Parameterization of Acyclic Diaminocarbene Ligands Applied to a Gold(I)-Catalyzed Enantioselective Tandem Rearrangement/Cyclization

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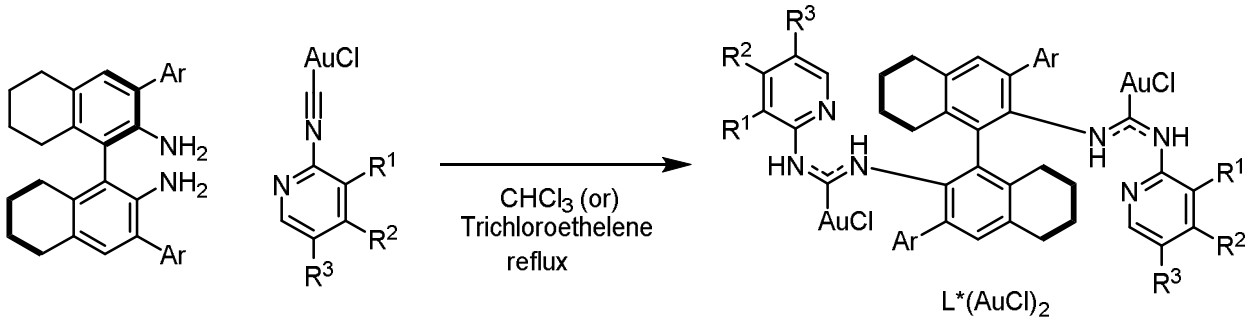
General Considerations:

Unless otherwise noted, reagents were obtained from commercial sources and used without further purification. Silver triflate (AgOTf) was obtained from Aldrich and stored amber bottle in desiccator. Dry tetrahydrofuran (THF), dichloromethane (DCM), and toluene were obtained by passage through activated alumina columns under argon. All other solvents used are HPLC grade. TLC analysis of reaction mixtures was performed on Merck silica gel 60 F254 TLC plates and visualized by ultraviolet light, iodine and/or potassiumpermanganate stain. Flash chromatography was carried out with ICN SiliTech 32-63 D60 Å silica gel. ^{1}H and ^{13}C NMR spectra were recorded with Bruker AVQ-400, AV-500, DRX-500, or AV-600 spectrometers and were referenced to residual ^{1}H and ^{13}C signals of the deuterated solvents, respectively (δH 7.26, δC 77.16 for chloroform and δH 5.32, δC54.00 for dichloromethane).^{19}F NMR spectra were recorded with Bruker AVQ-400spectrometer and were referenced to ^{19}F signal of the hexafluorobenzene (δF -164.9). Chemical shifts (δ) are given in parts per million (ppm) and coupling constants values (J)are given in Hertz (Hz). Abbreviations for multiplicities are as follows: (s) singlet, (brs) broad singlet, (d) doublet, (dd) doublet of doublets, (t) triplet, (q) quartet, (m) multiplet. Enantioselectivity was determined by chiral HPLC using Daicel Chiralpak IC column (0.46 cm x 25 cm). Generally, racemic samples were prepared by the procedure of Zhang using PPh_3AuCl or IPrAuCl (IPr = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene) and AgOTf.[15] Mass spectral data were obtained from the UC Berkeley Catalysis Center operated by usage of an Agilent Time of Flight (Q-TOF) mass spectrometer in ESI mode and micro-Mass/Analytical Facility operated by the College of Chemistry, University of California, Berkeley. X-ray crystallographic analysis was carried out at the College of Chemistry X-Ray Crystallographic Facility (CHEXRAY, University of California, Berkeley). Absolute stereochemistry was determined through VCD experiments at Merck facility.

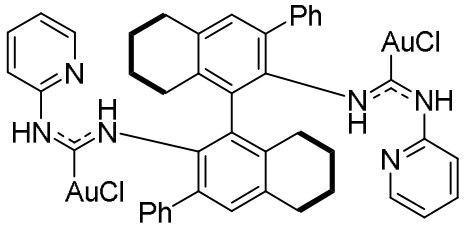
Catalyst Preparation:



General procedure for the preparation of Au (I) complexes:

5,5',6,6',7,7',8,8'-octahydro-3,3'-diido-2,2'-diamino-1,1'-binaphthyl and 5,5',6,6',7,7',8,8'-octahydro-3,3'-aryl substituted 2,2'-diamino-1,1'-binaphthyls[16,18] and Isocyanopyridyl gold(I) complexes[17], and were prepared by following the procedure that was reported by our group and others previously[18]. The general synthesis procedure is described as follows.

A round bottomed flask equipped with reflux condenser was loaded with 3,3'-disubstituted H8-BINAM derivative (1.0 equiv.) and dissolved in $CHCl_3$ or trichloroethelene. Substituted Isocyanopyridyl gold (I) complex[17] (2.0 equiv.) was added and heated to reflux for 6h. At this stage, the other portion of Isocyanopyridyl gold (I) complex (1.0 equiv.) was added and further continued heating until the TLC indicates the starting material consumed. The reaction mixture was concentrated in vacuo and purified by column chromatography (1:1 DCM/Hexanes→DCM). The isolated product was further purified by vapor diffusion recrystallization with $CHCl_3$/Pentane. The crystals were collected filtering through a fine frit Buchner filter funnel, and crystals were dissolved in DCM and dried in vacuo to give desired L*$(AuCl)_2$ complex as powdered compound. The mother liquor was crystallized again by following the same procedure to yield another crop of L*$(AuCl)_2$ complex.

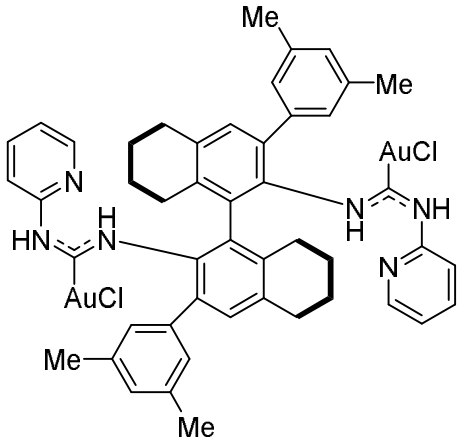


Complex L1*$(AuCl)_2$

0.0794 mmol scale, 73% yield (64.4 mg, 0.0576 mmol)

^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.44 (s, 2H), 8.36 (s, 2H), 8.29 – 8.22 (m, 2H), 7.80 – 7.66 (m, 2H), 7.31 (d, *J* = 7.5 Hz, 4H), 7.24 (dt, *J* = 14.5, 7.1 Hz, 6H), 7.18 – 7.07 (m, 4H), 6.86 (d, *J* = 8.3 Hz, 2H), 2.83 (d, *J* = 7.2 Hz, 4H), 2.61 (dt, *J* = 13.4, 6.5 Hz, 2H), 2.52 – 2.27 (m, 2H), 2.01 (d, *J* = 10.6 Hz, 2H), 1.87 (td, *J* = 14.8, 12.9, 6.6 Hz, 6H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.24, 155.17, 145.88, 139.79, 139.31, 138.51, 138.31, 135.26, 134.99, 133.40, 132.65, 130.59, 128.69,

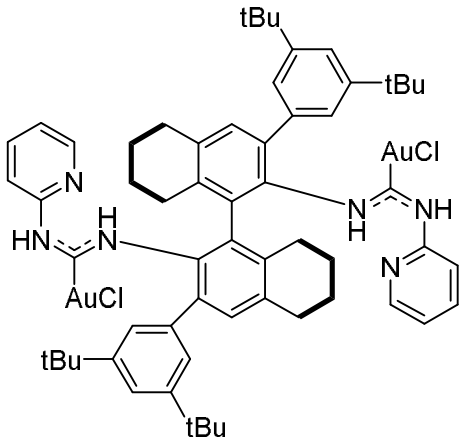
127.25, 120.12, 114.95, 30.10, 28.75, 23.87, 23.46; HRMS (ESI+): calc'd for $[C_{44}H_{40}N_6Au_2Cl_2]Na$: 1139.1915, found: 1139.1934



Complex L2*$(AuCl)_2$

0.287 mmol scale, 80% yield (269.5 mg, 0.230 mmol)

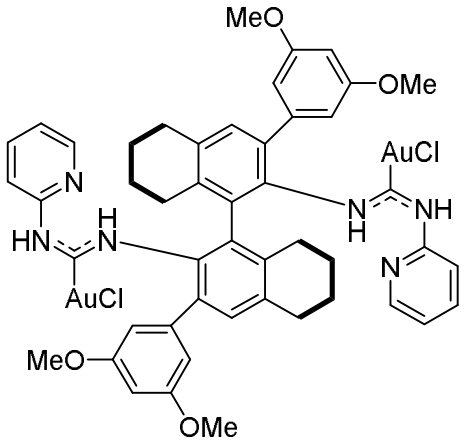
^{1}H NMR (400 MHz, CD_2Cl_2) δ 13.39 (s, 2H), 8.33 – 8.24 (m, 2H), 8.14 (s, 2H), 7.72 (ddd, *J* = 8.3, 7.4, 1.9 Hz, 2H), 7.15 (s, 2H), 7.12 (ddd, *J* = 7.4, 5.1, 1.0 Hz, 2H), 6.94 – 6.92 (m, 4H), 6.86 – 6.82 (m, 4H), 2.83 (t, *J* = 6.0 Hz, 4H), 2.72 – 2.52 (m, 2H), 2.37 (dt, *J* = 16.1, 5.1 Hz, 2H), 2.15 (s, 12H), 2.06 – 1.97 (m, 2H), 1.95 – 1.80 (m, 6H);^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.39, 155.07, 145.94, 139.43, 139.38, 138.55, 138.46, 138.13, 135.32, 134.74, 133.29, 132.29, 128.65, 128.56, 120.13, 114.64, 30.15, 28.75, 23.90, 23.49, 21.37; HRMS (ESI+): calc'd for $[C_{48}H_{48}N_6Au_2Cl_2]Na$: 1195.2541, found: 1195.2546.



Complex L3*$(AuCl)_2$

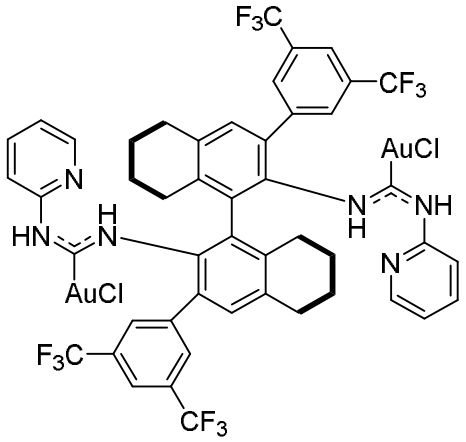
0.156 mmol scale, 64% yield (133.6 mg, 0.0995 mmol)

^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.44 (s, 2H), 8.27 (d, *J* = 4.2 Hz, 4H), 7.69 (t, *J* = 7.9 Hz, 2H), 7.24 (t, *J* = 2.0 Hz, 2H), 7.19 (s, 2H), 7.10 (d, *J* = 1.9 Hz, 6H), 6.79 (d, *J* = 8.3 Hz, 2H), 2.86 (t, *J* = 5.8 Hz, 4H), 2.66 (d, *J* = 17.0 Hz, 2H), 2.45 (dd, *J* = 14.1, 9.0 Hz, 2H), 2.05 (q, *J* = 7.7 Hz, 2H), 1.90 (dd, *J* = 20.1, 12.5 Hz, 6H), 1.13 (s, 36H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.54, 155.25, 150.99, 145.94, 139.63, 139.51, 138.69, 138.38, 135.35, 134.63, 133.52, 132.28, 125.25, 121.03, 120.12, 114.55, 35.14, 31.55, 30.24, 28.93, 23.98, 23.58; HRMS (ESI+): calc'd for $[C_{60}H_{72}N_6Au_2Cl_2]Na$: 1363.4419, found: 1363.4442.



Complex L4*$(AuCl)_2$

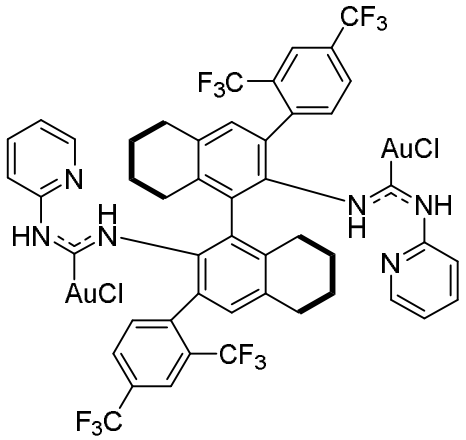
^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.39 (s, 2H), 8.42 (s, 2H), 8.24 (d, *J* = 5.1 Hz, 2H), 7.72 (t, *J* = 7.9 Hz, 2H), 7.16 (s, 2H), 7.15 – 7.01 (m, 2H), 6.88 (d, *J* = 8.3 Hz, 2H), 6.46 (d, *J* = 2.5 Hz, 4H), 6.30 (t, *J* = 2.5 Hz, 2H), 3.61 (s, 12H), 2.83 (s, 4H), 2.58 (d, *J* = 17.1 Hz, 2H), 2.38 (dd, *J* = 13.9, 8.8 Hz, 2H), 2.05 – 1.78 (m, 8H);^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.14, 160.96, 155.21, 145.82, 141.68, 139.41, 138.54, 138.45, 135.26, 135.13, 133.33, 132.32, 120.17, 114.96, 108.50, 100.32, 55.84, 30.12, 28.79, 23.86, 23.45;HRMS (ESI+): calc'd for $[C_{48}H_{48}O_4N_6Au_2Cl_2]Na$: 1259.2338, found: 1259.2367.



Complex L5*$(AuCl)_2$

0.268 mmol scale, 77% yield (287.7 mg, 0.207 mmol)

^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.57 (s, 2H), 8.78 (s, 2H), 8.25 (d, *J* = 5.0 Hz, 2H), 7.77 (s, 4H), 7.74 (d, *J* = 10.0 Hz, 4H), 7.25 (s, 2H), 7.19 – 7.08 (m, 2H), 6.90 (d, *J* = 8.3 Hz, 2H), 2.89 (t, *J* = 5.9 Hz, 4H), 2.70 – 2.57 (m, 2H), 2.43 (dt, *J* = 17.2, 5.1 Hz, 2H), 2.18 – 1.81 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.16, 155.05, 144.82, 141.08, 138.94, 138.26, 135.83, 135.45, 134.95, 133.56, 131.76, 131.40 (q, *J* = 33.1 Hz), 130.63, 123.28 (q, *J* = 273.4 Hz), 120.60, 119.82, 115.07, 29.82, 28.58, 23.38, 23.00; ^{19}F NMR (376 MHz, CD_2Cl_2) δ -63.54; HRMS (ESI+): calc'd for $[C_{48}H_{36}N_6Au_2Cl_2F_{12}]Na$: 1411.1410, found: 1411.1391.

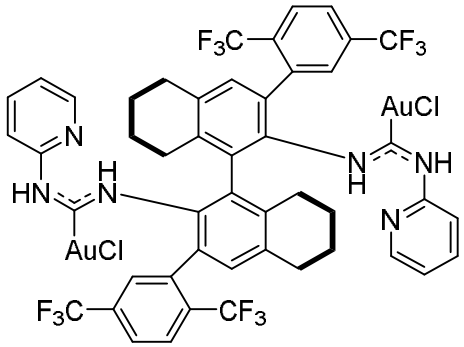


Complex L6*$(AuCl)_2$

0.0996 mmol scale, 56% yield (77.0 mg, 0.0554 mmol)

^{1}H NMR (600 MHz, CD_2Cl_2) δ 13.50 (s, 2H), 8.40 (s, 2H), 8.19 (dd, *J* = 5.2, 1.8 Hz, 2H), 8.07 (d, *J* = 8.5 Hz, 2H), 7.81 (s, 2H), 7.80 (s, 2H), 7.71 – 7.67 (m, 2H), 7.14 – 7.06 (m, 2H), 7.00 (s, 2H), 6.87 (d, *J* = 8.3 Hz, 2H), 2.96 – 2.70 (m, 4H), 2.54 (dt, *J* = 17.2, 6.5 Hz, 2H), 2.25 (dt, *J* = 17.1,

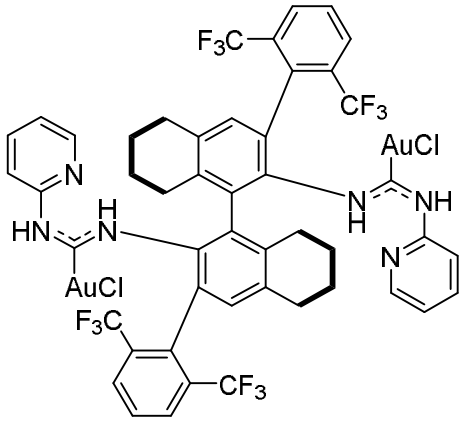
5.3 Hz, 2H), 2.06 – 1.70 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.26, 154.88, 145.65, 141.48, 139.21, 138.44, 137.49, 136.85, 135.17, 134.68, 134.09, 132.57, 130.50 (q, *J* = 33.3 Hz), 129.33 (q, *J* = 30.2 Hz), 128.66 – 128.21 (m), 124.02 (q, *J* = 273.2 Hz), 124.06 – 123.18 (m), 120.26, 114.78, 29.92, 28.18, 23.60, 23.21; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.63, -63.28; HRMS (ESI+): calc'd for $[C_{48}H_{36}N_6Au_2Cl_2F_{12}]Na$: 1411.1410, found: 1411.1427.



Complex L7*$(AuCl)_2$

0.101 mmol scale, 65% yield (90.2 mg, 0.0649 mmol)

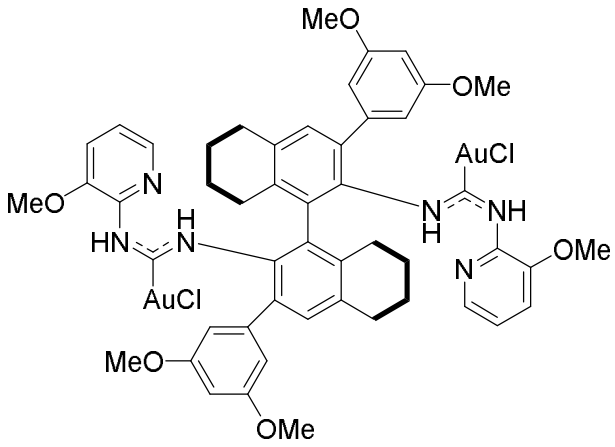
^{1}H NMR (500 MHz, $CDCl_3$) δ 13.50 (s, 2H), 8.69 (s, 2H), 8.31 – 8.09 (m, 4H), 7.86 – 7.45 (m, 6H), 7.08 (dd, *J* = 7.4, 5.2 Hz, 2H), 7.03 (s, 2H), 6.90 (d, *J* = 8.3 Hz, 2H), 2.81 (dh, *J* = 23.0, 5.9 Hz, 4H), 2.54 (dt, *J* = 14.5, 7.0 Hz, 2H), 2.25 (dt, *J* = 17.4, 5.3 Hz, 2H), 2.14 – 1.75 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.64, 154.94, 145.62, 139.21, 138.68, 138.42, 137.47, 135.15, 134.71, 134.41, 133.29 (q, *J* = 33.3 Hz), 132.84 – 132.76 (m), 132.69, 131.71 (q, *J* = 31.2, 30.8 Hz), 127.10 (q, *J* = 4.9 Hz), 125.28 (q, *J* = 3.8 Hz), 124.14 (q, *J* = 275.4 Hz), 123.82 (q, *J* = 274.3 Hz), 120.22, 114.88, 29.95, 28.20, 23.64, 23.26; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.61, -63.25; HRMS (ESI+): calc'd for $[C_{48}H_{36}N_6Au_2Cl_2F_{12}]Na$: 1411.1410, found: 1411.1432.



Complex L8*$(AuCl)_2$

0.0977 mmol scale, 53% yield (71.7 mg, 0.0516 mmol)

^{1}H NMR (500 MHz, $CDCl_3$) δ 13.50 (s, 2H), 8.54 (s, 2H), 8.19 (d, *J* = 4.3 Hz, 2H), 8.08 (d, *J* = 8.3 Hz, 2H), 7.80 (s, 4H), 7.68 (t, *J* = 8.2 Hz, 2H), 7.09 (dd, *J* = 7.6, 4.9 Hz, 2H), 7.00 (s, 2H), 6.88 (d, *J* = 8.3 Hz, 2H), 2.79 (tdd, *J* = 17.4, 14.4, 12.0, 7.8 Hz, 4H), 2.54 (dt, *J* = 14.4, 6.8 Hz, 2H), 2.25 (dt, *J* = 17.4, 5.2 Hz, 2H), 2.06 – 1.73 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 194.53, 154.82, 145.71, 141.45, 139.30, 138.52, 137.54, 136.86, 135.18, 134.72, 134.07, 132.58, 130.56 (q, *J* = 33.4 Hz), 129.38 (q, *J* = 30.3 Hz), 128.62 – 128.31 (m), 124.05 (q, *J* = 274.3 Hz), 123.79 – 123.18 (m), 120.33, 114.75, 29.94, 28.21, 23.61, 23.22; ^{19}F NMR (376 MHz, $CDCl_3$) δ -59.63, -63.28; HRMS (ESI+): calc'd for $[C_{48}H_{36}N_6Au_2Cl_2F_{12}]Na$: 1411.1410, found: 1411.1429.

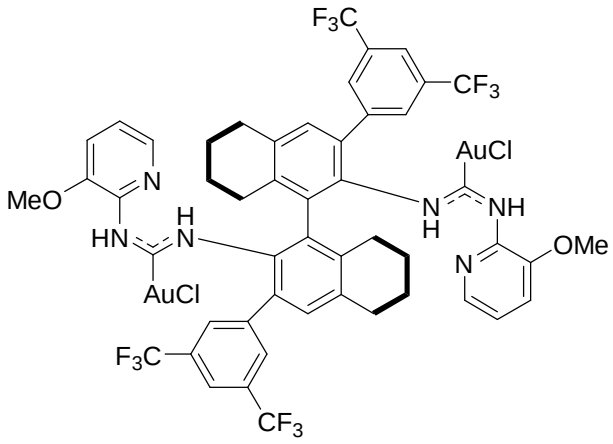


Complex L9*$(AuCl)_2$

0.179 mmol scale, 79% yield (183.5 mg, 0.141 mmol)

^{1}H NMR (4:1 rotamer ratio, asterisks denote minor rotamer peaks, 600 MHz, CD_2Cl_2) δ 13.66* (s, 0H), 13.56 (s, 2H), 8.54 (s, 2H), 8.51* (s, 0H), 7.73 (d, *J* = 5.1 Hz, 2H), 7.60* (d, *J* = 5.4 Hz, 0H), 7.32* (s, 0H), 7.20 (s, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.13* (s, 0H), 7.06 (dd, *J* = 8.3, 5.1 Hz, 2H), 7.03 – 6.96* (m, 0H), 6.47* (s, 0H), 6.45 (t, *J* = 1.8 Hz, 4H), 6.36* (d, *J* = 2.2 Hz, 0H), 6.29 (q, *J* = 2.0 Hz, 2H), 3.87* (s, 0H), 3.84 (s, 6H), 3.75* (s, 0H), 3.61 (s, 12H), 3.11 – 3.01* (m, 0H), 2.97 – 2.81 (m, 4H), 2.71* (dd, *J* = 15.8, 8.0 Hz, 0H), 2.58 (dt, *J* = 17.1, 6.6 Hz, 2H), 2.36 (dt, *J* = 16.9, 6.0 Hz, 2H), 2.16 – 1.66* (m, 8H, indistinguishable overlap of major and minor peaks); ^{13}C NMR (asterisks denote minor rotamer peaks, 126 MHz, $CDCl_3$) δ 195.07, 161.02*, 160.92, 145.87, 145.37*, 144.65, 144.14*, 141.87, 141.46*, 139.39*, 138.27, 138.14, 137.44*, 137.19*, 136.96*, 136.14, 135.14, 134.93, 133.57, 132.43, 132.26*, 120.81*, 120.27, 118.57*, 118.45, 108.87*,

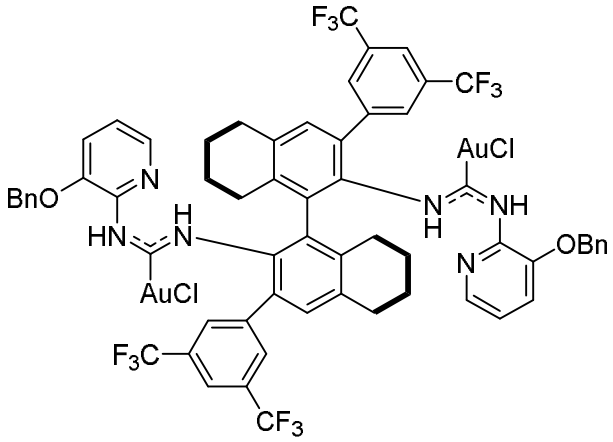
108.54, 100.17, 99.75*, 56.54, 56.02*, 55.78, 30.19, 29.28*, 28.69, 23.89, 23.50, 23.38*, 23.10*; HRMS (ESI+): calc'd for $[C_{50}H_{52}O_6N_6Au_2Cl_2]Na$: 1319.2549, found: 1319.2584.



Complex L10*$(AuCl)_2$

0.153 mmol scale, 51% yield (112.6 mg, 0.0777 mmol)

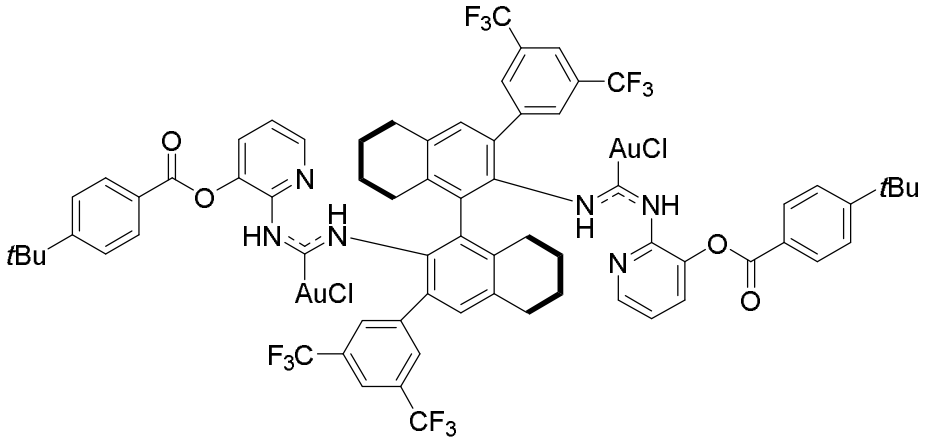
^{1}H NMR (5:1 rotamer ratio, asterisks denote minor rotamer peaks, 500 MHz, CD_2Cl_2) δ 13.93* (s, 0H), 13.72 (s, 2H), 8.58 (s, 2H), 7.83* (s, 0H), 7.82* (s, 0H), 7.78* (d, *J* = 1.4 Hz, 0H), 7.77 (t, *J* = 1.3 Hz, 4H), 7.73 (s, 2H), 7.71 – 7.68* (m, 0H), 7.29 (s, 2H), 7.26* (dd, *J* = 8.3, 1.3 Hz, 0H), 7.23* (s, 0H), 7.21 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.13 (dd, *J* = 8.2, 5.1 Hz, 2H), 7.11 – 7.07* (m, 0H), 3.87* (s, 0H), 3.83 (s, 6H), 3.10* (d, *J* = 17.3 Hz, 0H), 3.00 – 2.86 (m, 4H), 2.79* (d, *J* = 17.1 Hz, 0H), 2.64 (dt, *J* = 17.4, 6.4 Hz, 2H), 2.43 (dt, *J* = 17.5, 5.8 Hz, 2H), 2.16 – 1.69* (m, 8H, indistinguishable overlap of major and minor peaks); ^{13}C NMR (asterisks denote minor rotamer peaks, 151 MHz, CD_2Cl_2) δ 196.19, 194.94*, 145.76, 145.53*, 144.84, 144.60*, 142.07, 141.88*, 140.60*, 139.29, 139.07*, 136.96, 136.30, 135.77*, 135.21 (d, *J* = 4.3 Hz), 134.76*, 133.78, 132.51, 132.39*, 131.76 (q, *J* = 33.2 Hz), 131.48 – 130.80 (m), 124.85*, 127.01 – 121.13 (m), 121.62*, 120.98 (dd, *J* = 7.8, 3.9 Hz), 120.82, 118.96, 56.75, 30.25, 29.52*, 28.94, 23.78, 23.40, 23.24*, 22.97*; ^{19}F NMR (asterisks denote minor rotamer peaks, 376 MHz, $CDCl_3$) δ -63.32, -63.52*; HRMS (ESI+): calc'd for $[C_{50}H_{40}O_2N_6Au_2Cl_2F_{12}]Na$: 1471.1622, found: 1471.1649.



Complex L11*$(AuCl)_2$

0.093 mmol scale, 46% yield (68.6 mg, 0.0428 mmol)

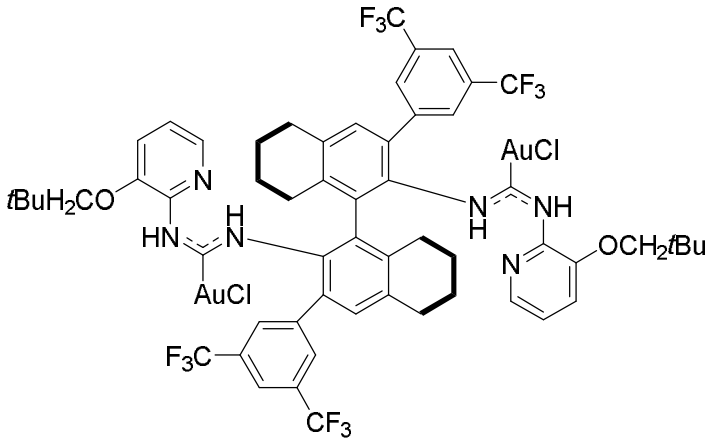
^{1}H NMR (7:1 rotamer ratio, asterisks denote minor rotamer peaks, 500 MHz, $CDCl_3$) δ 14.02* (s, 0H), 13.81 (s, 2H), 8.61 (d, *J* = 6.0 Hz, 2H), 8.56* (s, 0H), 7.83* (s, 0H), 7.79 (d, *J* = 5.2 Hz, 6H), 7.74 (s, 2H), 7.44 (d, *J* = 7.1 Hz, 4H), 7.39 – 7.34 (m, 4H), 7.33* (d, *J* = 7.3 Hz, 0H), 7.30 (d, *J* = 3.3 Hz, 2H), 7.21 (d, *J* = 8.1 Hz, 2H), 7.07 (dd, *J* = 8.3, 4.7 Hz, 2H), 5.22 – 5.06 (m, 4H), 3.08* (d, *J* = 17.1 Hz, 0H), 2.94 (t, *J* = 7.7 Hz, 4H), 2.79* (d, *J* = 16.6 Hz, 0H), 2.65 (dd, *J* = 15.5, 7.1 Hz, 2H), 2.45 (dt, *J* = 17.6, 5.8 Hz, 2H), 2.13 – 1.68* (m, 8H, indistinguishable overlap of major and minor peaks); ^{13}C NMR (asterisks denote minor rotamer peaks, 151 MHz, CD_2Cl_2) δ 196.40, 145.93, 143.83, 143.59*, 142.08, 141.89*, 139.33, 136.94, 136.51, 135.78, 135.33, 135.25, 133.81, 132.52, 131.77 (q, *J* = 33.0 Hz), 131.20, 129.28, 129.00, 128.42, 123.92 (q, *J* = 272.6 Hz), 121.50*, 121.05, 120.70, 120.26, 78.13*, 71.90, 30.26, 29.50*, 28.97, 23.79, 23.41, 23.23*, 22.97*; ^{19}F NMR (asterisks denote minor rotamer peaks, 376 MHz, $CDCl_3$) δ -63.35, -63.49*; HRMS (ESI+): calc'd for $[C_{62}H_{48}O_2N_6Au_2Cl_2F_{12}]$Na: 1623.2248, found: 1623.2308.



Complex L12*AuCl)$_2$

0.058 mmol scale, 27% yield (27.6 mg, 0.0158 mmol)

^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.74 (s, 2H), 8.40 (s, 2H), 8.16 (d, *J* = 5.2 Hz, 2H), 8.15 – 8.05 (m, 4H), 7.81 (s, 4H), 7.78 (dd, *J* = 8.1, 1.6 Hz, 2H), 7.74 (s, 2H), 7.60 – 7.46 (m, 4H), 7.32 (d, *J* = 3.2 Hz, 2H), 7.28 (dd, *J* = 8.2, 4.9 Hz, 2H), 2.94 (t, *J* = 6.7 Hz, 4H), 2.67 (dd, *J* = 16.4, 8.8 Hz, 2H), 2.49 (dt, *J* = 16.6, 4.8 Hz, 2H), 2.15 – 1.85 (m, 8H), 1.31 (s, 18H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 197.3, 163.9, 158.9, 147.4, 142.1, 141.6, 139.7, 136.8, 135.5, 135.3, 133.3, 132.7, 132.6, 131.7 (q, *J* = 35.2, 33.6 Hz), 131.1 – 131.0 (m), 131.0, 126.5, 125.6, 123.8 (q, *J* = 272.9 Hz), 121.5 – 121.0 (m), 120.7, 35.7, 31.3, 30.2, 29.1, 23.7, 23.3; ^{19}F NMR (376 MHz, CD_2Cl_2) δ -62.58; HRMS (ESI+): calc'd for $[C_{70}H_{60}N_6Au_2Cl_2F_{12}]Na$: 1763.3085, found: 1763.3063.

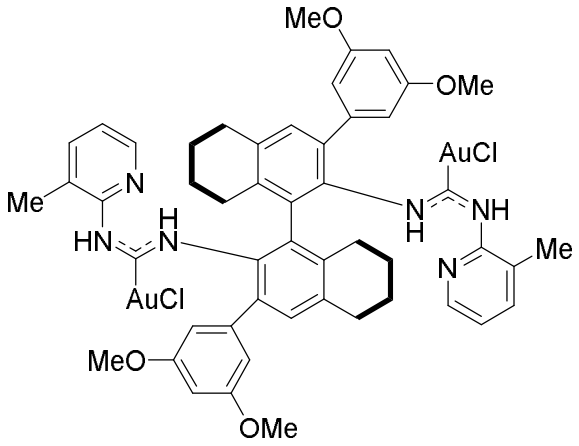


Complex L13*AuCl)$_2$

0.346 mmol scale, 43% yield (231.4 mg, 0.148 mmol)

^{1}H NMR (7:1 rotamer ratio, asterisks denote minor rotamer peaks, 600 MHz, CD_2Cl_2) δ 14.06* (s, 0H), 13.90 (s, 2H), 8.46 (s, 2H), 8.36* (s, 0H), 7.86* (s, 0H), 7.82* (s, 0H), 7.81 (d, *J* = 5.1 Hz,

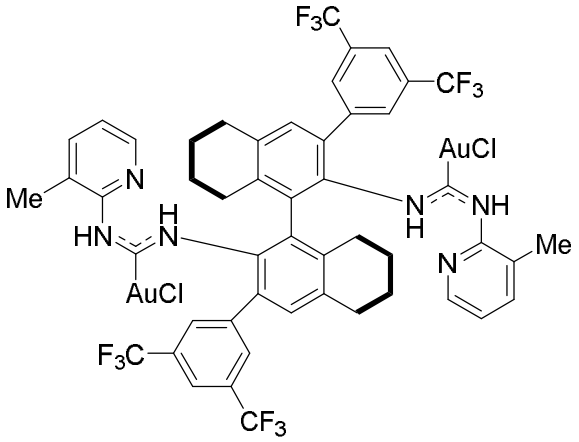
2H), 7.79 (s, 4H), 7.73 (s, 2H), 7.69* (d, *J* = 5.1 Hz, 0H), 7.30 (s, 2H), 7.27 (s, 0H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.13 (dd, *J* = 8.3, 5.0 Hz, 2H), 7.08* (dd, *J* = 8.3, 5.0 Hz, 0H), 3.73 (d, *J* = 8.4 Hz, 2H), 3.69* (d, *J* = 8.9 Hz, 0H), 3.62 (d, *J* = 8.5 Hz, 2H), 3.17 – 3.02* (m, 0H), 3.06 – 2.84 (m, 4H), 2.78* (dt, *J* = 13.9, 6.1 Hz, 0H), 2.75 – 2.61 (m, 2H), 2.46 (dt, *J* = 17.3, 5.3 Hz, 2H), 2.39* (d, *J* = 17.9 Hz, 0H), 2.10 – 1.70* (m, 8H, indistinguishable overlap of major and minor peaks), 1.02* (s, 0H), 1.01 (s, 18H); ^{13}C NMR (asterisks denote minor rotamer peaks, 151 MHz, CD_2Cl_2) δ 196.62, 195.10*, 155.55*, 145.90, 145.56*, 144.47, 144.36*, 142.00, 141.87*, 140.64*, 139.37, 139.11*, 137.72*, 136.95, 136.22*, 136.10, 135.73*, 135.40, 135.31, 134.67*, 133.61, 132.54, 132.47*, 131.75 (q, *J* = 33.0 Hz), 131.24 – 131.13* (m), 131.10 – 130.92 (m), 123.91 (q, *J* = 272.9 Hz), 121.70*, 121.16 – 120.93 (m), 120.85, 120.31*, 119.82, 80.07*, 79.84, 32.43*, 32.35, 30.31*, 30.25, 29.49*, 29.01, 27.00, 26.88*, 23.77, 23.36, 23.23*, 22.95*; ^{19}F NMR (asterisks denote minor rotamer peaks, 376 MHz, $CDCl_3$) δ -63.13*, -63.51; HRMS (ESI+): calc'd for $[C_{58}H_{56}O_2N_6Au_2Cl_2F_{12}]Na$: 1583.2874, found: 1583.2883.



Complex L14*$(AuCl)_2$

0.199 mmol scale, 13% yield (32.9 mg, 0.0260 mmol)

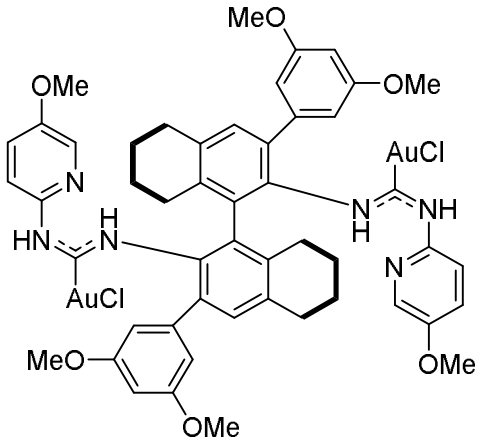
^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.94 (s, 2H), 8.24 – 8.04 (m, 2H), 7.92 (s, 2H), 7.54 (d, *J* = 7.5 Hz, 2H), 7.19 (s, 2H), 7.04 (dd, *J* = 7.5, 5.1 Hz, 2H), 6.46 (d, *J* = 2.3 Hz, 4H), 6.29 (t, *J* = 2.3 Hz, 2H), 3.58 (s, 12H), 2.86 (d, *J* = 6.5 Hz, 4H), 2.62 (dt, *J* = 14.3, 6.8 Hz, 2H), 2.40 (dt, *J* = 16.4, 5.6 Hz, 2H), 2.32 (s, 6H), 2.11 – 1.78 (m, 8H); ^{13}C NMR (151 MHz, CD_2Cl_2) δ 196.04, 161.04, 153.95, 143.20, 141.80, 140.59, 138.60, 138.57, 135.32, 135.23, 133.44, 132.44, 123.07, 120.25, 108.51, 100.64, 55.84, 30.24, 28.87, 23.94, 23.49, 17.33; HRMS (ESI+): calc'd for $[C_{50}H_{52}O_4N_6Au_2Cl_2F_{12}]Na$: 1287.2651, found: 1287.2666.



Complex L15*$(AuCl)_2$

0.265 mmol scale, 74% yield (280 mg, 0.197 mmol)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 14.15 (s, 2H), 8.12 (dd, *J* = 5.2, 1.8 Hz, 2H), 7.94 (s, 2H), 7.79 (d, *J* = 1.6 Hz, 4H), 7.73 (s, 2H), 7.58 (d, *J* = 7.4 Hz, 2H), 7.30 (s, 2H), 7.10 (dd, *J* = 7.5, 5.0 Hz, 2H), 2.91 (d, *J* = 5.6 Hz, 4H), 2.67 (dt, *J* = 13.8, 6.5 Hz, 2H), 2.47 (dt, *J* = 17.1, 5.0 Hz, 2H), 2.35 – 2.21 (m, 6H), 2.15 – 1.81 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 196.78, 153.65, 143.15, 141.79, 140.75, 139.39, 136.87, 135.35, 135.25, 133.49, 132.33, 131.66 (q, *J* = 33.2 Hz), 131.08, 123.81 (q, *J* = 272.8 Hz), 120.98 (q, *J* = 4.3 Hz), 30.18, 29.00, 23.70, 23.30, 17.15; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.62; HRMS (ESI+): calc'd for $[C_{50}H_{40}N_6Au_2Cl_2F_{12}]Na$: 1439.1723, found: 1439.1726.

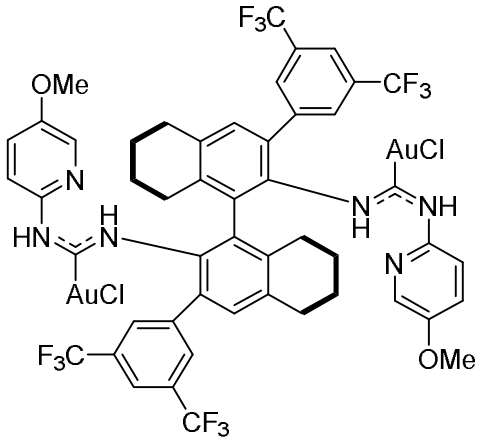


Complex L16*$(AuCl)_2$

0.187 mmol scale, 66% yield (161.2 mg, 0.124 mmol)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 13.04 (s, 2H), 8.19 (s, 2H), 7.89 (d, *J* = 3.0 Hz, 2H), 7.30 (dd, *J* = 9.0, 3.0 Hz, 2H), 7.15 (s, 2H), 6.86 (d, *J* = 9.0 Hz, 2H), 6.47 (d, *J* = 2.3 Hz, 4H), 6.31 (t, *J* = 2.3

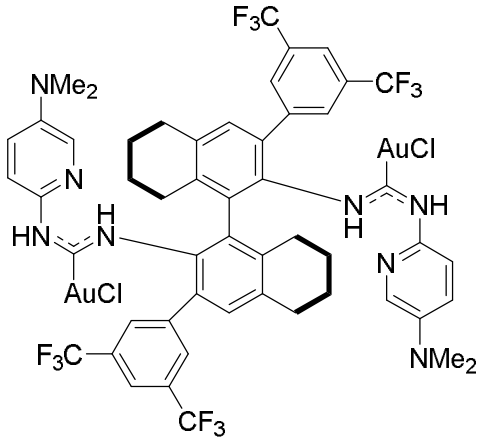
Hz, 2H), 3.86 (s, 6H), 3.63 (s, 12H), 2.83 (d, *J* = 6.4 Hz, 4H), 2.69 – 2.49 (m, 2H), 2.44 – 2.27 (m, 2H), 2.12 – 1.75 (m, 8H); ^{13}C NMR (151 MHz, CD_2Cl_2) δ 193.87, 161.02, 153.30, 149.11, 141.84, 138.70, 138.29, 135.44, 135.13, 133.50, 132.30, 131.53, 125.71, 115.79, 108.67, 100.31, 56.63, 55.92, 30.18, 28.81, 23.96, 23.54; HRMS (ESI+): calc'd for $[C_{50}H_{52}O_6N_6Au_2Cl_2]Na$: 1319.2549, found: 1319.2568.



Complex L17*$AuCl)_2$

0.447 mmol scale, 73% yield (473.2 mg, 0.326 mmol)

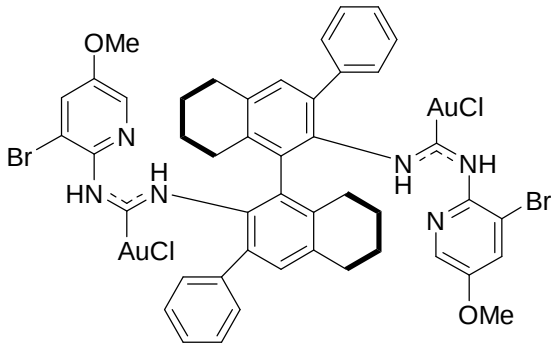
^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.22 (s, 2H), 9.17 – 8.40 (m, 2H), 7.89 (d, *J* = 3.0 Hz, 2H), 7.80 – 7.76 (m, 4H), 7.73 (s, 2H), 7.31 (dd, *J* = 9.0, 2.9 Hz, 2H), 7.25 (s, 2H), 6.90 (d, *J* = 9.0 Hz, 2H), 3.88 (d, *J* = 1.6 Hz, 6H), 2.90 (t, *J* = 6.0 Hz, 4H), 2.61 (dt, *J* = 16.2, 6.1 Hz, 2H), 2.43 (dt, *J* = 16.8, 5.4 Hz, 2H), 2.23 – 1.76 (m, 8H); ^{13}C NMR (126 MHz, CD_3CN) δ 194.09, 153.91, 149.39, 142.60, 139.56, 137.73, 136.10, 135.63, 134.35, 132.39, 131.82 – 131.75 (m), 131.72 (q, *J* = 33.2 Hz), 126.54, 124.37 (q, *J* = 272.3 Hz), 121.20 (dd, *J* = 7.4, 4.0 Hz), 118.31, 56.84, 30.23, 28.91, 23.89, 23.54; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.49; HRMS (ESI+): calc'd for $[C_{50}H_{40}O_2N_6Au_2Cl_2F_{12}]Na$: 1471.1622, found: 1471.1639.



Complex L18*AuCl)$_2$

0.101 mmol scale, 31% yield (46.4 mg, 0.0314 mmol)

^{1}H NMR (500 MHz, CD_2Cl_2) δ 13.38 (s, 2H), 8.27 (s, 2H), 7.81 (s, 4H), 7.73 (s, 2H), 7.70 – 7.61 (m, 2H), 7.23 (s, 2H), 7.12 (dt, *J* = 8.6, 2.1 Hz, 2H), 6.76 (d, *J* = 8.8 Hz, 2H), 3.09 – 2.97 (m, 12H), 2.90 (t, *J* = 6.3 Hz, 4H), 2.74 – 2.52 (m, 2H), 2.43 (dt, *J* = 17.2, 5.5 Hz, 2H), 2.10 – 1.82 (m, 8H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 193.07, 145.56, 144.22, 142.11, 138.66, 136.70, 135.58, 135.35, 133.83, 132.17, 131.52 (q, *J* = 33.2 Hz), 131.19 – 130.98 (m), 128.63, 123.90 (q, *J* = 272.8 Hz), 123.26, 121.00 – 120.75 (m), 114.97, 40.61, 30.11, 28.90, 23.78, 23.36; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.37; HRMS (ESI+): calc'd for $[C_{52}H_{46}N_8Au_2Cl_2F_{12}]Na$: 1497.2254, found: 1497.2255.

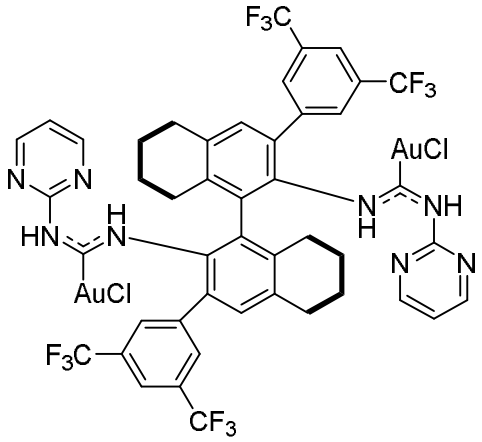


Complex L19*(AuCl)$_2$

0.112 mmol scale, 9% yield (13.1 mg, 0.0098 mmol)

^{1}H NMR (400 MHz, CD_2Cl_2) δ 13.23 (s, 2H), 8.25 (s, 2H), 7.83 (d, *J* = 2.7 Hz, 2H), 7.56 (d, *J* = 2.7 Hz, 2H), 7.32 – 7.19 (m, 12H), 3.88 (s, 6H), 3.05 – 2.81 (m, 5H), 2.67 – 2.22 (m, 5H), 2.13 – 1.74 (m, 2H), 1.54 (s, 4H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.0, 152.6, 145.1, 139.3, 138.0,

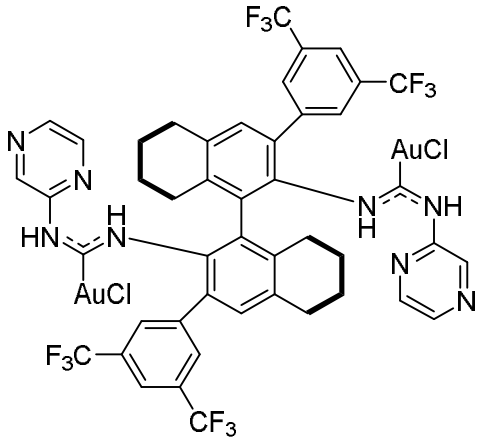
137.7, 134.4, 134.3, 133.0, 132.5, 130.5, 130.1, 128.2, 128.2, 126.8, 109.1, 56.4, 29.7, 28.2, 23.4, 23.0; HRMS (ESI+): calc'd for $[C_{46}H_{42}O_2N_6Au_2Br_2Cl_2]Na$: 1355. 0336, found: 1355.0353.



Complex L20*$(AuCl)_2$

0.100 mmol scale, 39% yield (53.9 mg, 0.0387 mmol)

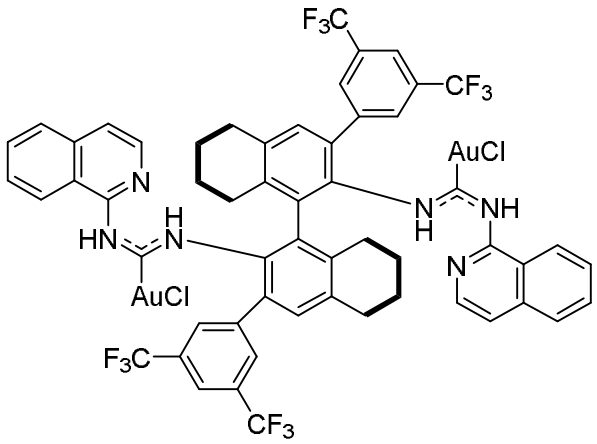
^{1}H NMR (500 MHz, CD_2Cl_2) δ 12.95 (s, 2H), 9.07 (s, 2H), 8.63 (s, 4H), 7.77 (s, 4H), 7.74 (s, 2H), 7.31 (s, 2H), 7.19 (t, *J* = 5.1 Hz, 2H), 2.92 (t, *J* = 6.1 Hz, 4H), 2.60 (dt, *J* = 16.9, 6.3 Hz, 2H), 2.44 (dt, *J* = 16.9, 5.3 Hz, 2H), 2.16 – 1.81 (m, 8H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 197.59, 159.04, 141.49, 139.73, 136.73, 135.47, 134.88, 133.34, 132.66, 131.75 (q, *J* = 33.2 Hz), 131.23 – 130.71 (m), 123.73 (q, *J* = 272.8 Hz), 121.27 – 121.03 (m), 118.13, 30.17, 29.04, 23.65, 23.34; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.53; HRMS (ESI+): calc'd for $[C_{46}H_{34}N_8Au_2Cl_2F_{12}]Na$: 1413.1315, found: 1413.1350.



Complex L21*$(AuCl)_2$

0.0953 mmol scale, 38% yield (51.0 mg, 0.0366 mmol)

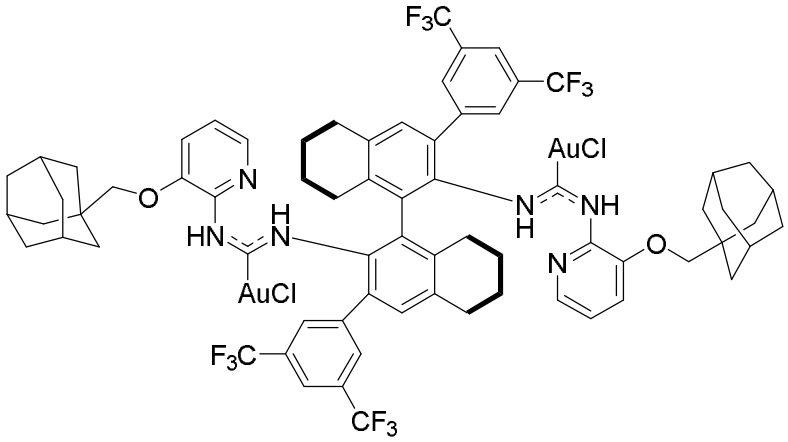
^{1}H NMR (500 MHz, CD_2Cl_2) δ 12.74 (s, 2H), 10.19 (s, 2H), 8.44 (s, 2H), 8.36 (d, *J* = 2.9 Hz, 2H), 8.15 – 8.01 (m, 2H), 7.72 (s, 2H), 7.65 (s, 4H), 7.26 (s, 2H), 2.94 (q, *J* = 6.2 Hz, 4H), 2.61 – 2.47 (m, 2H), 2.48 – 2.28 (m, 2H), 2.07 – 1.80 (m, 8H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 195.72, 151.11, 141.43, 140.20, 139.11, 138.95, 138.74, 136.54, 135.11, 134.61, 133.55, 132.50, 131.67 (q, *J* = 33.5 Hz), 131.07, 123.79 (q, *J* = 272.5 Hz), 121.39 – 120.83 (m), 30.11, 28.78, 23.73, 23.44; ^{19}F NMR (376 MHz, $CDCl_3$) δ -56.55; HRMS (ESI+): calc'd for $[C_{46}H_{34}N_8Au_2Cl_2F_{12}]Na$: 1413.1315, found: 1413.1339.



Complex L22*$(AuCl)_2$

0.105 mmol scale, 62% yield (92.0 mg, 0.062 mmol)

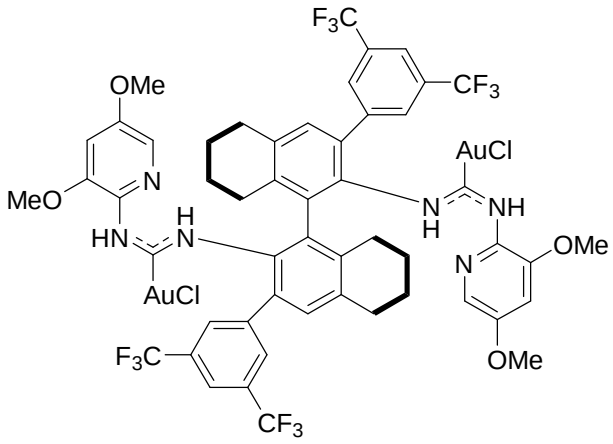
^{1}H NMR (400 MHz, CD_2Cl_2) δ 14.67 (s, 2H), 8.97 (s, 2H), 8.14 (t, *J* = 7.4 Hz, 4H), 7.89 (d, *J* = 8.1 Hz, 2H), 7.81 (d, *J* = 7.9 Hz, 6H), 7.73 – 7.65 (m, 4H), 7.56 (d, *J* = 5.9 Hz, 2H), 7.27 (s, 2H), 2.87 (d, *J* = 5.9 Hz, 4H), 2.85 – 2.69 (m, 2H), 2.53 (d, *J* = 17.4 Hz, 2H), 2.15 (d, *J* = 10.3 Hz, 2H), 2.03 – 1.85 (m, 6H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 197.6, 152.6, 144.4, 141.7, 139.6, 137.9, 137.5, 136.9, 135.4, 135.3, 133.4, 132.5, 132.2, 131.8, 131.5, 131.1, 128.9, 127.9, 124.8, 122.8, 122.7, 119.1, 119.0, 30.2, 29.2, 23.7, 23.3; ^{19}F NMR (376 MHz, CD_2Cl_2) δ -62.64; HRMS (ESI+): calc'd for $[C_{56}H_{40}N_6Au_2Cl_2F_{12}]H^+$: 1489.1904, found: 1489.1902.



Complex L23*$(AuCl)_2$

0.209 mmol scale, 51% yield (185 mg, 0.108 mmol)

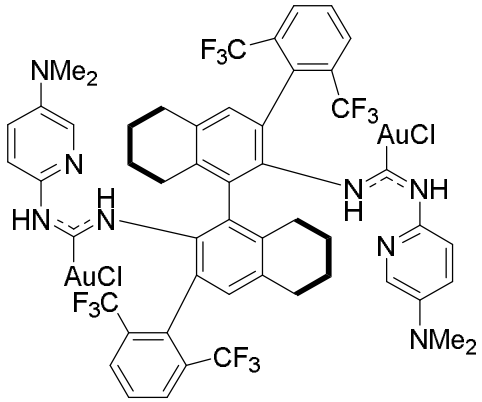
^{1}H NMR (asterisks denote minor rotamer peaks, 600 MHz, CD_2Cl_2) δ 14.09* (s, 0H), 13.97 (s, 1H), 8.46 (s, 1H), 8.37* (s, 0H), 7.84 (d, *J* = 18.2 Hz, 1H), 7.81 – 7.76 (m, 3H), 7.73 (s, 1H), 7.71* (dd, *J* = 5.2, 1.3 Hz, 0H), 7.31 – 7.22 (m, 3H), 7.12 (dd, *J* = 8.3, 5.0 Hz, 1H), 7.08* (dd, *J* = 8.3, 5.2 Hz, 0H), 3.66 (d, *J* = 9.2 Hz, 1H), 3.64 – 3.59* (m, 0H), 3.55 (d, *J* = 9.2 Hz, 1H), 3.09* (m, 0H), 2.92 (m, 2H), 2.80* (dd, *J* = 15.1, 8.4 Hz, 0H), 2.68 (m, 1H), 2.45 (m, 1H), 2.11 – 2.04 (m, 1H), 2.04 – 1.87 (m, 7H), 1.85 – 1.54* (m, indistinguishable overlap of major and minor peaks20H); ^{13}C NMR (asterisks denote minor rotamer peaks,126 MHz, $CDCl_3$) δ 196.4, 145.7, 144.4, 144.0*, 141.3, 138.6, 136.0, 135.3, 135.1, 135.0, 133.4, 132.2, 131.6, 131.3, 130.5, 124.4, 122.2, 120.3, 119.6, 80.1, 39.6*, 39.5, 37.0, 36.8*, 34.1*, 34.1, 29.9, 29.1*, 28.7, 28.1, 27.9, 23.3, 22.9, 22.8*, 22.5*; ^{19}F NMR (asterisks denote minor rotamer peaks, 376 MHz, CD_2Cl_2) δ -62.2*, -62.6; HRMS (ESI+): calc'd for $[C_{70}H_{68}O_2N_6Au_2Cl_2F_{12}]Na$: 1739.3818, found: 1739.3817.



Complex L24*$(AuCl)_2$

0.252 mmol scale, 46% yield (173.0 mg, 0.115 mmol)

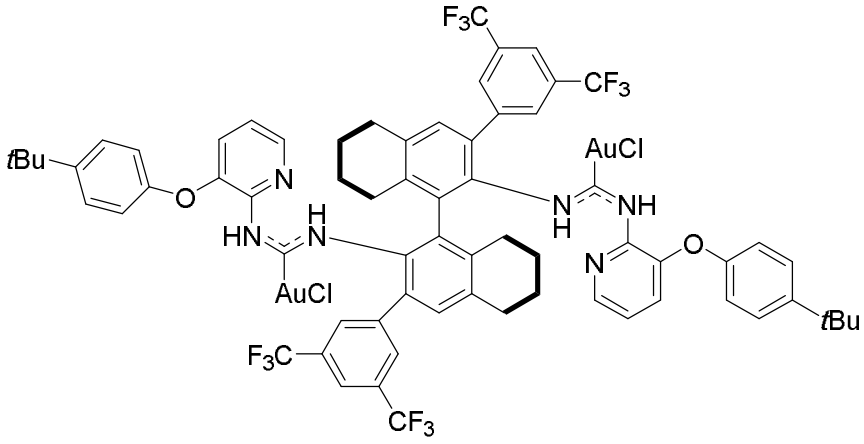
^{1}H NMR (9:1 rotamer ratio, asterisks denote minor rotamer peaks, 600 MHz, CD_2Cl_2) δ 13.45* (s, 0H), 13.41 (s, 2H), 8.42 (s, 2H), 7.88* (s, 0H), 7.82* (s, 0H), 7.78 (s, 4H), 7.73 (s, 2H), 7.41 (t, *J* = 1.9 Hz, 2H), 7.29 (s, 2H), 7.27* (d, *J* = 9.2 Hz, 0H), 6.87* (s, 0H), 6.85 – 6.76 (m, 2H), 3.89 (d, *J* = 1.6 Hz, 6H), 3.86* (s, 0H), 3.82 (d, *J* = 1.4 Hz, 6H), 3.67* (s, 0H), 3.09* (d, *J* = 17.4 Hz, 0H), 2.96 (p, *J* = 9.6, 8.2 Hz, 4H), 2.76* (d, *J* = 17.8 Hz, 0H), 2.63 (dt, *J* = 17.0, 6.6 Hz, 2H), 2.43 (dt, *J* = 17.2, 5.6 Hz, 2H), 2.15 – 1.69* (m, 8H, indistinguishable overlap of major and minor peaks); ^{13}C NMR (151 MHz, CD_2Cl_2) δ 194.58, 154.42, 145.77, 142.18, 139.87, 138.99, 136.85, 135.24, 133.89, 132.49, 131.71 (q, *J* = 33.3 Hz), 123.93 (q, *J* = 272.8 Hz), 121.01 – 120.84 (m), 120.77, 107.70, 56.85, 56.79, 30.27, 28.90, 23.84, 23.45; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.45; HRMS (ESI+): calc'd for $[C_{52}H_{44}O_4N_6Au_2Cl_2F_{12}]Na$: 1531.1833, found: 1531.1846.



Complex L25*$(AuCl)_2$

0.126 mmol scale, 84% yield (155.0 mg, 0.105 mmol)

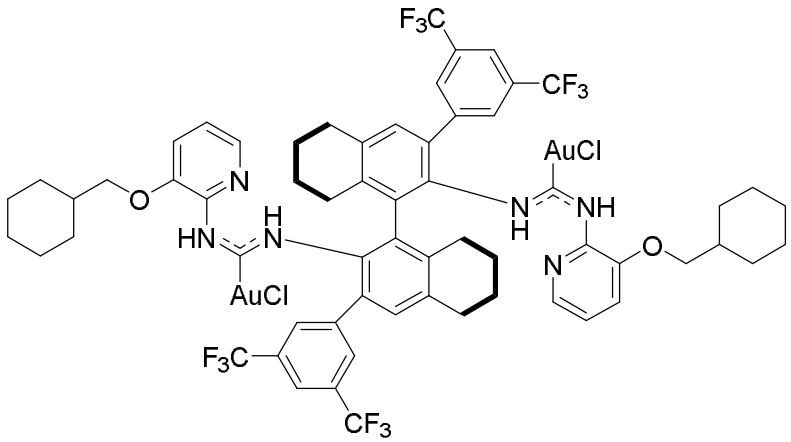
^{1}H NMR (400 MHz, CD_2Cl_2) δ 13.26 (s, 2H), 8.22 (s, 2H), 8.08 (s, 2H), 7.78 – 7.54 (m, 6H), 7.07 (dd, *J* = 9.1, 3.1 Hz, 2H), 7.01 (s, 2H), 6.74 (d, *J* = 9.0 Hz, 2H), 2.95 (s, 12H), 2.81 (q, *J* = 7.4, 6.4 Hz, 3H), 2.62 – 2.48 (m, 2H), 2.24 (d, *J* = 17.4 Hz, 2H), 2.15 – 1.63 (m, 9H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 192.4, 145.4, 144.2, 139.0, 138.0, 137.5, 135.5, 134.9, 134.7, 132.5, 128.7, 127.0, 125.2, 125.0, 123.2, 123.1, 114.8, 40.6, 29.9, 28.2, 23.7, 23.3; ^{19}F NMR (376 MHz, CD_2Cl_2) δ -58.67, -62.39; HRMS (ESI+): calc'd for [M-Cl] $[C_{52}H_{46}N_8Au_2ClF_{12}]$: 1439.2668, found: 1439.2680.



Complex L26*$(AuCl)_2$

0.0976 mmol scale, 73% yield (120 mg, 0.0712 mmol)

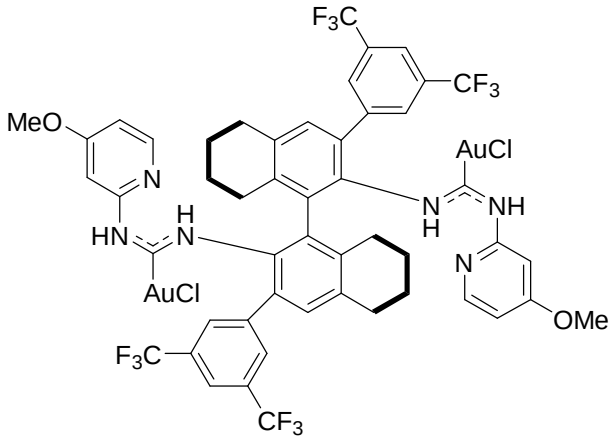
^{1}H NMR (asterisks denote minor rotamer peaks, 400 MHz, CD_2Cl_2) δ 14.00* (s, 0H), 13.77 (s, 2H), 8.75 (s, 2H), 7.98 – 7.70 (m, 7H), 7.50 – 7.31 (m, 5H), 7.19 – 7.11* (m, 0H), 7.03 (m, 7H), 6.95* (d, *J* = 8.8 Hz, 0H), 2.98 (m, 4H), 2.79 – 2.59 (m, 2H), 2.48 (dd, *J* = 14.6, 9.1 Hz, 2H), 2.16 – 1.80 (m, 8H), 1.31 (s, 18H); ^{13}C NMR (asterisks denote minor rotamer peaks, 126 MHz, CD_2Cl_2) δ 196.5, 151.8, 149.2, 146.0, 144.1, 142.0, 139.4, 138.0, 136.9, 135.3, 135.2, 133.8, 132.5, 132.2*, 131.9, 131.6, 131.4*, 131.2, 127.9*, 127.6, 127.2*, 125.0, 122.9, 122.8*, 121.0*, 120.7, 120.0*, 35.0*, 34.9, 31.7, 31.6, 30.3, 29.5*, 29.0, 23.8, 23.4, 23.2*, 22.9*; ^{19}F NMR (asterisks denote minor rotamer peaks, 376 MHz, CD_2Cl_2) δ -62.2*, -62.5; HRMS (ESI+): calc'd for $[C_{68}H_{60}O_2N_6Au_2Cl_2F_{12}]Na$: 1707.3192, found: 1707.3165.



Complex L27*$(AuCl)_2$

0.153 mmol scale, 87% yield (217.0 mg, 0.134 mmol)

^{1}H NMR (600 MHz, asterisks denote minor rotamer peaks, CD_2Cl_2) δ 14.08* (s, 0H), 13.86 (s, 1H), 8.50 (s, 1H), 8.44* (s, 0H), 7.83 (d, *J* = 1.6 Hz, 0H), 7.81* (s, 0H), 7.79 – 7.74 (m, 3H), 7.72 (m, 1H), 7.68* (dd, *J* = 5.2, 1.3 Hz, 0H), 7.27 (s, 1H), 7.25 – 7.22* (m, 0H), 7.19 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.10 (dd, *J* = 8.2, 5.0 Hz, 1H), 7.06* (dd, *J* = 8.2, 5.1 Hz, 0H), 3.88 – 3.80* (m, 0H), 3.77 (d, *J* = 6.5 Hz, 2H), 3.08* (d, *J* = 17.3 Hz, 0H), 3.02 – 2.85 (m, 2H), 2.82 – 2.73* (m, 0H), 2.66 (m, 1H), 2.44 (m, 1H), 2.05 (m, 1H), 2.00 – 1.58 (m, 6H), 1.54 (s, 1H), 1.35 – 0.82 (m, 6H); ^{13}C NMR (151 MHz, asterisks denote minor rotamer peaks, CD_2Cl_2) δ 196.5, 145.8, 145.6*, 144.4, 144.2*, 142.1, 141.9*, 140.6*, 139.3, 139.1*, 136.9, 136.0*, 135.9, 135.7*, 135.4, 135.4, 134.7*, 133.8, 132.6*, 132.5, 132.4*, 132.0*, 131.8, 131.8, 131.6, 131.4*, 131.1, 126.6*, 124.8, 123.0, 121.6*, 121.0*, 120.8, 120.0*, 119.5, 75.6, 37.4, 37.4*, 30.4, 30.4(d, *J* = 3.3 Hz), 30.3*, 30.3, 30.2, 29.5*, 29.0, 27.0, 26.9*, 26.1(d, *J* = 8.2 Hz)., 26.1*, 26.1*, 26.0, 23.8, 23.4, 23.2*, 23.0*; ^{19}F NMR (376 MHz, asterisk denote minor rotamer peak, CD_2Cl2) δ -62.19*, -62.57; HRMS (ESI+): calc'd for $[C_{62}H_{60}O_2N_6Au_2Cl_2F_{12}]Na$: 1635.3192, found: 1635.3245.

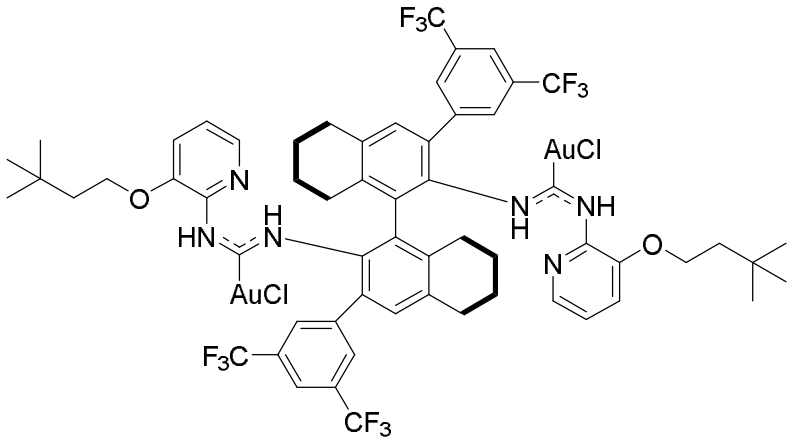


Complex L28*$(AuCl)_2$

0.237 mmol scale, 55% yield (190.0 mg, 0.131 mmol)

^{1}H NMR (500 MHz, $CDCl_3$) δ 13.75 (s, 2H), 8.92 (s, 2H), 8.03 (d, *J* = 6.0 Hz, 2H), 7.76 (s, 4H), 7.73 (s, 2H), 7.23 (s, 2H), 6.67 (dd, *J* = 5.9, 2.4 Hz, 2H), 6.45 (d, *J* = 2.5 Hz, 2H), 3.79 (s, 6H), 2.88 (t, *J* = 6.0 Hz, 4H), 2.60 (dt, *J* = 16.8, 6.6 Hz, 2H), 2.39 (dt, *J* = 16.7, 5.2 Hz, 2H), 2.15 – 1.76 (m, 8H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 195.44, 167.89, 156.98, 146.66, 141.85, 138.90, 136.66, 135.37, 133.71, 132.19, 131.57 (q, *J* = 33.1 Hz), 131.16 – 130.98 (m), 123.87 (q, *J* = 272.8 Hz), 121.25 – 120.80 (m), 108.74, 98.98, 56.13, 30.13, 28.86, 23.72, 23.35; ^{19}F NMR (376 MHz,

$CDCl_3$) δ -63.49; HRMS (ESI+): calc'd for $[C_{50}H_{40}O_2N_6Au_2Cl_2F_{12}]Na$: 1471.1622, found: 1471.1630.

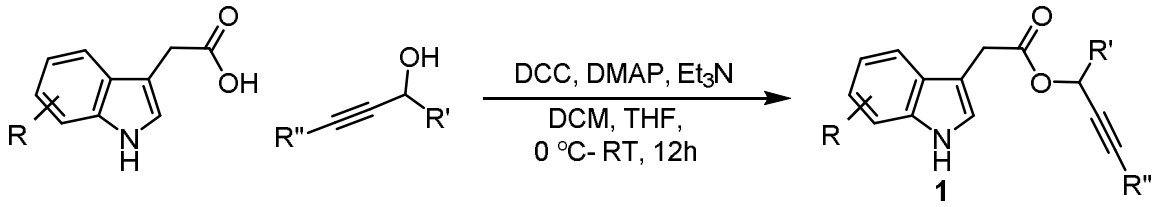


Complex L29*$(AuCl)_2$

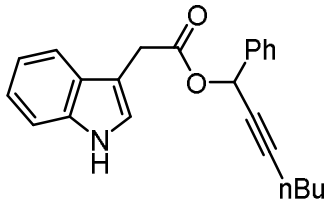
0.139 mmol scale, 62% yield (143.0 mg, 0.090 mmol)

^{1}H NMR (600 MHz, asterisks denote minor rotamer peaks, CD_2Cl_2) δ 13.98* (s, 0H), 13.76 (s, 2H), 8.54 (s, 2H), 8.49* (s, 0H), 7.84* (s, 1H), 7.82* (s, 1H), 7.79 – 7.76 (m, 6H), 7.73 (s, 2H), 7.68 (d, *J* = 5.1 Hz, 0H), 7.28 (s, 2H), 7.26* (d, *J* = 8.3 Hz, 0H), 7.23* (s, 0H), 7.22 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.11 (dd, *J* = 8.2, 5.0 Hz, 2H), 7.10 – 7.07* (m, 0H), 4.15 – 4.00 (m, 5H, indistinguishable overlap of major and minor peaks), 3.09* (d, *J* = 17.3 Hz, 0H), 3.03 – 2.86 (m, 4H), 2.83 – 2.74* (m, 0H), 2.73 – 2.59 (m, 2H), 2.48 – 2.36 (m, 2H), 2.09 – 2.03 (m, 2H), 2.00 – 1.84 (m, 2H), 1.85 – 1.68 (m, 5H, indistinguishable overlap of major and minor peaks), 1.54 (s, 3H, indistinguishable overlap of major and minor peaks), 0.96* (s, 4H), 0.94 (s, 18H); ^{13}C NMR (151 MHz, CD_2Cl2) δ 196.3, 194.9*, 145.8, 145.6*, 144.2, 144.0*, 142.1, 141.9*, 140.6*, 139.3, 139.1*, 136.9, 136.1*, 136.0, 135.7*, 135.3, 134.7*, 133.8, 132.6*, 132.5, 132.4*, 132.1*, 131.8, 131.8*, 131.6, 131.4*, 131.1, 126.6*, 124.8, 123.0, 121.6*, 121.0*, 121.0, 120.7, 119.7*, 119.4, 100.6, 67.8*, 67.7, 42.3*, 42.2, 31.2*, 30.3*, 30.2, 30.1*, 30.0, 29.9, 29.8, 29.5*, 29.0, 23.8, 23.4, 23.2*, 23.0*; ^{19}F NMR (376 MHz, CD_2Cl_2) δ -62.13*, -62.49; ; HRMS (ESI+): calc'd for $[C_{60}H_{60}O_2N_6Au_2Cl_2F_{12}]Na$: 1611.3192, found: 1611.3241.

Substrate Preparation:

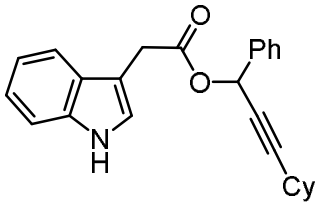


The synthesis of Indole propargyl acetates **1** was described before and the derivatives were prepared analogously.[15]



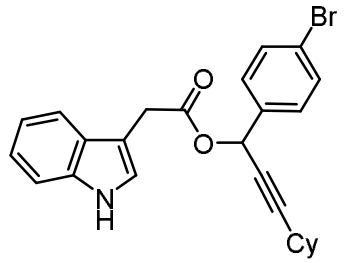
1a, 1-phenylhept-2-yn-1-yl 2-(1*H*-indol-3-yl)acetate

Compound 1a was obtained in 90% yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.58 (m,1H), 7.55 – 7.50 (m, 2H), 7.41 – 7.34 (m, 3H), 7.31 (m, 1H), 7.20 (m,1H), 7.12 (m, 1H), 7.06 (d, *J* = 2.4 Hz, 1H), 6.55 (t, *J* = 2.1 Hz, 1H), 3.97 – 3.66 (m, 2H), 2.28 (m, *J* = 7.1, 2.1 Hz, 2H), 1.53 (m, *J* = 8.5, 7.6, 6.2 Hz, 2H), 1.47 – 1.37 (m, 2H), 0.93 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.0, 137.6, 136.1, 128.7, 128.5, 127.7, 127.2, 123.2, 122.1, 119.5, 118.9, 111.1, 108.0, 88.6, 76.7, 66.5, 31.4, 30.5, 21.9, 18.5, 13.6; HRMS-TOF Calculated for [$C_{23}H_{23}NNaO_2$]: 368.1621; Found: 368.1636.



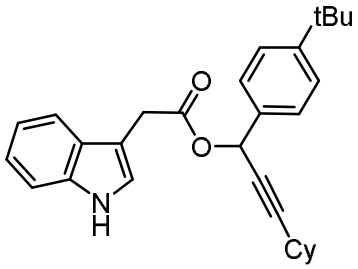
1b, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(1*H*-indol-3-yl)acetate

Compound 1b was obtained in 92% yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.08 (s, 1H), 7.60 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.57 – 7.54 (m, 2H), 7.43 – 7.34 (m, 3H), 7.30 (m, 1H), 7.24 – 7.16 (m, 1H), 7.15 – 7.09 (m, 1H), 7.02 (d, *J* = 2.3 Hz, 1H), 6.60 (d, *J* = 1.9 Hz, 1H), 3.91 – 3.78 (m, 2H), 2.62 – 2.32 (m, 1H), 1.88 – 1.79 (m, 2H), 1.77 – 1.66 (m, 2H), 1.60 – 1.43 (m, 3H), 1.42 – 1.26 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.1, 137.8, 136.2, 128.8, 128.6, 128.6, 127.9, 127.9, 127.3, 123.3, 122.2, 119.6, 119.0, 111.3, 108.0, 92.6, 76.8, 66.6, 32.4, 32.4, 31.5, 29.2, 25.9, 24.8; HRMS-TOF Calculated for [$C_{25}H_{25}NNaO_2$]: 394.1783; Found: 394.1802.



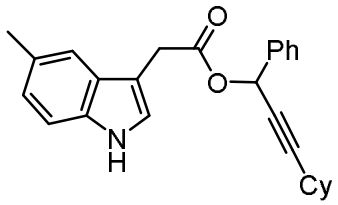
1c, 1-(4-bromophenyl)-3-cyclohexylprop-2-yn-1-yl 2-(1*H*-indol-3-yl)acetate

Compound 1c was obtained in 82% yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (s, 1H), 7.56 (m, 1H), 7.49 – 7.43 (m, 2H), 7.39 – 7.31 (m, 3H), 7.23 – 7.17 (m, 1H), 7.13 – 7.08 (m, 2H), 6.48 (d, *J* = 1.9 Hz, 1H), 3.91 – 3.74 (m, 2H), 2.45 (h, *J* = 4.1 Hz, 1H), 1.87 – 1.74 (m, 2H), 1.72 – 1.63 (m, 2H), 1.56 – 1.38 (m, 3H), 1.36 – 1.23 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.9, 136.9, 136.2, 131.7, 129.6, 127.3, 123.2, 122.9, 122.3, 119.8, 119.0, 111.3, 108.2, 93.0, 76.3, 65.9, 32.4, 32.4, 31.6, 29.2, 25.9, 24.9;HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.0910.



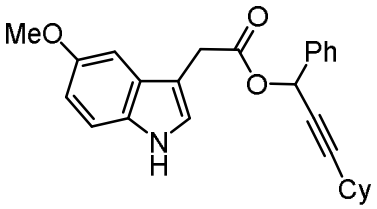
1d, 1-(4-(*tert*-butyl)phenyl)-3-cyclohexylprop-2-yn-1-yl 2-(1*H*-indol-3-yl)acetate

Compound 1d was obtained in 65% yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.58 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.51 – 7.46 (m, 2H), 7.43 – 7.36 (m, 2H), 7.32 (m, 1H), 7.21 – 7.17 (m, 1H), 7.13 – 7.09 (m, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 6.56 (d, *J* = 1.8 Hz, 1H), 3.91 – 3.74 (m, 2H), 2.56 – 2.35 (m, 1H), 1.87 – 1.76 (m, 2H), 1.70 (m, 2H), 1.59 – 1.43 (m, 4H), 1.35 (s, 13H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.2, 151.8, 136.2, 134.7, 127.7, 127.3, 125.6, 123.3, 122.2, 119.6, 119.1, 111.2, 108.2, 92.4, 76.9, 66.4, 34.7, 32.5, 32.5, 31.6, 31.4, 29.2, 26.0, 24.9; HRMS-TOF Calculated for [$C_{29}H_{33}NNaO_2$]: 450.2409; Found: 450.2457.



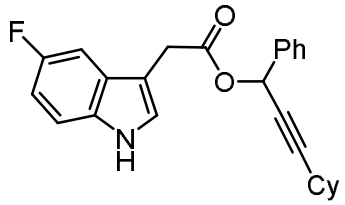
1e, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(5-methyl-1*H*-indol-3-yl)acetate

Compound 1e was obtained in 89% yield;^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 – 7.93 (m, 1H), 7.68 – 7.53 (m, 2H), 7.47 – 7.33 (m, 4H), 7.19 (d, *J* = 8.2 Hz, 1H), 7.05 (dd, *J* = 8.3, 1.6 Hz, 1H), 6.94 (d, *J* = 2.3 Hz, 1H), 6.63 (d, *J* = 1.8 Hz, 1H), 3.94 – 3.68 (m, 2H), 2.48 (s, 4H), 1.86 (m, 2H), 1.74 (m, 2H), 1.62 – 1.46 (m, 3H), 1.43 – 1.28 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.3, 137.7, 134.4, 128.7, 128.7, 128.6, 127.8, 127.4, 123.7, 123.5, 118.5, 111.0, 107.3, 92.6, 76.7, 66.5, 32.4, 32.4, 31.5, 29.1, 25.9, 24.8, 21.6;HRMS-TOF Calculated for [$C_{26}H_{27}NNaO_2$]: 408.1939; Found: 408.1978.



1f, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(5-methoxy-1*H*-indol-3-yl)acetate

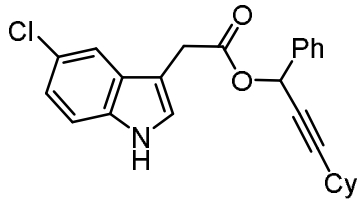
Compound 1f was obtained in 68% isolated yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.09 (s, 1H), 7.57 – 7.48 (m, 2H), 7.42 – 7.31 (m, 3H), 7.18 (d, *J* = 8.8 Hz, 1H), 7.02 (dd, *J* = 12.8, 2.4 Hz, 2H), 6.85 (dd, *J* = 8.8, 2.4 Hz, 1H), 6.56 (d, *J* = 1.8 Hz, 1H), 3.84 – 3.74 (m, 5H), 2.45 (q, *J* = 6.5, 4.2 Hz, 1H), 1.81 – 1.77 (m, 2H), 1.73 – 1.64 (m, 2H), 1.57 – 1.39 (m, 3H), 1.36 – 1.25 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.1, 171.1, 154.2, 154.1, 137.8, 131.3, 128.8, 128.7, 128.6, 127.8, 127.6, 127.6, 124.1, 112.6, 112.0, 112.0, 107.8, 107.8, 100.6, 92.6, 76.7, 66.5, 55.8, 32.4, 32.4, 31.6, 29.2, 25.9, 24.8; HRMS-TOF Calculated for [$C_{26}H_{27}NNaO_3$]: 424.1889; Found: 424.1935.



1g, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(5-fluoro-1*H*-indol-3-yl)acetate

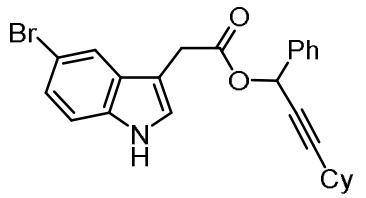
Compound 1g was obtained in 96% isolated yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.07 (s, 1H), 7.57 – 7.46 (m, 2H), 7.40 – 7.30 (m, 3H), 7.25 – 7.19 (m, 2H), 7.13 (d, *J* = 2.4 Hz, 1H), 6.96 – 6.88 (m, 1H), 6.53 (d, *J* = 1.9 Hz, 1H), 3.83 – 3.70 (m, 2H), 2.51 – 2.39 (m, 1H), 1.84 – 1.73 (m, 2H), 1.72 – 1.62 (m, 2H), 1.56 – 1.38 (m, 3H), 1.35 – 1.22 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.8, 158.8, 157.2, 137.7, 132.7, 128.9, 128.6, 127.9, 127.8, 127.7, 125.0, 111.9, 111.8, 110.8, 110.6, 108.6, 108.6, 104.3, 104.1, 92.8, 76.6, 66.7, 32.5, 32.4, 31.6, 29.2, 26.0, 24.9; ^{19}F NMR (376 MHz,

$CDCl_3$) δ -123.57 (td, *J* = 9.5, 4.3 Hz); HRMS-TOF Calculated for [$C_{25}H_{24}FNNaO_2$]: 412.1689; Found: 412.2082.



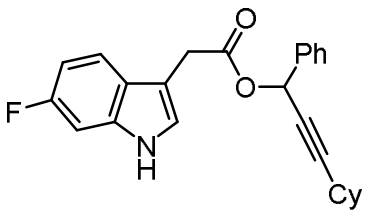
1h, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(5-chloro-1*H*-indol-3-yl)acetate

Compound 1h was obtained in 83% isolated yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.53 (d, *J* = 7.6 Hz, 3H), 7.42 – 7.31 (m, 3H), 7.17 (d, *J* = 8.6 Hz, 1H), 7.11 (m, 1H), 7.04 (d, *J* = 2.4 Hz, 1H), 6.53 (d, *J* = 1.8 Hz, 1H), 3.82 – 3.66 (m, 2H), 2.54 – 2.38 (m, 1H), 1.85 – 1.74 (m, 2H), 1.73 – 1.62 (m, 2H), 1.57 – 1.40 (m, 3H), 1.29 (t, *J* = 10.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.9, 137.6, 134.6, 128.9, 128.7, 128.4, 127.9, 125.5, 124.7, 122.6, 118.6, 112.3, 108.0, 92.8, 76.6, 66.8, 32.4, 32.4, 31.5, 29.2, 25.9, 24.9; HRMS-TOF Calculated for [$C_{25}H_{24}ClNNaO_2$]: 428.1393; Found: 428.1812.



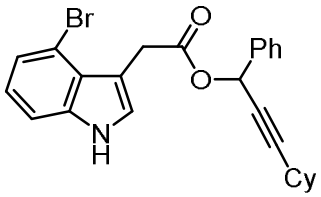
1i, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(5-bromo-1*H*-indol-3-yl)acetate

Compound 1i was obtained in 91% isolated yield;^{1}H NMR (600 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.70 (d, *J* = 1.8 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.43 – 7.34 (m, 3H), 7.22 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.06 (d, *J* = 8.6 Hz, 1H), 6.90 (d, *J* = 2.5 Hz, 1H), 6.56 (d, *J* = 1.8 Hz, 1H), 3.81 – 3.69 (m, 2H), 2.56 – 2.41 (m, 1H), 1.81 (dd, *J* = 10.9, 5.7 Hz, 2H), 1.69 (m, 2H), 1.59 – 1.22 (m, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.1, 137.6, 134.8, 128.9, 128.7, 127.9, 125.0, 124.7, 121.5, 112.9, 112.8, 107.5, 92.9, 76.6, 66.9, 32.4, 32.4, 31.4, 29.1, 25.9, 24.8; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.1345.



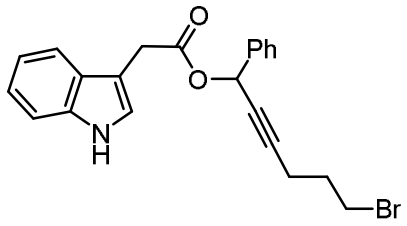
1j, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(6-fluoro-1*H*-indol-3-yl)acetate

Compound 1j was obtained in 80% isolated yield;[1]H NMR (600 MHz, $CDCl_3$) δ 8.32 – 8.17 (m, 1H), 7.65 – 7.53 (m, 2H), 7.46 (dd, *J* = 8.7, 5.2 Hz, 1H), 7.42 – 7.37 (m, 3H), 6.96 – 6.83 (m, 3H), 6.60 (d, *J* = 1.8 Hz, 1H), 3.86 – 3.75 (m, 2H), 2.58 – 2.42 (m, 1H), 1.91 – 1.78 (m, 2H), 1.71 (m, 2H), 1.61 – 1.43 (m, 3H), 1.40 – 1.25 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.2, 160.8, 159.3, 123.7, 123.7, 123.7, 119.7, 119.6, 108.4, 108.2, 107.9, 97.6, 97.4, 92.8, 77.4, 77.2, 76.9, 76.6, 66.8, 32.4, 32.4, 31.5, 29.1, 25.9, 24.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -120.44 (td, *J* = 9.6, 5.3 Hz); HRMS-TOF Calculated for [$C_{25}H_{24}FNNaO_2$]: 412.1689; Found: 412.2081.



1k, 3-cyclohexyl-1-phenylprop-2-yn-1-yl 2-(4-bromo-1*H*-indol-3-yl)acetate

Compound 1k was obtained in 92% isolated yield;[1]H NMR (500 MHz, $CDCl_3$) δ 8.46 (d, *J* = 2.6 Hz, 1H), 7.73 – 7.51 (m, 2H), 7.48 – 7.33 (m, 3H), 7.21 (d, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 8.1 Hz, 1H), 6.91 (t, *J* = 7.8 Hz, 1H), 6.67 (d, *J* = 2.2 Hz, 2H), 4.11 – 3.97 (m, 2H), 2.52 (m,1H), 1.94 – 1.80 (m, 2H), 1.74 (m, 2H), 1.53 (q, *J* = 10.3, 9.0 Hz, 3H), 1.34 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 172.4, 137.7, 137.6, 128.8, 128.6, 128.0, 125.8, 125.3, 123.6, 122.8, 113.8, 110.9, 108.1, 92.7, 76.7, 66.7, 32.5, 32.4, 32.3, 29.2, 25.9, 24.9; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.0880.

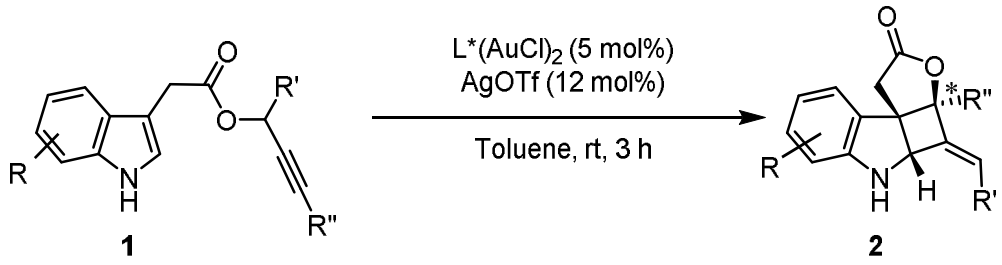


1l, 6-bromo-1-phenylhex-2-yn-1-yl 2-(1*H*-indol-3-yl)acetate

Compound 1l was obtained in 89% isolated yield;[1]H NMR (500 MHz, $CDCl_3$) δ 8.10 (s, 1H), 7.60 (d, *J* = 7.9 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.44 – 7.35 (m, 3H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.24 – 7.18 (m, 1H), 7.13 (m, 1 Hz, 1H), 7.05 (d, *J* = 2.4 Hz, 1H), 6.53 (t, *J* = 2.0 Hz, 1H), 3.97 – 3.72 (m, 2H), 3.44 (t, *J* = 6.5 Hz, 2H), 2.45 (m,1 Hz, 2H), 2.01 (m, 2H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 171.1, 137.3, 136.1, 128.9, 128.7, 127.7, 127.2, 123.3, 122.2, 119.6, 118.9, 111.3, 107.9, 86.3,

78.0, 66.4, 32.5, 31.5, 31.1, 17.6; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 432.0575; Found: 432.0580.

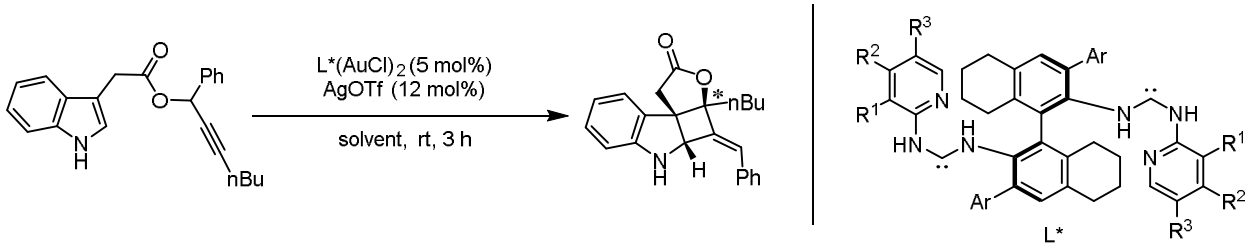
Enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction:



The corresponding gold(I) pre-catalyst L*$(AuCl)_2$ (0.0025 mmol, 0.05 equiv) and silver triflate (1.6 mg,0.006 mmol, 0.12 equiv) were weighed in a dram vial and toluene was added (1.0 mL). The heterogeneous mixture was sonicated for 5 min using a commercial ultrasonic cleaner, and then filtered through glass fiber into a second dram vial, which had been pre-weighed with substrate **1** (0.05 mmol, 1.0 equiv). The reaction vial was wrapped in aluminum foil and kept at room temperature for 3 h without stirring and then the reaction was quenched by addition of Et_3N (ca. 200 μL, 1.4 mmol). The reaction solvent was then removed in vacuo and the crude reaction mixture was re-dissolved in Et_2O and passed through a plug of silica gel to remove the catalyst. The solvent was again removed in vacuo and a solution of 1,3,5-trimethoxybenzene in $CDCl_3$ (1.0 mL, 0.03 M) was added via syringe for ^{1}HNMR analysis. A small portion of this sample was diluted with 85:15 hexanes:isopropanol and subjected to chiral HPLC analysis. For spectral data purpose, the crude mixture was purified by column chromatography Hexanes → 4:1 Hexanes/Ether.

Reaction optimization:

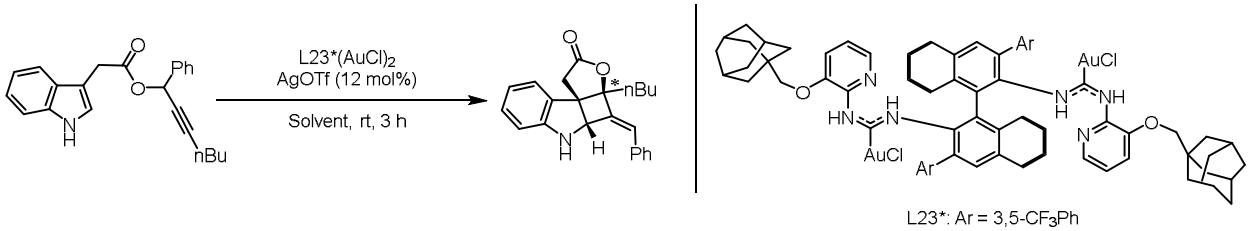
ee trends in DCM and Toluene



Pre-catalyst	Ar	R^1	R^2	R^3	% ee in DCM	% ee in Toluene
1	3,5-CH_3Ph	H	H	H	+30	+39
2	3,5-OMePh	H	H	H	+59	+50
3	3,5-CF_3Ph	H	H	H	+37	+35
4	3,5-CF_3Ph	Me	H	H	-9	-5
5	3,5-CF_3Ph	H	OMe	H	+52	+62
6	3,5-CF_3Ph	O(4-tBuPh)	H	H	-40	-44
7	3,5-CF_3Ph	OCH_2Cy	H	H	-63	-80
8	3,5-CF_3Ph	OCH_2tBu	H	H	-72	-80
9	3,5-CF_3Ph	OCH_2CH_2tButyl	H	H	-56	-79
10	3,5-CF_3Ph	OCH_2Adamantyl	H	H	-72	-81

ee was determined by chiral HPLC analysis and are averages from two runs. '+' sign represents (*R,R,R*)-isomer and '–' sign represents (*S,S,S*)- isomer.

Solvent optimization:

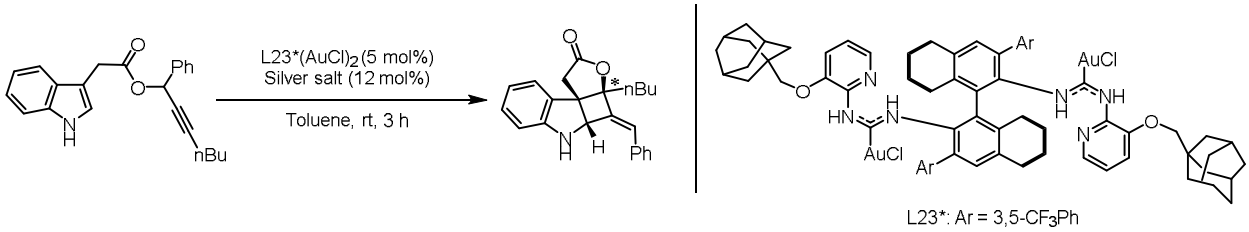


Entry	Solvent	% Yield	% ee
1	Benzene	89	-81
2	Cyclohexane	65	-69
3	Hexanes	ND	ND

4	Trichloroethelene	91	-75
5	Xylene	91	-81
6	Toluene	98	-82
7	Toluene:DCM (5:1)	96	-78
8	Toluene:DCM (1:5)	94	-79
9	DCM	95	-72

[a]Unless otherwise noted, all reactions were carried out with 1a (0.05 mmol) for 3 h. [b]Yields are determined by NMR spectroscopy with 1,3,5- trimethoxybenzene as internal standard. [c]ee was determined by chiral HPLC analysis and are averages from two runs. '+' sign represents (*R*,*R*,*R*)-isomer and '–' sign represents (*S*,*S*,*S*)- isomer.

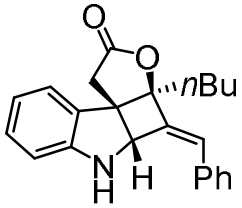
Silver salt optimization



Entry	Silver salt	% Yield	% ee
1	AgOAc	ND	ND
2	$AgBF_4$	74	-82
3	$AgNTf_2$	45	-26
4	AgONf	85	-75
5	AgPFBS	90	-77
6	AgONs	93	-80
7	4-CF_3-$PhSO_3Ag$	87	-80
8	3,5-CF_3-$PhSO_3Ag$	74	-80
9	AgOTf	98	-82

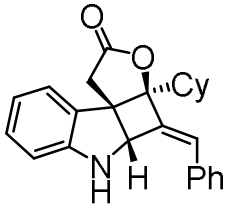
[a]Unless otherwise noted, all reactions were carried out with 1a (0.05 mmol) for 3 h. [b]Yields are determined by NMR spectroscopy with 1,3,5- trimethoxybenzene as internal standard. [c]ee was determined by chiral HPLC analysis and are averages from two runs. '+' sign represents (*R*,*R*,*R*)-isomer and '–' sign represents (*S*,*S*,*S*)- isomer.

Product Purification/Characterization Data



Product 2a

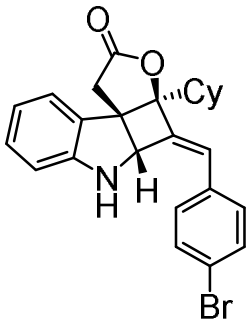
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2a, was isolated as white solid in 92% yield.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 4.4 Hz, 4H), 7.36 – 7.29 (m, 1H), 7.13 (m, 2H), 6.84 (m, 1H), 6.67 (d, *J* = 7.8 Hz, 1H), 6.62 (d, *J* = 1.8 Hz, 1H), 5.02 (d, *J* = 2.1 Hz, 1H), 4.40 (s, 1H), 3.19 – 3.02 (m, 2H), 1.84 (m, 1H), 1.69 – 1.54 (m, 1H), 1.51 – 1.36 (m, 2H), 1.27 (m, 2H), 0.86 (m, 3H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.7, 152.9, 144.2, 135.2, 129.5, 129.0, 128.9, 128.5, 128.4, 125.7, 124.3, 119.8, 111.5, 96.9, 67.1, 58.8, 39.3, 32.2, 25.5, 23.0, 14.0; $[\alpha]_D^{20}$ = –429 (c = 0.875,$CHCl_3$);HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 11.72 min,t_2 = major: 13.57 min. 82% ee; HRMS-TOF Calculated for [$C_{23}H_{23}NNaO_2$]: 368.1621; Found: 368.1614.



Product 2b

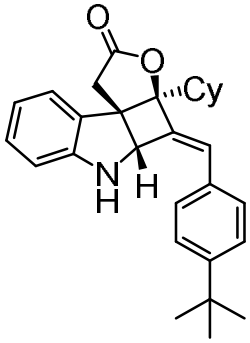
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2b, was isolated as white solid in 69% yield.^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 4.4 Hz, 4H), 7.36 – 7.28 (m, 1H), 7.20 – 7.11 (m, 2H), 6.83 (m, 1H), 6.73 – 6.64 (m, 2H), 4.92 (d, *J* = 1.8 Hz, 1H), 4.43 (s, 1H), 3.23 – 2.95 (m, 2H), 2.00 – 1.85 (m, 1H), 1.80 – 1.54 (m, 5H), 1.41 – 1.23 (m, 1H), 1.19 – 0.97 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.9, 153.4, 143.4, 135.4, 130.7, 129.5, 128.9, 128.4, 126.0, 124.8, 119.6, 111.2, 99.1, 67.8, 58.8, 41.1, 39.7, 26.7, 26.5, 26.2, 26.1, 26.0; $[\alpha]_D^{20}$ = –343 (c = 0.683, $CHCl_3$); HPLC:

IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 11.55 min,t_2 =major: 13.54 min. 91% ee; HRMS-TOF Calculated for [$C_{25}H_{25}NNaO_2$]: 394.1783; Found: 394.1794.



Product 2c

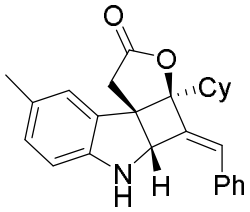
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2c, was isolated as white solid in 84% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.46 (m, 2H), 7.35 – 7.25 (m, 2H), 7.26 – 7.13 (m, 1H), 6.88 (m, 1H), 6.74 (d, *J* = 7.8 Hz, 1H), 6.64 (d, *J* = 1.7 Hz, 1H), 4.90 (s, 1H), 4.41 (s, 1H), 3.27 – 2.99 (m, 2H), 2.00 – 1.86 (m, 1H), 1.84 – 1.55 (m, 5H), 1.32 (m, 1H), 1.23 – 0.98 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.7, 153.3, 144.5, 134.3, 132.1, 129.9, 129.6, 129.6, 126.0, 124.9, 122.5, 119.9, 111.4, 98.9, 67.8, 59.0, 41.1, 39.7, 26.7, 26.5, 26.2, 26.1, 26.0; $[\alpha]_D^{20}$ = –289 (c = 0.43, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 10.48 min,t_2 = major: 12.99 min. 86% ee; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.0880.



Product 2d

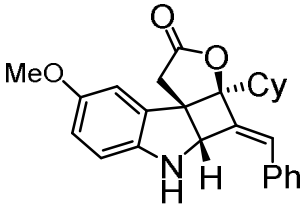
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reactionwith L23*$(AuCl)_2$ pre-catalyst, compound 2d, was isolated as white solid in 60% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.41 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.20 – 7.11 (m,

2H), 6.83 (m, 1H), 6.68 (d, *J* = 7.8 Hz, 1H), 6.64 (d, *J* = 1.7 Hz, 1H), 4.97 – 4.89 (m, 1H), 4.41 (s, 1H), 3.19 – 2.99 (m, 2H), 1.89 (m, 1H), 1.78 – 1.66 (m, 3H), 1.67 – 1.53 (m, 3H), 1.34 (s, 10H), 1.16 – 0.97 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 153.4, 151.7, 142.4, 132.6, 130.4, 129.5, 128.2, 126.2, 125.9, 124.8, 119.6, 111.2, 99.3, 67.8, 58.8, 41.2, 39.7, 34.9, 31.4, 26.7, 26.6, 26.3, 26.2, 26.1; $[\alpha]_D^{20}$ = –411 (c = 0.575, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 9.46 min,t_2 = major: 10.77 min. 94% ee; HRMS-TOF Calculated for [$C_{29}H_{33}NNaO_2$]: 450.2409; Found: 450.2394.



Product 2e

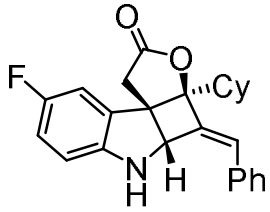
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reactionwith L23*$(AuCl)_2$ pre-catalyst, compound 2e, was isolated as white solid in 85% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 – 7.36 (m, 4H), 7.30 (m, 1H), 6.99 (d, *J* = 1.6 Hz, 1H), 6.96 (dd, *J* = 8.1, 1.7 Hz, 1H), 6.66 (d, *J* = 1.8 Hz, 1H), 6.62 (d, *J* = 7.9 Hz, 1H), 4.89 (d, *J* = 1.8 Hz, 1H), 4.29 (s, 1H), 3.21 – 2.93 (m, 2H), 2.30 (s, 3H), 1.90 (m, 1H), 1.79 – 1.55 (m, 6H), 1.39 – 1.24 (m, 1H), 1.15 – 1.01 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.9, 151.2, 143.6, 135.4, 130.7, 130.0, 129.3, 128.9, 128.5, 128.4, 126.5, 125.3, 111.4, 99.0, 68.1, 58.9, 41.2, 39.7, 26.8, 26.6, 26.3, 26.2, 26.0, 21.0; $[\alpha]_D^{20}$ = –344 (c = 0.65, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = major: 10.02 min,t_2 = minor: 11.58 min. 89% ee; HRMS-TOF Calculated for [$C_{26}H_{27}NNaO_2$]: 408.1939; Found: 408.1935.



Product 2f

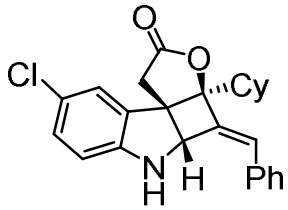
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2f, was isolated as white solid in 66% yield.

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 – 7.35 (m, 4H), 7.34 – 7.28 (m, 1H), 6.79 – 6.71 (m, 2H), 6.69 – 6.64 (m, 2H), 4.90 (d, *J* = 1.8 Hz, 1H), 4.18 (s, 1H), 3.77 (s, 3H), 3.20 – 2.97 (m, 2H), 1.90 (m, 1H), 1.80 – 1.55 (m, 5H), 1.40 – 1.23 (m, 1H), 1.20 – 0.98 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.8, 154.3, 147.2, 143.4, 135.3, 131.0, 128.9, 128.5, 128.4, 127.9, 115.1, 112.6, 111.0, 99.0, 68.5, 59.3, 56.3, 41.2, 39.6, 26.8, 26.7, 26.2, 26.2, 26.1; $[\alpha]_D^{20}$ = –351 (c = 1.025, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 18.48 min,t_2 = major: 20.42 min. 92% ee; HRMS-TOF Calculated for [$C_{26}H_{27}NNaO_3$]: 424.1889; Found: 424.1847.



Product 2g

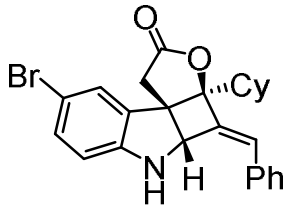
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2g, was isolated as white solid in 80% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39 (d, *J* = 4.4 Hz, 4H), 7.31 (m, 1H), 6.93 – 6.82 (m, 2H), 6.67 (d, *J* = 1.8 Hz, 1H), 6.63 (dd, *J* = 8.5, 4.3 Hz, 1H), 4.93 (s, 1H), 4.32 (s, 1H), 3.06 (s, 2H), 1.96 – 1.85 (m, 1H), 1.81 – 1.57 (m, 5H), 1.40 – 1.23 (m, 1H), 1.22 – 0.99 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.4, 158.3, 156.4, 149.5, 143.0, 135.2, 131.0, 128.9, 128.5, 128.5, 127.9, 127.8, 116.1, 116.0, 112.0, 111.9, 111.9, 111.8, 99.0, 68.6, 59.1, 59.1, 41.2, 39.6, 26.8, 26.7, 26.2, 26.1, 26.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -123.42 (td, *J* = 8.4, 4.2 Hz); $[\alpha]_D^{20}$ = –330 (c = 0.61, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 10.61 min,t_2 = major: 17.41 min. 92% ee; HRMS-TOF Calculated for [$C_{25}H_{24}FNNaO_2$]: 412.1689; Found: 412.1687.



Product 2h

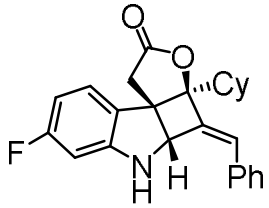
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2h, was isolated as white solid in 66% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 – 7.29 (m, 5H), 7.16 – 7.05 (m, 2H), 6.67 (d, *J* = 1.7 Hz, 1H), 6.59 (d, *J* = 8.4 Hz, 1H), 5.02 – 4.90 (m, 1H), 4.39 (d, *J* = 4.1 Hz, 1H), 3.06 (s, 2H), 1.96 – 1.85

(m, 1H), 1.81 – 1.50 (m, 5H), 1.37 – 1.22 (m, 2H), 1.20 – 0.96 (m, 4H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.3, 152.0, 142.8, 135.2, 131.0, 129.5, 129.0, 128.6, 128.4, 128.0, 124.9, 124.2, 111.9, 99.0, 68.3, 58.8, 41.3, 39.6, 26.8, 26.8, 26.3, 26.2, 26.0); $[\alpha]_D^{20}$ = –294 (c = 0.4, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 11.21 min,t_2 = major: 12.21 min. 88% ee; HRMS-TOF Calculated for [$C_{25}H_{24}ClNNaO_2$]: 428.1393; Found: 428.1384



Product 2i

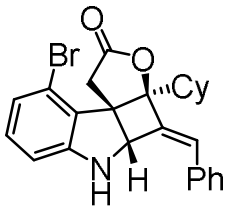
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2i, was isolated as white solid in 72% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.32 (m, 5H), 7.31 – 7.19 (m, 3H), 6.70 (s, 1H), 6.58 (d, *J* = 8.3 Hz, 1H), 4.97 (q, *J* = 1.8 Hz, 1H), 4.53 – 4.37 (m, 1H), 3.09 (s, 2H), 1.93 (d, *J* = 12.0 Hz, 1H), 1.84 – 1.56 (m, 5H), 1.43 – 0.97 (m, 5H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.3, 152.4, 142.8, 135.2, 132.3, 130.9, 129.0, 128.6, 128.4, 128.4, 127.8, 112.4, 110.9, 99.1, 68.2, 58.7, 41.2, 39.6, 26.8, 26.7, 26.2, 26.1, 26.0; $[\alpha]_D^{20}$ = –361 (c = 0.53, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = major: 11.22 min,t_2 = minor: 12.05 min. 90% ee; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.0884.



Product 2j

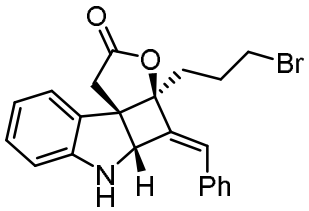
Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2j, was isolated as white solid in 80% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 – 7.29 (m, 5H), 7.06 (dd, *J* = 8.3, 5.4 Hz, 1H), 6.67 (d, *J* = 1.8 Hz, 1H), 6.55 – 6.43 (m, 1H), 6.42 – 6.24 (m, 1H), 4.97 (s, 1H), 4.49 (s, 1H), 3.19 – 2.95 (m, 2H), 1.91 (d, *J* = 12.6 Hz, 1H), 1.81 – 1.53 (m, 6H), 1.36 – 1.23 (m, 1H), 1.19 – 0.99 (m, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.5, 165.1, 163.5, 154.9, 154.8, 142.9, 135.3, 130.8, 129.0, 128.6, 128.4, 125.5, 125.5, 121.5, 121.5, 106.0, 105.8, 98.9, 98.5, 98.3, 68.5, 58.0, 41.2, 39.6, 26.8, 26.6, 26.3,

26.1, 26.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -111.79 (td, *J* = 9.2, 5.0 Hz); $[\alpha]_D^{20}$ = –303 (c = 0.5, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 9.72 min,t_2 = major: 13.50 min. 84% ee; HRMS-TOF Calculated for [$C_{25}H_{24}FNNaO_2$]: 412.1689; Found: 412.1685.



Product 2k

Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reaction with L23*$(AuCl)_2$ pre-catalyst, compound 2b, was isolated as white solid in 34% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 – 7.37 (m, 2H), 7.37 – 7.30 (m, 3H), 6.99 – 6.94 (m, 1H), 6.90 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.72 (d, *J* = 1.7 Hz, 1H), 6.57 (dd, *J* = 7.8, 1.1 Hz, 1H), 4.87 (dd, *J* = 4.0, 1.8 Hz, 1H), 4.49 (d, *J* = 4.1 Hz, 1H), 4.13 (d, *J* = 19.1 Hz, 1H), 2.83 (d, *J* = 19.1 Hz, 1H), 2.06 (m, 2H), 1.75 (d, *J* = 10.6 Hz, 1H), 1.65 – 1.57 (m, 2H), 1.56 (s, 1H), 1.46 – 1.35 (m, 1H), 1.21 – 1.03 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 175.6, 155.4, 142.8, 135.3, 131.0, 130.9, 129.0, 128.6, 128.4, 124.5, 124.1, 120.4, 109.6, 99.2, 68.5, 59.5, 42.5, 37.6, 28.4, 27.9, 26.6, 26.4, 26.4; $[\alpha]_D^{20}$ = –13.8 (c = 0.66, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = 8.54 min,t_2 = 9.23 min. 3% ee;HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 472.0888; Found: 472.0886.



Product 2l

Following the general procedure for enantioselective tandem 3,3-rearrangement-[2+2]cyclization reactionwith L23*$(AuCl)_2$ pre-catalyst, compound 2b, was isolated as white solid in 67% yield. ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.40 (d, *J* = 5.7 Hz, 4H), 7.36 – 7.30 (m, 1H), 7.18 – 7.09 (m, 2H), 6.86 (m, 1H), 6.69 (d, *J* = 7.9 Hz, 1H), 6.63 (d, *J* = 1.8 Hz, 1H), 5.02 (d, *J* = 1.8 Hz, 1H), 3.42 – 3.27 (m, 2H), 3.11 (d, *J* = 2.6 Hz, 2H), 2.03 – 1.90 (m, 3H), 1.79 (m, 1H); ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.8, 154.3, 147.2, 143.4, 135.3, 131.0, 128.9, 128.5, 128.4, 127.9, 115.1, 112.6, 111.0,

99.0, 68.5, 59.3, 56.3, 41.2, 39.6, 26.8, 26.7, 26.2, 26.2, 26.1; $[\alpha]_D^{20}$ = –388 (c = 0.38, $CHCl_3$); HPLC: IC column, 85:15 hexanes:isopropanol, 1.00 mL/min, t_1 = minor: 13.75 min, t_2 = major: 16.81 min. 84% ee; HRMS-TOF Calculated for [$C_{25}H_{24}BrNNaO_2$]: 432.0575; Found: 432.0570.

Determination of absolute stereochemistry through VCD experiment

1. **VCD Measurement and Calculations**
2. **Overlay of VCD and IR Spectra**
3. **Assigned Absolute Configuration**
4. **Conformations, Electronic Energies, and Coordinates of global and local minima**

VCD Measurements and Calculations

Sample was dissolved in $CDCl_3$ (48.5 mg/mL final concentration for compound **2g**, and 50 mg/mL for compound **2c**). All experiments were performed using a 0.10-mm path length cell with BaF_2 windows. The IR and VCD spectra were recorded using a Chiral*IR*™ VCD spectrometer equipped with the Dual PEM accessory (BioTools, Jupiter, FL), with 4 cm^{-1} resolution. A dry N_2 purge was used to eliminate water from the instrument. Data was collected in blocks, where the instrument recorded ~3000 scans over the course of 1 h and averaged those scans into one block. Each of the runs involved averaging eight blocks for each sample, as well as the solvent. The solvent background average was then subtracted from the sample average. Collection times for sample and solvent ranged were approximately eight hours each.

The general approach for VCD assignment at Merck, including the details computational workflow, has been published elsewhere.[1,2] A subset of the details of the computational methodology is provided here. Conformers of each test structure were geometry optimized at the B3LYP/6-31G** level and stationary points were confirmed by performing frequency calculations.[3-11] All calculations were performed using Gaussian 09.[12] Frequency calculations output the IR and VCD spectra.[13] Frequencies were scaled by a value of 0.98, but owing to the secondary scaling and shifting of the calculated VCD and IR spectra (during extraction of VCD by BioTools ViewVCD and during spectra alignment detailed below) in comparison to the experimental spectra, this initial scaling was, to some extent, arbitrary.

Output conformers were ranked according to DFT energy and a clustering was performed to remove duplicates. Initial identification of duplicates was performed solely on an electronic energy basis where compounds were considered identical if the difference in Hartrees was less

than 0.01. Rounding the differences led to inconsistencies in identification of duplicates. It became better to cluster the DFT minima by energy and then re-cluster each energy bucket by structure using an all atom RMS of 0.6 Å. This faithfully removed only identical compounds. Two Boltzmann distributions were calculated based on electronic energy (E) and free energy (G).

The in-house method for comparing VCD and IR spectra is based on published methodology.[14] We used the same formulas for calculating similarity for IR and VCD spectra of experimental and observed curves. Based on our experience in matching the curves by hand we introduced the following modifications to the algorithm: we scale the spectra (0 to 1 for IR, -1 to 1 for VCD) before comparing them; we isolate each peak for movement rather than groups of peaks; we isolate peaks independently for IR and VCD spectra; when looking for the best match we move the experimental peak only to higher frequencies with a maximum shift of 20 cm^{-1}; if the user sees that the baseline of the spectrum is not corrected the user can ask the program to correct the baseline. For all figures contained in the manuscript, the output intensities from Gaussian for IR $\Delta\varepsilon$ (molar absorptivity) and VCD $\Delta\varepsilon$ are D (10^{-40} esu^2 cm^2) and R (10^{-44} esu^2 cm^2), respectively. However, owing to scaling all peaks the intensities are labeled only as 'scaled'.

Calculations of the VCD and IR spectra involved modeling the *SSS* configuration (Figures S1-S2) provide the overlays of the calculated and measured IR and VCD spectra. A high degree of confidence is derived from the statistical and visual matching of the spectra. Assigned absolute configuration of the desired compounds is provided in Scheme S1.

Overlay of VCD and IR Spectra

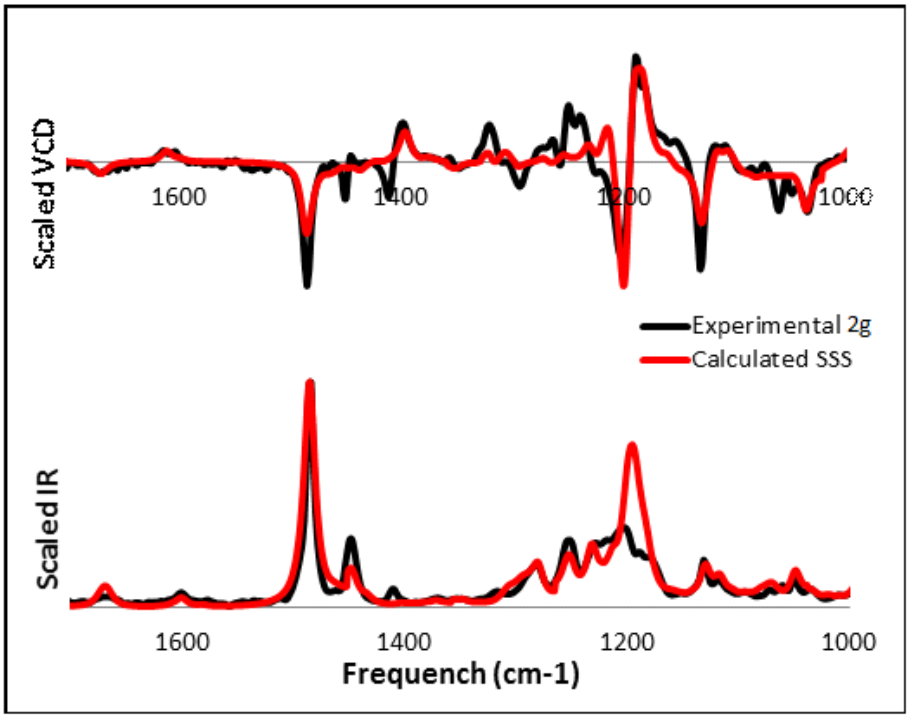


Figure S1: Overlay of measured (black) and calculated (red) VCD and IR spectra for compound **2g**.

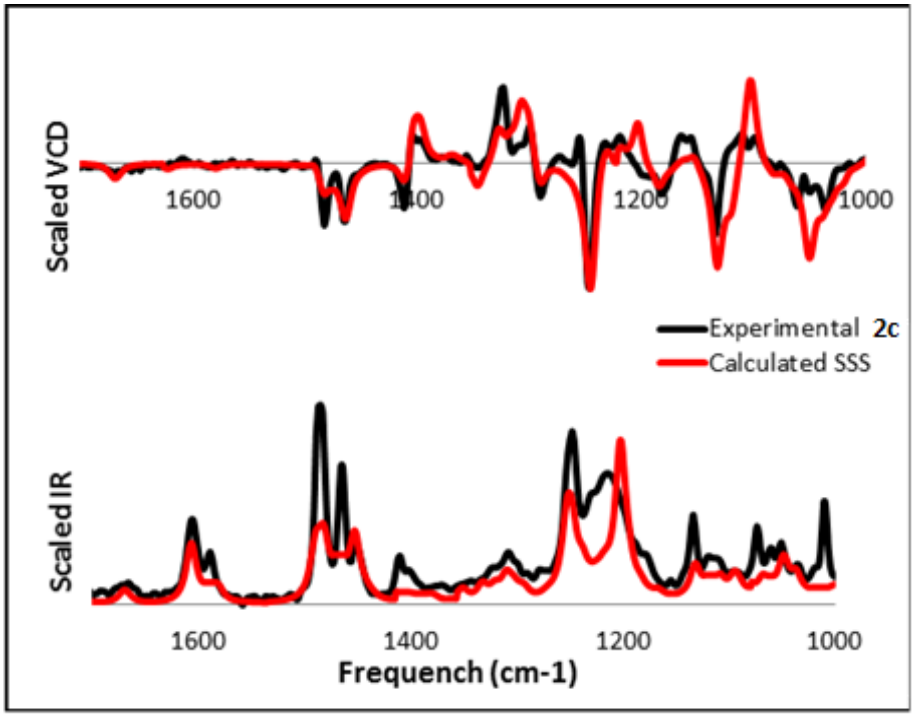
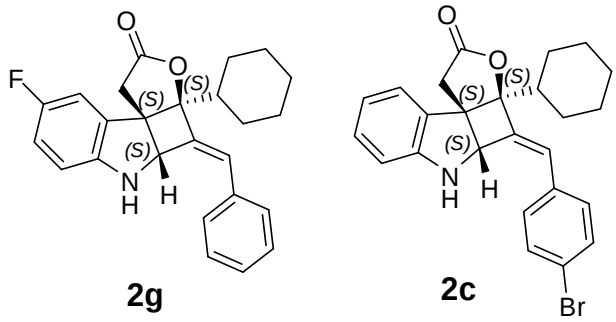


Figure S2: Overlay of measured (black) and calculated (red) VCD and IR spectra for compound **2c**.

Assigned Absolute Configuration



Scheme S1: Assigned absolute configuration of *SSS* for compounds **2g** and **2c**.

Conformations, Electronic Energies, and Coordinates of global and local minima
<u>Compound 2g:</u>

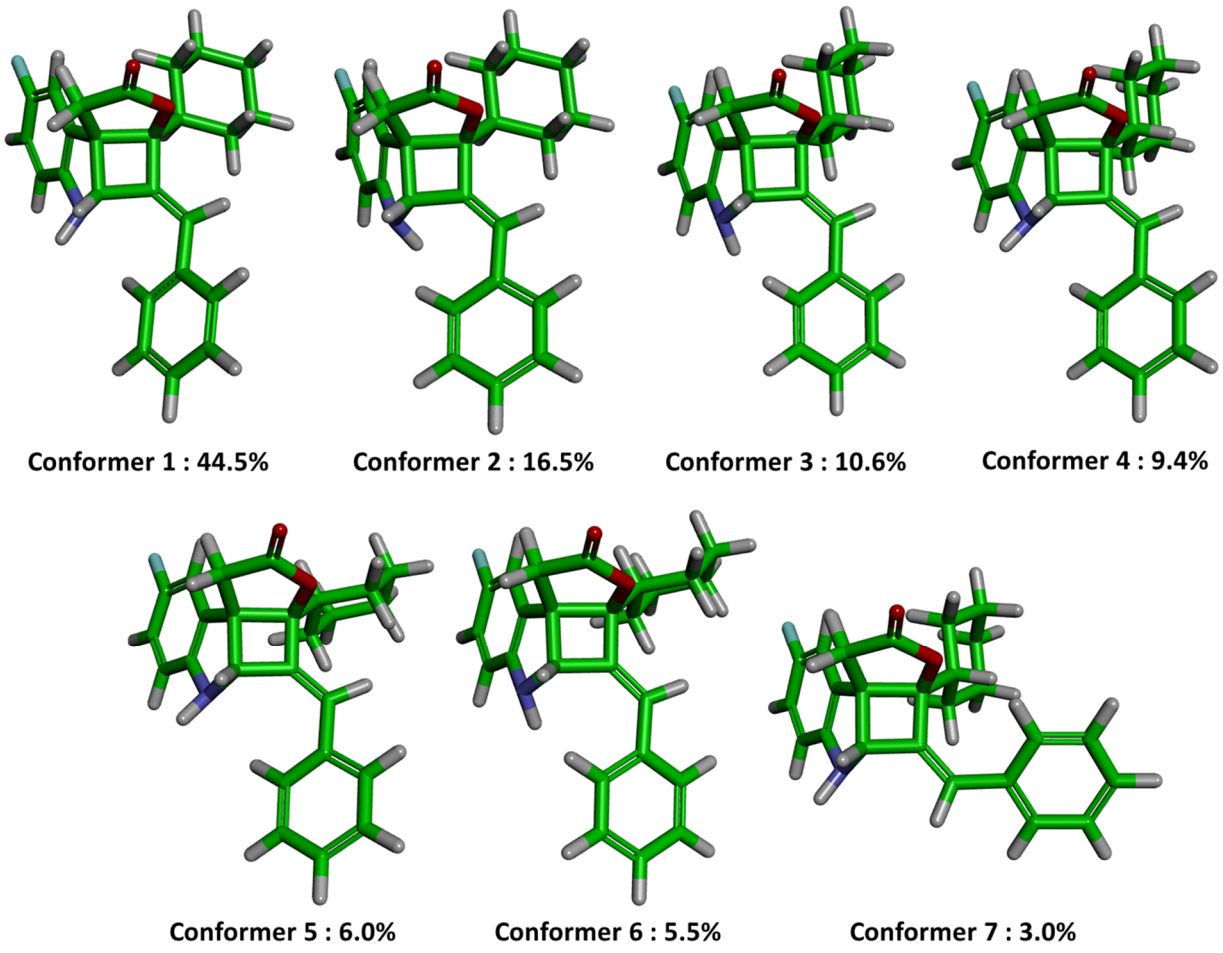


Figure S3: Conformers of the calculated *SSS* minima of compound **2g** contributing >2% to the Boltzmann distribution, percentages shown above based on *in vacuo* electronic energies.

Coordinates and electronic energies for B3LYP/6-31G conformational minima contributing >2% to the *in vacuo* Boltzmann distribution.**

Conformer 1
B3LYP/6-31G** Energy = -1272.170154 hartrees

6	3.0256	1.49541	0.550382
6	3.74825	2.40014	-0.22331
6	3.13757	3.24288	-1.14574
6	1.75146	3.19156	-1.31322
6	1.01161	2.29521	-0.53969
6	1.64495	1.43877	0.379057
7	-0.38338	2.11453	-0.55935
6	-0.75655	1.19775	0.536687
6	0.602932	0.617847	1.09058
6	-1.18596	-0.21304	0.168661
6	0.166766	-0.82176	0.538147
8	0.064321	-1.69133	1.69211
6	0.297698	-1.0366	2.86559
6	0.744235	0.398711	2.59341
6	-2.37261	-0.78396	-0.08081
6	-3.6535	-0.09575	-0.29673
6	-3.73213	1.18649	-0.87085
6	-4.96474	1.81214	-1.04746
6	-6.14304	1.17018	-0.66141
6	-6.08176	-0.11163	-0.11017
6	-4.85121	-0.74057	0.061788
8	0.175864	-1.57165	3.93566
1	-1.41967	1.69449	1.25603
6	0.994748	-1.51886	-0.55017
6	0.228902	-2.67774	-1.22249
6	1.06089	-3.34453	-2.32969
6	2.42373	-3.82332	-1.81244
6	3.18749	-2.67852	-1.13437
6	2.35268	-2.02657	-0.02078
9	5.09102	2.46341	-0.0656
1	1.782	0.496071	2.93014
1	0.149861	1.08582	3.20237
1	-0.71188	-2.31044	-1.64409
1	-0.02851	-3.42355	-0.45831
1	1.21649	-2.62344	-3.14488
1	0.49923	-4.18198	-2.76038

1	3.01645	-4.24426	-2.63331
1	2.27169	-4.63512	-1.08721
1	3.44669	-1.9189	-1.88528
1	4.13509	-3.04347	-0.72089
1	2.91901	-1.20589	0.429945
1	2.16786	-2.75921	0.773851
1	1.18728	-0.75456	-1.31705
1	3.55019	0.87456	1.26909
1	3.74816	3.93109	-1.71981
1	1.26139	3.8469	-2.02654
1	-2.41705	-1.87191	-0.08093
1	-2.82368	1.66387	-1.22222
1	-5.00769	2.79809	-1.50164
1	-7.10265	1.65858	-0.80234
1	-6.99433	-0.62311	0.181621
1	-4.80847	-1.7384	0.490292
1	-0.92262	2.97085	-0.59468

Conformer 2

B3LYP/6-31G** Energy = -1272.169216 hartrees

6	3.03663	1.52416	0.471026
6	3.7347	2.35085	-0.40745
6	3.09327	3.12343	-1.36856
6	1.69753	3.10378	-1.44991
6	0.982878	2.2887	-0.57147
6	1.65007	1.48069	0.366147
7	-0.41803	2.21285	-0.44077
6	-0.74263	1.24496	0.631386
6	0.631531	0.673311	1.12999
6	-1.16927	-0.14949	0.221613
6	0.184603	-0.7684	0.583479
8	0.067472	-1.62086	1.74866
6	0.343645	-0.96624	2.91453
6	0.814186	0.458285	2.62602
6	-2.3451	-0.70817	-0.10443
6	-3.65365	-0.06837	-0.29796
6	-4.77662	-0.90274	-0.45711
6	-6.05216	-0.37484	-0.63824
6	-6.23755	1.00785	-0.66962
6	-5.13509	1.85241	-0.52032
6	-3.85886	1.32553	-0.33939

8	0.233999	-1.49576	3.98826
1	-1.37652	1.71935	1.39175
6	1.01829	-1.48539	-0.48796
6	0.253049	-2.63734	-1.17271
6	1.10212	-3.32372	-2.25533
6	2.44702	-3.81565	-1.705
6	3.20991	-2.6749	-1.01938
6	2.35875	-2.00757	0.072253
9	5.0845	2.39758	-0.32095
1	1.86258	0.533769	2.93391
1	0.250652	1.16001	3.24771
1	-0.66954	-2.25889	-1.62369
1	-0.03722	-3.3737	-0.41126
1	1.28538	-2.61087	-3.07211
1	0.539288	-4.15695	-2.69261
1	3.05145	-4.2505	-2.50983
1	2.26891	-4.61951	-0.97705
1	3.49369	-1.92336	-1.76946
1	4.14417	-3.04783	-0.58347
1	2.92449	-1.19157	0.532483
1	2.14783	-2.73424	0.865574
1	1.24013	-0.72848	-1.25433
1	3.5872	0.938073	1.19937
1	3.68591	3.74746	-2.02841
1	1.18208	3.7296	-2.1716
1	-2.35848	-1.79064	-0.21448
1	-4.639	-1.98049	-0.43148
1	-6.90048	-1.04261	-0.75572
1	-7.22985	1.42455	-0.81353
1	-5.26889	2.92988	-0.54943
1	-3.02429	2.00953	-0.23825
1	-0.92899	2.07525	-1.3053

Conformer 3

B3LYP/6-31G** Energy = -1272.168797 hartrees

6	2.68434	1.61366	0.363366
6	3.01292	2.759	-0.35901
6	2.05074	3.66571	-0.78931
6	0.706608	3.4497	-0.47166
6	0.361165	2.31187	0.260096
6	1.34228	1.38013	0.646157

7	-0.90391	1.98129	0.767395
6	-0.84037	0.637408	1.35673
6	0.685923	0.239245	1.38218
6	-1.12008	-0.56629	0.465369
6	0.29291	-1.11252	0.625282
8	0.292507	-2.11154	1.69491
6	0.811631	-1.65406	2.87085
6	1.27662	-0.21199	2.70844
6	-2.15267	-1.00105	-0.26884
6	-3.49638	-0.42036	-0.40297
6	-4.30818	-0.84739	-1.46992
6	-5.5839	-0.32244	-1.66193
6	-6.08476	0.638781	-0.78274
6	-5.30023	1.06218	0.292691
6	-4.02325	0.539695	0.483241
8	0.872767	-2.34345	3.85483
1	-1.34569	0.614119	2.3306
6	1.02734	-1.73945	-0.56825
6	2.47354	-2.15696	-0.22753
6	3.13719	-2.89958	-1.39782
6	3.09149	-2.07762	-2.69295
6	1.65463	-1.65401	-3.02784
6	0.997881	-0.898	-1.86145
9	4.31393	2.99093	-0.65418
1	2.37274	-0.20326	2.69459
1	0.958172	0.385328	3.56662
1	2.47962	-2.78901	0.665471
1	3.06326	-1.25997	0.005067
1	2.61757	-3.85518	-1.55612
1	4.17271	-3.14952	-1.13871
1	3.5236	-2.6499	-3.52237
1	3.7141	-1.17957	-2.5746
1	1.05987	-2.54882	-3.26222
1	1.6415	-1.0279	-3.92769
1	-0.03236	-0.63382	-2.11982
1	1.53106	0.045092	-1.69945
1	0.468405	-2.66774	-0.77036
1	3.47213	0.93332	0.669008
1	2.36066	4.53862	-1.35337
1	-0.04921	4.16681	-0.77631
1	-1.98122	-1.88986	-0.87595
1	-3.92507	-1.59774	-2.1565
1	-6.18826	-0.66629	-2.49616

1	-7.07987	1.04813	-0.92789
1	-5.68814	1.79679	0.992367
1	-3.44669	0.860211	1.34393
1	-1.70352	2.16861	0.174639

Conformer 4

B3LYP/6-31G** Energy = -1272.168679 hartrees

6	2.95986	1.25742	0.606963
6	3.6038	2.31041	-0.03693
6	2.90602	3.34449	-0.65312
6	1.50943	3.33755	-0.63549
6	0.84794	2.29151	0.010314
6	1.56696	1.24671	0.617202
7	-0.54693	2.12851	0.134809
6	-0.80177	0.935205	0.963722
6	0.609991	0.289909	1.27626
6	-1.21558	-0.35352	0.265427
6	0.111577	-1.0468	0.555386
8	-0.05546	-2.01408	1.63551
6	0.310604	-1.53201	2.85517
6	0.910507	-0.13884	2.70776
6	-2.34601	-0.84965	-0.25466
6	-3.63876	-0.17393	-0.42912
6	-4.81492	-0.94592	-0.4341
6	-6.06453	-0.3466	-0.56954
6	-6.16367	1.03796	-0.72184
6	-5.00309	1.81433	-0.74603
6	-3.752	1.21773	-0.60357
8	0.175844	-2.1698	3.86665
1	-1.4275	1.18896	1.82808
6	0.83509	-1.77606	-0.58602
6	0.973611	-0.954	-1.88332
6	1.57498	-1.8072	-3.01158
6	2.92617	-2.41272	-2.60472
6	2.80762	-3.21106	-1.29865
6	2.19651	-2.3675	-0.16838
9	4.95657	2.32987	-0.05824
1	1.98795	-0.21377	2.89554
1	0.499772	0.528105	3.47048
1	1.62372	-0.09011	-1.70527
1	-0.0011	-0.55796	-2.18595

1	1.68772	-1.19834	-3.91627
1	0.876361	-2.61708	-3.26641
1	3.65677	-1.60293	-2.46829
1	3.31494	-3.05146	-3.40673
1	3.78946	-3.58982	-0.99116
1	2.17406	-4.0929	-1.46933
1	2.88663	-1.55027	0.079795
1	2.07803	-2.97713	0.732443
1	0.174306	-2.62858	-0.81462
1	3.55229	0.484882	1.08572
1	3.45895	4.1414	-1.13807
1	0.951076	4.13704	-1.11231
1	-2.32848	-1.89995	-0.54762
1	-4.74192	-2.02387	-0.31621
1	-6.96097	-0.95969	-0.56084
1	-7.13687	1.50659	-0.83421
1	-5.07293	2.88899	-0.8895
1	-2.84974	1.81557	-0.67303
1	-1.03822	2.96033	0.440069

Conformer 5

B3LYP/6-31G** Energy = -1272.168259 hartrees

6	3.19357	-1.13816	-0.4069
6	3.91129	-1.99787	0.420748
6	3.29257	-2.97683	1.19187
6	1.90182	-3.10847	1.15443
6	1.16644	-2.25646	0.32908
6	1.80855	-1.27463	-0.44589
7	-0.23547	-2.22657	0.177245
6	-0.57052	-1.20892	-0.83858
6	0.790821	-0.53524	-1.26823
6	-1.0746	0.155197	-0.37492
6	0.21152	0.870808	-0.78794
8	0.006971	1.62631	-2.01747
6	0.426378	0.971697	-3.1356
6	1.08504	-0.34715	-2.75134
6	-2.25401	0.643212	0.033931
6	-3.48894	-0.1006	0.31877
6	-4.72681	0.548985	0.159572
6	-5.92364	-0.12274	0.39515
6	-5.90784	-1.45494	0.813541

6	-4.6861	-2.10455	1.00177
6	-3.48716	-1.43678	0.759941
8	0.285208	1.42899	-4.23945
1	-1.17809	-1.64838	-1.63885
6	0.98646	1.7669	0.196849
6	0.456979	3.21994	0.217106
6	1.30376	4.11346	1.13608
6	1.38126	3.55535	2.56307
6	1.87591	2.10276	2.55915
6	1.02817	1.21238	1.63655
9	5.25785	-1.878	0.47286
1	2.15929	-0.26253	-2.95167
1	0.705956	-1.15154	-3.38747
1	-0.5817	3.22019	0.576616
1	0.439117	3.62684	-0.7964
1	0.893027	5.13005	1.14366
1	2.31941	4.19279	0.722785
1	0.382887	3.59503	3.02171
1	2.03449	4.18037	3.18362
1	1.86552	1.69291	3.57599
1	2.92293	2.07576	2.2253
1	0.002682	1.15944	2.02362
1	1.41959	0.1925	1.65164
1	2.02054	1.80395	-0.18264
1	3.72312	-0.39761	-0.99757
1	3.90158	-3.62203	1.81543
1	1.40658	-3.86192	1.75887
1	-2.33311	1.72588	0.126881
1	-4.74333	1.58602	-0.16525
1	-6.86885	0.394042	0.257085
1	-6.84005	-1.9783	1.00445
1	-4.66737	-3.133	1.3515
1	-2.53938	-1.92694	0.954644
1	-0.6602	-3.13214	0.015642

Conformer 6

B3LYP/6-31G** Energy = -1272.168182 hartrees

6	-2.96493	-1.47959	0.052887
6	-3.38145	-2.39866	-0.90886
6	-2.49839	-3.27816	-1.52464
6	-1.14651	-3.26942	-1.16525

6	-0.71296	-2.36021	-0.19913
6	-1.61558	-1.45454	0.387771
7	0.57057	-2.25281	0.357865
6	0.613145	-1.06514	1.2238
6	-0.8734	-0.56568	1.34934
6	0.993438	0.282139	0.615021
6	-0.38539	0.880528	0.886401
8	-0.34741	1.64033	2.13376
6	-0.91367	0.990499	3.1912
6	-1.44822	-0.36287	2.74228
6	2.08121	0.780799	0.011698
6	3.37898	0.134097	-0.23176
6	3.79738	-1.0499	0.406911
6	5.03761	-1.61552	0.1208
6	5.89284	-1.01482	-0.80598
6	5.50008	0.165818	-1.43798
6	4.26134	0.733416	-1.14965
8	-0.95828	1.47581	4.29085
1	1.11298	-1.29413	2.17346
6	-1.15573	1.71156	-0.1561
6	-1.03724	1.17484	-1.5992
6	-1.91001	1.98515	-2.57079
6	-1.56802	3.48036	-2.53055
6	-1.64611	4.02606	-1.09828
6	-0.77944	3.21174	-0.12576
9	-4.68937	-2.429	-1.25731
1	-2.54342	-0.31747	2.73515
1	-1.16305	-1.13618	3.46022
1	-1.31414	0.119179	-1.64648
1	0.010544	1.23753	-1.91896
1	-2.96825	1.84638	-2.30804
1	-1.79044	1.59307	-3.58762
1	-2.23697	4.04409	-3.19161
1	-0.5495	3.6277	-2.91761
1	-2.69074	3.9983	-0.75651
1	-1.34104	5.07886	-1.07231
1	-0.87824	3.60226	0.889424
1	0.277747	3.3279	-0.40341
1	-2.21565	1.64175	0.139221
1	-3.68861	-0.80285	0.495668
1	-2.87542	-3.97055	-2.26936
1	-0.45459	-3.96839	-1.62461
1	2.00477	1.79402	-0.3791

1	3.16609	-1.51892	1.15317
1	5.34139	-2.52532	0.630374
1	6.85878	-1.45894	-1.02643
1	6.16003	0.647138	-2.15367
1	3.96309	1.65483	-1.64293
1	1.35655	-2.37372	-0.2693

Conformer 7

B3LYP/6-31G** Energy = -1272.167594 hartrees

6	-3.38669	-0.0059	0.349514
6	-4.43623	0.379111	-0.48124
6	-4.46439	0.064766	-1.83555
6	-3.41014	-0.66026	-2.39748
6	-2.35176	-1.05774	-1.57774
6	-2.33136	-0.71922	-0.21153
7	-1.21407	-1.78527	-1.95773
6	-0.43425	-2.10991	-0.75248
6	-1.11025	-1.32051	0.43487
6	0.851316	-1.32535	-0.53183
6	0.260193	-0.50913	0.620588
8	0.795096	-0.96294	1.90016
6	-0.00105	-1.87205	2.5317
6	-1.30444	-2.04395	1.76311
6	2.0261	-1.40508	-1.17004
6	3.28467	-0.68617	-0.91418
6	4.14938	-0.42983	-1.9936
6	5.35138	0.247957	-1.80458
6	5.72392	0.66567	-0.52548
6	4.88876	0.392726	0.560074
6	3.68213	-0.27925	0.373121
8	0.326328	-2.40884	3.55709
1	-0.33768	-3.19566	-0.62278
6	0.377183	1.02361	0.596465
6	0.002921	1.66793	-0.75393
6	0.275961	3.18063	-0.73192
6	-0.46011	3.87335	0.423593
6	-0.11546	3.22255	1.77049
6	-0.37742	1.70752	1.75515
9	-5.466	1.07754	0.052242
1	-2.10782	-1.59749	2.36005
1	-1.53864	-3.10719	1.66154

1	-1.05894	1.50017	-0.96619
1	0.565945	1.19693	-1.56576
1	-0.01875	3.62336	-1.69065
1	1.3568	3.35165	-0.6283
1	-1.54403	3.80327	0.254809
1	-0.21638	4.9423	0.445088
1	-0.6892	3.68999	2.57955
1	0.945013	3.40079	1.99811
1	-0.07551	1.26698	2.71061
1	-1.45524	1.53525	1.64254
1	1.44728	1.21888	0.753335
1	-3.42155	0.250903	1.40306
1	-5.30829	0.385837	-2.43625
1	-3.42163	-0.91364	-3.453
1	2.05885	-2.08978	-2.01961
1	3.86506	-0.75751	-2.99034
1	5.99952	0.444979	-2.65358
1	6.66397	1.18787	-0.37377
1	5.1836	0.693351	1.5613
1	3.05741	-0.51883	1.22677
1	-1.37097	-2.54798	-2.60332

Compound 2c:

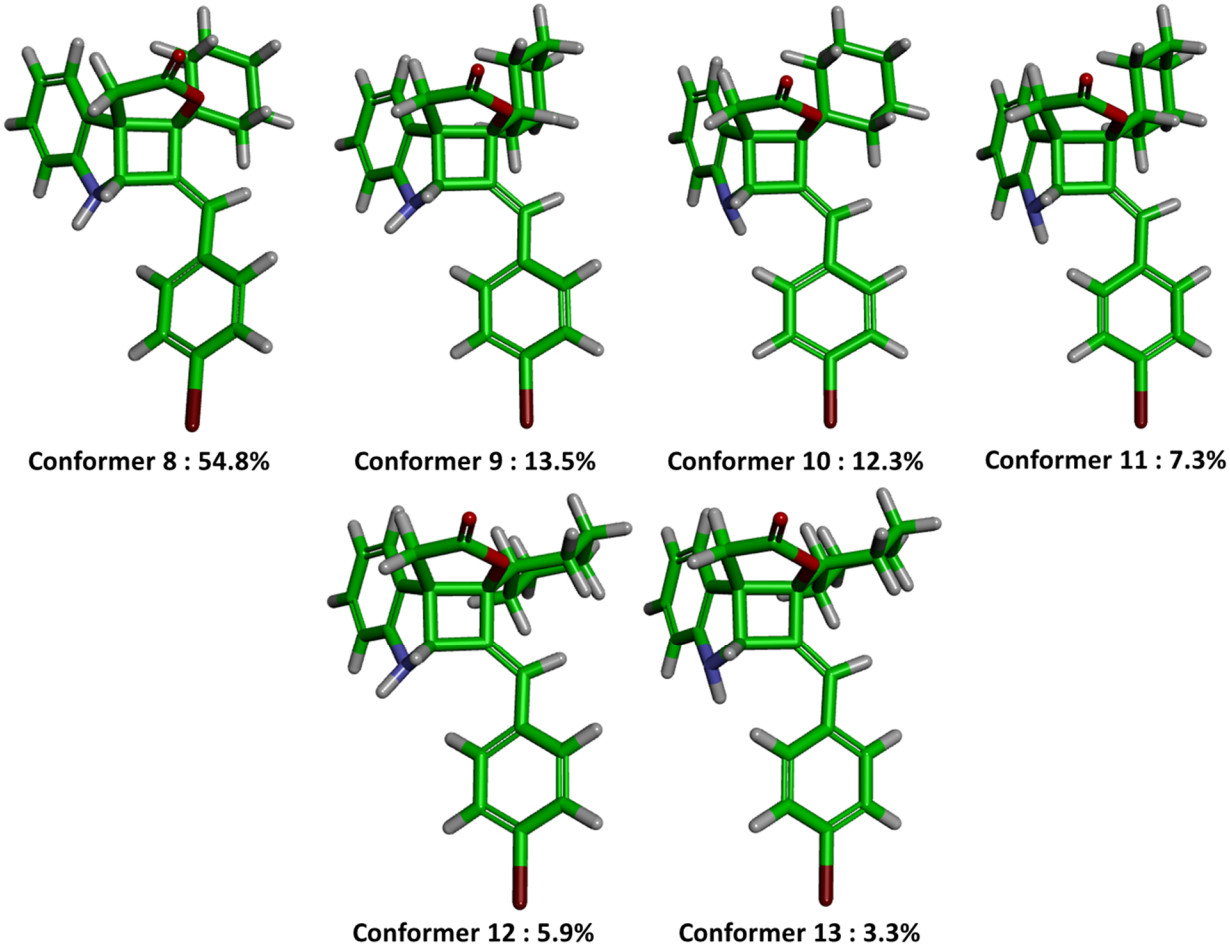


Figure S4: Conformers of the calculated *SSS* minima of compound **2c** contributing >2% to the Boltzmann distribution, percentages shown above based on *in vacuo* electronic energies.

Coordinates and electronic energies for B3LYP/6-31G conformational minima contributing >2% to the *in vacuo* Boltzmann distribution.**

Compound 2c

Conformer 8
B3LYP/6-31G** Energy = -3744.076920 hartrees

6	4.01874	2.19795	0.515595
6	4.53792	3.24503	-0.25674
6	3.71034	3.92961	-1.15202
6	2.36153	3.59052	-1.29455

6	1.85407	2.54531	-0.518368
6	2.68113	1.83996	0.377275
7	0.539859	2.06032	-0.513033
6	0.385466	1.09941	0.596252
6	1.85242	0.807822	1.09735
6	0.239624	-0.37032	0.232767
6	1.70869	-0.680272	0.522914
8	1.84443	-1.57401	1.66291
6	1.98013	-0.900854	2.83448
6	2.08166	0.596772	2.59168
6	-0.806856	-1.18766	0.047605
6	-2.22154	-0.80231	-0.060633
6	-2.63748	0.440672	-0.572265
6	-3.98791	0.77722	-0.640304
6	-4.93923	-0.139091	-0.195884
6	-4.56465	-1.38757	0.297648
6	-3.21189	-1.71246	0.353184
35	-6.79863	0.317241	-0.282661
8	2.02815	-1.47871	3.89466
1	-0.339014	1.46071	1.33551
6	2.61863	-1.16462	-0.612587
6	2.09432	-2.43775	-1.31013
6	3.00725	-2.85733	-2.47368
6	4.46262	-3.04436	-2.02409
6	4.9863	-1.79227	-1.30718
6	4.07159	-1.38647	-0.142093
1	1.36165	1.11812	3.2292
1	3.07997	0.919415	2.9068
1	2.03833	-3.25353	-0.576373
1	1.07876	-2.2716	-1.68325
1	2.62664	-3.78048	-2.92741
1	2.96636	-2.08575	-3.25575
1	4.52234	-3.90274	-1.34002
1	5.09809	-3.28544	-2.88507
1	6.00417	-1.9639	-0.93624
1	5.05023	-0.961221	-2.02352
1	4.08027	-2.17685	0.618575
1	4.46075	-0.482359	0.335905
1	2.61815	-0.355917	-1.35684
1	4.65716	1.68062	1.22686
1	5.58139	3.52693	-0.155487
1	4.11717	4.74382	-1.74552
1	1.71985	4.13142	-1.984

1	-0.613606	-2.25897	0.025246
1	-1.90135	1.1354	-0.961153
1	-4.29432	1.73541	-1.04526
1	-5.3142	-2.09614	0.631634
1	-2.91634	-2.68526	0.736227
1	-0.187014	2.76274	-0.583633

Conformer 9

B3LYP/6-31G** Energy = -3744.075598 hartrees

6	-3.9915	1.96874	-0.185257
6	-4.31605	3.12773	0.529531
6	-3.30226	3.98141	0.977418
6	-1.95737	3.69723	0.726992
6	-1.64428	2.53788	0.012963
6	-2.65461	1.6656	-0.433522
7	-0.357136	2.09602	-0.340059
6	-0.491122	0.874168	-1.14984
6	-2.03855	0.547935	-1.23574
6	-0.268398	-0.468194	-0.458846
6	-1.72884	-0.881845	-0.605027
8	-1.85493	-1.80563	-1.74227
6	-2.32667	-1.21199	-2.86618
6	-2.64004	0.249495	-2.60434
6	0.770618	-1.16916	0.017379
6	2.18713	-0.787815	0.090632
6	2.63188	0.54752	0.089329
6	3.98945	0.854155	0.144931
6	4.92022	-0.181722	0.20756
6	4.51526	-1.51469	0.231648
6	3.15458	-1.8061	0.181566
35	6.79	0.235608	0.277859
8	-2.46565	-1.82784	-3.89757
1	0.040229	0.975641	-2.10245
6	-2.46155	-1.5376	0.573963
6	-2.30608	-0.793754	1.9161
6	-2.95534	-1.58434	3.06343
6	-4.43347	-1.88621	2.78029
6	-4.60622	-2.6014	1.43331
6	-3.94962	-1.8217	0.282755
1	-2.24075	0.870235	-3.41112

1	-3.72972	0.37084	-2.60982
1	-1.24703	-0.620352	2.13249
1	-2.77946	0.192345	1.84867
1	-2.41285	-2.53029	3.20455
1	-2.85409	-1.02415	4.00081
1	-4.86026	-2.49194	3.58912
1	-4.9973	-0.942723	2.76444
1	-4.15239	-3.60088	1.49315
1	-5.67013	-2.75603	1.21634
1	-4.04974	-2.38551	-0.650335
1	-4.47991	-0.870507	0.144686
1	-1.9653	-2.51484	0.689031
1	-4.78157	1.31831	-0.550498
1	-5.35589	3.3667	0.730252
1	-3.56074	4.88163	1.5281
1	-1.17187	4.36335	1.07179
1	0.555476	-2.17869	0.36859
1	1.90766	1.35399	0.089585
1	4.31622	1.88822	0.151261
1	5.24591	-2.3134	0.291296
1	2.8361	-2.84468	0.201467
1	0.239279	2.81004	-0.743525

Conformer 10

B3LYP/6-31G** Energy = -3744.075509 hartrees

6	3.99806	2.21959	-0.025059
6	4.35102	3.17507	-0.9881
6	3.35714	3.80992	-1.73789
6	2.00245	3.5333	-1.52653
6	1.66165	2.59114	-0.552735
6	2.65695	1.90863	0.173648
7	0.375194	2.2591	-0.116539
6	0.460293	1.17403	0.877511
6	1.99497	0.911305	1.09506
6	0.286853	-0.258968	0.401736
6	1.76975	-0.593209	0.595672
8	1.93245	-1.41775	1.79046
6	2.29267	-0.697307	2.88455
6	2.49988	0.764734	2.52378
6	-0.766218	-1.03224	0.092368
6	-2.19273	-0.685212	0.024199
6	-2.72344	0.592086	0.295412

6	-4.09105	0.839012	0.211413
6	-4.95225	-0.195439	-0.152203
6	-4.4662	-1.47091	-0.42871
6	-3.09661	-1.70316	-0.337081
35	-6.83305	0.145318	-0.273117
8	2.42913	-1.21727	3.96675
1	-0.117274	1.42659	1.77516
6	2.62086	-1.1793	-0.539844
6	2.05079	-2.48731	-1.12887
6	2.92608	-3.03029	-2.27096
6	4.38726	-3.21516	-1.84295
6	4.95559	-1.91669	-1.25674
6	4.08594	-1.39783	-0.101956
1	1.98357	1.40085	3.2482
1	3.57083	0.981869	2.60755
1	1.97757	-3.24053	-0.332524
1	1.03838	-2.31956	-1.50743
1	2.51055	-3.97885	-2.63268
1	2.88416	-2.32972	-3.11724
1	4.44615	-4.00872	-1.08459
1	4.99324	-3.54868	-2.69414
1	5.982	-2.07447	-0.903685
1	5.00918	-1.15206	-2.04458
1	4.10531	-2.12653	0.717572
1	4.50928	-0.468509	0.291544
1	2.61247	-0.423771	-1.33784
1	4.7723	1.72489	0.554567
1	5.39636	3.41765	-1.15226
1	3.63644	4.54381	-2.48901
1	1.23238	4.05164	-2.09049
1	-0.560804	-2.07575	-0.133171
1	-2.07794	1.41312	0.58207
1	-4.48029	1.82774	0.427328
1	-5.1408	-2.27173	-0.709644
1	-2.71743	-2.69913	-0.548407
1	-0.346262	2.17539	-0.823357

Conformer 11

B3LYP/6-31G** Energy = -3744.075018 hartrees

6	-3.78642	2.1172	0.214692

6	-3.92786	3.16616	1.13371
6	-2.79905	3.86364	1.57378
6	-1.52194	3.55176	1.09676
6	-1.39421	2.51186	0.172009
6	-2.51946	1.77348	-0.24362
7	-0.235183	2.11628	-0.499631
6	-0.515739	0.905129	-1.28015
6	-2.07948	0.700103	-1.21001
6	-0.327693	-0.460118	-0.626044
6	-1.81176	-0.792616	-0.718059
8	-2.02857	-1.58975	-1.93728
6	-2.57666	-0.878729	-2.95578
6	-2.83065	0.554054	-2.52524
6	0.69027	-1.16419	-0.111339
6	2.11822	-0.822879	-0.052613
6	2.95852	-1.60391	0.762809
6	4.32128	-1.33967	0.873767
6	4.86301	-0.279543	0.150601
6	4.06607	0.508386	-0.679135
6	2.70458	0.233882	-0.776636
35	6.73594	0.097576	0.289572
8	-2.80947	-1.38734	-4.02755
1	-0.095556	0.982405	-2.29013
6	-2.52464	-1.53358	0.421737
6	-4.03916	-1.70494	0.177558
6	-4.68593	-2.57588	1.26647
6	-4.41396	-2.02625	2.67331
6	-2.91023	-1.8336	2.91356
6	-2.26787	-0.95403	1.8285
1	-2.50406	1.24738	-3.30475
1	-3.91138	0.687985	-2.39783
1	-4.52121	-0.718534	0.175685
1	-4.21491	-2.15259	-0.80594
1	-5.76542	-2.65016	1.08784
1	-4.28715	-3.59757	1.19219
1	-4.92451	-1.05948	2.78929
1	-4.83754	-2.69637	3.43133
1	-2.73675	-1.38699	3.90006
1	-2.41637	-2.81615	2.92424
1	-2.68424	0.057249	1.89317
1	-1.19238	-0.863318	2.0109
1	-2.0822	-2.54269	0.402516
1	-4.66226	1.57171	-0.12517

1	-4.91281	3.43424	1.50314
1	-2.9121	4.67176	2.29138
1	-0.651908	4.11355	1.42403
1	0.440006	-2.1216	0.345036
1	2.5344	-2.43199	1.32379
1	4.94912	-1.95168	1.51155
1	4.50086	1.32225	-1.24855
1	2.10537	0.842089	-1.44471
1	0.640519	2.15188	0.008205

Conformer 12

B3LYP/6-31G** Energy = -3744.074808 hartrees

6	-4.17691	1.99308	-0.064282
6	-4.5877	2.99424	0.824725
6	-3.63496	3.76669	1.49679
6	-2.26594	3.55484	1.3071
6	-1.86587	2.55068	0.422388
6	-2.81703	1.76972	-0.260772
7	-0.547106	2.17359	0.115366
6	-0.585133	1.13098	-0.926634
6	-2.11007	0.814626	-1.18414
6	-0.377404	-0.322617	-0.502408
6	-1.83743	-0.695796	-0.758243
8	-1.95123	-1.45299	-2.00771
6	-2.32862	-0.691954	-3.06476
6	-2.61074	0.730221	-2.62103
6	0.673758	-1.09766	-0.196746
6	2.08426	-0.711983	-0.056094
6	2.50379	0.595828	0.250983
6	3.85647	0.91253	0.353732
6	4.80726	-0.086864	0.152949
6	4.42787	-1.39739	-0.130554
6	3.07223	-1.70031	-0.225152
35	6.67005	0.345071	0.285685
8	-2.4231	-1.15589	-4.17727
1	0.013344	1.427	-1.79546
6	-2.69579	-1.40646	0.304656
6	-2.44767	-0.890806	1.73814
6	-3.38987	-1.56275	2.74921
6	-3.2702	-3.09152	2.70901
6	-3.47698	-3.6237	1.28463

6	-2.53884	-2.94457	0.274728
1	-2.13113	1.43834	-3.30225
1	-3.692	0.897965	-2.6886
1	-1.40773	-1.10357	2.01668
1	-2.56876	0.193908	1.78796
1	-3.17226	-1.18988	3.75729
1	-4.42641	-1.2717	2.5266
1	-2.27144	-3.3846	3.06308
1	-3.99206	-3.5502	3.39582
1	-3.3251	-4.70961	1.2561
1	-4.51875	-3.44749	0.980443
1	-2.73596	-3.32358	-0.731351
1	-1.49952	-3.20785	0.515443
1	-3.74129	-1.18102	0.041278
1	-4.91679	1.40454	-0.600833
1	-5.64595	3.17418	0.987254
1	-3.96042	4.54662	2.17968
1	-1.53016	4.15612	1.8332
1	0.481276	-2.16301	-0.077543
1	1.76548	1.36301	0.45394
1	4.164	1.92312	0.598796
1	5.17462	-2.17031	-0.273399
1	2.77359	-2.72125	-0.446306
1	0.085025	2.94335	-0.073861

Conformer 13

B3LYP/6-31G** Energy = -3744.074264 hartrees

6	3.90458	2.14038	-0.543297
6	4.05011	2.99608	-1.6446
6	2.92271	3.59064	-2.21832
6	1.64078	3.36997	-1.70206
6	1.50816	2.52662	-0.596348
6	2.63457	1.89251	-0.036274
7	0.345585	2.24915	0.12701
6	0.625681	1.19834	1.11548
6	2.18822	1.00332	1.09585
6	0.457769	-0.264313	0.707349
6	1.95116	-0.552349	0.843349
8	2.20003	-1.1468	2.16468
6	2.73687	-0.276914	3.05794
6	2.94225	1.0803	2.41503

6	-0.56313	-1.04826	0.331186
6	-1.99133	-0.718328	0.225858
6	-2.8354	-1.62076	-0.4483
6	-4.19808	-1.37583	-0.597276
6	-4.73633	-0.210959	-0.055174
6	-3.93593	0.699218	0.634323
6	-2.57442	0.441769	0.771926
35	-6.6087	0.142918	-0.251804
8	2.99571	-0.613301	4.18976
1	0.190747	1.45065	2.08971
6	2.75219	-1.35843	-0.195629
6	2.67302	-2.88628	0.036472
6	3.56749	-3.65187	-0.950282
6	3.23284	-3.31414	-2.40897
6	3.27543	-1.79917	-2.6475
6	2.37615	-1.03944	-1.65914
1	2.59392	1.87178	3.08383
1	4.01815	1.22803	2.26417
1	2.95876	-3.12659	1.06349
1	1.63327	-3.21909	-0.087386
1	4.61882	-3.39864	-0.751687
1	3.47013	-4.7303	-0.775282
1	3.92433	-3.82771	-3.08821
1	2.22639	-3.68846	-2.64526
1	4.30991	-1.44347	-2.54127
1	2.97114	-1.56555	-3.67491
1	2.4421	0.033793	-1.85209
1	1.33101	-1.32606	-1.8308
1	3.80339	-1.06363	-0.048714
1	4.77745	1.66605	-0.10219
1	5.03652	3.19114	-2.05382
1	3.04005	4.24696	-3.07635
1	0.772238	3.85158	-2.14175
1	-0.318719	-2.06929	0.043528
1	-2.41436	-2.53032	-0.867429
1	-4.82837	-2.08307	-1.12473
1	-4.3678	1.5956	1.06534
1	-1.97422	1.14757	1.3345
1	-0.52737	2.19108	-0.383739

Computational Details

Biaryl carboxylic acids used for parameterization were submitted to a geometry optimization in Gaussian 09[12] using the Def2TZVP basis set and M06-2x functional. This basis set and functional has been shown to be accurate for a large number of main group systems[19]. Input geometry for the unsubstituted biaryl carboxylic acid used a 90º dihedral angle between the two aryl rings, and a 0º dihedral angle between the carboxylic acid and the aryl ring. The –OH moiety of the carboxylic acid was pointed away from the second aryl ring. The optimized geometry of the unsubstituted biaryl carboxylic acid was used as the starting point for all subsequent calculations, with the 2-substitution being deemed the carbon closer in space to the carboxylic acid. Geometry optimization was then carried out on these structures.

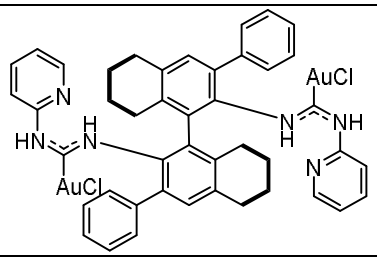
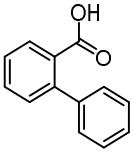
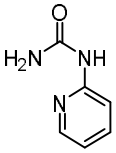
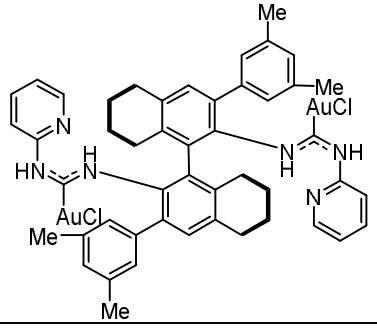
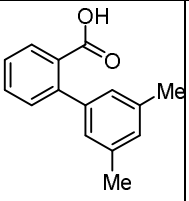
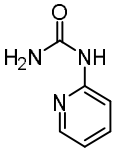
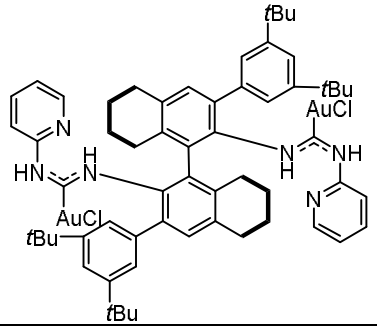
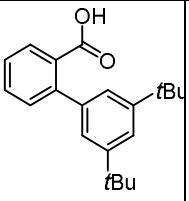
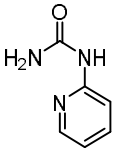
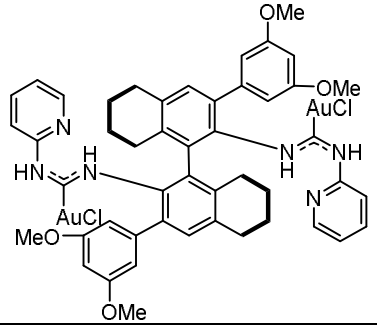
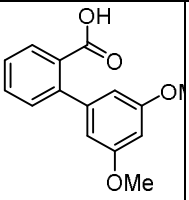
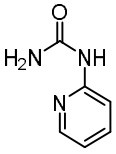
Urea molecules used for parameterization were submitted to a geometry optimization in Gaussian 09 using the Jun-CC-pVTZ basis set and M06-2x functional. This basis set was chosen as a compromise between computation efficiency and accuracy with possible hydrogen bonding interactions[20]. Input geometry for the unsubstituted pyridine-urea (R^2, R^3, R^4 = H) used a fully planar molecule. Output from this geometry optimization was used to build the input geometries for all subsequent molecules. Input geometries generally utilized planar molecules, with the exception of the $–NMe_2$ group, which had one bond in plane with the pyridine, and one 30º out of plane to conserve the sp^3 hybridization.

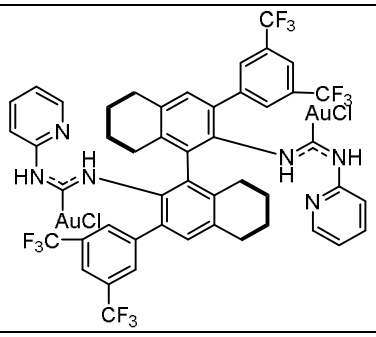
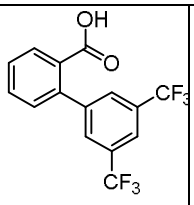
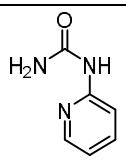
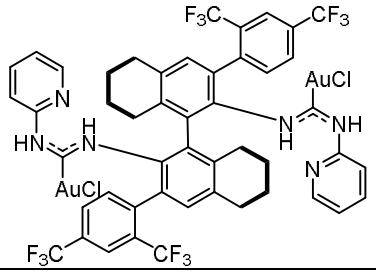
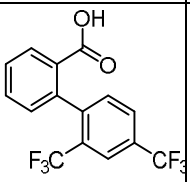
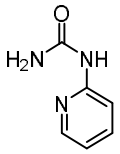
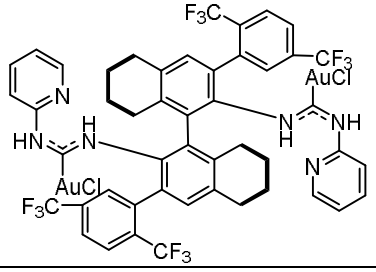
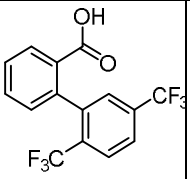
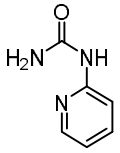
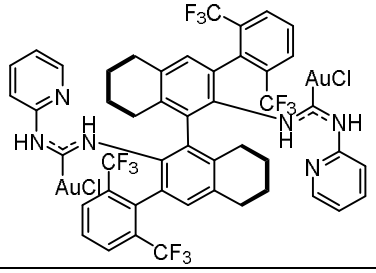
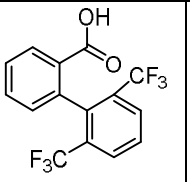
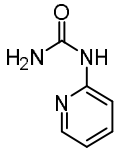
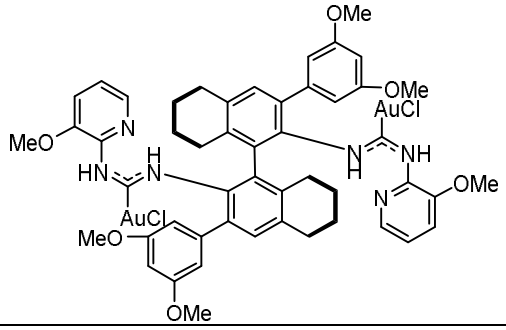
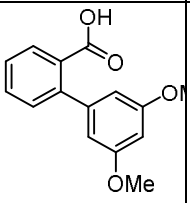
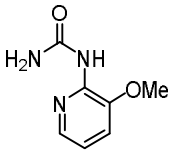
Triple zeta potential basis sets were chosen along with the M06-2x functional, as these generally lead to quantitative correlations. Infrared frequency and NBO charge distribution calculations were carried out on the optimized geometry. Linear scaling factors were not used as this would not affect the correlations[21]. All optimized structures lacked any imaginary frequencies and were thus deemed ground states and not transition states. Sterimol values were calculated using Molecular Modeling Pro[22]. Multivariate models were constructed and analyzed using Matlab Statistical toolbox version 2014a[23].

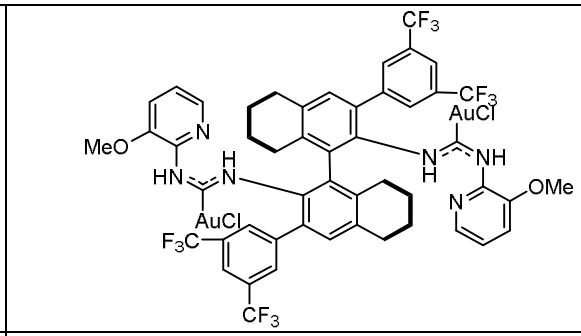
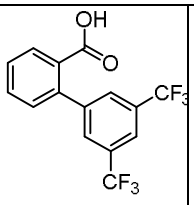
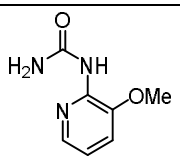
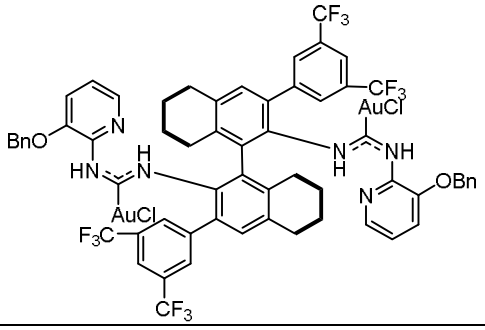
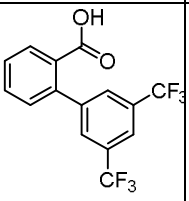
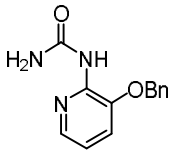
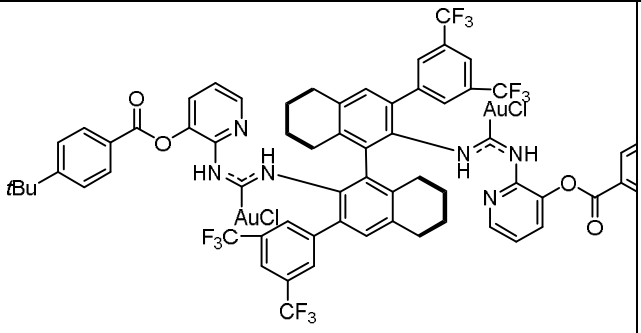
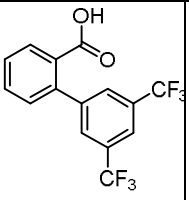
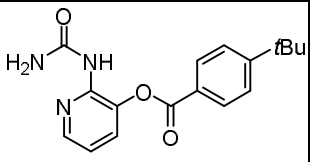
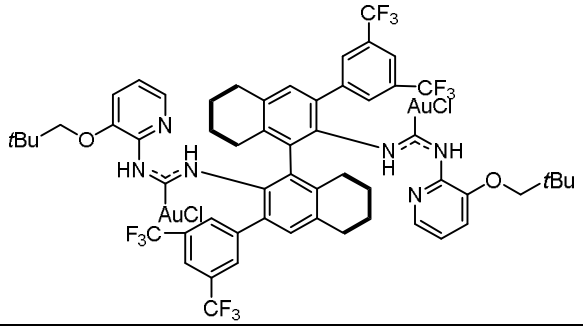
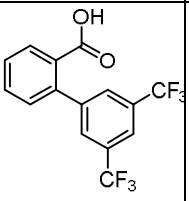
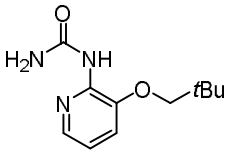
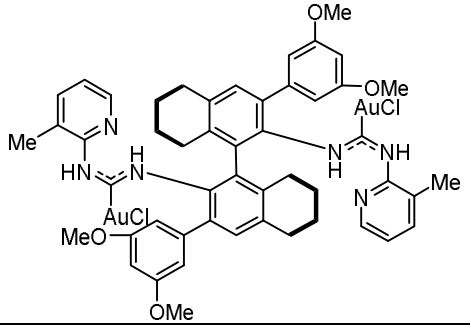
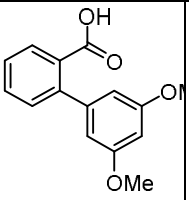
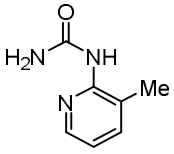
Catalyst Structures Versus Computed Structures

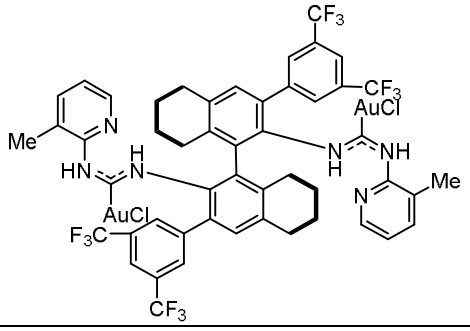
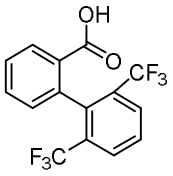
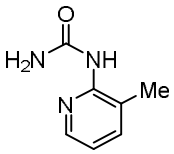
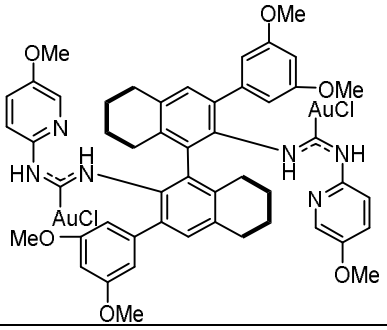
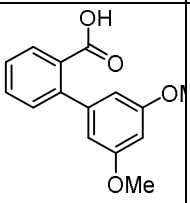
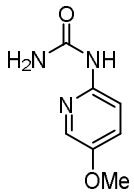
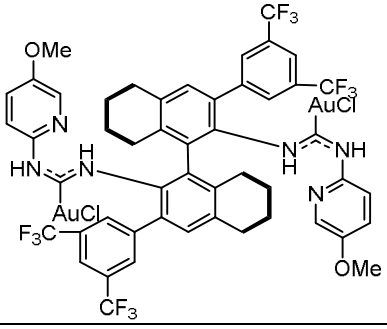
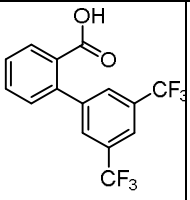
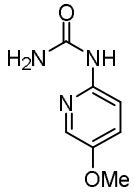
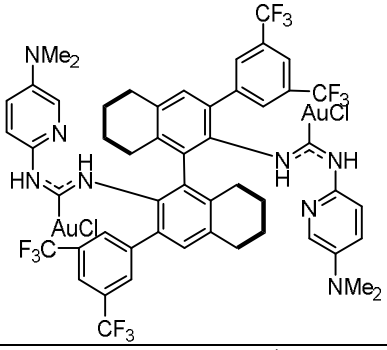
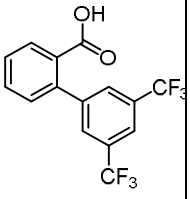
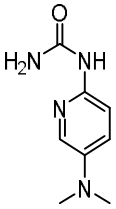
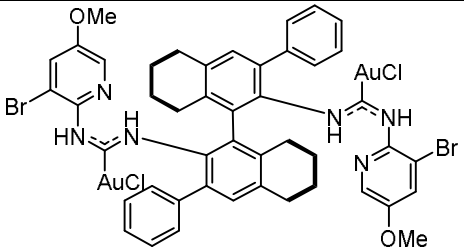
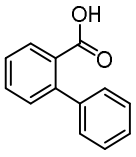
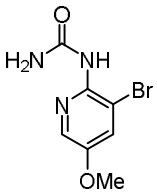
All catalysts utilized the H_8-*(S)*-BINAM backbone. The entire structure is listed below, as well as the computed structures that were used in modeling.

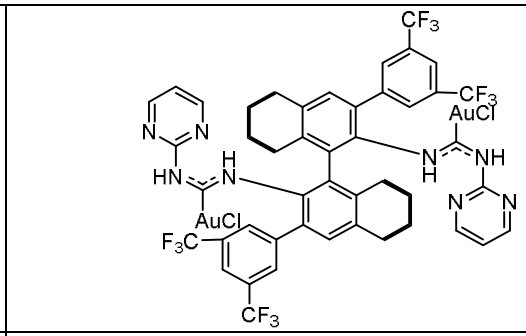
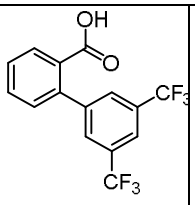
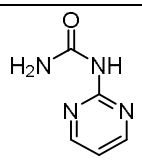
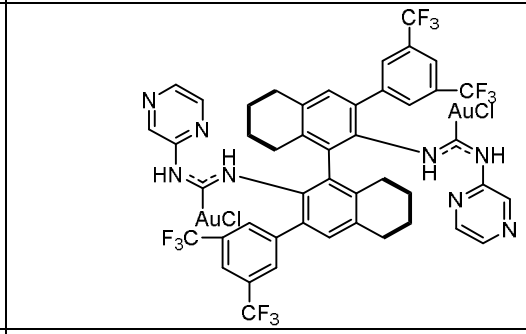
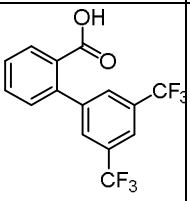
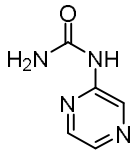
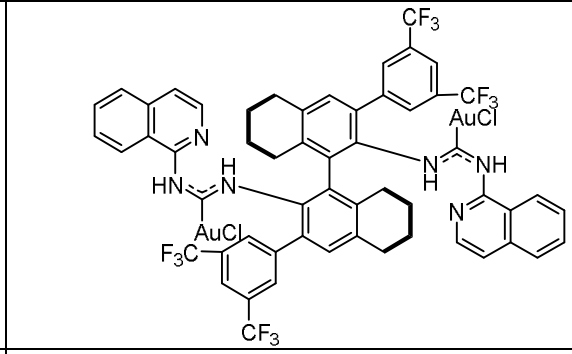
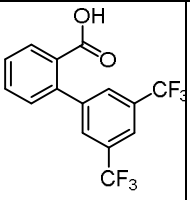
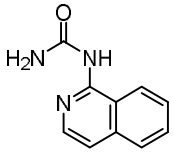
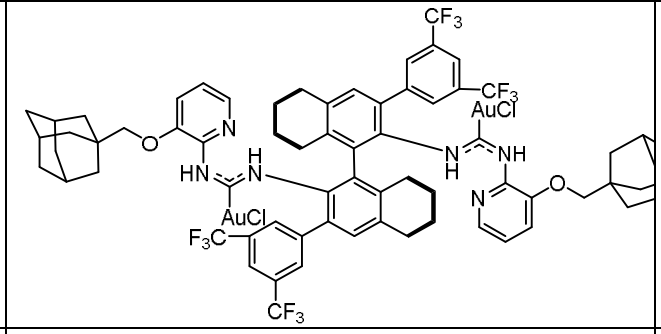
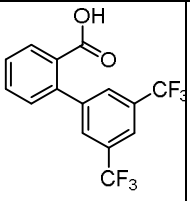
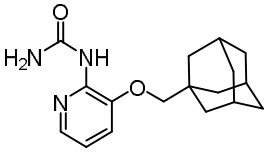
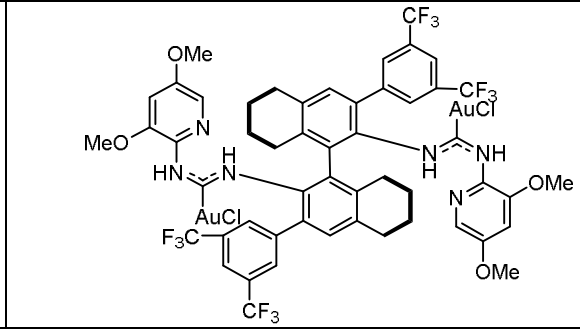
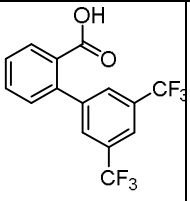
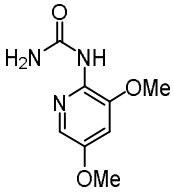
Table S1: Catalyst and computed structures

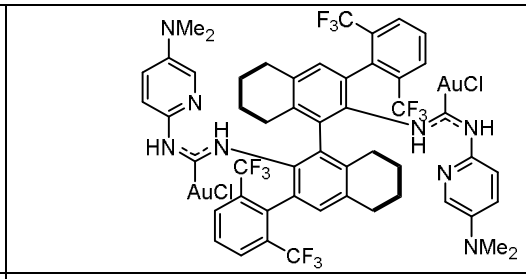
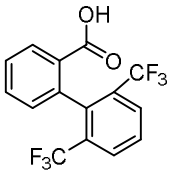
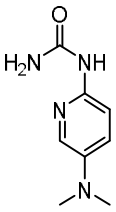
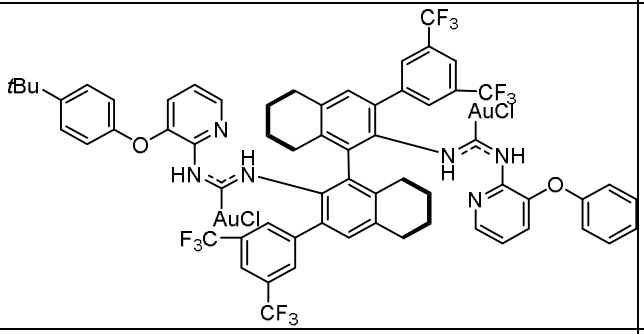
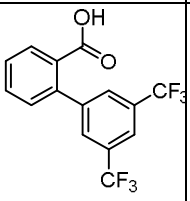
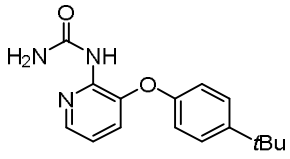
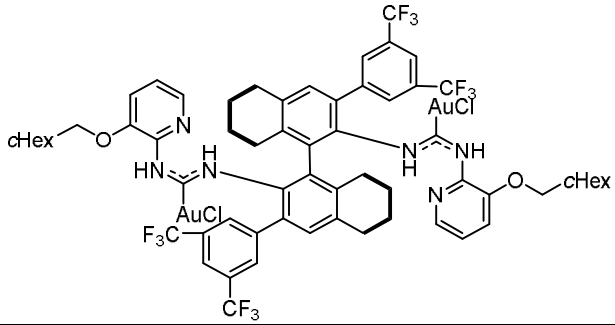
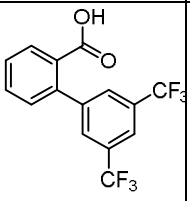
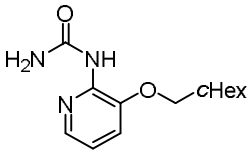
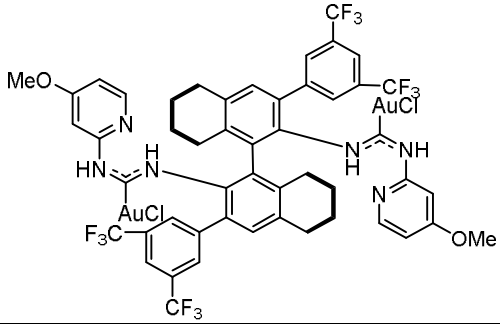
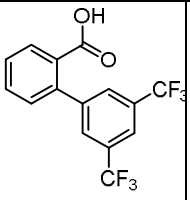
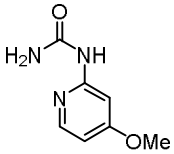
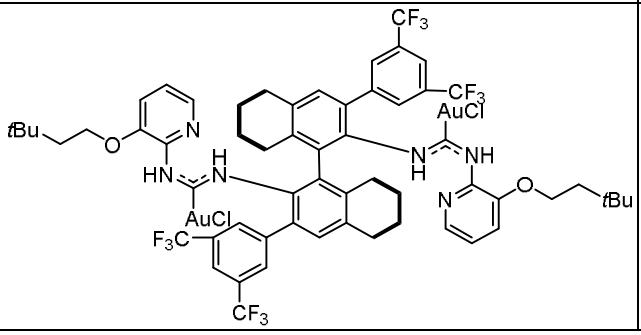
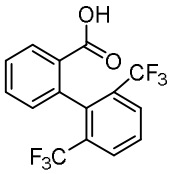
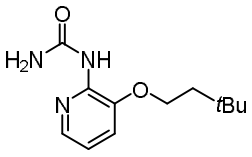
#	Structure	Aryl Group	Urea
1			
2			
3			
4			

5			
6			
7			
8			
9			

10			
11			
12			
13			
14			

15			
16			
17			
18			
19			

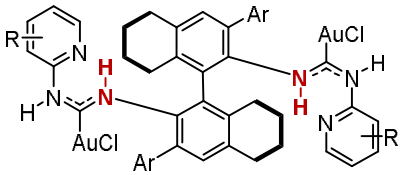
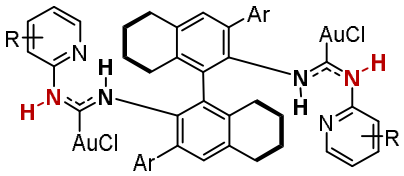
20			
21			
22			
23			
24			

25			
26			
27			
28			
29			

Parameters List

The ADC catalysts have two distinctive ^{1}H NMR shifts that correspond to the two NH shifts. Early modeling relied on these shifts and thus these are reported here. The first shift originates from the NH attached to the BINAM backbone. The second shift corresponds to the NH attached to the substituted aryl rings. These are highlighted in red for clarity.

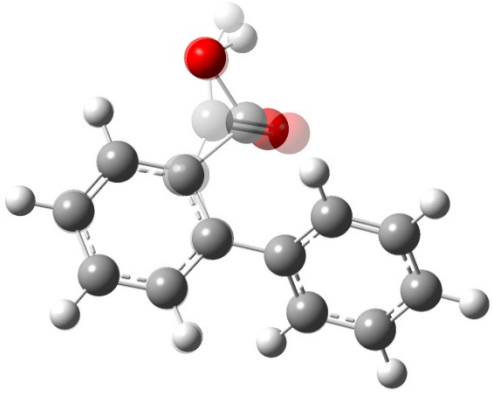
Table S2: NMR Parameters

#	 N-H Hydrogen Bonded	 N-H Aniline
1	13.44	8.36
2	13.39	8.14
3	13.44	8.27
4	13.39	8.42
5	13.57	8.78
6	13.50	8.26
7	13.49	8.32
8	13.50	8.26
9	13.55	8.54
10	13.72	8.59
11	13.81	8.61
12	13.73	8.40
13	13.90	8.45
14	13.94	7.92
15	14.16	7.94
16	13.23	8.25
17	13.22	8.76
18	13.36	8.05
19	13.23	8.25
20	12.91	8.73
21	12.74	10.04
22	14.67	8.96
23	13.97	8.46
24	13.41	8.42
25	13.26	8.22
26	13.77	8.75
27	13.86	8.50
28	13.75	8.92

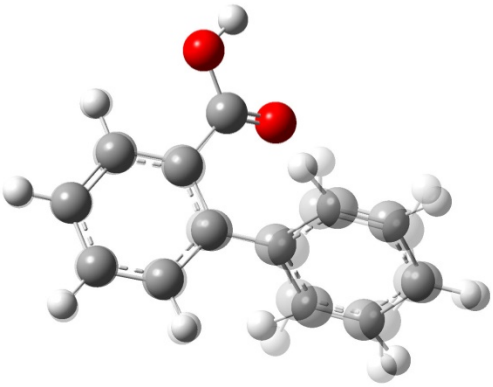
29	13.76	8.54

Aryl groups were simulated with biaryl carboxylic acids. Table S3 includes the biaryl carboxylic acid along with the parameters derived from these groups. A number of groups were calculated but never synthesized. Regardless, parameters from these groups are reported here. Representatives of each parameter are visualized for clarity.

C=O stretch:



2,3/5,6 stretch:



1,1’ stretch:

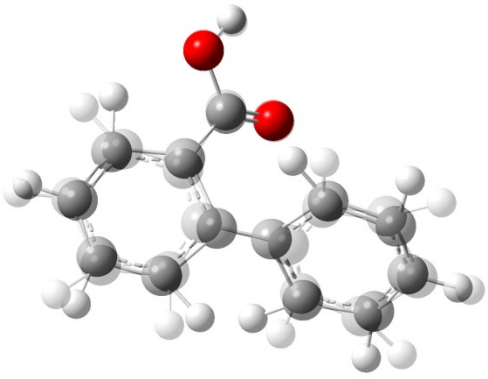
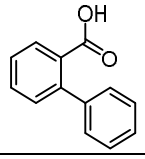
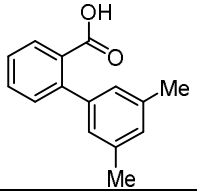
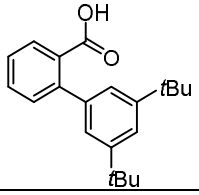
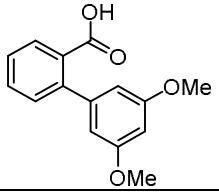
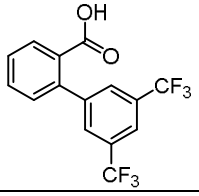
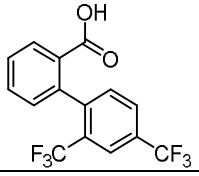
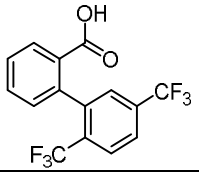
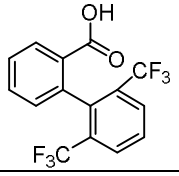
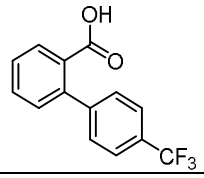
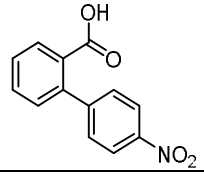
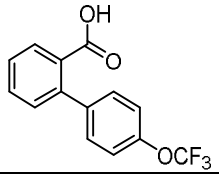
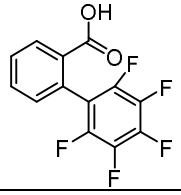
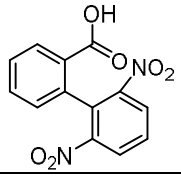
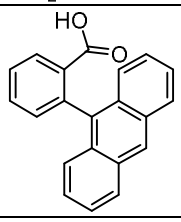
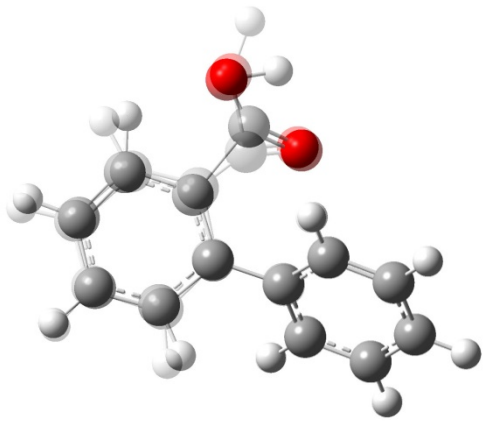


Table S3: Aryl group parameters

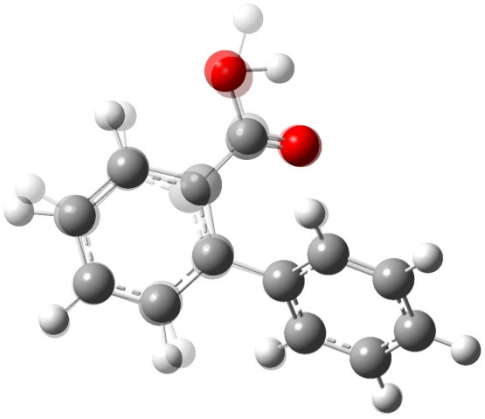
Biaryl Carboxylic acid	C=O stretch	C=O stretch int	2,3/5,6 stretch	2,3/5,6 stretch int	1,1’ stretch	1,1’ stretch int
	1858.34	341.1736	1688.33	1.0418	1558.90	2.7241
	1857.77	342.1896	1685.94	11.3233	1548.29	13.3398
	1859.04	336.3355	1677.51	25.8803	1545.59	31.9882
	1863.37	340.6566	1694.34	142.4133	1552.38	25.8095
	1855.24	355.1680	1701.23	5.3772	1678.04	6.5687
	1854.09	360.8599	1707.51	38.7875	1572.63	4.2720
	1851.38	362.8027	1705.8	2.1496	1544.48	13.6410
	1849.34	361.5283	1690.77	13.9801	1554.57	6.7959

	1857.43	350.8440	1702.61	25.1678	1578.33	6.2674
	1856.01	354.4442	1684.52	15.6907	1560.74	2.1364
	1857.54	343.5372	1696.09	26.9262	1576.25	59.5497
	1852.15	351.9194	1733.11	23.9773	1552.97	79.4397
	1843.36	362.7172	1675.62	220.6261	1556.1	15.0558
	1858.33	341.3035	1640.87	1.3125	1551.52	9.8598

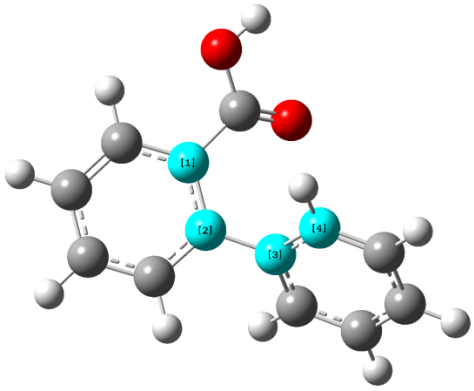
OCC sway:



OCOH bend:



Biaryl Dihedral:



O--C Distance:

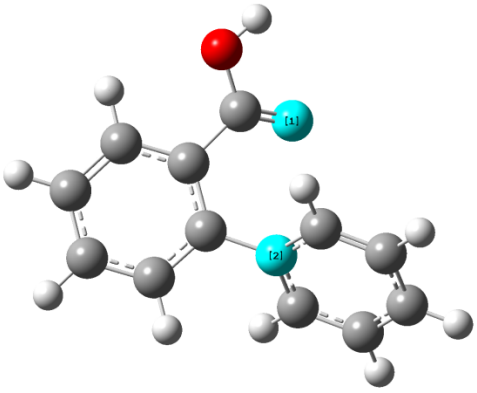
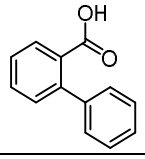
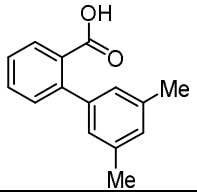
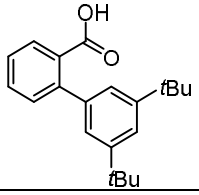
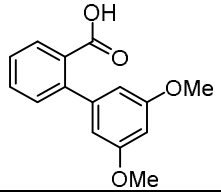
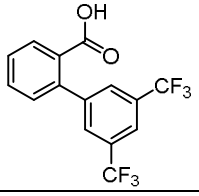
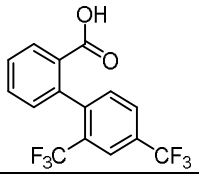
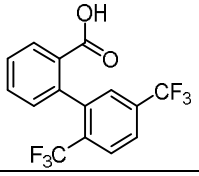
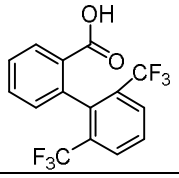
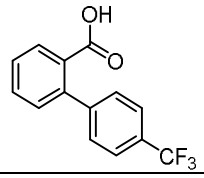
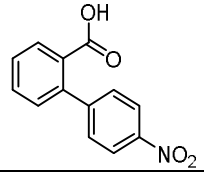
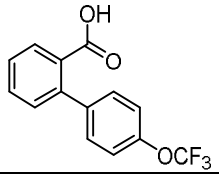
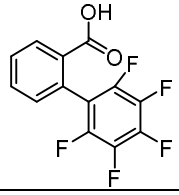
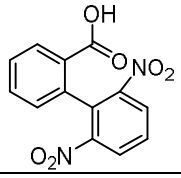
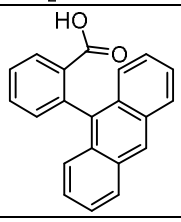
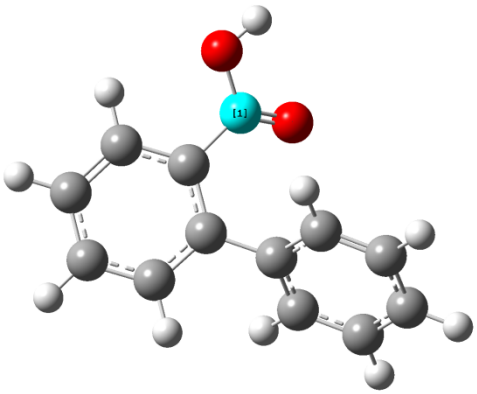


Table S3: Aryl group parameters continued

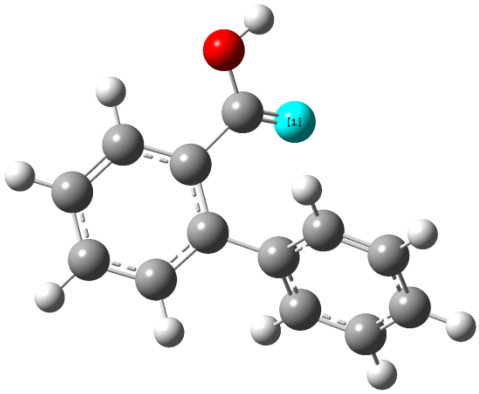
Biaryl Carboxylic acid	OCC sway	OCC sway int	OCOH bend	OCOH bend int	Biaryl dihedral	O--C distance
	1388.10	115.2057	1222.86	219.1623	54.40708	2.91940
	1385.48	115.2831	1218.27	193.8588	53.66714	2.93723
	1385.80	110.4202	1219.03	195.6319	50.94804	2.94753
	1386.55	113.5134	1224.03	168.2045	54.22598	2.94595
	1392.83	134.5383	1220.02	192.8528	55.51729	2.85557
	1398.04	145.8788	1222.42	189.9250	80.26448	2.76589
	1395.47	128.0073	1221.36	207.9752	82.19531	2.75754
	1396.24	142.4949	1220.61	181.7475	88.27557	2.72472

	1390.76	123.3926	1220.82	199.8589	56.67441	2.87293
	1390.70	132.8488	1217.93	195.9740	57.99285	2.85316
	1386.99	122.6394	1218.23	172.4381	52.55287	2.91879
	1395.63	141.2663	1221.84	208.4048	58.6311	2.80778
	1403.31	163.0516	1223.19	217.6446	94.28291	2.68418
	1388.40	122.9633	1215.86	187.6279	86.14638	2.76605

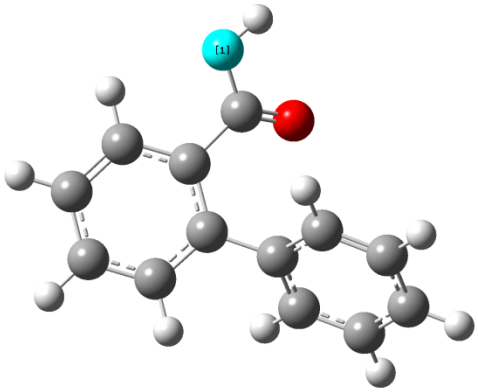
NBO_C



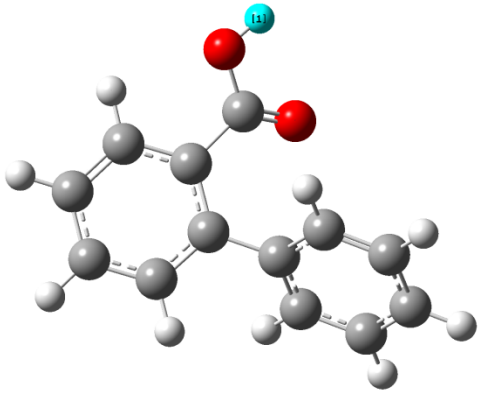
NBO_{O1}



NBO_{O2}



NBO_{H}



OCCC Dihedral

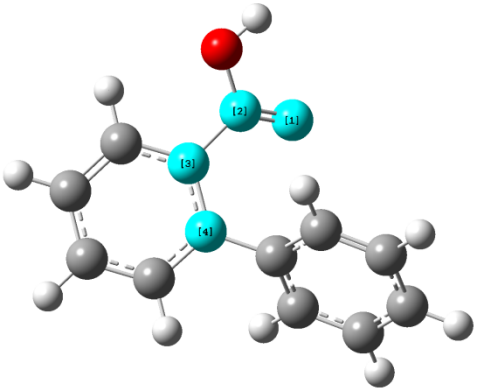
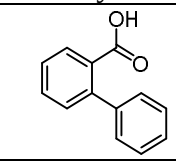
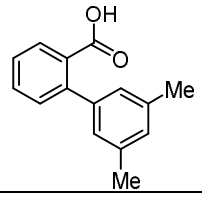
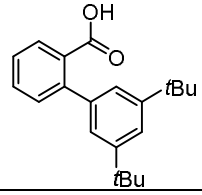
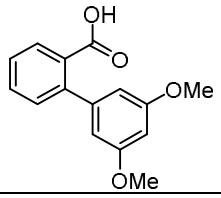
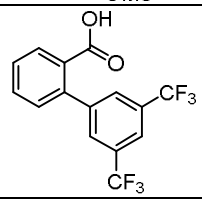
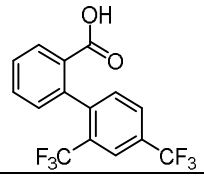
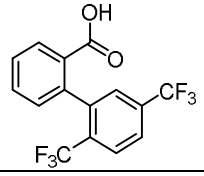
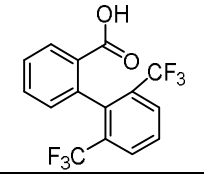
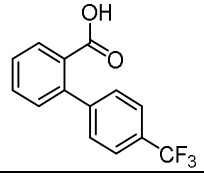
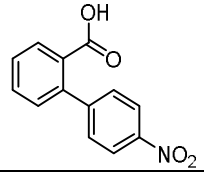
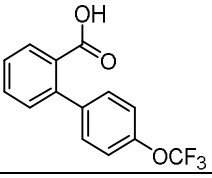
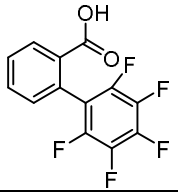
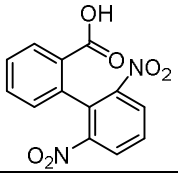
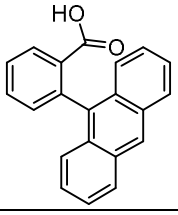


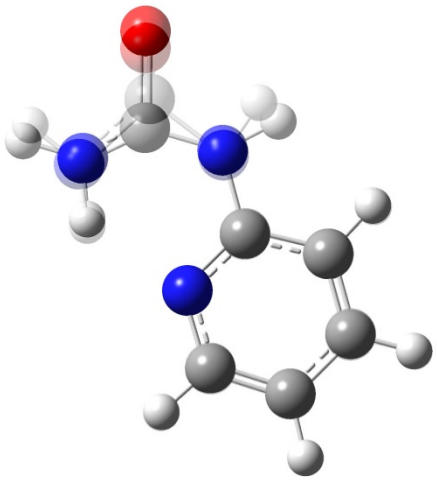
Table S3: Aryl Group Parameters Continued

Biaryl Carboxylic acid	NBO_C	NBO_{O1}	NBO_{O2}	NBO_H	OCCC Dihedral
	0.77962	-0.57415	-0.68885	0.49707	27.34645
	0.78035	-0.57490	-0.68901	0.49600	29.08915
	0.78037	-0.57616	-0.6884	0.49543	30.04504
	0.78022	-0.57290	-0.68806	0.49575	31.20879
	0.77732	-0.57847	-0.68341	0.50020	20.2494

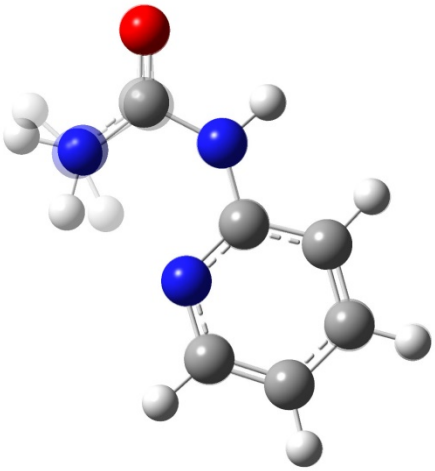
	0.78729	-0.58453	-0.68256	0.50066	16.35259
	0.78631	-0.58425	-0.68338	0.50080	13.75359
	0.78793	-0.58741	-0.68394	0.50060	4.15664
	0.77846	-0.57535	-0.68694	0.49919	22.54001
	0.77830	-0.57625	-0.68549	0.50020	21.00061
	0.77921	-0.57557	-0.68757	0.49812	26.94813
	0.78436	-0.58763	-0.68080	0.50070	17.68428
	0.79387	-0.59380	-0.67956	0.50104	0.01699
	0.77914	-0.57235	-0.69072	-0.49954	7.8812

Substitutions at the R groups on the pyridine moiety were simulated with ureas. Table S4 includes these ureas along with the parameters derived from these groups. A number of groups were calculated but never synthesized. Regardless, parameters from these groups are reported here. Representatives of each parameter are visualized for clarity.

C=O stretch:



NH_2 scissor:



C–N stretch:

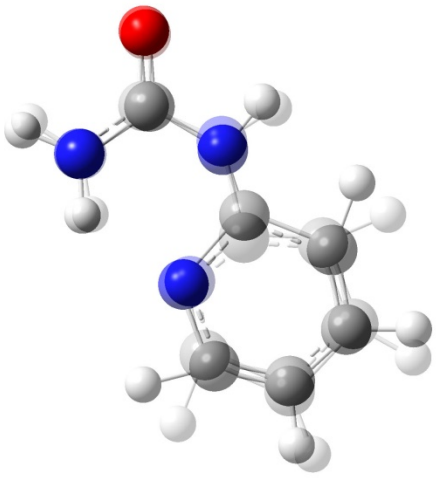
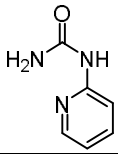
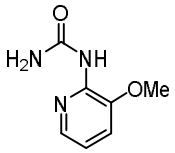
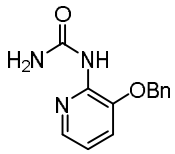
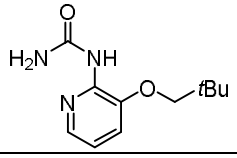
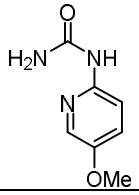
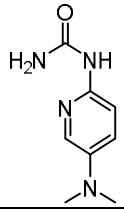
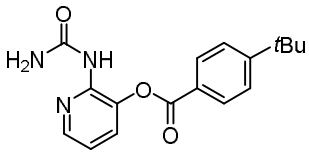
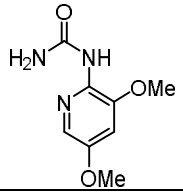
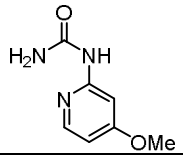
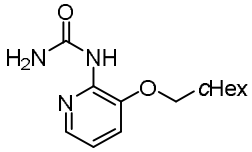
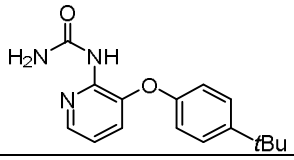
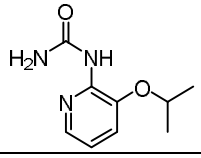
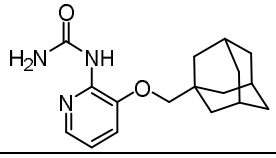
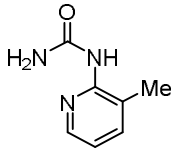
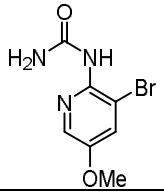
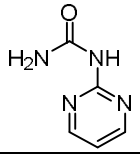
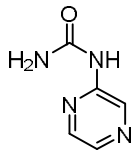
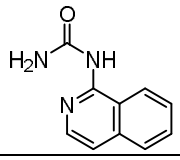
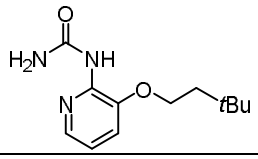
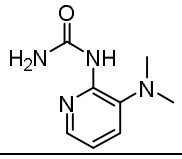
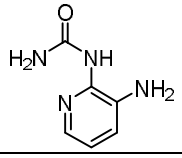
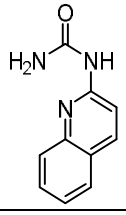
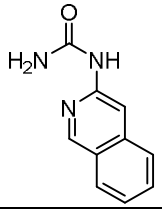


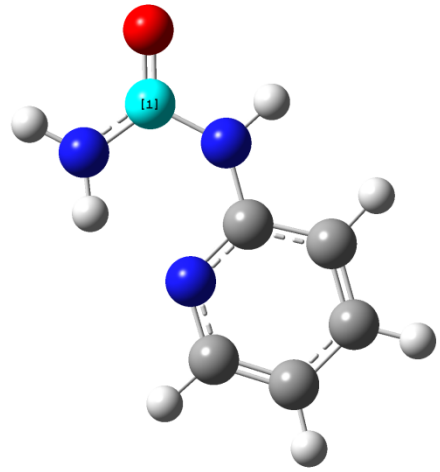
Table S4: Urea Parameters

Urea	C=O stretch	C=O stretch int	NH_2 scissor	NH_2 scissor int	C–N stretch	C–N stretch int
	1812.26	719.85	1593.91	420.2538	1539.53	134.5852
	1809.28	741.5668	1596.02	452.3287	1556.00	401.0913
	1810.35	670.8827	1596.60	463.4122	1555.41	378.9649
	1807.86	689.5108	1596.56	467.3407	1554.21	382.3888
	1806.80	764.7300	1596.51	346.2401	1559.79	487.5909
	1804.17	799.7262	1597.21	371.2573	1560.89	489.5687

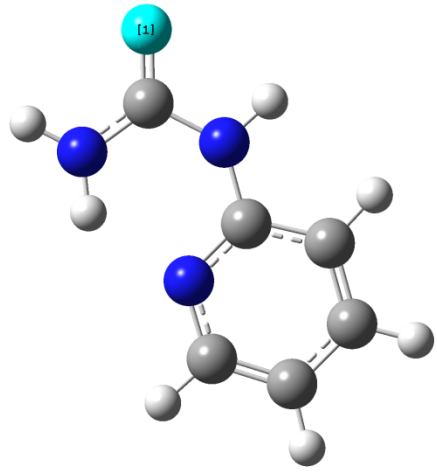
	1815.44	674.1773	1597.21	439.2809	1551.15	345.7587
	1805.51	780.7431	1598.50	404.5116	1563.21	581.6123
	1809.93	708.1454	1590.92	481.5817	1532.96	206.3635
	1807.63	686.7122	1595.65	473.4317	1554.28	384.1221
	1809.95	724.4114	1596.06	488.0869	1551.71	383.9920
	1807.18	718.5815	1595.37	475.1192	1552.70	392.0561
	1802.79	657.8325	1594.75	471.7443	1553.51	386.1295
	1809.05	695.9058	1591.84	438.1336	1537.68	255.3079
	1811.88	715.9719	1592.88	360.1643	1553.68	613.3307
	1818.21	703.7302	1598.82	394.2805	1545.92	464.3906

	1820.30	720.7243	1600.44	370.5854	1538.73	207.3897
	1817.63	697.1746	1591.14	391.2295	1523.99	158.5279
	1807.76	704.6705	1596.09	471.1118	1553.30	375.3427
	1804.24	699.0889	1595.23	448.9795	1544.48	340.9558
	1804.90	705.1149	1600.51	415.9014	1539.67	324.9853
	1815.72	792.8453	1592.58	347.0517	1511.82	183.0883
	1810.69	774.2148	1595.10	595.9699	1529.45	204.9642

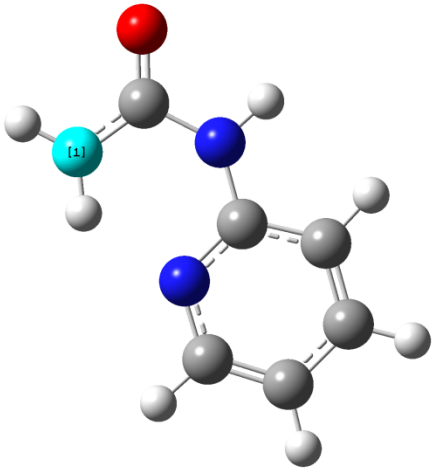
NBO_C



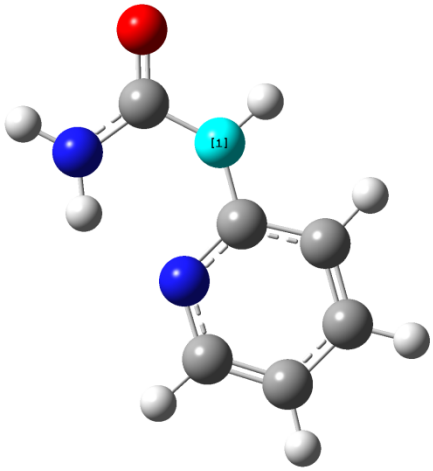
NBO_O



NBO_{N1}



NBO_{N2}



NBO_{Npyr}

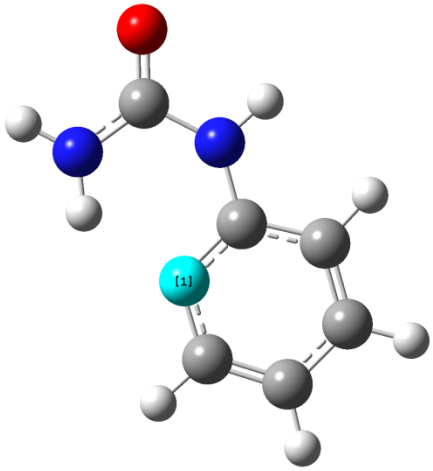
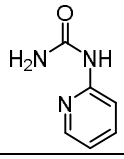
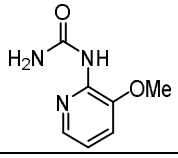
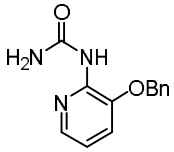
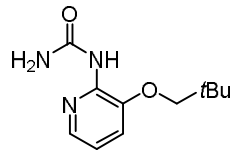
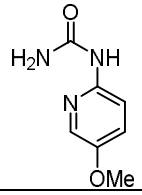
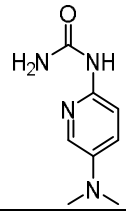
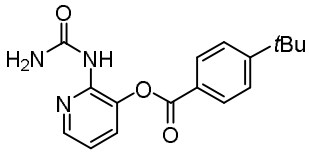
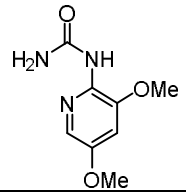
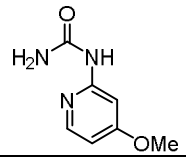
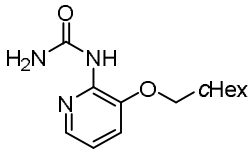
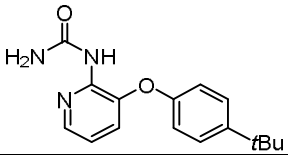
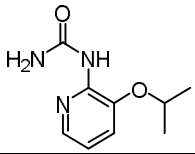
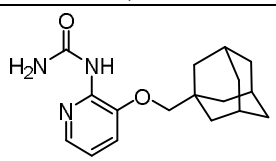
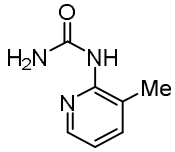
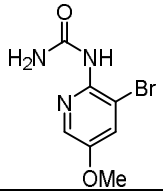
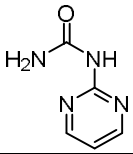
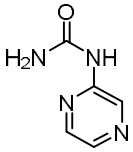
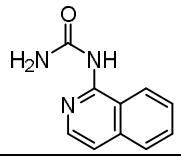
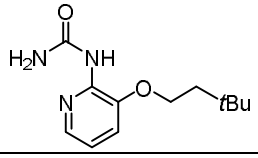
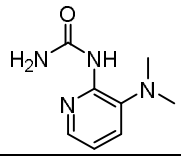
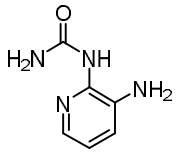
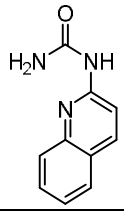
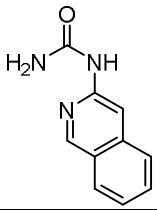


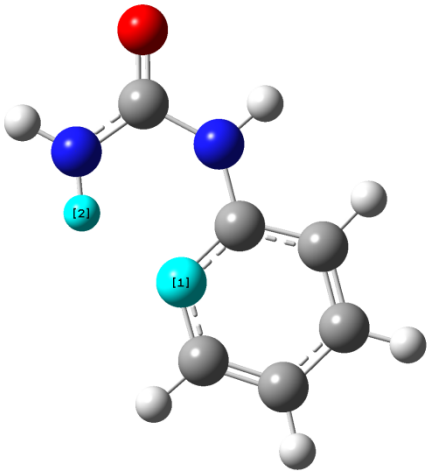
Table S4: Urea Parameters Continued

Urea	NBO_C	NBO_O	NBO_{N1}	NBO_{N2}	NBO_{Npyr}
	0.80419	-0.66130	-0.84622	-0.63986	-0.52532
	0.80474	-0.65987	-0.84750	-0.64497	-0.51350
	0.80503	-0.65970	-0.84751	-0.64573	-0.51214

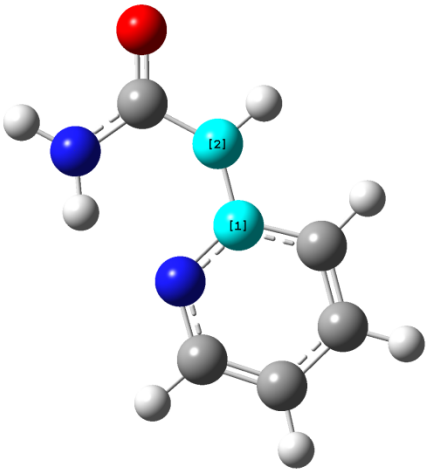
	0.80450	-0.66167	-0.84743	-0.64550	0.51400
	0.80293	-0.66560	-0.84855	-0.64282	-0.50787
	0.80280	-0.66756	-0.84910	-0.64218	-0.50936
	0.80453	-0.65350	-0.85649	-0.64740	-0.51634
	0.80395	-0.66432	-0.84986	-0.64810	-0.49508
	0.80446	-0.66320	-0.84730	-0.63916	-0.54708
	0.80483	-0.66200	-0.84776	-0.64553	-0.51317
	0.80405	-0.65940	-0.84796	-0.64418	-0.51433
	0.80402	-0.66191	-0.84803	-0.64485	-0.51539
	0.80517	-0.66255	-0.84759	-0.64551	-0.51244

	0.80597	-0.66282	-0.84551	-0.64834	-0.52275
	0.80536	-0.65673	-0.84631	-0.64884	-0.49558
	0.80379	-0.65054	-0.84546	-0.63834	-0.54423
	0.80401	-0.65253	-0.84395	-0.63838	-0.49172
	0.80624	-0.66026	-0.84272	-0.63995	-0.54222
	0.80425	-0.66133	-0.84790	-0.64539	-0.51487
	0.80581	-0.66125	-0.84778	-0.65241	-0.51960
	0.80673	-0.66008	-0.84784	-0.65754	-0.50856
	0.80402	-0.65896	-0.84509	-0.63750	-0.52893
	0.80395	-0.66389	-0.84777	-0.63908	-0.50851

N--H Distance:



C-N distance:



R_2--H distance:

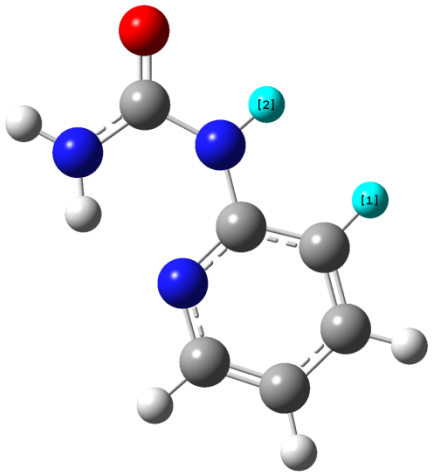
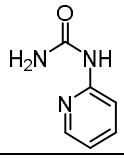
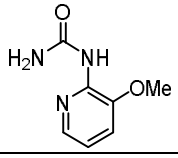
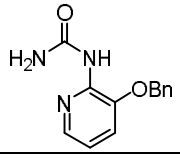
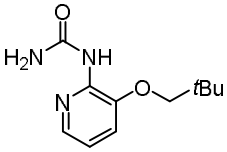
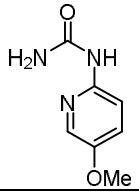
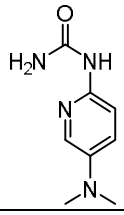
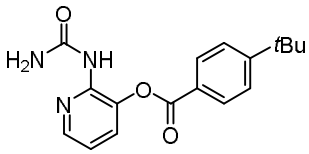
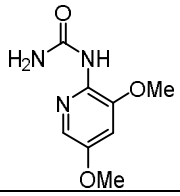
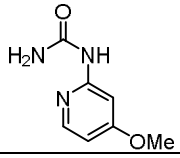
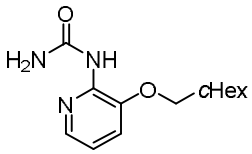
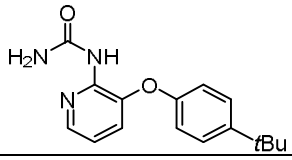
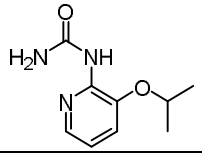
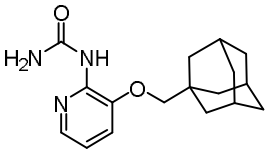
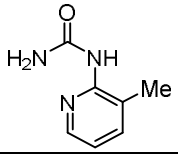
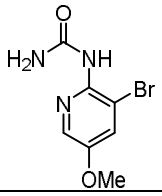
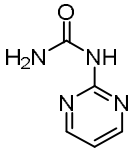
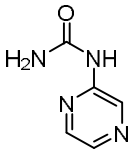
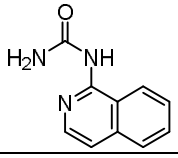
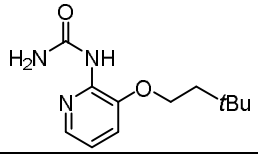
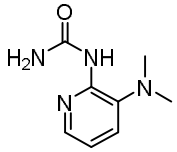
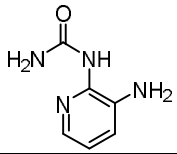
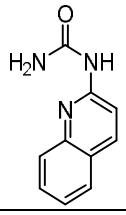
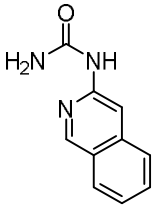


Table S4: Urea Parameters continued

Urea	N--H distance	C-N distance	R_2--H distance
	1.98775	1.38307	2.30744
	1.99172	1.3788	2.17126
	1.99116	1.37902	2.16650
	1.99233	1.37973	2.16393
	1.99361	1.38896	2.31721
	1.98966	1.38912	2.32234
	1.99477	1.37907	2.23116
	1.99704	1.38421	2.18394
	1.97941	1.38359	2.32458

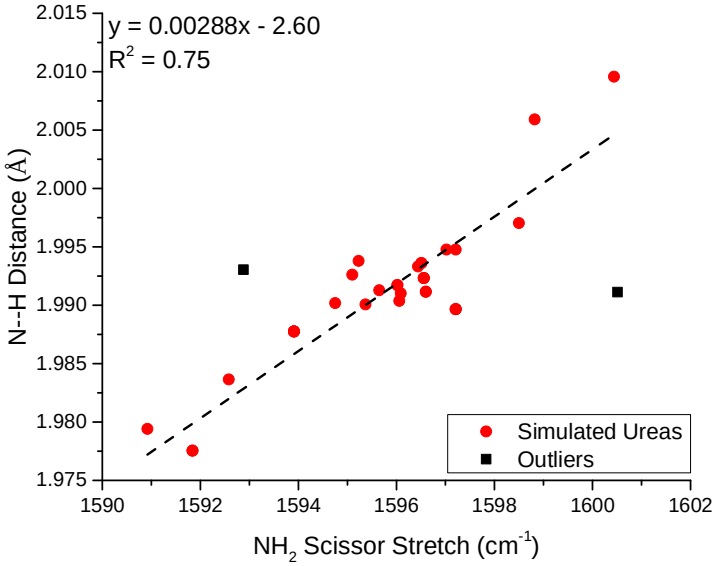
	1.99129	1.37965	2.16457
	1.99037	1.37929	2.18070
	1.99007	1.3795	2.15761
	1.99018	1.37997	2.15873
	1.97755	1.38484	2.39457
	1.99304	1.38070	2.56364
	2.00592	1.38421	*
	2.00957	1.37762	2.32280
	1.96433	1.37891	2.49283
	1.99102	1.37936	2.16452

	1.99380	1.38085	2.26409
	1.99112	1.38811	2.32791
	1.98365	1.38127	2.27462
	1.99261	1.38606	2.32573

*No R_2--H distance due to no substituent

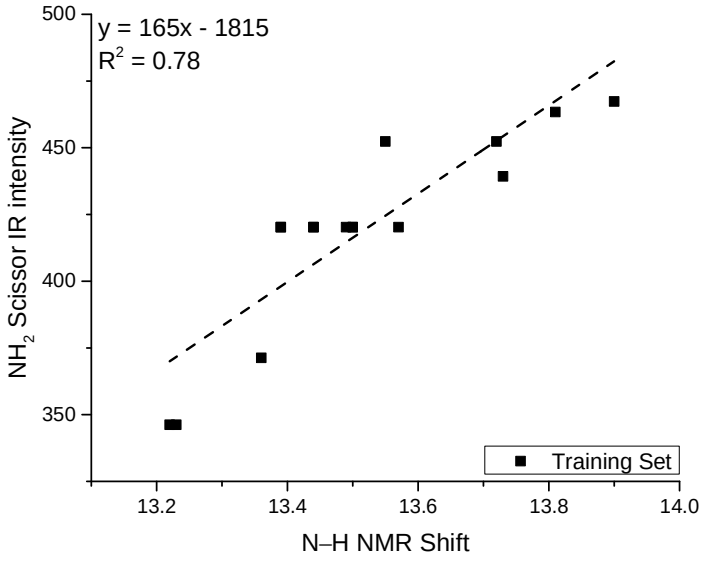
Parameter Trends

A number of trends were identified that help to explain the origin of a number of parameters. These are highlighted below.

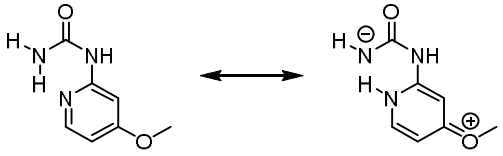


Further evidence of hydrogen bonding between the terminal hydrogen and the pyridine in the ureas

is shown between the relatively strong correlation between the distance of these two atoms and the IR scissoring frequency of the NH_2. Models built using the scissoring frequency in place of the N--H distance showed slightly decreased correlation coefficients compared to an optimal model. Two structures were identified as outliers in this trend. The first structure, derived from L19, includes a bromine atom that is unique to any other complex. The second structure includes $R^1 = NH_2$. The reason for this structure being an outlier is as yet unknown.



The intensity of the NH_2 scissor motion is correlated to the hydrogen bonded NMR shift**.** Small changes due to the variable aryl group are accounted for in the N-H hydrogen bonded NMR shift that cannot be accounted for in the NH_2 scissor IR intensity, as evidenced most clearly by the 8 complexes with varying aryl groups and a simulated intensity of 420.3. When comparing the entire set of complexes, three data points clearly become outliers from this trend. The first, from L28, contains a -OMe group on the pyridine ring that forms a resonance structure shown below, a likely cause of the lack of this correlation. The other two structures that are poorly correlated are the 1,3- and 1,4-pyrimidine structures (L20 and L21). The engagement of the second nitrogen in the aryl ring is a probable culprit for the origin of being off this trend line.



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X-ray analysis

Complex L23*(AuCl)$_2$ Crystallographic Data: The obtained crystal was twinned, which was treated with CELL_NOW and refined as a 2 component twin. Rotationally disordered CF_3 groups were restrained with ISOR and residual disordered solvent electron density was treated with SQUEEZE.

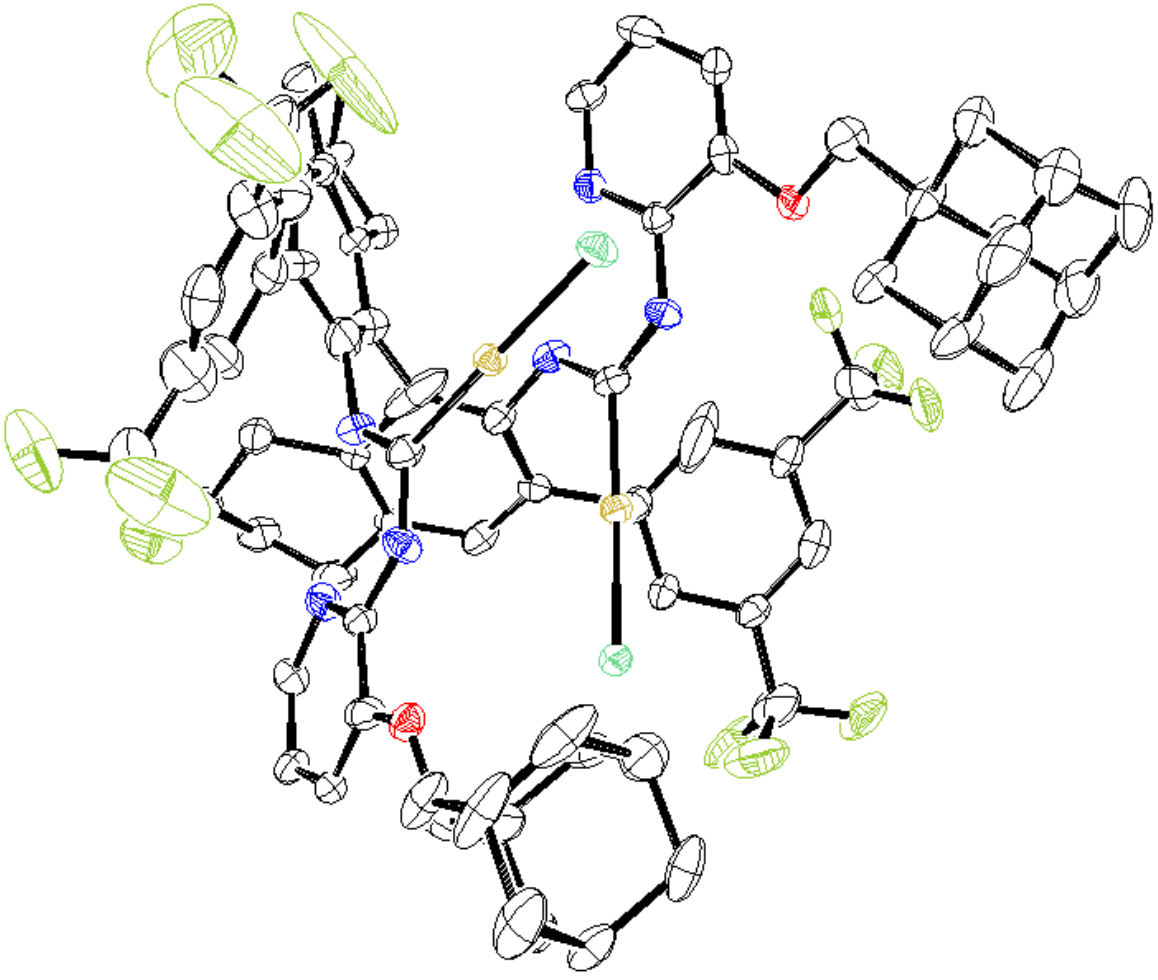


Table 1. Crystal data and structure refinement for cmh_sp_4.

Identification code	shelx	
Empirical formula	C70 H68 Au2 Cl2 F12 N6 O2	
Formula weight	1718.13	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P 1	
Unit cell dimensions	a = 11.2332(15) Å	a= 99.429(3)°.
	b = 13.4974(18) Å	b= 103.897(2)°.
	c = 13.5685(18) Å	g = 101.439(2)°.
Volume	1908.4(4) $Å^3$	
Z	1	
Density (calculated)	1.495 Mg/m^3	
Absorption coefficient	3.983 mm^{-1}	
F(000)	846	
Crystal size	0.100 x 0.100 x 0.100 mm^3	
Theta range for data collection	1.579 to 25.375°.	
Index ranges	-13<=h<=13, -16<=k<=16, -16<=l<=16	
Reflections collected	13583	
Independent reflections	13583 [R(int) = ?]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.745 and 0.504	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13583 / 95 / 824	
Goodness-of-fit on F^2	1.070	
Final R indices [I>2sigma(I)]	R1 = 0.0462, wR2 = 0.1116	
R indices (all data)	R1 = 0.0477, wR2 = 0.1129	
Absolute structure parameter	0.023(5)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.007 and -4.438 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for cmh_sp_4. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1054(16)	2554(18)	1289(18)	27(5)
C(2)	-1198(17)	2492(17)	1165(18)	25(5)
C(3)	-2296(17)	1880(20)	2272(19)	27(4)
C(4)	-3377(17)	2117(18)	1752(19)	26(4)
C(5)	-3370(15)	2590(16)	899(19)	28(5)
C(6)	-2280(20)	2770(20)	520(30)	31(7)
C(7)	-3055(17)	3800(20)	-560(20)	36(6)
C(8)	-2740(20)	4330(20)	-1360(20)	42(6)
C(9)	-3718(18)	4940(20)	-1650(20)	34(5)
C(10)	-1420(17)	5040(20)	-1058(19)	34(5)
C(11)	-2890(30)	3520(20)	-2340(20)	45(6)
C(12)	-3540(20)	5462(19)	-2506(18)	33(5)
C(13)	-3640(30)	4660(30)	-3560(30)	60(9)
C(14)	-2660(40)	4070(30)	-3270(30)	60(10)
C(15)	-2170(30)	6190(20)	-2200(20)	42(5)
C(16)	-1430(30)	4680(30)	-2970(20)	55(8)
C(17)	-1190(20)	5560(20)	-1920(20)	43(6)
C(18)	2130(20)	1600(20)	2460(30)	71(11)
C(19)	2637(19)	890(20)	1730(30)	49(8)
C(20)	3716(18)	677(18)	2360(20)	31(5)
C(21)	4178(15)	919(15)	3434(16)	24(4)
C(22)	3574(13)	1444(15)	4046(15)	21(4)
C(23)	2543(18)	1816(19)	3477(19)	33(5)
C(24)	4014(16)	1678(18)	5194(18)	29(4)
C(25)	4700(18)	893(17)	5601(16)	38(5)
C(26)	5787(15)	855(14)	5113(15)	34(4)
C(27)	5249(19)	460(20)	3900(20)	40(6)
C(28)	2298(12)	693(13)	722(10)	46(6)
C(29)	3152(9)	711(15)	130(12)	40(5)

C(30)	2711(13)	452(15)	-951(12)	44(5)
C(31)	1418(14)	173(16)	-1439(10)	50(6)
C(32)	564(9)	155(15)	-847(13)	70(8)
C(33)	1004(10)	415(13)	233(13)	67(7)
C(34)	3710(30)	550(20)	-1570(30)	47(7)
C(35)	-770(30)	-180(20)	-1550(20)	45(6)
C(36)	3332(15)	4646(17)	3326(16)	24(4)
C(37)	5558(16)	4719(17)	3367(18)	24(4)
C(38)	6735(18)	3650(20)	4032(18)	27(4)
C(39)	7768(18)	4070(20)	3780(20)	37(6)
C(40)	7663(18)	4948(18)	3260(20)	38(6)
C(41)	6630(20)	5240(20)	3060(20)	25(5)
C(42)	7283(19)	6410(20)	2090(20)	35(5)
C(43)	6920(20)	7313(19)	1596(19)	33(5)
C(44)	7010(30)	8280(20)	2380(30)	49(7)
C(45)	7890(20)	7520(20)	970(20)	38(5)
C(46)	5576(19)	6927(19)	837(19)	32(5)
C(47)	7570(30)	8380(20)	350(20)	47(6)
C(48)	7760(30)	9340(30)	1170(30)	61(9)
C(49)	6790(30)	9080(30)	1830(40)	65(11)
C(50)	5340(30)	8700(20)	960(30)	60(8)
C(51)	5320(30)	7790(20)	260(30)	48(7)
C(52)	6300(30)	7970(30)	-380(30)	60(8)
C(53)	2312(16)	3534(16)	4263(17)	28(4)
C(54)	2070(30)	2530(30)	4050(20)	84(14)
C(55)	948(15)	1995(17)	4463(19)	30(5)
C(56)	373(14)	2603(17)	5087(17)	30(5)
C(57)	765(18)	3671(19)	5246(19)	31(5)
C(58)	1710(13)	4143(15)	4871(16)	23(4)
C(59)	-684(18)	2070(20)	5460(20)	42(6)
C(60)	-636(17)	1060(15)	5603(14)	34(4)
C(61)	-650(17)	394(15)	4581(17)	34(4)
C(62)	542(17)	811(17)	4250(19)	32(5)
C(63)	1245(8)	5910(10)	5185(12)	25(4)
C(64)	2173(11)	5363(8)	5206(13)	30(4)
C(65)	3441(10)	5893(10)	5480(14)	105(12)

C(66)	3781(8)	6970(10)	5733(13)	32(4)
C(67)	2853(11)	7518(8)	5712(12)	35(4)
C(68)	1585(10)	6988(10)	5438(12)	28(4)
C(69)	530(30)	7530(30)	5560(30)	57(8)
C(70)	5130(20)	7590(30)	6000(30)	59(10)
N(1)	1088(13)	1967(15)	1949(14)	24(4)
N(2)	-79(13)	2752(16)	898(16)	26(4)
N(3)	-1185(13)	2047(15)	1981(16)	28(4)
N(4)	3345(13)	3945(15)	3948(14)	26(4)
N(5)	4422(13)	5014(17)	3119(15)	24(4)
N(6)	5643(14)	3919(15)	3824(15)	26(4)
O(1)	-2126(12)	3217(13)	-231(13)	27(3)
O(2)	6382(12)	6064(13)	2666(15)	30(4)
F(1)	3980(40)	-470(30)	-1790(30)	157(14)
F(2)	4660(30)	1080(40)	-1220(30)	230(30)
F(3)	3280(30)	210(40)	-2490(20)	180(20)
F(4)	-1070(20)	230(40)	-2450(30)	125(14)
F(5)	-1526(12)	158(16)	-913(15)	58(4)
F(6)	-1255(18)	-1190(20)	-1779(18)	85(7)
F(7)	-293(17)	7341(18)	4560(19)	85(8)
F(8)	980(17)	8554(14)	5737(16)	66(5)
F(9)	-160(20)	7206(15)	6043(19)	86(7)
F(10)	5628(15)	7896(16)	7035(15)	65(5)
F(11)	5269(14)	8353(16)	5620(30)	79(8)
F(12)	5847(11)	6993(12)	5674(15)	50(4)
Cl(1)	4382(4)	4040(4)	586(4)	30(1)
Cl(2)	-102(3)	5315(4)	1771(4)	24(1)
Au(1)	2577(1)	3219(1)	904(1)	21(1)
Au(2)	1746(1)	4991(1)	2637(1)	21(1)

Table 3. Bond lengths [Å] and angles [°] for cmh_sp_4.

C(1)-N(1)	1.29(3)
C(1)-N(2)	1.35(2)
C(1)-Au(1)	1.995(19)
C(2)-N(3)	1.34(3)
C(2)-N(2)	1.39(2)
C(2)-C(6)	1.47(3)
C(3)-C(4)	1.38(3)
C(3)-N(3)	1.38(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.41(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.43(3)
C(5)-H(5)	0.9500
C(6)-O(1)	1.30(3)
C(7)-O(1)	1.46(3)
C(7)-C(8)	1.47(4)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(9)	1.51(3)
C(8)-C(10)	1.52(3)
C(8)-C(11)	1.53(4)
C(9)-C(12)	1.49(4)
C(9)-H(9A)	0.9900
C(9)-H(9B)	0.9900
C(10)-C(17)	1.51(4)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(14)	1.61(5)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(15)	1.57(4)
C(12)-C(13)	1.61(4)
C(12)-H(12)	1.0000
C(13)-C(14)	1.50(4)

C(13)-H(13A)	0.9900
C(13)-H(13B)	0.9900
C(14)-C(16)	1.38(6)
C(14)-H(14)	1.0000
C(15)-C(17)	1.53(4)
C(15)-H(15A)	0.9900
C(15)-H(15B)	0.9900
C(16)-C(17)	1.62(4)
C(16)-H(16A)	0.9900
C(16)-H(16B)	0.9900
C(17)-H(17)	1.0000
C(18)-C(23)	1.31(5)
C(18)-N(1)	1.43(3)
C(18)-C(19)	1.56(5)
C(19)-C(28)	1.30(4)
C(19)-C(20)	1.41(3)
C(20)-C(21)	1.38(3)
C(20)-H(20)	0.9500
C(21)-C(22)	1.39(3)
C(21)-C(27)	1.52(3)
C(22)-C(23)	1.46(2)
C(22)-C(24)	1.48(3)
C(23)-C(54)	1.40(2)
C(24)-C(25)	1.53(3)
C(24)-H(24A)	0.9900
C(24)-H(24B)	0.9900
C(25)-C(26)	1.53(2)
C(25)-H(25A)	0.9900
C(25)-H(25B)	0.9900
C(26)-C(27)	1.57(3)
C(26)-H(26A)	0.9900
C(26)-H(26B)	0.9900
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.3900
C(28)-C(33)	1.3900

C(29)-C(30)	1.3900
C(29)-H(29)	0.9500
C(30)-C(31)	1.3900
C(30)-C(34)	1.55(3)
C(31)-C(32)	1.3900
C(31)-H(31)	0.9500
C(32)-C(33)	1.3900
C(32)-C(35)	1.51(3)
C(33)-H(33)	0.9500
C(34)-F(2)	1.11(4)
C(34)-F(3)	1.20(5)
C(34)-F(1)	1.47(4)
C(35)-F(6)	1.31(4)
C(35)-F(4)	1.42(4)
C(35)-F(5)	1.43(3)
C(36)-N(5)	1.34(3)
C(36)-N(4)	1.37(3)
C(36)-Au(2)	1.984(16)
C(37)-N(6)	1.34(3)
C(37)-N(5)	1.39(2)
C(37)-C(41)	1.46(3)
C(38)-N(6)	1.33(3)
C(38)-C(39)	1.34(3)
C(38)-H(38)	0.9500
C(39)-C(40)	1.48(4)
C(39)-H(39)	0.9500
C(40)-C(41)	1.28(3)
C(40)-H(40)	0.9500
C(41)-O(2)	1.36(3)
C(42)-O(2)	1.47(3)
C(42)-C(43)	1.56(3)
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900
C(43)-C(44)	1.51(4)
C(43)-C(46)	1.55(3)
C(43)-C(45)	1.55(3)

C(44)-C(49)	1.44(5)
C(44)-H(44A)	0.9900
C(44)-H(44B)	0.9900
C(45)-C(47)	1.58(4)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(51)	1.54(3)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(52)	1.47(5)
C(47)-C(48)	1.50(5)
C(47)-H(47)	1.0000
C(48)-C(49)	1.60(5)
C(48)-H(48A)	0.9900
C(48)-H(48B)	0.9900
C(49)-C(50)	1.69(5)
C(49)-H(49)	1.0000
C(50)-C(51)	1.42(5)
C(50)-H(50A)	0.9900
C(50)-H(50B)	0.9900
C(51)-C(52)	1.56(4)
C(51)-H(51)	1.0000
C(52)-H(52A)	0.9900
C(52)-H(52B)	0.9900
C(53)-C(54)	1.30(4)
C(53)-N(4)	1.38(3)
C(53)-C(58)	1.44(3)
C(54)-C(55)	1.59(5)
C(55)-C(56)	1.43(3)
C(55)-C(62)	1.53(3)
C(56)-C(57)	1.39(3)
C(56)-C(59)	1.50(3)
C(57)-C(58)	1.37(3)
C(57)-H(57)	0.9500
C(58)-C(64)	1.58(2)
C(59)-C(60)	1.41(3)

C(59)-H(59A)	0.9900
C(59)-H(59B)	0.9900
C(60)-C(61)	1.52(3)
C(60)-H(60A)	0.9900
C(60)-H(60B)	0.9900
C(61)-C(62)	1.54(2)
C(61)-H(61A)	0.9900
C(61)-H(61B)	0.9900
C(62)-H(62A)	0.9900
C(62)-H(62B)	0.9900
C(63)-C(64)	1.3900
C(63)-C(68)	1.3900
C(63)-H(63)	0.9500
C(64)-C(65)	1.3900
C(65)-C(66)	1.3900
C(65)-H(65)	0.9500
C(66)-C(67)	1.3900
C(66)-C(70)	1.51(3)
C(67)-C(68)	1.3900
C(67)-H(67)	0.9500
C(68)-C(69)	1.54(3)
C(69)-F(9)	1.20(5)
C(69)-F(8)	1.33(5)
C(69)-F(7)	1.39(4)
C(70)-F(11)	1.23(4)
C(70)-F(10)	1.34(4)
C(70)-F(12)	1.34(4)
N(1)-H(1)	0.8800
N(2)-H(2)	0.8800
N(4)-H(4A)	0.8800
N(5)-H(5A)	0.8800
F(1)-F(3)	1.60(6)
Cl(1)-Au(1)	2.283(4)
Cl(2)-Au(2)	2.289(4)

N(1)-C(1)-N(2)	116.1(17)

N(1)-C(1)-Au(1)	123.4(13)
N(2)-C(1)-Au(1)	120.4(16)
N(3)-C(2)-N(2)	118.1(16)
N(3)-C(2)-C(6)	127(2)
N(2)-C(2)-C(6)	115(2)
C(4)-C(3)-N(3)	123.2(19)
C(4)-C(3)-H(3)	118.4
N(3)-C(3)-H(3)	118.4
C(3)-C(4)-C(5)	119.8(17)
C(3)-C(4)-H(4)	120.1
C(5)-C(4)-H(4)	120.1
C(4)-C(5)-C(6)	121.1(17)
C(4)-C(5)-H(5)	119.5
C(6)-C(5)-H(5)	119.5
O(1)-C(6)-C(5)	128(2)
O(1)-C(6)-C(2)	119(2)
C(5)-C(6)-C(2)	113(2)
O(1)-C(7)-C(8)	109.8(16)
O(1)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7A)	109.7
O(1)-C(7)-H(7B)	109.7
C(8)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2
C(7)-C(8)-C(9)	108(2)
C(7)-C(8)-C(10)	115.3(19)
C(9)-C(8)-C(10)	110(2)
C(7)-C(8)-C(11)	109(2)
C(9)-C(8)-C(11)	107(2)
C(10)-C(8)-C(11)	108(2)
C(12)-C(9)-C(8)	112(2)
C(12)-C(9)-H(9A)	109.2
C(8)-C(9)-H(9A)	109.2
C(12)-C(9)-H(9B)	109.2
C(8)-C(9)-H(9B)	109.2
H(9A)-C(9)-H(9B)	107.9
C(17)-C(10)-C(8)	112(2)

C(17)-C(10)-H(10A)	109.3
C(8)-C(10)-H(10A)	109.3
C(17)-C(10)-H(10B)	109.3
C(8)-C(10)-H(10B)	109.3
H(10A)-C(10)-H(10B)	107.9
C(8)-C(11)-C(14)	111(2)
C(8)-C(11)-H(11A)	109.5
C(14)-C(11)-H(11A)	109.5
C(8)-C(11)-H(11B)	109.5
C(14)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	108.1
C(9)-C(12)-C(15)	110.5(18)
C(9)-C(12)-C(13)	113(2)
C(15)-C(12)-C(13)	104(2)
C(9)-C(12)-H(12)	109.7
C(15)-C(12)-H(12)	109.7
C(13)-C(12)-H(12)	109.7
C(14)-C(13)-C(12)	106(3)
C(14)-C(13)-H(13A)	110.5
C(12)-C(13)-H(13A)	110.5
C(14)-C(13)-H(13B)	110.5
C(12)-C(13)-H(13B)	110.5
H(13A)-C(13)-H(13B)	108.7
C(16)-C(14)-C(13)	113(3)
C(16)-C(14)-C(11)	109(3)
C(13)-C(14)-C(11)	110(3)
C(16)-C(14)-H(14)	108.3
C(13)-C(14)-H(14)	108.3
C(11)-C(14)-H(14)	108.3
C(17)-C(15)-C(12)	110(2)
C(17)-C(15)-H(15A)	109.7
C(12)-C(15)-H(15A)	109.7
C(17)-C(15)-H(15B)	109.7
C(12)-C(15)-H(15B)	109.7
H(15A)-C(15)-H(15B)	108.2
C(14)-C(16)-C(17)	111(2)

C(14)-C(16)-H(16A)	109.4
C(17)-C(16)-H(16A)	109.4
C(14)-C(16)-H(16B)	109.4
C(17)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(10)-C(17)-C(15)	109.6(19)
C(10)-C(17)-C(16)	109(2)
C(15)-C(17)-C(16)	105(2)
C(10)-C(17)-H(17)	110.8
C(15)-C(17)-H(17)	110.8
C(16)-C(17)-H(17)	110.8
C(23)-C(18)-N(1)	121(3)
C(23)-C(18)-C(19)	124(2)
N(1)-C(18)-C(19)	115(3)
C(28)-C(19)-C(20)	126(2)
C(28)-C(19)-C(18)	126(2)
C(20)-C(19)-C(18)	107(3)
C(21)-C(20)-C(19)	129(2)
C(21)-C(20)-H(20)	115.6
C(19)-C(20)-H(20)	115.6
C(20)-C(21)-C(22)	120.7(16)
C(20)-C(21)-C(27)	116.9(19)
C(22)-C(21)-C(27)	121.9(19)
C(21)-C(22)-C(23)	115.2(18)
C(21)-C(22)-C(24)	122.0(15)
C(23)-C(22)-C(24)	122.6(17)
C(18)-C(23)-C(54)	119(2)
C(18)-C(23)-C(22)	123(2)
C(54)-C(23)-C(22)	118(2)
C(22)-C(24)-C(25)	112.2(18)
C(22)-C(24)-H(24A)	109.2
C(25)-C(24)-H(24A)	109.2
C(22)-C(24)-H(24B)	109.2
C(25)-C(24)-H(24B)	109.2
H(24A)-C(24)-H(24B)	107.9
C(24)-C(25)-C(26)	108.6(16)

C(24)-C(25)-H(25A)	110.0
C(26)-C(25)-H(25A)	110.0
C(24)-C(25)-H(25B)	110.0
C(26)-C(25)-H(25B)	110.0
H(25A)-C(25)-H(25B)	108.3
C(25)-C(26)-C(27)	109.8(14)
C(25)-C(26)-H(26A)	109.7
C(27)-C(26)-H(26A)	109.7
C(25)-C(26)-H(26B)	109.7
C(27)-C(26)-H(26B)	109.7
H(26A)-C(26)-H(26B)	108.2
C(21)-C(27)-C(26)	113.0(18)
C(21)-C(27)-H(27A)	109.0
C(26)-C(27)-H(27A)	109.0
C(21)-C(27)-H(27B)	109.0
C(26)-C(27)-H(27B)	109.0
H(27A)-C(27)-H(27B)	107.8
C(19)-C(28)-C(29)	123.5(12)
C(19)-C(28)-C(33)	116.5(12)
C(29)-C(28)-C(33)	120.0
C(30)-C(29)-C(28)	120.0
C(30)-C(29)-H(29)	120.0
C(28)-C(29)-H(29)	120.0
C(31)-C(30)-C(29)	120.0
C(31)-C(30)-C(34)	122.1(16)
C(29)-C(30)-C(34)	117.7(16)
C(32)-C(31)-C(30)	120.0
C(32)-C(31)-H(31)	120.0
C(30)-C(31)-H(31)	120.0
C(31)-C(32)-C(33)	120.0
C(31)-C(32)-C(35)	110.1(15)
C(33)-C(32)-C(35)	129.8(15)
C(32)-C(33)-C(28)	120.0
C(32)-C(33)-H(33)	120.0
C(28)-C(33)-H(33)	120.0
F(2)-C(34)-F(3)	123(4)

F(2)-C(34)-F(1)	103(4)
F(3)-C(34)-F(1)	73(3)
F(2)-C(34)-C(30)	121(3)
F(3)-C(34)-C(30)	115(2)
F(1)-C(34)-C(30)	106(3)
F(6)-C(35)-F(4)	110(3)
F(6)-C(35)-F(5)	101(2)
F(4)-C(35)-F(5)	106(3)
F(6)-C(35)-C(32)	114(3)
F(4)-C(35)-C(32)	119(2)
F(5)-C(35)-C(32)	105(2)
N(5)-C(36)-N(4)	116.6(16)
N(5)-C(36)-Au(2)	121.1(16)
N(4)-C(36)-Au(2)	122.0(13)
N(6)-C(37)-N(5)	120.4(17)
N(6)-C(37)-C(41)	119.8(18)
N(5)-C(37)-C(41)	120(2)
N(6)-C(38)-C(39)	126(2)
N(6)-C(38)-H(38)	117.1
C(39)-C(38)-H(38)	117.1
C(38)-C(39)-C(40)	115.2(19)
C(38)-C(39)-H(39)	122.4
C(40)-C(39)-H(39)	122.4
C(41)-C(40)-C(39)	121(2)
C(41)-C(40)-H(40)	119.6
C(39)-C(40)-H(40)	119.6
C(40)-C(41)-O(2)	129(2)
C(40)-C(41)-C(37)	120(2)
O(2)-C(41)-C(37)	111(2)
O(2)-C(42)-C(43)	109.6(17)
O(2)-C(42)-H(42A)	109.8
C(43)-C(42)-H(42A)	109.8
O(2)-C(42)-H(42B)	109.8
C(43)-C(42)-H(42B)	109.8
H(42A)-C(42)-H(42B)	108.2
C(44)-C(43)-C(46)	110(2)

C(44)-C(43)-C(45)	111(2)
C(46)-C(43)-C(45)	109(2)
C(44)-C(43)-C(42)	114(2)
C(46)-C(43)-C(42)	109.2(19)
C(45)-C(43)-C(42)	102.7(17)
C(49)-C(44)-C(43)	109(3)
C(49)-C(44)-H(44A)	109.9
C(43)-C(44)-H(44A)	109.9
C(49)-C(44)-H(44B)	109.9
C(43)-C(44)-H(44B)	109.9
H(44A)-C(44)-H(44B)	108.3
C(43)-C(45)-C(47)	108.1(18)
C(43)-C(45)-H(45A)	110.1
C(47)-C(45)-H(45A)	110.1
C(43)-C(45)-H(45B)	110.1
C(47)-C(45)-H(45B)	110.1
H(45A)-C(45)-H(45B)	108.4
C(51)-C(46)-C(43)	108(2)
C(51)-C(46)-H(46A)	110.1
C(43)-C(46)-H(46A)	110.1
C(51)-C(46)-H(46B)	110.1
C(43)-C(46)-H(46B)	110.1
H(46A)-C(46)-H(46B)	108.4
C(52)-C(47)-C(48)	117(3)
C(52)-C(47)-C(45)	108(2)
C(48)-C(47)-C(45)	106(3)
C(52)-C(47)-H(47)	108.6
C(48)-C(47)-H(47)	108.6
C(45)-C(47)-H(47)	108.6
C(47)-C(48)-C(49)	108(3)
C(47)-C(48)-H(48A)	110.2
C(49)-C(48)-H(48A)	110.2
C(47)-C(48)-H(48B)	110.2
C(49)-C(48)-H(48B)	110.2
H(48A)-C(48)-H(48B)	108.5
C(44)-C(49)-C(48)	113(3)

C(44)-C(49)-C(50)	110(3)
C(48)-C(49)-C(50)	106(3)
C(44)-C(49)-H(49)	109.5
C(48)-C(49)-H(49)	109.5
C(50)-C(49)-H(49)	109.5
C(51)-C(50)-C(49)	107(2)
C(51)-C(50)-H(50A)	110.2
C(49)-C(50)-H(50A)	110.2
C(51)-C(50)-H(50B)	110.2
C(49)-C(50)-H(50B)	110.2
H(50A)-C(50)-H(50B)	108.5
C(50)-C(51)-C(46)	111(3)
C(50)-C(51)-C(52)	113(3)
C(46)-C(51)-C(52)	108.1(19)
C(50)-C(51)-H(51)	108.2
C(46)-C(51)-H(51)	108.2
C(52)-C(51)-H(51)	108.2
C(47)-C(52)-C(51)	109(3)
C(47)-C(52)-H(52A)	109.9
C(51)-C(52)-H(52A)	109.9
C(47)-C(52)-H(52B)	109.9
C(51)-C(52)-H(52B)	109.9
H(52A)-C(52)-H(52B)	108.3
C(54)-C(53)-N(4)	110(2)
C(54)-C(53)-C(58)	125(3)
N(4)-C(53)-C(58)	124.1(18)
C(53)-C(54)-C(23)	133(4)
C(53)-C(54)-C(55)	113(2)
C(23)-C(54)-C(55)	114(3)
C(56)-C(55)-C(62)	119.5(18)
C(56)-C(55)-C(54)	121(2)
C(62)-C(55)-C(54)	119.1(18)
C(57)-C(56)-C(55)	117.3(19)
C(57)-C(56)-C(59)	123.2(18)
C(55)-C(56)-C(59)	119(2)
C(58)-C(57)-C(56)	122.1(19)

C(58)-C(57)-H(57)	118.9
C(56)-C(57)-H(57)	118.9
C(57)-C(58)-C(53)	120.7(19)
C(57)-C(58)-C(64)	117.3(17)
C(53)-C(58)-C(64)	121.8(15)
C(60)-C(59)-C(56)	114.8(17)
C(60)-C(59)-H(59A)	108.6
C(56)-C(59)-H(59A)	108.6
C(60)-C(59)-H(59B)	108.6
C(56)-C(59)-H(59B)	108.6
H(59A)-C(59)-H(59B)	107.5
C(59)-C(60)-C(61)	108.9(17)
C(59)-C(60)-H(60A)	109.9
C(61)-C(60)-H(60A)	109.9
C(59)-C(60)-H(60B)	109.9
C(61)-C(60)-H(60B)	109.9
H(60A)-C(60)-H(60B)	108.3
C(60)-C(61)-C(62)	111.0(16)
C(60)-C(61)-H(61A)	109.4
C(62)-C(61)-H(61A)	109.4
C(60)-C(61)-H(61B)	109.4
C(62)-C(61)-H(61B)	109.4
H(61A)-C(61)-H(61B)	108.0
C(55)-C(62)-C(61)	113.8(16)
C(55)-C(62)-H(62A)	108.8
C(61)-C(62)-H(62A)	108.8
C(55)-C(62)-H(62B)	108.8
C(61)-C(62)-H(62B)	108.8
H(62A)-C(62)-H(62B)	107.7
C(64)-C(63)-C(68)	120.0
C(64)-C(63)-H(63)	120.0
C(68)-C(63)-H(63)	120.0
C(63)-C(64)-C(65)	120.0
C(63)-C(64)-C(58)	117.0(9)
C(65)-C(64)-C(58)	123.0(9)
C(66)-C(65)-C(64)	120.0

C(66)-C(65)-H(65)	120.0
C(64)-C(65)-H(65)	120.0
C(65)-C(66)-C(67)	120.0
C(65)-C(66)-C(70)	122.4(16)
C(67)-C(66)-C(70)	117.6(16)
C(68)-C(67)-C(66)	120.0
C(68)-C(67)-H(67)	120.0
C(66)-C(67)-H(67)	120.0
C(67)-C(68)-C(63)	120.0
C(67)-C(68)-C(69)	122.8(17)
C(63)-C(68)-C(69)	116.5(17)
F(9)-C(69)-F(8)	118(3)
F(9)-C(69)-F(7)	103(3)
F(8)-C(69)-F(7)	101(3)
F(9)-C(69)-C(68)	118(3)
F(8)-C(69)-C(68)	109(3)
F(7)-C(69)-C(68)	106(2)
F(11)-C(70)-F(10)	109(3)
F(11)-C(70)-F(12)	107(3)
F(10)-C(70)-F(12)	106(2)
F(11)-C(70)-C(66)	113.7(19)
F(10)-C(70)-C(66)	111(3)
F(12)-C(70)-C(66)	110(3)
C(1)-N(1)-C(18)	129(2)
C(1)-N(1)-H(1)	115.7
C(18)-N(1)-H(1)	115.7
C(1)-N(2)-C(2)	130(2)
C(1)-N(2)-H(2)	115.2
C(2)-N(2)-H(2)	115.2
C(2)-N(3)-C(3)	116.1(16)
C(36)-N(4)-C(53)	123.1(14)
C(36)-N(4)-H(4A)	118.5
C(53)-N(4)-H(4A)	118.5
C(36)-N(5)-C(37)	129(2)
C(36)-N(5)-H(5A)	115.3
C(37)-N(5)-H(5A)	115.3

C(38)-N(6)-C(37)	118.7(17)
C(6)-O(1)-C(7)	114.5(18)
C(41)-O(2)-C(42)	110.9(18)
C(34)-F(1)-F(3)	46(2)
C(34)-F(3)-F(1)	61(3)
C(1)-Au(1)-Cl(1)	175.9(7)
C(36)-Au(2)-Cl(2)	177.0(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for cmh_sp_4. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	32(8)	27(12)	28(12)	12(9)	13(7)	12(7)
C(2)	25(8)	22(11)	28(12)	6(9)	5(7)	8(7)
C(3)	27(7)	31(14)	24(13)	7(8)	10(7)	4(7)
C(4)	32(8)	23(11)	30(12)	10(9)	16(8)	11(7)
C(5)	21(7)	21(11)	39(13)	1(9)	4(7)	6(7)
C(6)	27(10)	32(15)	33(14)	-3(11)	5(9)	13(9)
C(7)	20(8)	52(17)	29(13)	-6(11)	7(7)	4(9)
C(8)	43(10)	50(16)	28(13)	-7(11)	5(8)	24(10)
C(9)	40(9)	31(13)	29(13)	-1(10)	6(8)	15(8)
C(10)	34(9)	43(15)	27(12)	2(11)	7(8)	20(9)
C(11)	74(14)	28(13)	34(14)	4(11)	9(11)	26(11)
C(12)	53(10)	31(12)	20(11)	6(9)	9(8)	24(9)
C(13)	95(19)	36(16)	33(16)	-10(12)	-6(13)	23(14)
C(14)	130(30)	35(14)	24(13)	8(11)	11(14)	44(15)
C(15)	83(15)	21(12)	21(12)	6(9)	14(10)	13(11)
C(16)	110(20)	54(16)	41(15)	27(13)	45(15)	58(17)
C(17)	45(10)	43(16)	49(16)	16(13)	22(10)	14(10)
C(18)	36(10)	28(14)	130(30)	32(17)	-10(14)	6(9)
C(19)	33(9)	50(16)	90(20)	52(16)	37(12)	25(10)
C(20)	42(9)	23(11)	41(13)	12(9)	27(9)	12(8)
C(21)	27(7)	21(9)	26(10)	6(7)	11(6)	5(6)

C(22)	22(6)	21(9)	20(9)	5(7)	6(6)	6(6)
C(23)	36(8)	39(12)	32(12)	20(10)	15(8)	16(8)
C(24)	31(8)	31(11)	33(11)	16(9)	14(7)	11(7)
C(25)	46(10)	47(13)	36(10)	23(9)	17(8)	29(9)
C(26)	30(8)	32(9)	45(10)	22(8)	12(7)	11(7)
C(27)	46(10)	37(13)	62(16)	30(12)	36(10)	25(9)
C(28)	41(10)	27(12)	63(15)	-11(10)	19(10)	4(8)
C(29)	46(10)	52(15)	27(10)	3(10)	17(8)	18(9)
C(30)	50(11)	51(16)	30(12)	17(10)	16(9)	-1(10)
C(31)	73(14)	30(13)	46(13)	14(10)	15(11)	7(11)
C(32)	58(12)	63(16)	87(15)	48(14)	1(12)	9(11)
C(33)	26(8)	38(11)	131(16)	49(12)	-6(10)	2(8)
C(34)	57(13)	28(13)	49(17)	-7(11)	15(12)	7(9)
C(35)	61(13)	45(16)	21(10)	8(10)	4(9)	3(11)
C(36)	26(7)	27(11)	20(11)	4(9)	5(7)	12(7)
C(37)	26(8)	20(11)	27(12)	6(9)	12(7)	6(7)
C(38)	32(8)	32(14)	20(13)	5(8)	7(7)	17(8)
C(39)	22(8)	51(16)	38(14)	4(12)	11(8)	10(9)
C(40)	33(9)	20(11)	64(18)	6(11)	22(10)	4(8)
C(41)	30(10)	22(11)	20(12)	4(9)	6(8)	0(8)
C(42)	42(10)	38(14)	33(14)	17(12)	19(9)	12(9)
C(43)	56(11)	27(12)	32(12)	13(10)	26(9)	20(9)
C(44)	80(15)	23(13)	60(19)	10(12)	46(14)	17(11)
C(45)	59(11)	28(13)	41(15)	10(11)	34(10)	12(9)
C(46)	50(10)	29(12)	28(12)	12(10)	17(8)	22(9)
C(47)	73(14)	36(14)	45(16)	7(12)	41(13)	16(11)
C(48)	100(20)	30(16)	60(20)	16(15)	46(17)	1(14)
C(49)	83(19)	30(17)	100(30)	0(18)	60(20)	16(15)
C(50)	110(20)	36(14)	67(19)	29(13)	55(17)	41(15)
C(51)	69(13)	43(16)	56(18)	29(14)	31(12)	36(12)
C(52)	100(20)	40(17)	60(20)	11(14)	54(17)	35(15)
C(53)	32(8)	24(9)	30(11)	5(8)	11(7)	11(7)
C(54)	100(20)	70(20)	51(18)	-36(15)	-44(15)	68(19)
C(55)	20(7)	20(10)	48(13)	6(9)	7(7)	5(6)
C(56)	20(7)	30(11)	32(11)	-7(8)	4(6)	7(7)
C(57)	40(9)	29(11)	31(12)	7(9)	15(8)	18(8)

C(58)	20(6)	27(10)	20(9)	3(8)	5(6)	7(6)
C(59)	33(9)	50(15)	48(15)	4(11)	17(9)	21(9)
C(60)	36(8)	45(10)	33(9)	15(8)	20(7)	17(8)
C(61)	36(8)	27(9)	46(12)	12(9)	22(8)	7(7)
C(62)	34(8)	28(11)	39(12)	6(9)	21(8)	8(7)
C(63)	34(8)	21(9)	24(10)	6(7)	13(7)	8(6)
C(64)	35(8)	23(9)	33(11)	11(8)	12(7)	8(7)
C(65)	140(20)	26(10)	150(30)	17(14)	28(19)	25(14)
C(66)	48(10)	21(8)	21(9)	3(6)	0(7)	11(7)
C(67)	61(11)	21(8)	26(10)	5(7)	16(9)	9(8)
C(68)	33(8)	26(9)	29(11)	7(8)	14(7)	13(7)
C(69)	65(16)	42(15)	60(20)	-14(14)	8(15)	27(13)
C(70)	32(11)	60(20)	70(20)	30(17)	-16(11)	3(11)
N(1)	26(6)	28(10)	22(9)	7(8)	8(6)	12(6)
N(2)	21(7)	34(11)	25(10)	12(9)	5(6)	4(6)
N(3)	27(7)	28(10)	30(11)	12(8)	9(6)	4(6)
N(4)	31(6)	30(10)	23(10)	10(8)	12(6)	15(6)
N(5)	20(6)	30(10)	20(10)	6(8)	6(6)	6(6)
N(6)	27(7)	21(10)	30(11)	2(8)	14(6)	3(6)
O(1)	31(6)	23(9)	28(9)	9(7)	7(5)	8(5)
O(2)	27(6)	22(9)	44(11)	4(8)	19(6)	4(6)
F(1)	200(20)	130(20)	150(20)	-29(16)	86(19)	56(18)
F(2)	118(19)	300(50)	140(30)	-170(30)	110(20)	-150(30)
F(3)	109(18)	340(60)	57(16)	-10(20)	63(15)	-30(30)
F(4)	73(13)	210(40)	100(20)	100(20)	19(13)	19(18)
F(5)	47(6)	74(11)	65(11)	40(9)	19(6)	15(7)
F(6)	77(10)	87(15)	58(11)	-6(10)	18(8)	-33(10)
F(7)	64(10)	76(13)	90(13)	-22(12)	-23(9)	46(10)
F(8)	74(9)	34(8)	74(11)	-13(7)	-8(8)	29(7)
F(9)	126(15)	72(12)	136(18)	63(13)	107(15)	76(12)
F(10)	60(8)	64(11)	44(9)	-15(8)	-1(6)	-3(7)
F(11)	39(7)	42(10)	140(20)	49(13)	-8(10)	-10(6)
F(12)	37(5)	27(6)	78(11)	2(7)	17(6)	-6(5)
Cl(1)	23(2)	35(3)	34(3)	11(2)	12(2)	6(2)
Cl(2)	23(2)	23(2)	30(3)	9(2)	7(1)	7(1)
Au(1)	22(1)	22(1)	22(1)	7(1)	8(1)	7(1)

Au(2)	22(1)	22(1)	22(1)	6(1)	7(1)	7(1)

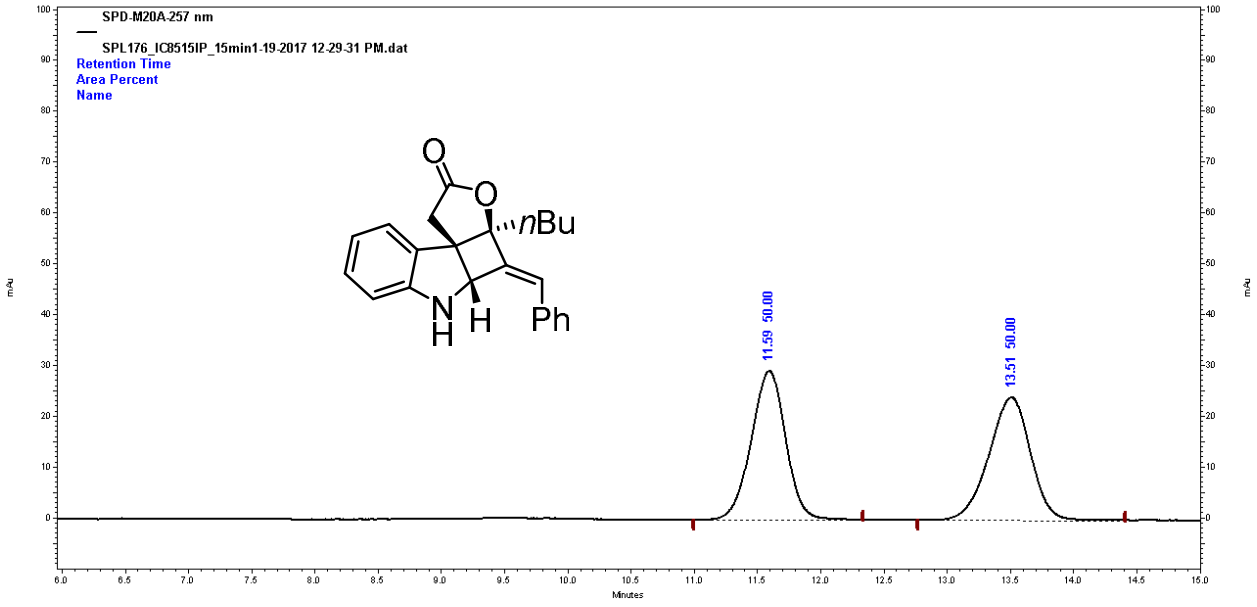
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for cmh_sp_4.

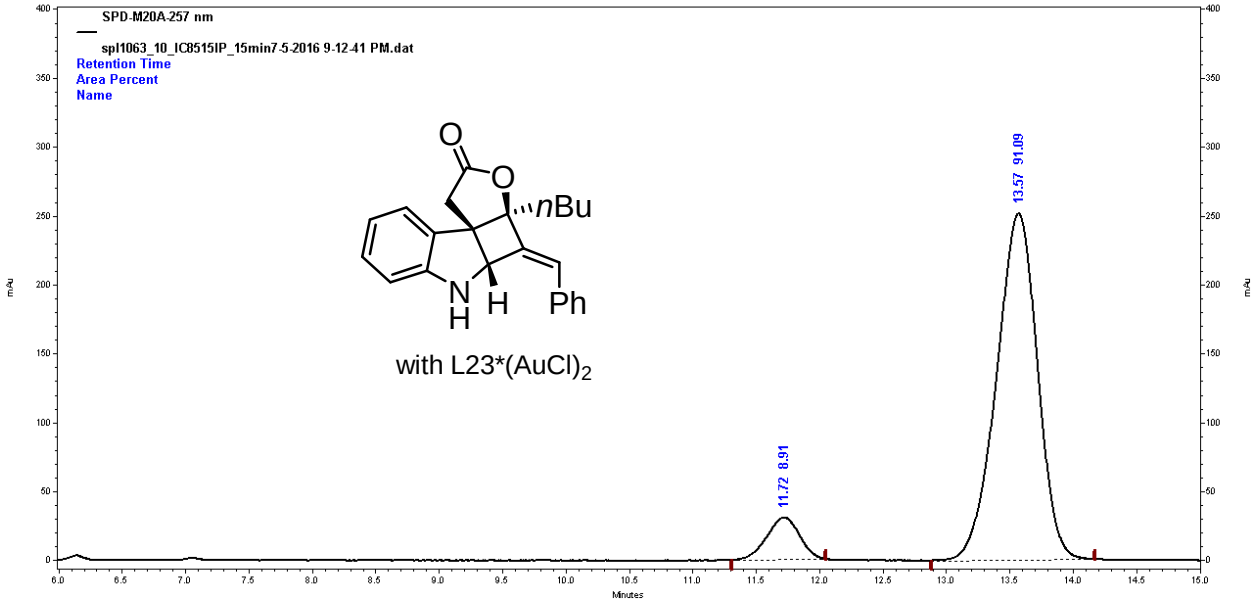
	x	y	z	U(eq)
H(3)	-2314	1580	2858	32
H(4)	-4125	1965	1967	31
H(5)	-4100	2796	572	34
H(7A)	-3057	4318	51	44
H(7B)	-3910	3323	-834	44
H(9A)	-4574	4465	-1870	41
H(9B)	-3661	5467	-1031	41
H(10A)	-1310	5580	-429	41
H(10B)	-787	4635	-884	41
H(11A)	-3752	3054	-2563	54
H(11B)	-2274	3094	-2184	54
H(12)	-4173	5880	-2653	39
H(13A)	-4492	4180	-3834	73
H(13B)	-3471	5034	-4101	73
H(14)	-2748	3515	-3893	72
H(15A)	-2042	6498	-2792	50
H(15B)	-2056	6754	-1599	50
H(16A)	-1281	5024	-3537	66
H(16B)	-827	4246	-2839	66
H(17)	-309	6016	-1718	52
H(20)	4188	322	1997	38
H(24A)	3277	1678	5474	35
H(24B)	4592	2380	5448	35
H(25A)	4105	199	5414	45
H(25B)	5033	1100	6369	45

H(26A)	6280	386	5406	40
H(26B)	6361	1556	5278	40
H(27A)	5941	631	3578	48
H(27B)	4940	-307	3737	48
H(29)	4036	901	464	48
H(31)	1117	-4	-2178	60
H(33)	421	402	638	80
H(38)	6787	3106	4394	32
H(39)	8515	3830	3919	45
H(40)	8371	5299	3080	46
H(42A)	7260	5823	1533	41
H(42B)	8152	6644	2565	41
H(44A)	6372	8132	2761	59
H(44B)	7860	8503	2887	59
H(45A)	7835	6877	470	46
H(45B)	8761	7763	1441	46
H(46A)	5512	6285	333	39
H(46B)	4946	6774	1226	39
H(47)	8192	8523	-55	56
H(48A)	7609	9919	837	73
H(48B)	8644	9538	1625	73
H(49)	6838	9725	2343	78
H(50A)	4679	8547	1322	71
H(50B)	5183	9247	586	71
H(51)	4450	7536	-247	58
H(52A)	6255	7311	-843	72
H(52B)	6099	8471	-815	72
H(57)	368	4090	5627	38
H(59A)	-671	2498	6127	50
H(59B)	-1499	2019	4947	50
H(60A)	-1374	753	5829	41
H(60B)	144	1095	6149	41
H(61A)	-1415	387	4032	41
H(61B)	-688	-327	4659	41
H(62A)	1249	556	4626	38
H(62B)	377	527	3496	38

H(63)	379	5548	4998	30
H(65)	4075	5519	5494	126
H(67)	3085	8254	5885	42
H(1)	375	1764	2105	29
H(2)	-110	3097	399	31
H(4A)	4047	3747	4157	31
H(5A)	4419	5514	2777	28

HPLC traces:

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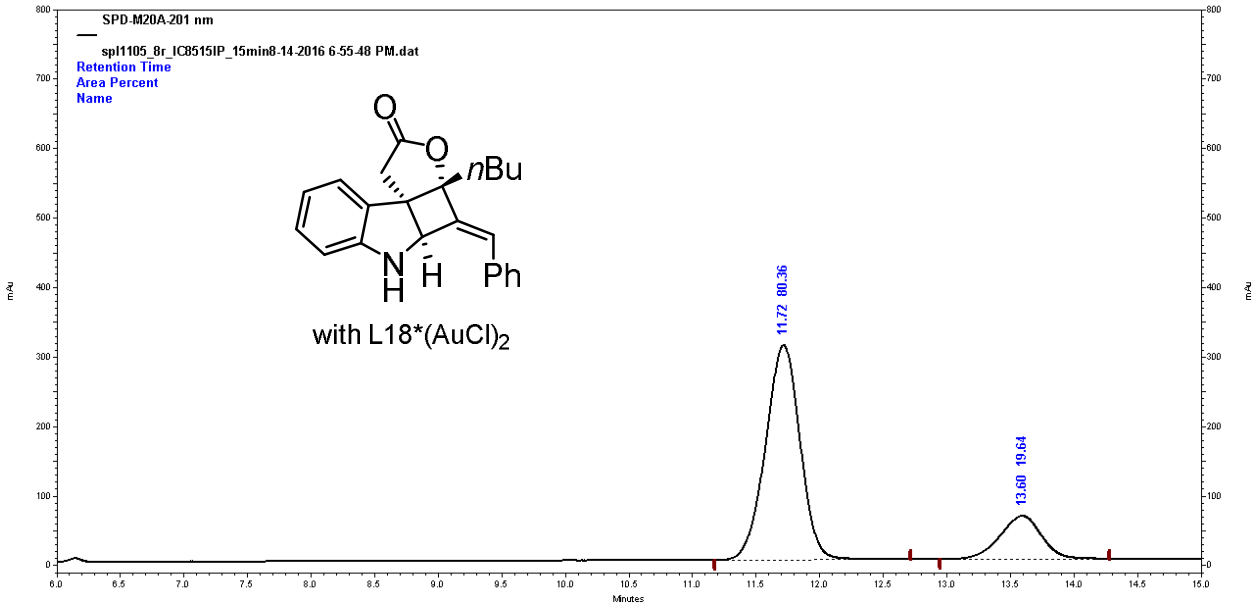
Retention Time
Area Percent
Name
O
O
nBu
N
H
H
Ph
with L23*(AuCl)2
11.72 8.91
13.57 91.09
mAu
Minutes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Retention Time
Area Percent
Name
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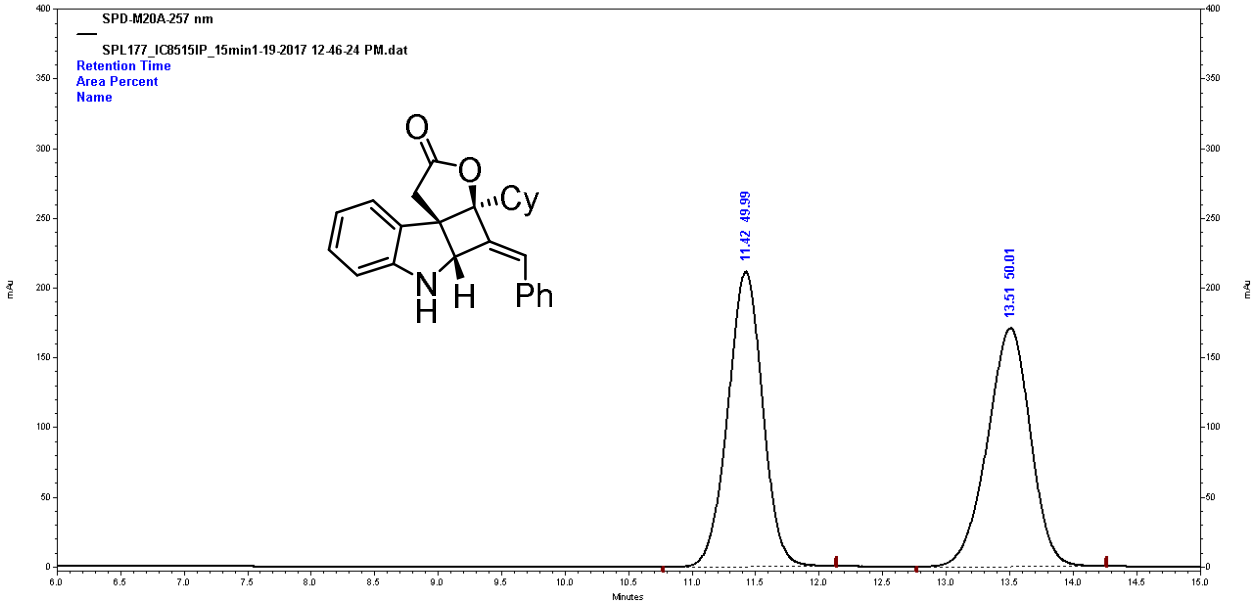
nBu
N
H
H
Ph
with L18*(AuCl)2
11.72 80.36
13.60 19.64
mAu
Minutes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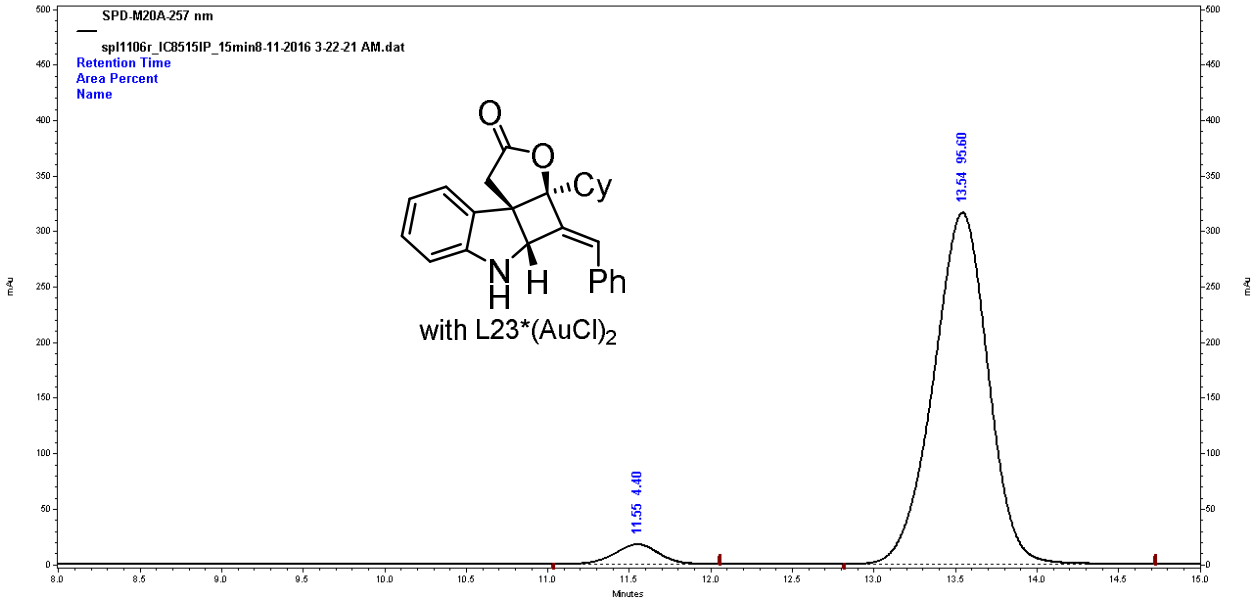
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Ph
11.42 49.99
13.51 50.01
mAu
Minutes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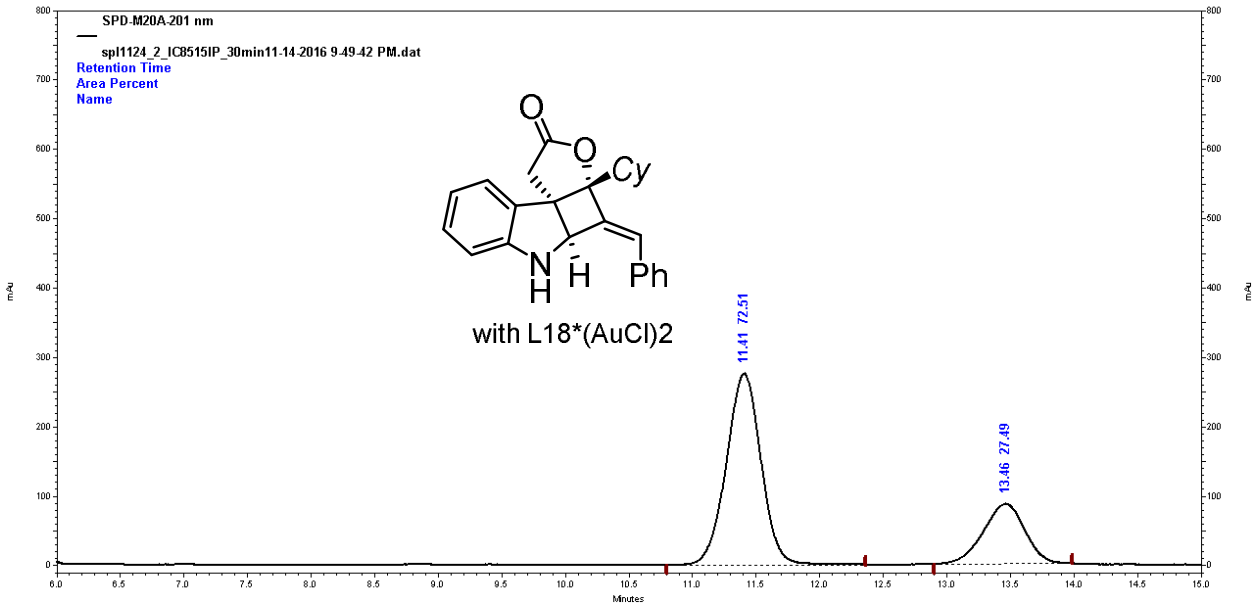
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Ph
with L23*(AuCl)2
11.55 4.40
13.54 95.60
mAu
Minutes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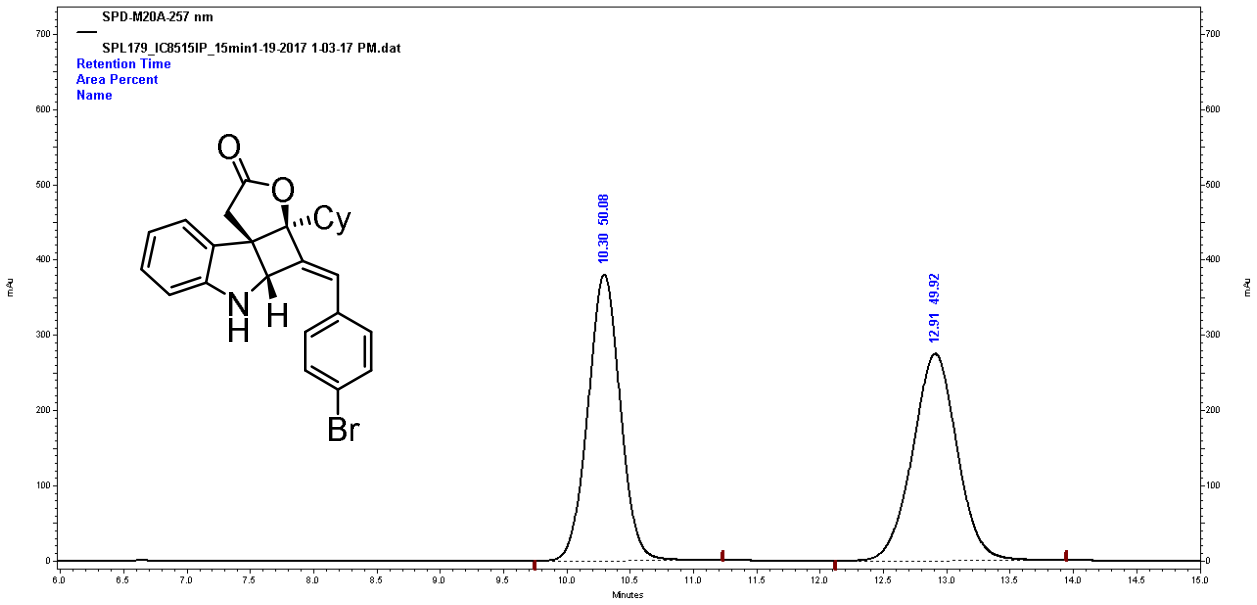
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Ph
with L18*(AuCl)2
11.41 72.51
13.46 27.49
mAu
Minutes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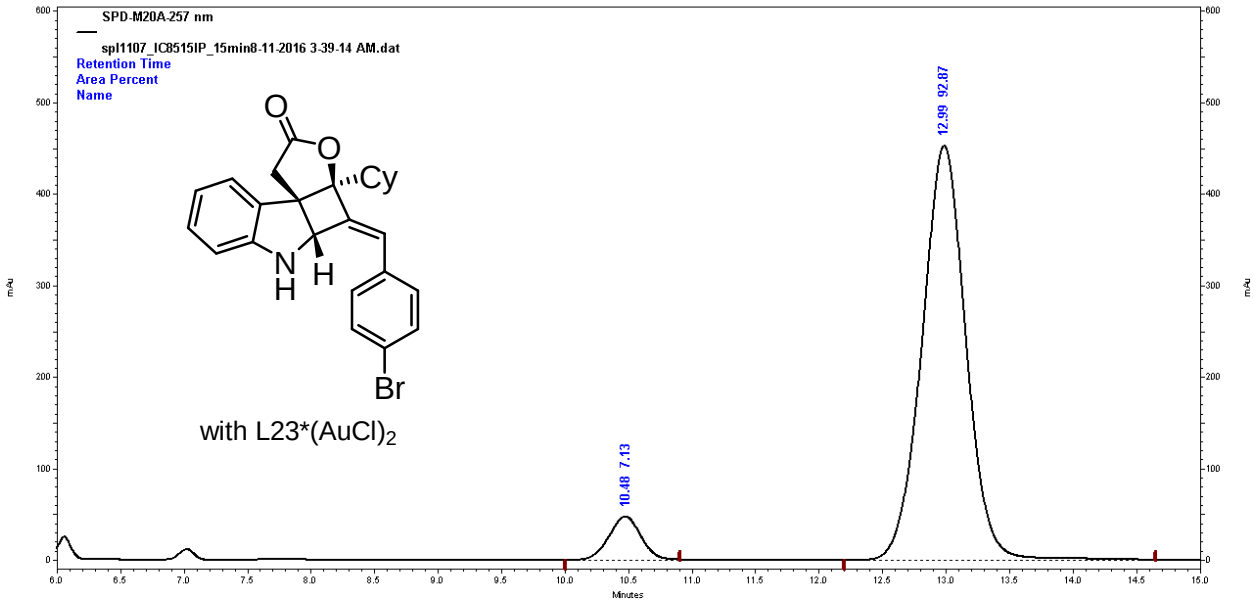
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Br
10.30 50.08
12.91 49.92
mAu
Minutes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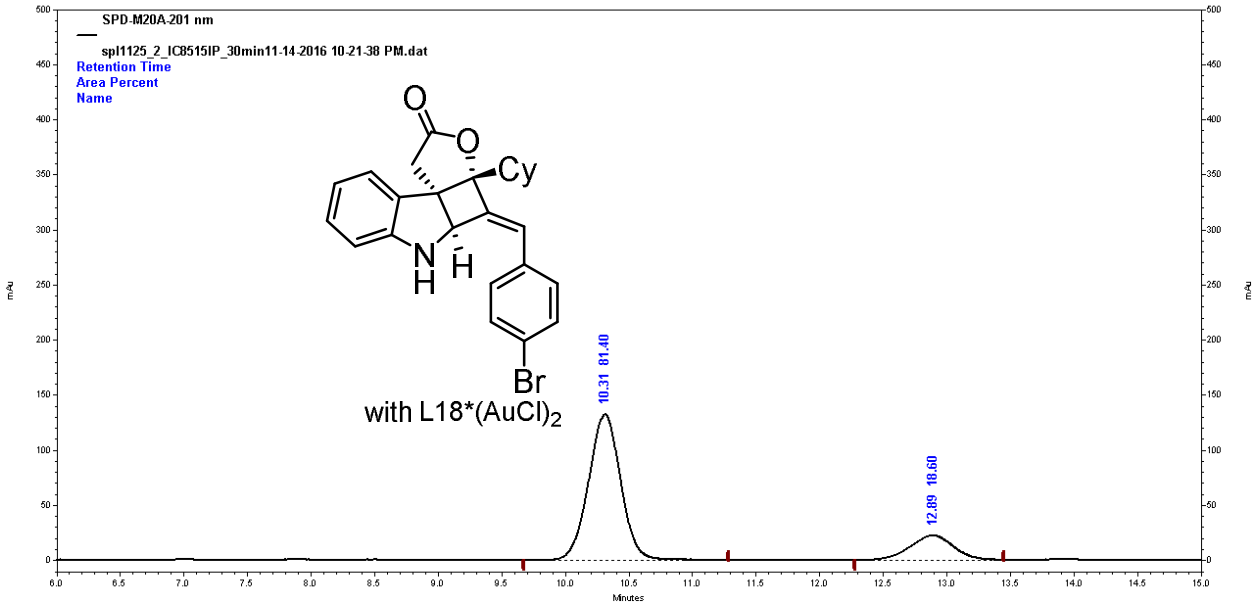
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Br
with L23*(AuCl)2
10.48 7.13
12.99 92.87
mAu
Minutes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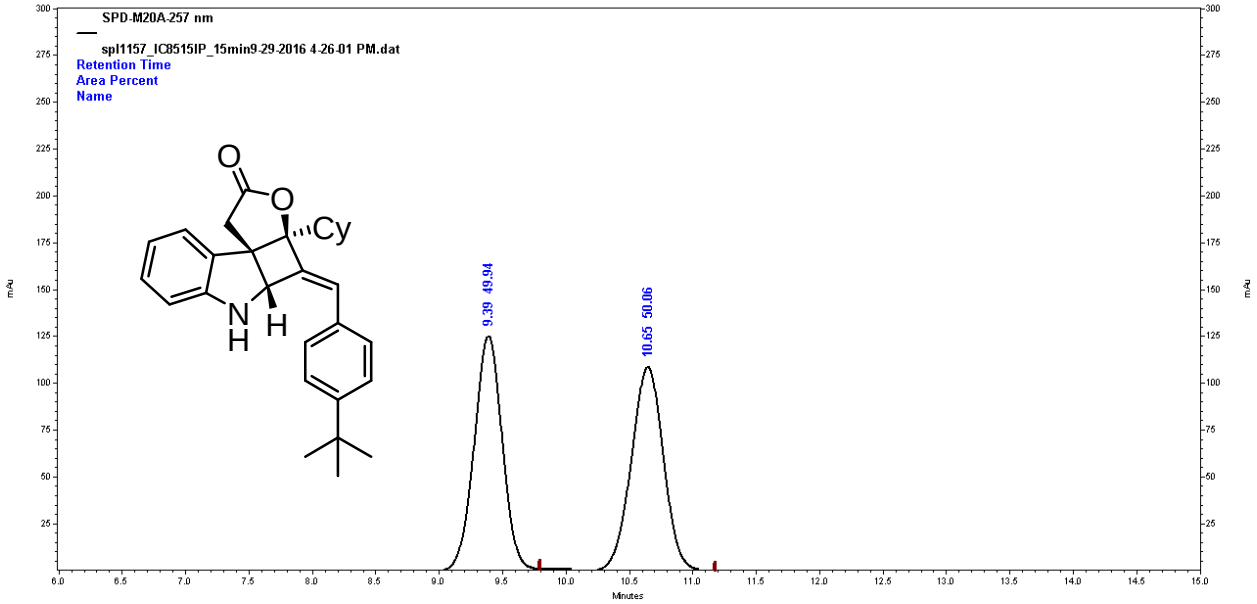
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
Br
with L18*(AuCl)2
10.31 81.40
12.89 18.60
mAu
Minutes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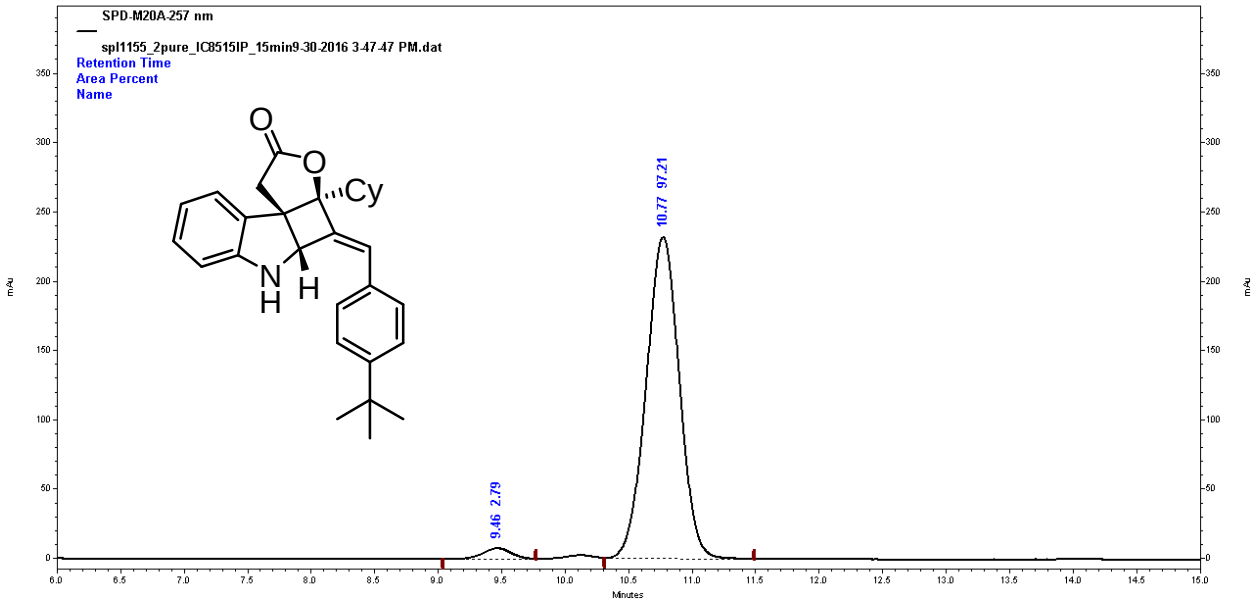
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
9.39 49.94
10.65 50.06
mAu
Minutes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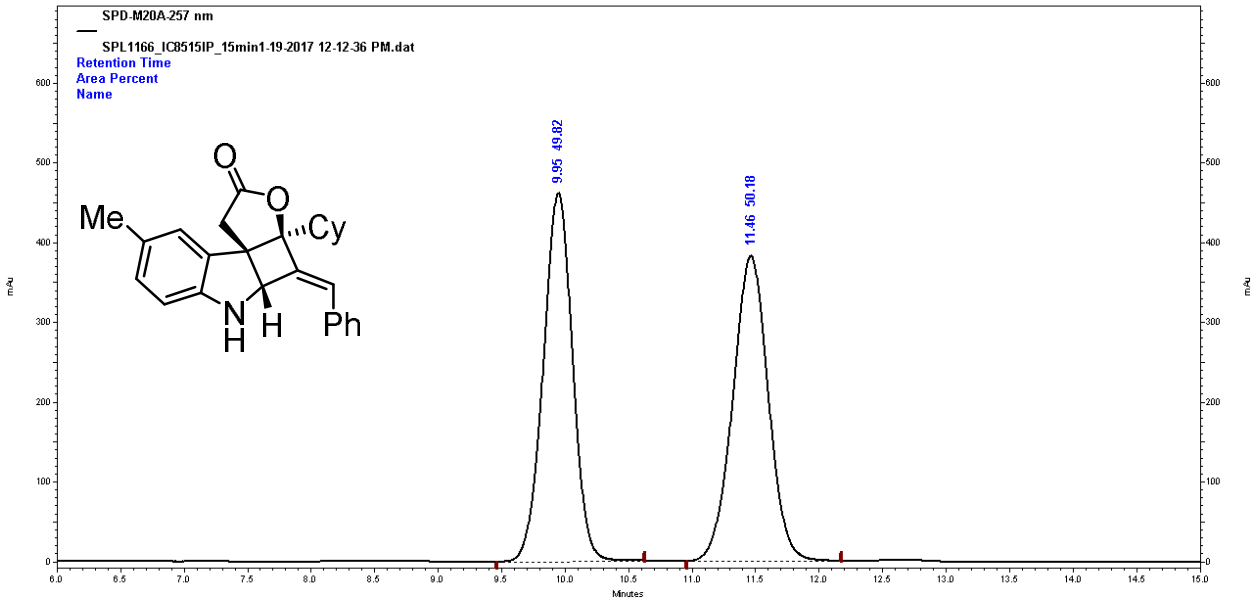
Retention Time
Area Percent
Name
O
O
Cy
N
H
H
9.46 2.79
10.77 97.21
mAu
Minutes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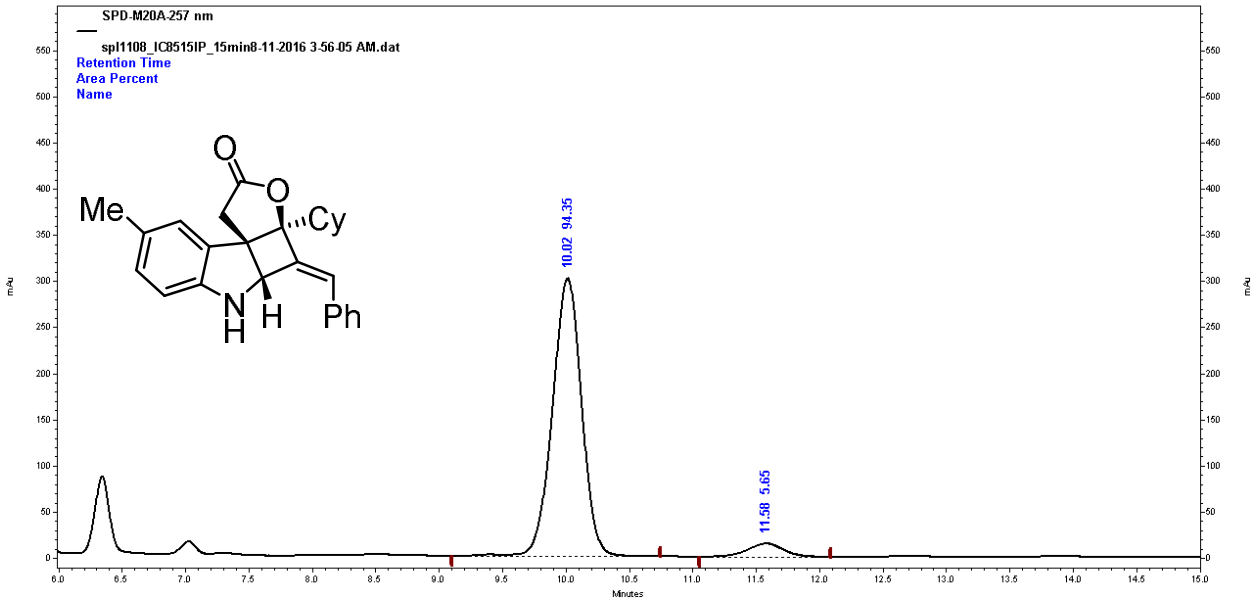
Retention Time
Area Percent
Name
9.95 49.82
11.46 50.18
mAu
Minutes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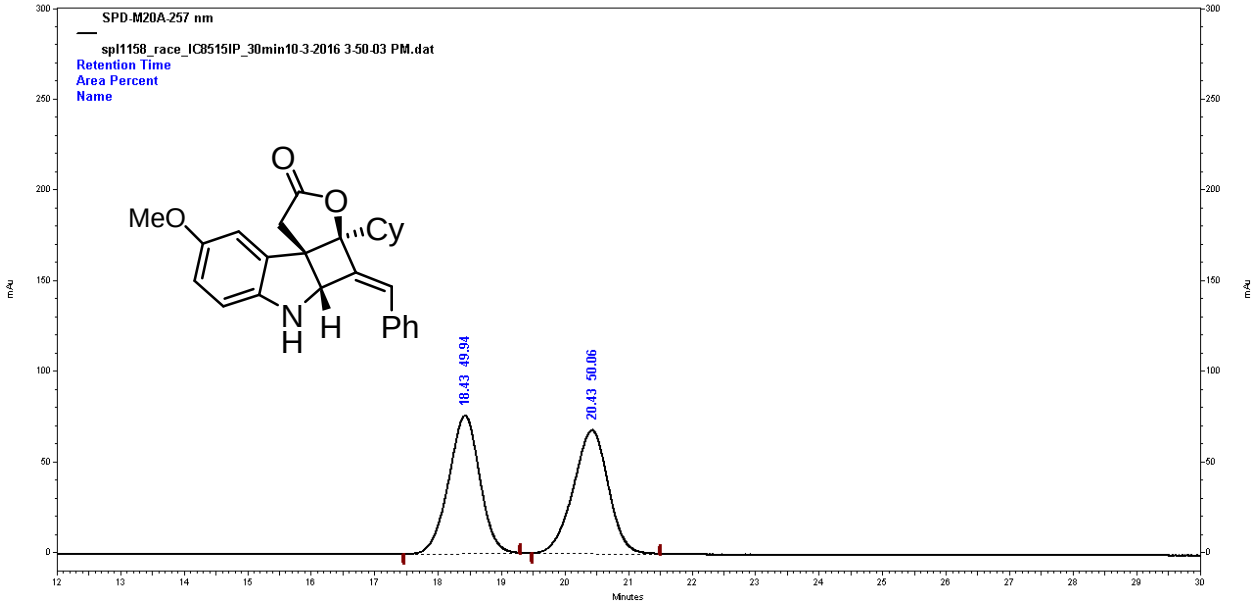
Retention Time
Area Percent
Name
10.02 94.35
11.58 5.65
mAu
Minutes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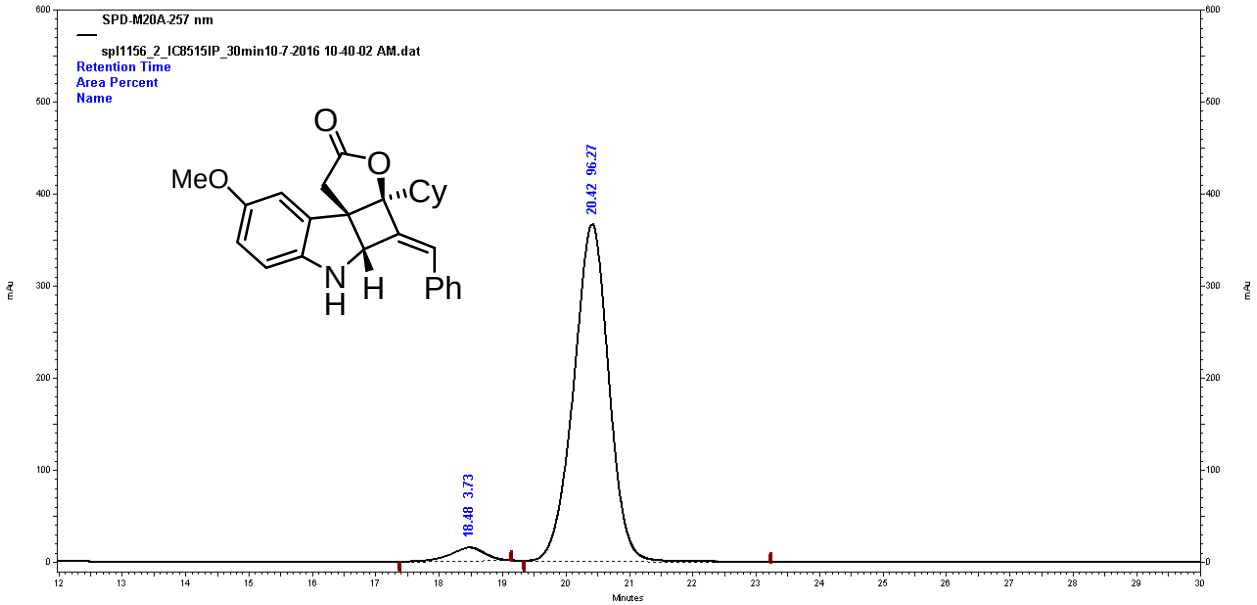
Retention Time
Area Percent
Name
MeO
O
O
Cy
N
H
H
Ph
18.43 49.94
20.43 50.06
mAu
Minutes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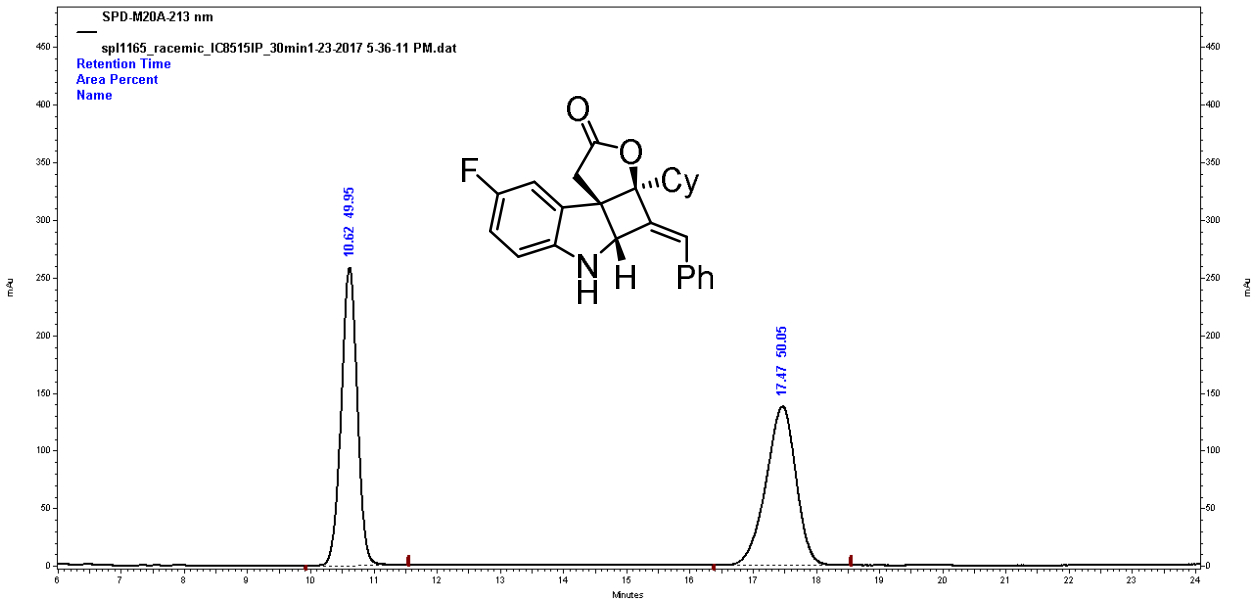
Retention Time
Area Percent
Name
MeO
O
O
Cy
N
H
H
Ph
18.48 3.73
20.42 96.27
mAu
Minutes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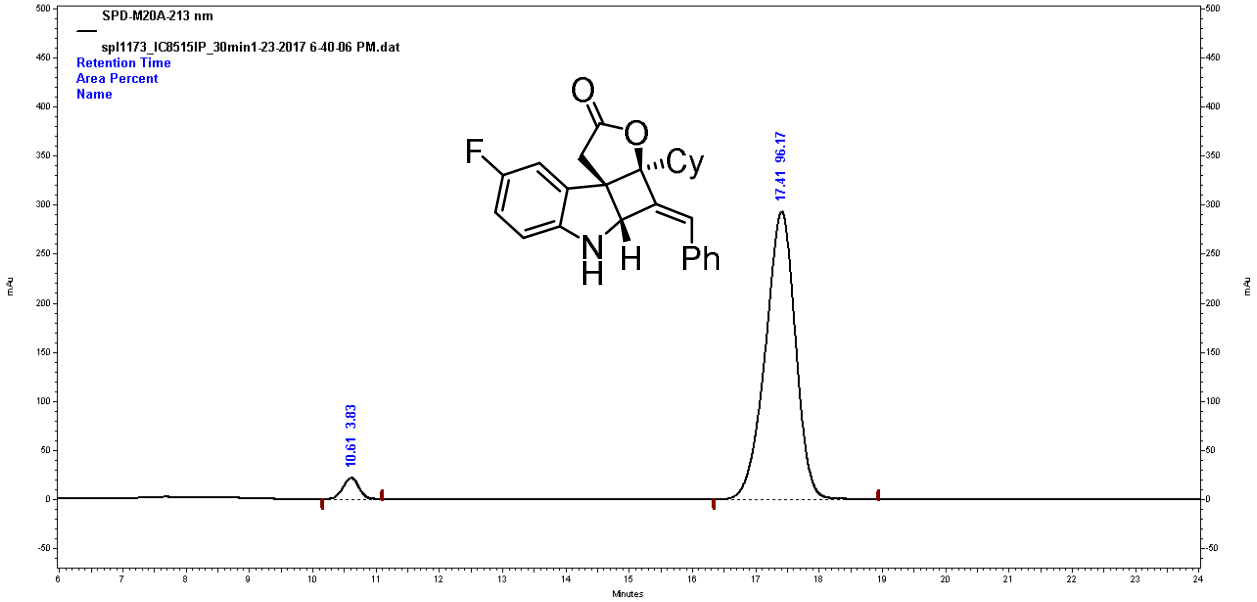
Retention Time
Area Percent
Name
10.62 49.95
17.47 50.05
mAu
Minutes
O
O
F
Cy
N
H
H
Ph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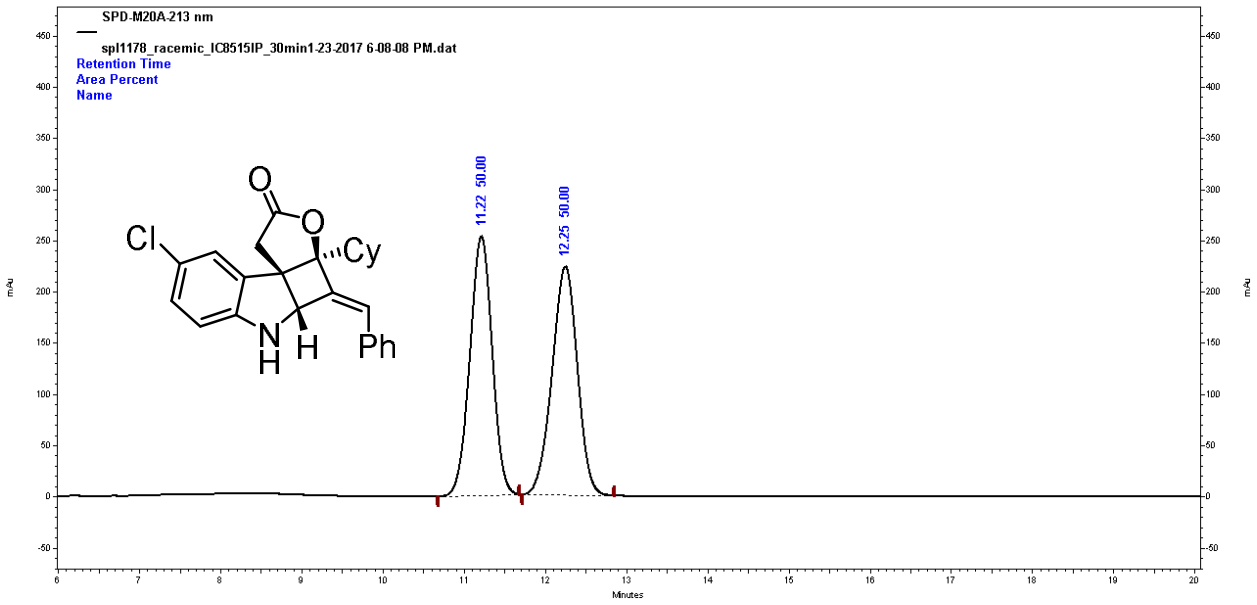
Retention Time
Area Percent
Name
10.61 3.83
17.41 96.17
mAu
Minutes
O
O
F
Cy
N
H
H
Ph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Retention Time
Area Percent
Name
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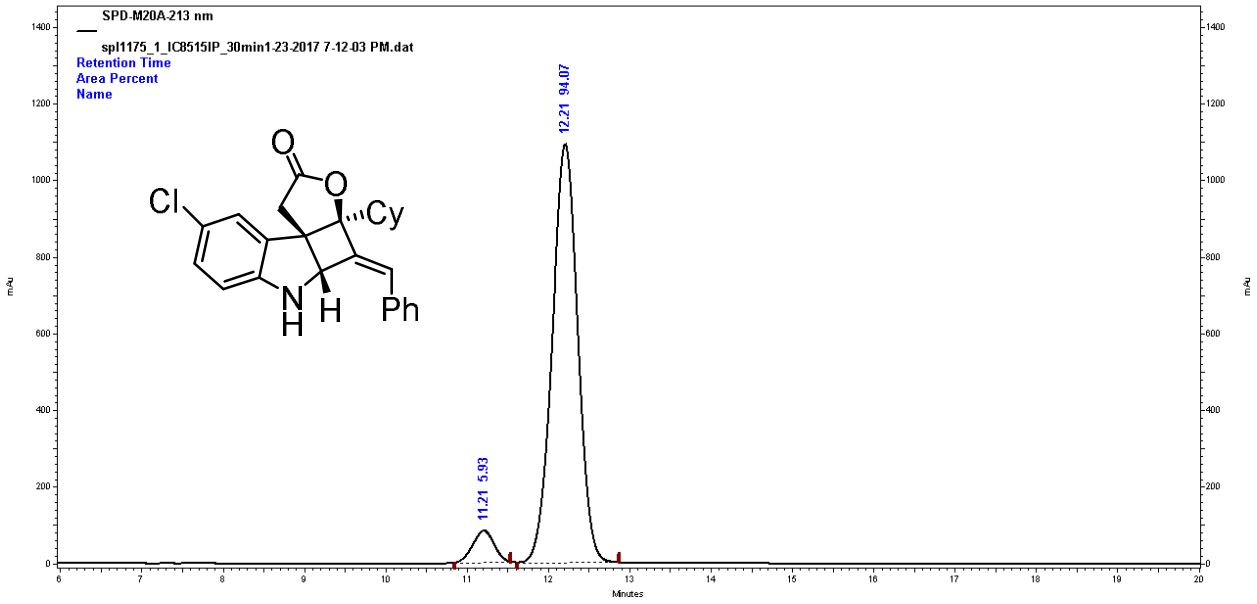
12.25 50.00
Cl
O
O
Cy
N
H
H
Ph
mAu
Minutes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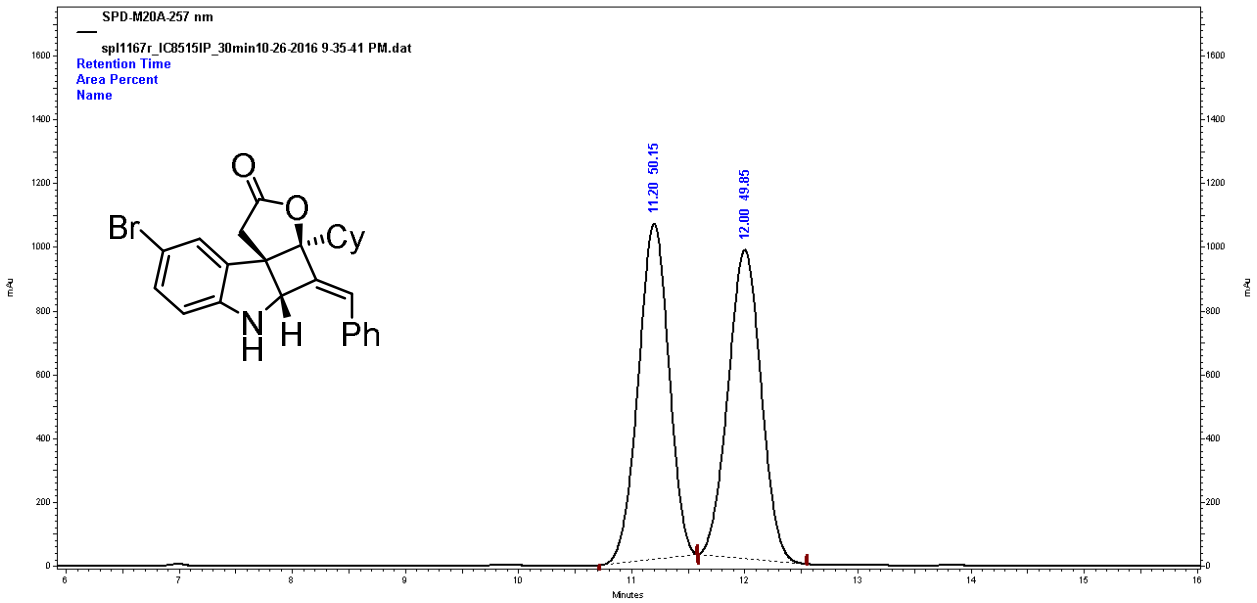
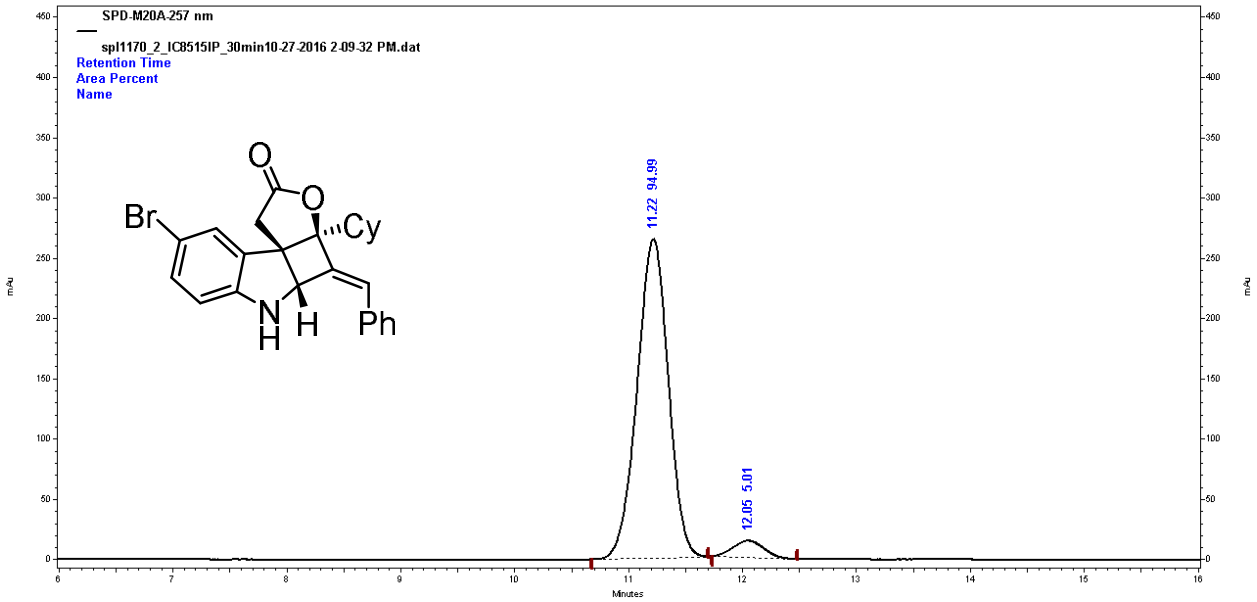
Retention Time
Area Percent
Name
11.21 5.93
12.21 94.07
Cl
O
O
Cy
N
H
H
Ph
mAu
Minutes


SPD-M20A-257 nm
spl1167r_IC8515IP_30min10-26-2016 9-35-41 PM.dat
Retention Time
Area Percent
Name
11.20 50.15
12.00 49.85
mAu
Minutes
Br
O
O
Cy
N
H
H
Ph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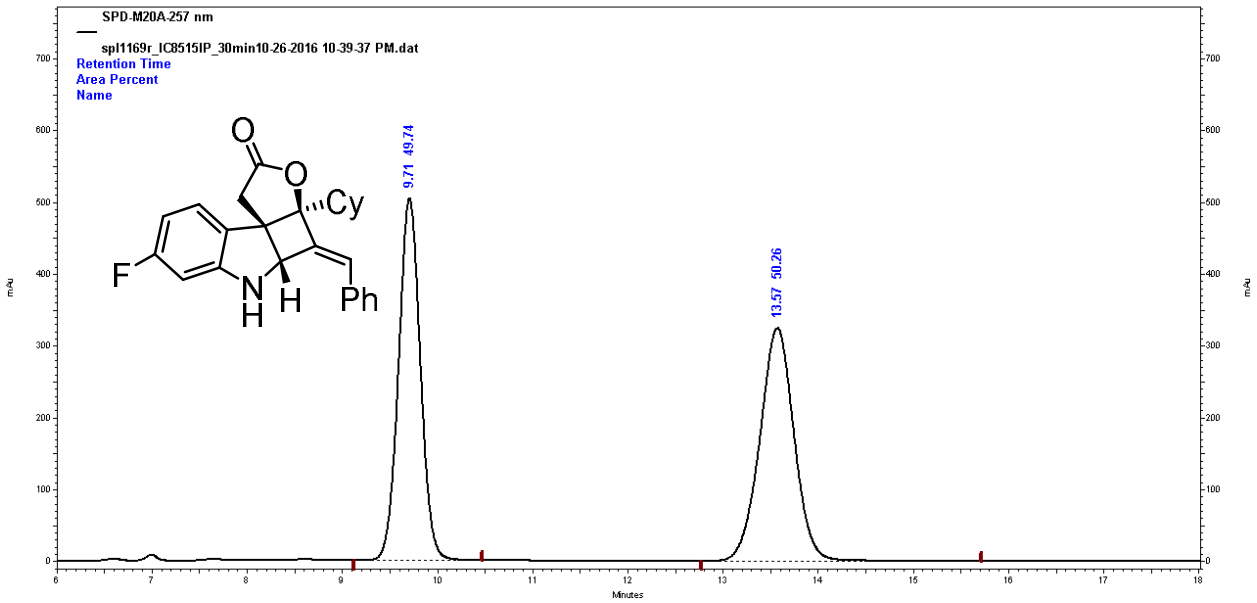
spl1170_2_IC8515IP_30min10-27-2016 2-09-32 PM.dat
Retention Time
Area Percent
Name
11.22 94.99
12.05 5.01
mAu
Minutes
Br
O
O
Cy
N
H
H
Ph


SPD-M20A-257 nm
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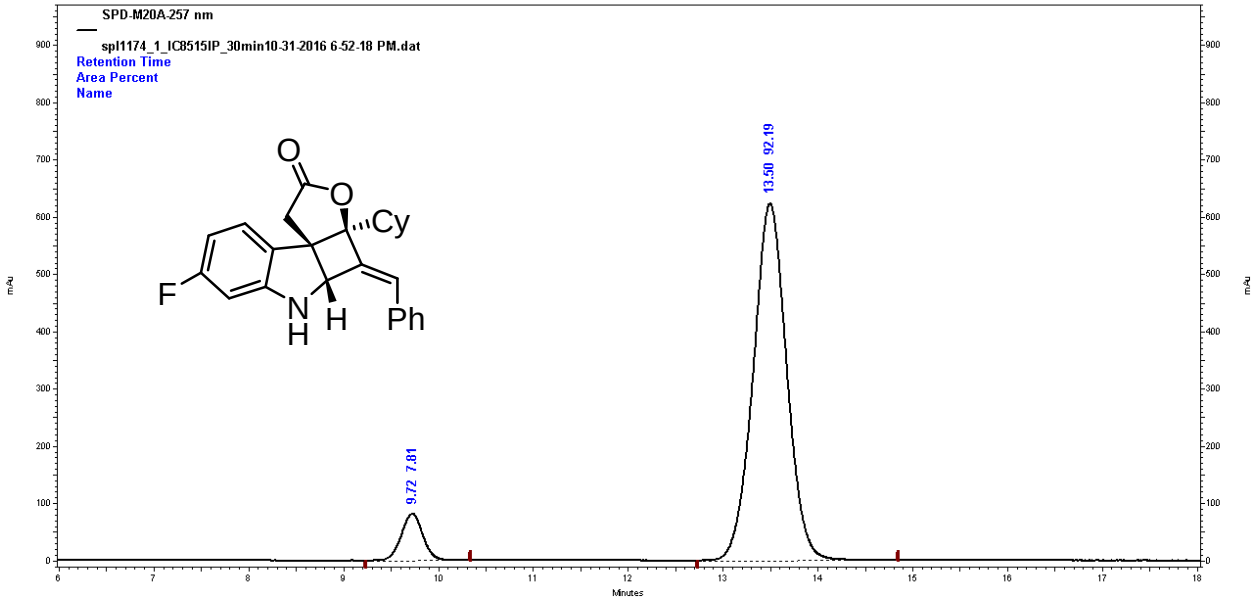
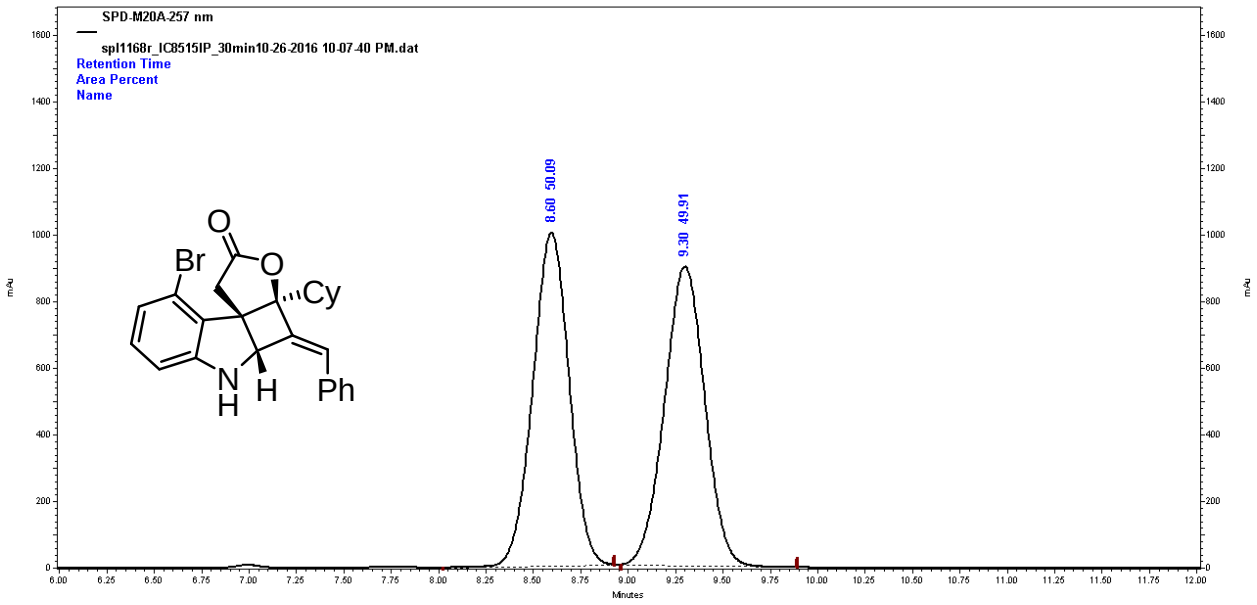
Retention Time
Area Percent
Name
9.71 49.74
13.57 50.26
mAu
Minutes


SPD-M20A-257 nm
spl1174_1_IC8515IP_30min10-31-2016 6-52-18 PM.dat
Retention Time
Area Percent
Name
9.72 7.81
13.50 92.19
mAu
Minutes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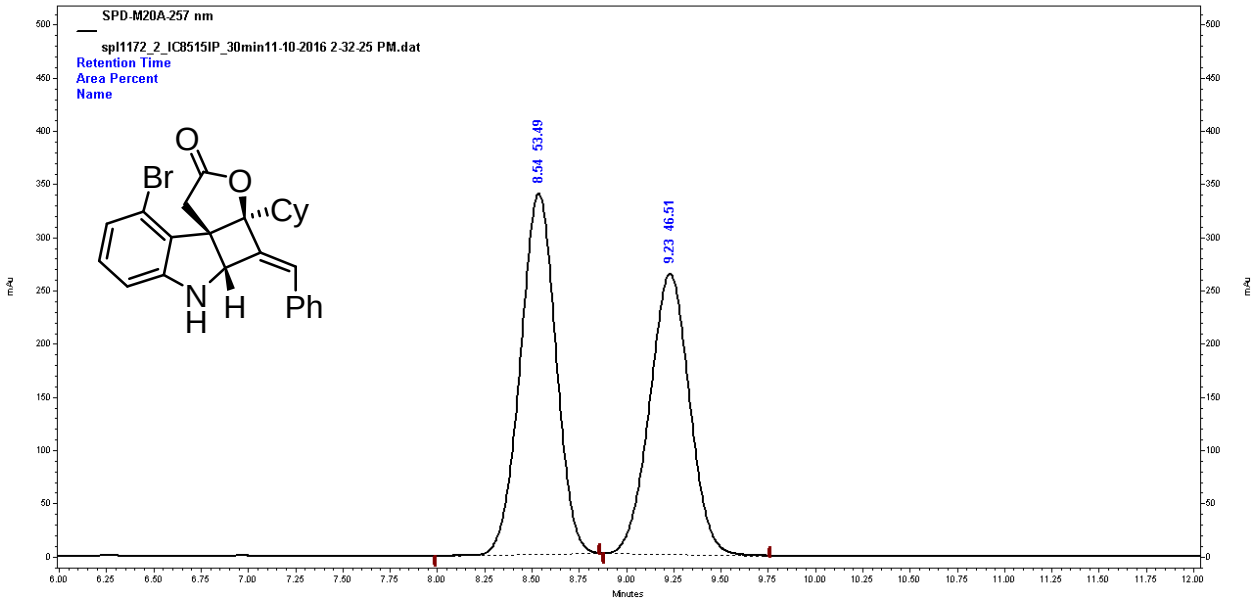
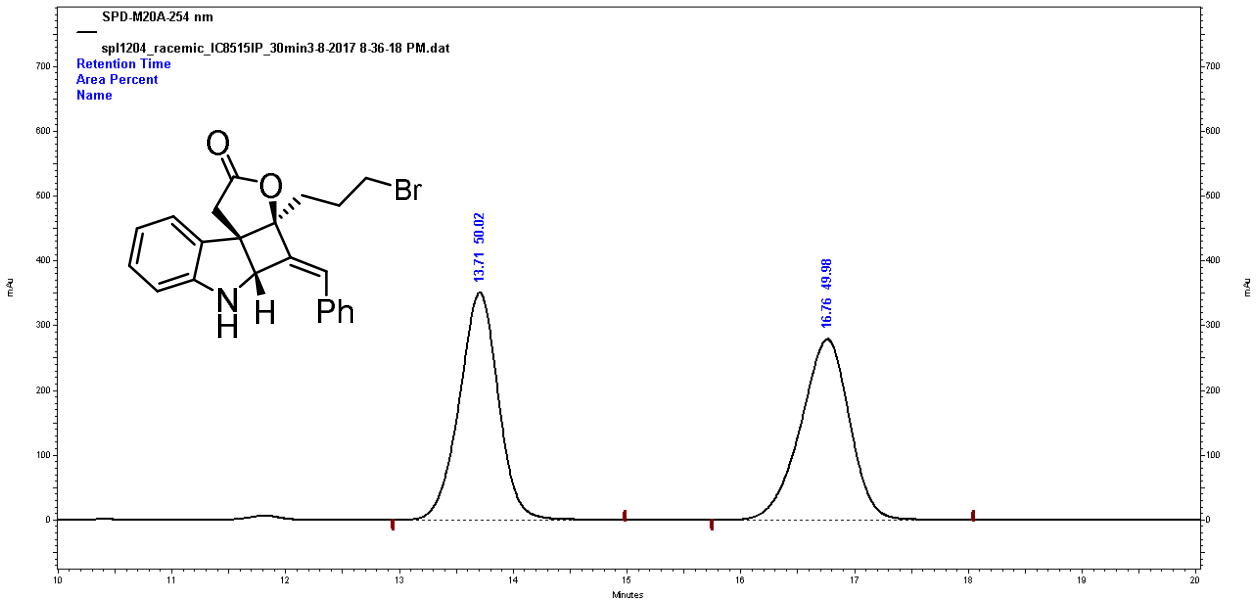
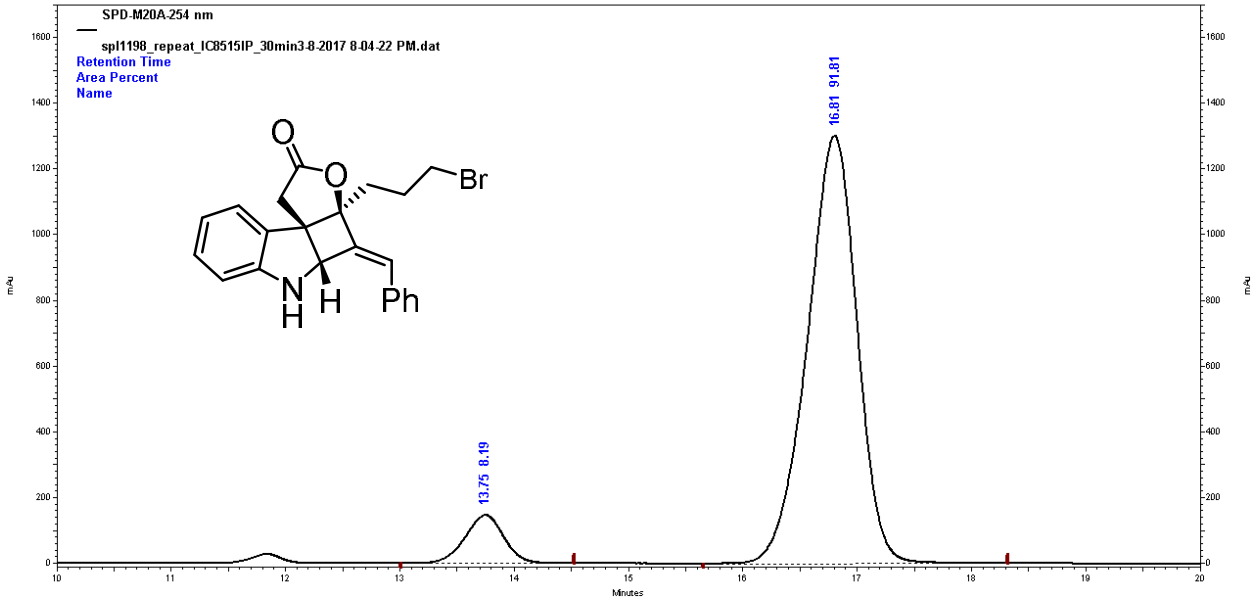
spl1168r_IC8515IP_30min10-26-2016 10-07-40 PM.dat
Retention Time
Area Percent
Name
8.60 50.09
9.30 49.91
mAu
Minutes
O
Br
O
Cy
N
H
H
Ph

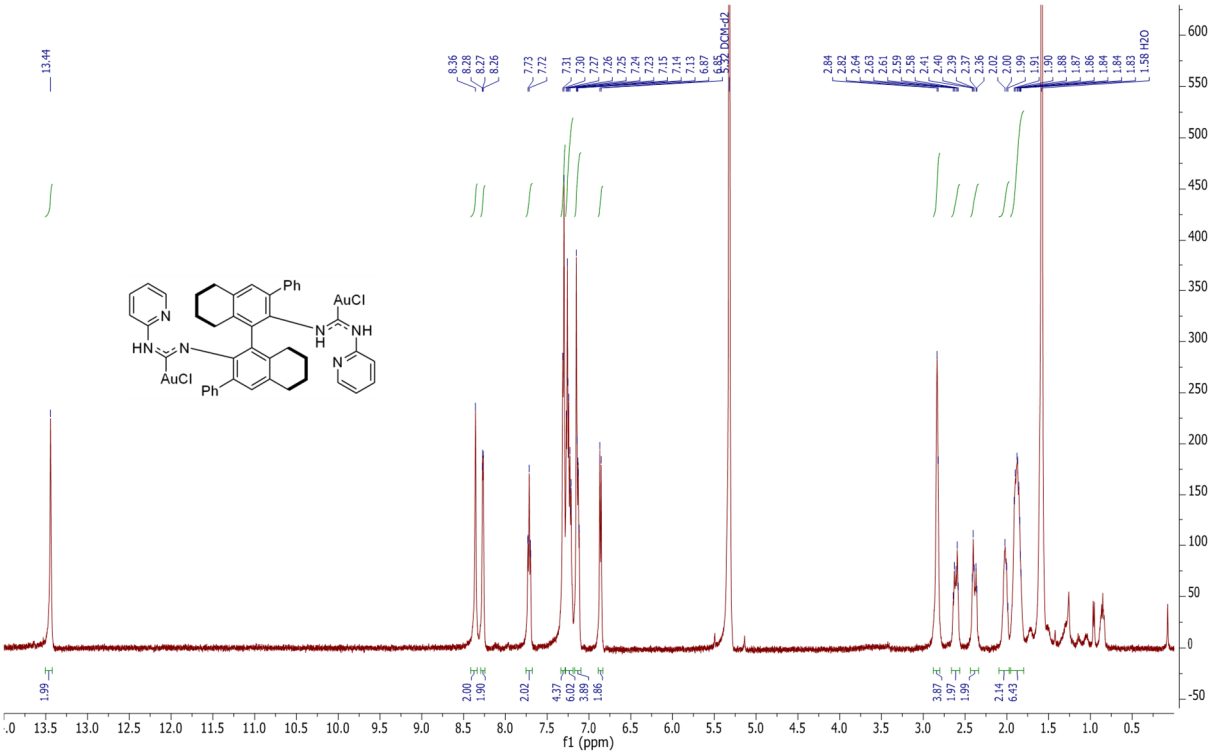

SPD-M20A-257 nm
spl1172_2_IC8515IP_30min11-10-2016 2-32-25 PM.dat
Retention Time
Area Percent
Name
8.54 53.49
9.23 46.51
mAu
Minutes
O
Br
O
Cy
N
H
H
Ph

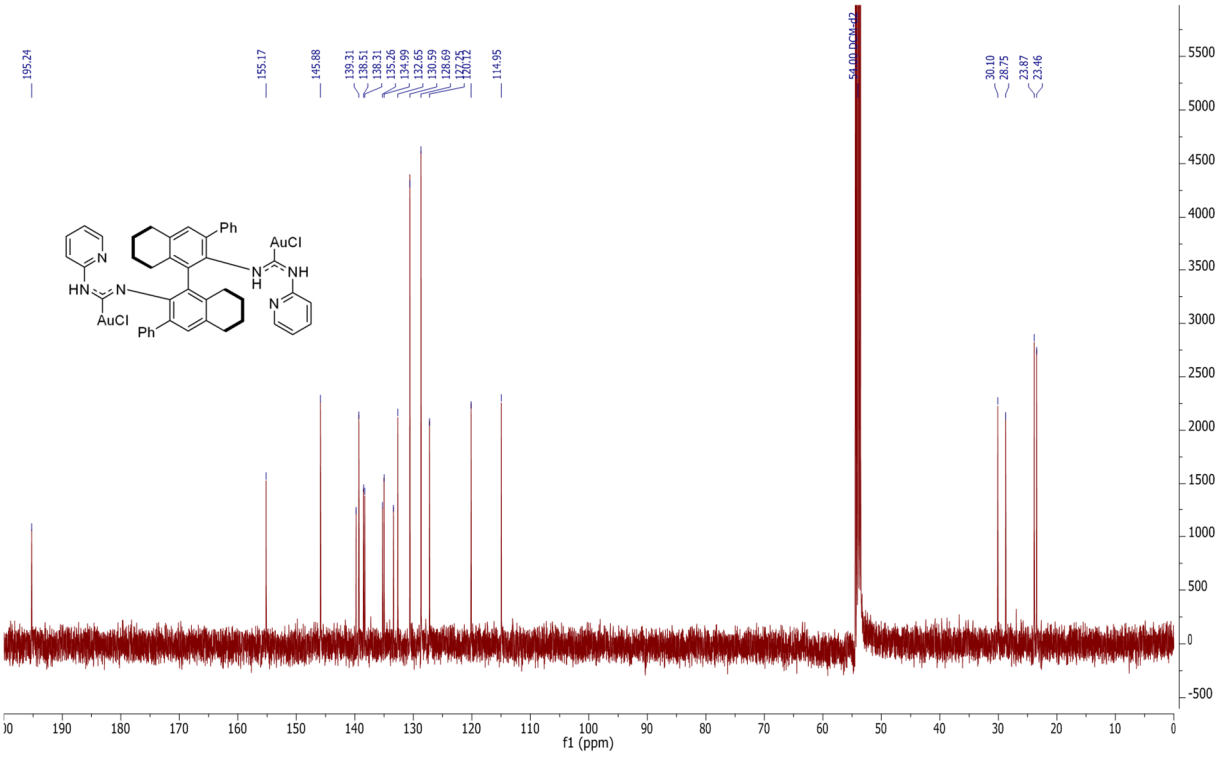

SPD-M20A-254 nm
spl1204_racemic_IC8515IP_30min3-8-2017 8-36-18 PM.dat
Retention Time
Area Percent
Name
13.71 50.02
16.76 49.98
mAu
Minutes


SPD-M20A-254 nm
spl1198_repeat_IC8515IP_30min3-8-2017 8-04-22 PM.dat
Retention Time
Area Percent
Name
13.75 8.19
16.81 91.81
mAu
Minutes

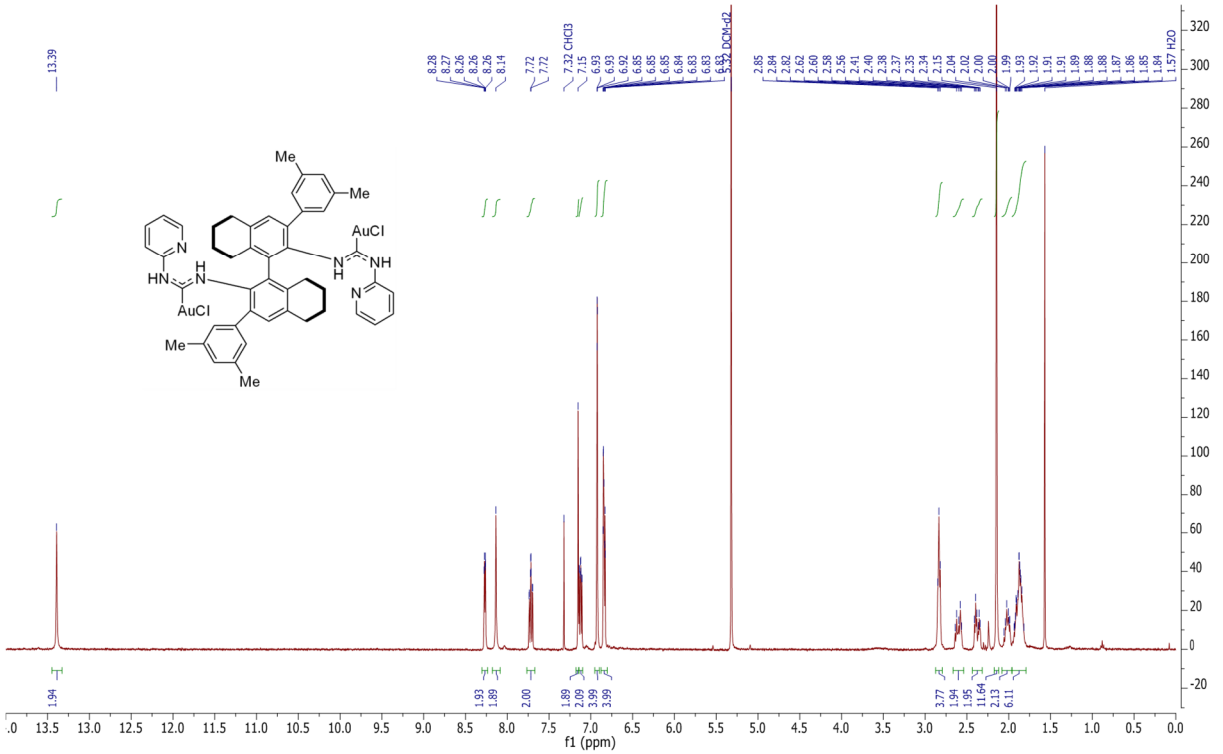
^{1}H and ^{13}C NMR Spectra:

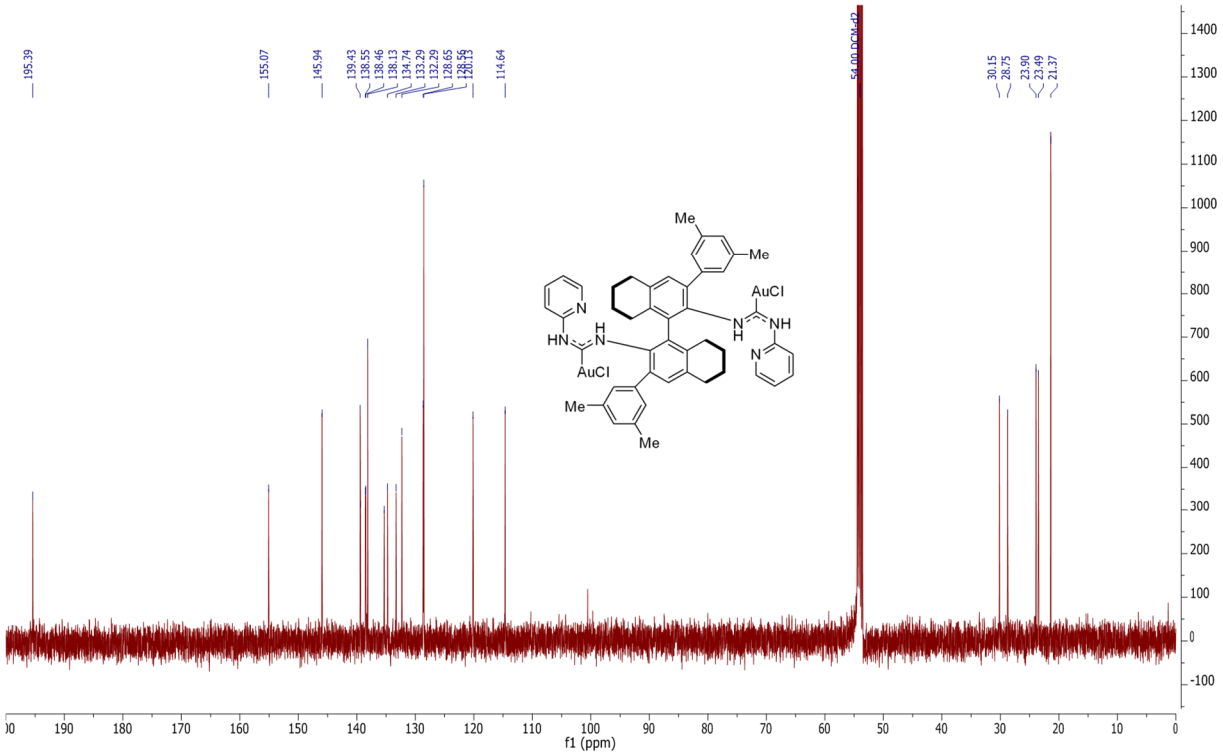
Complex L1*$(AuCl)_2$



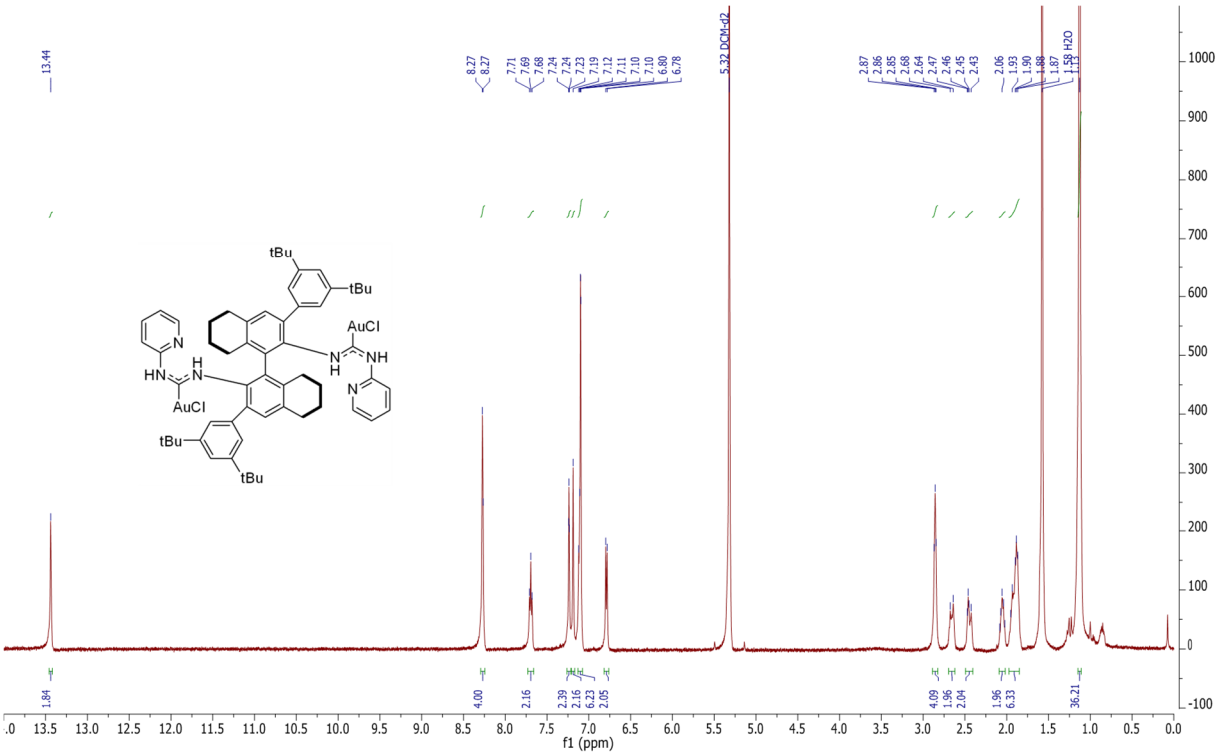


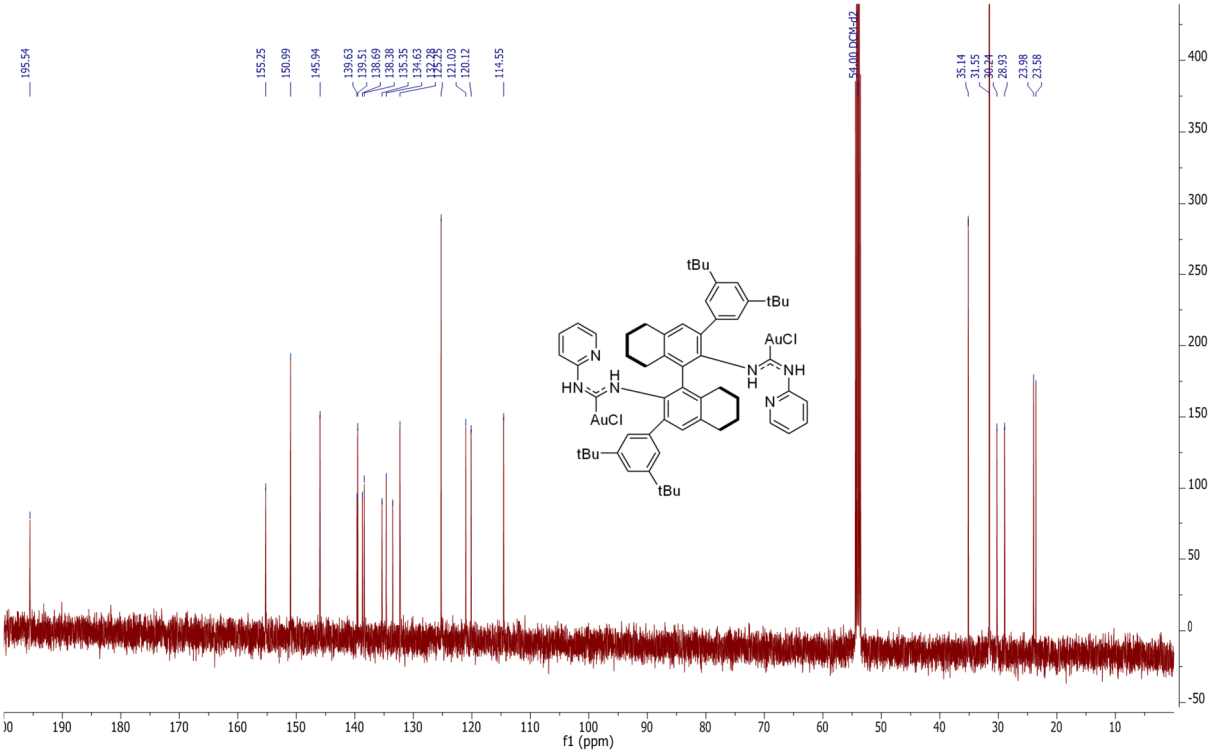
Complex L2*$(AuCl)_2$



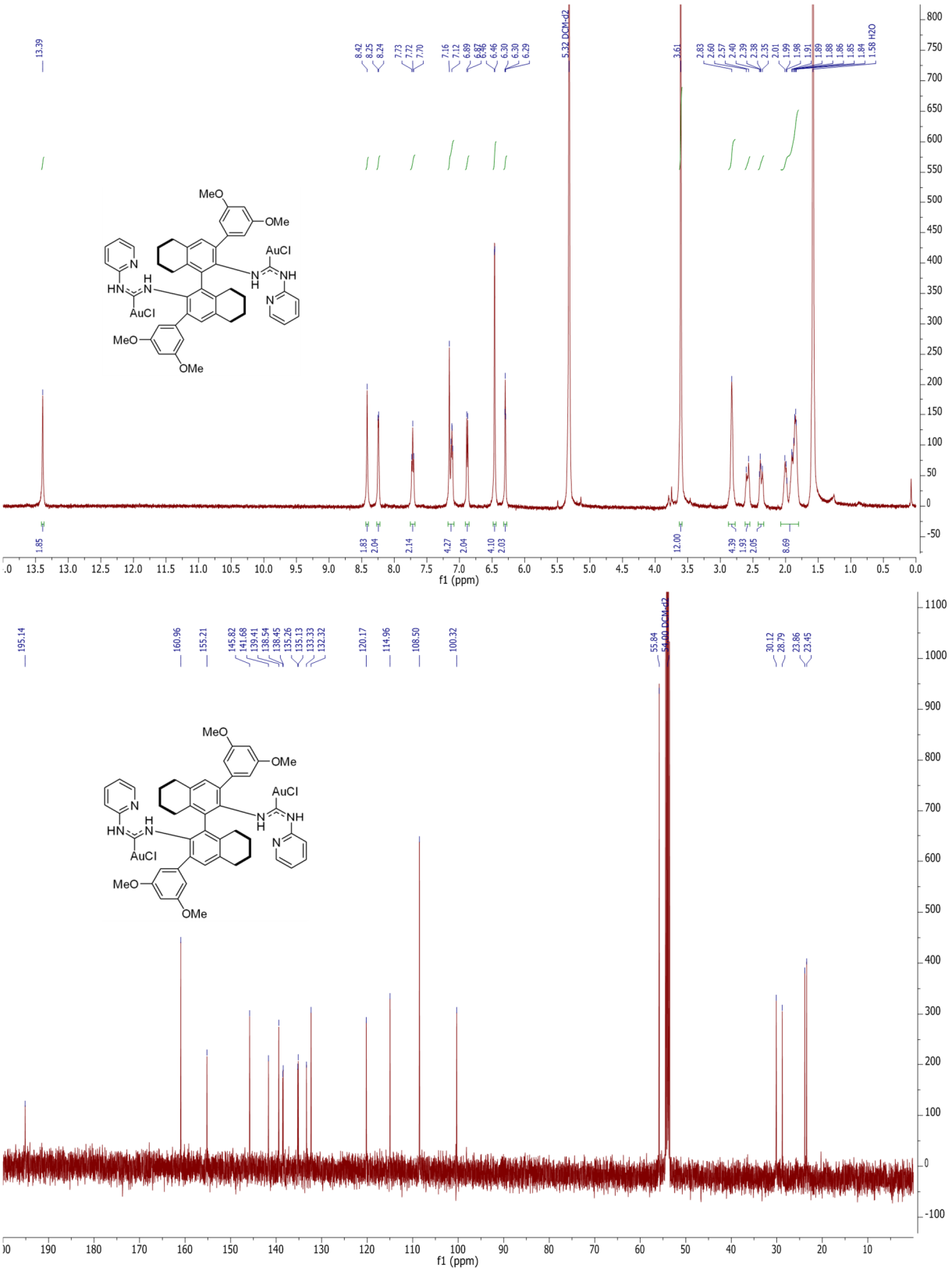


Complex L3*$(AuCl)_2$

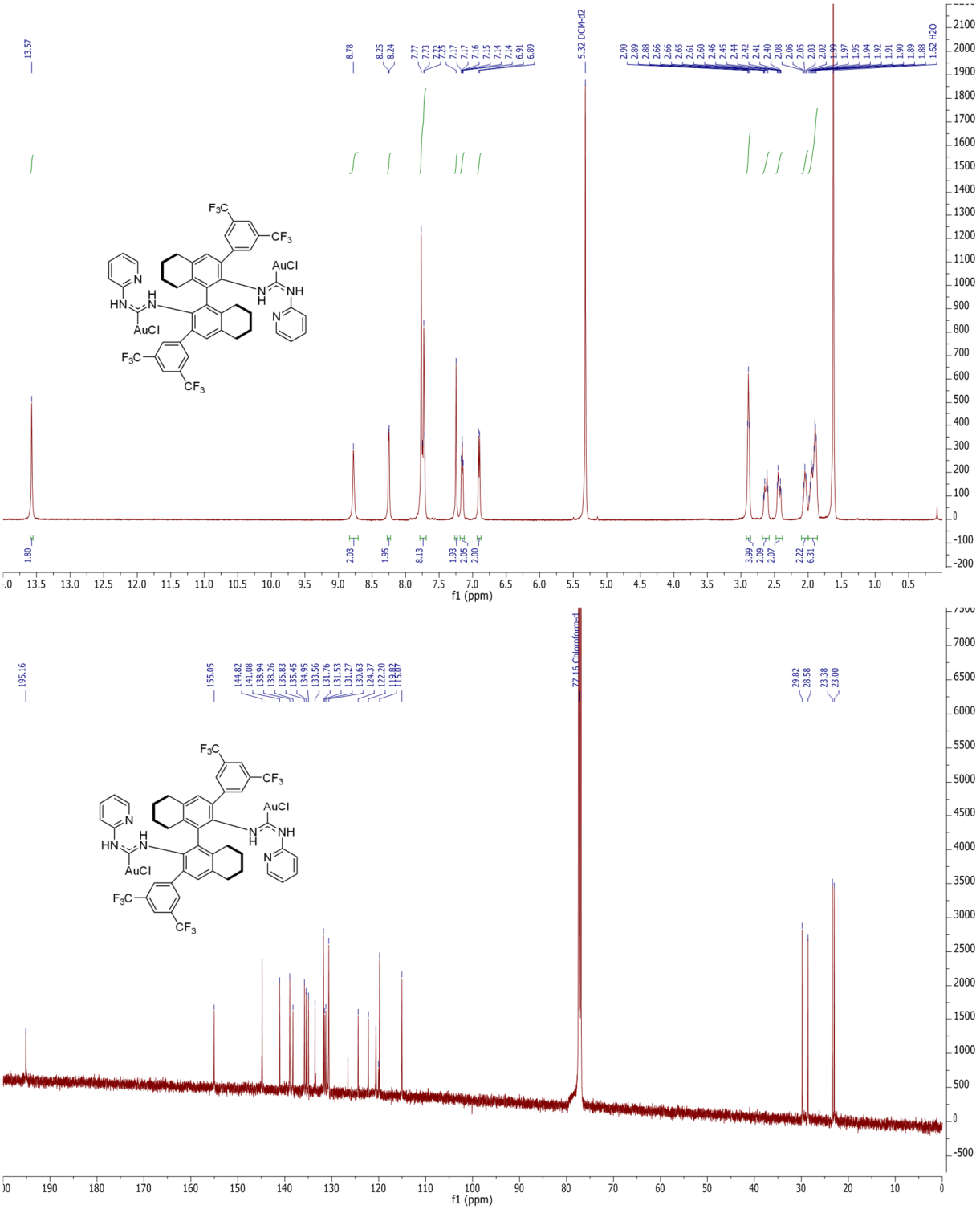




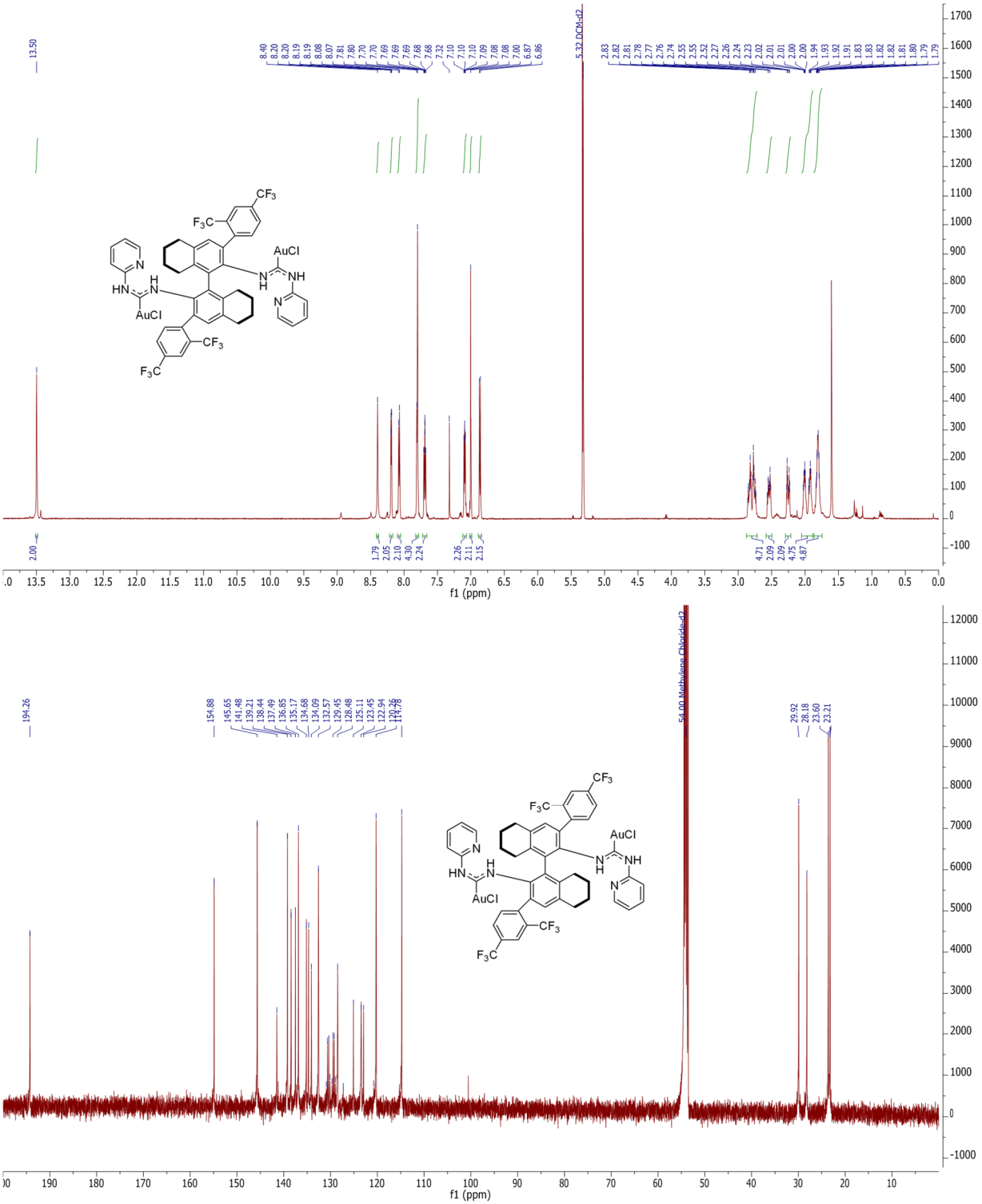
Complex L4*$(AuCl)_2$



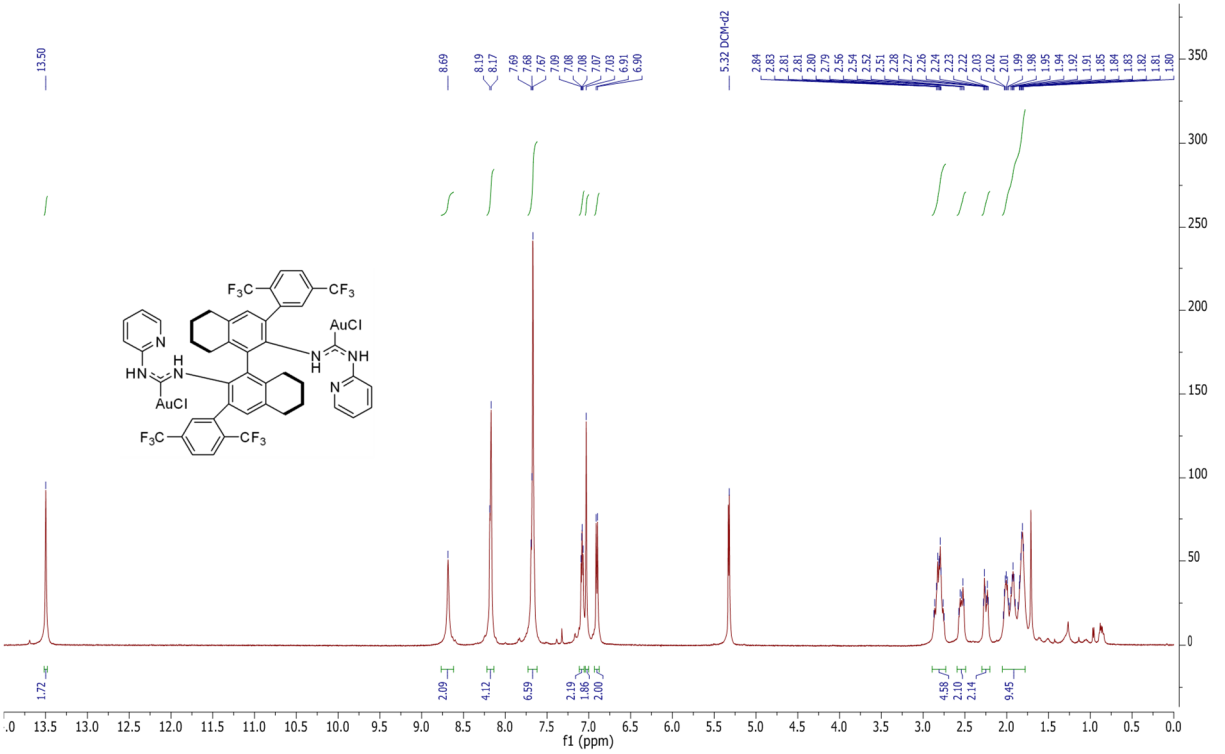
Complex L5*$(AuCl)_2$

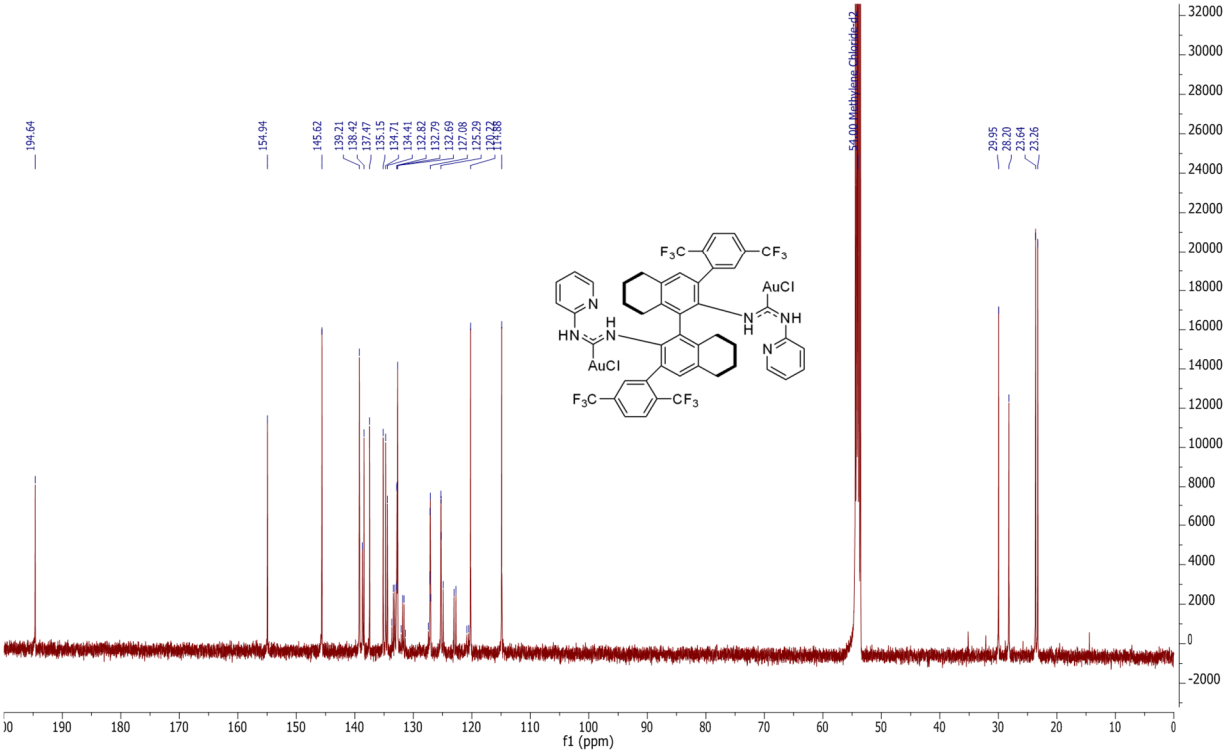


Complex L6*$(AuCl)_2$

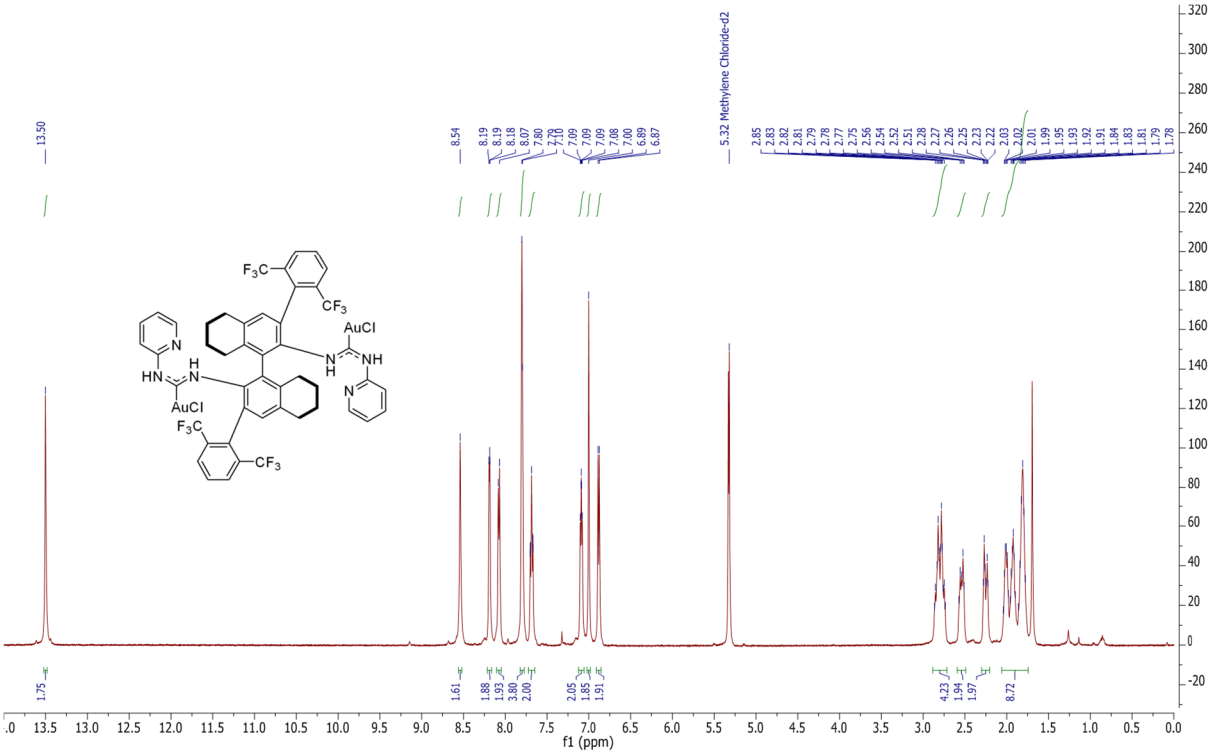


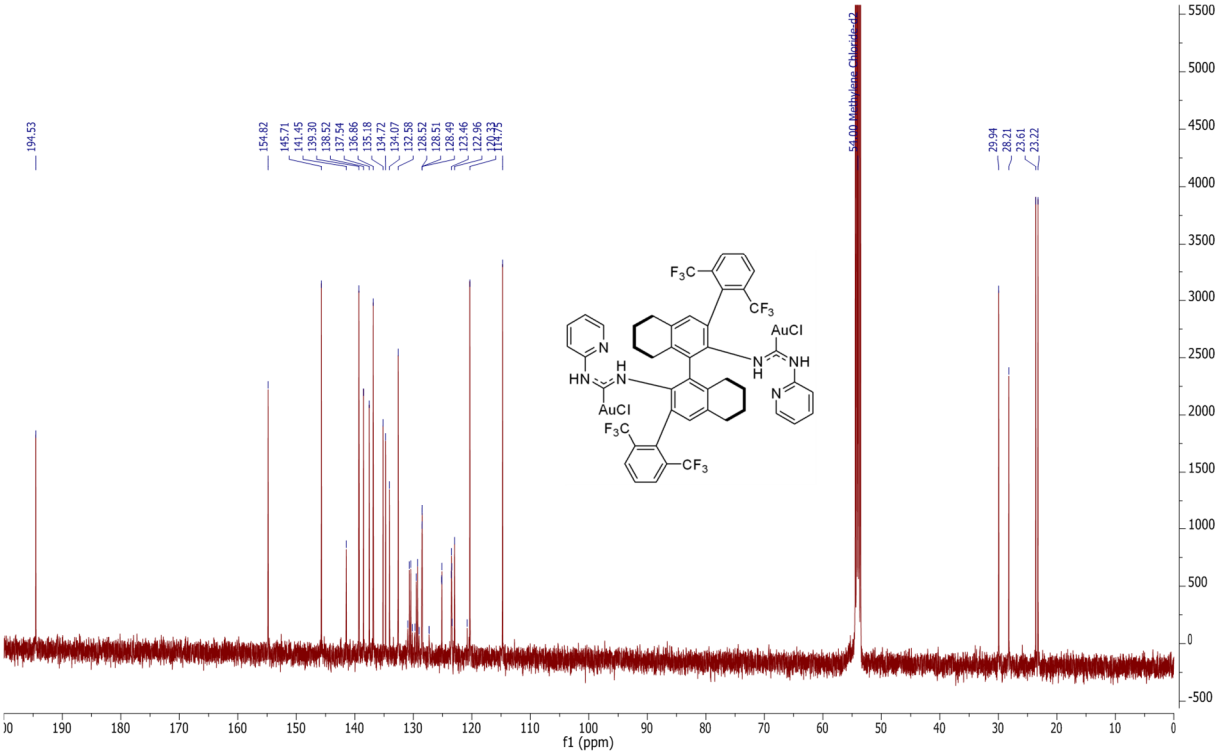
Complex L7*$(AuCl)_2$



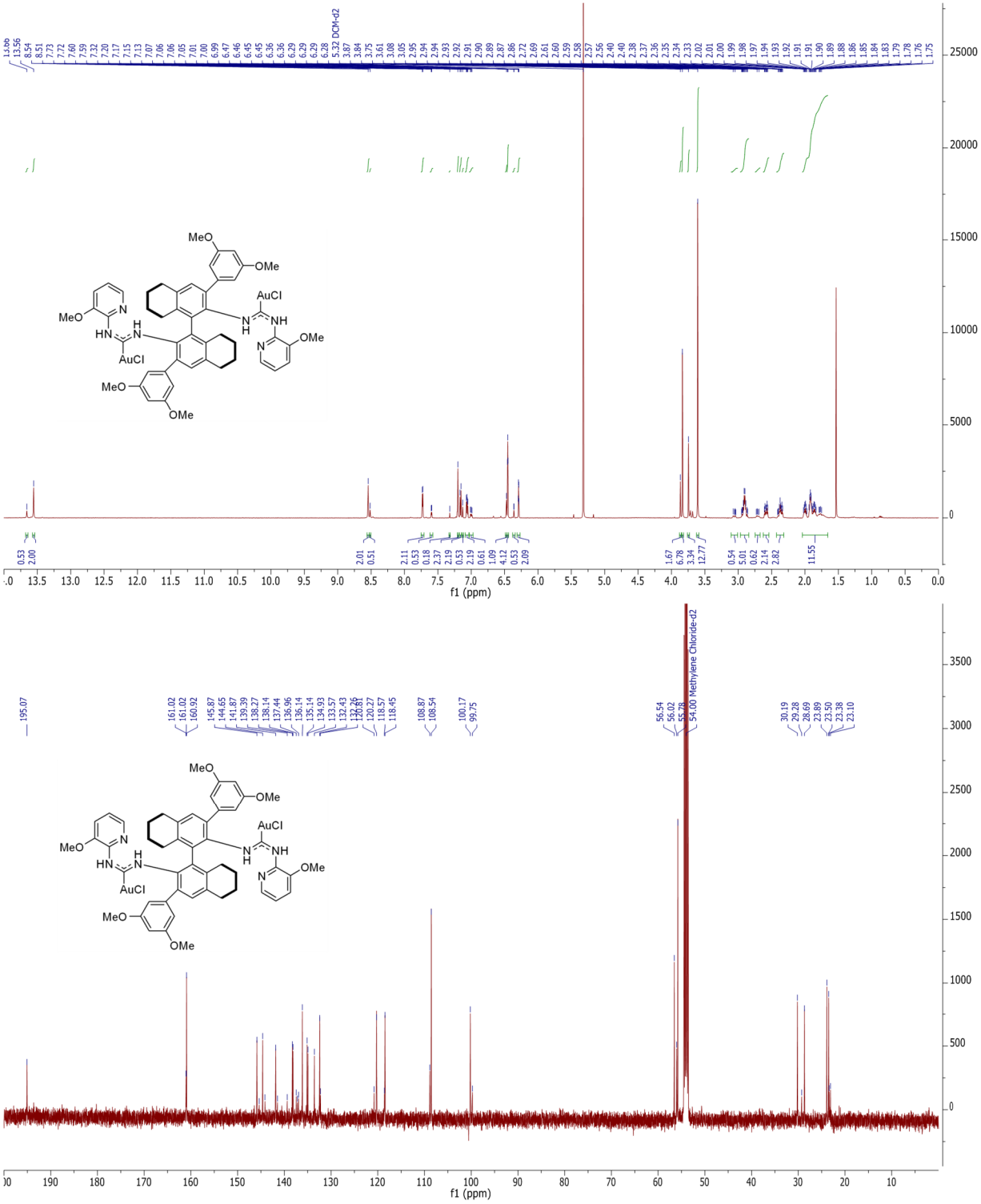


Complex L8*$(AuCl)_2$

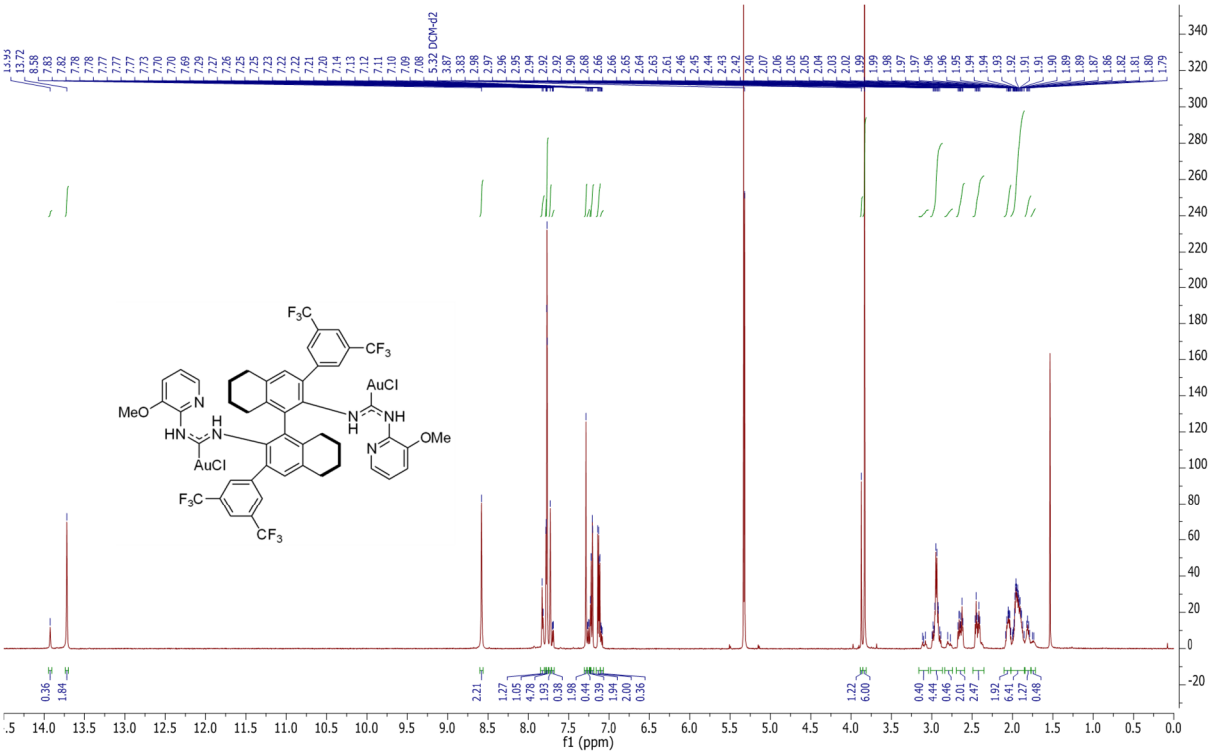


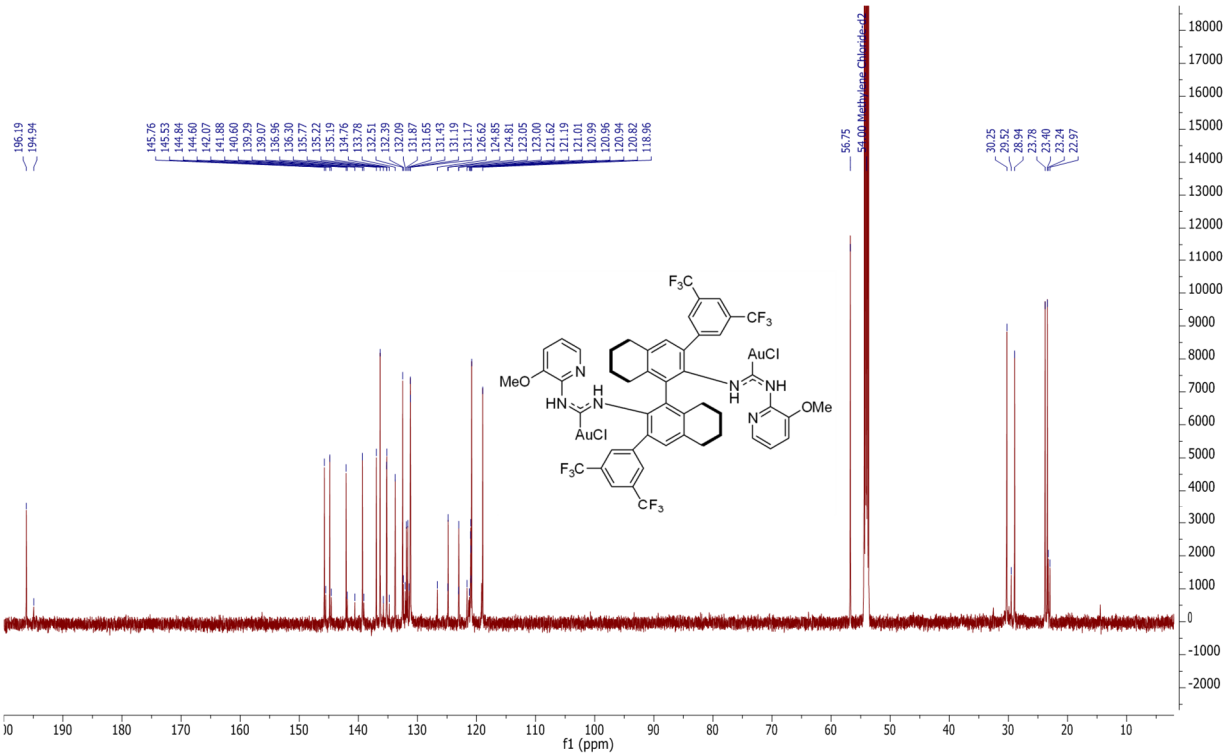


Complex L9*$(AuCl)_2$

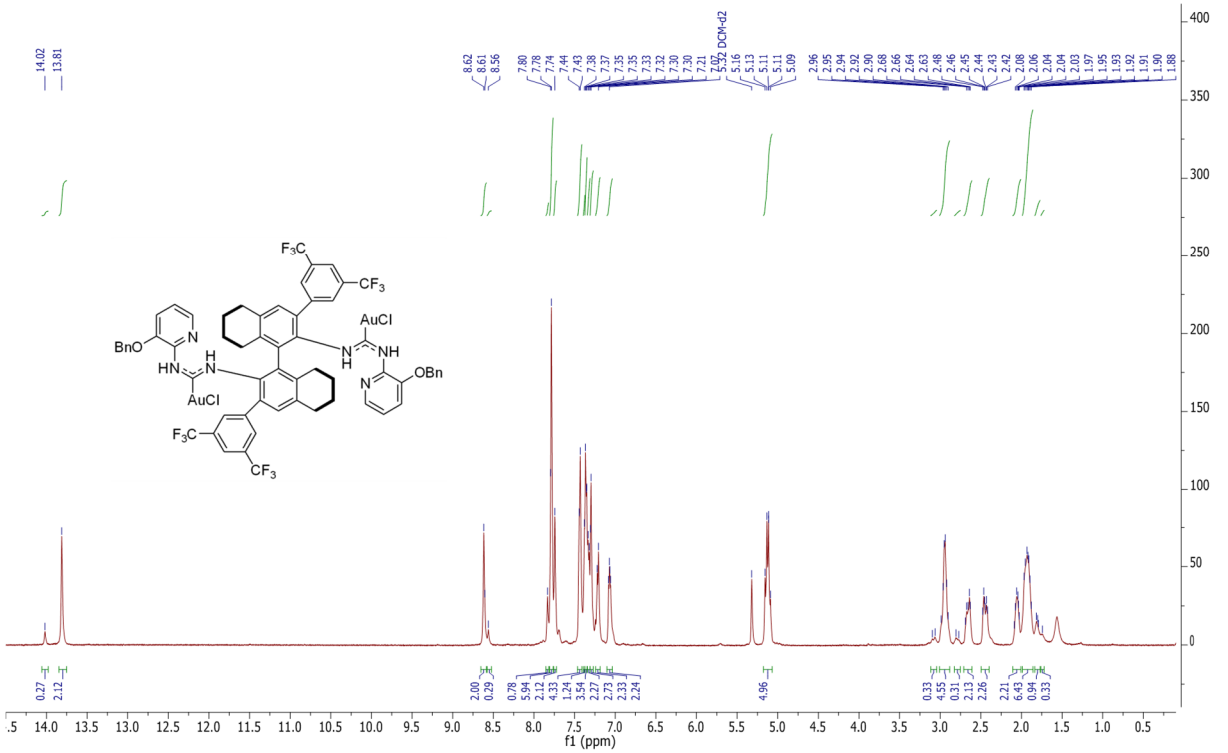


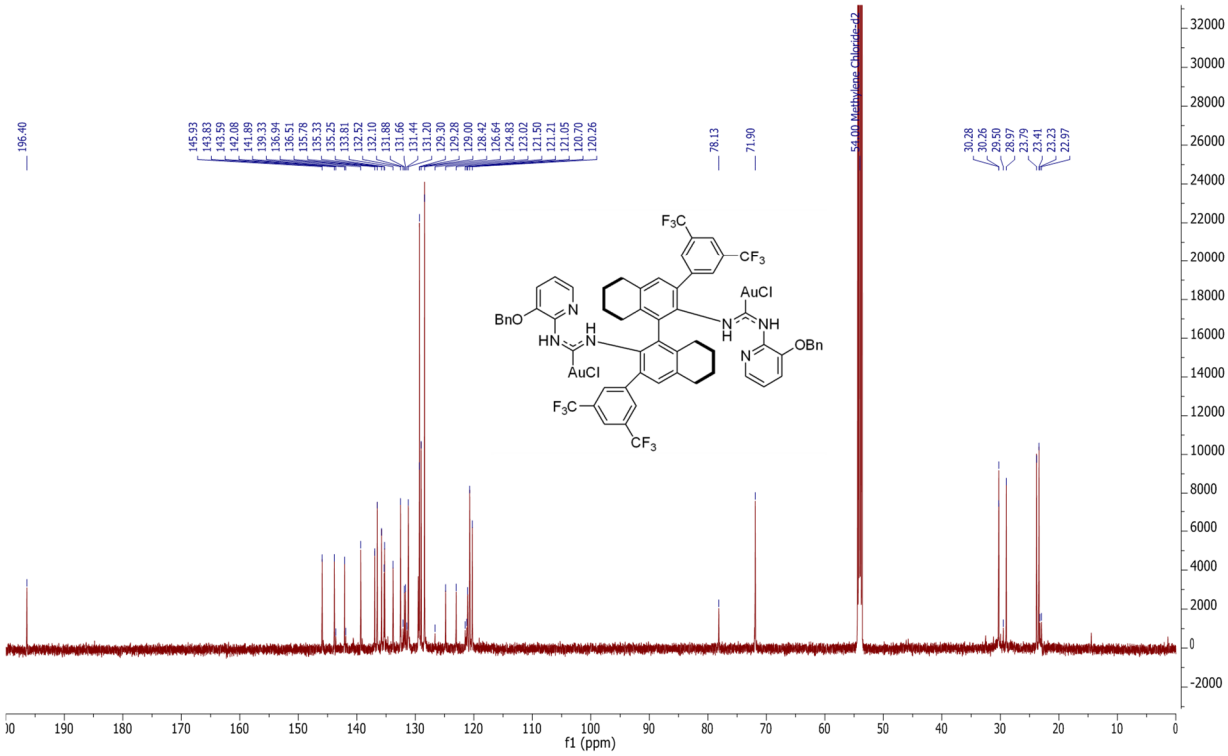
Complex L10*$(AuCl)_2$



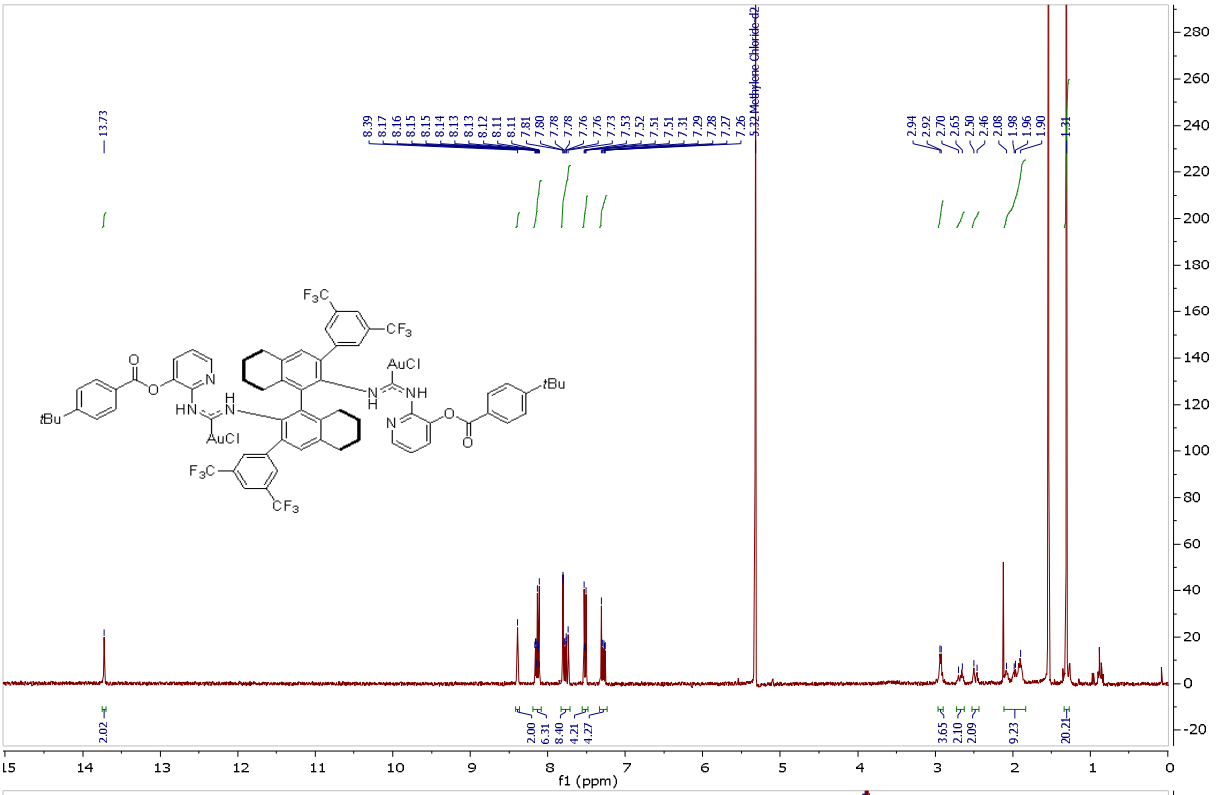


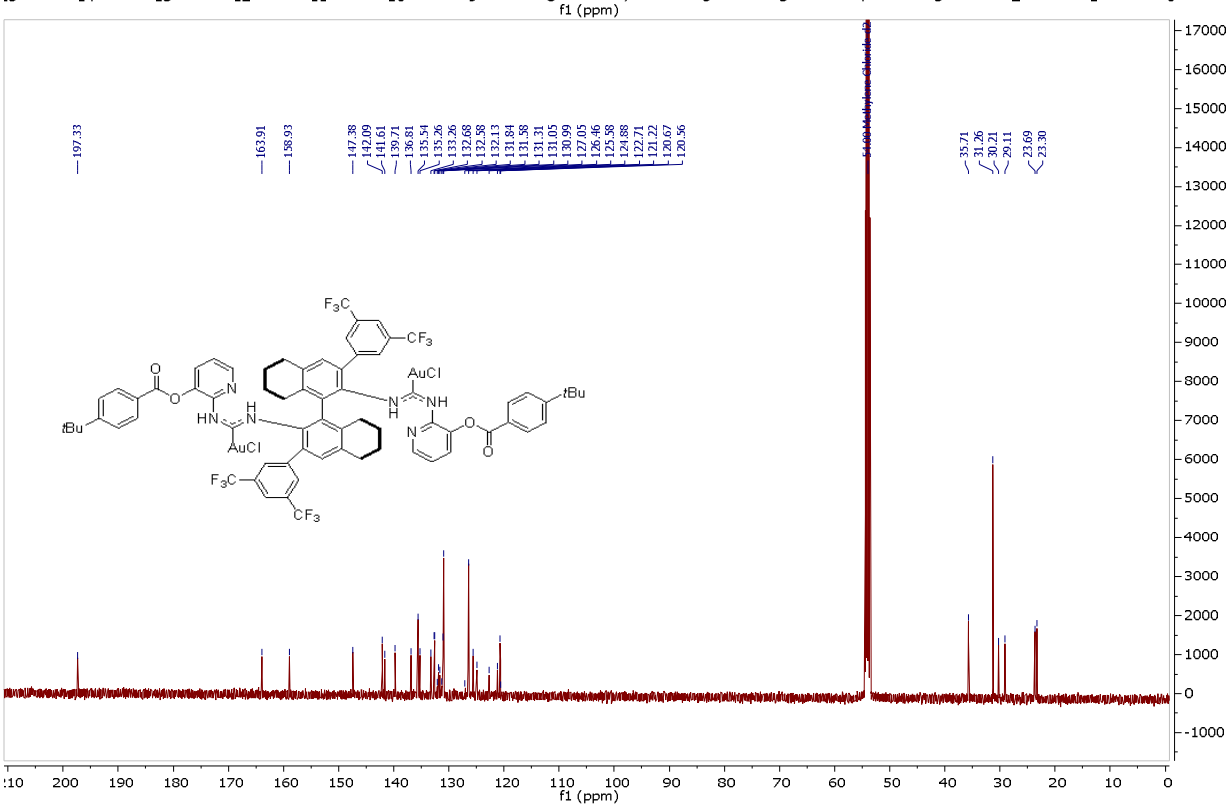
Complex L11*$(AuCl)_2$



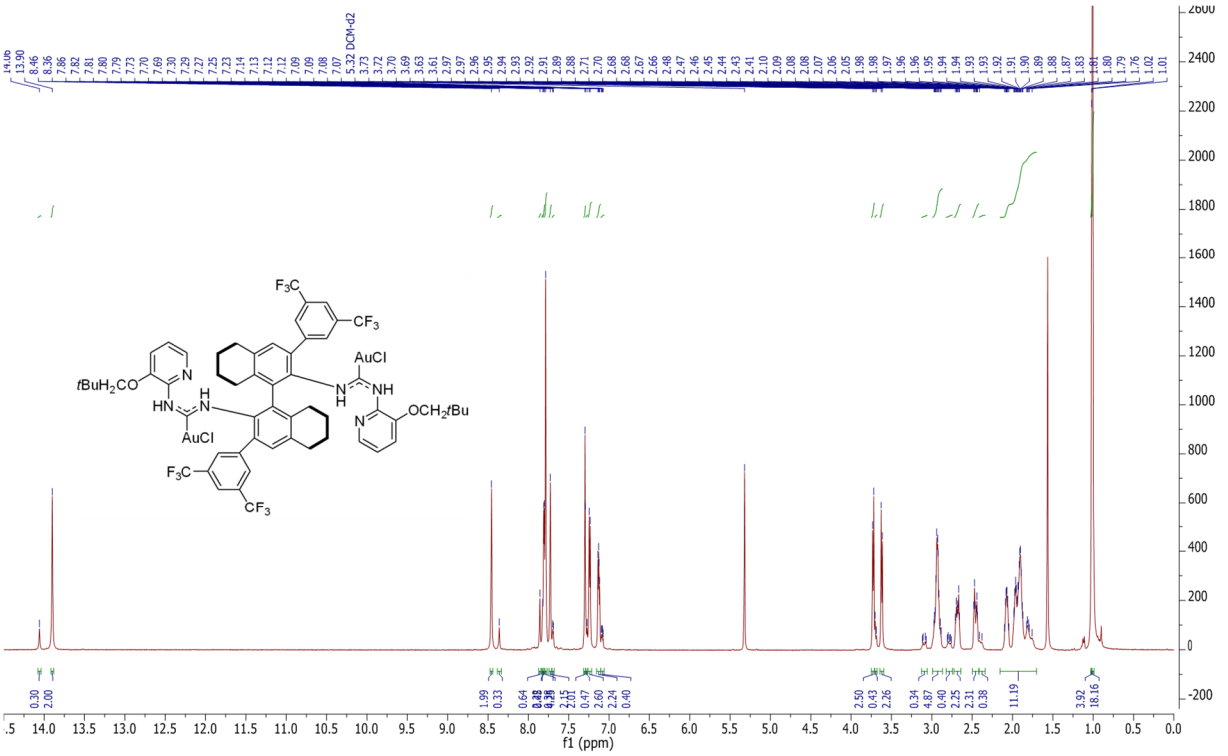


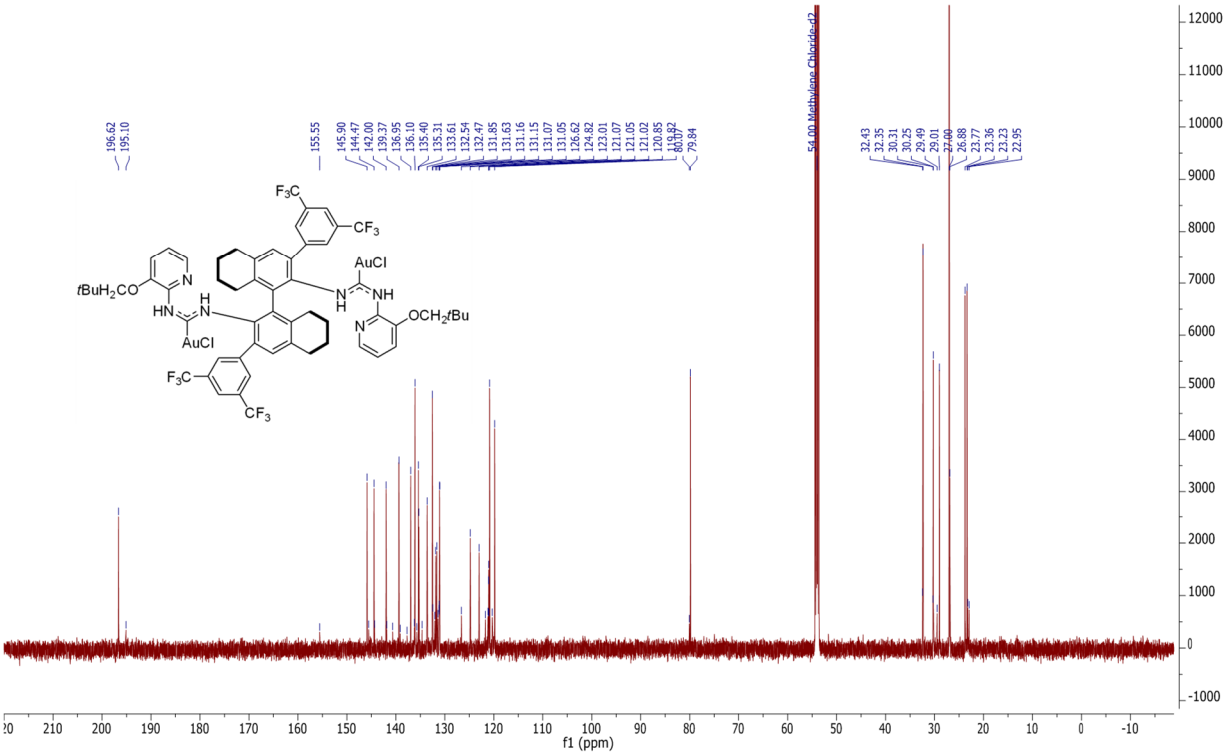
Complex L12*$(AuCl)_2$



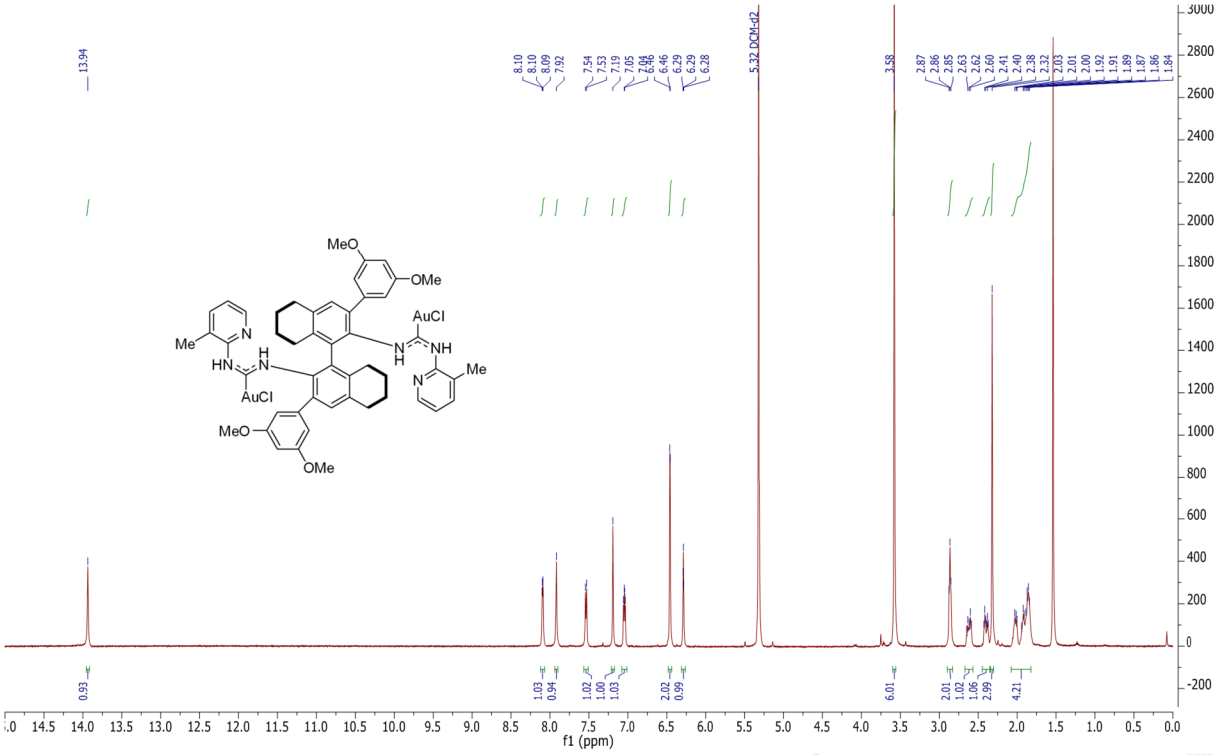


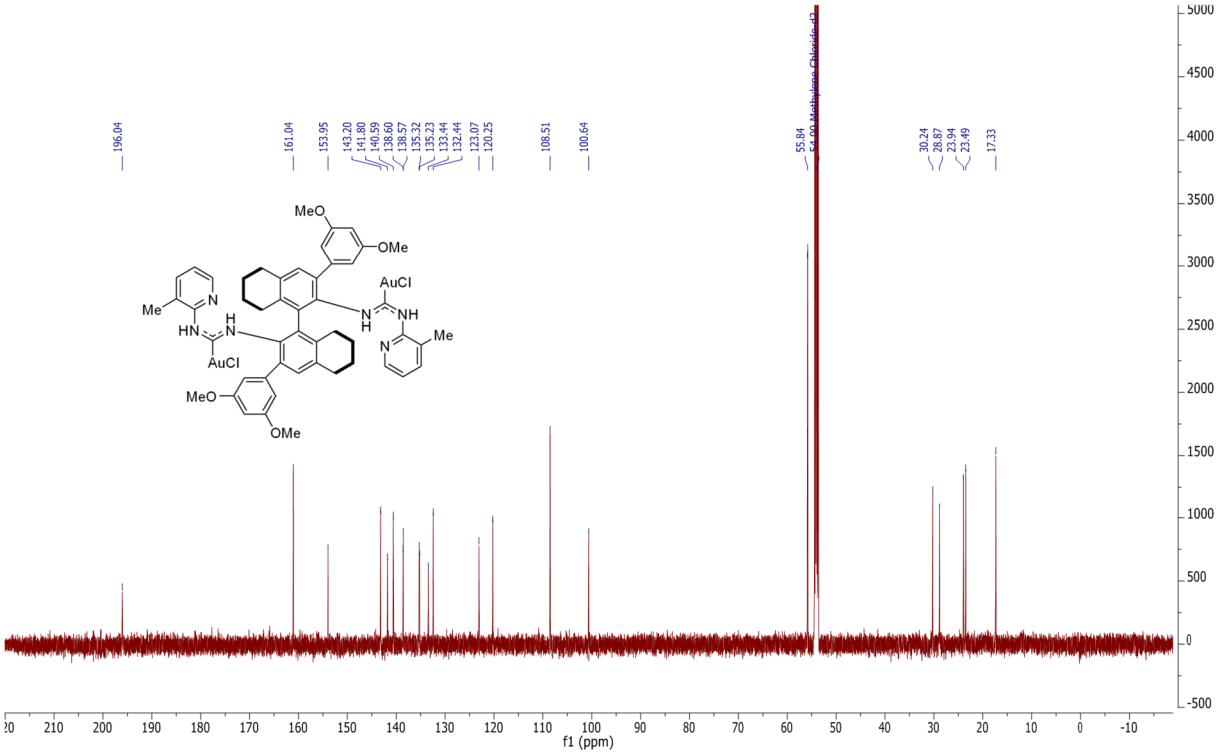
Complex L13*$(AuCl)_2$



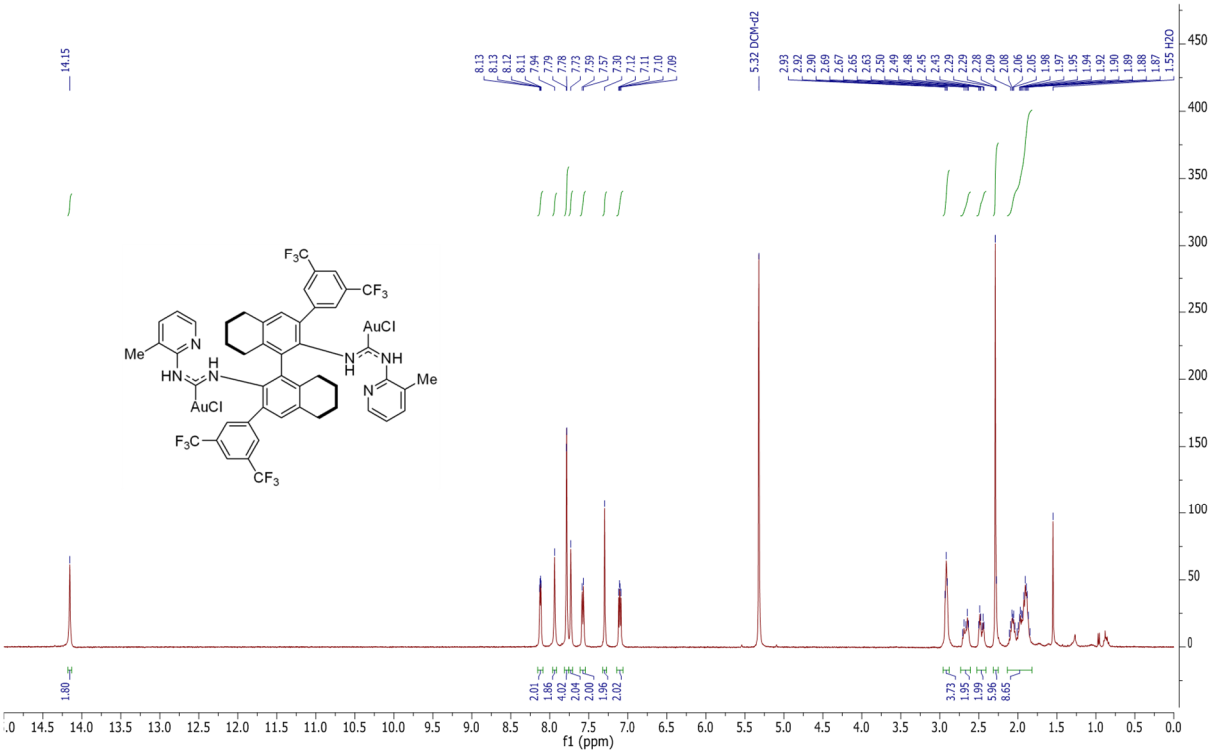


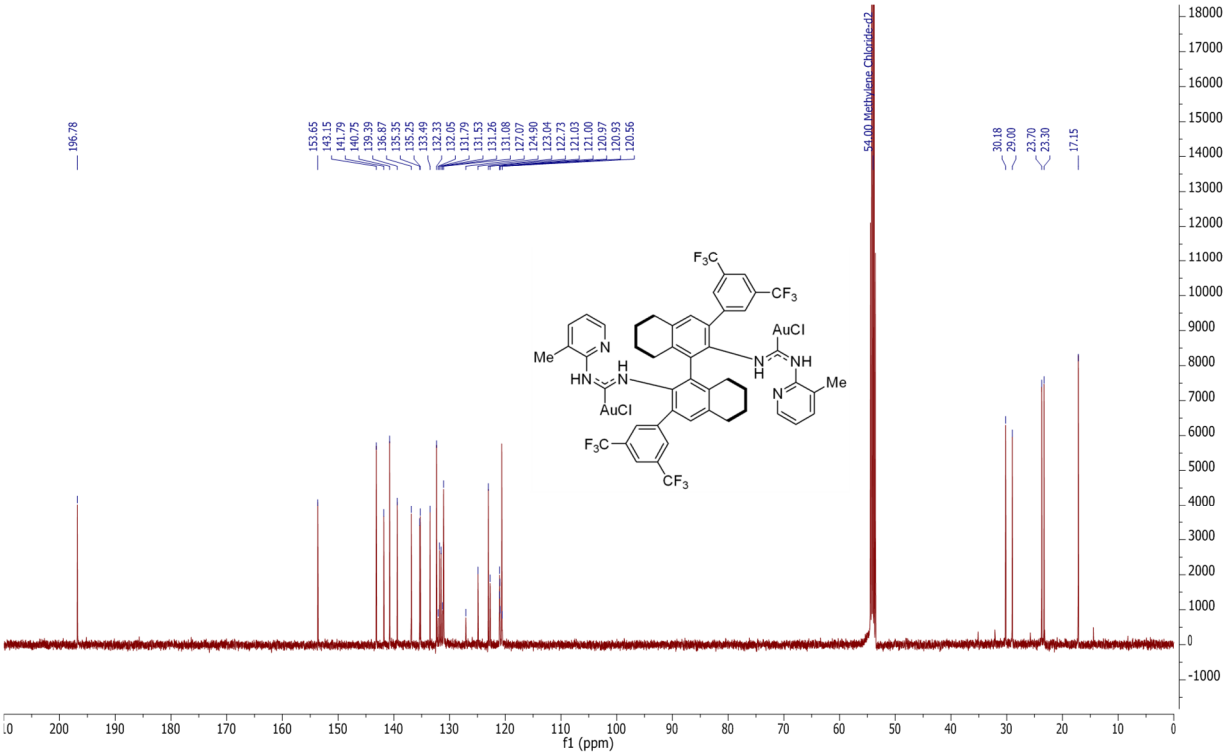
Complex L14*$(AuCl)_2$



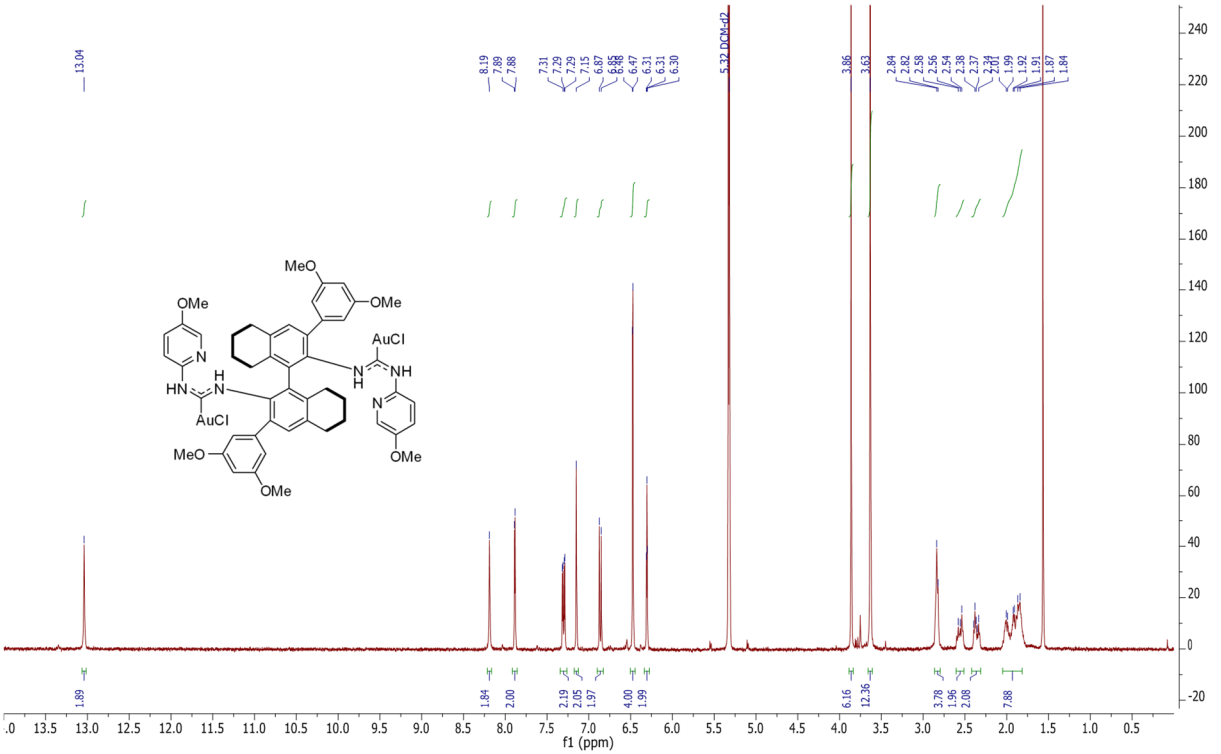


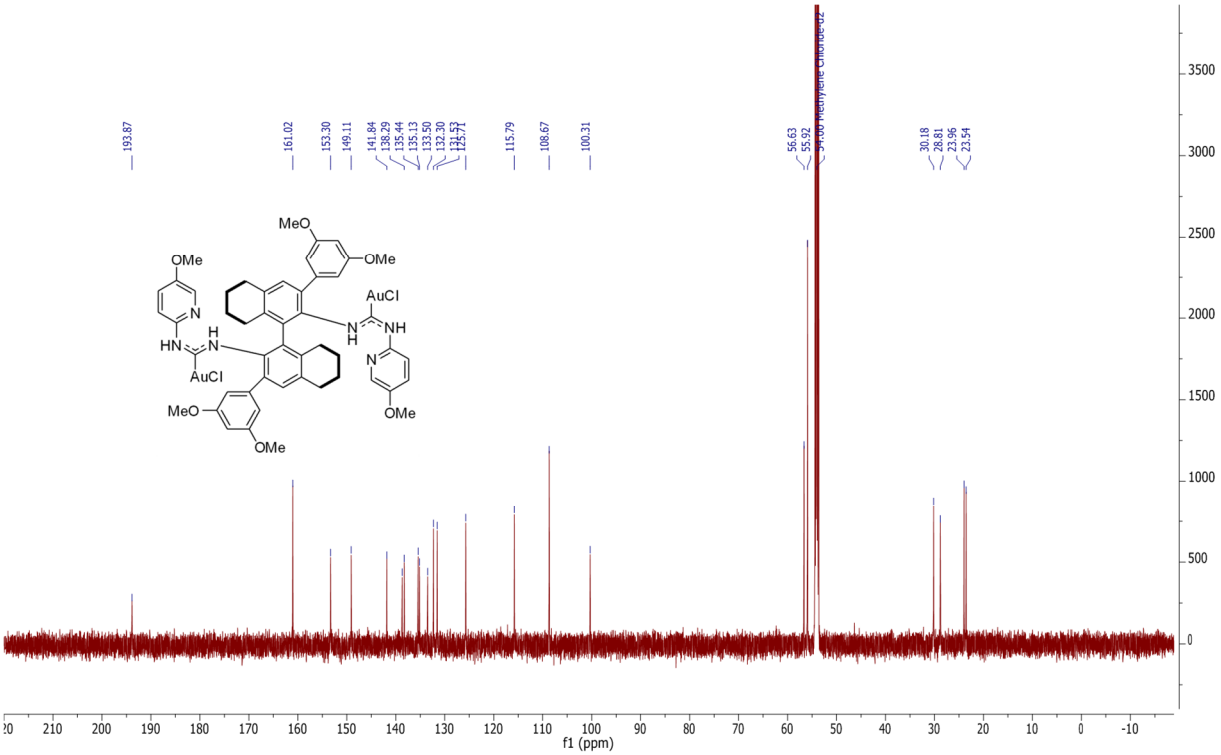
Complex L15*$(AuCl)_2$



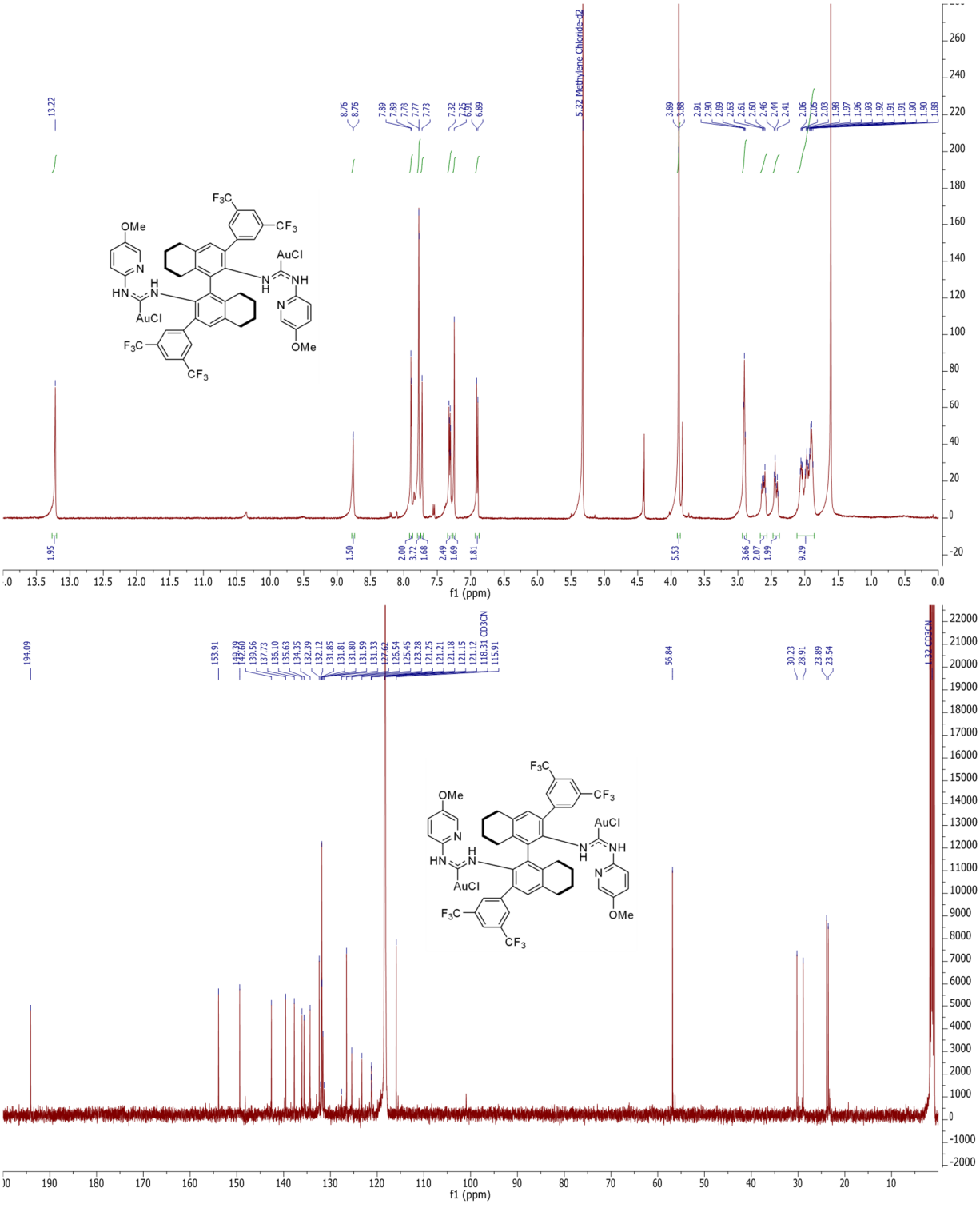


Complex L16*$(AuCl)_2$

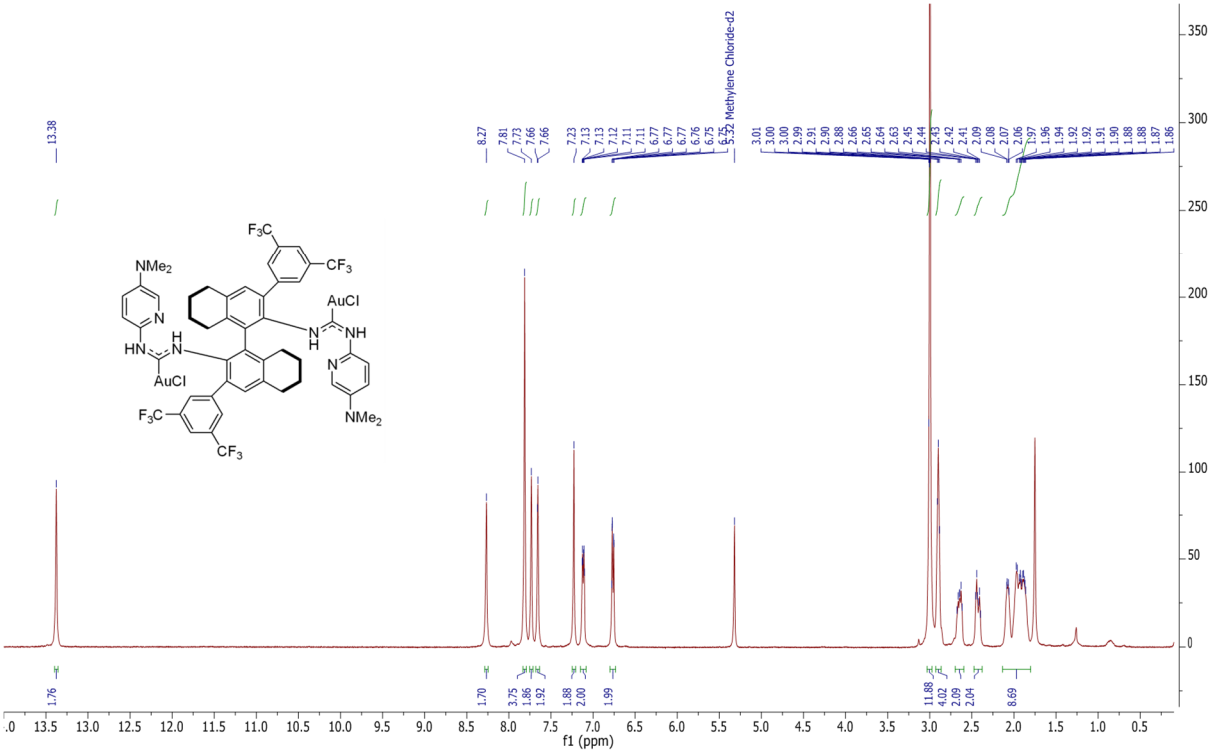


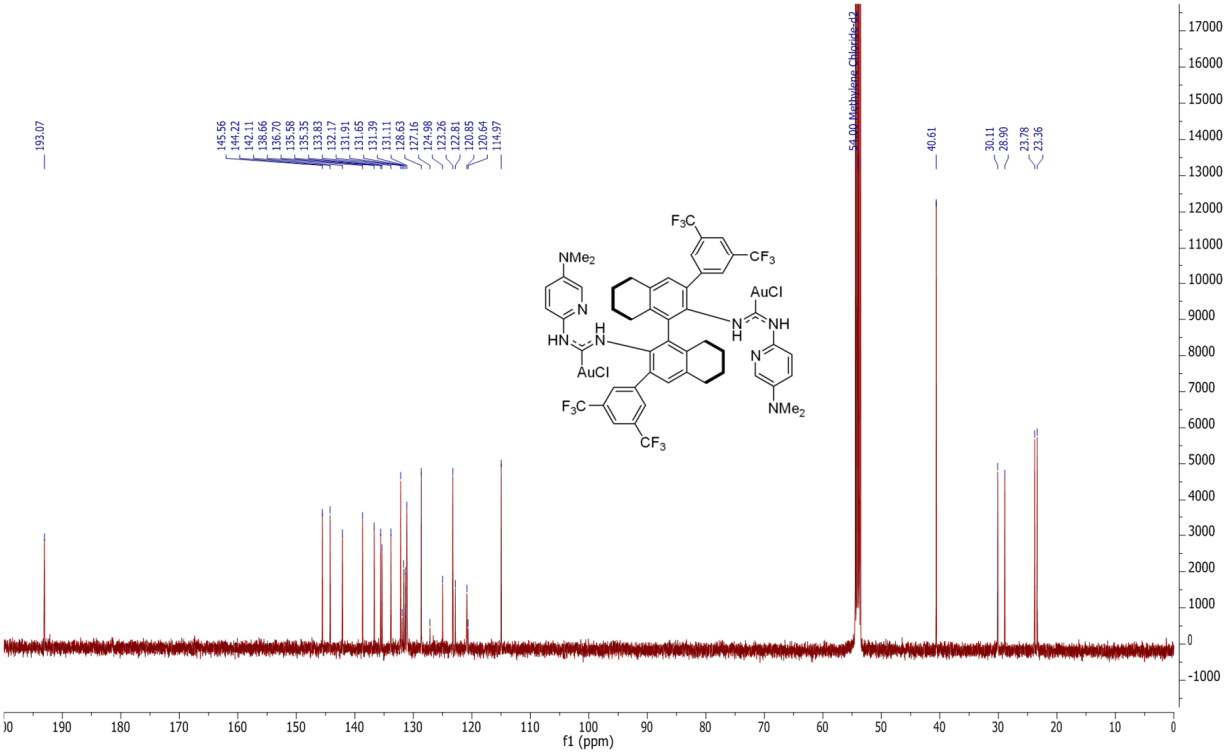


Complex L17*$(AuCl)_2$

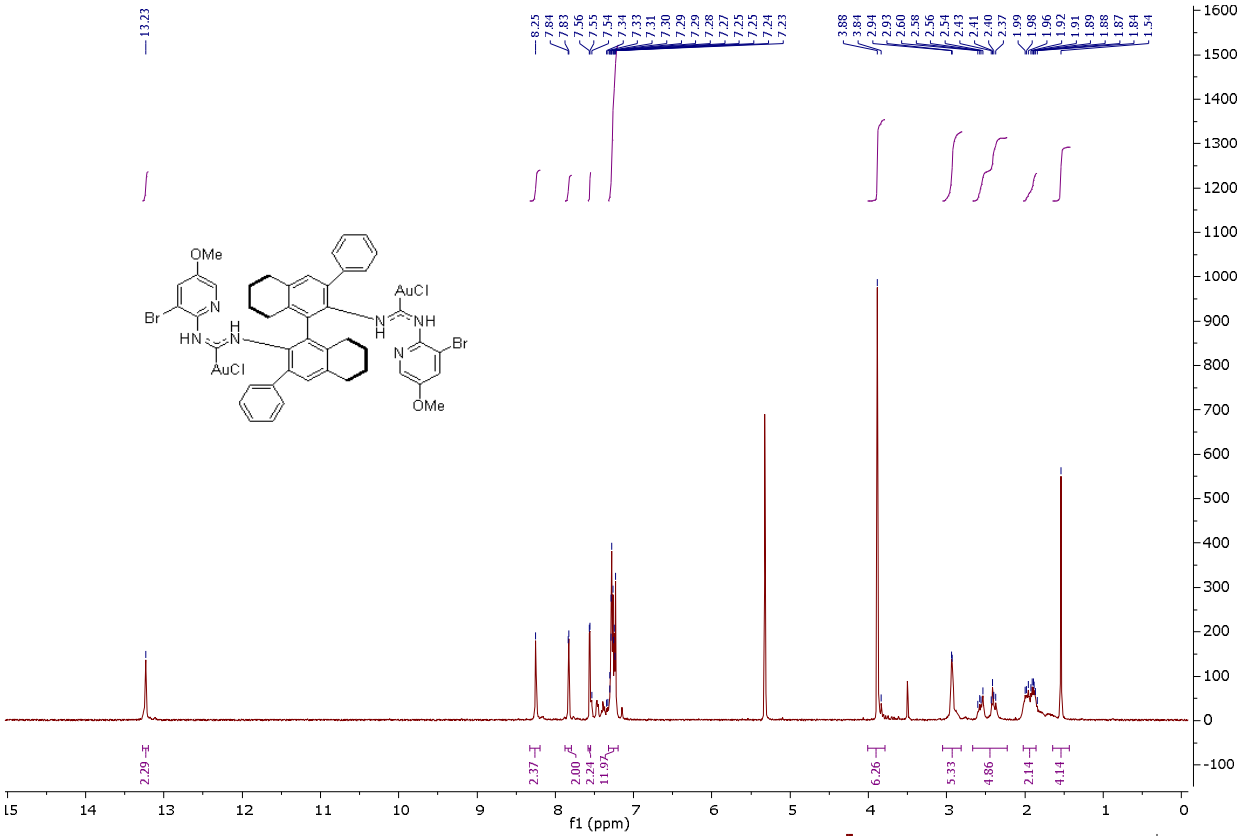


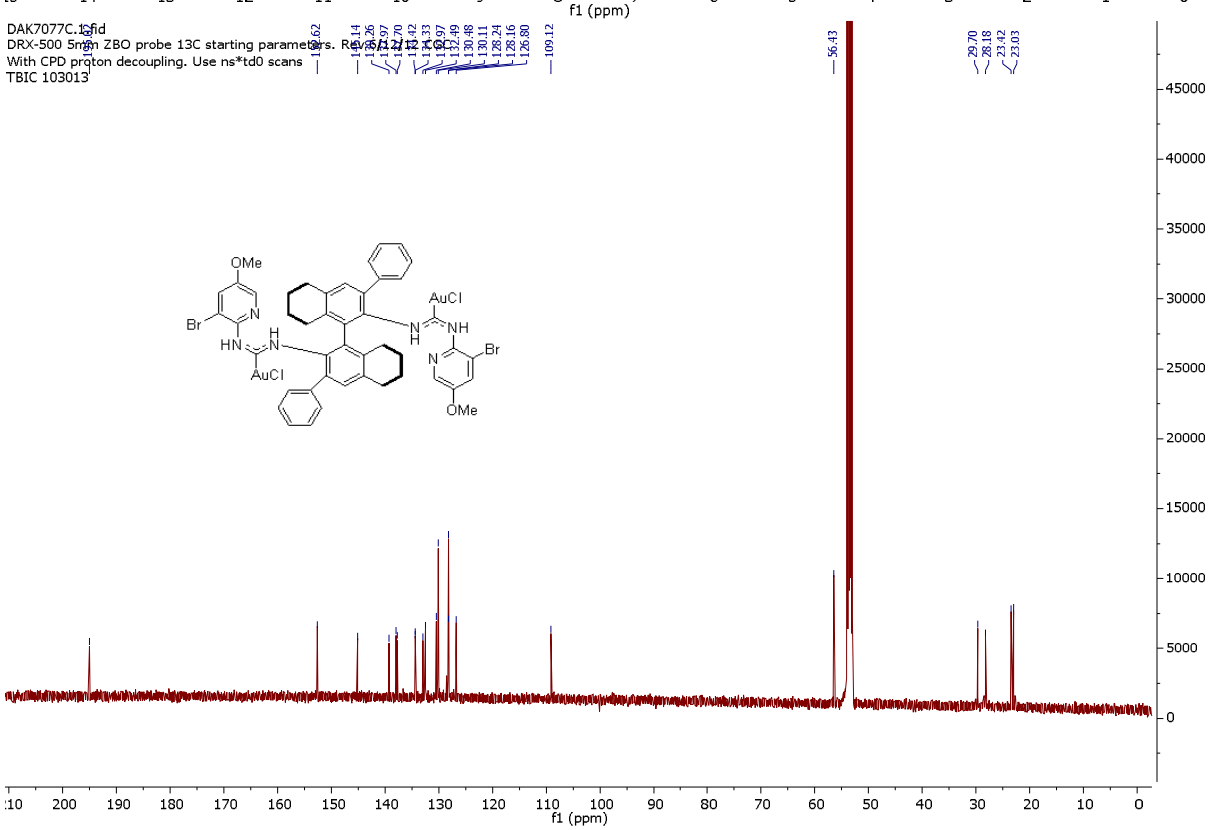
Complex L18*$(AuCl)_2$



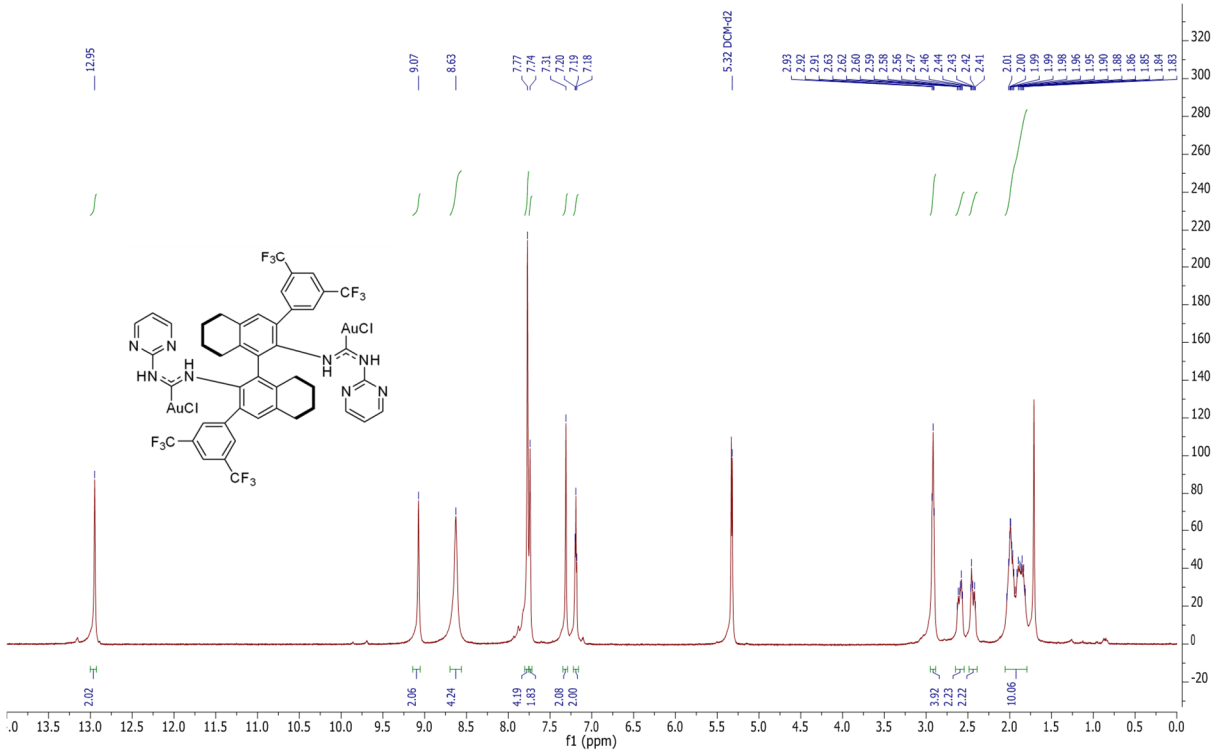


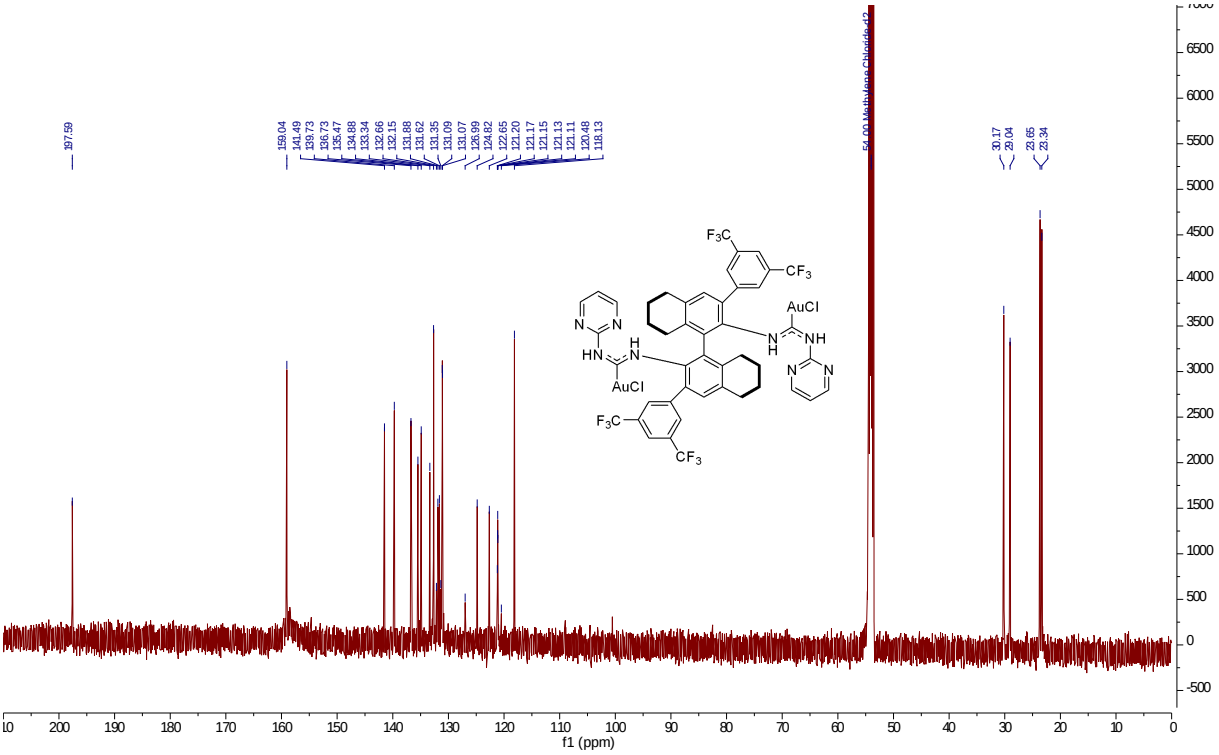
Complex L19*(AuCl)$_2$



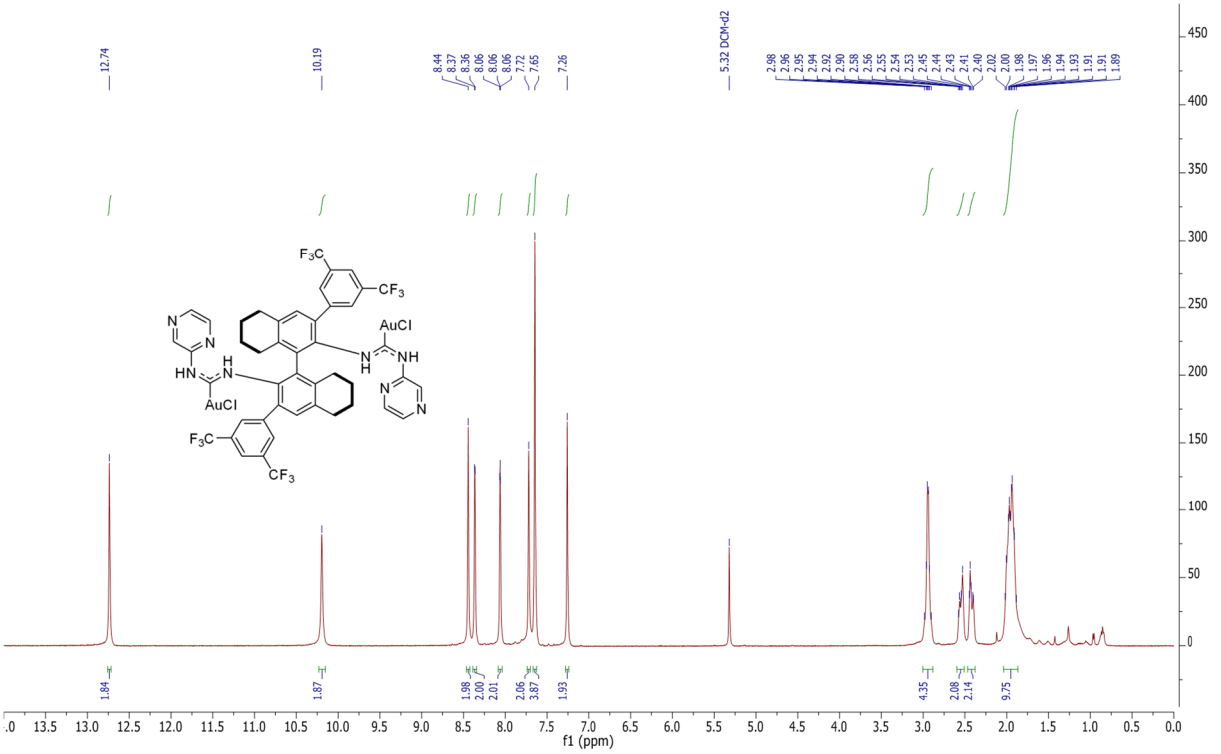


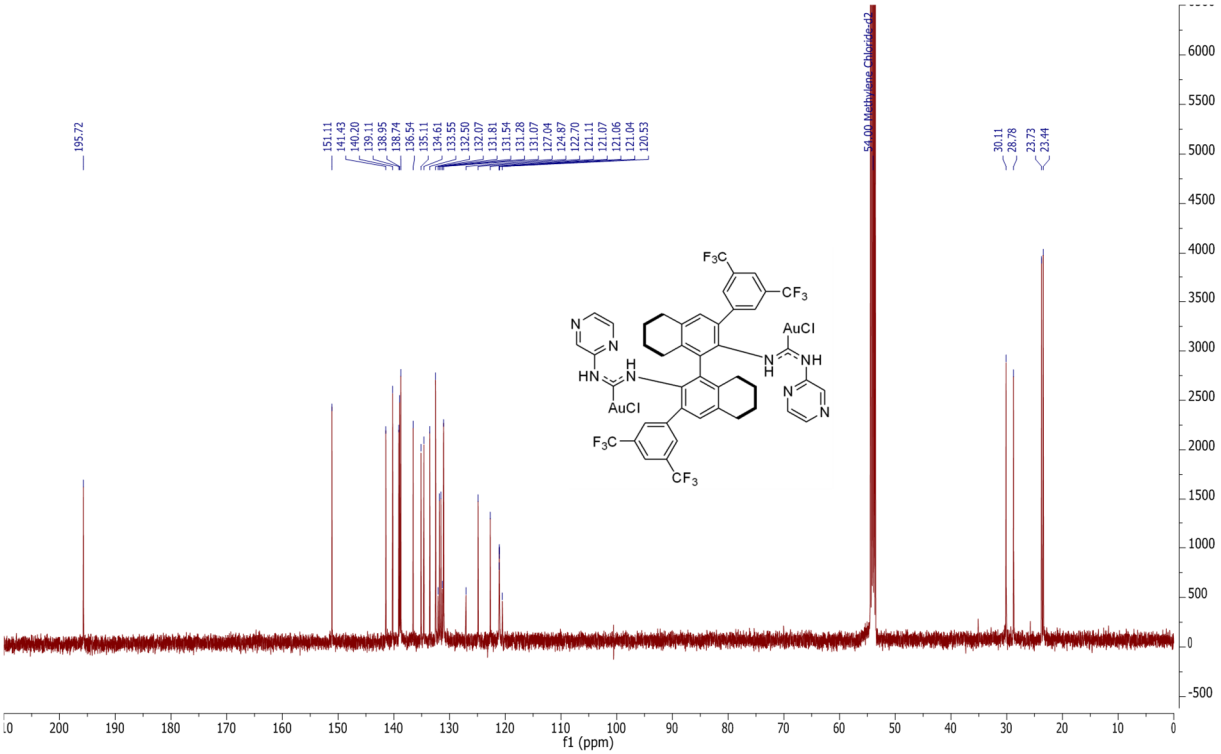
Complex L20*$(AuCl)_2$



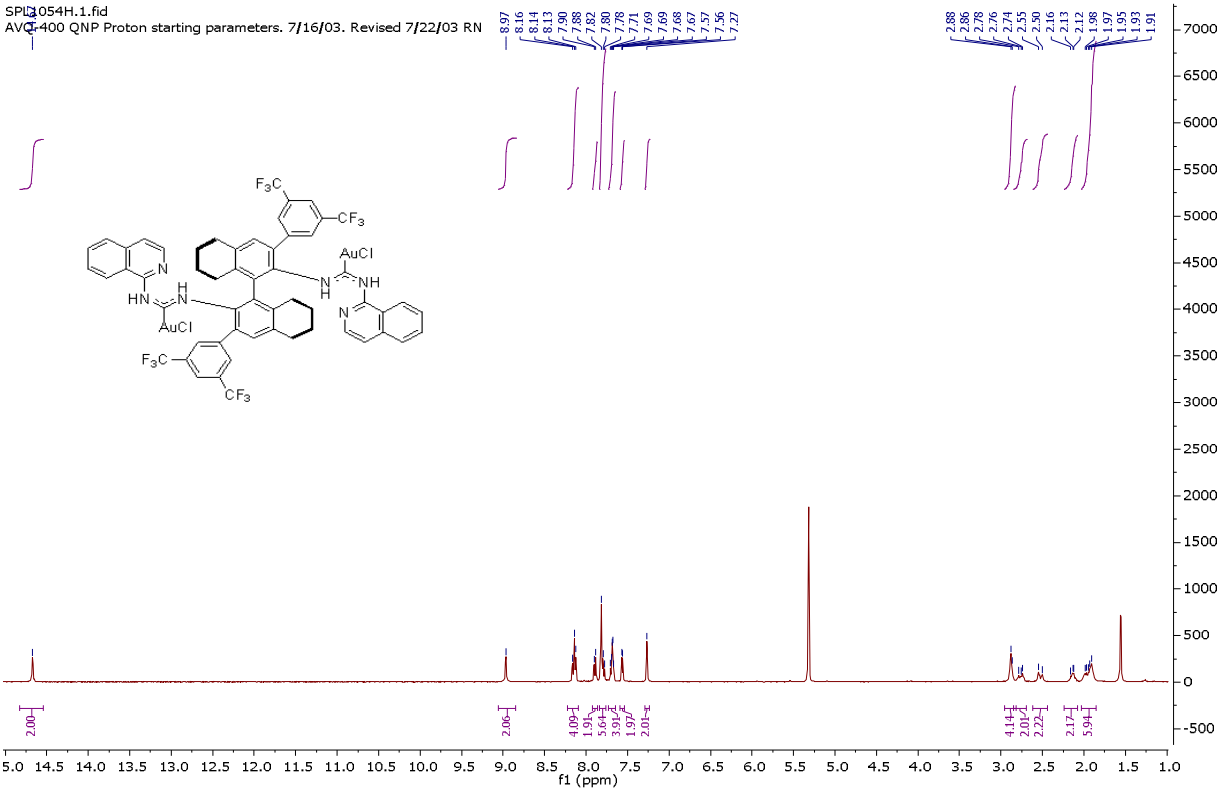


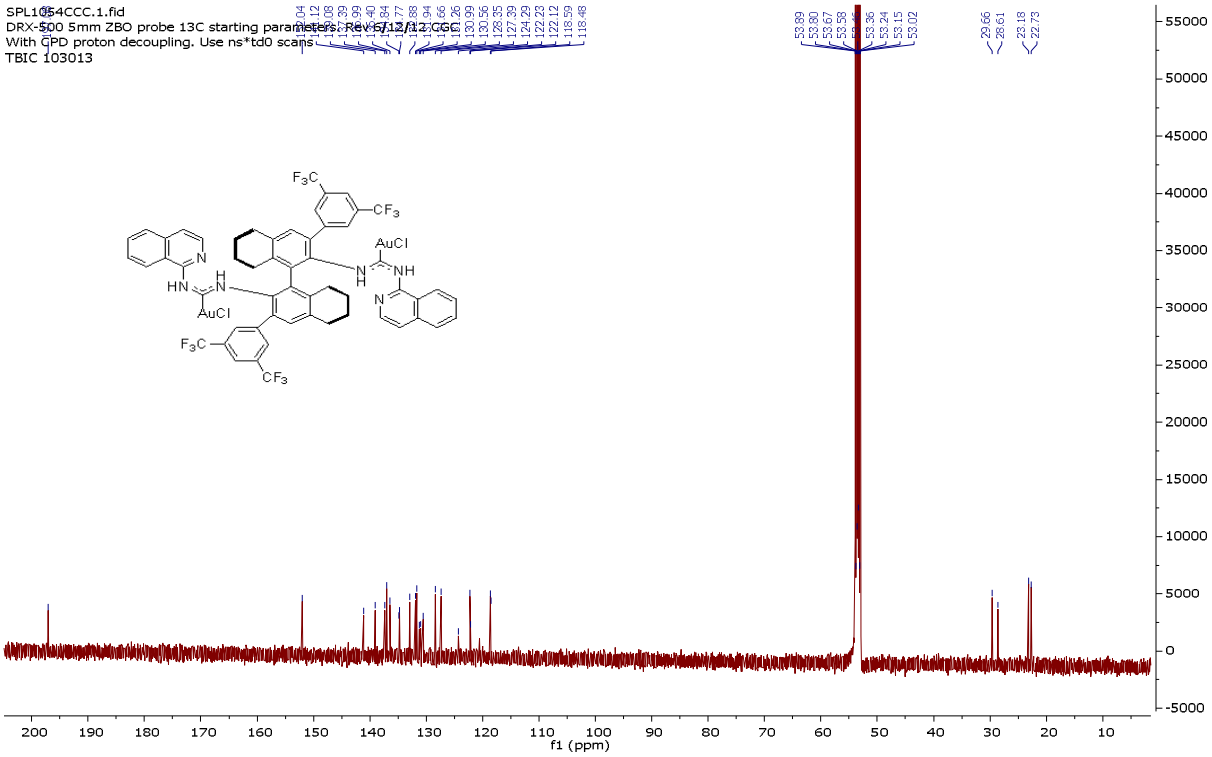
Complex L21*$(AuCl)_2$



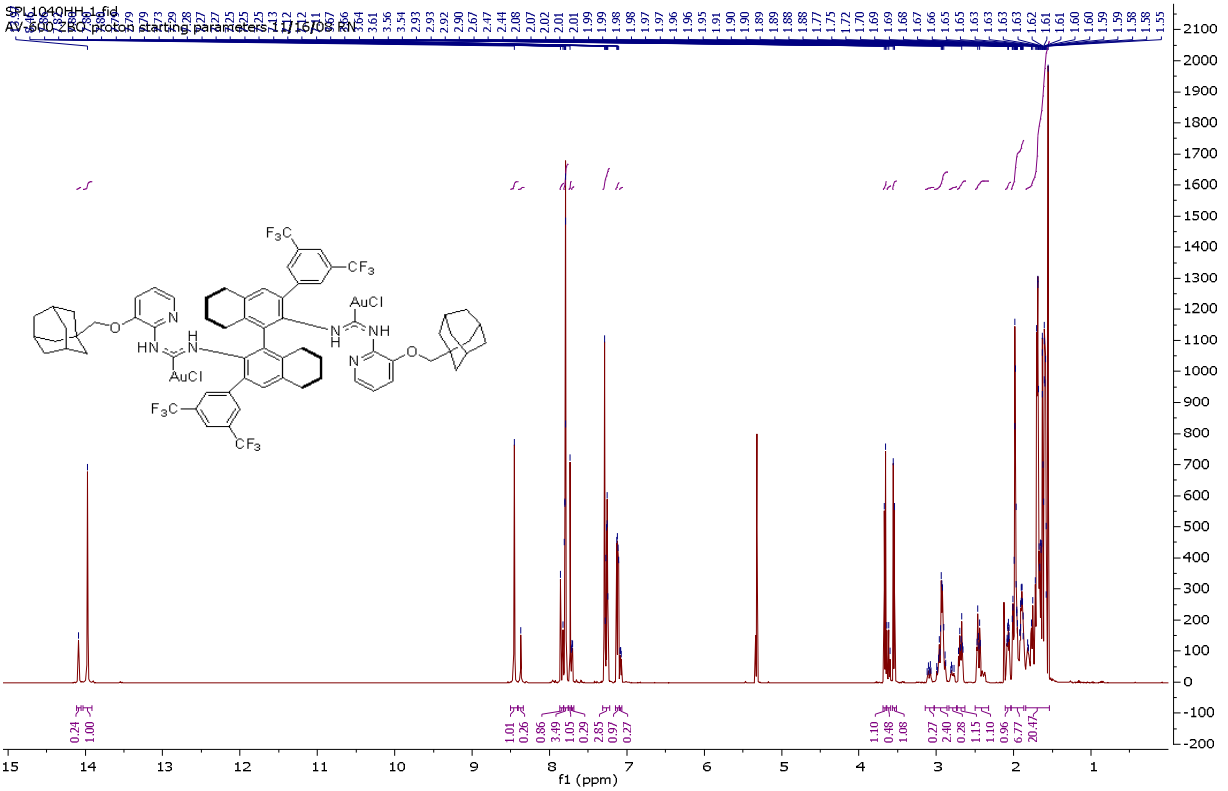


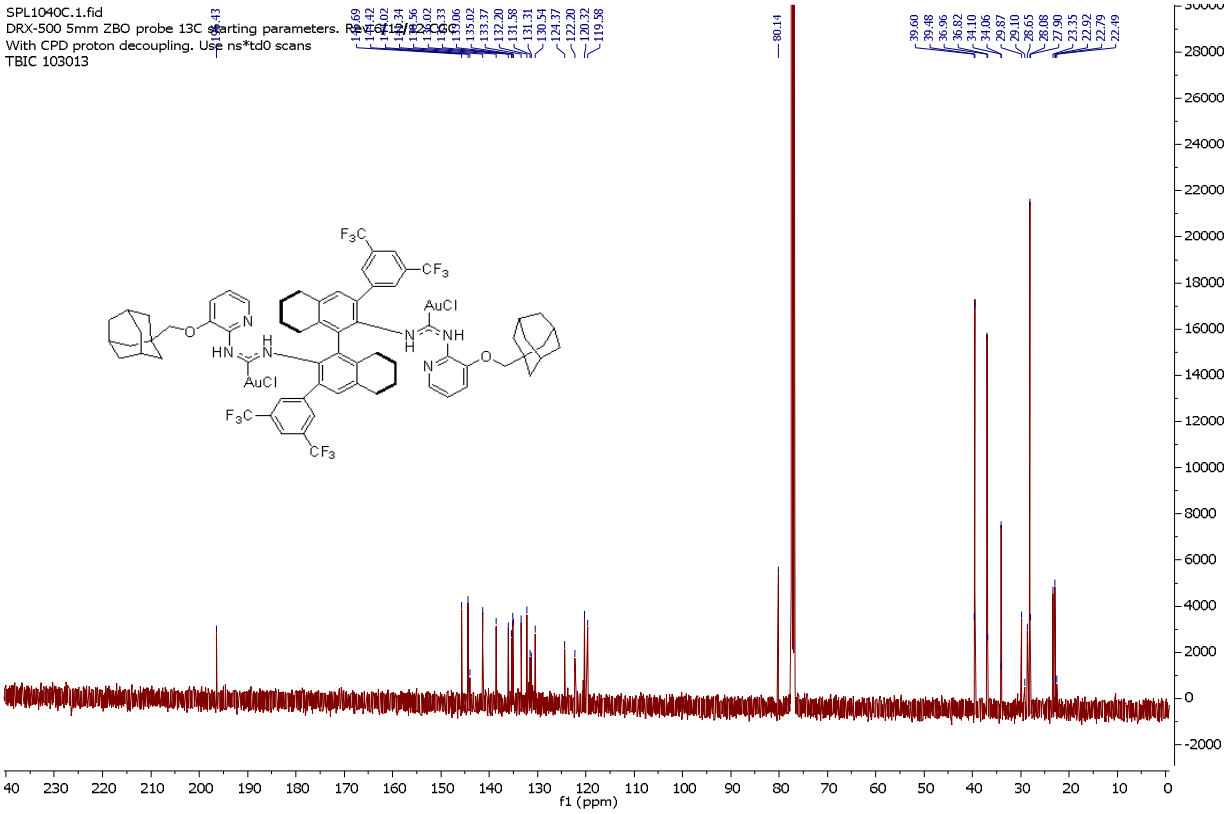
Complex L22*(AuCl)$_2$



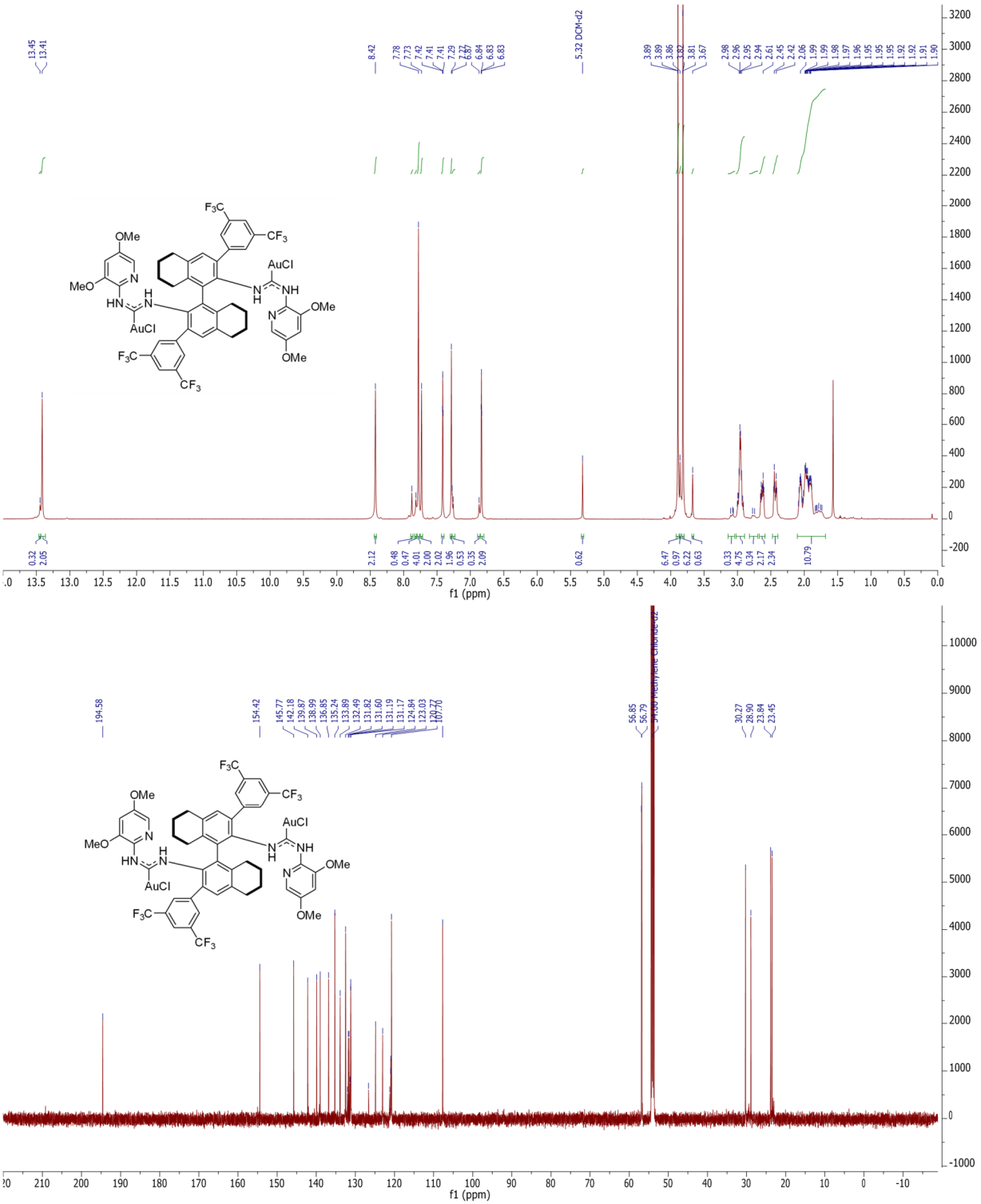


Complex L23*$(AuCl)_2$

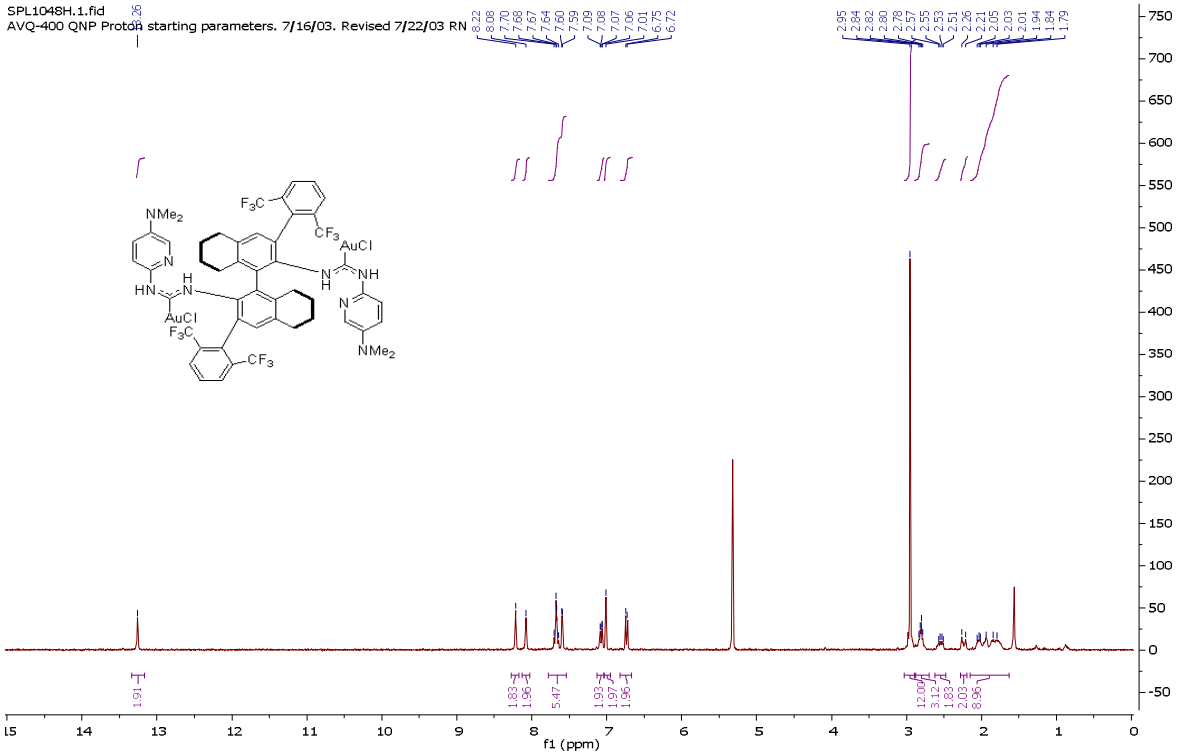


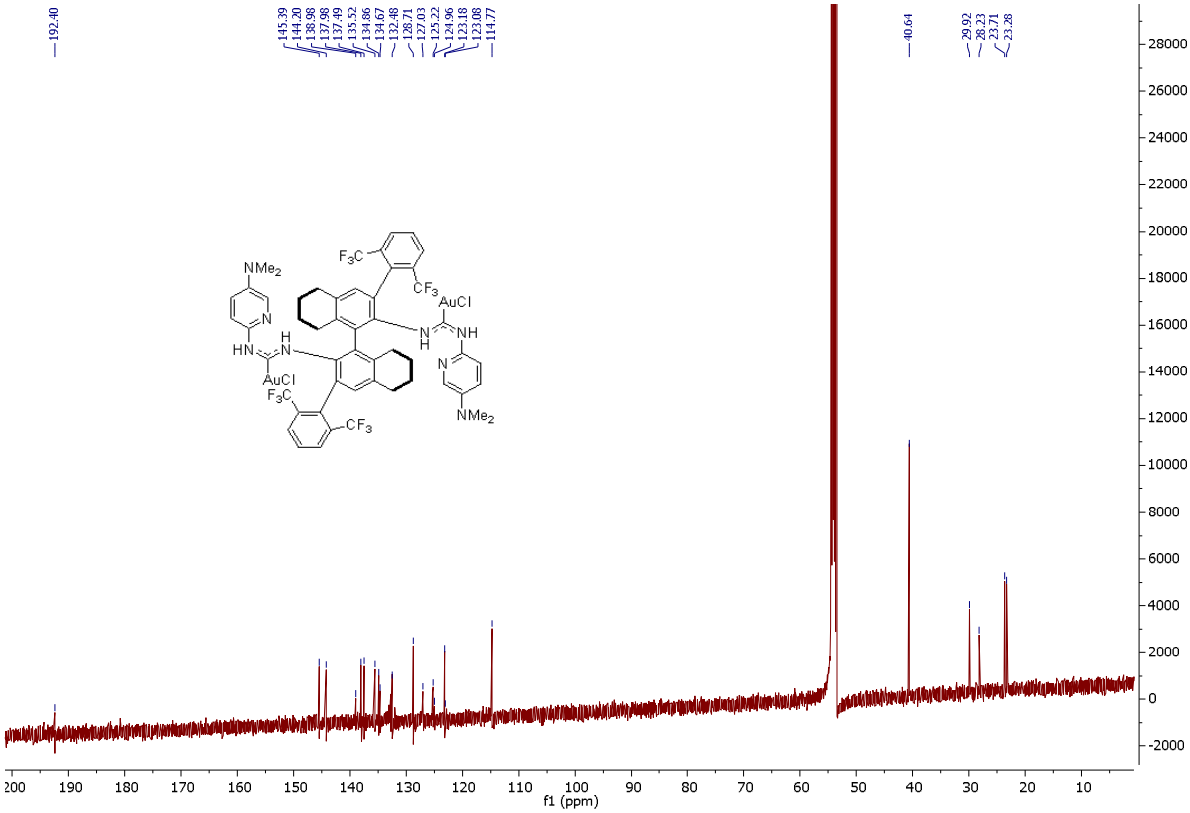


Complex L24*$(AuCl)_2$

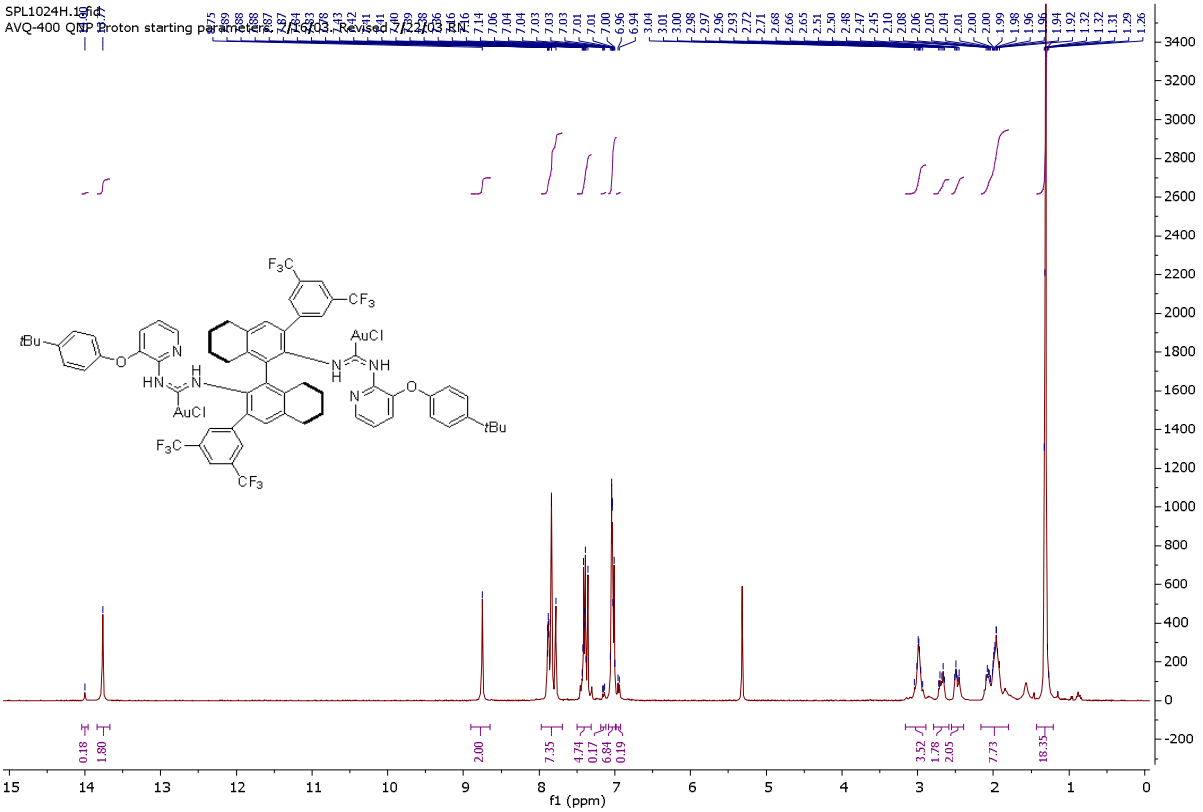


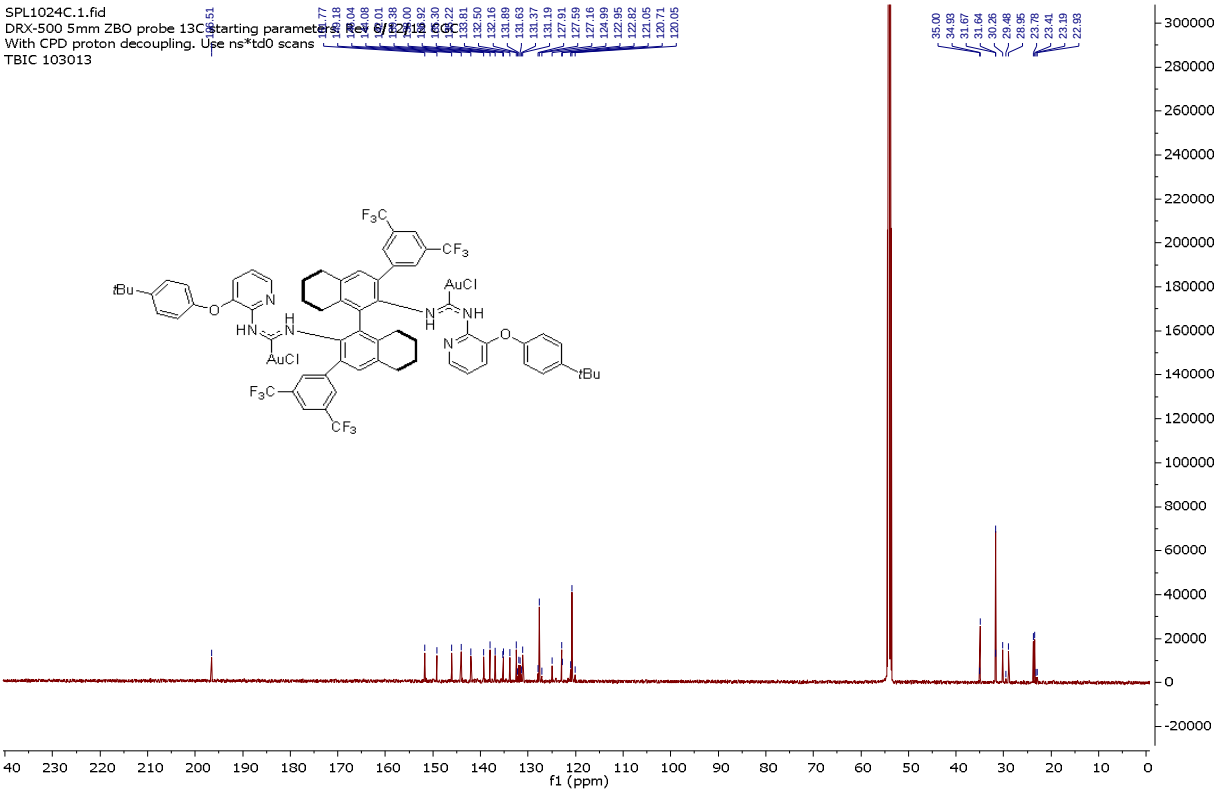
Complex L25*$(AuCl)_2$



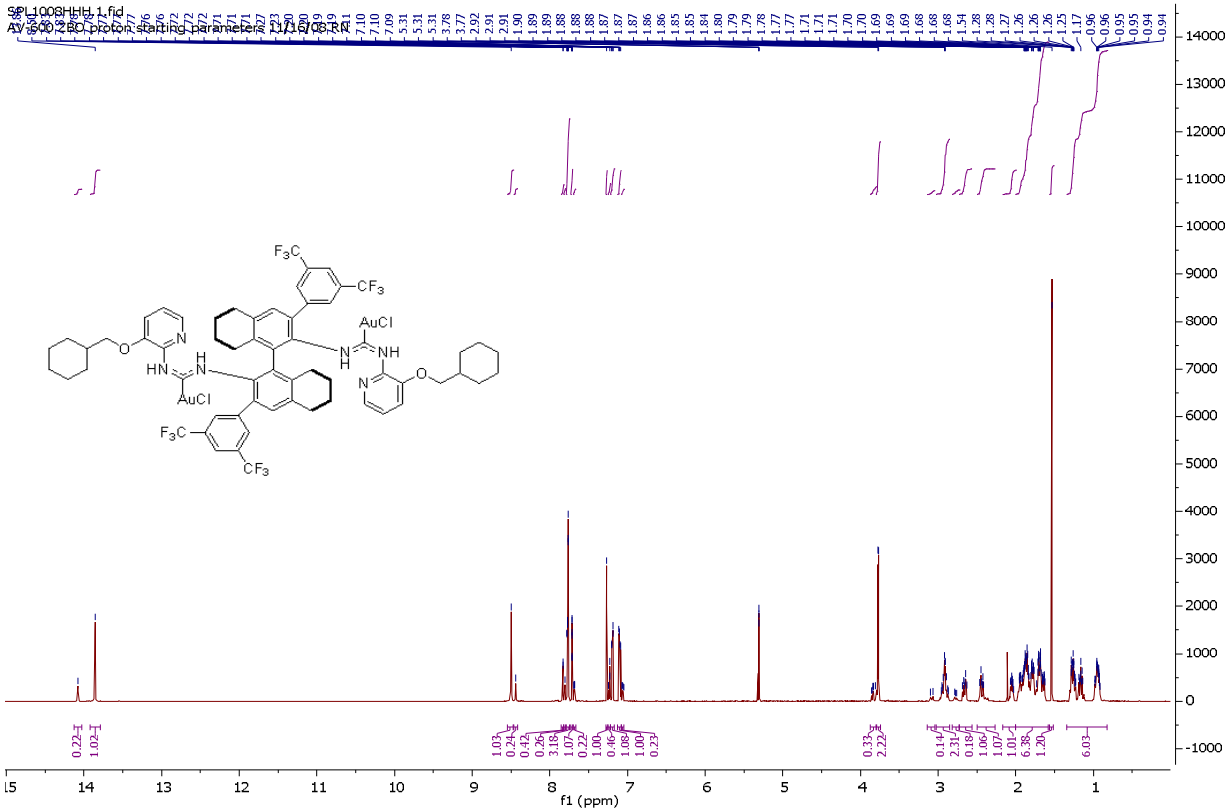


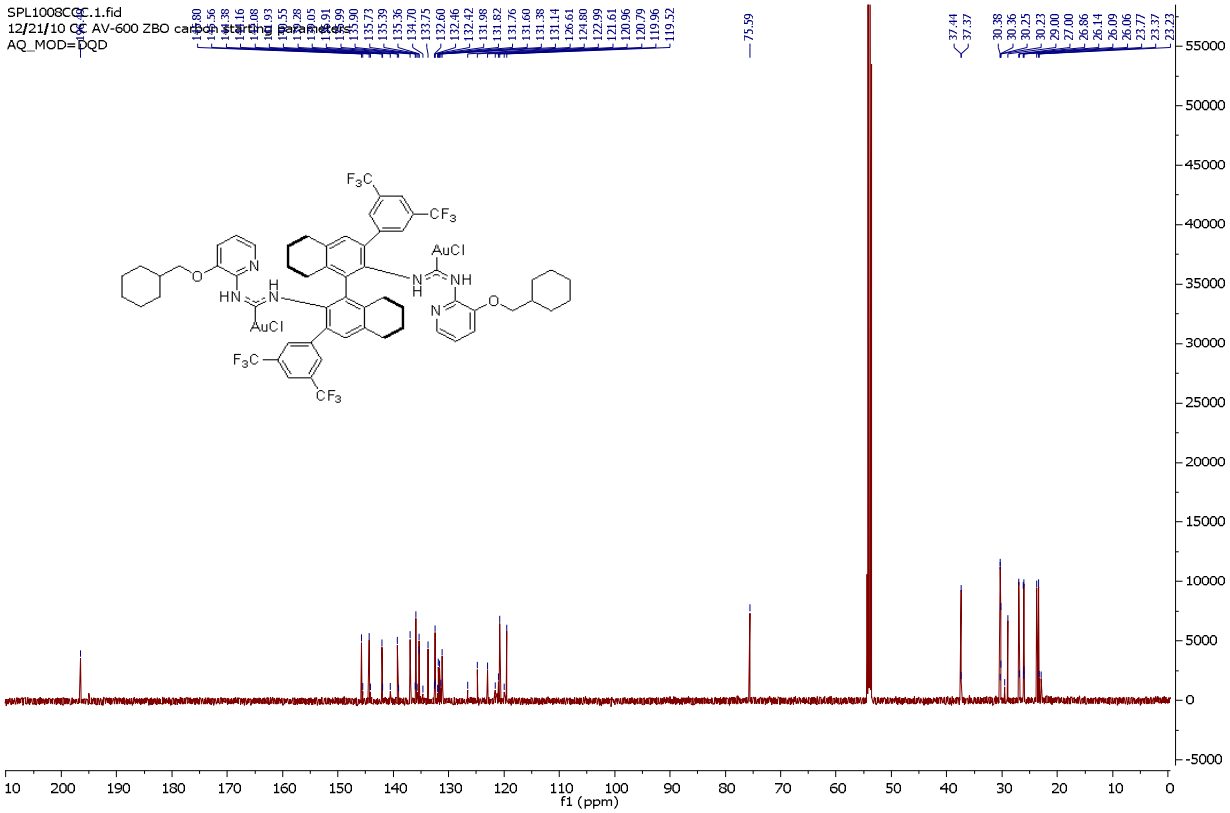
Complex L26*(AuCl)$_2$



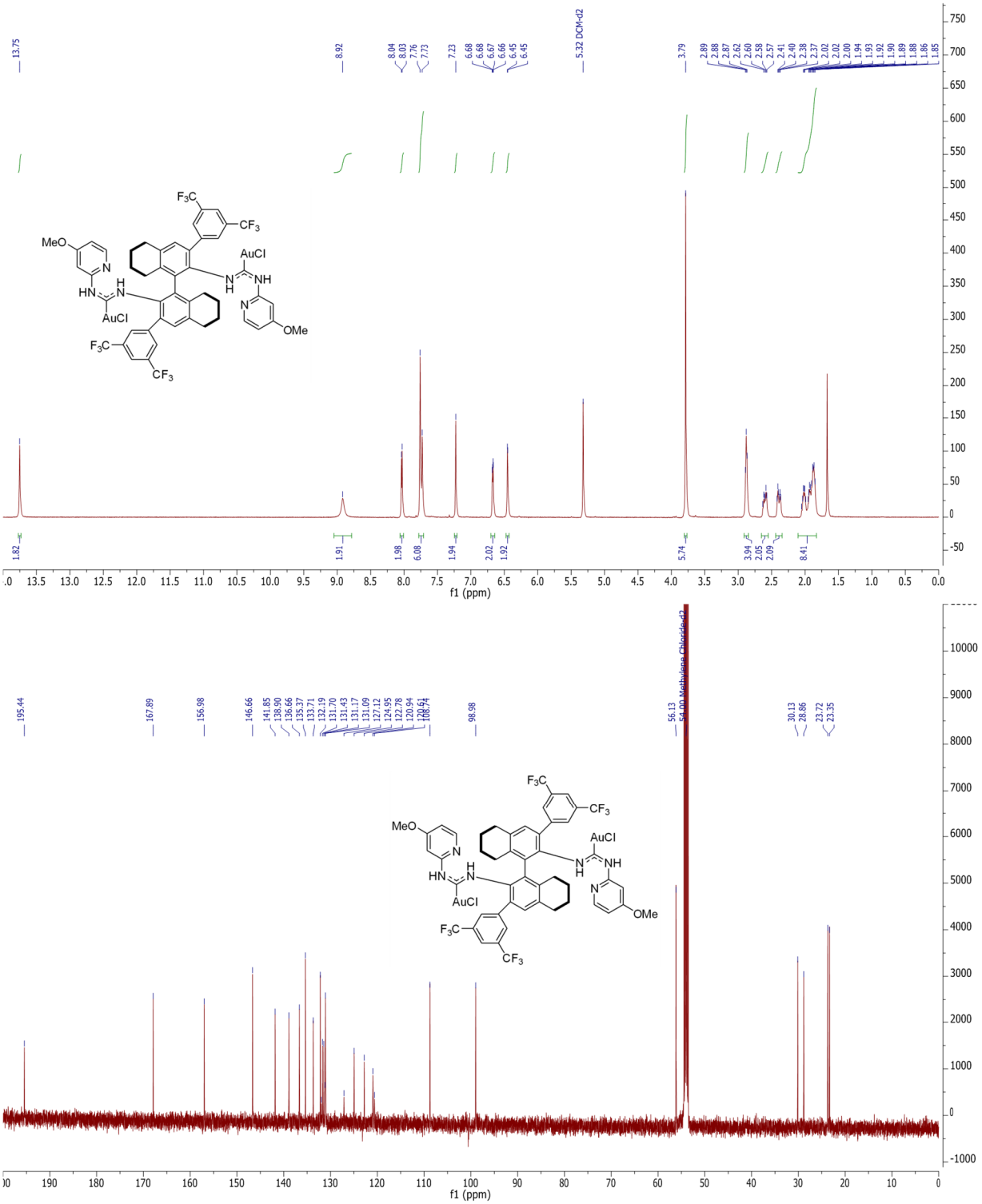


Complex L27*$(AuCl)_2$

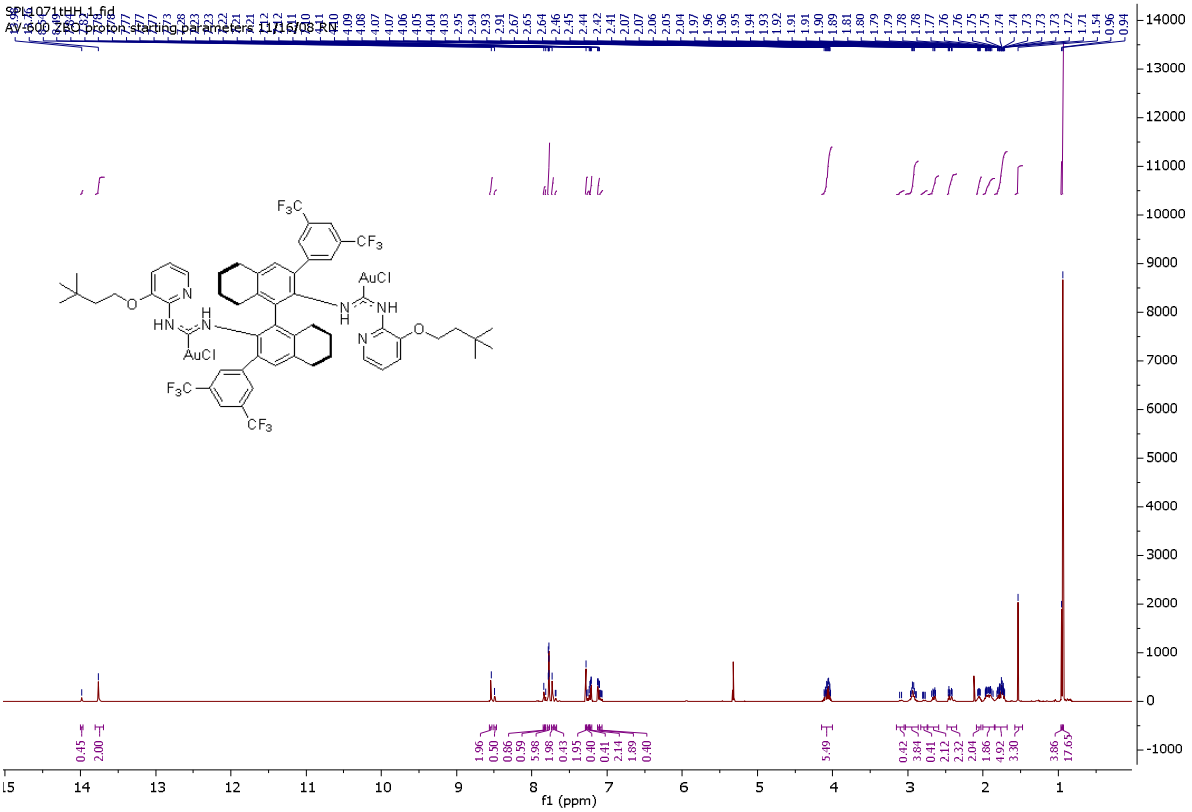


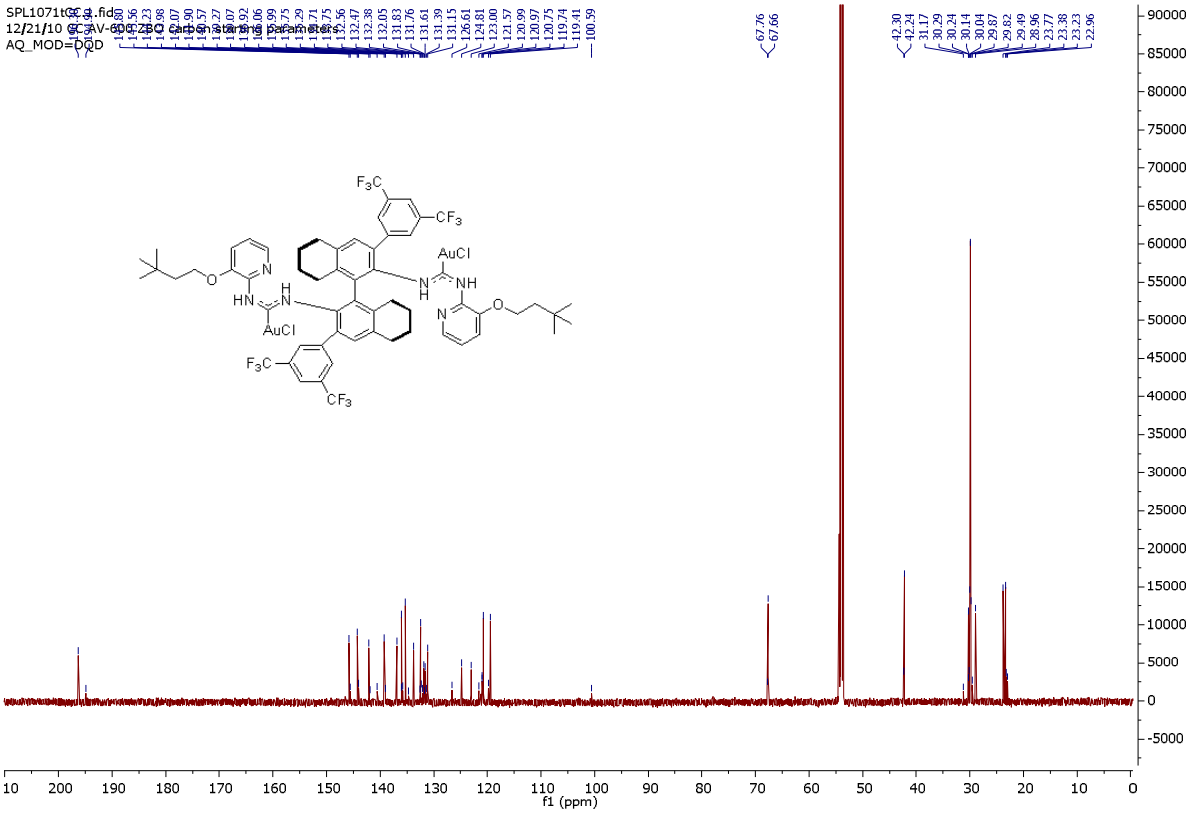


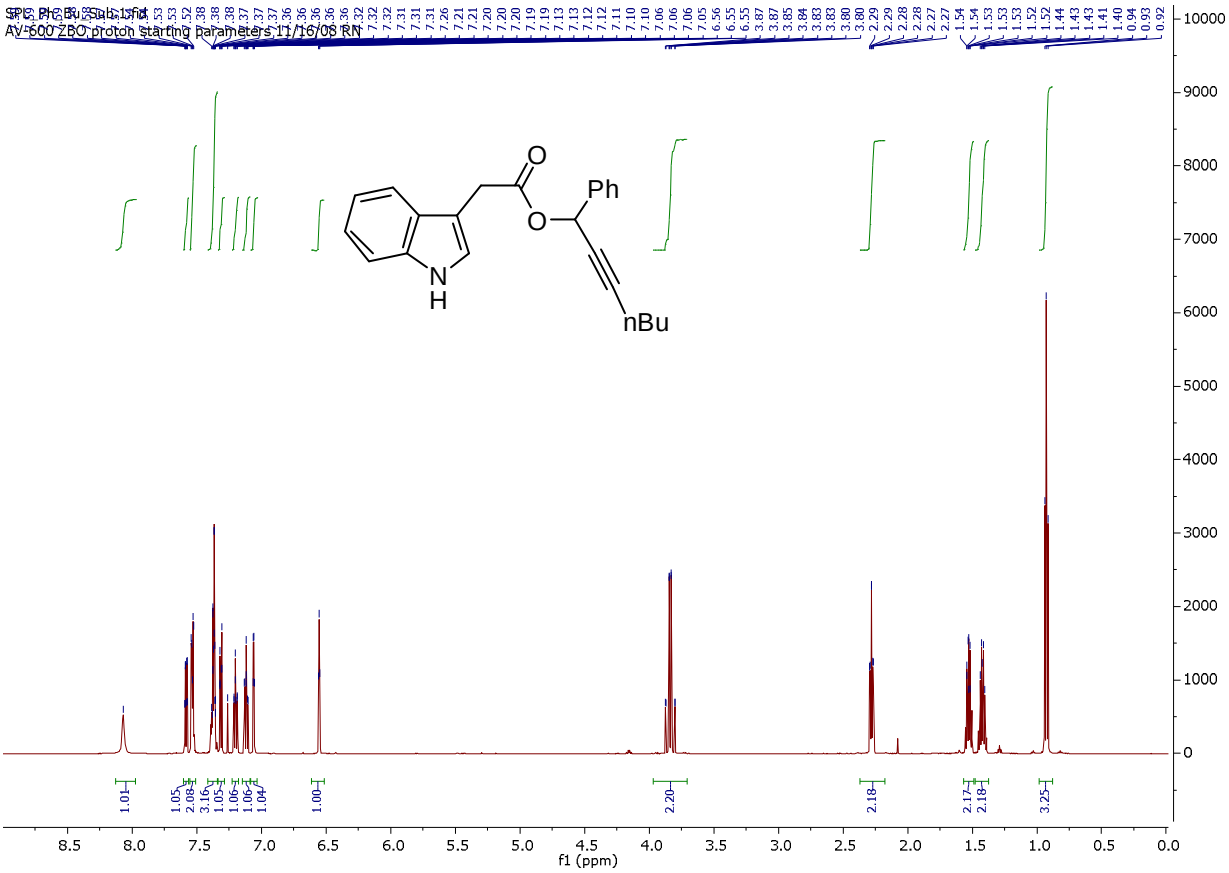
Complex L28*$(AuCl)_2$

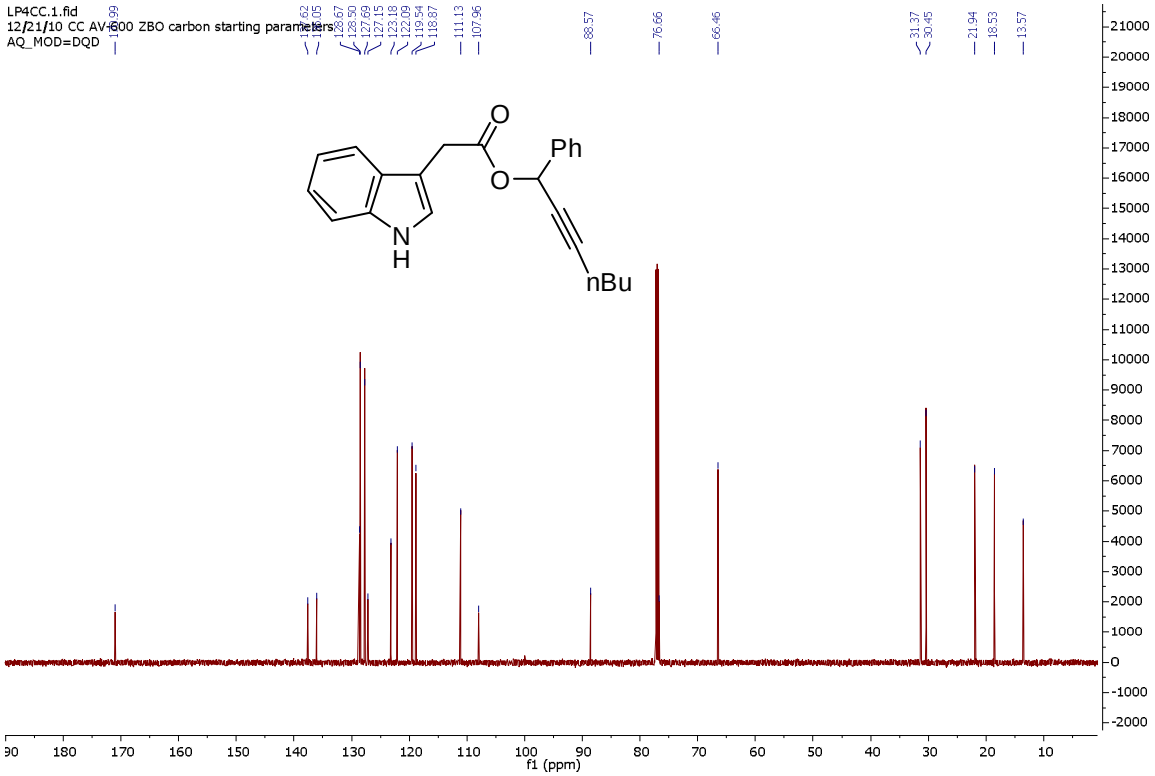


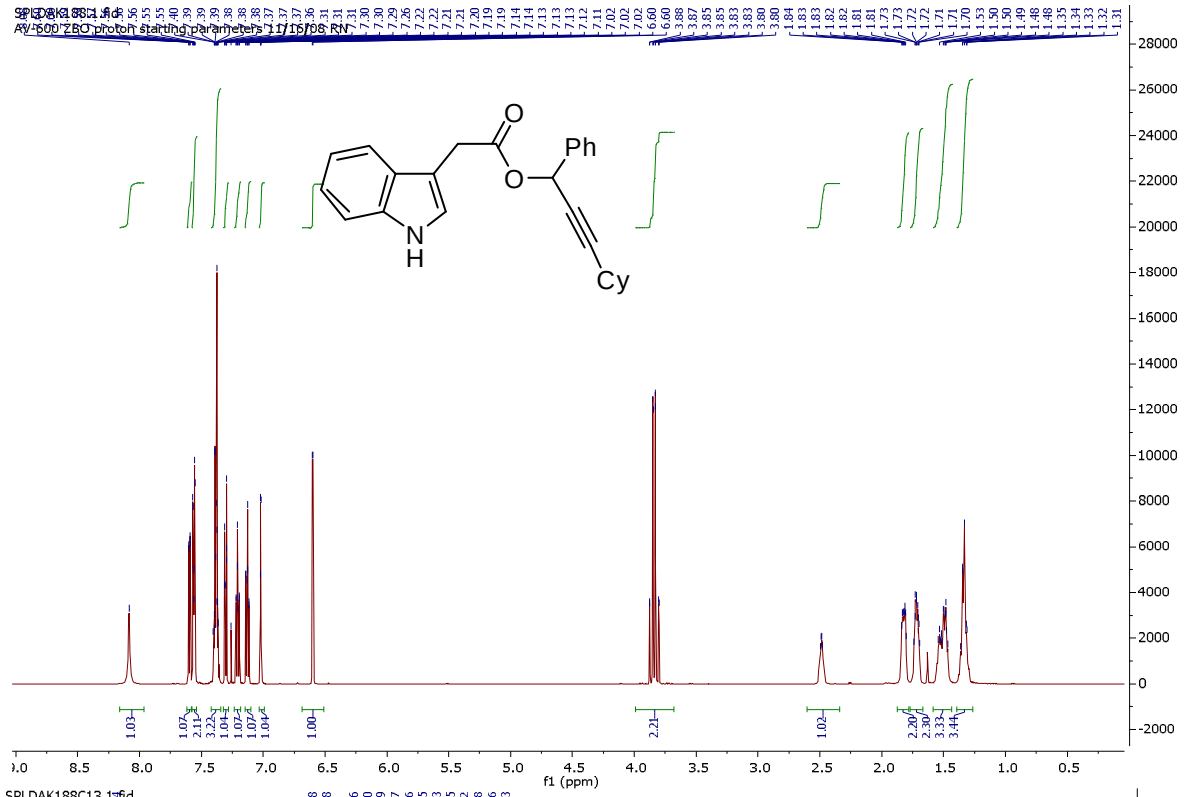
Complex L29*(AuCl)$_2$

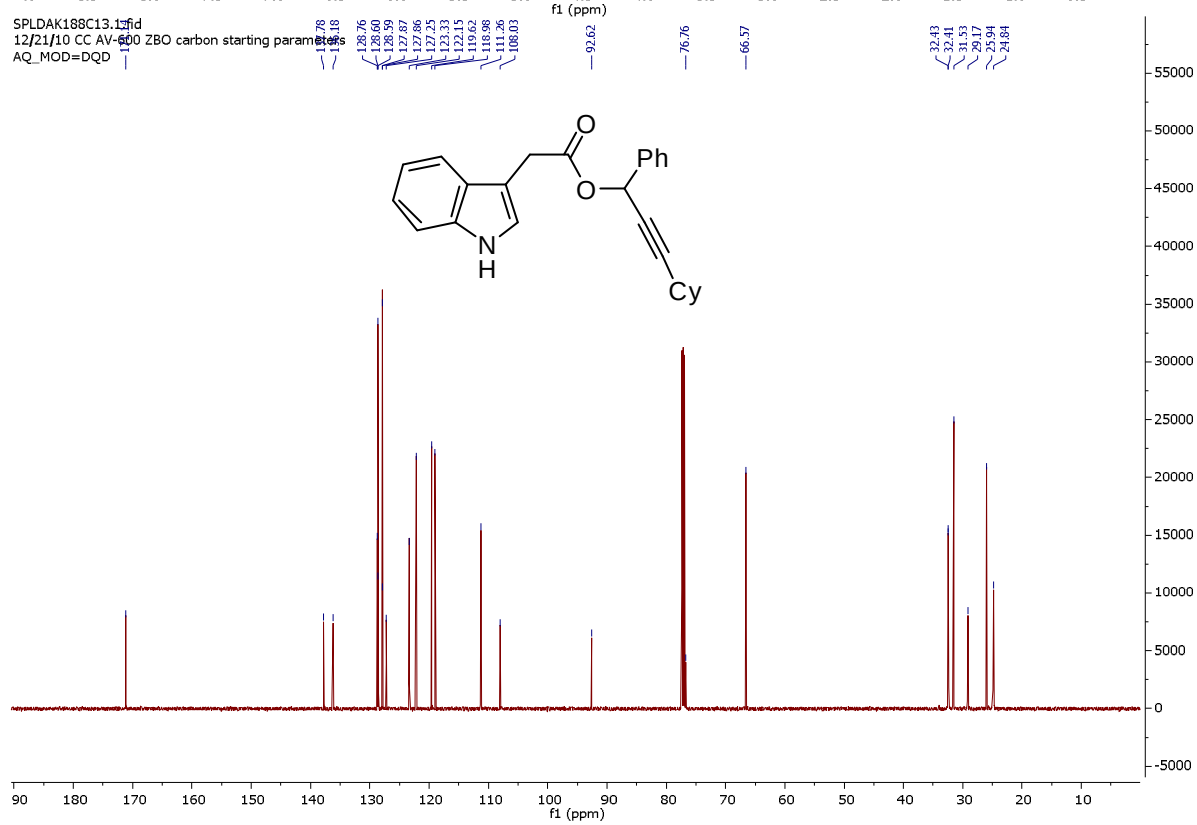


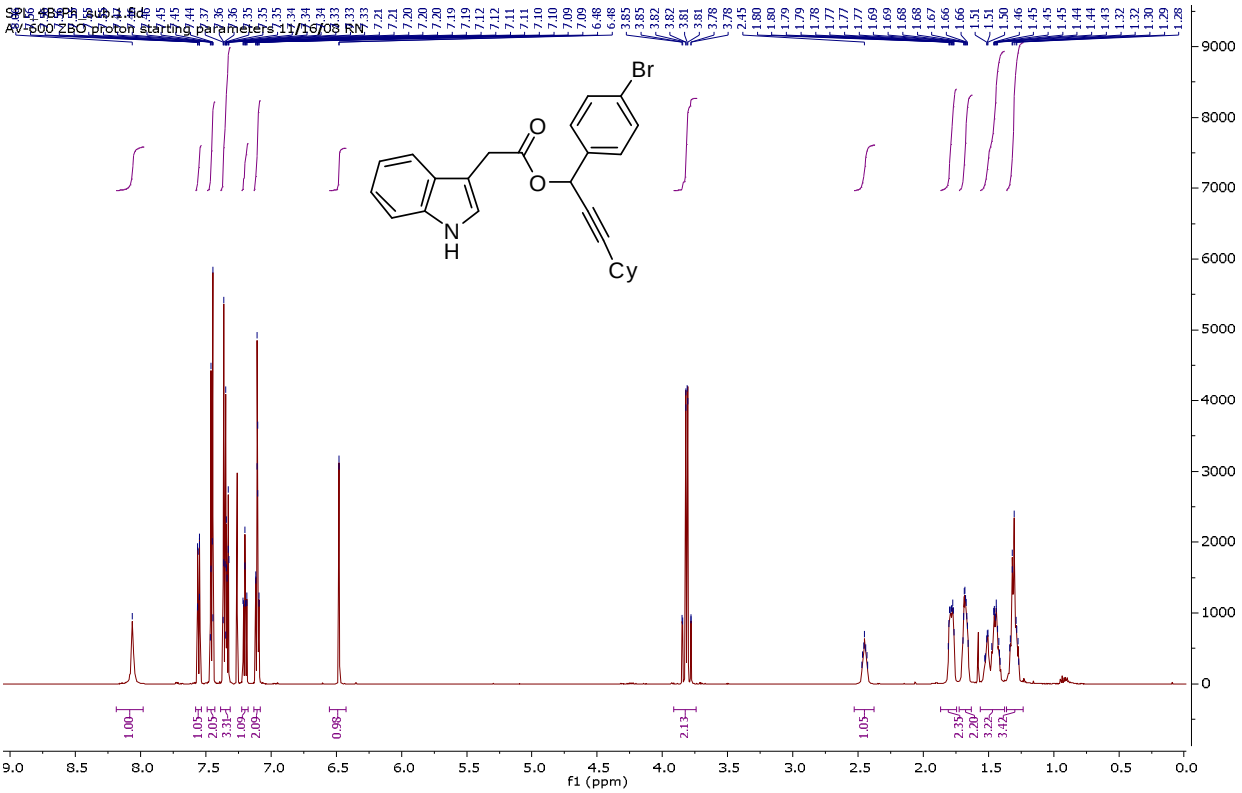


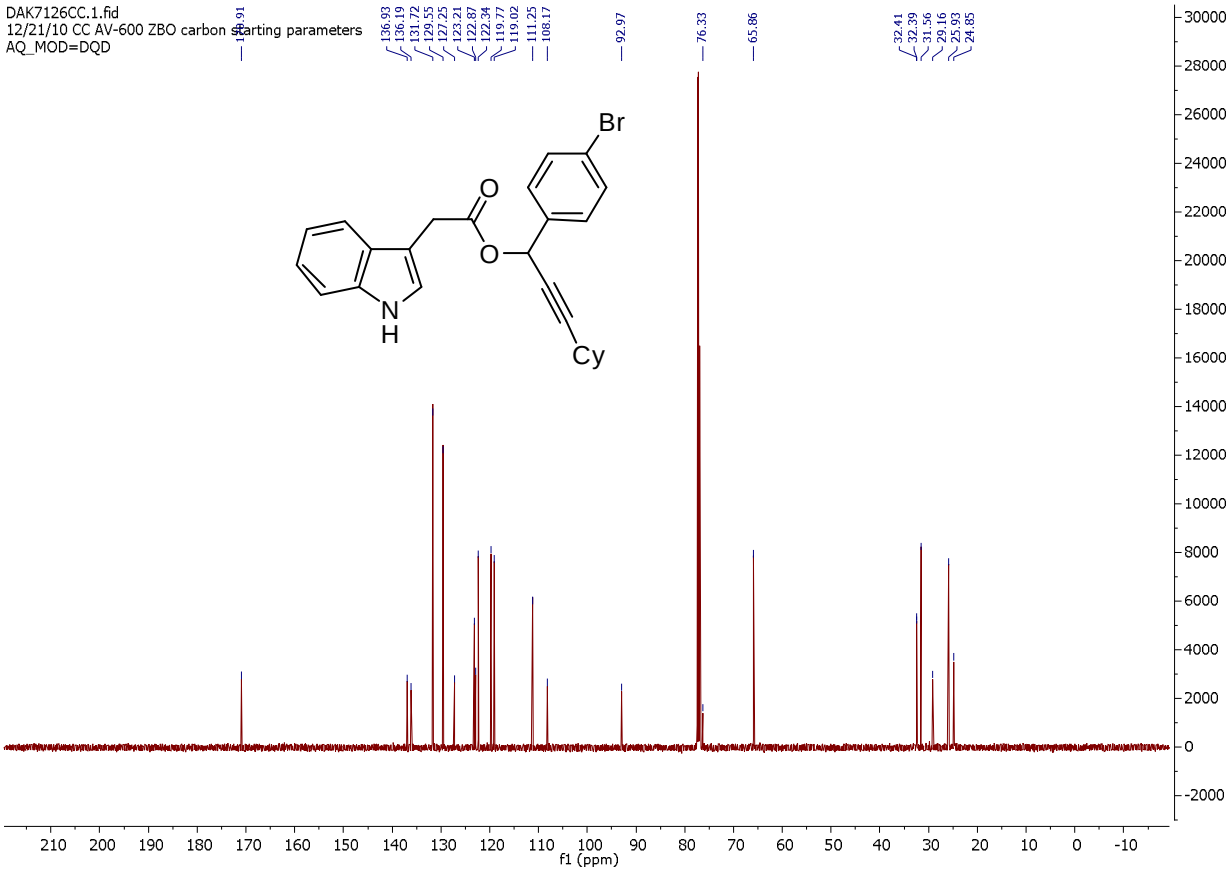

AV-600 ZBO proton starting parameters 11/16/08 RN
O
Ph
O
N
H
nBu
f1 (ppm)

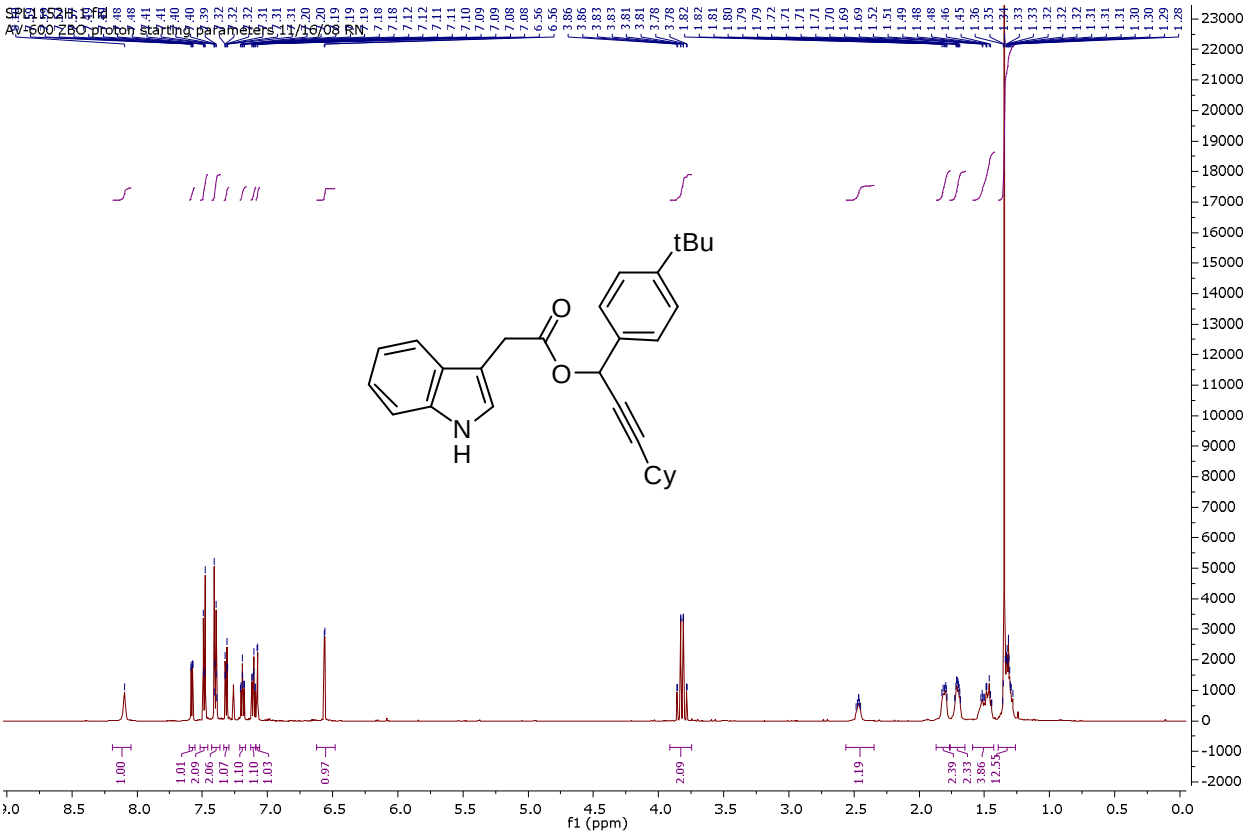

LP4CC.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
O
Ph
O
N
H
nBu
f1 (ppm)

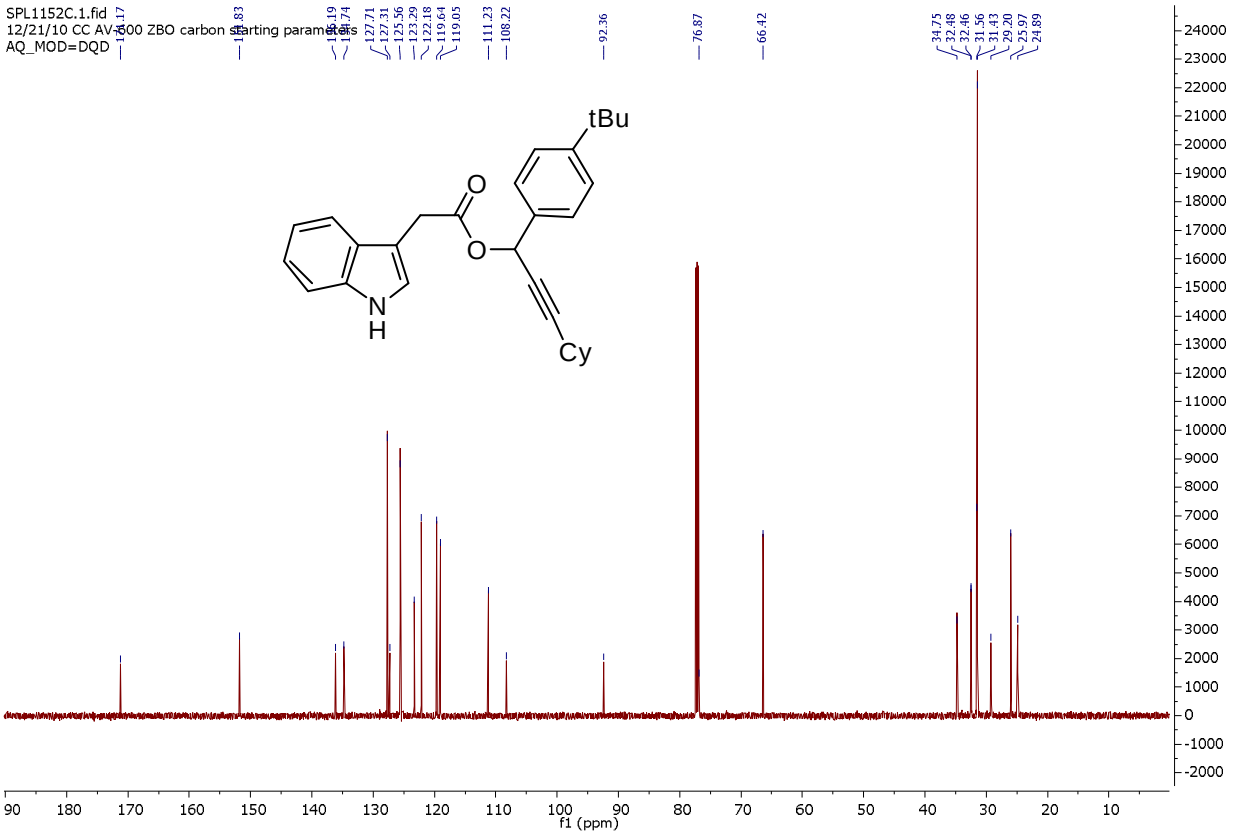

AV-500 ZBO proton starting parameters 11/15/08 RN
O
Ph
O
N
H
Cy
f1 (ppm)

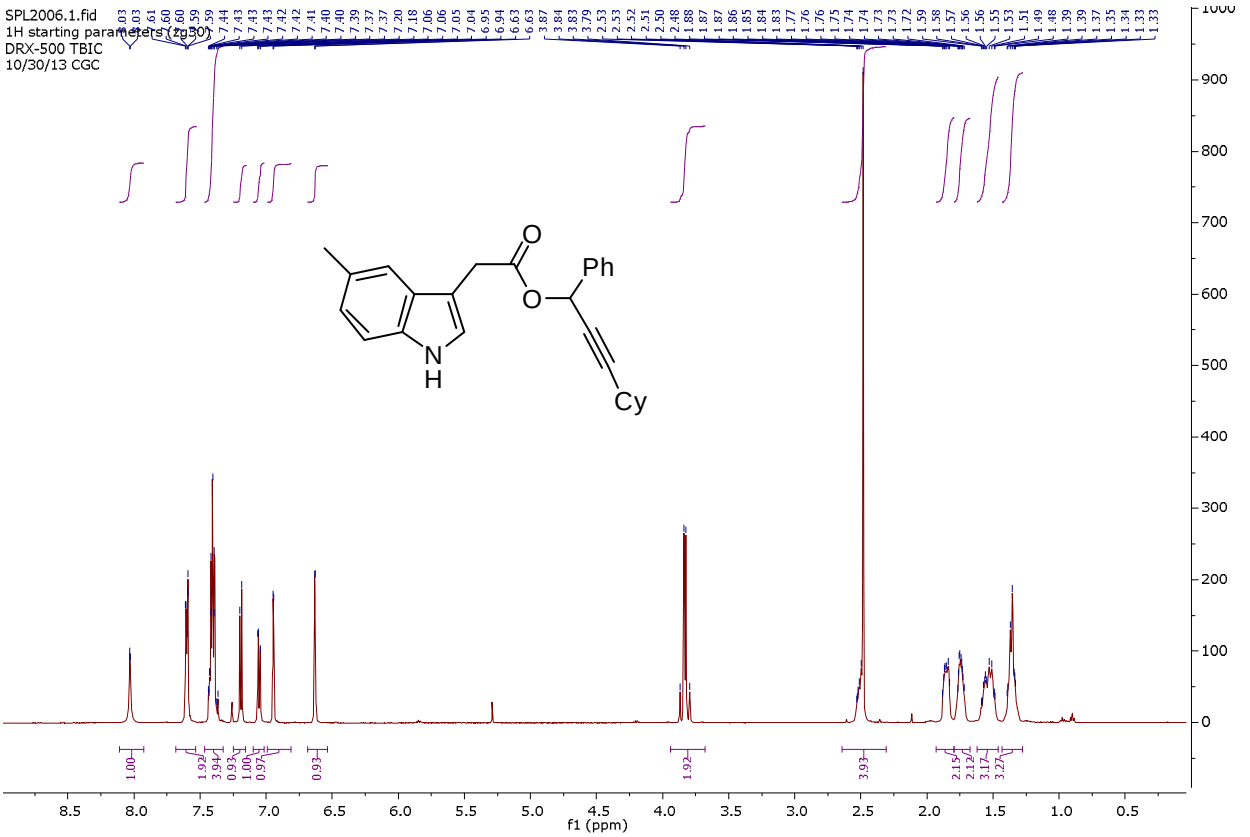

SPLDAK188C13.12.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
O
Ph
O
N
H
Cy
f1 (ppm)

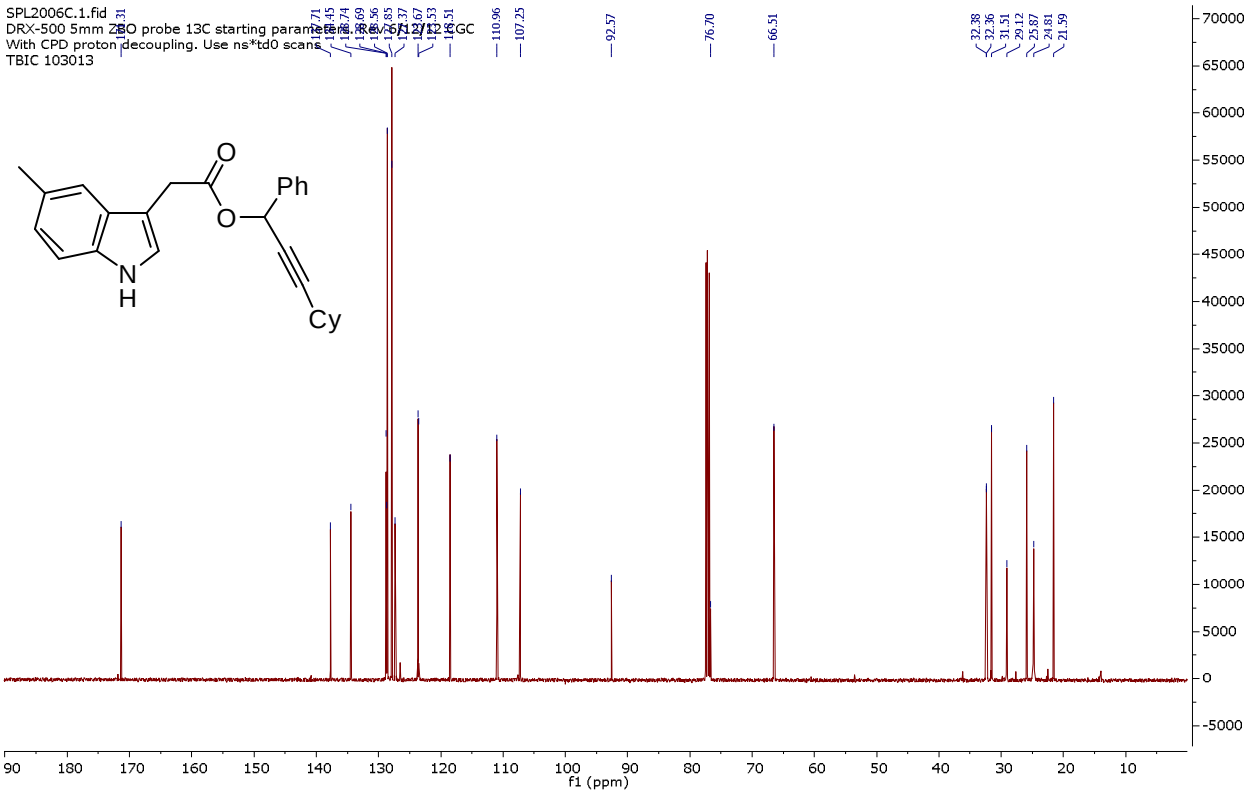

Br
O
O
N
H
Cy
f1 (ppm)

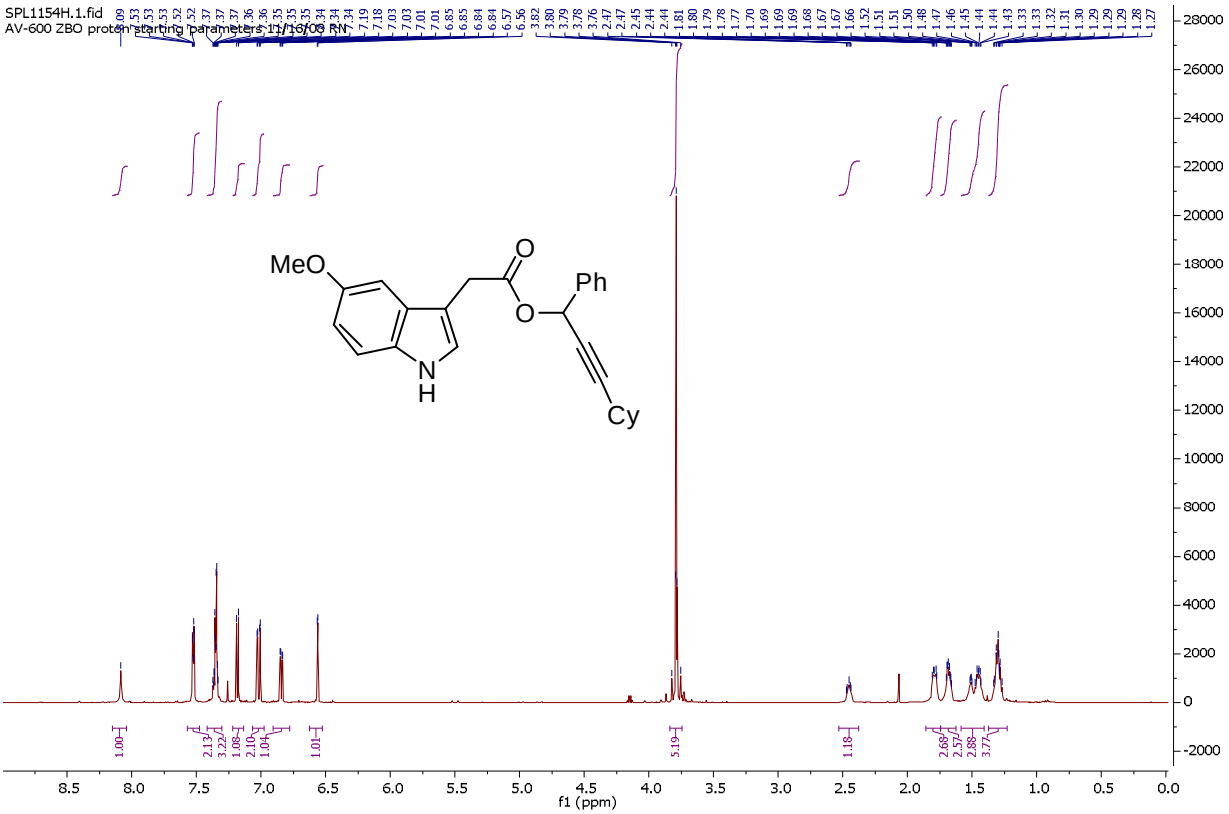

DAK7126CC.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
Br
O
O
N
H
Cy
f1 (ppm)

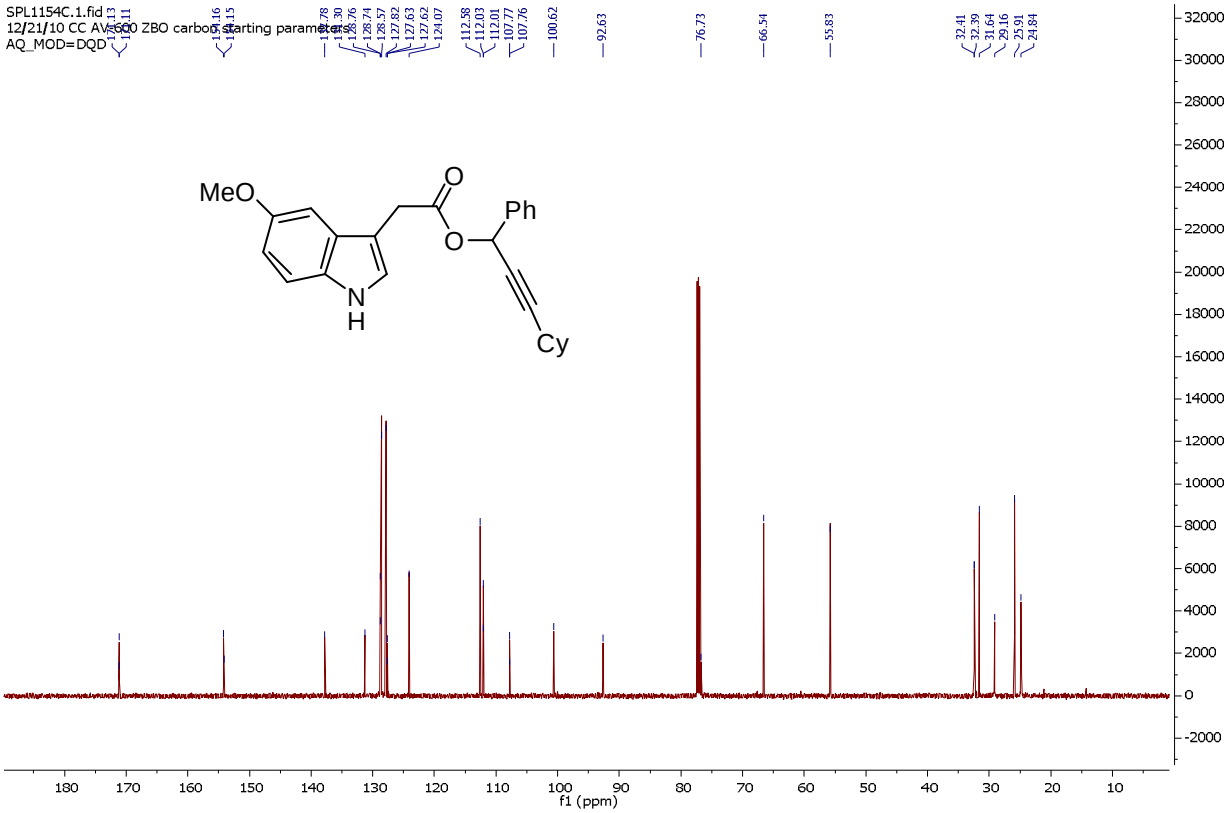

tBu
O
O
N
H
Cy
f1 (ppm)

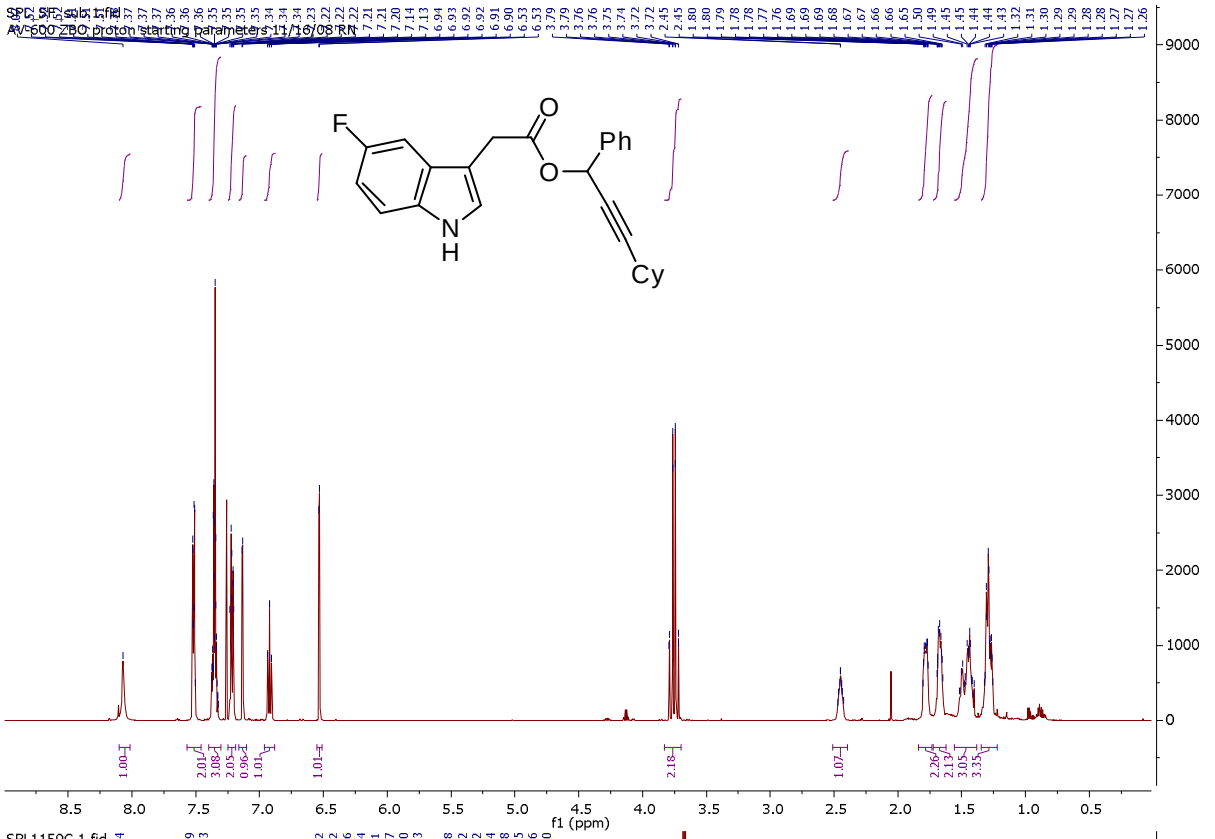

SPL1152C.1.fid
12/21/10 CC AV-500 ZBO carbon starting parameters
AQ_MOD=DQD
tBu
O
O
N
H
Cy
f1 (ppm)

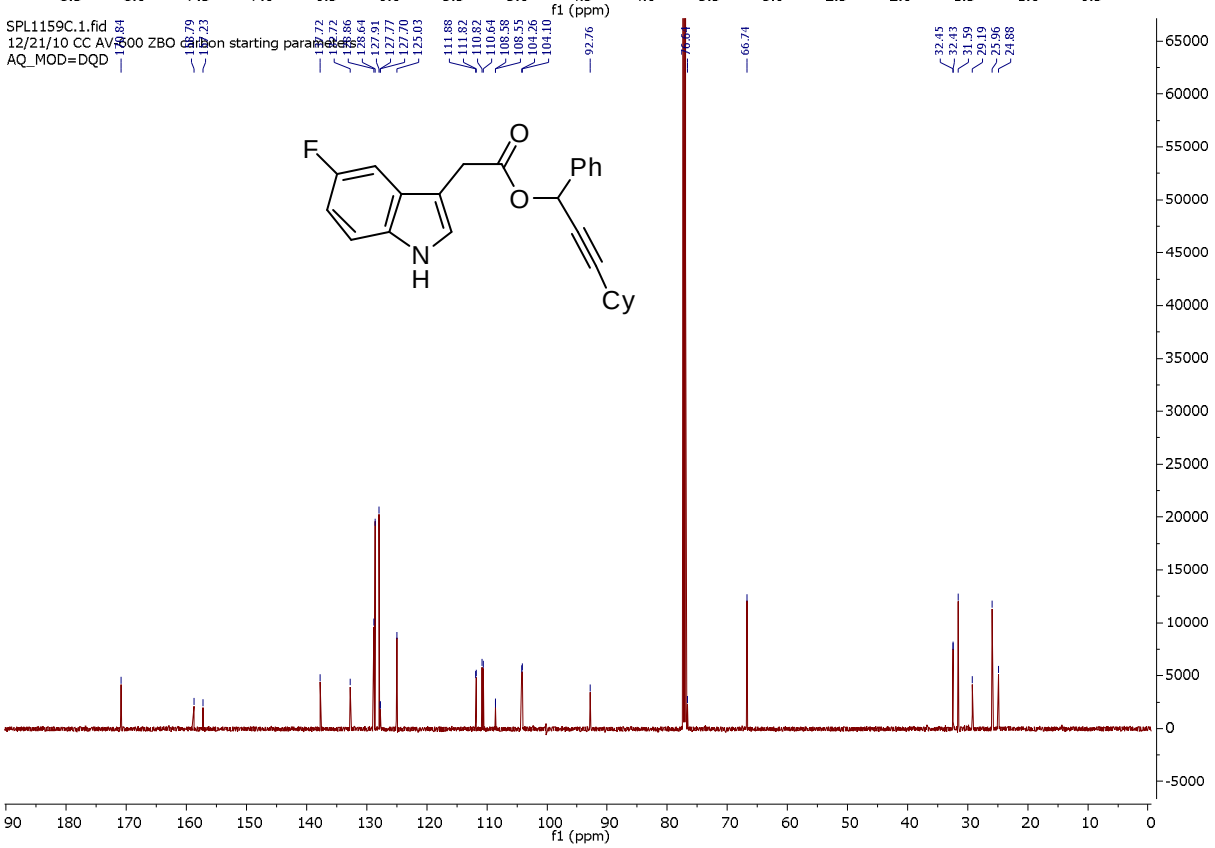

SPL2006.1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
Ph
O
N
H
Cy
f1 (ppm)

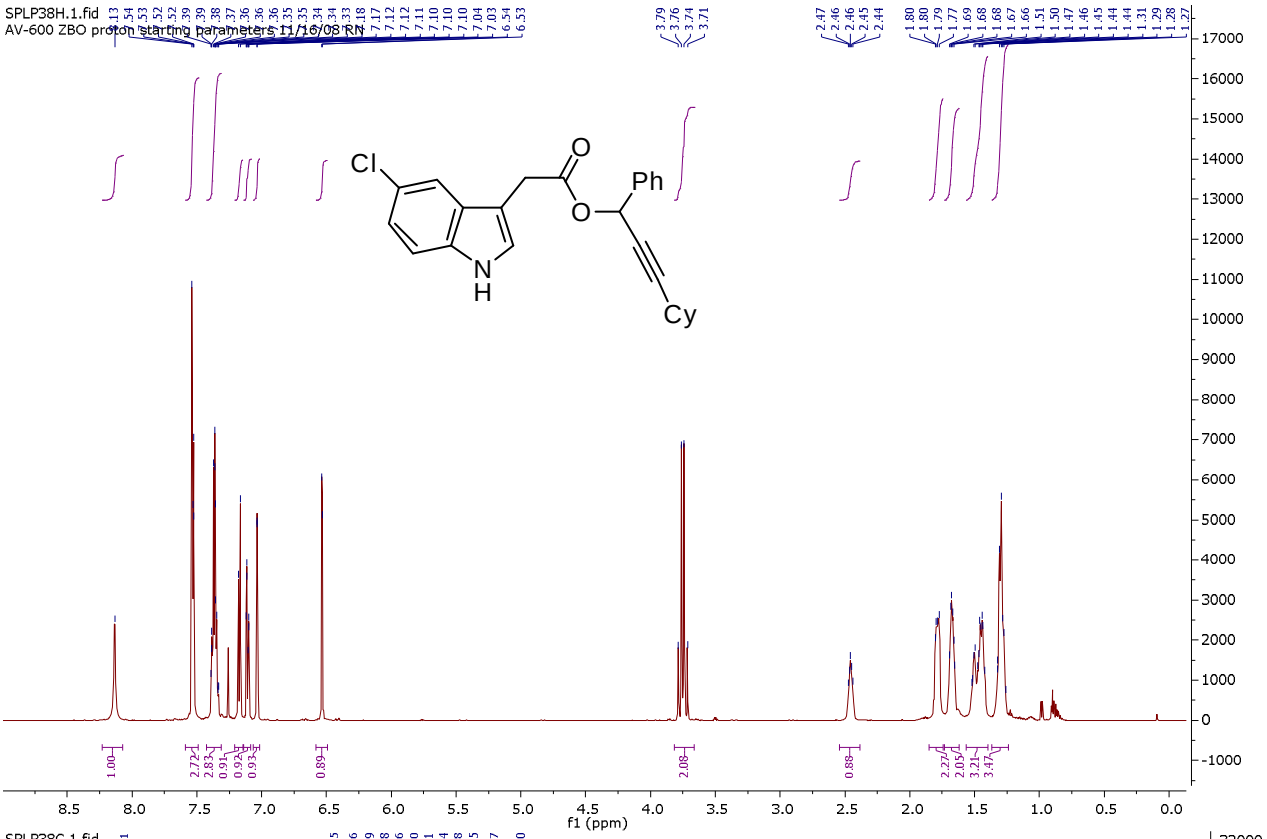

SPL2006C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters (zgpg30) 6/11/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
O
Ph
O
N
H
Cy
f1 (ppm)

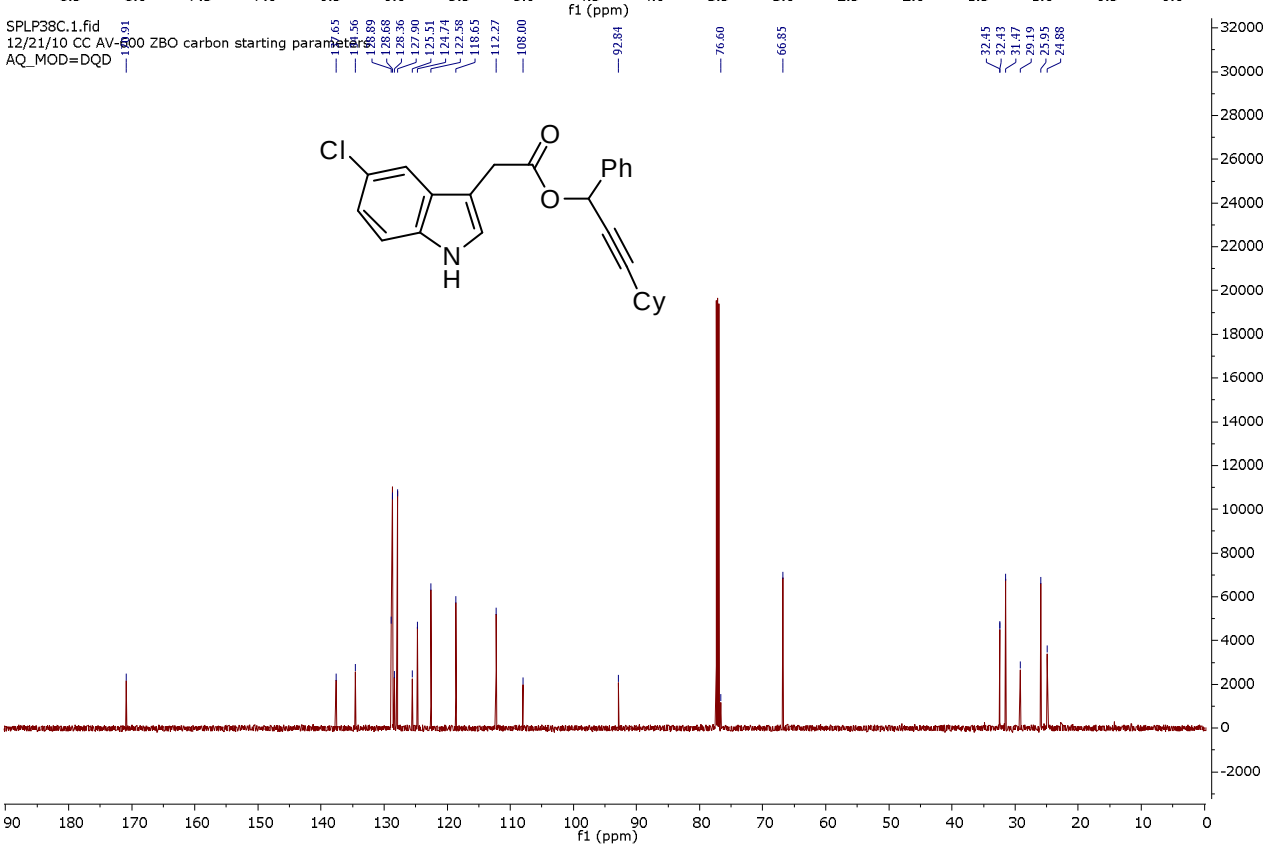

SPL1154H.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN
MeO
O
O
Ph
N
H
Cy
f1 (ppm)

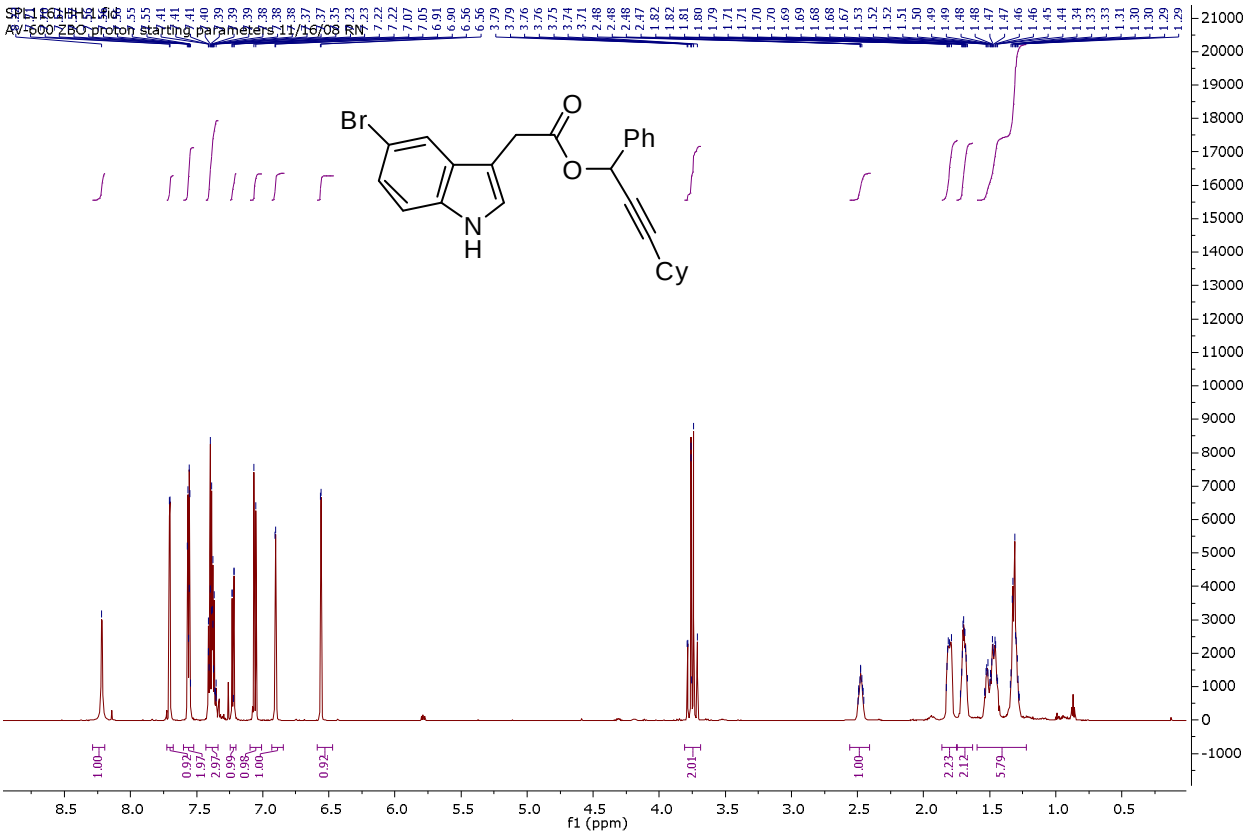

SPL1154C.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
MeO
O
O
Ph
N
H
Cy
f1 (ppm)

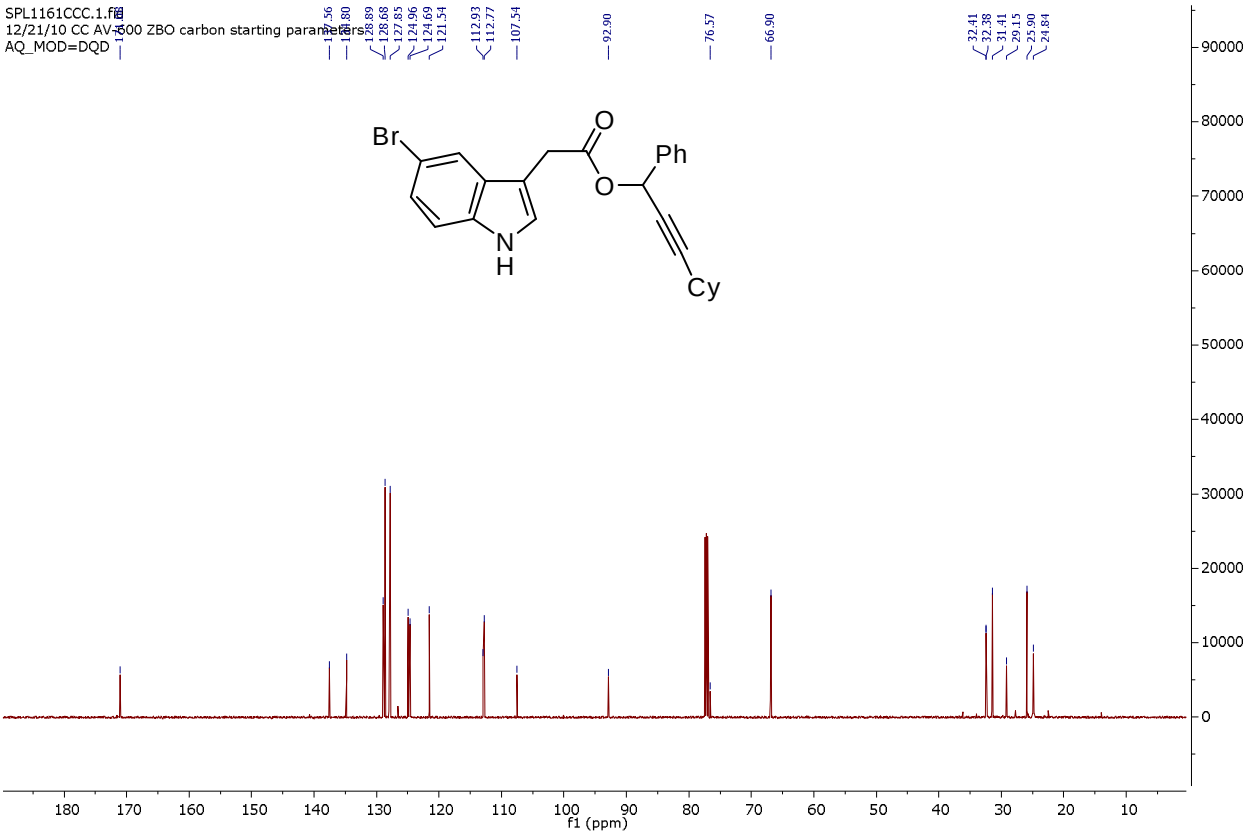

F
O
O
Ph
N
H
Cy
f1 (ppm)

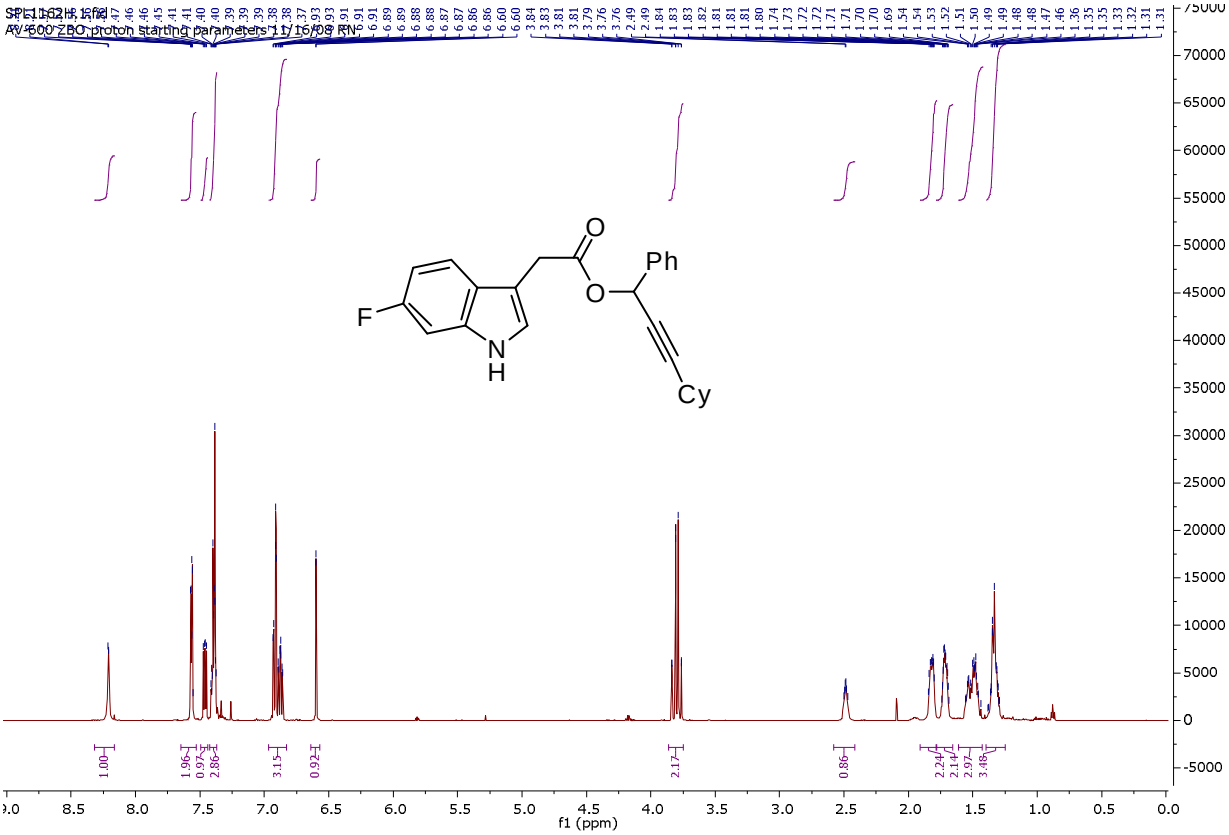

SPL1159C.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
F
O
O
Ph
N
H
Cy
f1 (ppm)

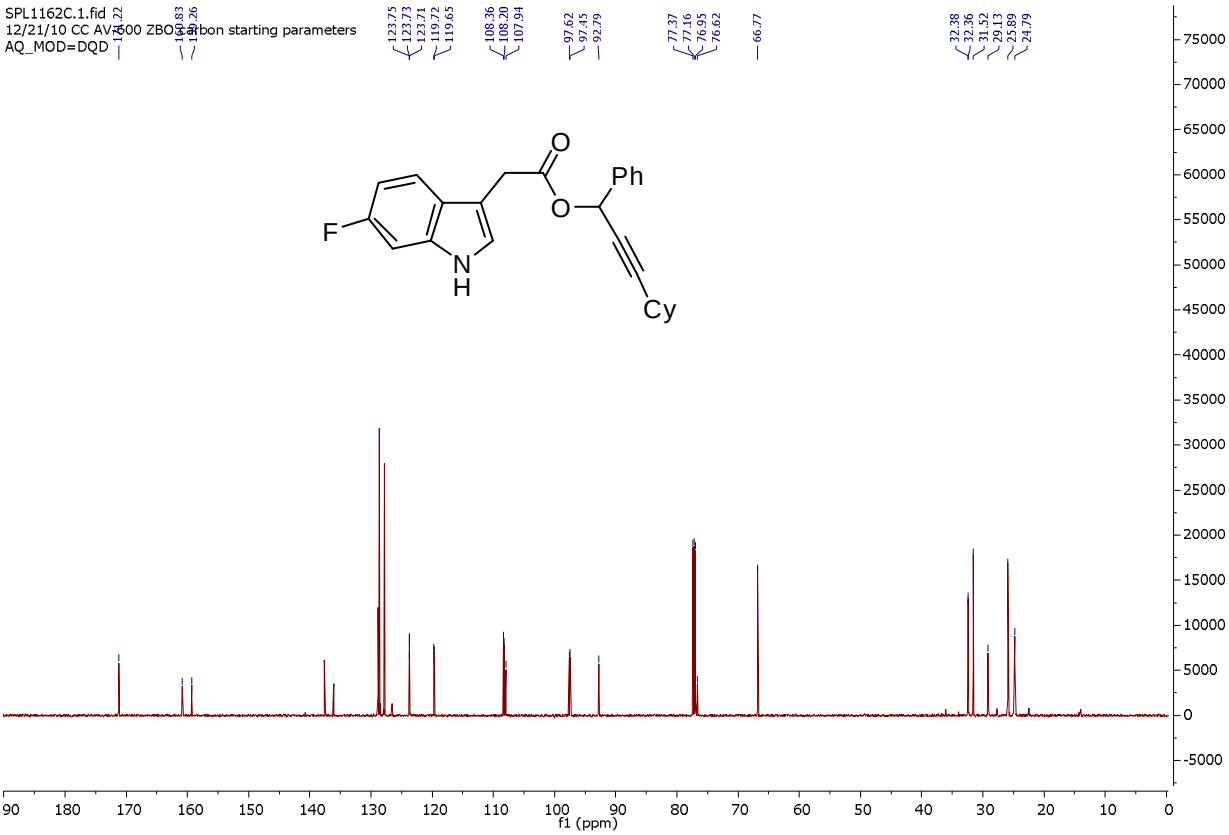

SPLP38H.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN
Cl
O
O
Ph
N
H
Cy
f1 (ppm)

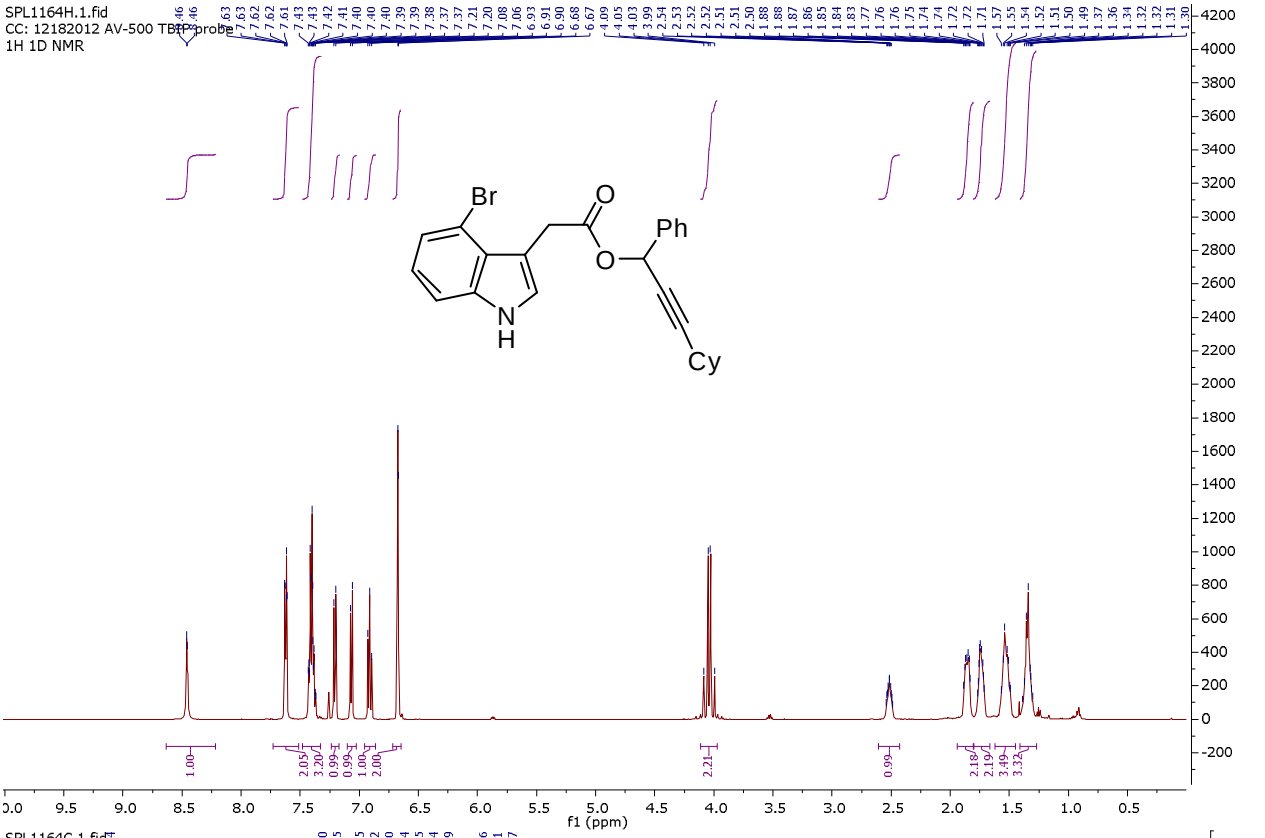

SPLP38C.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
Cl
O
O
Ph
N
H
Cy
f1 (ppm)

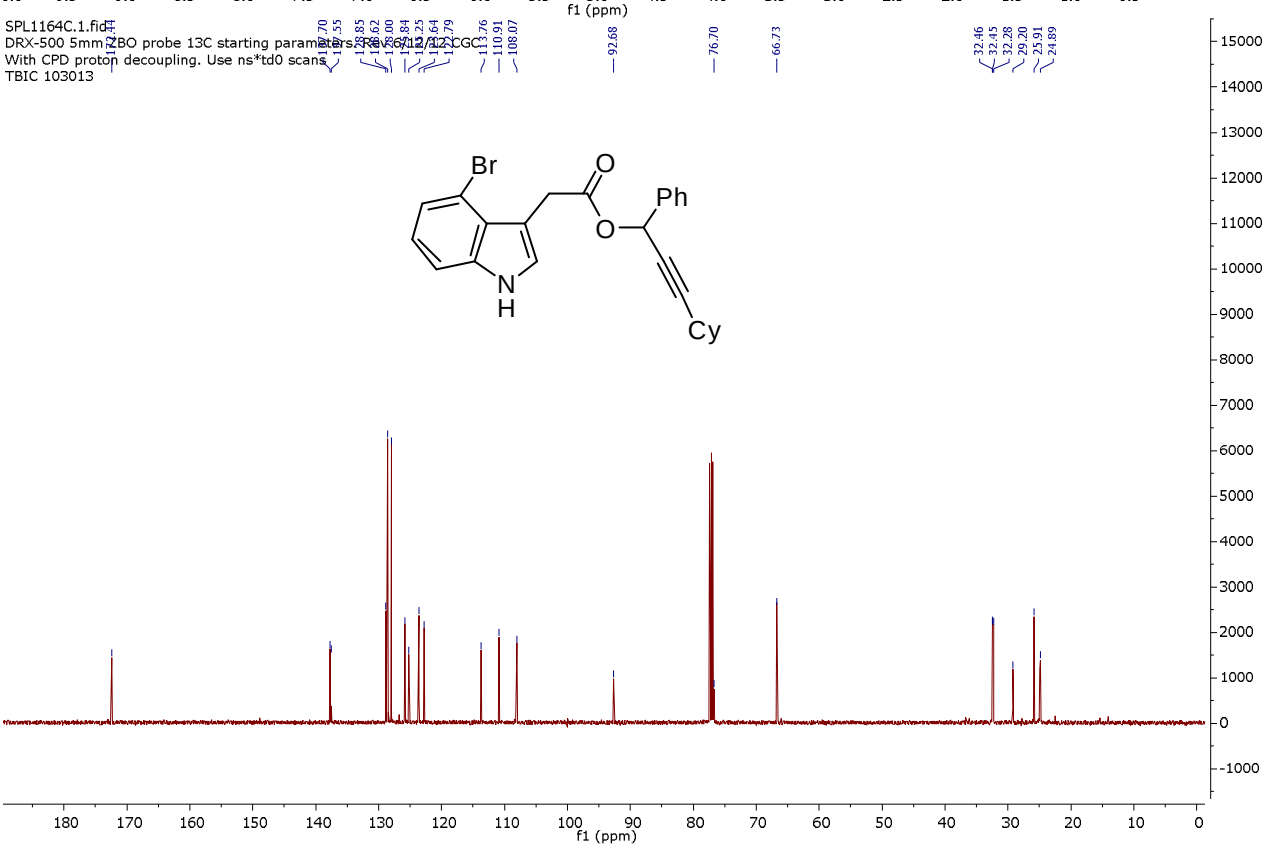

SPL1161H.1.fid
AV-500 ZBO proton starting parameters 11/16/08 RM
Br
O
Ph
O
N
H
Cy
f1 (ppm)

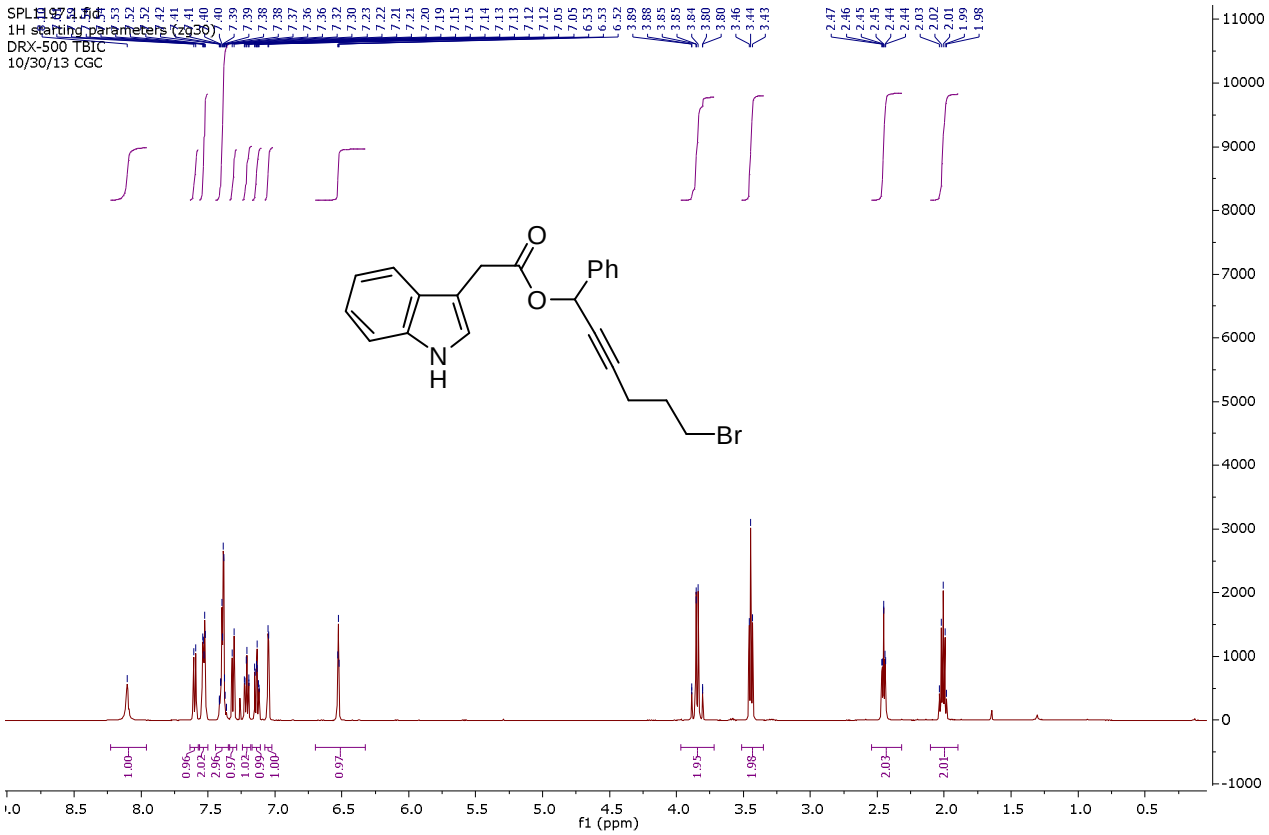

SPL1161CCC.1.fid
12/21/10 CC AV-500 ZBO carbon starting parameters
AQ_MOD=DQD
Br
O
Ph
O
N
H
Cy
f1 (ppm)

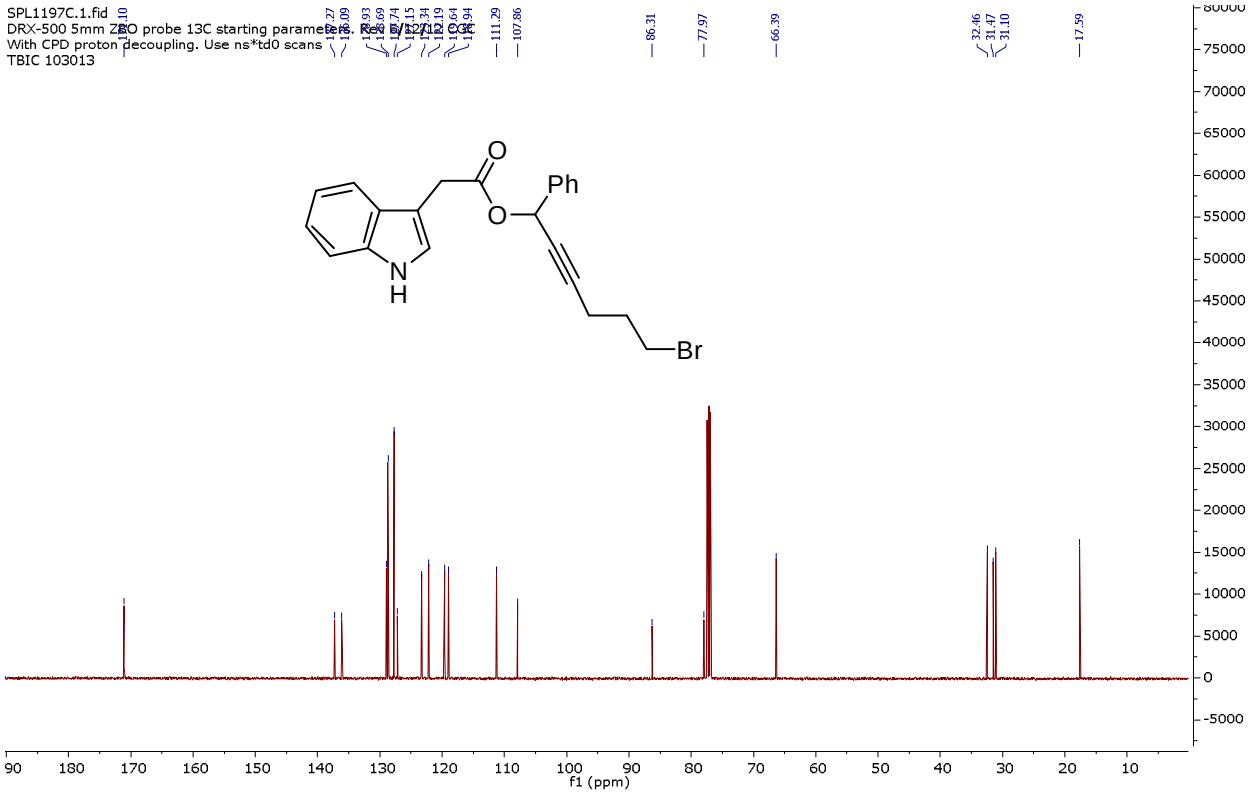

F
N
H
O
O
Ph
Cy
f1 (ppm)

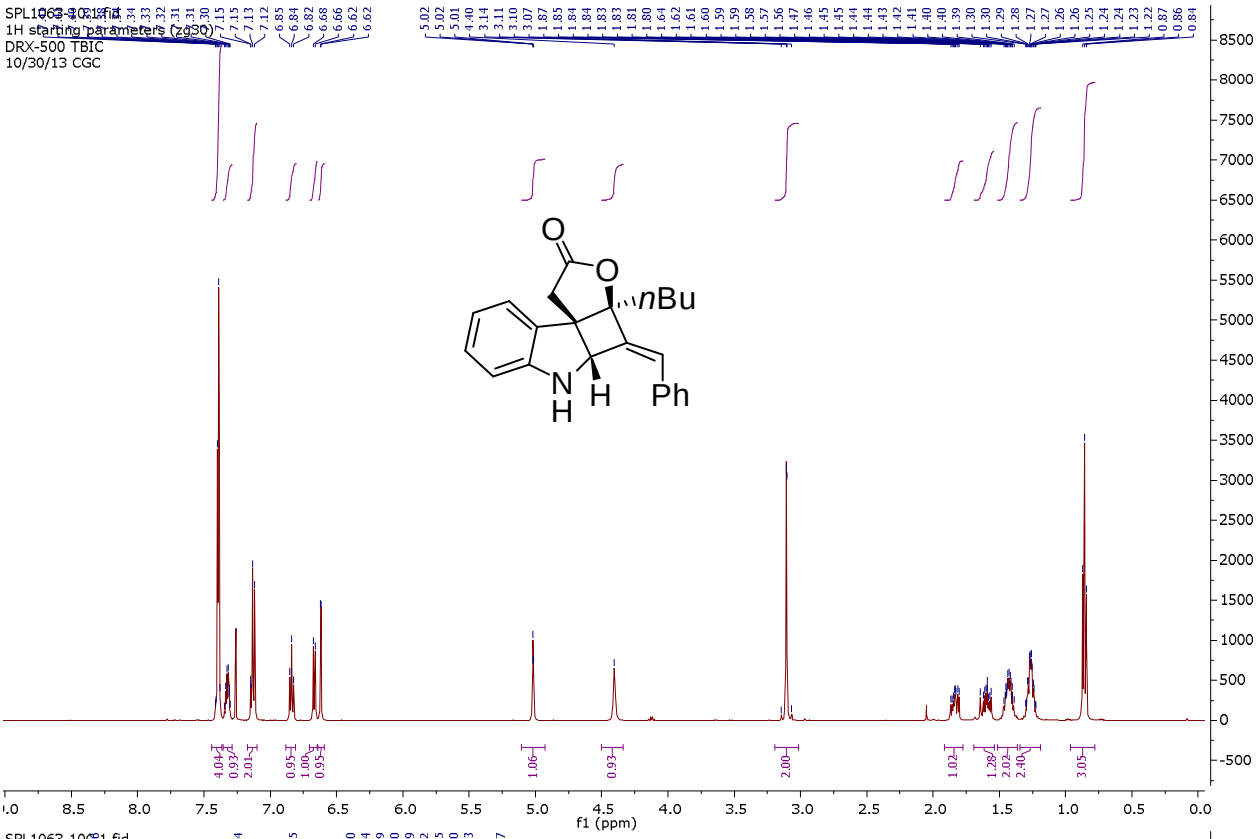

SPL1162C.1.fid
12/21/10 CC AV-500 ZBO carbon starting parameters
AQ_MOD=DQD
F
N
H
O
O
Ph
Cy
f1 (ppm)

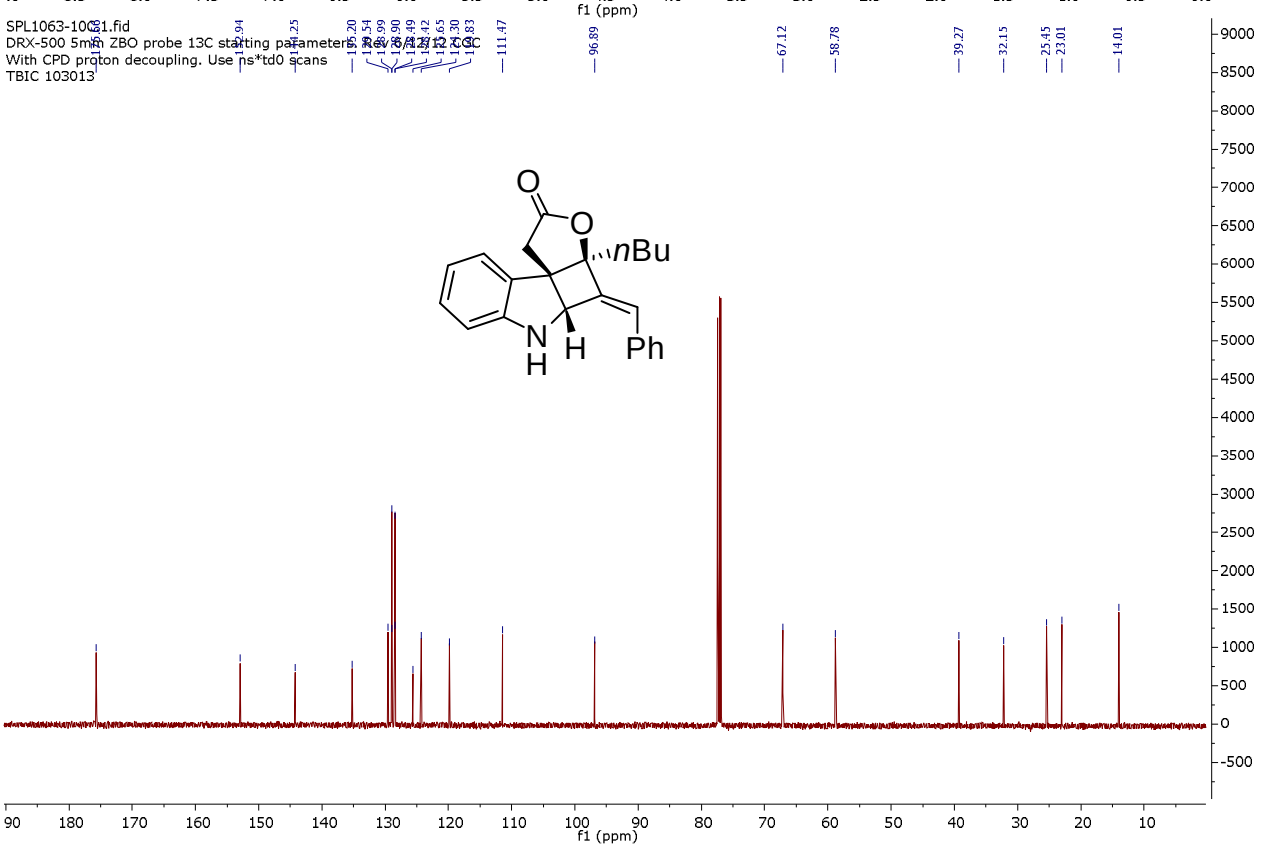

SPL1164H.1.fid
CC: 12182012 AV-500 TBIP probe
1H 1D NMR
Br
O
Ph
O
N
H
Cy
f1 (ppm)

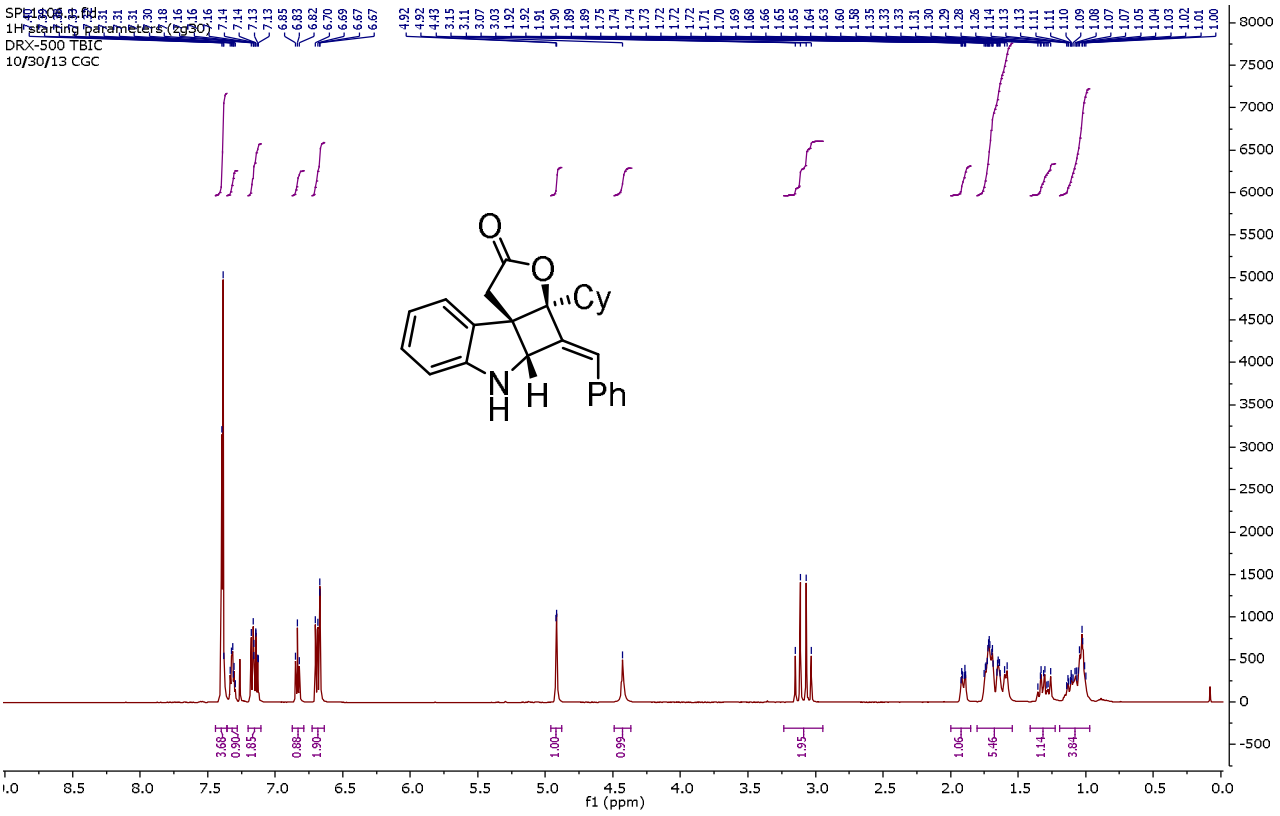

SPL1164C.1.fid
DRX-500 5mm PABBO probe 13C starting parameters zgdc30 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
Br
O
Ph
O
N
H
Cy
f1 (ppm)

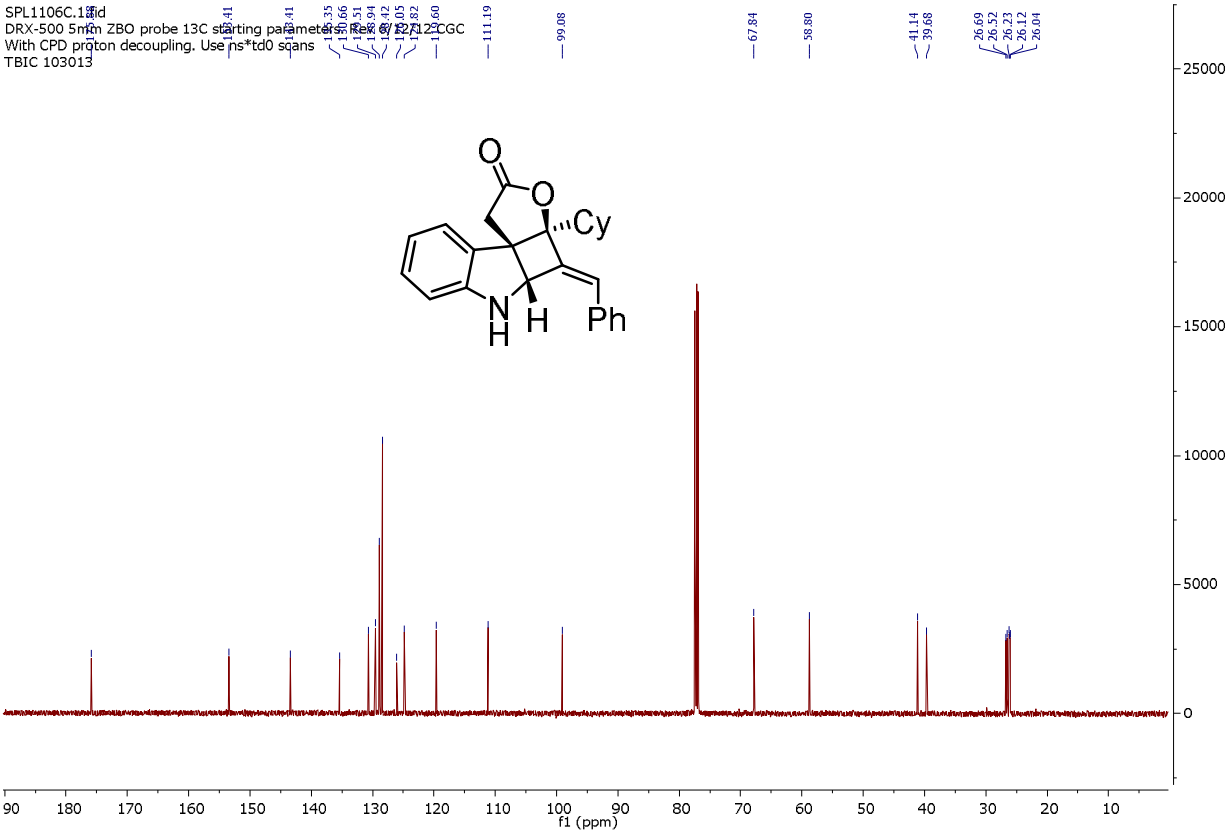

SPL1197.1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
Ph
O
N
H
Br
f1 (ppm)

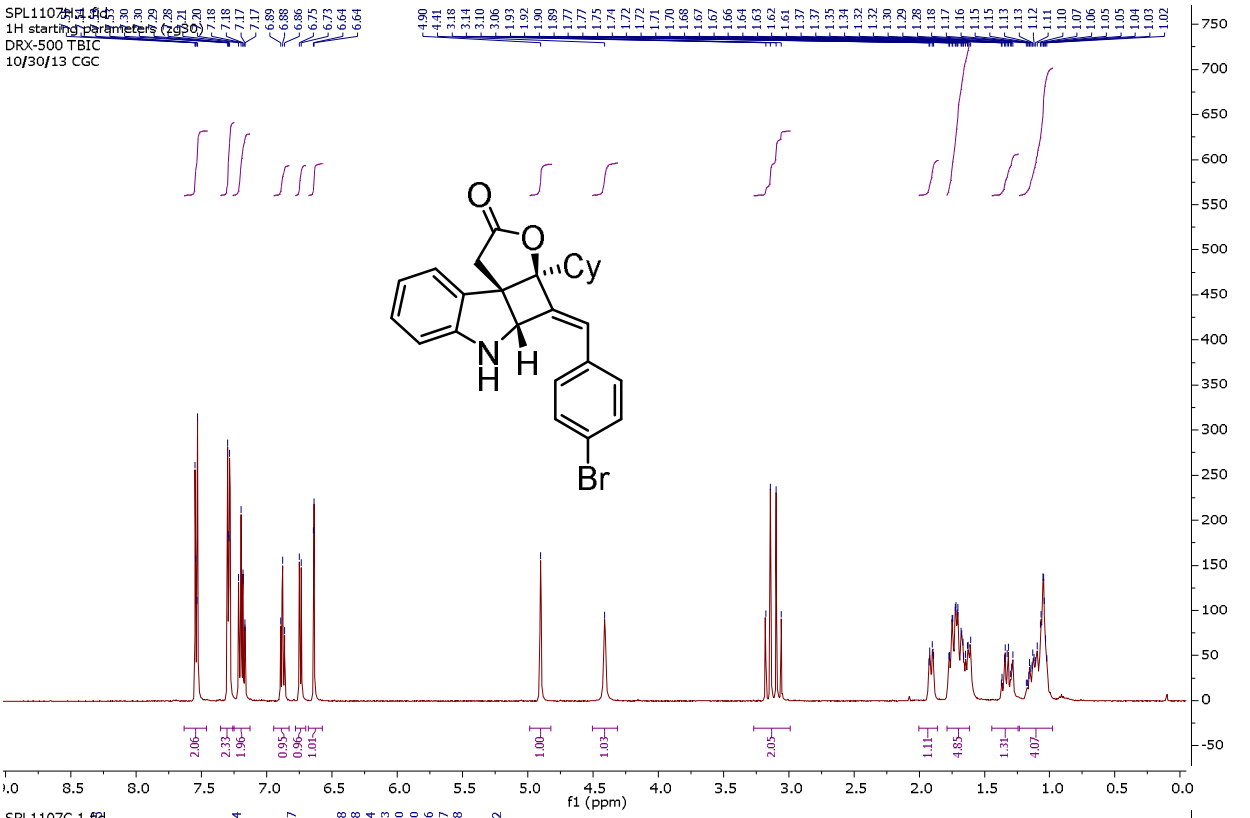

SPL1197C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
O
Ph
O
N
H
Br
f1 (ppm)

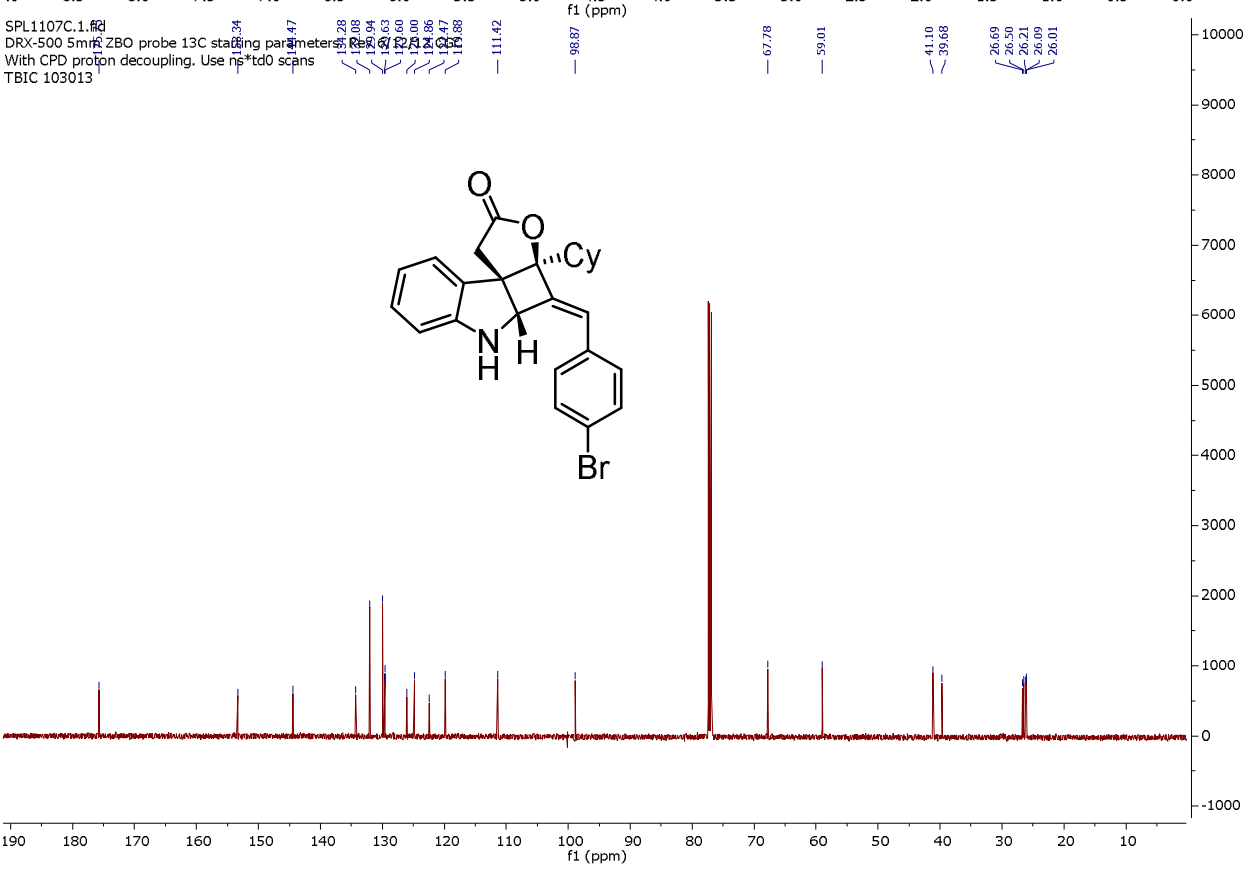

SPL1063-10C1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
O
nBu
N
H
H
Ph
f1 (ppm)

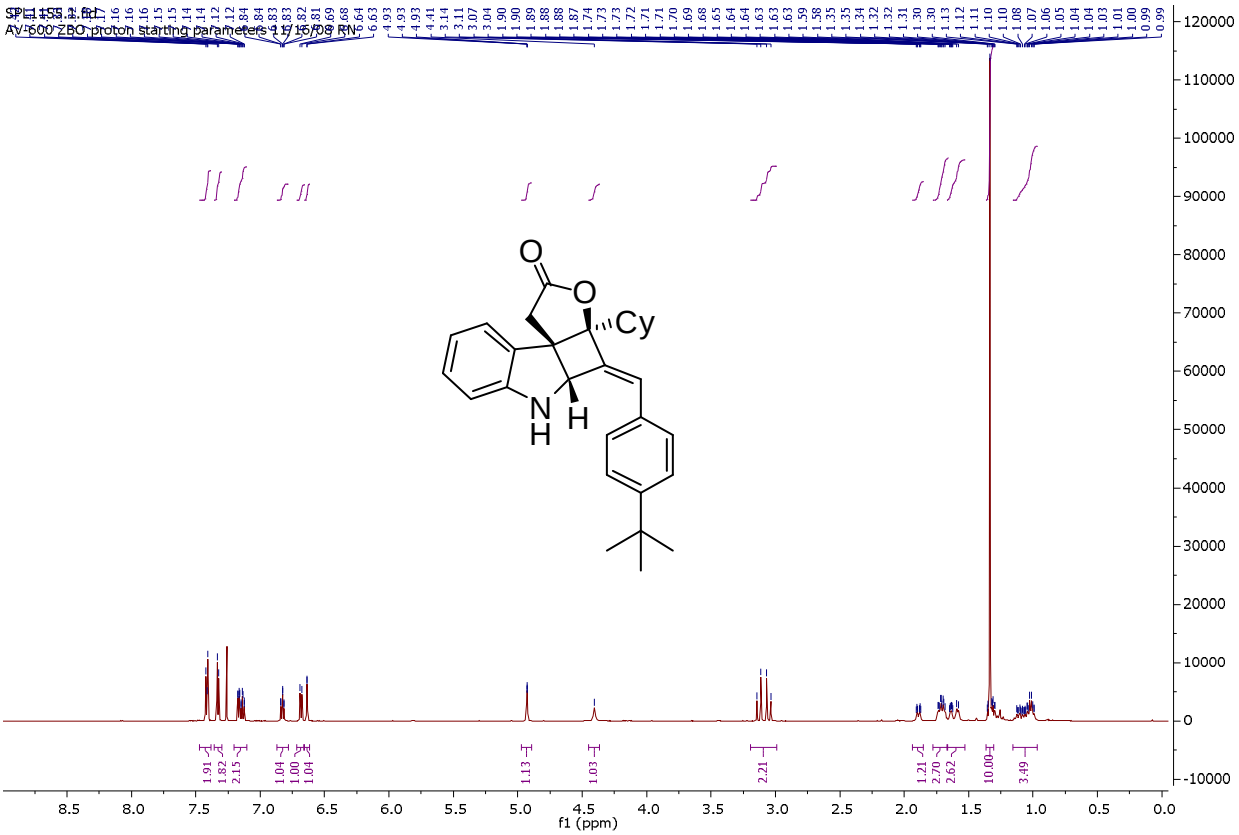

SPL1063-10C1.fid
DRX-500 5mm ZBO probe 13C starting parameters
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
O
O
nBu
N
H
H
Ph
f1 (ppm)

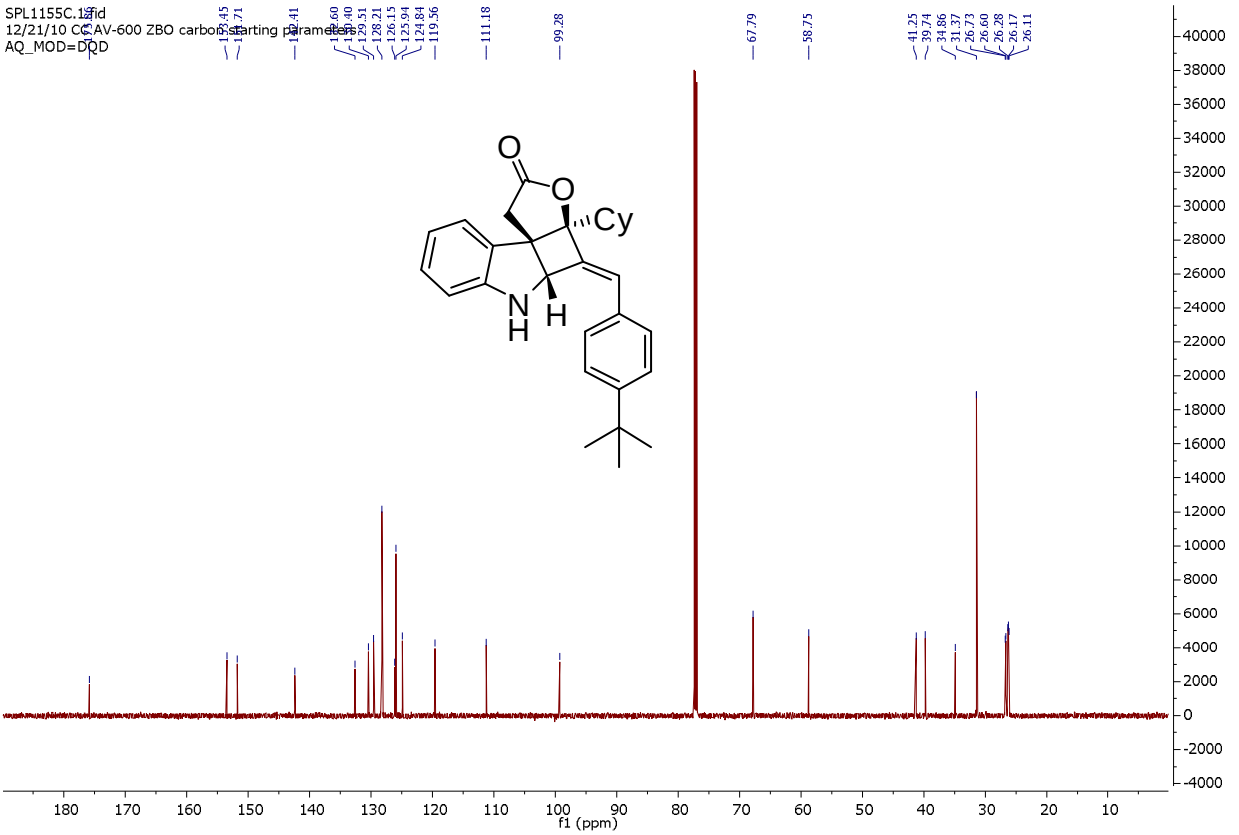

DRX-500 TBIC
10/30/13 CGC
O
O
Cy
N
H
H
Ph
f1 (ppm)

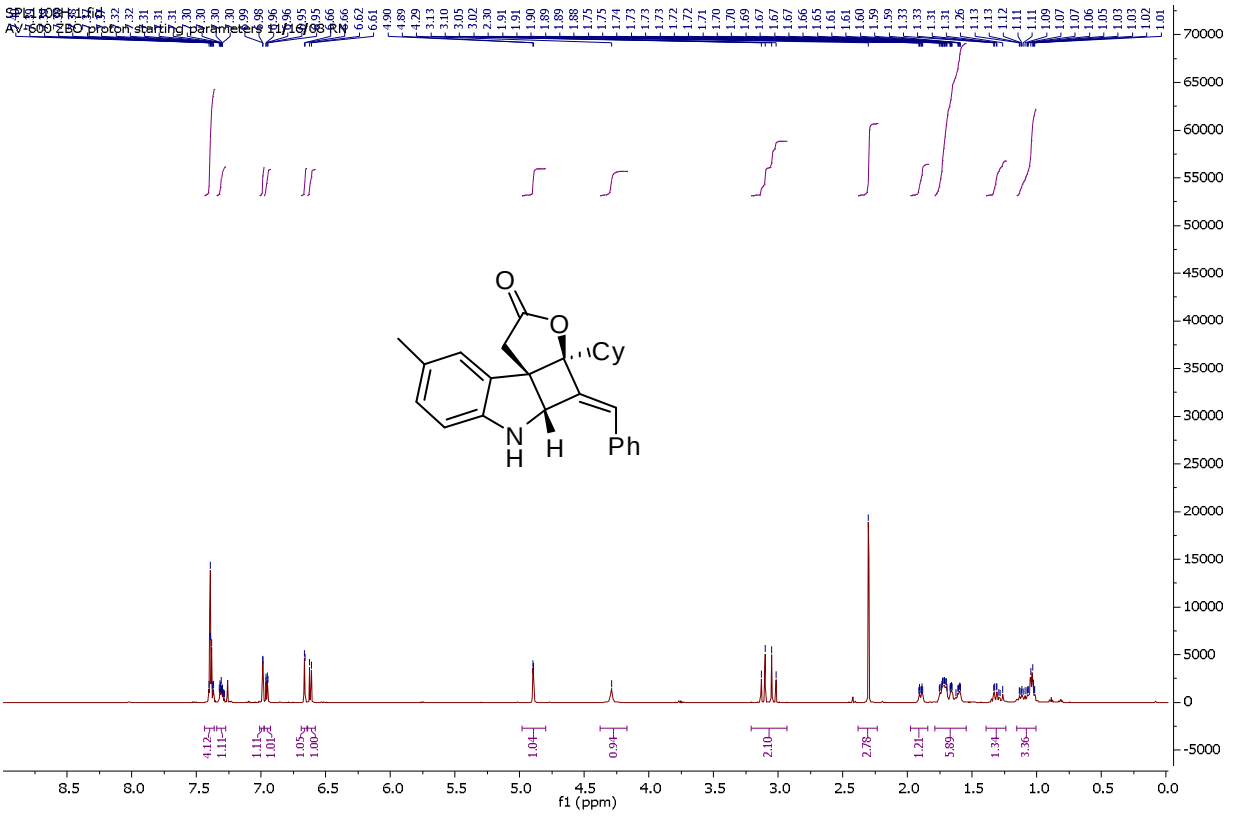

DRX-500 5mm ZBO probe 13C starting parameters: Rex 8/12/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
O
O
Cy
N
H
H
Ph
f1 (ppm)

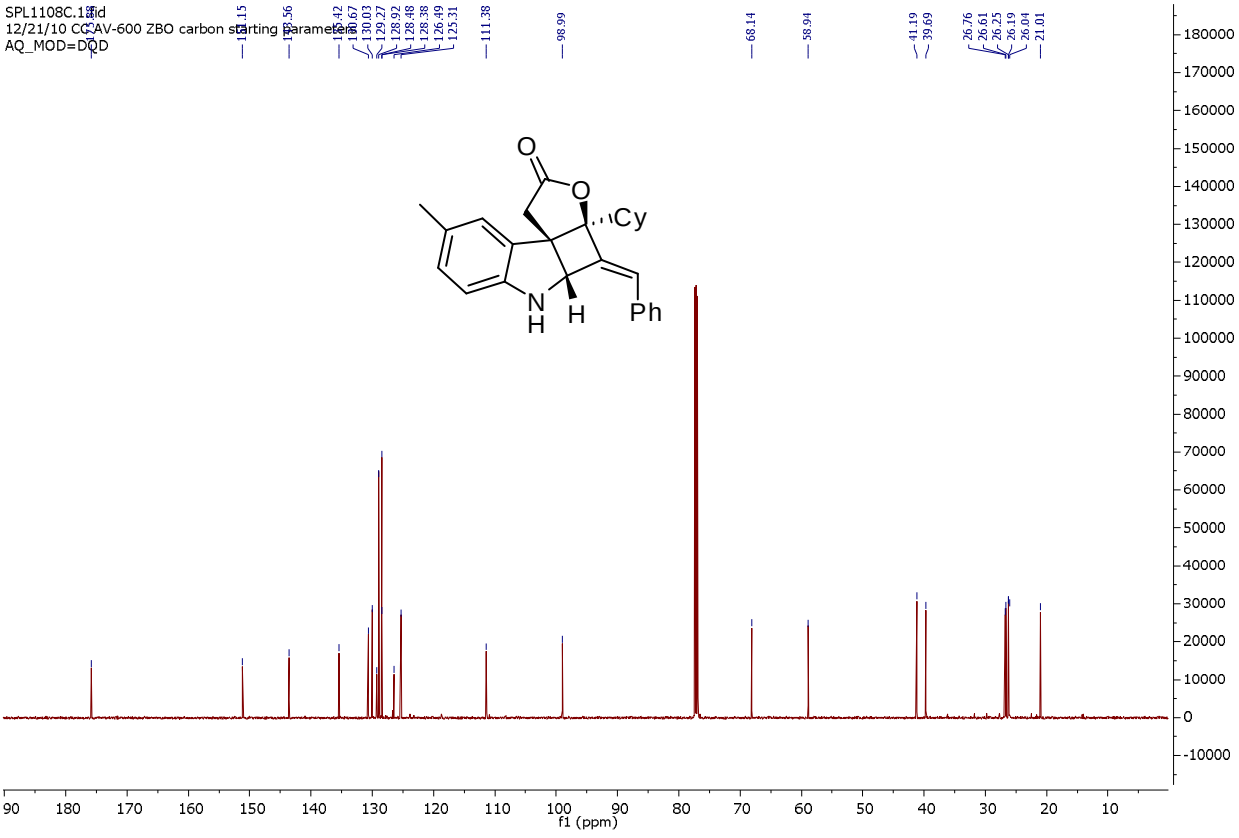

SPL1107H.1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
O
Cy
N
H
H
Br
f1 (ppm)

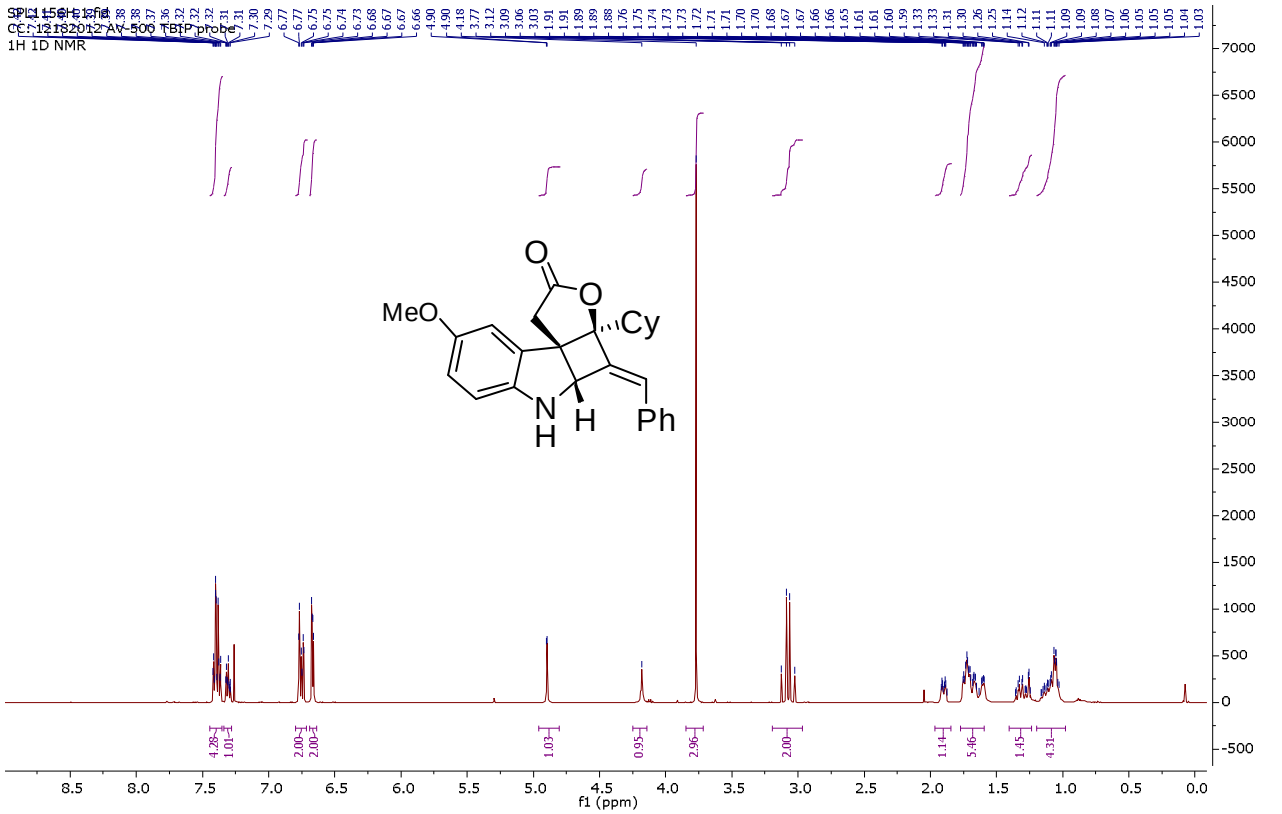

SPL1107C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters (zgpg30)
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
O
O
Cy
N
H
H
Br
f1 (ppm)

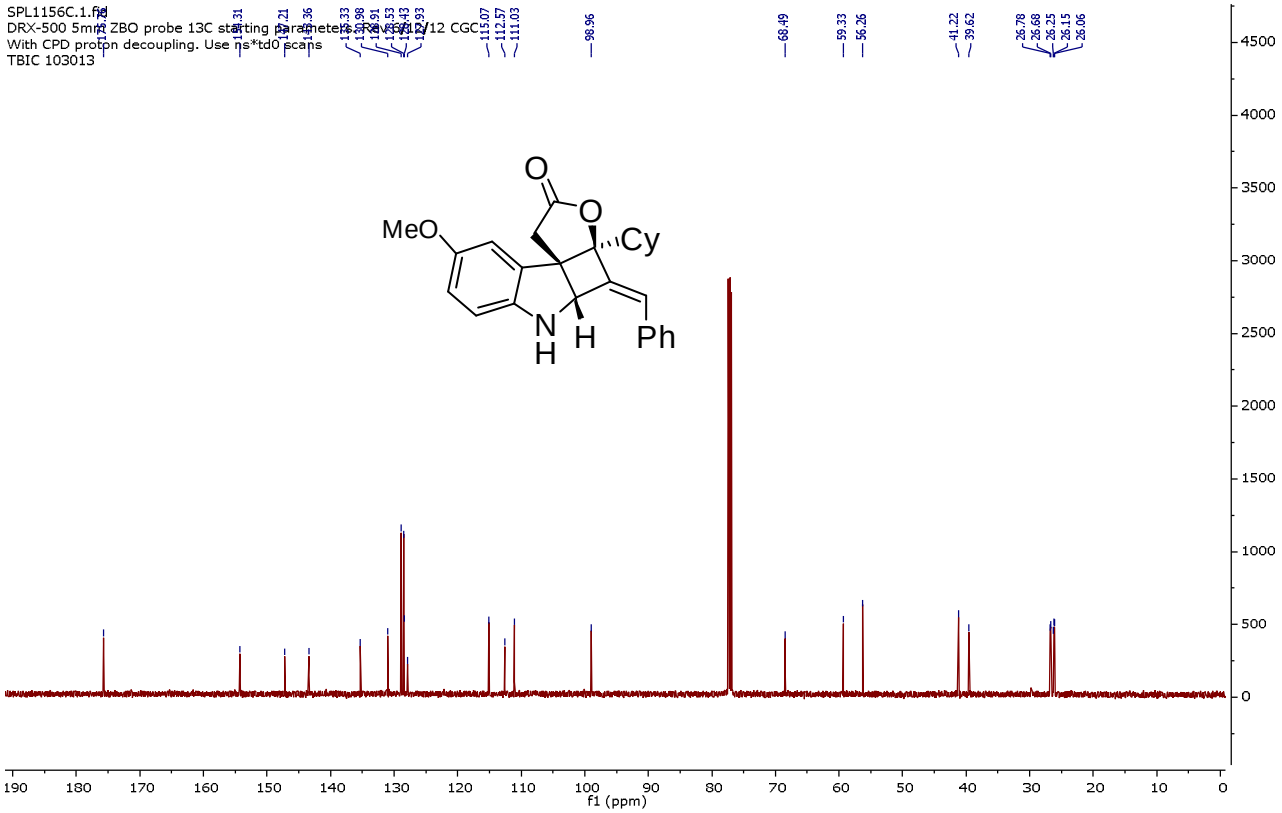

AV-600 ZBO proton starting parameters 11/16/08 RN
O
O
Cy
N
H
H
f1 (ppm)

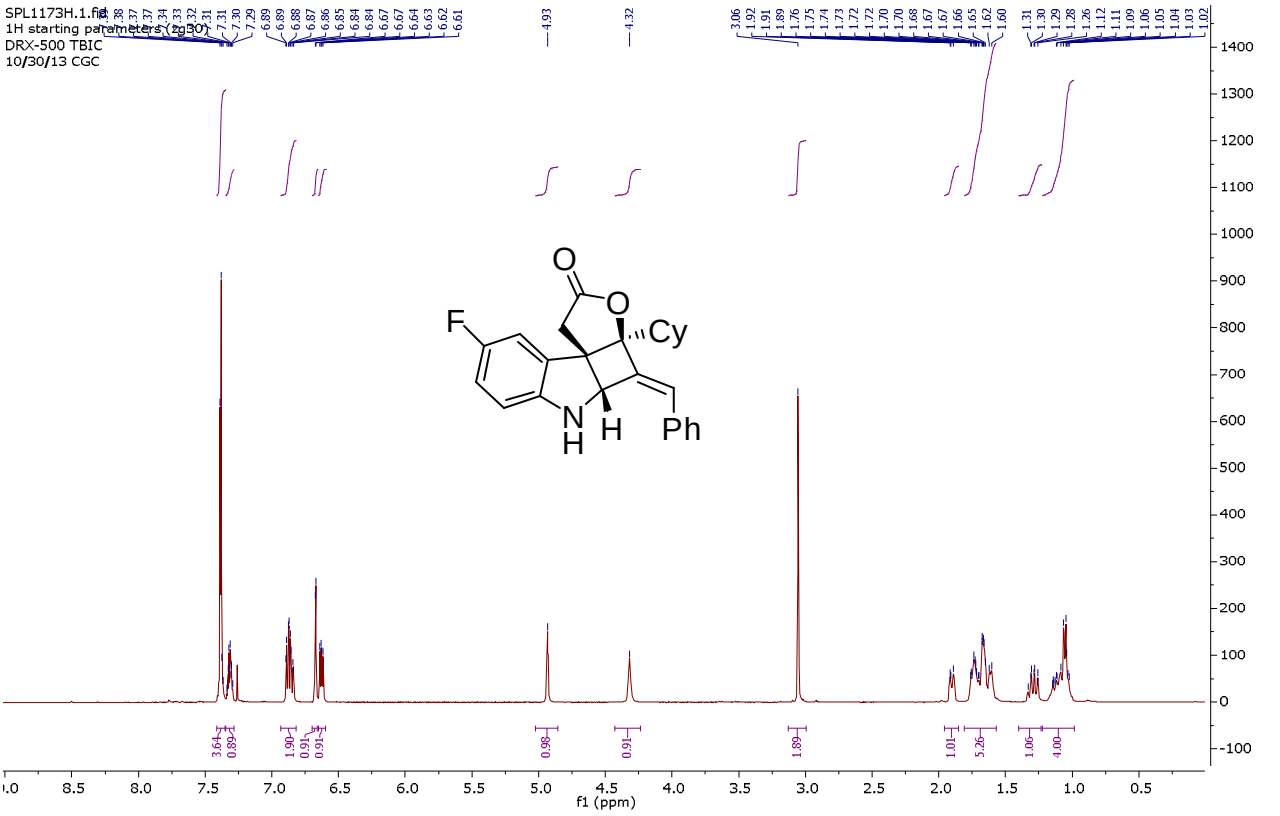

12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
O
O
Cy
N
H
H
f1 (ppm)

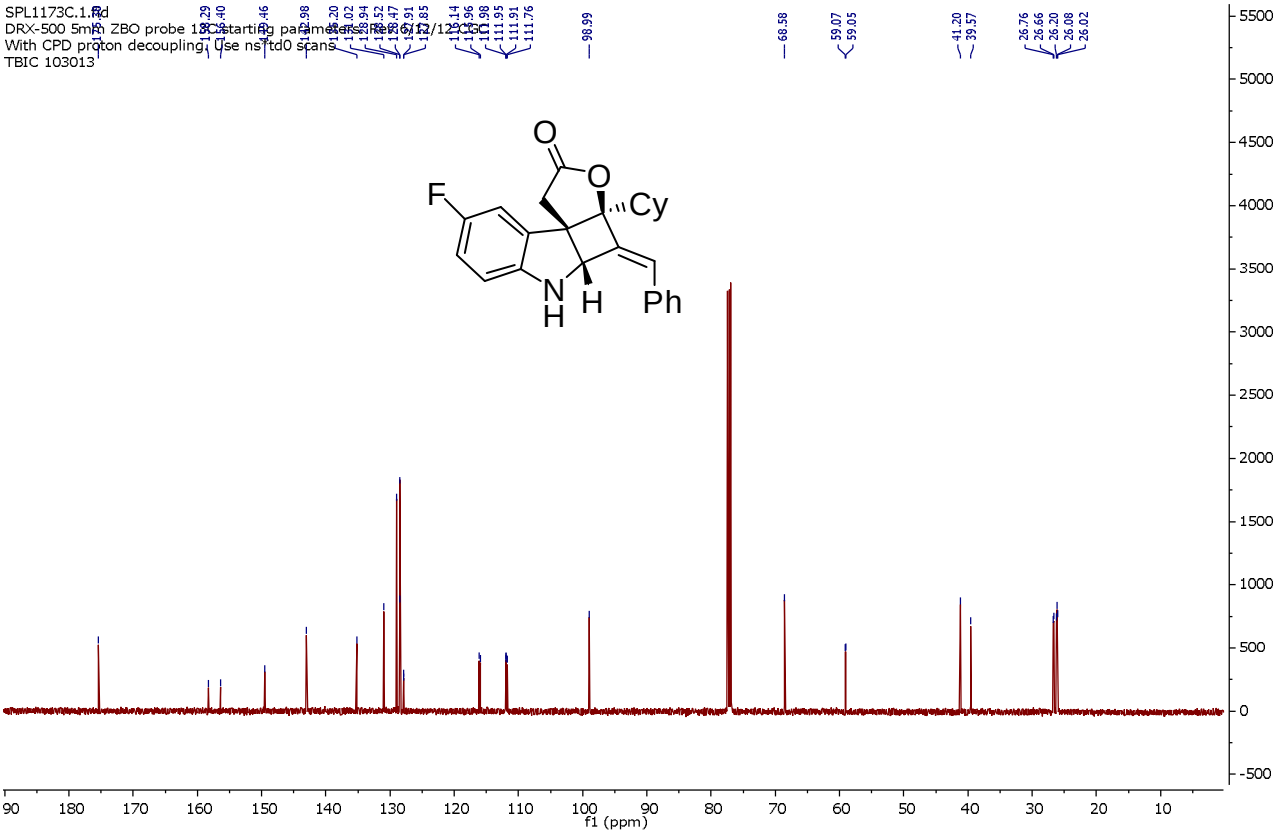

SPL1108H.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN
O
O
Cy
N
H
H
Ph
f1 (ppm)

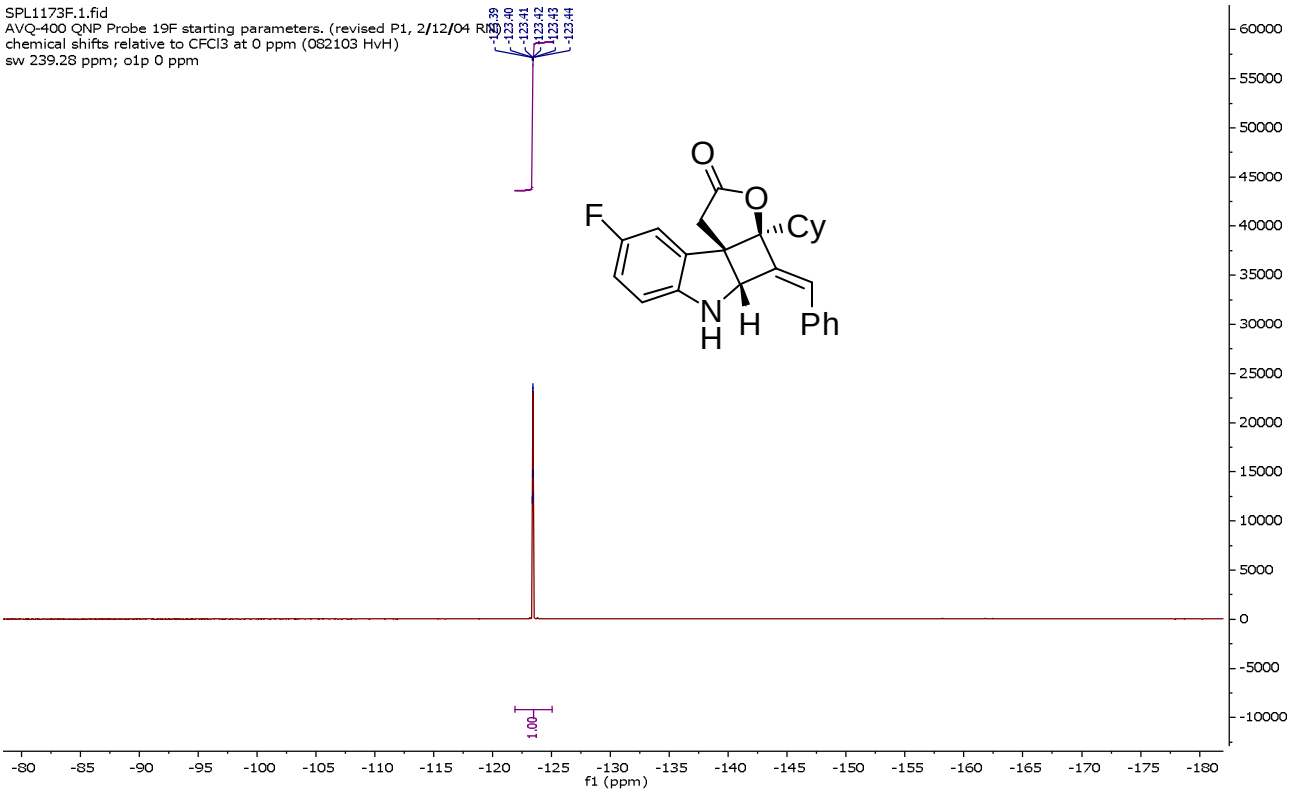

SPL1108C.1.fid
12/21/10 CC AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
O
O
Cy
N
H
H
Ph
f1 (ppm)

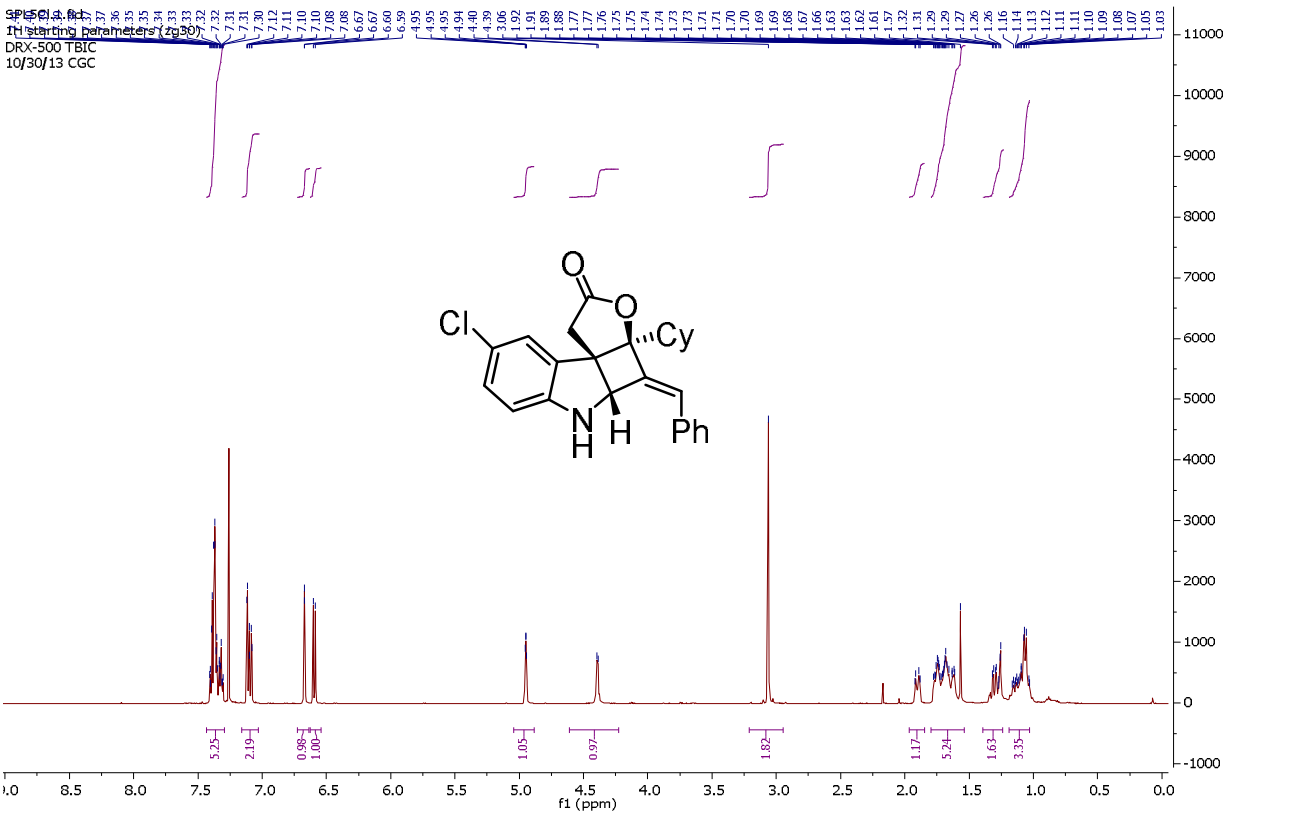

SPL1156H.1.fid
CC, 12182012 AV-500 TBIP probe
1H 1D NMR
MeO
O
O
Cy
N
H
H
Ph
f1 (ppm)

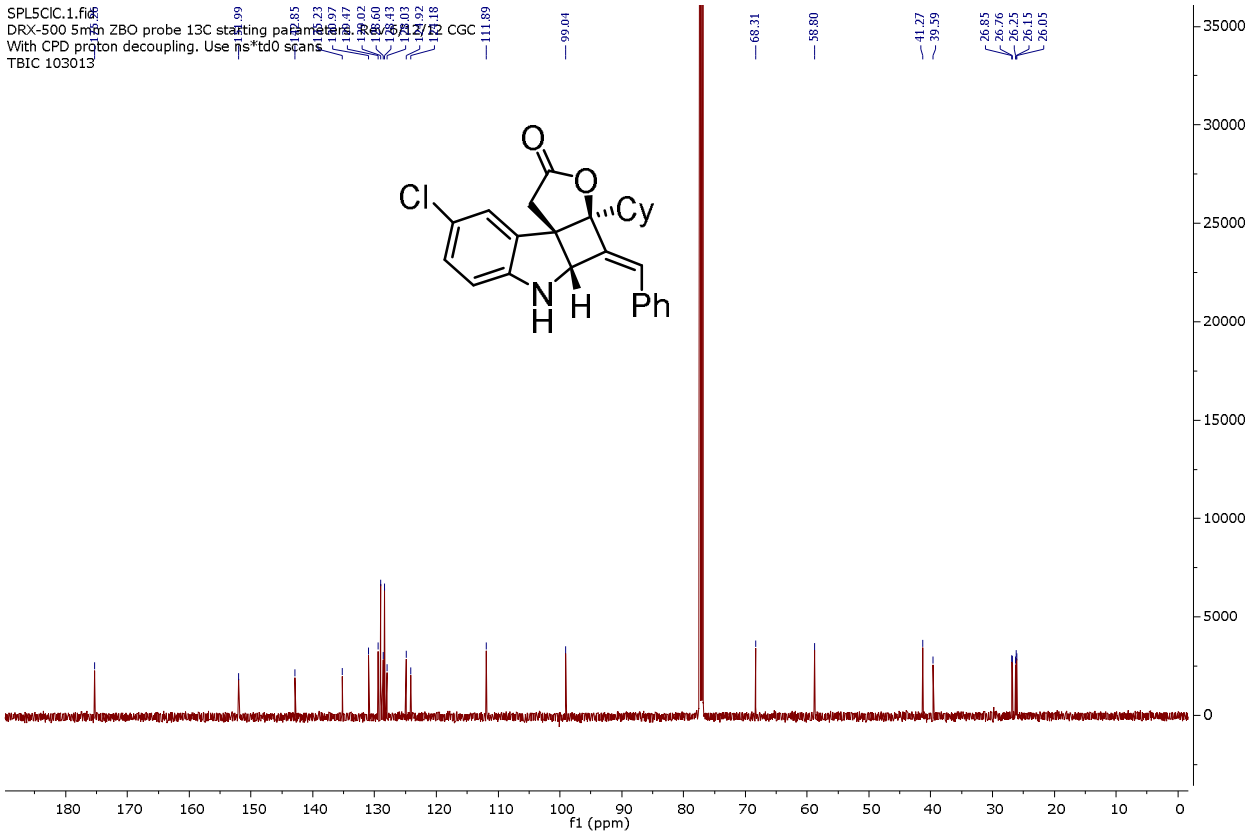

SPL1156C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
MeO
O
O
Cy
N
H
H
Ph
f1 (ppm)

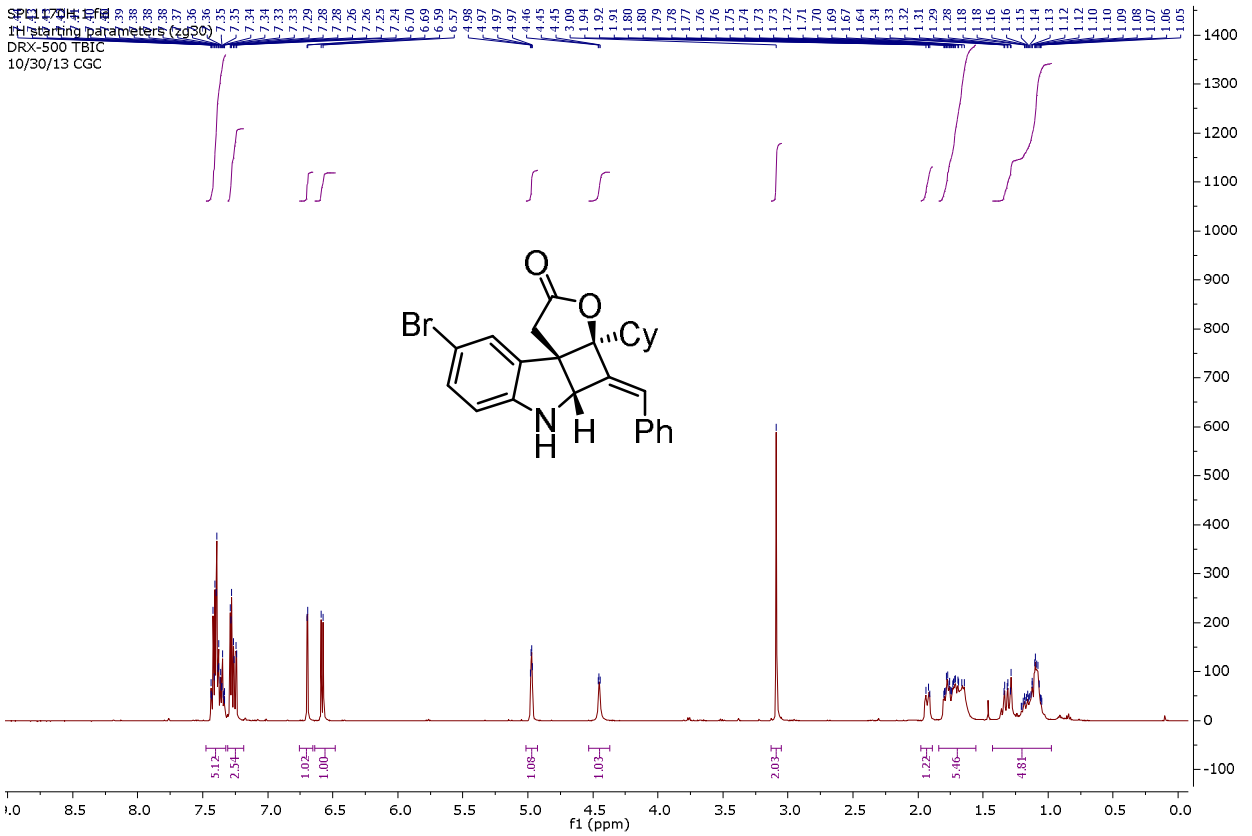

SPL1173H.1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
O
Cy
F
N
H
H
Ph
f1 (ppm)


SPL1173C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters 12/12/12 CGC
With CPD proton decoupling, use ns*td0 scans
TBIC 103013
O
O
Cy
F
N
H
H
Ph
f1 (ppm)


SPL1173F.1.fid
AVQ-400 QNP Probe 19F starting parameters. (revised P1, 2/12/04 RM)
chemical shifts relative to CFCl3 at 0 ppm (082103 HvH)
sw 239.28 ppm; o1p 0 ppm
-123.39
-123.40
-123.41
-123.42
-123.43
-123.44
O
O
F
Cy
N
H
H
Ph
1.00
f1 (ppm)


SPL5Cl4.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
O
O
Cl
Cy
N
H
H
Ph
5.25
2.19
0.98
1.00
1.05
0.97
1.82
1.17
5.24
1.63
3.35
f1 (ppm)


SPL5ClC.1.fid
DRX-500 5mm ZBO probe 13C starting parameters (zgpg30) 10/12/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
Cl
O
O
Cy
N
H
H
Ph
f1 (ppm)


SPL1170H-1.fid
1H starting parameters (zg30)
DRX-500 TBIC
10/30/13 CGC
Br
O
O
Cy
N
H
H
Ph
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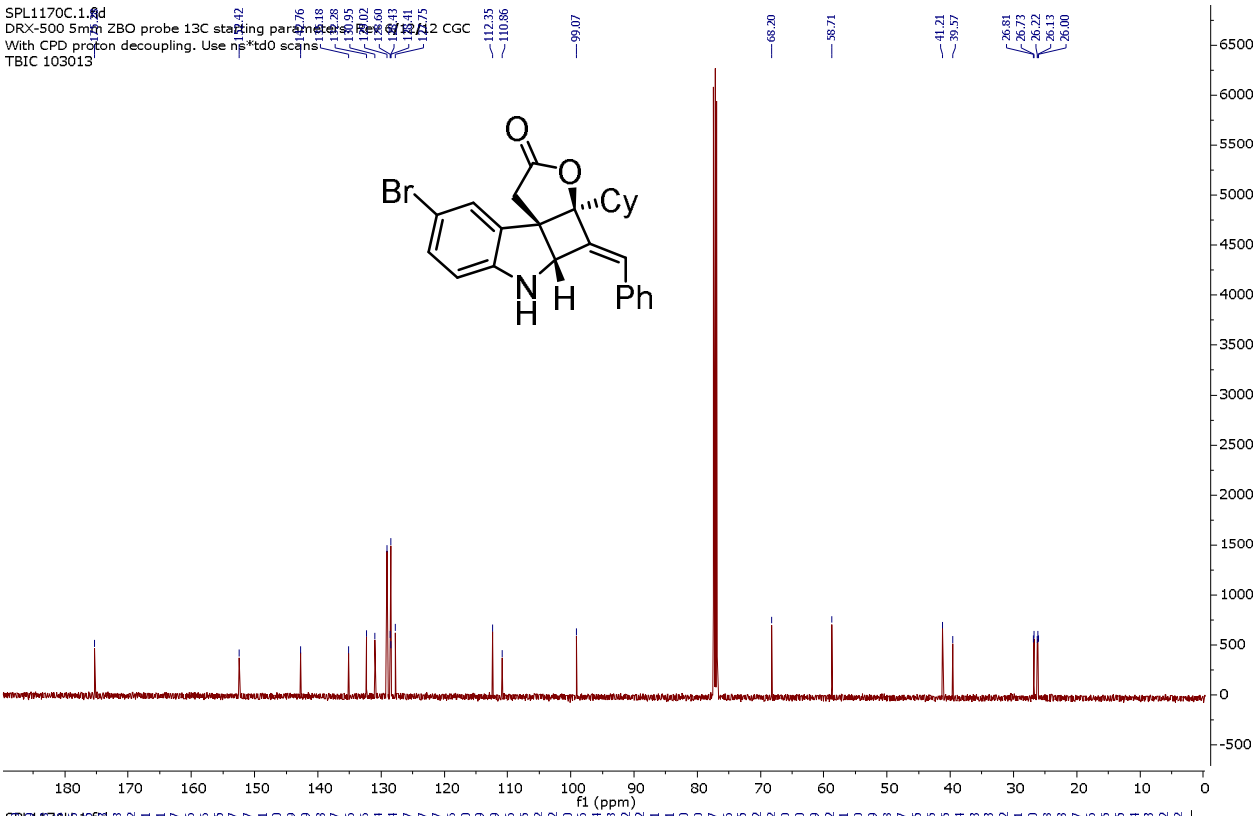
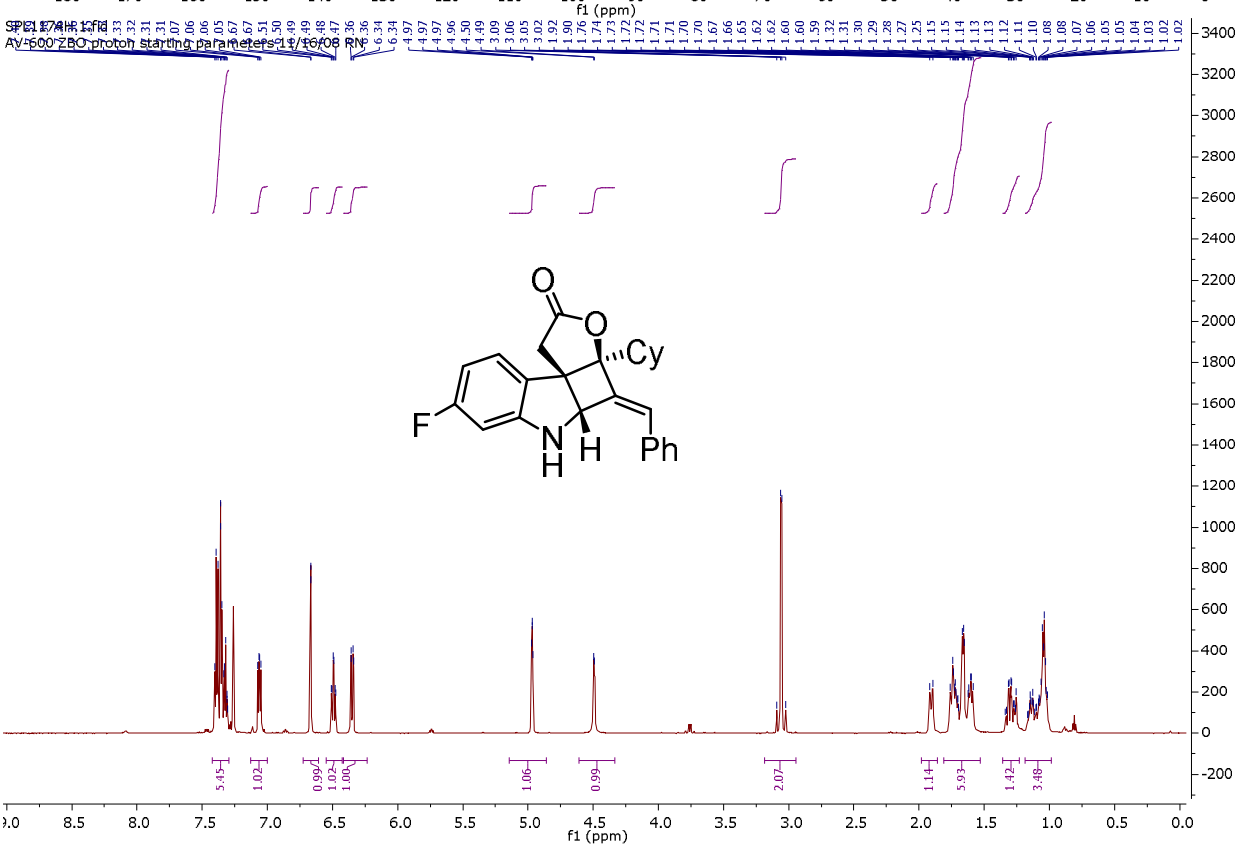
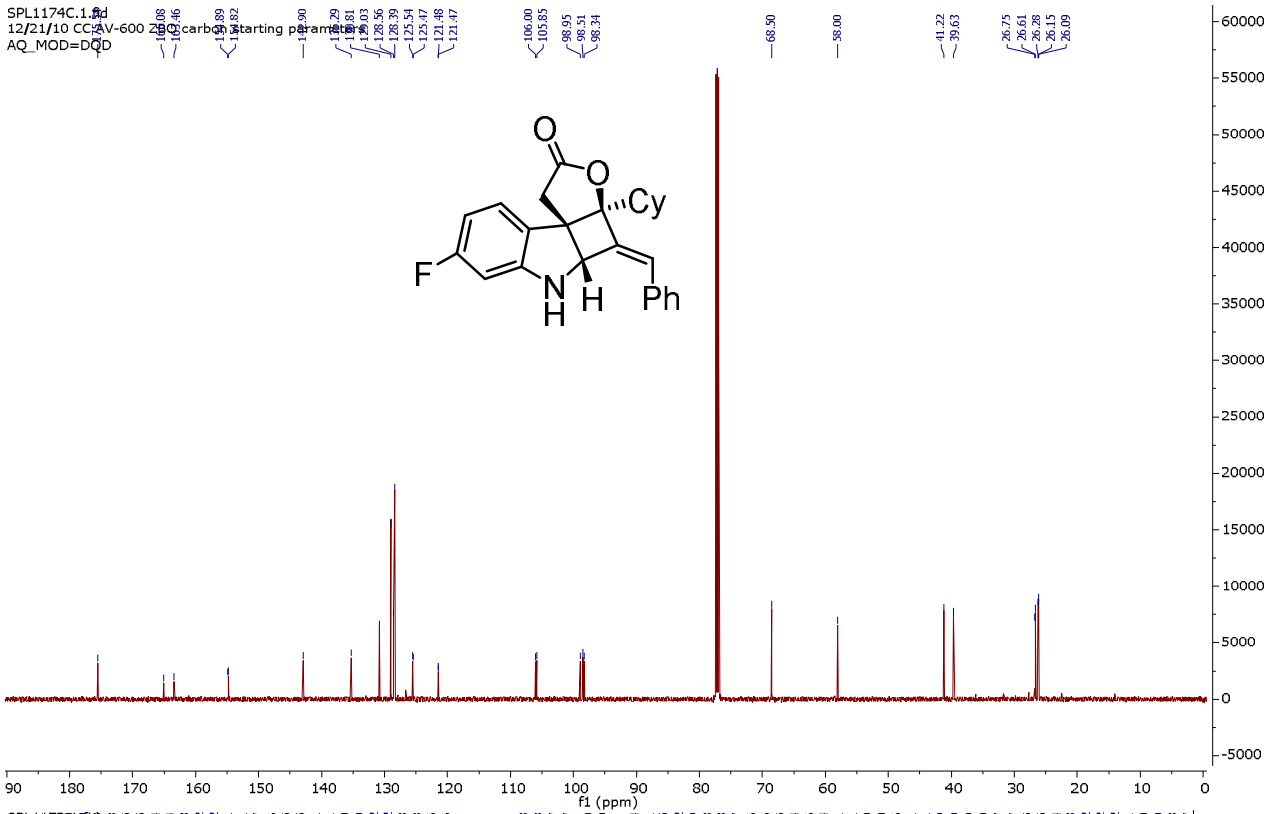
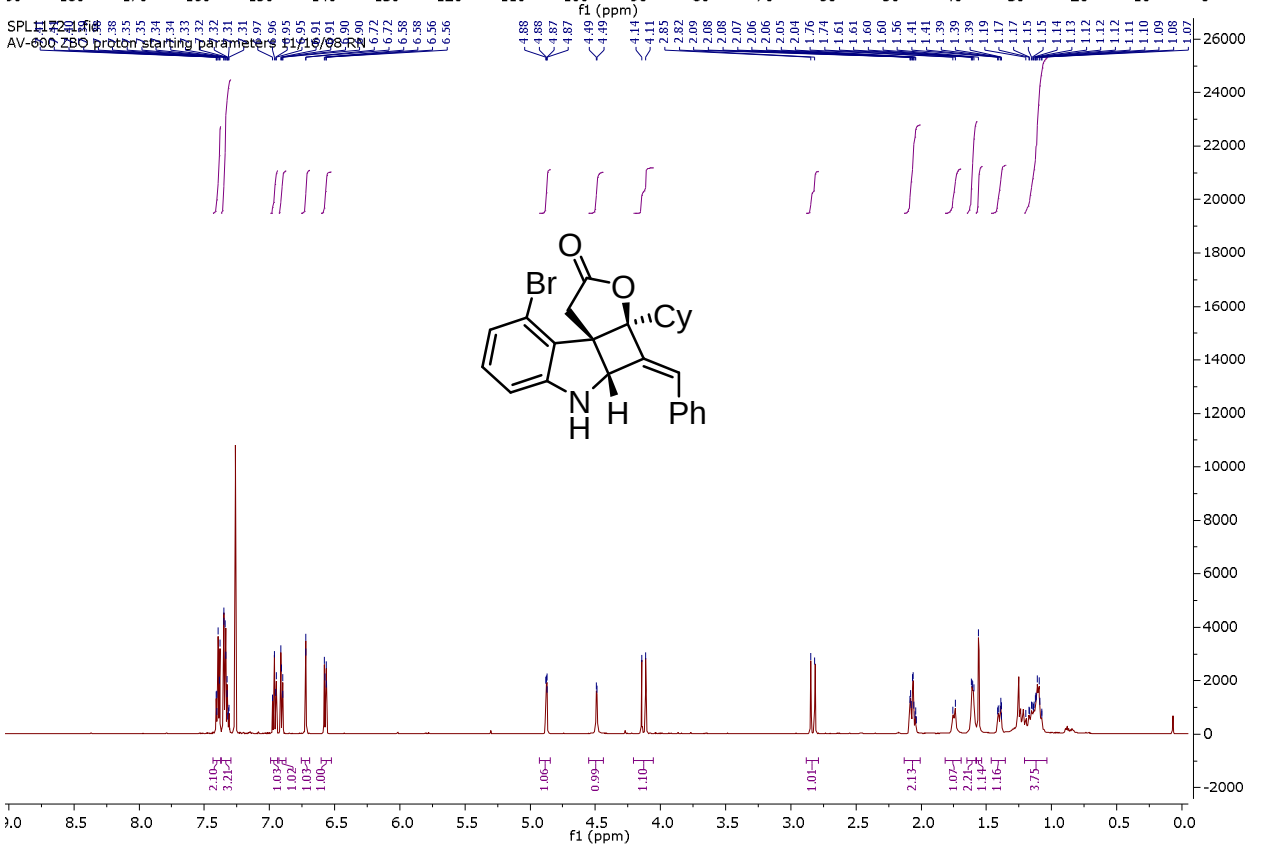
2.54
1.02
1.00
1.08
1.03
2.03
1.22
5.46
4.81
f1 (ppm)


SPL1170C.1.fid
DRX-500 5mm ZBO probe 13C starting parameters 11/16/12 CGC
With CPD proton decoupling. Use ns*td0 scans
TBIC 103013
Br
O
O
Cy
N
H
H
Ph
f1 (ppm)


SPL1174H.1.fid
AV-500 ZBO proton starting parameters 11/16/08 RM
F
O
O
Cy
N
H
H
Ph
f1 (ppm)


SPL1174C.1.fid
12/21/10 CC:AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
O
O
Cy
F
N
H
H
Ph
f1 (ppm)


SPL1172.1.fid
AV-600 ZBO proton starting parameters 11/16/09 RN
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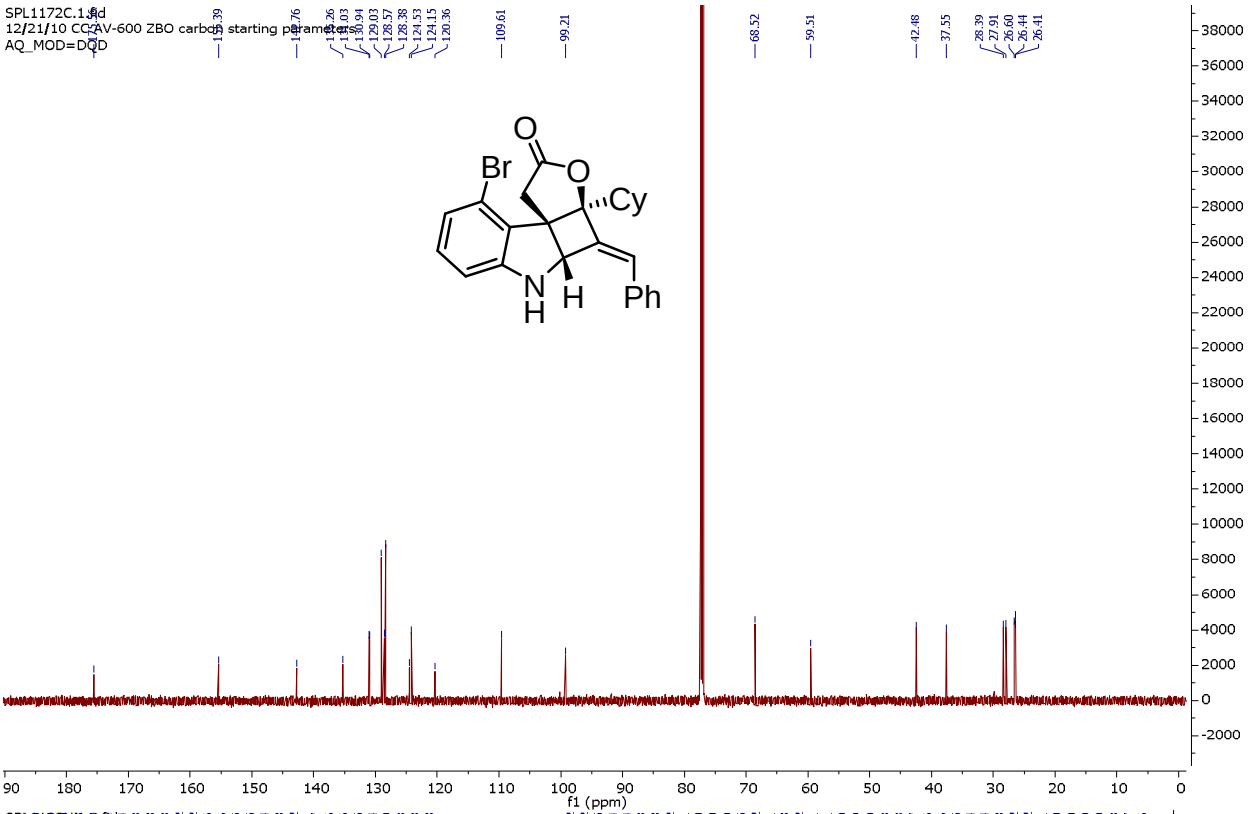
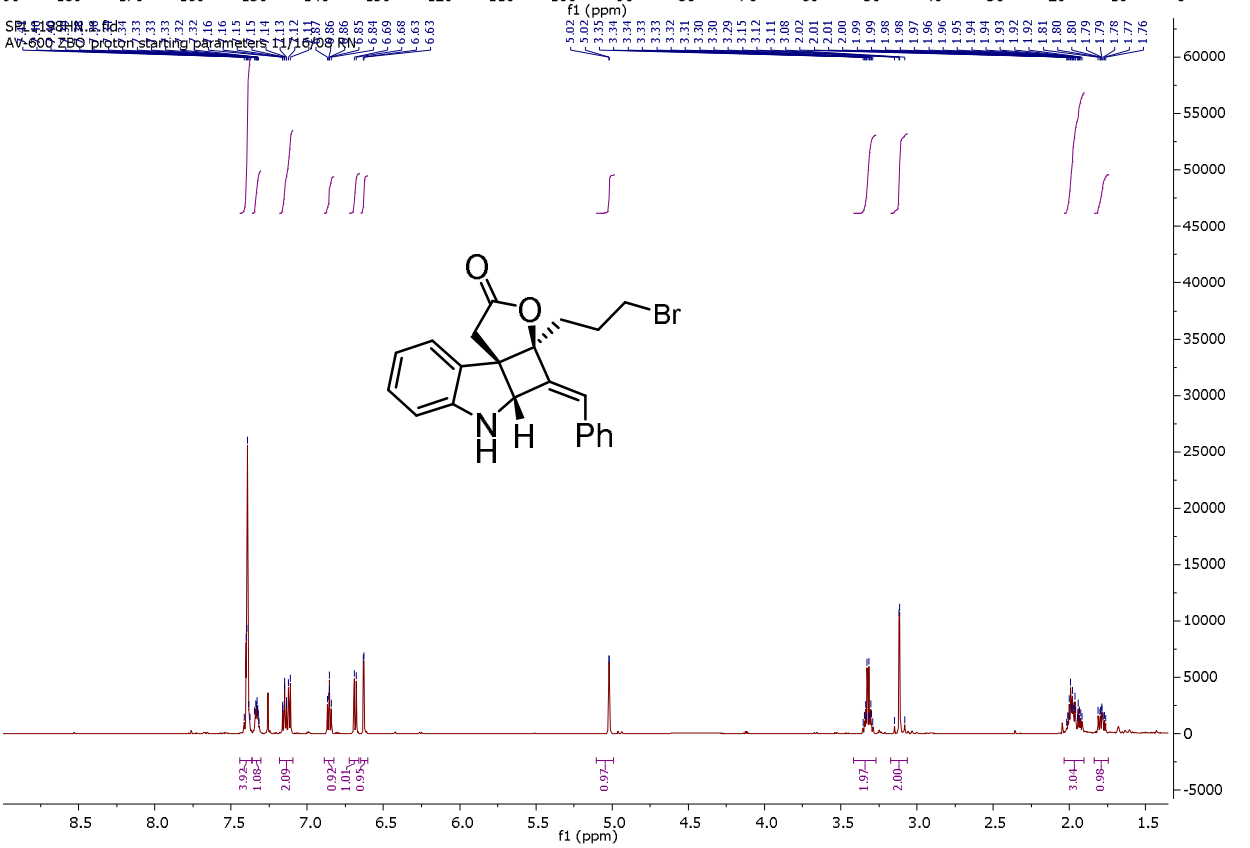
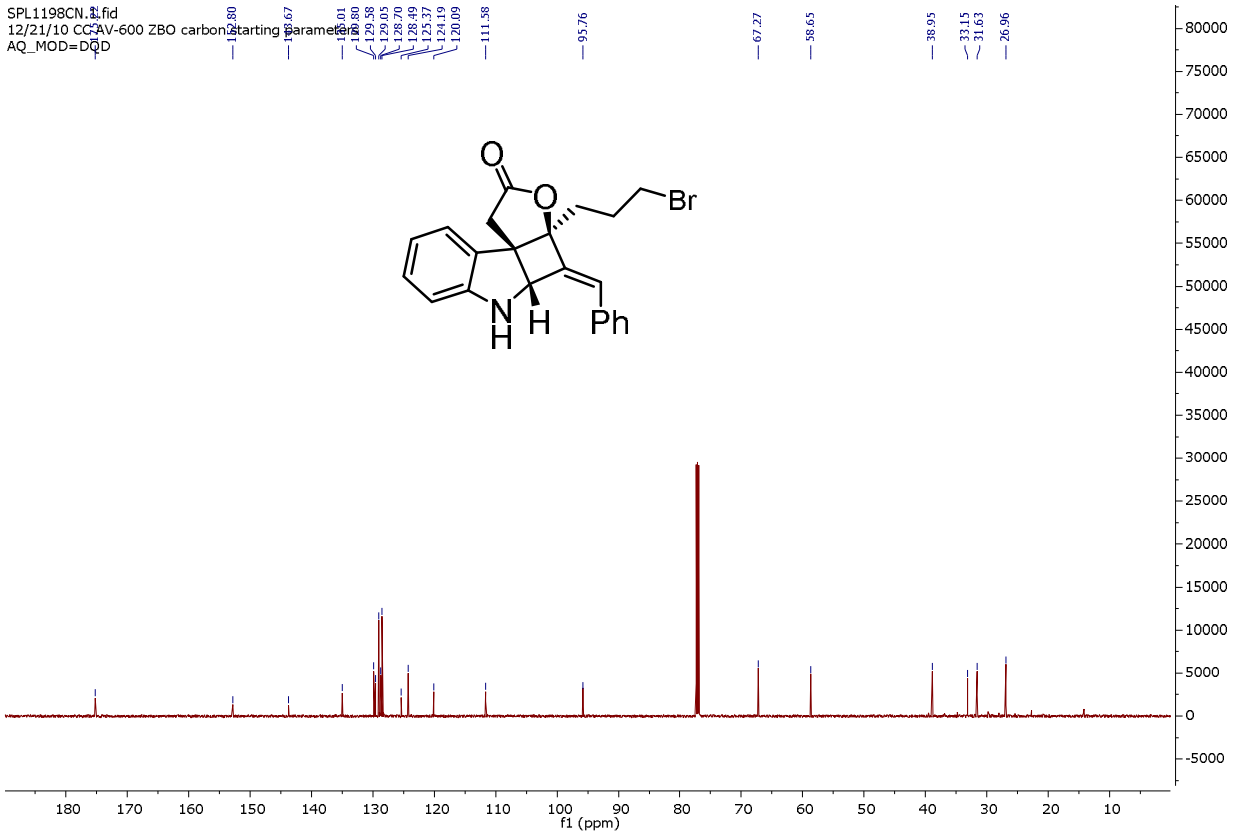
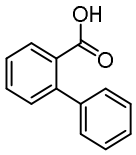
Br
O
Cy
N
H
H
Ph
f1 (ppm)


SPL1172C.1.fid
12/21/10 CC-AV-600 ZBO carbon starting parameters
AQ_MOD=DQD
Br
O
O
Cy
N
H
H
Ph
f1 (ppm)

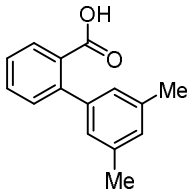

SPL1193HN.1.fid
AV-600 ZBO proton starting parameters 11/16/08 RN
O
O
Br
N
H
H
Ph
f1 (ppm)


SPL1198CN.1.fid
12/21/10 CC-AV-600 ZBO carbon2 starting parameters
AQ_MOD=DQD
172.80
159.67
136.01
130.80
129.58
129.05
128.70
128.49
125.37
124.19
120.09
111.58
95.76
67.27
58.65
38.95
33.15
31.63
26.96
O
O
Br
N
H
H
Ph
f1 (ppm)

Computed Geometry Coordinates

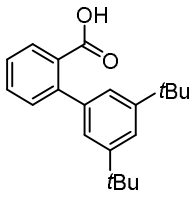


C	-2.24798100	-2.31010000	0.21151600
C	-1.42131500	0.32817700	-0.05000000
C	-0.45659100	-0.68594900	0.03297000
C	-0.89759700	-2.00189900	0.15987900
H	-2.56018900	-3.34173100	0.31203200
H	-0.15853500	-2.78885500	0.24495100
C	3.76482600	-0.03304500	0.15712900
C	2.93087100	0.63163400	1.04685700
C	1.56112300	0.43597200	0.99420600
C	1.00544100	-0.42905400	0.05447100
C	1.84804400	-1.09965300	-0.82666700
C	3.22016400	-0.89811300	-0.78022700
H	4.83501900	0.12342300	0.19507200
H	0.91187500	0.95247000	1.69147100
H	1.42132700	-1.76814700	-1.56470000
C	-2.77717800	0.01644300	0.02728600
H	-3.50222700	0.81618900	-0.03401800
C	-3.19398300	-1.29777700	0.15309500
H	-4.24970500	-1.52890600	0.20177100
H	3.34967500	1.30486500	1.78369700
H	3.86332400	-1.41649400	-1.47970600
C	-1.03618800	1.74166300	-0.33042700
O	-0.06717300	2.09795200	-0.93883700
O	-1.94123500	2.62174600	0.14822500
H	-1.64111000	3.49982400	-0.12619300



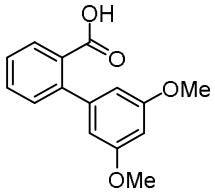
C	2.72238200	-2.22932100	-0.81305100
C	1.94643700	0.25389500	0.15711100
C	0.96201900	-0.67717700	-0.20193900
C	1.37836700	-1.91789600	-0.68250900
H	3.01499100	-3.20105600	-1.18992600
H	0.62411000	-2.63567500	-0.98028300
C	-3.22632400	0.06594800	-0.14727900
C	-2.39036400	0.95801800	-0.80863500
C	-1.02187900	0.71532500	-0.80472600
C	-0.49391900	-0.39192500	-0.15304900
C	-1.35396700	-1.27404900	0.49504900

C	-2.72485800	-1.05201700	0.51253000
H	-4.29685300	0.24377900	-0.14780900
H	-0.35714100	1.39458300	-1.32866900
H	-0.94256300	-2.13693100	1.00712900
C	3.29644100	-0.05337000	0.00026400
H	4.03664700	0.68426400	0.27822700
C	3.68815600	-1.29218100	-0.47781000
H	4.73941400	-1.52390700	-0.58501500
C	-2.94300300	2.17344900	-1.50090200
H	-2.49422000	2.30249600	-2.48656300
H	-4.02320100	2.10269400	-1.62282000
H	-2.72801800	3.07433800	-0.92229300
C	-3.64634000	-1.97982400	1.25538500
H	-3.20488300	-2.96974400	1.36685900
H	-3.85281900	-1.59399900	2.25620100
H	-4.60108500	-2.08438400	0.73968500
C	1.59096800	1.54534200	0.81382600
O	0.64229100	1.73825600	1.51987600
O	2.50239900	2.51060900	0.56503500
H	2.22340200	3.28731700	1.07041300



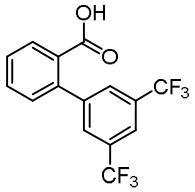
C	3.63252700	-2.11413000	-1.49593500
C	2.97514100	-0.06077000	0.25373100
C	1.94763900	-0.75280400	-0.40426600
C	2.30545200	-1.78080000	-1.27510700
H	3.87800800	-2.91763200	-2.17862400
H	1.51915200	-2.30553200	-1.80353900
C	-2.17108800	0.22437800	-0.09321300
C	-1.25304400	1.24580800	-0.36909500
C	0.08625100	0.91056400	-0.45806300
C	0.51130700	-0.40518800	-0.26761000
C	-0.42170200	-1.39216300	-0.00199500
C	-1.78373500	-1.09372100	0.09229800
H	-3.21914800	0.48147700	-0.02403200
H	0.83134600	1.66383800	-0.67722400
H	-0.07446900	-2.40656100	0.15722100
C	4.30886100	-0.38049400	0.00827100
H	5.08306100	0.17255300	0.52202600
C	4.64151400	-1.40725500	-0.85877300
H	5.68022800	-1.65370300	-1.03406600
C	-1.75942000	2.67609000	-0.54847500
C	-2.77396000	-2.21469200	0.40475500
C	-2.75526400	2.72704200	-1.71510200
H	-3.61287100	2.07680200	-1.53951400
H	-3.12706700	3.74562100	-1.84700500

H	-2.27678400	2.41166500	-2.64416800
C	-2.45995900	3.12692500	0.74090800
H	-2.81860400	4.15309200	0.63308700
H	-3.31704300	2.49464000	0.97602400
H	-1.77007100	3.08721900	1.58575100
C	-0.62453200	3.65697400	-0.84163600
H	0.09849700	3.68526400	-0.02393300
H	-0.09717000	3.39965700	-1.76211600
H	-1.03522900	4.66100700	-0.96104500
C	-4.22002300	-1.72066200	0.43682000
H	-4.36969100	-0.96538000	1.21056100
H	-4.52165500	-1.29784400	-0.52362600
H	-4.88385800	-2.55857500	0.65674000
C	-2.43919500	-2.81504900	1.77713500
H	-3.13465900	-3.62384800	2.01272700
H	-1.42734700	-3.22063300	1.80074000
H	-2.51511100	-2.05566700	2.55732400
C	-2.66362200	-3.30630100	-0.66859200
H	-1.66175600	-3.73563500	-0.70345600
H	-3.36834400	-4.11359400	-0.45699000
H	-2.89184500	-2.89988700	-1.65580500
C	2.68113900	0.95378600	1.30730200
O	1.73678800	0.95004000	2.04528500
O	3.64364500	1.89795000	1.38664200
H	3.40324400	2.47250500	2.12737600

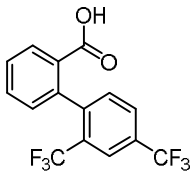


C	3.30900600	-2.04478900	-1.13939600
C	2.47609300	0.23485400	0.20862400
C	1.51510900	-0.65163300	-0.29507900
C	1.95766000	-1.79068900	-0.96413000
H	3.62339400	-2.93758000	-1.66476600
H	1.21995100	-2.47150400	-1.36993800
C	-2.70417500	0.00979800	-0.11825700
C	-1.85485300	0.98203600	-0.64667900
C	-0.48361700	0.77810900	-0.69454000
C	0.05288600	-0.40580200	-0.20655800
C	-0.77776600	-1.38939600	0.31215100
C	-2.14966900	-1.17551100	0.35953900
H	-3.76856000	0.17254200	-0.08126900
H	0.14611000	1.55090900	-1.11541000
C	3.83255100	-0.01040600	0.00797900
H	4.55519000	0.69232700	0.39958500
C	4.25252300	-1.14889800	-0.65896400
H	5.30871300	-1.33600000	-0.79990700
H	-0.37775300	-2.31316300	0.70778100
O	-2.29693900	2.16461600	-1.14462200

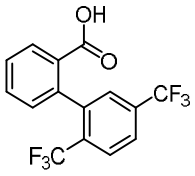
O	-2.88758100	-2.18185700	0.89309200
C	-3.67923000	2.42889500	-1.10436600
H	-4.05249400	2.43448800	-0.07637500
H	-3.81288200	3.41535200	-1.54066800
H	-4.24186800	1.69608800	-1.69009400
C	-4.28234400	-2.01051000	0.97968900
H	-4.67255900	-2.91805900	1.43294600
H	-4.53913300	-1.15269400	1.60761400
H	-4.72914800	-1.88073300	-0.01024500
C	2.08820200	1.39510900	1.06268100
O	1.15643600	1.43152000	1.81459600
O	2.94967700	2.42746100	0.93975200
H	2.65403400	3.10709700	1.56202800



C	3.63613800	-1.93068400	-1.63025400
C	2.96873300	-0.00570900	0.26129900
C	1.94837900	-0.66664100	-0.43853200
C	2.30614800	-1.63036700	-1.37760100
H	3.88519500	-2.68324400	-2.36728800
H	1.52283900	-2.13286400	-1.93151500
C	-2.23127800	0.19058200	-0.06039000
C	-1.32260100	1.20362800	-0.35089200
C	0.02674600	0.93892400	-0.45518800
C	0.50464100	-0.35936100	-0.27090900
C	-0.39819300	-1.37237000	0.00732400
C	-1.75709200	-1.09248100	0.11554200
H	-3.28818800	0.40577900	0.02327700
H	0.71792300	1.74013800	-0.68139200
H	-0.04326300	-2.38504400	0.15879800
C	4.30309500	-0.29834500	-0.01087800
H	5.07533600	0.22262300	0.53719900
C	4.63975800	-1.25768300	-0.95089000
H	5.67985000	-1.48041200	-1.14797400
C	-1.85453100	2.59383900	-0.56361500
C	-2.69252400	-2.22534100	0.43439400
F	-2.57195600	3.01143000	0.48575600
F	-2.66568300	2.64789100	-1.62888200
F	-0.88037600	3.48471100	-0.76256000
F	-3.96782700	-1.83505200	0.47326100
F	-2.40674300	-2.77799200	1.61952500
F	-2.60126200	-3.20450500	-0.47668000
C	2.65526300	0.93978300	1.37227600
O	3.68302300	1.76426100	1.64942400
H	3.40883100	2.30691000	2.40264800
O	1.62823000	0.97338000	1.99087100



C	3.51696500	-1.30158600	-1.99382100
C	2.61946400	-0.53744400	0.52229500
C	1.69331200	-0.76190300	-0.50223800
C	2.16013500	-1.14745900	-1.75460100
H	3.85786800	-1.60070000	-2.97641900
H	1.44439100	-1.31136300	-2.55040800
C	-2.54544600	-0.45739800	-0.02947900
C	-1.80531100	0.69956300	-0.19888800
C	-0.42906400	0.61978700	-0.34825400
C	0.21945500	-0.61614900	-0.32122800
C	-0.54755000	-1.76658200	-0.16803400
C	-1.92047700	-1.69447700	-0.01891100
C	3.98195200	-0.68143500	0.27293200
H	4.68353400	-0.49727500	1.07411400
C	4.43184700	-1.06486300	-0.97894700
H	5.49212900	-1.17861800	-1.16105800
H	-0.04868500	-2.72668800	-0.14585100
C	0.35512000	1.89369800	-0.54328100
C	-4.04138200	-0.39467400	0.09459200
F	-4.47393700	0.83315100	0.39144900
F	-4.49299100	-1.22144800	1.04490200
F	-4.64283800	-0.75862200	-1.04761300
F	-0.44324500	2.95950600	-0.64736900
F	1.19180500	2.13592400	0.47598200
F	1.10106900	1.85511800	-1.65439700
H	-2.29781600	1.66107900	-0.21579700
H	-2.50473500	-2.59611800	0.11354400
C	2.15378200	-0.18387400	1.89317300
O	1.03658600	-0.33107900	2.30578100
O	3.13934200	0.31622300	2.65904400
H	2.75030300	0.50464300	3.52482400



C	2.60466500	-1.85011800	-2.19493200
C	2.06919000	-1.09936800	0.42662000
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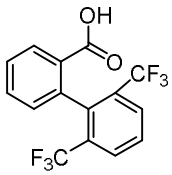
C	1.46087400	-1.12574100	-1.89645600
H	2.80521900	-2.13807800	-3.21881900
H	0.77704400	-0.83913100	-2.68550900
C	-2.49977700	1.37897500	0.05138900
C	-1.30989900	2.08570000	-0.01658100

C	-0.11098000	1.42015500	-0.21902400
C	-0.07823700	0.02896800	-0.34599400
C	-1.27792400	-0.66674200	-0.29518700
C	-2.47494400	0.00345100	-0.09720500
C	3.22171900	-1.81864200	0.11921900
H	3.90106800	-2.08405900	0.91655300
C	3.48958300	-2.19646800	-1.18522400
H	4.38526800	-2.75881600	-1.41272600
H	-1.27089400	-1.74389900	-0.40258900
C	1.16357100	2.22238500	-0.30878100
F	0.93224900	3.53695300	-0.24805000
F	2.01479300	1.93334500	0.68464400
F	1.81473500	1.99432100	-1.45662800
H	-1.31409200	3.16161300	0.08142900
H	-3.43730300	1.89489100	0.20479700
C	-3.74976800	-0.78898300	0.00274500
F	-4.82136300	-0.05508900	-0.31435500
F	-3.94409400	-1.24959100	1.24447000
F	-3.73822200	-1.85215200	-0.80891200
C	1.77698600	-0.74661800	1.84513800
O	0.71795700	-0.36821300	2.26405100
O	2.84371200	-0.91158200	2.64787000
H	2.55745700	-0.67221200	3.54061400



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C	-0.26358300	-1.14648300	-1.85923000
H	-0.72384500	-2.71133200	-3.24418100
H	0.05209900	-0.45380700	-2.62887500
C	1.15706400	3.25728100	0.26229400
C	2.06019500	2.21336600	0.17300500
C	1.61392700	0.92390200	-0.07626700
C	0.25408700	0.64807900	-0.23617700
C	-0.63959300	1.71879200	-0.15469200
C	-0.19345300	3.00818800	0.09575400
C	-1.07524100	-2.90755000	0.11104500
H	-1.38877200	-3.58686600	0.89046900
C	-1.10909700	-3.29982600	-1.21655200
H	-1.45137700	-4.29202900	-1.47842000
C	2.63405400	-0.18582500	-0.16907400
F	3.86245700	0.24395400	0.13911400
F	2.36244800	-1.20277500	0.65479300
F	2.70546800	-0.69307500	-1.40845900
H	3.11755700	2.39560100	0.30111300
H	1.50462800	4.26175100	0.46046300

C	-2.12262800	1.48825200	-0.32172800
F	-2.61223700	0.64637000	0.59646500
F	-2.81660000	2.62585200	-0.20954300
F	-2.42044100	0.97412500	-1.52215700
H	-0.90810800	3.81584500	0.16250100
C	-0.58628400	-1.23855600	1.89720300
O	-0.14866400	-0.20369800	2.32045900
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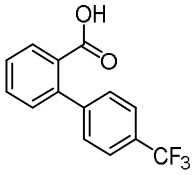
H	-1.01470800	-1.83595900	3.61391500



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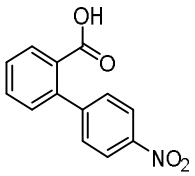
C	-2.27807000	-1.99128800	0.16647600
H	-3.96808500	-3.29036900	0.36387200
H	-1.55638400	-2.79622400	0.22965800
C	2.42006700	-0.16483400	0.01356900
C	1.64675000	0.49846200	0.95978000
C	0.27451500	0.34594700	0.95101100
C	-0.34172500	-0.47027800	0.00317000
C	0.44466400	-1.13569500	-0.92937300
C	1.82404900	-0.98113200	-0.93148200
H	-0.33086500	0.86145100	1.68616800
H	-0.02813100	-1.76465500	-1.67318500
C	-4.11159200	0.07217100	0.07834400
H	-4.81896800	0.88826800	0.03258200
C	-4.55581000	-1.23186500	0.21762500
H	-5.61513100	-1.43769200	0.29264800
H	2.12280600	1.13258600	1.69697200
H	2.42983600	-1.48982300	-1.66857100
C	3.91057000	0.00691100	0.05648700
F	4.26031200	1.29961600	0.08714100
F	4.44234200	-0.55555200	1.15307800
F	4.51810300	-0.54371600	-0.99887300
C	-2.33151400	1.75594400	-0.31167700
O	-1.32218400	2.08579900	-0.86797000
O	-3.24527600	2.65687400	0.10268300
H	-2.91529600	3.52686400	-0.16335700



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C	-1.45385300	-0.67970800	0.06105800
C	-1.91456700	-1.98018600	0.25146000
H	-3.60095500	-3.27675900	0.49193600
H	-1.18998300	-2.77844800	0.35365500
C	2.75013100	-0.14761600	0.06173400
C	1.99264800	0.54199300	0.99283500
C	0.62054100	0.38083300	0.97363200
C	0.01488700	-0.45820600	0.03961300
C	0.80778500	-1.14505700	-0.87593000
C	2.18413000	-0.98929800	-0.87634600
H	0.00797300	0.90958200	1.69280100
H	0.34004100	-1.79296700	-1.60612900
C	-3.75646200	0.06984000	0.05726500
H	-4.46749300	0.87907400	-0.03185600
C	-4.19569200	-1.22913300	0.25078000
H	-5.25469300	-1.43656200	0.32553200
H	2.48069400	1.18546700	1.70986700
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N	4.21440000	0.01951800	0.07341700
O	4.68745700	0.75185700	0.91224900
O	4.85385800	-0.58694500	-0.75562000
C	-1.97548300	1.74237200	-0.38780500
O	-0.94788500	2.04868300	-0.92427100
O	-2.90635000	2.65641900	-0.05099400
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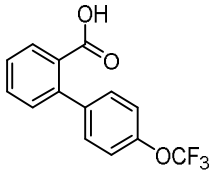

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C	-2.78467800	-1.92610400	0.25915300
H	-4.57548900	-3.03294200	0.64661500
H	-2.14763700	-2.80103300	0.29743400
C	2.04528300	-0.57281600	-0.33592100
C	1.42354600	0.25385900	0.58659600
C	0.04150400	0.22079500	0.68068900
C	-0.72342800	-0.61796400	-0.12187100
C	-0.06905600	-1.44309700	-1.03206000
C	1.30939400	-1.42063200	-1.14608000
H	-0.44911100	0.86095200	1.40370100
H	-0.64802900	-2.09621800	-1.67310400
C	-4.39631700	0.31565600	0.24454400
H	-5.01666000	1.20093400	0.22899400
C	-4.95917200	-0.92867700	0.47183800
H	-6.02305600	-1.01875200	0.64575900
H	1.98982100	0.91336900	1.22647200
H	1.82868300	-2.04731800	-1.85808000

O	3.41876500	-0.63994200	-0.53594300
C	4.25981300	0.11819900	0.18672400
F	4.04866300	1.42516700	0.01877300
F	4.17909700	-0.12993900	1.49627400
F	5.48871700	-0.15731500	-0.21021500
C	-2.50639100	1.78842300	-0.38160900
O	-1.57338000	1.99554900	-1.10496800
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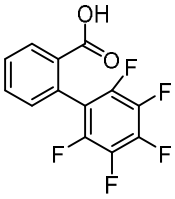

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C	-1.71258800	1.74064600	-0.96008000
H	-3.37000800	2.91171700	-1.63777000
H	-0.97206400	2.41485300	-1.37067200
C	2.93925700	-0.08778800	-0.07996600
C	2.11387900	-1.02179000	-0.68518400
C	0.75350000	-0.79352300	-0.73681800
C	0.17485200	0.34857500	-0.20069100
C	1.02745000	1.26803700	0.39051900
C	2.39506800	1.06199400	0.46097900
C	-3.60081800	-0.00131700	0.06004800
H	-4.32975500	-0.68840200	0.46547100
C	-4.01033500	1.14104200	-0.60731400
H	-5.06540700	1.34640000	-0.72926800
F	-0.01509700	-1.71267900	-1.31526800
F	2.63599800	-2.12329100	-1.20766800
F	4.24562500	-0.29534200	-0.02390600
F	3.18204000	1.95852700	1.04141100
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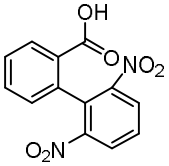
C	-1.84455800	-1.46692100	1.03602800
O	-0.77360800	-1.62840000	1.55305900
O	-2.83753900	-2.36505300	1.15726800
H	-2.49712900	-3.08301200	1.70975400



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C	-1.00906800	-0.00003400	-1.93995700
H	-2.54138400	-0.00014800	-3.43760400

H	-0.19913000	0.00018500	-2.65908600
C	3.52154100	0.00098300	0.28314400
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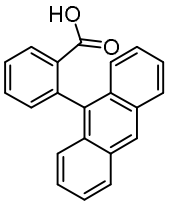
C	1.47277000	1.17139800	-0.08861800
C	0.72616600	0.00015900	-0.19840600
C	1.47348600	-1.17065800	-0.08887400
C	2.83648600	-1.19250600	0.14521700
C	-3.07454900	-0.00051600	-0.09865500
H	-3.87274300	-0.00074100	0.62978300
C	-3.36227200	-0.00042000	-1.45703000
H	-4.39105600	-0.00053800	-1.79114800
H	3.33658300	2.14920000	0.21430700
H	3.33790500	-2.14732800	0.21391300
C	-1.44885600	-0.00068100	1.79560800
O	-0.34204000	-0.00101600	2.26406200
O	-2.54852200	-0.00061600	2.56657700
H	-2.24489200	-0.00099200	3.48510000
N	0.81769900	2.49010500	-0.21218500
O	-0.31256900	2.60139100	0.19465700
O	1.47725300	3.38040100	-0.69933000
H	4.58342100	0.00128300	0.48361400
N	0.81922700	-2.48975800	-0.21268100
O	1.47963600	-3.37979700	-0.69914000
O	-0.31127900	-2.60161500	0.19333700



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C	-0.42068300	-2.50362000	-0.25011000
C	-2.39001300	-1.06064400	-0.00296800
C	-2.19284700	1.35297300	-0.09927800
C	-0.02030500	2.43390100	-0.46484300
C	-1.20419300	-3.60327100	-0.09929800
H	0.64579400	-2.61540200	-0.39869700
C	-3.17672600	-2.24205300	0.14814700
C	-2.96181300	0.20515200	0.05284400
C	-2.77676100	2.65441500	-0.04656100
H	1.04699700	2.35980800	-0.63035300
C	-0.61479100	3.65421900	-0.40826300
C	-2.60672400	-3.47295400	0.10107300
H	-0.76164300	-4.59066700	-0.12910400
H	-4.24327900	-2.13071900	0.30420800
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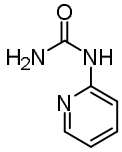
H	-3.84530500	2.73029200	0.11671500

H	-0.02053800	4.55138100	-0.52528900
H	-3.21358900	-4.36160500	0.21753300
H	-2.47120800	4.75048500	-0.15128300
C	1.26630200	-0.16459900	-0.60799300
C	2.23718400	-0.09958700	0.40015900
C	1.68892700	-0.33779700	-1.92336000
C	3.59002600	-0.20242600	0.07636200
C	3.03448900	-0.44535300	-2.23969100
H	0.93951000	-0.38734000	-2.70373400
C	3.99062100	-0.37668900	-1.23672400
H	4.32375100	-0.14571900	0.86770400
H	3.33513600	-0.58040100	-3.27085600
H	5.04274400	-0.45790700	-1.47515300
C	1.83657200	0.06818300	1.82698800
O	0.71712600	0.02709300	2.25320400
O	2.89582700	0.27304200	2.63882700
H	2.53869600	0.35610000	3.53404000



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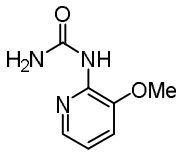
C	-1.28644200	-1.33302500	0.00001900
C	-0.28115700	-0.35181000	-0.00000500
H	-2.01957900	2.38632300	0.00009000
H	-3.91739900	0.78918900	0.00013500
H	-3.39091300	-1.66633700	0.00008900
N	-0.56024400	0.94648700	0.00002100
C	2.24937500	-0.06357000	-0.00005900
N	2.16550500	1.28113100	-0.00012300
H	3.03325400	1.78482500	-0.00004900
H	1.26422500	1.73543900	-0.00004100
O	3.28831900	-0.69235900	-0.00002600
N	1.03781700	-0.76797700	-0.00005600
H	1.20283700	-1.76170200	-0.00004800
H	-1.02010700	-2.38042400	-0.00000200



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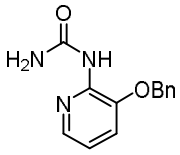
C	1.22476900	-0.30875900	-0.00013600
C	-0.08188200	0.24738500	-0.00017700
H	0.55477700	3.43027200	0.00016700

H	2.90059700	2.61724300	0.00021700
H	3.31128900	0.15535800	0.00003400
N	-0.28131000	1.55052800	-0.00006200
C	-2.52111800	-0.44013700	0.00002300
N	-2.94076300	0.84145900	0.00006600
H	-2.27247100	1.59781400	0.00006800
H	-3.93314300	0.98871700	0.00029600
O	-3.25593300	-1.40674000	0.00025100
N	-1.13574400	-0.64169400	-0.00034300
H	-0.89224200	-1.62002800	-0.00050900
O	1.27858500	-1.66324800	-0.00028500
C	2.55849800	-2.26211600	0.00028900
H	2.39328800	-3.33454900	0.00028400
H	3.12064400	-1.97775000	-0.89158900
H	3.11987700	-1.97765100	0.89261300



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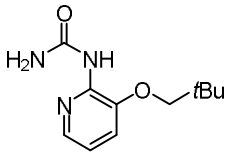
C	0.94121000	-1.08744500	0.01803000
C	2.03719600	-0.18539900	-0.02879400
H	4.56718300	-2.20912000	0.16575800
H	2.76483500	-3.91391500	0.25050300
H	0.39138700	-3.14947500	0.15045400
N	3.28527900	-0.60627400	0.02481600
C	2.55068800	2.29161200	-0.17948000
N	3.88066300	2.07654300	-0.11969500
H	4.24404400	1.13682000	-0.05961900
H	4.46869000	2.88842100	-0.16005700
O	2.03206000	3.38594500	-0.26706700
N	1.73353800	1.15581500	-0.13197700
H	0.75365200	1.38733800	-0.18965800
O	-0.28311200	-0.50935800	-0.04335300
C	-1.41792800	-1.35537800	0.05308500
H	-1.42683900	-2.06091300	-0.78220600
H	-1.35364900	-1.92824000	0.98468100
C	-2.65823400	-0.50894300	0.03820100
C	-3.77432200	-0.92287500	-0.67693500
C	-2.71402700	0.67593200	0.76524700
C	-4.93937100	-0.16806900	-0.66116100
H	-3.73188100	-1.83747900	-1.25539100
C	-3.87333300	1.43529200	0.77343000
H	-1.84389100	1.00587900	1.31707200
C	-4.98989300	1.01312400	0.06316900
H	-5.80213900	-0.49831300	-1.22312800
H	-3.90582900	2.35885800	1.33482800
H	-5.89339800	1.60703500	0.07045800



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C	0.24923700	0.99496600	-0.00023300
C	1.51589100	0.35245400	-0.00002900
H	3.54642000	2.88391200	0.00039800
H	1.41650900	4.15853100	0.00002000
H	-0.73518400	2.89200800	-0.00040100
N	2.64331300	1.03506400	0.00019400
C	2.55151400	-1.96124000	-0.00002900
N	3.80414700	-1.46193000	0.00002600
H	3.95572200	-0.46392200	0.00048700
H	4.55353800	-2.12891600	0.00054100
O	2.28028900	-3.14521200	-0.00008800
N	1.50986900	-1.02726500	-0.00010700
H	0.60257300	-1.46657800	-0.00011900
O	-0.81942200	0.16452800	-0.00043800
C	-2.11524600	0.74248400	-0.00021500
H	-2.23004800	1.37146600	0.88962700
H	-2.23041900	1.37132500	-0.89010900
C	-3.16115900	-0.36499200	0.00009100
C	-3.00789300	-1.22649200	1.25320500
H	-3.77838000	-1.99809100	1.27406900
H	-2.03565600	-1.71739200	1.27804000
H	-3.10927300	-0.62260200	2.15700400
C	-3.00827400	-1.22682700	-1.25283100
H	-3.77878200	-1.99841700	-1.27324600
H	-3.10991600	-0.62317900	-2.15676400
H	-2.03605100	-1.71774500	-1.27781800
C	-4.53247000	0.31033600	0.00020800
H	-5.32041900	-0.44321600	0.00048700
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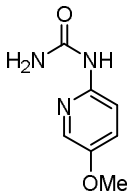

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C	2.08473500	0.26601400	-0.00004000
C	1.52269300	1.54648200	0.00047700
C	0.16135300	1.68469400	0.00017600
C	-0.63983000	0.52747100	-0.00084000
H	1.59214200	-1.83012700	-0.00188400

H	2.17886600	2.40610300	0.00129000
N	-0.11056500	-0.68116600	-0.00153800
C	-3.06897500	-0.23707600	0.00032000
N	-2.72413100	-1.54113800	0.00128500
H	-1.75230600	-1.81217700	-0.00081300
H	-3.47688700	-2.20432500	-0.00010000
O	-4.21295400	0.17305200	0.00082300
N	-2.01971500	0.68601900	-0.00094600
H	-2.37050500	1.62990500	-0.00172200
O	3.43897000	0.19185100	0.00054000
C	4.01156400	-1.09833000	0.00065100
H	5.08745100	-0.95512400	0.00104300
H	3.71825900	-1.65807100	0.89206200
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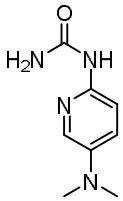

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C	1.73690700	-0.11360900	-0.15263200
C	1.20626400	-1.41092700	-0.24913400
C	-0.14735700	-1.61109600	-0.20681700
C	-0.99711800	-0.49937200	-0.07731600
H	1.12884800	1.94163800	0.04641800
H	1.86577100	-2.25712600	-0.38220300
N	-0.51614500	0.72703400	0.00078200
C	-3.45208300	0.15565500	0.07619800
N	-3.15884300	1.46910600	0.16735900
H	-3.93658900	2.09803100	0.24403900
H	-2.19838200	1.77889600	0.15044300
O	-4.57869000	-0.30112000	0.08585600
N	-2.36822800	-0.71831600	-0.03517900
H	-2.68008500	-1.67364300	-0.09804400
H	-0.56183400	-2.60675700	-0.28662700
N	3.12299500	0.10085000	-0.23681000
C	3.94237900	-0.70185700	0.65977800
H	4.98508500	-0.61833300	0.35765000
H	3.85159800	-0.36816200	1.70240500
H	3.66314700	-1.74984300	0.61018200
C	3.55349000	1.48284000	-0.26564200
H	4.62477400	1.50860500	-0.45550100
H	3.05103500	2.01604700	-1.07092400
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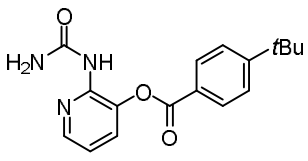

C	2.07117900	-1.30367800	2.39528400
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C	0.37322500	-2.11795100	0.94725800
C	0.90560800	-1.33100400	-0.04088200
C	2.04370100	-0.54565300	0.23284000
H	2.56680600	-1.25844300	3.35619200
H	0.57602500	-2.70447800	3.01546600
H	-0.49299600	-2.73174500	0.73556200
N	2.60303200	-0.54358600	1.43211700
O	0.41469200	-1.30032000	-1.32361200
C	3.61699300	1.13017700	-0.84128400
N	4.28774600	1.32610000	0.31243900
H	5.08627000	1.93225000	0.26587300
H	4.06480000	0.78000800	1.13136000
O	3.87013100	1.68294200	-1.89061000
N	2.54065600	0.23168100	-0.79240400
H	2.10116800	0.11874100	-1.69370100
C	-0.95581000	-1.27675400	-1.52791500
O	-1.42528200	-2.00127700	-2.34644700
C	-1.72258900	-0.27969500	-0.73422500
C	-1.13302700	0.88119900	-0.25352800
C	-3.07916900	-0.51899900	-0.53597700
C	-1.89467500	1.81855400	0.43694400
H	-0.08242500	1.07678500	-0.43021900
C	-3.85305400	0.39090900	0.16764800
H	-3.51579500	-1.42304500	-0.93978500
C	-3.24203300	1.54978000	0.64528700
H	-3.84080400	2.26832700	1.19476400
C	-1.27221400	3.09879100	0.92001200
H	-1.24217400	3.83669700	0.11682600
H	-1.84051700	3.52617100	1.74404400
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C	-5.31537100	0.14644100	0.41635700
H	-5.64997000	-0.76782700	-0.06904000
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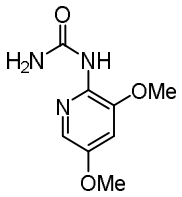

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C	0.17000900	1.12523700	-0.00010000
C	-0.63528000	-0.04786200	0.00017000
H	1.61177100	-2.39596100	0.00011900
H	2.19720400	1.84178200	-0.00024600
N	-0.09591800	-1.24180900	0.00014600
C	-3.06155300	-0.77838400	-0.00003200

N	-2.72088200	-2.08465400	0.00024400
H	-1.75034400	-2.36030400	0.00016500
H	-3.47602100	-2.74500500	-0.00014100
O	-4.20479100	-0.36683300	-0.00034000
N	-2.00712200	0.13679400	0.00018400
H	-2.32751400	1.09234100	0.00012600
O	-0.50584200	2.29696200	-0.00048800
C	0.25724900	3.48730600	0.00027600
H	-0.45507700	4.30573000	0.00047200
H	0.88387700	3.54469100	0.89246300
H	0.88428200	3.54559000	-0.89157500
O	3.44463700	-0.35353300	0.00028400
C	4.02912400	-1.63841700	-0.00036500
H	5.10376000	-1.48551200	-0.00154600
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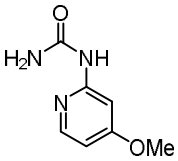

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C	-0.67195300	-0.90929600	-0.00032200
C	0.49279200	-0.14207300	-0.00051000
H	-0.68990900	2.87351500	0.00006700
N	0.47724300	1.19205200	-0.00037100
C	3.03166900	-0.34452900	0.00015000
N	3.20968200	0.99105600	-0.00004900
H	2.41202000	1.61001700	0.00061900
H	4.15854200	1.31683600	0.00197300
O	3.93076700	-1.16153200	0.00081200
N	1.70815500	-0.80330200	-0.00080300
H	1.67926600	-1.81016000	-0.00116500
H	-0.63840800	-1.98921700	-0.00035000
H	-2.84417000	1.69757000	0.00025200
O	-2.98933100	-1.04528700	-0.00003500
C	-4.25635500	-0.41437500	0.00059700
H	-4.99007200	-1.21384500	0.00217200
H	-4.38573600	0.20152100	0.89217400
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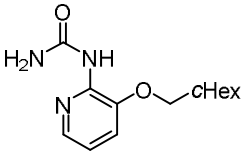

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C	1.11174000	-1.05601500	-0.03764600
C	2.26047000	-0.22096100	-0.01393000
H	4.64566500	-2.38161900	0.40459600
H	2.74399200	-3.97675300	0.38365500
H	0.43288200	-3.07844400	0.09150300
N	3.47438200	-0.71051200	0.14109700
C	2.92677800	2.21871500	-0.18024200
N	4.23560300	1.92932000	-0.03181100
H	4.53673300	0.97273100	0.08346000
H	4.87145800	2.70516200	-0.04551500
O	2.48009800	3.33886500	-0.32564000
N	2.04401000	1.13365200	-0.16092600
H	1.08426600	1.41839700	-0.27980600
O	-0.06746800	-0.41273100	-0.20336200
C	-1.25609000	-1.19009000	-0.21735000
H	-1.33589600	-1.74771100	0.72326500
H	-1.20903500	-1.90822100	-1.04244400
C	-2.44213200	-0.26275000	-0.37872400
C	-3.72534800	-1.08238000	-0.52171300
C	-2.55794900	0.71736600	0.78874800
H	-2.29284100	0.31044600	-1.30059900
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H	-3.84690800	-1.70694100	0.37076800
H	-3.64584600	-1.75920600	-1.37530900
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H	-2.64529300	0.14138200	1.71763900
H	-1.64878100	1.31329400	0.86894000
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H	-5.85241300	-0.78661100	-0.74768700
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H	-3.85318900	2.29439500	1.49250100
H	-3.65359900	2.24793600	-0.24886600
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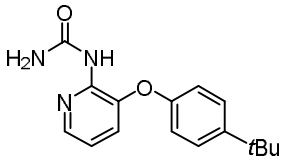
H	-5.23004500	0.23783900	1.41873000



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C	-1.13474500	1.83599600	0.20581500
C	-1.60246700	0.54788200	0.15480300
C	-2.99473800	0.32371300	0.02932600
H	-4.13308400	3.36244400	-0.06622100
H	-1.72208400	3.91331400	0.16152100
H	-0.07508000	2.02456300	0.30563100
N	-3.85063400	1.32638600	-0.04481000
C	-4.69737500	-1.54736000	-0.12344200
N	-5.72618800	-0.67978200	-0.21188700
H	-5.55847600	0.31534200	-0.19527400

H	-6.64327200	-1.07847300	-0.29253600
O	-4.81155000	-2.75601200	-0.13615000
N	-3.41892100	-0.98814800	-0.00995800
H	-2.69928800	-1.69174700	0.05232800
O	-0.83302000	-0.57928100	0.23913600
C	0.54339100	-0.43882800	0.16557400
C	1.29815000	-0.61078400	1.30608100
C	1.14992300	-0.17325000	-1.05246700
C	2.68434600	-0.51954200	1.22690800
H	0.80269800	-0.82118500	2.24377500
C	2.52837400	-0.08121900	-1.11200900
H	0.53896200	-0.04517100	-1.93605800
C	3.32754800	-0.25183400	0.02308500
H	3.25723900	-0.66319600	2.13091200
H	2.99085500	0.12166100	-2.06892800
C	4.84588300	-0.14622000	-0.10147900
C	5.21772000	1.24661500	-0.62873900
H	6.30142500	1.33260600	-0.72304700
H	4.77986100	1.43544200	-1.60863000
H	4.86932900	2.02293200	0.05357400
C	5.34989800	-1.21255000	-1.08402000
H	6.43483900	-1.14740400	-1.18095400
H	5.09496500	-2.21258900	-0.73159900
H	4.91575700	-1.08251000	-2.07504900
C	5.54910900	-0.35616300	1.23896200
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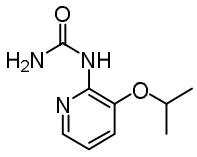

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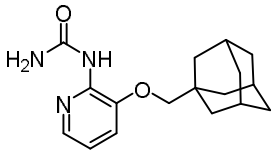
C	-0.30700100	2.90749400	-0.15502100
C	-1.16472800	1.80283600	-0.19066900
C	-0.62820700	0.53905300	-0.13998700
C	0.78446000	0.41031900	-0.05001100
H	1.74470300	3.51118200	-0.03417800
H	-0.70110400	3.91181100	-0.19246400
H	-2.23238700	1.95063600	-0.25368700
N	1.58149300	1.46017900	-0.01575800
C	2.59818300	-1.35504500	0.08220000
N	3.57670300	-0.42806600	0.13065300
H	3.34984500	0.55512700	0.10340700
H	4.51746600	-0.77129300	0.19038700
O	2.78402700	-2.55513400	0.10813000
N	1.28760600	-0.87329300	-0.00305700
H	0.60739900	-1.61649900	-0.03744000
O	-1.30708000	-0.63250500	-0.18518400
C	-2.73916600	-0.62045700	-0.19778600

H	-3.06949300	0.13077600	-0.92027900
C	-3.27736900	-0.30622700	1.18750000
H	-2.90774300	0.64697900	1.56128400
H	-4.36611500	-0.26869600	1.16468300
H	-2.97173800	-1.08866500	1.88213400
C	-3.16120400	-1.99304600	-0.67770600
H	-4.24776500	-2.05552000	-0.71950200
H	-2.75870400	-2.19506600	-1.66836300
H	-2.79570100	-2.75546800	0.01013800



C	-4.46967600	-1.87185900	-0.00910000
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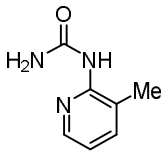
C	-2.16079500	-2.46271100	0.00239500
C	-1.85608200	-1.12398100	0.03026200
C	-2.92091800	-0.18437400	0.02919500
H	-5.52169100	-2.12421800	-0.02239900
H	-3.77991400	-3.89247000	-0.03459800
H	-1.37799100	-3.20671300	-0.00466900
N	-4.18350800	-0.56123700	0.01123600
C	-3.33985200	2.31497900	-0.00255900
N	-4.67738600	2.14632300	-0.03648900
H	-5.07408000	1.21802200	-0.03264800
H	-5.23435300	2.97944200	-0.08178200
O	-2.77940000	3.39270800	-0.01010200
N	-2.56797800	1.14960300	0.04536100
H	-1.57923900	1.34523100	0.05922800
O	-0.61540500	-0.58638300	0.05788900
C	0.49890700	-1.45935500	-0.05566400
H	0.49022700	-2.17255400	0.77675000
H	0.42111600	-2.01747500	-0.99625700
C	1.77761700	-0.64425600	-0.02711900
C	1.93463200	0.07723500	1.31974000
C	2.96327600	-1.60200800	-0.21787700
C	1.79483100	0.39555900	-1.15803500
H	1.91720200	-0.65878300	2.13037200
H	1.09167300	0.75432000	1.47563600
C	3.25199000	0.85842600	1.34769200
H	2.85963200	-2.12948100	-1.17142300
H	2.95870400	-2.35608800	0.57601500
C	4.28373700	-0.82464500	-0.19296500
H	0.95152200	1.08009100	-1.04553500
H	1.67615700	-0.11122000	-2.12141900
C	3.11133200	1.17831600	-1.13224000
H	3.34953600	1.36582100	2.30898300
C	4.42493400	-0.10826900	1.15438200
C	3.25126800	1.89314800	0.21636600
H	5.11311300	-1.52081700	-0.32958000

C	4.28420700	0.21183800	-1.32282900
H	3.10722200	1.91372800	-1.93855300
H	4.44449100	-0.83951800	1.96709400
H	5.36985500	0.43995400	1.18698500
H	2.42759000	2.59812800	0.35342900
H	4.18016700	2.46862300	0.23710200
H	5.22765000	0.76344100	-1.32086400
H	4.20162800	-0.28944600	-2.29098400



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C	-1.30242700	0.92565700	0.00006100
C	-0.20103400	0.03875900	0.00007000
H	-1.62662500	-2.87798900	-0.00020000
H	-3.68833100	-1.48733800	-0.00018700
H	-3.42672000	1.00169300	-0.00003500
N	-0.33881100	-1.28052600	-0.00002300
C	2.34754800	0.00114700	-0.00003400
N	2.39825300	-1.34461100	0.00034500
H	3.31163500	-1.75985900	0.00023100
H	1.54451100	-1.88367600	0.00017200
O	3.31911500	0.73052800	-0.00039600
N	1.07199000	0.58392100	0.00012200
H	1.14627500	1.58758600	0.00018000
C	-1.10193800	2.41189600	0.00009400
H	-0.54715900	2.74087400	0.88181800
H	-0.54738300	2.74091700	-0.88175400
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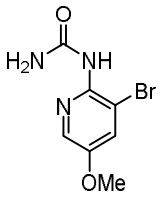

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C	1.53746400	0.92422400	0.00009700
C	0.17592100	0.78421000	0.00002900
C	-0.39943600	-0.50749700	-0.00005900
H	2.27241800	-2.37032800	-0.00006500
H	1.99987700	1.90092000	0.00014600
N	0.38191200	-1.57204700	-0.00006300
C	-2.59206000	-1.78827300	-0.00004100
N	-1.97158700	-2.98546900	0.00051300
H	-0.96504200	-3.04103500	0.00063200

H	-2.56328200	-3.79574000	0.00060000
O	-3.79629100	-1.63779800	-0.00031700
N	-1.77261600	-0.65139600	-0.00046700
H	-2.32338000	0.19293900	0.00048900
O	3.68194900	-0.01465500	0.00006900
C	4.50430100	-1.16353500	-0.00016100
H	5.52841200	-0.80464600	-0.00082500
H	4.33075400	-1.76970600	0.89197800
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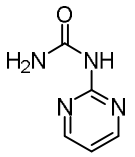

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C	2.88209500	0.35710600	0.00018200
C	2.47452900	-0.97104400	0.00026200
C	0.30355000	-0.33811400	-0.00020800
H	2.08860200	2.35686700	-0.00023900
N	0.58168100	0.96603400	-0.00030900
C	-2.22328900	-0.06955100	-0.00000500
N	-2.15622000	1.27676100	0.00037700
H	-3.03091400	1.76841000	0.00039700
H	-1.26536700	1.74843300	-0.00017100
O	-3.25307500	-0.70938300	0.00013700
N	-1.00173100	-0.76068100	-0.00047700
H	-1.12239900	-1.76229300	-0.00001600
H	3.92318900	0.63711100	0.00035200
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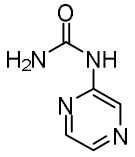
N	1.20337500	-1.33065800	0.00005200



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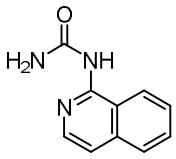
H	2.11159100	2.34131900	0.00030700
N	0.58255500	0.95937300	0.00013900
C	-2.23953700	-0.05934300	-0.00005400
N	-2.15935600	1.28561000	-0.00022300
H	-3.02940500	1.78589400	0.00014400
H	-1.26475100	1.75046300	-0.00015700
O	-3.27344100	-0.69266700	0.00023900
N	-1.02196800	-0.75896200	-0.00023300
H	-1.17917300	-1.75474000	0.00020300
H	3.92030100	0.61177600	-0.00018600
N	2.58127000	-0.97127100	-0.00002800

C	1.31291300	-1.30208100	0.00003300
H	1.06396100	-2.35784300	0.00003300



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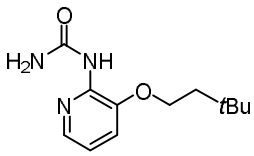
H	2.84000300	1.44209900	0.00003600
O	3.64743800	-1.61113200	0.00034000
N	1.57760400	-0.72516300	0.00005100
H	1.32281500	-1.69699200	0.00051600
C	0.56685000	0.21279800	-0.00006600
C	-0.79919600	-0.25515700	-0.00008400
C	-1.16873800	-1.61713500	-0.00025300
C	-1.81229500	0.72764200	0.00006500
C	-0.11820000	2.40824700	-0.00002500
C	-2.48807200	-1.98361200	-0.00015000
H	-0.42405100	-2.40047700	-0.00055800
C	-3.16520800	0.32306400	0.00017100
C	-1.43793600	2.09541400	0.00008900
H	0.21195000	3.43878700	-0.00007100
C	-3.49686200	-1.00309700	0.00009700
H	-2.75542700	-3.03102200	-0.00028300
H	-3.93357800	1.08525900	0.00030400
H	-2.19471800	2.86677200	0.00015600
H	-4.53573400	-1.30389300	0.00018900
N	0.87612700	1.48426300	-0.00004500



C	3.05894200	2.37253500	-0.01188900
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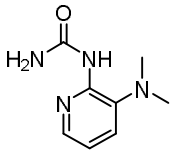
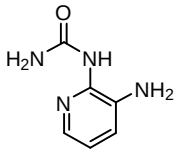
C	0.68073600	2.23063100	0.01175000
C	0.79758300	0.86261200	0.01467600
C	2.09819800	0.29179700	0.00496900
H	3.98397900	2.93352800	-0.02336600
H	1.78593500	4.08691100	-0.00519600
H	-0.29065900	2.70227300	0.02045300
N	3.18559100	1.03717900	-0.00810000
C	3.26246400	-1.95920400	-0.00043900
N	4.48472700	-1.38940300	-0.01587000
H	4.57939600	-0.38455700	-0.02048900
H	5.27053300	-2.01281800	-0.02445100
O	3.05995300	-3.15663500	0.00519400
N	2.16948200	-1.08571400	0.00944100

H	1.28778300	-1.57448200	0.02001500
O	-0.22413900	-0.02553900	0.02552300
C	-1.55129300	0.48512300	0.00732800
H	-1.71082800	1.10122600	0.89709000
H	-1.67876100	1.11409400	-0.87814900
C	-3.98455900	-0.36403900	-0.00566200
C	-2.48652200	-0.70518100	-0.02213100
H	-2.25452800	-1.34159300	0.83572200
H	-2.26203800	-1.28727700	-0.91967700
C	-4.35175900	0.53713700	-1.18664700
H	-5.43343300	0.67195100	-1.23592000
H	-3.90276900	1.52739300	-1.09631600
H	-4.02328100	0.09791900	-2.13095300
C	-4.37523300	0.32282300	1.30451000
H	-5.45436000	0.48127100	1.33888800
H	-4.09776100	-0.29027500	2.16401700
H	-3.89975200	1.29848400	1.41378900
C	-4.75854900	-1.67797900	-0.12214700
H	-5.83385300	-1.49404500	-0.10119400
H	-4.52034200	-2.19053700	-1.05573900
H	-4.51320000	-2.34775000	0.70397900



C	0.31319800	2.64493100	0.09992400
C	1.66249100	2.39010100	0.03115600
C	2.07519900	1.05992400	-0.05014800
C	1.14167000	0.04667700	-0.06954100
C	-0.22807800	0.42385500	-0.04663500
H	-0.06049600	3.65774400	0.18038500
H	2.37848200	3.19792900	0.05020100
H	3.12941400	0.82227400	-0.09083300
N	-0.61646600	1.68442100	0.05459800
C	-2.55935100	-0.57825700	-0.12833500
N	-3.14768600	0.60410700	0.15249600
H	-4.14995600	0.62142900	0.10453600
H	-2.59223000	1.44685900	0.17766200
O	-3.15902200	-1.61564400	-0.32742900
N	-1.16111100	-0.58839000	-0.15414000
H	-0.78565200	-1.49205000	-0.40327000
N	1.45721900	-1.33305700	-0.13803400
C	1.29452900	-2.01848900	1.14496600
H	1.36596200	-3.09404400	0.98698700
H	2.07030100	-1.71369200	1.85953800
H	0.32080300	-1.79472800	1.57595200
C	2.74195400	-1.64701300	-0.73633800
H	3.58990500	-1.38005400	-0.09060400
H	2.78751000	-2.71975600	-0.91903800
H	2.84477900	-1.12669500	-1.68681200



C	1.59923600	-1.76754700	-0.04921200
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C	2.55315700	0.40791500	-0.00584300
C	1.28439900	0.94396400	0.02722700
C	0.19467000	0.04200100	-0.02649300
H	1.67600500	-2.84677100	-0.06137400
H	3.70912500	-1.41278700	-0.07857500
H	3.41108400	1.06863300	0.02222300
N	0.35868900	-1.26819500	-0.04059800
C	-2.34596600	0.00011400	-0.01769900
N	-2.38031500	-1.32355000	0.24903400
H	-3.28569500	-1.75491500	0.20279300
H	-1.52780600	-1.86230000	0.18908000
O	-3.32640100	0.69726100	-0.18197600
N	-1.07835700	0.59442800	-0.05947400
H	-1.13837100	1.56139100	-0.34053200
N	1.02675500	2.32235400	0.04976000
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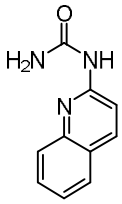

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H	1.78920500	-1.76056500	-0.00006700
O	4.46654000	-0.08050100	0.00018400
N	2.34600200	0.68175300	-0.00015300
H	2.80485600	1.57823600	0.00007100
C	0.96472900	0.67947100	-0.00008000
C	0.32352800	1.95799400	-0.00003400
C	-1.06094700	-0.40775700	-0.00003500
C	-1.02930800	2.00811100	0.00001500
H	0.92390800	2.85727100	-0.00004200
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C	-1.77484700	-1.62403900	-0.00003700
H	-1.54727300	2.95914800	0.00005200
C	-3.19193400	0.78059000	0.00006800
C	-3.14429400	-1.62243000	0.00001300
H	-1.21113200	-2.54673600	-0.00007800
C	-3.86405700	-0.41193500	0.00006700

H	-3.73109500	1.71970700	0.00011000
H	-3.68200700	-2.56086700	0.00001100
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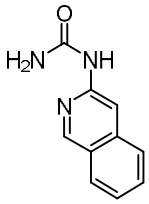

C	-3.49028800	-0.17094300	0.00001200
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H	-2.65382500	1.70399900	0.00000000
O	-4.48137900	-0.87411900	0.00004500
N	-2.23324100	-0.78570100	-0.00006300
H	-2.33108100	-1.78824100	-0.00001600
C	-0.93944100	-0.28845400	-0.00003400
C	0.12405200	-1.16699600	-0.00001900
C	1.43438900	-0.66695600	-0.00000400
H	-0.04870200	-2.23521700	-0.00001900
C	0.44945900	1.53075800	-0.00002200
C	1.61191100	0.73726400	-0.00000600
C	2.58814800	-1.49361800	0.00001200
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C	3.83240000	-0.93442600	0.00002500
H	2.46421100	-2.56866200	0.00001200
C	4.00444000	0.47174500	0.00002300
H	3.02655700	2.36729400	0.00000700
H	4.70638700	-1.57201700	0.00003600
H	5.00219300	0.88714800	0.00003500
N	-0.76989600	1.05492300	-0.00003700