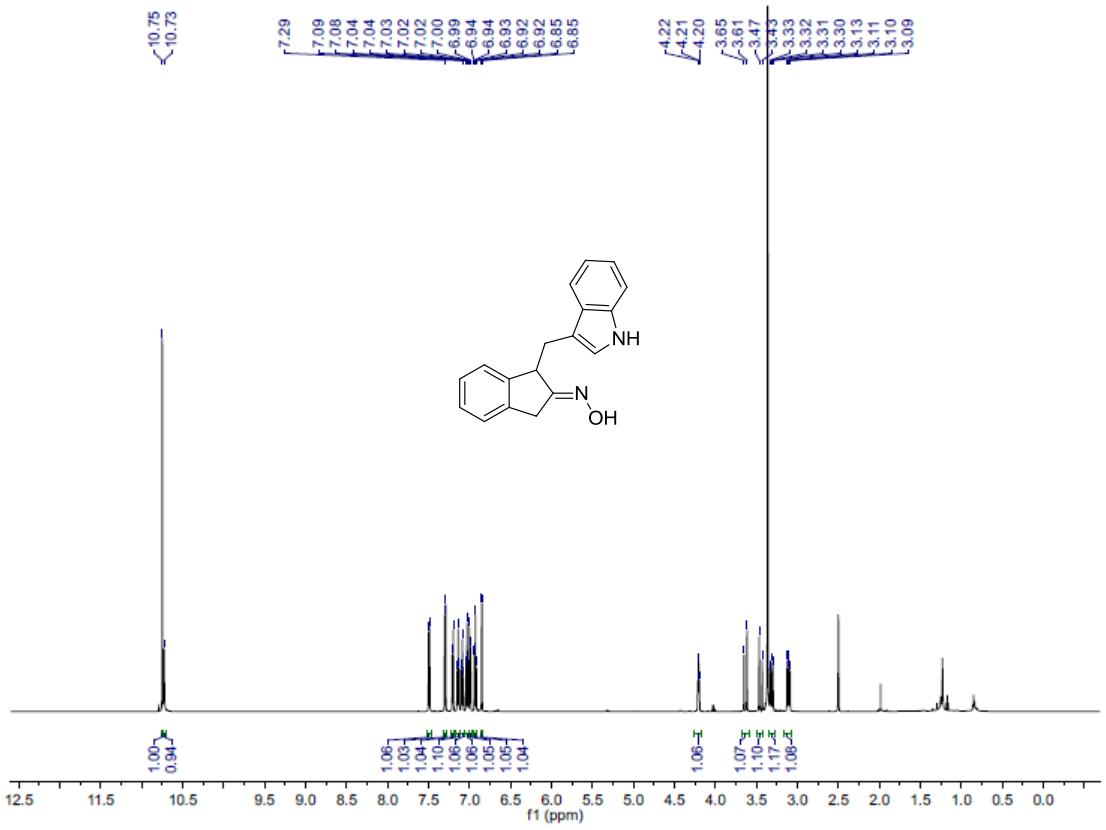
150
100
50
0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7.03
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7.02
7.00
6.99
6.94
6.94
6.93
6.92
6.92
6.85
6.85
4.22
4.21
4.20
3.65
3.61
3.47
3.43
3.33
3.32
3.31
3.30
3.13
3.11
3.10
3.09
NH
N
OH
1.00
0.94
1.06
1.03
1.04
1.10
1.06
1.06
1.05
1.05
1.04
1.06
1.07
1.10
1.17
1.08
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
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2.5
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1.0
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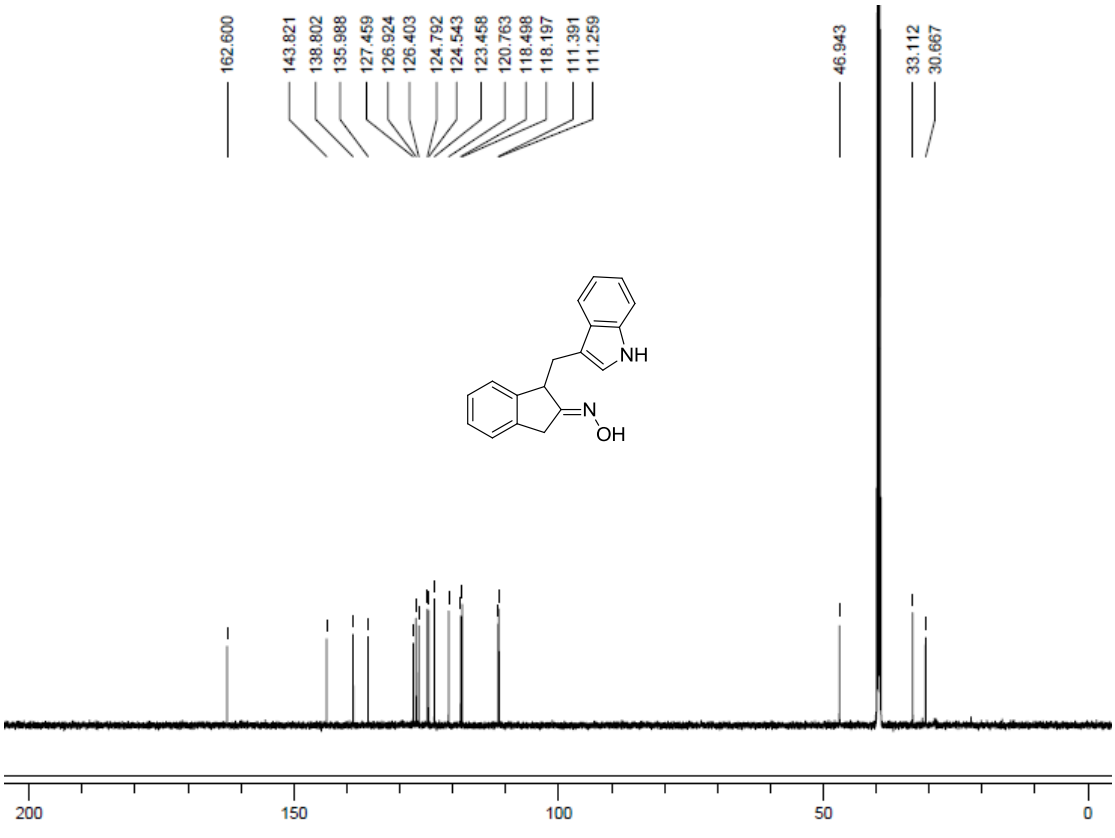
0.0
f1 (ppm)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111.391
111.259
46.943
33.112
30.667
NH
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OH
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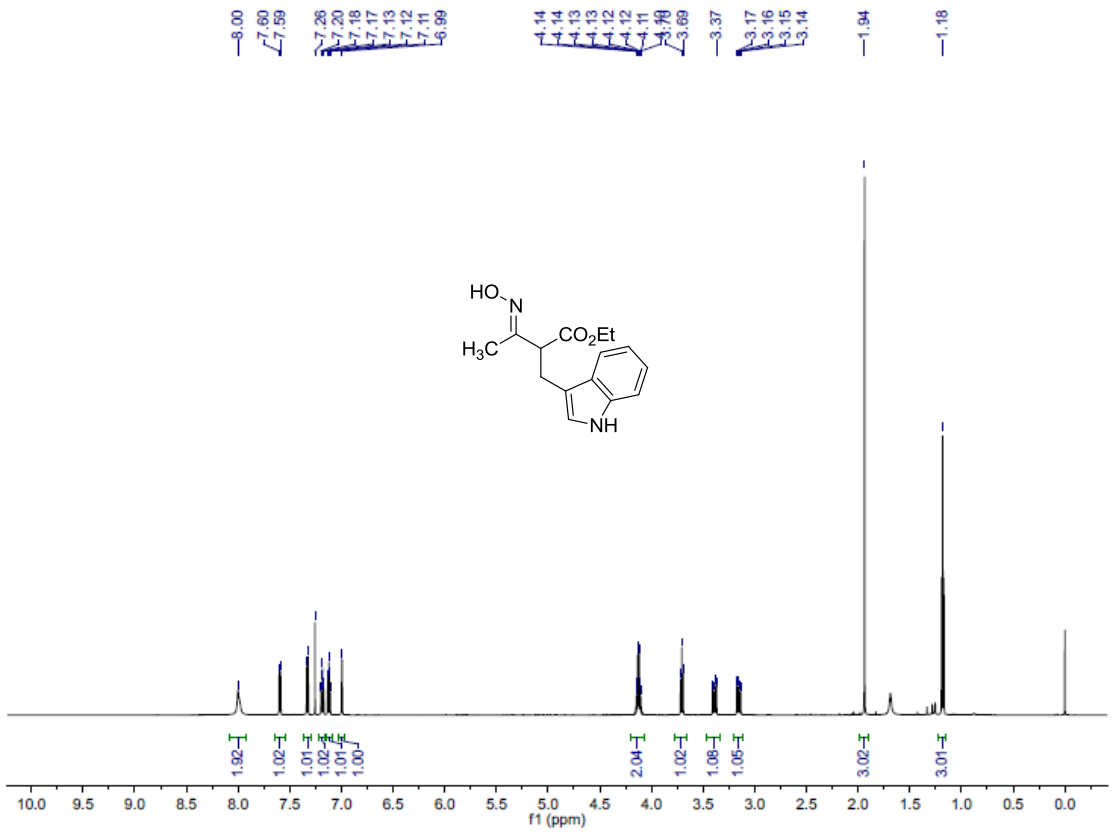
150
100
50
0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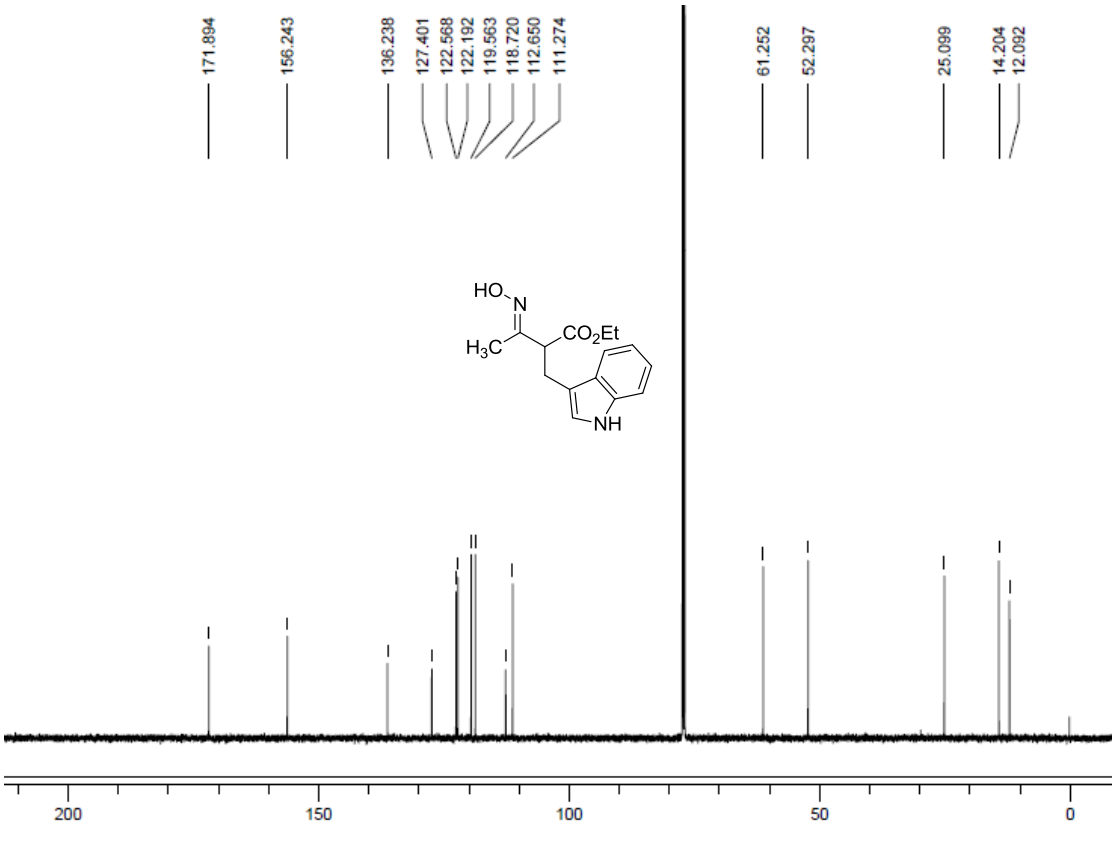
7.17
7.13
7.12
7.11
6.99
4.14
4.14
4.13
4.13
4.12
4.12
4.11
3.69
3.37
3.17
3.16
3.15
3.14
1.94
1.18
HO
N
H3C
CO2Et
NH
1.92
1.02
1.01
1.02
1.01
1.00
2.04
1.02
1.08
1.05
3.02
3.01
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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122.192
119.563
118.720
112.650
111.274
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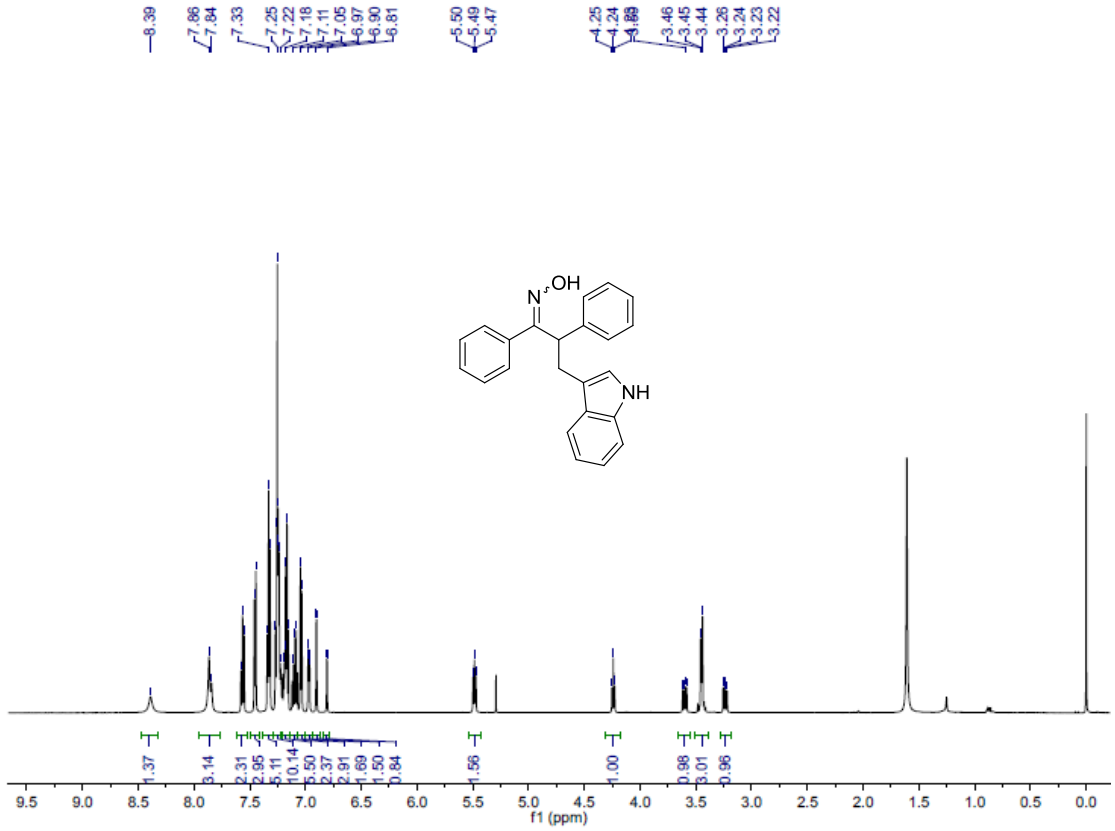
25.099
14.204
12.092
HO
N
H3C
CO2Et
NH
200
150
100
50
0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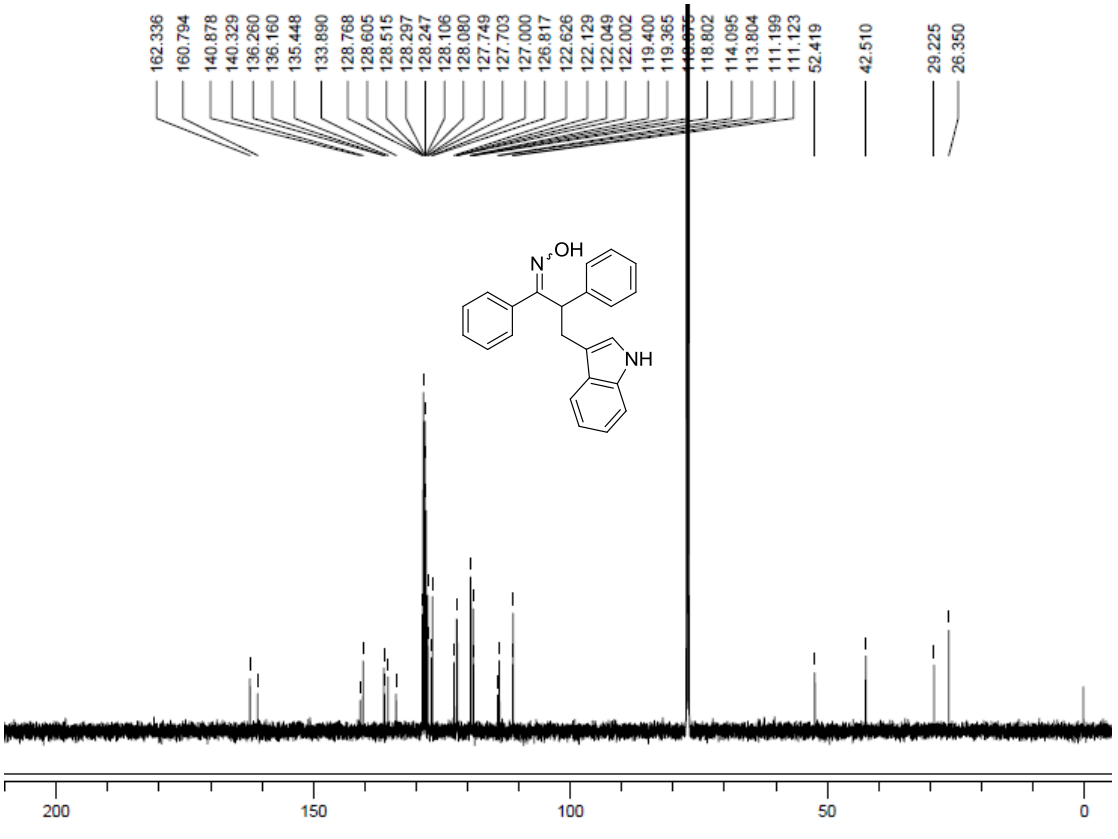
7.22
7.18
7.11
7.05
6.97
6.90
6.81
5.50
5.49
5.47
4.25
4.24
3.46
3.45
3.44
3.26
3.24
3.23
3.22
N
OH
NH
1.37
3.14
2.31
2.95
5.11
10.14
5.50
2.37
2.91
1.69
1.50
0.84
1.56
1.00
0.98
3.01
0.96
f1 (ppm)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128.515
128.297
128.247
128.106
128.080
127.749
127.703
127.000
126.817
122.626
122.129
122.049
122.002
119.400
119.365
118.802
114.095
113.804
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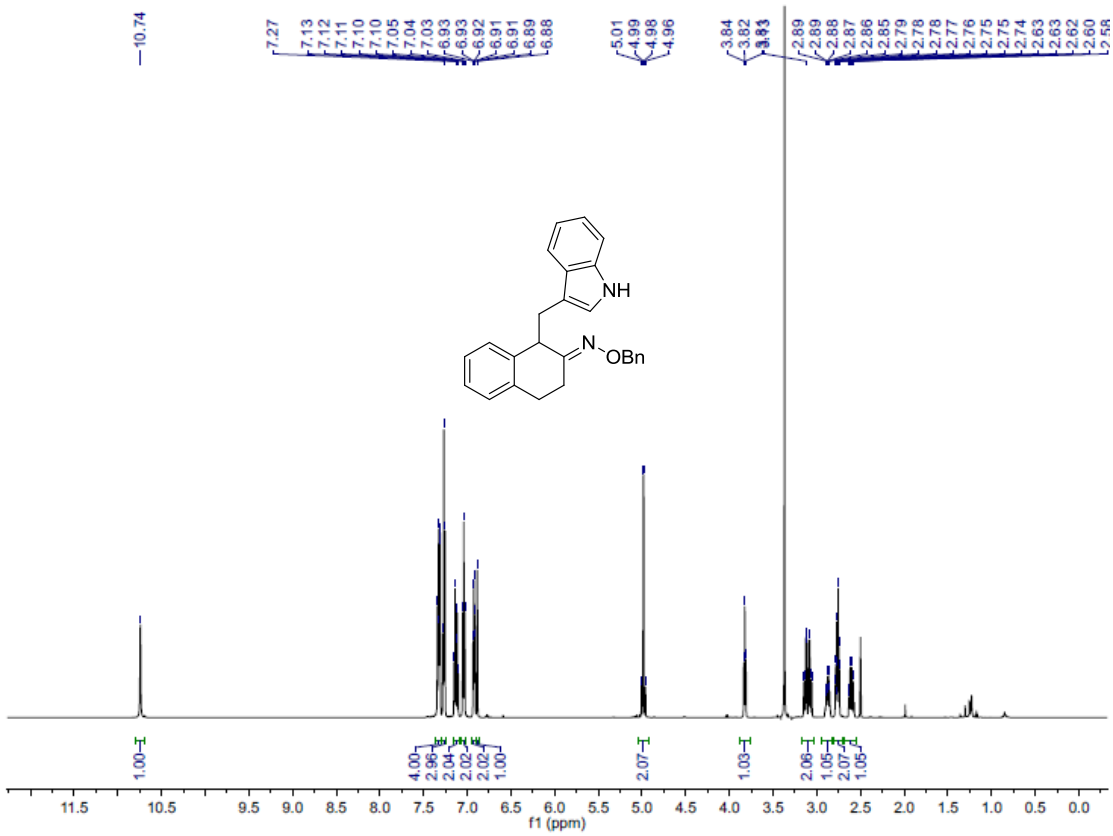
111.123
52.419
42.510
29.225
26.350
N
OH
NH
200
150
100
50
0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7.05
7.04
7.03
6.93
6.93
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6.91
6.91
6.89
6.88
5.01
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4.98
4.96
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3.82
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2.89
2.88
2.87
2.86
2.85
2.79
2.78
2.78
2.77
2.76
2.75
2.75
2.74
2.63
2.62
2.60
NH
N
OBn
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4.00
2.96
2.04
2.02
2.02
1.00
2.07
1.03
2.06
1.05
2.07
1.05
11.5
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.0
2.5
2.0
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1.0
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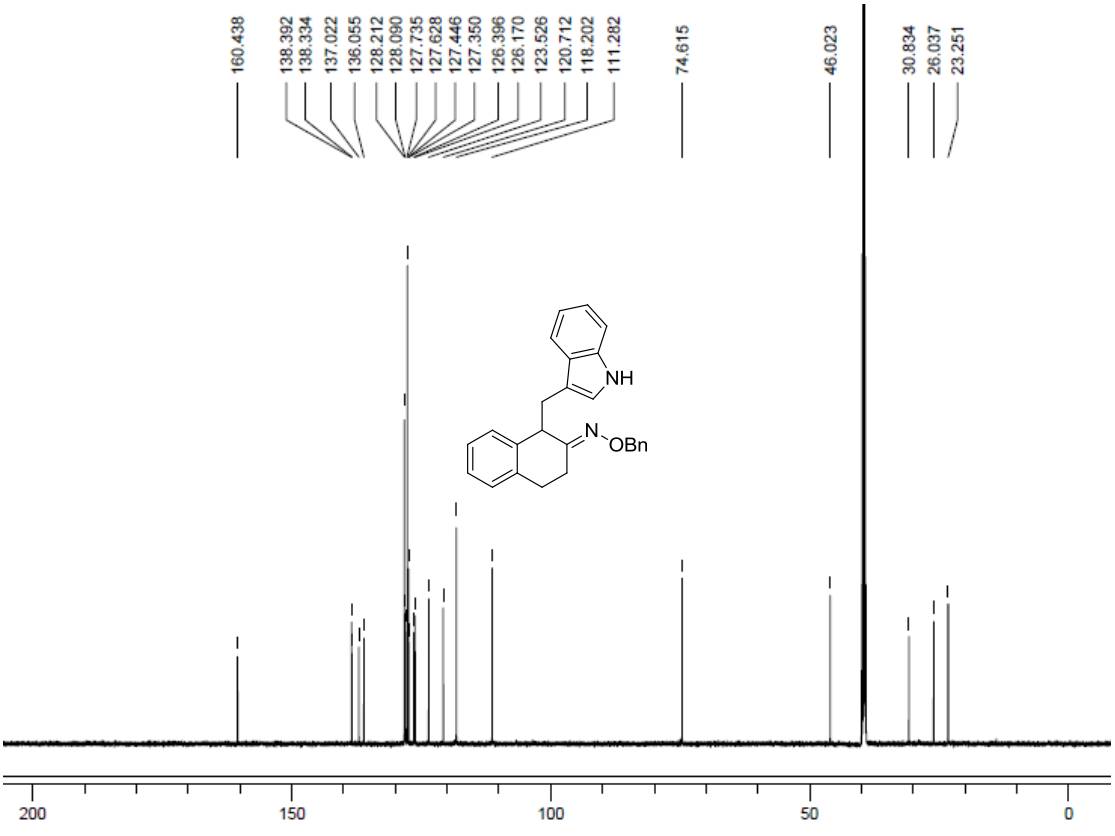
0.0
f1 (ppm)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127.735
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127.446
127.350
126.396
126.170
123.526
120.712
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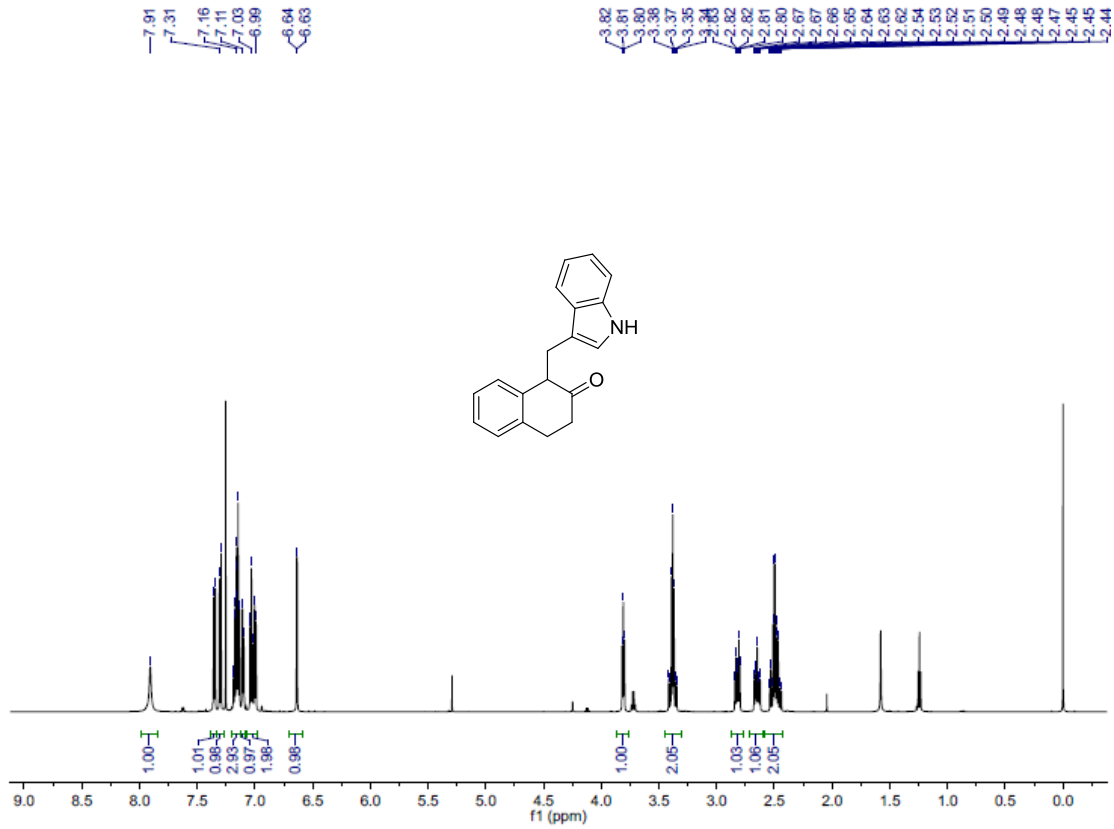
46.023
30.834
26.037
23.251
NH
N
OBn
200
150
100
50
0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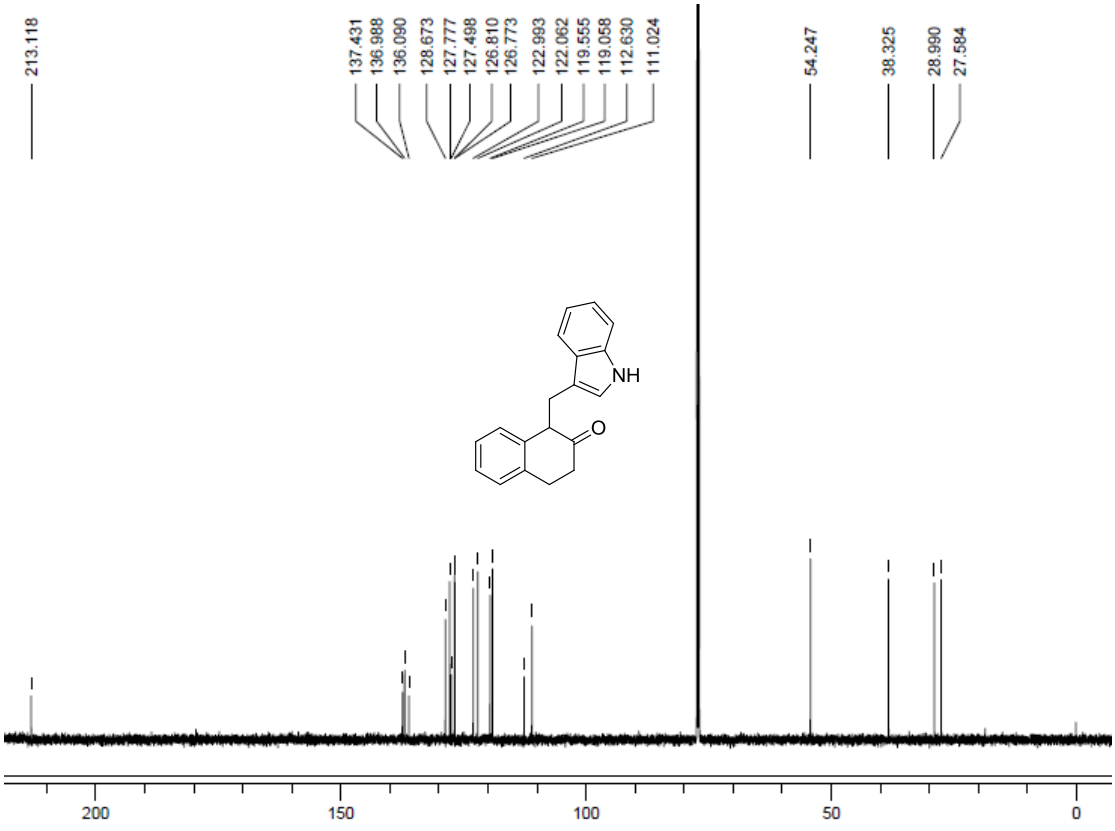
7.11
7.03
6.99
6.64
6.63
3.82
3.81
3.80
3.38
3.37
3.35
2.82
2.81
2.80
2.67
2.66
2.65
2.64
2.63
2.62
2.54
2.53
2.52
2.51
2.50
2.49
2.48
2.47
2.45
2.44
NH
O
1.00
1.01
0.98
2.93
0.97
1.98
0.98
1.00
2.05
1.03
1.06
2.05
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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126.810
126.773
122.993
122.062
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119.058
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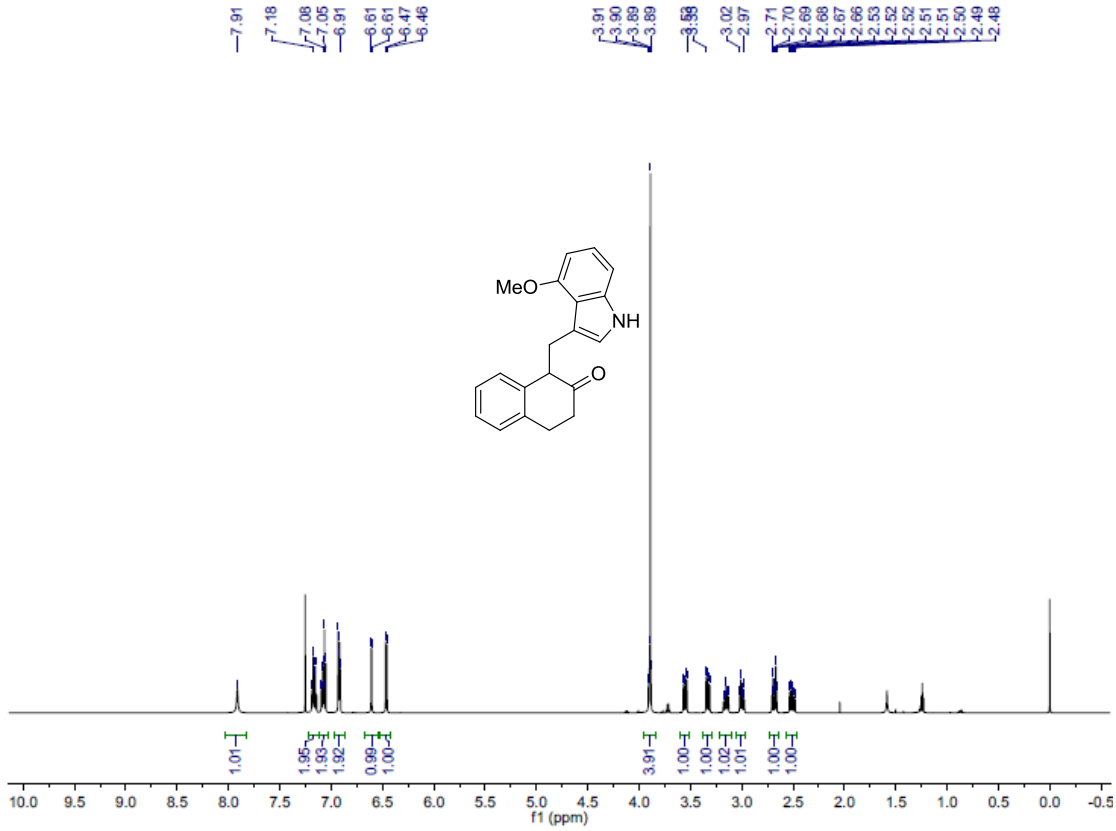
111.024
54.247
38.325
28.990
27.584
NH
O
200
150
100
50
0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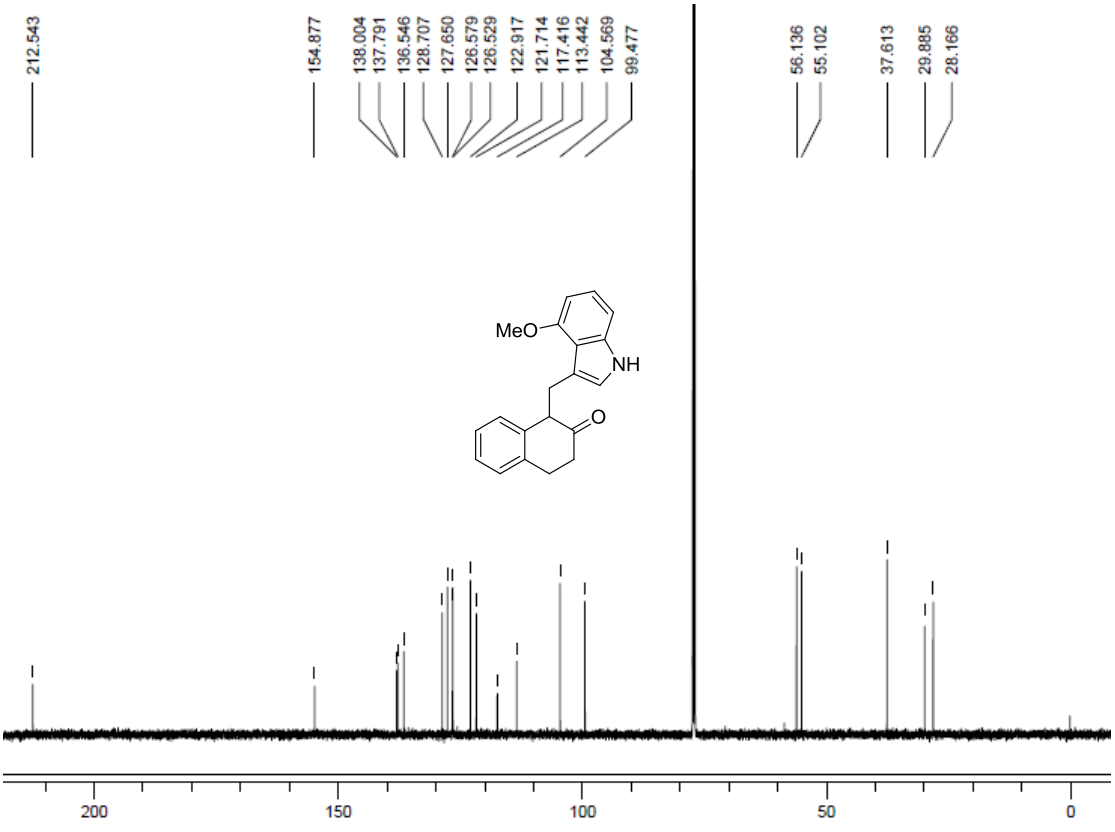
7.05
6.91
6.61
6.61
6.47
6.46
3.91
3.90
3.89
3.89
3.02
2.97
2.71
2.70
2.69
2.68
2.67
2.66
2.53
2.52
2.52
2.51
2.51
2.50
2.49
2.48
MeO
NH
O
1.01
1.95
1.93
1.92
0.99
1.00
3.91
1.00
1.00
1.02
1.01
1.00
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.529
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117.416
113.442
104.569
99.477
56.136
55.102
37.613
29.885
28.166
MeO
NH
O
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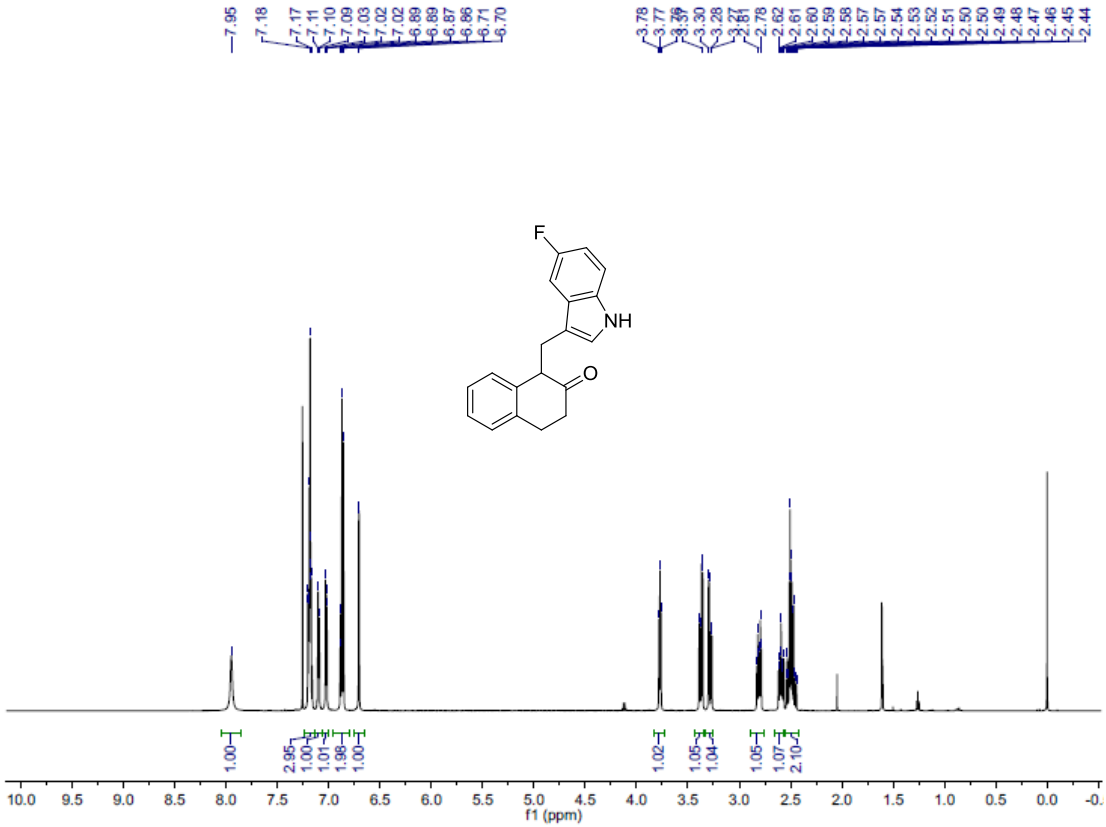
150
100
50
0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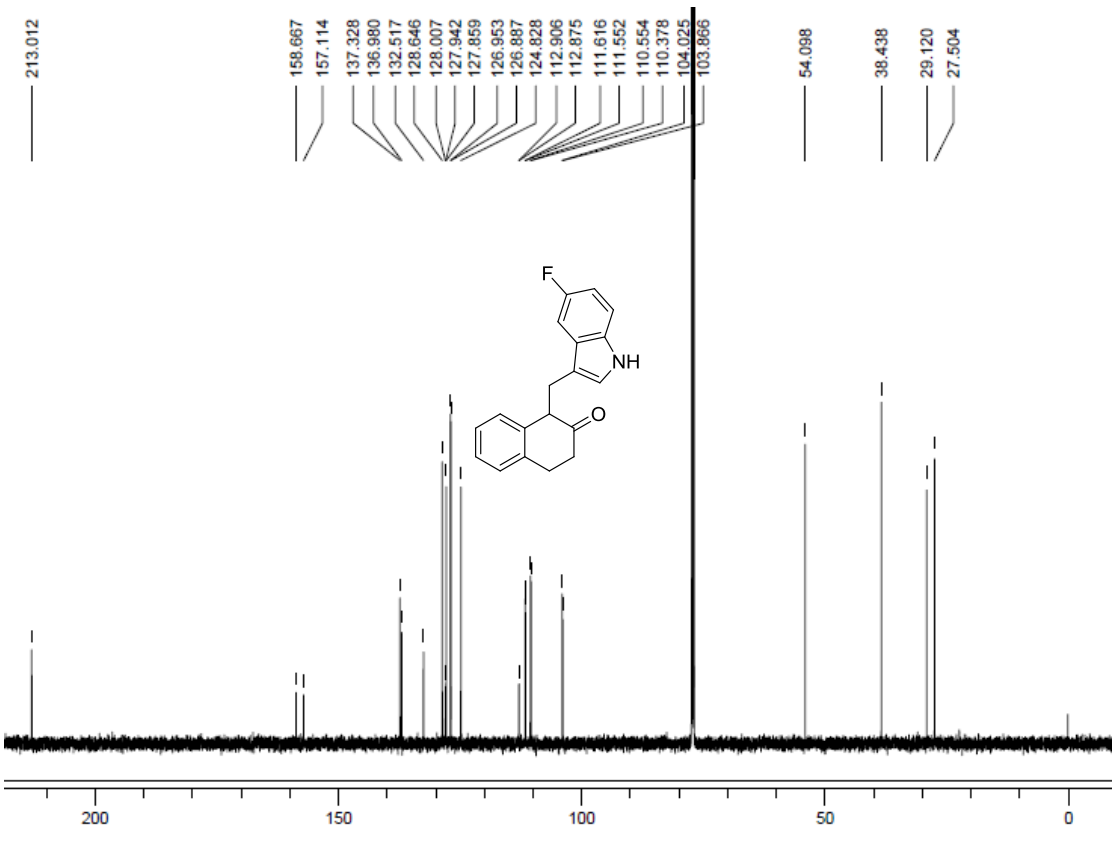
7.11
7.10
7.09
7.03
7.02
7.02
6.89
6.89
6.87
6.86
6.71
6.70
3.78
3.77
3.30
3.28
2.78
2.62
2.61
2.60
2.59
2.58
2.57
2.54
2.53
2.52
2.51
2.50
2.50
2.49
2.48
2.47
2.46
2.45
2.44
F
NH
O
1.00
2.95
1.00
1.01
1.98
1.00
1.02
1.05
1.04
1.05
1.07
2.10
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.859
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126.887
124.828
112.906
112.875
111.616
111.552
110.554
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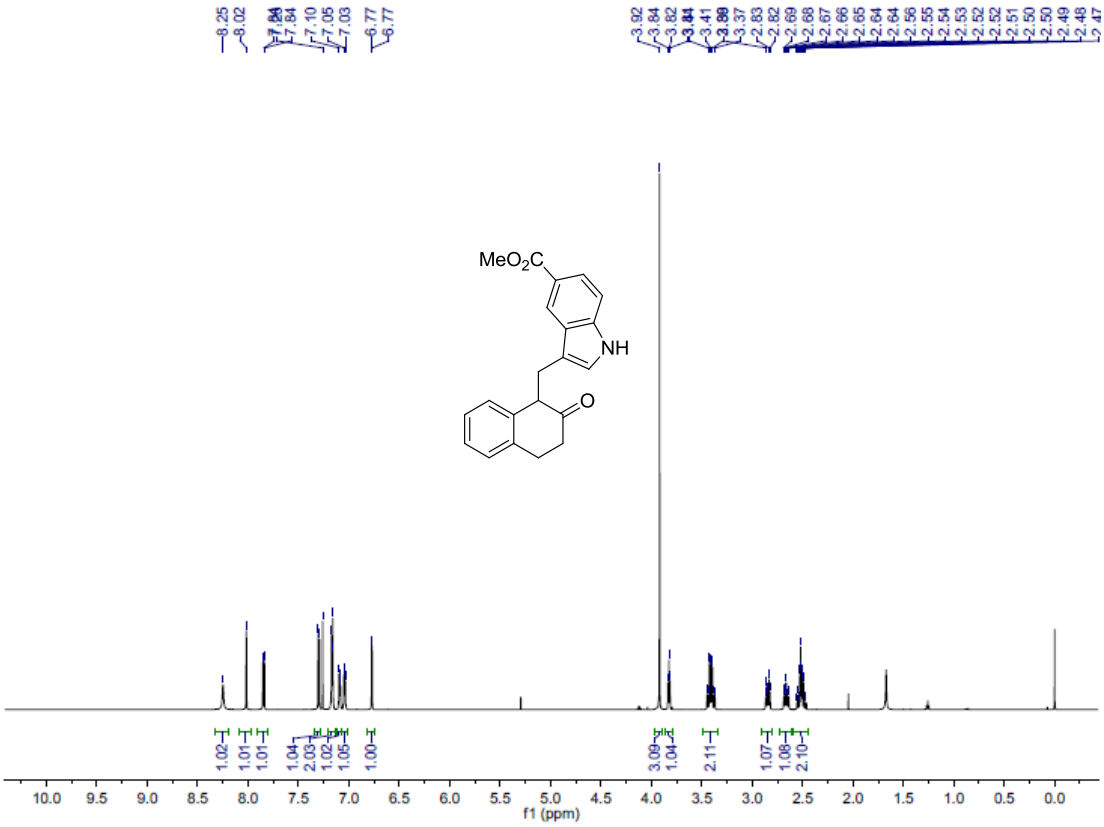
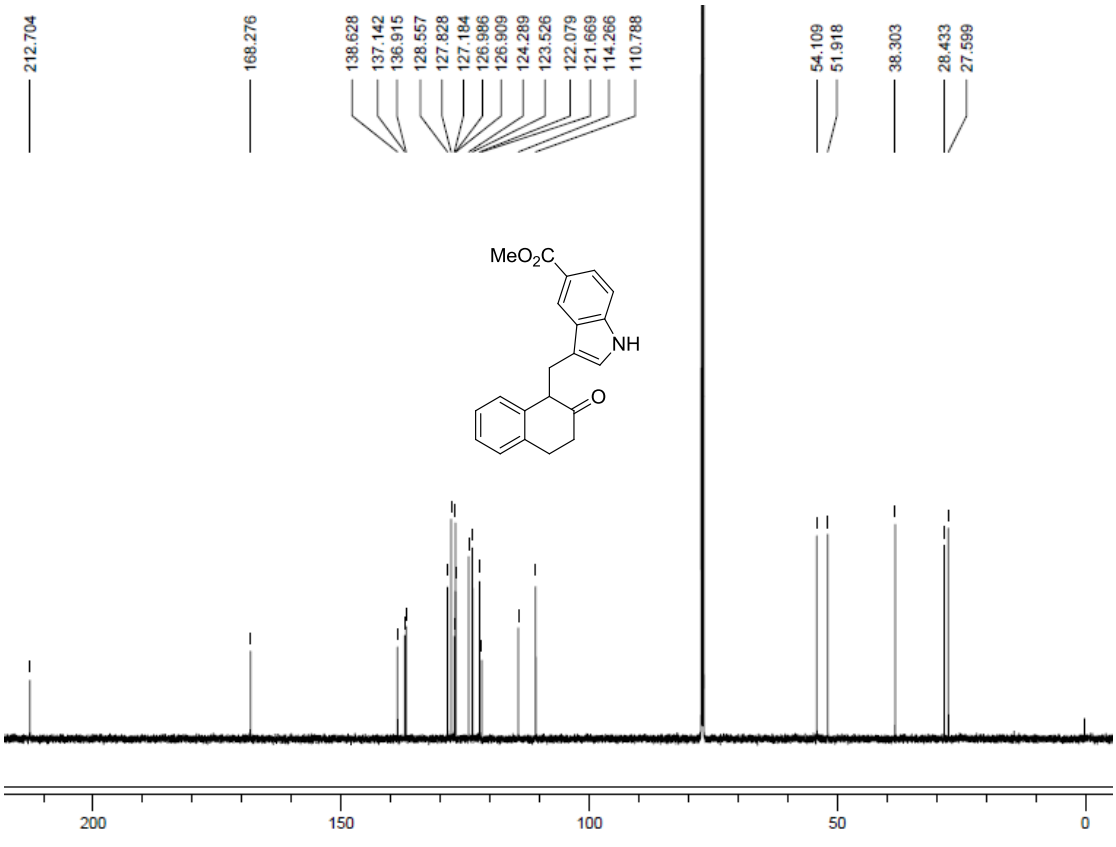
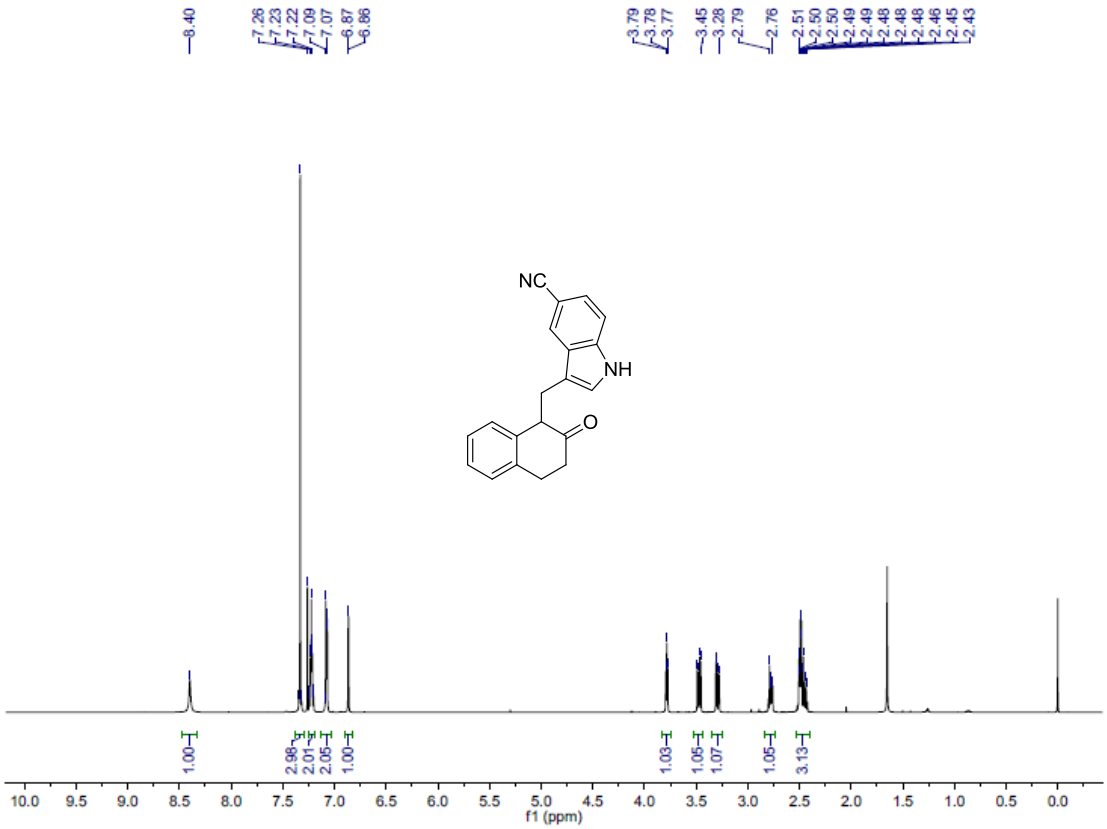
103.866
54.098
38.438
29.120
27.504
F
NH
O
200
150
100
50
0


MeO2C
NH
O
f1 (ppm)


MeO2C
NH
O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3.45
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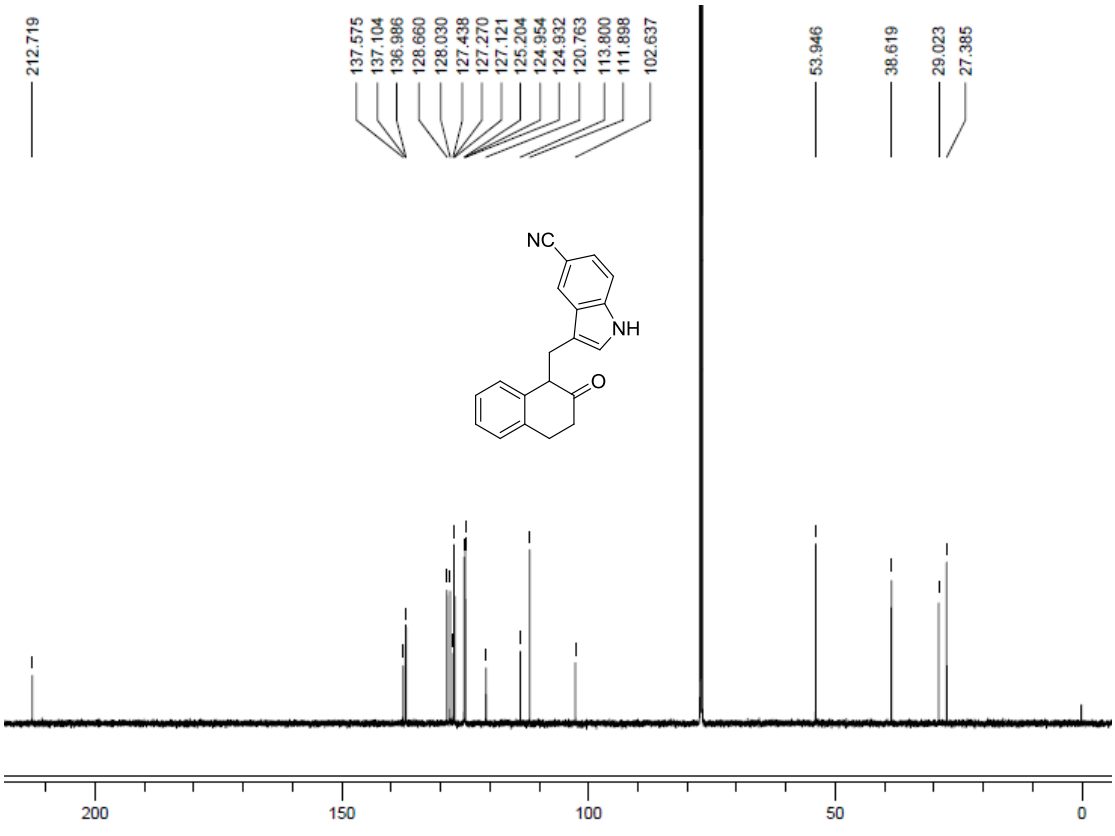
2.50
2.50
2.49
2.49
2.48
2.48
2.48
2.46
2.45
2.43
NC
NH
O
1.00
2.98
2.01
2.05
1.00
1.03
1.05
1.07
1.05
3.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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124.932
120.763
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NC
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O
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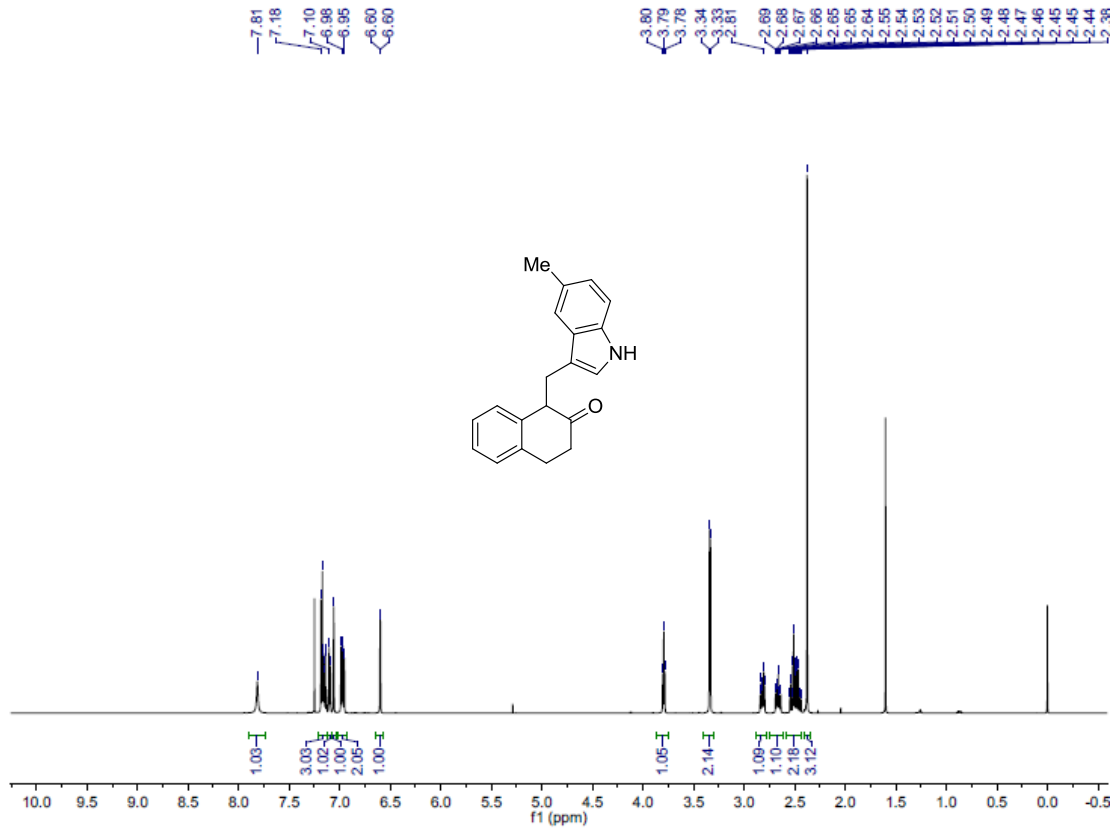
150
100
50
0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6.60
3.80
3.79
3.78
3.34
3.33
2.81
2.69
2.68
2.67
2.66
2.65
2.65
2.64
2.55
2.54
2.53
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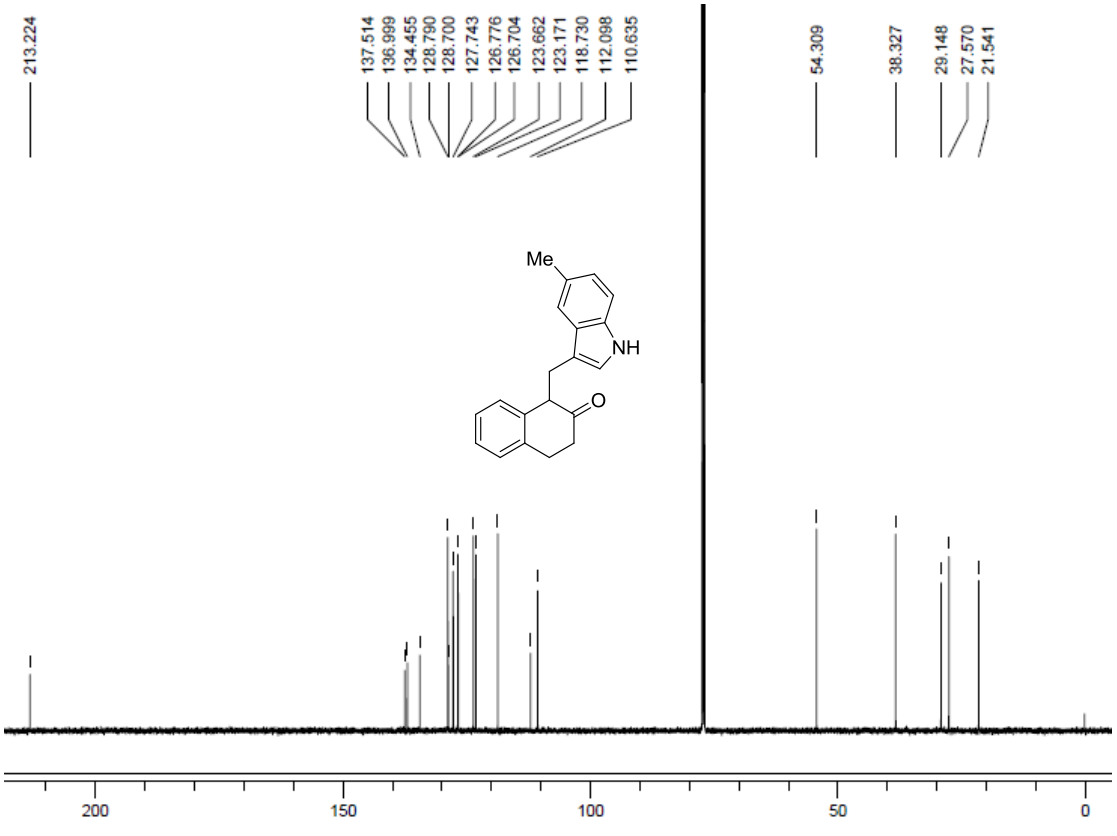
2.51
2.50
2.49
2.48
2.47
2.46
2.45
2.45
2.44
Me
NH
O
1.03
3.03
1.02
1.00
2.05
1.00
1.05
2.14
1.09
1.10
2.18
3.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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126.776
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118.730
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38.327
29.148
27.570
21.541
Me
NH
O
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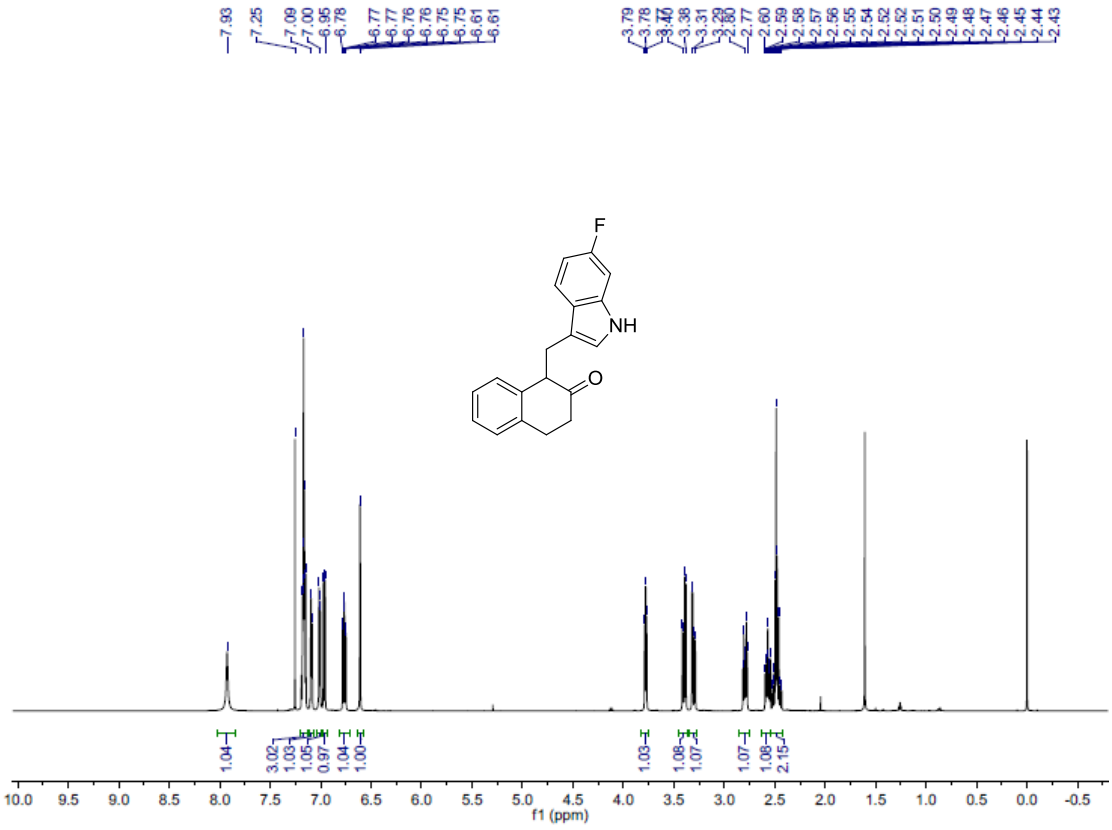
150
100
50
0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6.77
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6.76
6.75
6.75
6.61
6.61
3.79
3.78
3.47
3.46
3.38
3.31
3.29
3.28
2.80
2.77
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2.59
2.58
2.57
2.56
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2.54
2.52
2.52
2.51
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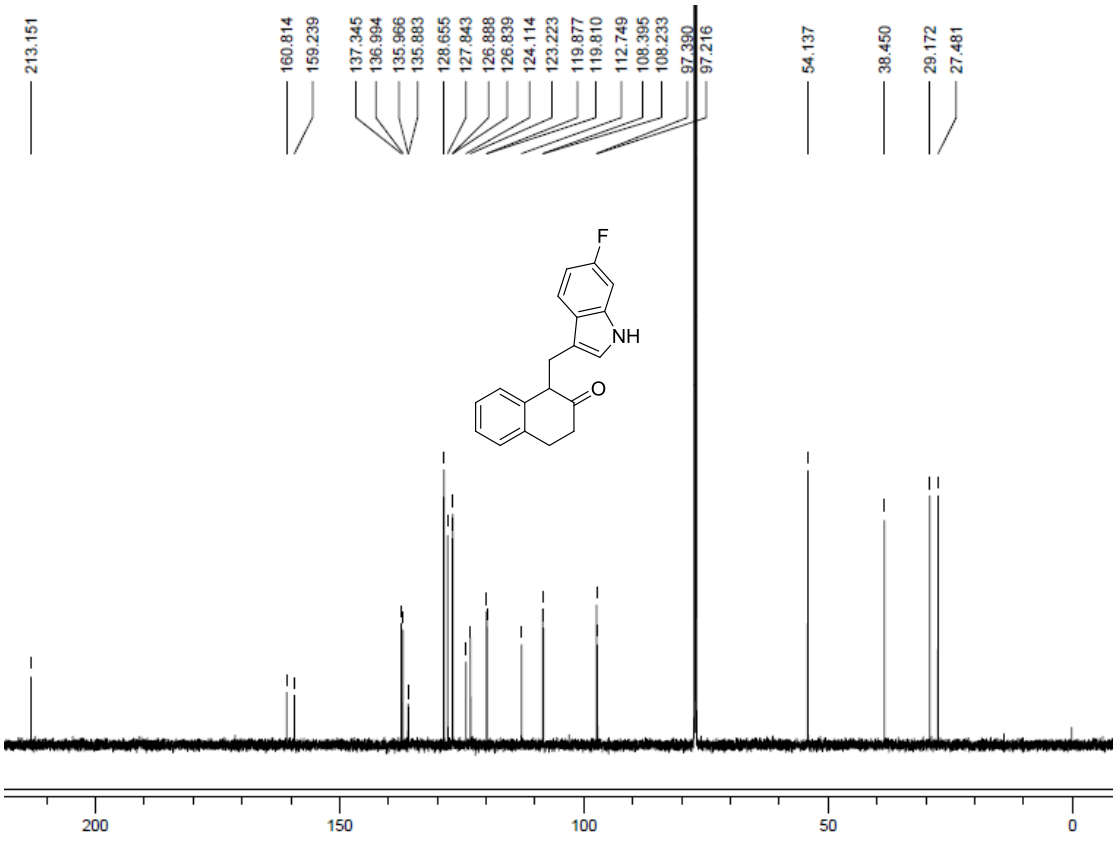
2.48
2.47
2.46
2.45
2.44
2.43
F
NH
O
1.04
3.02
1.03
1.05
0.97
1.04
1.00
1.03
1.08
1.07
1.07
1.08
2.15
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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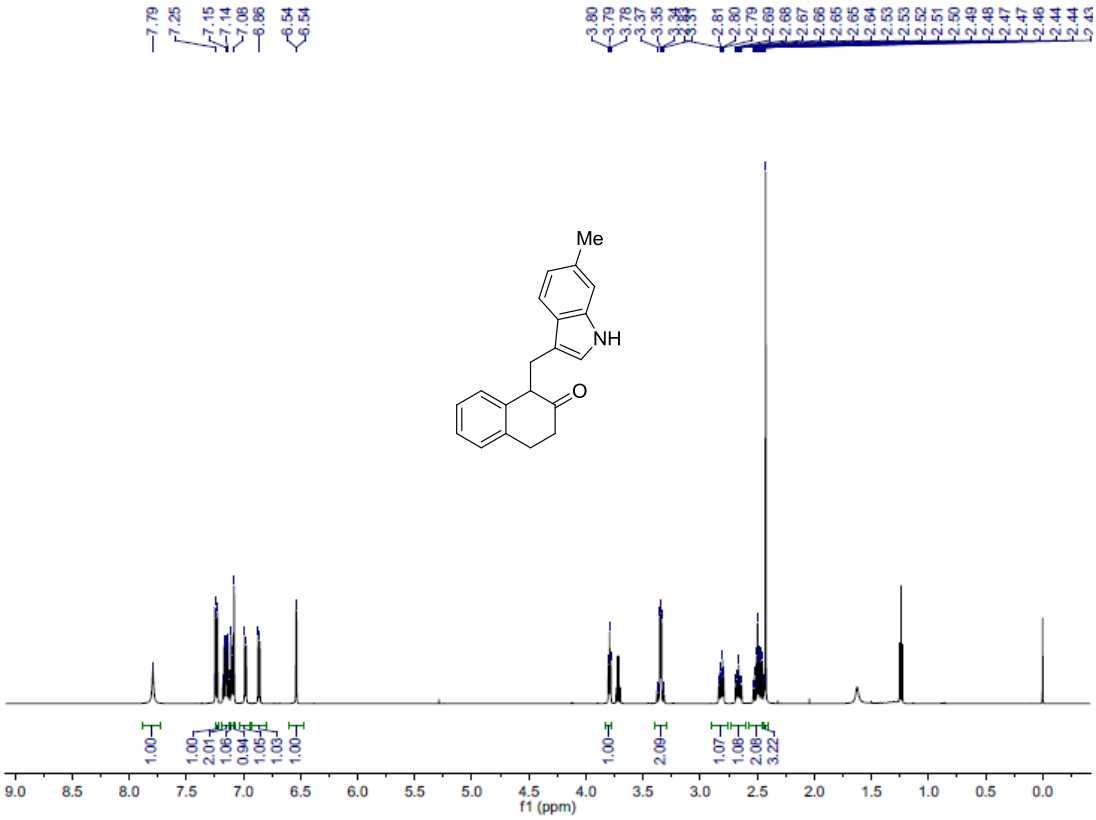
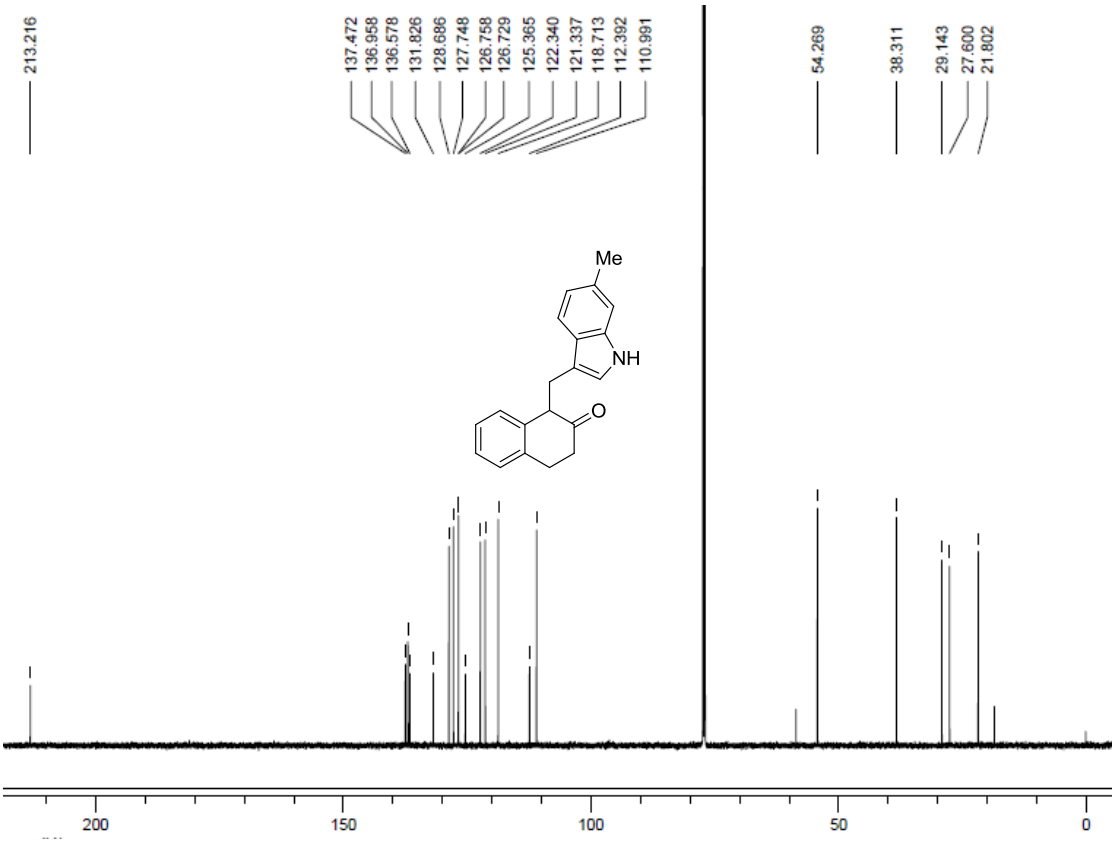
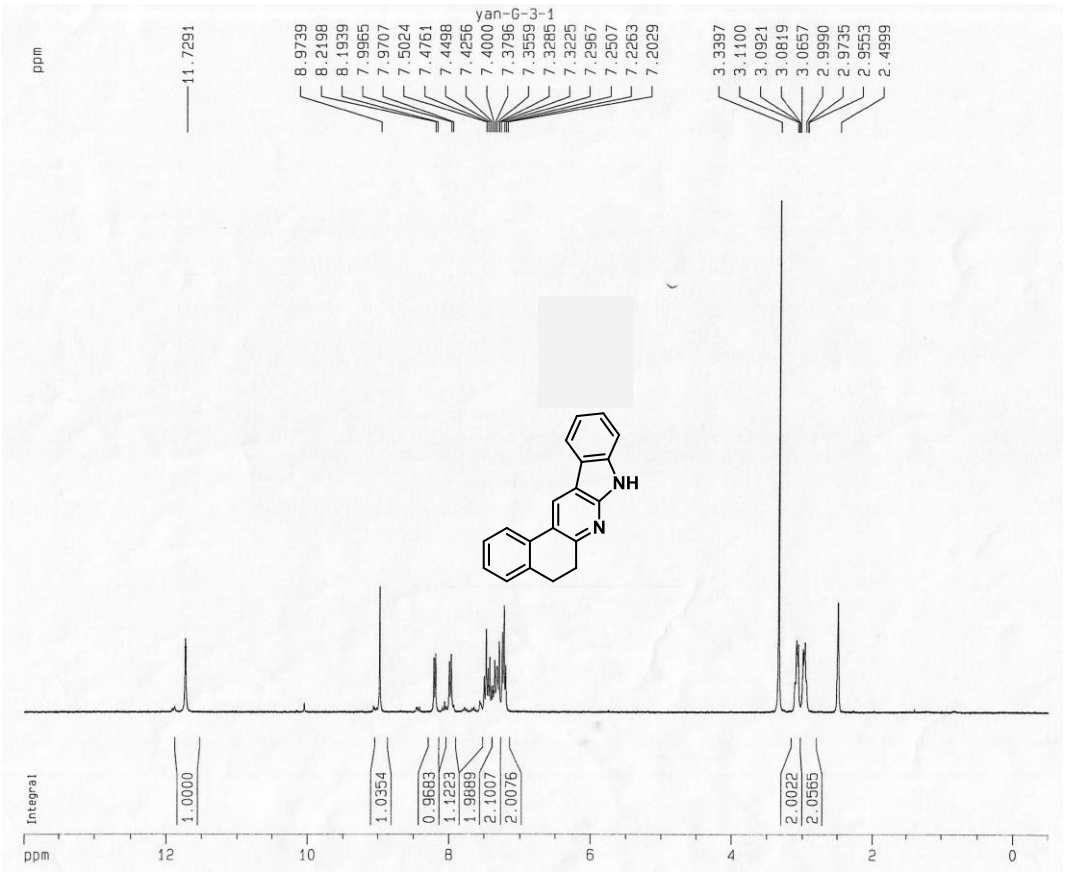
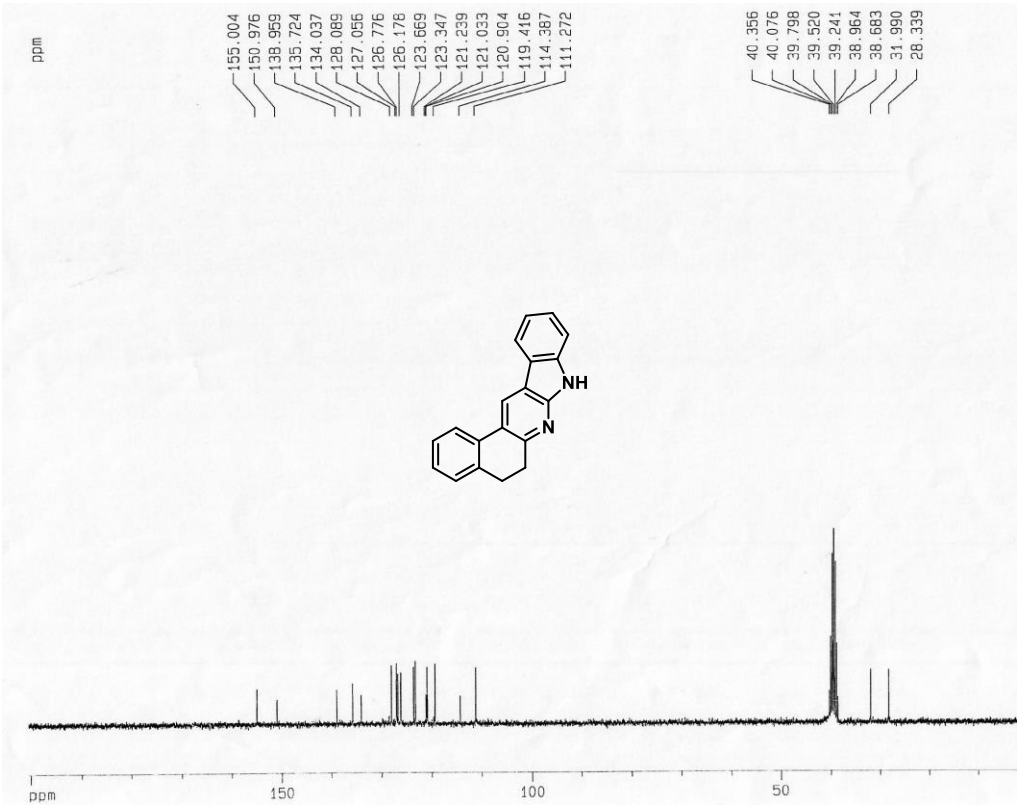
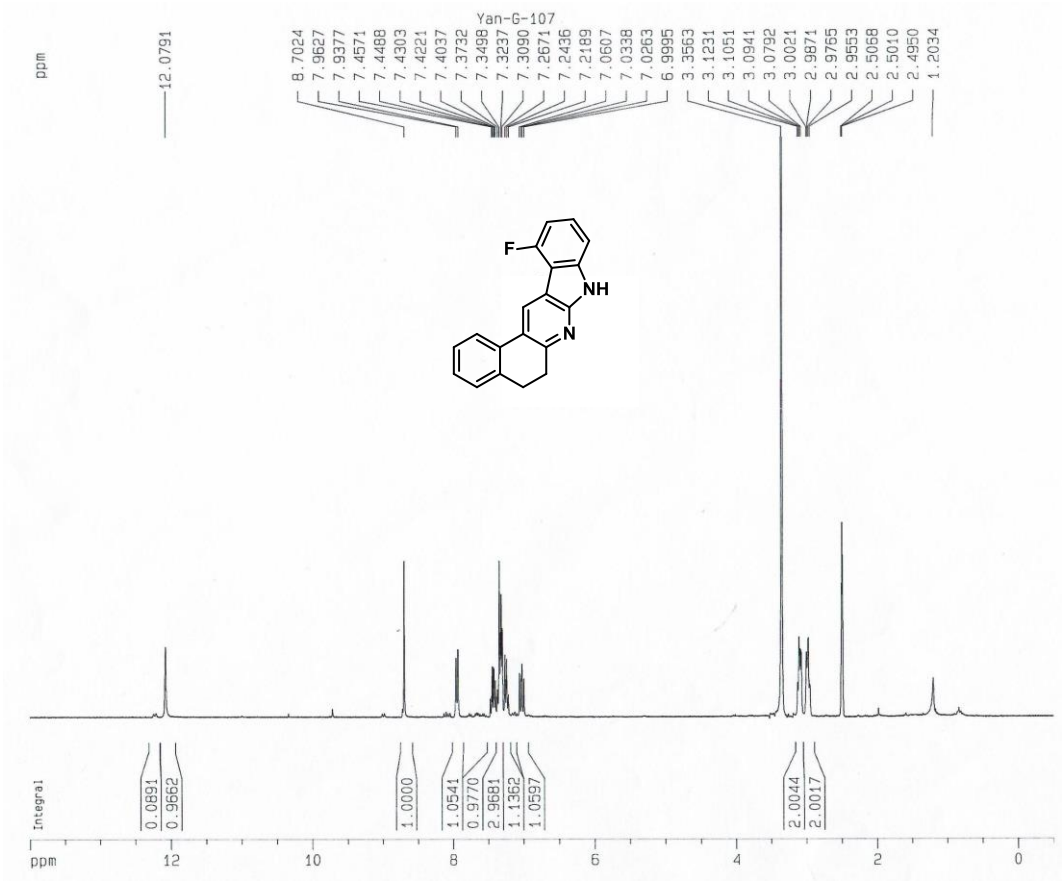
126.888
126.839
124.114
123.223
119.877
119.810
112.749
108.395
108.233
97.390
97.216
54.137
38.450
29.172
27.481
F
NH
O
200
150
100
50
0

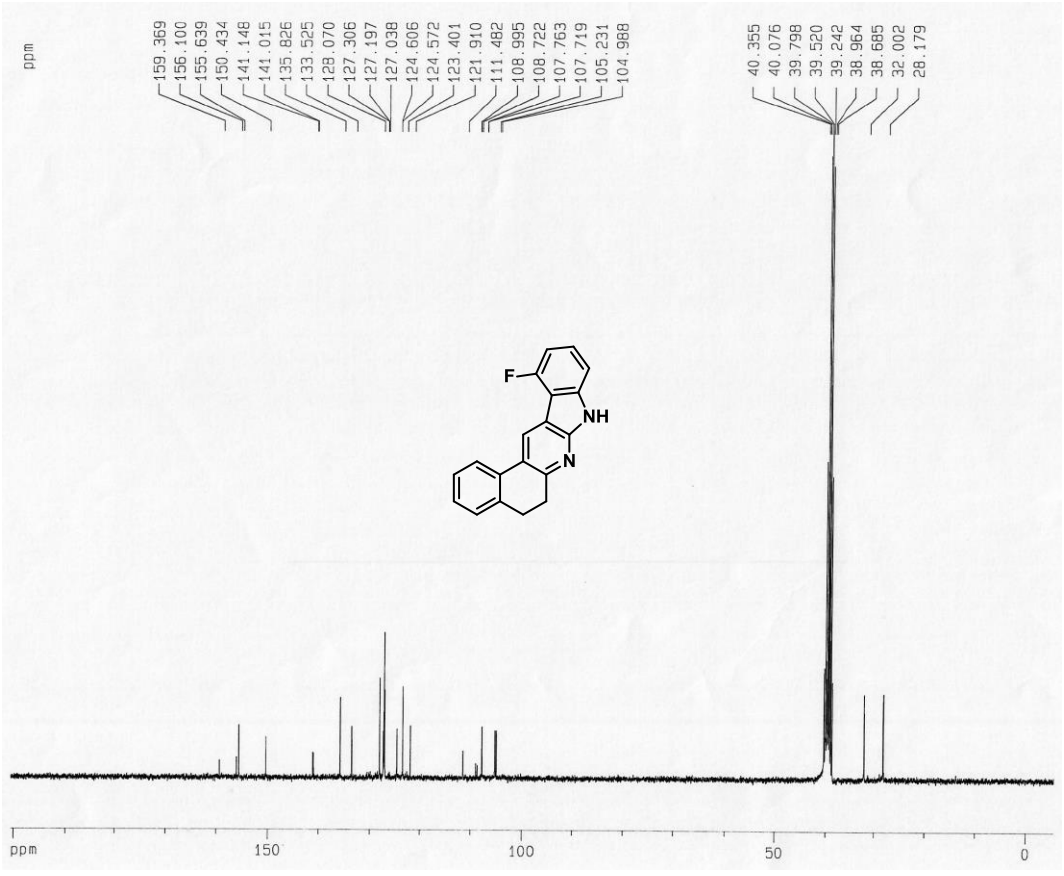

7.79
7.25
7.15
7.14
7.08
6.86
6.54
6.54
3.80
3.79
3.78
3.37
3.35
2.81
2.80
2.79
2.69
2.68
2.67
2.66
2.65
2.64
2.53
2.52
2.51
2.50
2.49
2.48
2.47
2.46
2.44
Me
NH
O
1.00
1.00
2.01
1.06
0.94
1.05
1.03
1.00
1.00
2.09
1.07
1.08
2.08
3.22
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

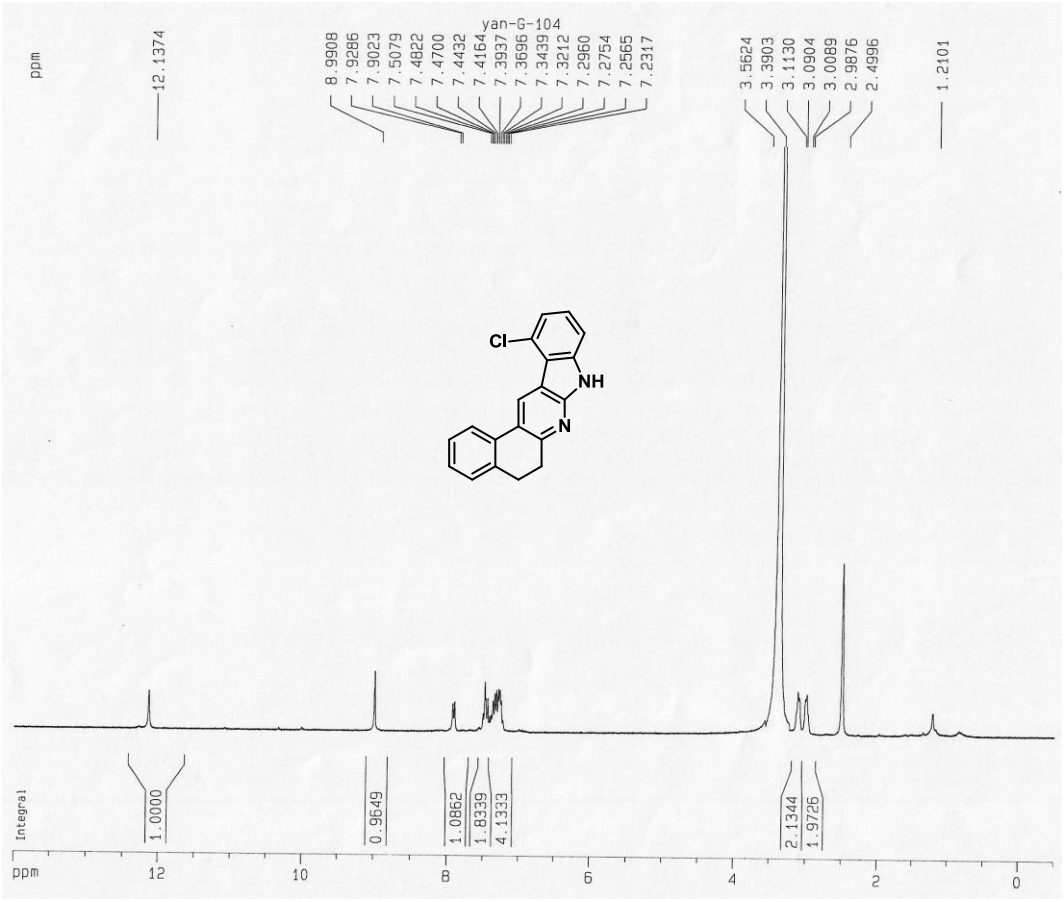

213.216
137.472
136.958
136.578
131.826
128.686
127.748
126.758
126.729
125.365
122.340
121.337
118.713
112.392
110.991
54.269
38.311
29.143
27.600
21.802
Me
NH
O
200
150
100
50
0

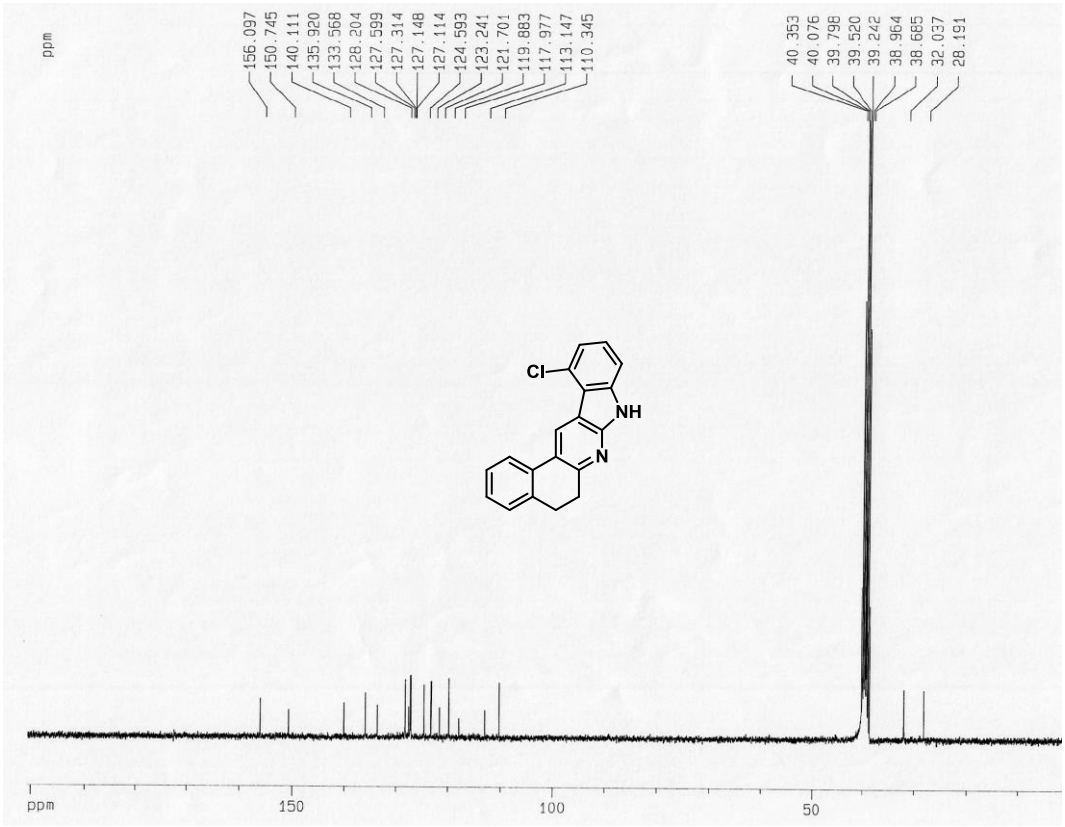

yan-G-3-1
ppm
11.7291
8.9739
8.2198
8.1939
7.9965
7.9707
7.5024
7.4761
7.4498
7.4256
7.4000
7.3796
7.3559
7.3285
7.3225
7.2967
7.2507
7.2263
7.2029
3.3397
3.1100
3.0921
3.0819
3.0657
2.9990
2.9735
2.9553
2.4999
NH
N
Integral
1.0000
1.0354
0.9683
1.1223
1.9889
2.1007
2.0076
2.0022
2.0565
ppm
12
10
8
6
4
2
0

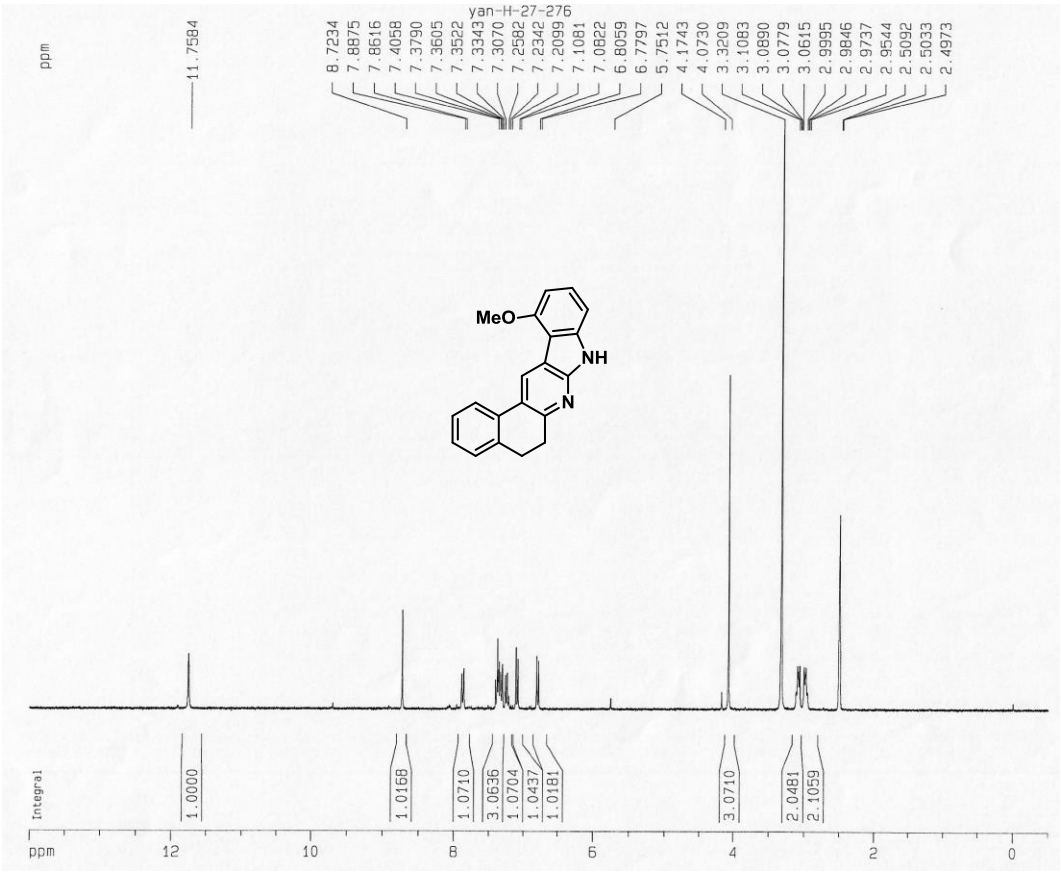

ppm
155.004
150.976
138.959
135.724
134.037
128.089
127.056
126.776
126.176
123.669
123.347
121.239
121.033
120.904
119.416
114.387
111.272
40.356
40.076
39.798
39.520
39.241
38.964
38.683
31.990
28.339
NH
N
ppm
150
100
50

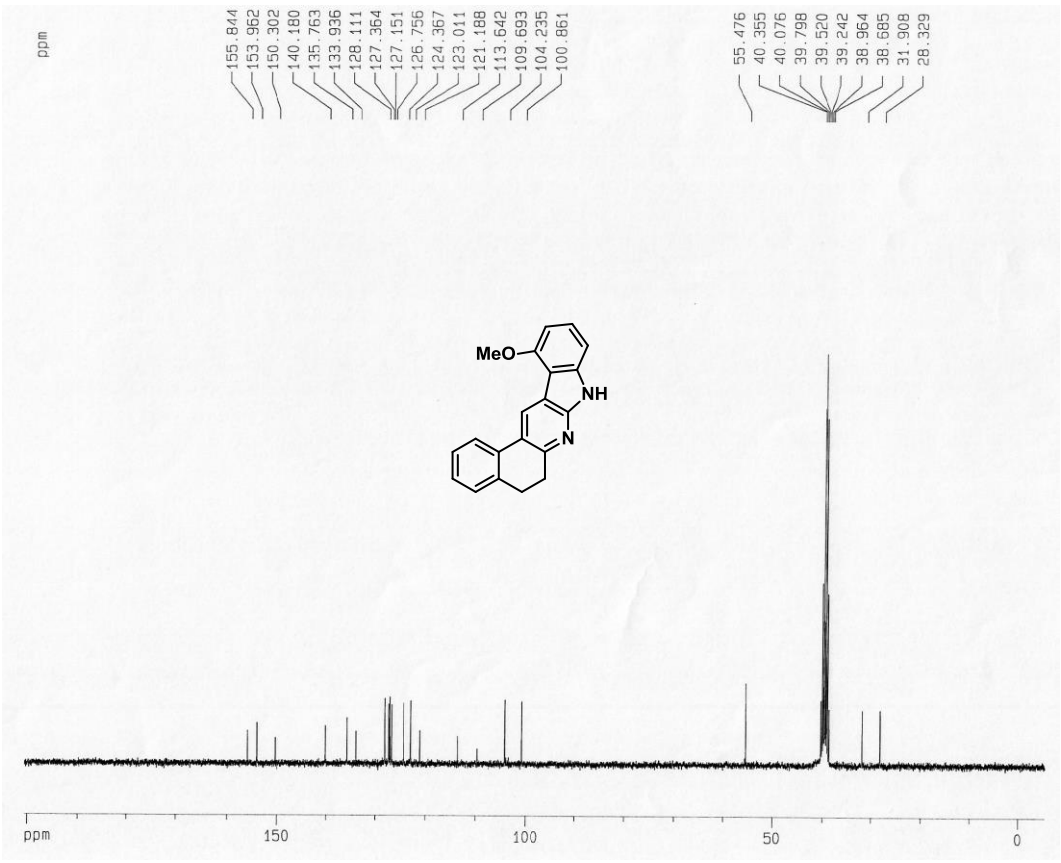

Yan-G-107
ppm
12.0791
8.7024
7.9627
7.9377
7.4571
7.4488
7.4303
7.4221
7.4037
7.3732
7.3498
7.3237
7.3090
7.2671
7.2436
7.2189
7.0607
7.0338
7.0263
6.9995
3.3563
3.1231
3.1051
3.0941
3.0792
3.0021
2.9871
2.9765
2.9553
2.5068
2.5010
2.4950
1.2034
F
NH
N
Integral
0.0891
0.9662
1.0000
1.0541
0.9770
2.9681
1.1362
1.0597
2.0044
2.0017
ppm
12
10
8
6
4
2
0


ppm
159.369
156.100
155.639
150.434
141.148
141.015
135.826
133.525
128.070
127.306
127.197
127.038
124.606
124.572
123.401
121.910
111.482
108.995
108.722
107.763
107.719
105.231
104.988
40.355
40.076
39.798
39.520
39.242
38.964
38.685
32.002
28.179
F
NH
N
ppm
150
100
50
0

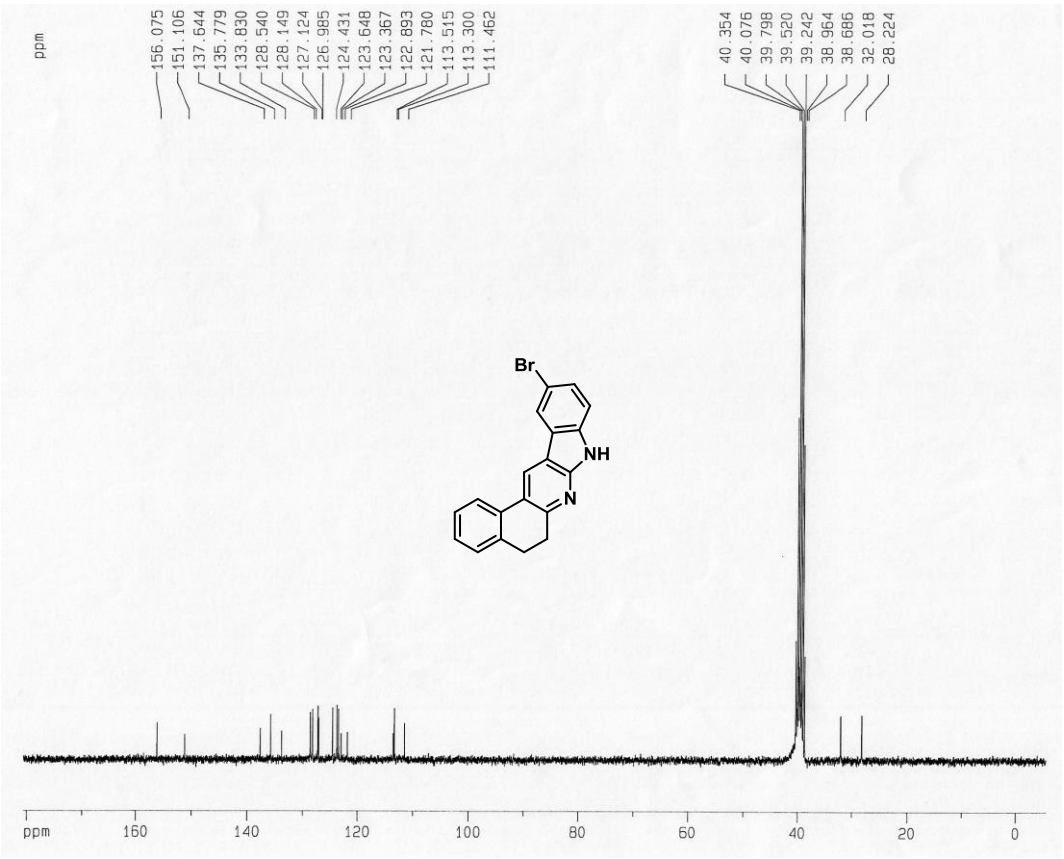

yan-G-104
ppm
12.1374
8.9908
7.9286
7.9023
7.5079
7.4822
7.4700
7.4432
7.4164
7.3937
7.3696
7.3439
7.3212
7.2960
7.2754
7.2565
7.2317
3.5624
3.3903
3.1130
3.0904
3.0089
2.9876
2.4996
1.2101
Cl
NH
N
Integral
1.0000
0.9649
1.0862
1.8339
4.1333
2.1344
1.9726
ppm
12
10
8
6
4
2
0

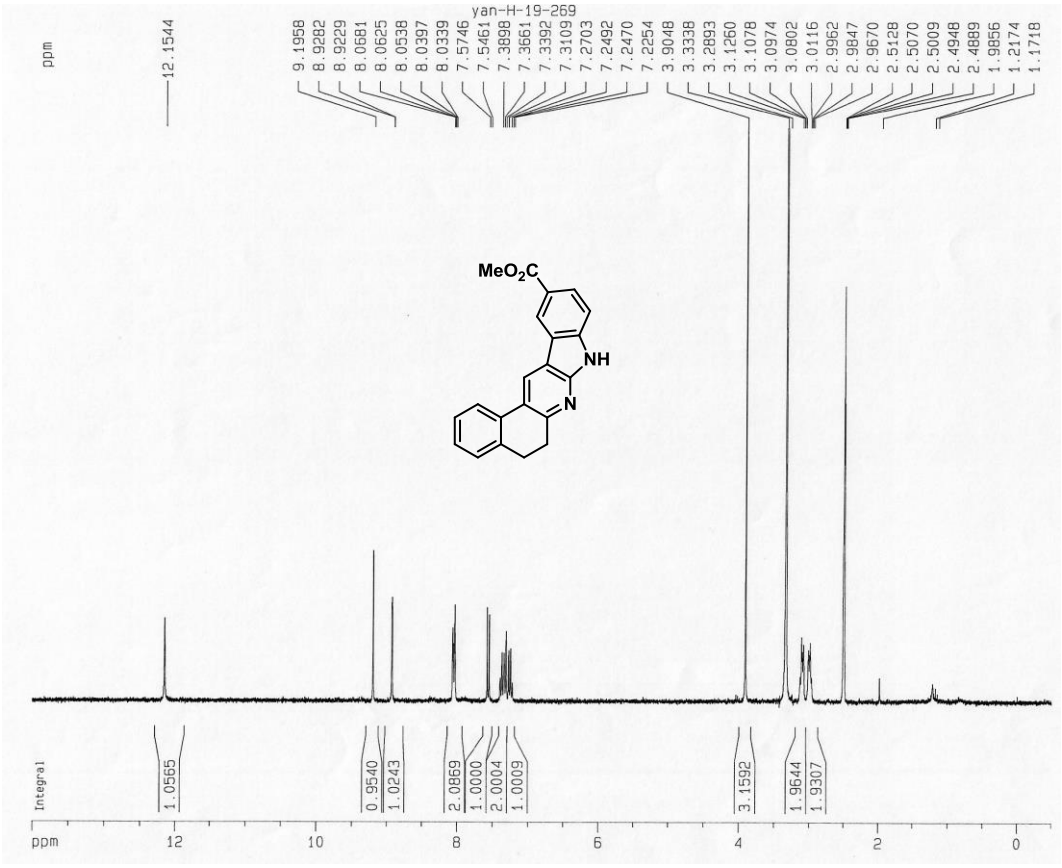

ppm
156.097
150.745
140.111
135.920
133.568
128.204
127.599
127.314
127.148
127.114
124.593
123.241
121.701
119.883
117.977
113.147
110.345
40.353
40.076
39.798
39.520
39.242
38.964
38.665
32.037
28.191
Cl
NH
N
ppm
150
100
50

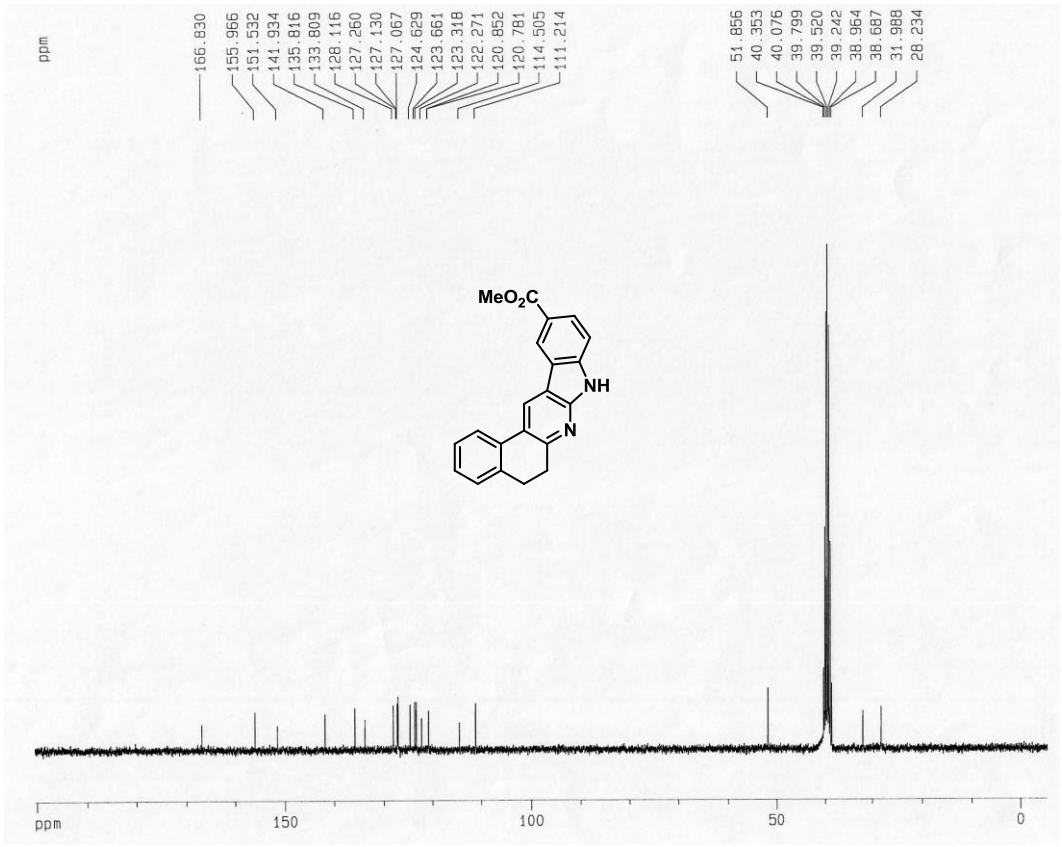

yan-H-27-276
ppm
11.7584
8.7234
7.8875
7.8616
7.4058
7.3790
7.3605
7.3522
7.3343
7.3070
7.2582
7.2342
7.2099
7.1081
7.0822
6.8059
6.7797
5.7512
4.1743
4.0730
3.3209
3.1083
3.0890
3.0779
3.0615
2.9995
2.9846
2.9737
2.9544
2.5092
2.5033
2.4973
MeO
NH
N
Integral
1.0000
1.0168
1.0710
3.0636
1.0704
1.0437
1.0181
3.0710
2.0481
2.1059
ppm
12
10
8
6
4
2
0

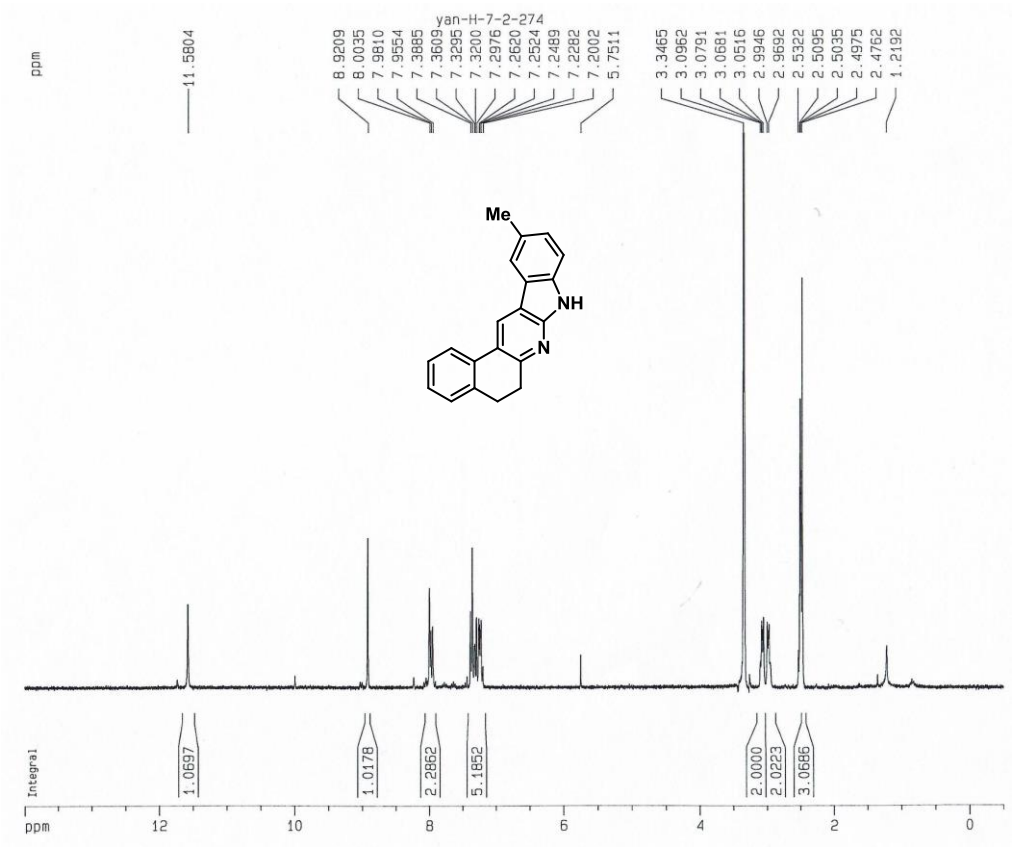

ppm
155.844
153.962
150.302
140.180
135.763
133.936
128.111
127.364
127.151
126.756
124.367
123.011
121.188
113.642
109.693
104.235
100.861
55.476
40.355
40.076
39.798
39.520
39.242
38.964
38.685
31.908
28.329
MeO
NH
N
ppm
150
100
50
0

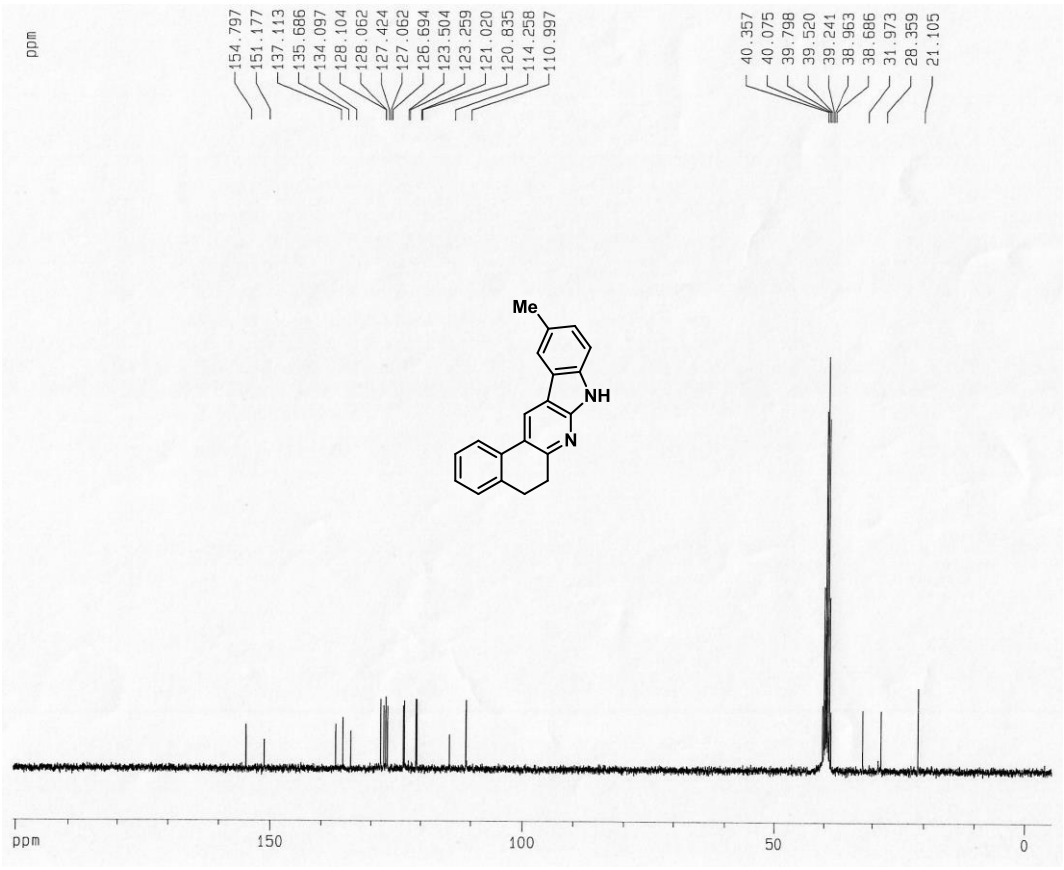

yan-G-112-2
ppm
11.9072
9.0658
8.4598
8.4535
7.9644
7.9387
7.5689
7.5622
7.5401
7.5336
7.4612
7.4332
7.3958
7.3707
7.3441
7.3323
7.3099
7.2693
7.2434
7.2195
3.3290
3.1152
3.0964
3.0864
3.0700
3.0052
2.9892
2.9786
2.9590
2.5057
2.4999
2.4940
1.2241
Br
NH
N
Integral
1.0000
0.9930
1.0177
1.1017
1.0597
1.0197
2.0534
1.0281
1.9588
1.9666
ppm
12
10
8
6
4
2
0

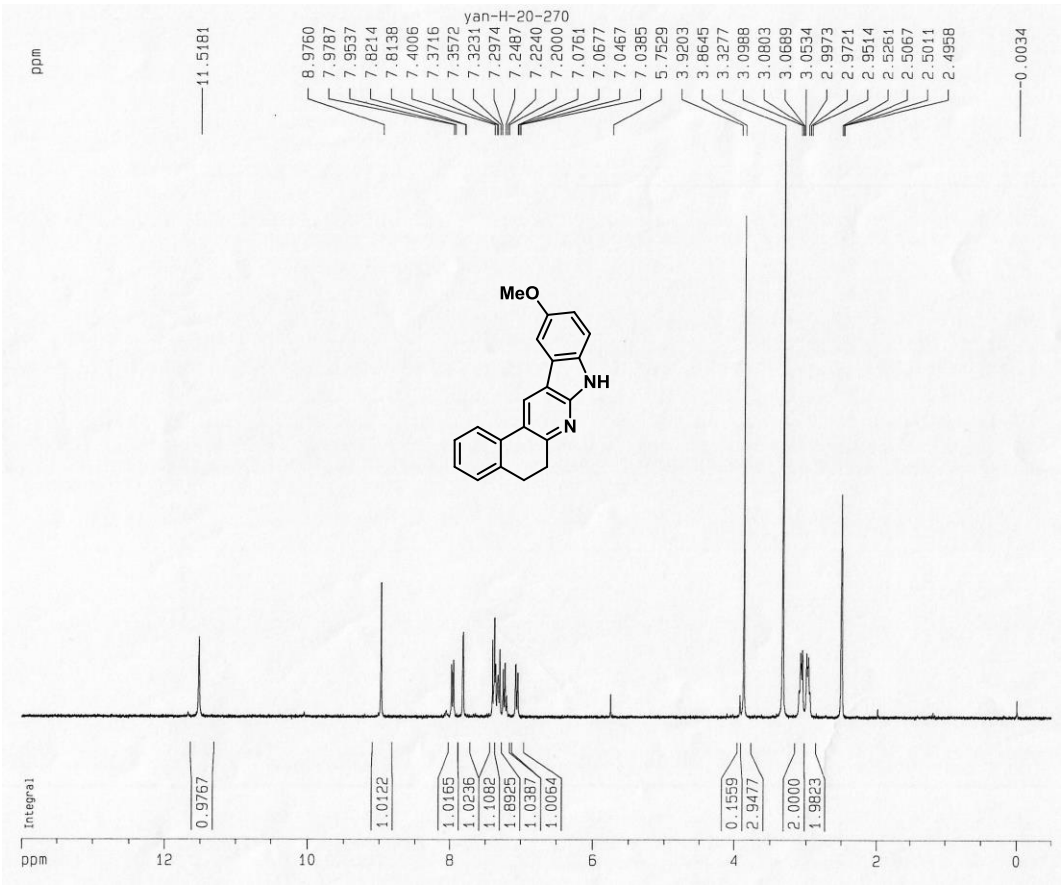

ppm
156.075
151.106
137.644
135.779
133.830
128.540
128.149
127.124
126.985
124.431
123.648
123.367
122.893
121.780
113.515
113.300
111.462
40.354
40.076
39.798
39.520
39.242
38.964
38.686
32.018
28.224
Br
NH
N
ppm
160
140
120
100
80
60
40
20
0

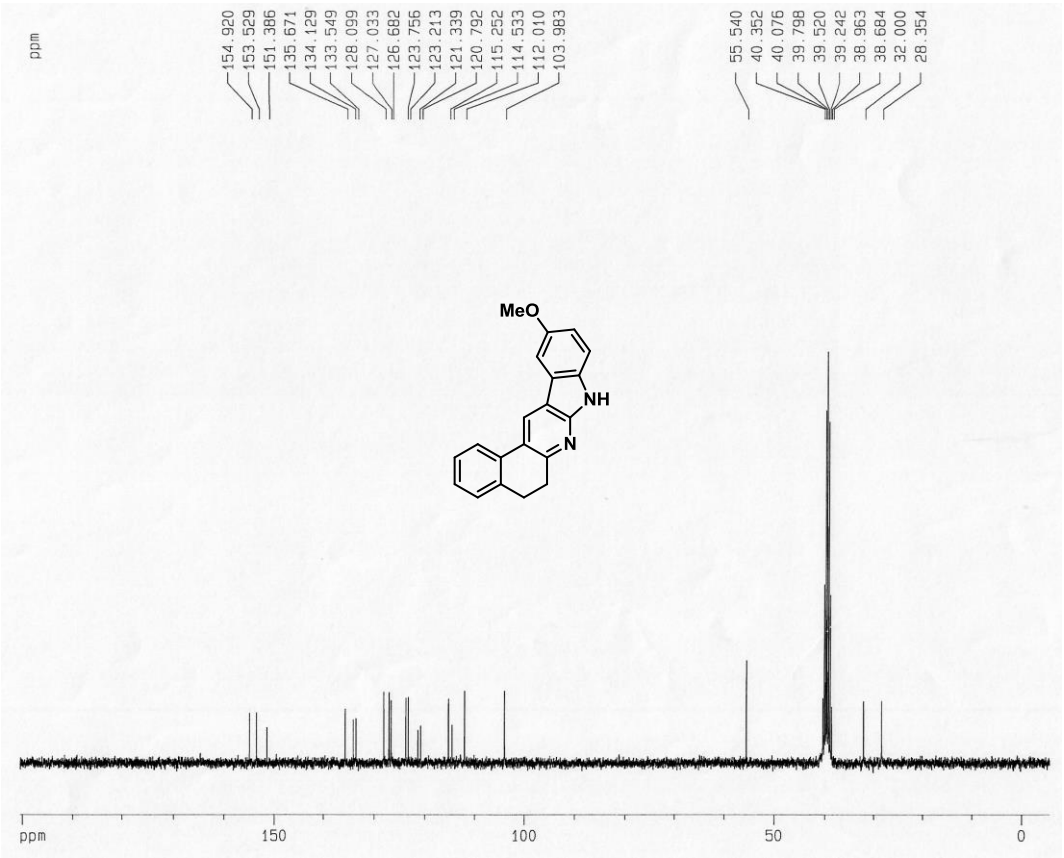

yan-H-19-269
ppm
12.1544
9.1958
8.9282
8.9229
8.0681
8.0625
8.0538
8.0397
8.0339
7.5746
7.5461
7.3898
7.3661
7.3392
7.3109
7.2703
7.2492
7.2470
7.2254
3.9048
3.3338
3.2893
3.1260
3.1078
3.0974
3.0802
3.0116
2.9962
2.9847
2.9670
2.5128
2.5070
2.5009
2.4948
2.4889
1.9856
1.2174
1.1718
MeO2C
NH
N
Integral
1.0565
0.9540
1.0243
2.0869
1.0000
2.0004
1.0009
3.1592
1.9644
1.9307
ppm
12
10
8
6
4
2
0


ppm
166.830
155.966
151.532
141.934
135.816
133.809
128.116
127.260
127.130
127.067
124.629
123.661
123.318
122.271
120.852
120.781
114.505
111.214
51.856
40.353
40.076
39.799
39.520
39.242
38.964
38.687
31.988
28.234
MeO2C
NH
N
ppm
150
100
50
0

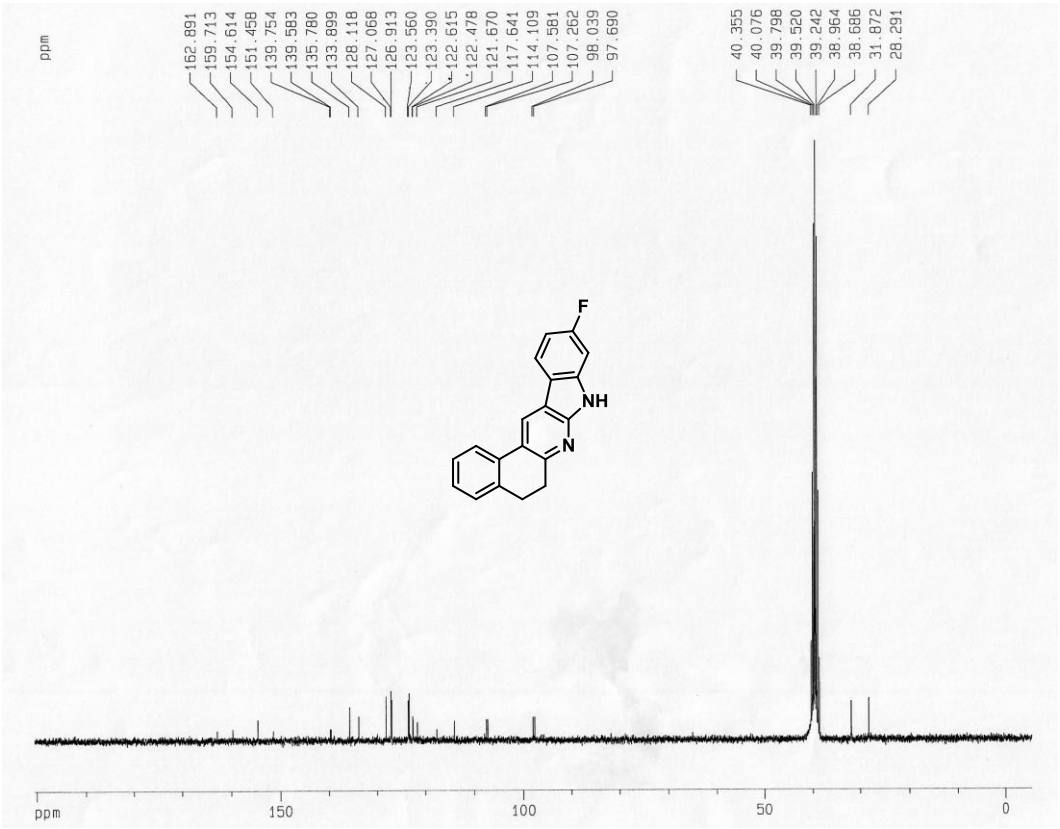

yan-H-7-2-274
ppm
11.5804
8.9209
8.0035
7.9810
7.9554
7.3885
7.3609
7.3295
7.3200
7.2976
7.2620
7.2524
7.2489
7.2282
7.2002
5.7511
3.3465
3.0962
3.0791
3.0681
3.0516
2.9946
2.9692
2.5322
2.5095
2.5035
2.4975
2.4762
1.2192
Me
NH
N
Integral
1.0697
1.0178
2.2862
5.1852
2.0000
2.0223
3.0686
ppm
12
10
8
6
4
2
0

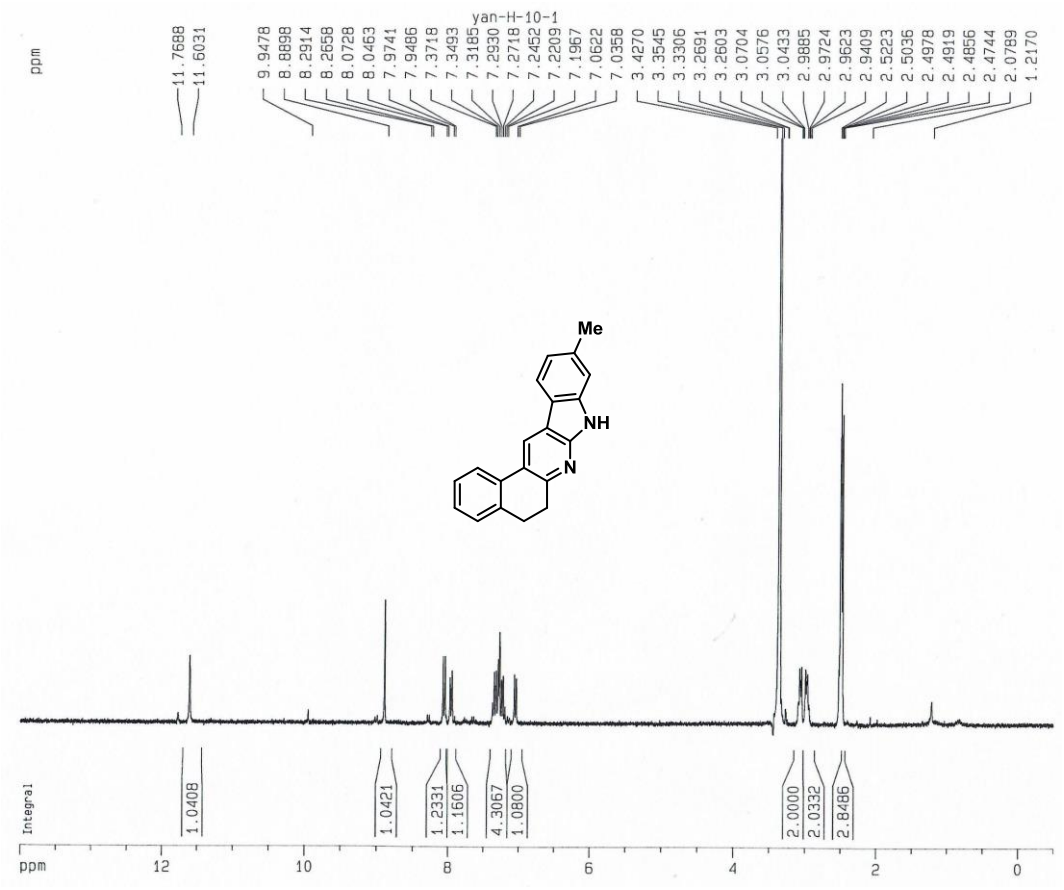

ppm
154.797
151.177
137.113
135.686
134.097
128.104
128.062
127.424
127.062
126.694
123.504
123.259
121.020
120.835
114.258
110.997
40.357
40.075
39.798
39.520
39.241
38.963
38.686
31.973
28.359
21.105
Me
NH
N
ppm
150
100
50
0

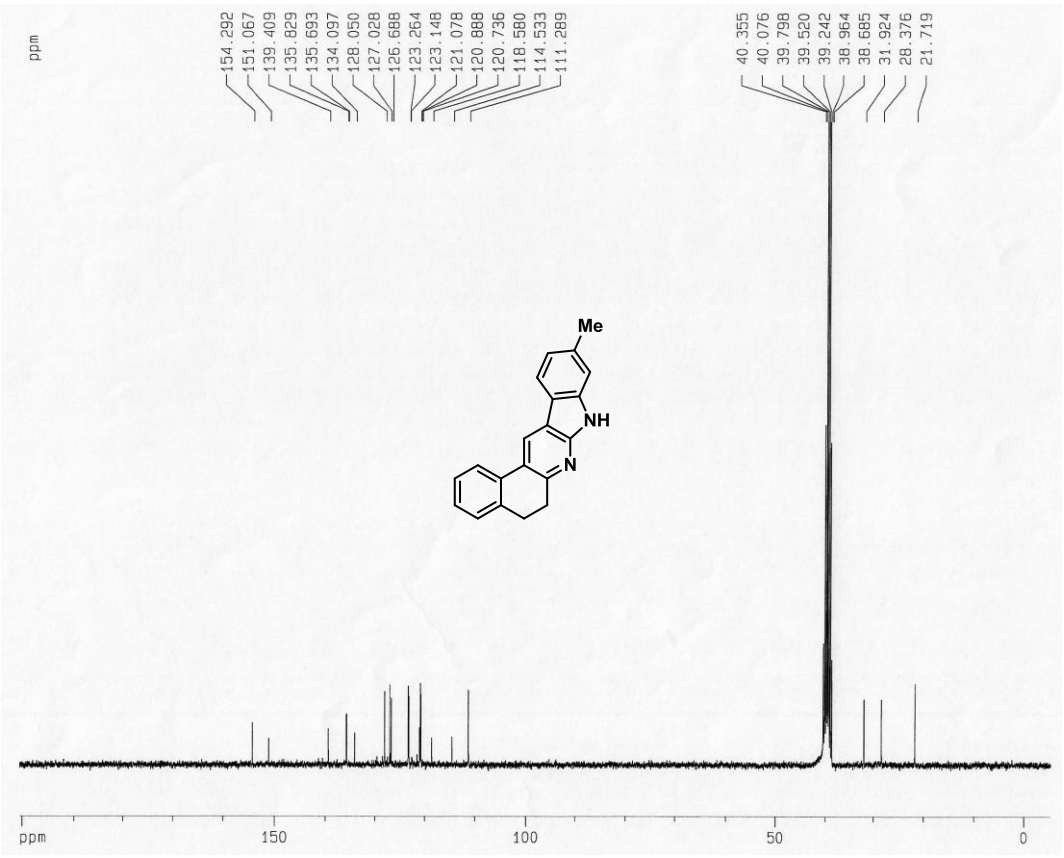

yan-H-20-270
ppm
11.5181
8.9760
7.9787
7.9537
7.8214
7.8138
7.4006
7.3716
7.3572
7.3231
7.2974
7.2487
7.2240
7.2000
7.0761
7.0677
7.0467
7.0385
5.7529
3.9203
3.8645
3.3277
3.0988
3.0803
3.0689
3.0534
2.9973
2.9721
2.9514
2.5261
2.5067
2.5011
2.4958
0.0034
MeO
NH
N
Integral
0.9767
1.0122
1.0165
1.0236
1.1082
1.8925
1.0387
1.0064
0.1559
2.9477
2.0000
1.9823
ppm
12
10
8
6
4
2
0

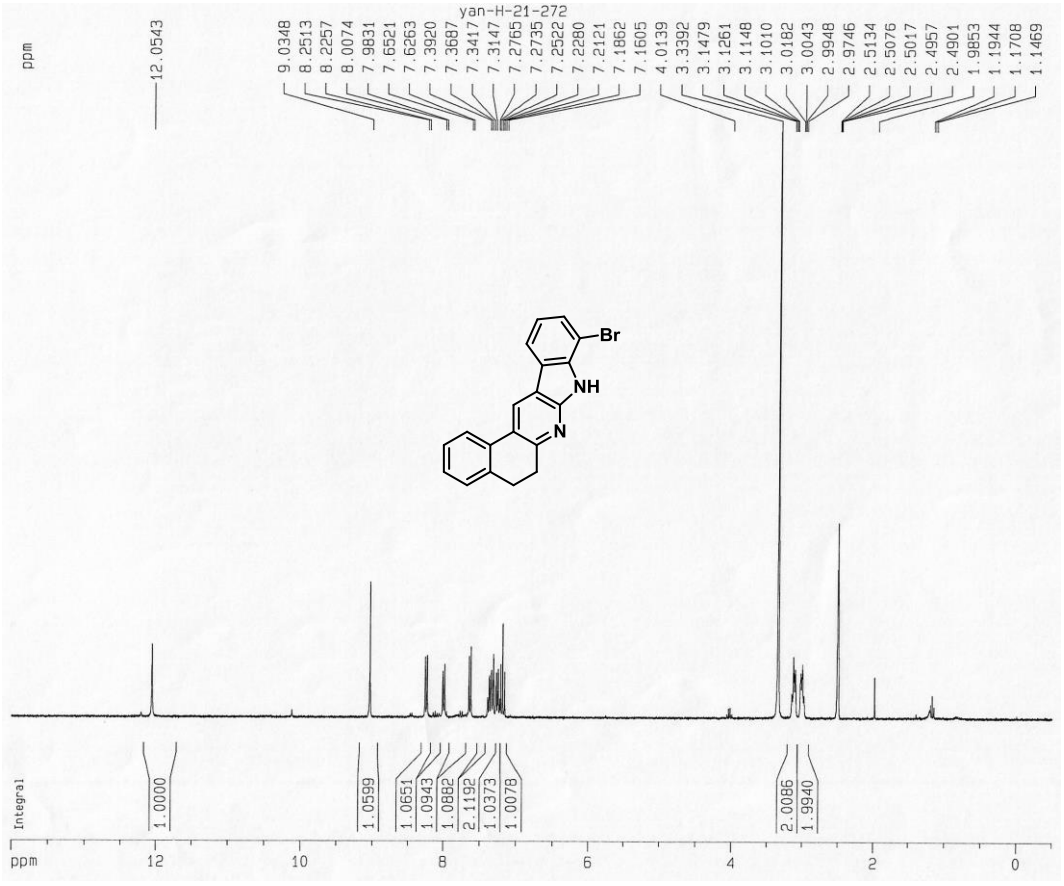

ppm
154.920
153.529
151.386
135.671
134.129
133.549
128.099
127.033
126.682
123.756
123.213
121.339
120.792
115.252
114.533
112.010
103.983
55.540
40.352
40.076
39.798
39.520
39.242
38.963
38.684
32.000
28.354
MeO
NH
N
ppm
150
100
50
0

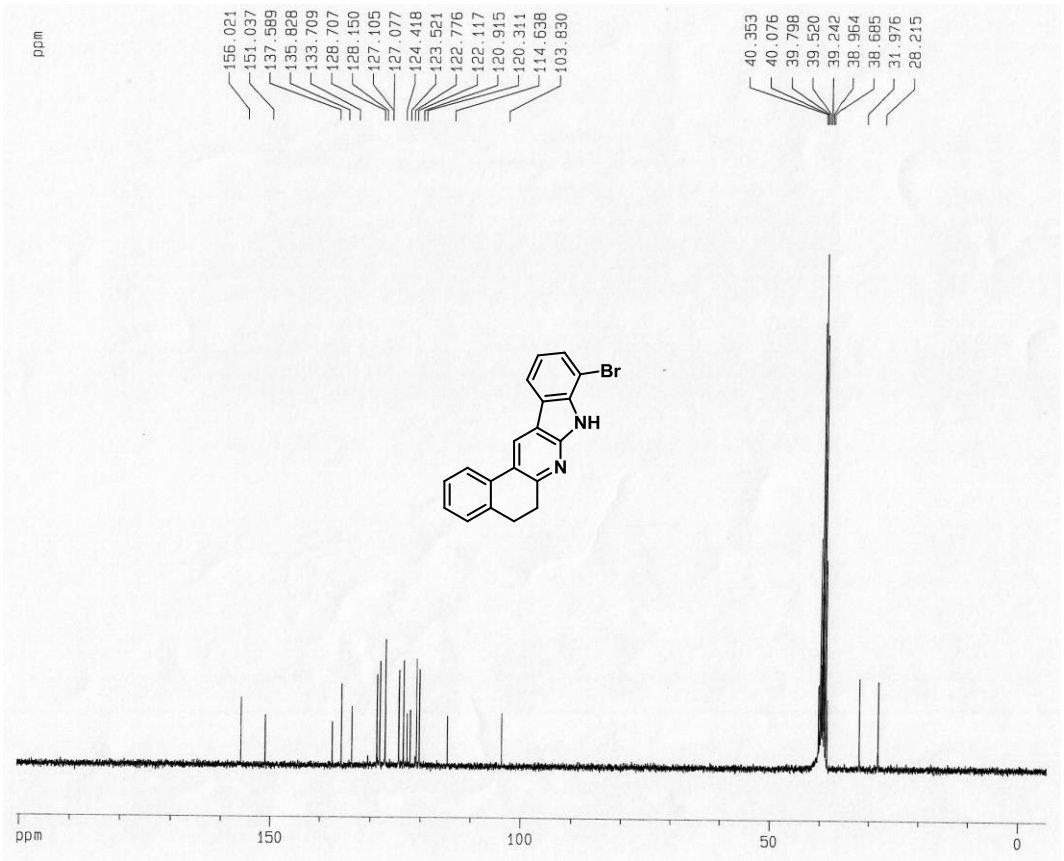

Yan-H-17-268
ppm
11.8531
8.9744
8.2440
8.2252
8.2155
8.1967
7.9841
7.9578
7.3864
7.3606
7.3351
7.3073
7.2584
7.2499
7.2391
7.2248
7.2170
7.1087
7.1017
7.0755
7.0472
3.3202
3.1035
3.0857
3.0737
3.0594
3.0005
2.9854
2.9739
2.9527
2.5068
2.5010
2.4953
-0.0014
F
NH
N
Integral
1.0000
1.0088
1.0155
1.0658
2.0358
1.9855
0.9677
1.9661
1.9629
ppm
12
10
8
6
4
2
0

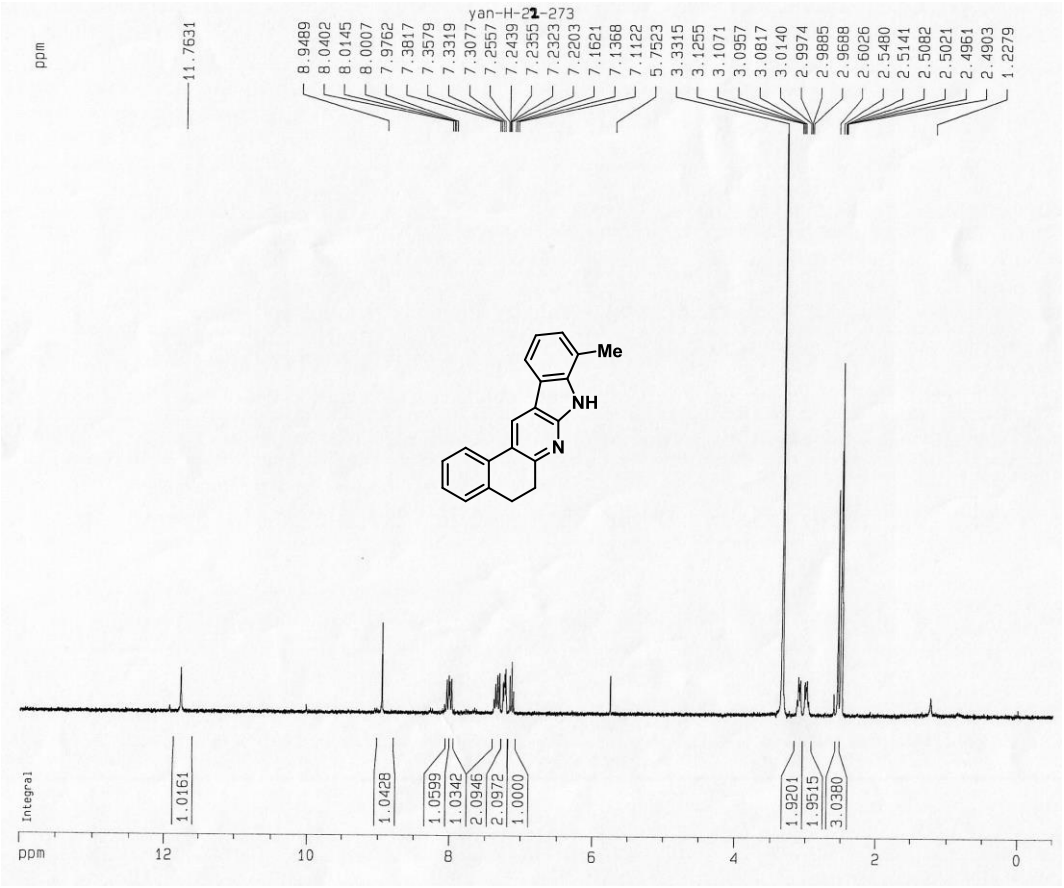

ppm
162.891
159.713
154.614
151.458
139.754
139.583
135.780
133.899
128.118
127.068
126.913
123.560
123.390
122.615
122.478
121.670
117.641
114.109
107.581
107.262
98.039
97.690
40.355
40.076
39.798
39.520
39.242
38.964
38.686
31.872
28.291
F
NH
N
ppm
150
100
50
0

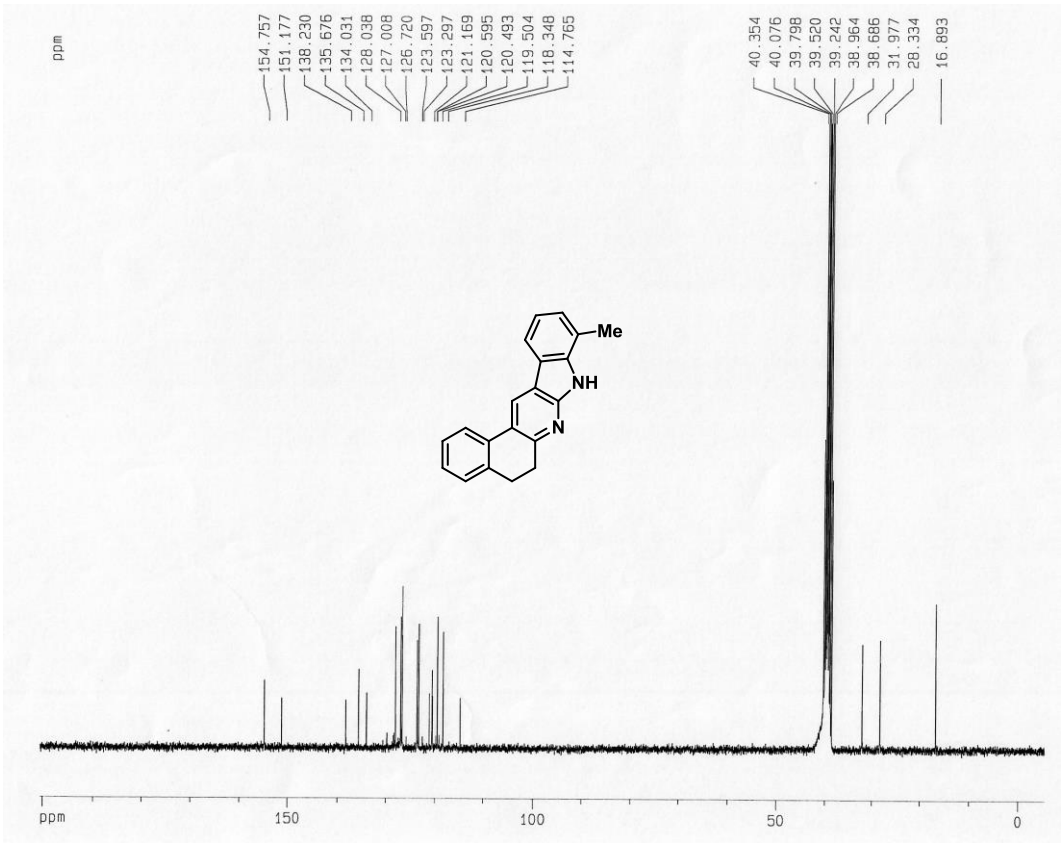

yan-H-10-1
ppm
11.7688
11.6031
9.9478
8.8898
8.2914
8.2658
8.0728
8.0463
7.9741
7.9486
7.3718
7.3493
7.3185
7.2930
7.2718
7.2452
7.2209
7.1967
7.0622
7.0358
3.4270
3.3545
3.3306
3.2691
3.2603
3.0704
3.0576
3.0433
2.9885
2.9724
2.9623
2.9409
2.5223
2.5036
2.4978
2.4919
2.4856
2.4744
2.0789
1.2170
Me
NH
N
Integral
1.0408
1.0421
1.2331
1.1606
4.3067
1.0800
2.0000
2.0332
2.8486
ppm
12
10
8
6
4
2
0

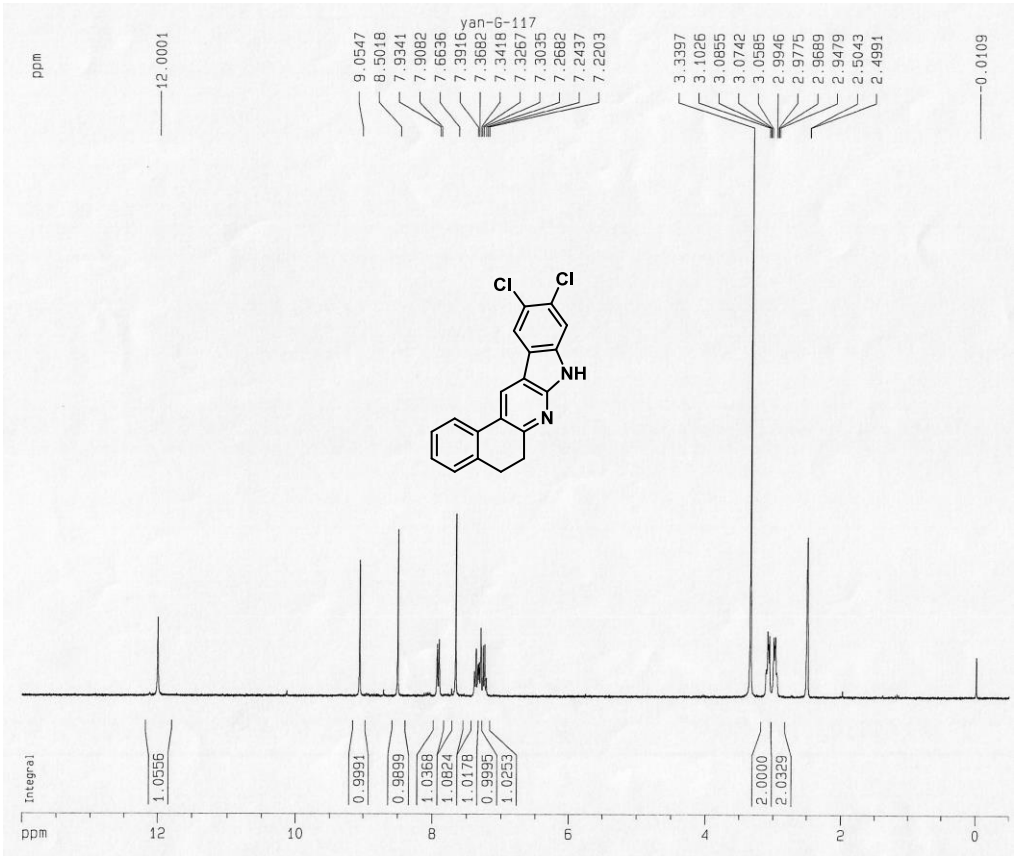

ppm
154.292
151.067
139.409
135.829
135.693
134.097
128.050
127.028
126.688
123.264
123.148
121.078
120.888
120.736
118.580
114.533
111.289
40.355
40.076
39.798
39.520
39.242
38.964
38.685
31.924
28.376
21.719
Me
NH
N
ppm
150
100
50
0

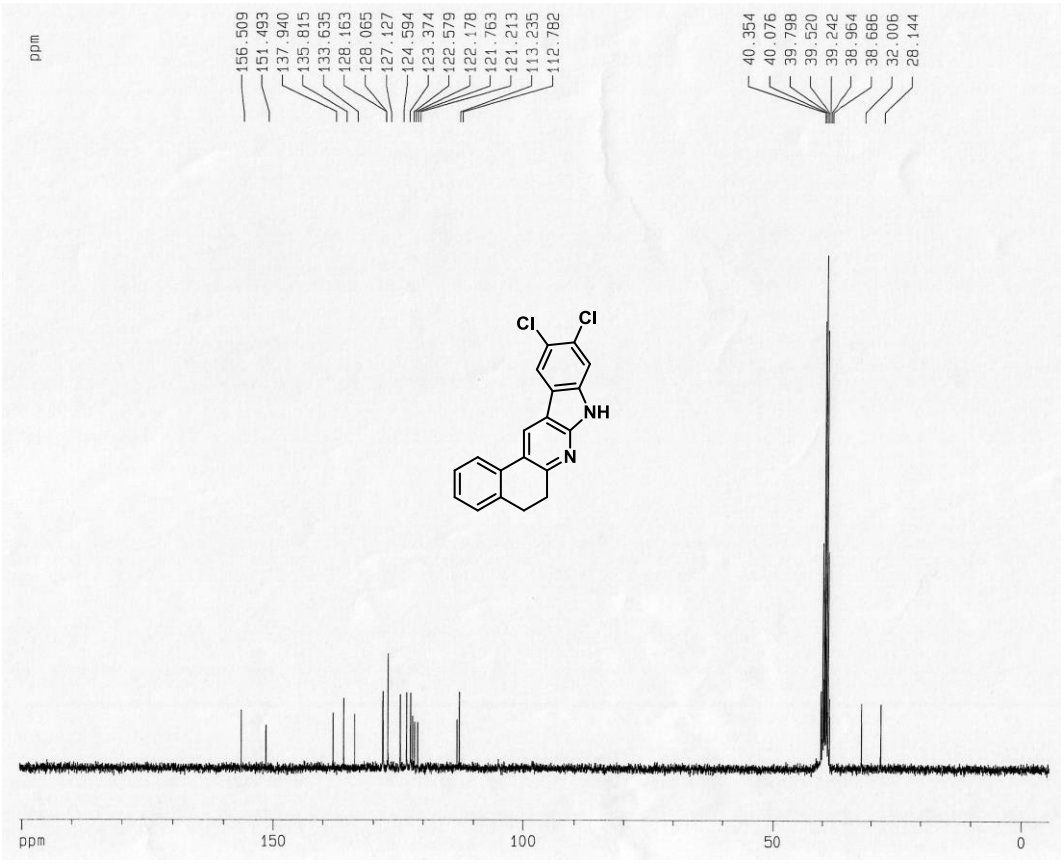

yan-H-21-272
ppm
12.0543
9.0348
8.2513
8.2257
8.0074
7.9831
7.6521
7.6263
7.3920
7.3687
7.3417
7.3147
7.2765
7.2735
7.2522
7.2280
7.2121
7.1862
7.1605
4.0139
3.3392
3.1479
3.1261
3.1148
3.1010
3.0182
3.0043
2.9948
2.9746
2.5134
2.5076
2.5017
2.4957
2.4901
1.9853
1.1944
1.1708
1.1469
Br
NH
N
Integral
1.0000
1.0599
1.0651
1.0943
1.0882
2.1192
1.0373
1.0078
2.0086
1.9940
ppm
12
10
8
6
4
2
0

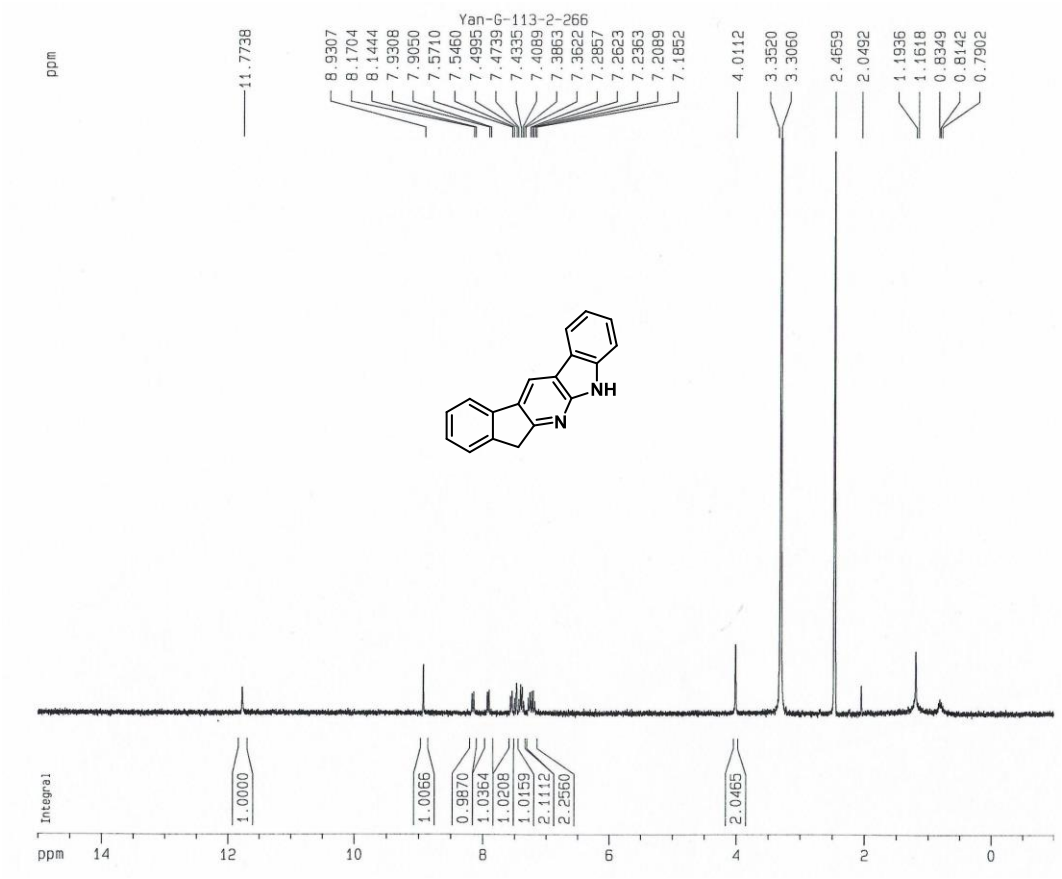

ppm
156.021
151.037
137.589
135.828
133.709
128.707
128.150
127.105
127.077
124.418
123.521
122.776
122.117
120.915
120.311
114.638
103.830
40.353
40.076
39.798
39.520
39.242
38.964
38.685
31.976
28.215
Br
NH
N
ppm
150
100
50
0

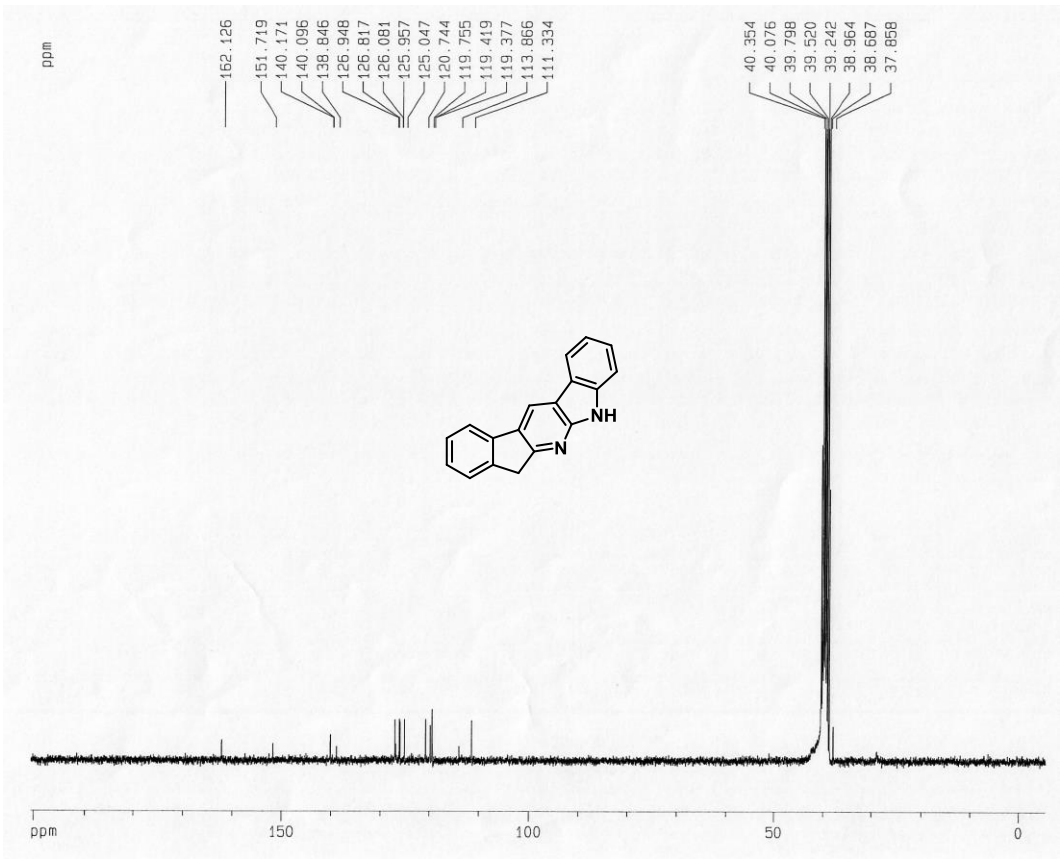

yan-H-21-273
ppm
11.7631
8.9489
8.0402
8.0145
8.0007
7.9762
7.3817
7.3579
7.3319
7.3077
7.2557
7.2439
7.2355
7.2323
7.2203
7.1621
7.1368
7.1122
5.7523
3.3315
3.1255
3.1071
3.0957
3.0817
3.0140
2.9974
2.9885
2.9688
2.6026
2.5480
2.5141
2.5082
2.5021
2.4961
2.4903
1.2279
Me
NH
N
Integral
1.0161
1.0428
1.0599
1.0342
2.0946
2.0972
1.0000
1.9201
1.9515
3.0380
ppm
12
10
8
6
4
2
0

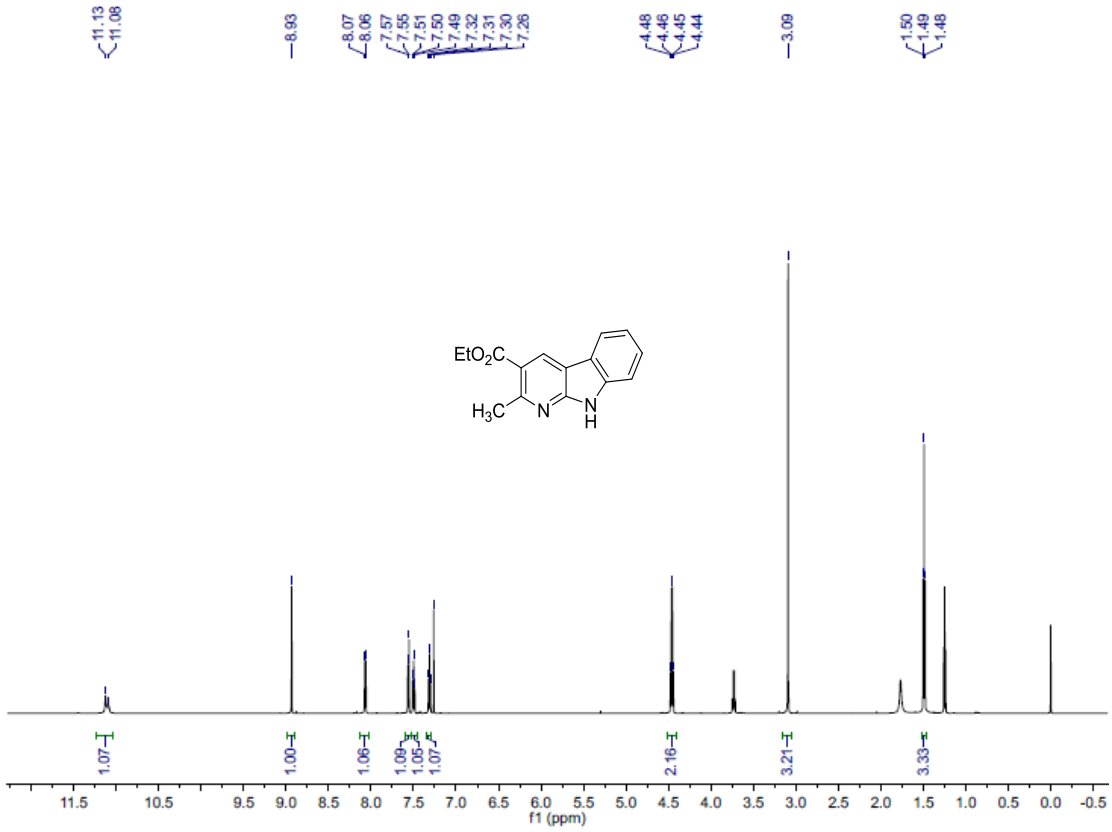

ppm
154.757
151.177
138.230
135.676
134.031
128.038
127.008
126.720
123.597
123.297
121.169
120.595
120.493
119.504
118.348
114.765
40.354
40.076
39.798
39.520
39.242
38.964
38.686
31.977
28.334
16.893
Me
NH
N
ppm
150
100
50
0

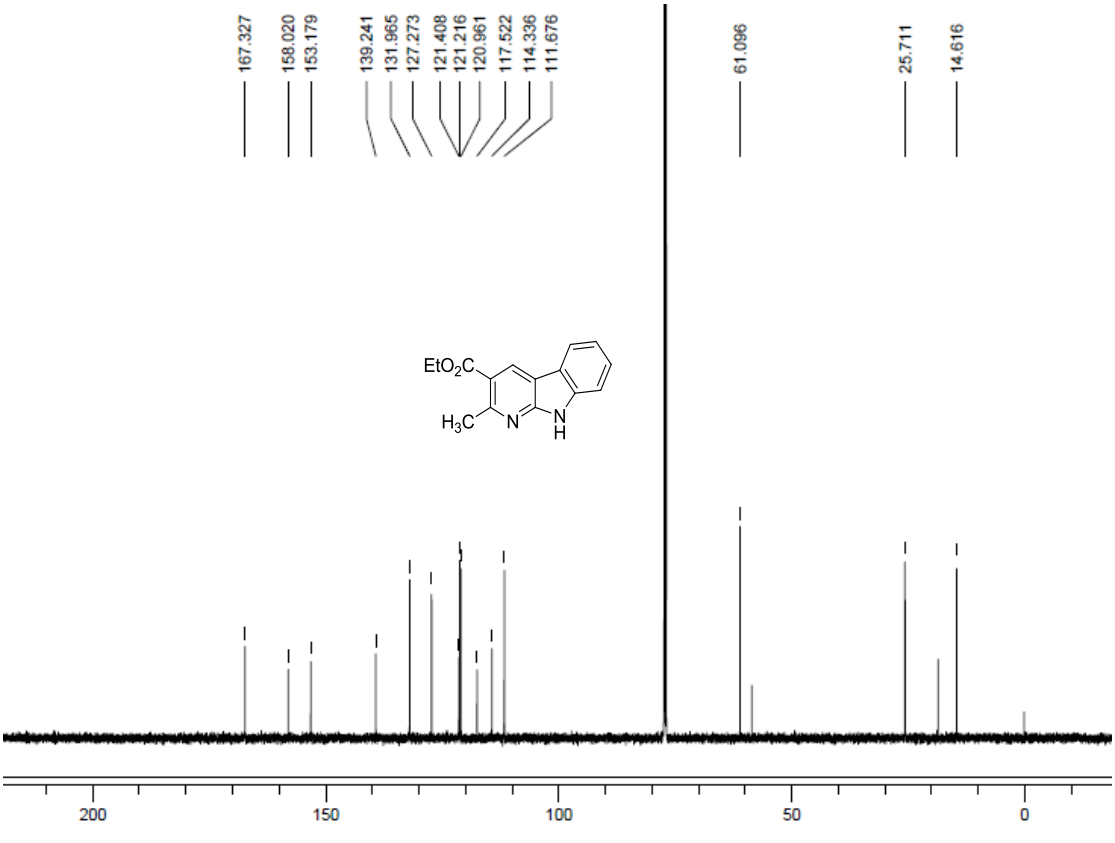

yan-6-117
ppm
12.0001
9.0547
8.5018
7.9341
7.9082
7.6636
7.3916
7.3682
7.3418
7.3267
7.3035
7.2682
7.2437
7.2203
3.3397
3.1026
3.0855
3.0742
3.0585
2.9946
2.9775
2.9689
2.9479
2.5043
2.4991
-0.0109
Cl
Cl
NH
N
Integral
1.0556
0.9991
0.9899
1.0368
1.0824
1.0178
0.9995
1.0253
2.0000
2.0329
ppm
12
10
8
6
4
2
0

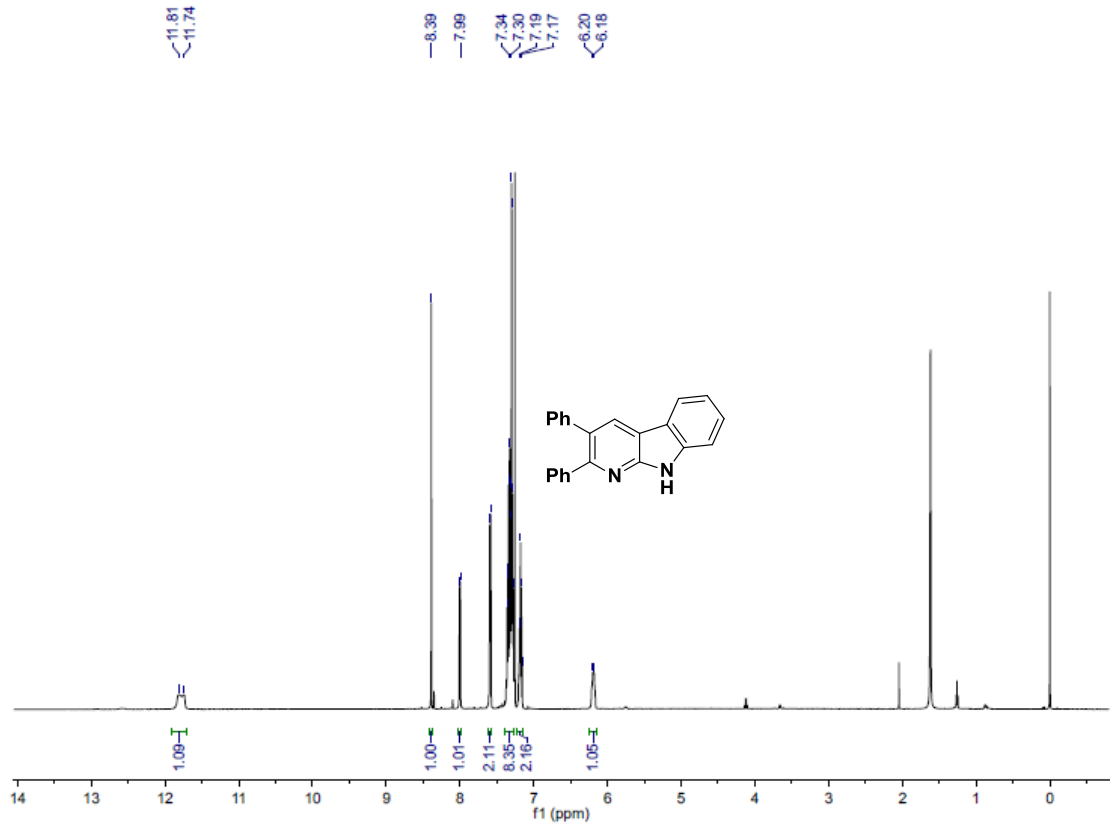

ppm
156.509
151.493
137.940
135.815
133.635
128.163
128.065
127.127
124.594
123.374
122.579
122.178
121.763
121.213
113.235
112.782
40.354
40.076
39.798
39.520
39.242
38.964
38.686
32.006
28.144
Cl
Cl
NH
N
ppm
150
100
50
0

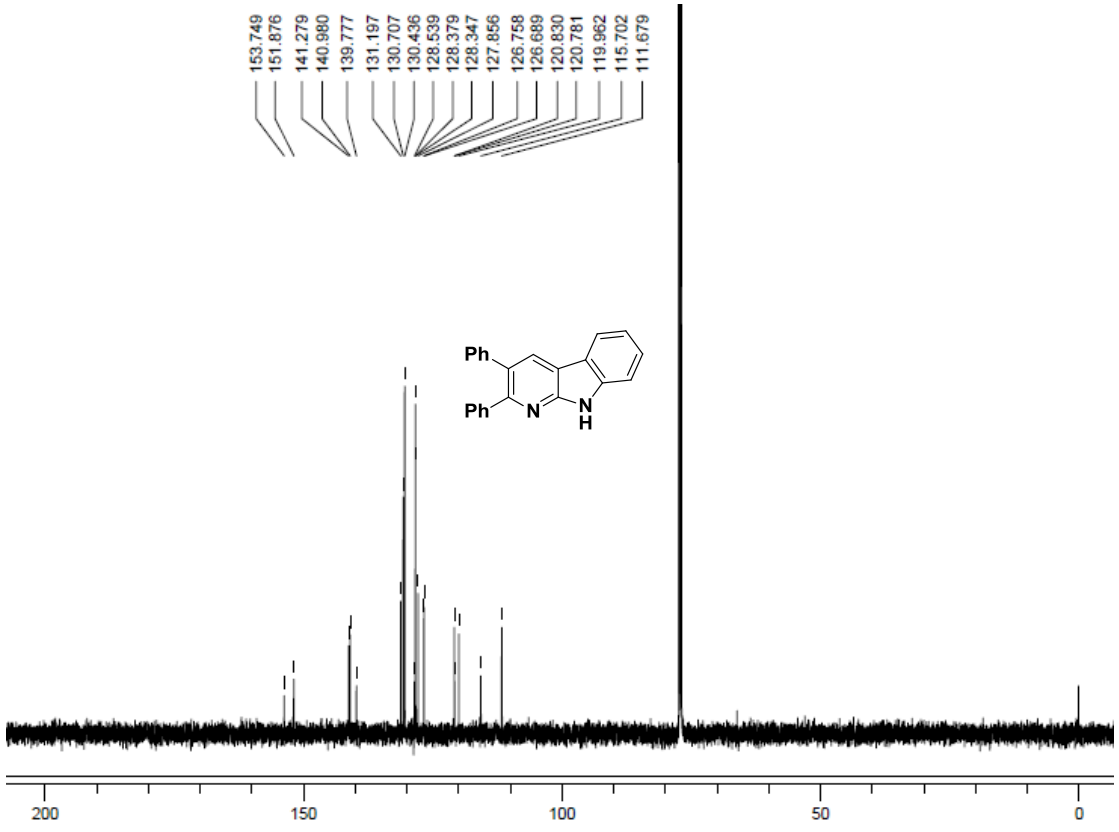

Yan-G-113-2-266
ppm
11.7738
8.9307
8.1704
8.1444
7.9308
7.9050
7.5710
7.5460
7.4995
7.4739
7.4335
7.4089
7.3863
7.3622
7.2857
7.2623
7.2363
7.2089
7.1852
4.0112
3.3520
3.3060
2.4659
2.0492
1.1936
1.1618
0.8349
0.8142
0.7902
NH
N
Integral
1.0000
1.0066
0.9870
1.0364
1.0208
1.0159
2.1112
2.2560
2.0465
ppm
14
12
10
8
6
4
2
0

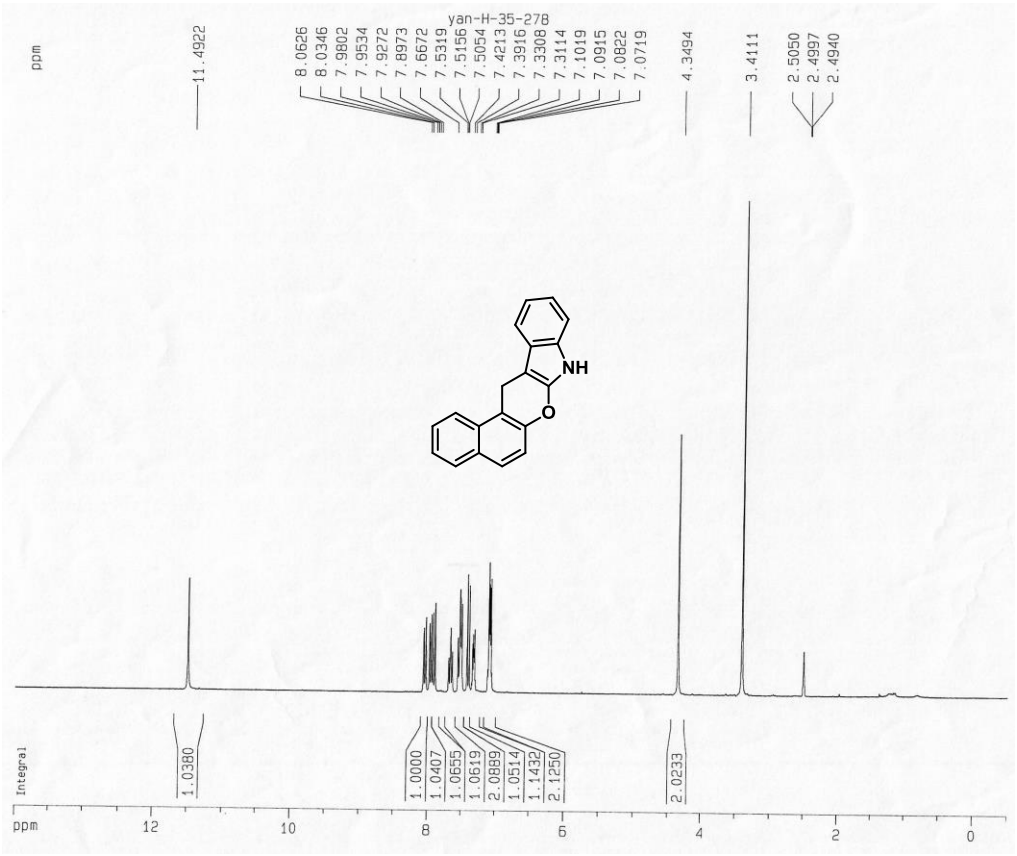

ppm
162.126
151.719
140.171
140.096
138.846
126.948
126.817
126.081
125.957
125.047
120.744
119.755
119.419
119.377
113.866
111.334
40.354
40.076
39.798
39.520
39.242
38.964
38.687
37.858
NH
N
ppm
150
100
50
0

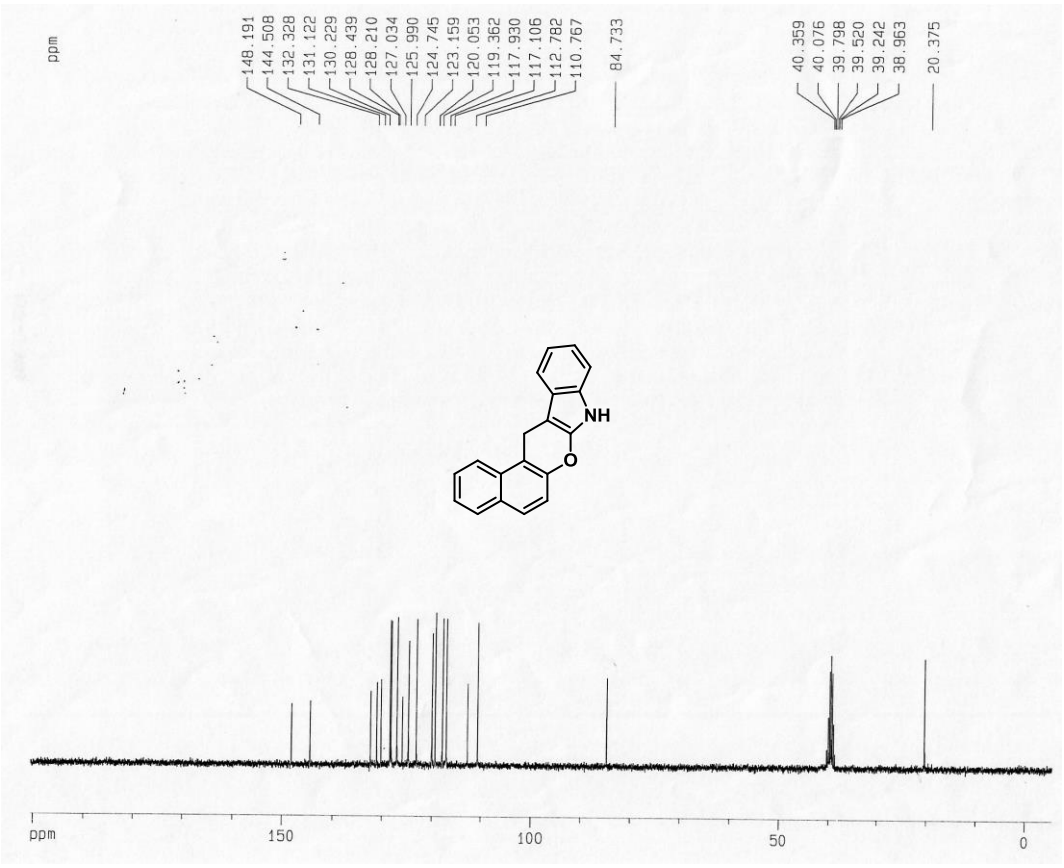

11.13
11.08
8.93
8.07
8.06
7.57
7.55
7.51
7.50
7.49
7.32
7.31
7.30
7.26
4.48
4.46
4.45
4.44
3.09
1.50
1.49
1.48
EtO2C
H3C
N
H
1.07
1.00
1.06
1.09
1.05
1.07
2.16
3.21
3.33
f1 (ppm)

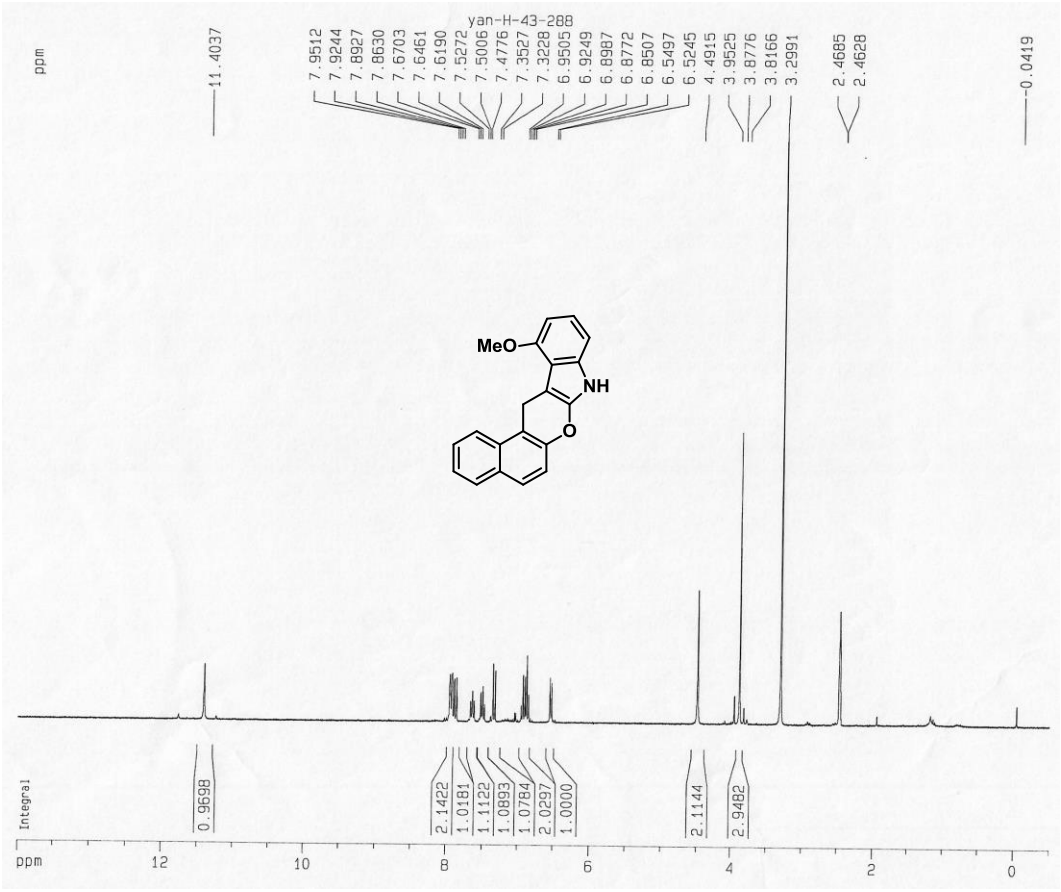

167.327
158.020
153.179
139.241
131.965
127.273
121.408
121.216
120.961
117.522
114.336
111.676
61.096
25.711
14.616
EtO2C
H3C
N
H
200
150
100
50
0

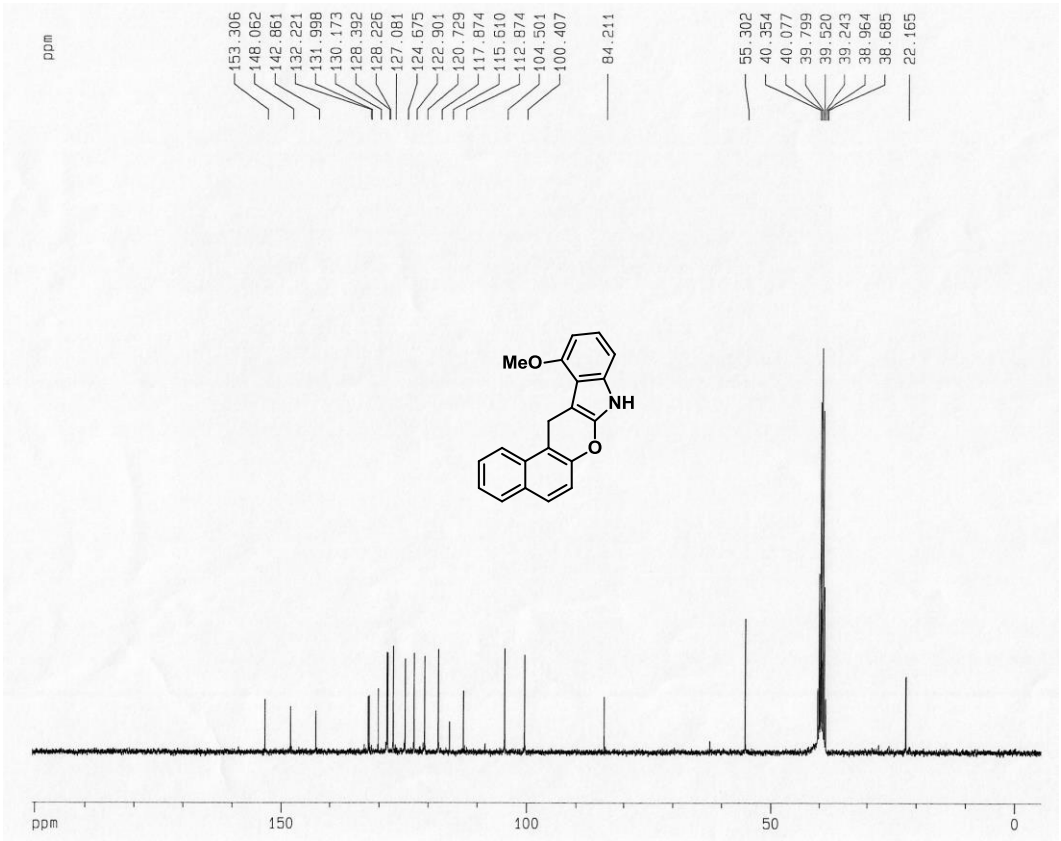

11.81
11.74
8.39
7.99
7.34
7.30
7.19
7.17
6.20
6.18
Ph
Ph
N
H
1.09
1.00
1.01
2.11
8.35
2.16
1.05
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0
f1 (ppm)

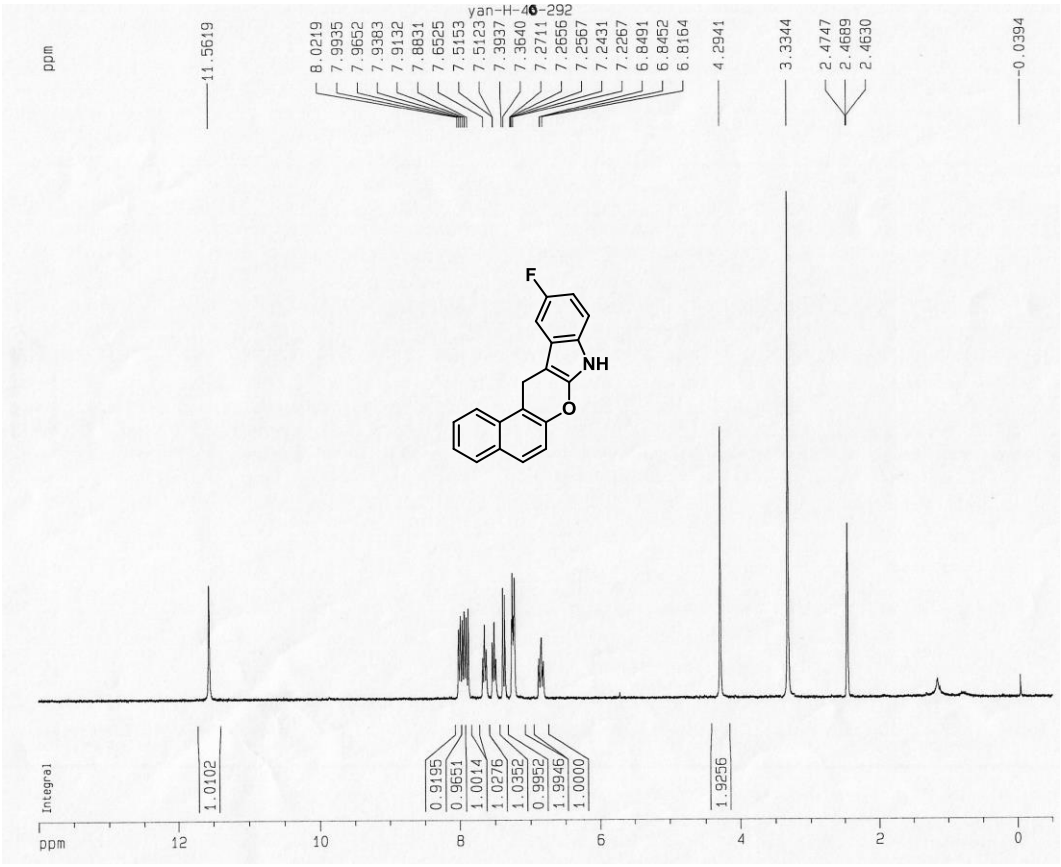

153.749
151.876
141.279
140.980
139.777
131.197
130.707
130.436
128.539
128.379
128.347
127.856
126.758
126.689
120.830
120.781
119.962
115.702
111.679
Ph
Ph
N
H
200 150 100 50 0

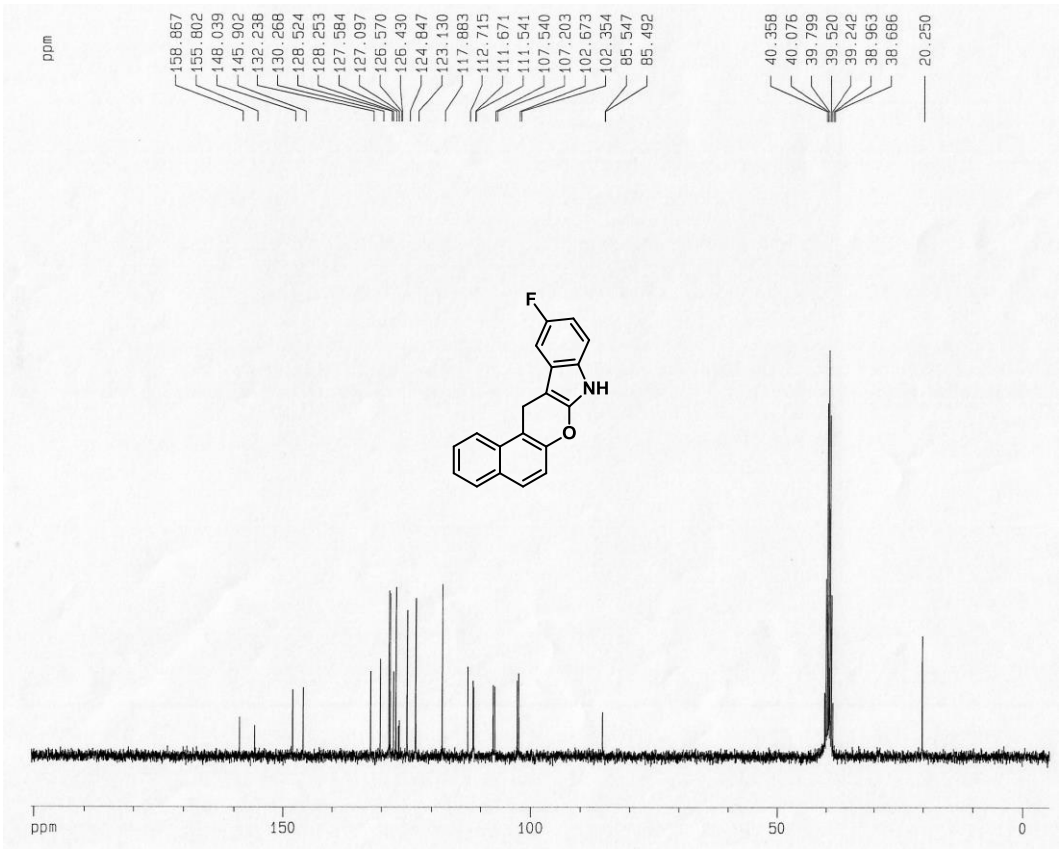

yan-H-35-278
ppm
11.4922
8.0626
8.0346
7.9802
7.9534
7.9272
7.8973
7.6672
7.5319
7.5156
7.5054
7.4213
7.3916
7.3308
7.3114
7.1019
7.0915
7.0822
7.0719
4.3494
3.4111
2.5050
2.4997
2.4940
NH
O
Integral
1.0380
1.0000
1.0407
1.0655
1.0619
2.0889
1.0514
1.1432
2.1250
2.0233
ppm
12
10
8
6
4
2
0

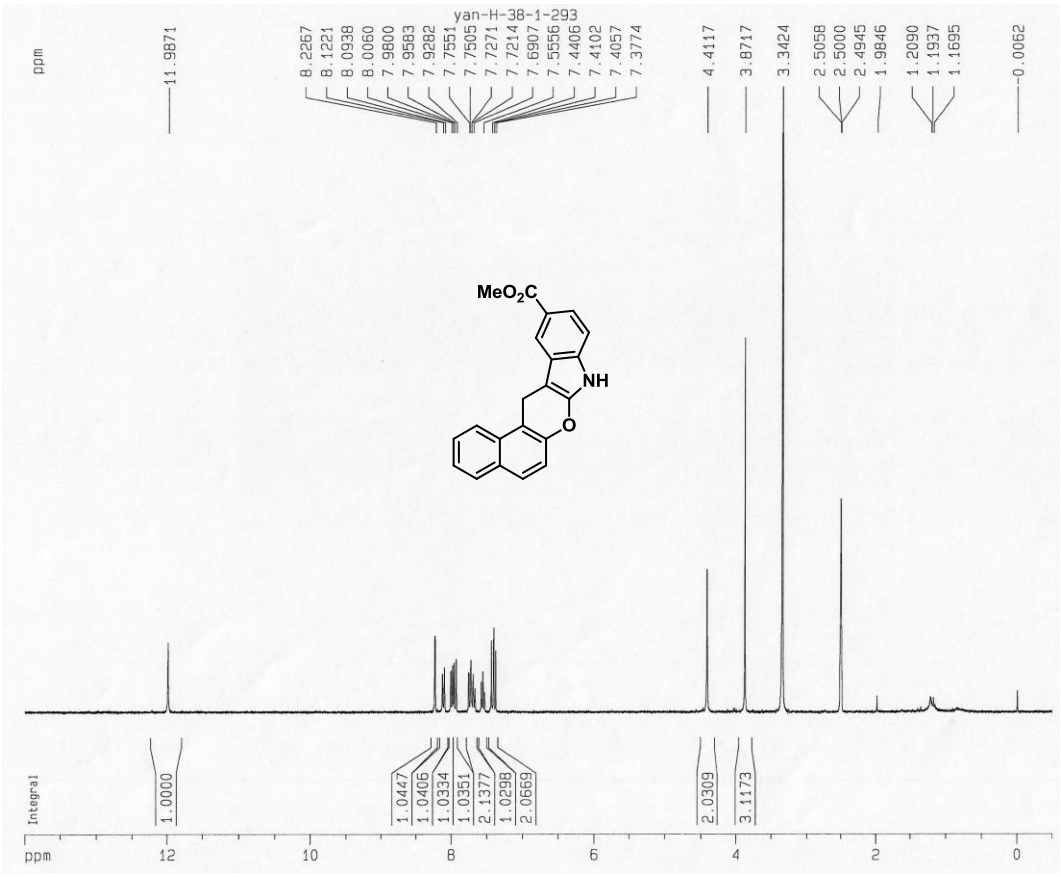

ppm
148.191
144.508
132.328
131.122
130.229
128.439
128.210
127.034
125.990
124.745
123.159
120.053
119.362
117.930
117.106
112.782
110.767
84.733
40.359
40.076
39.798
39.520
39.242
38.963
20.375
NH
O
ppm
150
100
50
0

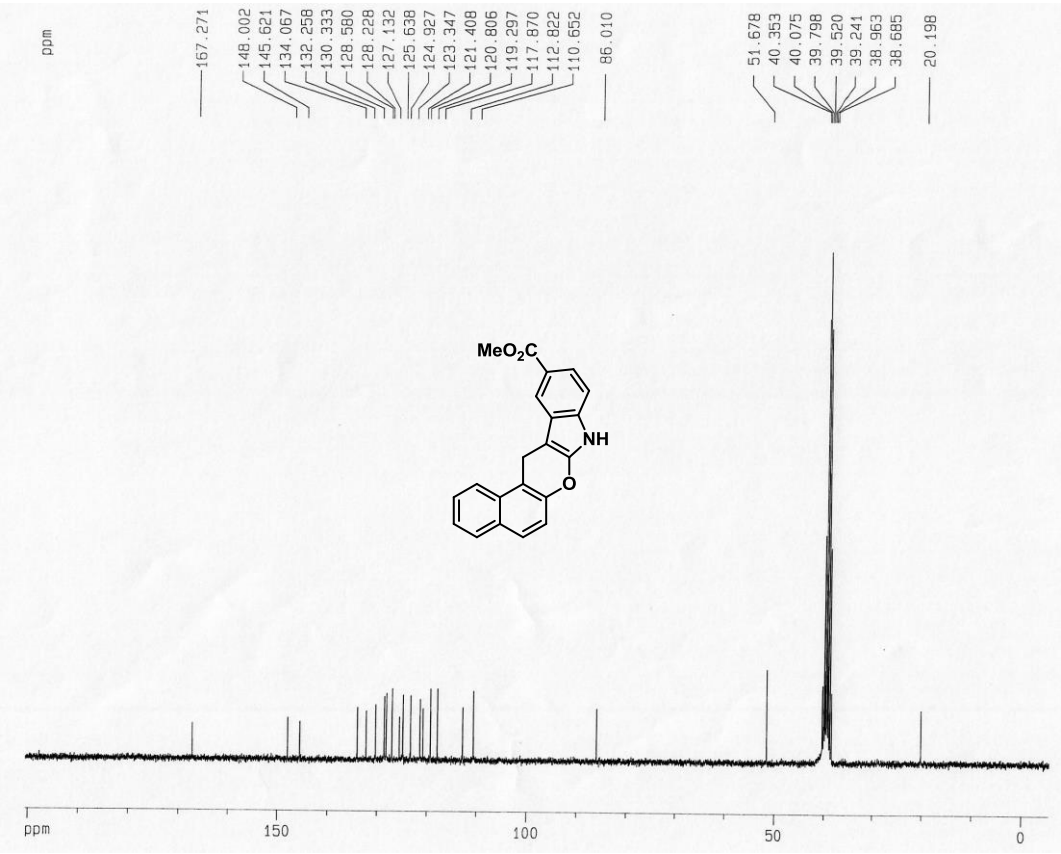

yan-H-43-288
ppm
11.4037
7.9512
7.9244
7.8927
7.8630
7.6703
7.6461
7.6190
7.5272
7.5006
7.4776
7.3527
7.3228
6.9505
6.9249
6.8987
6.8772
6.8507
6.5497
6.5245
4.4915
3.9525
3.8776
3.8166
3.2991
2.4685
2.4628
-0.0419
MeO
NH
O
Integral
0.9698
2.1422
1.0181
1.1122
1.0893
1.0784
2.0297
1.0000
2.1144
2.9482
ppm
12
10
8
6
4
2
0

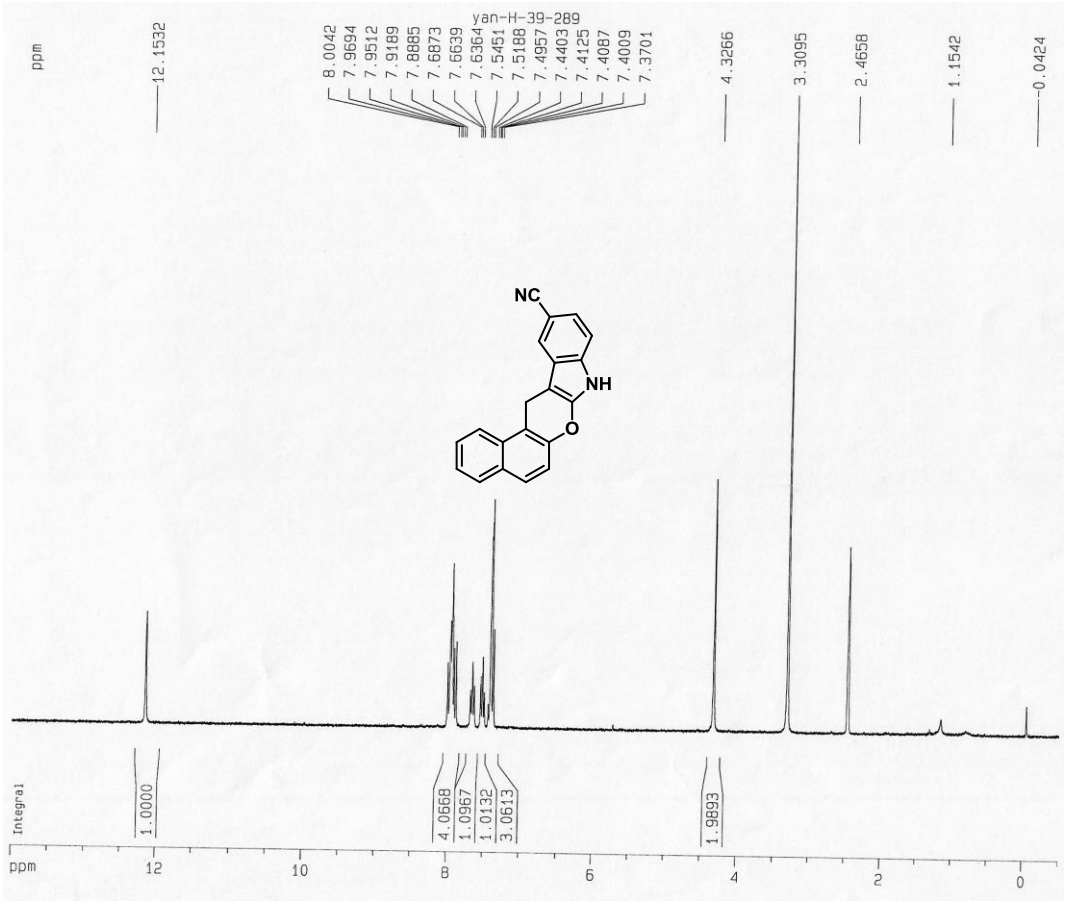

ppm
153.306
148.062
142.861
132.221
131.998
130.173
128.392
128.226
127.081
124.675
122.901
120.729
117.874
115.610
112.874
104.501
100.407
84.211
55.302
40.354
40.077
39.799
39.520
39.243
38.964
38.685
22.165
MeO
NH
O
ppm
150
100
50
0

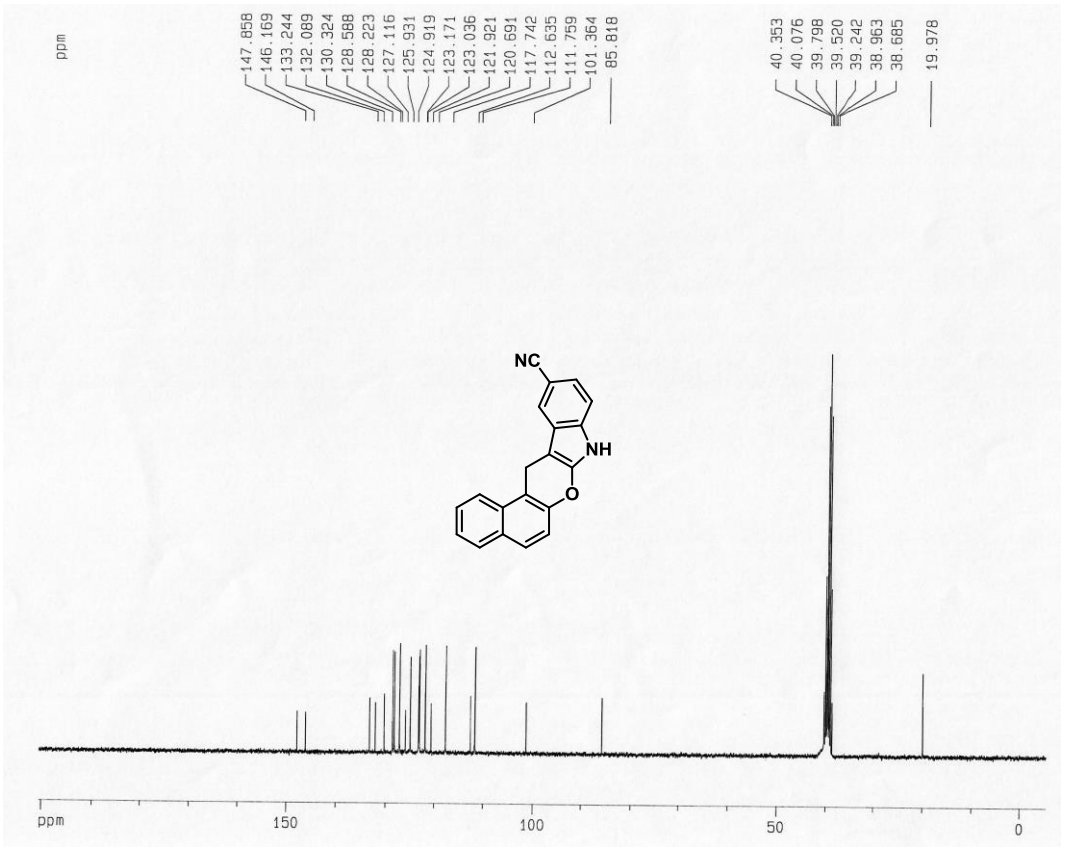

yan-H-40-292
ppm
11.5619
8.0219
7.9935
7.9652
7.9383
7.9132
7.8831
7.6525
7.5153
7.5123
7.3937
7.3640
7.2711
7.2656
7.2567
7.2431
7.2267
6.8491
6.8452
6.8164
4.2941
3.3344
2.4747
2.4689
2.4630
0.0394
F
NH
O
Integral
1.0102
0.9195
0.9651
1.0014
1.0276
1.0352
0.9952
1.9946
1.0000
1.9256
ppm
12
10
8
6
4
2
0

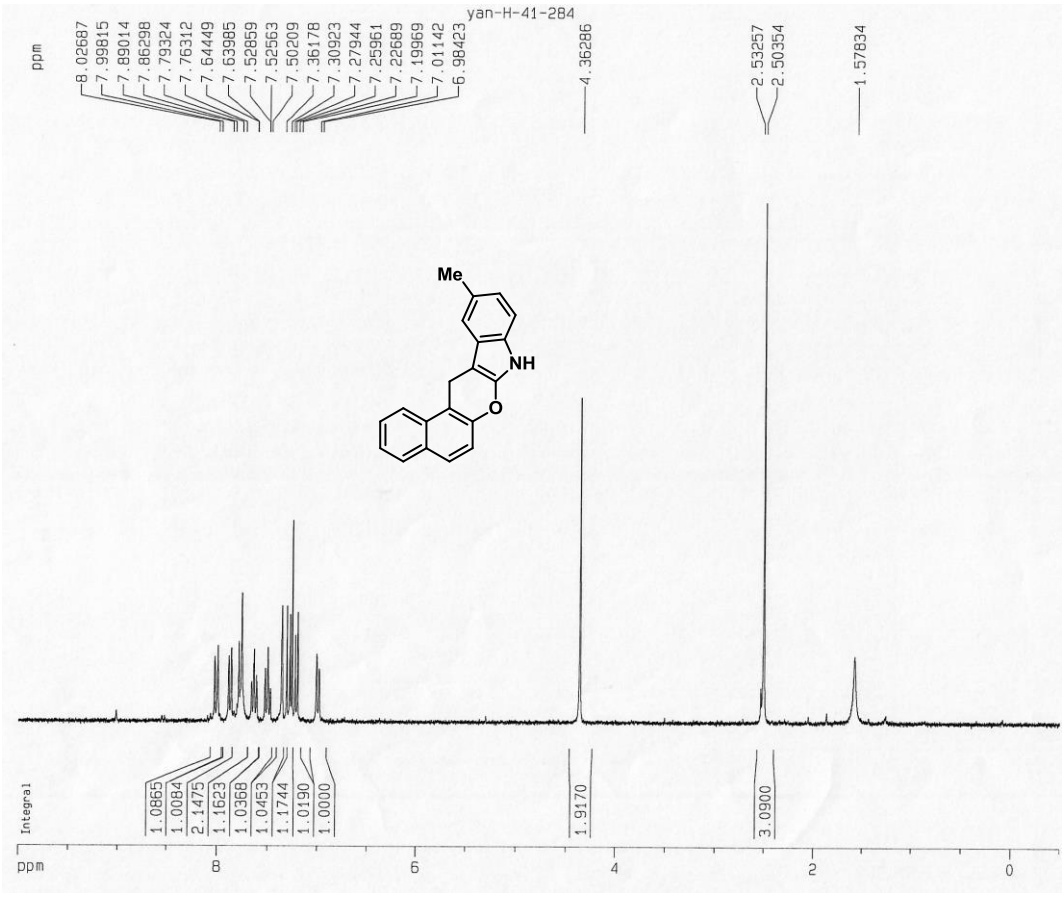

ppm
158.867
155.802
148.039
145.902
132.238
130.268
128.524
128.253
127.584
127.097
126.570
126.430
124.847
123.130
117.883
112.715
111.671
111.541
107.540
107.203
102.673
102.354
85.547
85.492
40.358
40.076
39.799
39.520
39.242
38.963
38.686
20.250
F
NH
O
ppm
150
100
50
0

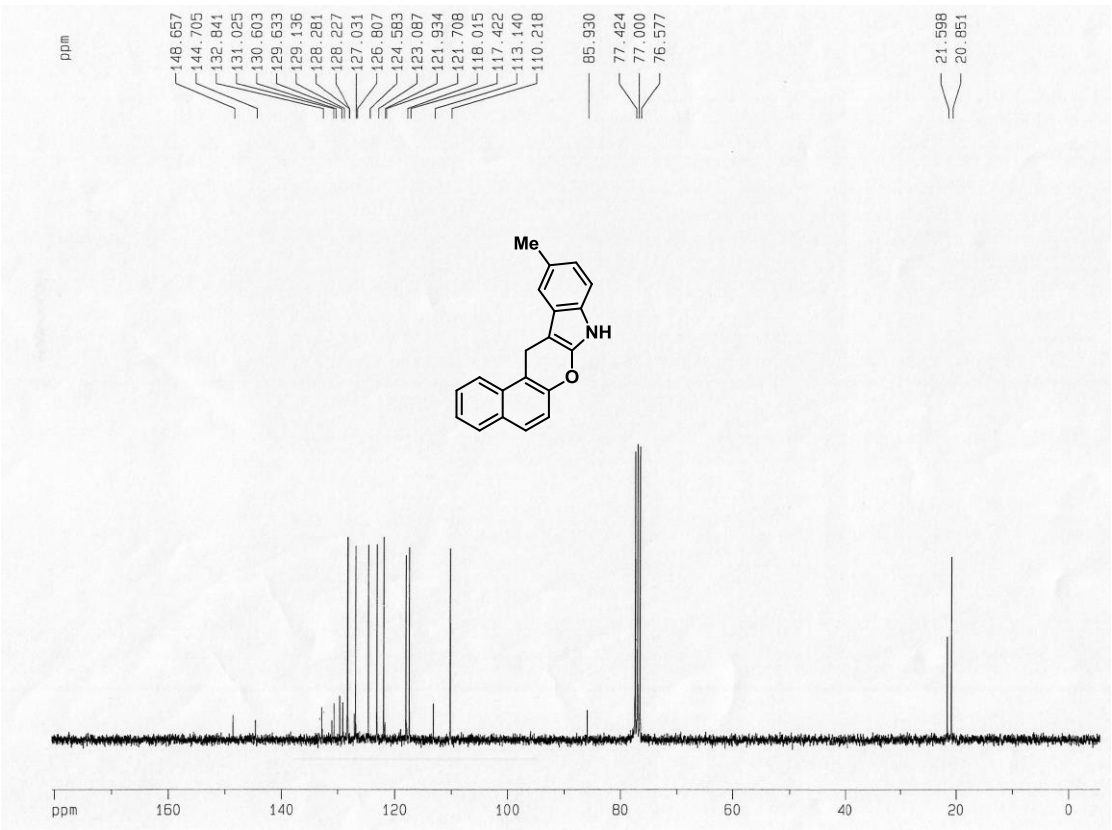

yan-H-38-1-293
ppm
11.9871
8.2267
8.1221
8.0938
8.0060
7.9800
7.9583
7.9282
7.7551
7.7505
7.7271
7.7214
7.6907
7.5556
7.4406
7.4102
7.4057
7.3774
4.4117
3.8717
3.3424
2.5058
2.5000
2.4945
1.9846
1.2090
1.1937
1.1695
0.0062
MeO2C
NH
O
Integral
1.0000
1.0447
1.0406
1.0334
1.0351
2.1377
1.0298
2.0669
2.0309
3.1173
ppm
12
10
8
6
4
2
0

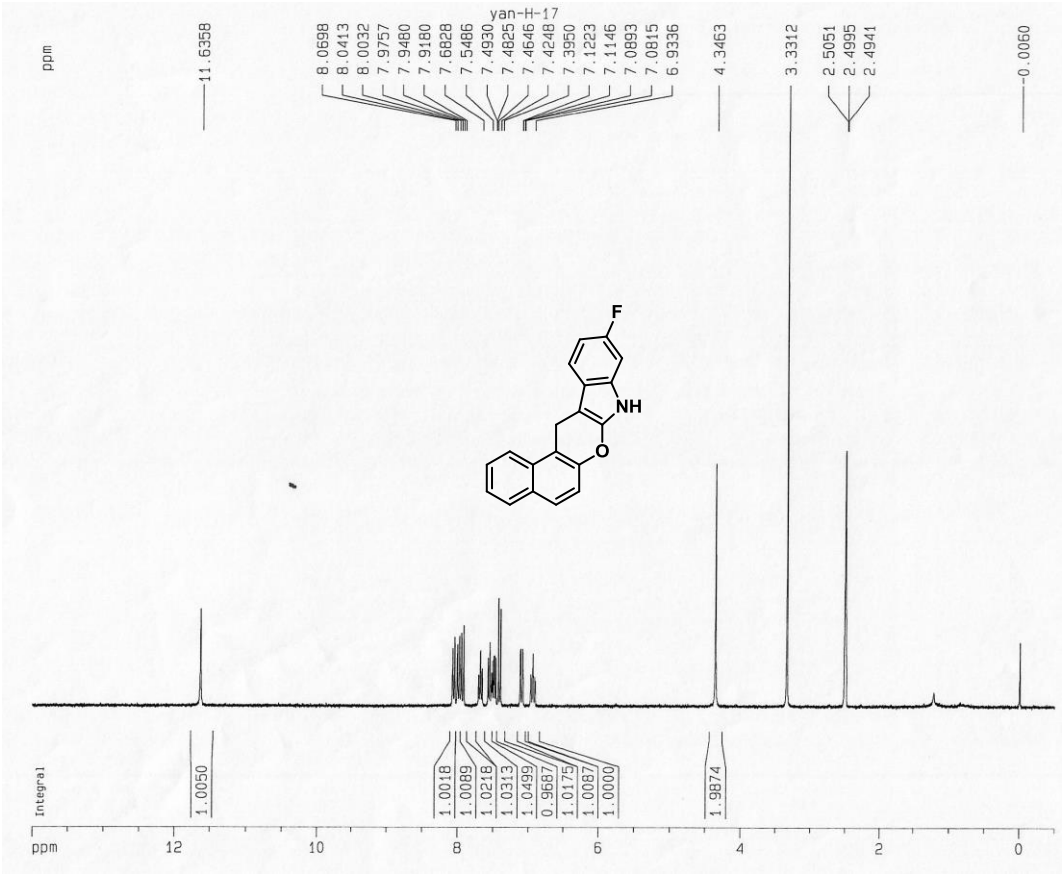

ppm
167.271
148.002
145.621
134.067
132.258
130.333
128.580
128.228
127.132
125.638
124.927
123.347
121.408
120.806
119.297
117.870
112.822
110.652
86.010
51.678
40.353
40.075
39.798
39.520
39.241
38.963
38.685
20.198
MeO2C
NH
O
ppm
150
100
50
0

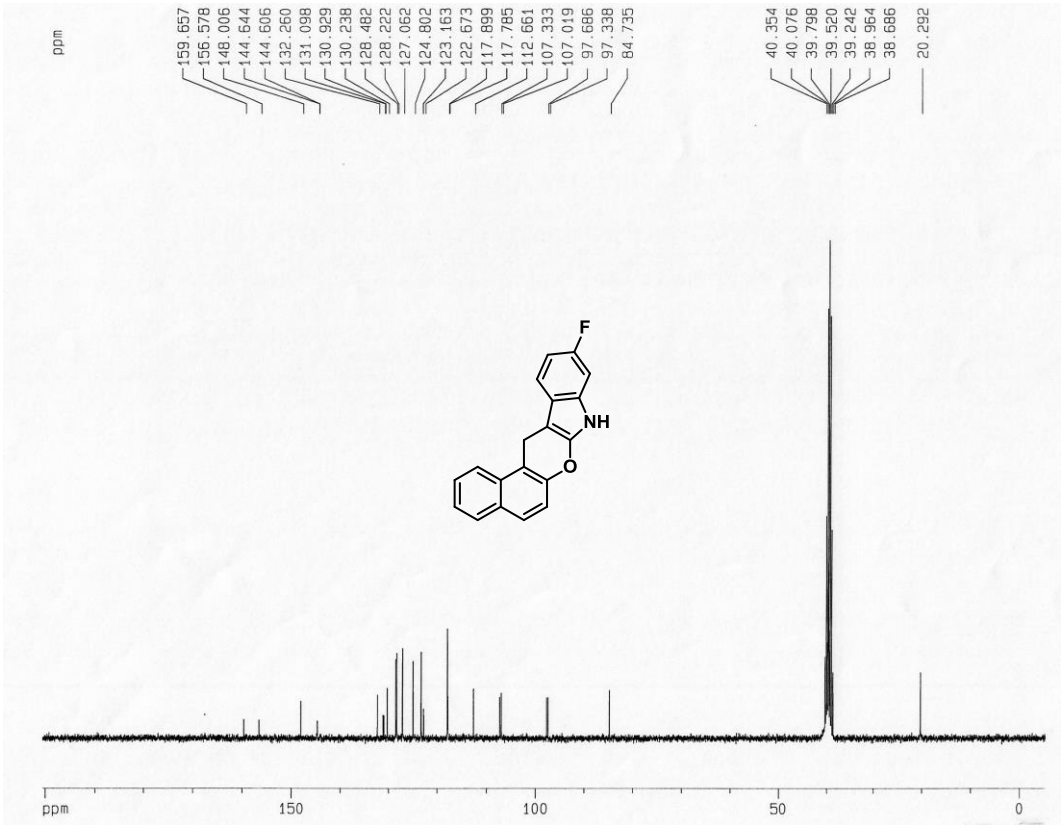

yan-H-39-289
ppm
12.1532
8.0042
7.9694
7.9512
7.9189
7.8885
7.6873
7.6639
7.6364
7.5451
7.5188
7.4957
7.4403
7.4125
7.4087
7.4009
7.3701
4.3266
3.3095
2.4658
1.1542
0.0424
NC
NH
O
Integral
1.0000
4.0668
1.0967
1.0132
3.0613
1.9893
ppm
12
10
8
6
4
2
0

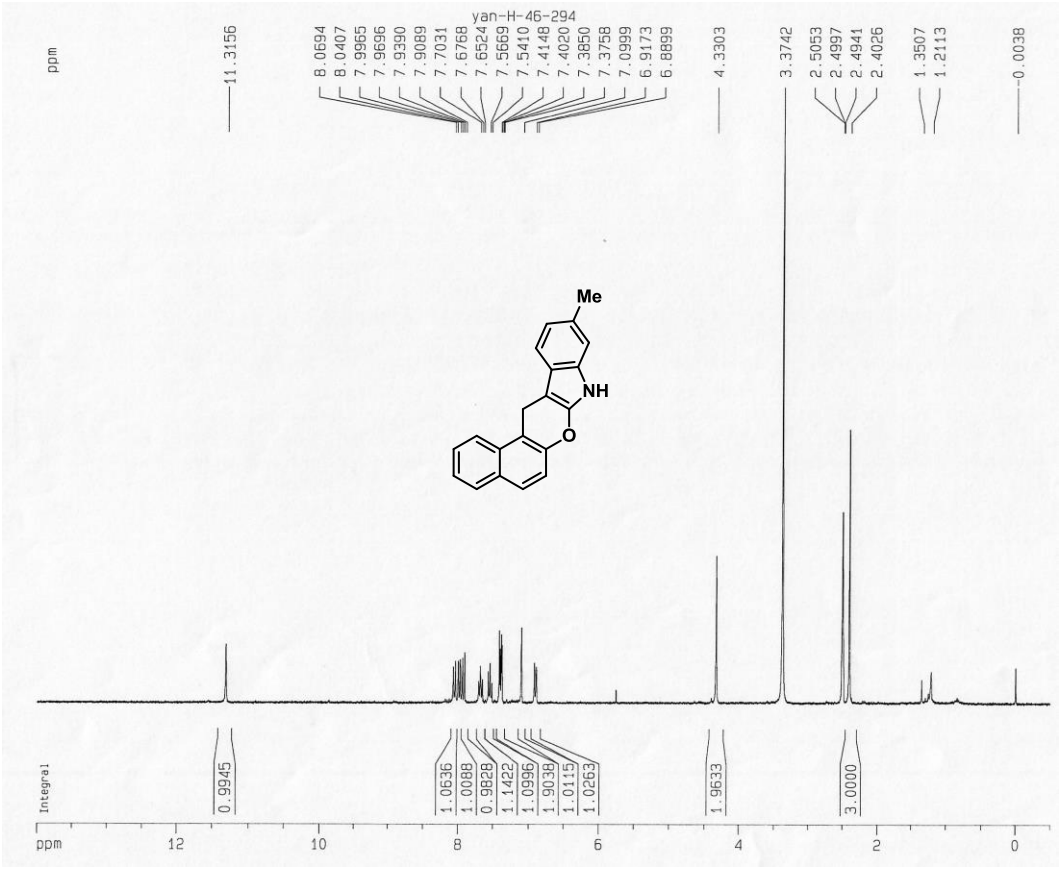

ppm
147.858
146.169
133.244
132.089
130.324
128.588
128.223
127.116
125.931
124.919
123.171
123.036
121.921
120.691
117.742
112.635
111.759
101.364
85.818
40.353
40.076
39.798
39.520
39.242
38.963
38.685
19.978
NC
NH
O
ppm
150
100
50
0

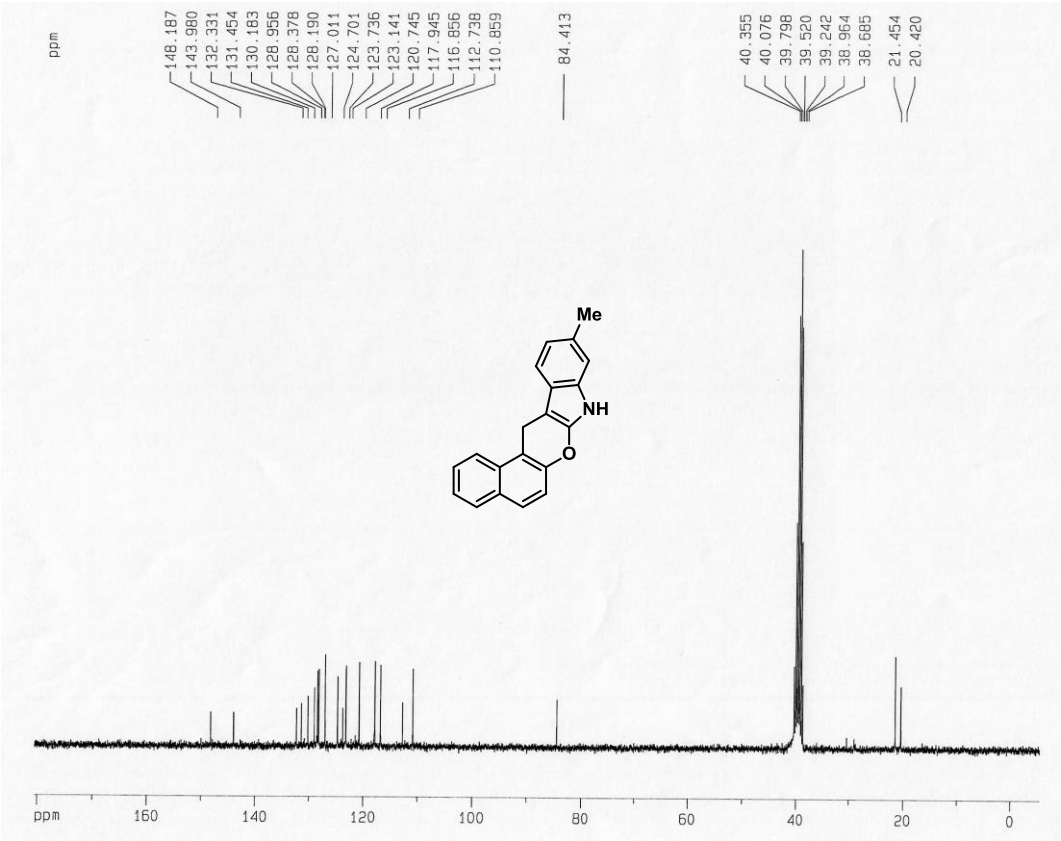

yan-H-41-284
ppm
8.02687
7.99815
7.89014
7.86298
7.79324
7.76312
7.64449
7.63985
7.52859
7.52563
7.50209
7.36178
7.30923
7.27944
7.25961
7.22689
7.19969
7.01142
6.98423
4.36286
2.53257
2.50354
1.57834
Me
NH
O
Integral
1.0865
1.0084
2.1475
1.1623
1.0368
1.0453
1.1744
1.0190
1.0000
1.9170
3.0900
ppm
8
6
4
2
0

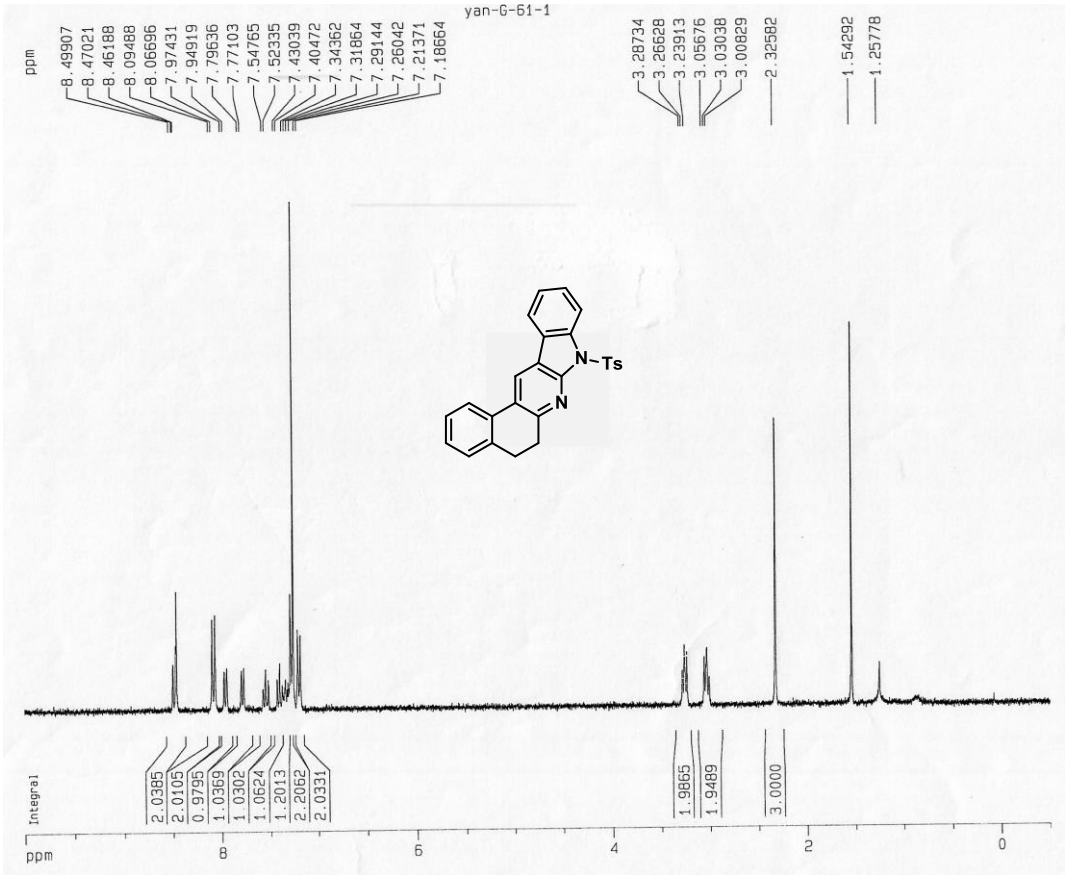

ppm
148.657
144.705
132.841
131.025
130.603
129.633
129.136
128.281
128.227
127.031
126.807
124.583
123.087
121.934
121.708
118.015
117.422
113.140
110.218
85.930
77.424
77.000
76.577
21.598
20.851
Me
NH
O
ppm
160
140
120
100
80
60
40
20
0

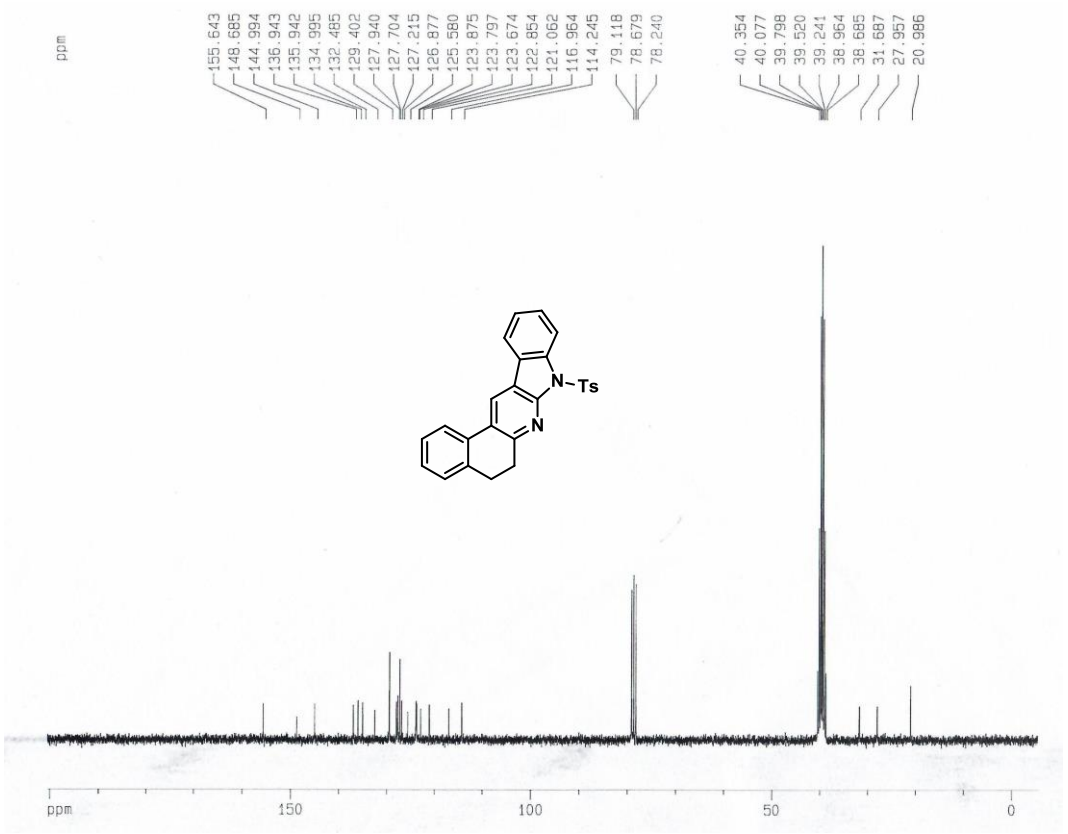

yan-H-17
ppm
11.6358
8.0698
8.0413
8.0032
7.9757
7.9480
7.9180
7.6828
7.5486
7.4930
7.4825
7.4646
7.4248
7.3950
7.1223
7.1146
7.0893
7.0815
6.9336
4.3463
3.3312
2.5051
2.4995
2.4941
-0.0060
F
NH
O
integral
1.0050
1.0018
1.0089
1.0218
1.0313
1.0499
0.9687
1.0175
1.0087
1.0000
1.9874
ppm
12
10
8
6
4
2
0

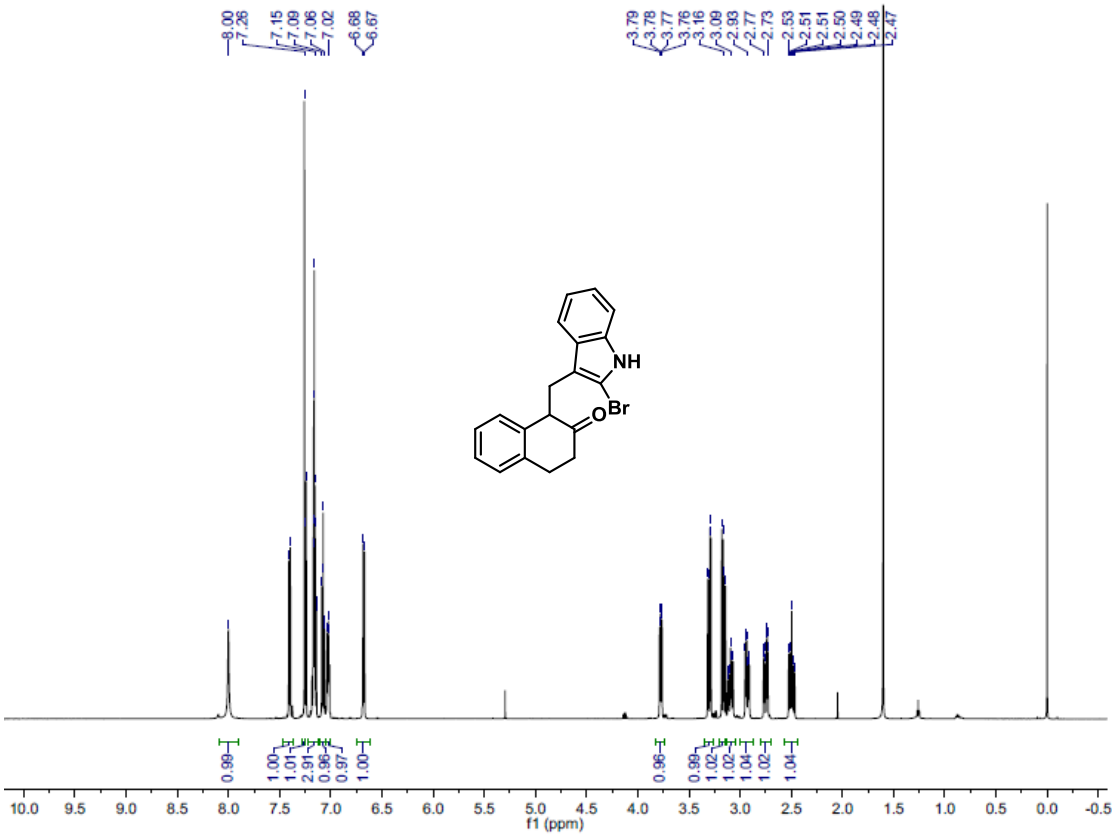

ppm
159.657
156.578
148.006
144.644
144.606
132.260
131.098
130.929
130.238
128.482
128.222
127.062
124.802
123.163
122.673
117.899
117.785
112.661
107.333
107.019
97.686
97.338
84.735
40.354
40.076
39.798
39.520
39.242
38.964
38.686
20.292
F
NH
O
ppm
150
100
50
0

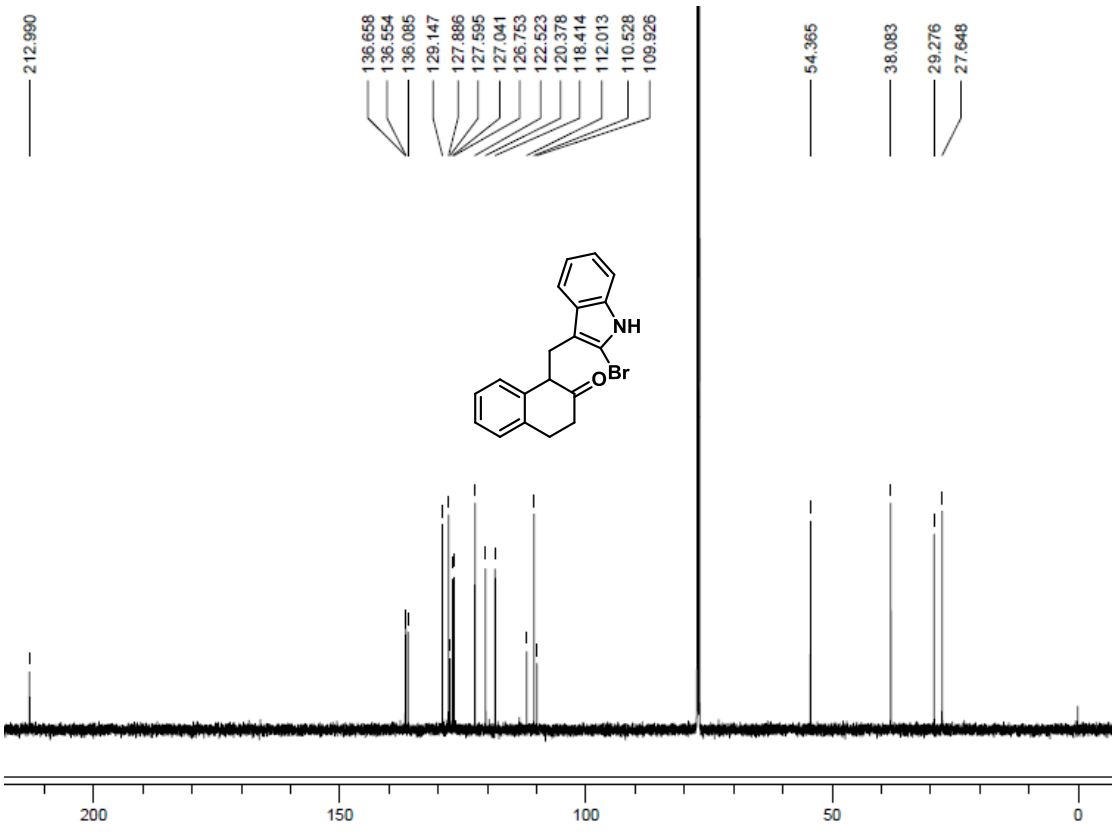

yan-H-46-294
ppm
11.3156
8.0694
8.0407
7.9965
7.9696
7.9390
7.9089
7.7031
7.6768
7.6524
7.5669
7.5410
7.4148
7.4020
7.3850
7.3758
7.0999
6.9173
6.8899
4.3303
3.3742
2.5053
2.4997
2.4941
2.4026
1.3507
1.2113
0.0038
Me
NH
O
Integral
0.9945
1.0636
1.0088
0.9828
1.1422
1.0996
1.9038
1.0115
1.0263
1.9633
3.0000
ppm
12
10
8
6
4
2
0


ppm
148.187
143.980
132.331
131.454
130.183
128.956
128.378
128.190
127.011
124.701
123.736
123.141
120.745
117.945
116.856
112.738
110.859
84.413
40.355
40.076
39.798
39.520
39.242
38.964
38.685
21.454
20.420
Me
NH
O
ppm
160
140
120
100
80
60
40
20
0


yan-G-61-1
ppm
8.49907
8.47021
8.46188
8.09488
8.06696
7.97431
7.94919
7.79636
7.77103
7.54765
7.52335
7.43039
7.40472
7.34362
7.31864
7.29144
7.26042
7.21371
7.18664
3.28734
3.26628
3.23913
3.05676
3.03038
3.00829
2.32582
1.54292
1.25778
N-Ts
N
Integral
2.0385
2.0105
0.9795
1.0369
1.0302
1.0624
1.2013
2.2062
2.0331
1.9865
1.9489
3.0000
ppm
8
6
4
2
0


ppm
155.643
148.685
144.994
136.943
135.942
134.995
132.485
129.402
127.940
127.704
127.215
126.877
125.580
123.875
123.797
123.674
122.854
121.062
116.964
114.245
79.118
78.679
78.240
40.354
40.077
39.798
39.520
39.241
38.964
38.685
31.687
27.957
20.986
N-Ts
N
ppm
150
100
50
0


8.00
7.26
7.15
7.09
7.06
7.02
6.68
6.67
3.79
3.78
3.77
3.76
3.16
3.08
2.93
2.77
2.73
2.53
2.51
2.51
2.50
2.49
2.48
2.47
NH
O
Br
0.99
1.00
1.01
2.91
0.96
0.97
1.00
0.96
0.99
1.02
1.02
1.04
1.02
1.04
f1 (ppm)


212.990
136.658
136.554
136.085
129.147
127.886
127.595
127.041
126.753
122.523
120.378
118.414
112.013
110.528
109.926
54.365
38.083
29.276
27.648
NH
O
Br