

Supporting information for

**Potassium Iodide Catalyzed Simultaneous C3-Formylation and N-Aminomethylation of
Indoles with 4-Substituted-N, N-dimethylanilines**

Lan-Tao Li, Hong-Ying Li, Li-Juan Xing, Li-Juan Wen, Peng Wang*, and Bin Wang*^[a]

State Key Laboratory of Medicinal Chemical Biology, College of Pharmacy, Nankai University, 94 Weijin Road, Tianjin 300071, China; Fax: (+86)-22-23507760; Tel: (+86)-22-23506290; E-mail: wangbin@nankai.edu.cn, pwang@nankai.edu.cn

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General remarks

^1H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE AV400 (400MHz for H and 100MHz for C). Signal positions were recorded in ppm with the abbreviations s, d, t, and m denoting singlet, doublet, triplet, and multiplet respectively. NMR spectra were recorded in $(\text{CD}_3)_2\text{SO}$, and chemical shifts were referenced to residual $(\text{CD}_2\text{H})\text{SO}(\text{CD}_3)$ at 2.50 ppm for ^1H or 39.52 ppm for ^{13}C unless otherwise noted. NMR spectra recorded in CDCl_3 were referenced to residual CHCl_3 at 7.26 ppm for ^1H or 77.0 ppm for ^{13}C . NMR spectra recorded in CD_3OD were referenced to residual CH_3OH at 3.34 ppm for ^1H or 49.86 ppm for ^{13}C . All coupling constants J were quoted in Hz. Data were reported as follows: chemical shift, multiplicity, coupling constant and integration. High resolution mass spectrometry was conducted using a Varian 7.0 T FTICR-MS by ESI or MALDI technique unless otherwise noted. Reactions were monitored by thin-layer chromatography (TLC) on 0.25mm silica gel glass plates coated with 60 F_{254} . Column chromatography was performed on silica gel (200-300 mesh) using a mixture of petroleum ether (60-90°C)/ethyl acetate as eluant. Commercially available indoles, 4-methyl-N, N-dimethylaniline, and 4-bromo-N, N-dimethylaniline and were used as received without further purification, and other 4-substituted-N, N-dimethylanilines were prepared according to reported method.^[1]

Representative Procedure

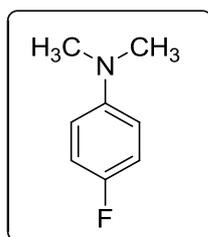
Preparation of 4-substituted N, N-dimethylanilines

To trimethylphosphate (2.1 g, 15 mmol) was added aniline (10 mmol). The mixture was stirred at 110 °C for 2 h and then cooled to room temperature, neutralized with aqueous NaOH (6 mL, 20%). After additional stirring at 110 °C for 12 h, the mixture was diluted with water to dissolve Na_3PO_4 . The resulting mixture was extracted with ethyl acetate for three times. The combined organic phase was dried over anhydrous Na_2SO_4 , filtrated, and concentrated under reduced pressure. The residue was purified on a silica gel column to afford N, N-dimethylanilines (petroleum ether /ethyl acetate, 100:1, v/v).

Preparation of indoles derivatives

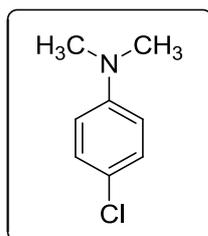
To a mixture of indole (0.50 mmol, 1 equiv), KI (16.6 mg, 0.10 mmol, 0.2 equiv) PivOH (255.3 mg, 2.5 mmol, 5 equiv) in a 50 mL tube were added DMSO (1 mL) under air. Then N, N-dimethylaniline (2.0 mmol, 4 equiv) and TBPB (560 μ L, 3.0 mmol, 6 equiv) were added separately. The mixture was stirred at 60 °C for 16 h, and then quenched with saturated NaHCO₃ solution (10 mL). The mixture was extracted with ethyl acetate for three times. The combined organic phase was washed with brine and dried with anhydrous Na₂SO₄, filtrated, and concentrated under reduced pressure. The residue was purified by silica gel column chromatography (petroleum ether /ethyl acetate, 5:1, v/v) to give the products.

Characterization Data of Compounds



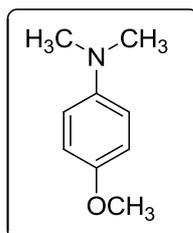
¹H-NMR (CDCl₃, 400 MHz): 6.93-6.99 (m, 2H), 6.68-6.72(m, 2H), 2.91(s, 6H).

¹³C-NMR (CDCl₃, 100 MHz): 155.6 (d, 234Hz), 147.4, 115.3 (d, 22Hz), 113.9 (d, 7.3Hz), 41.4



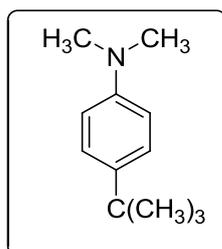
¹H-NMR (CDCl₃, 400 MHz): 7.09 (d, 8.8Hz, 2H), 6.55(d, 8.8Hz, 2H), 2.84(s, 6H).

¹³C-NMR (CDCl₃, 100 MHz): 149.1, 128.8, 121.4, 113.6, 40.6.



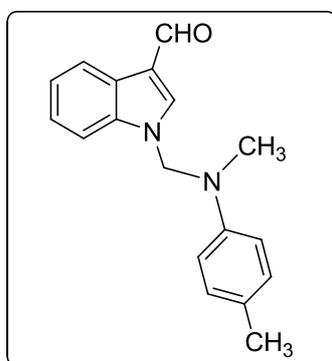
¹H-NMR (CDCl₃, 400 MHz): 6.87 (d, 9.2Hz, 2H), 6.78 (d, 9.2Hz, 2H), 3.77 (s, 3H),

2.88 (s, 6H). $^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz): 151.9, 145.6, 114.8, 114.5, 55.5, 41.7.



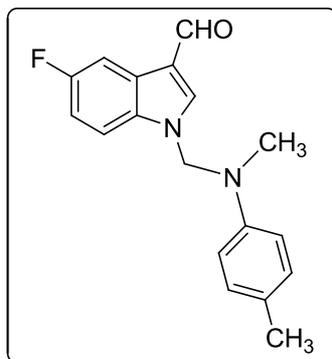
$^1\text{H-NMR}$ (CDCl_3 , 400 MHz): 7.36 (d, 8.8Hz, 2H), 6.80 (d, 9.2Hz, 2H), 2.99 (s, 6H), 1.38 (s, 9H). $^{13}\text{C-NMR}$ (CDCl_3 , 100 MHz): 148.5, 139.3, 125.8, 112.6, 40.8, 33.7, 31.5

3a



$^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 400MHz): 9.88(s, 1H), 8.17(s, 1H), 8.09(dd, 2.2Hz, 6.6Hz, 1H), 7.60-7.58(m, 1H), 7.22-7.28(m, 2H), 7.04(d, 8.4Hz, 2H), 6.87(d, 8.4Hz, 2H), 5.88(s, 2H), 2.99(s, 3H), 2.20(s, 3H), $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 100MHz): 185.03, 145.38, 139.51, 136.79, 129.67, 127.26, 124.77, 123.58, 122.55, 120.94, 117.24, 114.22, 111.62, 64.14, 37.63, 19.98, HRMS (ESI): calculated for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{ONa}$ $[\text{M}+\text{Na}]^+$: 301.1311, found: 301.1308.

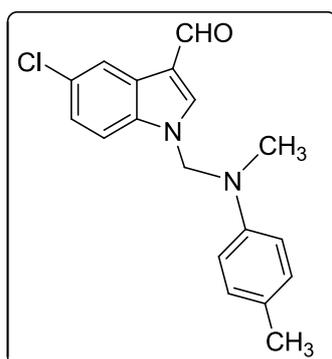
3b



$^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 400MHz): 9.86(s, 1H), 8.24(s, 1H), 7.76(dd, 2.2Hz, 9.4Hz, 1H),

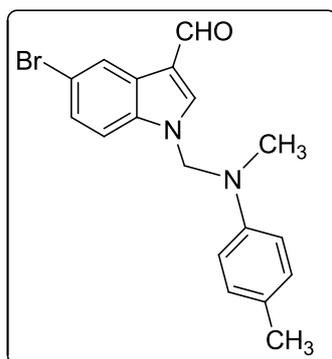
7.61(dd, 4.4Hz, 9.2Hz, 1H), 7.15(td, 2.0Hz, 9.2Hz, 1H), 7.04(d, 8.2Hz, 2H), 6.87(d, 8.2Hz, 2H), 5.89(s, 2H), 2.99(s, 3H), 2.19(s, 3H). ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.10, 158.90(d, 235Hz), 145.29, 140.52, 133.36, 129.72, 127.38, 125.41(d, 11Hz), 117.03(d, 4Hz), 114.25, 113.16(d, 10Hz), 111.70(d, 26Hz), 105.86(d, 24Hz), 64.46, 37.64, 20.01; HRMS (ESI): calculated for: $\text{C}_{18}\text{H}_{17}\text{FN}_2\text{ONa}$, $[\text{M}+\text{Na}]^+$: 319.1217, found: 319.1215

3c



^1H -NMR (DMSO- d_6 , 400MHz): 9.87(s, 1H), 8.24(s, 1H), 8.06(s, 1H), 7.63(d, 8.8Hz, 1H), 7.30(d, 8.8Hz, 1H), 7.04(d, 8.0Hz, 2H), 6.87(d, 8.4Hz, 2H), 5.89(s, 2H), 2.99(s, 3H), 2.19(s, 3H); ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.25, 145.25, 140.37, 135.29, 129.72, 127.45, 127.32, 125.90, 123.57, 119.99, 116.58, 114.31, 113.45, 64.44, 37.67, 20.01; HRMS (ESI): calculated for $\text{C}_{18}\text{H}_{17}^{35}\text{ClN}_2\text{ONa}$, $[\text{M}+\text{Na}]^+$: 335.0922, found: 335.0920; calculated for $\text{C}_{18}\text{H}_{17}^{37}\text{ClN}_2\text{ONa}$, $[\text{M}+\text{Na}]^+$: 337.0892, found: 337.0899

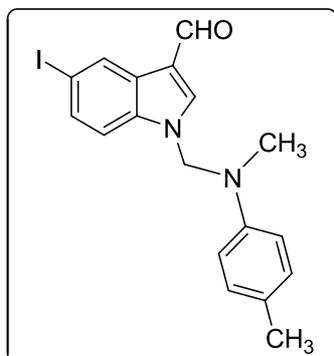
3d



^1H -NMR (DMSO- d_6 , 400MHz): 9.87(s, 1H), 8.22(s, 2H), 7.58(d, 8.8Hz, 1H), 7.42(d, 8.8Hz, 1H), 7.04(d, 8.0Hz, 2H), 6.86(d, 8.0Hz, 2H), 5.89(s, 2H), 2.98(s, 3H), 2.19(s, 3H); ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.21, 145.22, 140.15, 135.54, 129.68, 127.44, 126.47, 126.11, 123.02, 116.46, 115.34, 114.30, 113.81, 64.42, 37.64, 19.98; HRMS

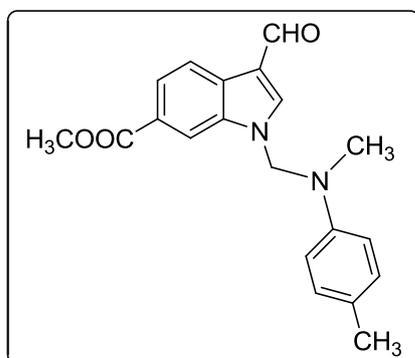
(ESI): calculated for $C_{18}H_{17}^{79}BrN_2ONa$, $[M+Na]^+$: 379.0417, found: 379.0417;
calculated for $C_{18}H_{17}^{81}BrN_2ONa$, $[M+Na]^+$: 381.0396, found: 381.0399

3e



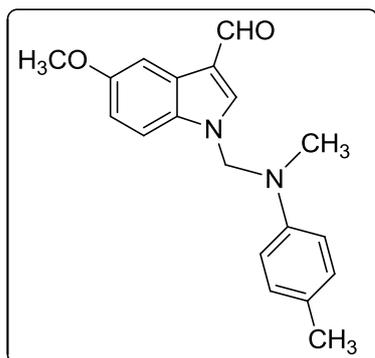
1H -NMR (DMSO- d_6 , 400MHz): 9.86(s, 1H), 8.42(s, 1H), 8.17(s, 1H), 7.55(d, 8.6Hz, 1H), 7.46(d, 8.6Hz, 1H), 7.04(d, 7.4Hz, 2H), 6.86(d, 7.4Hz, 2H), 5.88(s, 2H), 2.98(s, 3H), 2.19(s, 3H). ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.27, 145.24, 139.86, 135.98, 131.59, 129.71, 129.22, 127.44, 127.13, 116.21, 114.32, 114.17, 87.23, 64.34, 37.68, 20.01. HRMS (ESI): calculated for $C_{18}H_{17}IN_2ONa$, $[M+Na]^+$: 427.0278, found: 427.0272

3f



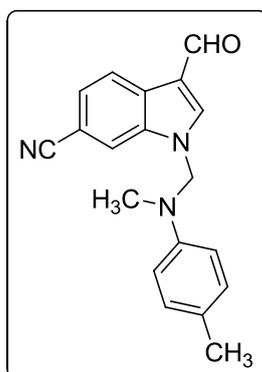
1H -NMR (DMSO- d_6 , 400MHz): 9.92(s, 1H), 8.38(s, 1H), 8.18-8.16(m, 2H), 7.83(d, 8.4Hz, 1H), 7.05(d, 8.0Hz, 2H), 6.88(d, 8.0Hz, 2H), 5.98(s, 2H), 3.85(s, 3H), 2.98(s, 3H), 2.20(s, 3H); ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.29, 166.52, 145.40, 141.92, 136.10, 129.69, 128.47, 127.59, 124.62, 123.16, 120.73, 116.99, 114.50, 113.78, 64.81, 52.06, 37.46, 20.01. HRMS (ESI): calculated for $C_{20}H_{20}N_2O_3Na$ $[M+Na]^+$: 359.1366, found: 359.1372

3g



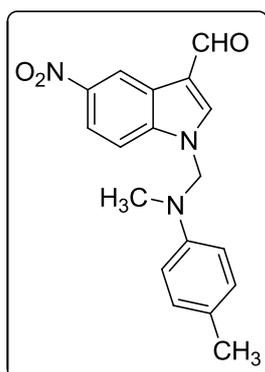
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.83(s, 1H), 8.11(s, 1H), 7.57(s, 1H), 7.47(d, 9.2Hz, 1H), 7.04(d, 7.6Hz, 2H), 6.89-6.85(m, 3H), 5.84(s, 2H), 3.77(s, 3H), 2.98(s, 3H), 2.19(s, 3H); $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 184.87, 155.89, 145.37, 139.45, 131.60, 129.66, 127.24, 125.62, 116.96, 114.22, 113.21, 112.48, 102.64, 64.25, 55.32, 37.59, 19.99; HRMS (ESI): calculated for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2\text{Na}$, $[\text{M}+\text{Na}]^+$: 331.1417, found: 331.1419

3h



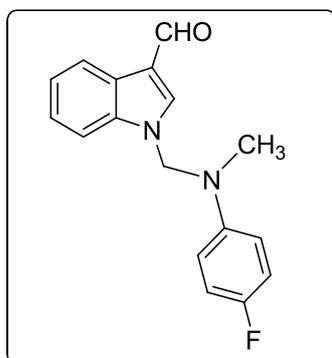
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.93(s, 1H), 8.39(s, 1H), 8.22(d, 8.0Hz, 1H), 8.12(s, 1H), 7.60(d, 8.0Hz, 1H), 7.06(d, 7.4Hz, 2H), 6.88(d, 7.4Hz, 2H), 5.96(s, 2H), 3.00(s, 3H), 2.20(s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.50, 145.26, 141.86, 135.77, 129.71, 127.86, 125.31, 121.80, 119.67, 117.17, 116.94, 115.65, 114.66, 105.19, 64.87, 37.60, 19.98. HRMS (ESI): calculated for $\text{C}_{19}\text{H}_{17}\text{N}_3\text{ONa}$, $[\text{M}+\text{Na}]^+$: 326.1264, found: 326.1260.

3i



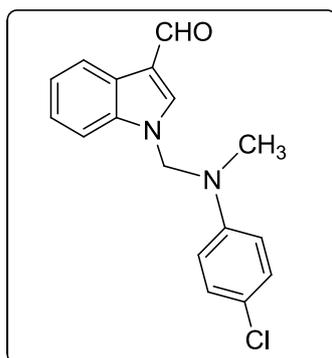
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.97(s, 1H), 8.93(d, 2.4Hz, 1H), 8.42(s, 1H), 8.16(dd, 1.8Hz, 9.0Hz, 1H), 7.84(d, 9.2Hz, 1H), 7.05(d, 8.4Hz, 2H), 6.88(d, 8.4Hz, 2H), 5.98(s, 2H), 3.02(s, 3H), 2.19(s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.69, 145.07, 143.11, 142.22, 139.68, 129.74, 127.65, 124.14, 118.74, 118.16, 117.07, 114.35, 112.52, 64.83, 37.74, 19.98. HRMS (ESI): calculated for $\text{C}_{18}\text{H}_{17}\text{N}_3\text{O}_3\text{Na}$, $[\text{M}+\text{Na}]^+$: 346.1162, found: 346.1160.

3j



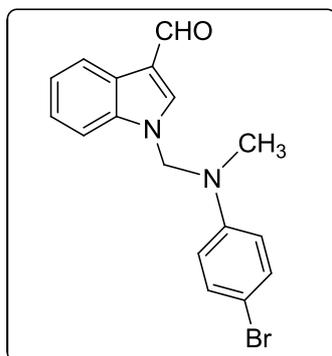
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.89 (s, 1H), 8.21(s, 1H), 8.09(dd, 1.6Hz, 7.2Hz, 1H), 7.55(d, 7.2Hz, 1H), 7.25(t, 5.4Hz, 2H), 7.08(t, 8.8Hz, 2H), 6.96-7.00(m, 2H), 5.89 (s, 2H), 2.99 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.06, 155.91 (d, 234Hz), 144.45, 139.62, 136.78, 124.76, 123.59, 122.57, 120.95, 117.30, 115.85 (d, 7.5Hz), 115.59 (d, 21.9Hz), 111.58, 64.53, 37.87. HRMS (ESI): calculated for $\text{C}_{17}\text{H}_{15}\text{FN}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 305.1061, found: 305.1058.

3k



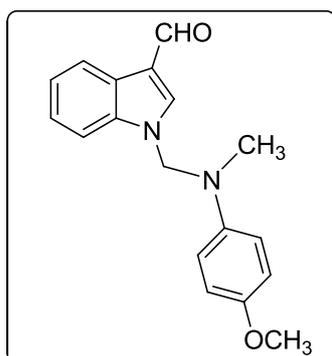
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.89 (s, 1H), 8.22(s, 1H), 8.10 (d, 7.6Hz, 1H), 7.60 (d, 7.6Hz, 1H), 7.27-7.31(m, 2H), 7.26(d, 8.8Hz, 2H), 6.98 (d, 8.8Hz, 2H), 5.93 (s, 2H), 3.04 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.11, 146.50, 139.46, 136.67, 128.90, 124.81, 123.69, 122.66, 122.23, 121.02, 117.40, 115.45, 111.56, 63.69, 37.74. HRMS (ESI): calculated for $\text{C}_{17}\text{H}_{15}^{35}\text{ClN}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 321.0765, found: 321.0762; calculated for $\text{C}_{17}\text{H}_{15}^{37}\text{ClN}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 323.0736, found: 323.0740.

3l



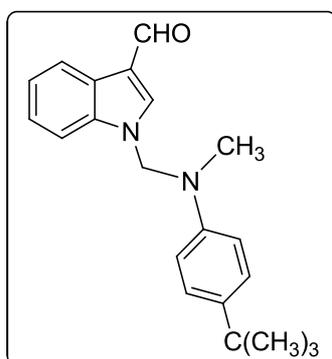
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.89(s, 1H), 8.22(s, 1H), 8.10(d, 7.6Hz, 1H), 7.61(d, 7.6Hz, 1H), 7.38(d, 8.8Hz, 2H), 7.27(t, 8.8Hz, 2H), 6.94(d, 8.8Hz, 2H), 5.93(s, 2H), 3.04(s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.10, 146.84, 139.41, 136.64, 131.74, 124.81, 123.69, 122.65, 121.02, 117.40, 115.87, 111.54, 109.83, 63.55, 37.69. HRMS (ESI): calculated for $\text{C}_{17}\text{H}_{16}^{79}\text{BrN}_2\text{O}$, $[\text{M}+\text{H}]^+$: 343.0441, found: 343.0442; calculated for $\text{C}_{17}\text{H}_{16}^{81}\text{BrN}_2\text{O}$, $[\text{M}+\text{H}]^+$: 345.0420, found: 345.0422. This high resolution mass spectrometry was conducted using a VG ZAB-HS by ESI technique

3m



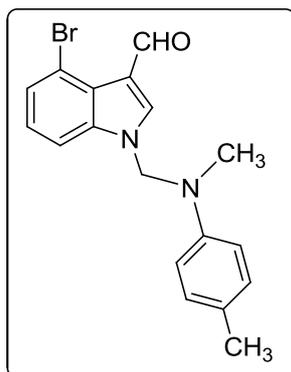
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.88 (s, 1H), 8.16 (s, 1H), 8.08 (dd, 6.0Hz, 2.8Hz, 1H), 7.53 (dd, 6.0Hz, 2.4Hz, 1H), 7.27-7.22 (m, 2H), 6.93 (d, 9.2Hz, 2H), 6.84 (d, 9.2Hz, 2H), 5.83 (s, 2H), 3.67 (s, 3H), 2.93 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.03, 152.78, 141.80, 139.78, 136.94, 124.71, 123.54, 122.51, 120.90, 117.19, 116.38, 114.57, 111.66, 65.04, 55.20, 37.84. HRMS (ESI): calculated for $\text{C}_{18}\text{H}_{18}\text{N}_2\text{NaO}_2$, $[\text{M}+\text{Na}]^+$: 317.1261, found: 317.1265

3n



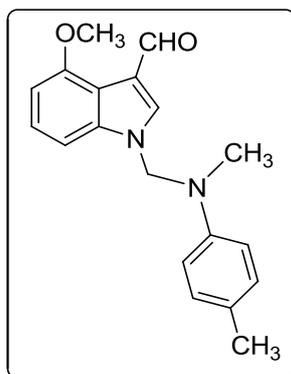
$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 9.89 (s, 1H), 8.22 (s, 1H), 8.11 (dd, 6.2Hz, 2.4Hz, 1H), 7.60 (dd, 6.4Hz, 2.4Hz, 1H), 7.28-7.26 (m, 2H), 7.24 (d, 8.8Hz, 2H), 6.87 (d, 8.8Hz, 2H), 5.87 (s, 2H), 3.04 (s, 3H), 1.22 (s, 9H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 185.01, 145.20, 140.74, 139.40, 136.69, 125.83, 124.85, 123.56, 122.57, 120.97, 117.29, 113.57, 111.57, 64.27, 37.74, 33.54, 31.30. HRMS (ESI): calculated for $\text{C}_{21}\text{H}_{24}\text{N}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 343.1781, found: 343.1785.

3o



$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 10.66 (s, 1H), 8.11 (s, 1H), 7.67 (d, 8.0Hz, 1H), 7.50 (d, 8.0Hz, 1H), 7.20 (t, 8.0Hz, 2H), 7.05 (d, 8.2Hz, 2H), 6.88 (d, 8.2Hz, 2H), 5.94 (s, 2H), 2.96 (s, 3H), 2.20 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 184.43, 145.18, 137.82, 134.73, 129.84, 129.71, 127.55, 126.41, 123.84, 121.70, 116.92, 114.38, 111.67, 64.40, 37.51, 19.98. HRMS (ESI): calculated for $\text{C}_{18}\text{H}_{17}^{35}\text{BrN}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 379.0416, found: 379.0438; calculated for $\text{C}_{18}\text{H}_{17}^{37}\text{BrN}_2\text{NaO}$, $[\text{M}+\text{Na}]^+$: 381.0396, found: 381.0367. This high resolution mass spectrometry was conducted using a VG ZAB-HS by ESI technique.

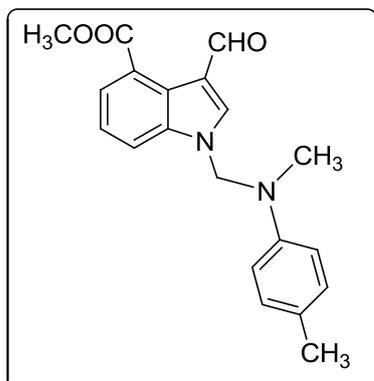
3p



$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 10.27 (s, 1H), 7.87 (s, 1H), 7.22-7.17 (m, 2H), 7.04 (d, 8.6Hz, 2H), 6.87 (d, 8.6Hz, 2H), 6.79 (d, 7.2Hz, 1H), 5.86 (s, 2H), 3.92 (s, 3H), 2.94 (s, 3H), 2.20 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 186.28, 153.79, 145.33, 137.67, 130.88, 129.67, 127.31, 123.74, 117.20, 115.98, 114.29, 104.98, 102.77, 64.10, 55.43, 37.49, 19.98. HRMS (ESI): calculated for $\text{C}_{19}\text{H}_{20}\text{N}_2\text{NaO}_2$, $[\text{M}+\text{Na}]^+$: 331.1417, found: 331.1422. This high resolution mass spectrometry was conducted

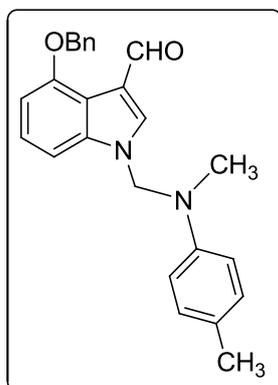
using a VG ZAB-HS by ESI technique.

3q



$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 10.11 (s, 1H), 8.18 (s, 1H), 7.83 (d, 8.0Hz, 1H), 7.59 (d, 6.8Hz, 1H), 7.34 (t, 8.0Hz, 1H), 7.05 (d, 8.6Hz, 2H), 6.88 (d, 8.6Hz, 2H), 5.94 (s, 2H), 3.85 (s, 3H), 2.97 (s, 3H), 2.20 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 186.13, 168.49, 145.28, 137.85, 137.46, 129.70, 127.50, 124.82, 123.51, 122.57, 119.10, 117.22, 115.50, 114.38, 64.33, 52.01, 37.56, 19.98. HRMS (ESI): calculated for $\text{C}_{20}\text{H}_{20}\text{N}_2\text{NaO}_3$, $[\text{M}+\text{Na}]^+$: 359.1366, found: 359.1367. This high resolution mass spectrometry was conducted using a VG ZAB-HS by ESI technique.

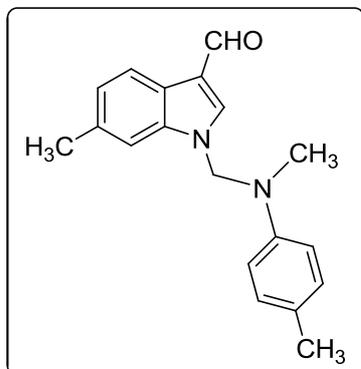
3r



$^1\text{H-NMR}$ (DMSO- d_6 , 400MHz): 10.27 (s, 1H), 7.88 (s, 1H), 7.51 (d, 7.4Hz, 2H), 7.41 (t, 7.4Hz, 2H), 7.24-7.22 (m, 2H), 7.16 (t, 8.0Hz, 1H), 7.04 (d, 8.6Hz, 2H), 6.90 (d, 7.4Hz, 1H), 6.87 (d, 8.6Hz, 2H), 5.87 (s, 2H), 5.27 (s, 2H), 2.94 (s, 3H), 2.20 (s, 3H). $^{13}\text{C-NMR}$ (DMSO- d_6 , 100MHz): 186.14, 152.72, 145.32, 137.80, 137.08, 131.07, 129.85, 129.68, 128.53, 127.91, 127.63, 123.69, 121.71, 117.18, 114.30, 105.21, 104.07, 69.58, 64.12, 37.50, 19.98. HRMS (ESI): calculated for $\text{C}_{25}\text{H}_{25}\text{N}_2\text{O}_2$, $[\text{M}+\text{H}]^+$:

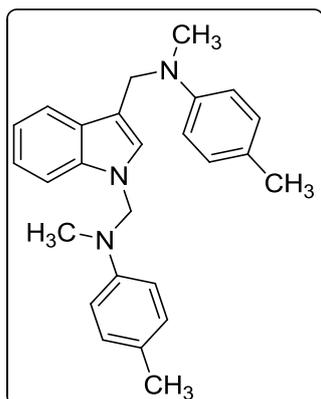
385.1911, found: 385.1904. This high resolution mass spectrometry was conducted using a VG ZAB-HS by ESI technique.

3s



$^1\text{H-NMR}$ (CD_3OD , 400MHz): 9.76 (s, 1H), 8.05-8.02 (m, 1H), 7.89 (s, 1H), 7.17 (s, 1H), 7.10 (d, 8.4Hz, 3H), 6.86 (d, 8.4Hz, 2H), 5.72 (s, 2H), 2.96 (s, 3H), 2.40 (s, 3H), 2.28 (s, 3H). $^{13}\text{C-NMR}$ (CD_3OD , 100MHz): 187.93, 148.39, 141.64, 139.95, 136.09, 131.74, 130.21, 126.43, 123.09, 120.02, 117.45, 116.44, 113.17, 67.58, 38.77, 22.71, 21.32. HRMS (ESI): calculated for $\text{C}_{19}\text{H}_{21}\text{N}_2\text{O}$, $[\text{M}+\text{H}]^+$: 293.1648, found: 293.1648. This high resolution mass spectrometry was conducted using a VG ZAB-HS by ESI technique.

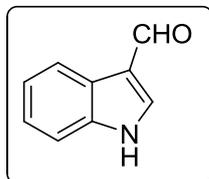
4



$^1\text{H-NMR}$ ($\text{DMSO-}d_6$, 400MHz): 7.46(d, 8.0Hz, 1H), 7.42(d, 8.0Hz, 1H), 7.09(s, 1H), 7.05(d, 7.2Hz, 1H), 7.00(d, 8.0Hz, 2H), 6.97(s, 1H), 6.94(d, 7.6Hz, 2H), 6.83(d, 7.6Hz, 2H), 6.71(d, 7.6Hz, 2H), 5.68(s, 2H), 4.50(s, 2H), 2.79(s, 3H), 2.77(s, 3H), 2.20(s, 3H), 2.17(s, 3H). $^{13}\text{C-NMR}$ ($\text{DMSO-}d_6$, 100MHz): 147.71, 146.07, 136.26, 129.48, 129.31, 127.35, 126.90, 124.59, 121.32, 119.06, 118.89, 114.63, 113.28,

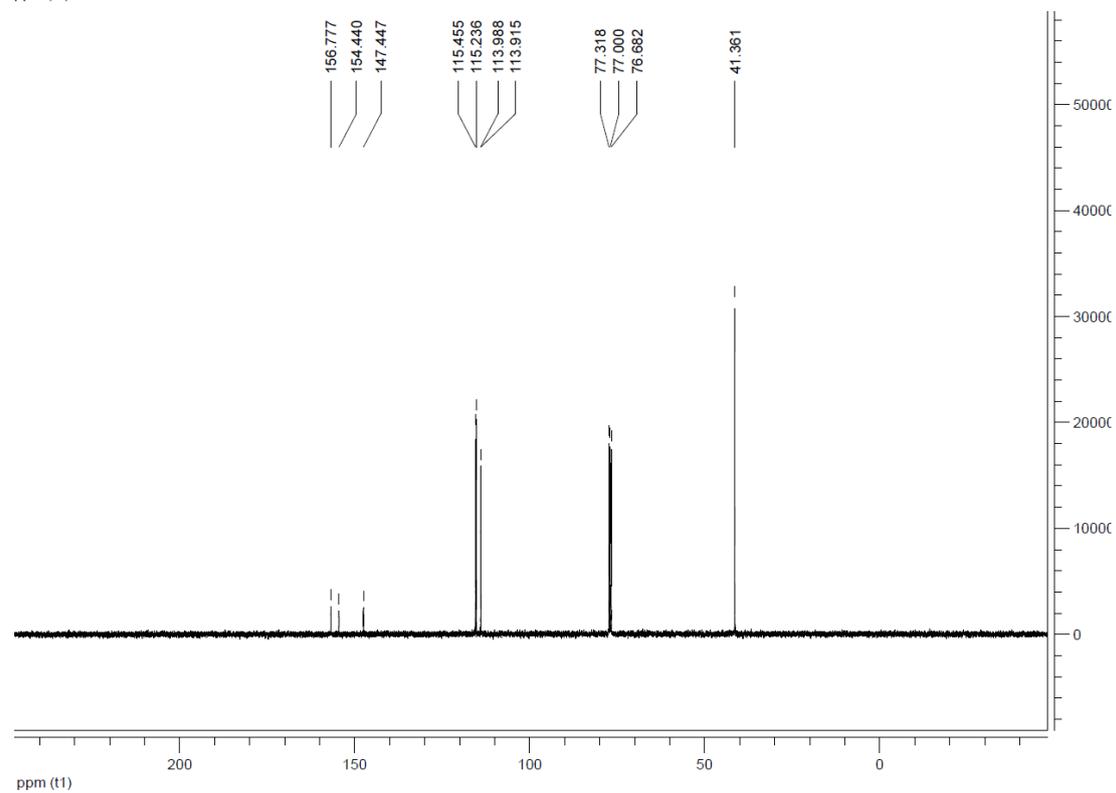
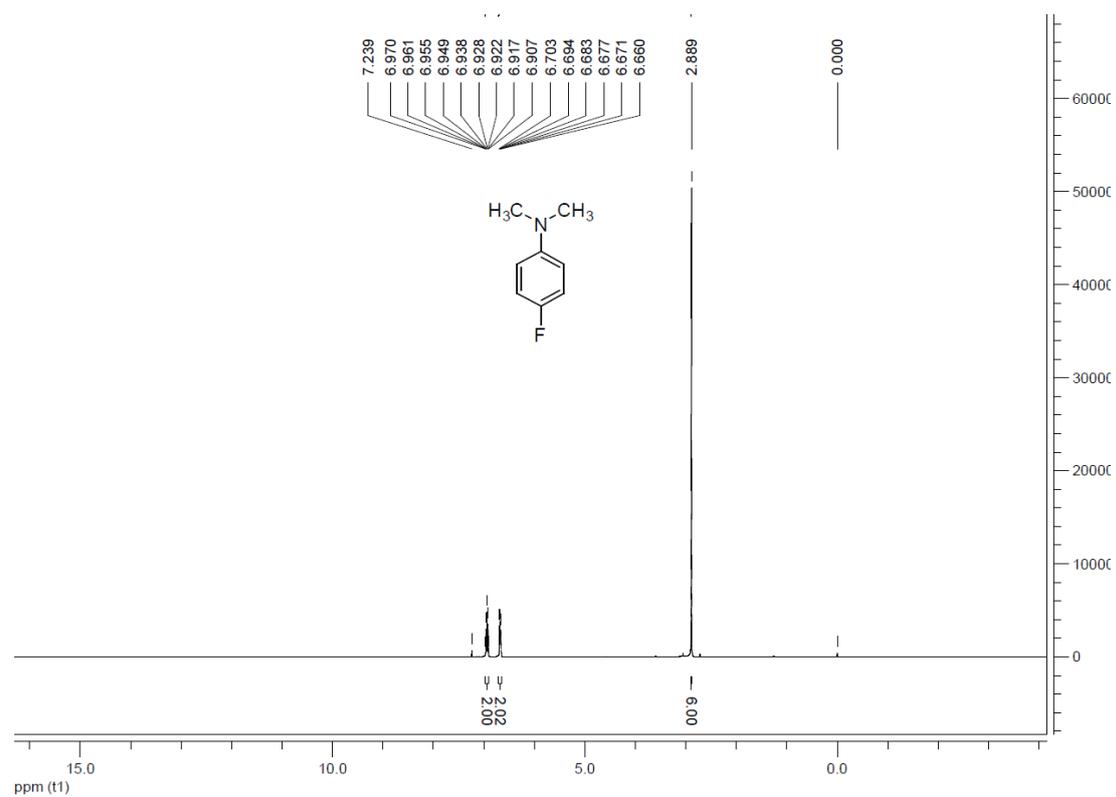
111.76, 111.36, 110.48, 63.14, 47.77, 37.82, 37.18, 20.02, 20.02; HRMS (ESI):
calculated for $C_{26}H_{29}N_3Na$, $[M+Na]^+$: 406.2254, found: 406.2260

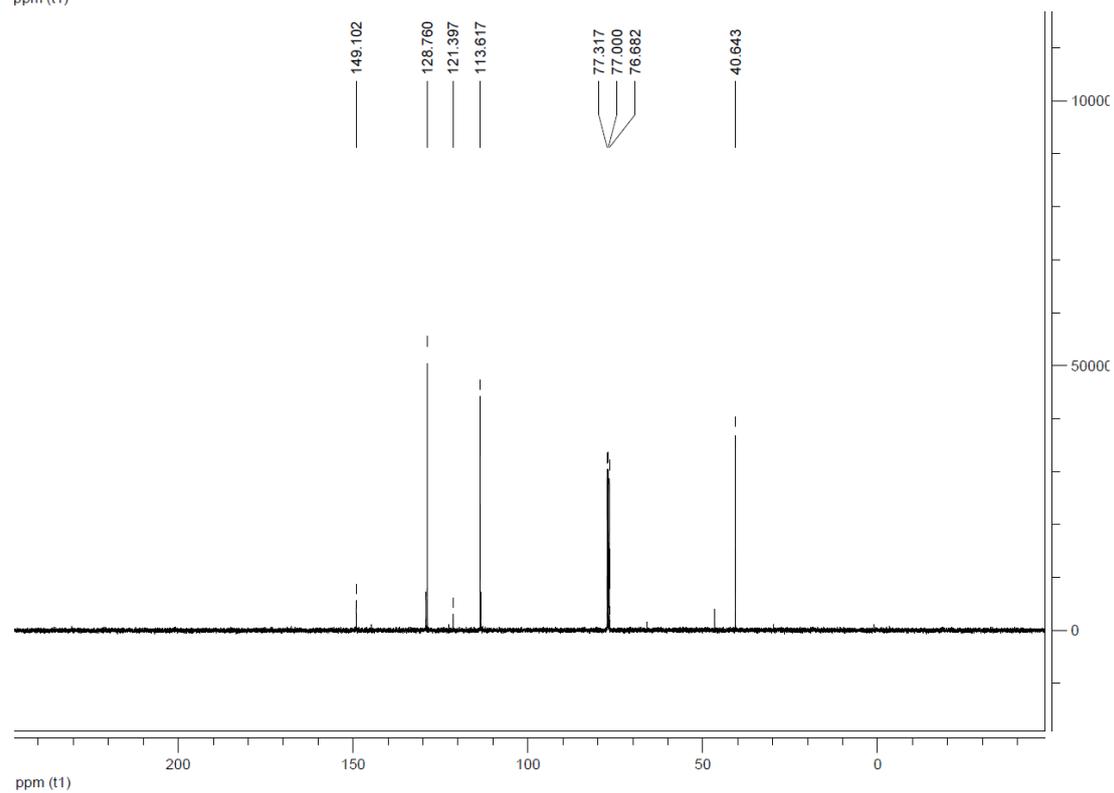
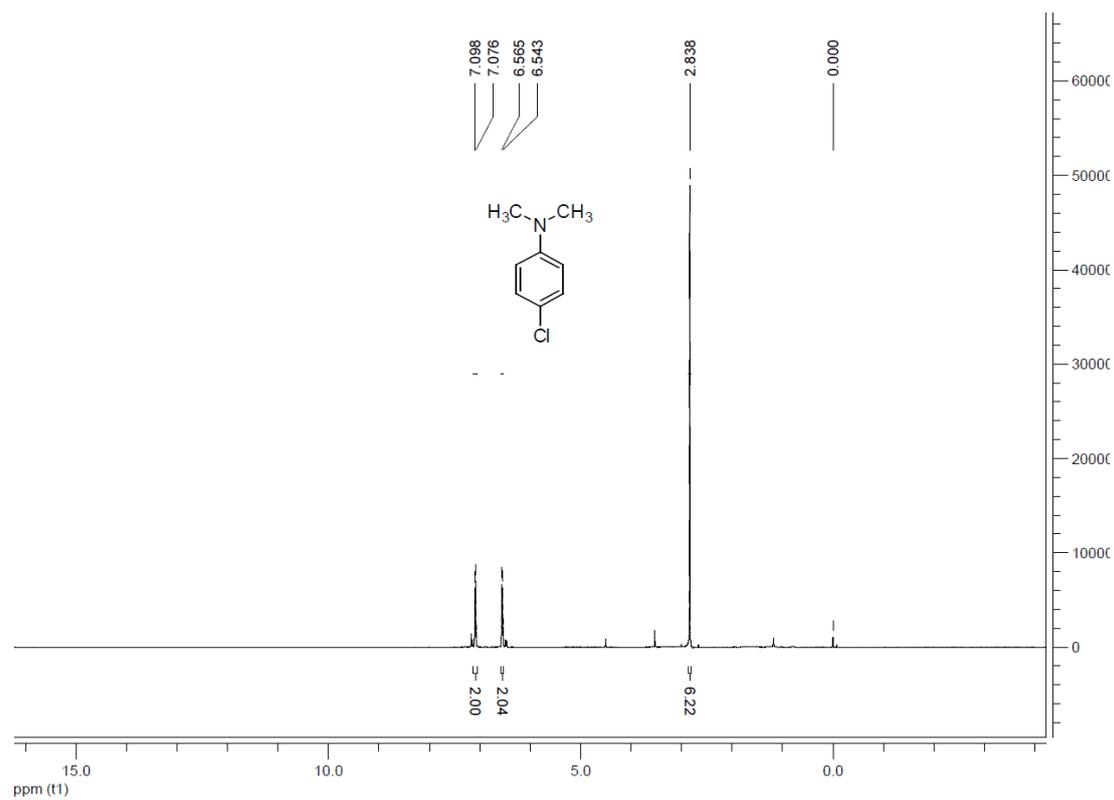
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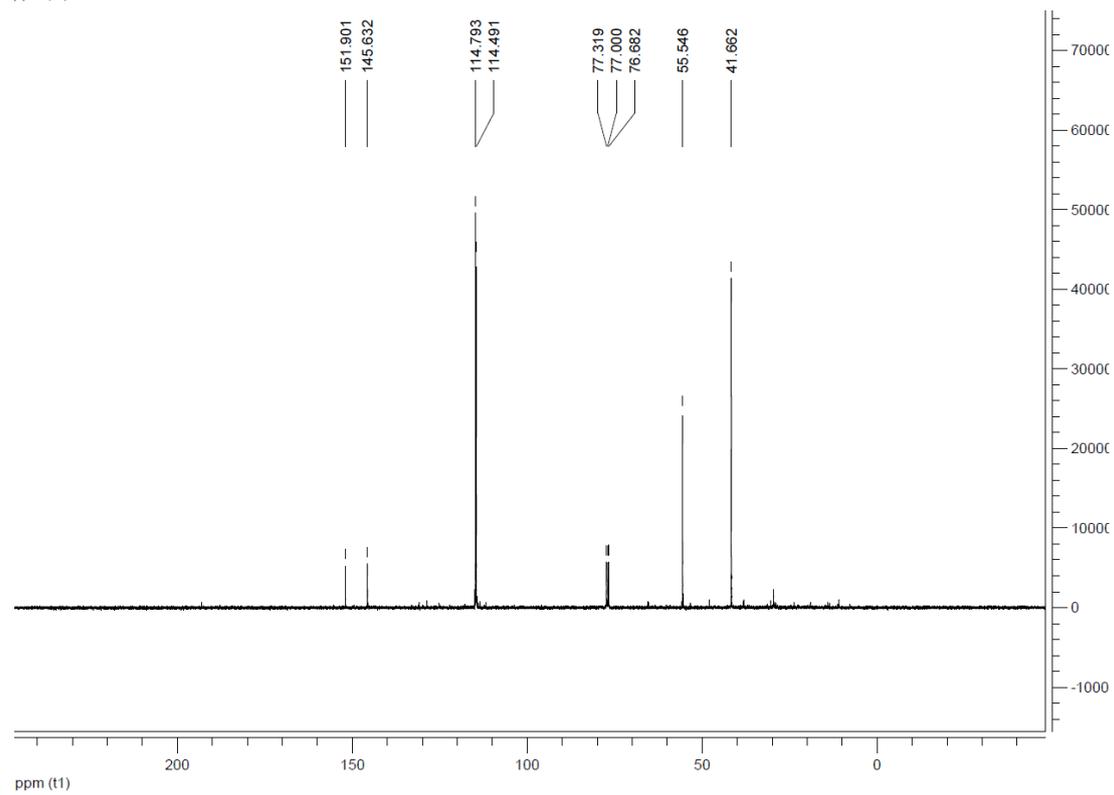
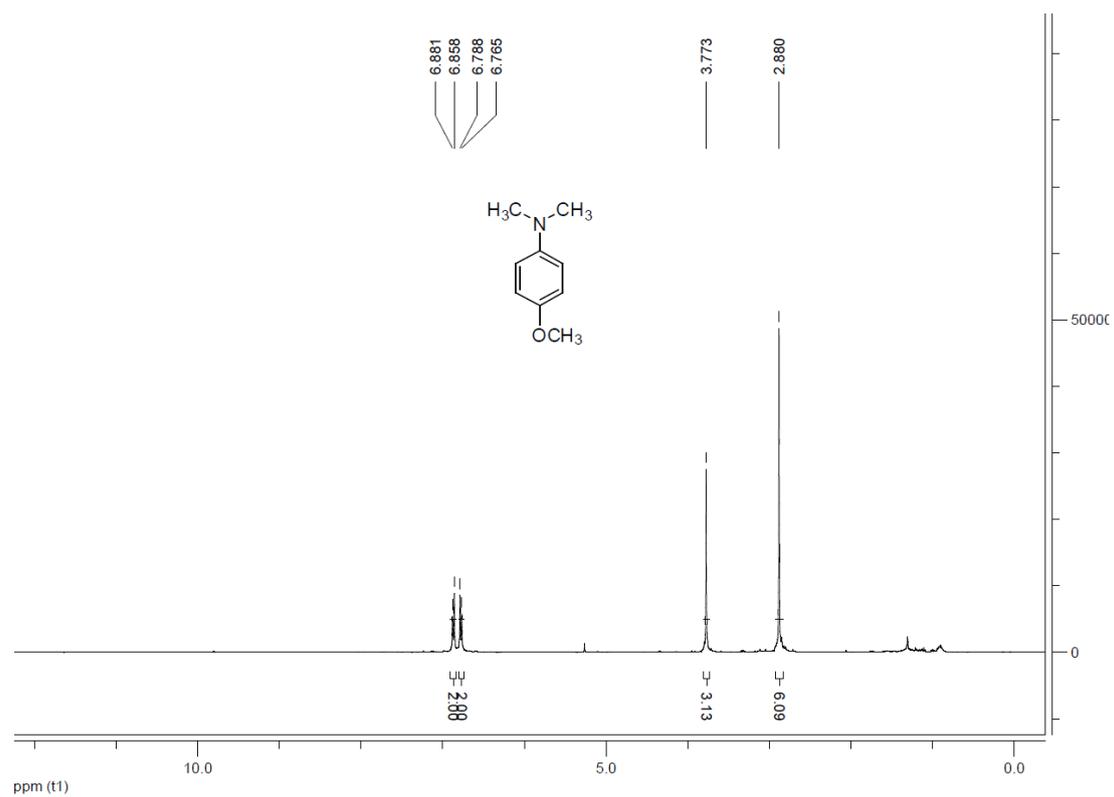


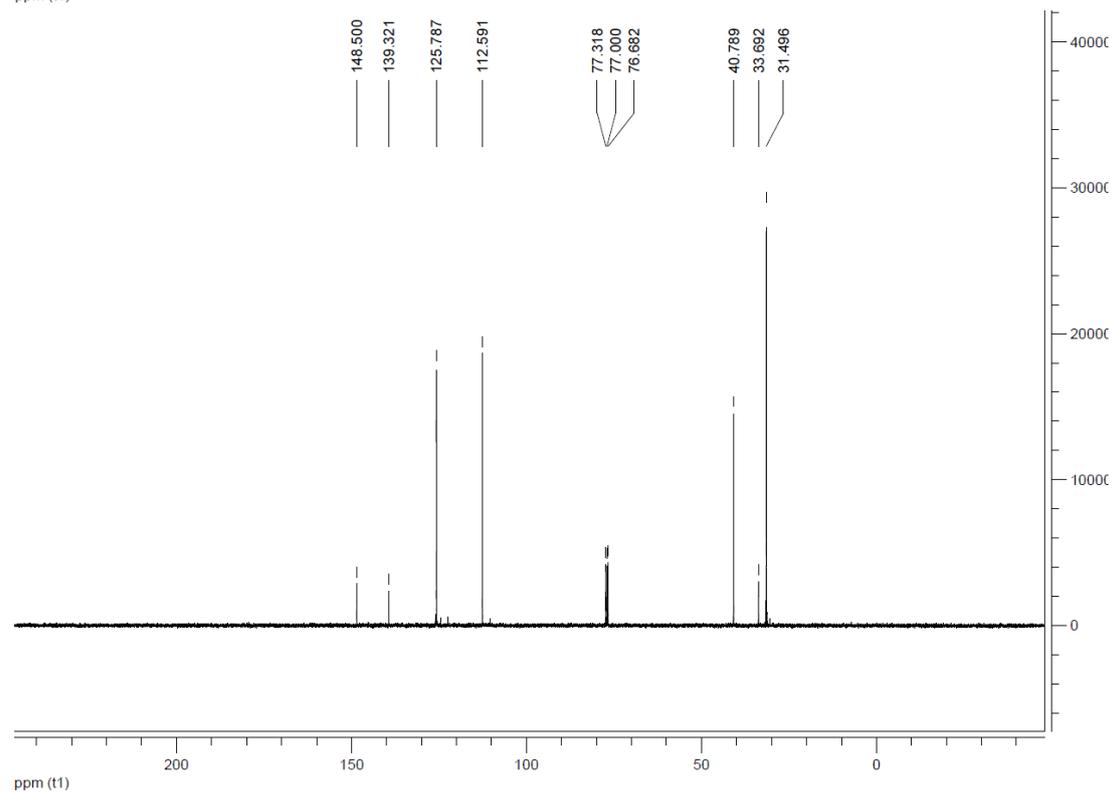
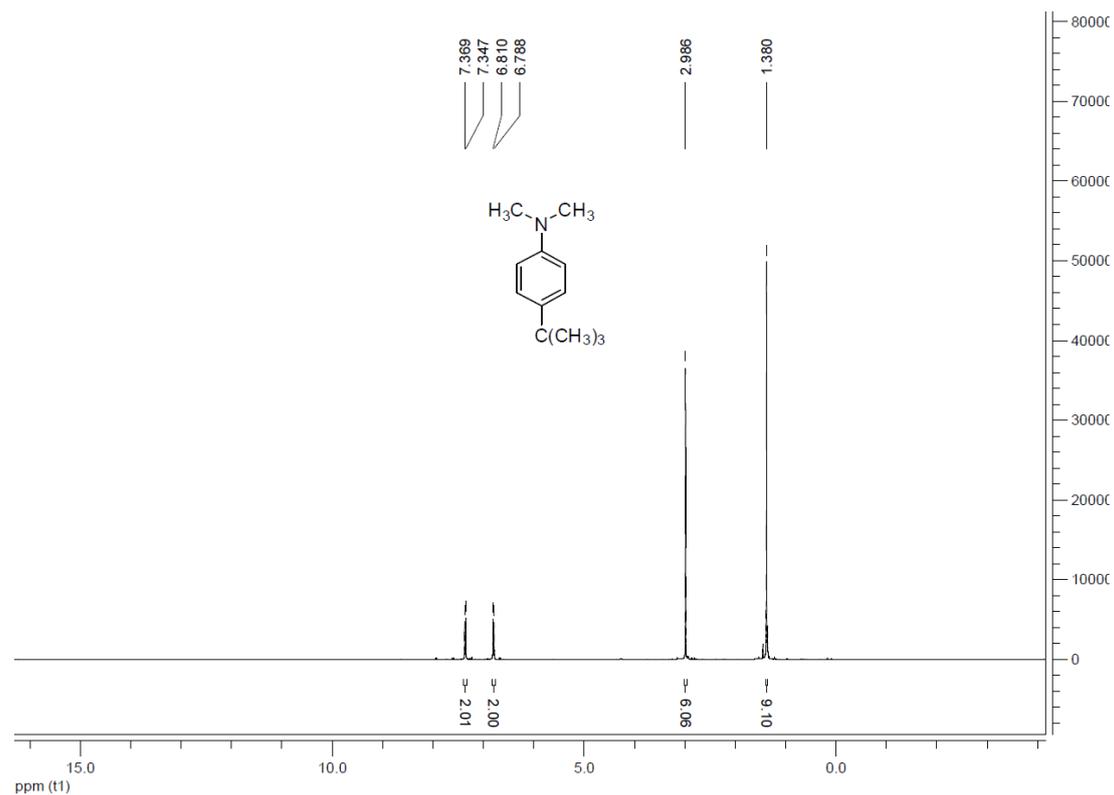
1H -NMR (DMSO- d_6 , 400MHz): 12.1 (b, 1H), 9.94(s, 1H), 8.29(s, 1H), 8.10(d, 7.2Hz, 1H), 7.51(d, 8.0Hz, 1H), 7.28-7.20(m, 2H). ^{13}C -NMR (DMSO- d_6 , 100MHz): 185.00, 138.53, 137.07, 124.14, 123.49, 122.16, 120.85, 118.18, 112.45

^1H and ^{13}C NMR charts of the products



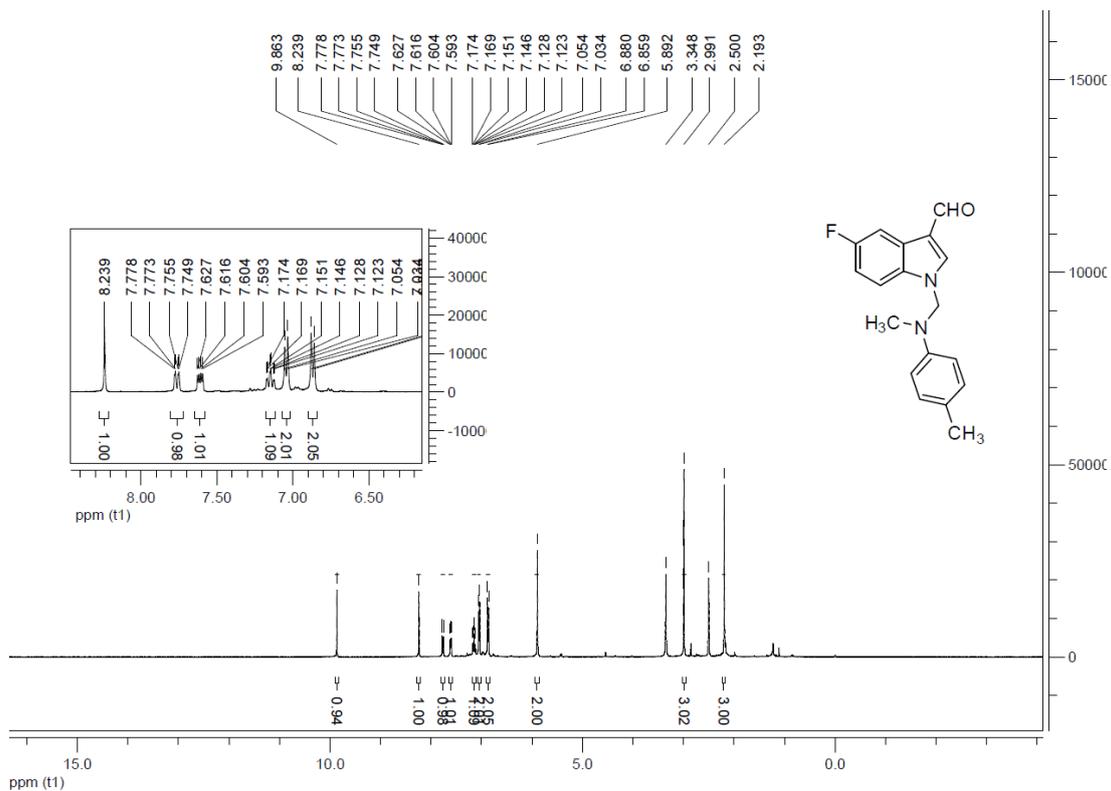
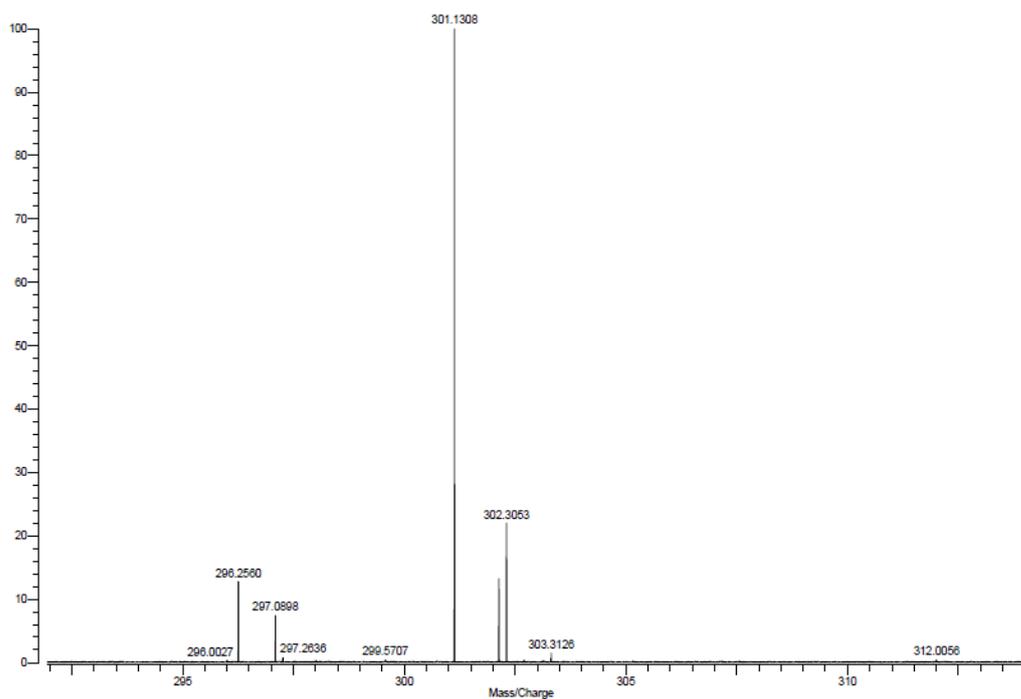


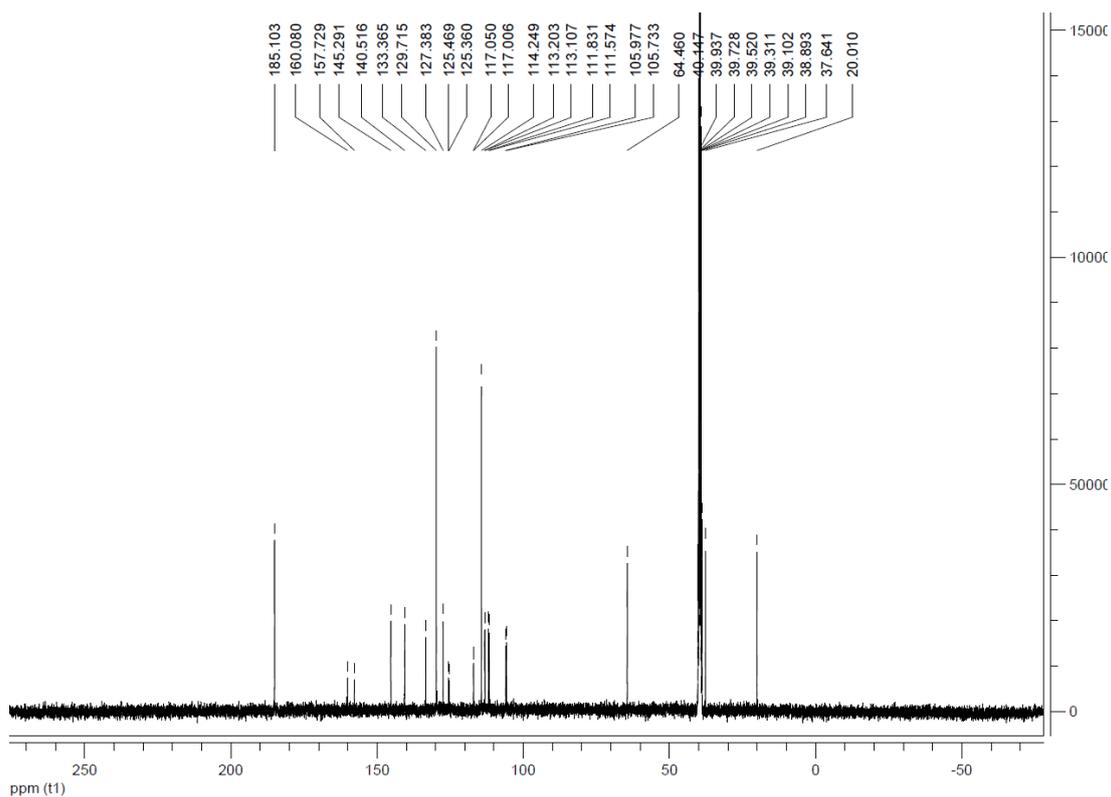




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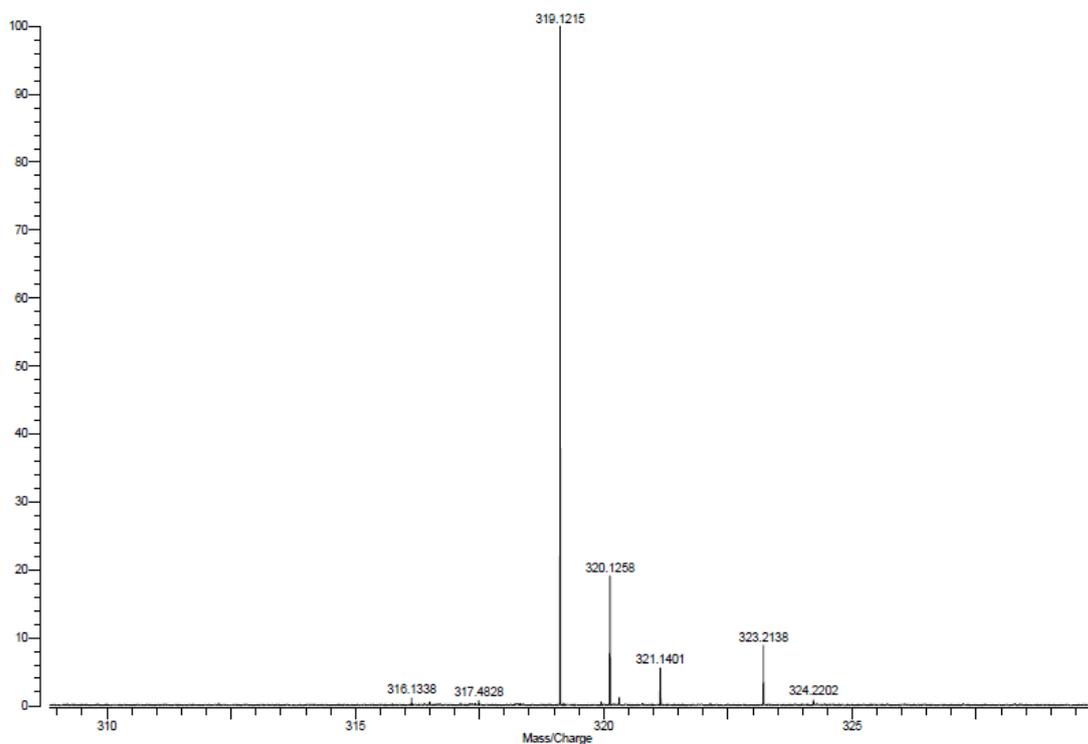
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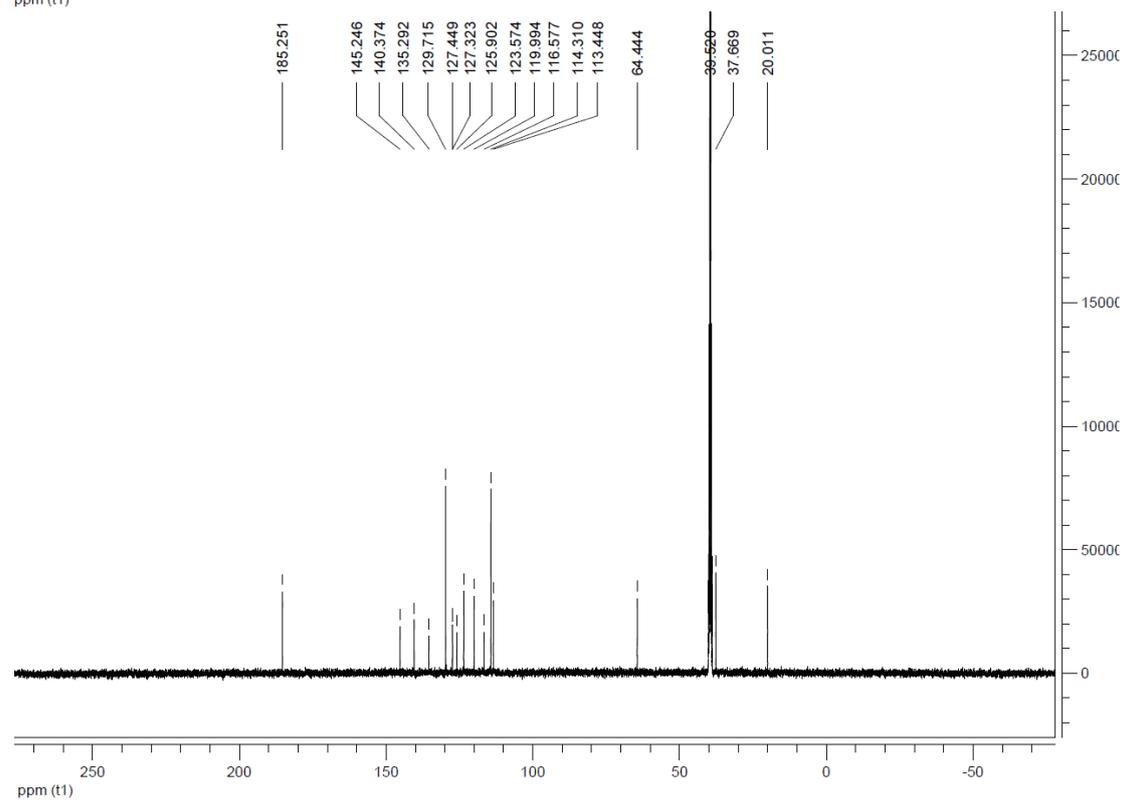
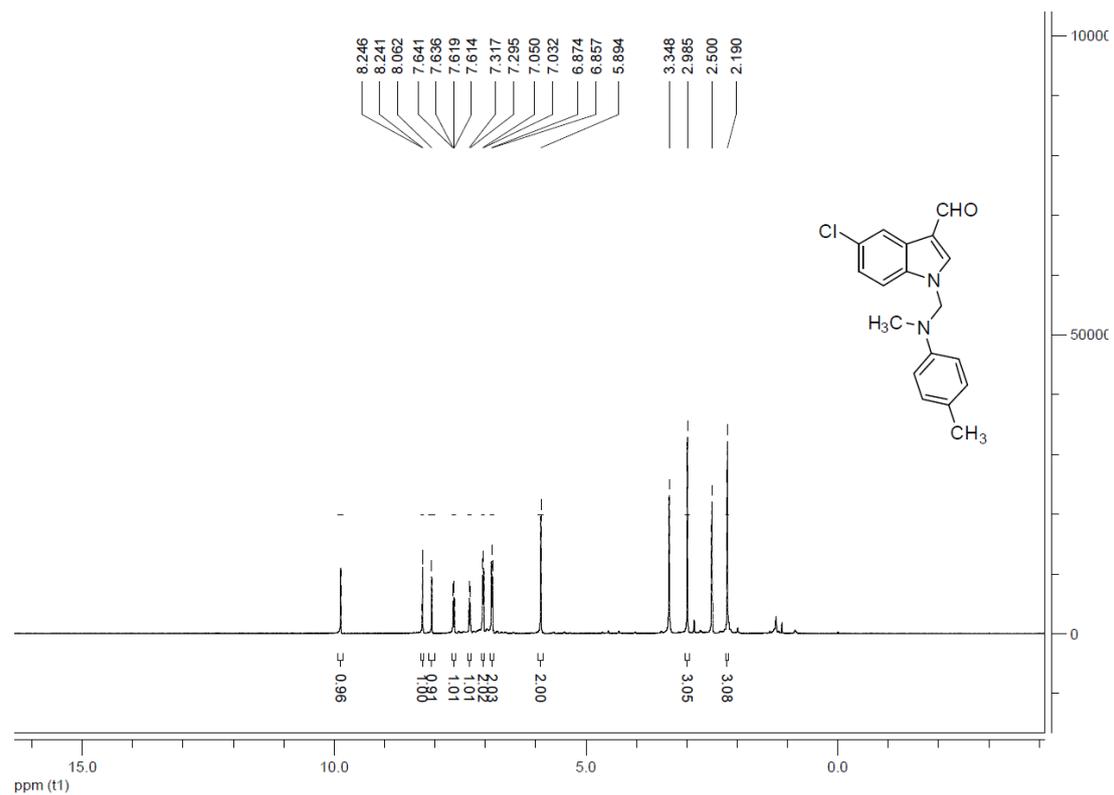




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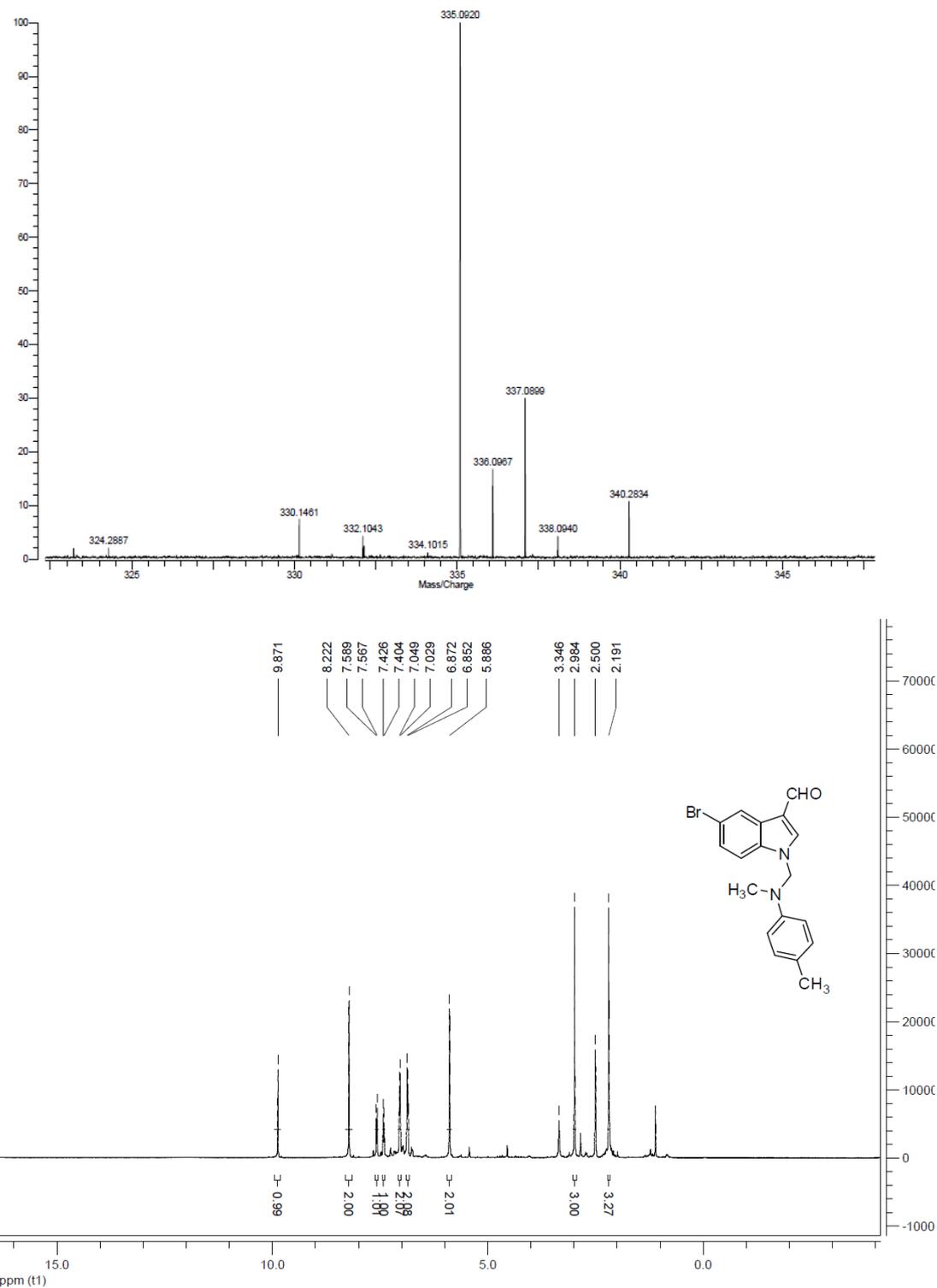
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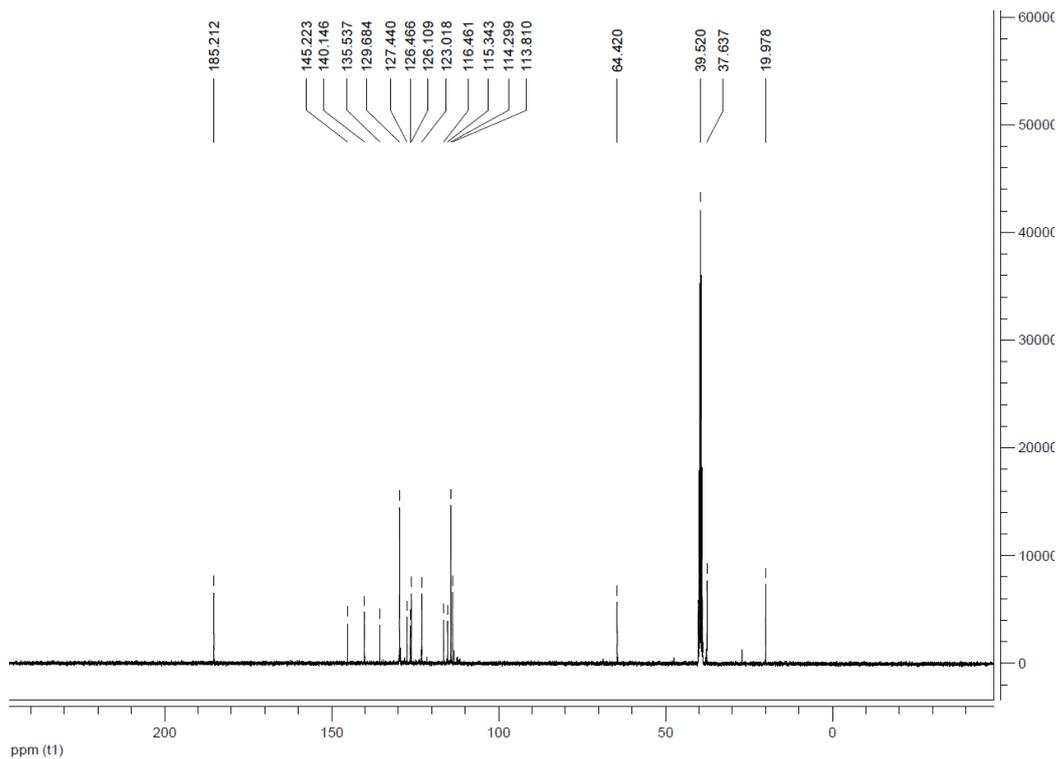




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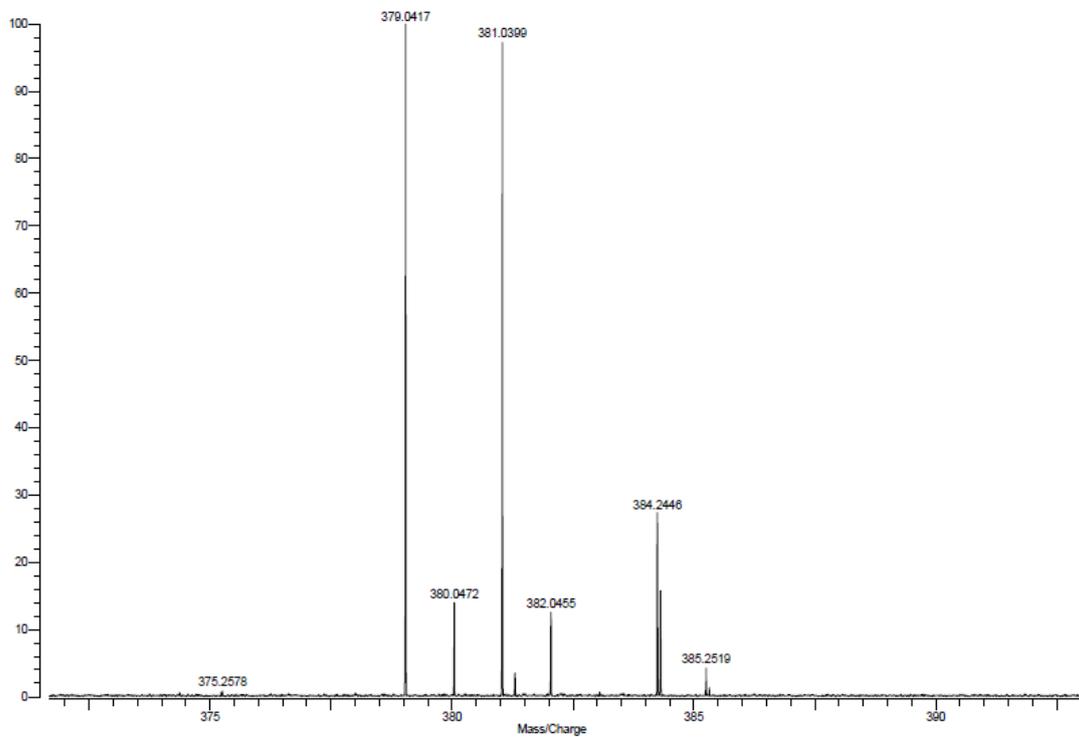
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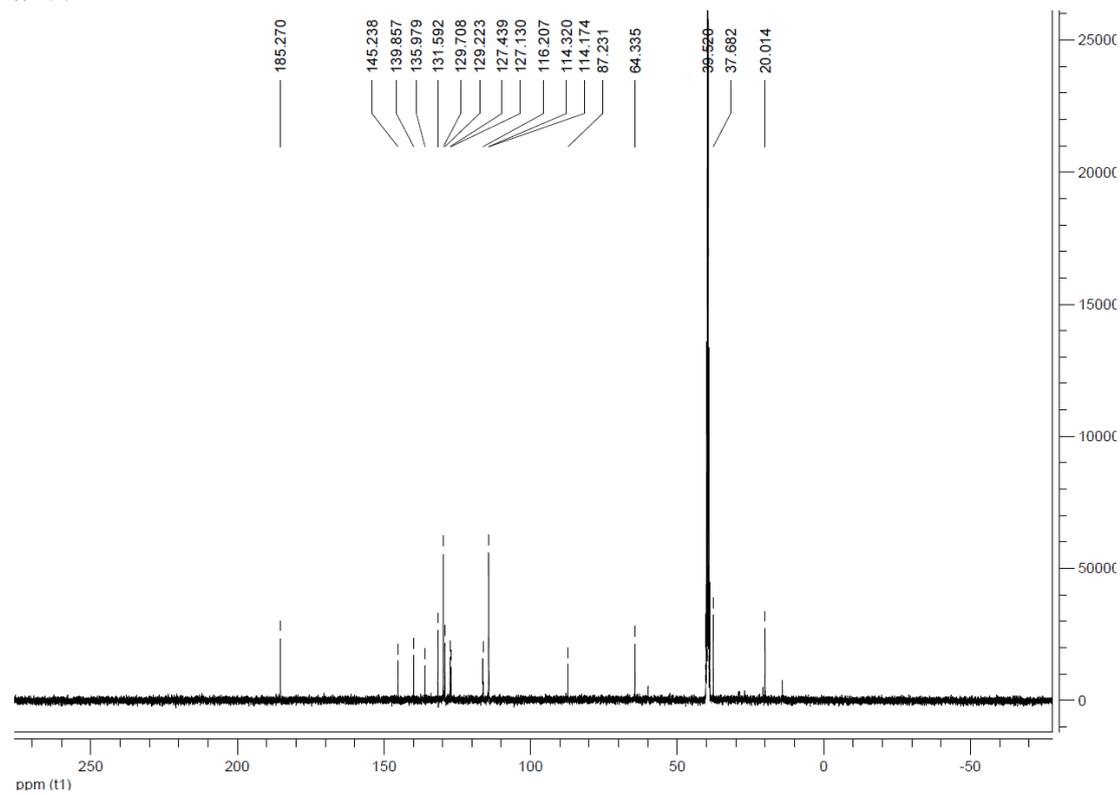
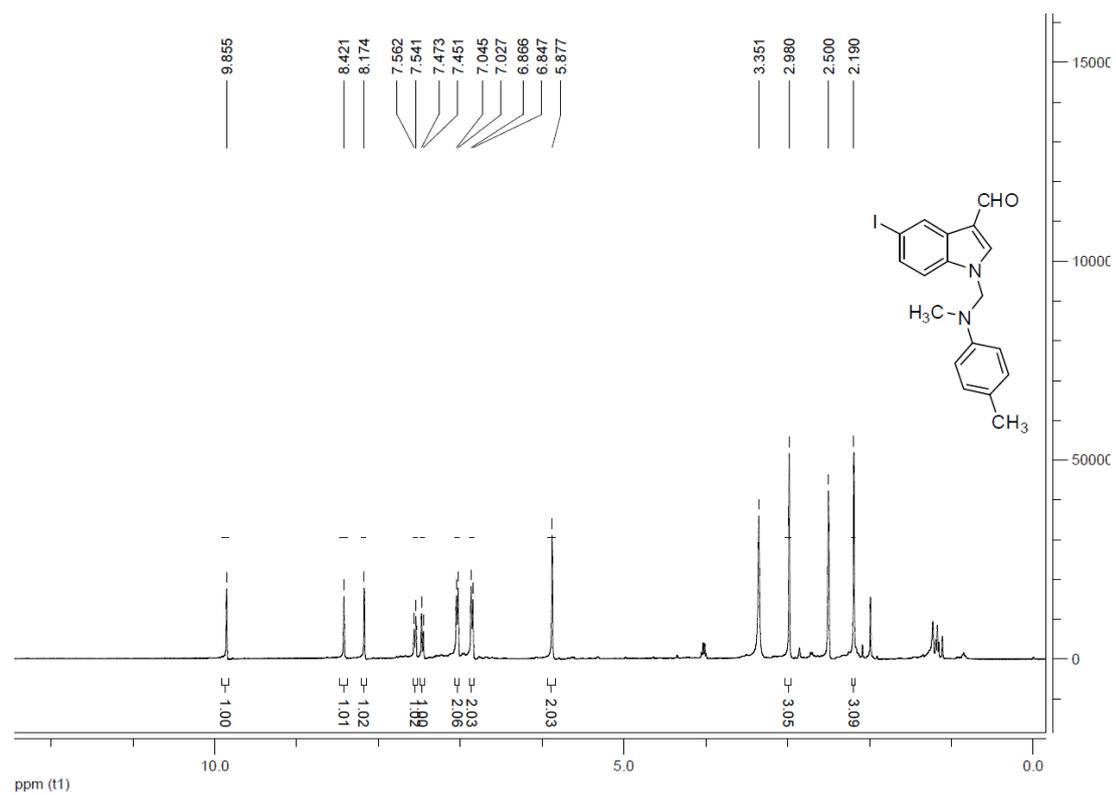




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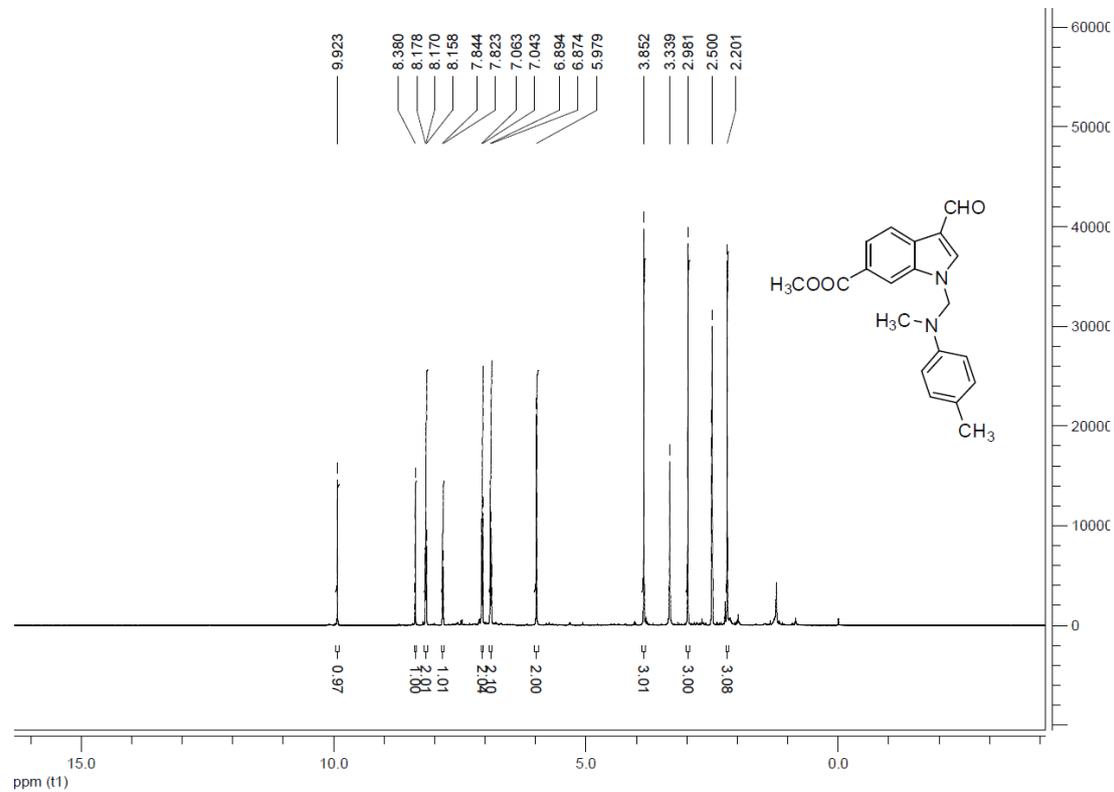
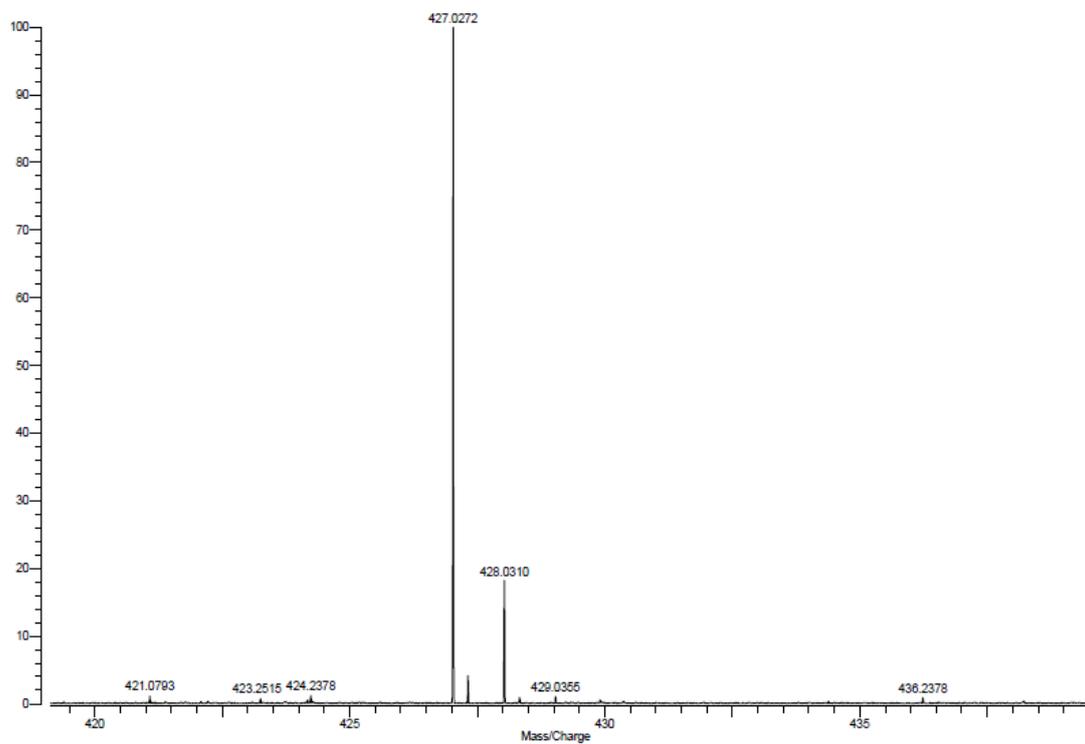


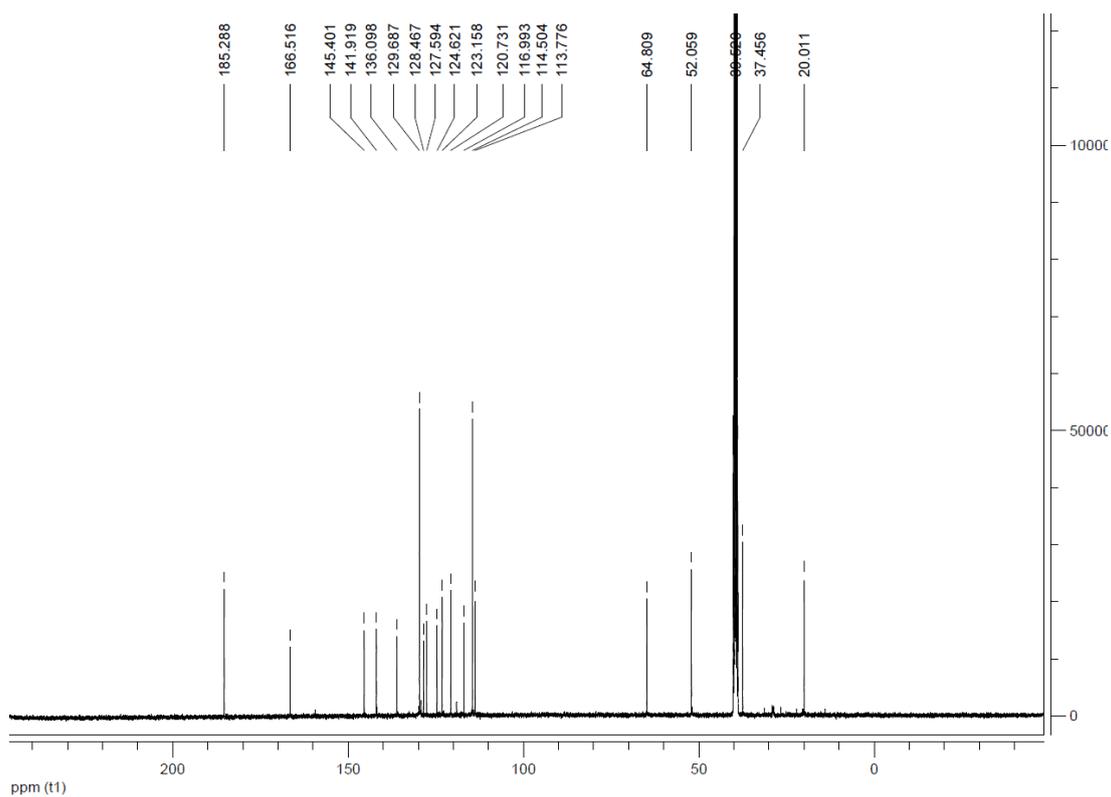


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Mode: Positive
Scans: 1

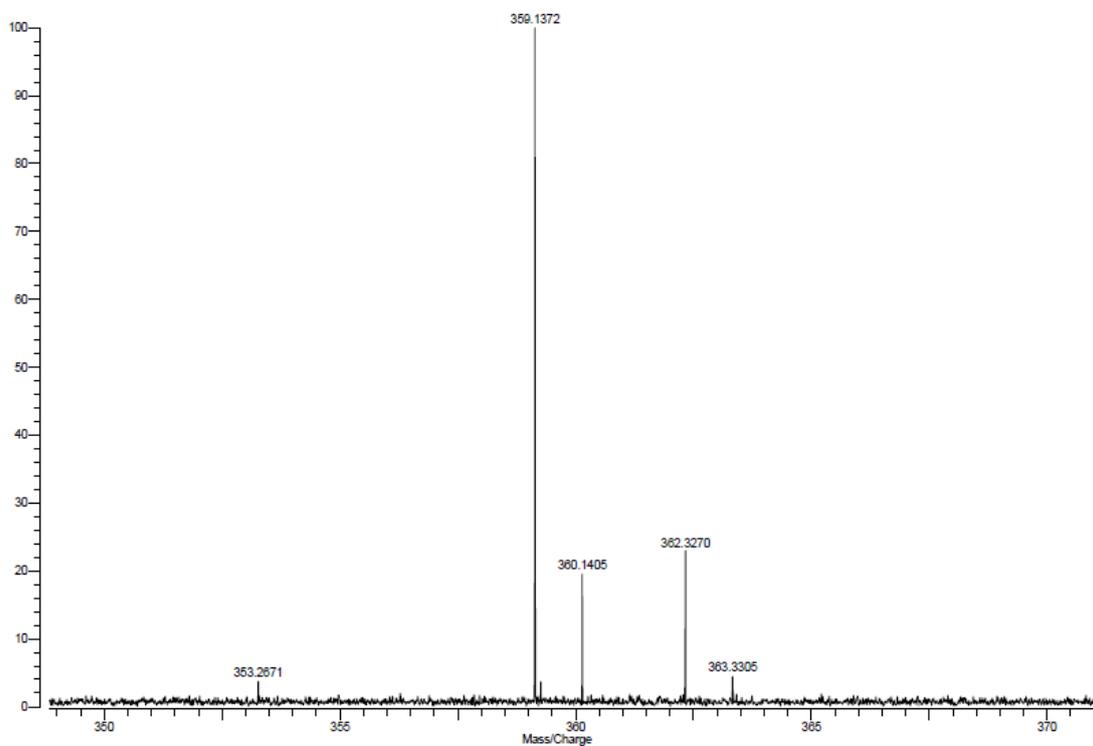
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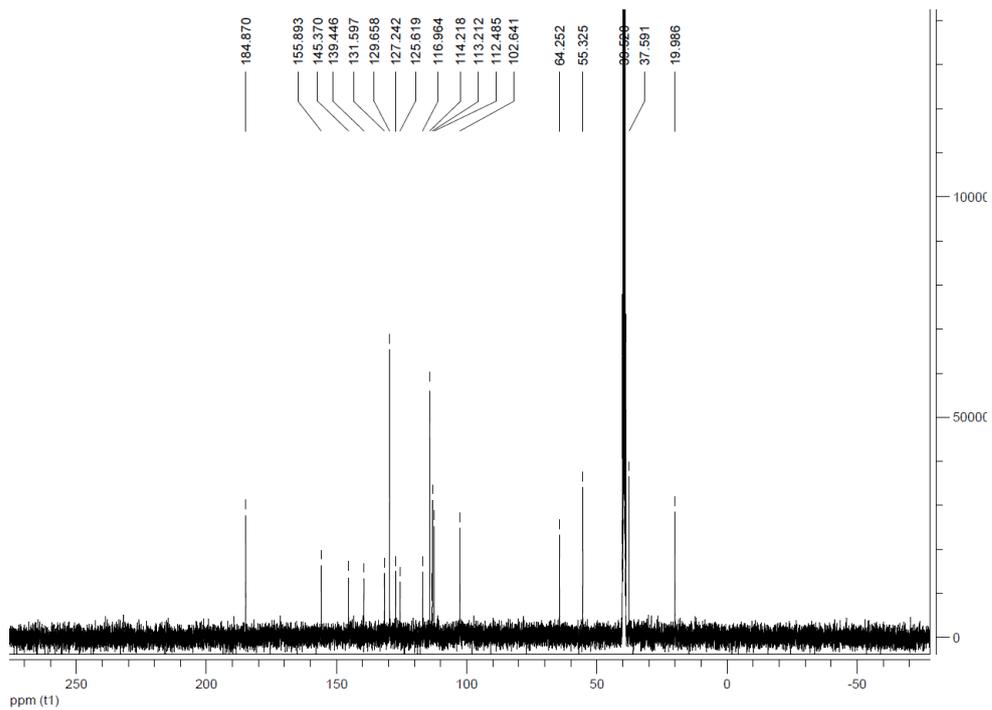
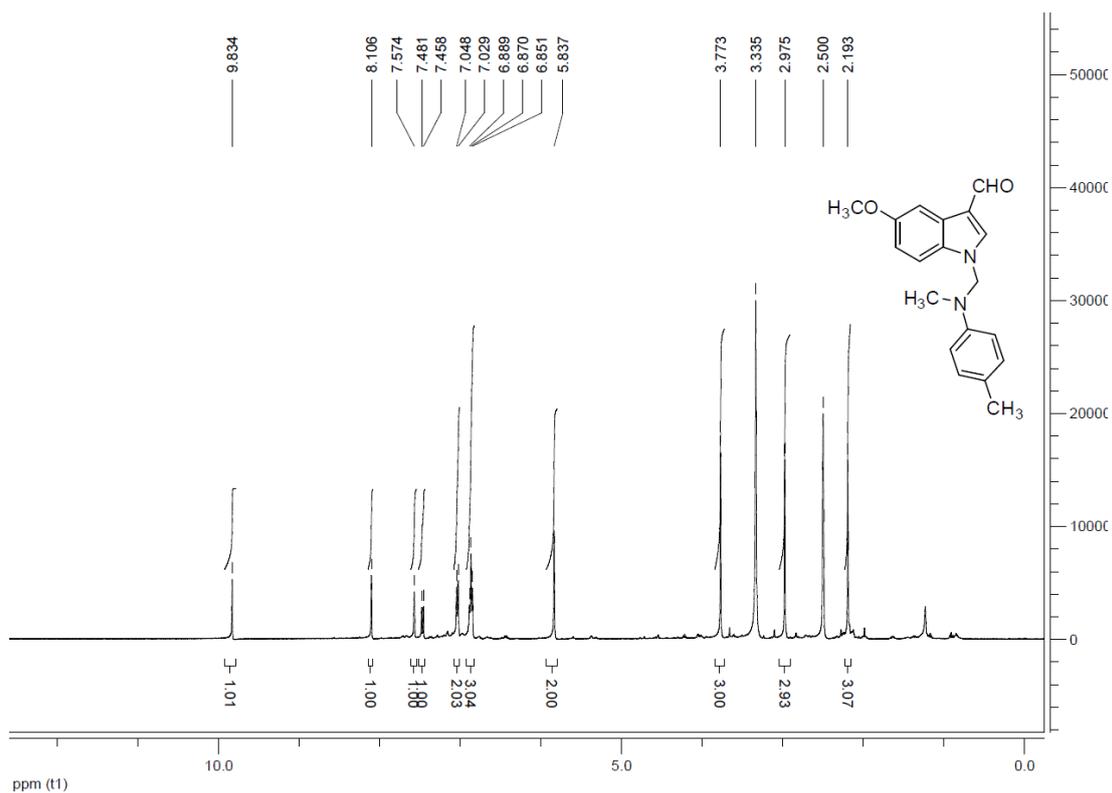




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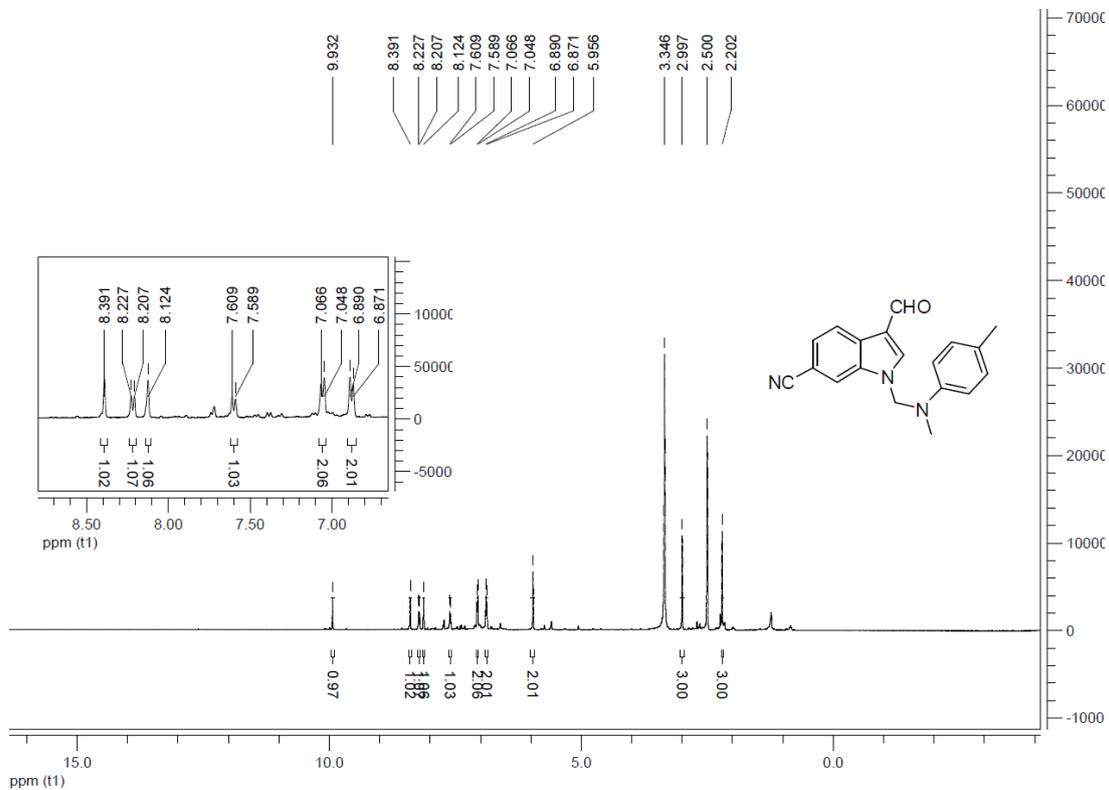
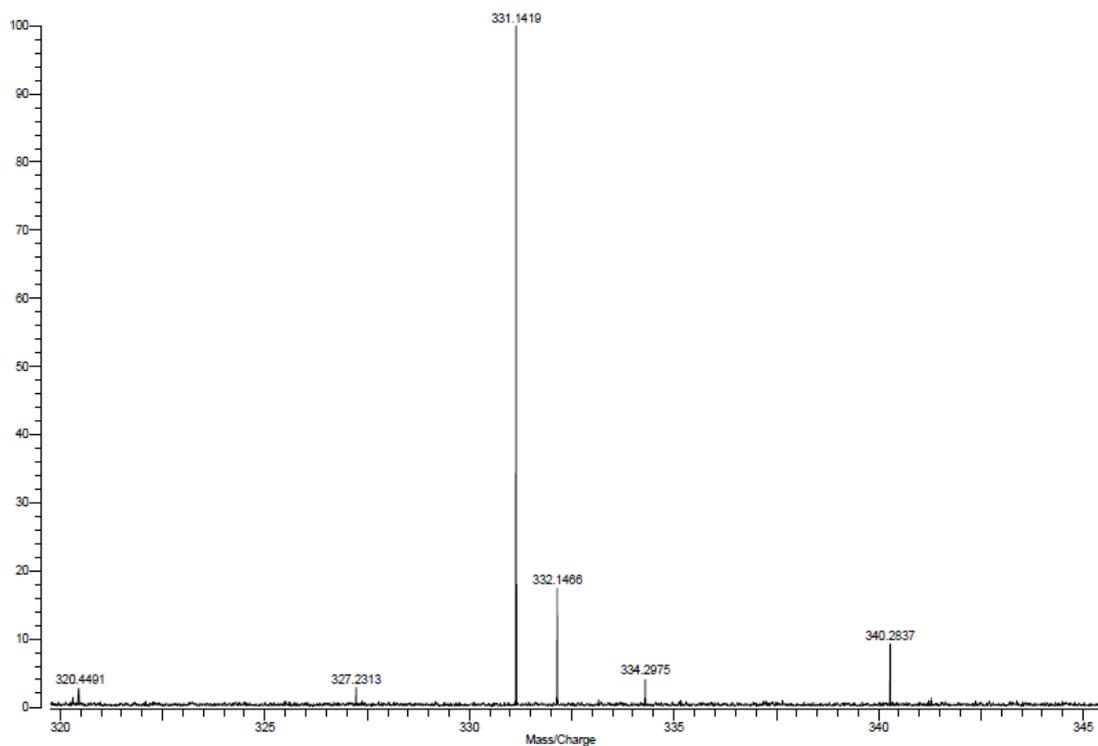


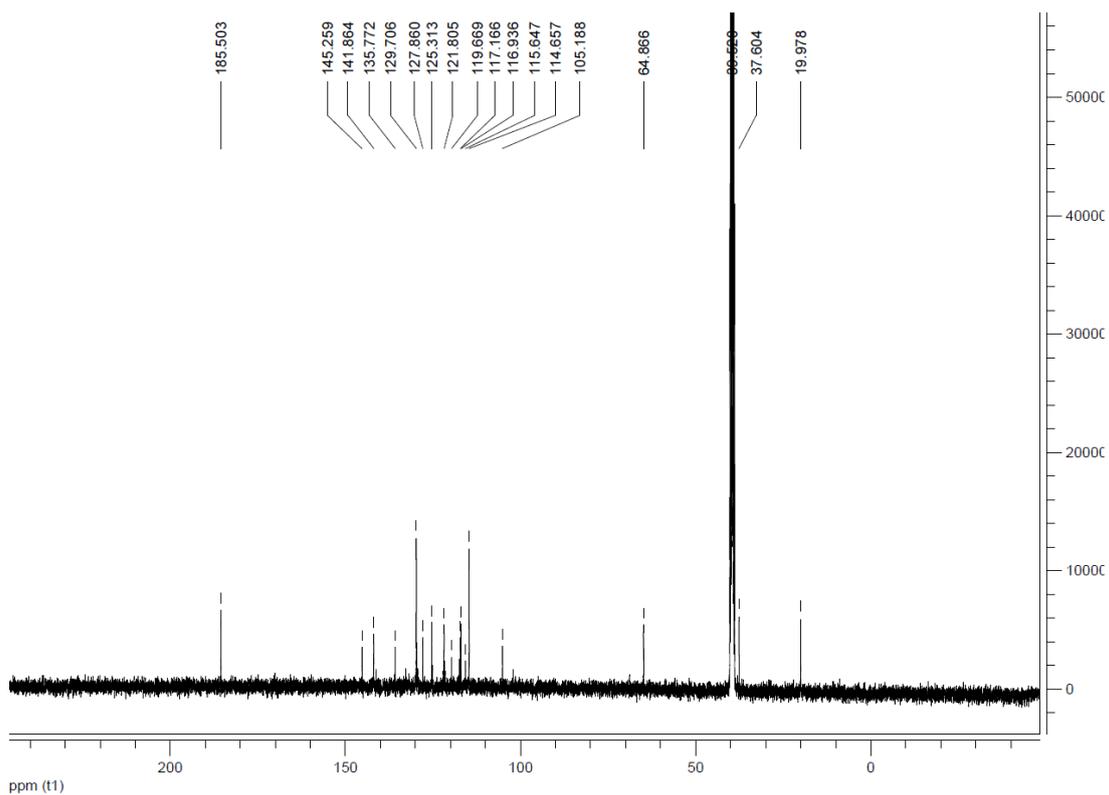


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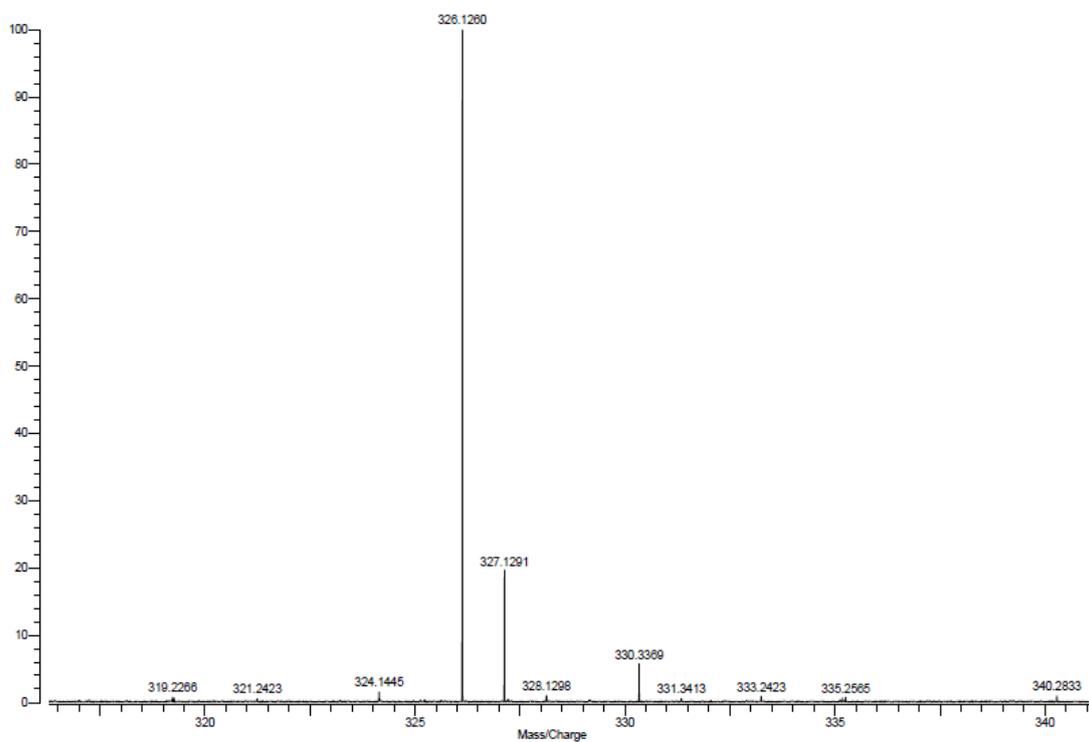
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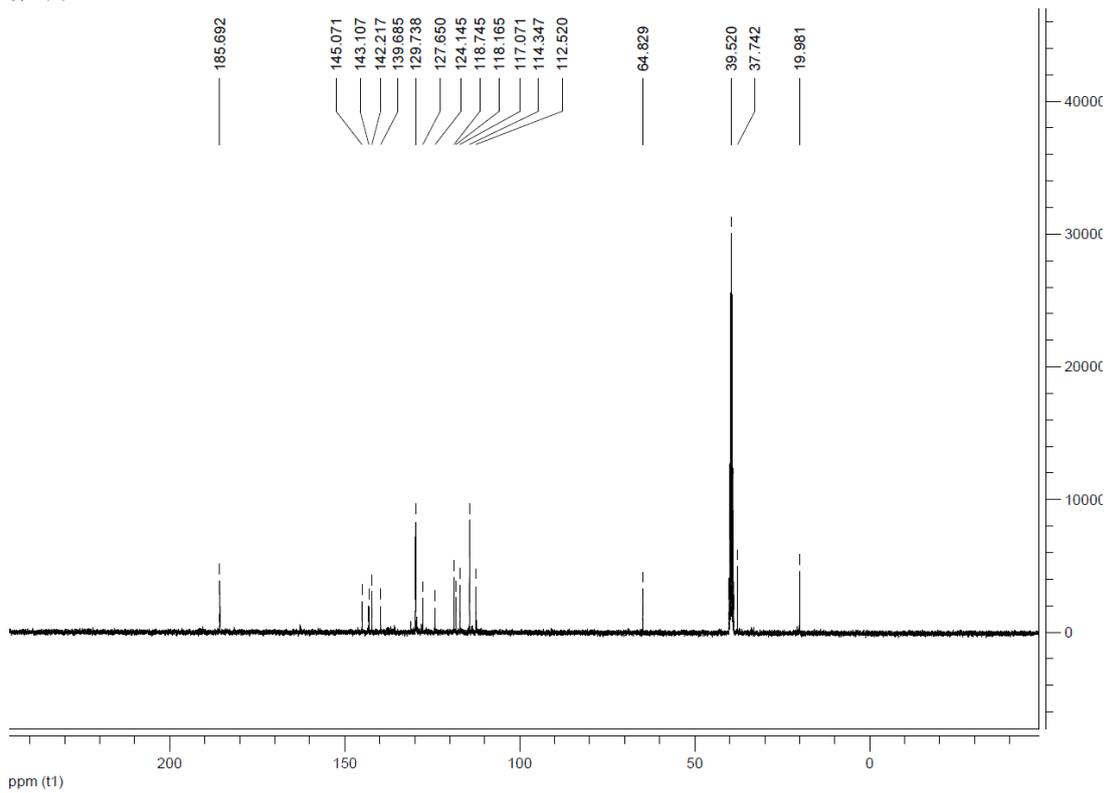
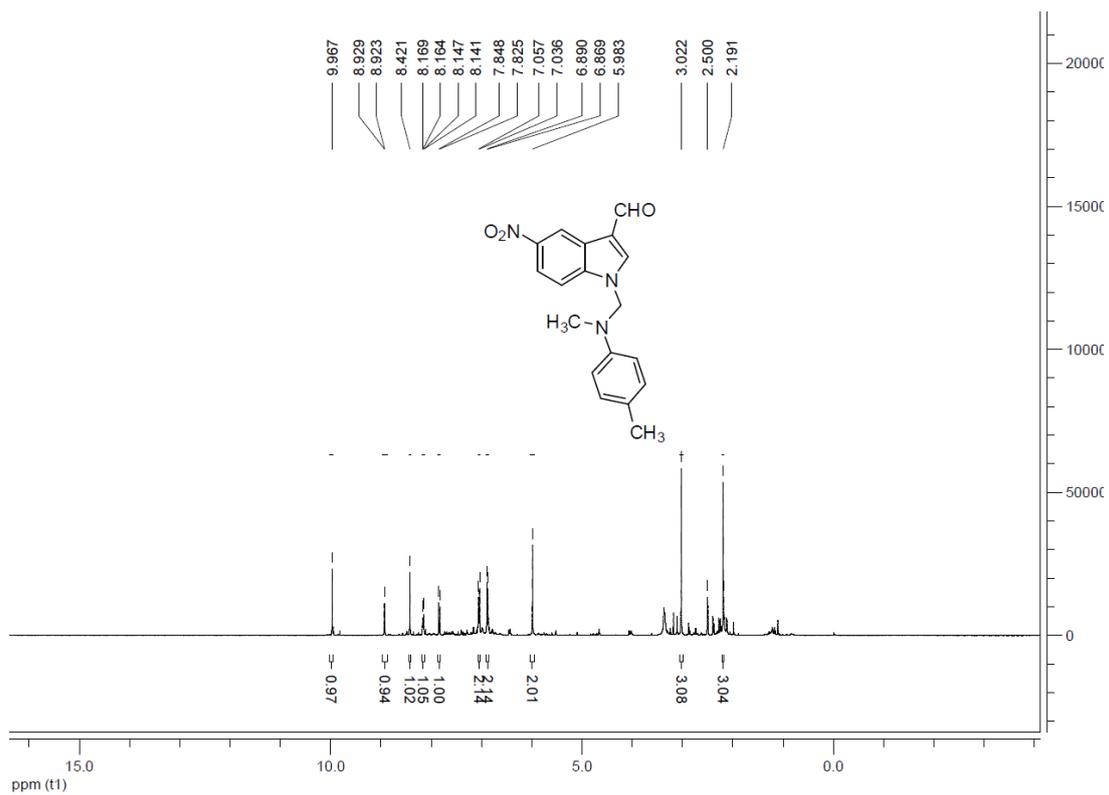




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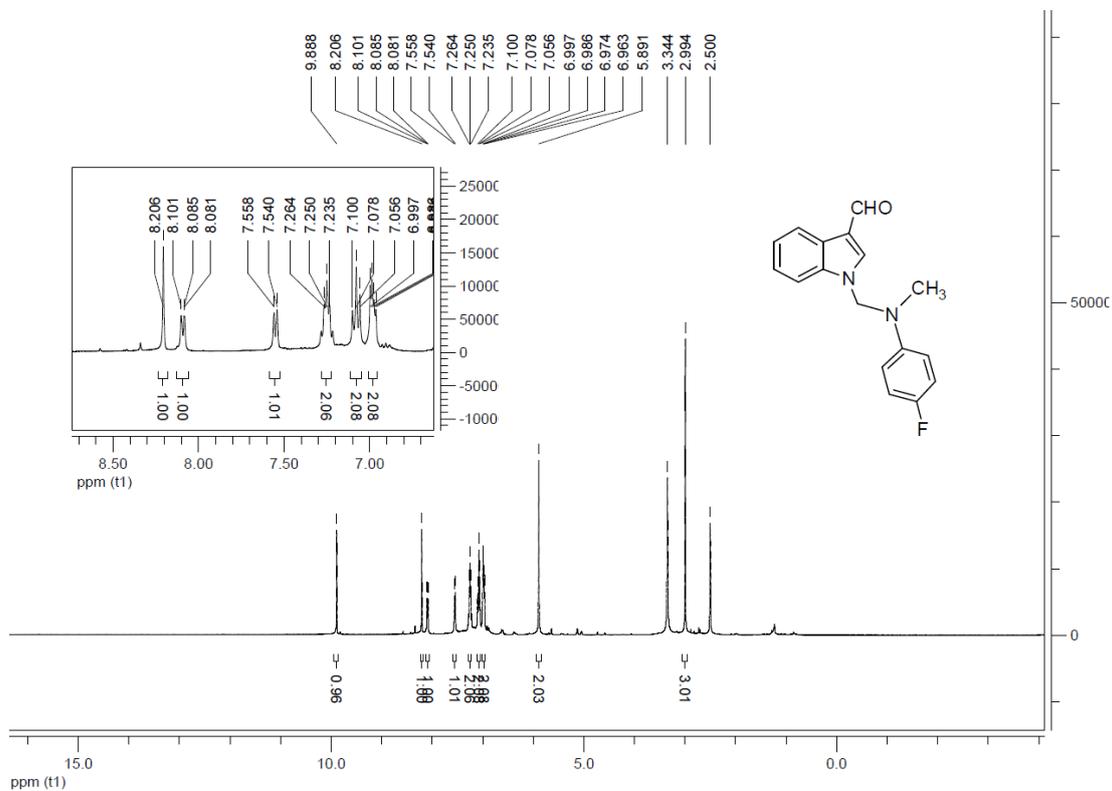
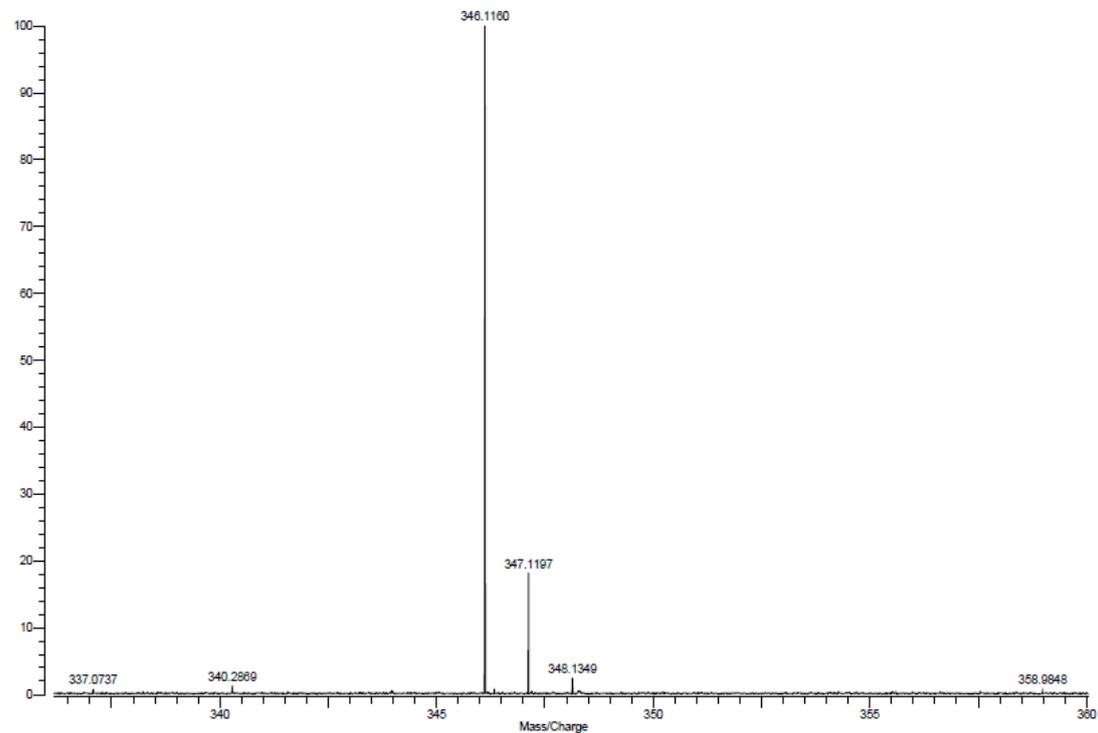


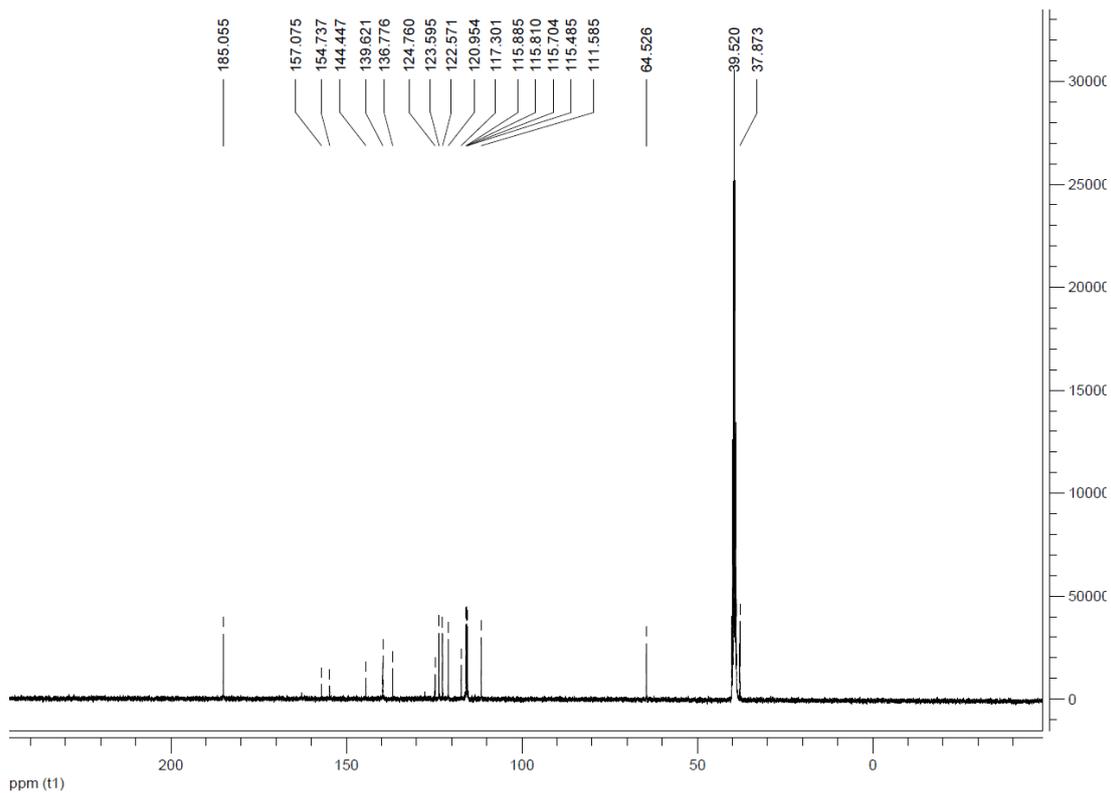


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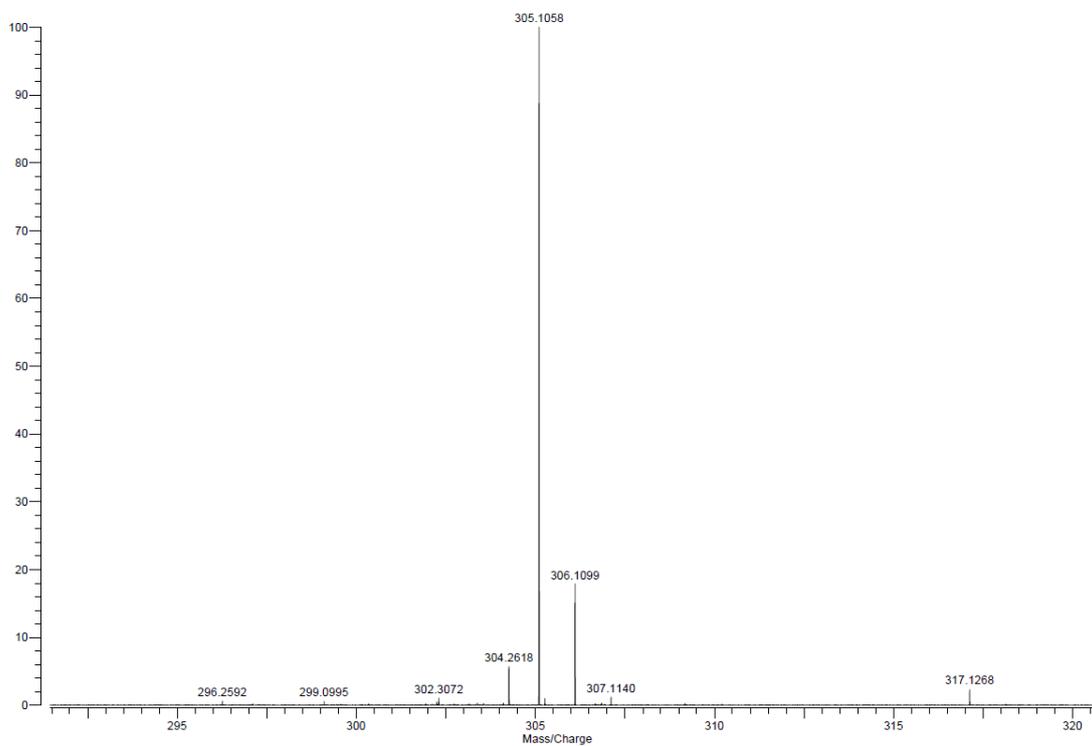
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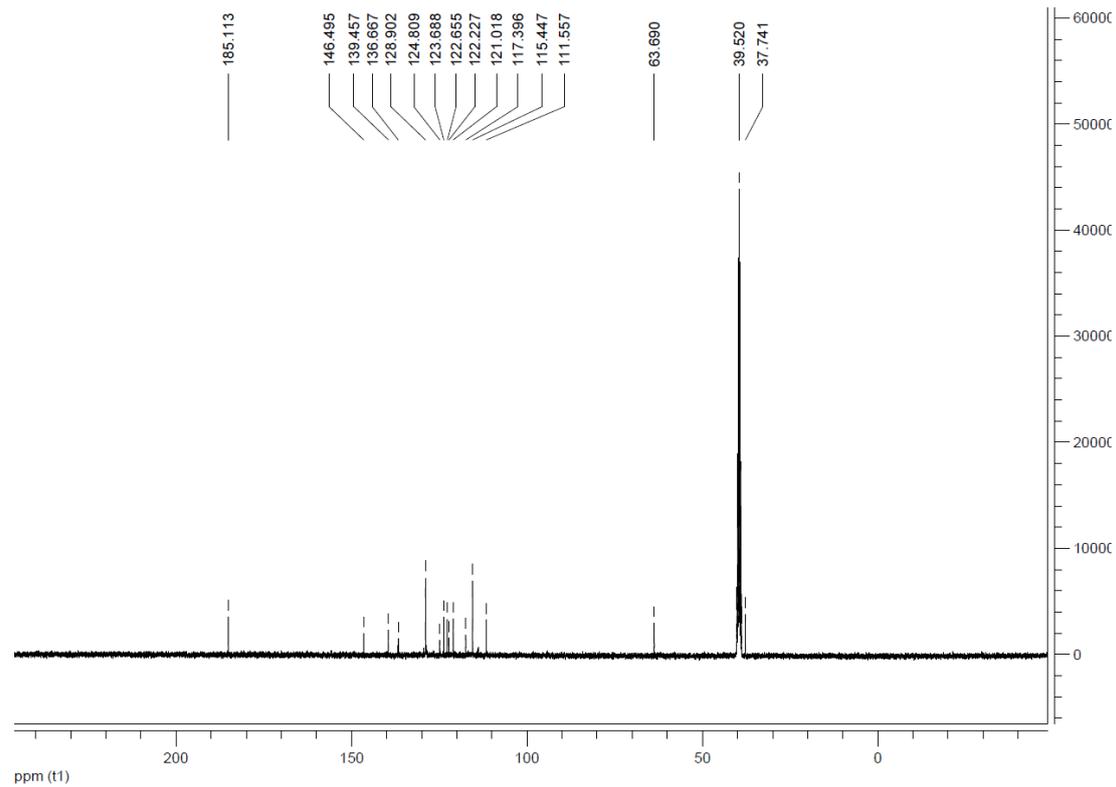
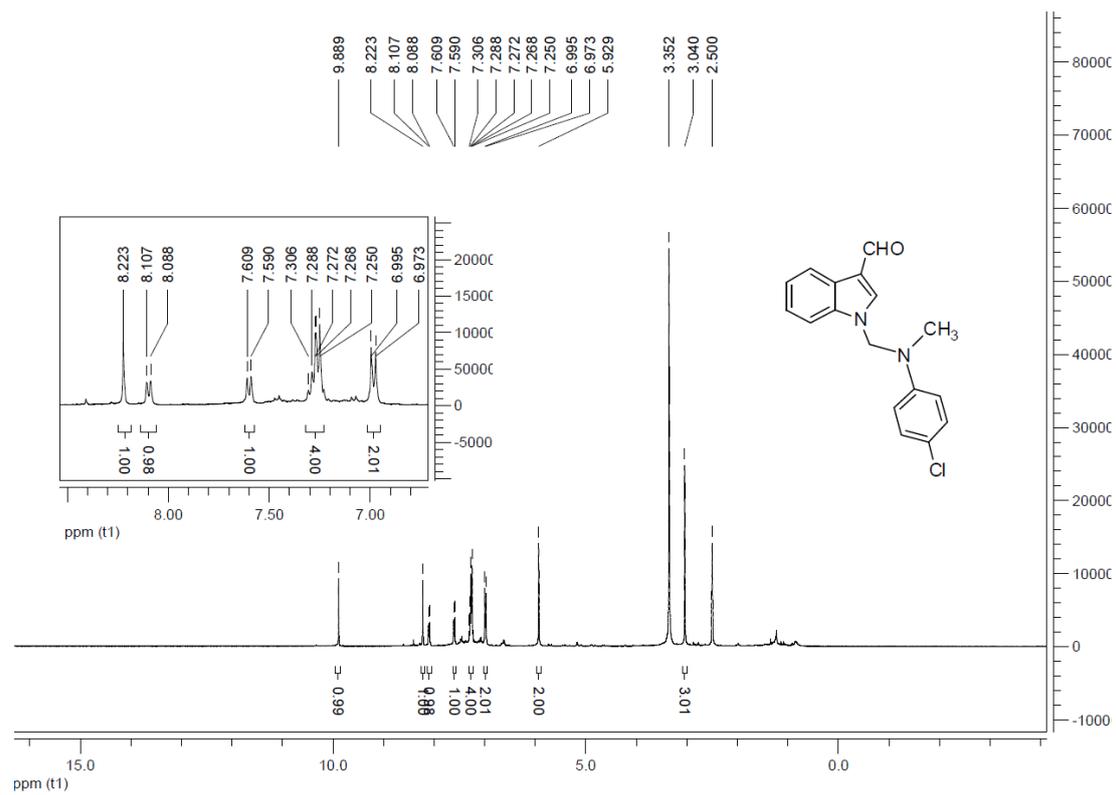




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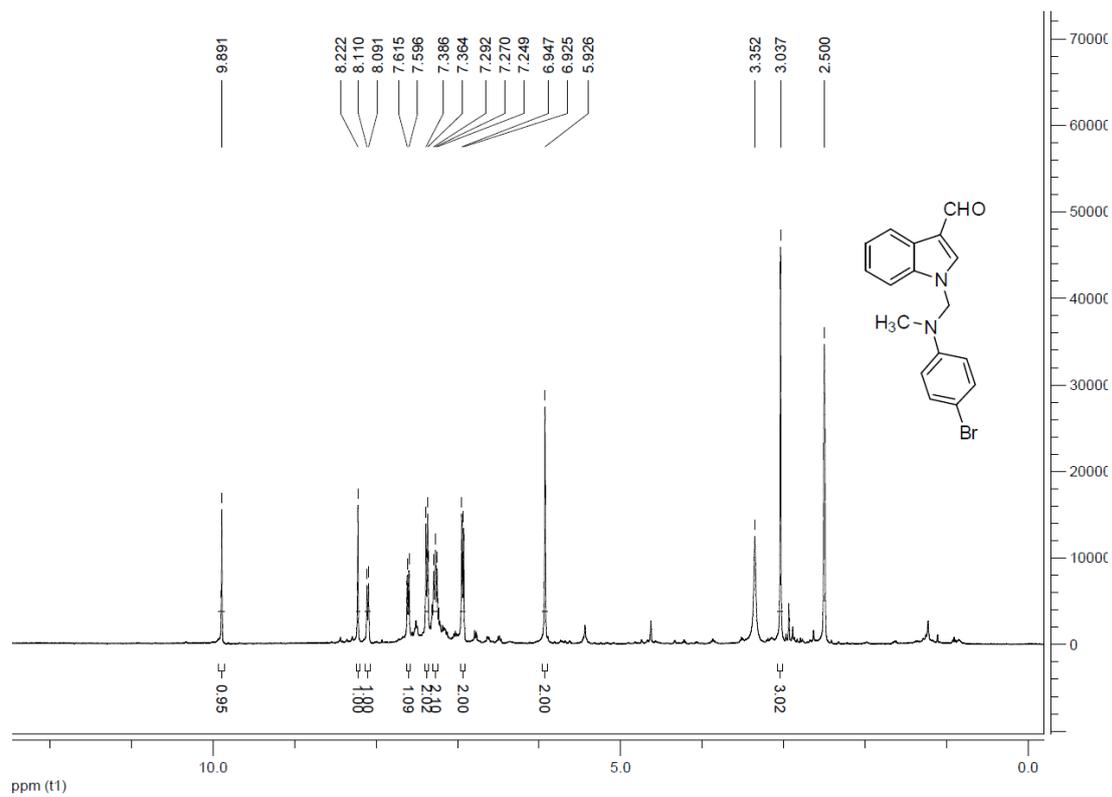
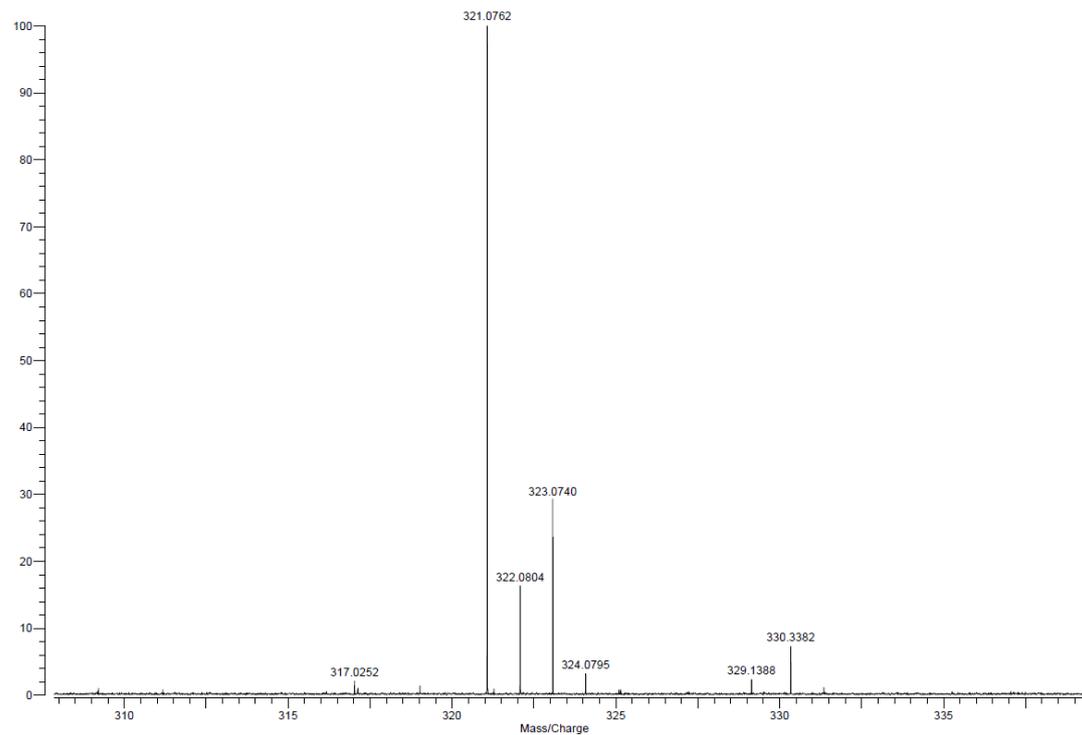


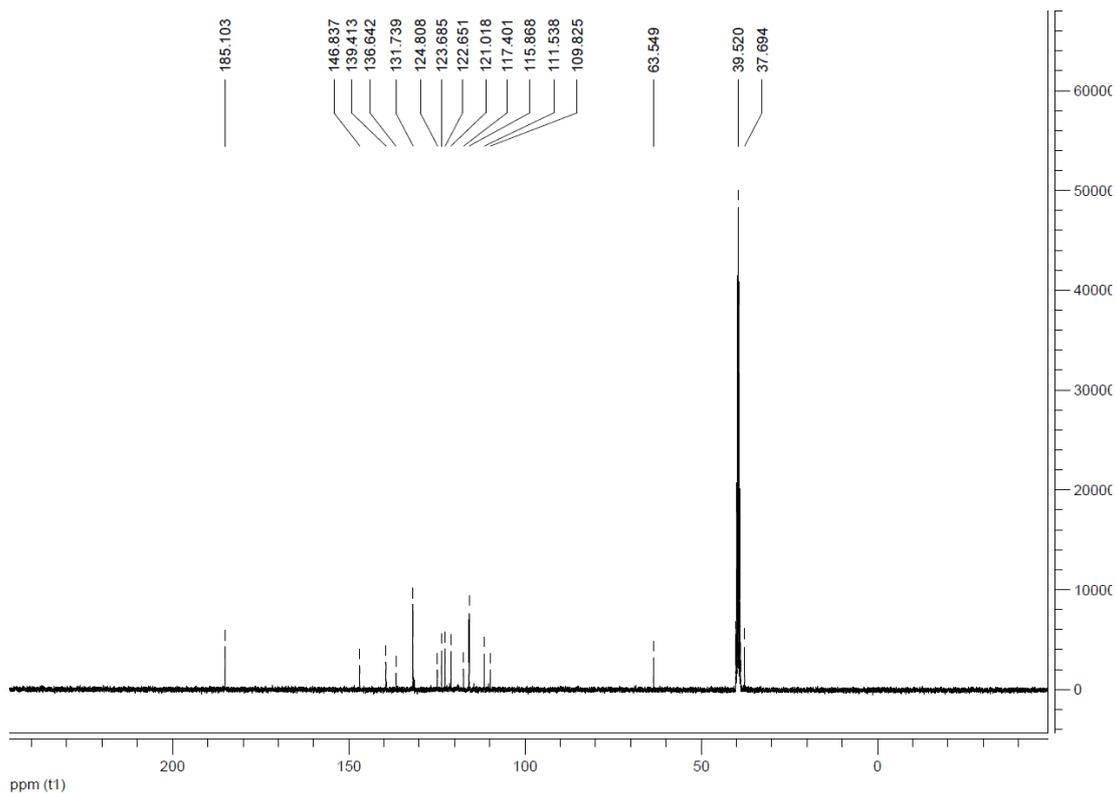


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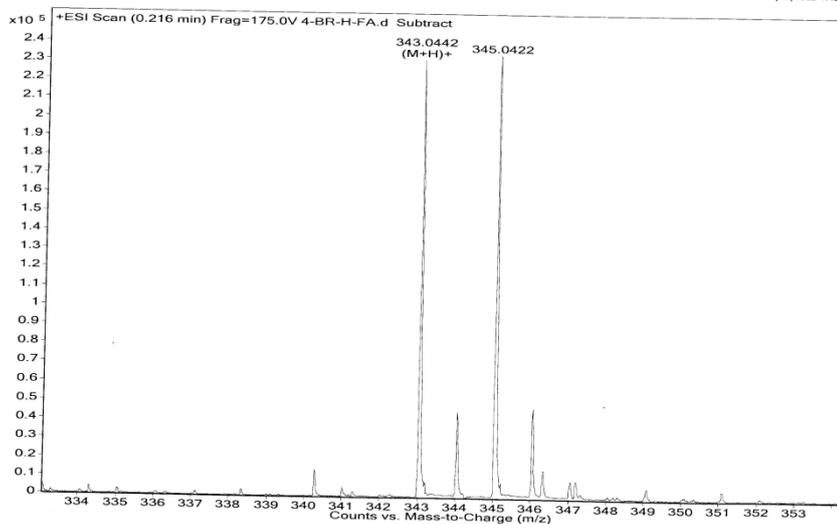
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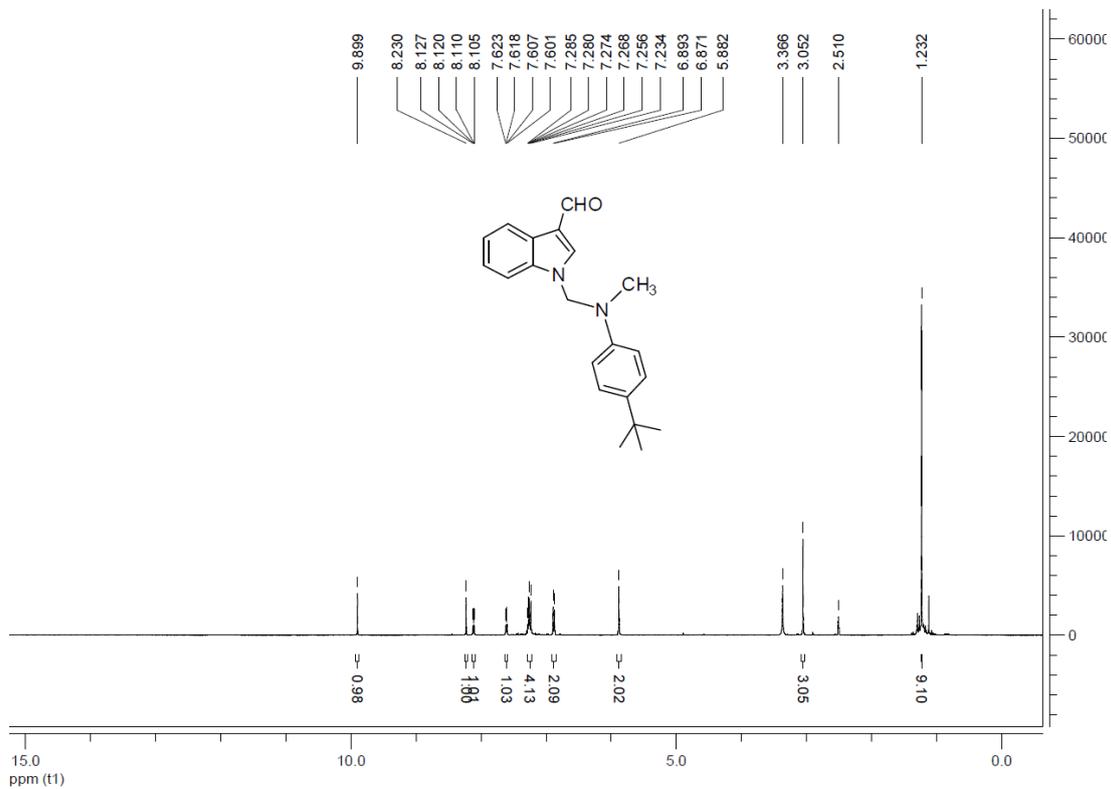
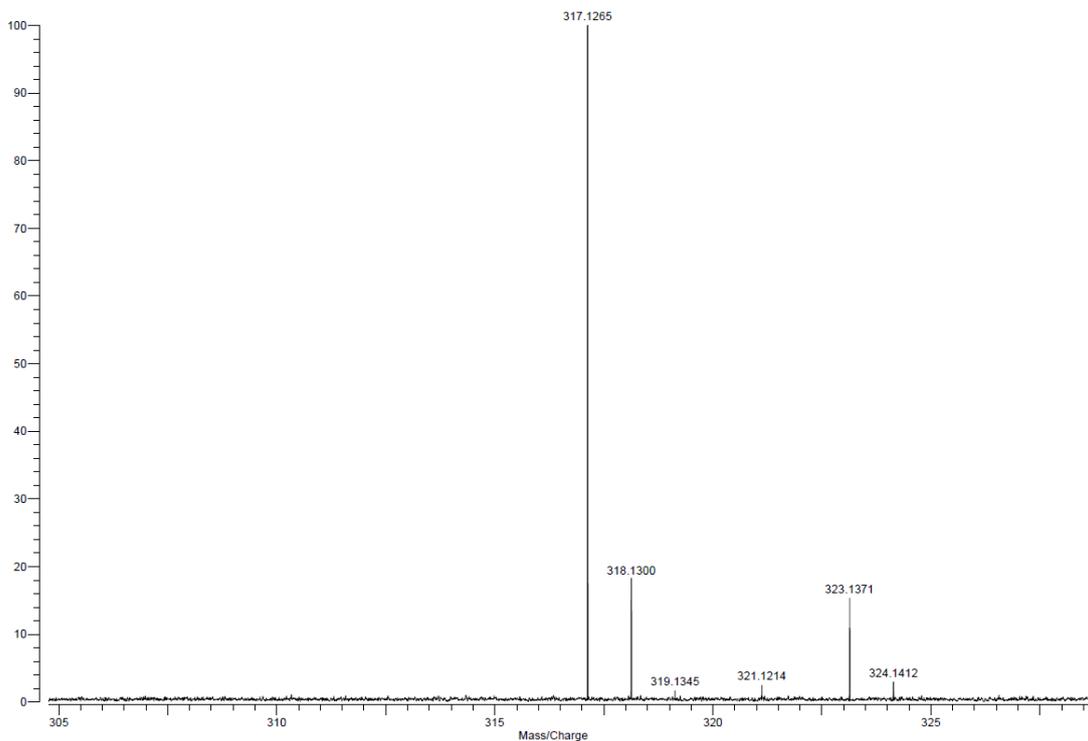
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Inj Vol	-1	InjPosition		SampleType	Sample	IRM Calibration Status
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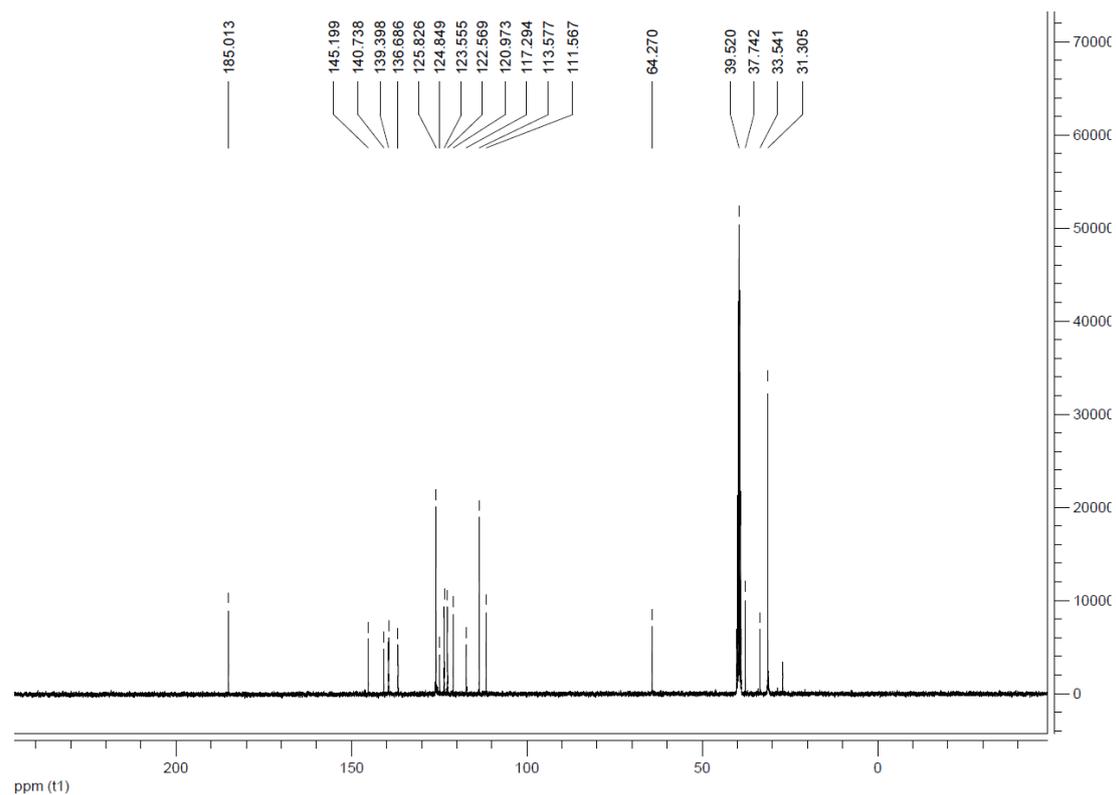


Varian QFT-ESI
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Scans: 1

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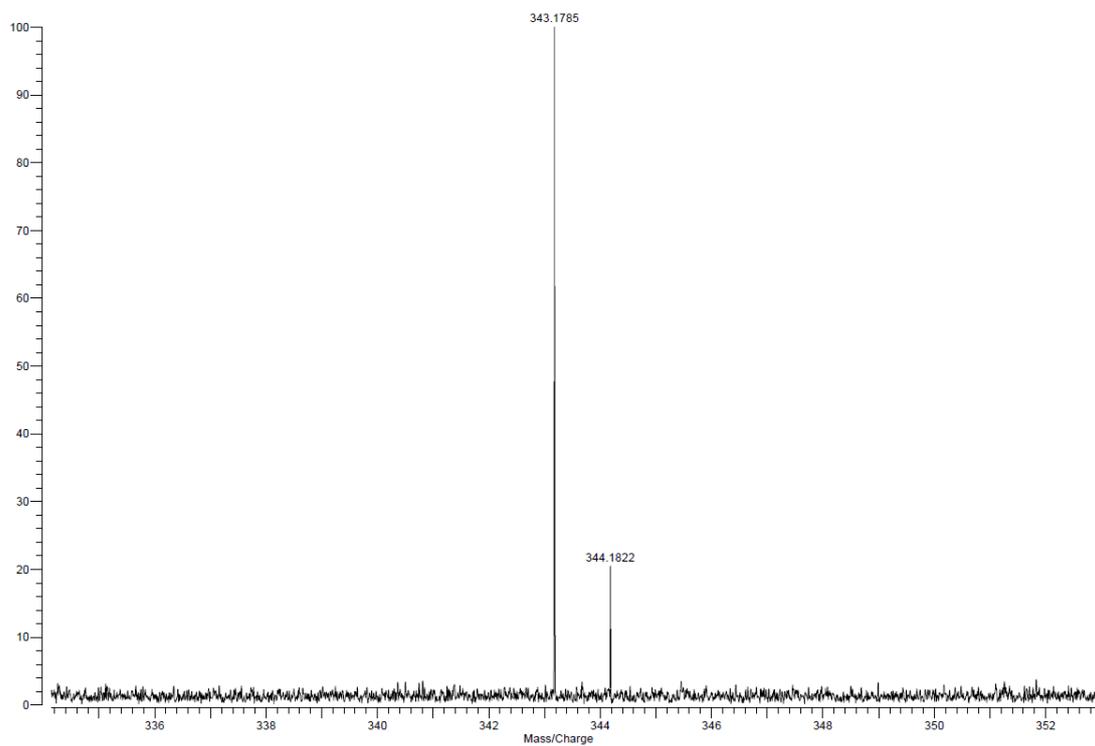


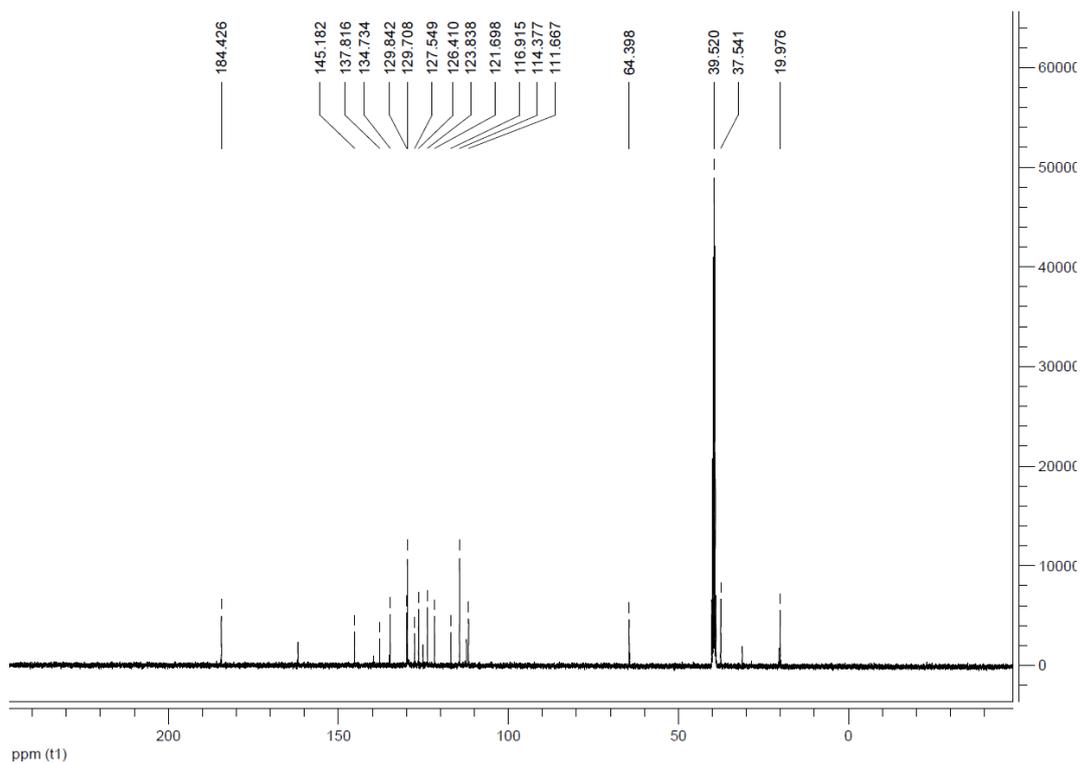
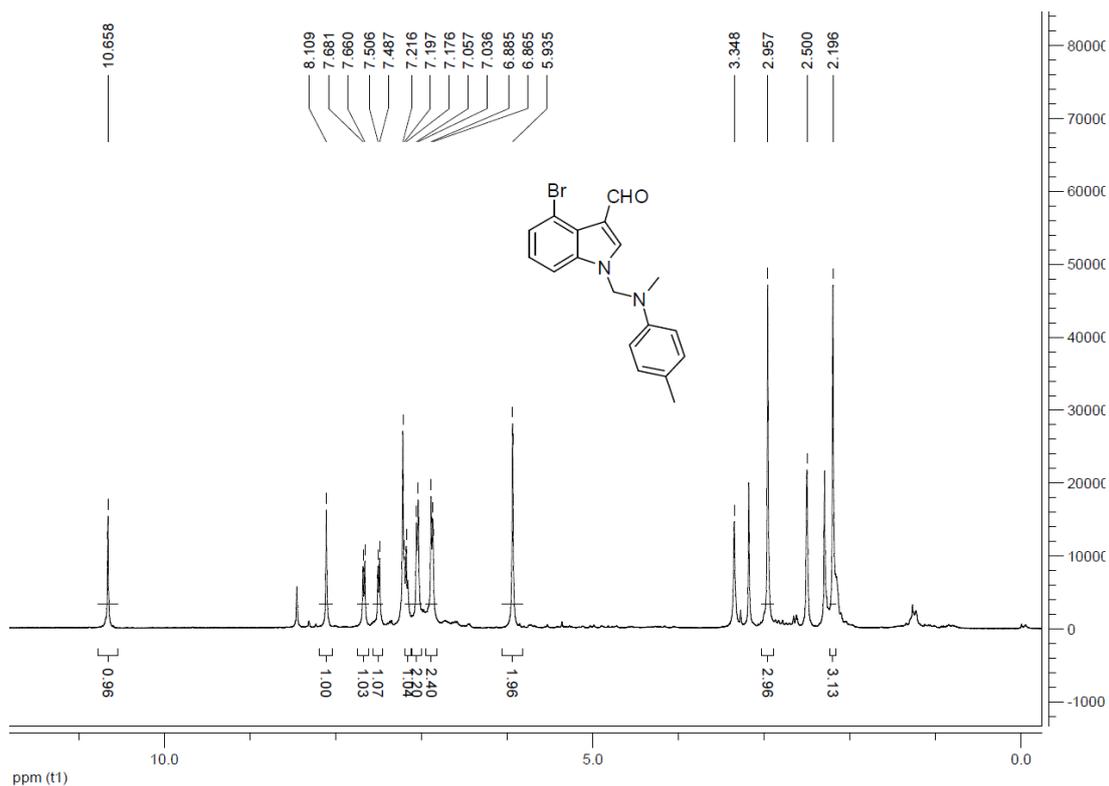


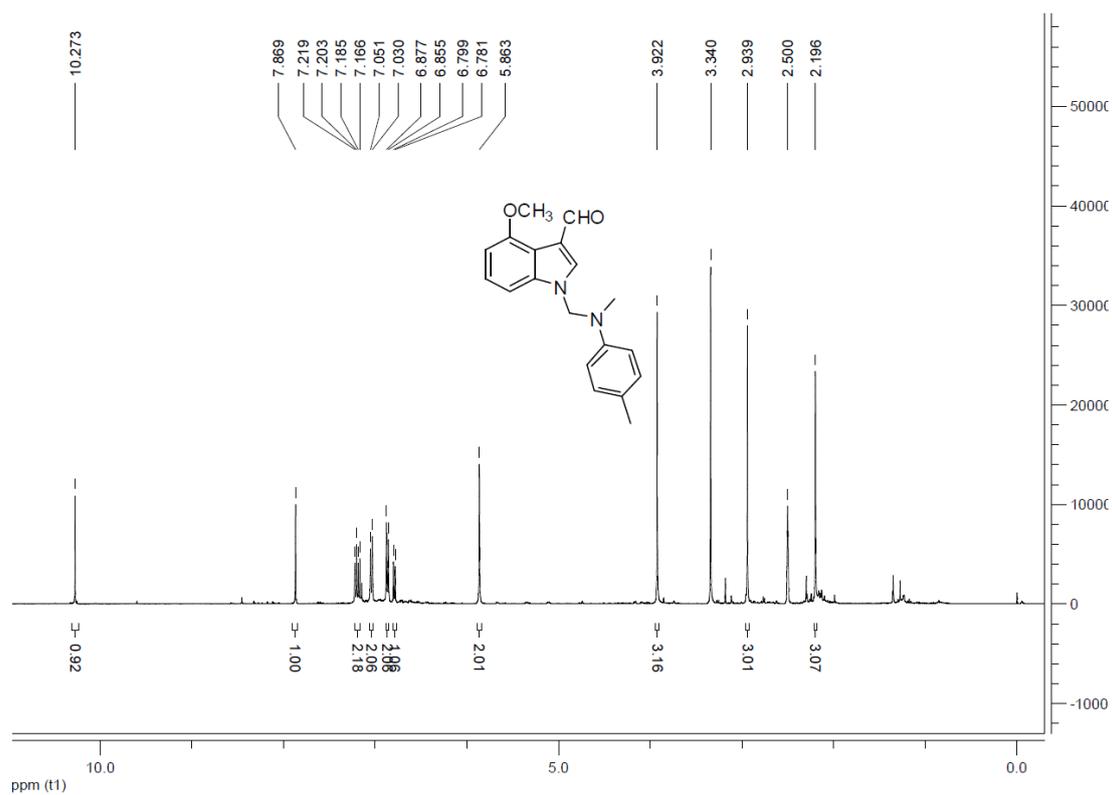
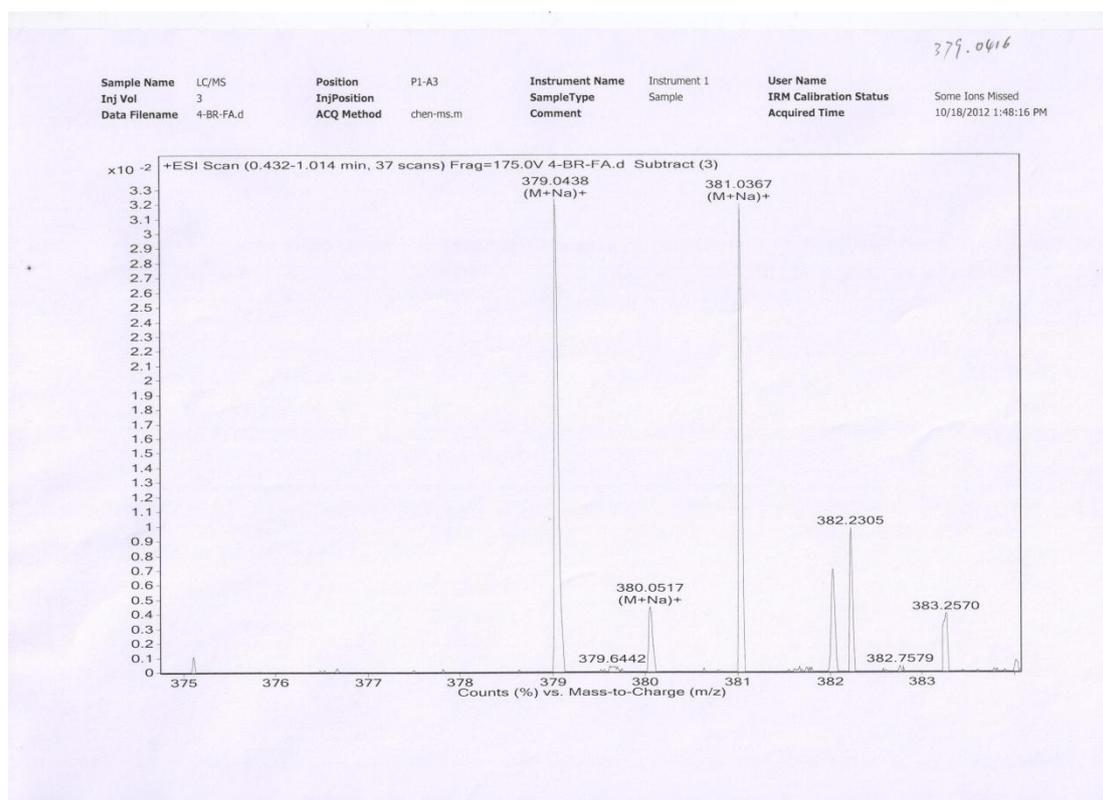
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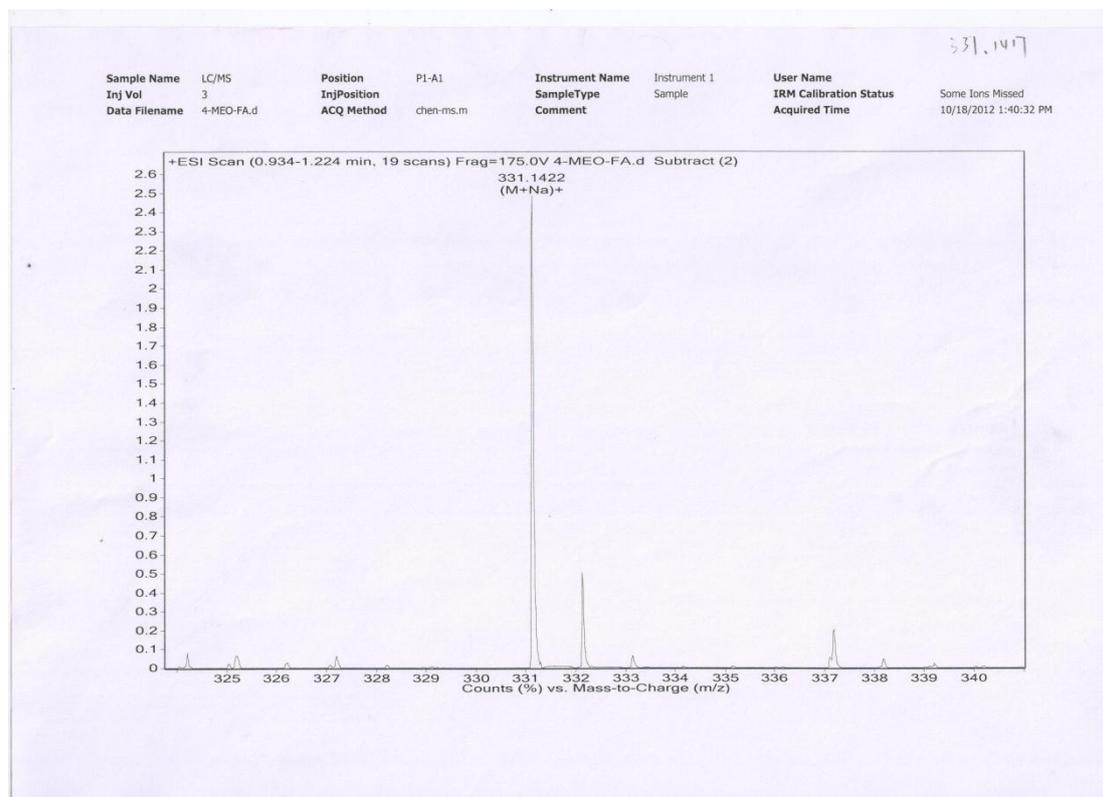
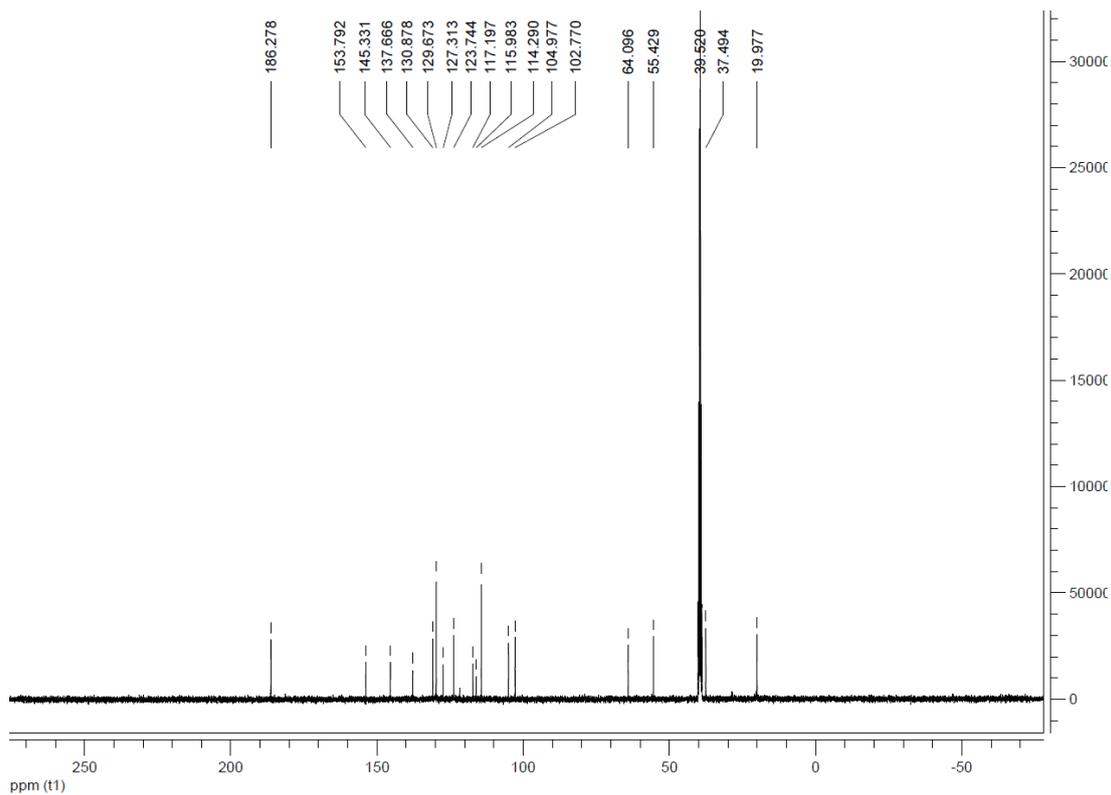
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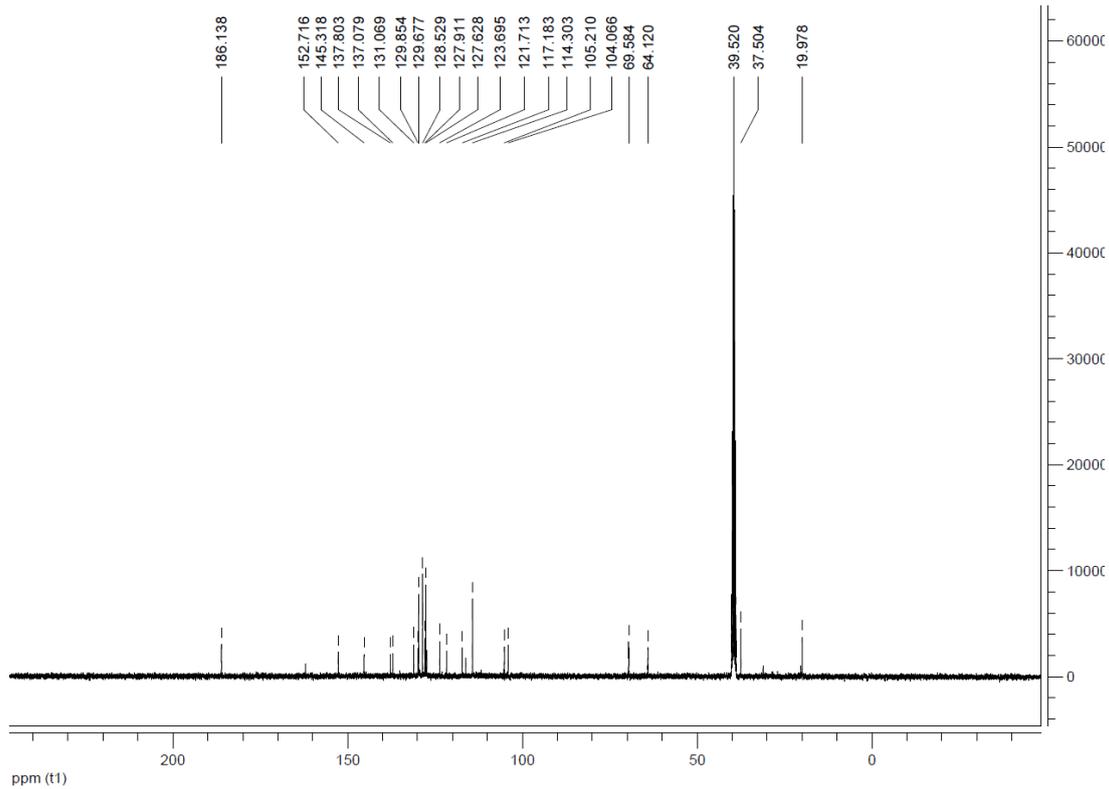
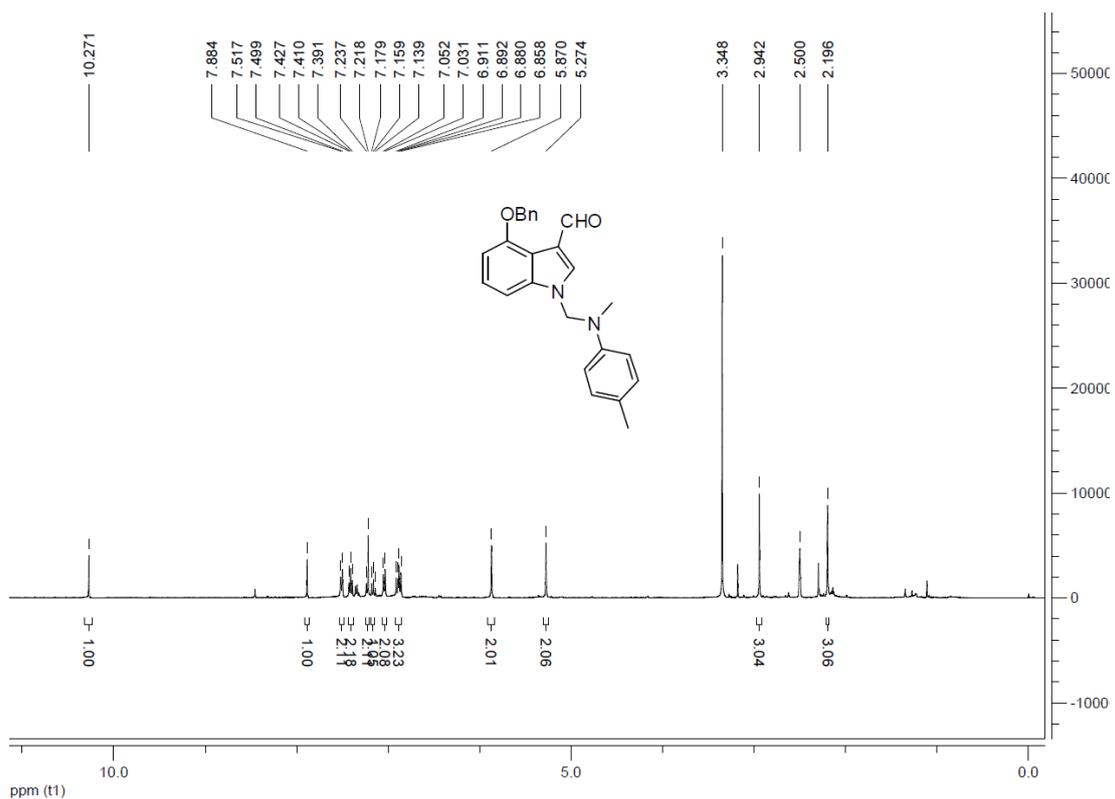
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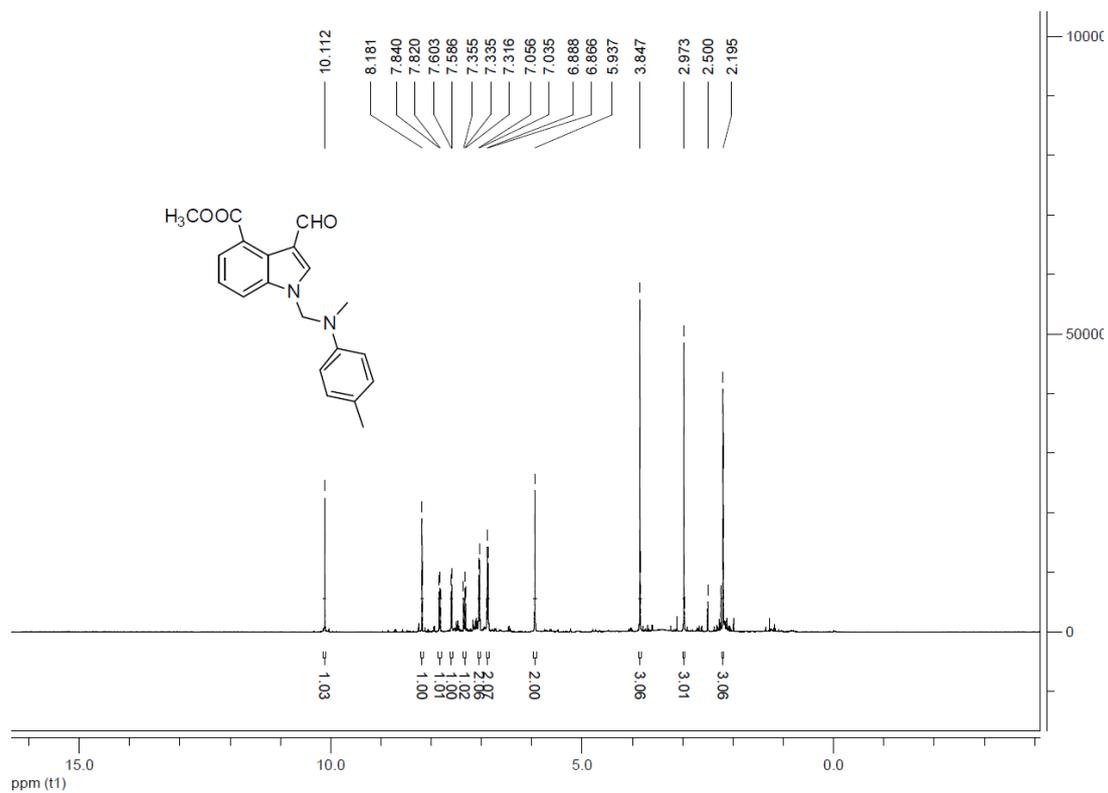
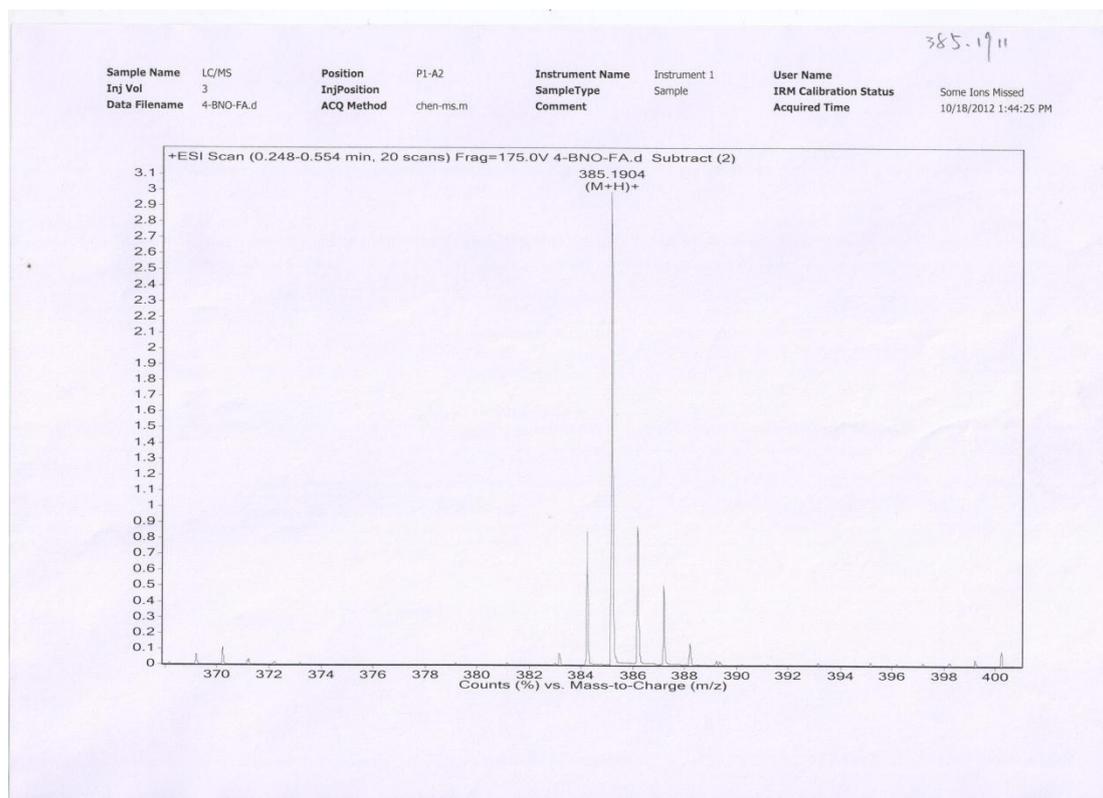


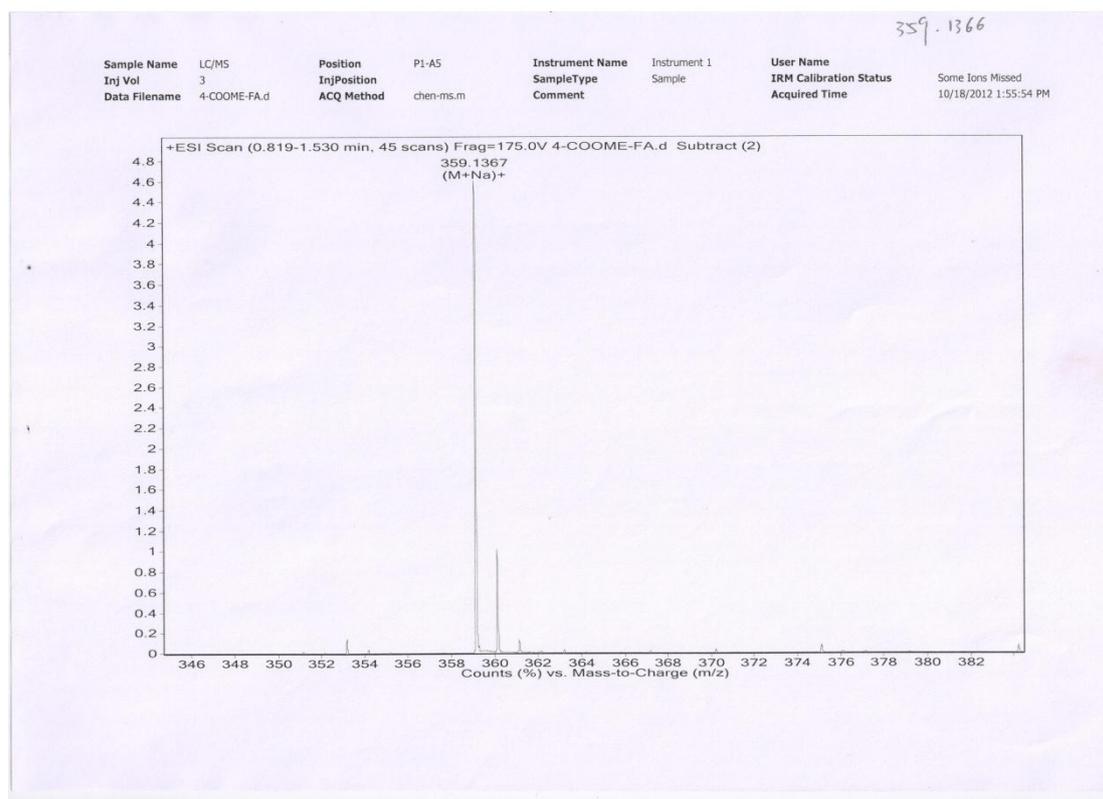
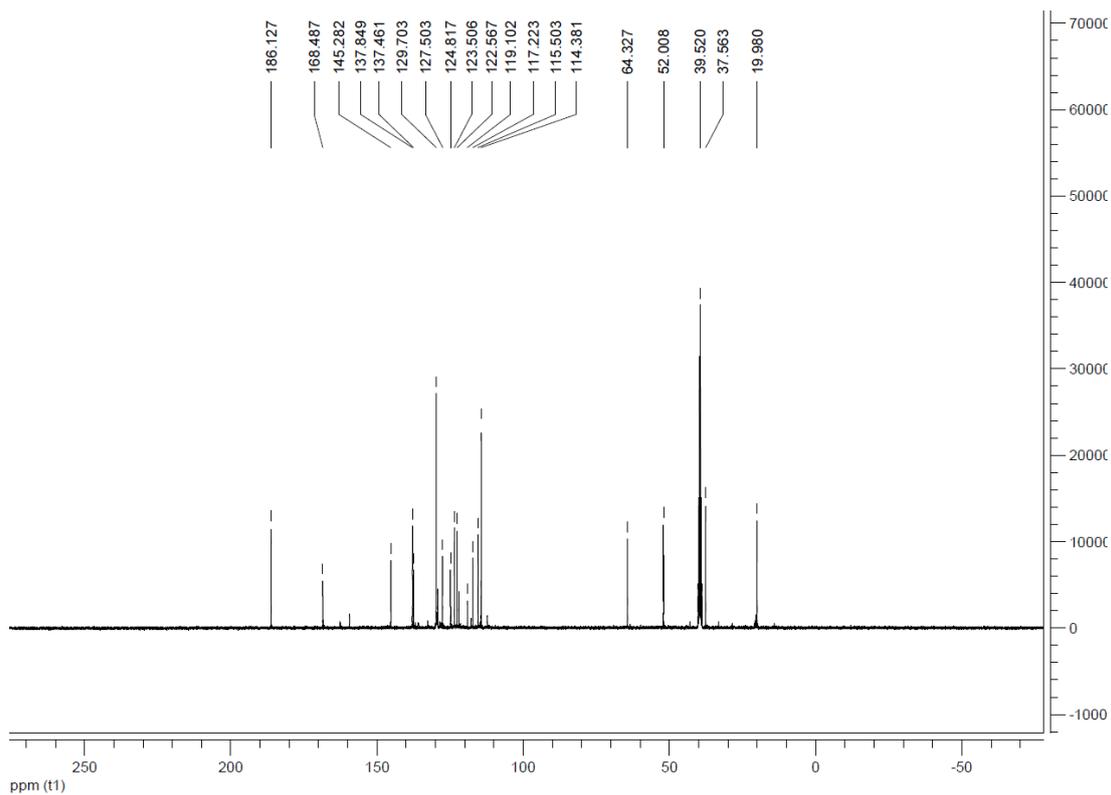


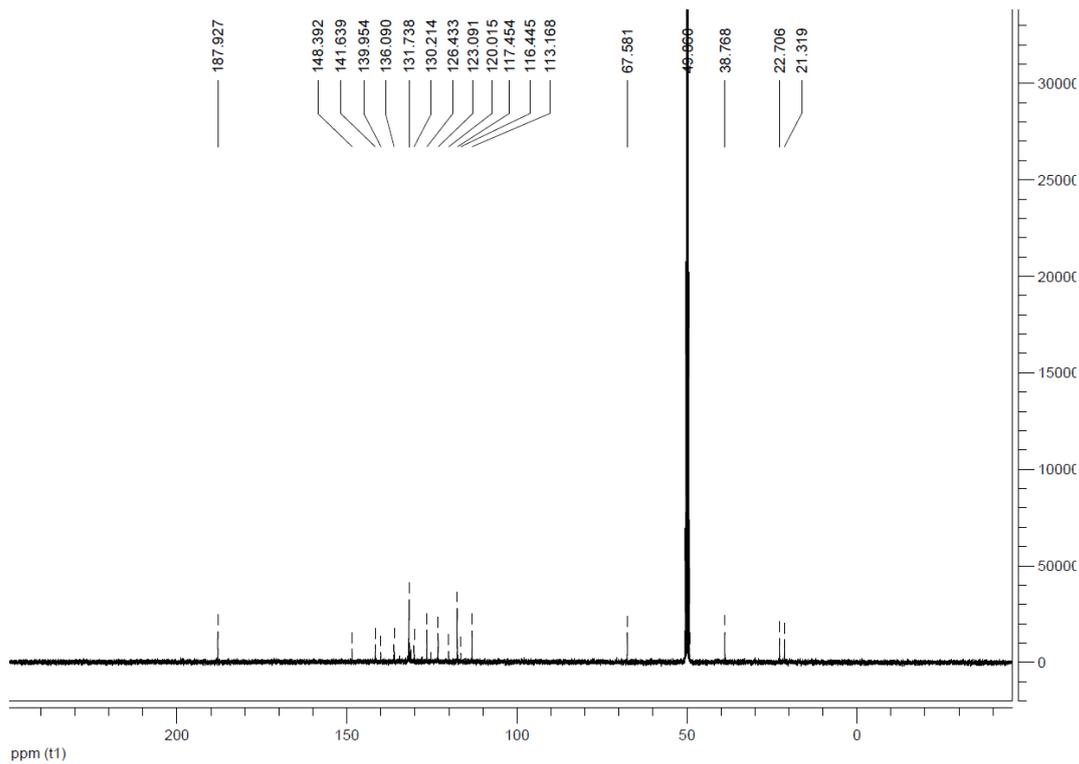
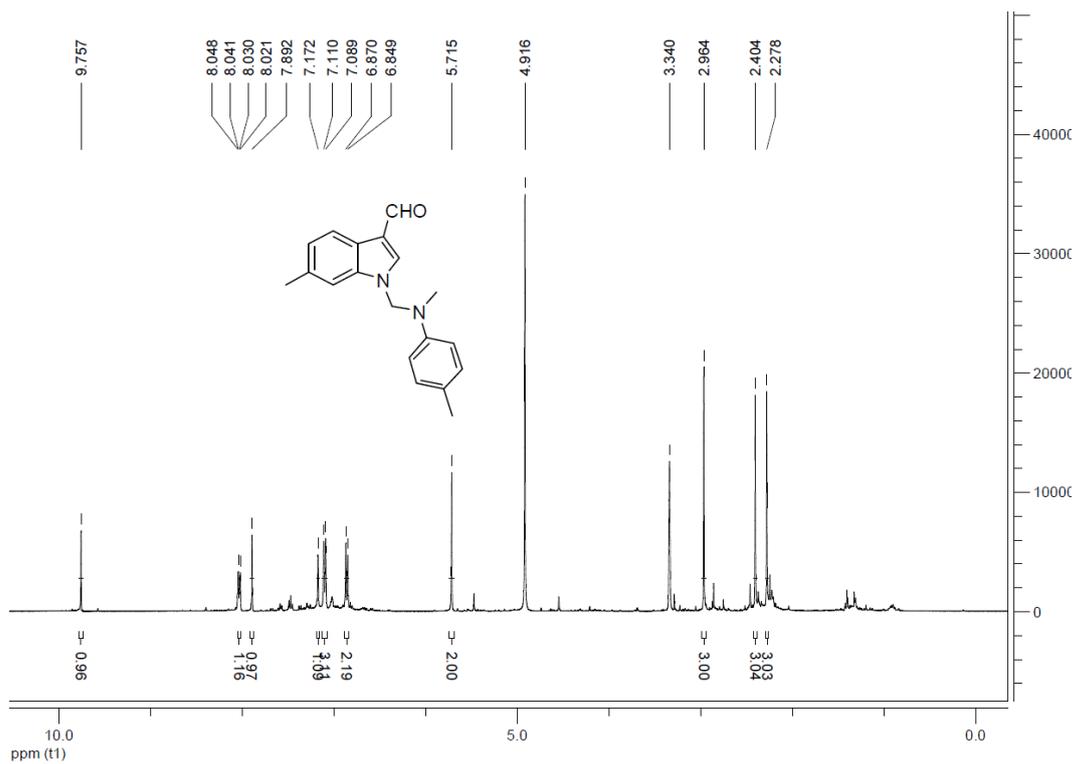


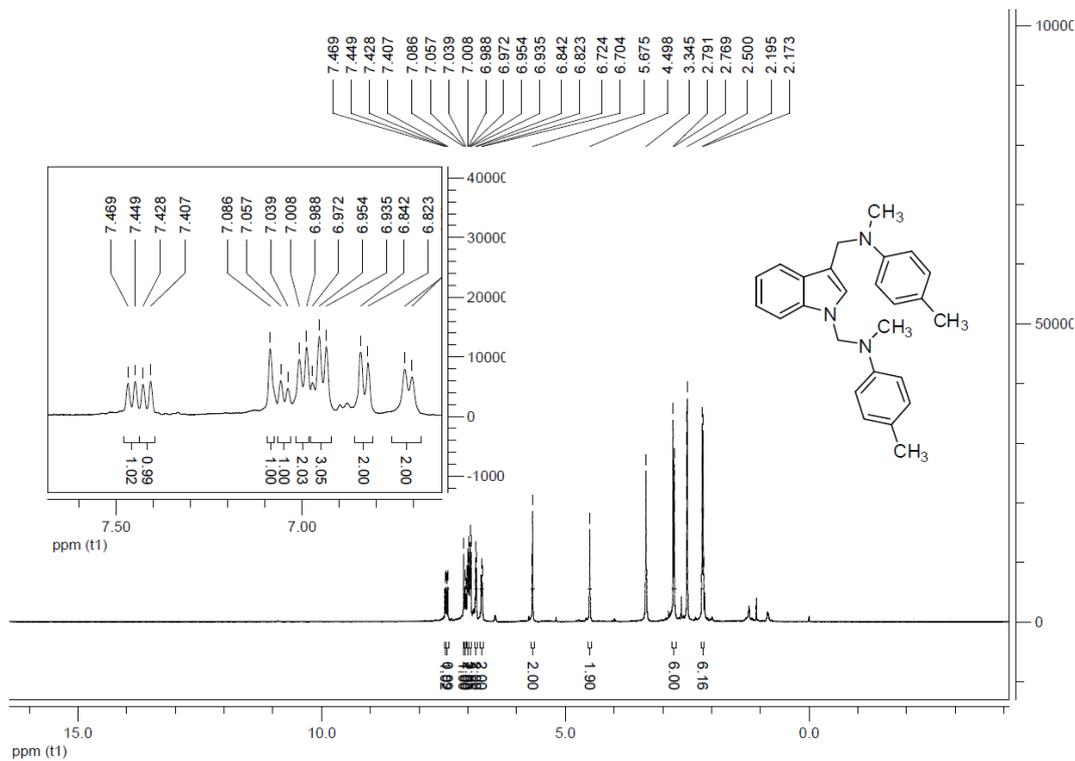
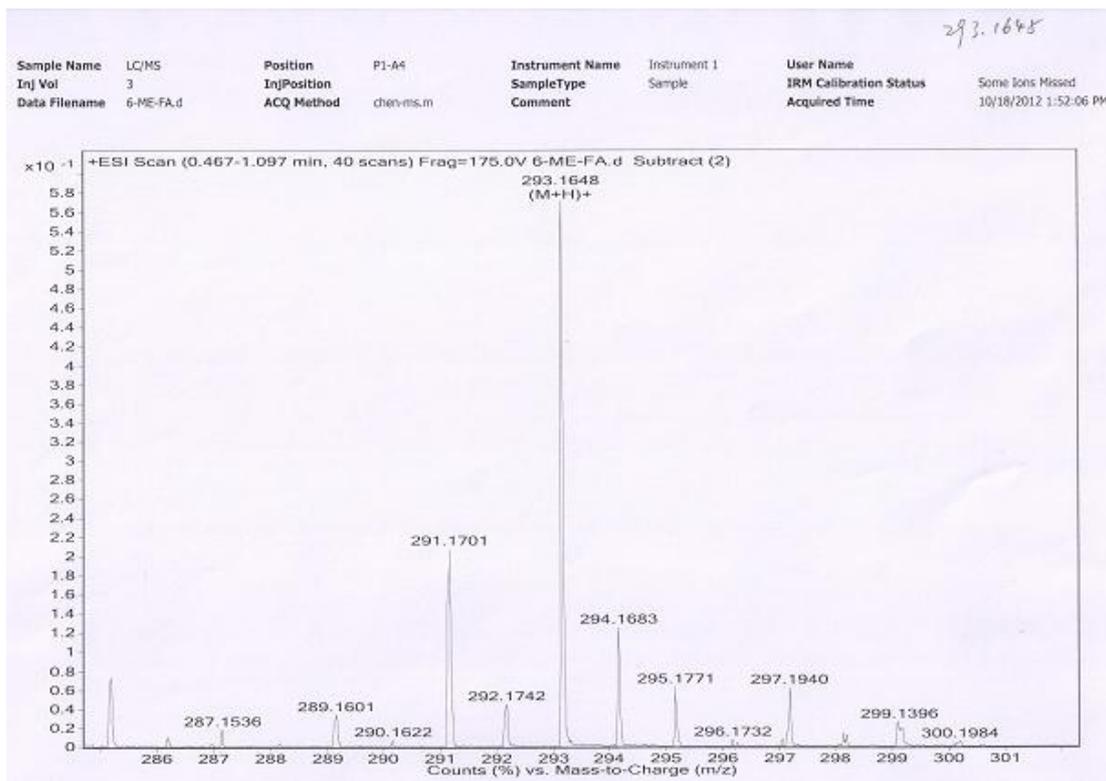


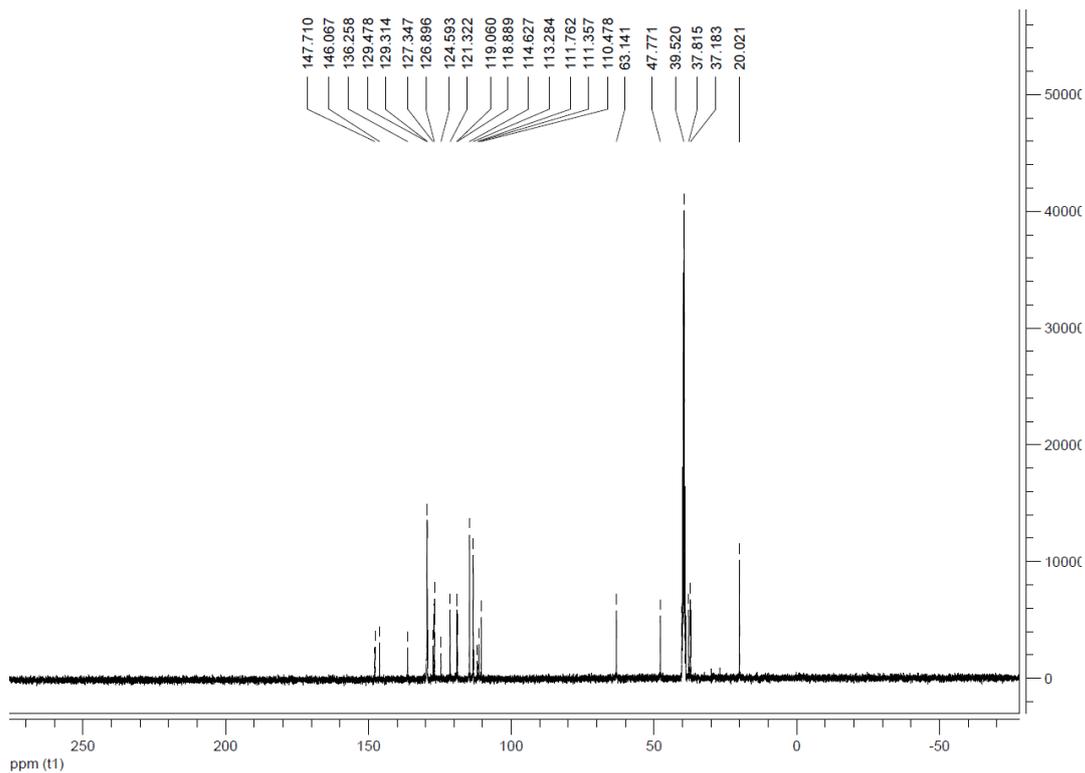






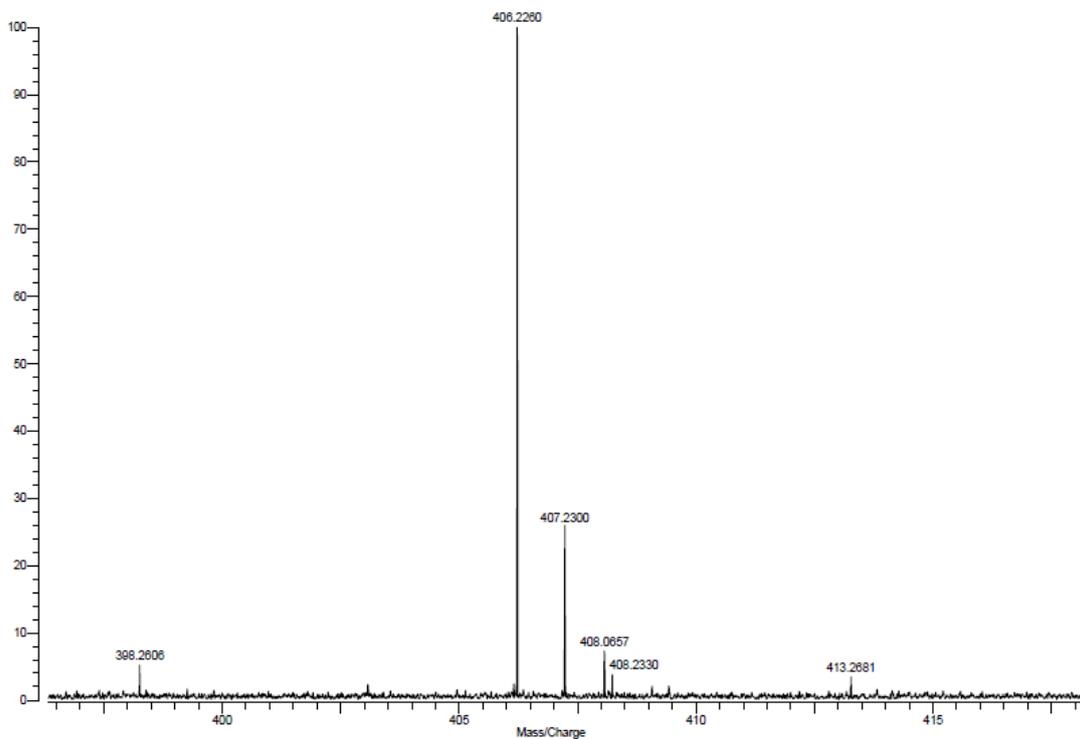


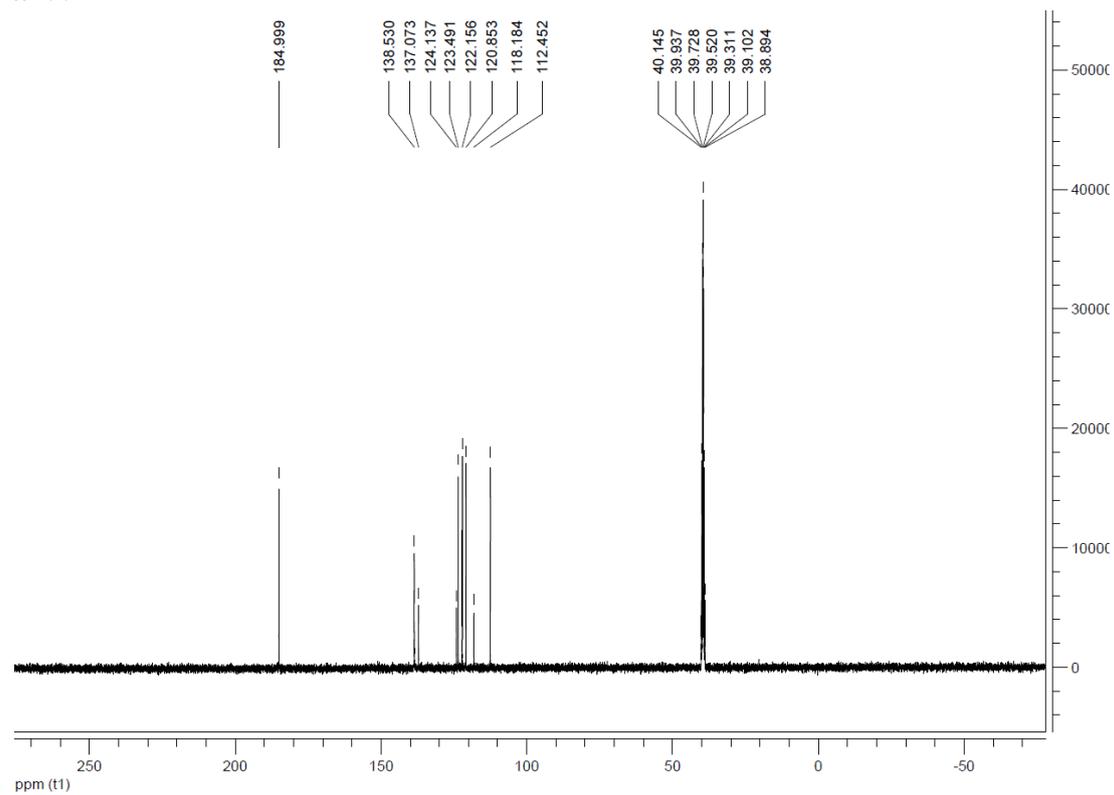
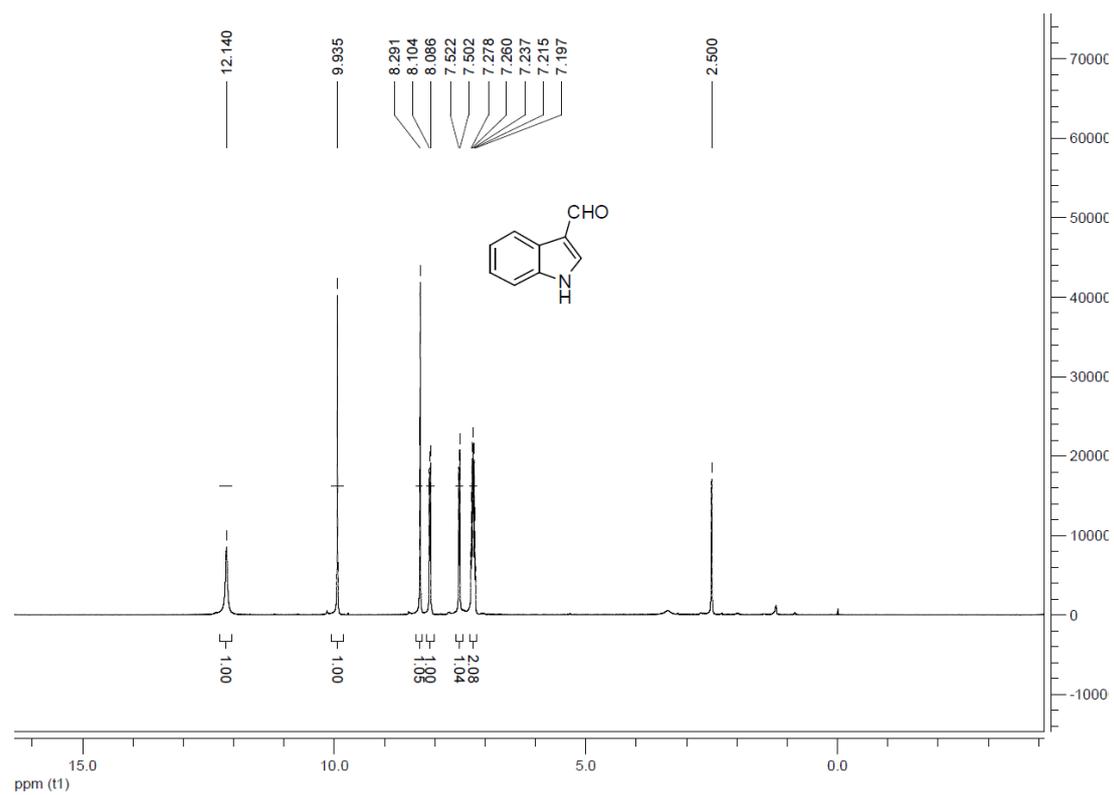




Varian QFT-ESI
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Mode: Positive
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Reference

- [1] L. Huang, T. Niu, J. Wu, Y. Zhang, *The Journal of Organic Chemistry* **2011**, *76*, 1759-1766.