DMSO as Oxidant and Sulfenylating Agent for Metal-free Oxidation and Methylthiolation of Alcohol-containing Indoles

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Supporting Information

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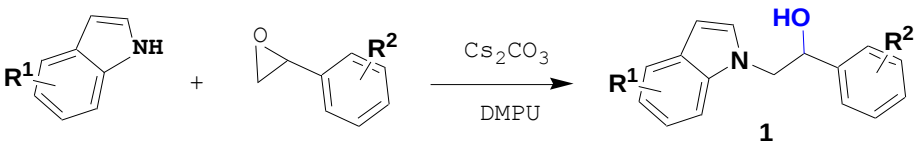
1. General information

Commercially available organic and inorganic reagents were used without further purification except for the solvent and DMSO, which was distilled by the known method before use. Flash column chromatography was performed over silica (200-300 mesh). ^{1}H-NMR was recorded at 400 MHz or 500 MHz: chemical shifts are reported in ppm relative to tetramethylsilane (TMS) with the solvent resonance employed as the internal standard ($CDCl_3$ at 7.26 ppm, DMSO at 2.50 ppm). ^{13}C-NMR was recorded at 100 MHz or 125 MHz: chemical shifts are reported in ppm from tetramethylsilane (TMS) with the solvent resonance as the internal standard ($CDCl_3$ at 77.20 ppm, DMSO at 39.52 ppm). ^{19}F-NMR NMR was recorded on a Varian Inova 400 instrument in $CDCl_3$ at 376 MHz with CF_3COOH as external standard. Chemical shifts (δ) are expressed in ppm and coupling constants J are given in Hz. Attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopy was performed on VERTEX70 IR (Bruker). The data were collected over 32 scans with a resolution of 4 cm-1 at room temperature. HRMS (Analyzer: TOF) was reported in units of mass of charge ratio (m/z). GC-MS experiments were performed with an Agilent 6890N GC system equipped with a 5973N mass-selective detector, high resolution mass spectra (HRMS) were obtained on a Waters GCT Premier TOF MS with EI or CI source.

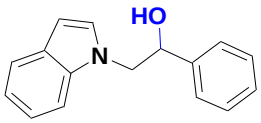
2. Synthesis of Starting Materials[1]

2.1

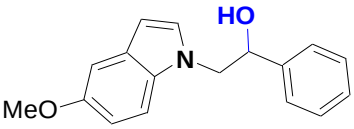


The starting substrates 1 were known compounds and prepared according to previous report[1]: A typical procedure to prepare the substituted indoles **1** is as follows: to a mixture of indole (10 mmol, 1.17 g) and styrene oxide (12 mmol, 1.44 g), cesium carbonate (20 mmol, 7.1 g) was added, then DMPU (20 mL) was added, and

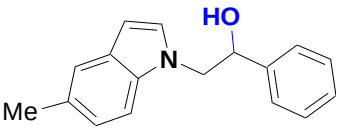
the resulting solution was stirred at 90 ^{o}C for 12 h (monitored by TLC). The mixture was allowed to cool to ambient temperature, and reaction mixture was diluted with EtOAc (150 mL) and washed thoroughly with brine, dried over anhydrous Na_2SO_4, The residue was purified by silica gel column chromatography (hexanes/acetate, 10/1) to give 2.2 g (>90 % yield) of the targeted product **1** as a yellow solid.



1a: Pale yellow solid, 92 % Yield. ^{1}H-NMR (500MHz, $CDCl_3$): δ (ppm) 7.70 (d, J = 8.0, 1H), 7.43-7.39 (m, 6H), 7.29 (t, J = 7.5, 1H), 7.19 (t, J = 7.0, 1H), 7.12 (d, J = 3.0, 1H), 6.55 (d, J = 3.0, 1H), 5.05-5.02 (m, 1H), 4.38-4.27 (m, 2H), 2.23 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 141.2, 136.3, 128.8, 128.7, 128.3, 125.9, 121.7, 121.1, 119.6, 109.5, 101.6, 73.6, 54.2; GC-MS Calcd for $C_{16}H_{15}NO$: 237.1; found: 237.1.

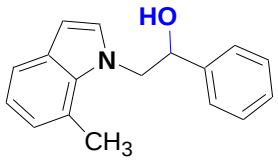


1b: Pale white solid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.43-7.37 (m, 5H), 7.29-7.27 (m, 1H), 7.13 (d, J = 2.5, 1H), 7.07 (d, J = 3.0, 1H), 6.93-6.91 (m, 1H), 6.44 (d, J = 3.0, 1H), 5.02 (t, J = 4.0, 1H), 4.33-4.22 (m, 2H), 3.89 (s, 3H), 2.27-2.25 (m, 1H); ^{13}C-NMR (125MHz, $CDCl_3$) δ (ppm) 154.2, 141.2, 131.6, 129.2, 129.1, 128.7, 128.2, 125.9, 112.1, 110.2, 102.8, 101.1, 73.6, 55.9, 54.4; GC-MS Calcd for $C_{17}H_{17}NO_2$: 267.1; found: 267.1.

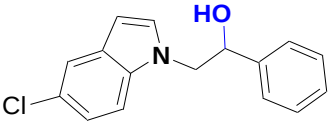


1c: Pale white solid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.6 (s, 1H), 7.53-7.49 (m, 3H), 7.42 (t, J = 8.0, 3H), 7.26 (d, J = 8.5, 1H), 7.12 (d, J = 3.0, 1H), 6.56 (d, J = 3.0, 1H), 4.96-4.94 (m, 1H), 4.34-4.25 (m, 2H), 2.69 (s, 3H); ^{13}C-NMR

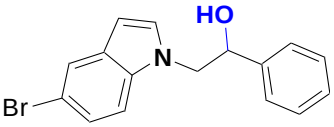
(125 MHz, $CDCl_3$) δ (ppm) 141.4, 134.8, 129.2, 129.0, 128.9, 128.8, 128.3, 126.1, 123.8, 121.0, 109.4, 101.0, 73.5, 54.3, 21.6; GC-MS Calcd for $C_{17}H_{17}NO$: 251.1; found: 251.2;



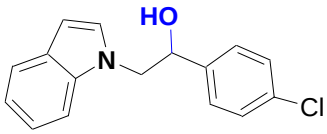
1d: Light green solid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.54 (d, J = 8.0, 1H), 7.46-7.39 (m, 5H), 7.09-7.08 (m, 3H), 6.54-6.53 (m, 1H), 4.93-4.91 (m, 1H), 4.63-4.60 (m, 1H), 4.47-4.42 (m, 1H), 2.81 (s, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 140.9, 134.8, 130.2, 130.0, 128.8, 128.3, 126.0, 125.0, 120.8, 119.9, 119.4, 102.0, 75.0, 56.2, 20.5; GC-MS Calcd for $C_{17}H_{17}NO$: 251.1; found: 251.1.



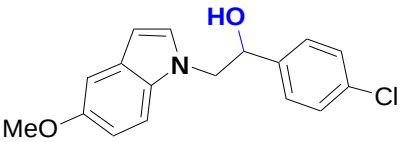
1e: Pale yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.62 (d, J = 2.0, 1H), 7.42-7.38 (m, 3H), 7.31 (d, J = 6.5, 2H), 7.25 (d, J = 9.0, 1H), 7.21-7.19 (m, 1H), 7.08 (d, J = 3.0,1H), 6.44 (d, J = 3.0, 1H), 4.92 (t, J = 4.5, 1H), 4.29-4.21 (m, 2H), 2.48-2.44 (m, 1H); ^{13}C-NMR (125MHz, $CDCl_3$) δ (ppm) 141.0, 134.8, 130.1, 129.6, 128.8, 128.4, 125.9, 125.3, 122.0, 120.4, 110.6, 101.1, 73.5, 54.1; GC-MS Calcd for $C_{16}H_{14}ClNO$: 271.1; found: 271.1.



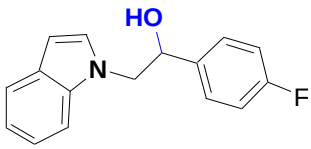
1f: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.77 (s, 1H), 7.41-7.28 (m, 6H), 7.21 (d, J = 8.5, 1H), 7.07 (s, 1H), 6.44 (s, 1H), 4.95 (t, J = 6.5, 1H), 4.30-4.22 (m, 2H), 2.34 (s, 1H); ^{13}C-NMR (125MHz, $CDCl_3$) δ (ppm) 141.0, 135.0, 130.3, 129.9, 128.8, 128.4, 125.8, 124.5, 123.8, 112.9, 111.0, 101.1, 73.6, 54.1; Calcd for $C_{16}H_{14}BrNO$: 315.0; found: 315.1.



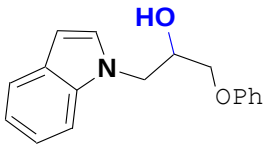
1g: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.68 (d, J = 7.5, 1H), 7.40-7.33 (m, 3H), 7.31-7.23 (m, 3H), 7.19 (t, J = 8.0, 1H), 7.05 (d, J = 3.5, 1H), 6.53 (d, J = 3.0, 1H), 4.93-4.91 (m, 1H), 4.29-4.19 (m, 2H), 2.47 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 139.6, 136.2, 134.0,128.9, 128.8, 127.3, 121.8, 121.2, 119.8, 109.4, 101.7, 72.8, 54.0; GC-MS Calcd for $C_{16}H_{14}ClNO$: 271.1; found: 271.1.



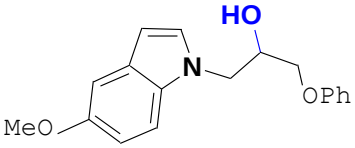
1h: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.35 (d, J = 8.5, 2H), 7.25 (t, J = 8.5, 3H), 7.11 (d, J = 2.5, 1H), 7.01 (d, J = 3.0, 1H), 6.92-6.89 (m, 1H), 6.42 (d, J = 3.0, 1H), 4.95-4.93 (m, 1H), 4.27-4.16 (m, 2H), 3.87 (s, 3H), 2.38 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 154.2, 139.6, 133.9, 131.5, 129.1, 128.8, 127.2, 110.1, 102.9, 101.2, 72.9, 55.9; GC-MS Calcd for $C_{17}H_{16}ClNO_2$: 301.1; found: 301.1.



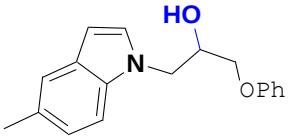
1i: Light yellow liquid, 90 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.70 (d, J = 8, 1H), 7.38 (d, J = 8.0, 1H), 7.29 (t, J = 5.5, 3H), 7.22-7.18 (m, 1H), 7.11-7.06 (m, 3H), 6.54 (d, J = 3.0, 1H), 4.94 (s, 1H), 4.30-4.21 (m, 2H), 2.45 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 163.6, 161.6, 136.9, 136.2, 128.7, 127.6 (d, J = 32.5), 121.8, 121.2, 119.7, 115.6 (d, J = 86), 109.4, 101.6, 72.8, 54.1; F-NMR (80 MHz, CD_3Cl) δ (ppm) -113.8; GC-MS Calcd for $C_{17}H_{16}FNO$: 255.1; found: 255.1.



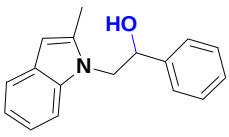
1j: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.70 (d, J = 8, 1H), 7.45 (d, J = 8.0, 1H), 7.35 (t, J = 7.5, 2H), 7.26 (t, J = 8.0, 1H), 7.18 (t, J = 7.5, 2H), 7.05 (t, J = 7.5, 1H), 6.95 (d, J = 8.0, 2H), 6.57 (d, J = 3.0, 1H), 4.47-4.32 (m, 3H), 3.96-3.88 (m, 2H), 2.45 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 158.3, 136.4, 129.7, 128.7, 128.6, 121.9, 121.5, 121.1, 119.7, 114.7, 109.4, 101.9, 69.5, 68.9, 48.8; GC-MS Calcd for $C_{17}H_{17}NO_2$: 267.1; found: 267.1.



1k: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, $CDCl_3$) δ (ppm) 7.39-7.32 (m, 3H), 7.18-7.16 (m, 2H), 7.08 (t, J = 7.5, 1H), 6.95 (d, J = 9.0, 3H), 6.51 (d, J = 3.0, 1H), 4.40-4.24 (m, 3H), 3.92-3.84 (m, 5H, 2.87 (s, 1H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 158.3, 154.2, 131.9, 129.7, 129.3, 129.1, 121.5, 114.7, 112.2, 110.3, 102.9, 101.4, 69.5, 68.9, 56.0, 49.0; GC-MS Calcd for $C_{18}H_{19}NO_3$: 297.1; found: 297.1.



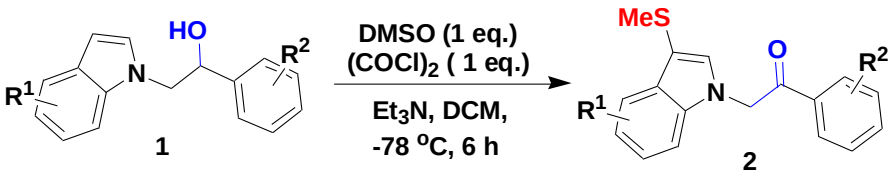
1l: Light yellow liquid, 90 % Yield. ^{1}H-NMR (500 MHz, CDC_3l) δ (ppm) 7.37 (s, 1H), 7.27-7.21 (m, 3H), 7.01-6.93 (m, 3H), 6.83 (d, J = 8.0, 2H), 6.37 (d, J = 3.2, 1H), 4.30-4.13 (m, 3H), 3.81-3.72 (m, 2H), 2.50 (s, 1H), 2.41 (s, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 158.3, 134.9, 129.7, 129.0, 128.9, 128.8, 123.6, 121.5, 120.8, 114.7, 109.2, 101.4, 69.5, 48.8, 21.5; GC-MS Calcd for $C_{18}H_{19}NO_2$: 281.1; found: 281.1;



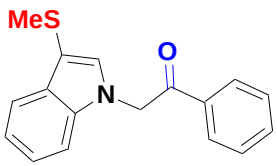
1m: Deep brown liquid, 80 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.51-7.07 (m, 10H), 5.01-4.98 (m, 1H), 4.23-4.07 (m, 2H), 2.24 (s, 2H), 2.01 (s, 1H), 1.24 (s, 1H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 141.4, 137.4, 136.9, 128.7, 128.2, 128.3, 125.8, 120.7, 119.8, 109.3, 100.3, 73.2, 51.1, 12.9; GC-MS Calcd for $C_{17}H_{17}NO$: 251.1; found: 251.1.

3. Preparation of 3-Sulfenylindoles under the Swern Oxidation Reaction conditions[2]

3.1

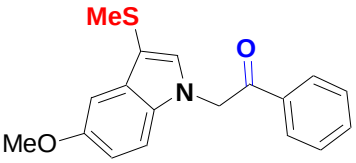


At -78 °C, under N_2, DMSO (0.74 mL, 1 equiv.) was added dropwise to a solution of oxalyl chloride (0.355 mL, 1 equiv.) in 10 mL of CH_2Cl_2. The mixture was stirred for 30 min before a solution of indole **1** (0.474 g, 2 mmol, 1 equiv.) in 10 mL of CH_2Cl_2 was added slowly over a period of time of 15 min. After 1 h at -78 °C, dry NEt_3 (2.47 mL, 5 equiv.) was added. The mixture was left 15 min at -78 °C and 1 h at rt. The reaction was then quenched by the addition of 25 mL of brine and 10 mL of H_2O. The aqueous phase was extracted by 3×25 mL of CH_2Cl_2. The combined organic phases were dried on Na_2SO_4, filtered, and evaporated under vacuum. The crude was purified by chromatography on silica (petroleum ether/acetate: 10/1). The precipitate was recrystallized and dried to give **2** as a white solid.

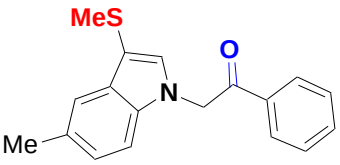


2a: A pale white solid, mp: 148-152 °C, 63 % Yield. ^{1}H-NMR (400 MHz, DMSO-D_6) δ (ppm) 8.11 (d, J = 7.6, 2H), 7.72 (d, J = 7.6, 1H), 7.66-7.60 (m, 3H), 7.51 (s, 1H), 7.43 (d, J = 8, 1H), 7.17-7.14 (m, 2H), 5.93 (s, 2H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz,

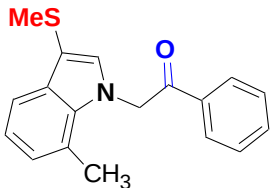
DMSO-D_6) δ (ppm) 194.1, 137.3, 134.7, 133.8, 132.9, 128.9, 128.7, 128.0, 121.9, 119.7, 118.5, 110.6, 105.4, 52.4, 19.5; IR (ν_{max}/cm^{-1}): 2922.2, 1694.4, 1511.6, 1499.8, 1224.9, 1167.1, 977.9, 757.7, 688.7; GC-MS Calcd for $C_{17}H_{15}NOS$: 281.1; found: 281.1; HRMS (MALDI-TOF) Calcd for $C_{17}H_{15}NOS$ [$M+H^+$]: 282.0908; found: 282.0960.



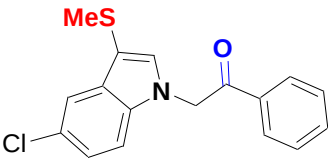
2b: A pale white solid, mp: 108-110 ^oC, 65 % Yield. ^{1}H-NMR(500 MHz, DMSO-D_6) δ (ppm) 8.09 (d, J = 7.5, 2H), 7.72 (t, J = 7.5, 1H), 7.61 (t, J = 8, 2H), 7.47 (d, J = 5.5, 1H), 7.34-7.32 (m, 1H), 7.11-7.09 (m, 1H), 6.82-6.80 (m, 1H), 5.87 (s, 2H), 3.82 (s, 3H), 2.33 (s, 3H); ^{13}C-NMR (125MHz, DMSO-D_6) δ (ppm) 194.7, 154.7, 135.2, 134.3, 134.2, 132.9, 129.8, 129.3, 128.6, 112.4, 112.0, 105.2, 110.7, 55.9, 53.0, 20.2; IR (ν_{max}/cm^{-1}): 2915.3, 1696.4, 1481.8, 1290.9, 1224.5, 1034.1, 848.6, 762.4, 617.1; GC-MS Calcd for $C_{18}H_{17}NO_2S$: 311.1; found: 311.1; HRMS (MALDI-TOF) Calcd for $C_{18}H_{17}NO_2S$ [$M+ H^+$]: 312.1014; found: 312.1054.



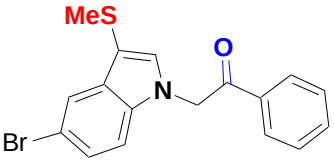
2c: A pale white solid, mp: 142-145 ^oC, 60 % Yield. ^{1}H-NMR(500 MHz, DMSO-D_6) δ (ppm) 8.10 (d, J = 7.5, 2H), 7.72 (t, J = 7, 1H), 7.61 (t, J = 7.5, 2H), 7.44 (d, J = 6.5, 2H), 7.30 (d, J = 8.5, 1H), 6.99 (d, J = 8.5, 1H), 5.87 (s, 2H), 2.43 (s, 3H), 2.34 (s, 3H); ^{13}C-NMR (125 MHz, DMSO-D6) δ (ppm) 194.6, 136.2, 135.2, 134.3, 133.5, 129.4, 129.3, 128.9, 128.6, 123.9, 118.6, 110.8, 105.2, 52.9, 21.6, 20.1; IR (ν_{max}/cm^{-1}): 3114.3, 2198.6, 1695.0, 1594.9, 1508.9, 1347.8, 1224.9, 1183.9, 785.6; GC-MS Calcd for $C_{18}H_{17}NOS$: 295.1; found: 295.1; HRMS (MALDI-TOF) Calcd for$C_{18}H_{17}NOS$[$M+ H^+$]: 296.1064; found: 296.1118.



2d: A pale white solid, mp: 155-158 ^{o}C, 58 % Yield. ^{1}H-NMR(500 MHz, $CDCl_3$) δ (ppm) 7.99 (d, J = 7.5, 2H), 7.66 (d, J = 7.5, 2H), 7.54 (t, J = 8, 2H), 7.09 (t, J = 8, 2H), 7.05 (s, 1H), 6.94 (d, J = 7.5, 1H), 5.66 (s, 2H), 2.46 (s, 3H), 2.39 (s, 3H); ^{13}C-NMR (125 MHz, $CDCl_3$) δ (ppm) 193.5, 136.1, 134.3, 134.2, 133.6, 130.6, 129.1, 128.0, 125.7, 120.8, 120.5, 117.9, 107.8, 55.1, 20.2, 19.4; IR (ν_{max}/cm^{-1}): 3040.2, 2945.3, 2360.5, 1686.7, 1435.2, 1227.8, 1168.6, 783.9, 752.7, 689.2; GC-MS Calcd for $C_{18}H_{17}NOS$: 295.1; found: 295.1; HRMS (MALDI-TOF)Calcd for $C_{18}H_{17}NOS$ [M+ H^{+}]: 296.1064; found: 296.1113.

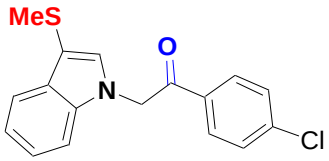


2e: A pale white solid, mp: 170-173 ^{o}C, 66 % Yield. ^{1}H-NMR(400 MHz, DMSO-D_6) δ (ppm) 8.09 (d, J = 7.6, 2H), 7.73-7.49 (m, 6H), 7.18 (d, J = 8.8, 1H), 5.95 (s, 2H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz, DMSO-D_6) δ (ppm) 193.8, 135.9, 134.8, 134.6, 133.9, 129.9, 128.8, 128.1, 124.7, 121.9, 117.6, 112.5, 105.3, 52.7,19.6; IR (ν_{max}/cm^{-1}): 2920.9, 1693.6, 1579.7, 1466.0, 1333.4, 1226.6, 756.9, 688.8, 620.4; GC-MS Calcd for $C_{17}H_{14}ClNOS$: 315.0; found: 315.1; HRMS (MALDI-TOF)Calcd for $C_{17}H_{14}ClNOS$ [M+ H^{+}]: 316.0518; found: 316.0557.

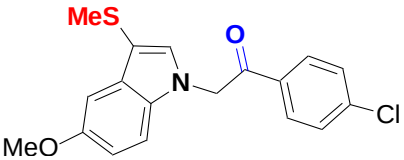


2f: A pale white solid, mp: 165-167 ^{o}C, 53 % Yield. ^{1}H-NMR(400 MHz, DMSO-D_6) δ (ppm) 8.09 (d, J = 7.6, 2H), 7.74 (d, J = 12.8, 2H), 7.63-7.57 (m, 3H), 7.46 (d, J = 8.8, 1H), 7.32 (d, J = 1.2, 1H), 5.94 (s, 2H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, DMSO-D_6) δ (ppm) 193.8, 136.2, 134.6, 133.9, 130.5, 128.9, 128.1, 124.5, 120.7,

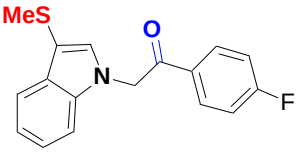
112.9, 112.6, 105.2, 52.6, 19.7; IR (ν_{max}/cm^{-1}): 2920.4, 1694.0, 1462.9, 1345.8, 1225.4, 1170.0, 756.1, 688.6, 606.1; GC-MS Calcd for $C_{17}H_{14}BrNOS$: 361.0; found: 361.0; HRMS (MALDI-TOF) Calcd for$C_{17}H_{14}BrNOS$ [M+H$^+$]: 360.0013; found: 360.0057.



2g: A pale white solid, mp: 168-170 ^{o}C, 57 % Yield. ^{1}H-NMR(400 MHz,$CDCl_3$) δ (ppm) 7.86 (d, J = 8.4, 3H), 7.45 (d, J= 8.4, 2H), 7.17 (d, J = 28, 4H), 5.33 (s, 2H), 2.37 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 191.6, 140.7, 137.2, 132.9, 131.9, 129.5, 129.4, 129.4, 122.8, 120.4, 119.7, 109.4, 108.2, 52.2, 20.3; IR (ν_{max}/cm^{-1}): 2921.2, 1693.7, 1595.6, 1466.1, 1345.6, 1226.6, 1171.5, 757.1, 689.1, 620.5; GC-MS Calcd for $C_{17}H_{14}ClNOS$: 315.0; found: 315.1; HRMS (MALDI-TOF)Calcd for $C_{17}H_{14}ClNOS$ [M+ H$^+$]: 316.0518; found: 316.0568.

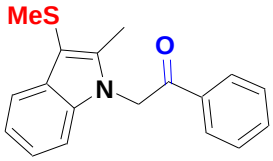


2h: A pale white solid, mp: 124-125 ^{o}C, 63 % Yield. ^{1}H-NMR(400 MHz, $CDCl_3$) δ (ppm) 7.84 (d, J = 8, 2H), 7.44 (d, J = 8, 2H), 7.19-6.86 (m, 4H), 5.28 (s, 2H), 3.86 (s, 3H), 2.35 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 191.8, 154.9, 140.7, 132.9, 132.7, 132.3, 130.2, 129.4, 129.4, 113.4, 110.3, 107.4, 101.3, 55.9, 52.4, 20.4; IR (ν_{max}/cm^{-1}): 2960.5, 1692.5, 1589.0, 1480.2, 1287.3, 1210.6, 1035.9, 978.4, 784.0; GC-MS Calcd for $C_{18}H_{16}ClNO_2S$: 345.1; found: 345.1; HRMS (MALDI-TOF)Calcd for $C_{18}H_{16}ClNO_2S$ [M+ H$^+$]: 346.0624; found: 346.0678.



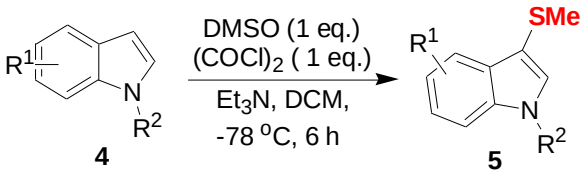
2i: A pale white solid, mp: 143-145 ^{o}C, 60 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.94-7.75 (m, 3H), 7.19-7.11 (m, 6H), 5.28 (s, 2H), 2.35 (s, 3H); ^{13}C-NMR

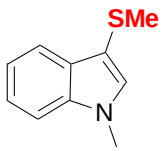
(100 MHz, $CDCl_3$) δ (ppm) 191.3, 167.6, 165.0, 137.3, 132.0, 130.8 (d, J = 9.4), 129.5, 122.8, 120.4, 119.7, 116.3 (d, J = 22), 109.5, 108.0, 52.1, 20.2; ^{19}F-NMR (80 MHz, $CDCl_3$) δ (ppm) -102.8; IR (ν_{max}/cm^{-1}): 2918.3, 1690.0, 1597.0, 1507.3, 1228.4, 1159.3, 824.5, 739.8, 576.8; GC-MS Calcd for $C_{17}H_{14}FNOS$: 299.1; found: 299.1; HRMS (MALDI-TOF) Calcd for $C_{17}H_{14}FNOS$ [M+ H$^+$]: 300.0814; found: 300.0868.



2j: A pale white solid, mp: 180-183 ^{o}C, 54 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.03 (d, J = 8, 2H), 7.77 (d, J = 7.6, 1H), 7.68 (t, J = 7.6, 1H), 7.55 (t, J = 7.6, 2H), 7.18 (t, J = 7.6, 2H), 7.08 (d, J = 8, 1H), 5.41 (s, 2H), 2.44 (s, 3H), 2.30 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 192.8, 141.0, 136.8, 134.6, 134.2, 129.8, 129.1, 128.0, 121.8, 120.4, 119.0, 108.5, 104.6, 49.8, 20.0, 10.7; IR (ν_{max}/cm^{-1}): 3058.1, 2918.7, 1686.6, 1596.6, 1463.9, 1227.2, 1174.3, 985.3; GC-MS Calcd for $C_{18}H_{17}NOS$: 295.1; found: 295.1; HRMS (MALDI-TOF)Calcd for $C_{18}H_{17}NOS$ [M+ H$^+$]: 296.1064; found: 296.1107.

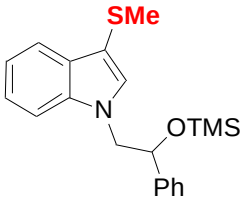
3.2



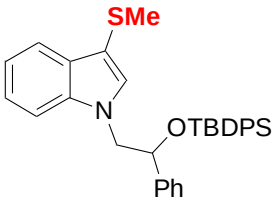


5b: A Yellow liquid, 56 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.67 (d, J = 8, 1H), 7.24-7.06 (m, 4H), 3.66 (s, 3H), 2.27 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 136.3, 131.5, 128.4, 121.2, 118.9, 118.3, 108.6, 105.1, 31.8, 19.6; IR (ν_{max}/cm^{-1}): 2918.9, 2849.8, 2361.6, 1740.4, 1499.9, 1239.5, 1011.5, 740.0, 668.9; GC-MS Calcd for $C_{10}H_{11}NS$: 177.1; found: 177.1; HRMS (MALDI-TOF)Calcd for

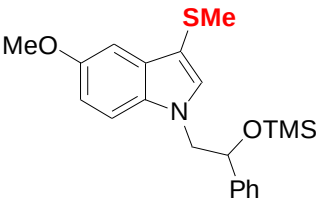
$C_{10}H_{11}NS$ [M+H^+]: 178.0646; found: 178.0702.



5c: A light yellow liquid, 82 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.99 (d, J = 7.6, 1H), 7.63-7.39 (m, 9H), 5.16-5.13 (m, 1H), 4.46-4.33 (m, 2H), 2.56 (s, 3H), 0.00 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 141.1, 136.9, 132.3, 129.5, 128.8, 128.4, 125.9, 122.5, 120.2, 119.5, 110.0, 106.7, 73.4, 54.1, 20.5; IR (ν_{max}/cm^{-1}): 2918.7, 1508.6, 1275.6, 1163.3, 749.4, 700.8; GC-MS Calcd for $C_{20}H_{25}NOSSi$: 355.1; found: 355.2;

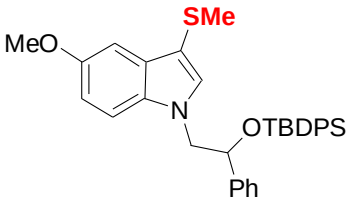


5d: A white liquid, 80 % Yield. ^{1}H-NMR(400 MHz, $CDCl_3$) δ (ppm) 7.69 (d, J = 8, 1H), 7.41-7.32 (m, 5H), 7.24-7.19 (m, 3H), 7.14-7.08 (m, 6H), 7.03-6.98 (m, 3H), 6.75 (s, 1H), 6.66 (d, J = 8, 1H), 4.92 (t, J = 6.4, 1H), 4.25-4.20 (m, 1H), 4.03-3.98 (m, 1H), 2.16 (s, 3H), 1.01 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 141.6, 136.7, 136.0, 135.9, 133.4, 132.9, 132.7, 130.0, 129.8, 129.5, 128.4, 128.0, 127.8, 127.6, 126.4, 122.2, 120.0, 119.4, 109.9, 106.3, 74.4, 55.0, 27.2, 20.6, 19.4; IR (ν_{max}/cm^{-1}): 2929.8, 2856.5, 1459.4, 1275.7, 1111.5, 749.6, 700.6, 486.5; GC-MS Calcd for $C_{33}H_{35}NOSSi$: 521.2; found: 521.3; HRMS (MALDI-TOF) Calcd for $C_{33}H_{35}NOSSi$ [M+ H^+]: 522.2242; found: 522.2278.

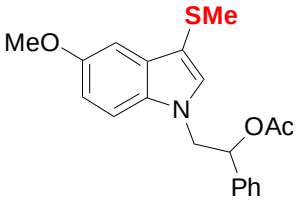


5e: A light yellow liquid, 83 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.56-7.35

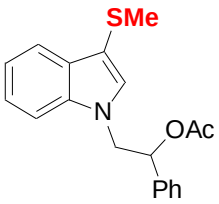
(m, 9H), 7.14-7.11 (m, 1H), 5.13-5.10 (m, 1H), 4.40-4.28 (m, 2H), 4.11 (s, 3H), 2.54 (s, 3H), 0.00 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 155.0, 142.2, 133.8, 132.3, 130.6, 128.9, 128.3, 126.2, 112.9, 111.3, 105.2, 101.2, 74.5, 56.3, 55.8, 21.1; IR (ν_{max}/cm^{-1}): 3445.0, 2919.1, 1619.3, 1485.2, 1449.7, 1217.1, 1033.0, 795.4, 704.1; GC-MS Calcd for $C_{21}H_{27}NO_2SSi$: 385.2; found: 385.2;



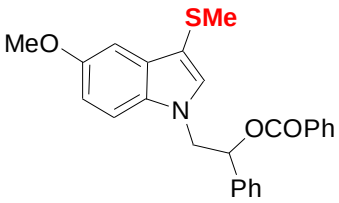
5f: A white liquid, 78 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.44 (d, J = 6.8, 2H), 7.35 (t, J = 6.4, 3H), 7.26-7.22 (m, 3H), 7.15-7.09 (m, 6H), 6.99-6.97 (m, 2H), 6.71-6.66 (m, 2H), 6.49 (d, J = 8.8, 1H), 4.90 (t, J = 6.4, 1H), 4.20-4.15 (m, 1H). 3.98-3.93 (m, 1H), 3.82 (s, 3H), 2.15 (s, 3H), 1.01 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 154.7, 141.6, 136.0, 135.9, 133.4, 133.3, 132.9, 131.8, 130.2, 130.0, 129.8, 128.3, 128.0, 127.8, 127.6, 126.3, 112.6, 110.8, 105.5, 100.8, 74.3, 56.0, 55.1, 27.2, 20.7, 19.3; IR (ν_{max}/cm^{-1}): 2931.3, 2857.5, 1619.8, 1485.3, 1218.1, 1111.3, 749.1, 702.3, 503.3; GC-MS Calcd for $C_{34}H_{37}NO_2SSi$: 551.2; found: 551.3; HRMS (MALDI-TOF)Calcd for $C_{34}H_{37}NO_2SSi$ [M+H$^+$]: 552.2348; found: 552.2383.



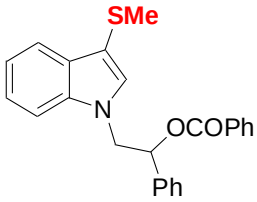
5g: A light white liquid, 81 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.17-7.05 (m, 7H), 6.79-6.76 (m, 2H), 5.89-5.86 (m, 1H), 4.29-4.23 (m, 1H), 4.14-4.09 (m, 1H), 3.74 (s, 3H), 2.15 (s, 3H), 1.85 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 169.7, 154.8, 137.4, 132.6, 132.0, 130.1, 128.8, 128.7, 126.4, 112.9, 110.9, 106.5, 100.9, 74.5, 55.9, 51.5, 21.0, 20.7; IR (ν_{max}/cm^{-1}): 2919.3, 1743.7, 1484.9, 1372.2, 1218.2, 1034.2, 797.4, 721.6; GC-MS Calcd for $C_{20}H_{21}NO_3S$: 355.1; found: 355.2; HRMS (MALDI-TOF)Calcd for $C_{20}H_{21}NO_3S$ [M+ H$^+$]: 356.1276; found: 356.1331.



5h: A light yellow liquid, 73 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.71 (d, J = 7.6, 1H), 7.34-7.12 (m, 8H), 6.89 (s, 1H), 6.00-5.94 (m, 1H), 4.23-4.18 (m, 1H), 2.25 (s, 3H), 1.90 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 169.7, 137.5, 137.1, 132.0, 129.5, 128.9, 128.8, 126.5, 122.6, 120.3, 119.6, 110.0, 107.3, 74.5, 51.3, 21.0, 20.6; IR (ν_{max}/cm^{-1}): 3637.0, 2919.6, 1745.5, 1459.8, 1231.5, 1026.9, 742.5, 700.2; GC-MS Calcd for $C_{19}H_{19}NO_2S$:325.1; found: 325.1; HRMS (MALDI-TOF) Calcd for $C_{19}H_{19}NO_2S$ [M+ H^{+}]: 326.1170; found: 326.1214.

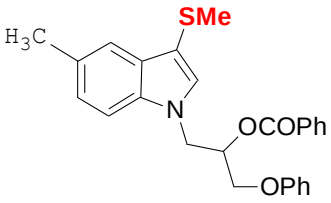


5i: A light white liquid, 79 % Yield. ^{1}H-NMR (400 MHz,$CDCl_3$) δ (ppm) 7.97 (d, J = 7.6, 2H), 7.45 (t, J = 7.2, 1H), 7.33 (t, J = 7.6, 2H), 7.27-7.16 (m, 7H), 6.88 (d, J = 9.2, 2H), 6.23 (t, J = 6, 1H), 4.49-4.44 (m, 1H), 4.35-4.30 (m, 1H), 3.80 (s, 3H), 2.17 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 165.5, 154.9, 137.5, 133.4, 132.9, 132.1, 130.2, 111.1, 106.5, 101.0, 75.0, 55.9, 51.6, 20.7; IR (ν_{max}/cm^{-1}): 2924.8, 1712.5, 1486.7, 1276.0, 1216.3, 1115.4, 960.3, 756.0, 711.4; GC-MS Calcd for $C_{25}H_{23}NO_3S$: 417.1; found: 417.2; HRMS (MALDI-TOF) Calcd for $C_{25}H_{23}NO_3S$ [M+H^{+}]: 418.1432; found: 418.1472;

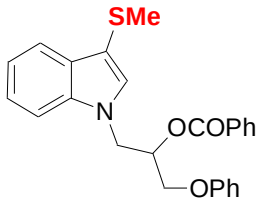


5j: A light white liquid, 82 % Yield. ^{1}H-NMR(400 MHz, $CDCl_3$) δ (ppm) 7.95 (d, J = 7.6, 1H), 7.71 (d, J = 7.6, 1H), 7.42-7.28 (m, 4H), 7.20-7.12 (m, 7H), 6.89 (s, 1H),

6.23 (t, J = 6.4, 1H), 4.51-4.45 (m, 1H), 4.36-4.32 (m, 1H), 2.17 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 165.5, 137.6, 133.5, 132.2, 129.9, 129.8, 129.6, 128.9, 128.8, 128.6, 126.5, 122.7, 120.4, 119.6, 110.2, 107.4, 75.1, 51.5, 20.6; IR (ν_{max}/cm^{-1}): 3052.1, 2921.8, 1703.4, 1459.6, 1262.2, 1113.7, 962.8, 742.4, 525.0; GC-MS Calcd for $C_{24}H_{21}NO_2S$: 387.1; found: 387.2; HRMS (MALDI-TOF) Calcd for $C_{24}H_{21}NO_2S$ [M+H$^+$]: 388.1327; found: 388.1375.

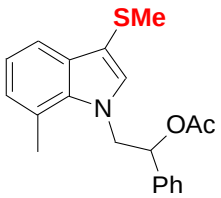


5k: A yellow liquid, 93 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.65 (d, J = 7.2, 2H), 7.50 (d, J = 6, 3H), 7.40 (t, J = 6.8, 2H), 7.33-7.26 (m, 4H), 7.20-7.16 (m, 2H), 7.09 (s, 1H), 6.92-6.83 (m, 3H), 6.64 (d, J = 8, 2H), 4.34 (d, J = 10, 2H), 4.21-4.16 (m, 1H), 3.66 (t, J = 4, 2H), 2.44 (s, 3H), 2.25 (s, 3H), 1.03 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 158.3, 135.9, 135.8, 135.4, 133.6, 132.9, 132.6, 130.1, 130.0, 129.6, 129.5, 129.3, 127.9, 127.8, 123.9, 121.1, 119.0, 114.6, 109.7, 106.1, 70.5, 68.3, 49.3, 27.0, 21.5, 20.4, 19.3; IR (ν_{max}/cm^{-1}): 3446.2, 2930.5, 2867.7, 1599.2, 1495.4, 1243.6, 1112.6, 703.4, 612.8, 507.8; GC-MS Calcd for $C_{35}H_{39}NO_2SSi$: 565.2; found: 565.4; HRMS (MALDI-TOF) Calcd for $C_{35}H_{39}NO_2SSi$ [M+H$^+$]: 566.2504; found: 566.2547.



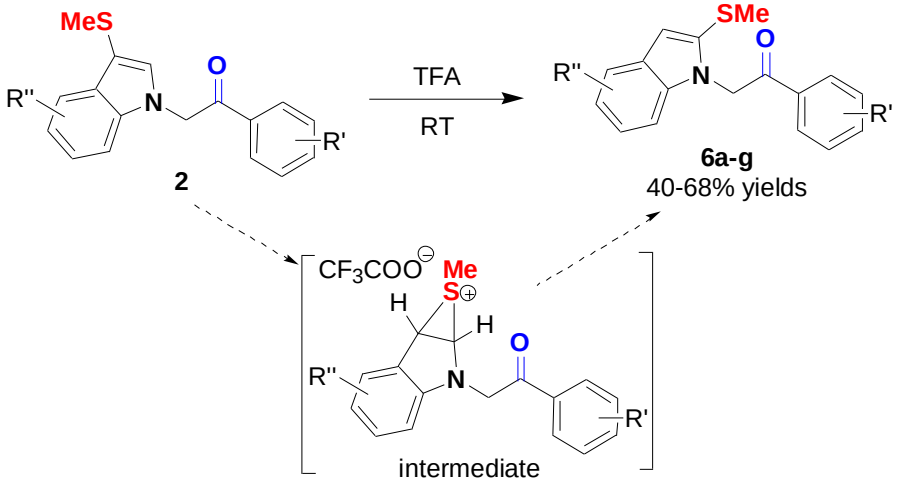
5l: A yellow liquid, 89 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.72 (d, J = 7.6, 1H), 7.64 (d, J = 7.6, 2H), 7.46 (d, J = 7.6, 2H), 7.39 (t, J = 7.6, 2H), 7.32-7.24 (m, 4H), 7.20-7.05 (m, 5H), 6.98 (d, J = 8, 1H), 6.90 (t, J = 7.2, 1H), 6.64 (d, J = 8, 2H), 4.38 (d, J = 10.8, 2H), 4.23 (t, J = 8.8, 1H), 3.66 (s, 2H), 2.66 (s, 3H), 1.02 (s, 9H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 158.3, 137.0, 135.9, 135.8, 133.6, 132.8, 132.5, 130.1, 129.5, 129.4, 127.9, 127.8, 122.4, 121.1, 120.0, 119.4, 114.6, 110.0, 106.9,

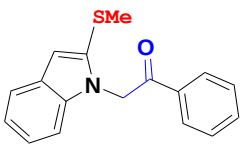
70.5, 68.4, 49.3, 27.0, 20.3, 19.3; IR (ν_{max}/cm^{-1}): 3456.0, 2930.8, 1588.9, 1460.7, 1243.5, 1112.2, 822.3, 740.0, 702.9, 508.3; GC-MS Calcd for$C_{34}H_{37}NO_2SSi$: 551.2; found: 551.3; HRMS (MALDI-TOF) Calcd for $C_{34}H_{37}NO_2SSi$ [M+H$^+$]: 522.2348; found: 522.2383.



5m: A light yellow liquid, 79 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.58 (d, J = 8, 1H), 7.26-7.19 (m, 5H), 7.03 (t, J = 7.6, 1H), 6.92 (d, J = 7.6, 2H), 5.96-5.93 (m, 1H), 4.57-4.52 (m, 1H), 4.43-4.38 (m, 1H), 2.66 (s, 3H), 2.24 (s, 3H), 1.83 (s, 3H);^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm)169.4, 137.4, 135.6, 133.5, 130.7, 129.0, 128.9, 126.6, 125.9, 121.2, 120.5, 117.8, 107.5, 75.6, 53.3, 20.5, 20.3; IR (ν_{max}/cm^{-1}): 2921.4, 1743.8, 1406.0, 1231.0, 1023.7, 941.4, 746.7, 697.3, 525.6; GC-MS Calcd for$C_{20}H_{21}NO_2S$: 339.1; found: 339.2; HRMS (MALDI-TOF) Calcd for $C_{20}H_{21}NO_2S$ [M+H$^+$]: 340.1327; found: 340.1374.

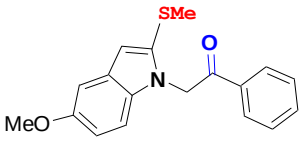
3.3



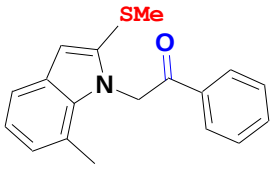


6a: A red solid, mp: 152-155 ^{o}C, 40 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm)

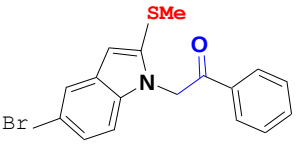
7.96 (d, J = 8, 2H), 7.56-7.42 (m, 4H), 7.07-6.96 (m, 3H), 6.68 (s, 1H), 5.57 (s, 2H), 2.25 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 193.4, 138.2, 134.9, 134.0, 133.7, 129.0, 128.1, 128.0, 122.6, 120.5, 120.2, 109.3, 107.9, 49.8, 20.4; IR (ν_{max}/cm^{-1}): 2923.5, 1686.5, 1457.1, 1349.6, 1227.1, 988.9, 739.4, 621.6; GC-MS Calcd for $C_{17}H_{15}NOS$: 281.1; found: 281.1; HRMS (MALDI-TOF)Calcd for $C_{17}H_{15}NOS$ [M+Na$^+$]: 282.0908; found: 282.0963.



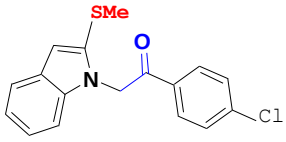
6b: A pale white solid, mp: 133-136 ^{o}C, 68 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.96(d, J = 8, 2H), 7.56 (t, J = 7.6, 1H), 7.44 (t, J = 7.6, 2H), 6.97 (s, 1H), 6.87 (d, J = 8.8, 1H), 6.74 (d, J = 8, 1H), 6.61 (s, 1H), 5.54 (s, 2H), 3.74 (s, 3H), 2.25 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 191.4, 152.5, 132.9, 132.8, 131.9, 131.8, 131.5, 127.0, 126.2, 126.0, 110.8, 108.0, 105.6, 100.2, 53.9, 47.8, 18.4; IR (ν_{max}/cm^{-1}): 2921.9, 1687.0, 1460.0, 1221.0, 971.4, 779.9, 688.2; GC-MS Calcd for $C_{18}H_{17}NO_2S$: 311.1; found: 311.1; HRMS (MALDI-TOF) Calcd for $C_{18}H_{17}NO_2S$ [M+Na$^+$]: 312.1014; found: 312.1072.



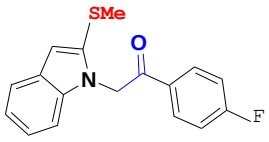
6c: A pale white solid, mp: 170-173 ^{o}C, 65 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.08 (d, J = 7.6, 2H), 7.68 (t, J = 7.2, 1H), 7.57 (t, J = 7.6, 2H), 7.46 (d, J = 8, 1H), 7.00 (t, J = 7.6, 1H), 6.90 (d, J = 7.2, 1H), 6.80 (s, 1H), 5.99 (s, 2H), 2.47 (s, 3H), 2.33 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 194.2, 137.3, 134.6, 134.1, 134.0, 129.1, 128.7, 128.1, 125.6, 120.2, 120.1, 118.8, 108.8, 52.0, 20.5, 19.7; IR (ν_{max}/cm^{-1}): 2922.6, 1449.3, 1226.0, 999.6, 783.6, 737.8, 688.8; GC-MS Calcd for $C_{18}H_{17}NOS$: 295.1; found: 295.1; HRMS (MALDI-TOF)Calcd for $C_{18}H_{17}NOS$ [M+Na$^+$]: 296.1064; found: 296.1107.



6d: A light red solid, mp: 144-148 ^{o}C, 53 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.95 (d, J = 8, 2H), 7.62-7.56 (m, 2H), 7.46 (t, J = 7.6, 2H), 7.15 (t, J = 8.8, 1H), 6.83 (d, J = 8.8, 1H), 6.57 (s, 1H), 5.52 (s, 2H), 2.28 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 192.8, 136.8, 135.6, 134.7, 134.2, 129.6, 129.1, 128.1, 125.1, 122.8, 113.5, 110.6, 106.5, 49.8, 19.9; IR (ν_{max}/cm^{-1}): 2923.3, 1683.6, 1594.8, 1459.6, 1224.6, 793.8, 752.1, 687.2; GC-MS Calcd for $C_{17}H_{14}BrNOS$: 361.0; found: 361.0; HRMS (MALDI-TOF)Calcd for $C_{17}H_{14}BrNOS$ [M+Na^{+}]: 360.0013; found: 360.0038.

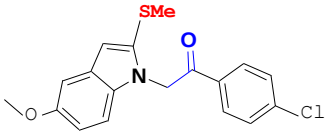


6e: A yellow solid, mp: 142-145 ^{o}C, 46 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.05 (d, J = 8, 2H), 7.64 (t, J = 7.6, 1H), 7.55 (t, J = 7.6, 3H), 7.11 (d, J = 8.8, 1H), 6.96 (d, J = 8.4, 1H), 6.97 (s, 1H), 5.60 (s, 2H), 2.37 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 192.9, 136.6, 135.8, 134.7, 134.2, 129.1, 129.0, 128.1, 125.9, 122.6, 119.7, 110.2, 106.6, 49.8, 19.9; IR (ν_{max}/cm^{-1}): 2924.7, 1685.8, 1595.3, 1459.4, 1322.1, 1224.9, 754.2, 687.7; GC-MS Calcd for $C_{17}H_{14}ClNOS$: 315.0; found: 315.1; HRMS (MALDI-TOF)Calcd for $C_{17}H_{14}ClNOS$ [M+Na^{+}]: 316.0518; found: 316.0569.

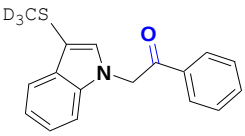


6f: A red solid, mp: 124-127 ^{o}C, 60 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.10-8.07 (m, 2H), 7.60 (d, J = 7.6, 1H), 7.23-7.06 (m, 5H), 6.78 (s, 1H), 5.65 (s, 2H), 3.37 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 190.6, 166.1, 163.6, 136.8, 132.4, 130.0 (d, J = 3), 129.5 (d, J = 9.3), 126.7, 121.2, 119.1 (d, J = 21.3), 114.9 (d, J = 21.9), 107.9, 106.4, 48.3, 18.9; ^{19}F-NMR (80 MHz, $CDCl_3$) δ (ppm) -103.2; IR

(ν_{max}/cm^{-1}): 2922.1, 1692.0, 1594.5, 1457.6, 1228.8, 1158.3, 991.4; GC-MS Calcd for $C_{17}H_{14}FNOS$: 299.1; found: 299.1; HRMS (MALDI-TOF)Calcd for $C_{17}H_{14}FNOS$ [M+Na^+]: 300.0814; found: 300.0862.



6g: A light yellow solid, mp: 168-170 ^oC, 57 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 7.96 (d, J = 8.8, 2H), 7.49 (d, J = 8.4, 2H), 7.06 (d, J = 2.4, 1H), 6.96 (d, J = 9.2, 1H), 6.85-6.82 (m, 1H), 6.69 (s, 1H), 5.58 (s, 2H), 3.84 (s, 3H), 2.34 (s, 3H); ^{13}C-NMR (100 MHz, $CDCl_3$) δ (ppm) 192.5, 154.5, 140.5, 133.8, 129.5, 129.3, 128.3, 112.9, 109.9, 107.7, 102.3, 55.9, 49.9, 29.7, 20.4; IR (ν_{max}/cm^{-1}): 2921.6, 1692.8, 1589.1, 1455.9, 1218.9, 990.7, 822.9; GC-MS Calcd for $C_{18}H_{16}ClNO_2S$: 345.1; found: 345.1; HRMS (MALDI-TOF)Calcd for $C_{18}H_{16}ClNO_2S$ [M+Na^+]: 346.0264; found: 346.0664.



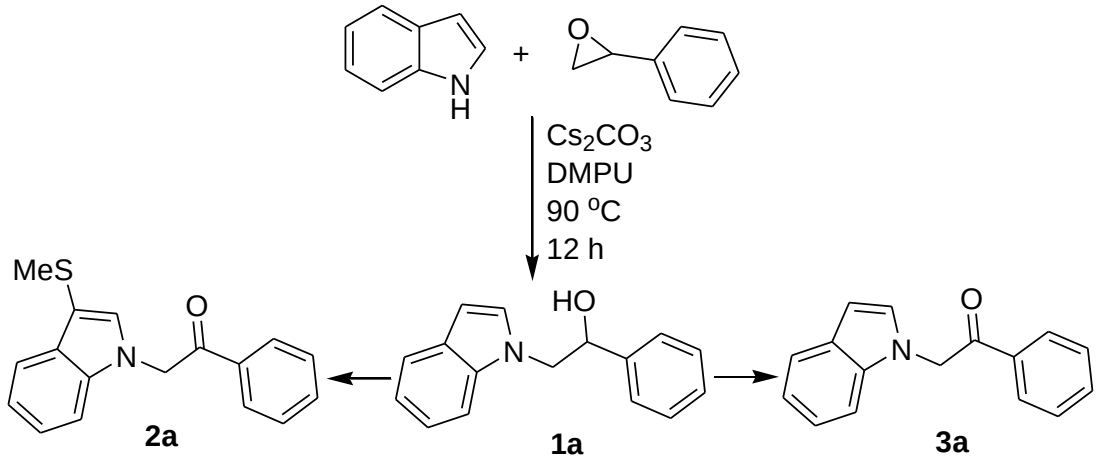
D_3-2a: A deep yellow solid, 55 % Yield. ^{1}H-NMR (400 MHz, $CDCl_3$) δ (ppm) 8.00 (d, J = 8, 2H), 7.78 (d, J = 6.8, 1H), 7.65 (t, J = 7.2, 1H), 7.54-7.47 (m, 2H), 7.25-7.17 (m, 4H), 5.46 (s, 2H); GC-MS Calcd for $C_{17}H_{12}NOSD_3$: 284.1; found: 284.1.

References

[1] Fink, D. W. *Synlett* **2004**, 2394

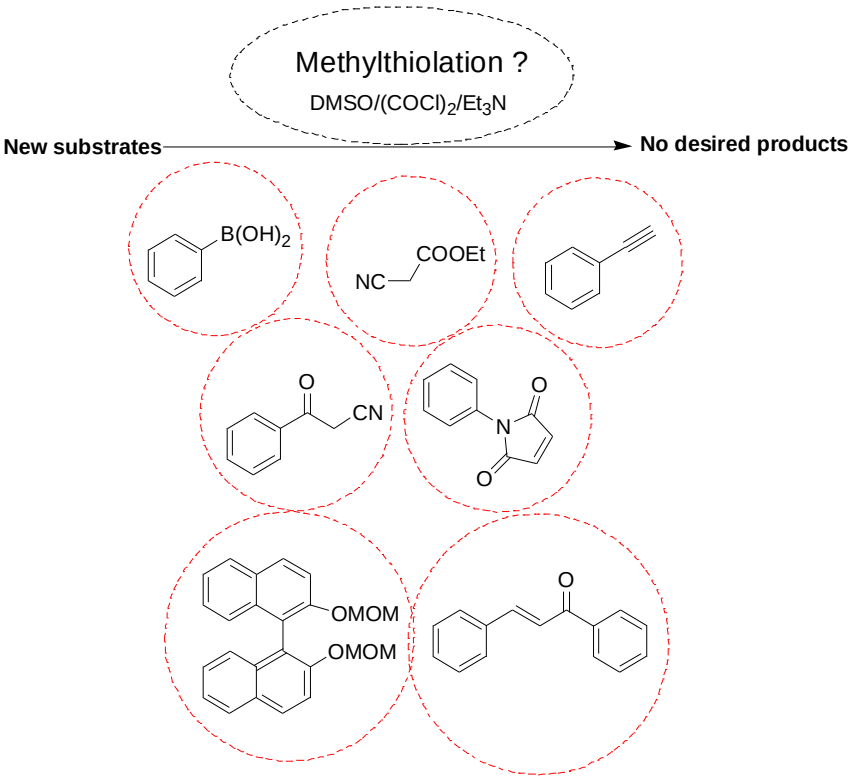
[2] (a) Mancuso, A. J.; Swern, D. *Synthesis* **1981**, 165. (b) Tidwell, T. T. *Org. React.* **1990**, *39*, 297; c) Giagou, T.; Meyer, M. P. *J. Org. Chem.* **2010**, *75*, 8088.

Table S1. Optimization studies for synchronous oxidation of and methylthiolation of indole 1a with DMSO under Swern Oxidation Conditions[a]



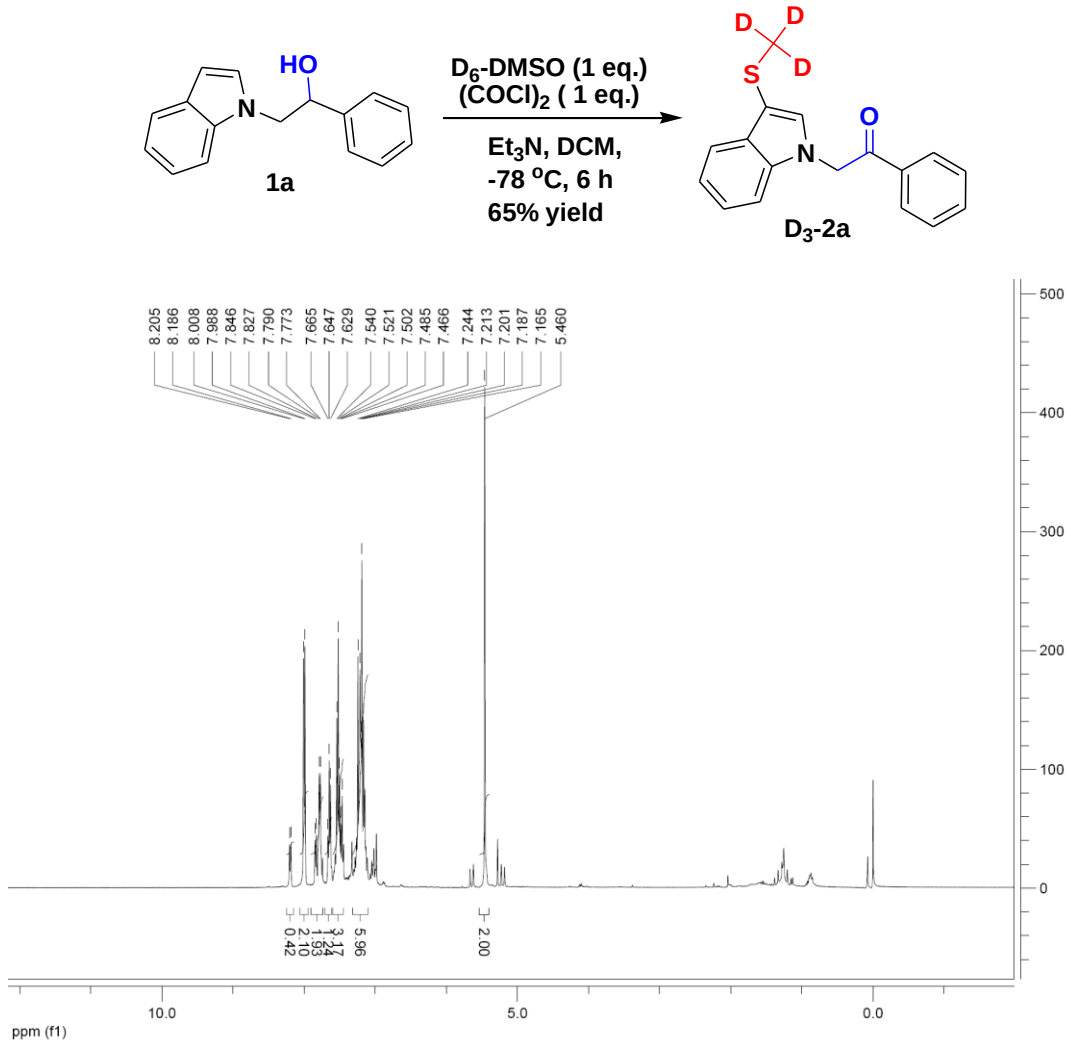
Entry	DMSO	$(COCl)_2$	Additive	Yield of **2a** (%)[b]
1	1 eq.	1 eq.	-	63
2	2 eq.	2 eq.	-	37[c]
3	4 eq.	4 eq.	-	56[c]
4	1 eq.	1 eq.	$InCl_3$[d]	50[c]
5	1 eq.	-	CH_3SiCl_3[e]	<5
6	1 eq.	-	TMSCl[e]	<5

[a] General reaction conditions: Alcohol-containing indole 1 (2 mmol), DMSO (1 eq.), oxalyl dichloride or other activator (1 eq.), Et_3N (5 eq.), DCM (20 mL), at -78 °C to room temperature for totally 6 h. [b] Isolated yields except specified note. [c] The yield of **2a** was calculated by GC because of the existence of unidentified byproducts, in which these side-products could not be isolated by flash column chromatography. [d] The amount of $InCl_3$ was 10 mol%. [e] The amount of silane activator was 1 equiv.

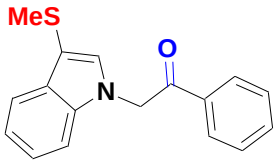


Scheme S1. The unsuccessful tries on the methylthiolation of other types of molecules

Figure S1. The oxidation and methylthiolation of substituted indole 1a with deuterated DMSO



Crude ^{1}H-NMR spectrum of the product **D_3-2a** from the oxidation and methylthiolation of substituted indole **1a** with deuterated DMSO: The S-CD_3 was introduced to the desired product because of the disappearance of δ = 2. 35 ppm (s, 3H).

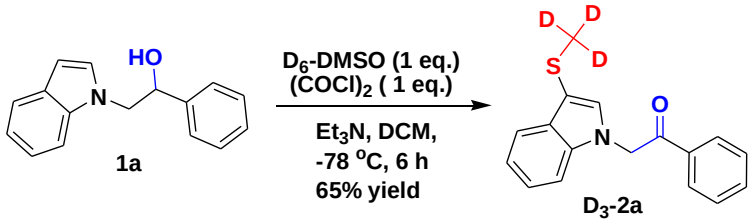


C17H15NOS

Exact Mass: 281.09

Mol. Wt.: 281.37

m/e: 281.09 (100.0%), 282.09 (19.4%), 283.08 (4.5%), 283.09 (2.0%)



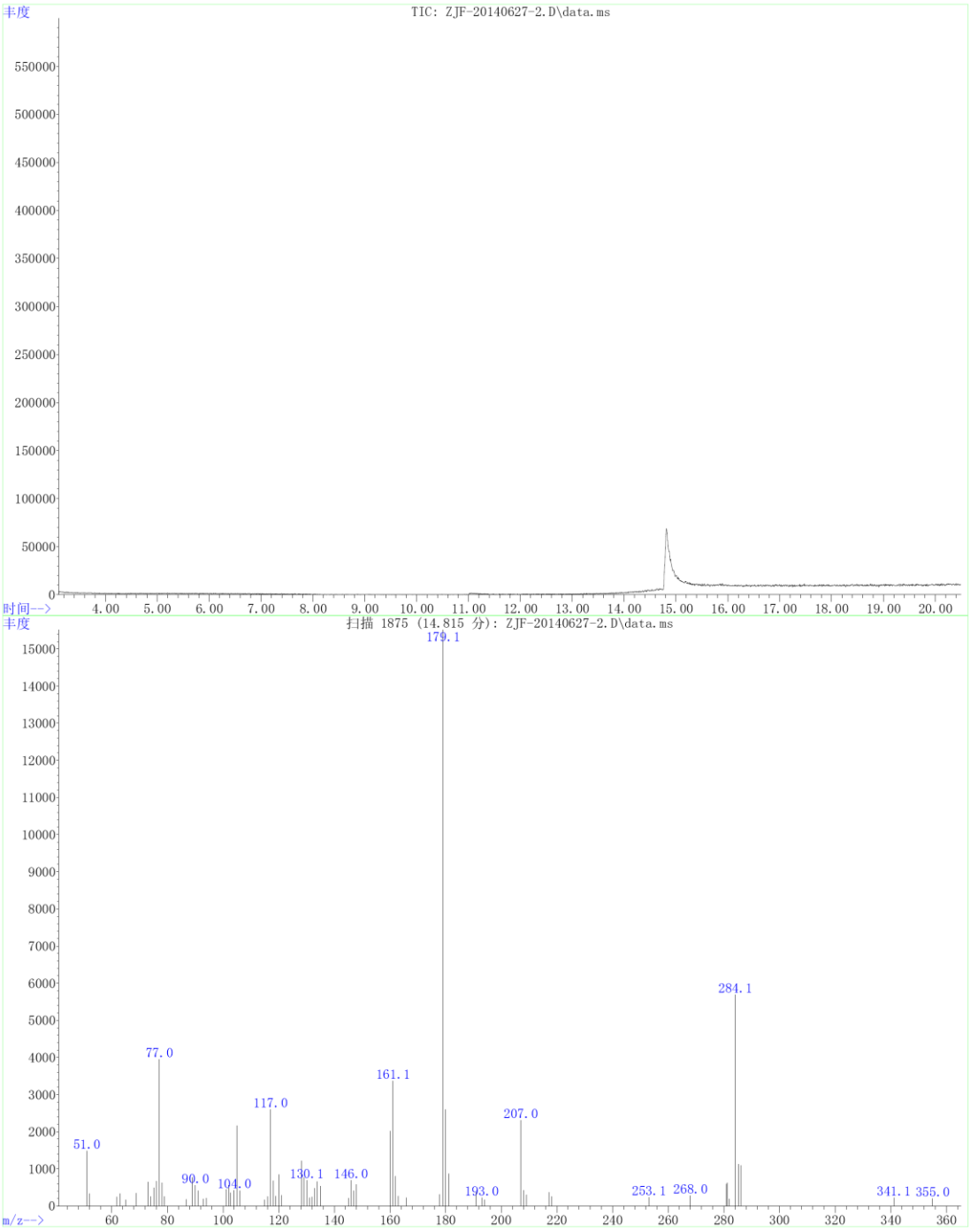
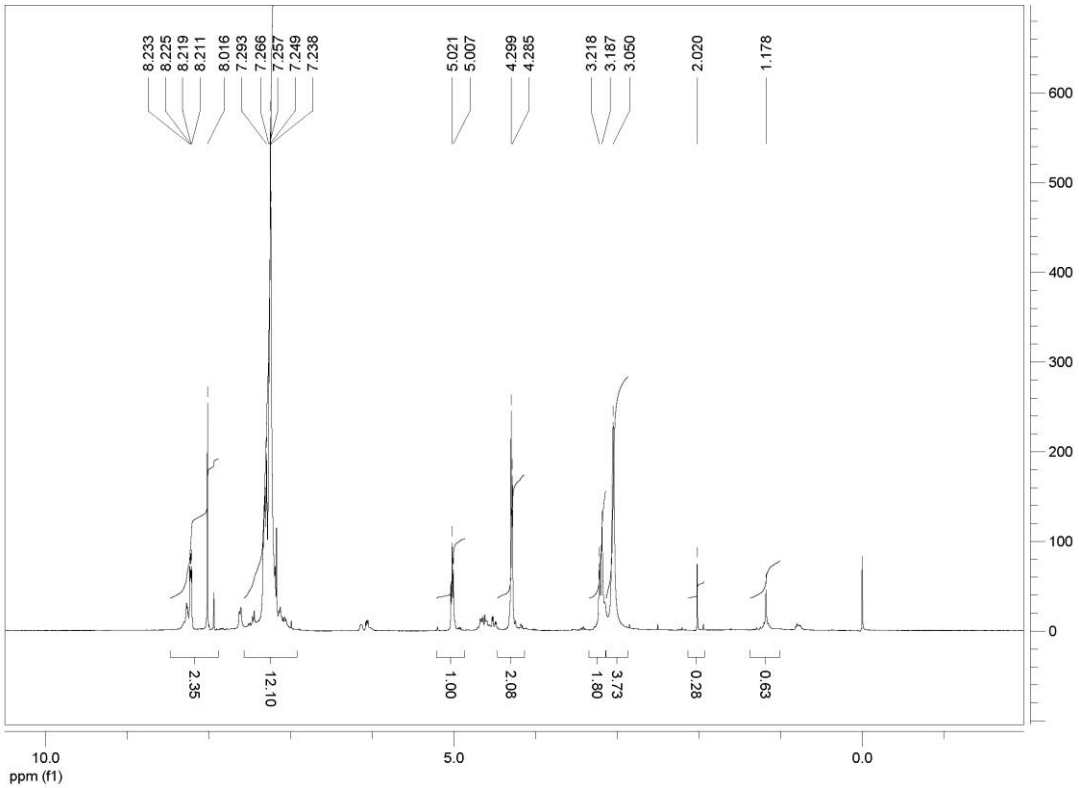
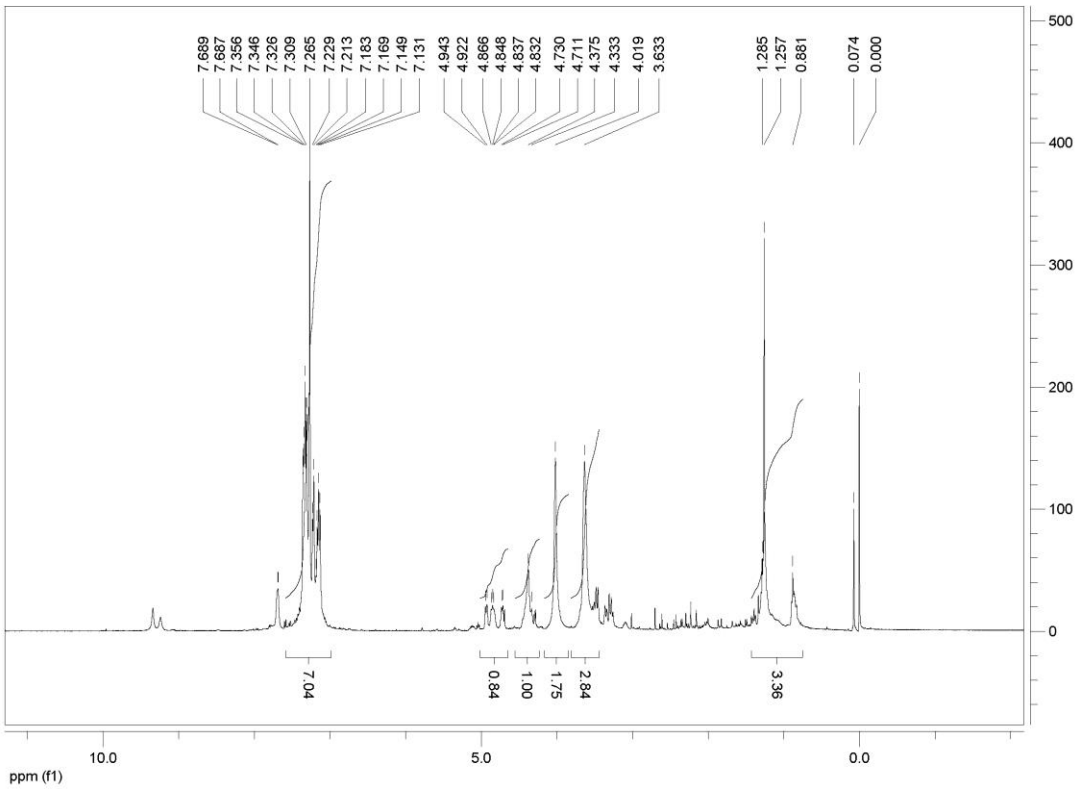


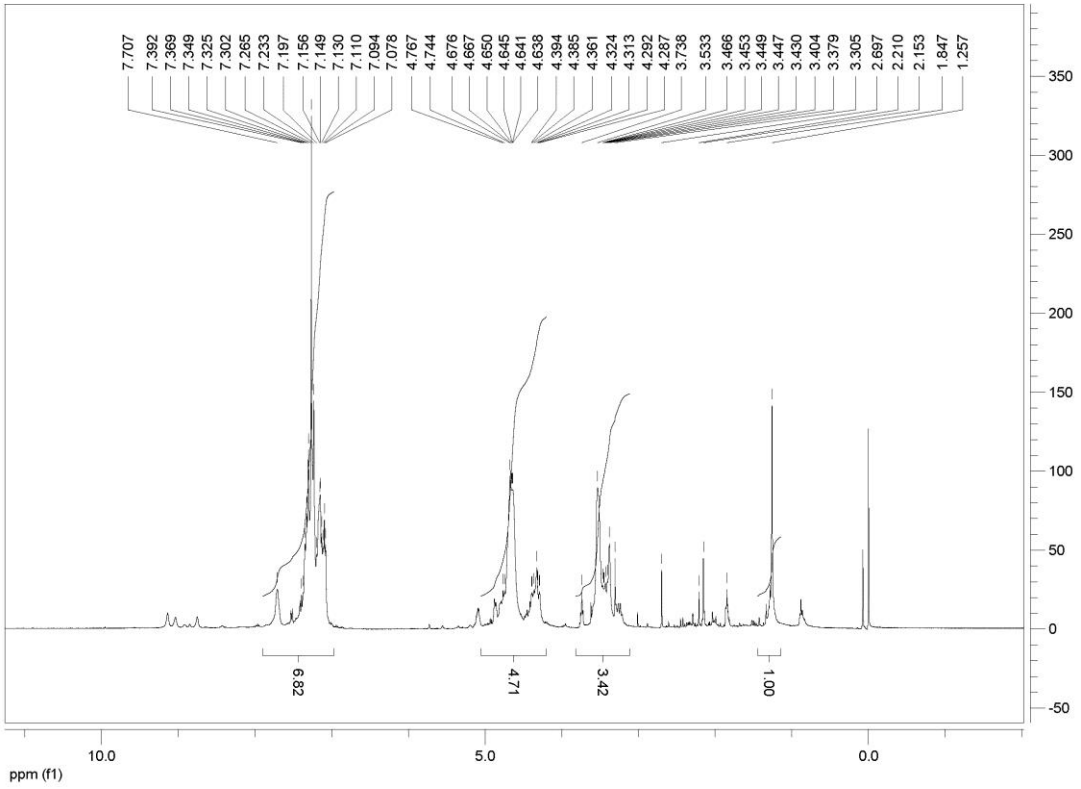
Figure S2. In-situ ^{1}H-NMR analysis of the methylthiolation of substituted indole 1a under different conditions:



(a) In-situ NMR spectrum of DMSO/$(COCl)_2$/indole 1a = 1:1:1 in $CDCl_3$



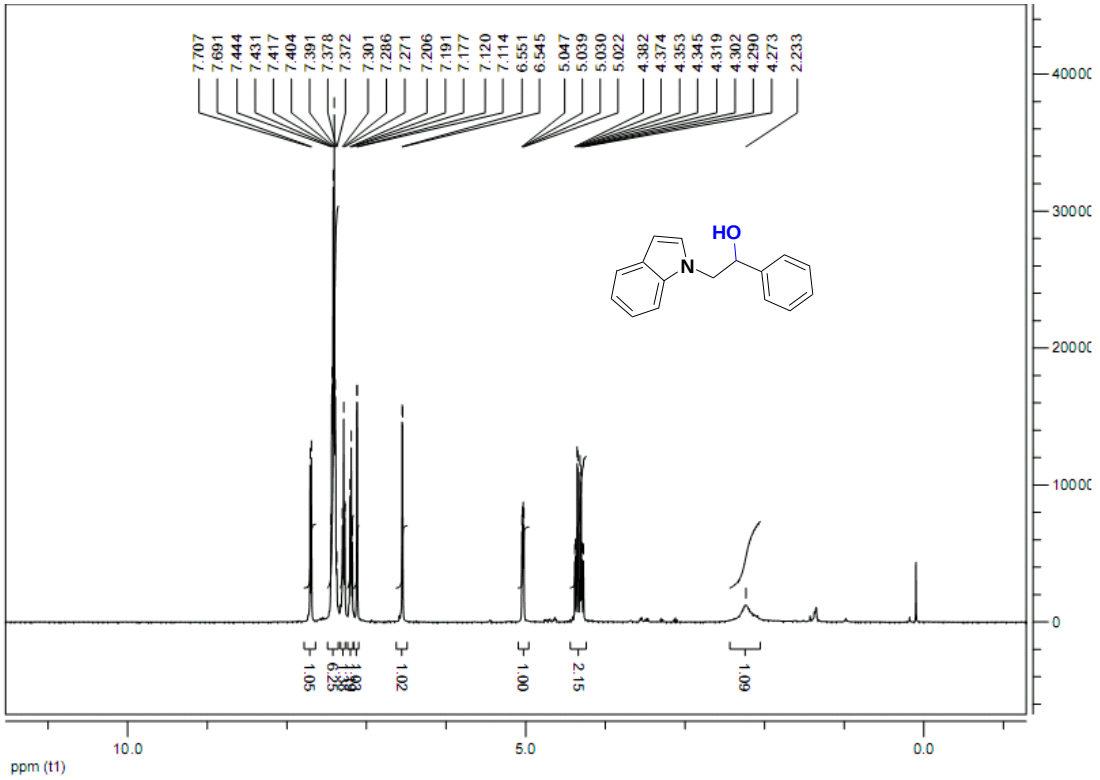
(b)Reaction mixtures from DMSO/$(COCl)_2$/indole 1a/Et_3N = 1:1:1:1

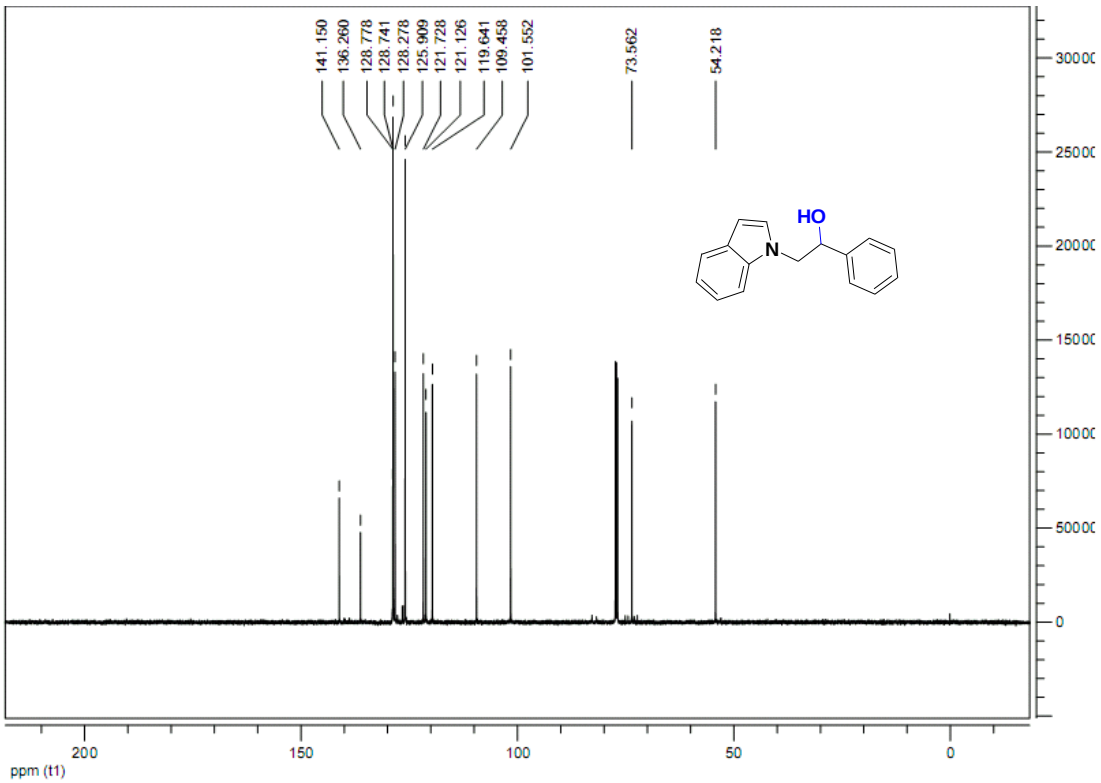


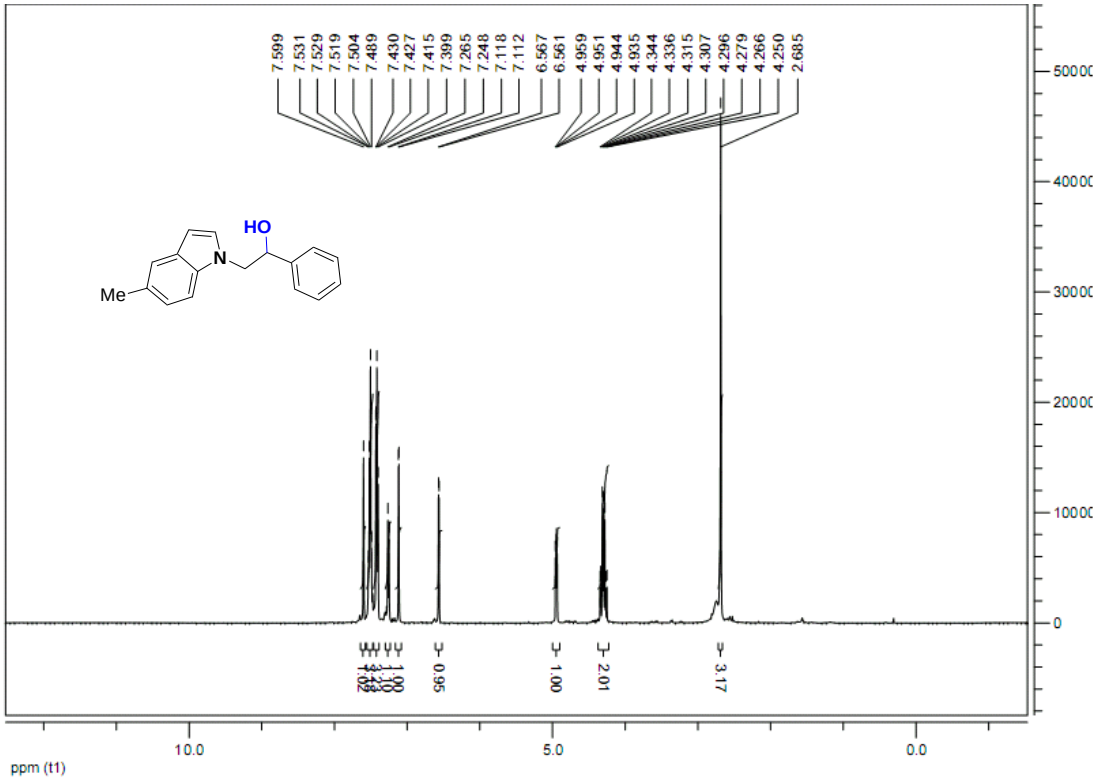
(c) Reaction mixtures from DMSO/$(COCl)_2$/indole 1a = 1:1:1

4. NMR Spectra

a. NMR Spectra Copies of Starting Materials






7.599
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7.529
7.519
7.504
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7.415
7.399
7.265
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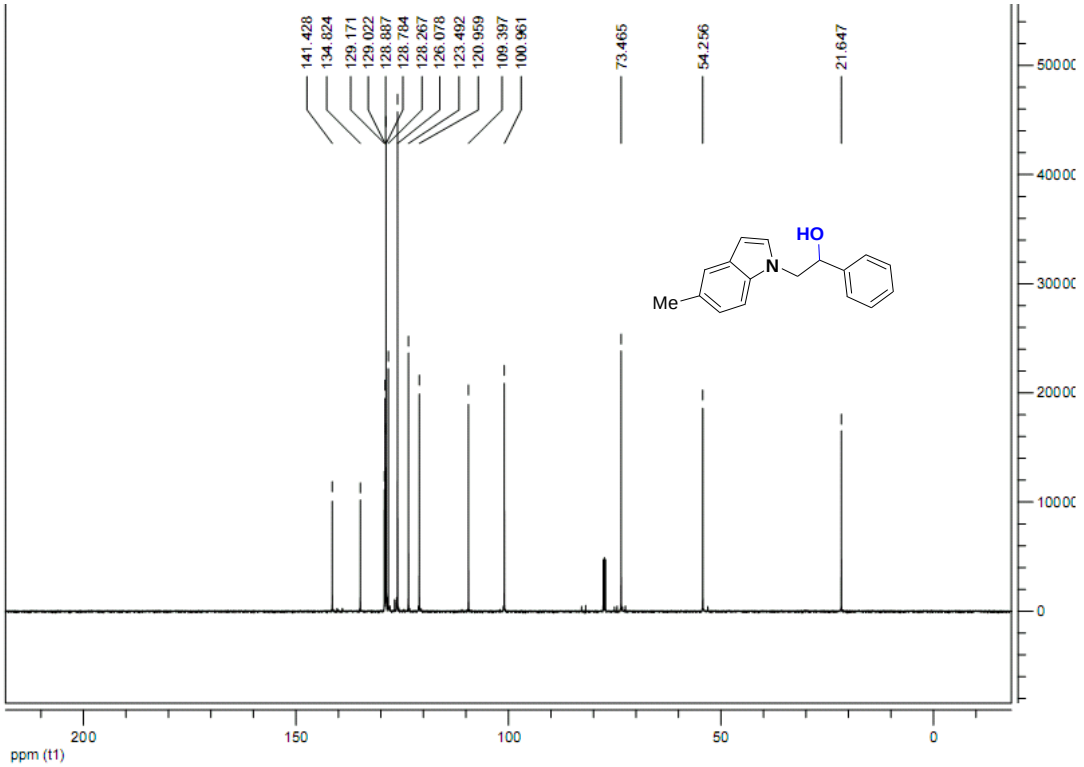
7.118
7.112
6.567
6.561
4.959
4.951
4.944
4.935
4.344
4.336
4.315
4.307
4.296
4.279
4.266
4.250
2.685
HO
N
Me
0.95
1.00
2.01
3.17
10.0
5.0
0.0
ppm (t1)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134.824
129.171
129.022
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128.784
128.267
126.078
123.492
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73.465
54.256
21.647
HO
N
Me
200
150
100
50
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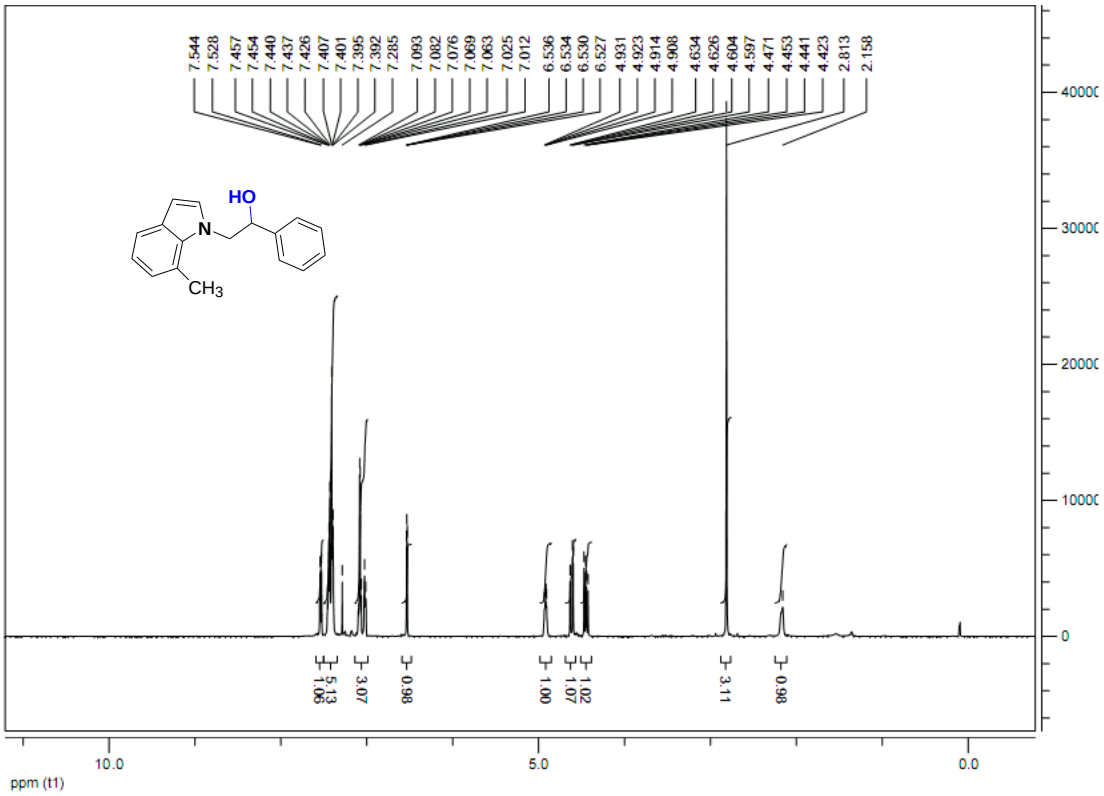
ppm (t1)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7.528
7.457
7.454
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7.407
7.401
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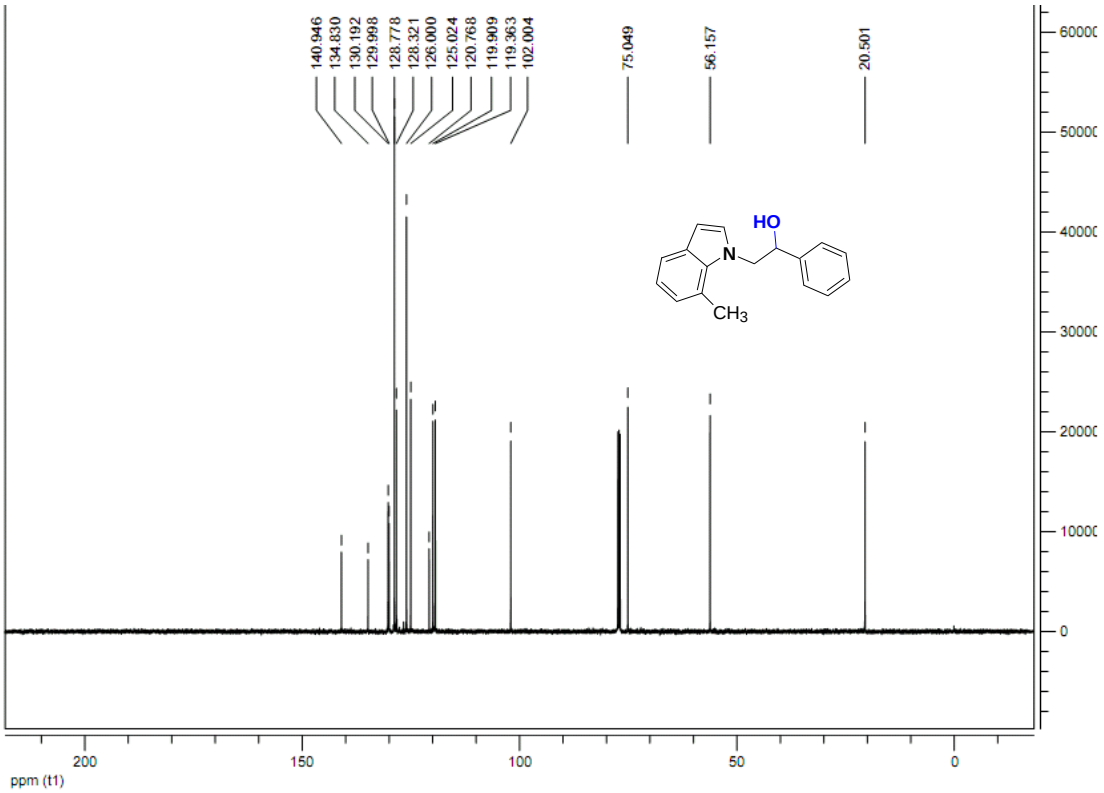
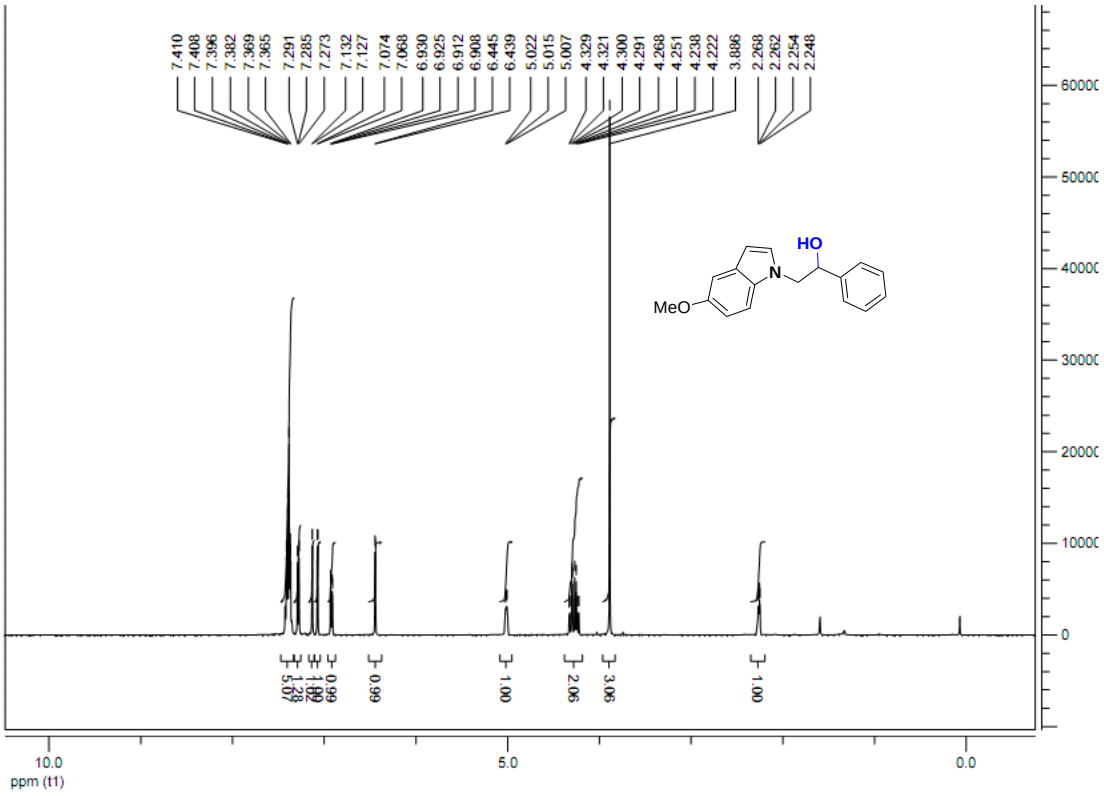
7.392
7.285
7.093
7.082
7.076
7.069
7.063
7.025
7.012
6.536
6.534
6.530
6.527
4.931
4.923
4.914
4.908
4.634
4.626
4.604
4.597
4.471
4.453
4.441
4.423
2.813
2.158
HO
N
CH3
5.13
3.07
0.98
1.00
1.07
1.02
3.11
0.98
10.0
5.0
0.0
ppm (t1)


140.946
134.830
130.192
129.998
128.778
128.321
126.000
125.024
120.768
119.909
119.363
102.004
75.049
56.157
20.501
HO
N
CH3
200
150
100
50
0
ppm (t1)


7.410
7.408
7.396
7.382
7.369
7.365
7.291
7.285
7.273
7.132
7.127
7.074
7.068
6.930
6.925
6.912
6.908
6.445
6.439
5.022
5.015
5.007
4.329
4.321
4.300
4.291
4.268
4.251
4.238
4.222
3.886
2.268
2.262
2.254
2.248
HO
N
MeO
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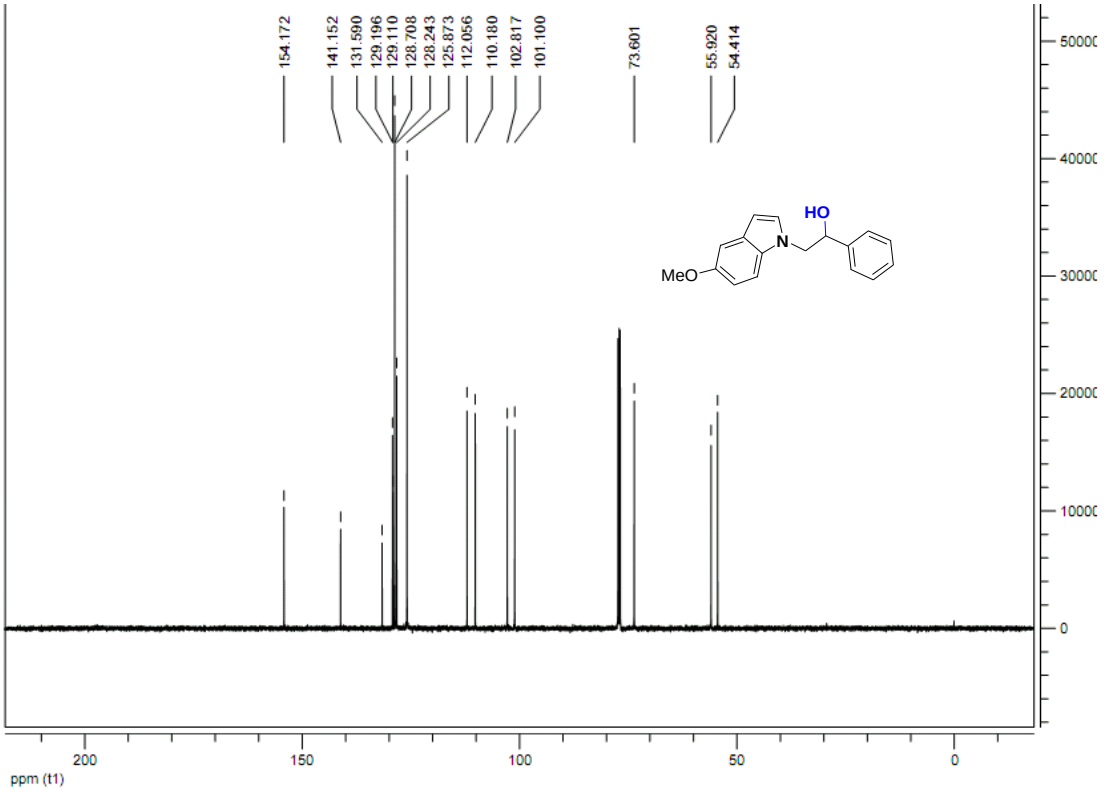
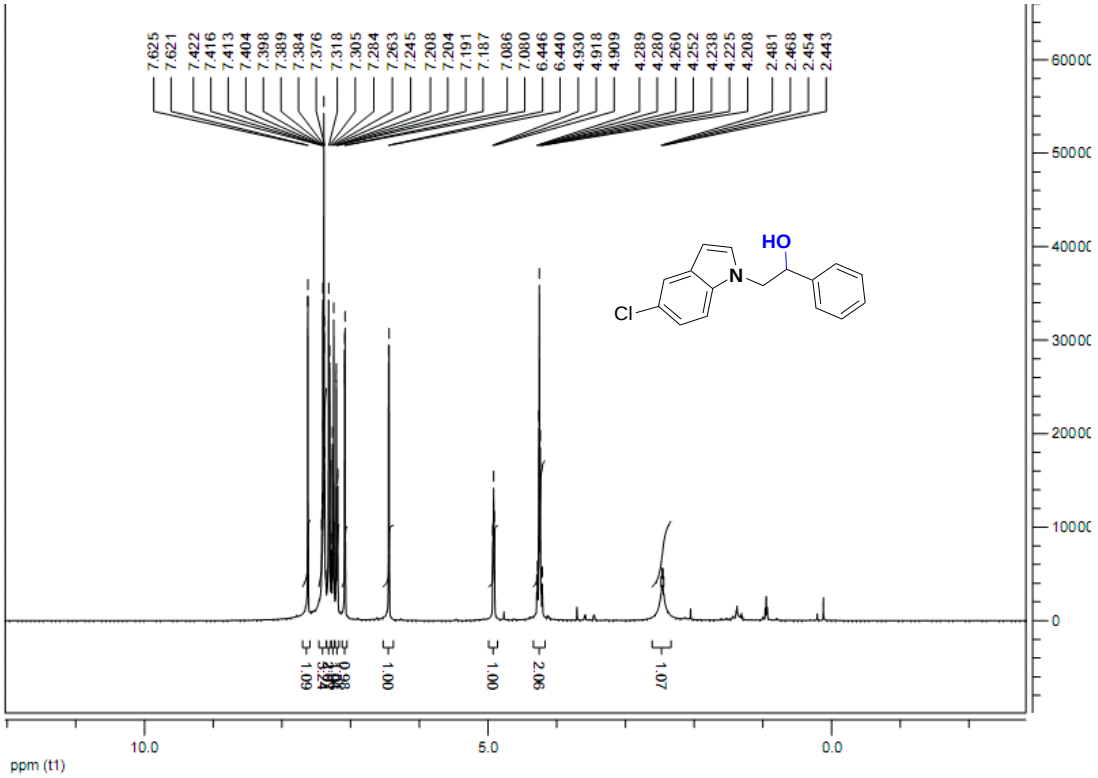
0.99
1.00
2.06
3.06
1.00
10.0
5.0
0.0
ppm (t1)


154.172
141.152
131.590
129.196
129.110
128.708
128.243
125.873
112.056
110.180
102.817
101.100
73.601
55.920
54.414
HO
N
MeO
200
150
100
50
0
ppm (t1)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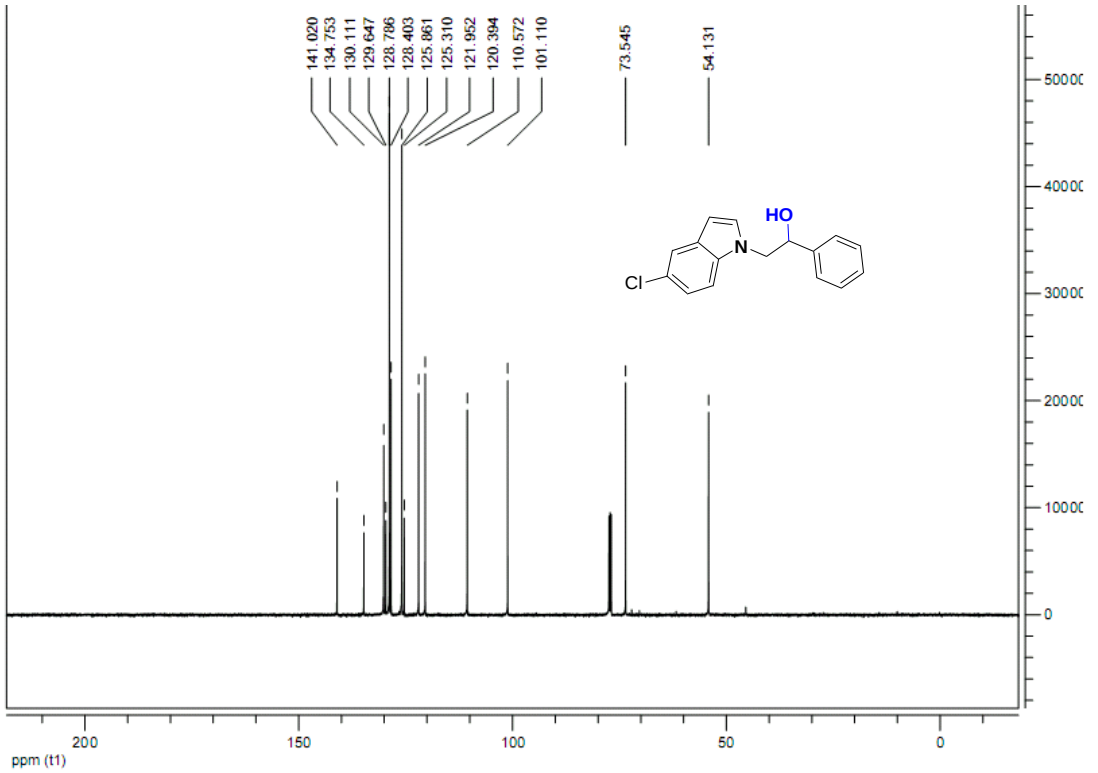
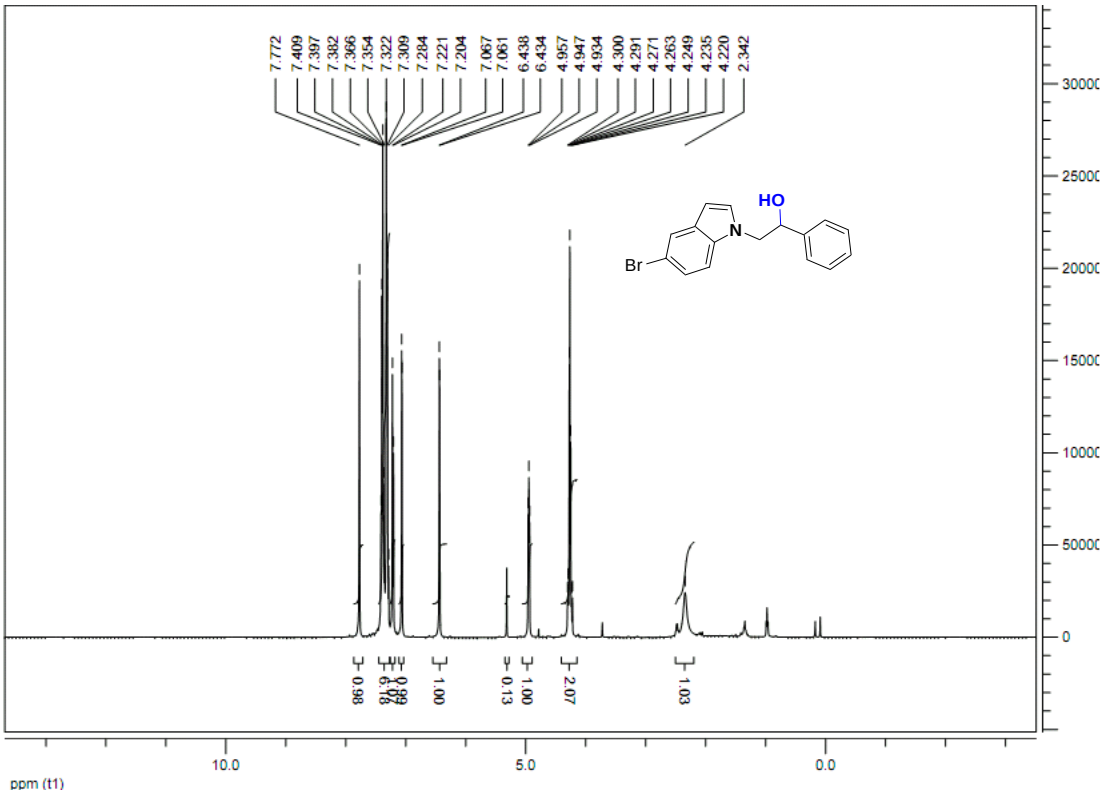
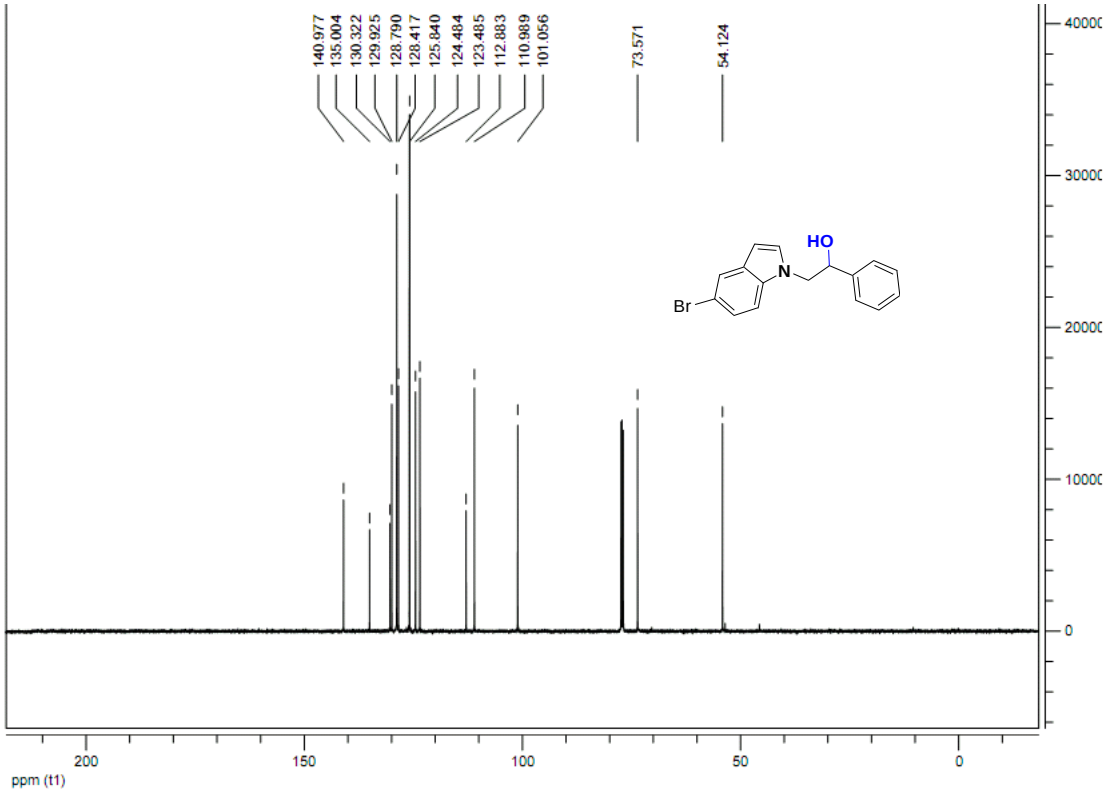
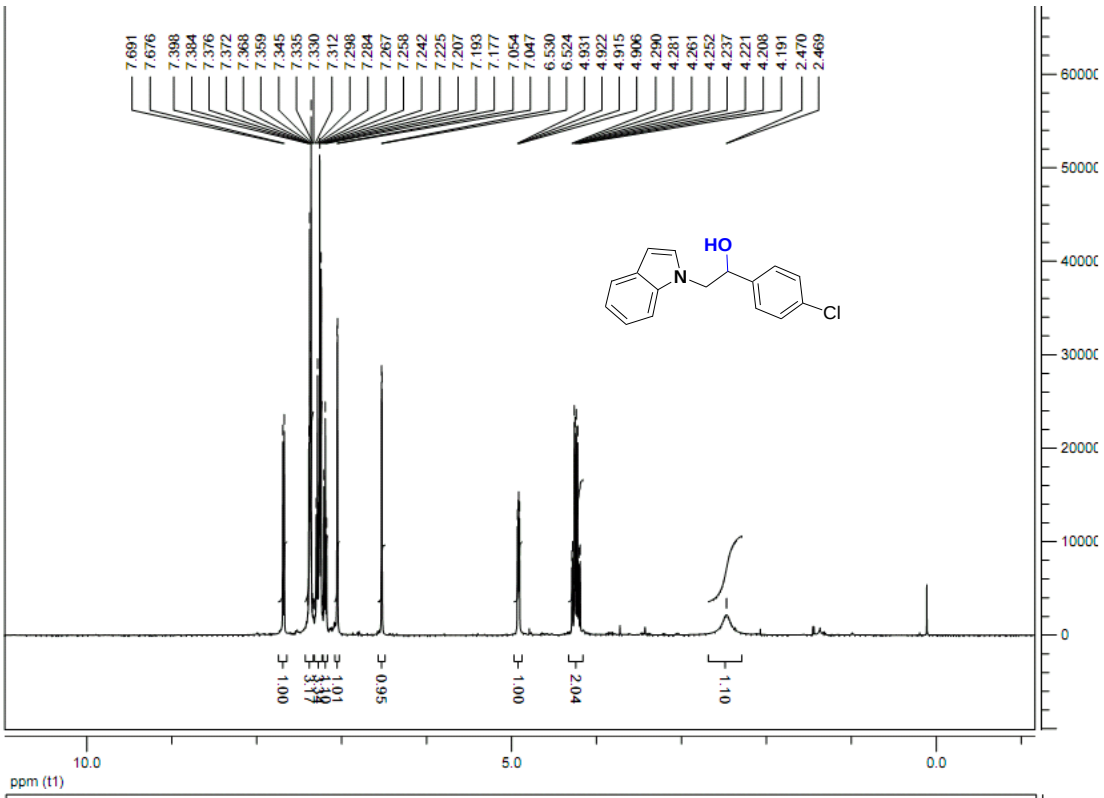
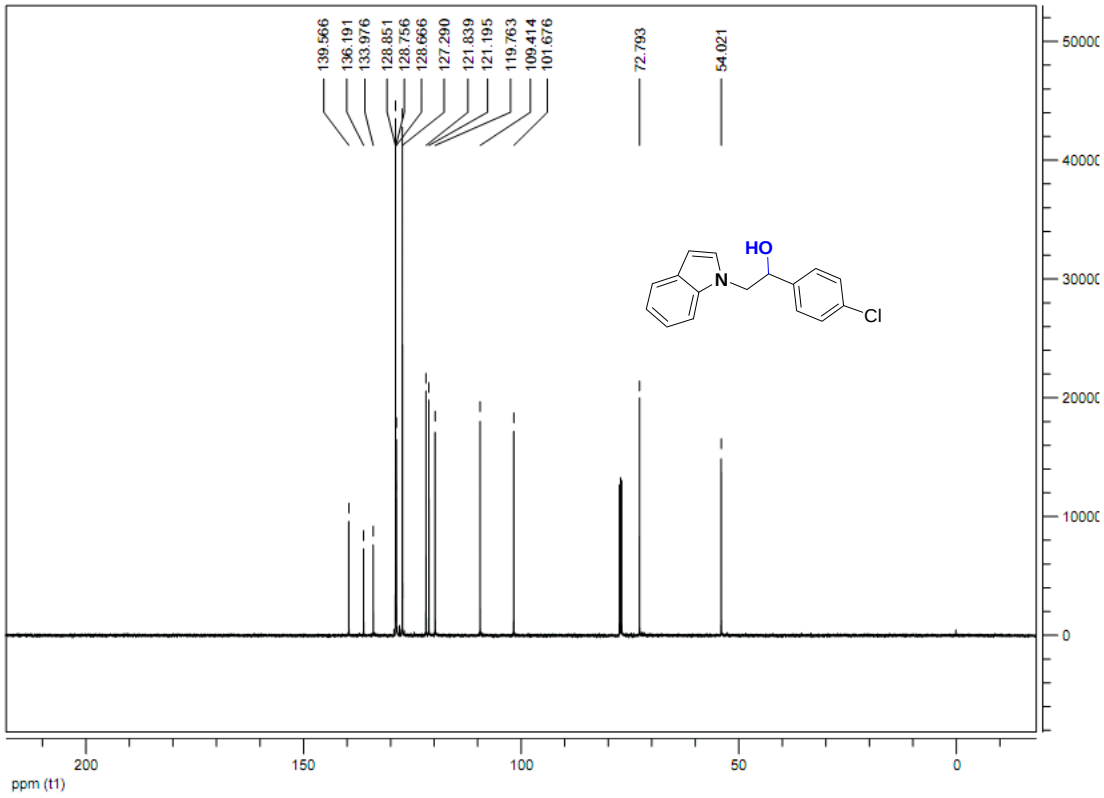
7.621
7.422
7.416
7.413
7.404
7.398
7.389
7.384
7.376
7.318
7.305
7.284
7.263
7.245
7.208
7.204
7.191
7.187
7.086
7.080
6.446
6.440
4.930
4.918
4.909
4.289
4.280
4.260
4.252
4.238
4.225
4.208
2.481
2.468
2.454
2.443
HO
N
Cl
1.09
1.00
1.00
2.06
1.07
10.0
5.0
0.0
ppm (t1)

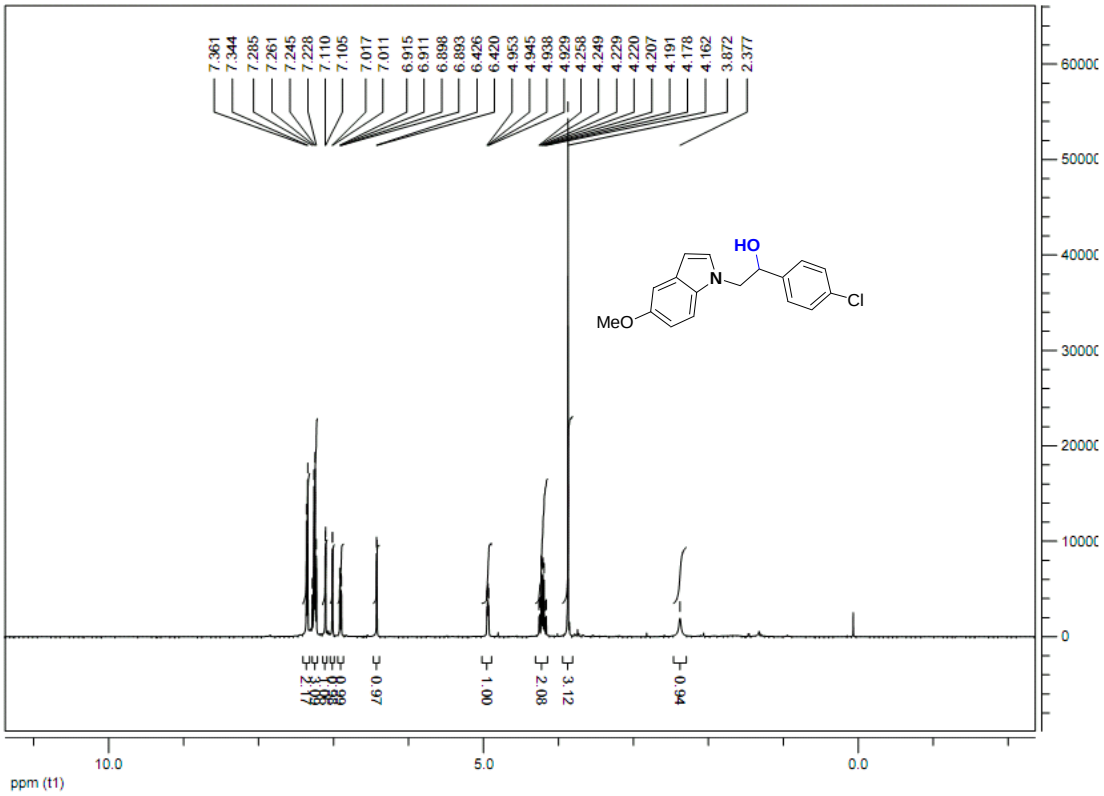

141.020
134.753
130.111
129.647
128.786
128.403
125.861
125.310
121.952
120.394
110.572
101.110
73.545
54.131
HO
N
Cl
200
150
100
50
0
ppm (t1)

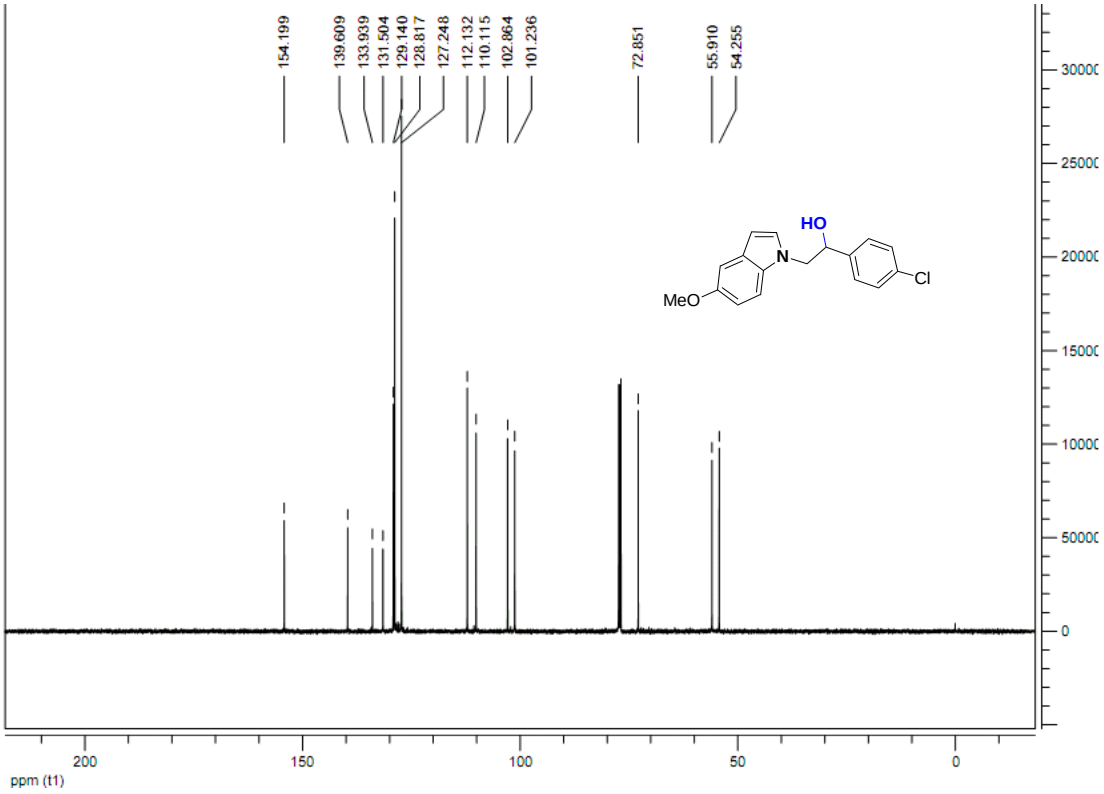

7.772
7.409
7.397
7.392
7.366
7.354
7.322
7.309
7.284
7.221
7.204
7.067
7.061
6.438
6.434
4.957
4.947
4.934
4.300
4.291
4.271
4.263
4.249
4.235
4.220
2.342
HO
N
Br
0.98
0.89
0.89
1.00
0.13
1.00
2.07
1.03
10.0
5.0
0.0
ppm (t1)

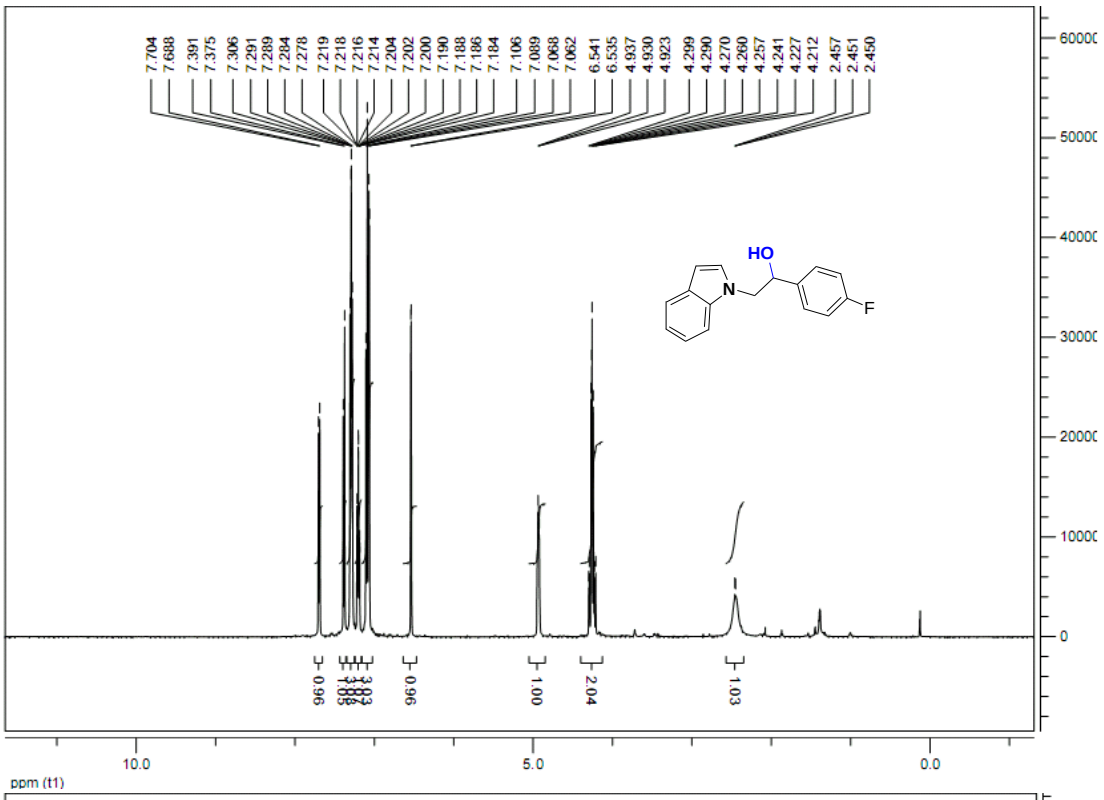

140.977
135.004
130.322
129.925
128.790
128.417
125.840
124.484
123.485
112.883
110.989
101.056
73.571
54.124
HO
N
Br
200
150
100
50
0
ppm (t1)

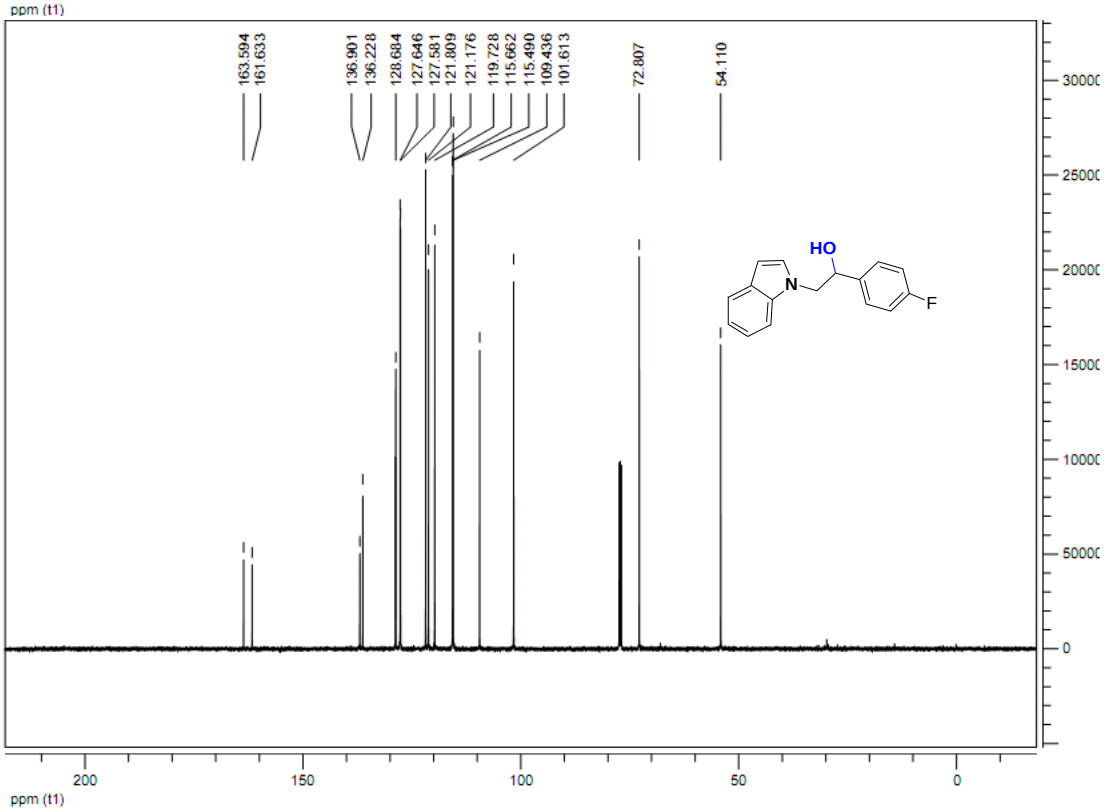

7.691
7.676
7.398
7.384
7.376
7.372
7.368
7.359
7.345
7.335
7.330
7.312
7.298
7.284
7.267
7.258
7.242
7.225
7.207
7.193
7.177
7.054
7.047
6.530
6.524
4.931
4.922
4.915
4.906
4.290
4.281
4.261
4.252
4.237
4.221
4.208
4.191
2.470
2.469
HO
N
Cl
1.00
0.95
1.00
2.04
1.10
ppm (t1)

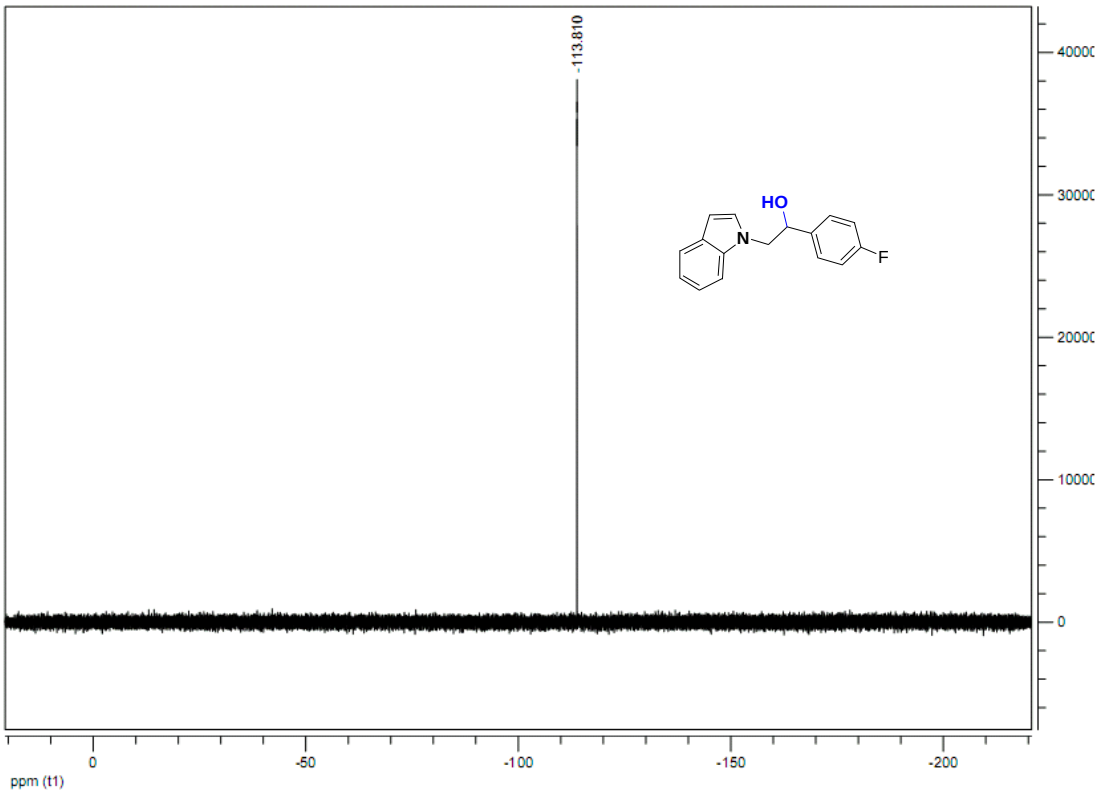

139.566
136.191
133.976
128.851
128.756
128.666
127.290
121.839
121.195
119.763
109.414
101.676
72.793
54.021
HO
N
Cl
ppm (t1)

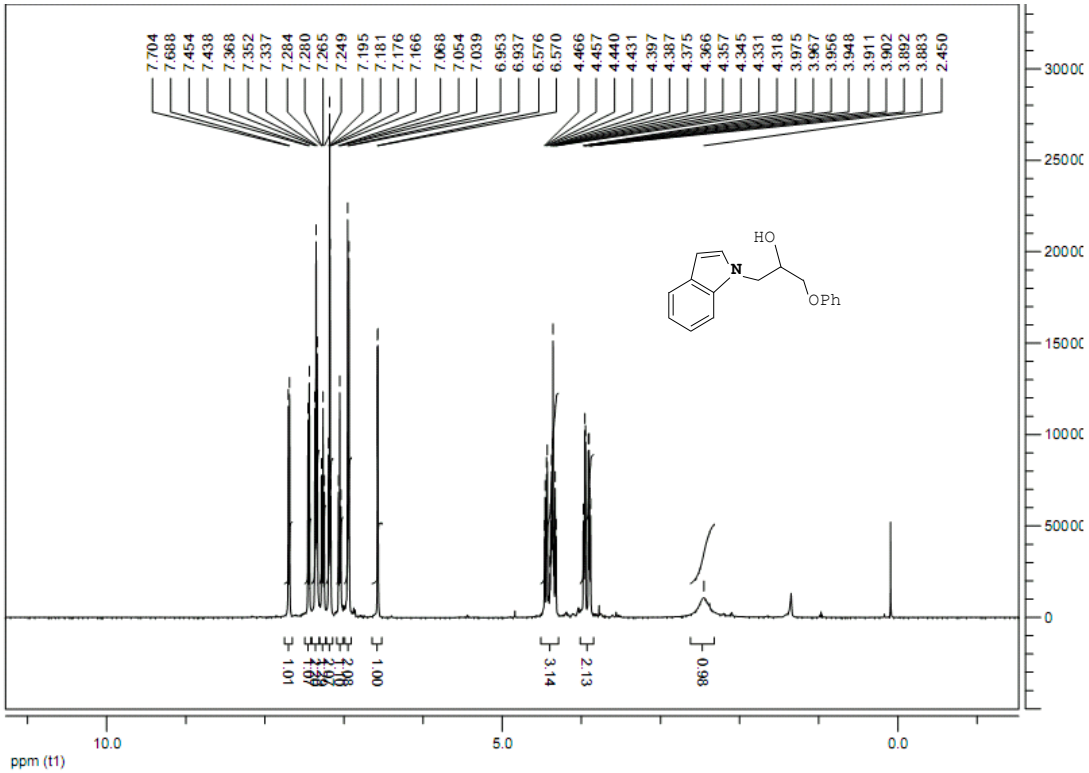

7.361
7.344
7.285
7.261
7.245
7.228
7.110
7.105
7.017
7.011
6.915
6.911
6.898
6.893
6.426
6.420
4.953
4.945
4.938
4.929
4.258
4.249
4.229
4.220
4.207
4.191
4.178
4.162
3.872
2.377
HO
N
Cl
MeO
0.97
1.00
2.08
3.12
0.94
10.0
5.0
0.0
ppm (t1)

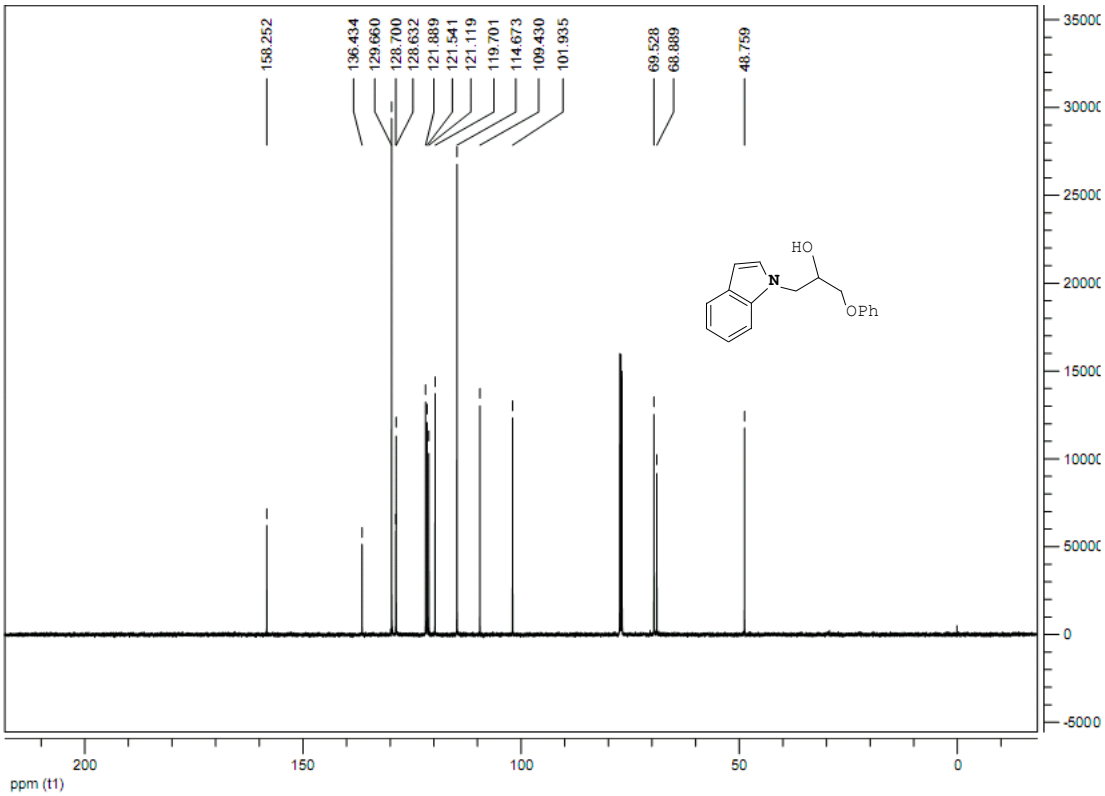

154.199
139.609
133.939
131.504
129.140
128.817
127.248
112.132
110.115
102.864
101.236
72.851
55.910
54.255
HO
N
Cl
MeO
200
150
100
50
0
ppm (t1)

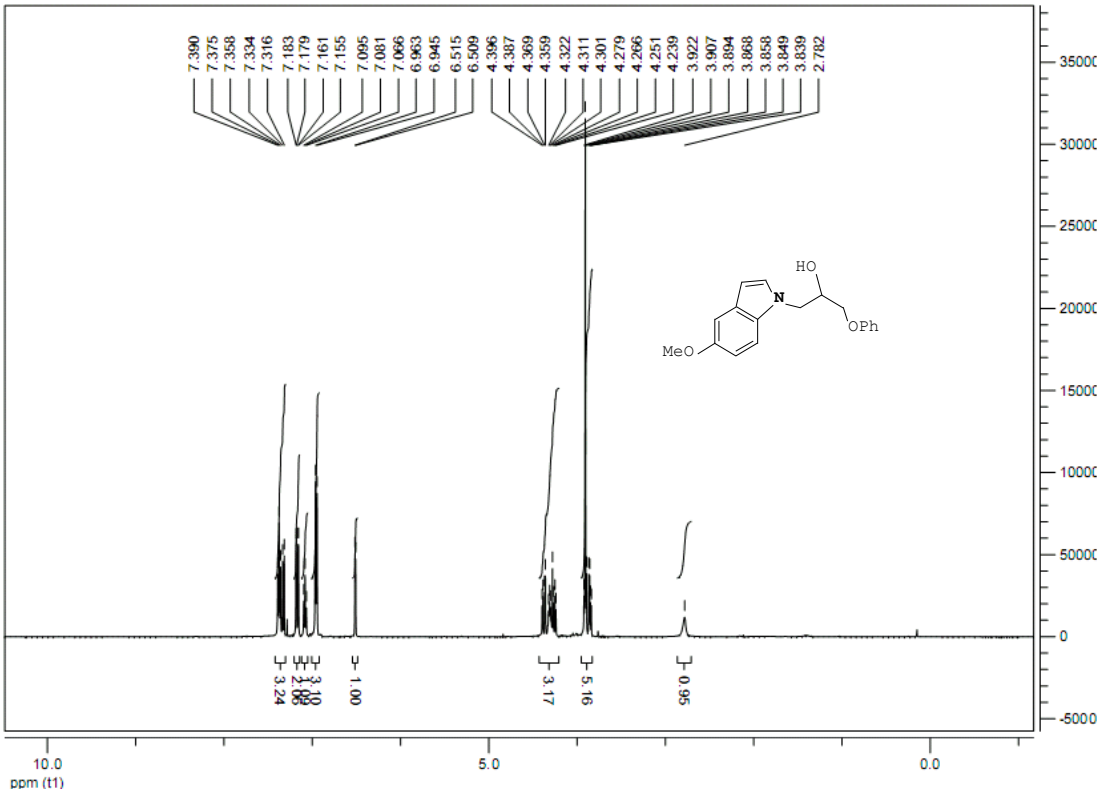

7.704
7.688
7.391
7.375
7.306
7.291
7.289
7.284
7.278
7.219
7.218
7.216
7.214
7.204
7.202
7.200
7.190
7.188
7.186
7.184
7.106
7.089
7.068
7.062
6.541
6.535
4.937
4.930
4.923
4.299
4.290
4.270
4.260
4.257
4.241
4.227
4.212
2.457
2.451
2.450
HO
N
F
0.96
0.96
1.00
2.04
1.03
10.0
5.0
0.0
ppm (t1)


163.594
161.633
136.901
136.228
128.684
127.646
127.581
121.809
121.176
119.728
115.662
115.490
109.436
101.613
72.807
54.110
HO
N
F
200
150
100
50
0
ppm (t1)


-113.810
HO
N
F
4000
3000
2000
1000
0
0
-50
-100
-150
-200
ppm (t1)


7.704
7.688
7.454
7.438
7.368
7.352
7.337
7.284
7.280
7.265
7.249
7.195
7.181
7.176
7.166
7.068
7.054
7.039
6.953
6.937
6.576
6.570
4.466
4.457
4.440
4.431
4.397
4.387
4.375
4.366
4.357
4.345
4.331
4.318
3.975
3.967
3.956
3.948
3.911
3.902
3.892
3.883
2.450
HO
N
OPh
1.01
1.00
3.14
2.13
0.98
3000
2500
2000
1500
1000
5000
0
10.0
5.0
0.0
ppm (t1)


158.252
136.434
129.660
128.700
128.632
121.889
121.541
121.119
119.701
114.673
109.430
101.935
69.528
68.889
48.759
HO
N
OPh
ppm (t1)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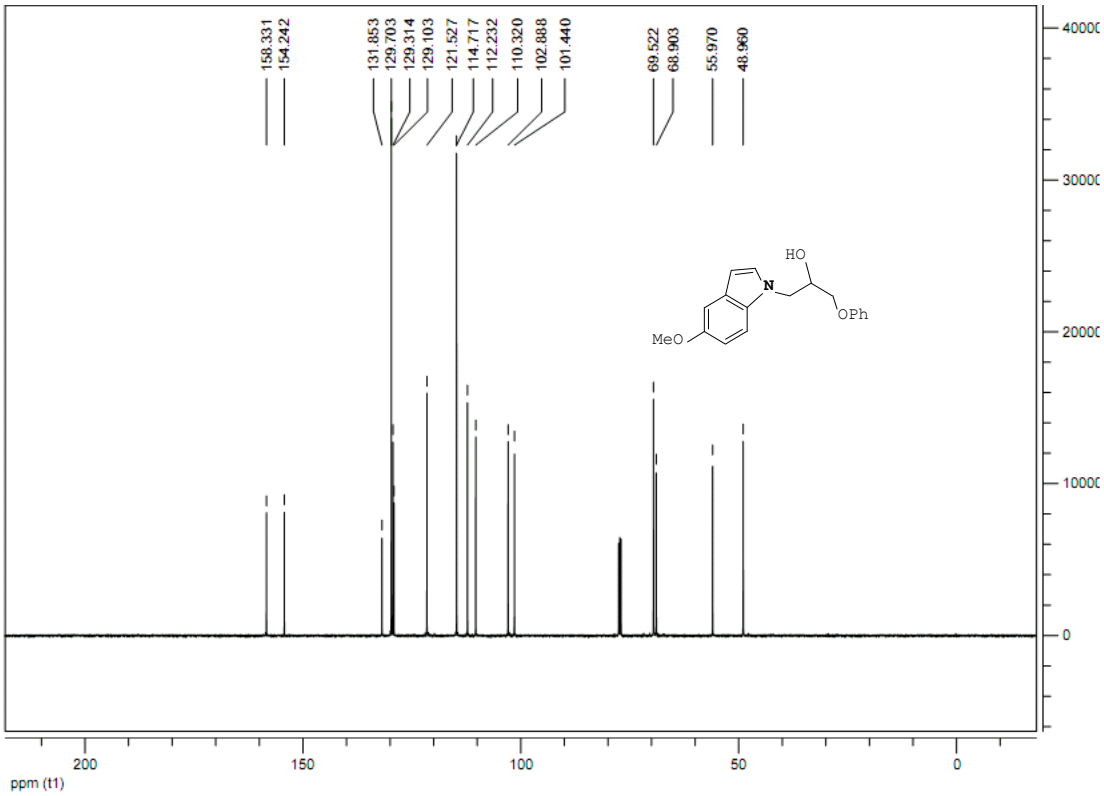
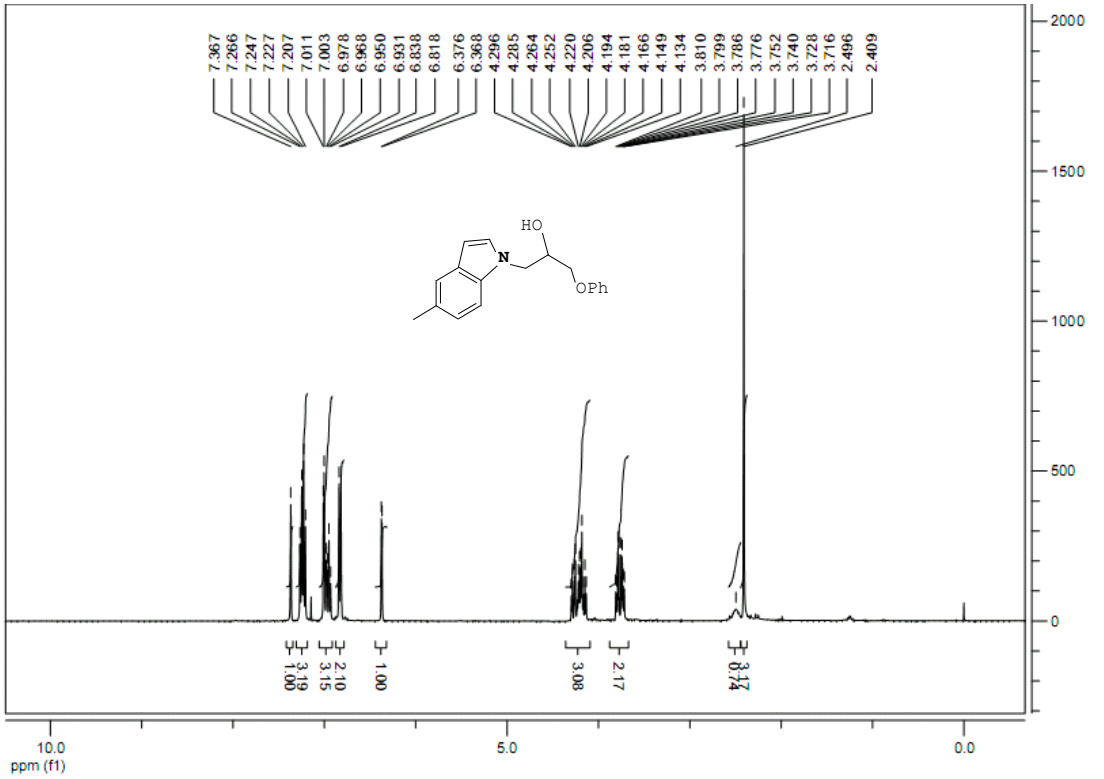
7.375
7.358
7.334
7.316
7.183
7.179
7.161
7.155
7.095
7.081
7.066
6.963
6.945
6.515
6.509
4.396
4.387
4.369
4.359
4.322
4.311
4.301
4.279
4.266
4.251
4.239
3.922
3.907
3.894
3.868
3.858
3.849
3.839
2.782
HO
N
OPh
MeO
3.24
1.00
3.17
5.16
0.95
ppm (t1)


158.331
154.242
131.853
129.703
129.314
129.103
121.527
114.717
112.232
110.320
102.888
101.440
69.522
68.903
55.970
48.960
HO
N
OPh
MeO
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)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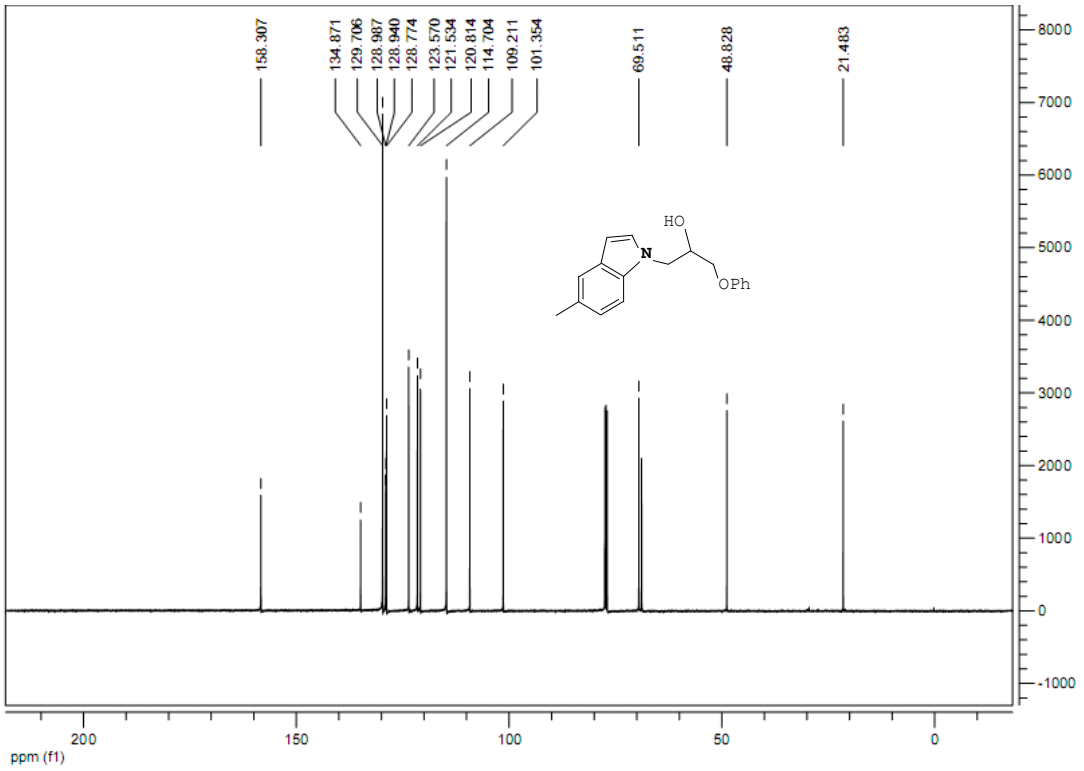
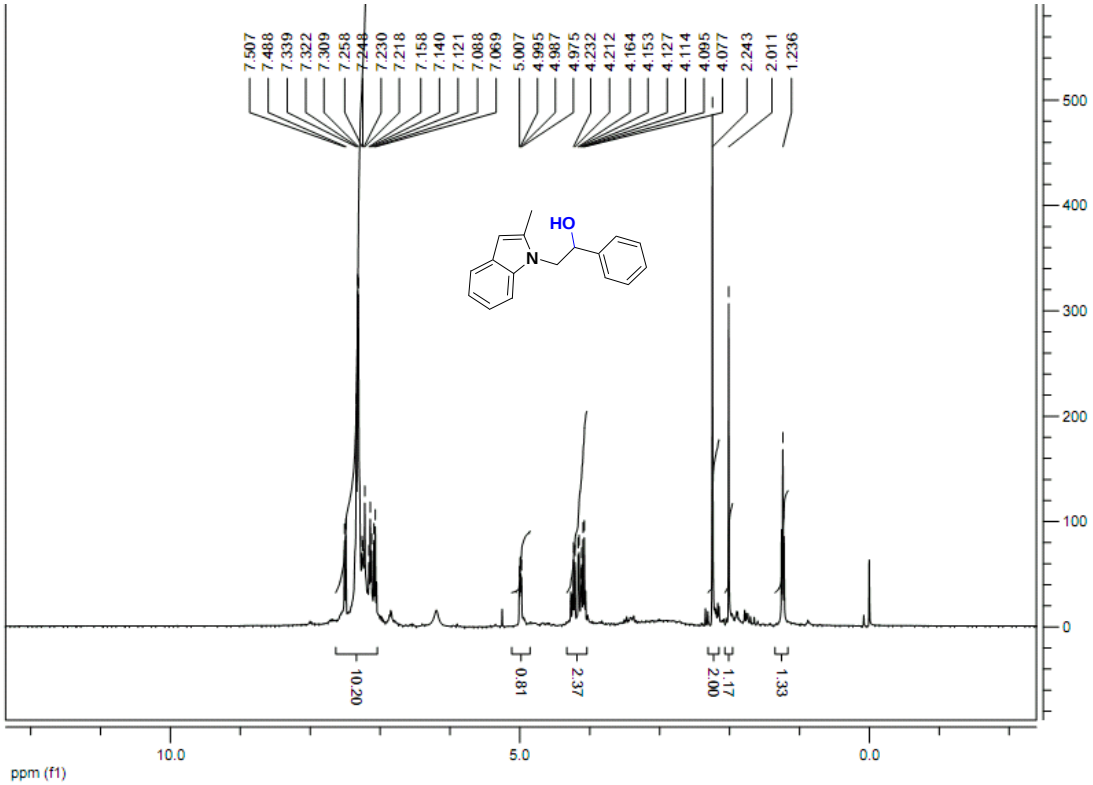
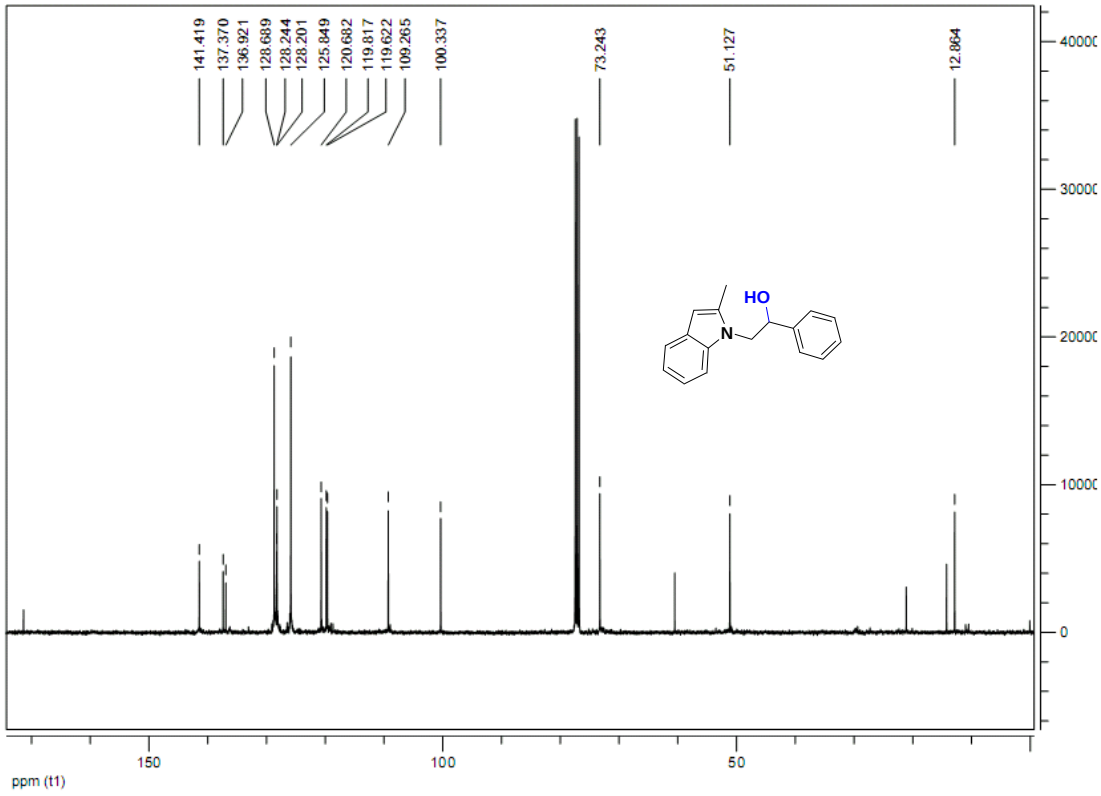
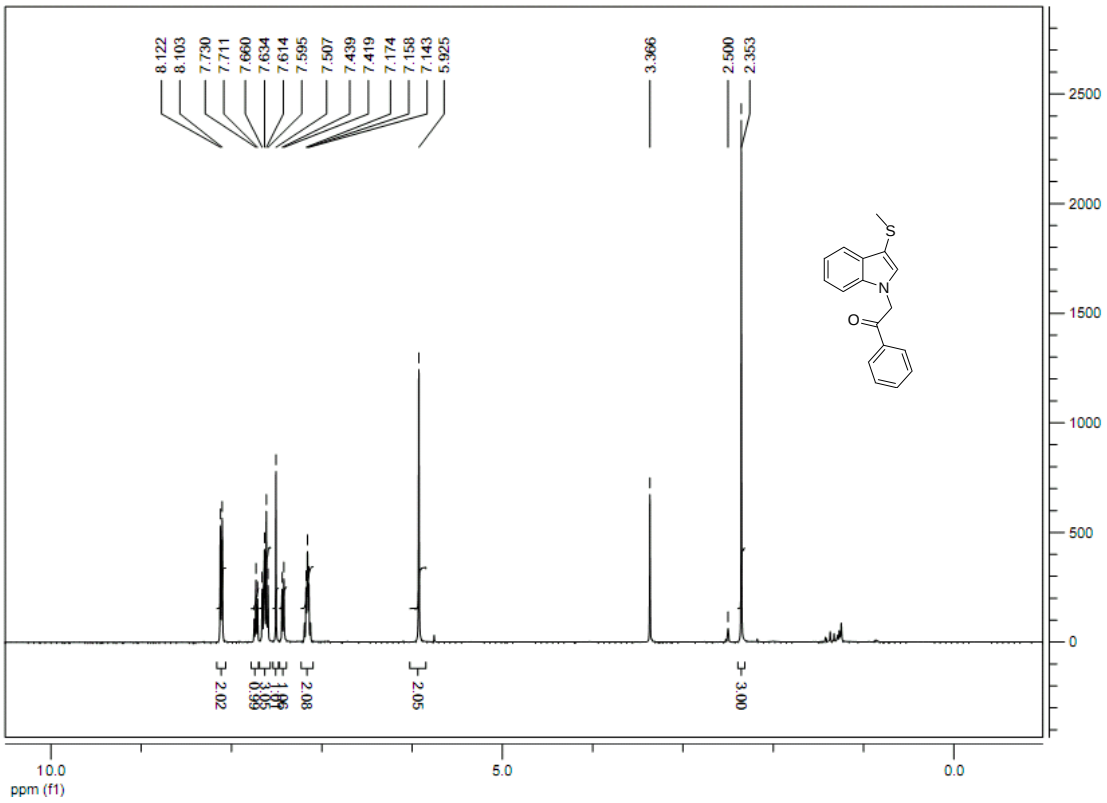
7.266
7.247
7.227
7.207
7.011
7.003
6.978
6.968
6.950
6.931
6.838
6.818
6.376
6.368
4.296
4.285
4.264
4.252
4.220
4.206
4.194
4.181
4.166
4.149
4.134
3.810
3.799
3.786
3.776
3.752
3.740
3.728
3.716
2.496
2.409
HO
N
OPh
1.00
3.19
3.15
2.10
1.00
3.08
2.17
3.17
3.74
2000
1500
1000
500
0
10.0
5.0
0.0
ppm (f1)

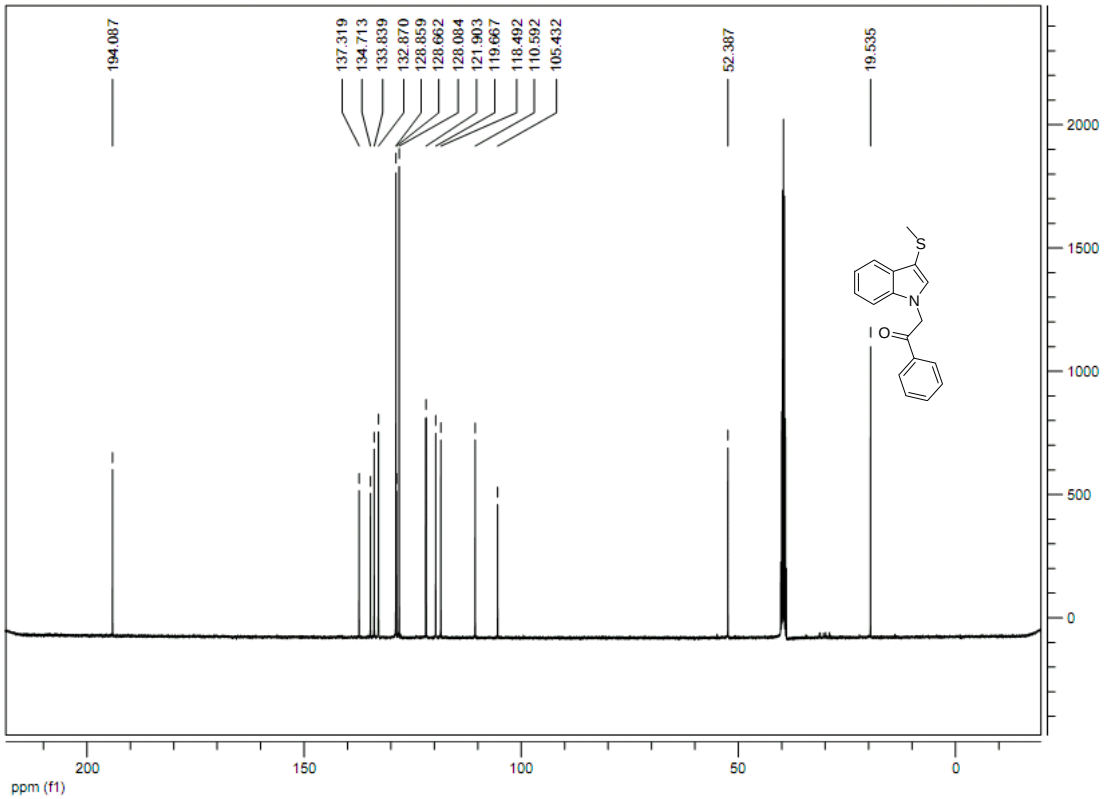

158.307
134.871
129.706
128.987
128.940
128.774
123.570
121.534
120.814
114.704
109.211
101.354
69.511
48.828
21.483
HO
N
OPh
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
200
150
100
50
0
ppm (f1)

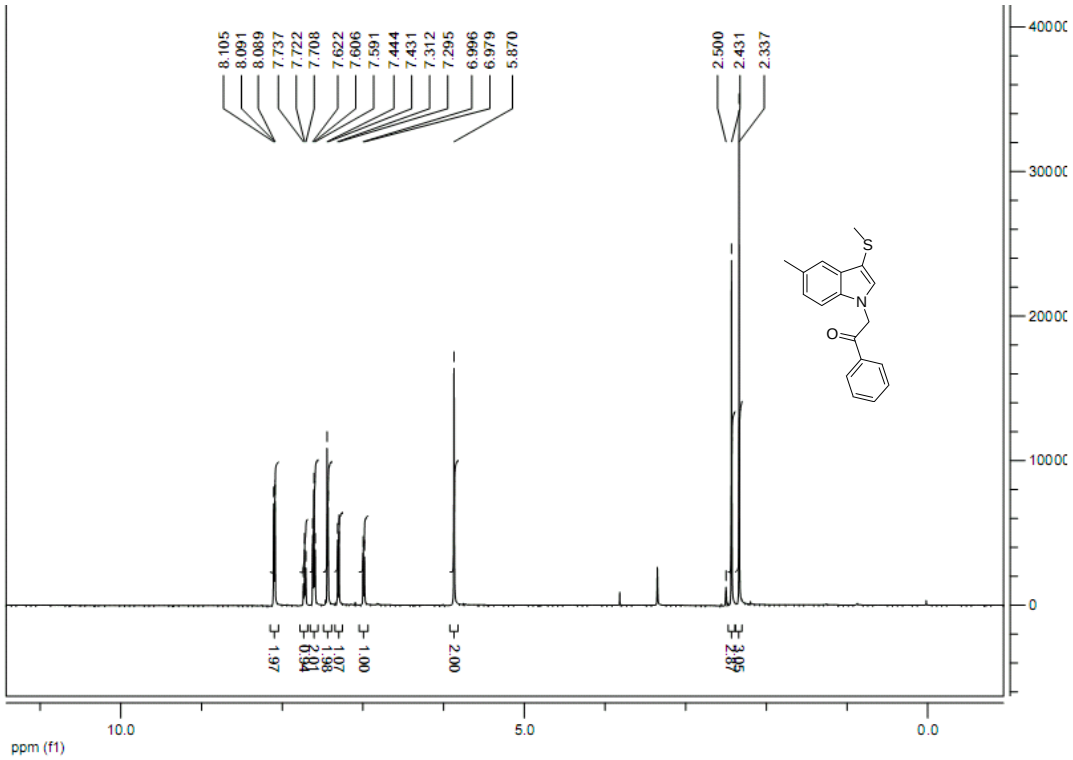

7.507
7.488
7.339
7.322
7.309
7.258
7.248
7.230
7.218
7.158
7.140
7.121
7.088
7.069
5.007
4.995
4.987
4.975
4.232
4.212
4.164
4.153
4.127
4.114
4.095
4.077
2.243
2.011
1.236
HO
N
10.20
0.81
2.37
2.00
1.17
1.33
500
400
300
200
100
0
10.0
5.0
0.0
ppm (f1)

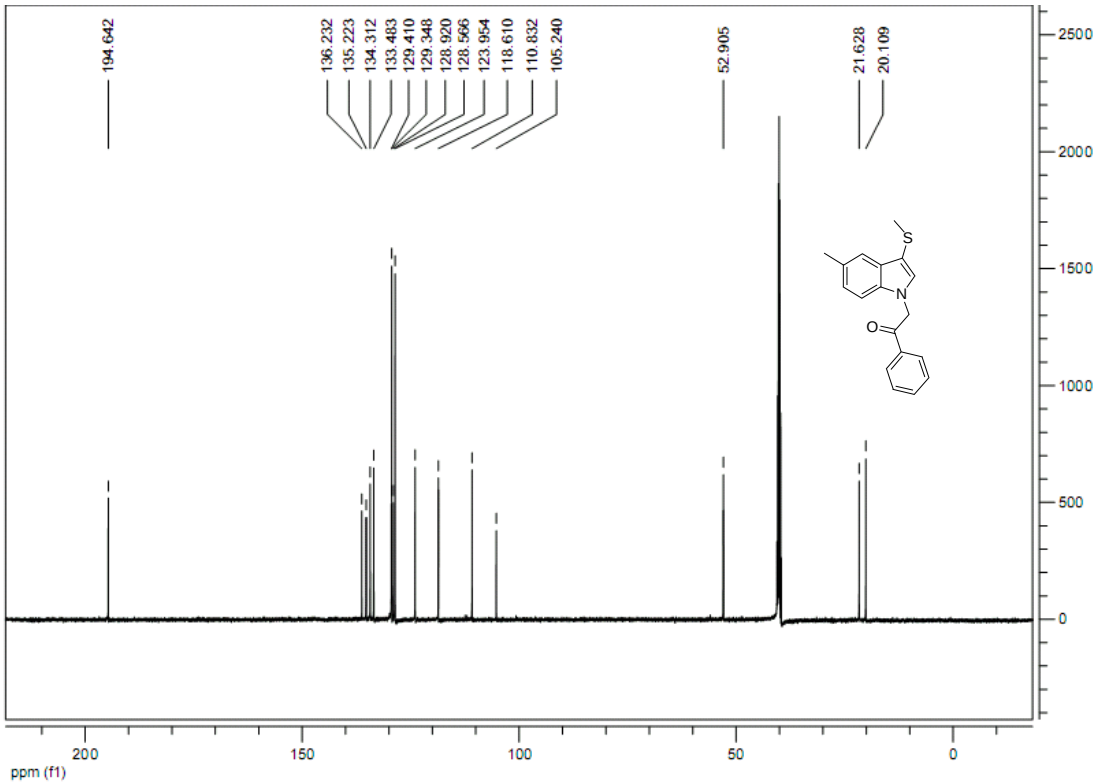


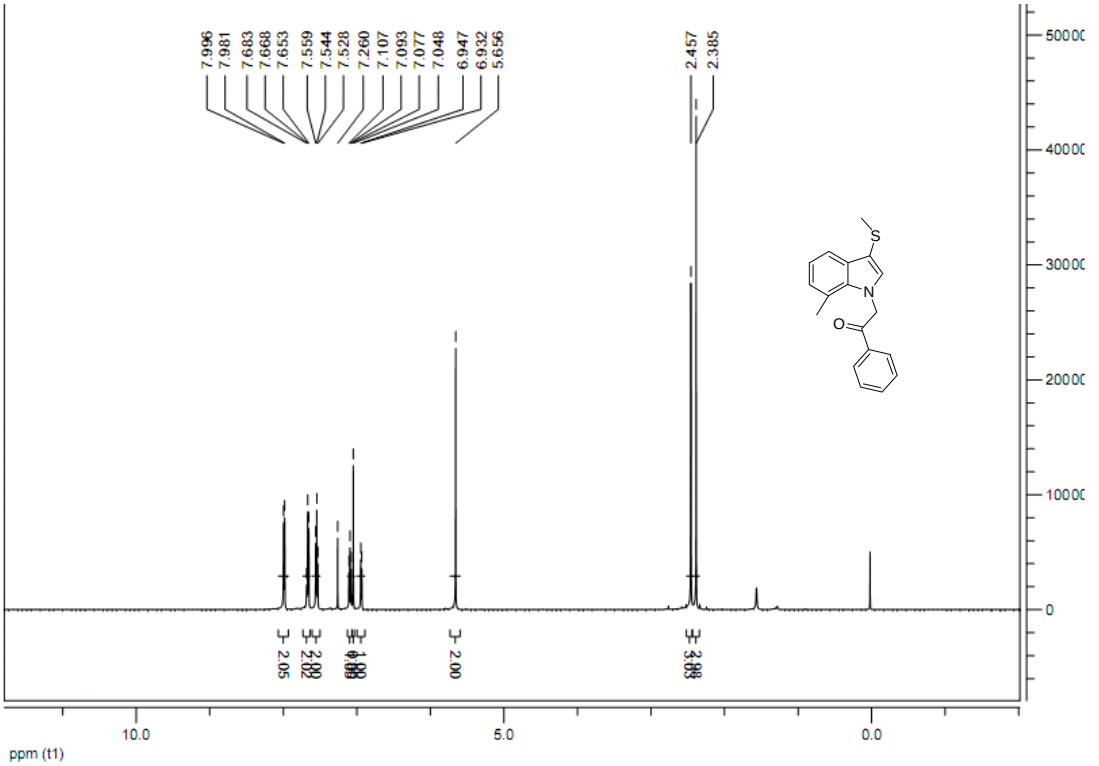
b. NMR Spectra Copies of Oxidation products

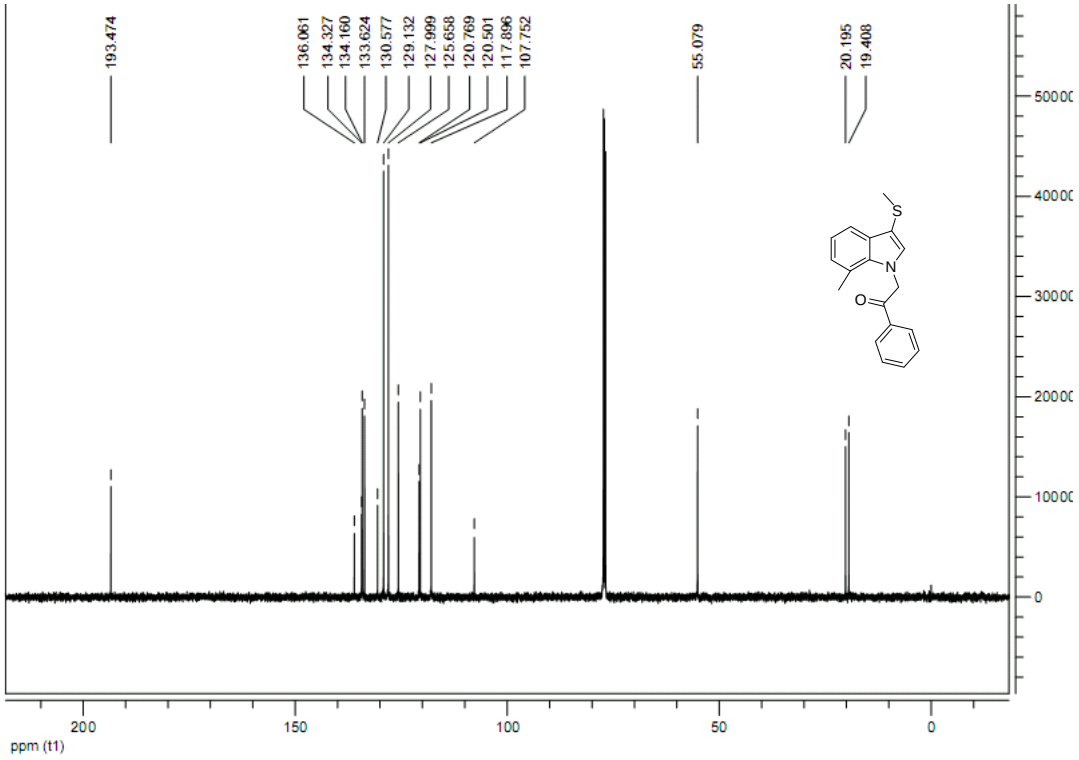



194.087
137.319
134.713
133.839
132.870
128.859
128.662
128.084
121.903
119.667
118.492
110.592
105.432
52.387
19.535
S
N
O
2000
1500
1000
500
0
200
150
100
50
0
ppm (f1)


8.105
8.091
8.089
7.737
7.722
7.708
7.622
7.606
7.591
7.444
7.431
7.312
7.295
6.996
6.979
5.870
2.500
2.431
2.337
S
N
O
40000
30000
20000
10000
0
1.97
2.00
3.95
10.0
5.0
0.0
ppm (f1)


194.642
136.232
135.223
134.312
133.483
129.410
129.348
128.920
128.566
123.954
118.610
110.832
105.240
52.905
21.628
20.109
2500
2000
1500
1000
500
0
200
150
100
50
0
ppm (f1)


7.996
7.981
7.683
7.668
7.653
7.559
7.544
7.528
7.260
7.107
7.093
7.077
7.048
6.947
6.932
5.656
2.457
2.385
10.0
5.0
0.0
ppm (t1)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136.061
134.327
134.160
133.624
130.577
129.132
127.999
125.658
120.769
120.501
117.896
107.752
55.079
20.195
19.408
S
N
O
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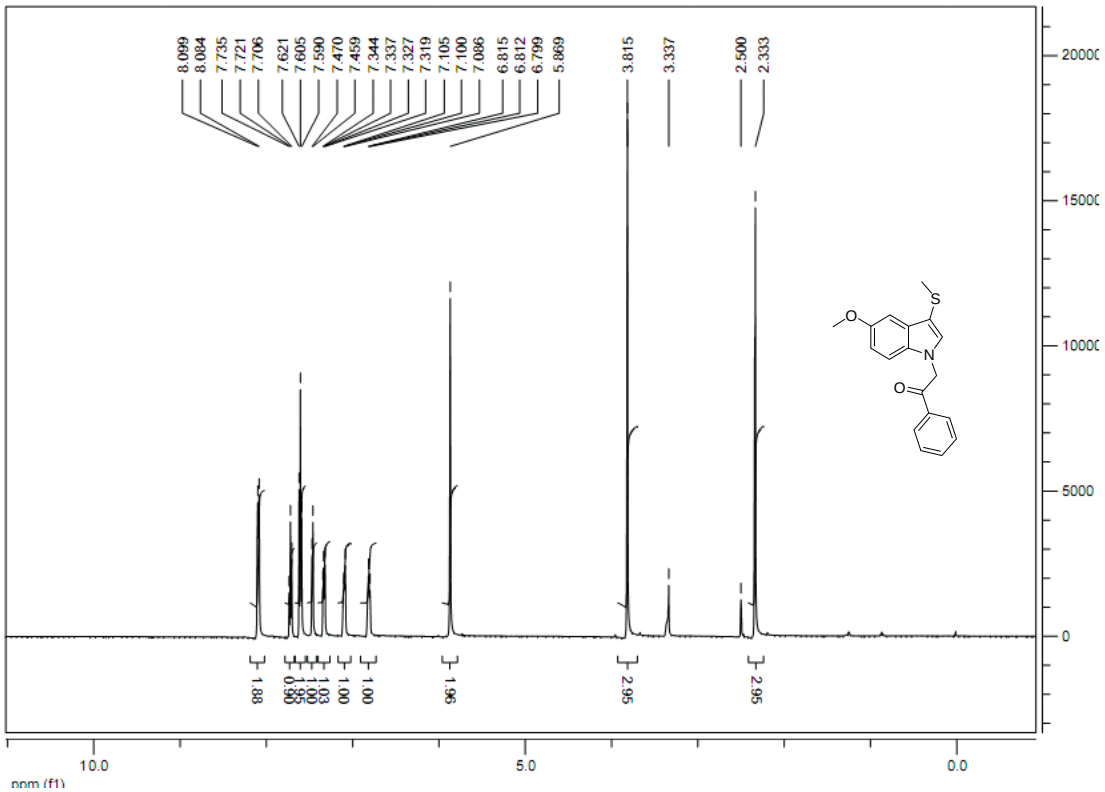
4000
3000
2000
1000
0
200
150
100
50
0
ppm (t1)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8.084
7.735
7.721
7.706
7.621
7.605
7.590
7.470
7.459
7.344
7.337
7.327
7.319
7.105
7.100
7.086
6.815
6.812
6.799
5.869
3.815
3.337
2.500
2.333
1.88
1.00
1.03
1.00
1.00
1.96
2.95
2.95
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O
N
O
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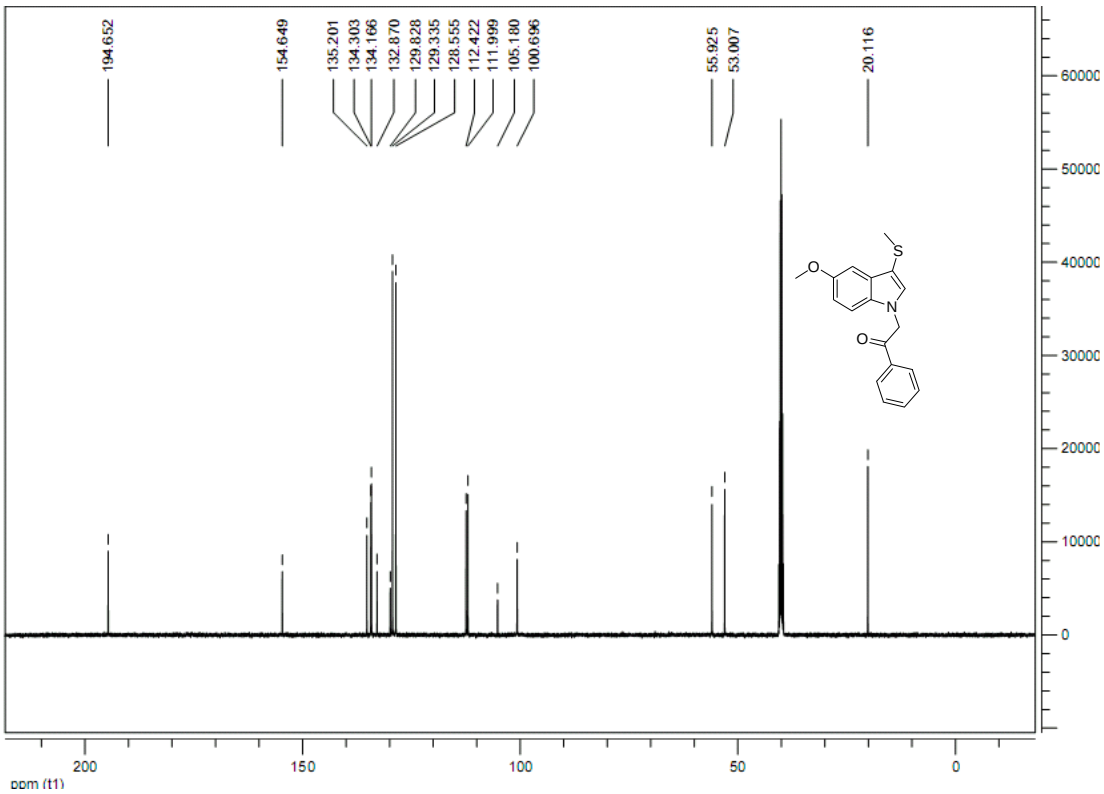
15000
10000
5000
0
10.0
5.0
0.0
ppm (f1)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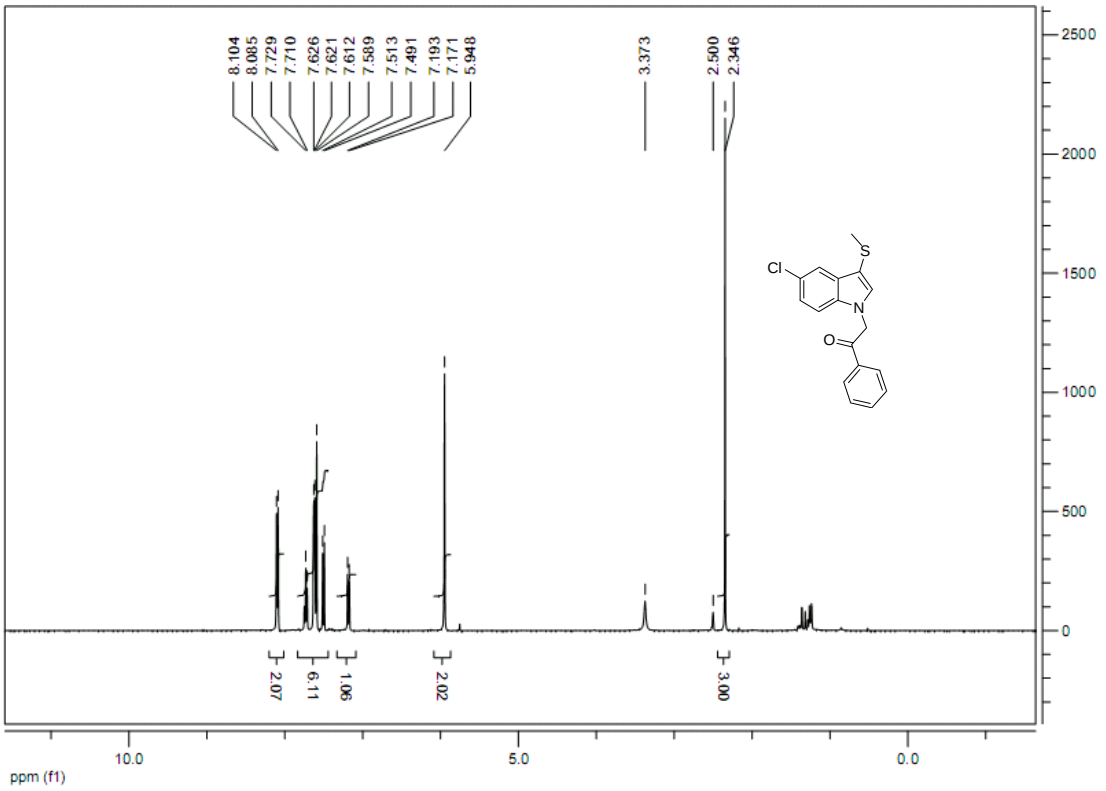
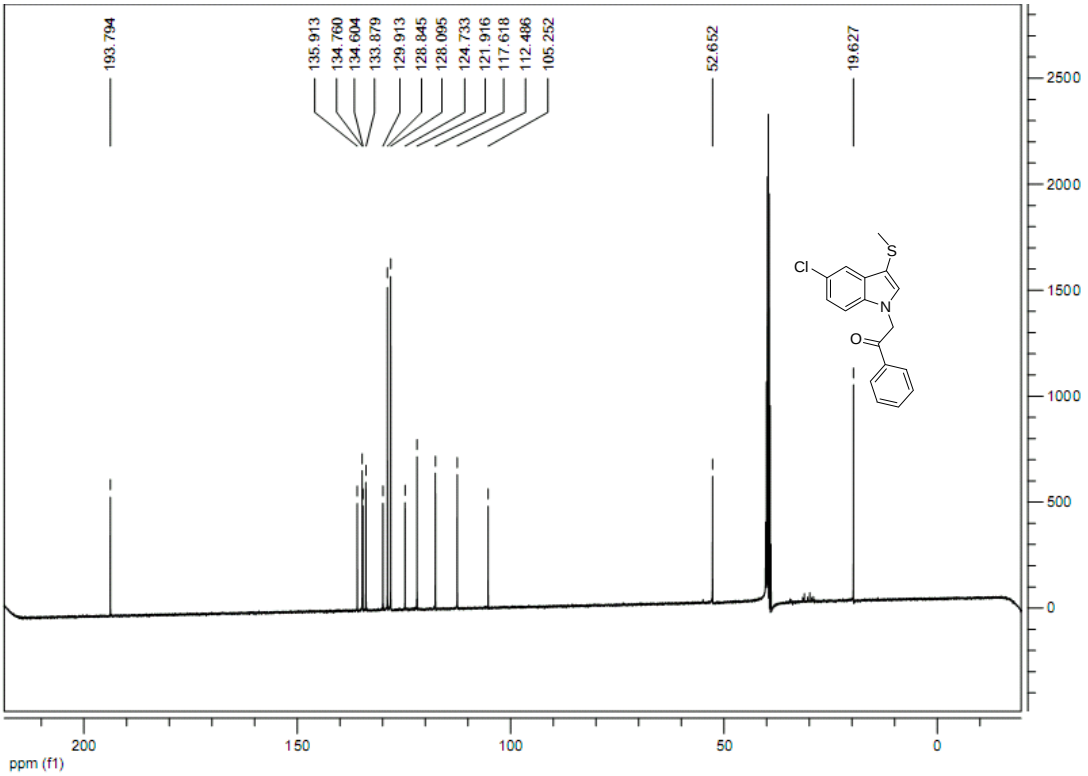
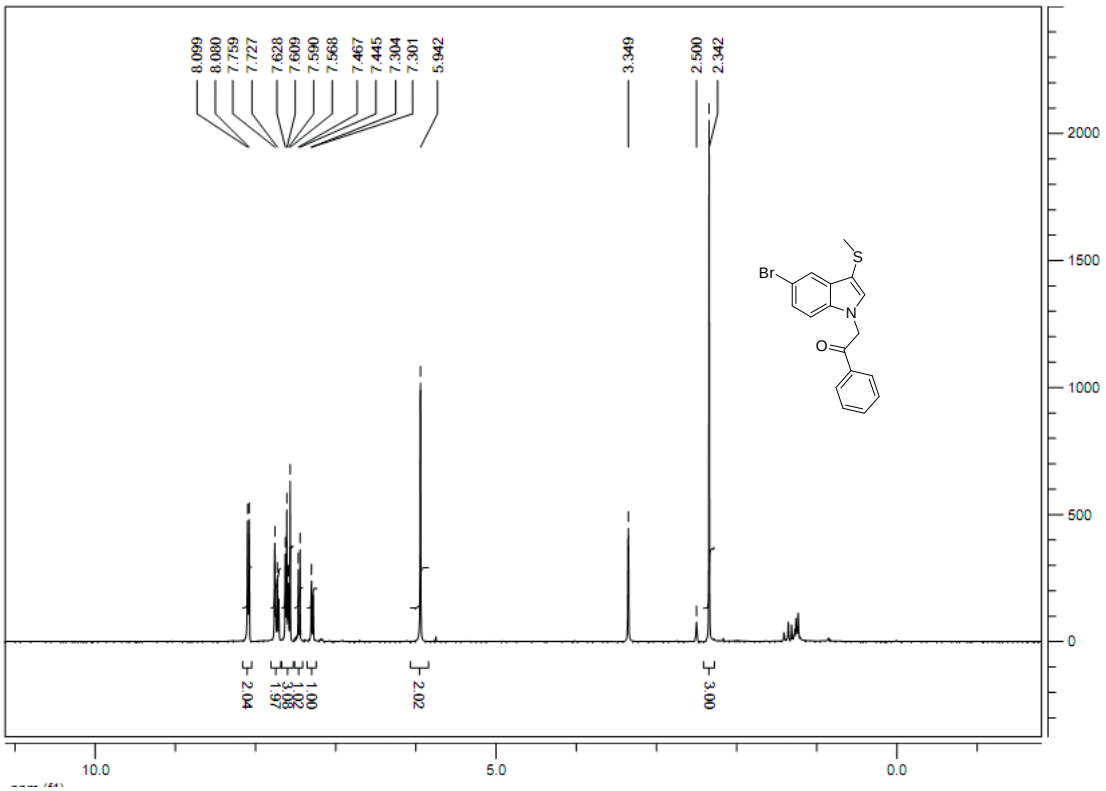
154.649
135.201
134.303
134.166
132.870
129.828
129.335
128.555
112.422
111.999
105.180
100.696
55.925
53.007
20.116
60000
50000
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)
S
O
N
O


8.104
8.085
7.729
7.710
7.626
7.621
7.612
7.589
7.513
7.491
7.193
7.171
5.948
3.373
2.500
2.346
2500
2000
1500
1000
500
0
2.07
6.11
1.06
2.02
3.00
10.0
5.0
0.0
ppm (f1)
S
Cl
N
O


193.794
135.913
134.760
134.604
133.879
129.913
128.845
128.095
124.733
121.916
117.618
112.486
105.252
52.652
19.627
Cl
S
N
O
2500
2000
1500
1000
500
0
200
150
100
50
0
ppm (f1)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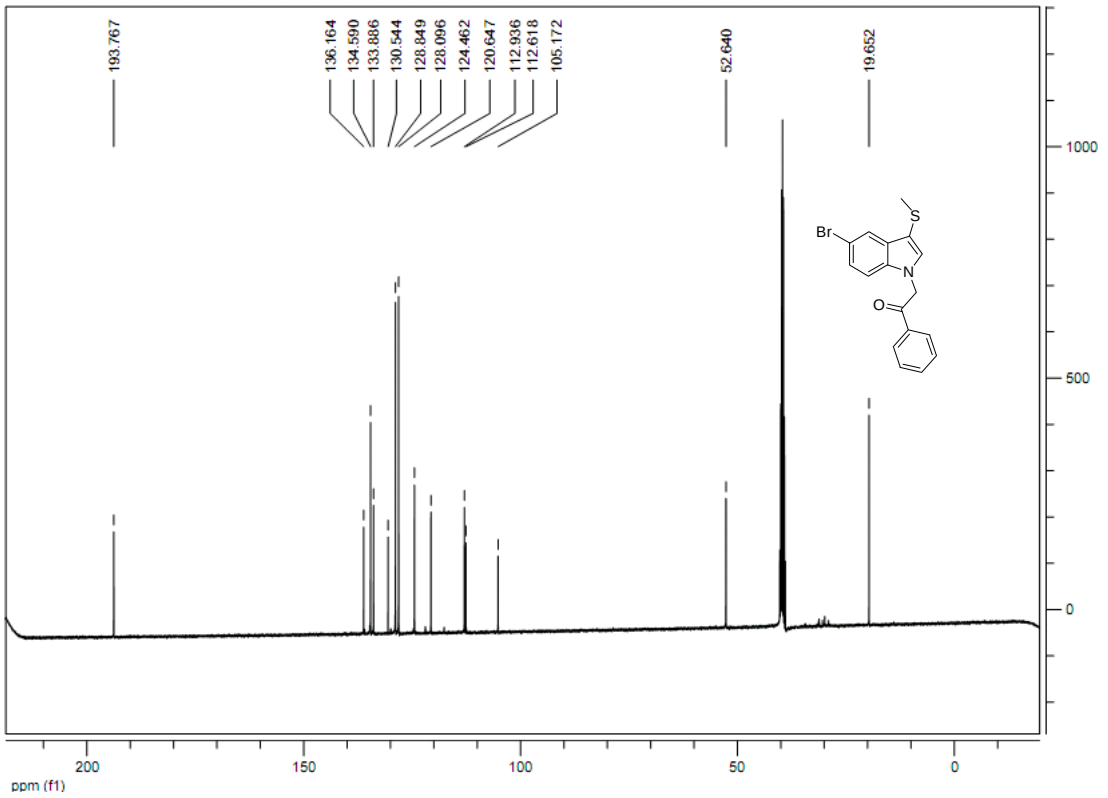
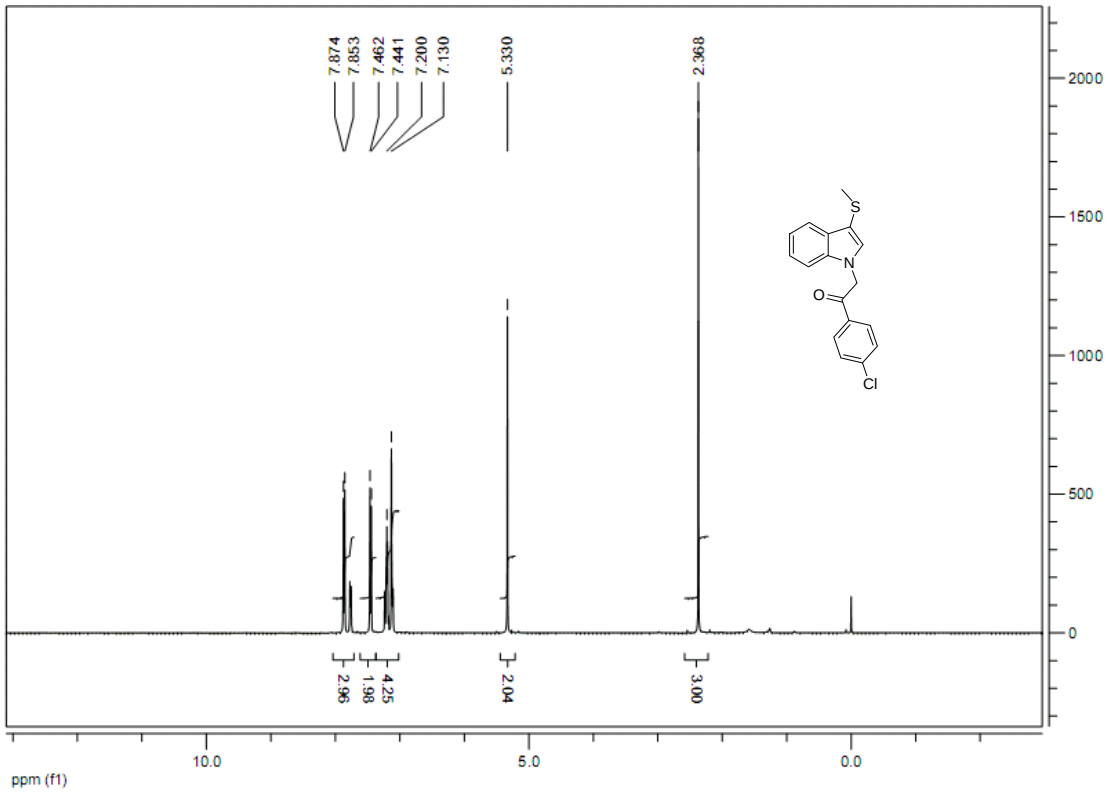
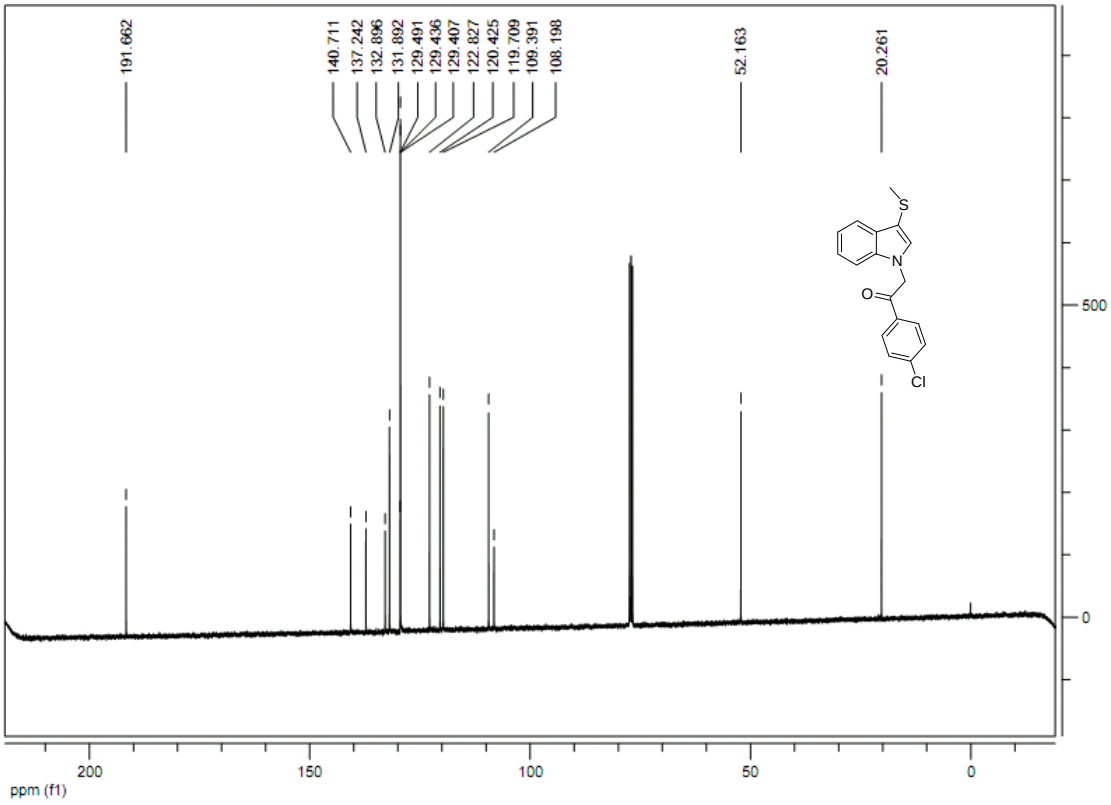
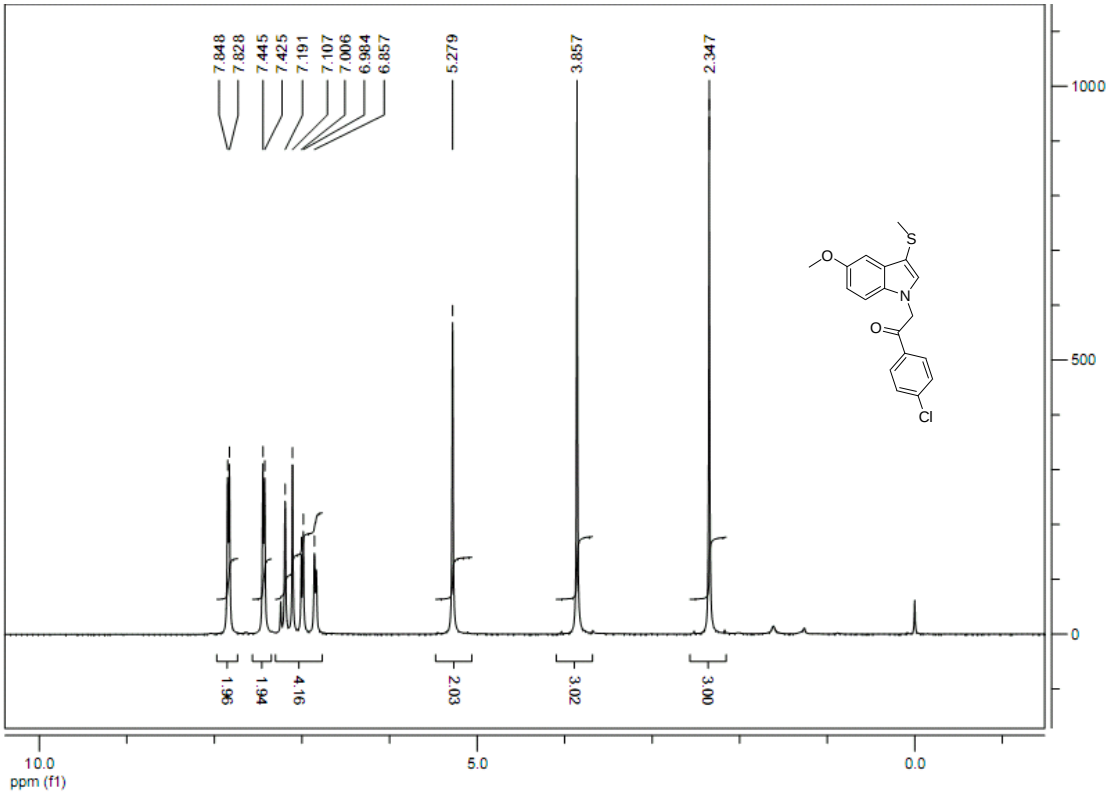
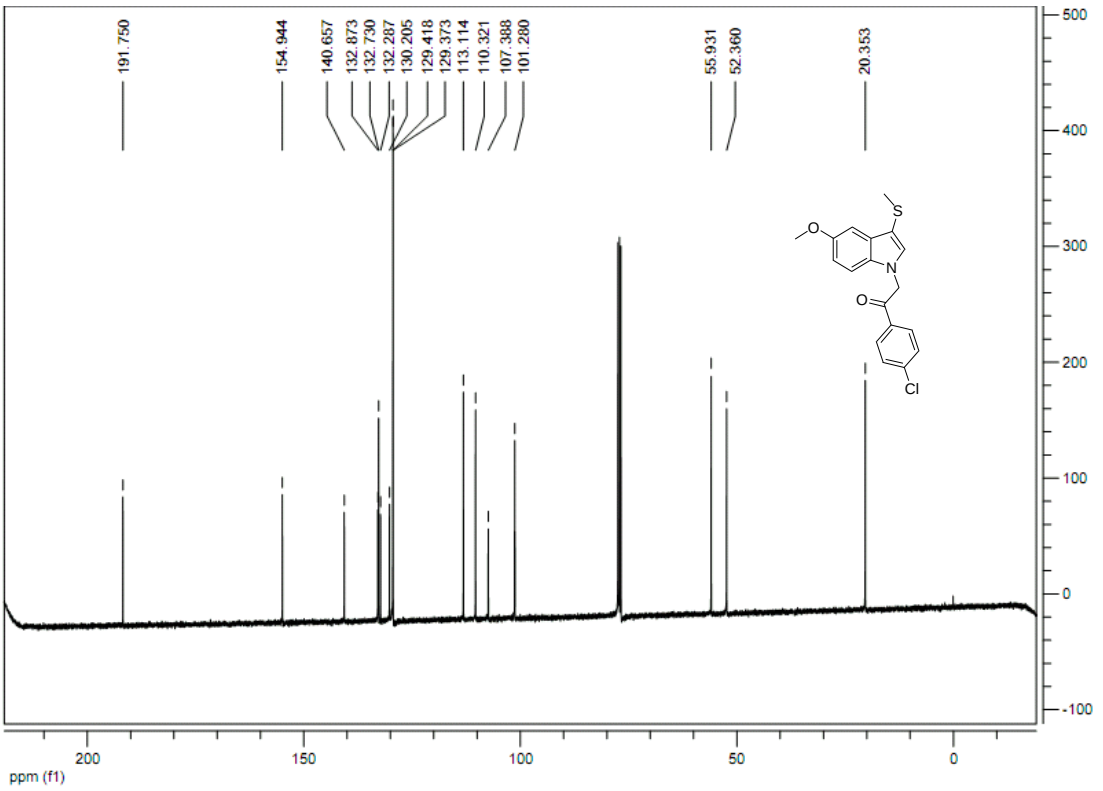
8.080
7.759
7.727
7.628
7.609
7.590
7.568
7.467
7.445
7.304
7.301
5.942
3.349
2.500
2.342
Br
S
N
O
2.04
1.97
1.00
2.02
3.00
2000
1500
1000
500
0
10.0
5.0
0.0


193.767
136.164
134.590
133.886
130.544
128.849
128.096
124.462
120.647
112.936
112.618
105.172
52.640
19.652
Br
S
N
O
1000
500
0
200
150
100
50
0
ppm (f1)


7.874
7.853
7.462
7.441
7.200
7.130
5.330
2.368
S
N
O
Cl
2000
1500
1000
500
0
2.96
1.98
4.25
2.04
3.00
10.0
5.0
0.0
ppm (f1)


191.662
140.711
137.242
132.896
131.892
129.491
129.436
129.407
122.827
120.425
119.709
109.391
108.198
52.163
20.261
S
N
O
Cl
500
0
200
150
100
50
0
ppm (f1)


7.848
7.828
7.445
7.425
7.191
7.107
7.006
6.984
6.857
5.279
3.857
2.347
S
O
N
O
Cl
1000
500
0
1.96
1.94
4.16
2.03
3.02
3.00
10.0
5.0
0.0
ppm (f1)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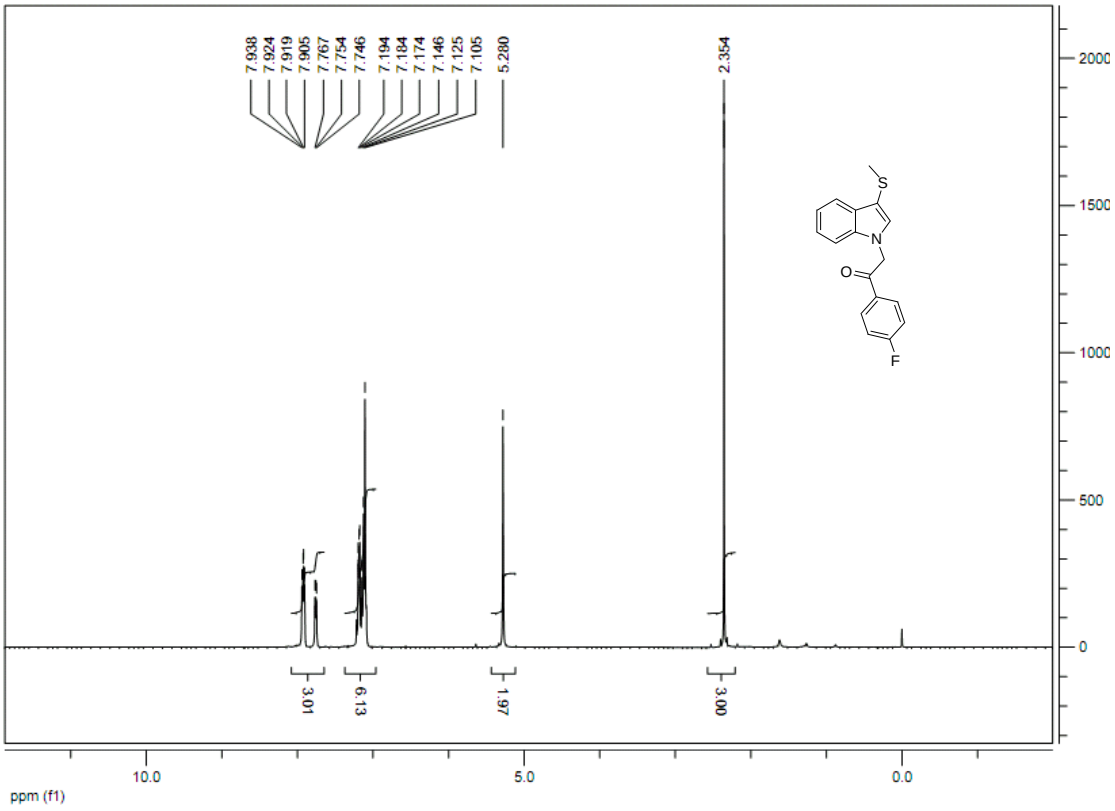
140.657
132.873
132.730
132.287
130.205
129.418
129.373
113.114
110.321
107.388
101.280
55.931
52.360
20.353
O
S
N
O
Cl
500
400
300
200
100
0
-100
200
150
100
50
0
ppm (f1)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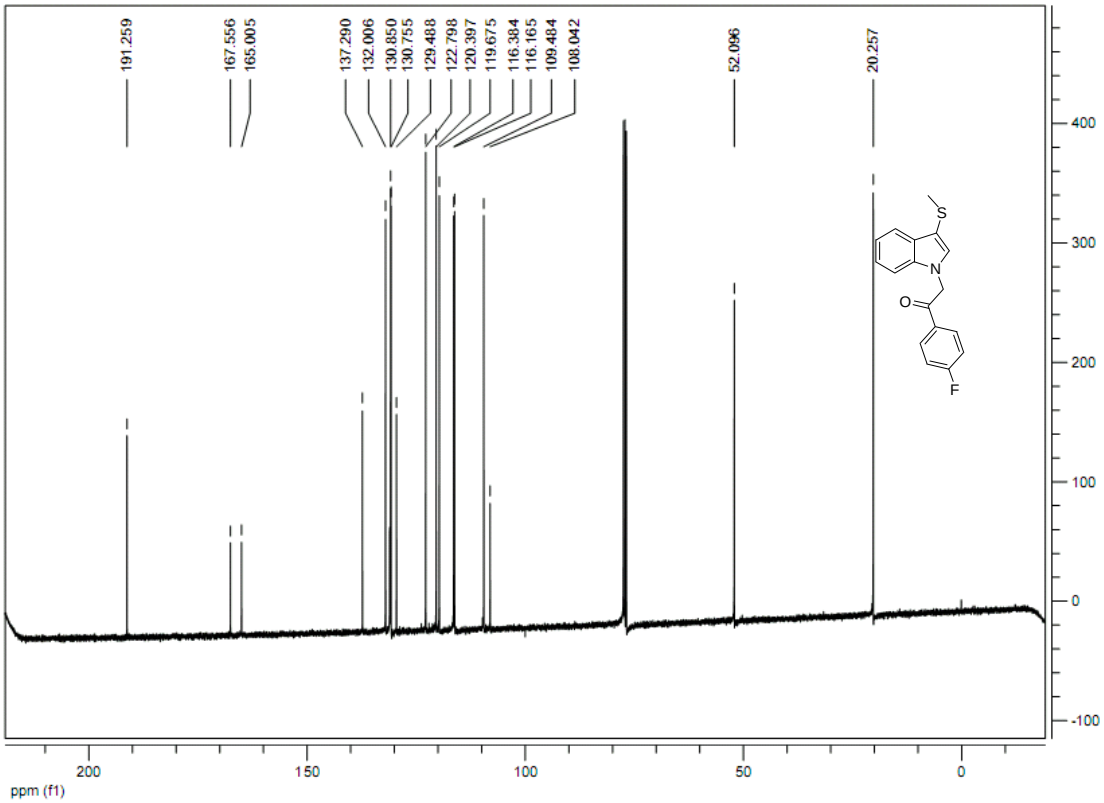
7.924
7.919
7.905
7.767
7.754
7.746
7.194
7.184
7.174
7.146
7.125
7.105
5.280
2.354
S
N
O
F
3.01
6.13
1.97
3.00
2000
1500
1000
500
0
10.0
5.0
0.0
ppm (f1)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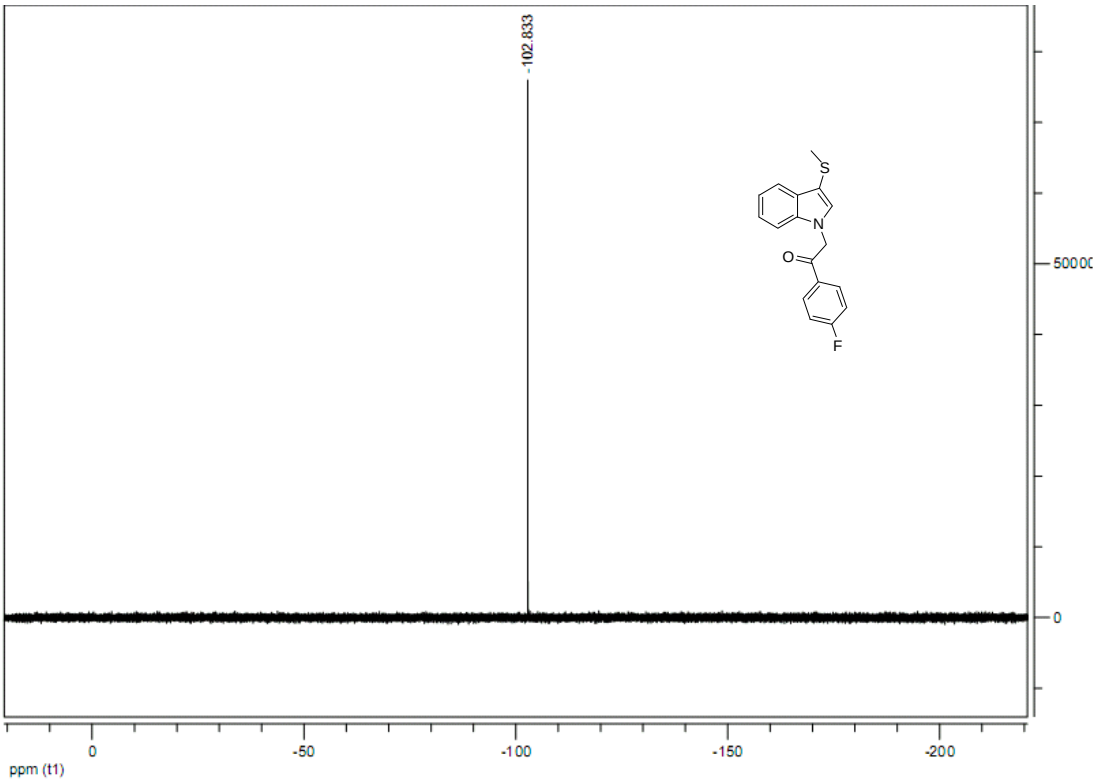
167.556
165.005
137.290
132.006
130.850
130.755
129.488
122.798
120.397
119.675
116.384
116.165
109.484
108.042
52.096
20.257
S
N
O
F
400
300
200
100
0
-100
200
150
100
50
0
ppm (f1)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S
N
O
F
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0
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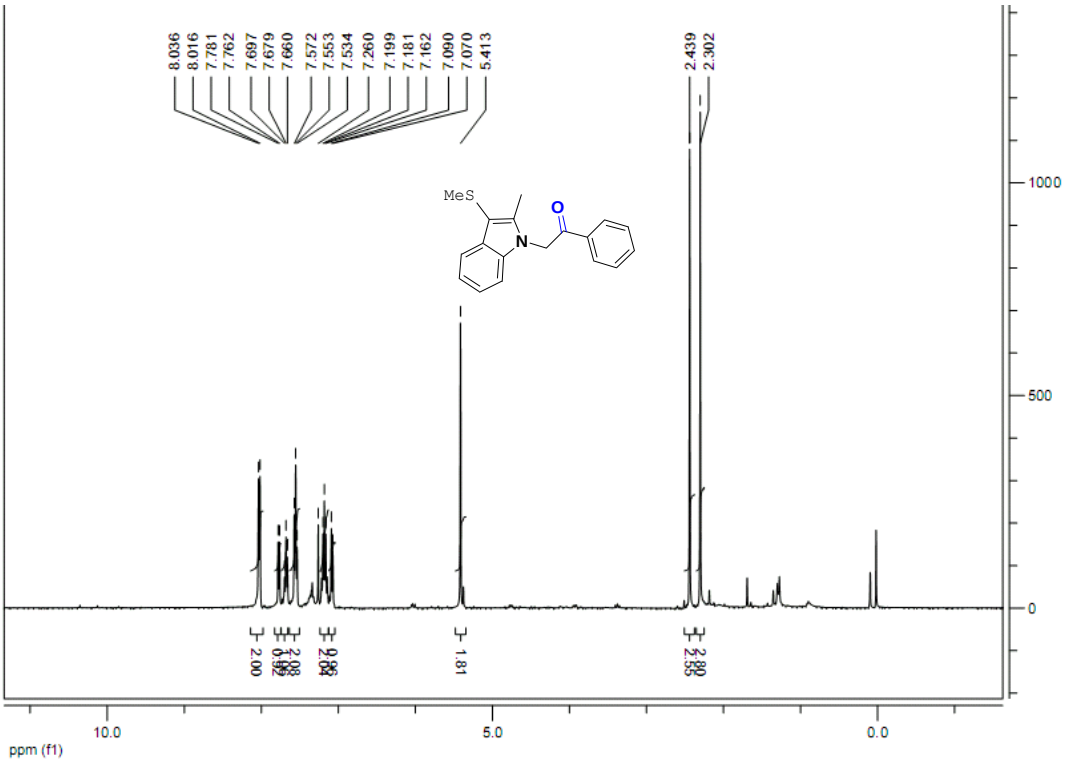
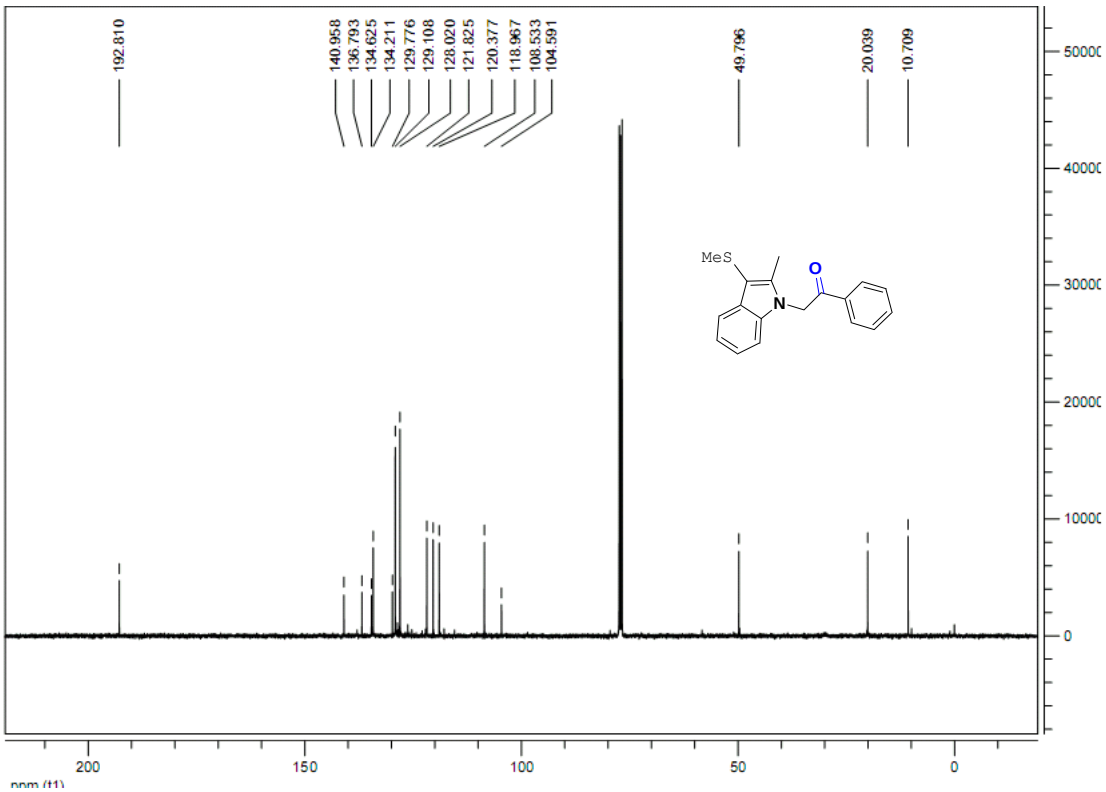
-150
-200
ppm (f1)


8.036
8.016
7.781
7.762
7.697
7.679
7.660
7.572
7.553
7.534
7.260
7.199
7.181
7.162
7.090
7.070
5.413
2.439
2.302
MeS
O
N
1000
500
0
2.00
1.81
10.0
5.0
0.0
ppm (f1)


192.810
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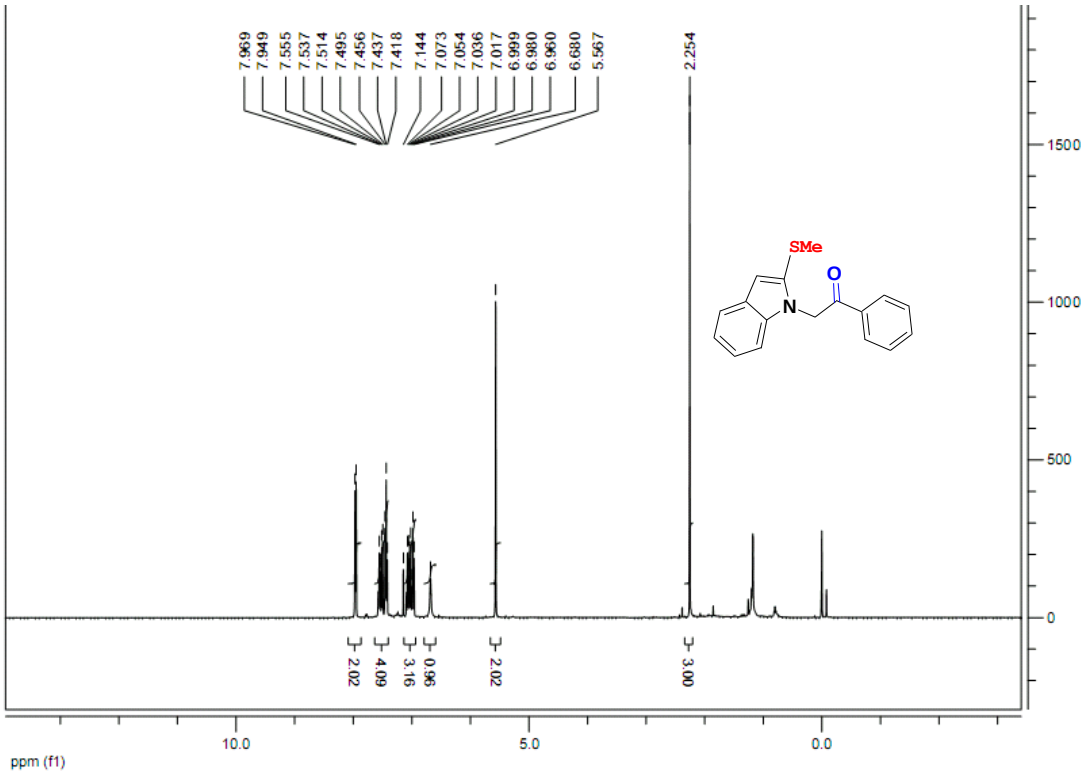
134.211
129.776
129.108
128.020
121.825
120.377
118.967
108.533
104.591
49.796
20.039
10.709
MeS
O
N
50000
40000
30000
20000
10000
0
200
150
100
50
0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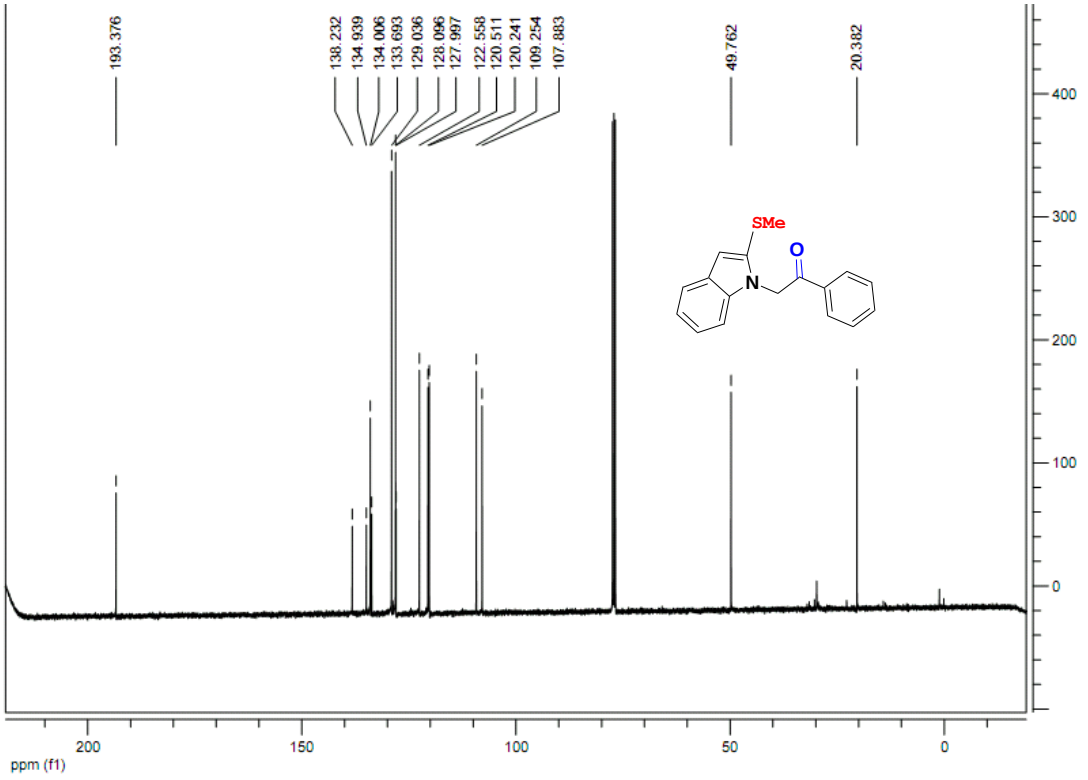
7.949
7.555
7.537
7.514
7.495
7.456
7.437
7.418
7.144
7.073
7.054
7.036
7.017
6.999
6.980
6.960
6.680
5.567
2.254
SMe
O
N
1500
1000
500
0
2.02
4.09
3.16
0.96
2.02
3.00
10.0
5.0
0.0
ppm (f1)


193.376
138.232
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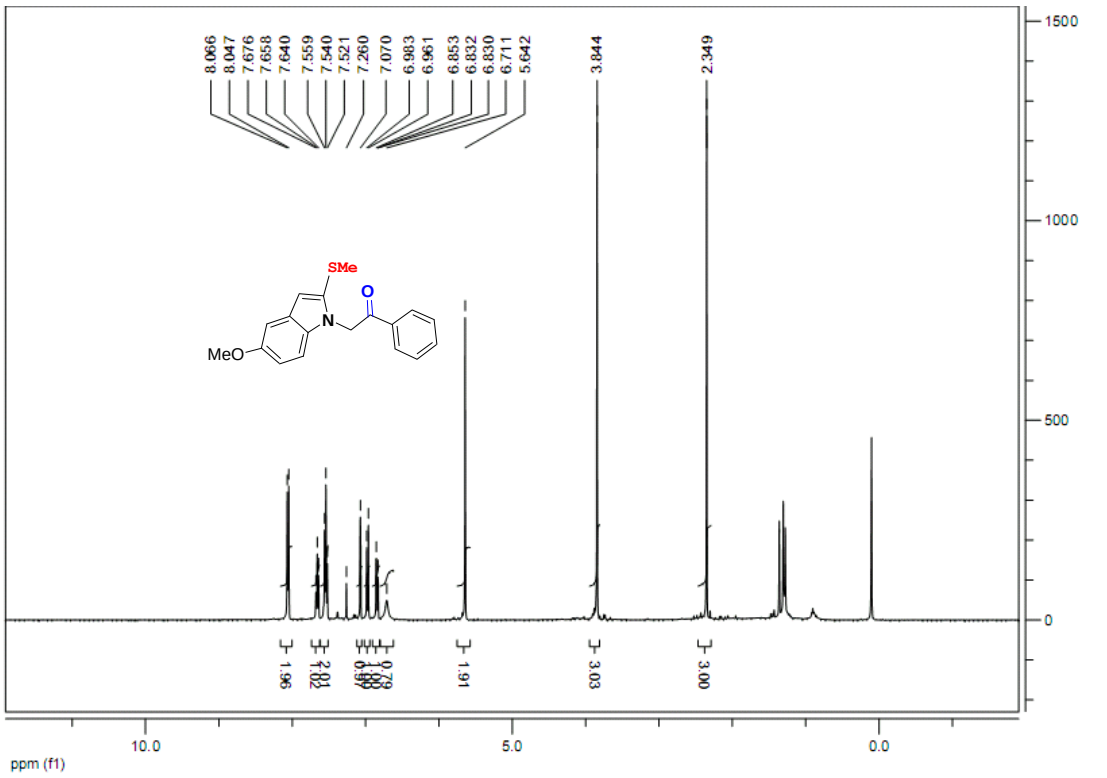
134.006
133.693
129.036
128.096
127.997
122.558
120.511
120.241
109.254
107.883
49.762
20.382
SMe
O
N
400
300
200
100
0
200
150
100
50
0
ppm (f1)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8.047
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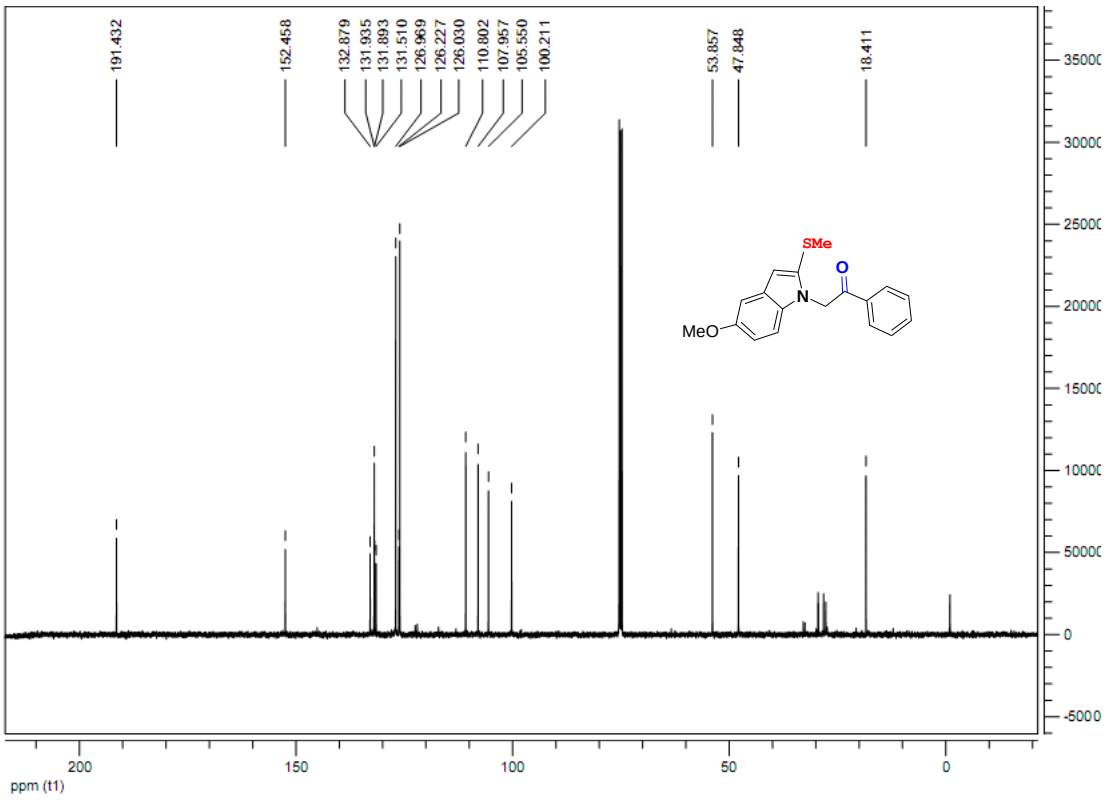
7.559
7.540
7.521
7.260
7.070
6.983
6.961
6.853
6.832
6.830
6.711
5.642
3.844
2.349
SMe
O
N
MeO
1.96
2.02
1.91
3.03
3.00
1500
1000
500
0
10.0
5.0
0.0
ppm (f1)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131.893
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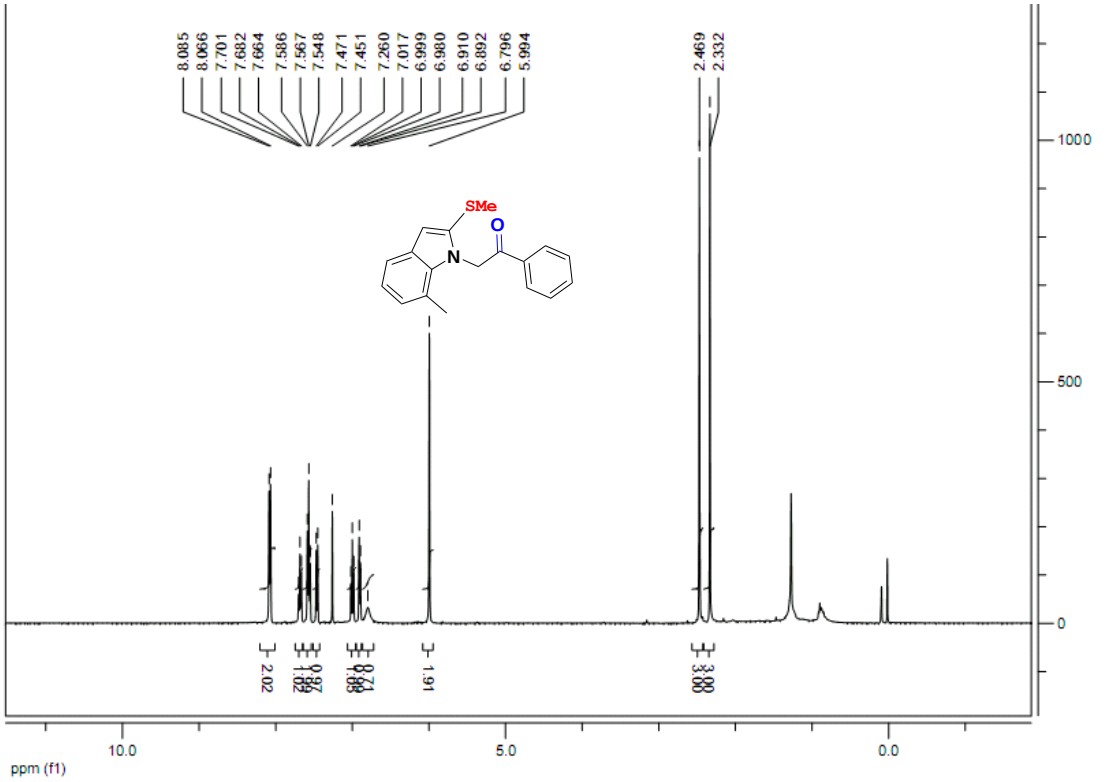
126.969
126.227
126.030
110.802
107.957
105.550
100.211
53.857
47.848
18.411
SMe
O
N
MeO
35000
30000
25000
20000
15000
10000
5000
0
-5000
200
150
100
50
0
ppm (t1)


8.085
8.066
7.701
7.682
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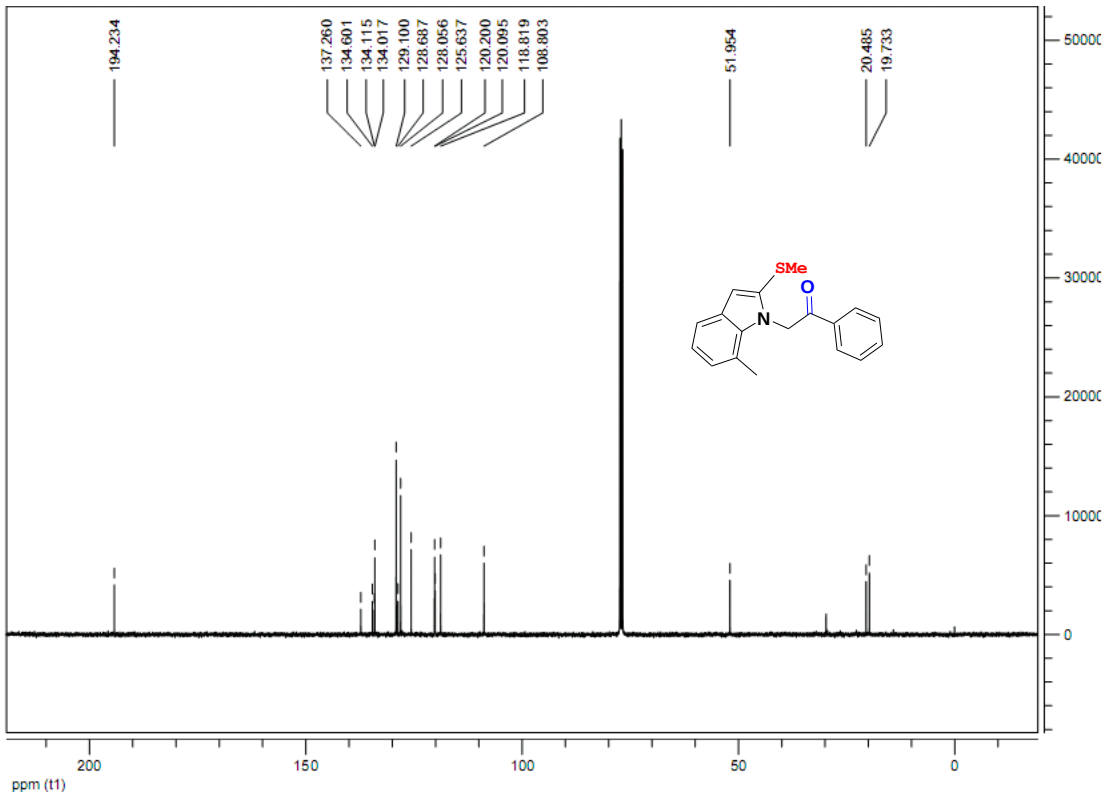
7.586
7.567
7.548
7.471
7.451
7.260
7.017
6.999
6.980
6.910
6.892
6.796
5.994
2.469
2.332
SMe
O
N
1000
500
0
2.02
1.91
3.00
10.0
5.0
0.0
ppm (f1)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137.260
134.601
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134.017
129.100
128.687
128.056
125.637
120.200
120.095
118.819
108.803
51.954
20.485
19.733
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N
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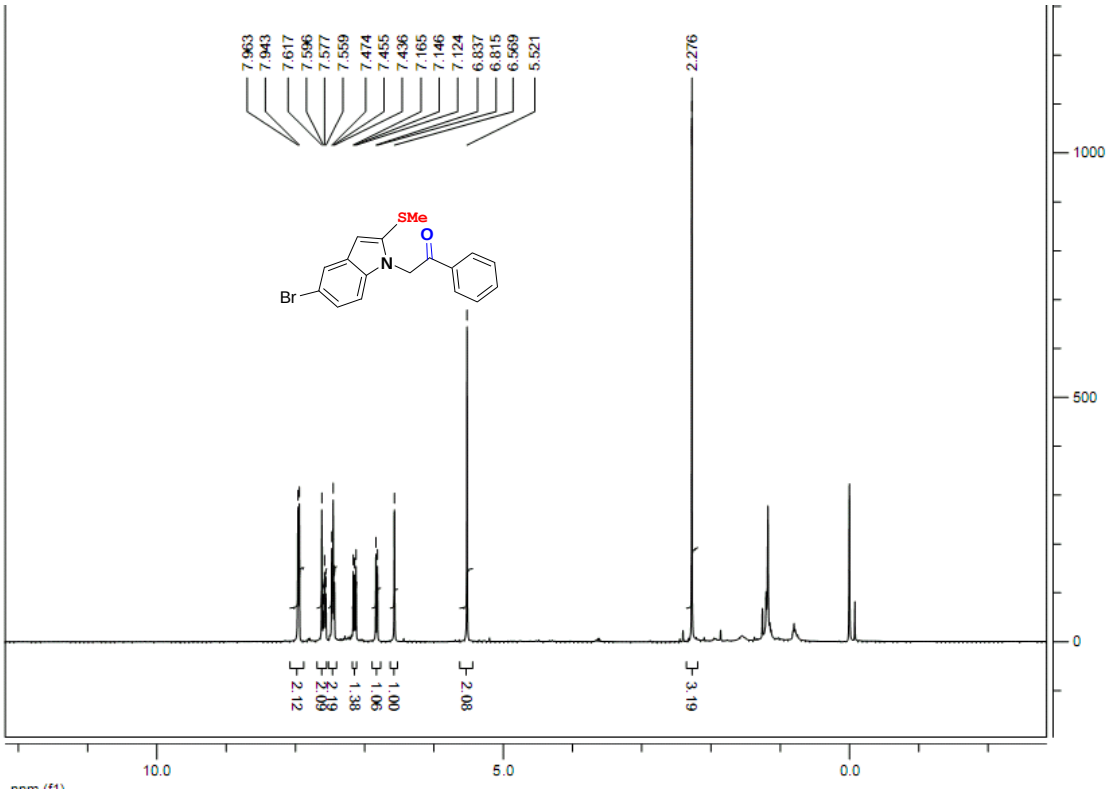
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)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7.455
7.436
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7.146
7.124
6.837
6.815
6.569
5.521
2.276
SMe
O
N
Br
1000
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2.00
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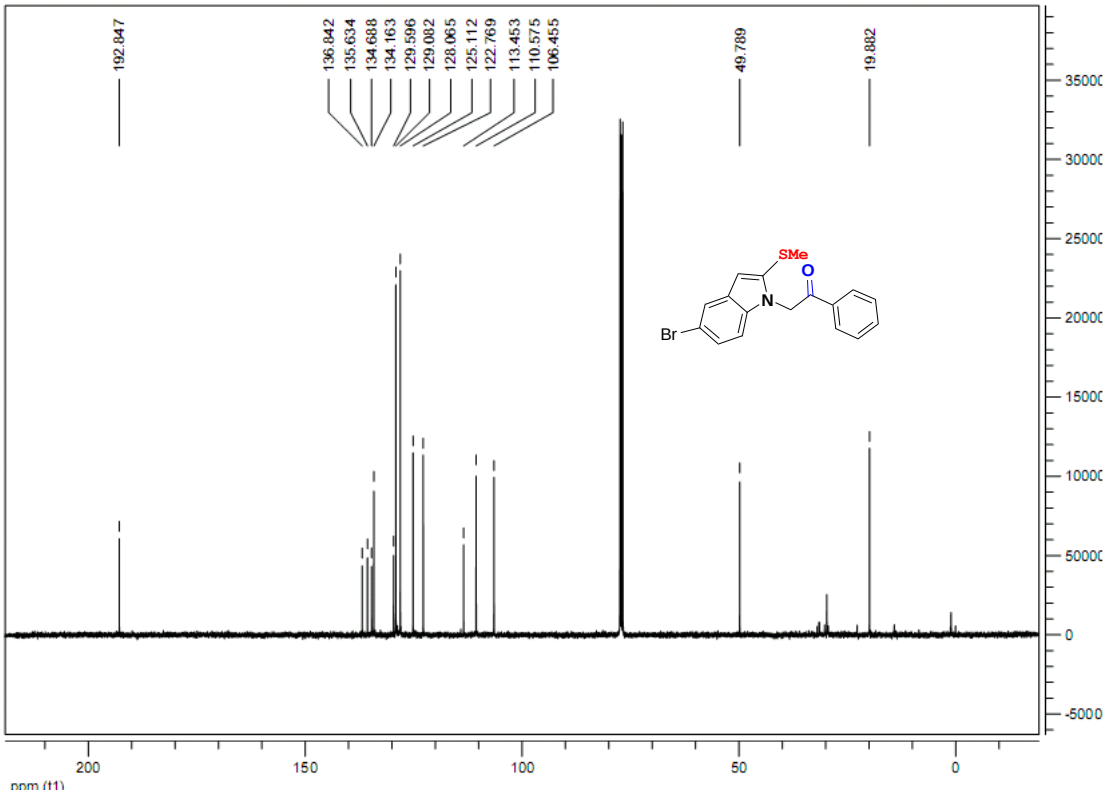
1.90
1.00
2.08
3.19
10.0
5.0
0.0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134.163
129.596
129.082
128.065
125.112
122.769
113.453
110.575
106.455
49.789
19.882
SMe
O
N
Br
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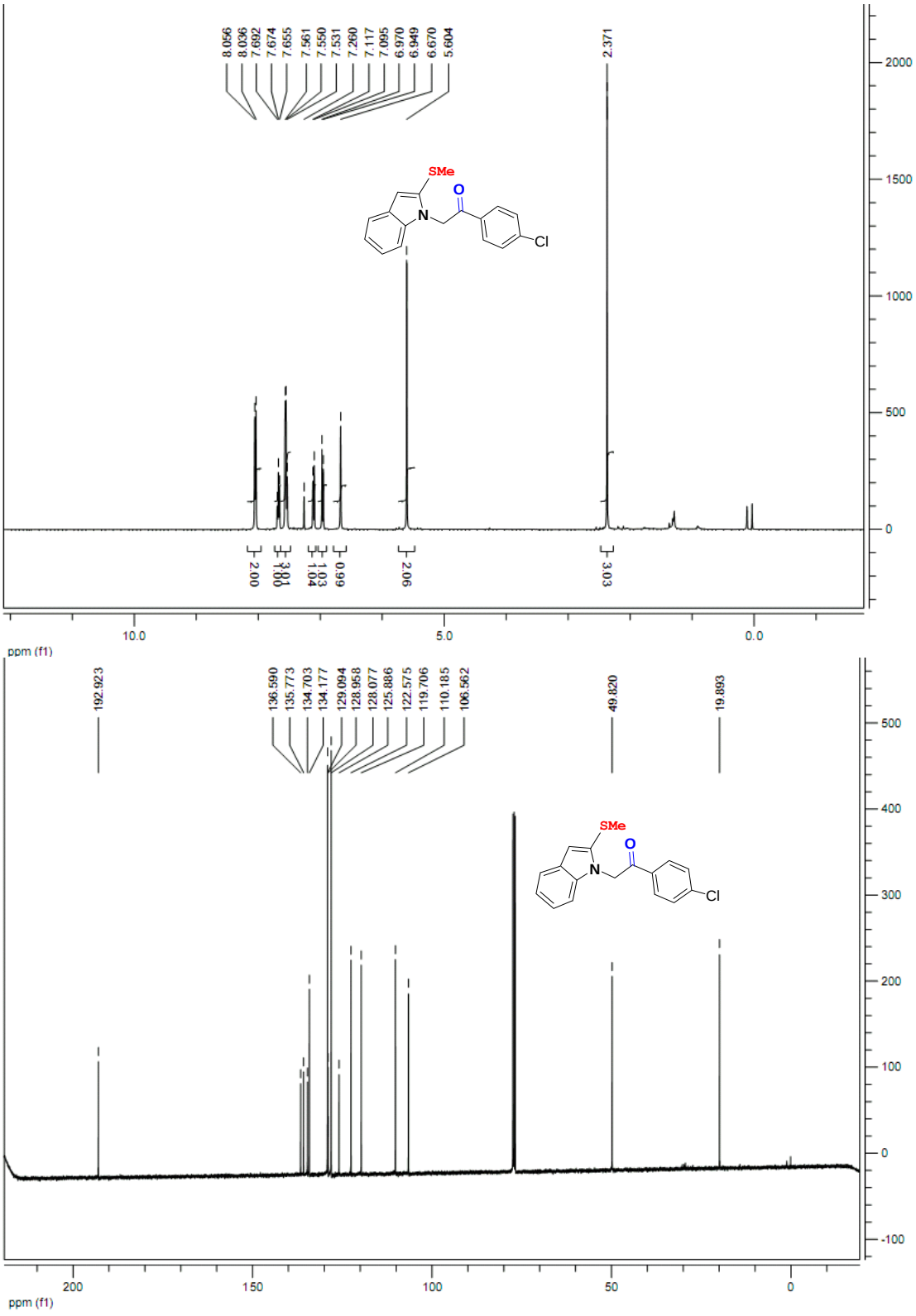
25000
20000
15000
10000
5000
0
-5000
200
150
100
50
0
ppm (f1)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7.561
7.550
7.531
7.260
7.117
7.095
6.970
6.949
6.670
5.604
2.371
SMe
O
N
Cl
2.00
3.01
1.04
1.03
0.99
2.06
3.03
ppm (f1)
192.923
136.590
135.773
134.703
134.177
129.094
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128.077
125.886
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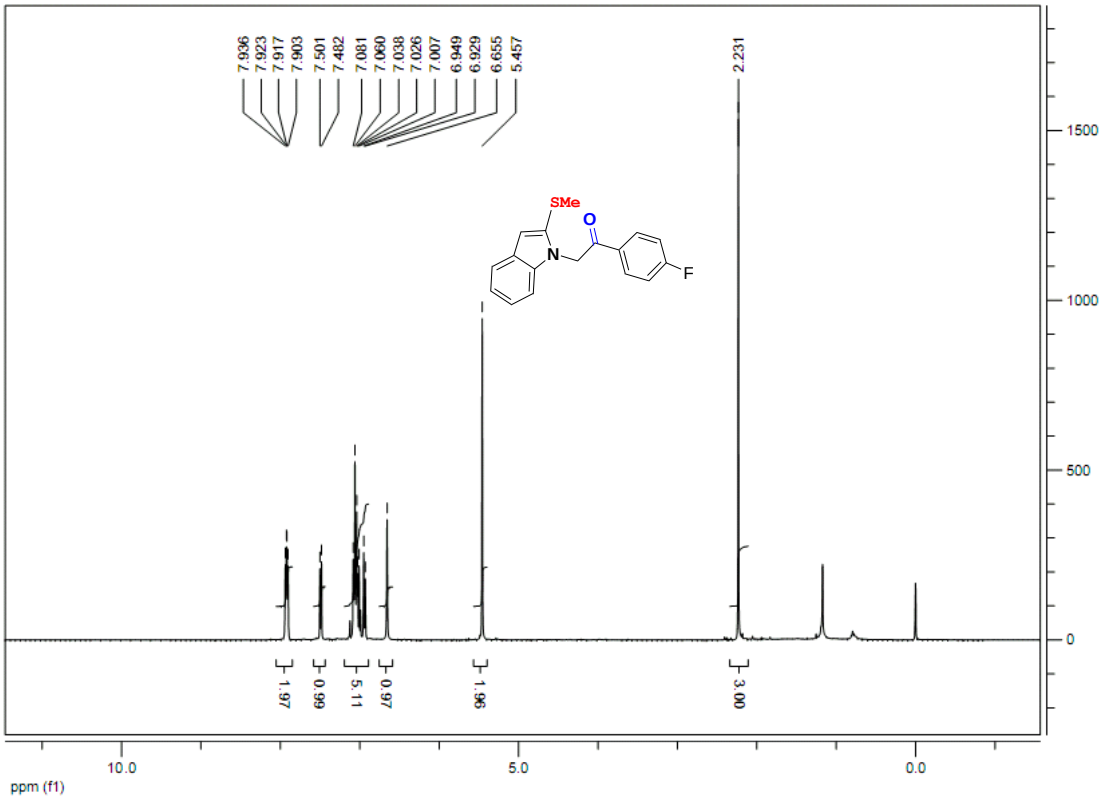
110.185
106.562
49.820
19.893
ppm (f1)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7.903
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7.482
7.081
7.060
7.038
7.026
7.007
6.949
6.929
6.655
5.457
2.231
SMe
O
N
F
1.97
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5.11
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1.96
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1500
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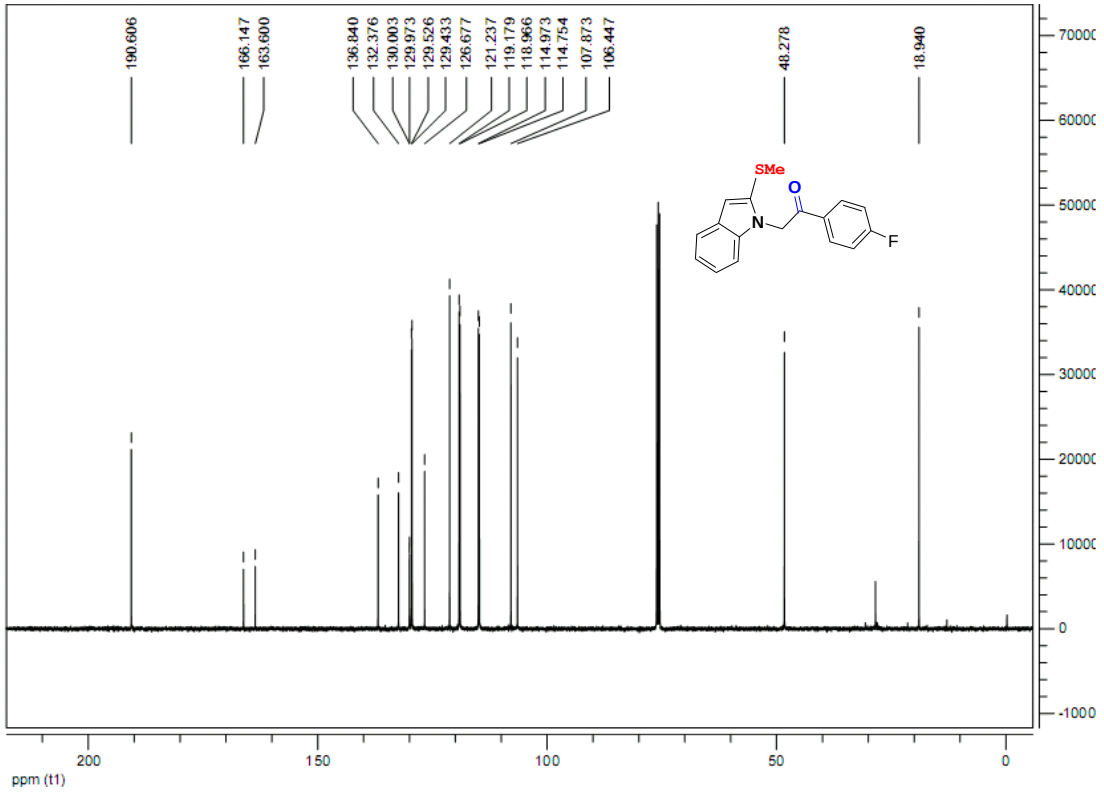
500
0
10.0
5.0
0.0
ppm (f1)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166.147
163.600
136.840
132.376
130.003
129.973
129.526
129.433
126.677
121.237
119.179
118.966
114.973
114.754
107.873
106.447
48.278
18.940
SMe
O
N
F
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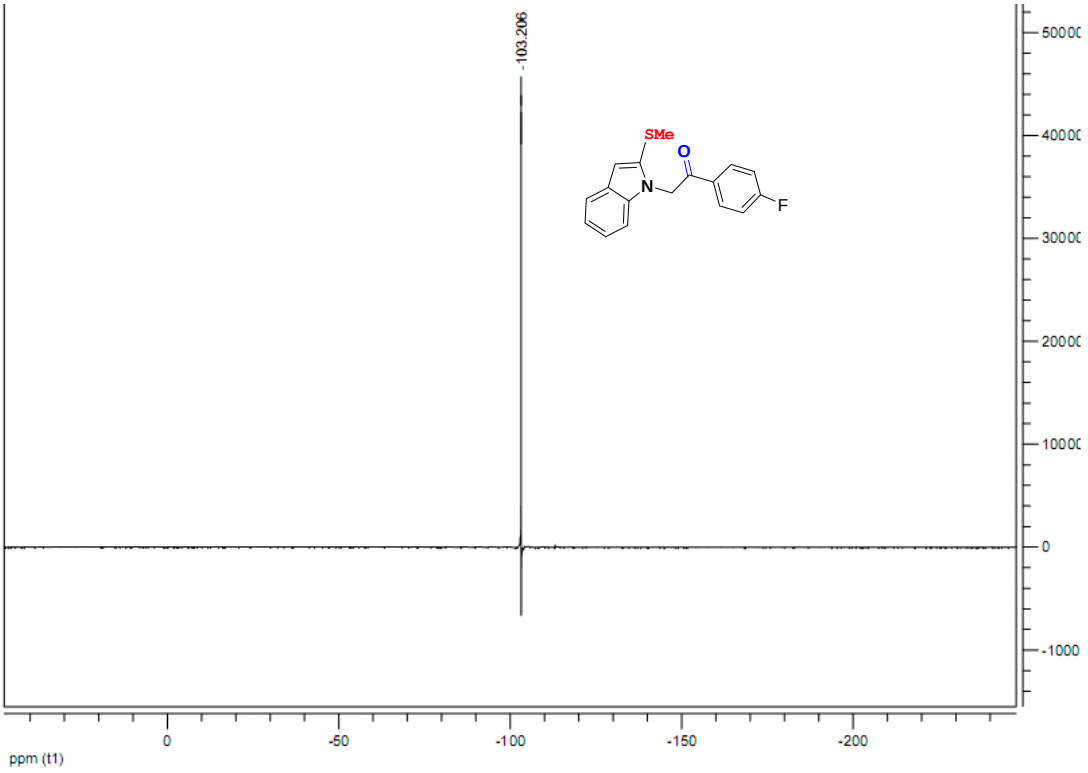
60000
50000
40000
30000
20000
10000
0
-10000
200
150
100
50
0
ppm (t1)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O
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F
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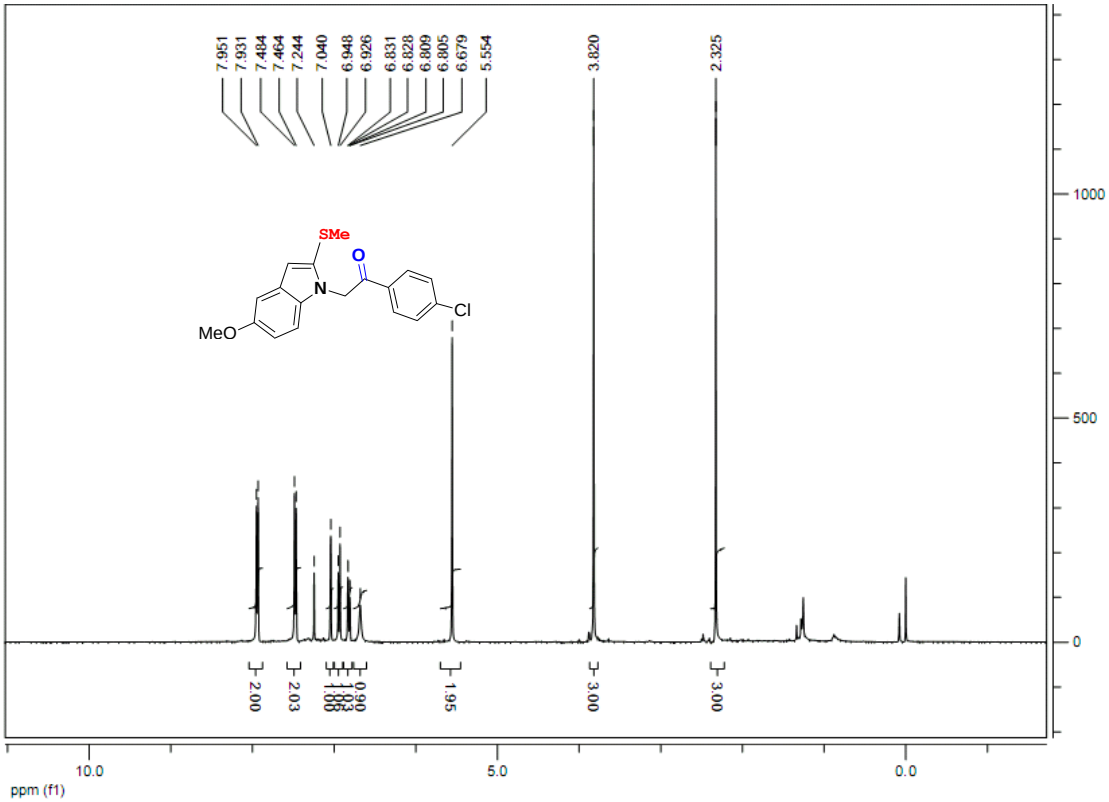
40000
30000
20000
10000
0
-10000
0
-50
-100
-150
-200
ppm (t1)


7.951
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7.464
7.244
7.040
6.948
6.926
6.831
6.828
6.809
6.805
6.679
5.554
3.820
2.325
SMe
O
N
MeO
Cl
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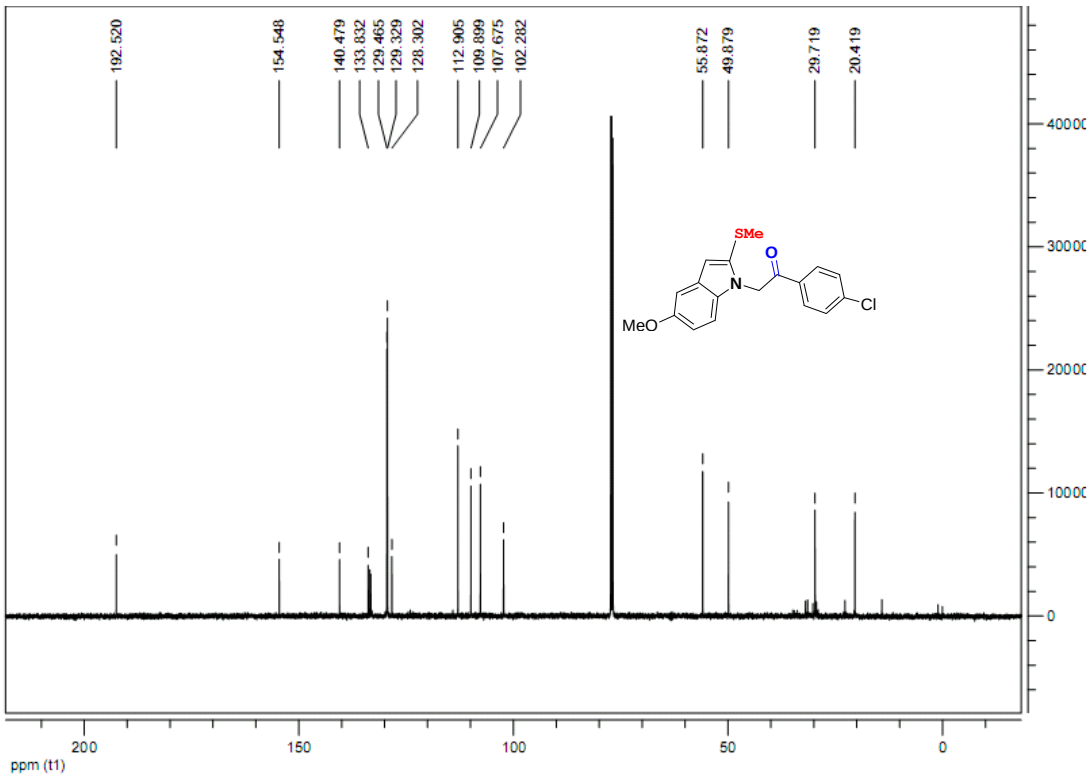
2.03
0.90
1.95
3.00
3.00
10.0
5.0
0.0
ppm (f1)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129.329
128.302
112.905
109.899
107.675
102.282
55.872
49.879
29.719
20.419
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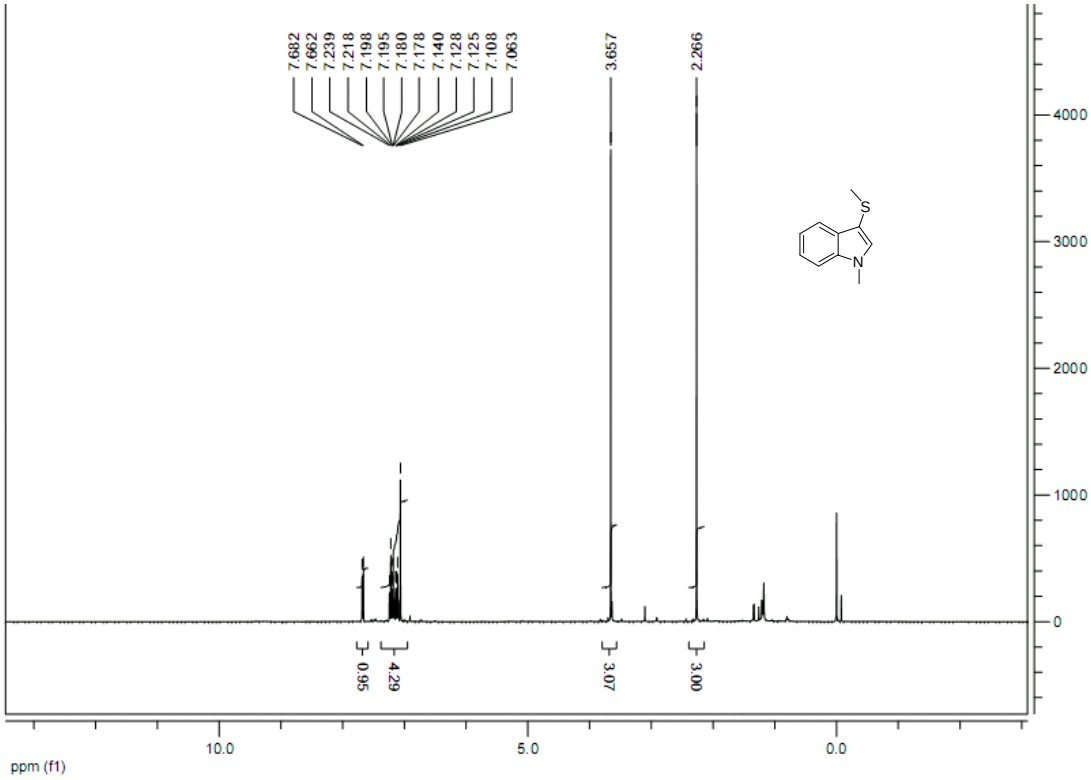
O
N
Cl
MeO
4000
3000
2000
1000
0
200
150
100
50
0
ppm (t1)


7.682
7.662
7.239
7.218
7.198
7.195
7.180
7.178
7.140
7.128
7.125
7.108
7.063
3.657
2.266
S
N
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3.00
4000
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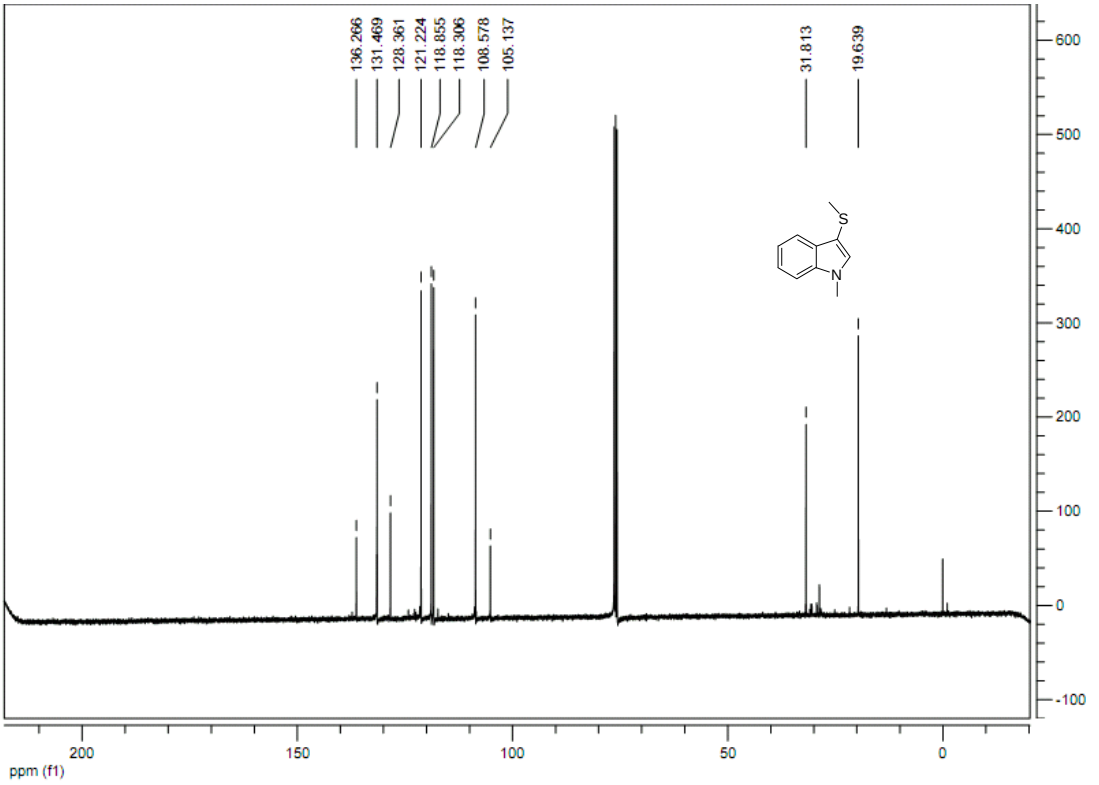
0.0
ppm (f1)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131.469
128.361
121.224
118.855
118.306
108.578
105.137
31.813
19.639
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50
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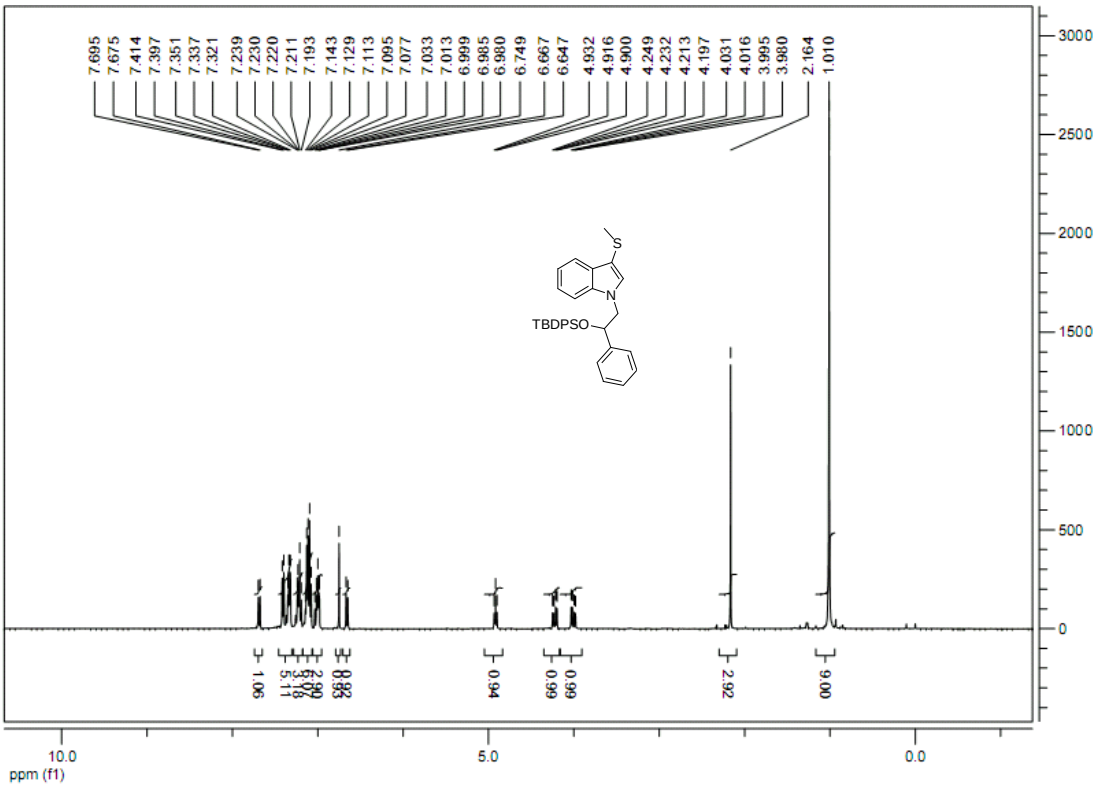
ppm (f1)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7.414
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7.337
7.321
7.239
7.230
7.220
7.211
7.193
7.143
7.129
7.113
7.095
7.077
7.033
7.013
6.999
6.985
6.980
6.749
6.667
6.647
4.932
4.916
4.900
4.249
4.232
4.213
4.197
4.031
4.016
3.995
3.980
2.164
1.010
S
N
TBDPSO
1.06
5.11
2.90
0.83
0.94
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0.99
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9.00
3000
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2000
1500
1000
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0
10.0
5.0
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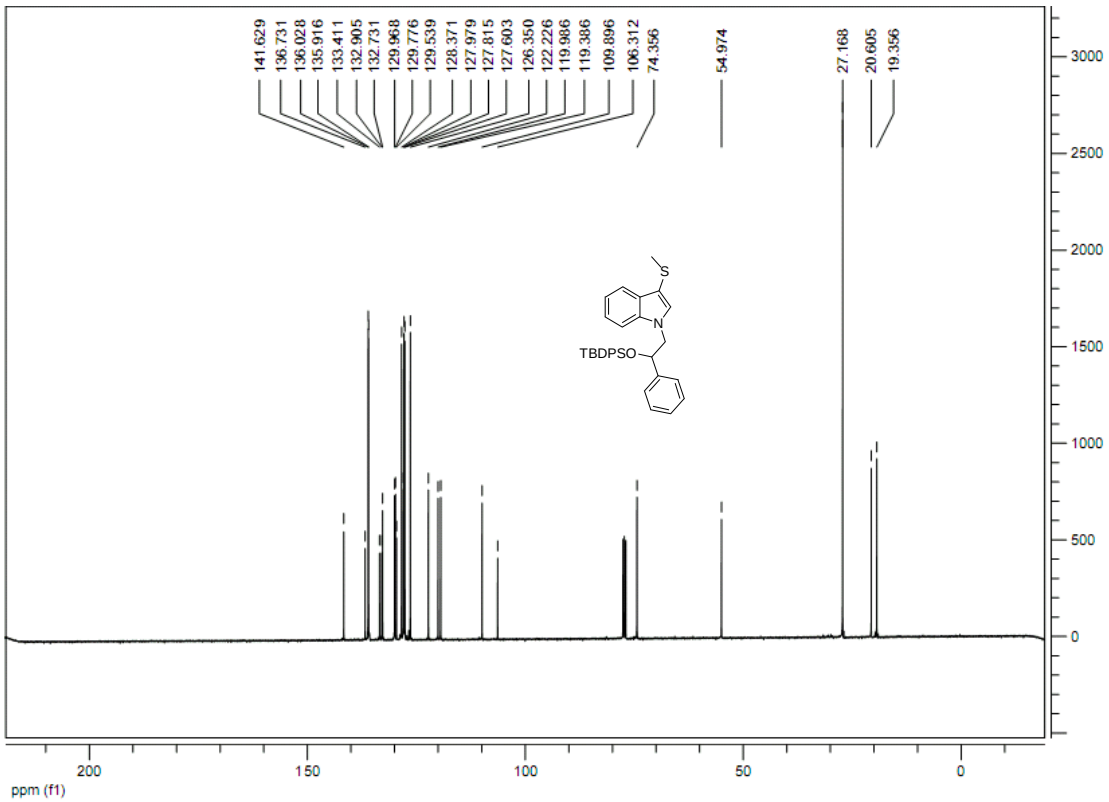
ppm (f1)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136.028
135.916
133.411
132.905
132.731
129.968
129.776
129.539
128.371
127.979
127.815
127.603
126.350
122.226
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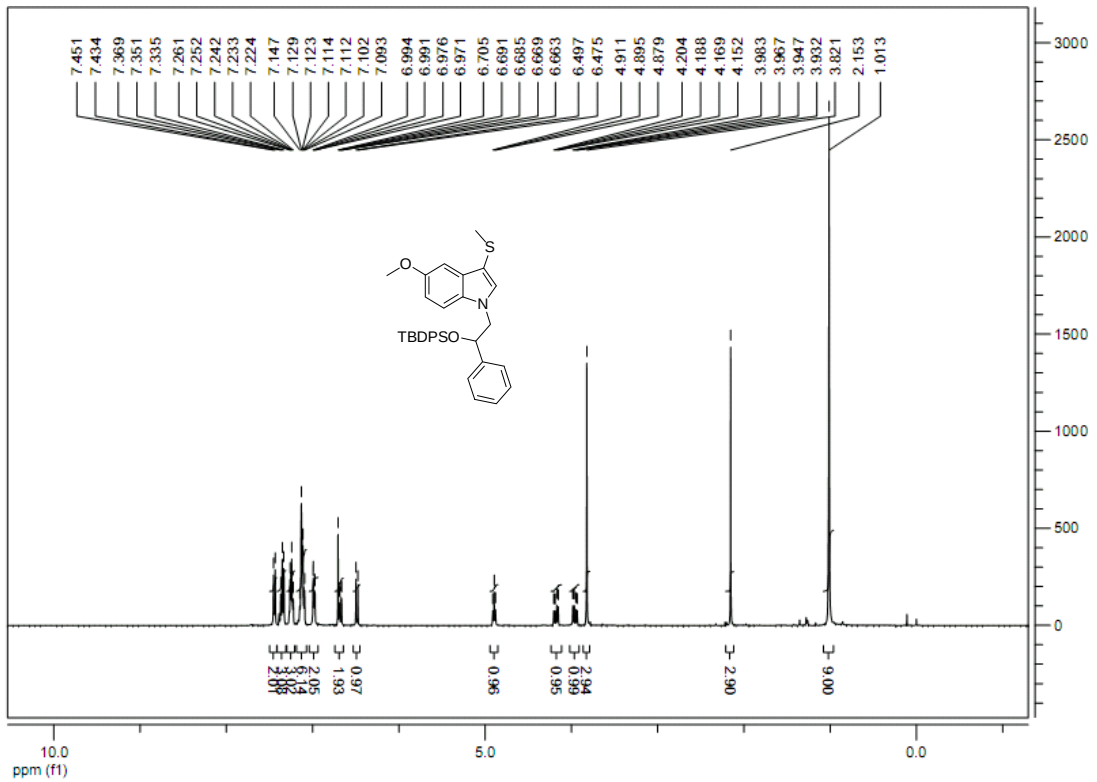
109.896
106.312
74.356
54.974
27.168
20.605
19.356
TBDPSO
ppm (f1)


7.451
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7.369
7.351
7.335
7.261
7.252
7.242
7.233
7.224
7.147
7.129
7.123
7.114
7.112
7.102
7.093
6.994
6.991
6.976
6.971
6.705
6.691
6.685
6.669
6.663
6.497
6.475
4.911
4.895
4.879
4.204
4.188
4.169
4.152
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3.967
3.947
3.932
3.821
2.153
1.013
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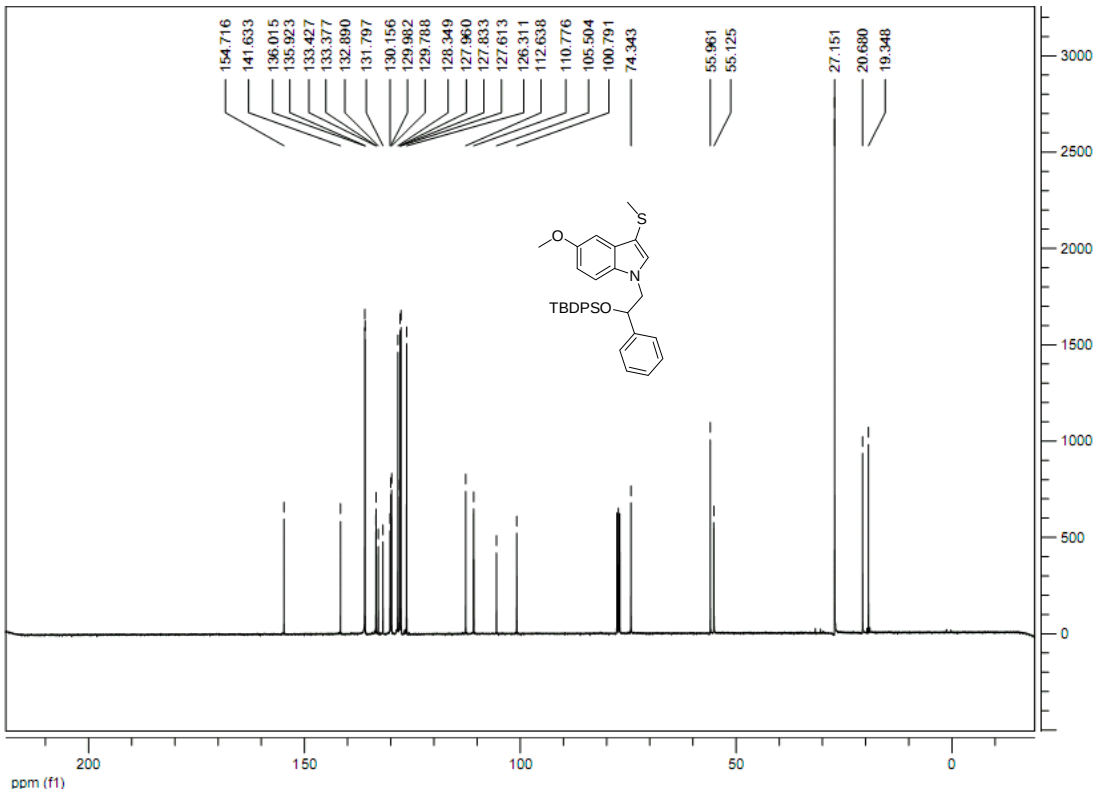
ppm (f1)


154.716
141.633
136.015
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133.377
132.890
131.797
130.156
129.982
129.788
128.349
127.960
127.833
127.613
126.311
112.638
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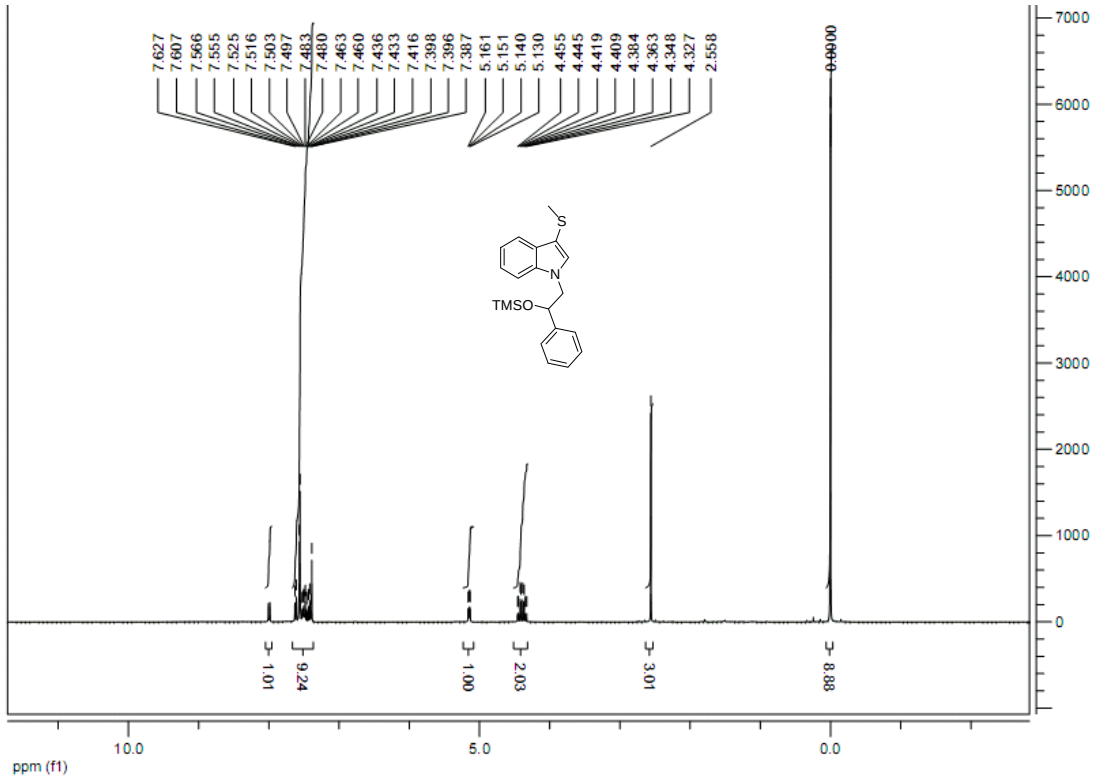
100.791
74.343
55.961
55.125
27.151
20.680
19.348
TBDPSO
ppm (f1)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7.607
7.566
7.555
7.525
7.516
7.503
7.497
7.483
7.480
7.463
7.460
7.436
7.433
7.416
7.398
7.396
7.387
5.161
5.151
5.140
5.130
4.455
4.445
4.419
4.409
4.384
4.363
4.348
4.327
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0.0000
TMSO
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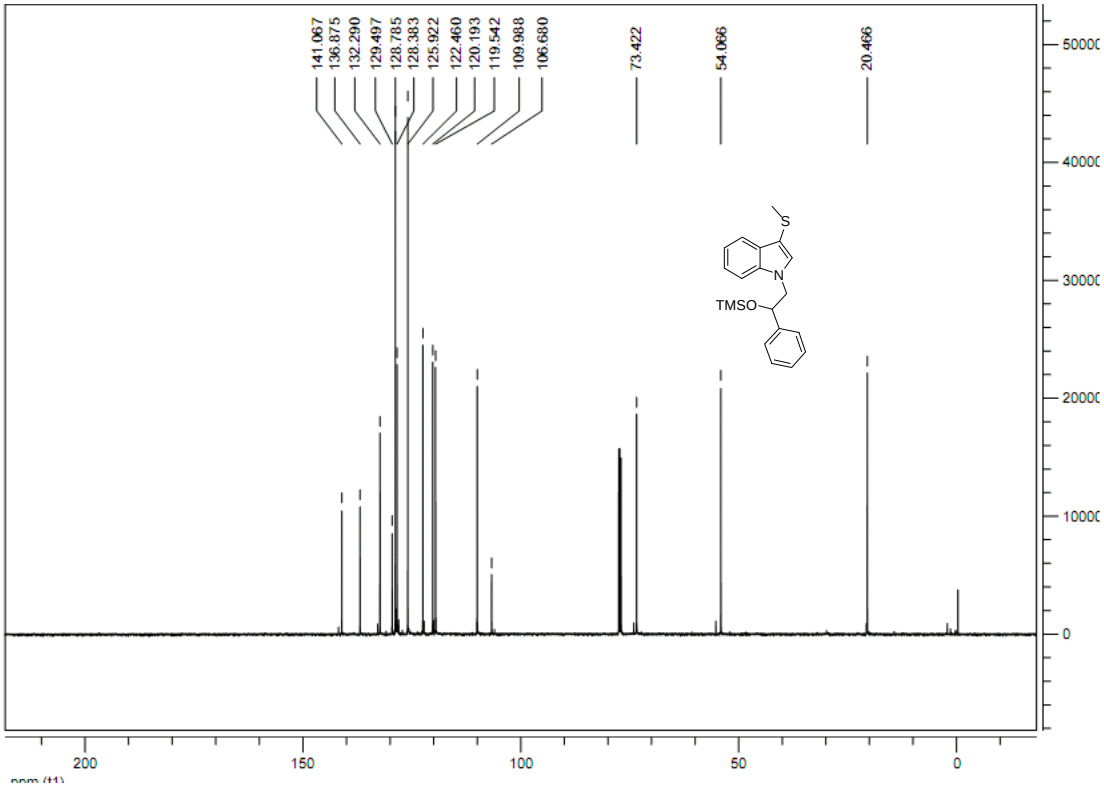
9.24
1.00
2.03
3.01
8.88
ppm (f1)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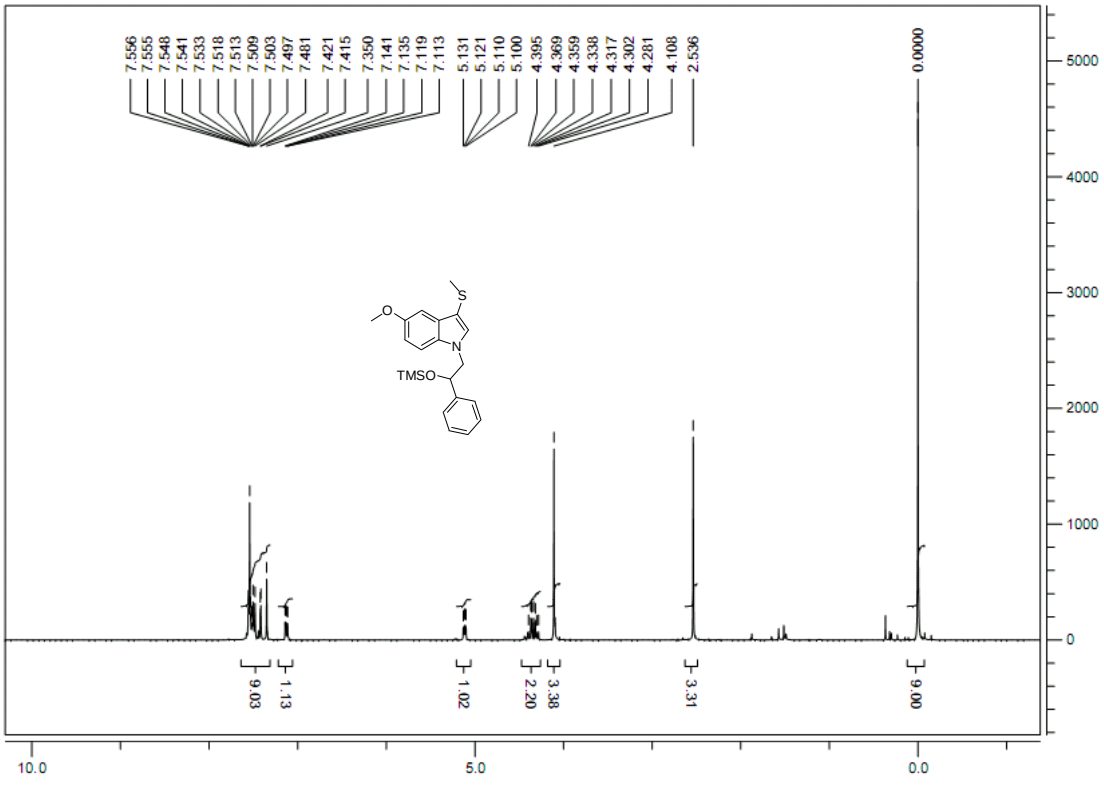
136.875
132.290
129.497
128.785
128.383
125.922
122.460
120.193
119.542
109.988
106.680
73.422
54.066
20.466
TMSO
S
N
200
150
100
50
0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7.555
7.548
7.541
7.533
7.518
7.513
7.509
7.503
7.497
7.481
7.421
7.415
7.350
7.141
7.135
7.119
7.113
5.131
5.121
5.110
5.100
4.395
4.369
4.359
4.338
4.317
4.302
4.281
4.108
2.536
0.0000
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O
S
N
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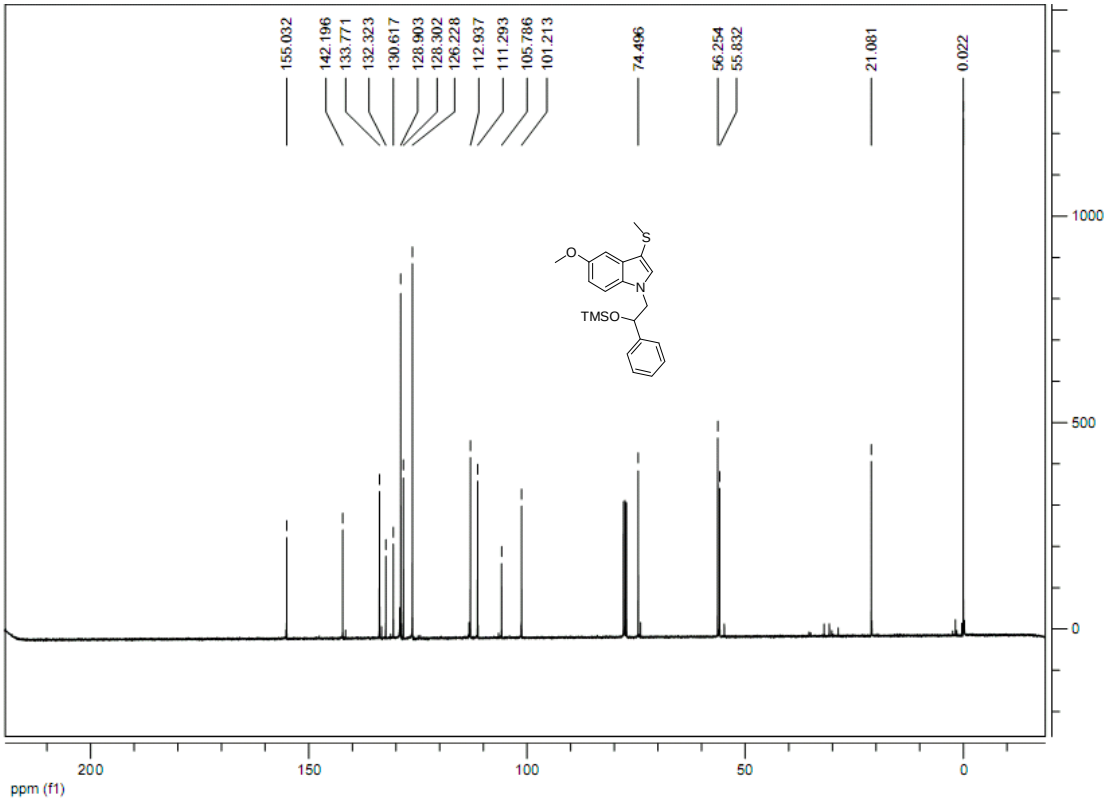
1.13
1.02
2.20
3.38
3.31
9.00
10.0
5.0
0.0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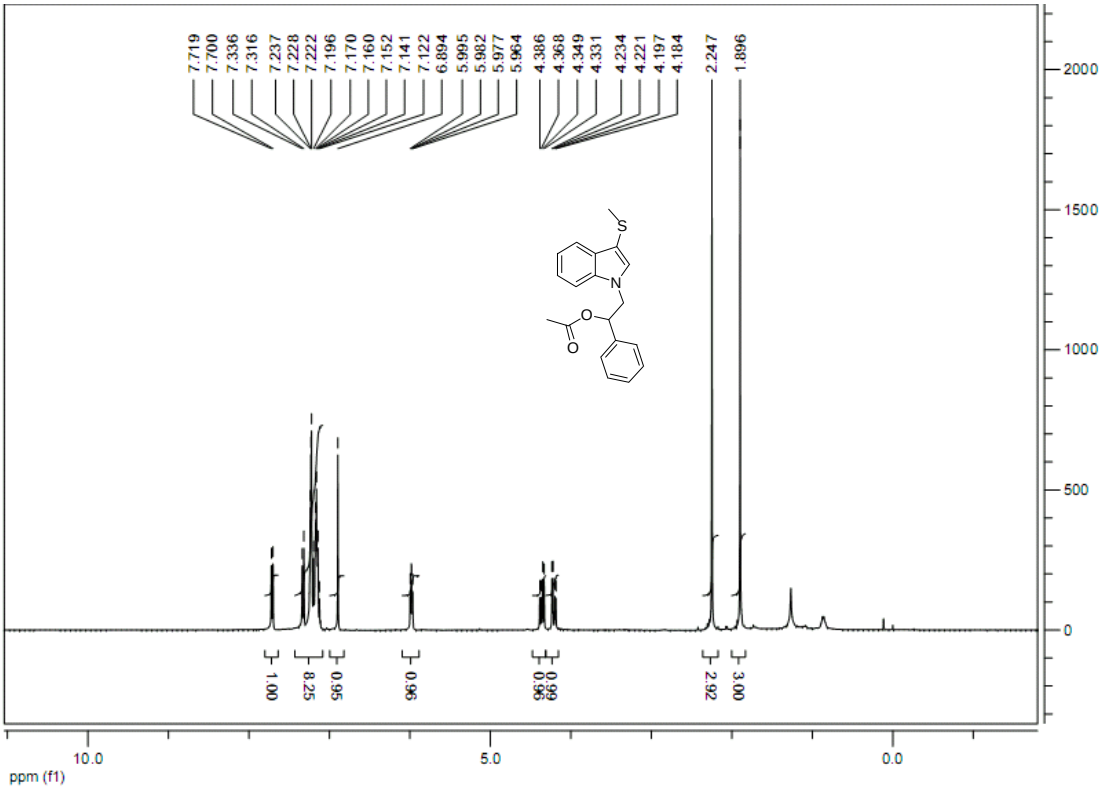
142.196
133.771
132.323
130.617
128.903
128.302
126.228
112.937
111.293
105.786
101.213
74.496
56.254
55.832
21.081
0.022
TMSO
1000
500
0
200
150
100
50
0
ppm (f1)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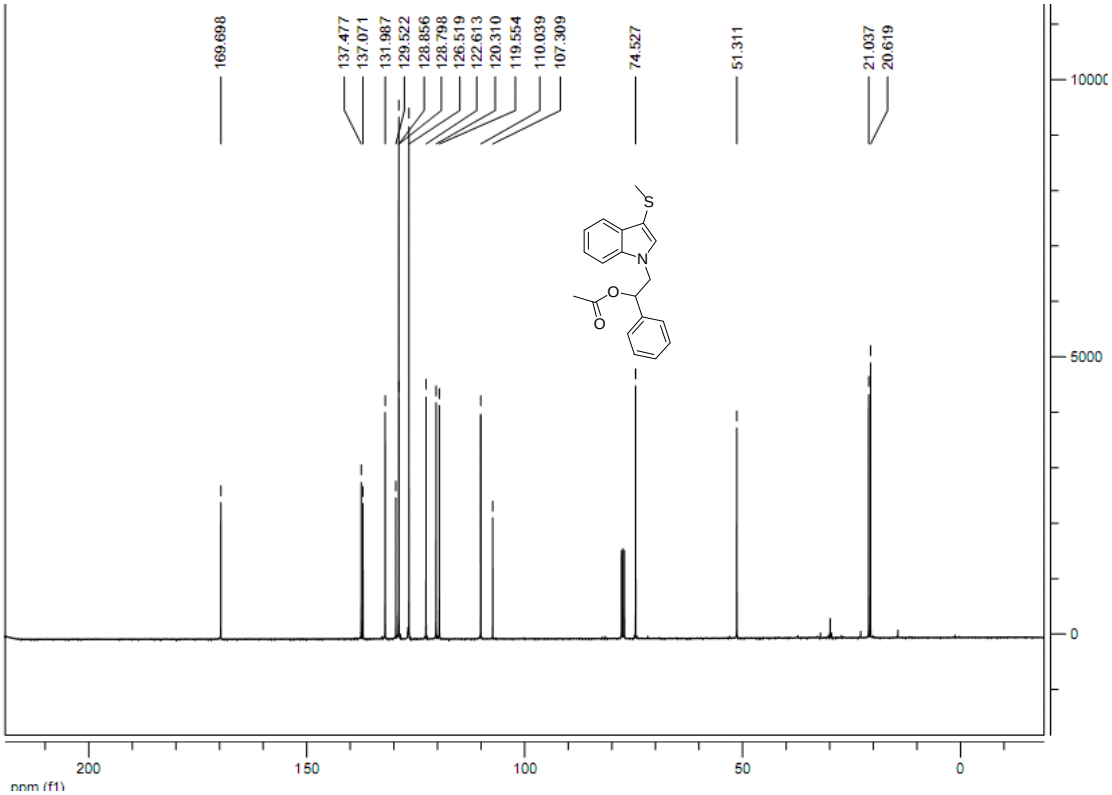
7.700
7.336
7.316
7.237
7.228
7.222
7.196
7.170
7.160
7.152
7.141
7.122
6.894
5.995
5.982
5.977
5.964
4.386
4.368
4.349
4.331
4.234
4.221
4.197
4.184
2.247
1.896
1.00
8.25
0.95
0.96
0.99
0.99
2.92
3.00
2000
1500
1000
500
0
10.0
5.0
0.0
ppm (f1)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128.856
128.798
126.519
122.613
120.310
119.554
110.039
107.309
74.527
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20.619
S
N
O
O
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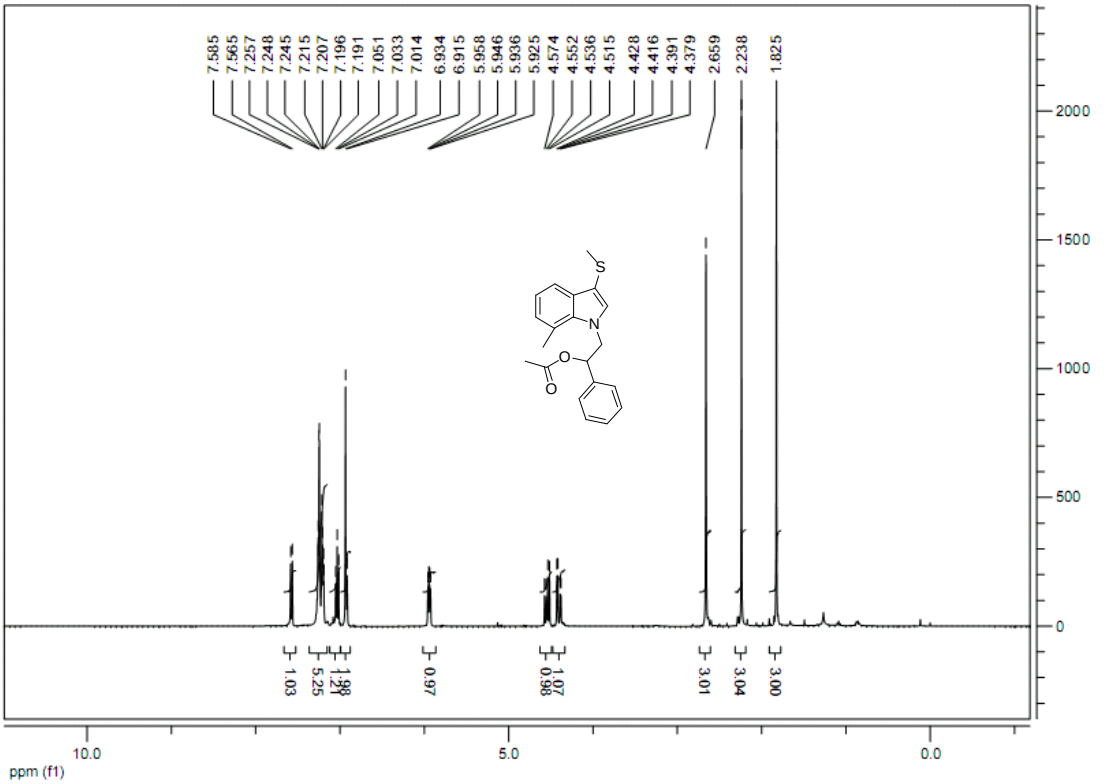
100
50
0
ppm (f1)


7.585
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7.245
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7.196
7.191
7.051
7.033
7.014
6.934
6.915
5.958
5.946
5.936
5.925
4.574
4.552
4.536
4.515
4.428
4.416
4.391
4.379
2.659
2.238
1.825
S
N
O
O
2000
1500
1000
500
0
1.03
5.25
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1.21
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0.98
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3.04
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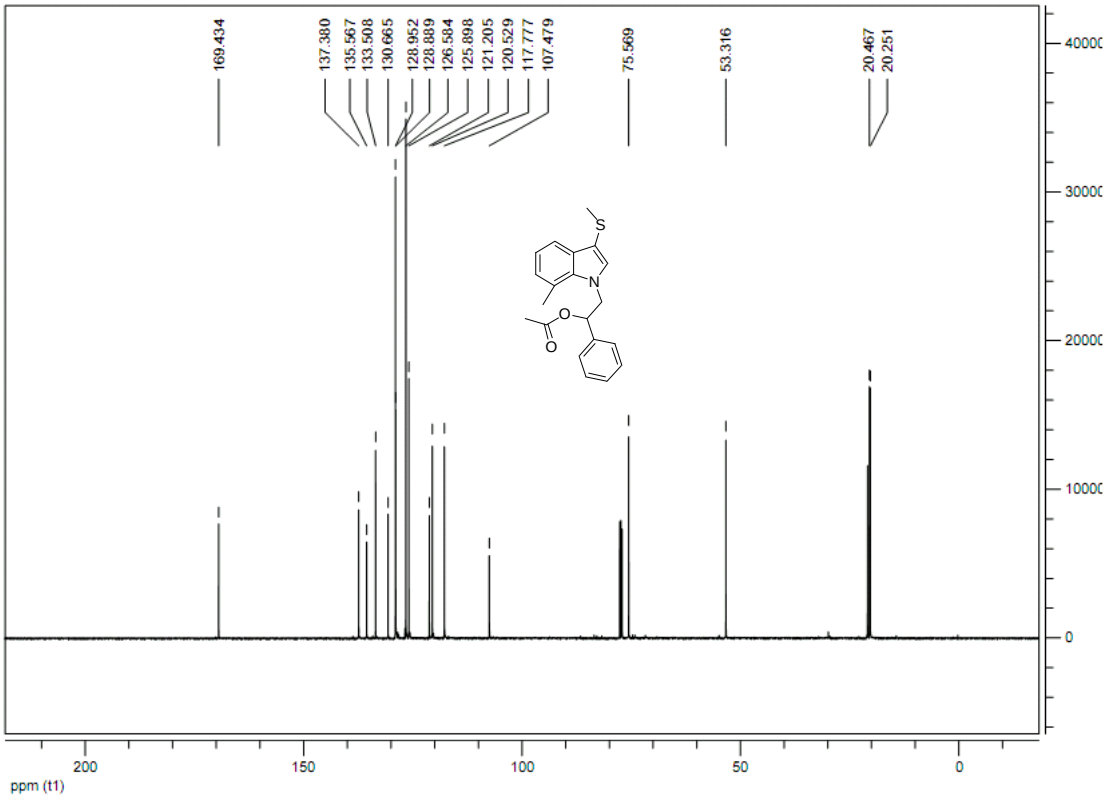
ppm (f1)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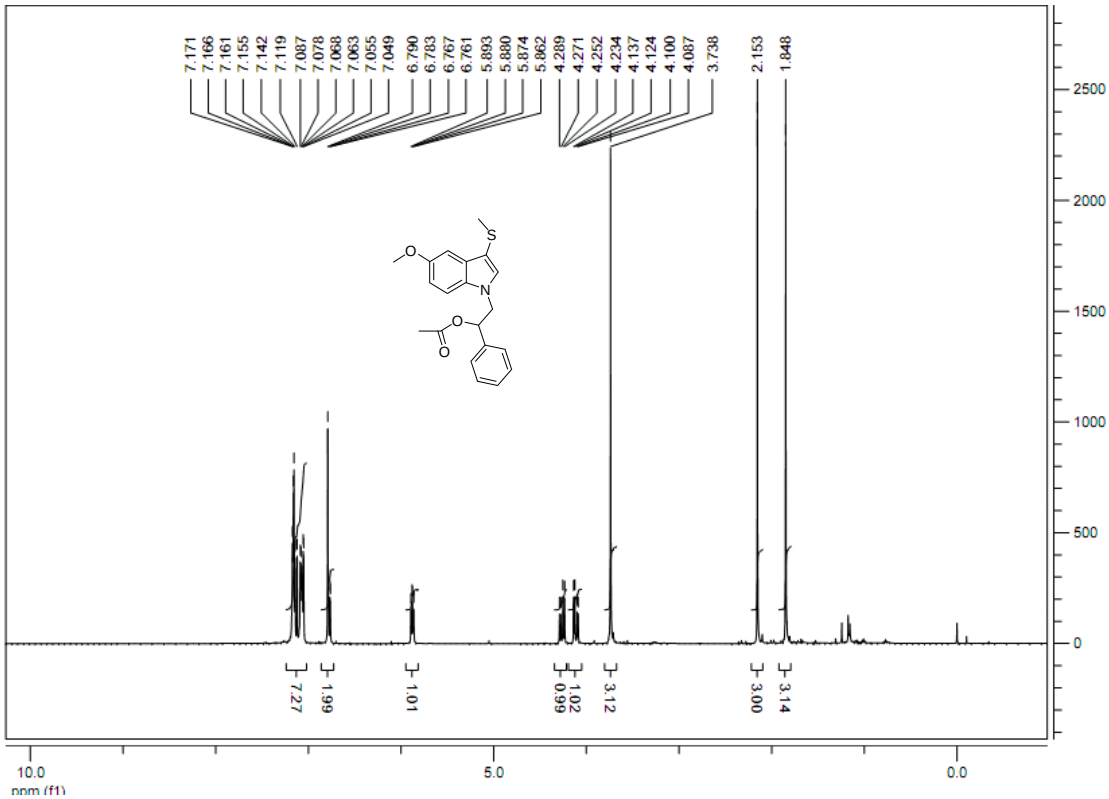
128.889
126.584
125.898
121.205
120.529
117.777
107.479
75.569
53.316
20.467
20.251
S
N
O
O
4000
3000
2000
1000
0
200
150
100
50
0
ppm (t1)


7.171
7.166
7.161
7.155
7.142
7.119
7.087
7.078
7.068
7.063
7.055
7.049
6.790
6.783
6.767
6.761
5.893
5.880
5.874
5.862
4.289
4.271
4.252
4.234
4.137
4.124
4.100
4.087
3.738
2.153
1.848
S
O
N
O
O
2500
2000
1500
1000
500
0
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0.99
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10.0
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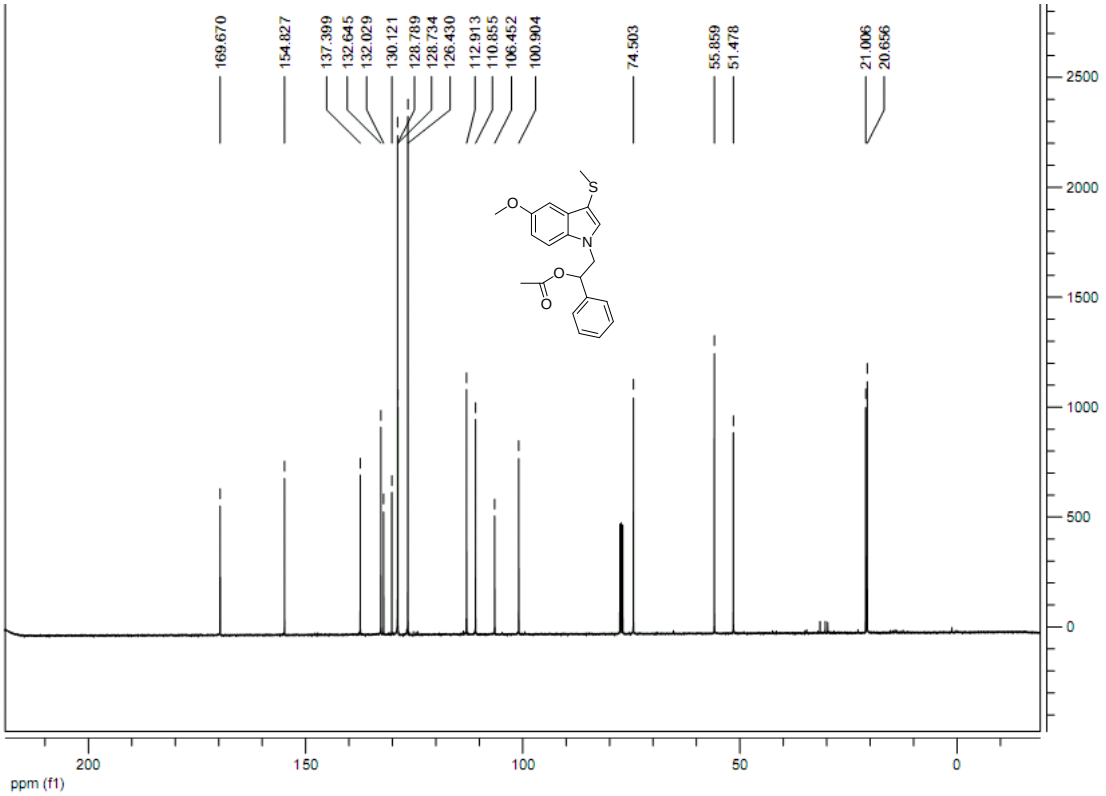
0.0
ppm (f1)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128.789
128.734
126.430
112.913
110.855
106.452
100.904
74.503
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1000
500
0
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100
50
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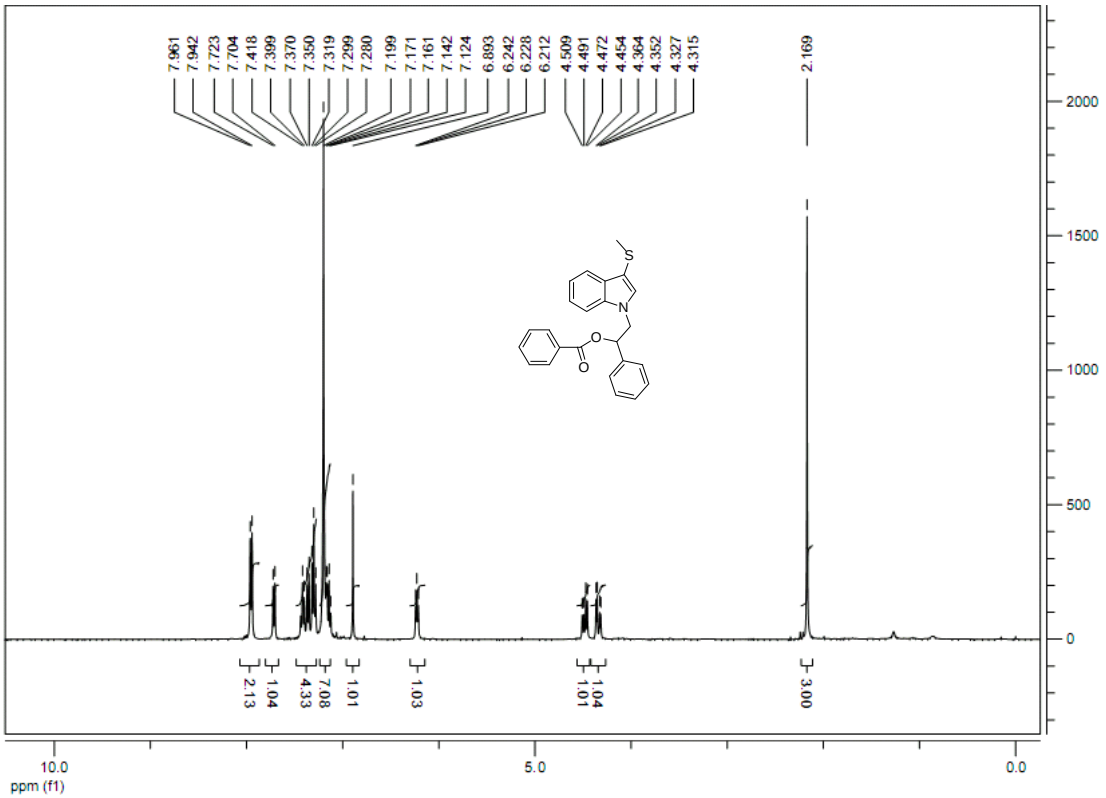
ppm (f1)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7.299
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7.199
7.171
7.161
7.142
7.124
6.893
6.242
6.228
6.212
4.509
4.491
4.472
4.454
4.364
4.352
4.327
4.315
2.169
2000
1500
1000
500
0
2.13
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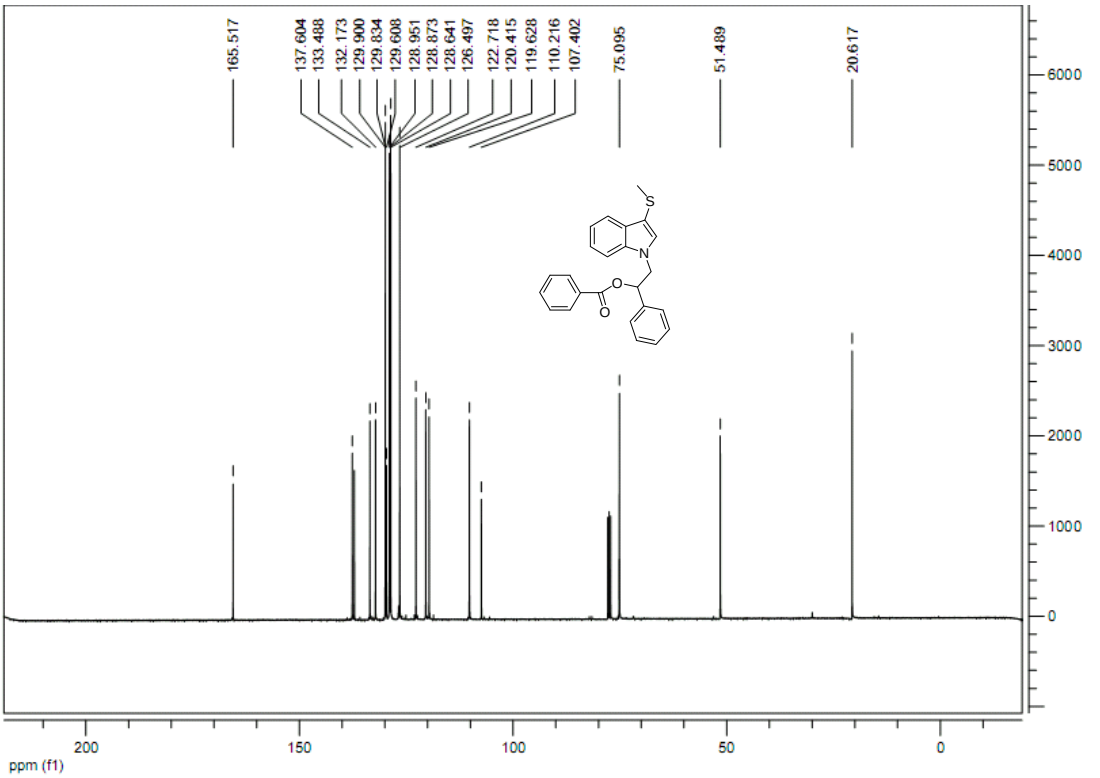
ppm (f1)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129.608
128.951
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128.641
126.497
122.718
120.415
119.628
110.216
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20.617
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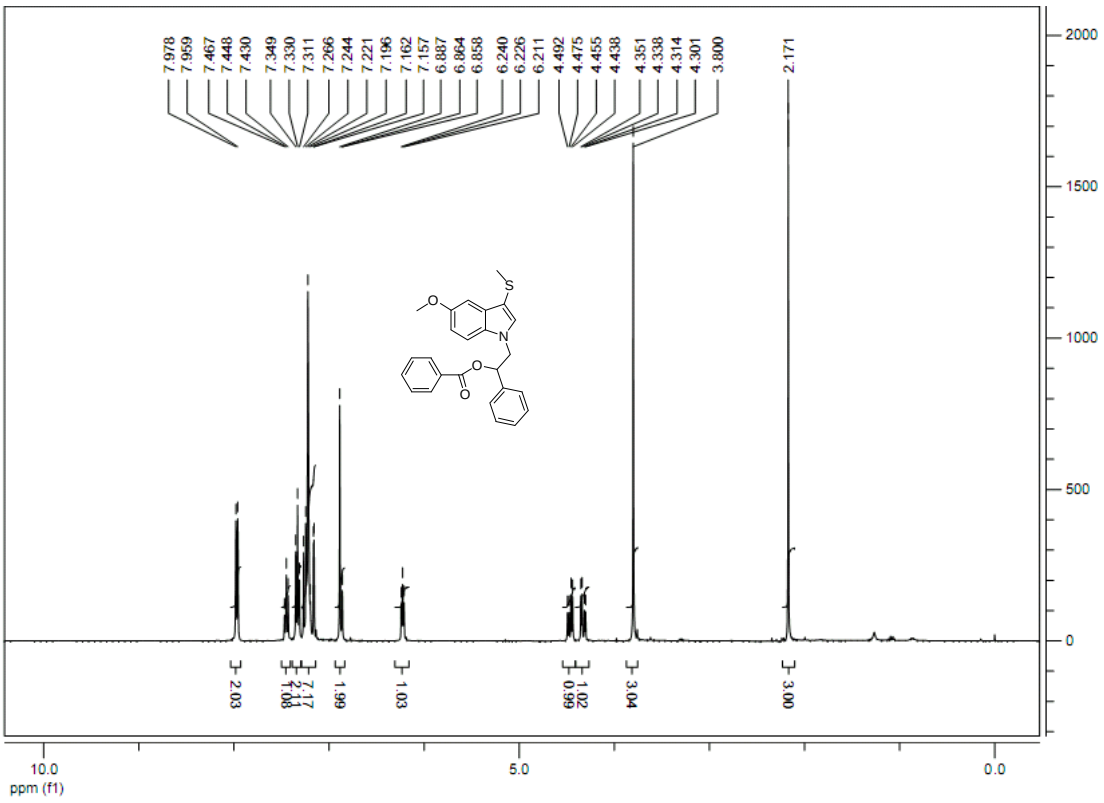
ppm (f1)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7.311
7.266
7.244
7.221
7.196
7.162
7.157
6.887
6.864
6.858
6.240
6.226
6.211
4.492
4.475
4.455
4.438
4.351
4.338
4.314
4.301
3.800
2.171
2000
1500
1000
500
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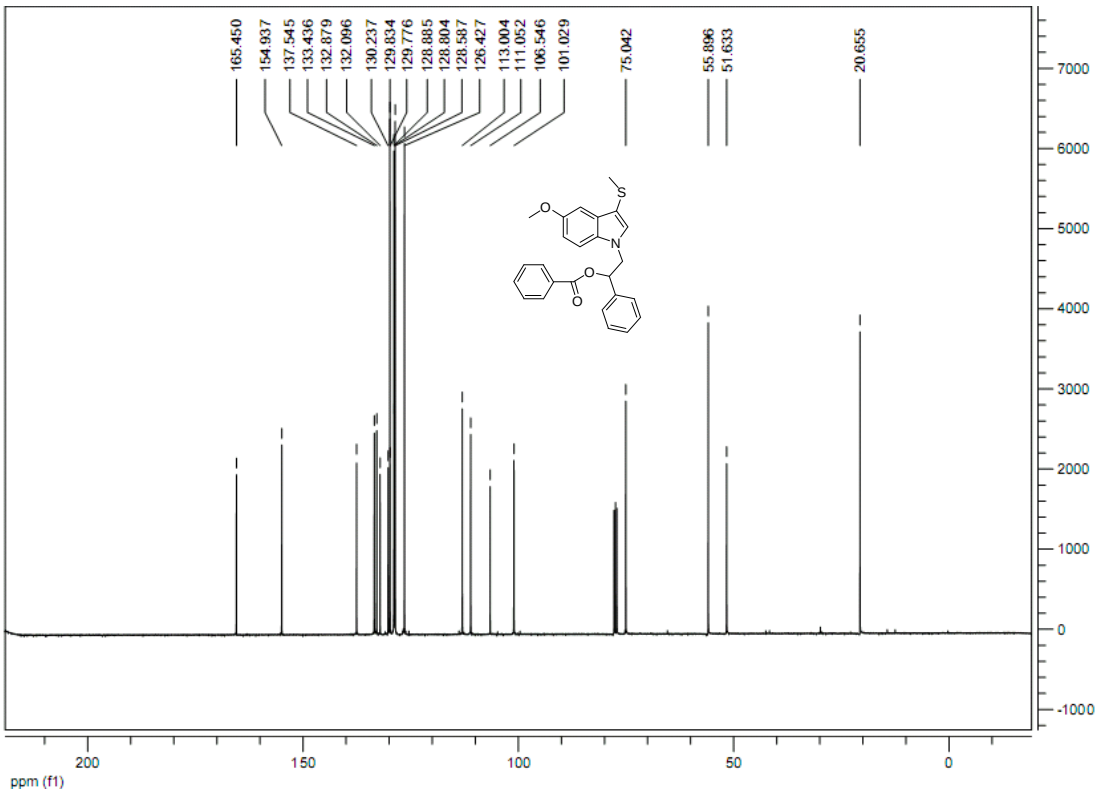
1.99
1.03
0.99
1.02
3.04
3.00
10.0
5.0
0.0
ppm (f1)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128.885
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128.587
126.427
113.004
111.052
106.546
101.029
75.042
55.896
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1000
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200
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100
50
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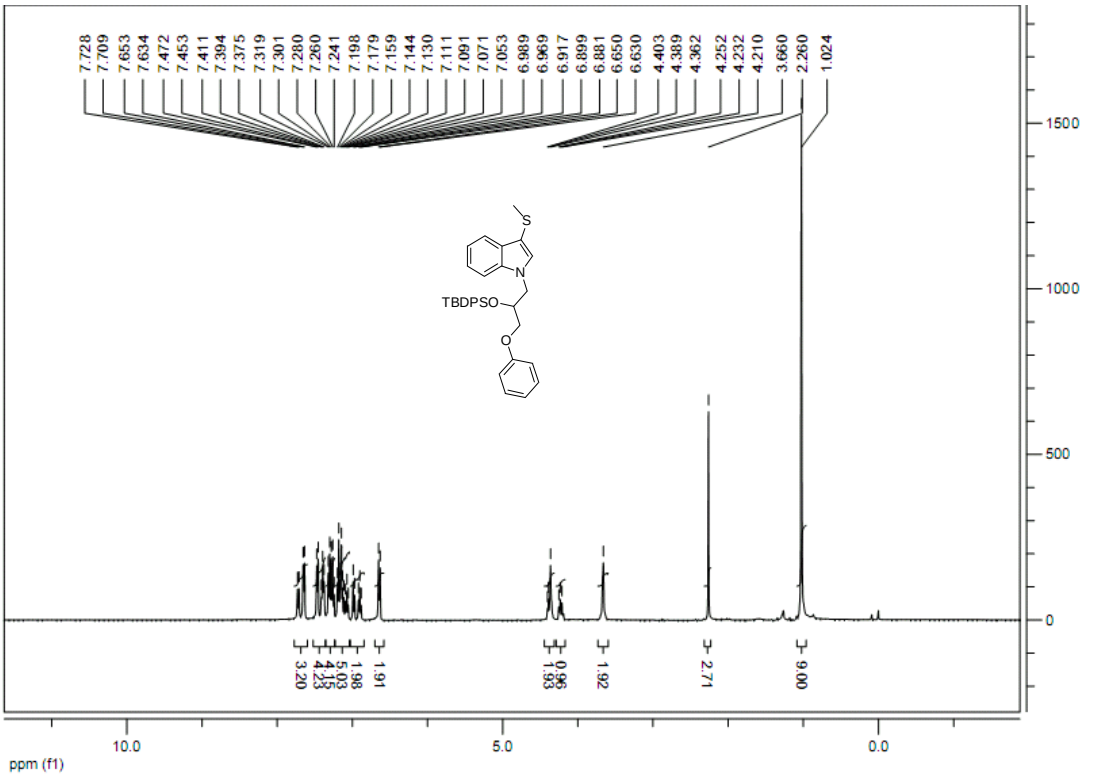
ppm (f1)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7.241
7.198
7.179
7.159
7.144
7.130
7.111
7.091
7.071
7.053
6.989
6.969
6.917
6.899
6.881
6.650
6.630
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4.389
4.362
4.252
4.232
4.210
3.660
2.260
1.024
TBDPSO
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1.61
1.68
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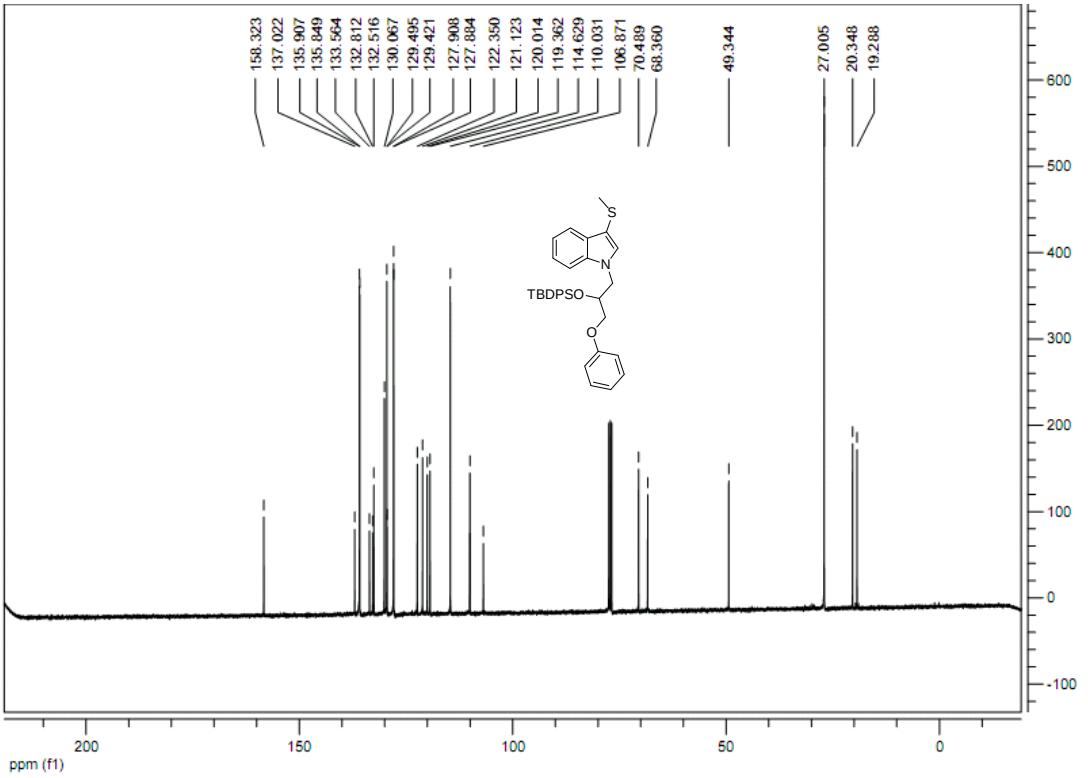
0.0
ppm (f1)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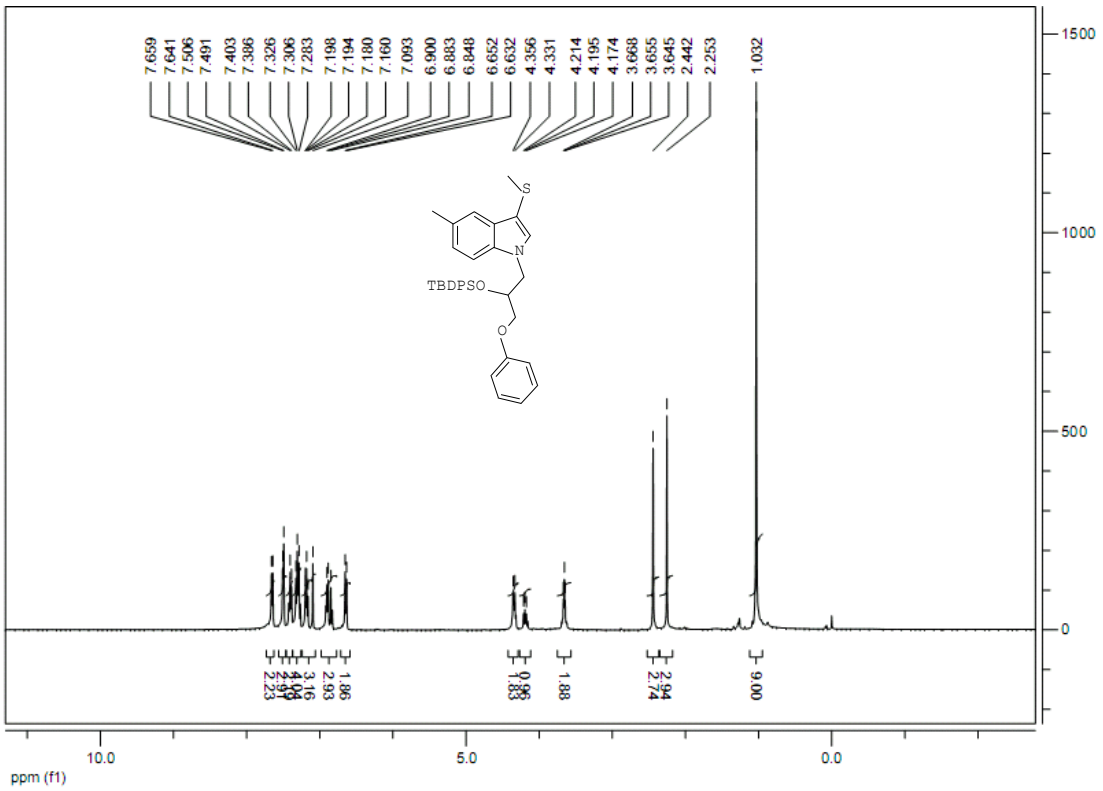
129.421
127.908
127.884
122.350
121.123
120.014
119.362
114.629
110.031
106.871
70.489
68.360
49.344
27.005
20.348
19.288
S
N
TBDPSO
O
600
500
400
300
200
100
0
-100
200
150
100
50
0
ppm (f1)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7.283
7.198
7.194
7.180
7.160
7.093
6.900
6.883
6.848
6.652
6.632
4.356
4.331
4.214
4.195
4.174
3.668
3.655
3.645
2.442
2.253
1.032
S
N
TBDPSO
O
2.23
2.91
4.09
3.16
2.63
1.86
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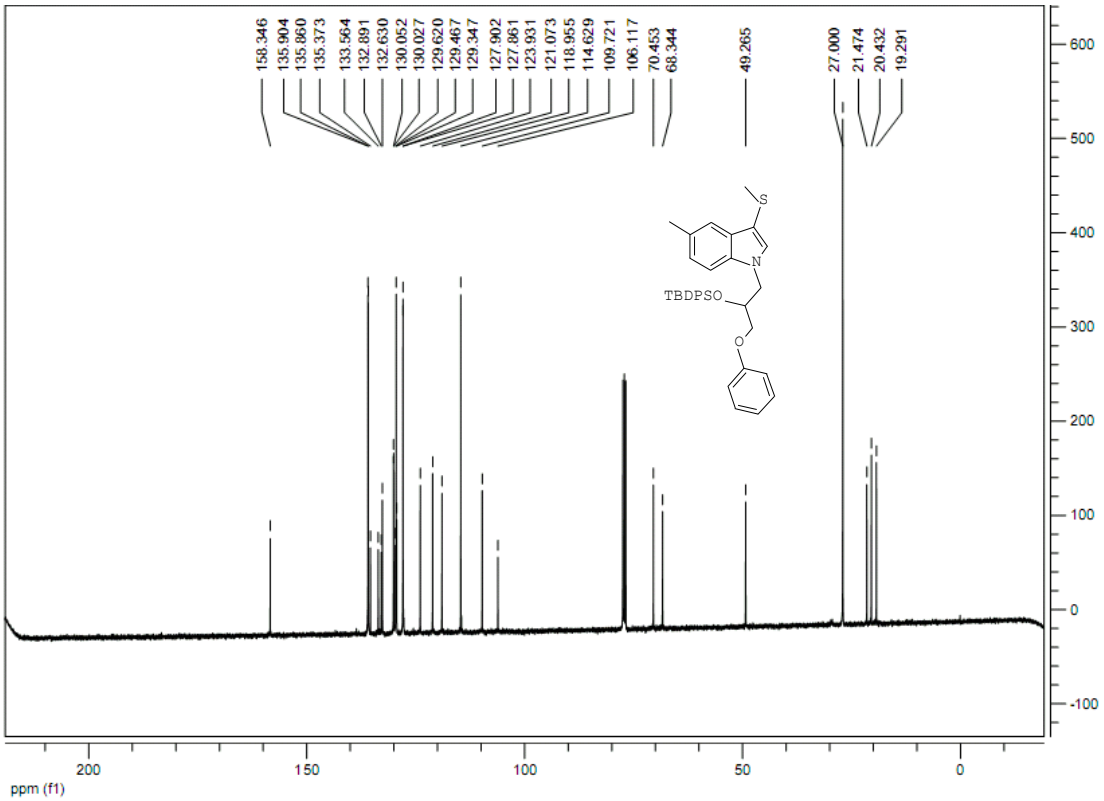
ppm (f1)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129.620
129.467
129.347
127.902
127.861
123.931
121.073
118.955
114.629
109.721
106.117
70.453
68.344
49.265
27.000
21.474
20.432
19.291
S
N
TBDPSO
O
600
500
400
300
200
100
0
-100
200
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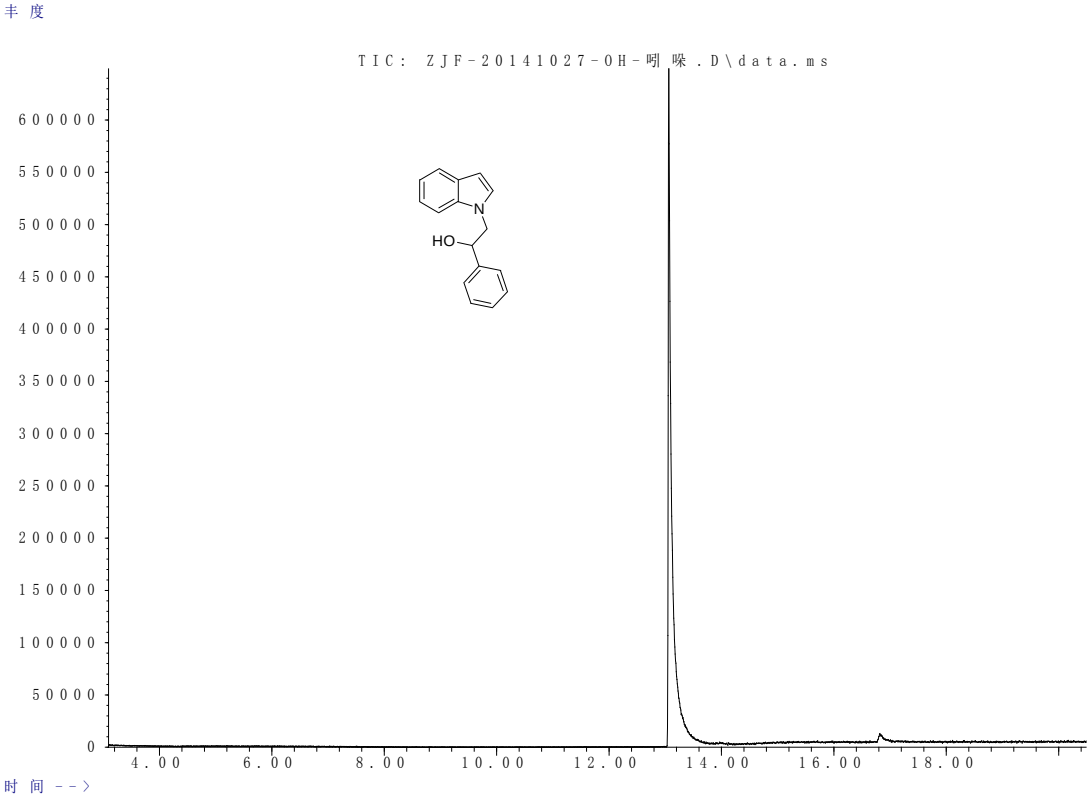
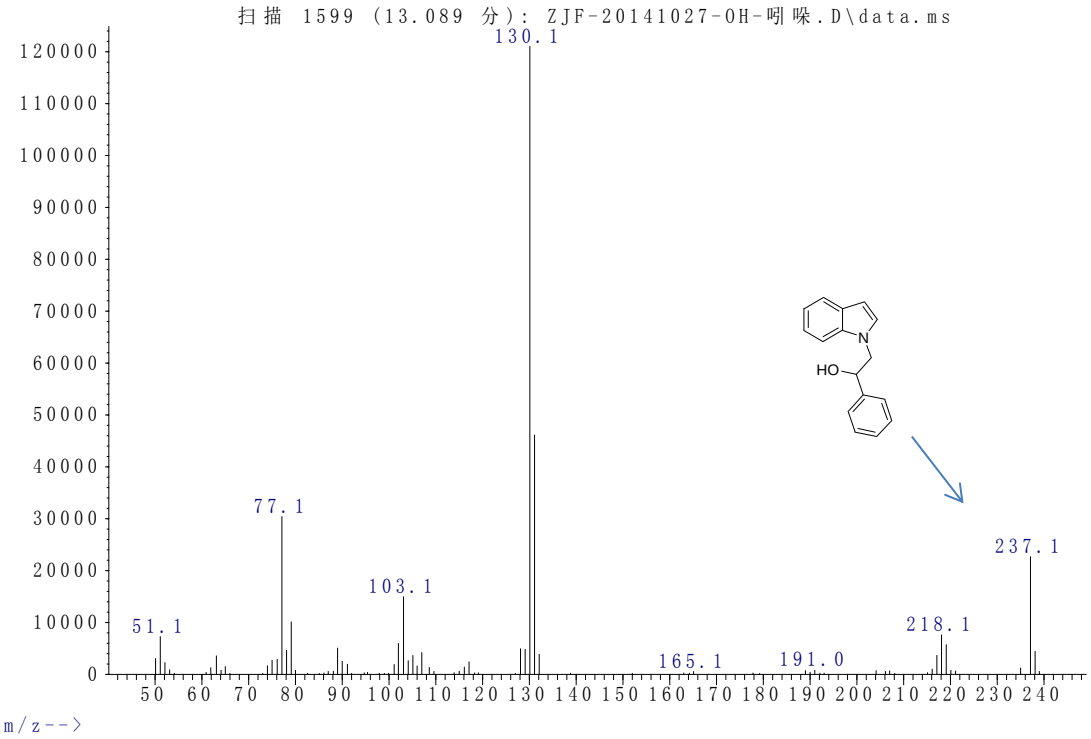
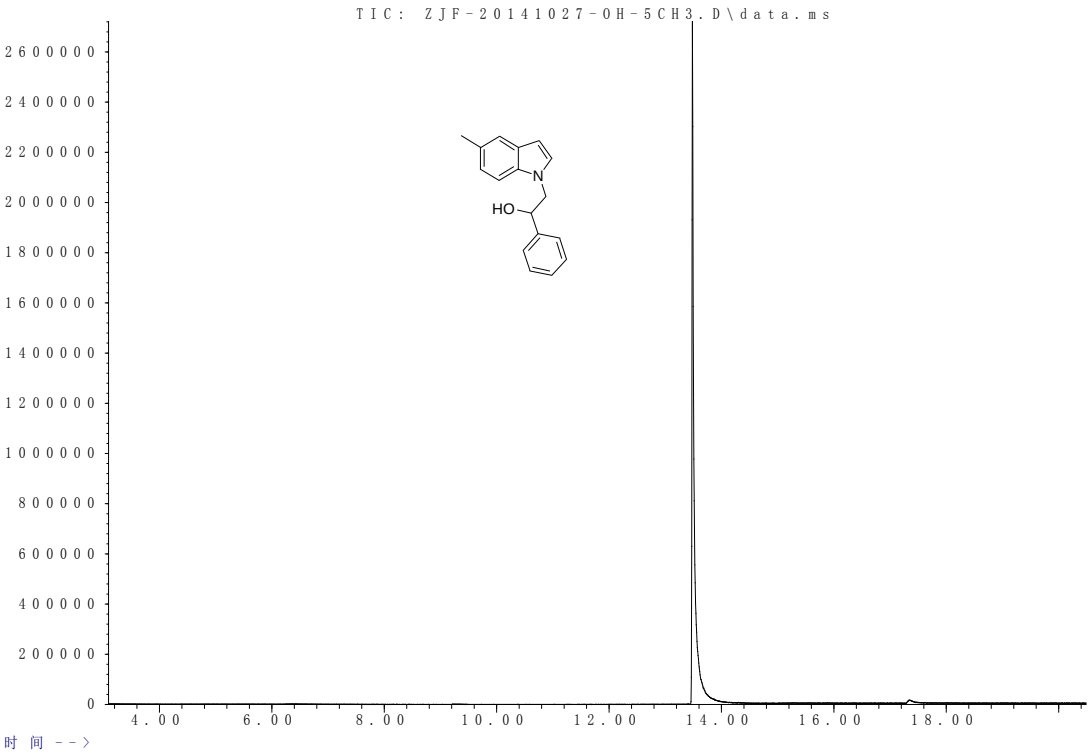
100
50
0
ppm (f1)

5. GC-MS Spectra of the starting material and 3-sulfenylindoles

a. GC-MS Spectra of Starting Materials



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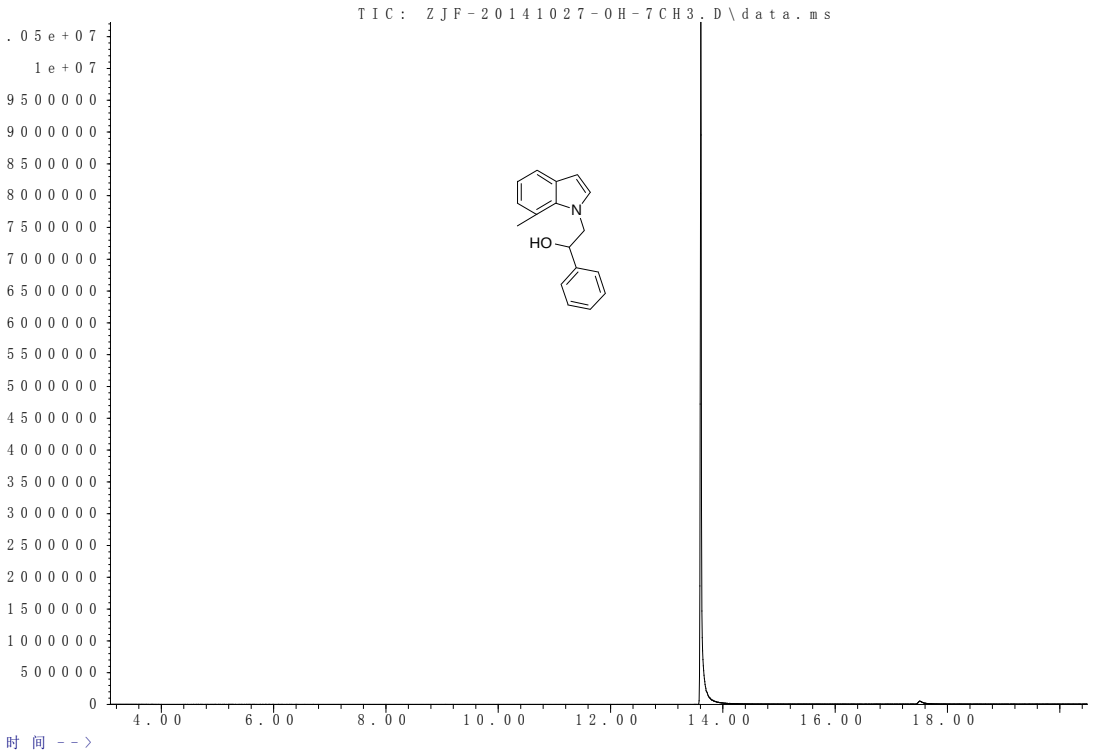
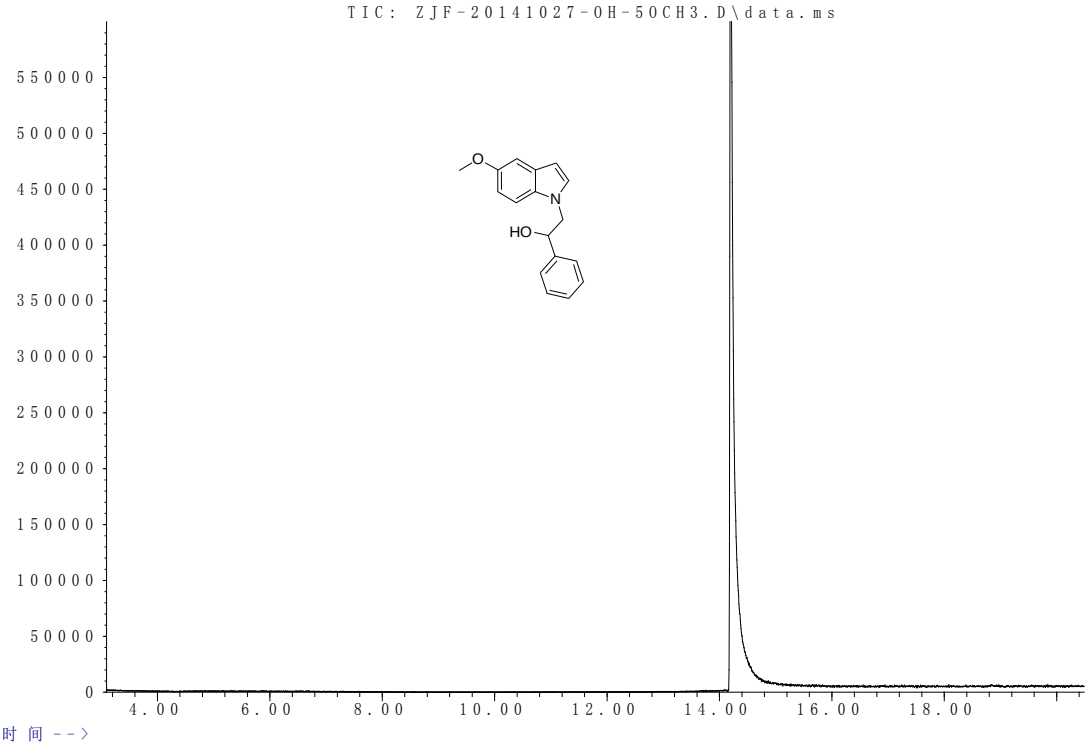
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
HO
N
时 间 -->
丰度
扫描 1662 (13.483 分): ZJF-20141027-OH-5CH3.D\data.ms
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
144.1
251.2
77.1
115.1
51.1
95.6
178.1
204.1
232.1
281.1
60
80
100
120
140
160
180
200
220
240
260
280
HO
N
m/z-->

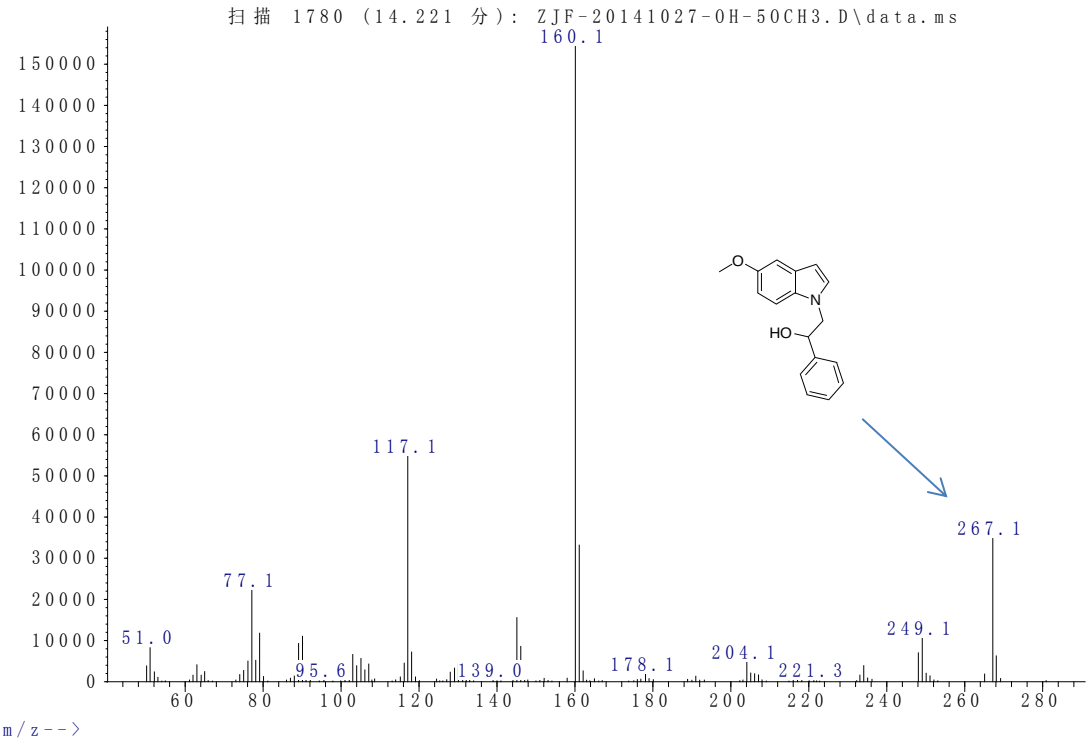

丰 度
TIC: ZJF-20141027-OH-7CH3.D\data.ms
1.05e+07
1e+07
9500000
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
HO
N
时 间 -->
丰 度
扫 描 1679 (13.589 分): ZJF-20141027-OH-7CH3.D\data.ms
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
144.1
77.1
115.1
51.1
95.3
178.0
204.0
233.1
251.1
281.0
60
80
100
120
140
160
180
200
220
240
260
280
HO
N
m/z-->
72

丰 度


TIC: ZJF-20141027-OH-5OCH3.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
O
N
HO

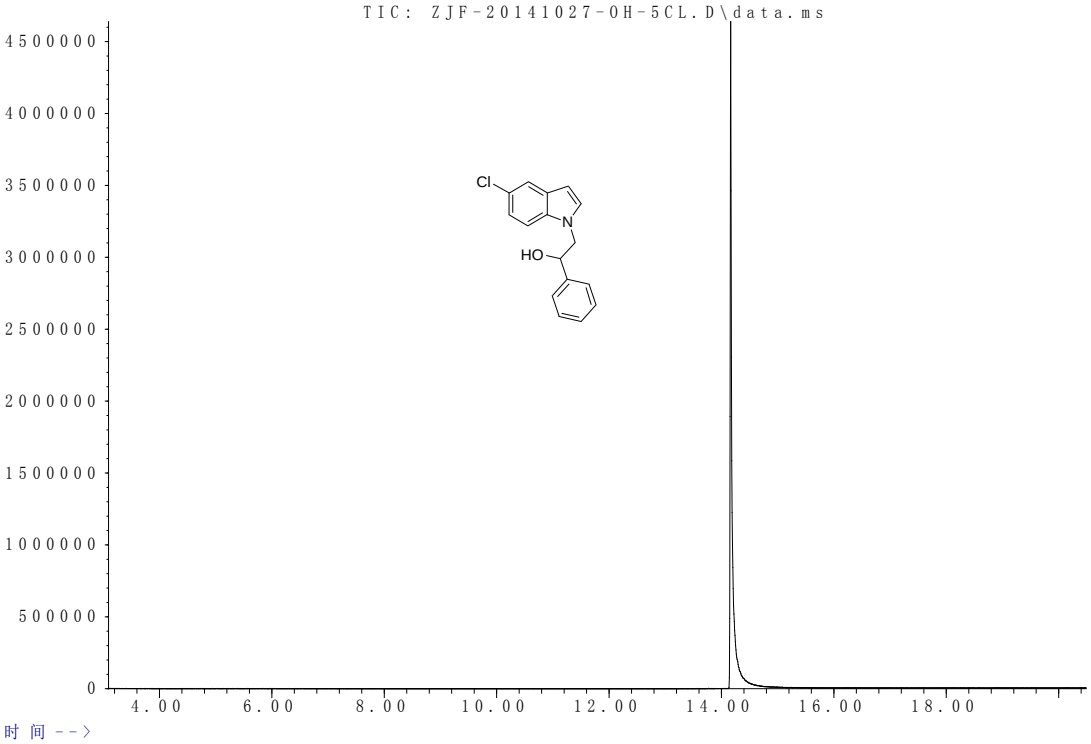
时 间 -->

丰 度


扫 描 1780 (14.221 分): ZJF-20141027-OH-5OCH3.D\data.ms
160.1
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
117.1
77.1
51.0
95.6
139.0
178.1
204.1
221.3
249.1
267.1
60
80
100
120
140
160
180
200
220
240
260
280
O
N
HO

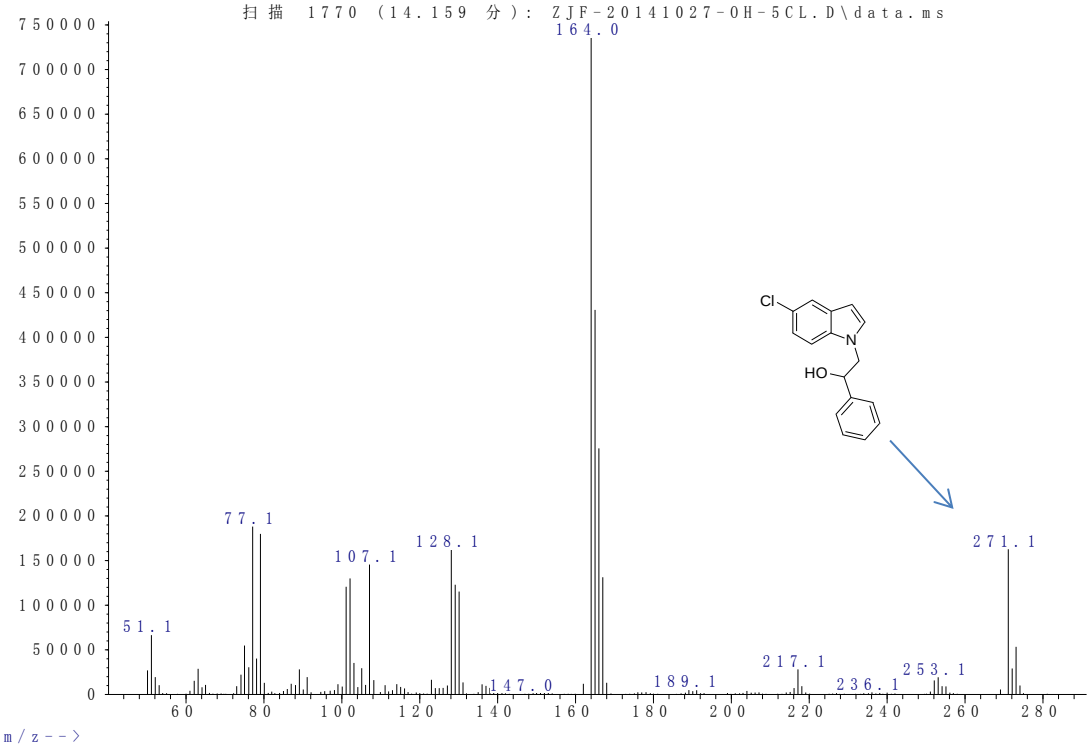
m/z-->

丰 度


TIC: ZJF-20141027-0H-5CL.D\data.ms
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
Cl
N
HO

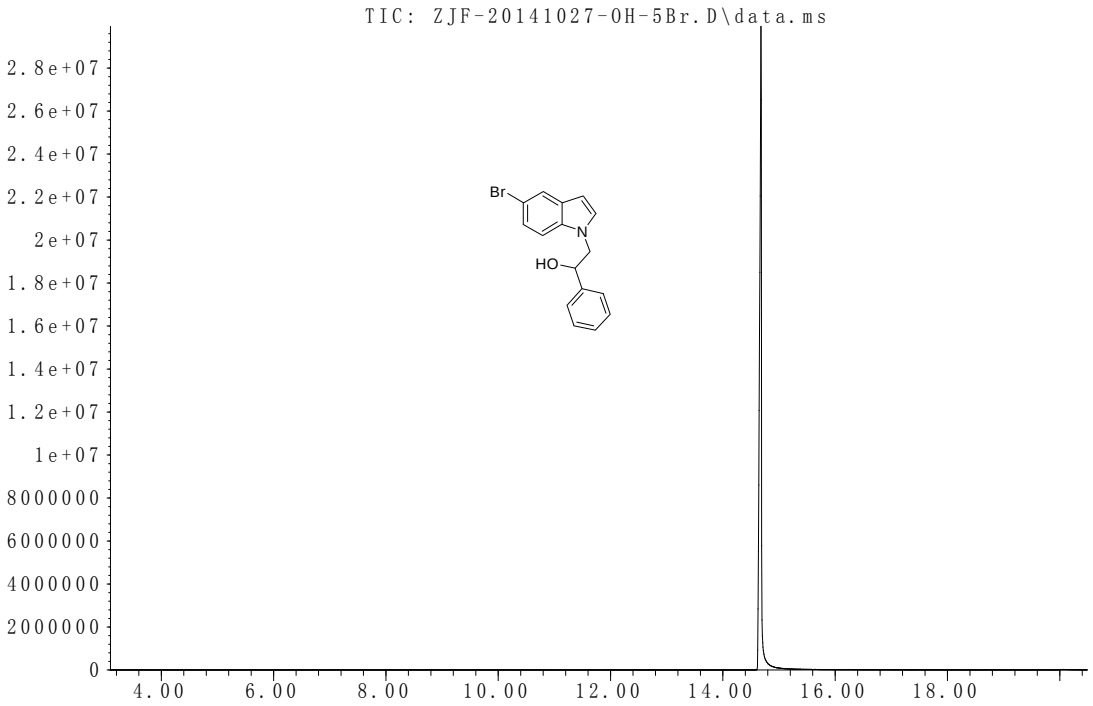
时 间 -->

丰 度


扫 描 1770 (14.159 分): ZJF-20141027-0H-5CL.D\data.ms
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
164.0
77.1
107.1
128.1
51.1
147.0
189.1
217.1
236.1
253.1
271.1
60
80
100
120
140
160
180
200
220
240
260
280
Cl
N
HO

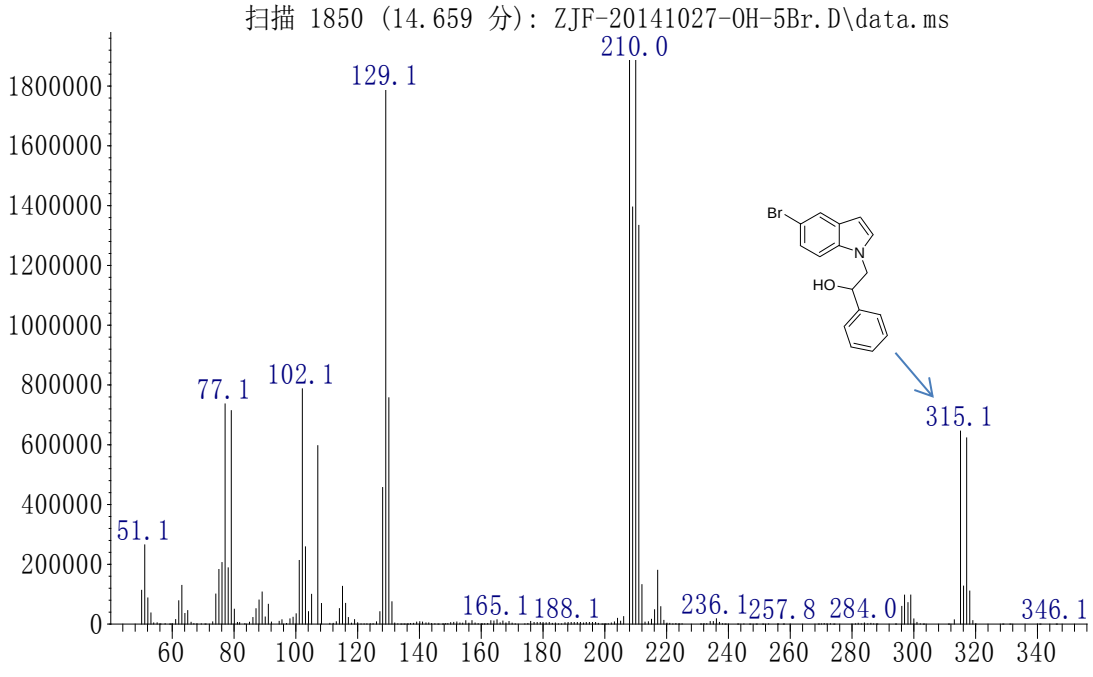
m/z -->

丰度


TIC: ZJF-20141027-OH-5Br.D\data.ms
2.8e+07
2.6e+07
2.4e+07
2.2e+07
2e+07
1.8e+07
1.6e+07
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
Br
N
HO

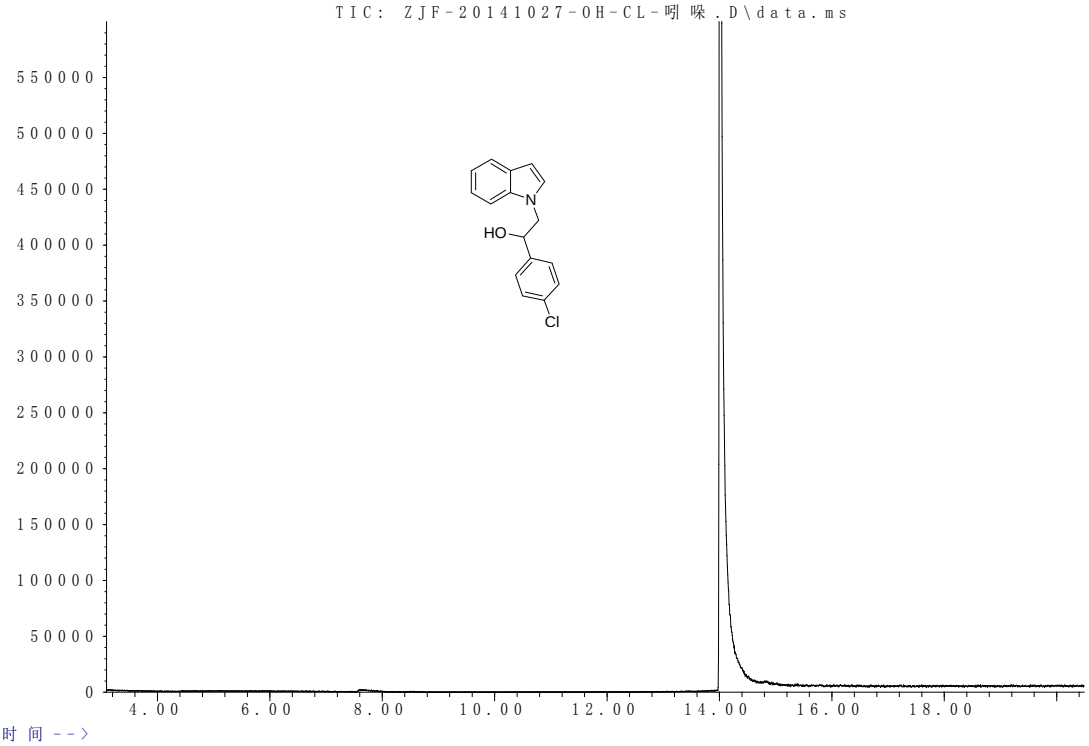
时间-->

丰度

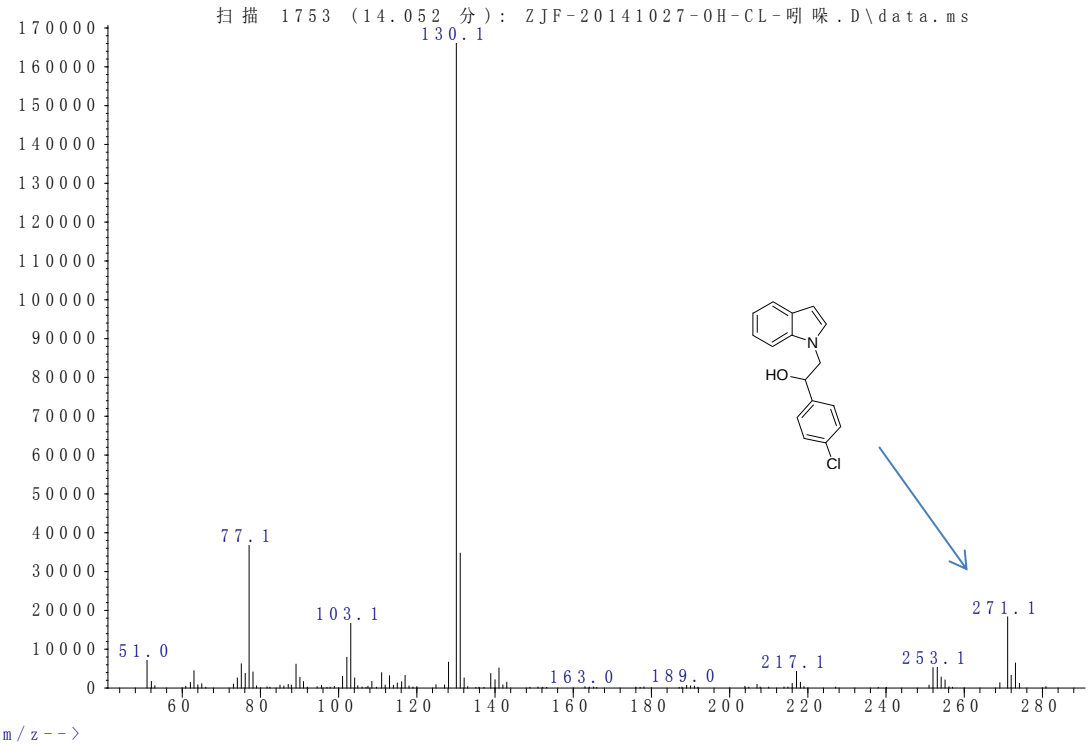

扫描 1850 (14.659 分): ZJF-20141027-OH-5Br.D\data.ms
210.0
129.1
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
77.1
102.1
51.1
165.1
188.1
236.1
257.8
284.0
315.1
346.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
Br
N
HO

m/z-->

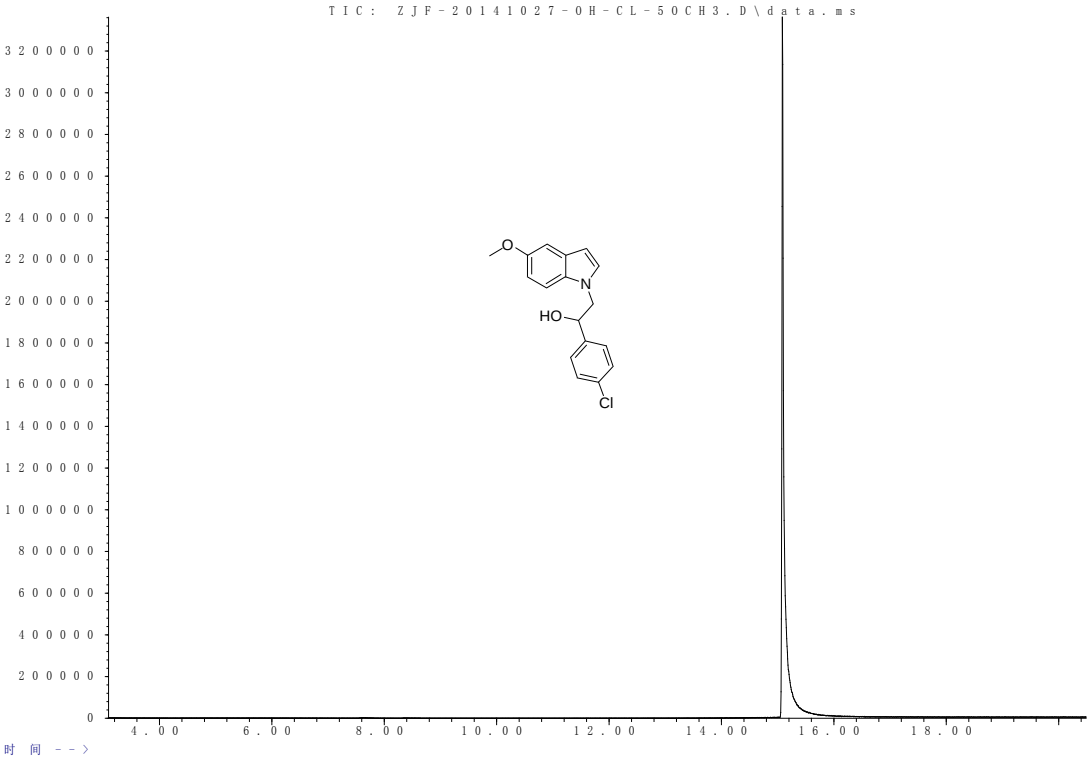
丰 度


TIC: ZJF-20141027-OH-CL-吲 哚 .D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
HO
N
Cl
时 间 -->

丰 度

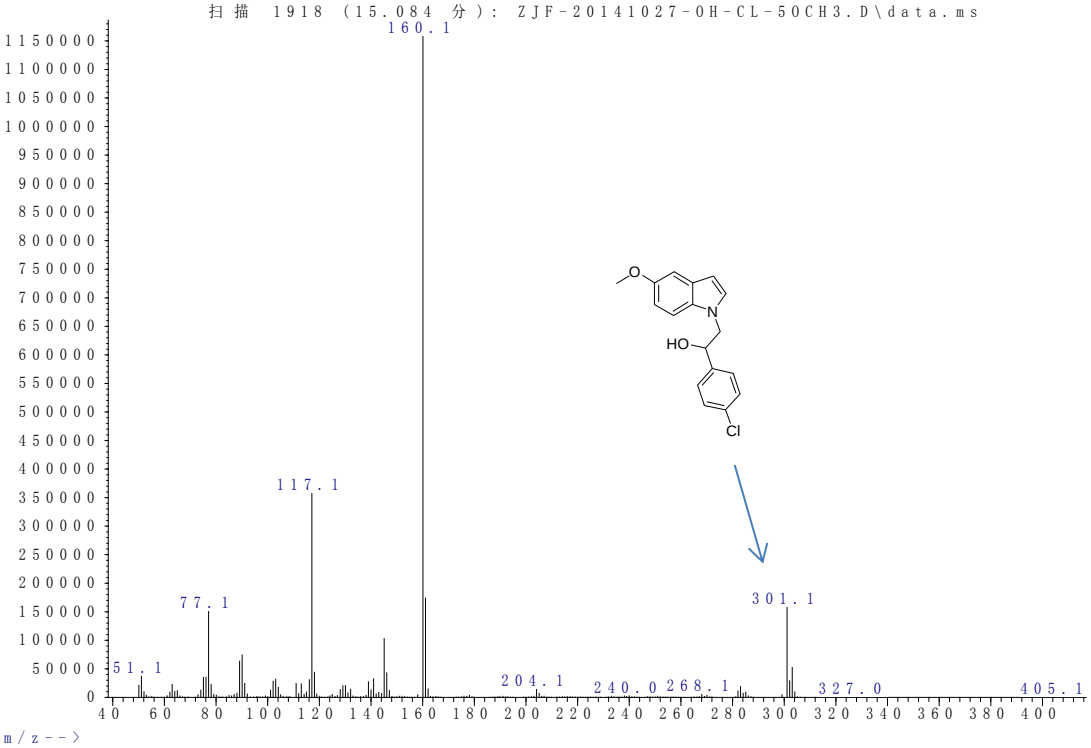

扫 描 1753 (14.052 分): ZJF-20141027-OH-CL-吲 哚 .D\data.ms
170000
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
130.1
77.1
103.1
51.0
163.0
189.0
217.1
253.1
271.1
60
80
100
120
140
160
180
200
220
240
260
280
HO
N
Cl
m/z-->

丰 度

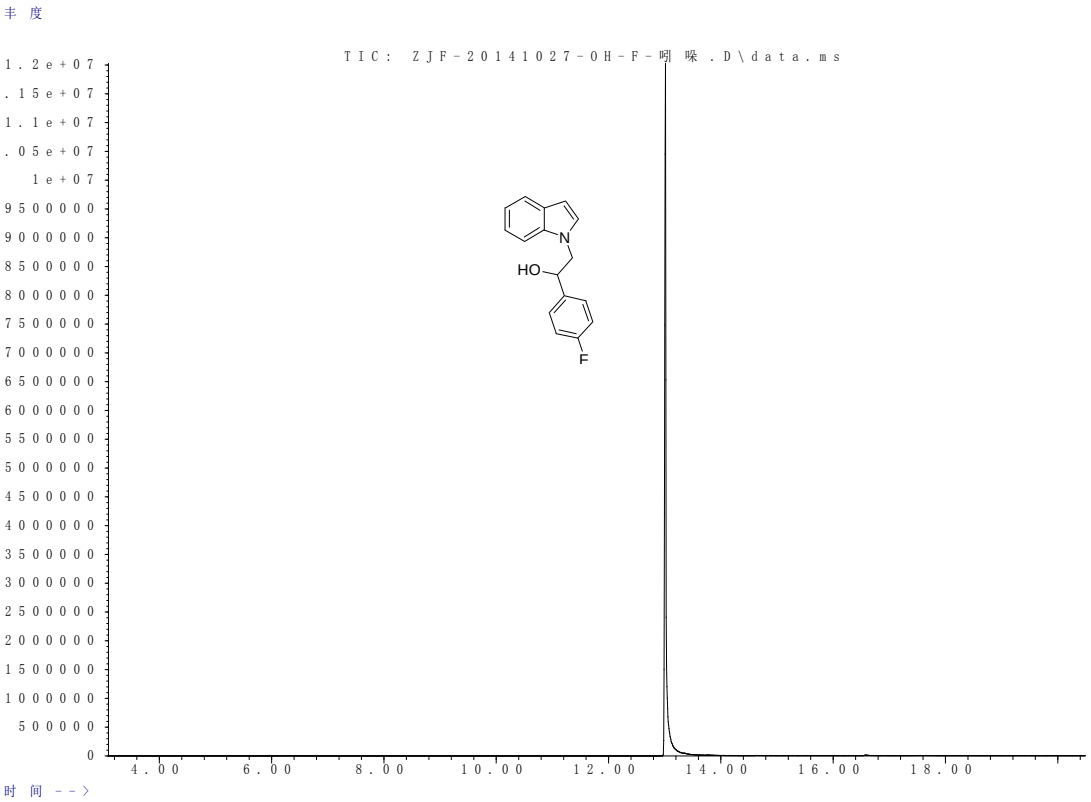

TIC: ZJF-20141027-OH-CL-50CH3.D\data.ms
32000000
30000000
28000000
26000000
24000000
22000000
20000000
18000000
16000000
14000000
12000000
10000000
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
O
N
HO
Cl

时 间 -->

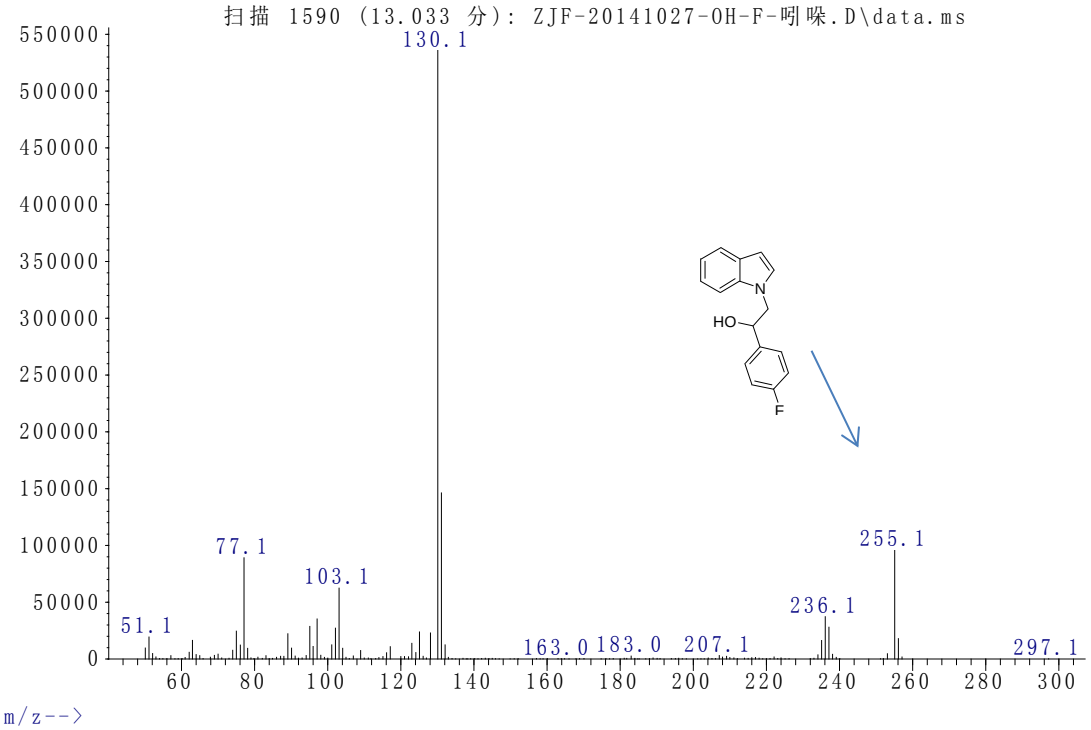
丰 度

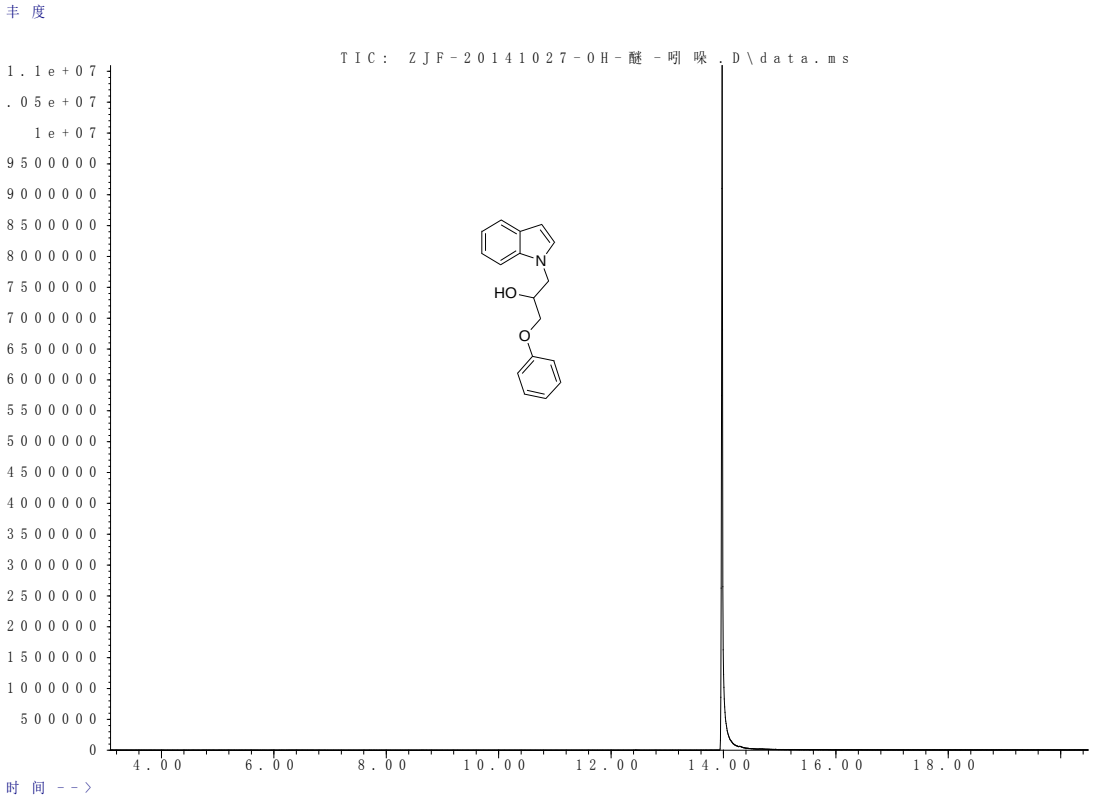

扫 描 1918 (15.084 分): ZJF-20141027-OH-CL-50CH3.D\data.ms
160.1
117.1
77.1
51.1
204.1
240.0
268.1
301.1
327.0
405.1
11500000
11000000
10500000
10000000
9500000
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400
O
N
HO
Cl

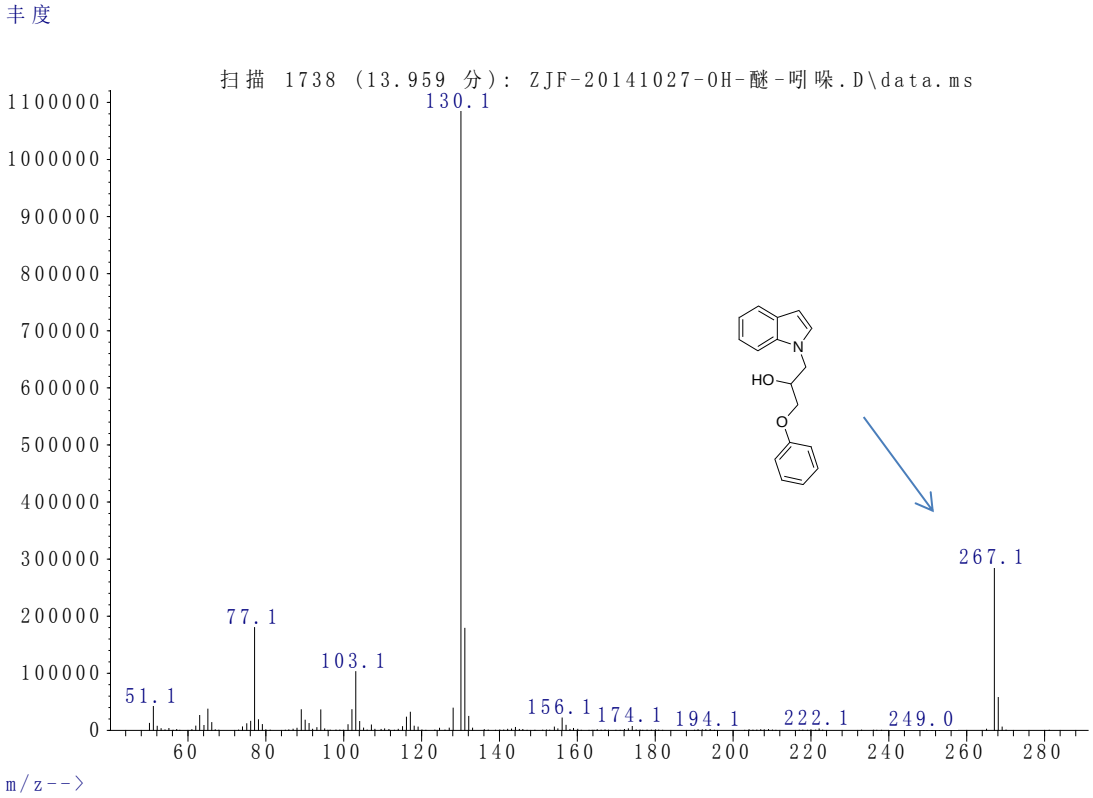
m/z-->

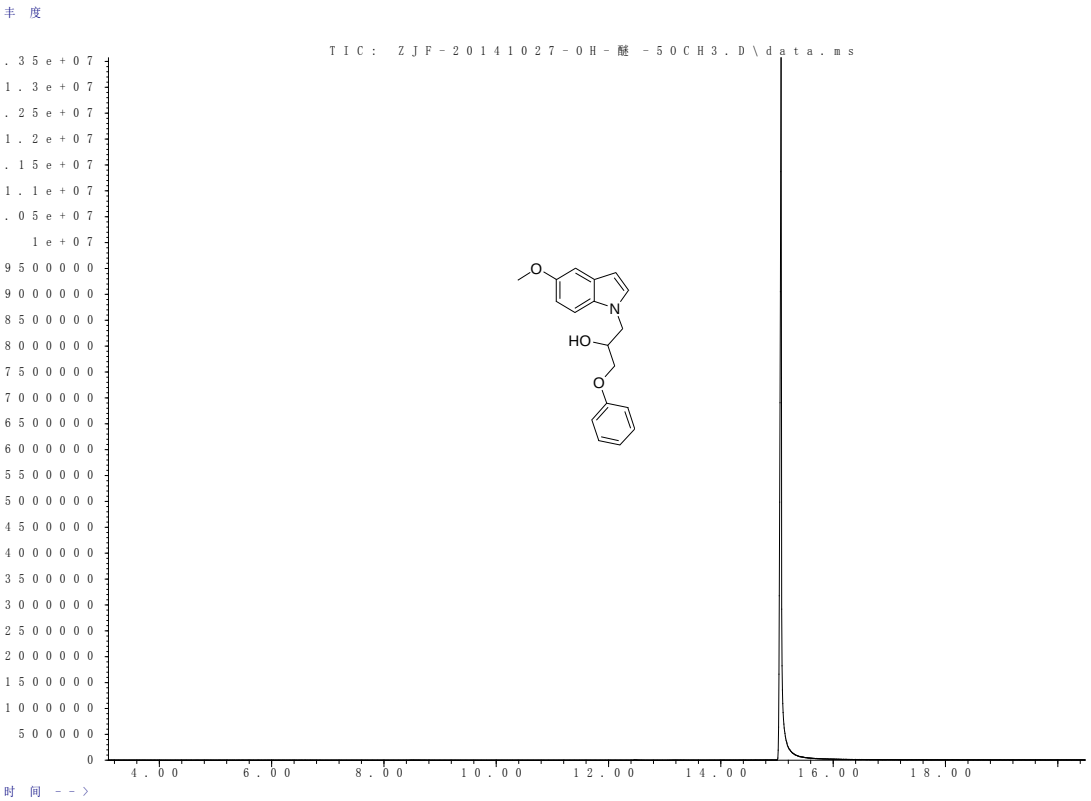

丰 度
TIC: ZJF-20141027-OH-F-吲 哚 .D\data.ms
1.2e+07
.15e+07
1.1e+07
.05e+07
1e+07
95000000
90000000
85000000
80000000
75000000
70000000
65000000
60000000
55000000
50000000
45000000
40000000
35000000
30000000
25000000
20000000
15000000
10000000
5000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
HO
N
F

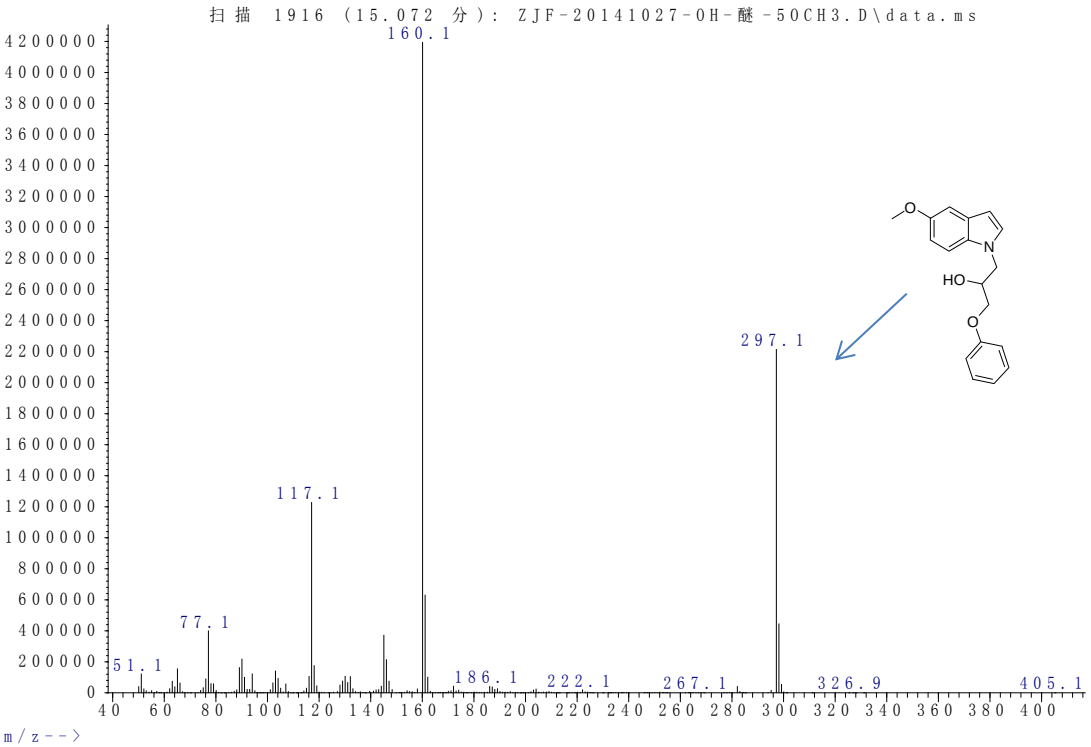
丰度

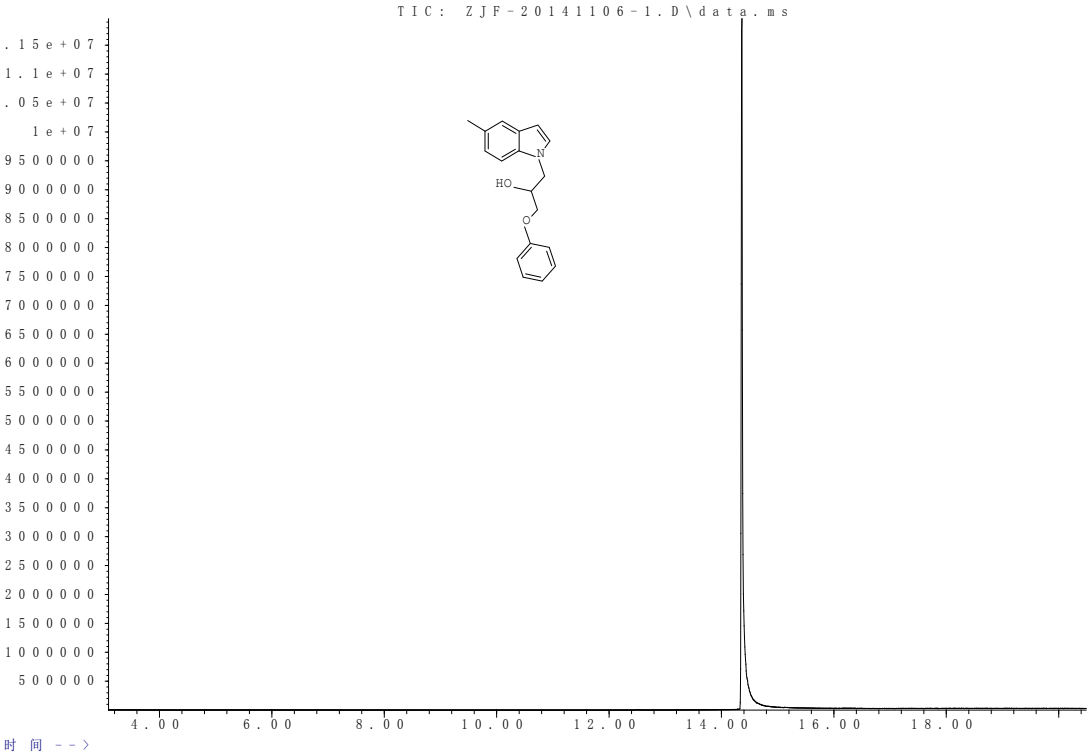

扫描 1590 (13.033 分): ZJF-20141027-OH-F-吲哚.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
130.1
77.1
103.1
51.1
163.0
183.0
207.1
236.1
255.1
297.1
60
80
100
120
140
160
180
200
220
240
260
280
300
m/z-->
HO
N
F

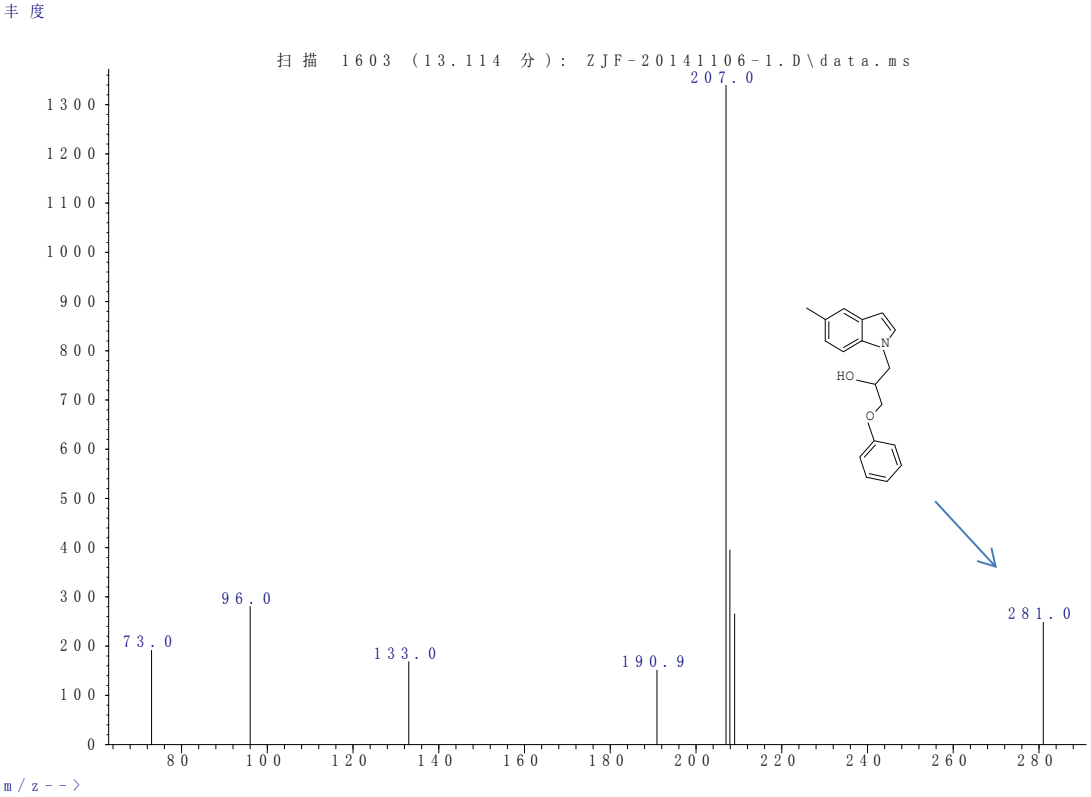

丰 度
TIC: ZJF-20141027-OH-醚 -吲 哚 .D\data.ms
1.1e+07
.05e+07
1e+07
95000000
90000000
85000000
80000000
75000000
70000000
65000000
60000000
55000000
50000000
45000000
40000000
35000000
30000000
25000000
20000000
15000000
10000000
5000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
N
HO
O

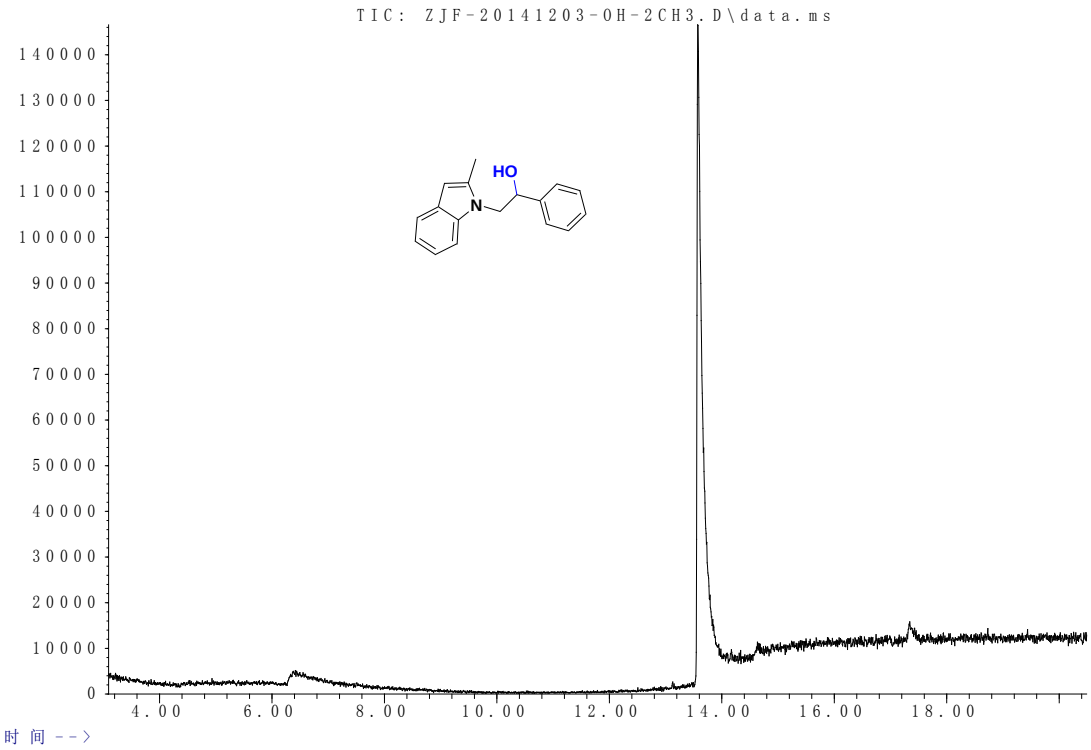

丰 度
扫描 1738 (13.959 分): ZJF-20141027-OH-醚-吲哚.D\data.ms
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
130.1
267.1
77.1
103.1
51.1
156.1
174.1
194.1
222.1
249.0
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->
N
HO
O


丰 度
TIC: ZJF-20141027-0H-醚 -50CH3.D\data.ms
.35e+07
1.3e+07
.25e+07
1.2e+07
.15e+07
1.1e+07
.05e+07
1e+07
95000000
90000000
85000000
80000000
75000000
70000000
65000000
60000000
55000000
50000000
45000000
40000000
35000000
30000000
25000000
20000000
15000000
10000000
5000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
O
N
HO
O

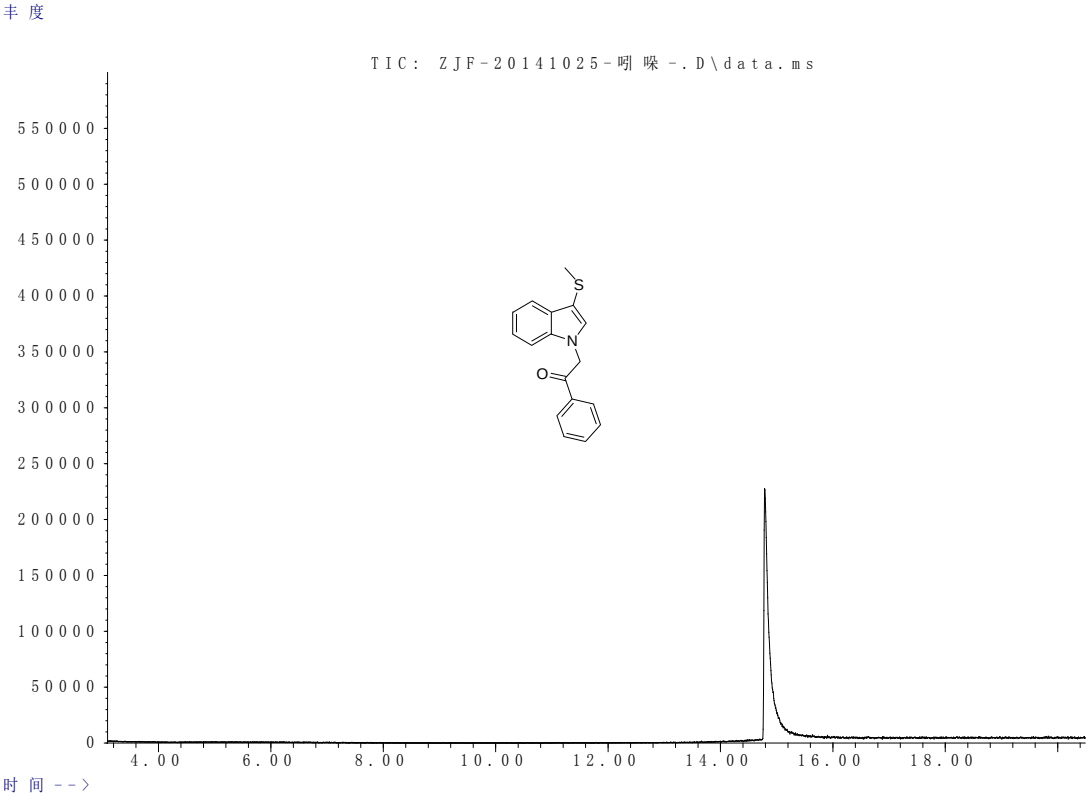

丰 度
扫 描 1916 (15.072 分): ZJF-20141027-0H-醚 -50CH3.D\data.ms
42000000
40000000
38000000
36000000
34000000
32000000
30000000
28000000
26000000
24000000
22000000
20000000
18000000
16000000
14000000
12000000
10000000
8000000
6000000
4000000
2000000
0
160.1
297.1
117.1
77.1
51.1
186.1
222.1
267.1
326.9
405.1
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400
m/z-->
O
N
HO
O

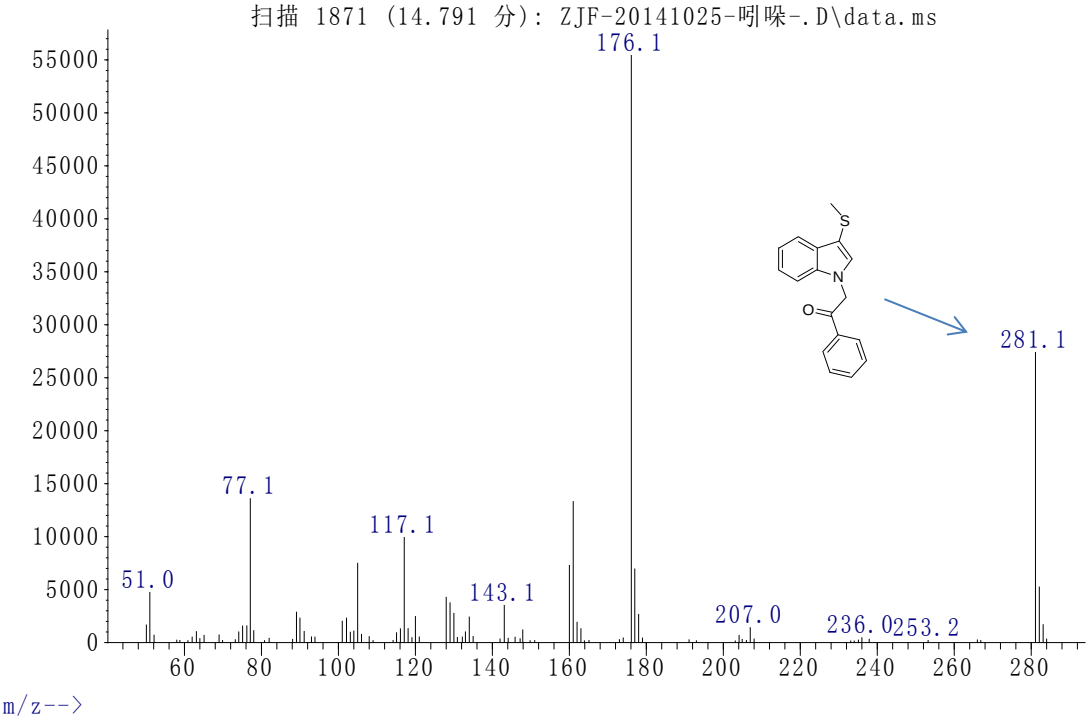

丰 度
TIC: ZJF-20141106-1.D\data.ms
.15e+07
1.1e+07
.05e+07
1e+07
95000000
90000000
85000000
80000000
75000000
70000000
65000000
60000000
55000000
50000000
45000000
40000000
35000000
30000000
25000000
20000000
15000000
10000000
5000000
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
HO
N
O

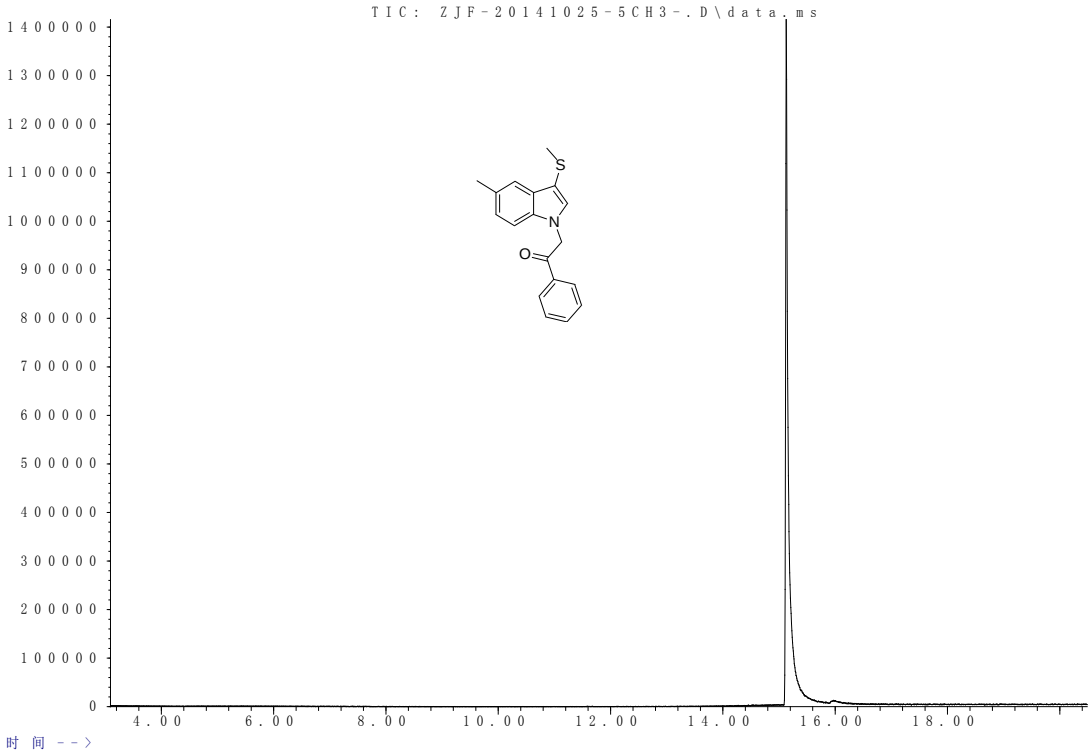

丰 度
扫 描 1603 (13.114 分): ZJF-20141106-1.D\data.ms
207.0
96.0
73.0
133.0
190.9
281.0
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
80
100
120
140
160
180
200
220
240
260
280
m/z-->
HO
N
O


丰 度
TIC: ZJF-20141203-OH-2CH3.D\data.ms
HO
N
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
丰 度
扫 描 1675 (13.565 分): ZJF-20141203-OH-2CH3.D\data.ms
144.1
HO
N
40000
35000
30000
25000
20000
15000
10000
5000
0
77.1
115.0
51.0
95.9
165.0
189.0
207.1
233.1
251.1
281.1
60
80
100
120
140
160
180
200
220
240
260
280
m/z-->
82

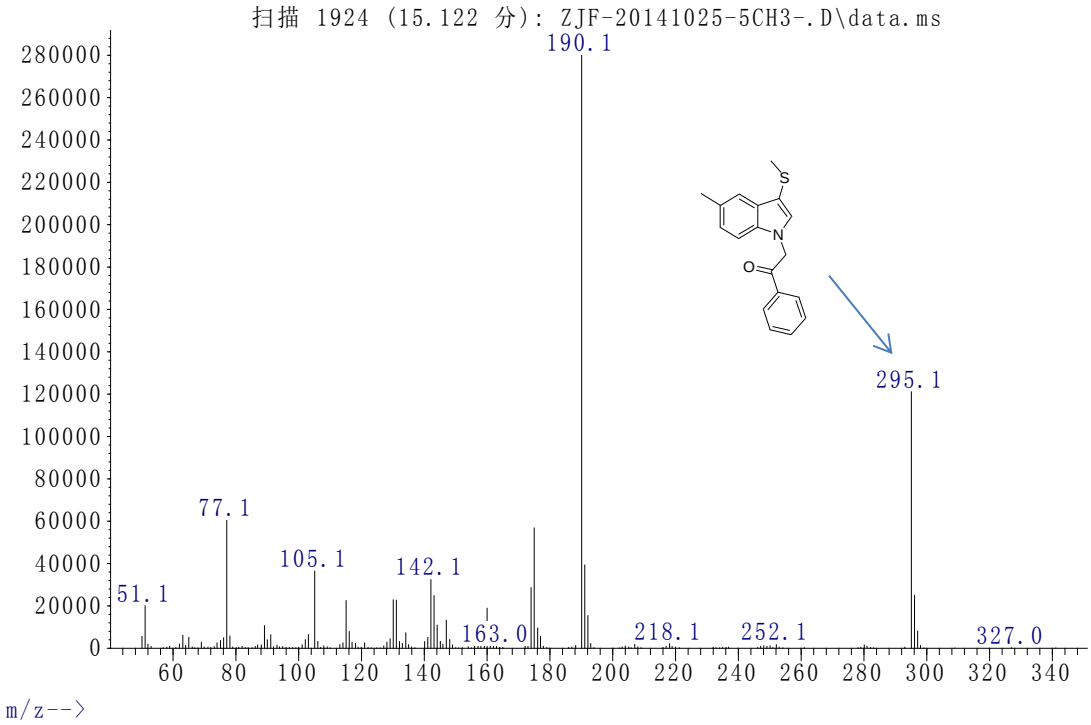
b. GC-MS Spectra of the 3-sulfenylindole products



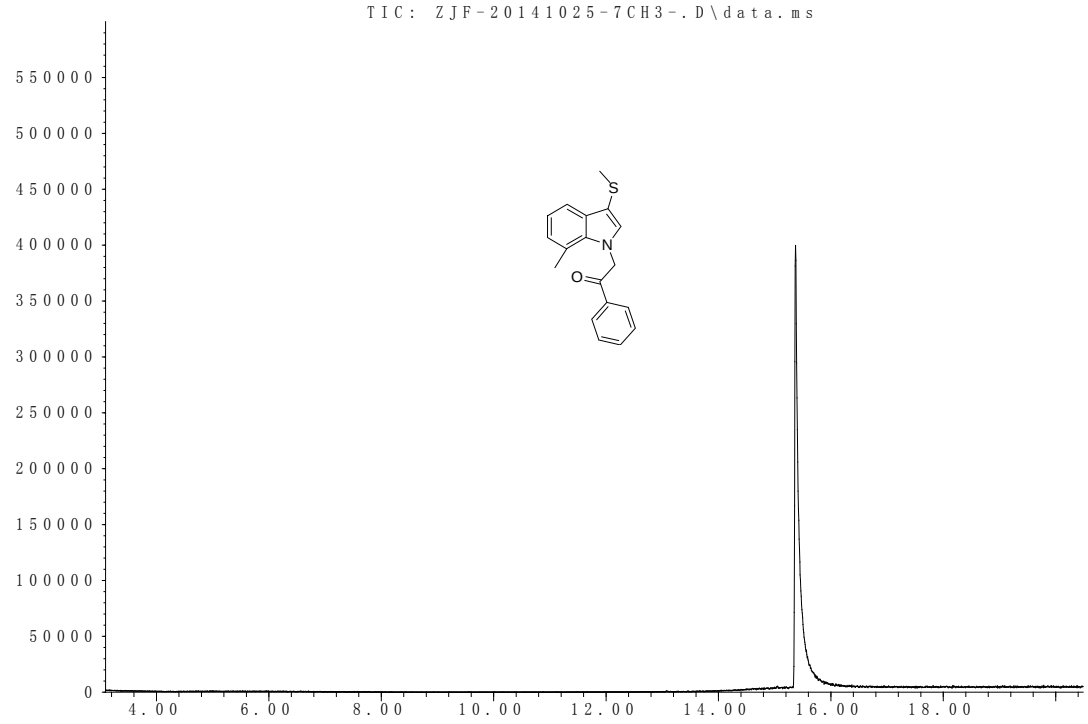



丰 度
TIC: ZJF-20141025-5CH3-.D\data.ms
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
S
N
O

丰度

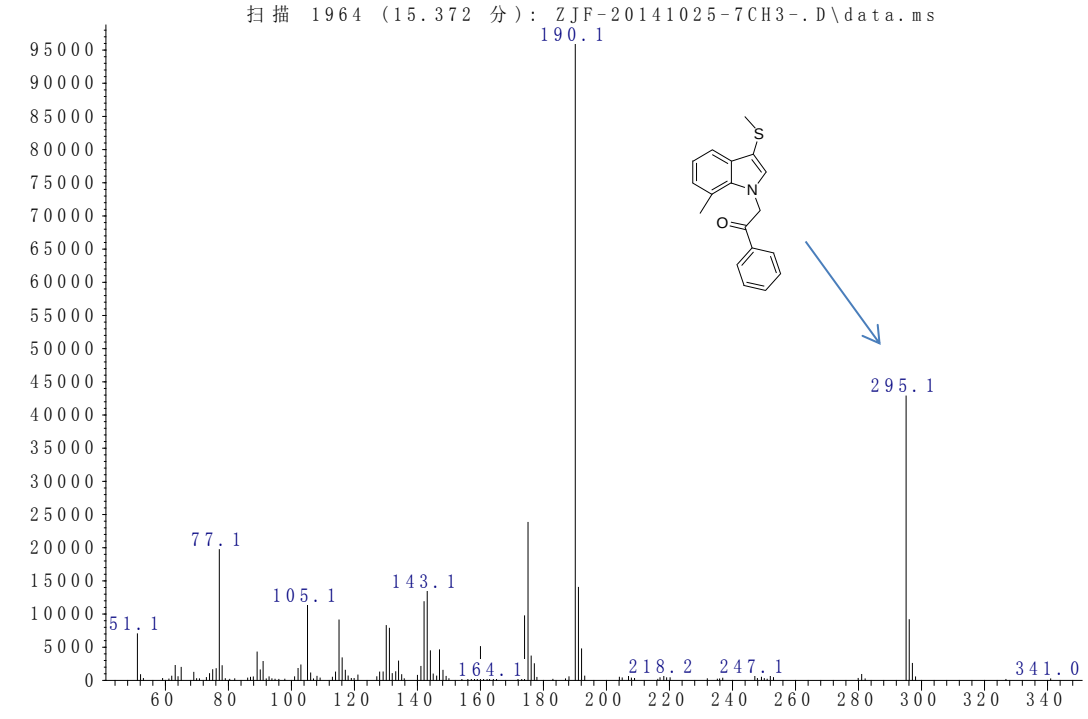

扫描 1924 (15.122 分): ZJF-20141025-5CH3-.D\data.ms
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
190.1
295.1
77.1
105.1
142.1
51.1
163.0
218.1
252.1
327.0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->
S
N
O

丰 度


TIC: ZJF-20141025-7CH3-.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
S
N
O

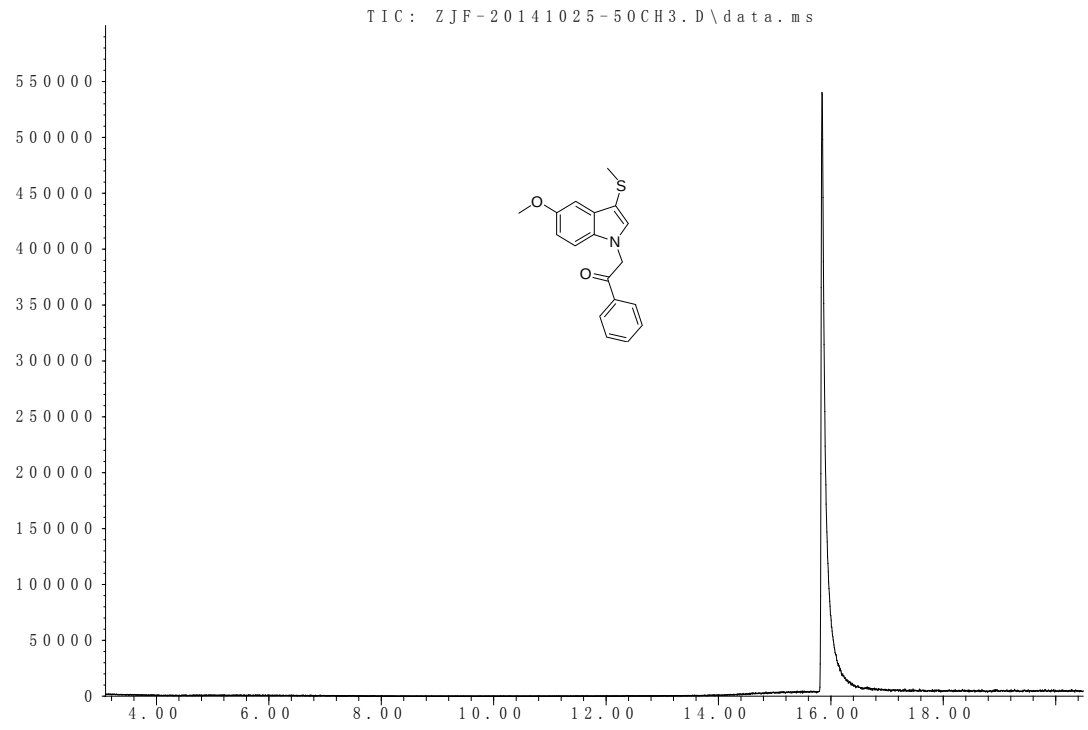
时 间 -->

丰 度


扫描 1964 (15.372 分): ZJF-20141025-7CH3-.D\data.ms
190.1
295.1
77.1
105.1
143.1
51.1
164.1
218.2
247.1
341.0
95000
90000
85000
80000
75000
70000
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
S
N
O

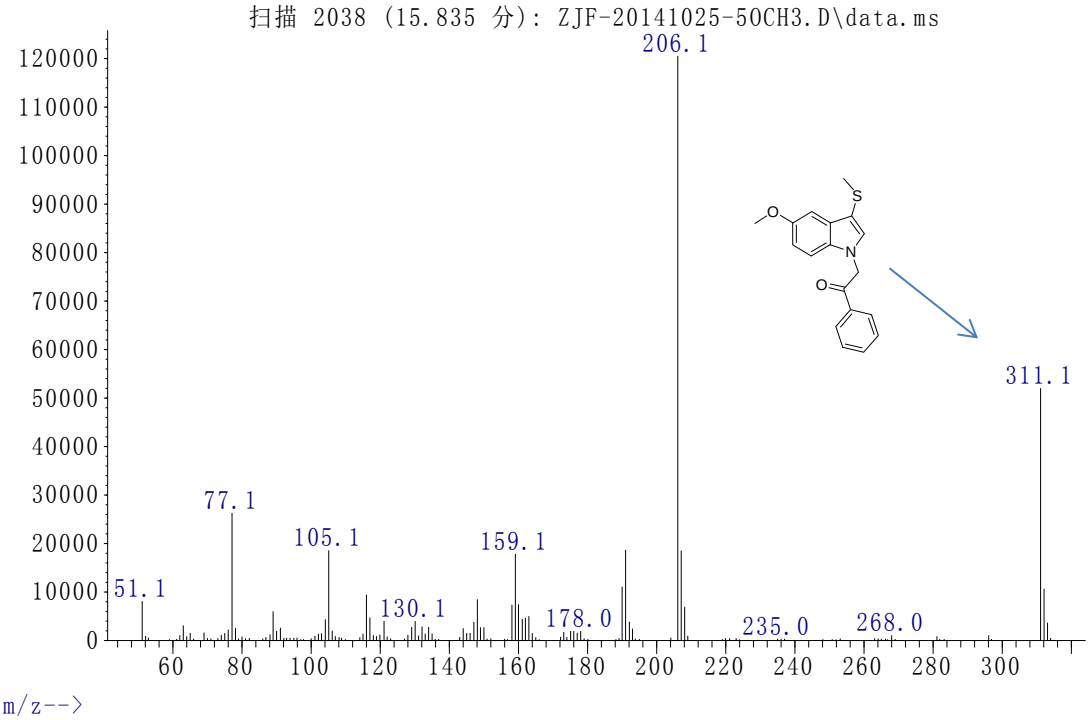
m/z-->

丰 度


TIC: ZJF-20141025-5OCH3.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
O
S
N
O

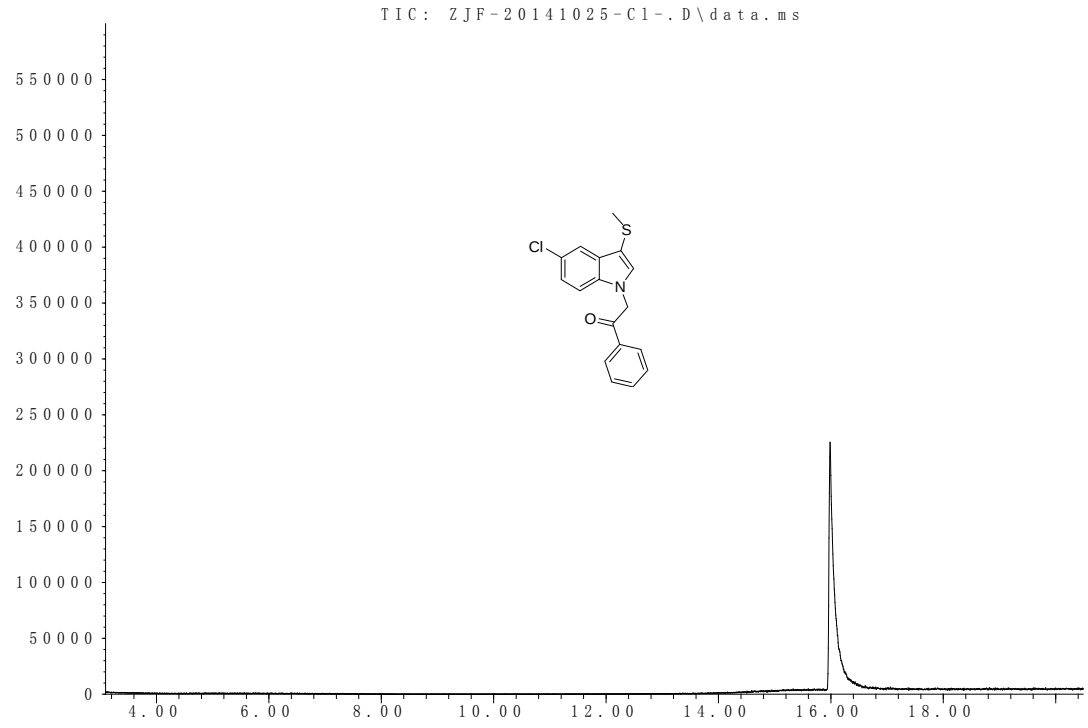
时 间 -->

丰度


扫描 2038 (15.835 分): ZJF-20141025-5OCH3.D\data.ms
206.1
311.1
77.1
105.1
159.1
51.1
130.1
178.0
235.0
268.0
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
O
S
N
O

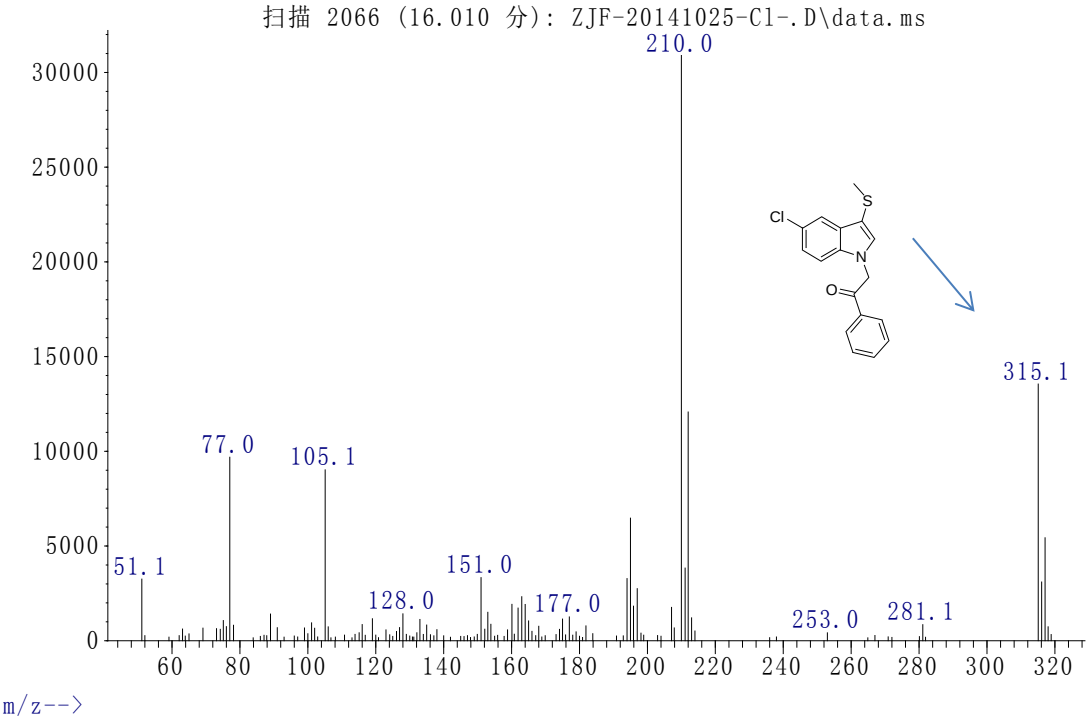
m/z-->

丰 度

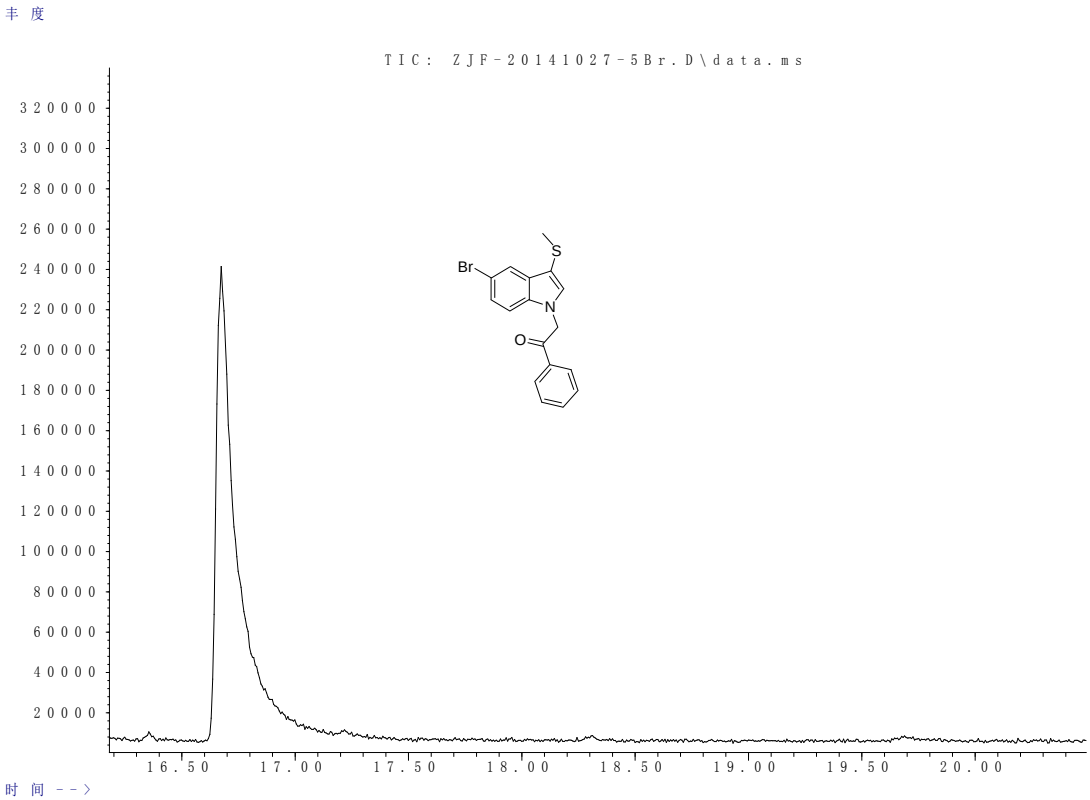

TIC: ZJF-20141025-Cl-.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
Cl
S
N
O

时 间 -->

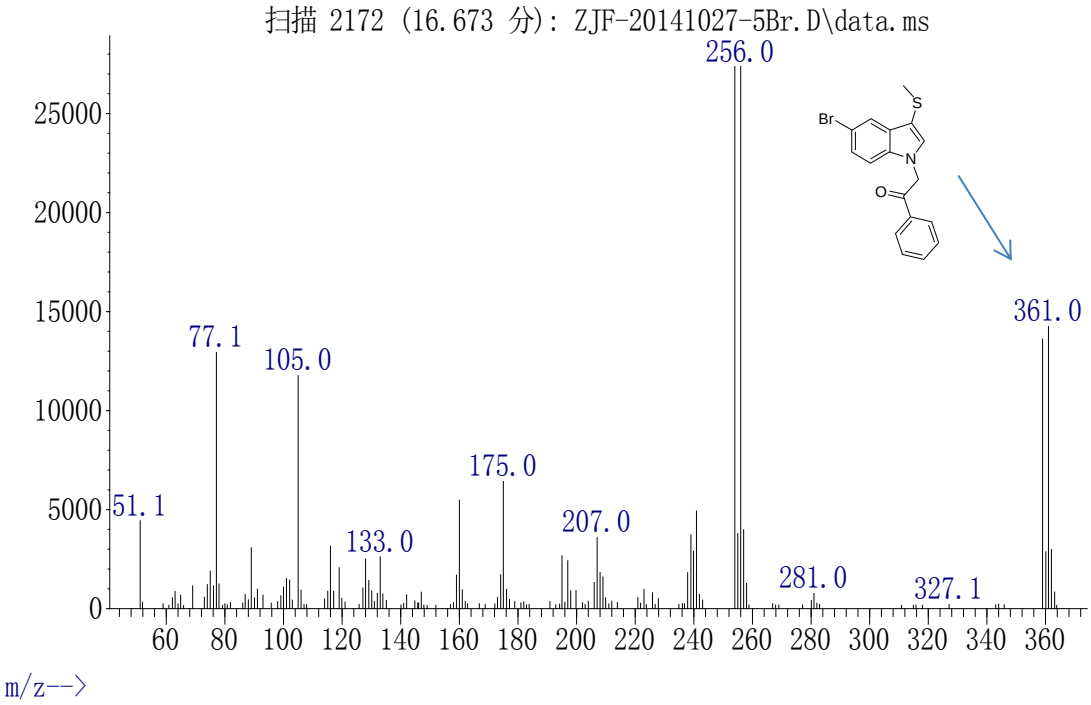
丰度

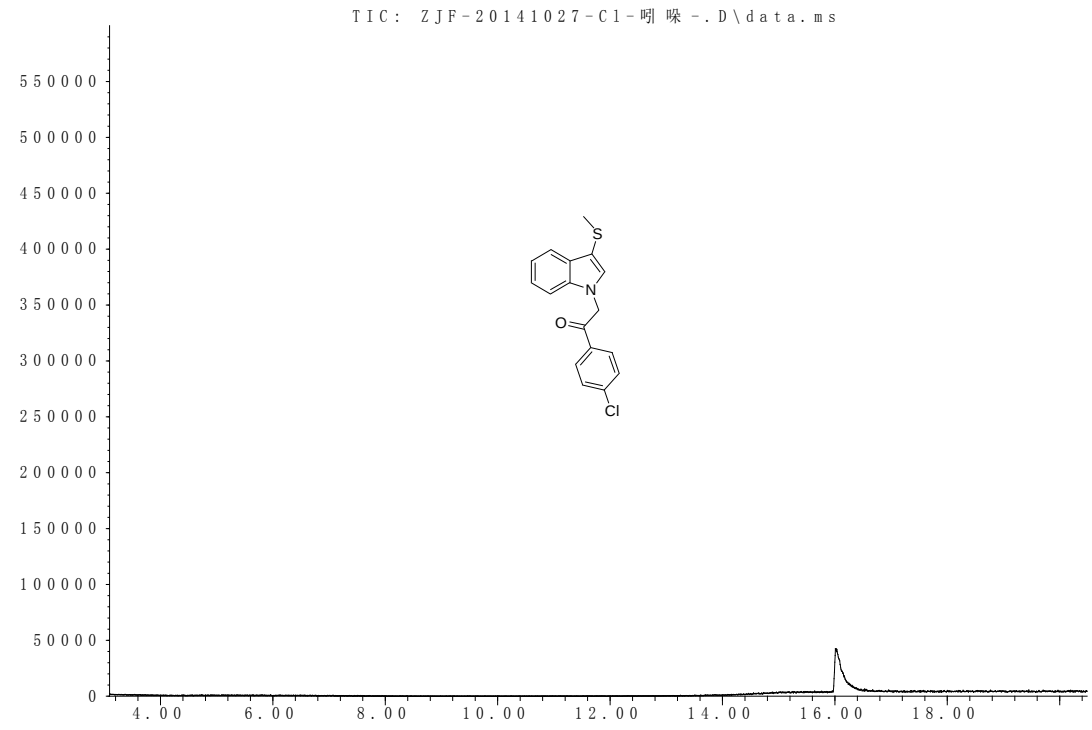

扫描 2066 (16.010 分): ZJF-20141025-Cl-.D\data.ms
30000
25000
20000
15000
10000
5000
0
210.0
315.1
77.0
105.1
51.1
151.0
128.0
177.0
253.0
281.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
Cl
S
N
O

m/z-->

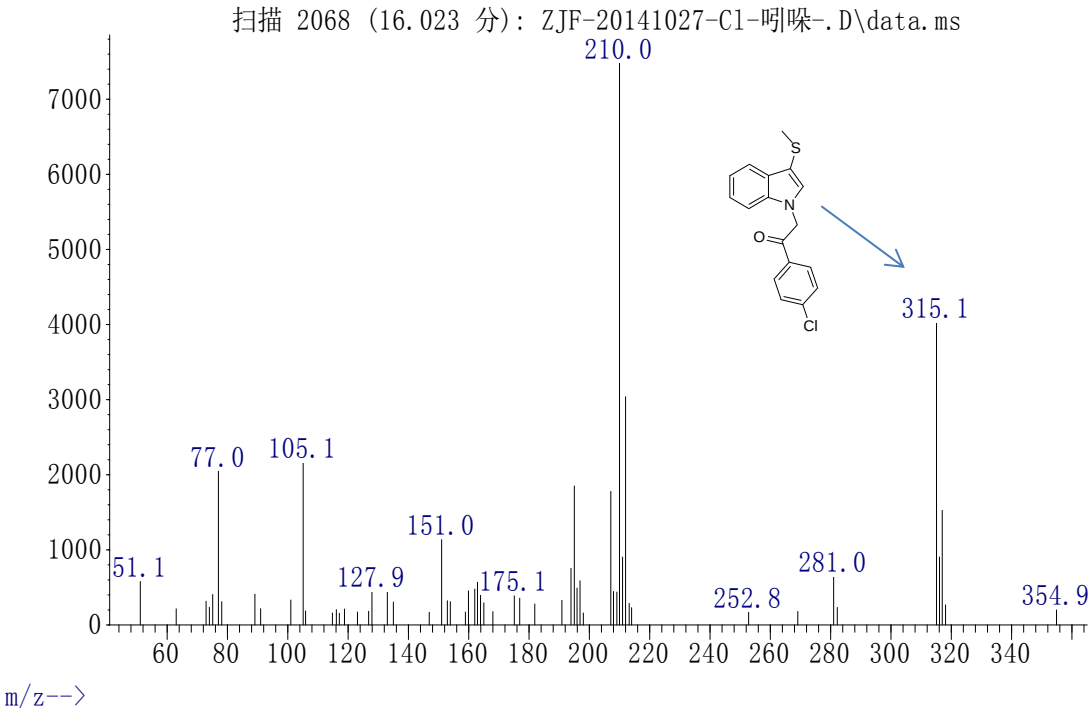

丰 度
TIC: ZJF-20141027-5Br.D\data.ms
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
16.50
17.00
17.50
18.00
18.50
19.00
19.50
20.00
时 间 -->
Br
S
N
O

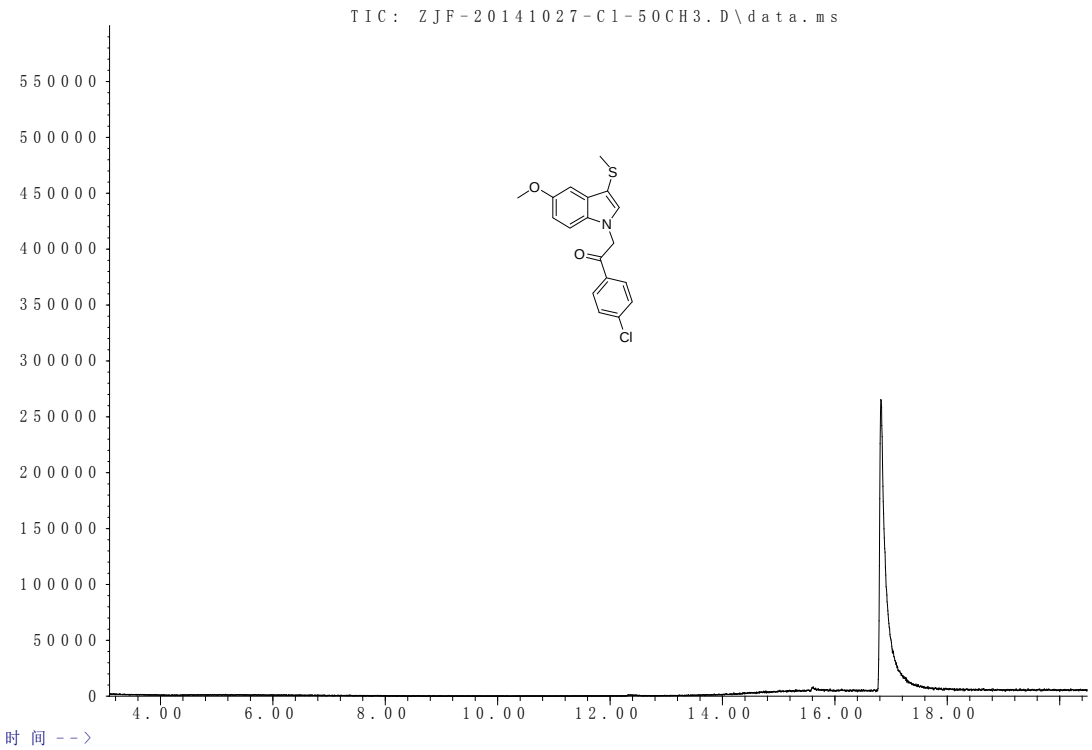
丰度


扫描 2172 (16.673 分): ZJF-20141027-5Br.D\data.ms
256.0
361.0
77.1
105.0
175.0
51.1
133.0
207.0
281.0
327.1
25000
20000
15000
10000
5000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
m/z-->
Br
S
N
O

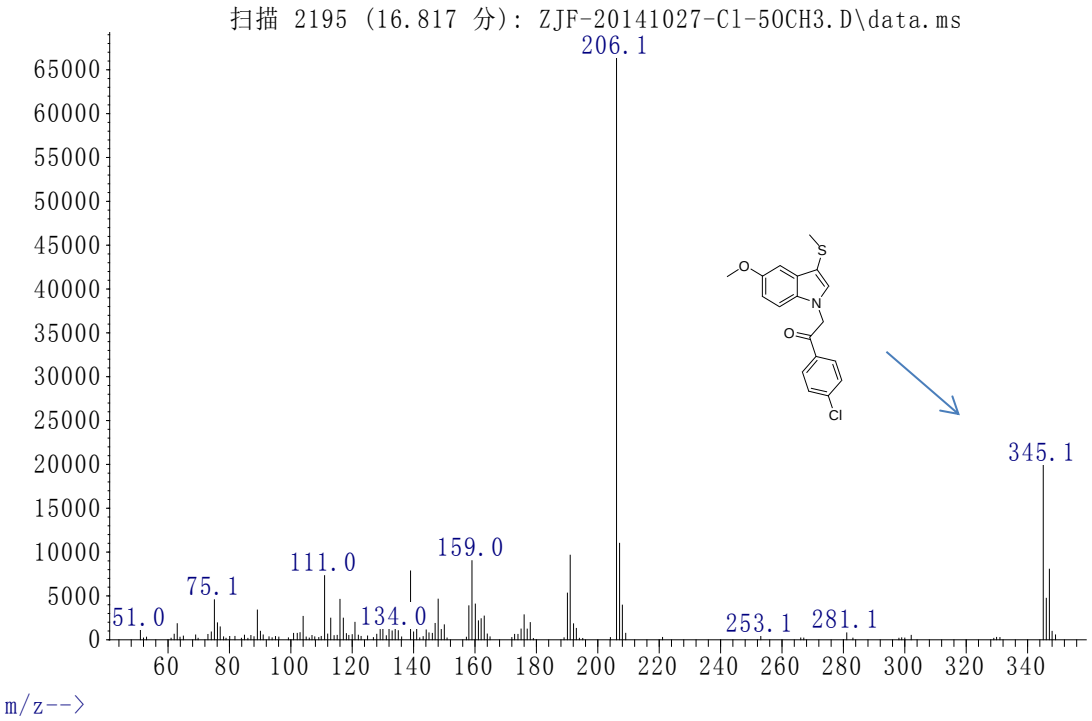

丰 度
TIC: ZJF-20141027-Cl-吲 哚 -.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
S
N
O
Cl

丰度

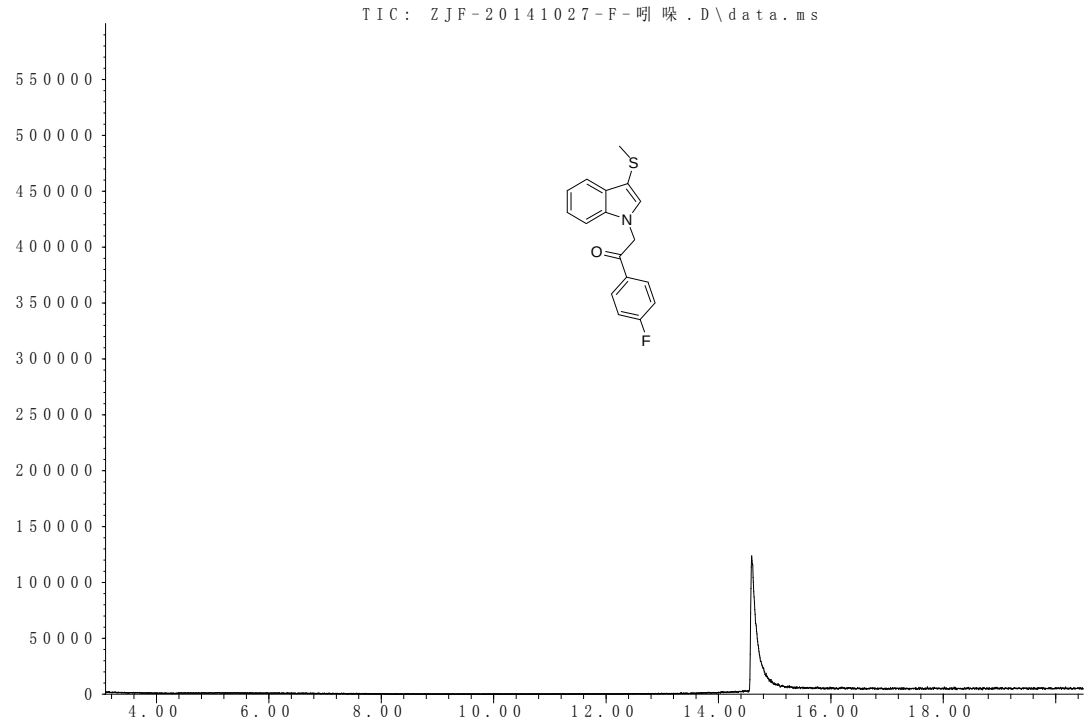

扫描 2068 (16.023 分): ZJF-20141027-Cl-吲哚-.D\data.ms
210.0
315.1
77.0
105.1
151.0
51.1
127.9
175.1
281.0
252.8
354.9
7000
6000
5000
4000
3000
2000
1000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->
S
N
O
Cl


丰 度
TIC: ZJF-20141027-Cl-5OCH3.D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
O
S
N
O
Cl

丰度

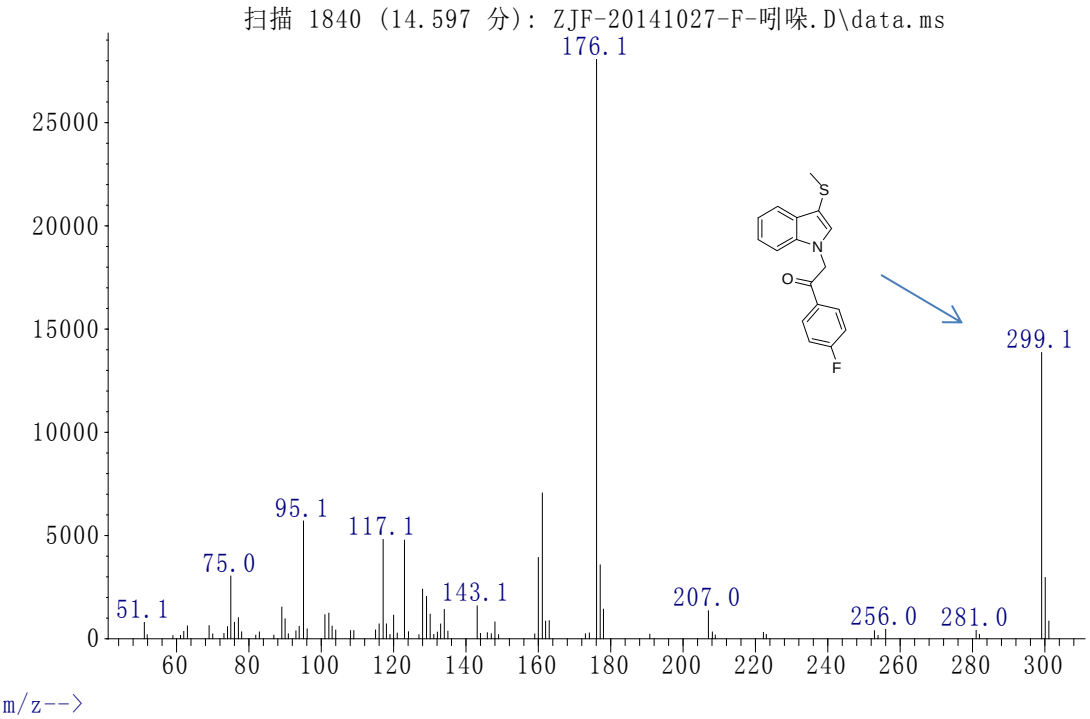

扫描 2195 (16.817 分): ZJF-20141027-Cl-5OCH3.D\data.ms
206.1
345.1
159.0
111.0
75.1
51.0
134.0
253.1
281.1
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->
O
S
N
O
Cl

丰 度

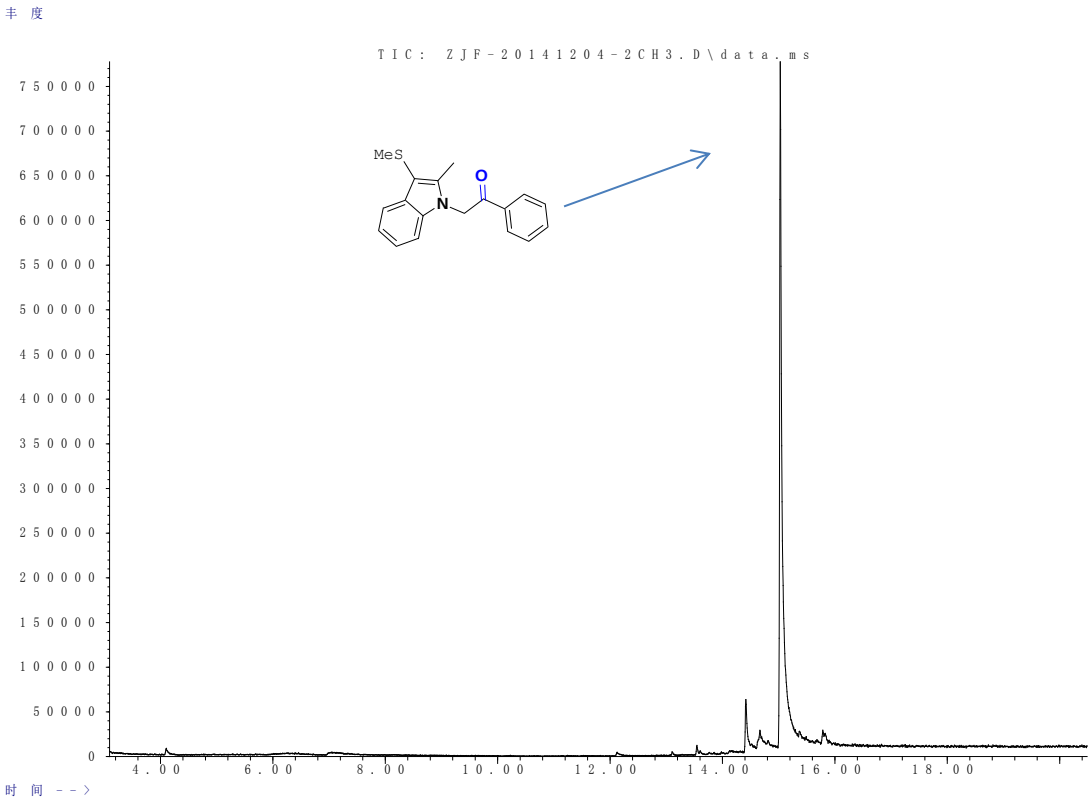

TIC: ZJF-20141027-F-吲 哚 .D\data.ms
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
S
N
O
F

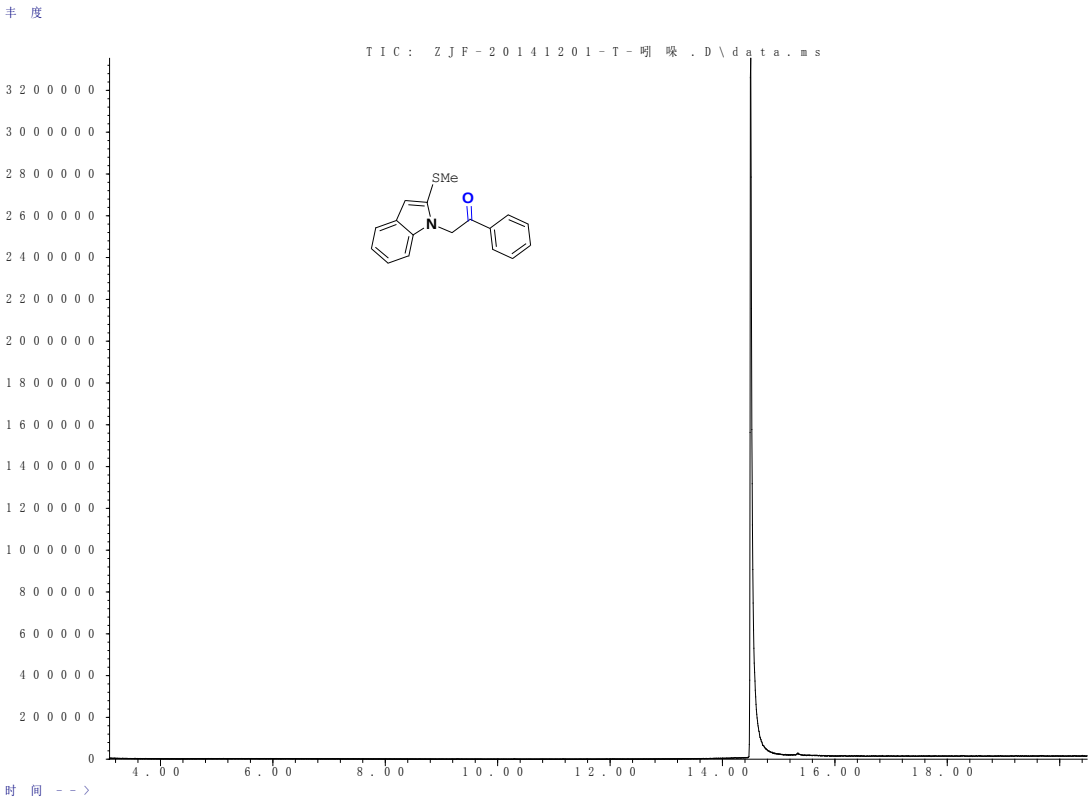
时 间 -->

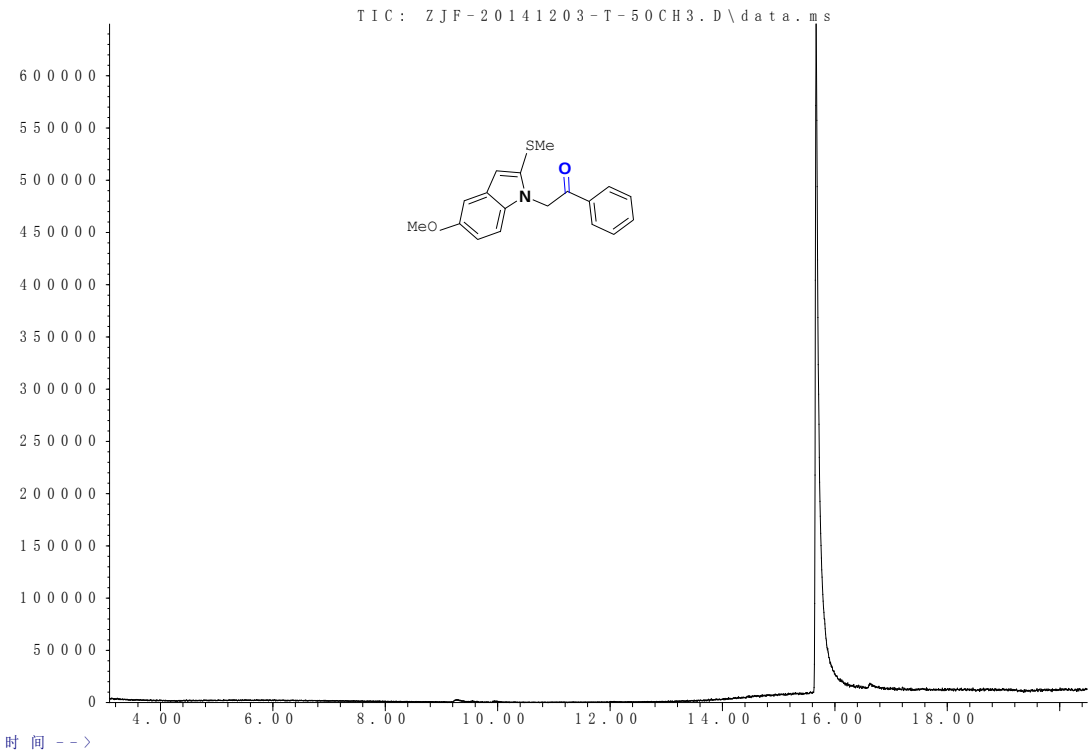
丰度

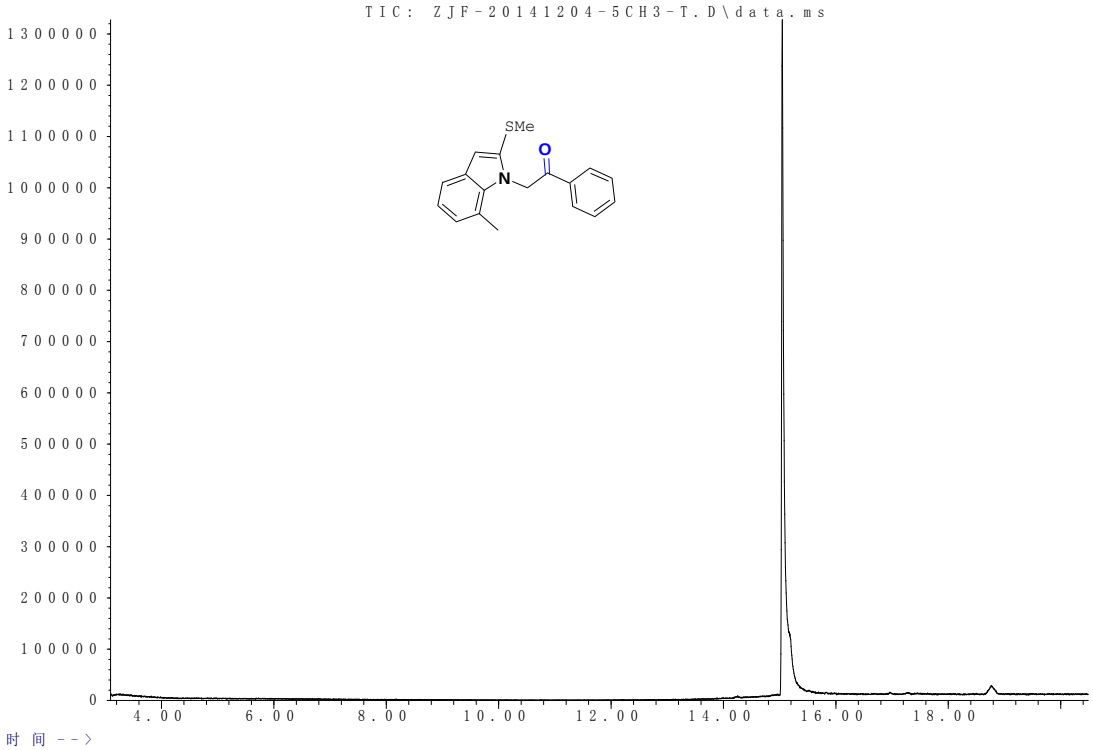

扫描 1840 (14.597 分): ZJF-20141027-F-吲哚.D\data.ms
176.1
25000
20000
15000
10000
5000
0
95.1
117.1
75.0
143.1
51.1
207.0
256.0
281.0
299.1
60
80
100
120
140
160
180
200
220
240
260
280
300
S
N
O
F

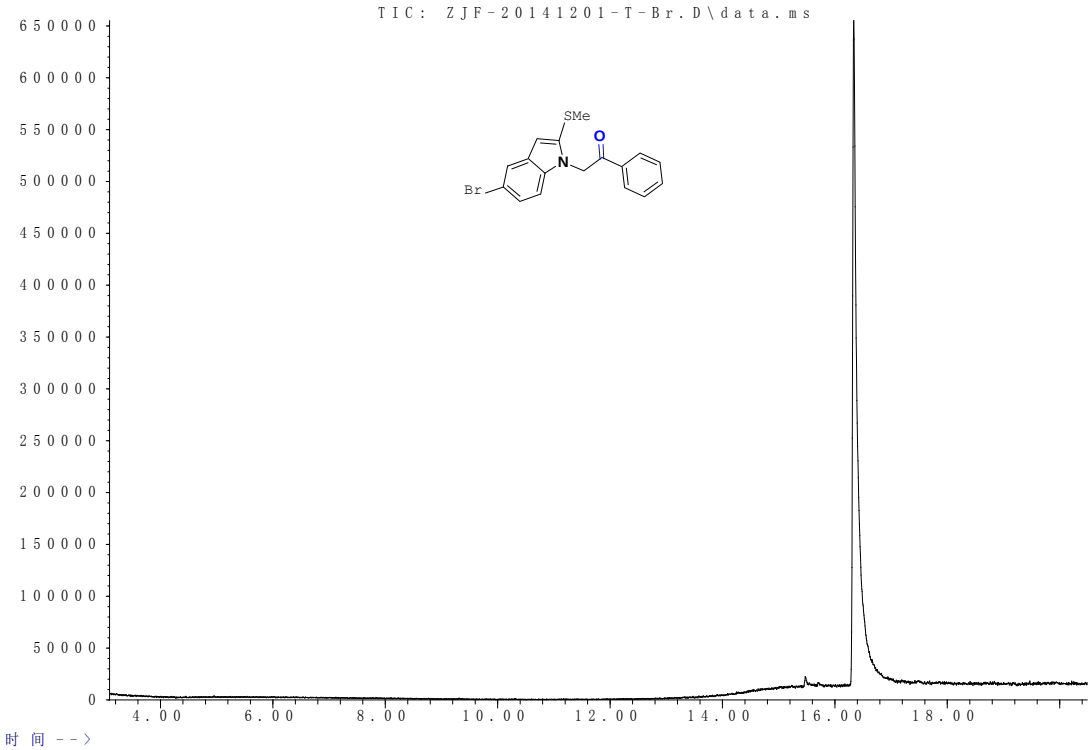
m/z-->


丰 度
TIC: ZJF-20141204-2CH3.D\data.ms
MeS
O
N
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
丰度
扫描 1909 (15.028 分): ZJF-20141204-2CH3.D\data.ms
190.1
MeS
O
N
295.1
77.0
105.0
142.1
51.0
231.1
264.1
165.0
327.0
355.0
160000
150000
140000
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->

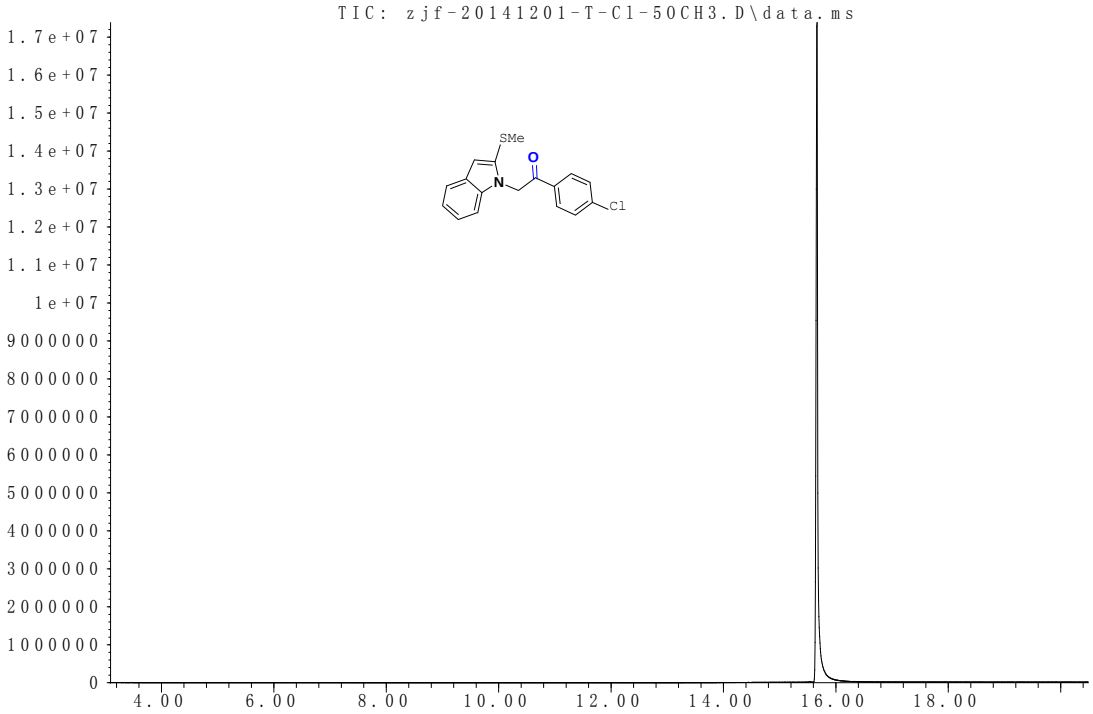

丰 度
TIC: ZJF-20141201-T-吲 哚 .D\data.ms
SMe
O
N
32000000
30000000
28000000
26000000
24000000
22000000
20000000
18000000
16000000
14000000
12000000
10000000
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
丰度
扫描 1827 (14.515 分): ZJF-20141201-T-吲哚.D\data.ms
176.0
SMe
O
N
281.1
117.1
77.1
51.0
143.1
204.1
238.0
340.9
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->


丰 度
TIC: ZJF-20141203-T-5OCH3.D\data.ms
SMe
O
N
MeO
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
丰度
扫描 2013 (15.679 分): ZJF-20141203-T-5OCH3.D\data.ms
206.1
311.1
77.1
105.0
147.1
51.0
176.0
236.1
281.0
354.8
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->


丰 度
TIC: ZJF-20141204-5CH3-T.D\data.ms
SMe
O
N
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
丰度
扫描 1909 (15.028 分): ZJF-20141204-5CH3-T.D\data.ms
190.1
SMe
O
N
295.1
77.0
131.1
105.1
51.0
160.1
219.0
252.0
340.9
65000
60000
55000
50000
45000
40000
35000
30000
25000
20000
15000
10000
5000
0
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->

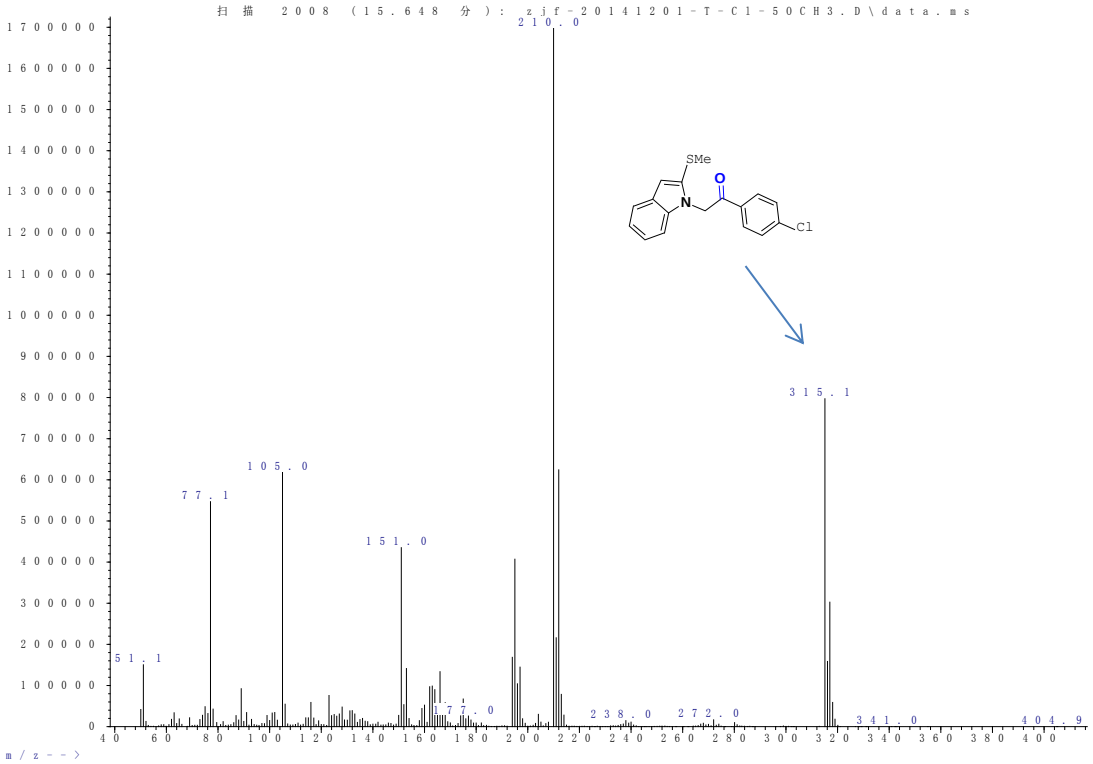

丰 度
TIC: ZJF-20141201-T-Br.D\data.ms
SMe
O
N
Br
6 5 0 0 0 0
6 0 0 0 0 0
5 5 0 0 0 0
5 0 0 0 0 0
4 5 0 0 0 0
4 0 0 0 0 0
3 5 0 0 0 0
3 0 0 0 0 0
2 5 0 0 0 0
2 0 0 0 0 0
1 5 0 0 0 0
1 0 0 0 0 0
5 0 0 0 0
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 - - >
丰 度
扫 描 2123 (16.367 分): ZJF-20141201-T-Br.D\data.ms
254.0
SMe
O
N
Br
105.0
77.0
361.0
175.0
207.0
133.0
281.1
315.9
405.2
4 2 0 0 0
4 0 0 0 0
3 8 0 0 0
3 6 0 0 0
3 4 0 0 0
3 2 0 0 0
3 0 0 0 0
2 8 0 0 0
2 6 0 0 0
2 4 0 0 0
2 2 0 0 0
2 0 0 0 0
1 8 0 0 0
1 6 0 0 0
1 4 0 0 0
1 2 0 0 0
1 0 0 0 0
8 0 0 0
6 0 0 0
4 0 0 0
2 0 0 0
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420
m / z - - >

丰 度

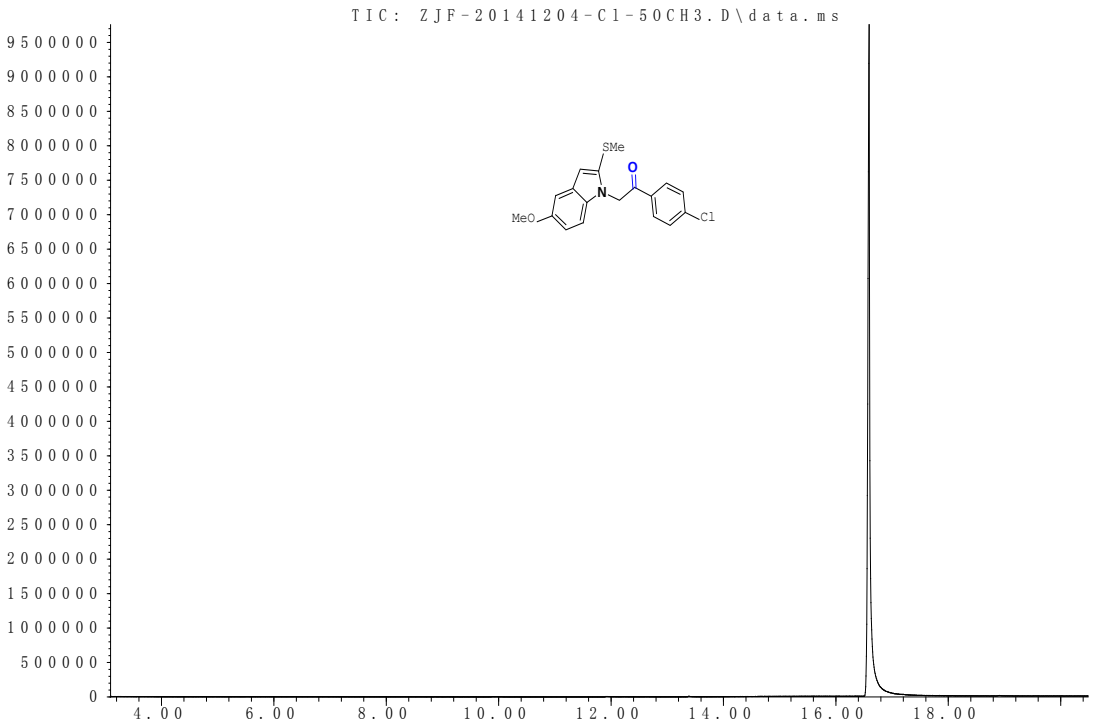

TIC: zjf-20141201-T-Cl-50CH3.D\data.ms
1.7e+07
1.6e+07
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
SMe
O
N
Cl

时 间 - - >

丰 度

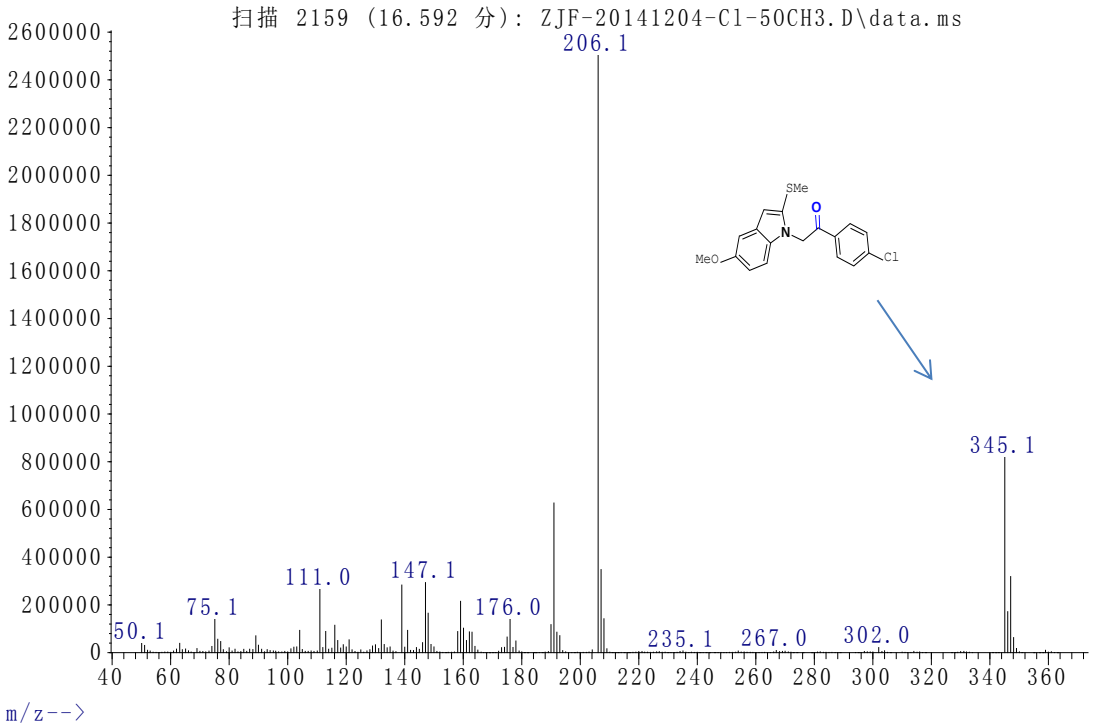

扫 描 2008 (15.648 分): zjf-20141201-T-Cl-50CH3.D\data.ms
210.0
315.1
105.0
77.1
151.0
51.1
177.0
238.0
272.0
341.0
404.9
SMe
O
N
Cl
m/z - - >

丰 度


TIC: ZJF-20141204-Cl-5OCH3.D\data.ms
SMe
O
N
MeO
Cl
95000000
90000000
85000000
80000000
75000000
70000000
65000000
60000000
55000000
50000000
45000000
40000000
35000000
30000000
25000000
20000000
15000000
10000000
5000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

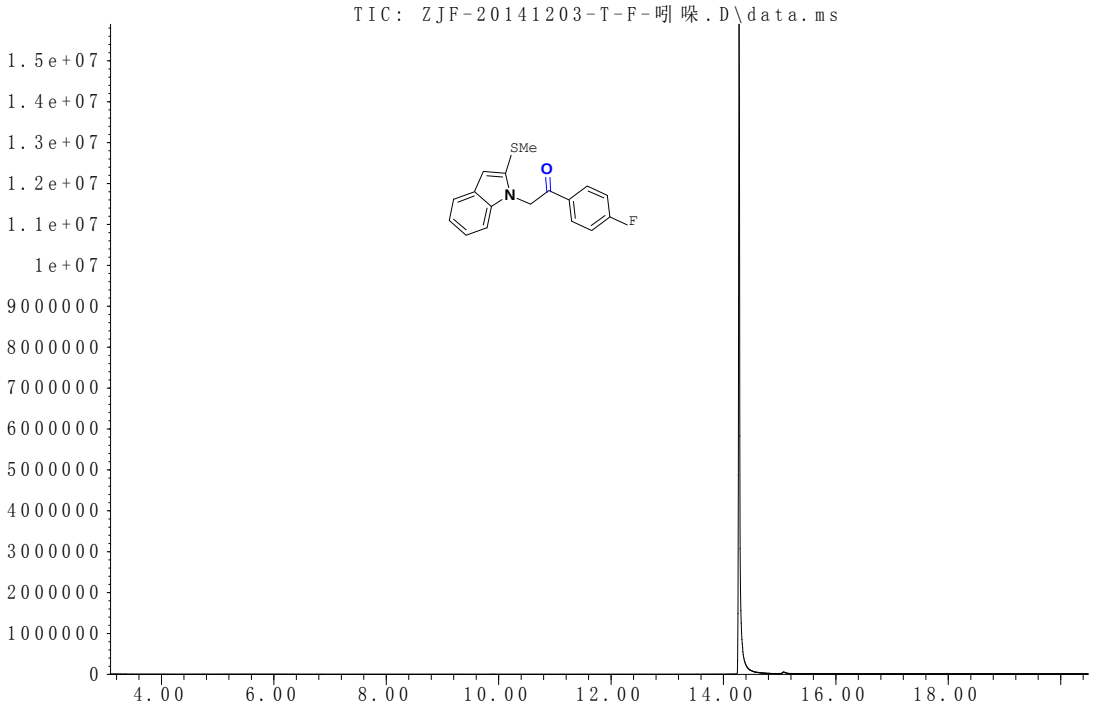
时 间 -->

丰度


扫描 2159 (16.592 分): ZJF-20141204-Cl-5OCH3.D\data.ms
206.1
SMe
O
N
MeO
Cl
345.1
111.0
147.1
75.1
176.0
50.1
235.1
267.0
302.0
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360

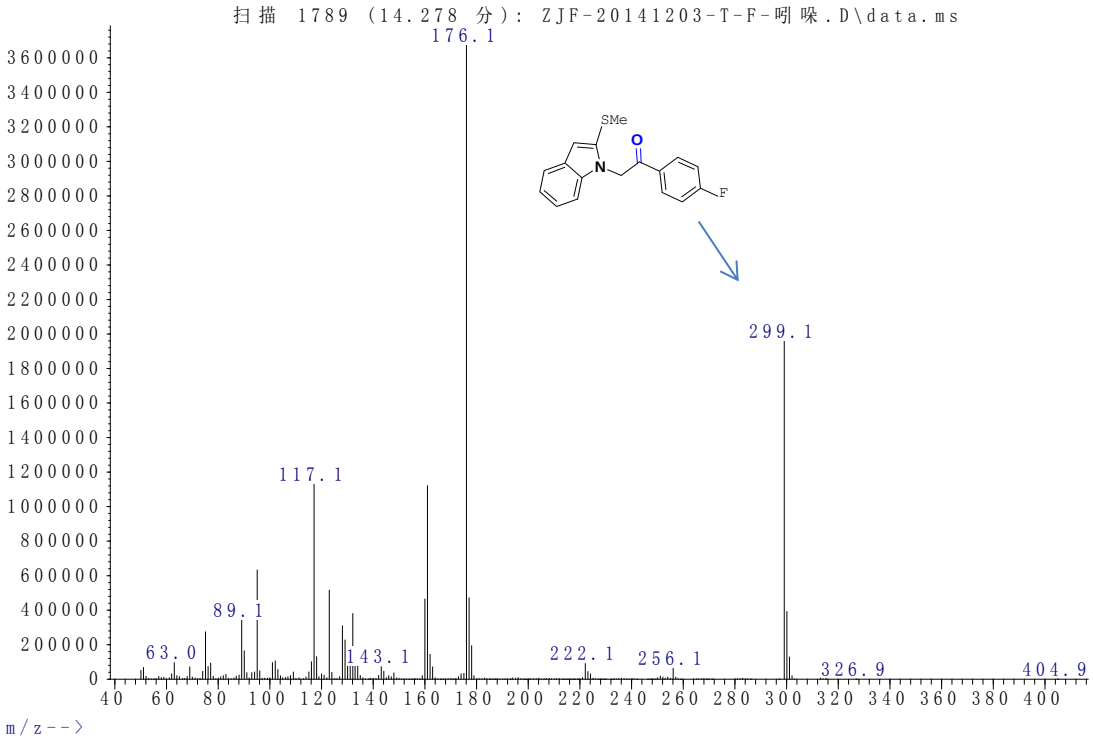
m/z-->

丰度


TIC: ZJF-20141203-T-F-吲哚.D\data.ms
SMe
O
N
F
1.5e+07
1.4e+07
1.3e+07
1.2e+07
1.1e+07
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00

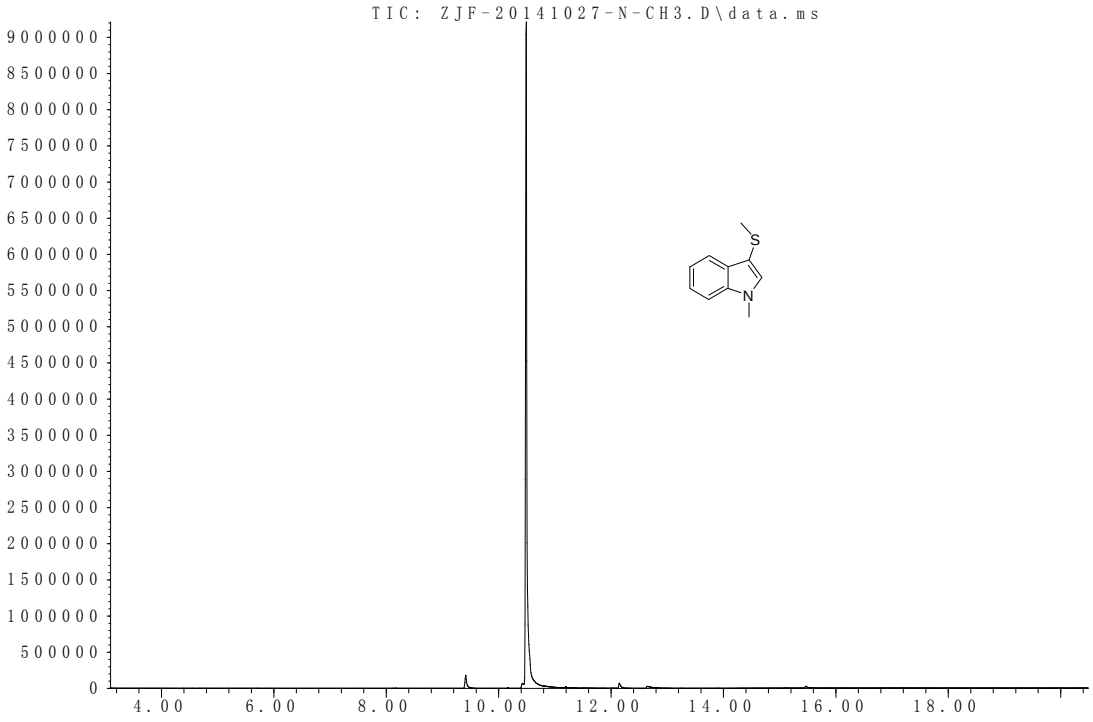
时间-->

丰度


扫描 1789 (14.278 分): ZJF-20141203-T-F-吲哚.D\data.ms
176.1
SMe
O
N
F
299.1
117.1
89.1
63.0
143.1
222.1
256.1
326.9
404.9
3600000
3400000
3200000
3000000
2800000
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400

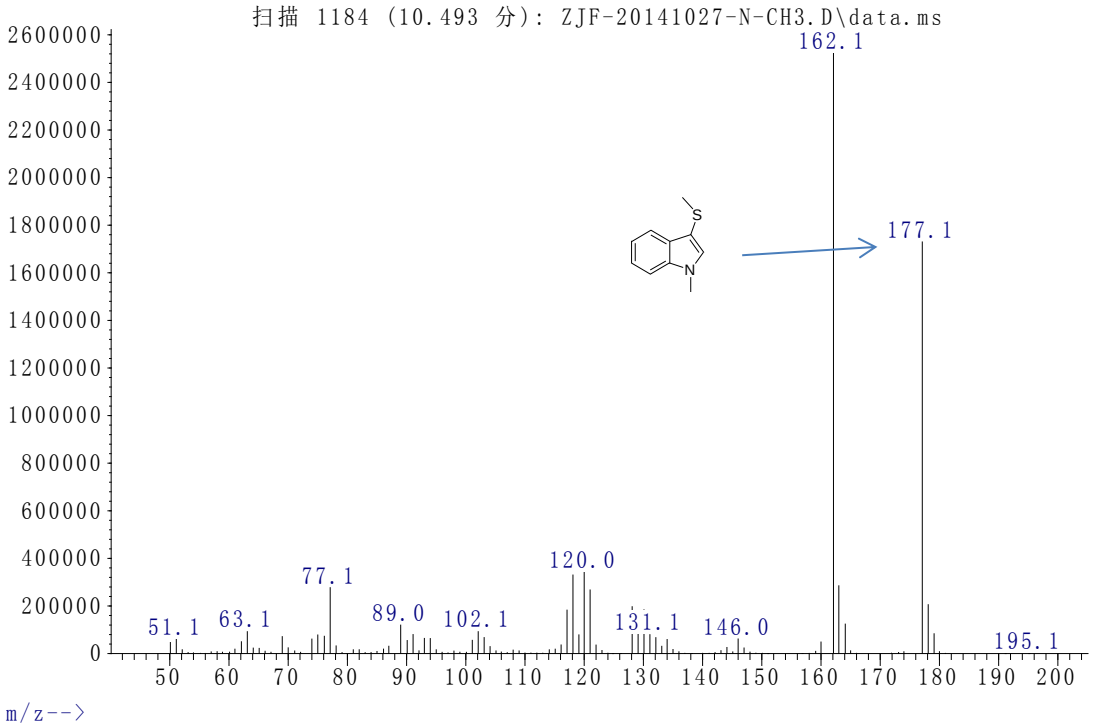
m/z-->

丰 度


TIC: ZJF-20141027-N-CH3.D\data.ms
9000000
8500000
8000000
7500000
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
S
N

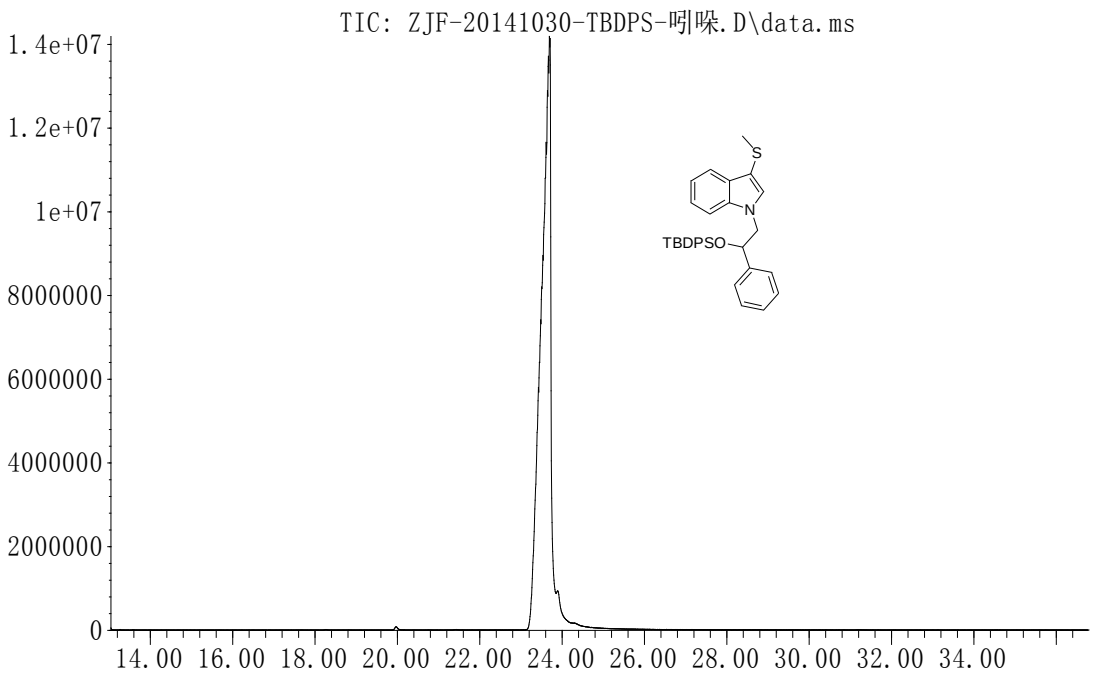
时 间 -->

丰度


扫描 1184 (10.493 分): ZJF-20141027-N-CH3.D\data.ms
2600000
2400000
2200000
2000000
1800000
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
162.1
177.1
120.0
77.1
89.0
102.1
131.1
146.0
51.1
63.1
195.1
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
S
N

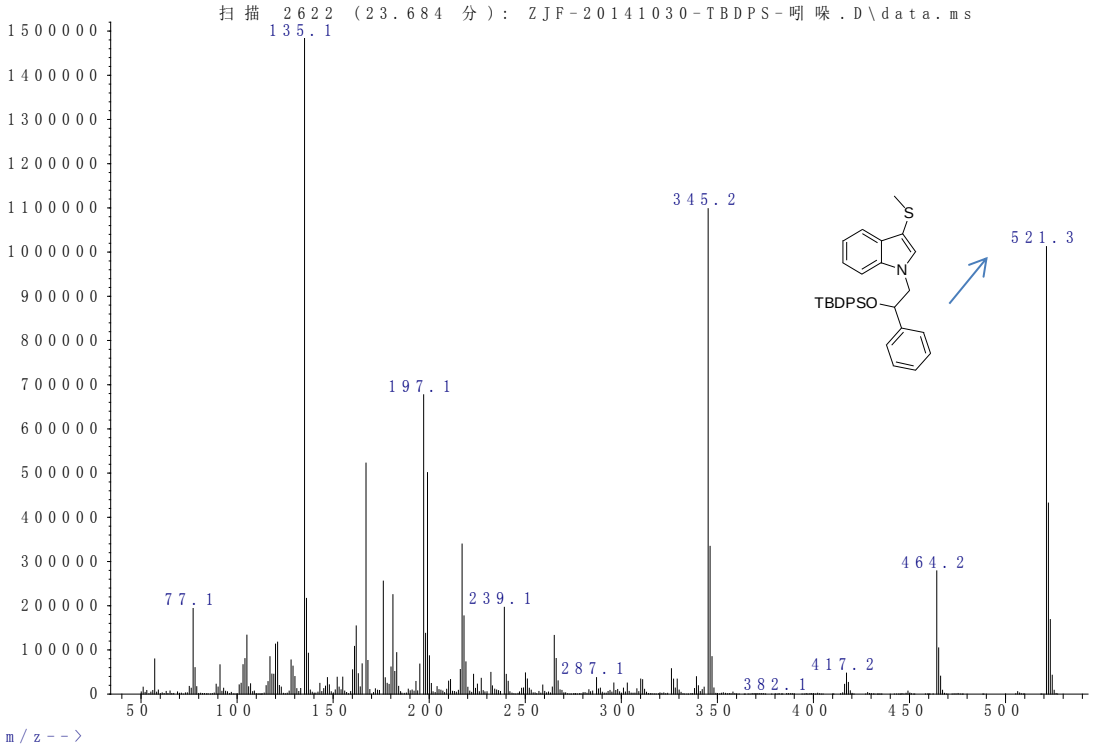
m/z-->

丰度


TIC: ZJF-20141030-TBDPS-吲哚.D\data.ms
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
14.00 16.00 18.00 20.00 22.00 24.00 26.00 28.00 30.00 32.00 34.00
S
N
TBDPSO

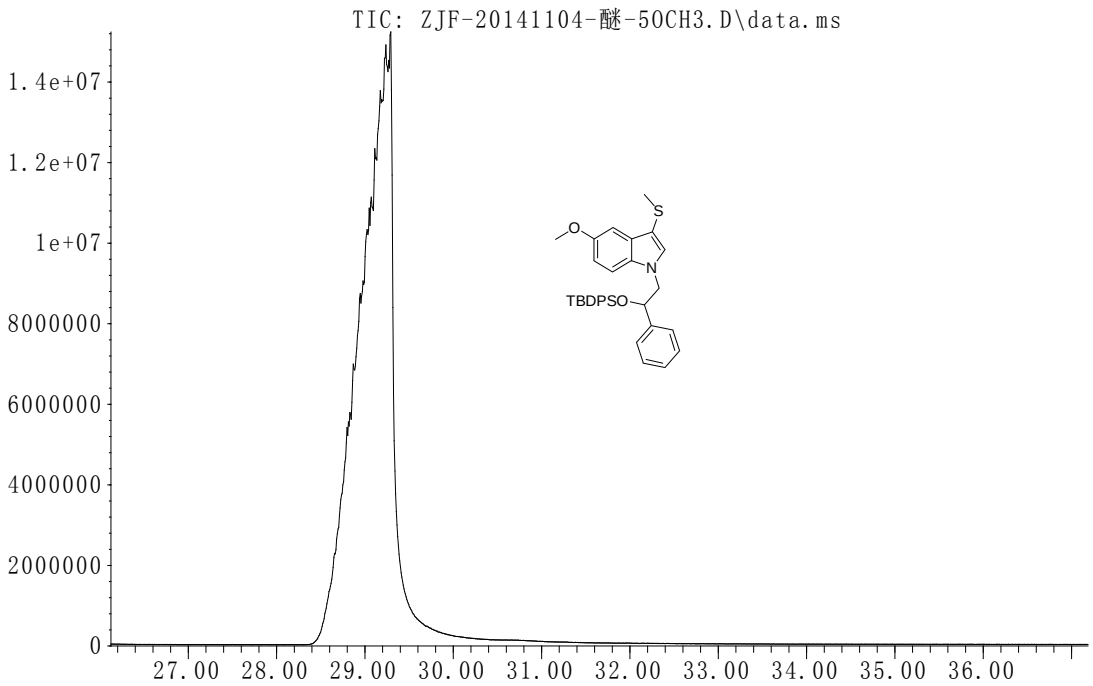
时间-->

丰 度


扫 描 2622 (23.684 分): ZJF-20141030-TBDPS-吲 哚 .D\data.ms
135.1
345.2
521.3
197.1
464.2
77.1
239.1
287.1
382.1
417.2
S
N
TBDPSO
50 100 150 200 250 300 350 400 450 500

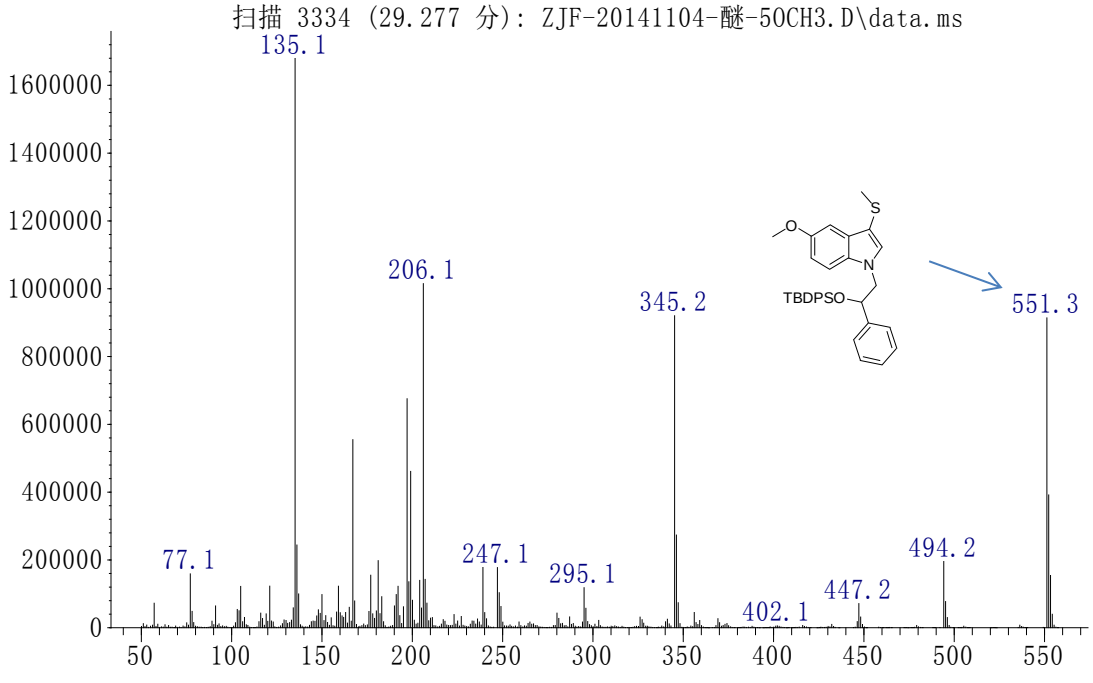
m/z-->

丰度

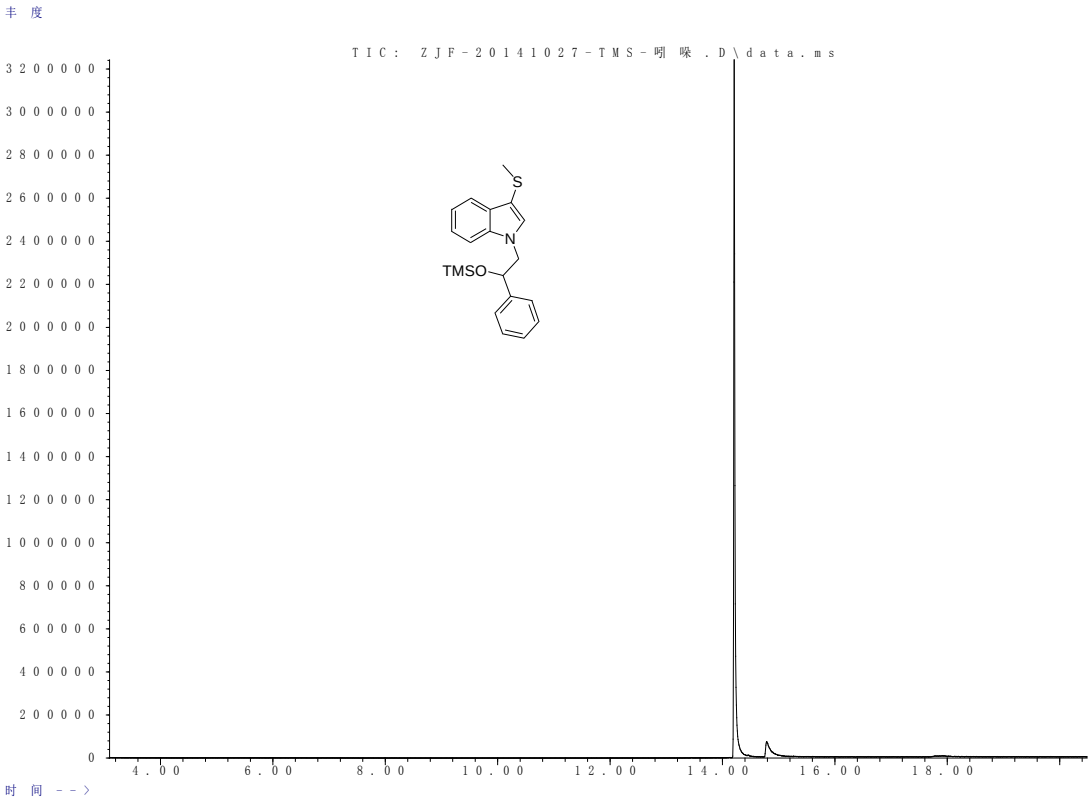

TIC: ZJF-20141104-醚-5OCH3.D\data.ms
1.4e+07
1.2e+07
1e+07
8000000
6000000
4000000
2000000
0
27.00
28.00
29.00
30.00
31.00
32.00
33.00
34.00
35.00
36.00
S
O
N
TBDPSO

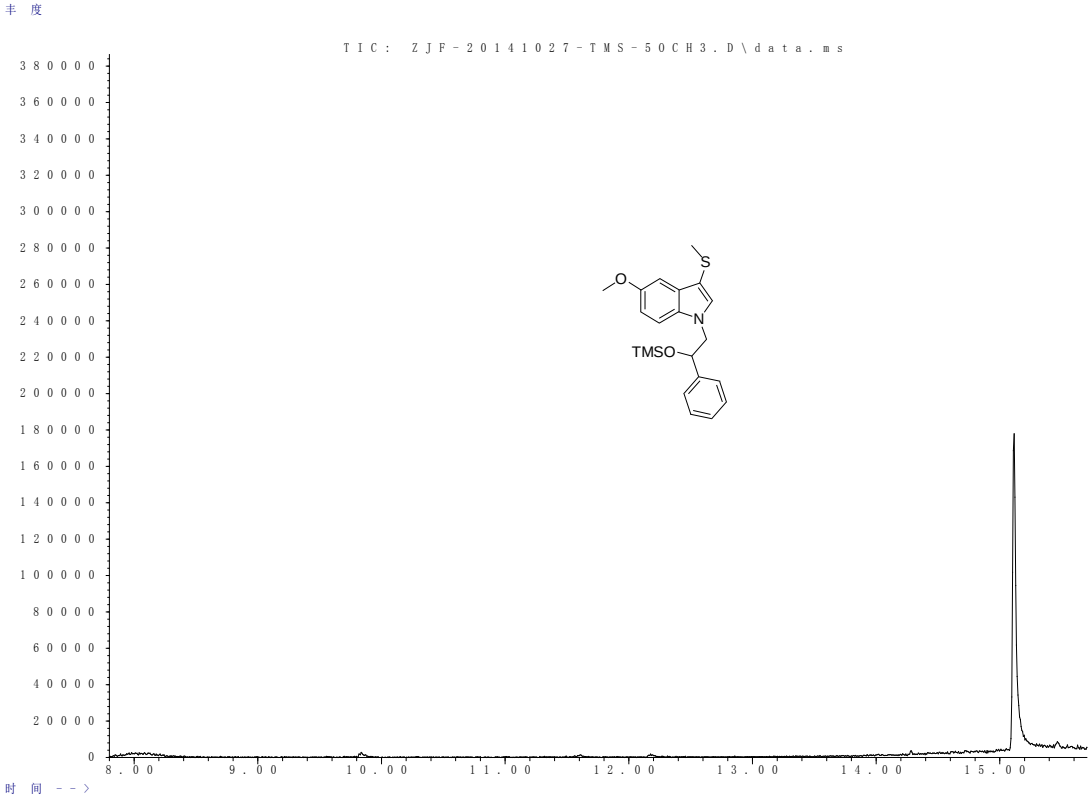
时间-->

丰度

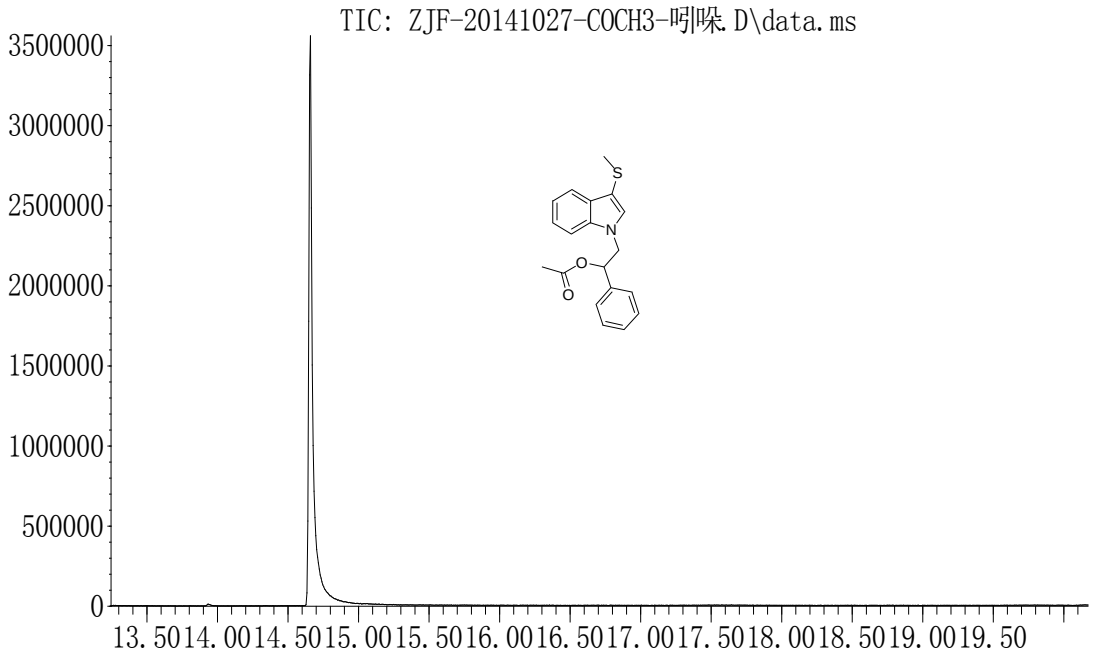

扫描 3334 (29.277 分): ZJF-20141104-醚-5OCH3.D\data.ms
135.1
206.1
345.2
551.3
77.1
247.1
295.1
402.1
447.2
494.2
1600000
1400000
1200000
1000000
800000
600000
400000
200000
0
50
100
150
200
250
300
350
400
450
500
550
S
O
N
TBDPSO

m/z-->


丰 度
TIC: ZJF-20141027-TMS-吲 哚 .D\data.ms
32000000
30000000
28000000
26000000
24000000
22000000
20000000
18000000
16000000
14000000
12000000
10000000
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
S
N
TMSO
时 间 -->
丰度
扫描 1778 (14.209 分): ZJF-20141027-TMS-吲哚.D\data.ms
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
179.1
73.1
355.2
217.1
117.1
143.0
51.1
265.1
293.1
322.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
S
N
TMSO
m/z-->

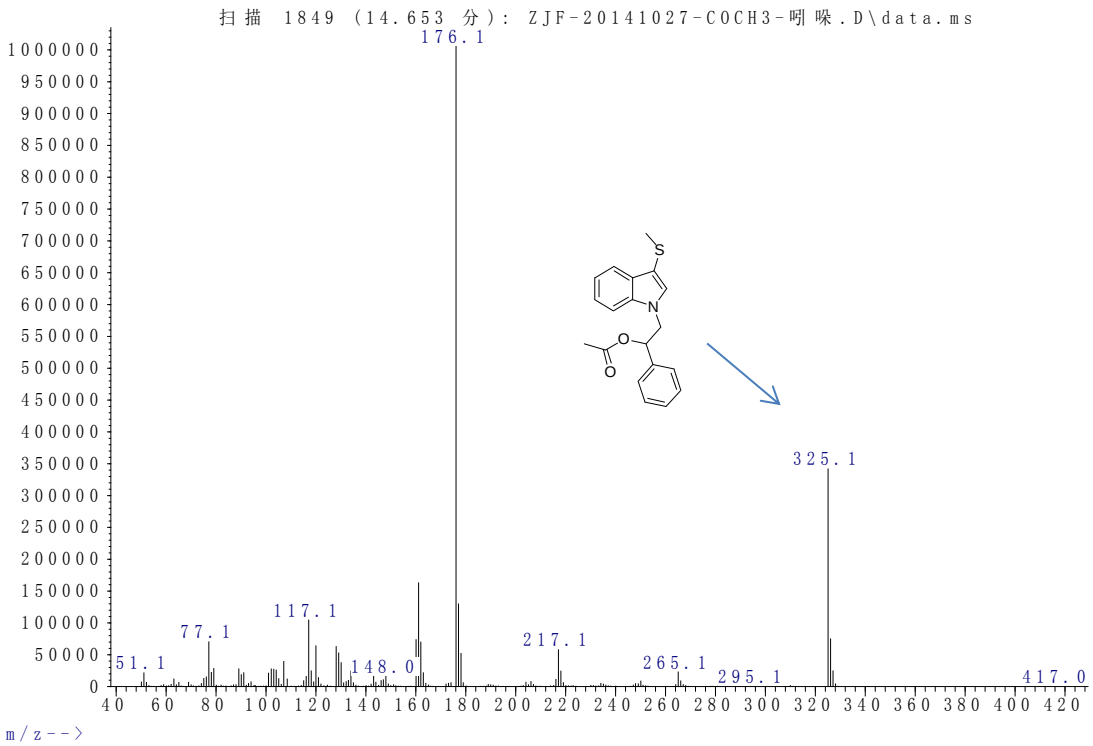

丰 度
TIC: ZJF-20141027-TMS-50CH3.D\data.ms
380000
360000
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
8.00
9.00
10.00
11.00
12.00
13.00
14.00
15.00
O
S
N
TMSO
时 间 -->
丰 度
扫 描 1923 (15.116 分): ZJF-20141027-TMS-50CH3.D\data.ms
38000
36000
34000
32000
30000
28000
26000
24000
22000
20000
18000
16000
14000
12000
10000
8000
6000
4000
2000
0
206.1
179.1
73.1
385.2
116.0
150.0
247.1
281.1
323.1
355.1
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
380
O
S
N
TMSO
m/z -->

丰度

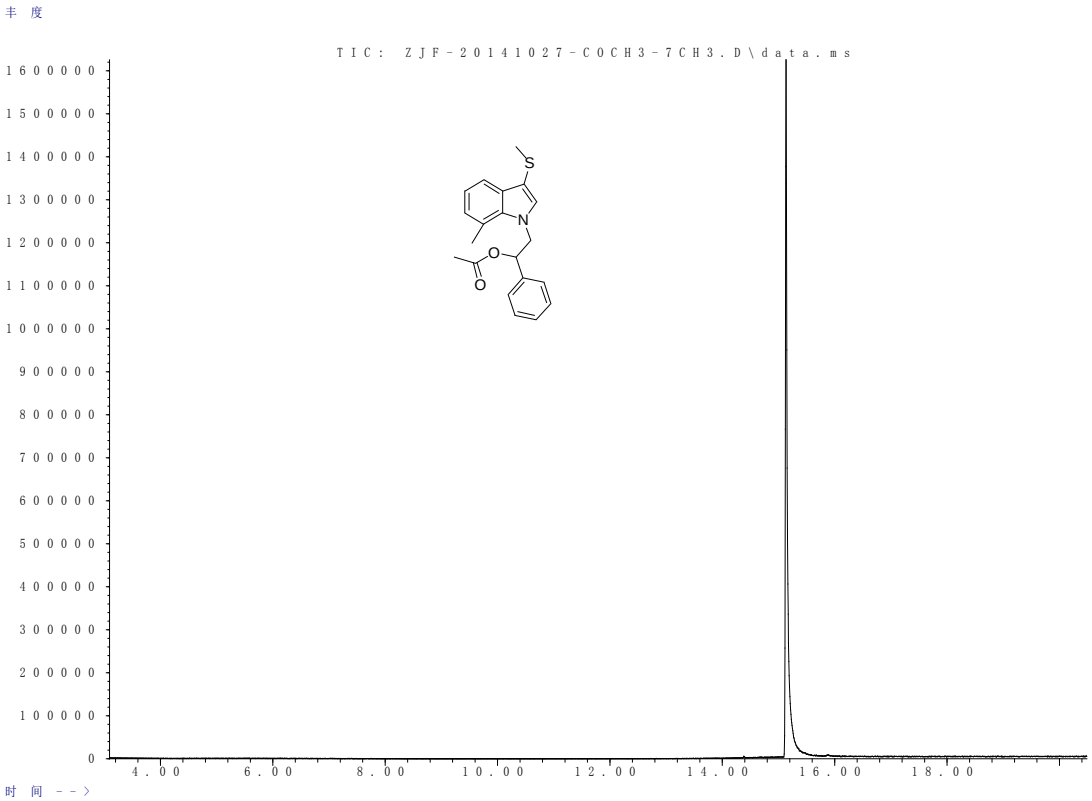

TIC: ZJF-20141027-COCH3-吲哚.D\data.ms
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
13.50 14.00 14.50 15.00 15.50 16.00 16.50 17.00 17.50 18.00 18.50 19.00 19.50
S
N
O
O

时间-->

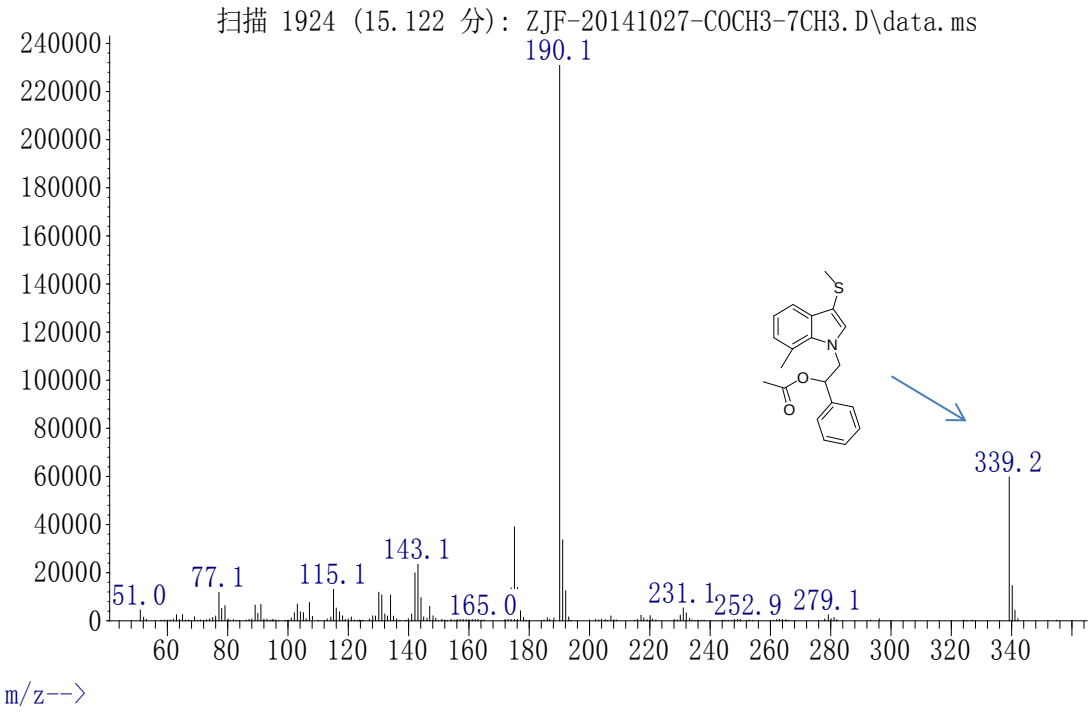
丰 度

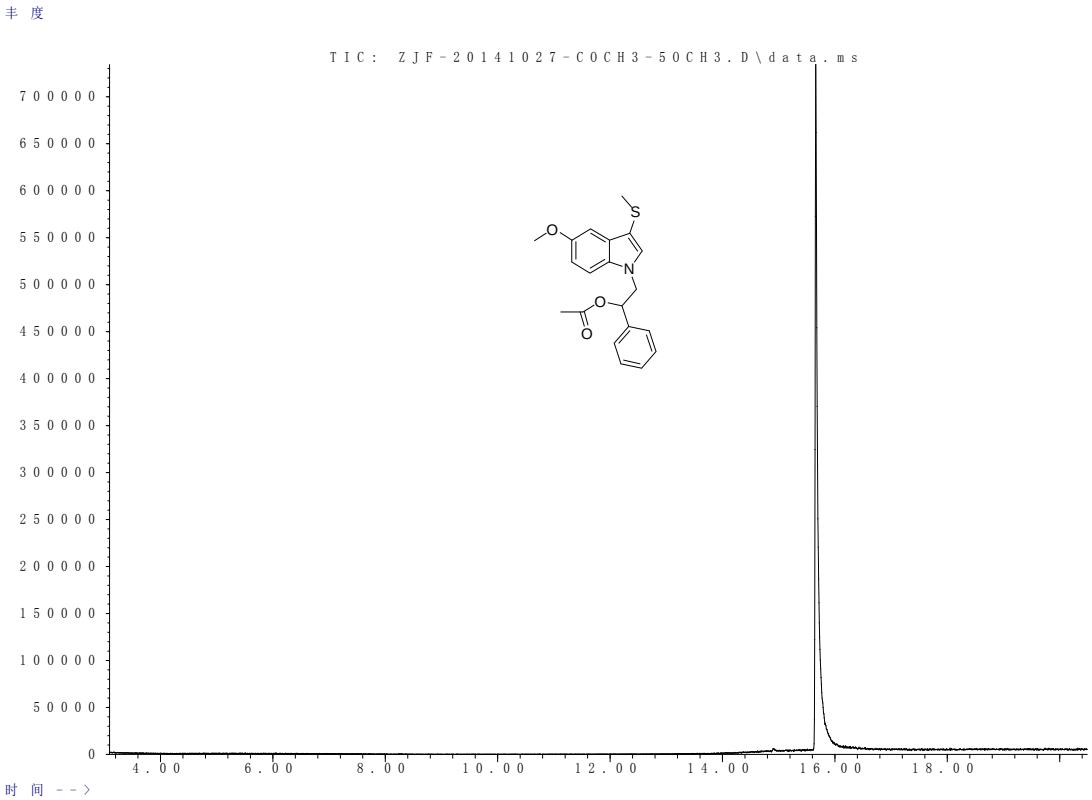

扫 描 1849 (14.653 分): ZJF-20141027-COCH3-吲 哚 .D\data.ms
176.1
325.1
117.1
77.1
217.1
51.1
148.0
265.1
295.1
417.0
1000000
950000
900000
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420
S
N
O
O

m/z-->

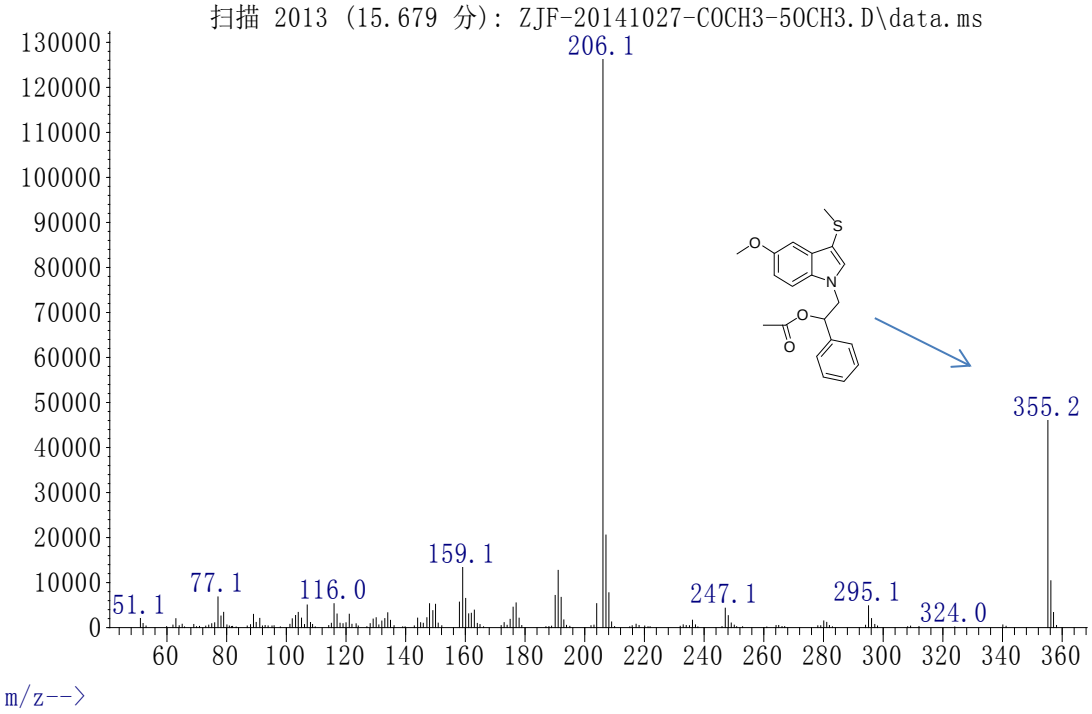

丰 度
TIC: ZJF-20141027-COCH3-7CH3.D\data.ms
16000000
15000000
14000000
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
S
N
O
O

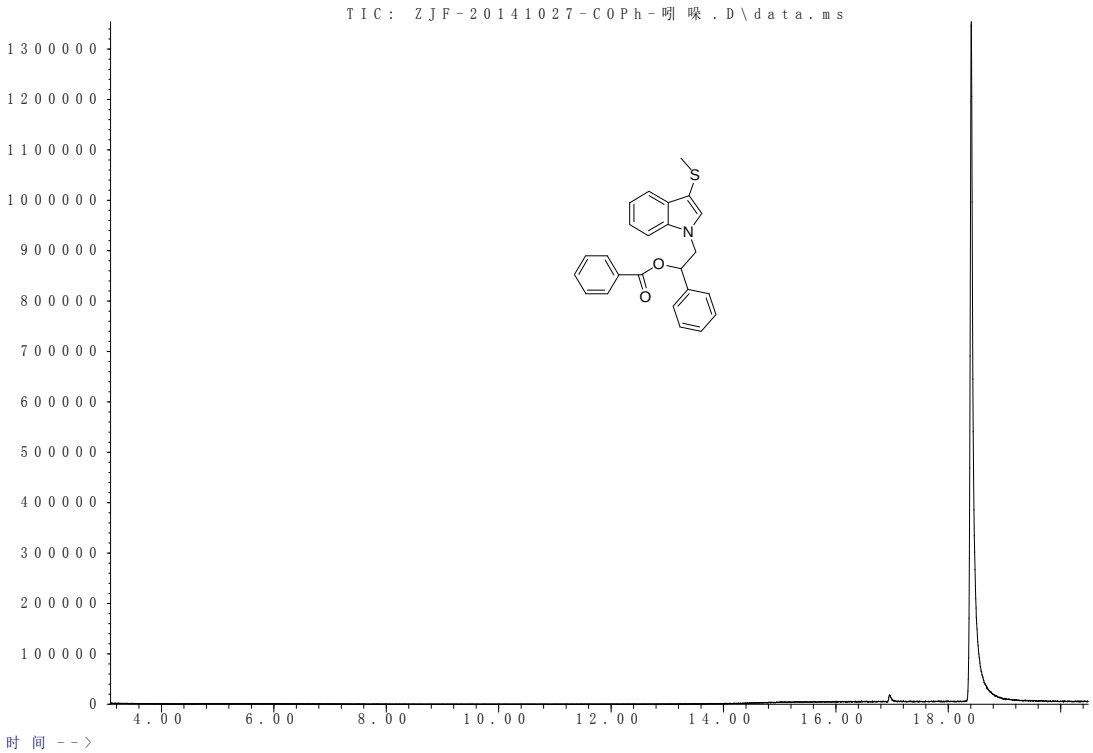
丰度

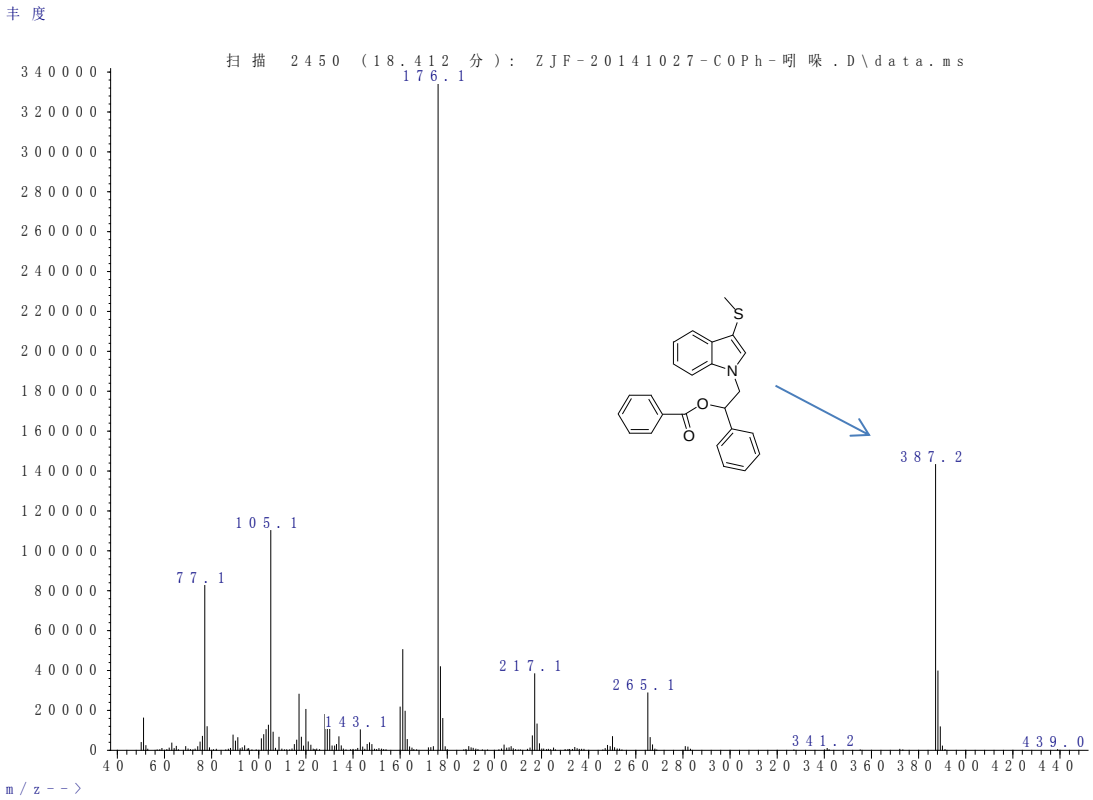

扫描 1924 (15.122 分): ZJF-20141027-COCH3-7CH3.D\data.ms
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
190.1
339.2
143.1
77.1
115.1
51.0
165.0
231.1
252.9
279.1
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
m/z-->
S
N
O
O

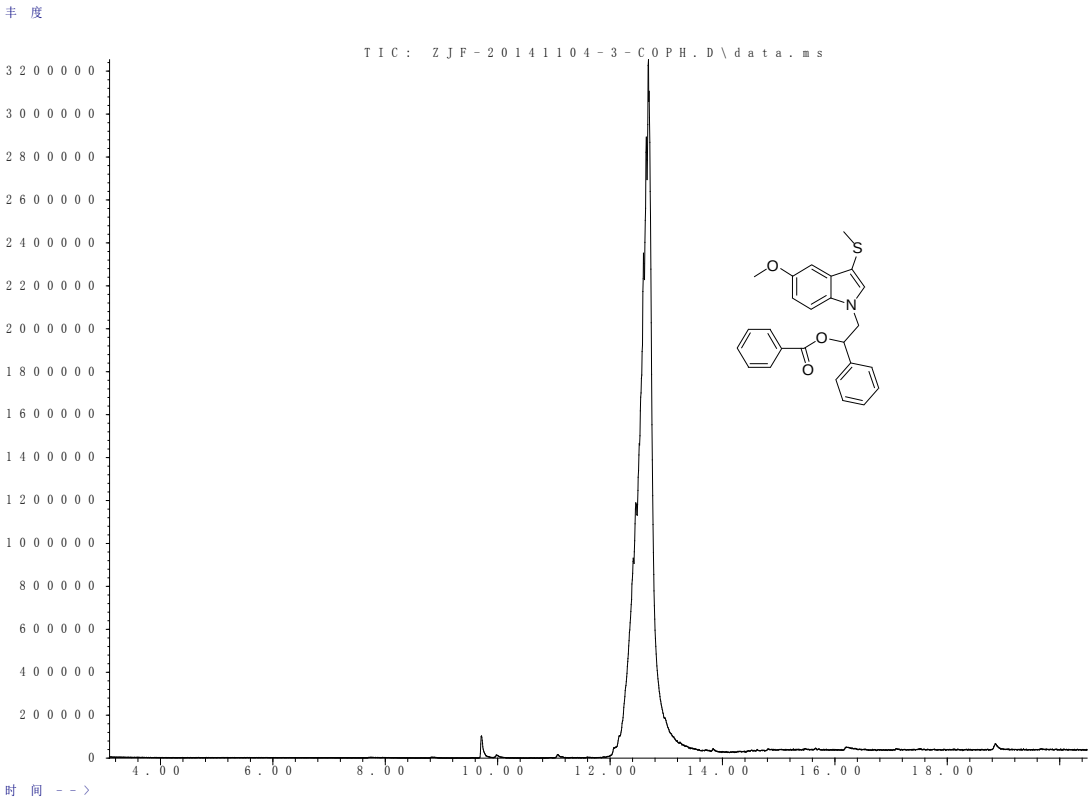

丰 度
TIC: ZJF-20141027-COCH3-5OCH3.D\data.ms
7000000
6500000
6000000
5500000
5000000
4500000
4000000
3500000
3000000
2500000
2000000
1500000
1000000
500000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
O
S
N
O
O

丰度

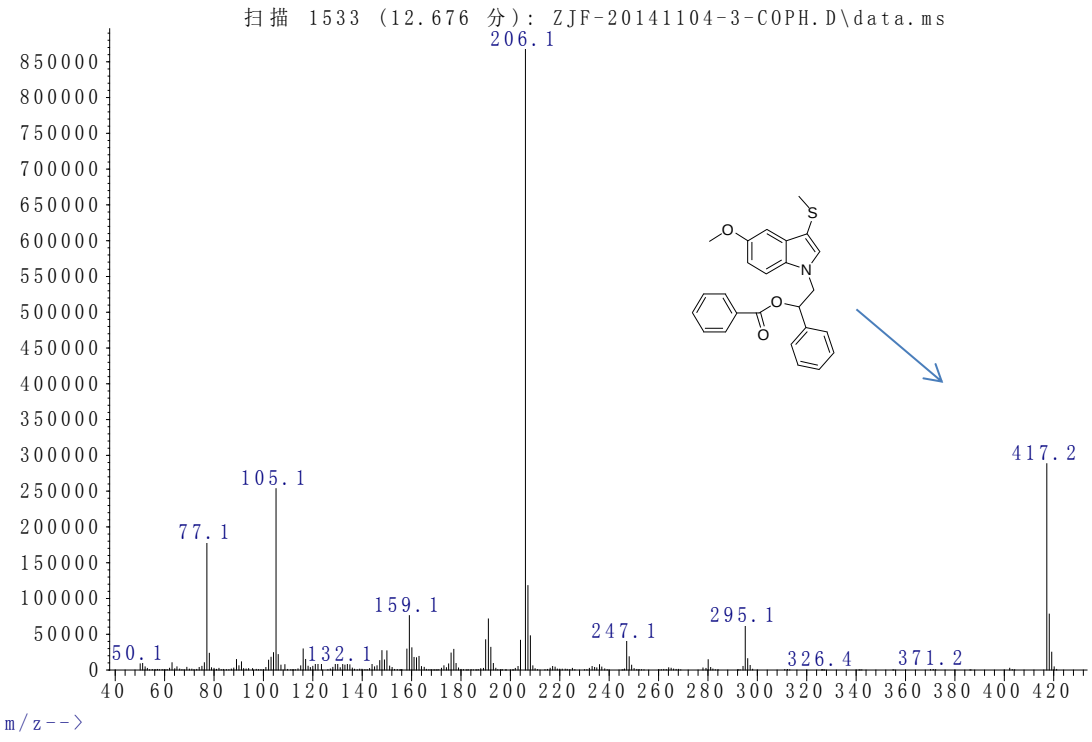

扫描 2013 (15.679 分): ZJF-20141027-COCH3-5OCH3.D\data.ms
206.1
355.2
159.1
77.1
116.0
51.1
247.1
295.1
324.0
130000
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340
360
m/z-->
O
S
N
O
O


丰 度
TIC: ZJF-20141027-COPh-吲 哚 .D\data.ms
13000000
12000000
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
S
N
O
O

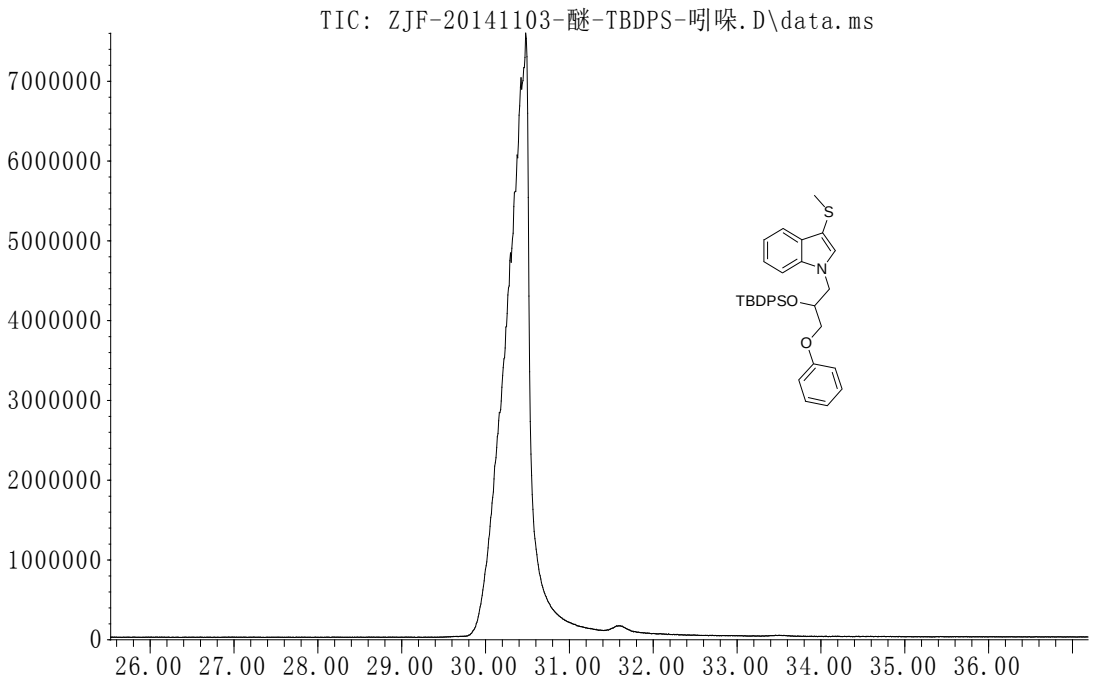

丰 度
扫 描 2450 (18.412 分): ZJF-20141027-COPh-吲 哚 .D\data.ms
340000
320000
300000
280000
260000
240000
220000
200000
180000
160000
140000
120000
100000
80000
60000
40000
20000
0
176.1
105.1
77.1
143.1
217.1
265.1
341.2
387.2
439.0
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440
m/z -->
S
N
O
O


丰 度
TIC: ZJF-20141104-3-COPH.D\data.ms
32000000
30000000
28000000
26000000
24000000
22000000
20000000
18000000
16000000
14000000
12000000
10000000
8000000
6000000
4000000
2000000
0
4.00
6.00
8.00
10.00
12.00
14.00
16.00
18.00
时 间 -->
O
S
N
O
O

丰度

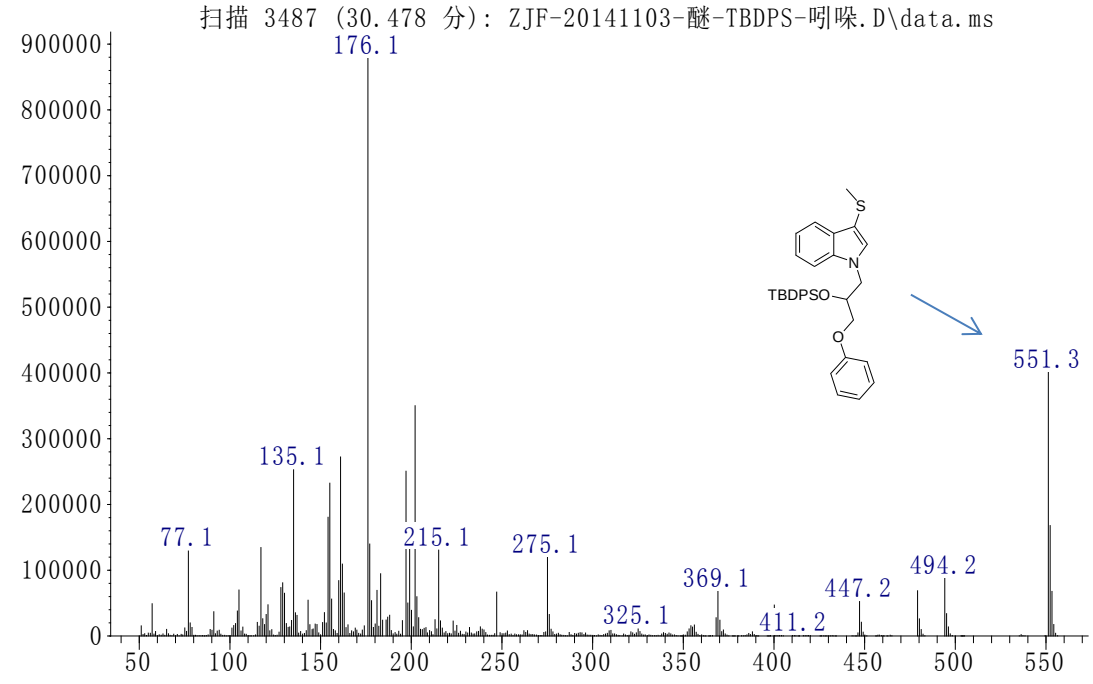

扫描 1533 (12.676 分): ZJF-20141104-3-COPH.D\data.ms
206.1
850000
800000
750000
700000
650000
600000
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
105.1
77.1
159.1
247.1
295.1
417.2
50.1
132.1
326.4
371.2
40 60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420
m/z-->
O
S
N
O
O

丰度


TIC: ZJF-20141103-醚-TBDPS-吲哚.D\data.ms
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
26.00 27.00 28.00 29.00 30.00 31.00 32.00 33.00 34.00 35.00 36.00
S
N
TBDPSO
O

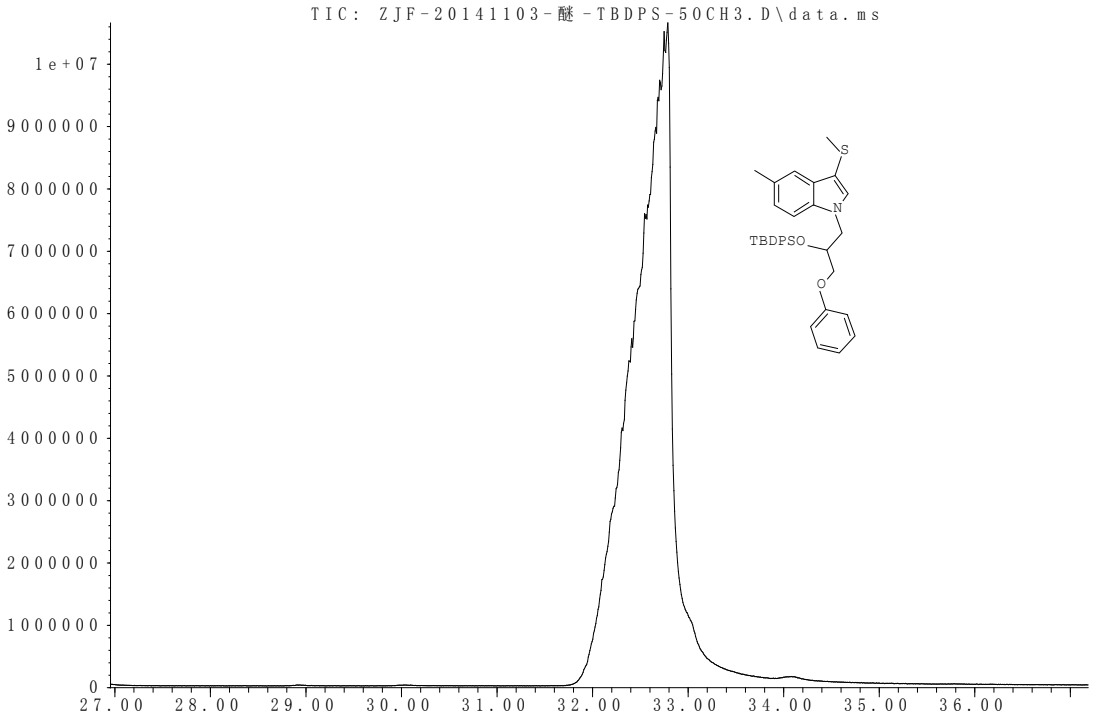
时间-->

丰度


扫描 3487 (30.478 分): ZJF-20141103-醚-TBDPS-吲哚.D\data.ms
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
176.1
135.1
77.1
215.1
275.1
325.1
369.1
411.2
447.2
494.2
551.3
50 100 150 200 250 300 350 400 450 500 550
S
N
TBDPSO
O

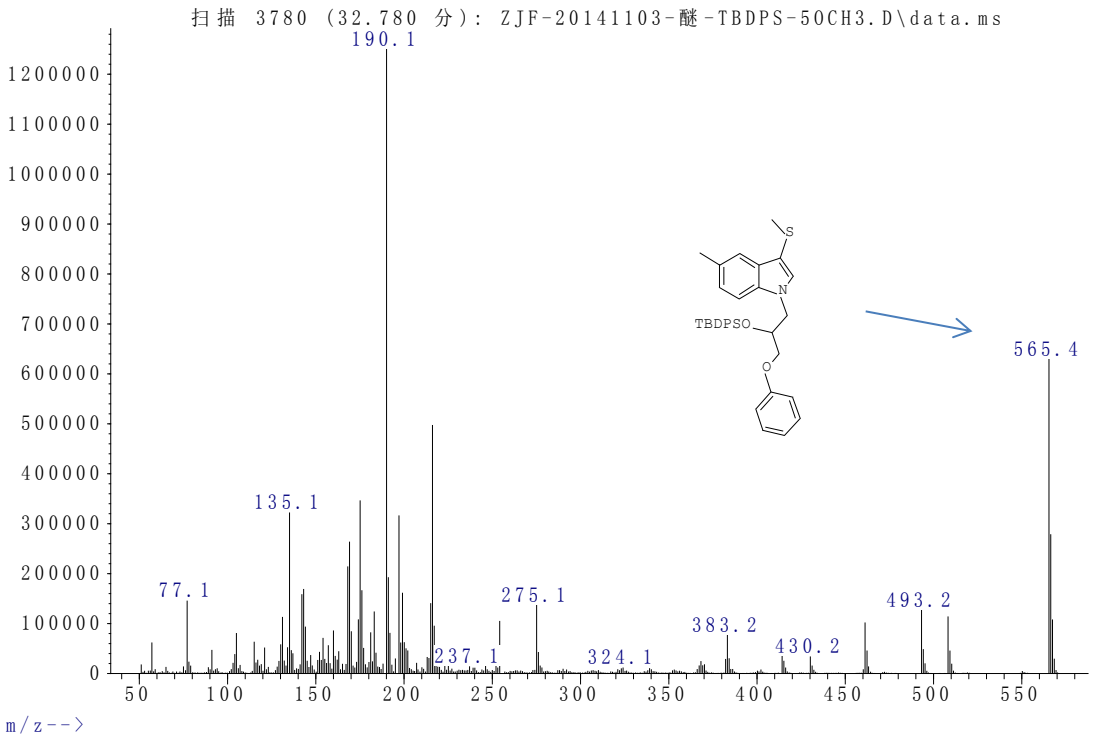
m/z-->

丰 度


TIC: ZJF-20141103-醚-TBDPS-5OCH3.D\data.ms
1e+07
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
27.00
28.00
29.00
30.00
31.00
32.00
33.00
34.00
35.00
36.00
S
N
TBDPSO
O

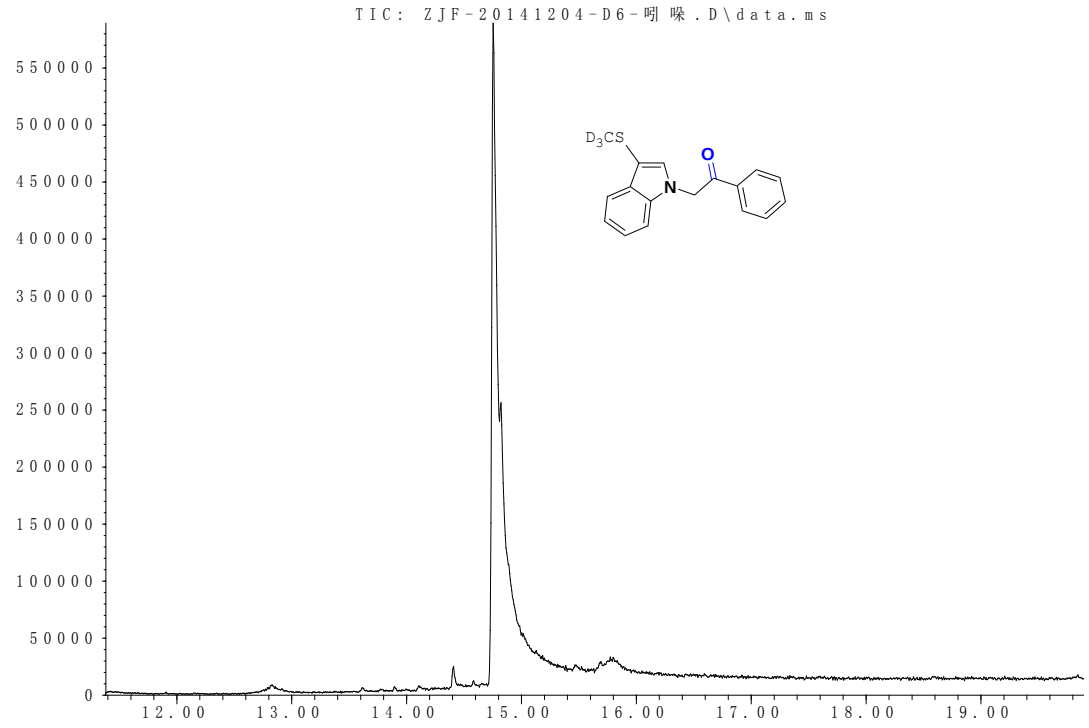
时 间 -->

丰 度

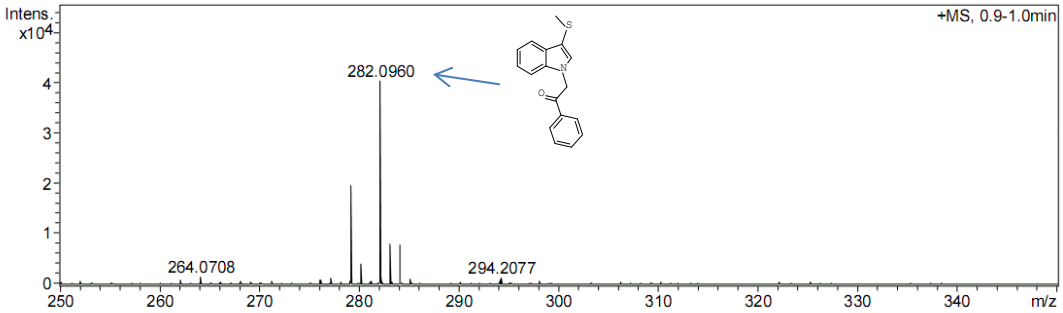

扫描 3780 (32.780 分): ZJF-20141103-醚-TBDPS-5OCH3.D\data.ms
190.1
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
0
135.1
77.1
275.1
237.1
324.1
383.2
430.2
493.2
565.4
50
100
150
200
250
300
350
400
450
500
550
S
N
TBDPSO
O

m/z-->

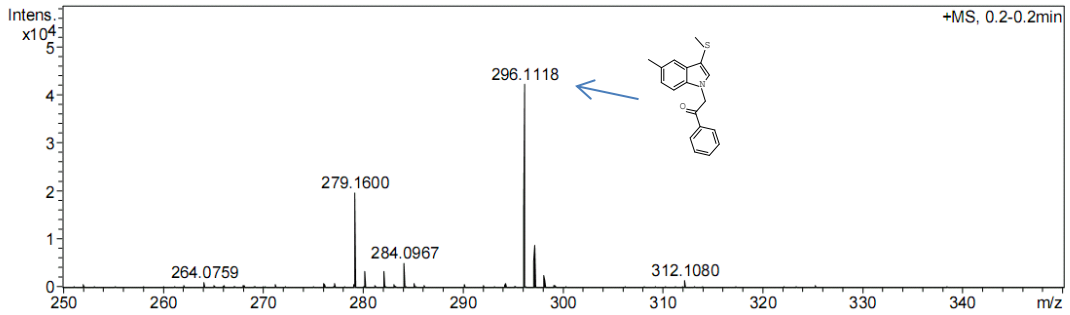
丰 度


TIC: ZJF-20141204-D6-吲 哚 .D\data.ms
D3CS
O
N
550000
500000
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
12.00
13.00
14.00
15.00
16.00
17.00
18.00
19.00
时 间 -->
丰度
扫描 1864 (14.747 分): ZJF-20141204-D6-吲哚.D\data.ms
179.1
284.1
77.1
105.0
161.0
51.0
128.0
207.0
236.0
266.1
120000
110000
100000
90000
80000
70000
60000
50000
40000
30000
20000
10000
0
60
80
100
120
140
160
180
200
220
240
260
280
300
m/z-->

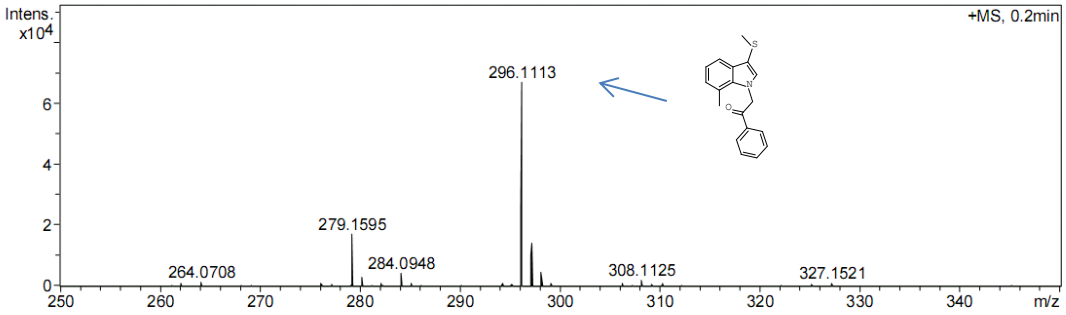
6. MALDI-TOF analysis of 3-sulfenylindole products



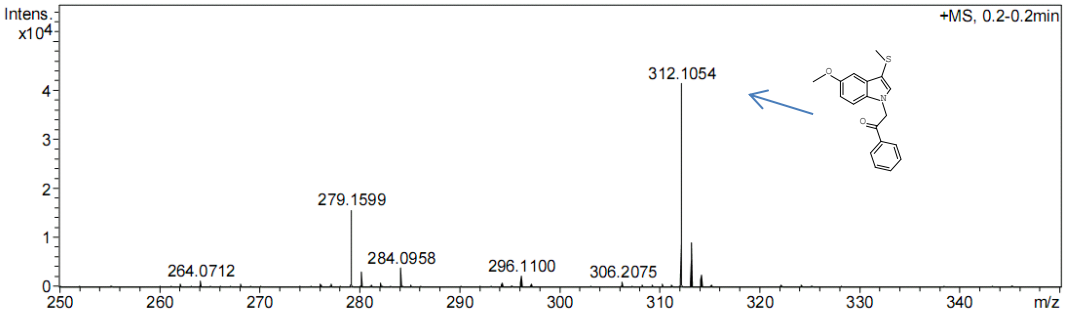
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
282.0960	1	C 17 H 16 N O S	100.00	282.0947	-1.3	-4.4	65.4	10.5	even	ok



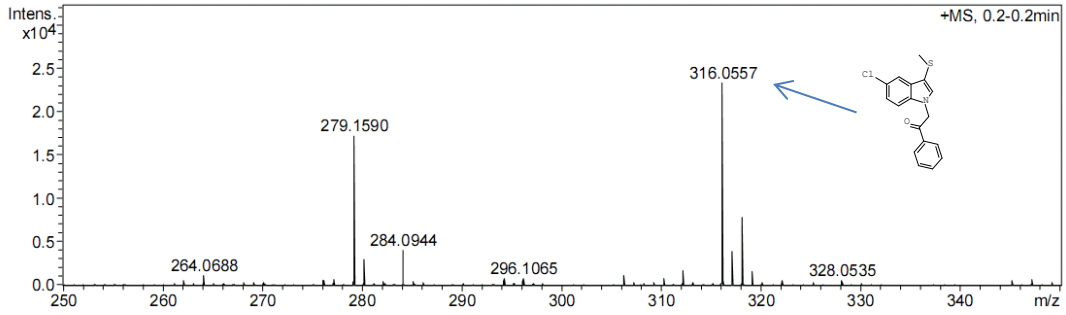
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
296.1118	1	C 18 H 18 N O S	100.00	296.1104	-1.4	-4.8	2.8	10.5	even	ok
	2	C 15 H 22 N O S 2	44.34	296.1137	1.9	6.5	26.1	5.5	even	ok



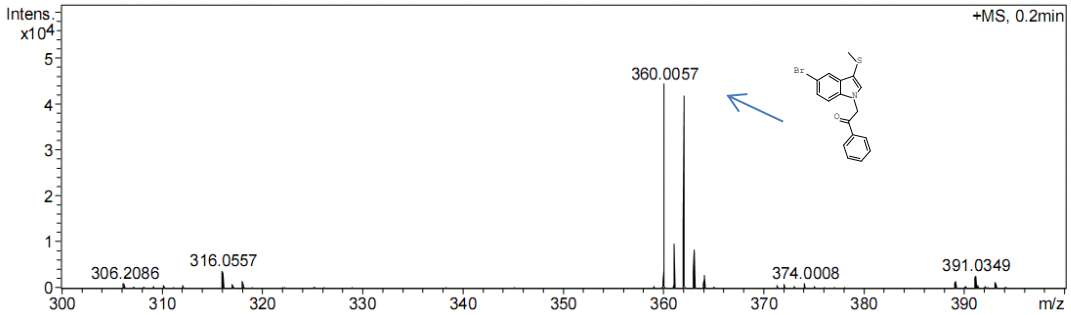
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
296.1113	1	C 18 H 18 N O S	100.00	296.1104	-0.9	-3.1	4.5	10.5	even	ok



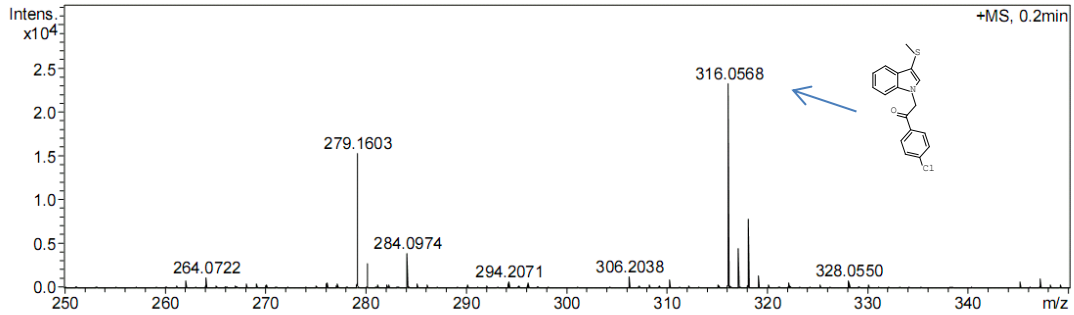
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
312.1054	1	C 18 H 18 N O 2 S	100.00	312.1053	-0.1	-0.4	7.6	10.5	even	ok



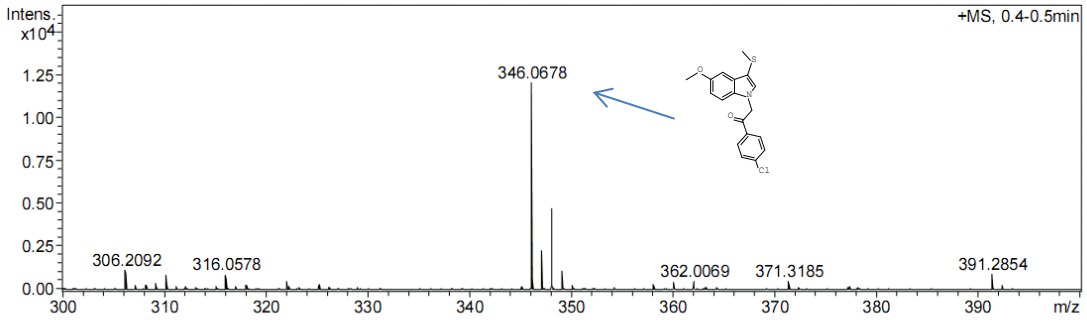
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
316.0557	1	C 17 H 15 Cl N O S	100.00	316.0557	0.1	0.3	25.0	10.5	even	ok
	2	C 11 H 21 Cl O 4 S 2	42.73	316.0564	0.8	2.5	45.3	1.0	odd	ok
	3	C 9 H 19 Cl N 3 O 3 S 2	46.67	316.0551	-0.6	-1.8	46.0	1.5	even	ok



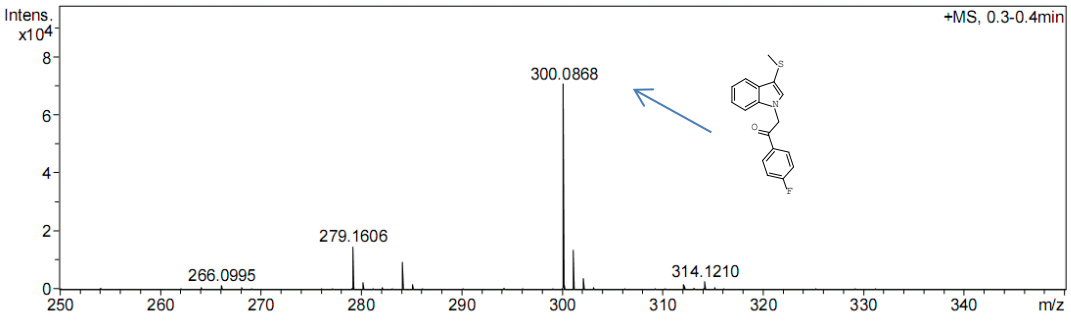
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
360.0057	1	C 17 H 15 Br N O S	100.00	360.0052	-0.5	-1.3	31.0	10.5	even	ok



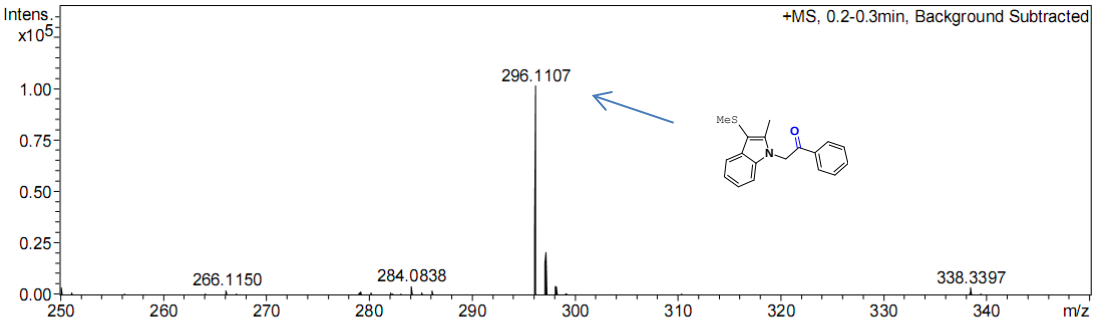
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
316.0568	1	C 17 H 15 Cl N O S	100.00	316.0557	-1.1	-3.4	21.4	10.5	even	ok



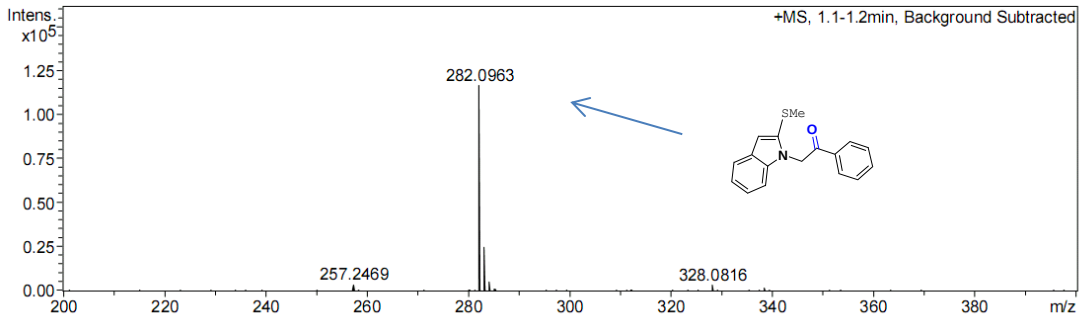
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
346.0678	1	C 18 H 17 Cl N O 2 S	93.52	346.0663	-1.5	-4.5	9.7	10.5	even	ok



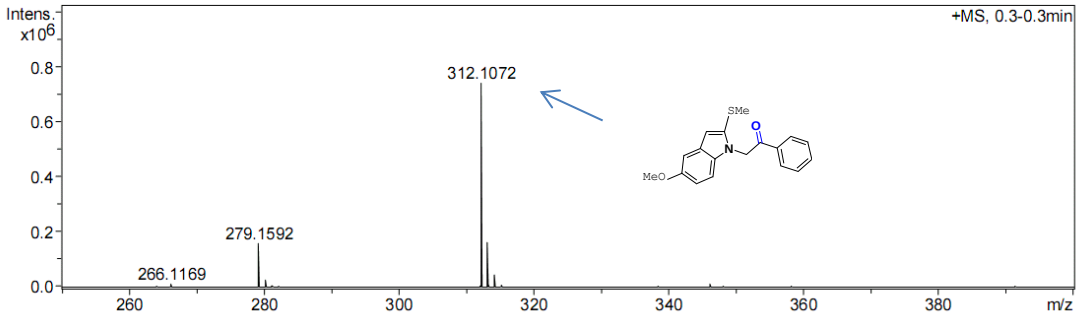
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
300.0868	1	C 17 H 15 F N O S	100.00	300.0853	-1.5	-5.0	4.0	10.5	even	ok
	2	C 14 H 19 F N O S 2	48.00	300.0887	1.9	6.3	27.0	5.5	even	ok



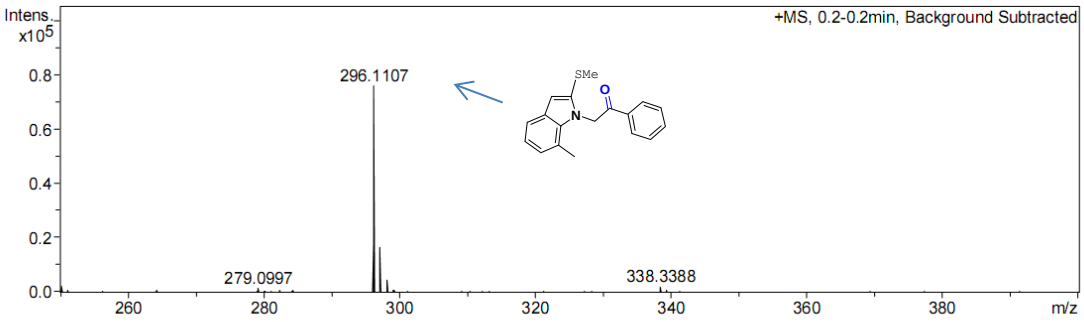
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
296.1107	1	C 18 H 18 N O S	100.00	296.1104	-0.4	-1.3	11.2	10.5	even	ok



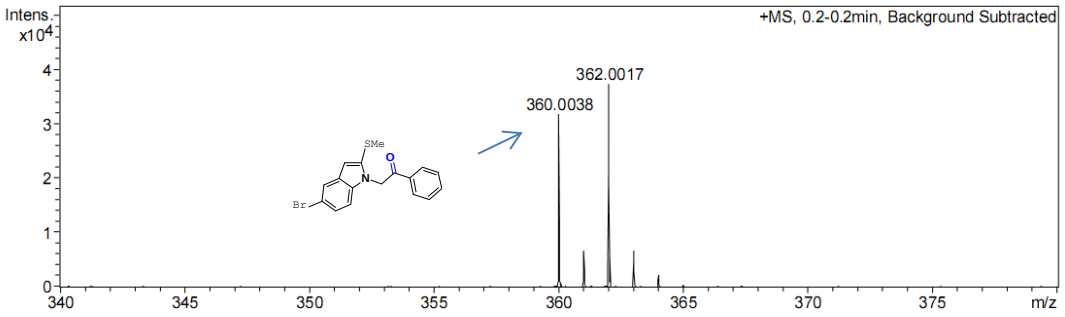
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
282.0963	1	C 17 H 16 N O S	100.00	282.0947	-1.6	-5.7	12.0	10.5	even	ok
	2	C 14 H 20 N O S 2	52.68	282.0981	1.8	6.3	35.6	5.5	even	ok



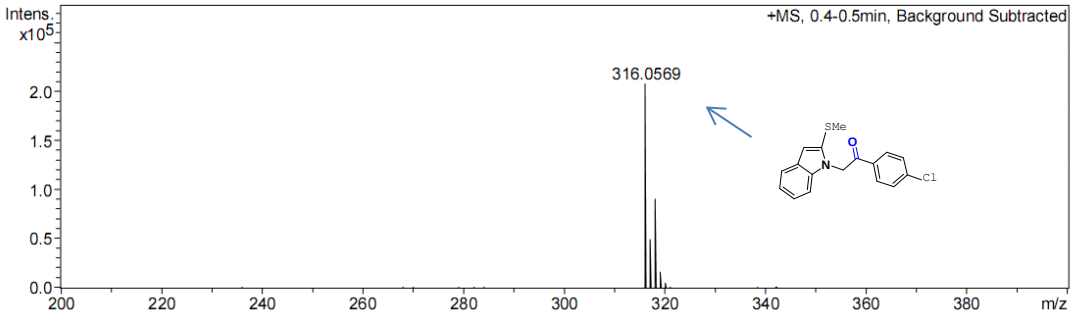
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
312.1072	1	C 18 H 18 N O 2 S	100.00	312.1053	-1.9	-6.1	7.0	10.5	even	ok
	2	C 15 H 22 N O 2 S 2	83.77	312.1086	1.5	4.7	30.1	5.5	even	ok



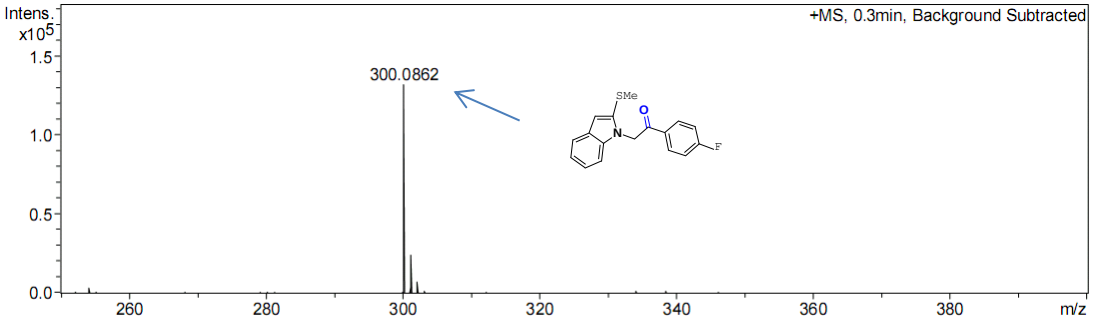
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
296.1107	1	C 18 H 18 N O S	100.00	296.1104	-0.3	-1.1	7.8	10.5	even	ok



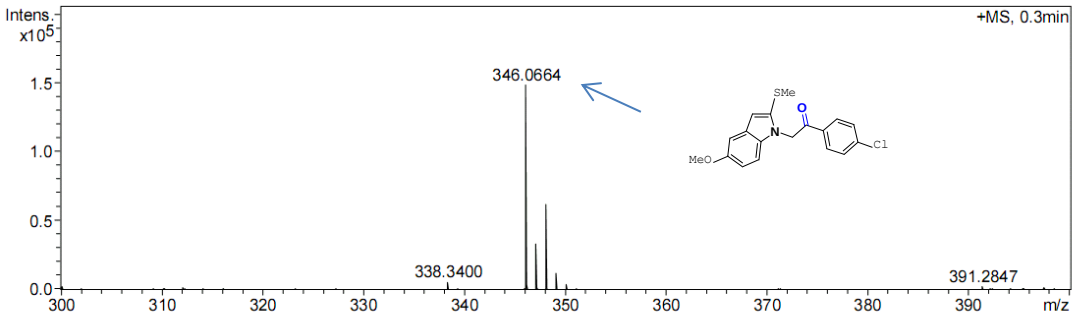
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
360.0038	1	C 17 H 15 Br N O S	100.00	360.0052	1.5	4.0	48.0	10.5	even	ok
362.0017	1	C 17 H 15 Br N O S	100.00	360.0052	1.5	4.0	48.0	10.5	even	ok



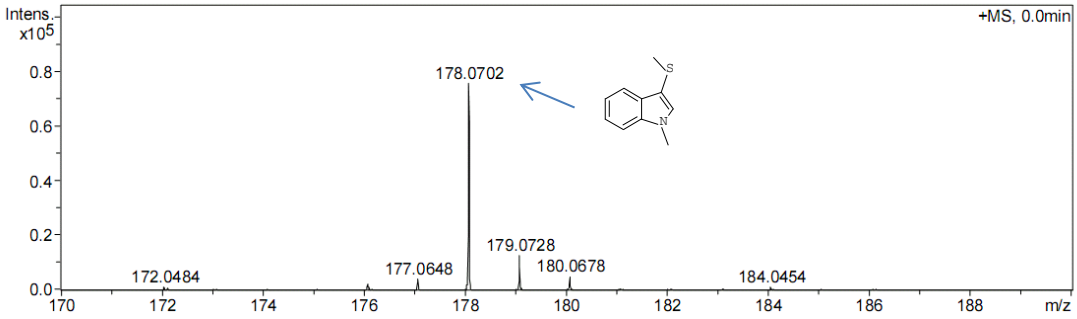
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
316.0569	1	C 17 H 15 Cl N O S	100.00	316.0557	-1.2	-3.8	29.8	10.5	even	ok



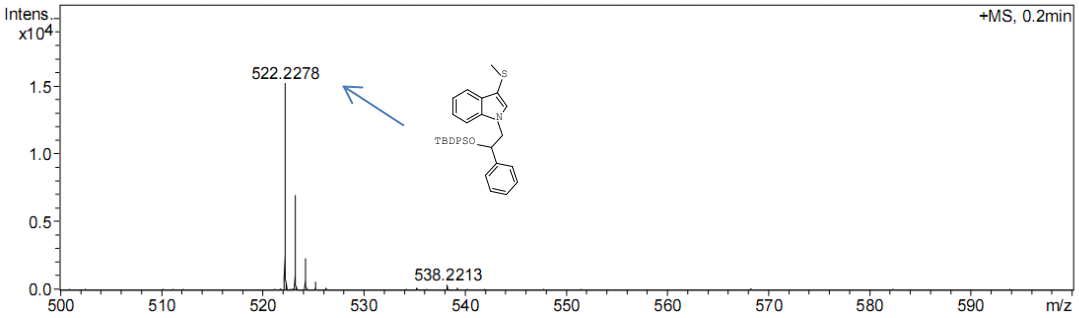
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
300.0862	1	C 17 H 15 F N O S	74.63	300.0853	-0.9	-3.1	7.3	10.5	even	ok
	2	C 14 H 16 F 2 N O 2 S	100.00	300.0864	0.2	0.7	11.2	6.5	even	ok



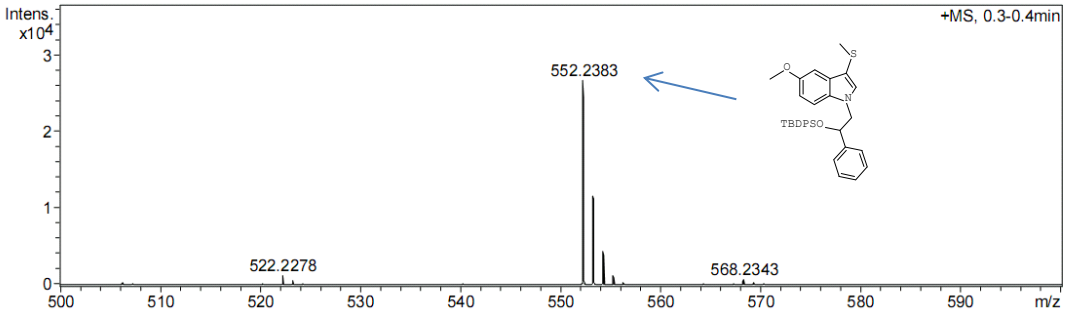
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
346.0664	1	C 18 H 17 Cl N O 2 S	100.00	346.0663	-0.1	-0.4	14.6	10.5	even	ok



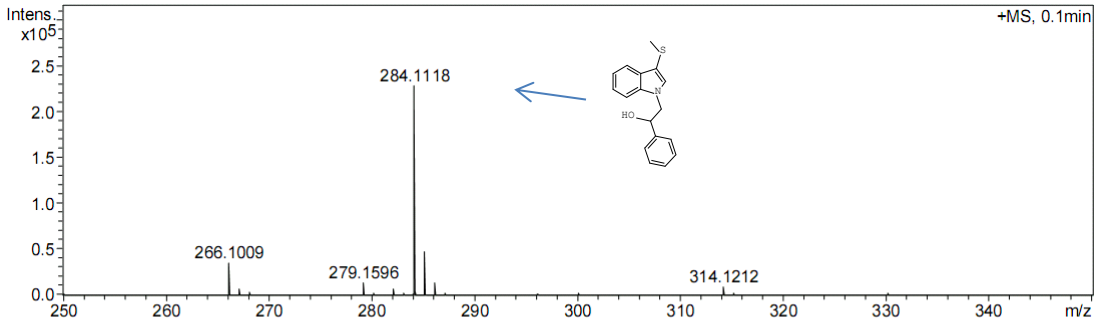
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
178.0702	1	C 10 H 12 N S	100.00	178.0685	-1.7	-9.6	26.9	5.5	even	ok
	2	C 7 H 16 N S 2	74.16	178.0719	1.7	9.3	40.2	0.5	even	ok



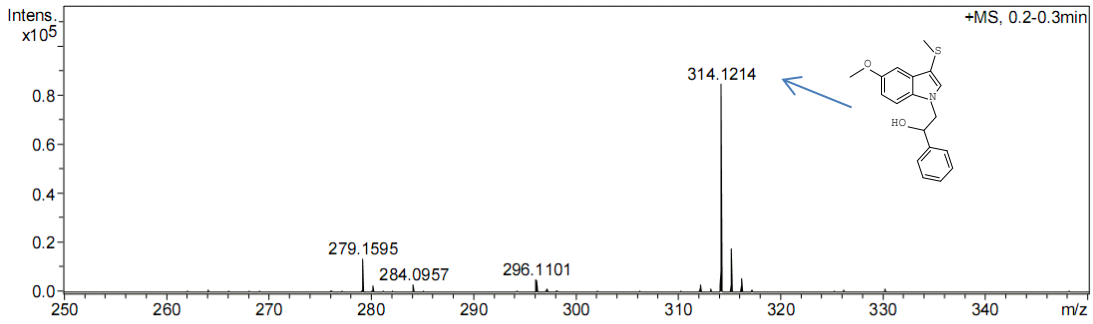
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
522.2278	1	C 33 H 36 N O S Si	100.00	522.2281	0.3	0.6	19.2	17.5	even	ok
	2	C 30 H 38 O 4 S Si	18.34	522.2255	-2.4	-4.5	36.3	13.0	odd	ok



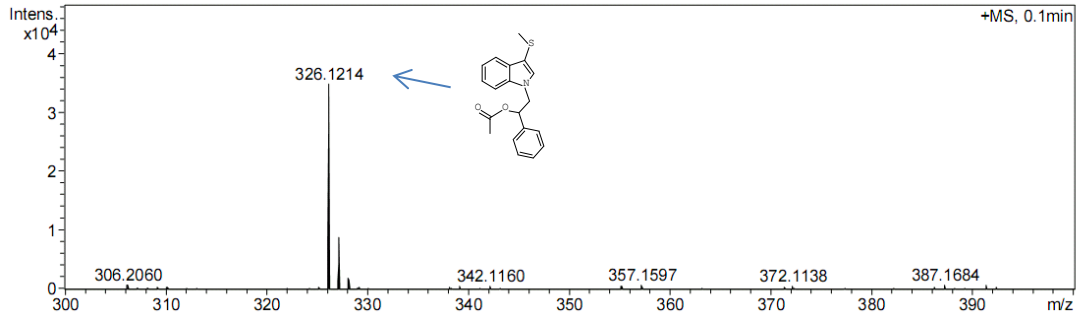
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
552.2383	1	C 34 H 38 N O 2 S Si	100.00	552.2387	0.4	0.7	4.7	17.5	even	ok
	2	C 32 H 36 N 4 O S Si	73.20	552.2374	-1.0	-1.8	5.1	18.0	odd	ok



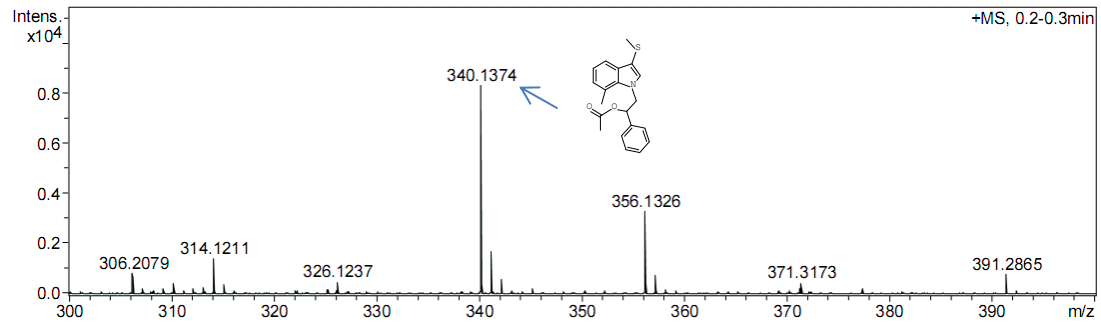
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
284.1118	1	C 17 H 18 N O S	100.00	284.1104	-1.4	-5.0	6.1	9.5	even	ok
	2	C 15 H 16 N 4 S	31.91	284.1090	-2.8	-9.8	11.0	10.0	odd	ok
	3	C 14 H 22 N O S 2	43.55	284.1137	1.9	6.8	28.9	4.5	even	ok



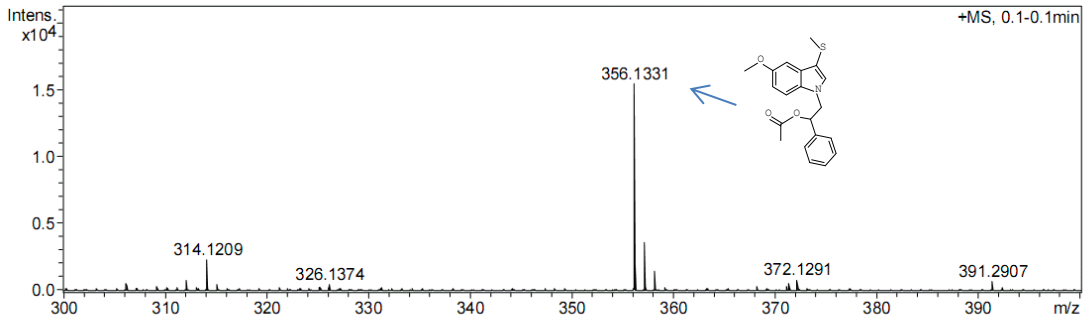
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
314.1214	1	C 18 H 20 N O 2 S	100.00	314.1209	-0.5	-1.5	3.5	9.5	even	ok



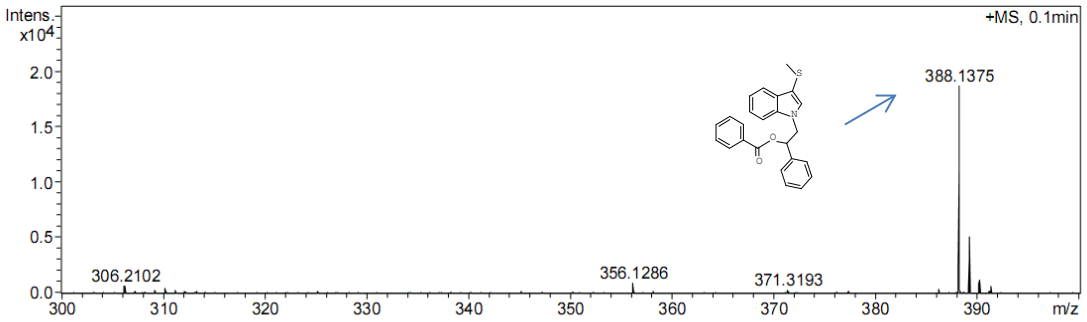
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
326.1214	1	C 19 H 20 N O 2 S	100.00	326.1209	-0.5	-1.5	19.7	10.5	even	ok



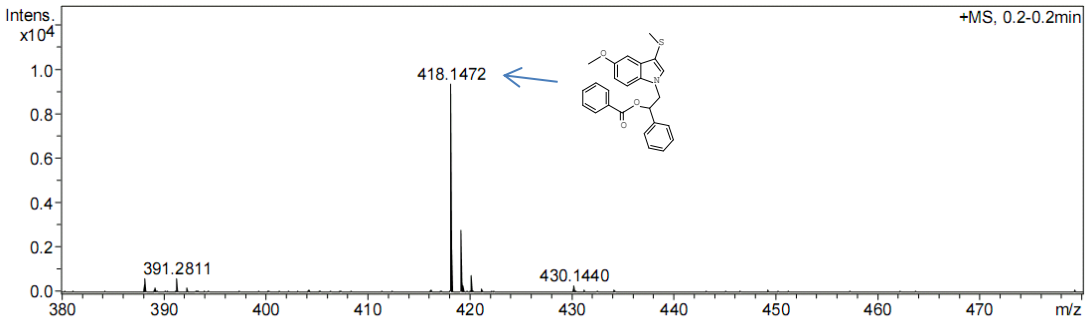
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
340.1374	1	C 20 H 22 N O 2 S	100.00	340.1366	-0.8	-2.3	11.2	10.5	even	ok



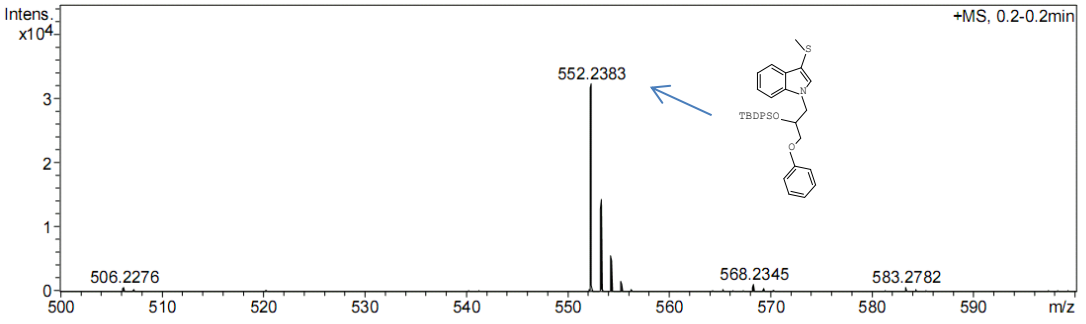
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
356.1331	1	C 20 H 22 N O 3 S	100.00	356.1315	-1.6	-4.6	9.4	10.5	even	ok
	2	C 17 H 26 N O 3 S 2	76.92	356.1349	1.7	4.9	18.2	5.5	even	ok



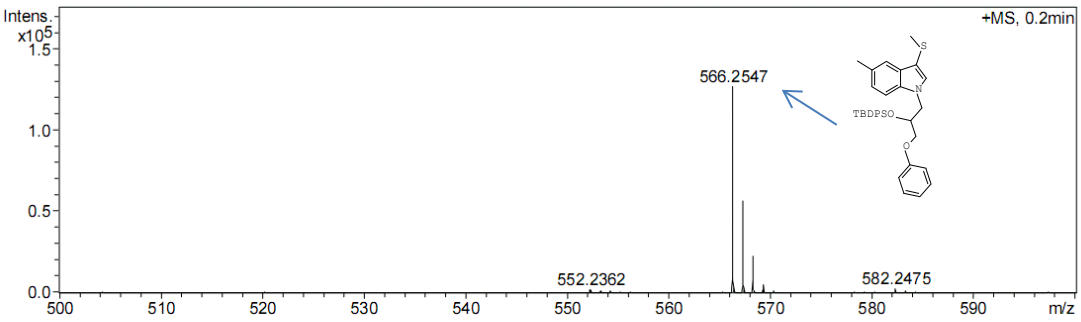
Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
388.1375	1	C 24 H 22 N O 2 S	100.00	388.1366	-1.0	-2.5	10.1	14.5	even	ok
	2	C 19 H 24 N 4 O S 2	58.01	388.1386	1.1	2.7	32.4	10.0	odd	ok



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
418.1472	1	C 25 H 24 N O 3 S	100.00	418.1471	-0.1	-0.2	7.8	14.5	even	ok
	2	C 23 H 22 N 4 O 2 S	45.23	418.1458	-1.4	-3.5	12.1	15.0	odd	ok
	3	C 20 H 34 O S 4	11.51	418.1487	1.5	3.5	63.0	4.0	odd	ok



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
552.2383	1	C 34 H 38 N O 2 S Si	100.00	552.2387	0.4	0.7	5.4	17.5	even	ok



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e¯ Conf	N-Rule
566.2547	1	C 35 H 40 N O 2 S Si	100.00	566.2544	-0.4	-0.6	3.2	17.5	even	ok
	2	C 33 H 38 N 4 O S Si	42.45	566.2530	-1.7	-3.0	7.9	18.0	odd	ok