Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Electronic Supplementary information

Cu–Catalyzed Sequential C–N Bond Formations: Expeditious Synthesis of Tetracyclic Indoloindol-3-ones

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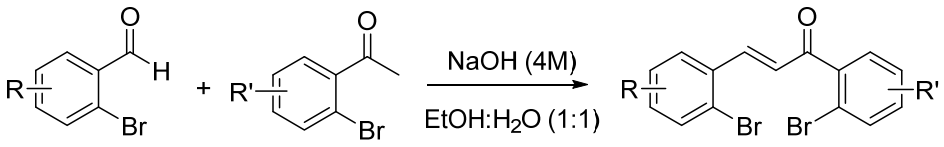
General Remarks: All reactions were carried out in anhydrous solvents under an atmosphere of argon in oven–dried glassware. Commercial reagents and solvents were used without purification. Column chromatography was carried out by using spectrochem silica gel (60–120, 100–200, 230–400 mesh size). ^{1}H and ^{13}C NMR spectroscopy measurements were carried out on Bruker AC 200 MHz, Bruker DRX 400, DRX 500 MHz and JEOL 400 spectrometers, and TMS was used as an internal standard. ^{1}H and ^{13}C NMR chemical shifts are reported in ppm downfield from $CDCl_3$ (δ = 7.25) or TMS and coupling constants (J) are reported in Hertz (Hz). The following abbreviations are used to designate signal multiplicity: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet, b = broad. The Multiplicity of ^{13}C NMR signals was assigned with the help of DEPT spectra and the abbreviations used: s = singlet d = doublet t = triplet q = quartet, represent C (quaternary), CH, CH_2 and CH_3 respectively. Mass spectroscopy was carried out on PI QStar Pulsar (Hybrid Quadrupole–TOF LC/MS/MS) and 4800 plus MALDI TOF/TOF Applied Biosystem spectrometeror UPLC coupled Mass Spectrometer. HRMS mass spectra were recorded on a Thermo Scientific Q–Exactive, Accela 1250 pump.

General Procedure for the synthesis of chalcone (1a-1l):



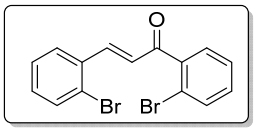
1

Compound **1** was prepared according to known procedure. 4N NaOH (0.25 mol L^{-1}) was added dropwise to a mixture of 2–bromobenzaldehyde (0.1 mmol), 2-bromoacetophenone (0.1 mmol) in ethanol (4 mL) at ambient temperature. After 12 h, the reaction was quenched with the addition of sat. NaCl (20 mL) and diluted with CH_2Cl_2.The organic layer was separated and aqueous layer was extracted with CH_2Cl_2 (2×20 mL). The extract was washed with water (2×30 mL), dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by silica gel chromatography (10→30% EtOAc in petroleum ether) to give **1**.

General procedure for the Cu (I)-catalyzed indoloindol-3-one preparation: All the reactions have been carried out employing 100 mg of the chalcone and a general procedure as follows:

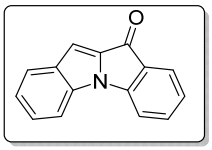
To a solution of **1** (1 equiv; 100 mg scale) in DMF (3 mL) was added L-proline (0.2 equiv) K_2CO_3 (4 equiv), CuI (0.2 equiv.) and NaN_3 (1.2 equiv) sequentially. The mixture was stirred at 140 °C for 20h. After completion ofthe reaction as indicated by TLC, reaction mixture was cooled and diluted with water (30 mL) and extracted with EtOAc (3×30 mL). Combined organic layer was dried over Na_2SO_4 and evaporated under reduced pressure. The crude product was purified by silica gel chromatography (20→40% EtOAc in petroleum ether) to give **2**.

(*E*)-1,3-bis(2-bromophenyl)prop-2-en-1-one (1a):



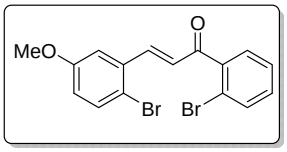
Reaction of 2-bromobenzaldehyde (3 g) with 2'-bromoacetophenone(3 g) gave **1a** (5.5 g, 92%) as yellow liquid; R_f 0.4 (2:8 v/v ethyl acetate/petroleum ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.02 (d, J = 16 Hz, 1H), 7.28–7.53 (m, 5H), 7.54–7.76 (m, 3H), 7.83 (d, J=16 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 119.5 (s), 126.0 (s), 127.4 (d), 127.8 (d), 128.0 (d), 128.5 (d), 129.3 (d), 131.6 (d), 131.7 (d), 133.5 (d), 133.5 (d), 134.5 (s), 140.8 (s), 144.9 (d), 194.5 (s) ppm; HRMS (ESI+) calculated for $C_{15}H_{11}OBr_2$ 364.9171; found 364.9174**.**

10*H*-Indolo[1,2-a]indol-10-one (2a):



2a (31 mg, 52%) was obtained as orange solid; R_f 0.3 (1:9 v/v ethyl acetate/petroleum ether);mp: 155–156 °C;^{1}H NMR (500 MHz, Acetone-d6) :δ 7.19 (m,2H), 7.24 (d, J=0.6 Hz, 1H) ,7.49 (ddd, J=1.2, 7.3, 8.2 Hz, 1H), 7.60–7.69 (m, 2H), 7.71–7.78 (m, 2H), 7.83 (dd, J= 0.9, 8.2 Hz, 1H); ^{13}C NMR (125 MHz, Acetone-d6): δ 108.2 (d), 112.7 (d), 112.9 (d), 123.0 (d), 125.1 (d), 125.5 (d), 125.9 (d), 129.1 (d), 130.2 (s), 133.7 (s), 135.2 (s), 136.7 (s), 136.9 (d), 146.4 (s), 181.7 (s)ppm; HRMS (ESI+) calculated for $C_{15}H_9ONNa$ 242.0576; found 242.0572**.**

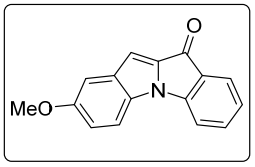
(*E*)-3-(2-Bromo-5-methoxyphenyl)-1-(2-bromophenyl)prop-2-en-1-one (1b):



Reaction of 2-bromo-5-methoxybenzaldehyde(0.5 g)with 1-(2-bromophenyl)ethan-1-one (0.46 g) gave **1b**(0.85 g, 93%) as pale yellow solid; R_f 0.4 (2:8 v/v ethyl acetate/petroleum ether); mp: 97–99 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.84 (s, 3H), 6.84 (dd, J = 2.4, 8.8 Hz, 1H), 7.00 (d, J = 16.0 Hz, 1H), 7.20 (d, J = 3.0 Hz, 1H), 7.30–7.42 (m, 1H), 7.42–7.53 (m, 3H), 7.67 (dd, J= 1.1,7.3 Hz, 1H), 7.77 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz,

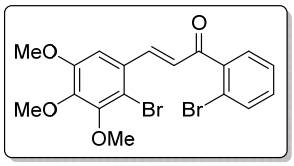
$CDCl_3$): δ 55.6 (q), 112.7 (d), 116.6 (s), 118.2 (s), 119.5 (s), 127.3 (d), 128.5 (d), 129.3 (d), 131.6 (d), 133.5 (d), 134.0 (d), 135.0 (s), 140.7 (s), 145.0 (d), 159.0 (s), 194.5 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{13}O_2Br_2$ 394.9282; found 394.9279**.**

2-Methoxy-10*H*-indolo[1,2-*a*]indol-10-one (**2b):**



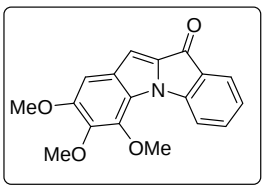
2b (34 mg, 54%) was obtained as light orange solid; R_f 0.4 (1:9v/v ethyl acetate/petroleum ether); mp: 162–164 °C; ^{1}H NMR (400 MHz, $CDCl_3$):δ 3.85 (s, 3H), 7.09 (d, *J* = 2.7Hz, 1H), 7.11–7.16 (m, 2H), 7.22 (d, *J* = 2.2 Hz, 1H), 7.30 (d, *J* = 8.6 Hz, 1H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.48 (d, *J* = 8.3 Hz 1H), 7.66 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 55.7 (q), 108.0 (d), 109.5 (d), 110.8 (d), 112.1 (d), 121.6 (d), 121.8 (d), 125.1 (d), 128.1 (d), 129.3 (s), 129.8 (s), 130.4 (s), 132.3 (s), 133.2 (s), 155.3 (s), 181.7 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{12}ON$ 250.0863; found 250.0864**.**

(*E*)-3-(2-Bromo-3,4,5-trimethoxyphenyl)-1-(2-bromophenyl)prop-2-en-1-one (1c):



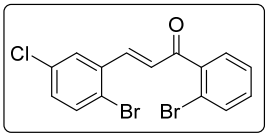
Reaction of 2-bromo-3,4,5-trimethoxybenzaldehyde (0.6 g) and 1-(2-bromophenyl) ethan-1-one (0.4 g) gave **1c** (0.85 g, 86%) as white solid; R_f0.4 (2:8v/v ethyl acetate/petroleum ether); mp: 78–80 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.88 (s, 3H), 3.90 (s, 3H), 3.93 (s, 3H), 6.92 (d, J = 15.9 Hz, 1H), 7.03 (s, 1H), 7.36 (d, J = 3.4 Hz, 1H), 7.44 (d, J = 4.0 Hz, 2H), 7.67 (d, J = 7.9 Hz, 1H), 7.79 (d, J = 15.9 Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$):δ 56.2 (q), 61.0 (q), 61.3 (q), 105.9 (d), 113.7 (s), 119.4 (s), 127.3 (d), 127.7 (d), 129.2 (d), 129.6 (s), 131.5 (d), 133.4 (d), 140.6 (s), 145.3 (s), 145.6 (d), 151.1 (s), 152.8 (s), 194.8 (s) ppm; HRMS (ESI+) calculated for $C_{18}H_{17}O_4Br_2$, 454.9494; found 454.9483.

2,3,4-Trimethoxy-10*H*-indolo[1,2-*a*]indol-10-one (2c):



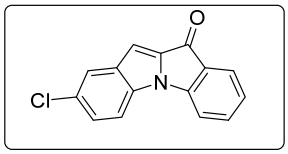
2c (32 mg, 47%) was obtained as orange solid; R_f 0.6 (2:8v/v ethyl acetate/petroleum ether); mp: 200–202 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.89 (s,3H), 3.97 (s, 3H), 4.06 (s, 3H), 6.81 (s, 1H), 7.01–7.07 (m, 2H), 7.45–7.50 (m, 1H), 7.59 (d, *J* = 7.3 Hz, 1H), 7.78 (d, *J* = 7.9 Hz, 1H); ^{13}C NMR (125MHz, $CDCl_3$): δ 56.2 (q), 61.4 (q), 61.9 (q), 100.9 (d), 108.0 (d), 114.2 (d), 123.8 (d), 124.6 (d),128.9 (s), 129.4 (s), 135.8 (d), 136.9 (s), 139.7 (s), 141.8 (s), 144.1 (s), 146.1 (s), 150.6 (s), 181.6 (s) ppm; HRMS (ESI+) calculated for $C_{18}H_{16}O_4N$, 310.1074; found 310.1075**.**

(*E*)-3-(2-Bromo-5-chlorophenyl)-1-(2-bromophenyl)prop-2-en-1-one (1d):



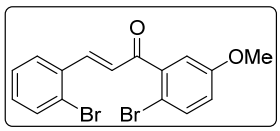
Reaction of 2-bromo-5-chlorobenzaldehyde (0.2 g) and 1-(2-bromophenyl) ethan-1-one (0.18 g) gave **1d** (0.32 g, 88%) as white solid; R_f 0.5 (1:9v/v ethyl acetate/petroleum ether); mp: 90–92 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.04 (d, J = 16.0 Hz, 1H), 7.20–7.26 (m, 1H), 7.32–7.42 (m, 1H), 7.42–7.50 (m, 2H), 7.55 (d, J = 8.6 Hz, 1H), 7.64–7.83 (m, 3H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 119.5 (s), 123.5 (s), 127.4 (d), 127.7 (d), 129.3 (d), 129.4 (d), 131.4 (d), 131.8 (d), 133.5 (d), 133.9 (s), 134.5 (d), 136.0 (s), 140.6 (s), 142.9 (d), 193.7 (s) ppm; HRMS (ESI+) calculated for $C_{15}H_{10}OCl\ Br_2$ 398.8787; found 398.8784**.**

2-Chloro-10*H*-indolo[1,2-*a*]indol-10-one (**2d):**



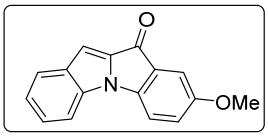
2d (33 mg, 55%) was obtained as orange solid; R_f 0.3 (1:9v/v ethyl acetate/petroleum ether); mp: 154–156 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.07 (s, 1H), 7.12 (t, J = 7.6 Hz, 1H), 7.33–7.41 (m, 2H), 7.45–7.50 (m, 1H), 7.54 (t, J= 7.8 Hz, 1H), 7.62–7.70 (m, 2H);^{13}C NMR (125 MHz, $CDCl_3$):δ 106.9 (d), 111.3 (d), 112.2 (d), 124.3 (d, 2C),125.4 (d), 127.6 (s), 128.4 (d), 129.2 (s), 132.5 (s), 133.5 (s), 135.7 (d), 136.7 (s), 145.3 (s), 181.4 (s) ppm; HRMS (ESI+) calculated for $C_{15}H_9ONCl$ 254.0367; found 254.0363.

(*E*)-1-(2-Bromo-5-methoxyphenyl)-3-(2-bromophenyl)prop-2-en-1-one (1e):



Reaction of 2-bromobenzaldehyde (0.47g) and 1-(2-bromo-5-methoxyphenyl)ethan-1-one (0.58 g) gave **1e** (0.96g, 96%) as pale yellow solid; R_f 0.4 (3:7v/v ethyl acetate/petroleum ether); mp: 94–96 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 4.11 (s, 3H), 7.19 (dd, J = 3.0, 8.7 Hz, 1H), 7.32 (d, J = 13.1 Hz, 1H), 7.38–7.69 (m, 3H), 7.76–8.02 (m, 3H), 8.15 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.7 (q), 109.8 (s), 114.3 (d), 118.0 (d), 126.0 (s), 127.8 (d), 128.0 (d), 128.3 (d), 131.7 (d), 133.5 (d), 134.2 (d), 134.5 (s), 141.5 (s), 144.9 (d), 158.8 (s), 194.2 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{13}O_2Br_2$ 394.9282; found 394.9276.

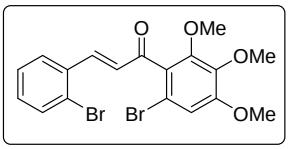
8-Methoxy-10*H*-indolo [1, 2-*a*] indol-10-one (2e):



2e (33 mg, 53%) was obtained as pale orange solid; R_f 0.5 (1:9 v/v ethyl acetate/petroleum ether); mp 161–163 °C; ^{1}H NMR (500 MHz, $CDCl_3$):δ 3.89 (s, 3H), 7.12 (dd, J = 2.4, 8.2 Hz, 1H), 7.13–7.18 (m, 2H), 7.25 (s, 1H), 7.31–7.34 (m, 1H), 7.46 (t, J = 7.9 Hz, 1H), 7.50 (d, J = 8.5 Hz, 1H), 7.69

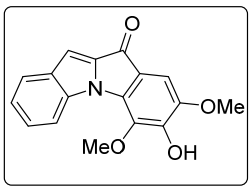
(d, J = 8.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$):δ 55.9 (q), 108.0 (d), 109.5 (d), 111.0 (d), 112.1 (d), 121.6 (d), 121.7 (d), 125.1 (d), 127.7 (s), 128.1 (d), 132.3 (s), 132.6 (s), 134.3 (s), 139.7 (s), 156.7 (s), 181.7 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{11}O_2NNa$ 272.0682; found 272.0680**.**

(*E*)-1-(6-Bromo-2,3,4-trimethoxyphenyl)-3-(2-bromophenyl)prop-2-en-1-one (1f):



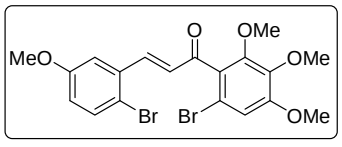
Reaction of 2-bromobenzaldehyde (0.52 g) and 1-(2-bromo-3,4,5-trimethoxyphenyl)ethan-1-one (0.82 g) gave **1f** (1.17g, 90%) as white solid; R_f 0.5 (1:9 v/v ethyl acetate/petroleum ether); mp: 73–75 °C; ^{1}H NMR (200 MHz, $CDCl_3$):δ 3.91 (s, 3H), 3.95 (s, 3H), 3.97 (s, 3H), 6.87 (s, 1H), 7.07 (d, J = 16.0 Hz, 1H), 7.21–7.42 (m, 2 H), 7.59–7.75 (m, 2H), 7.90 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 56.3 (q), 61.2 (q), 61.2 (q), 106.7 (s), 108.3 (d), 125.9 (s), 127.8 (d), 128.0 (d), 128.4 (d), 131.6 (d), 133.5 (d), 134.5 (s), 136.3 (s), 144.2 (d), 144.9 (s), 151.1 (s), 153.0 (s), 193.6 (s) ppm; HRMS (ESI+) calculated for $C_{18}H_{17}O_4Br_2$ 453.9494; found 454.9490**.**

7-Hydroxy-6,8-dimethoxy-10*H*-indolo [1, 2-*a*] indol-10-one (**2f):**



2f (36 mg, 56%) was obtained as orange solid; R_f 0.5 (3:7 v/v ethyl acetate/petroleum ether); mp: 196–198 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.92 (s, 3H), 4.06 (s, 3H), 6.27 (s, 1H), 7.00 (s, 1H), 7.07 (t, J = 7.4 Hz, 1H), 7.11 (s, 1H), 7.37 (t, J = 7.8 Hz, 1H), 7.57 (d, J = 8.2 Hz, 1H), 7.94 (d, J = 8.5 Hz, 1H); ^{13}C NMR (125 MHz,$CDCl_3$):δ 56.8 (q), 61.7 (q), 103.0 (d), 108.3 (d), 113.8 (d), 120.9 (s), 121.6 (d), 124.4 (d), 128.1 (d), 132.4 (s), 133.5 (s), 135.0 (s), 135.2 (s), 137.0 (s), 144.4 (s), 146.5 (s), 181.0 (s) ppm; HRMS (ESI+) calculated for $C_{17}H_{13}O_4NNa$ 318.0737; found 318.0732.

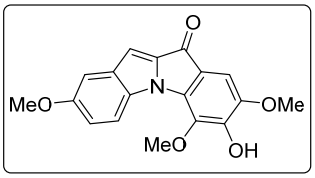
(*E*)-1-(6-Bromo-2,3,4-trimethoxyphenyl)-3-(2-bromo-5-methoxyphenyl)prop-2-en-1-one(1g):



Reaction of 2-bromo-5-methoxybenzaldehyde (0.3 g) and 1-(2-bromo-3,4,5-trimethoxyphenyl)ethan-1-one (0.4 g) gave **1g** (0.64 g, 95%) as white solid; R_f 0.4 (2:8 v/v ethyl acetate/petroleum ether); mp: 86–88 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.83 (s, 3H), 3.89 (s, 3H), 3.94 (s, 3H), 3.95 (s, 3H), 6.78–6.88 (m, 2H), 7.02 (d, J = 15.9 Hz, 1H), 7.20 (d, J = 3.0Hz, 1H), 7.50 (d, J = 8.7 Hz, 1H), 7.82 (d, J = 16.0 Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 55.6 (q), 56.3 (q),

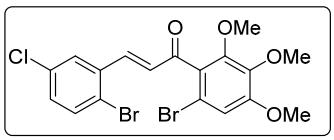
61.2 (q), 61.2 (q), 106.7 (s), 108.3 (d), 112.7 (d), 116.6 (s), 118.1 (d), 128.5 (d), 134.0 (d), 135.1 (s), 136.3 (s), 144.3 (d), 144.9 (s), 151.2 (s), 153.0 (s), 159.1 (s), 193.6 (s) ppm; HRMS (ESI+) calculated for $C_{19}H_{19}O_5Br_2$, 484.9599; found 484.9595**.**

7-Hydroxy-2,6,8-trimethoxy-10*H*-indolo[1,2-*a*]indol-10-one (**2g**)**:**



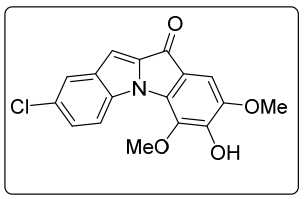
2g (36 mg, 54%) was obtained as orange solid; R_f 0.4 (4:6 v/v ethyl acetate/petroleum ether); mp: 208–210 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.83 (s, 3H), 3.91 (s, 3H), 4.04 (s, 3H), 6.96–7.06 (m, 4 H), 7.75–7.85 (d, j = 8.8 Hz, 1 H);^{13}C NMR (100 MHz, $CDCl_3$):δ 56.2 (q), 61.4 (q), 61.9 (q), 100.9 (d), 108.0 (d), 114.2 (d), 123.7 (d), 124.6 (d), 128.9 (s), 129.3 (s), 135.8 (d), 136.9 (s), 139.7 (s), 141.8 (s), 144.1 (s), 146.1 (s), 150.6 (s), 181.6 (s) ppm.

(*E*)-1-(6-Bromo-2,3,4-trimethoxyphenyl)-3-(2-bromo-5-chlorophenyl)prop-2-en-1-one (1h):



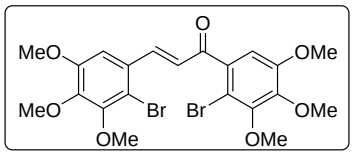
Reaction of 2-bromo-5-chlorobenzaldehyde (0.25g) and 1-(2-bromo-3,4,5-trimethoxyphenyl)ethan-1-one (0.32g) gave **1h**(0.48 g, 87%) as pale yellow solid; R_f 0.2 (1:9 v/v ethyl acetate/petroleum ether); mp: 166–168 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.89 (s, 3H), 3.94 (s, 3H), 3.95 (s, 3H), 6.84 (s, 1H), 7.06 (d, *J* = 16.0Hz, 1H), 7.13–7.25 (m, 1H), 7.55 (d, *J* = 8.5Hz, 1H), 7.65 (d, *J* = 2.5 Hz, 1H), 7.81 (d, *J* = 15.9 Hz, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 56.3 (q), 61.2 (q, 2C),106.8 (s), 108.4 (d), 123.6 (s), 127.7 (d), 129.3 (d), 131.4 (d), 133.2 (s), 134.0 (s), 134.5 (d), 136.2 (s), 142.0(s), 145.1 (d), 151.2 (s), 153.1 (s), 193.0 (s) ppm; HRMS (ESI+) calculated for $C_{18}H_{16}O_4Br_2Cl$ 488.9104; found 488.9027.

2-Chloro-7-hydroxy-6,8-dimethoxy-10*H*-indolo[1,2-*a*]indol-10-one (2h):



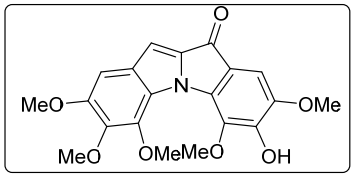
2h (37 mg, 55%) was obtained as red solid; R_f 0.4 (3:7 v/v ethyl acetate/petroleum ether); mp: 162–163 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.92 (s, 3H), 4.05 (s, 3H), 7.03 (s, 1H), 7.00 (s, 1H), 7.31 (d, *J* = 8.8 Hz, 1H), 7.55 (s, 1H), 7.87 (d, *J* = 8.8Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 56.8 (q), 61.6 (q), 103.0 (d), 107.2 (d), 114.9 (d), 120.6 (s), 123.5 (d), 127.1 (s), 128.3 (d), 133.3 (s), 133.5 (s), 133.5 (s), 134.6 (s), 137.9 (s), 144.7 (s), 146.6 (s), 180.8 (s) ppm; HRMS (ESI+) calculated for $C_{17}H_{13}ClNO_4$ 330.0528; found 330.0529**.**

(*E*)-1,3-Bis(2-bromo-3,4,5-trimethoxyphenyl)prop-2-en-1-one (1i):



Reaction of 2-bromo-3,4,5-trimethoxybenzaldehyde (0.7 g) and 1-(2-bromo-3,4,5-trimethoxyphenyl)ethan-1-one (0.73 g) gave **1i** (1.2 g, 95%) as white solid; R_f 0.6 (1:9 v/v ethyl acetate/petroleum ether); mp: 150–152 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.88–3.92 (m, 9H), 3.93–3.97 (m, 9H), 6.83 (s, 1H), 6.94 (d, J = 16.0 Hz, 1H), 7.03 (s, 1H), 7.86 (d, J = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 56.2 (q), 56.3 (q), 61.0 (s), 61.2 (s), 61.2 (q, 2C), 106.1 (d), 106.7 (s), 108.2 (d), 113.7 (s), 127.7 (d), 129.8 (s), 136.3 (s), 144.7 (s), 144.8 (d), 145.3 (s), 151.1 (s), 151.2 (s), 152.9 (s), 153.0 (s), 193.8 (s) ppm. HRMS (ESI+) calculated for $C_{21}H_{23}O_7Br_2$ 544.9811; found 544.9796.

7-Hydroxy-2,3,4,6,8-pentamethoxy-10*H*-indolo[1,2-*a*]indol-10-one (2i):



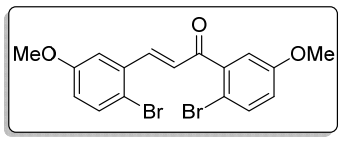
2i (46 mg, 65%) was obtained as red solid; R_f 0.4 (4:6 v/v ethyl acetate/petroleum ether);mp: 162–163°C; ^{1}H NMR (400 MHz, $CDCl_3$):δ 3.87–3.88 (m, 3H), 3.89 (s, 3H), 3.91 (s, 3H), 3.94 (s, 3H), 3.99 (s, 3H), 6.36 (br. s., 1H), 6.80 (s, 1H), 7.06 (d, J = 8.3 Hz, 2H);^{13}C NMR (125 MHz,$CDCl_3$): δ 56.2 (q), 56.6 (q), 61.7 (q), 62.2 (q), 62.4 (q), 100.7 (d), 103.7 (d), 108.7 (d), 122.2 (s), 125.8 (s), 129.7 (s), 134.6 (s), 134.8 (s), 139.3 (s), 141.2 (s), 144.3 (s), 144.9 (s), 146.8 (s), 150.1 (s), 180.3 (s)ppm; HRMS (ESI+) calculated for $C_{20}H_{19}O_7NNa$ 408.1054; found 408.1046

Crystal strucuture: Single crystal X–ray diffraction data of compound **2i** was collected on a Bruker SMART APEX II CCD diffractometer with graphite–monochromatized (MoK_α= 0.71073 Å) radiation. The X–ray generator was operated at 50 kV and 30 mA. A preliminary set of cell constants and an orientation matrix were calculated from three sets of 36 frames. Data were collected with ωscan width of 0.5° at different settings of φ and $2\theta$with a frame time of 10, seckeeping the sampledetector distance fixed at 5.00 cm. The X–ray data collection was monitored by APEX2 program (Bruker, 2006).All the data were corrected for Lorentzian, polarization and absorption effects using SAINT and SADABS programs (Bruker, 2006). SHELX–97 was used for structure solution and full matrix leastsquares refinement on F^2.All the hydrogen atoms were placed in geometrically idealized positionand constrained to ride on their parent atoms. ORTEP views of seven compounds were drawn with 30% probability displacement ellipsoids and H atoms are shown as small spheres of arbitrary radii.CCDC: 1410863 contain the supplementary crystallographic data for this

paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Structure Code.	2i	Observed Refln.	2764
CCDC No.	1410863	R_{int}	0.0249
Mol. Formula	$C_{20}H_{19}NO_7$	No. of Parameter	259
Mr	385.36	R_1_obs, R_1 _*all*	0.0435,0.0518
Temp. (K)	299(2)	wR_2_obs, wR_2_*all*	0.1130, 0.1195
Crystal System	monoclinic	GoF	1.053
Space group	$P2_1/c$	$\Delta\rho_{max}$,$\Delta\rho_{min}$/eÅ^{-3}	0.178, -0.247
a/Å	11.3454(4)	No. of Parameter	259
b/Å	13.0130(5)	R_1_obs, R_1 _*all*	0.0435,0.0518
c/Å	12.3899(4)	wR_2_obs, wR_2_*all*	0.1130, 0.1195
α/°	90	GoF	1.053
β/°	91.009(2)	$\Delta\rho_{max}$,$\Delta\rho_{min}$/eÅ^{-3}	0.178, -0.247
γ/°	90°		
V/Å^3	1828.93(11)		
Z,D_{calc}/g cm^{-3}	4, 1.400		
μ/mm^{-1}	0.107		
F (000)	808		
θ max/°	25.00		
Absor.correction	multi-scan		
Refln. collected	26312		
Unique Refln.	3228		

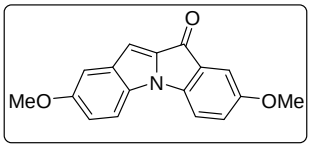
(*E*)-1,3-Bis(2-bromo-5-methoxyphenyl)prop-2-en-1-one (1j):



Reaction of 2-bromo-5-methoxybenzaldehyde (0.4 g) and 1-(2-bromo-5-methoxyphenyl)ethan-1-one (0.42 g) gave **1j** (0.63 g, 80%) as pale yellow solid; R_f 0.4 (2:8 v/v ethyl acetate/petroleum ether); mp: 74–75 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 4.07 (s, 6H), 7.04–7.24 (m, 4H), 7.43 (d, J = 3.0 Hz, 1H), 7.74 (dd, J = 6.8,8.7 Hz, 2H), 8.04 (d, J = 16.0 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 55.6 (q, 2C), 113.5 (d),113.8 (d),114.1 (d), 114.7 (s), 114.8 (s), 117.8 (d),

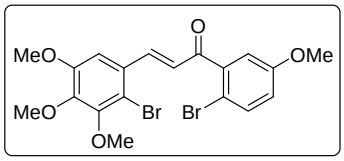
118.0 (d), 133.8 (d), 134.3 (d), 134.5 (d), 141.8 (s), 142.2 (s), 158.7 (s), 159.0 (s), 191.8 (s)ppm; HRMS (ESI+) calculated for $C_{17}H_{15}O_3Br_2$,424.9382; found424.9375**.**

2,8-Dimethoxy-10*H*-indolo[1,2-*a*]indol-10-one (**2j**)**:**



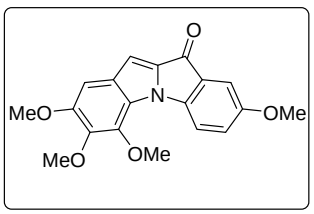
2j (35 mg, 53%) was obtained as light orange solid; R_f0.3 (1:9v/v ethyl acetate/petroleum ether); mp: 204–206 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.84 (s, 3H), 3.82 (s, 3H), 6.99–7.09 (m, 4H), 7.15–7.23 (m, 2H), 7.36 (d, J = 8.6 Hz, 1H);^{13}C NMR (100 MHz, $CDCl_3$):δ 55.7 (q), 55.9 (q), 105.4 (d), 107.4 (d), 109.7 (d), 111.5 (d), 111.8 (d), 119.2 (d), 120.1 (s), 121.4 (d), 130.4 (s), 132.8 (s), 139.7 (s), 151.5 (s), 155.1 (s), 156.6 (s)ppm; HRMS (ESI+) calculated for $C_{17}H_{13}O_3NNa$ 302.0788; found 302.0783

(*E*)-3-(2-Bromo-3,4,5-trimethoxyphenyl)-1-(2-bromo-5-methoxyphenyl)prop-2-en-1-one(1k):



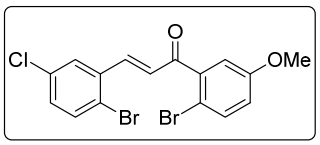
Reaction of 2-bromo-3,4,5-trimethoxybenzaldehyde (0.55 g) and 1-(2-bromo-5-methoxyphenyl)ethan-1-one (0.45 g) gave **1k** (0.87 g, 90%) as pale yellow solid; R_f 0.7 (2:8 v/v ethyl acetate/petroleum ether); mp: 89–91°C; ^{1}H NMR (200 MHz, $CDCl_3$): δ3.84 (s, 3H), 3.89 (s, 3H), 3.92 (s, 3H), 3.94 (s, 3H), 6.86–6.93 (m, 1H), 6.93–6.99 (m, 2H), 7.03 (s, 1H), 7.53 (d, J = 8.7 Hz, 1H), 7.83 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.7 (q), 56.2 (q), 61.0 (q), 61.2 (q), 106.2 (d), 109.7 (s), 113.7 (s), 114.3 (s), 117.9 (d), 127.6 (d), 129.7 (s), 134.2 (d), 141.5 (s), 145.4 (s), 145.5 (d), 151.2 (s), 152.9 (s), 158.8 (s), 194.4 (s)ppm. HRMS (ESI+) calculated for $C_{19}H_{19}O_5Br_2$ 484.9599; found 484.9589.

2,3,4,8-Tetramethoxy-10*H*-indolo[1,2-*a*]indol-10-one (2k):



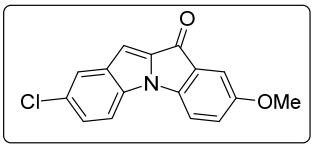
2k (43 mg, 62%) was obtained as pale orange solid; R_f 0.5 (1:9v/v ethyl acetate/petroleum ether); mp: 205–207 °C; ^{1}H NMR (200 MHz, $CDCl_3$):δ 3.85 (s, 3H), 3.88 (s, 3H), 4.01 (s, 3H), 4.04 (s, 3H), 6.99–7.08 (m, 4H), 7.82 (d, J = 8.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$):δ55.6(q), 56.5 (q), 61.3 (q), 62.1 (q), 104.3 (s), 104.9 (d), 104.9 (d), 108.1 (d), 114.8 (d), 119.1 (d), 124.5 (s), 130.7 (s), 132.8 (s), 134.1 (s), 137.1 (s), 139.7 (s), 150.6 (s), 155.1 (s), 181.1 (s)ppm; HRMS (ESI+) calculated for $C_{19}H_{17}O_5NNa$ 362.0999; found 362.0994**.**

(*E*)-3-(2-Bromo-5-chlorophenyl)-1-(2-bromo-5-methoxyphenyl)prop-2-en-1-one(1l):



Reaction of 2-bromo-5-chlorobenzaldehyde (0.2 g) and 1-(2-bromo-5-methoxyphenyl) ethan-1-one (0.2 g) gave **1l** (0.32 g, 84%) as white solid; R_f 0.5 (2:8 v/v ethyl acetate/petroleum ether); mp: 111–113 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 4.04 (s, 3H), 6.95–7.21 (m, 2H), 7.35–7.48 (m, 1H), 7.58–8.04 (m, 5H);^{13}C NMR (125 MHz, $CDCl_3$): δ 55.7 (q), 114.4 (d), 118.2 (d), 127.8 (d), 129.1 (d), 131.4 (d), 133.5 (s), 133.9 (s), 134.3 (s), 134.5 (d), 136.1 (s), 141.3 (s), 142.9 (d), 158.9 (s), 179.8 (s), 193.6 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{12}O_2ClBr_2$ 428.8893; found 428.8877**.**

2-Chloro-8-methoxy-10*H*-indolo[1,2-*a*]indol-10-one (**2l**):



2l (32 mg, 49%) was obtained as orange solid; R_f 0.6 (2:8 v/v ethyl acetate/petroleum ether); mp: 158–160 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.87 (s, 3H), 7.07–7.11 (m, 2H), 7.12 (d, J = 2.4 Hz, 1H), 7.24 (d, J = 8.3 Hz, 1H), 7.39 (d, J = 8.8 Hz, 1H), 7.47 (dd, J = 2.2, 8.3 Hz, 1H), 7.60 (d, J = 2.2Hz, 1H);^{13}C NMR (125 MHz, $CDCl_3$): δ 55.7 (q), 105.7 (d), 108.4 (d), 111.7 (d), 112.0 (d), 119.5 (d), 125.3 (d), 129.4 (s), 129.7 (s), 130.7 (s), 133.3 (s), 134.8 (d), 136.2 (s), 143.8 (s), 155.5 (s), 180.1 (s) ppm; HRMS (ESI+) calculated for $C_{16}H_{11}O_2NCl$ 284.0473; found 284.0473**.**

Acquisition Time (sec)	3.9584	***Comment***	anand	***Date***	28 May 2014 15:45:12
Date Stamp	28 May 2014 15:45:12			***Solvent***	CHLOROFORM-d
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Wed5av2#025\1\PDATA\1\1r			***Frequency (MHz)***	200.13

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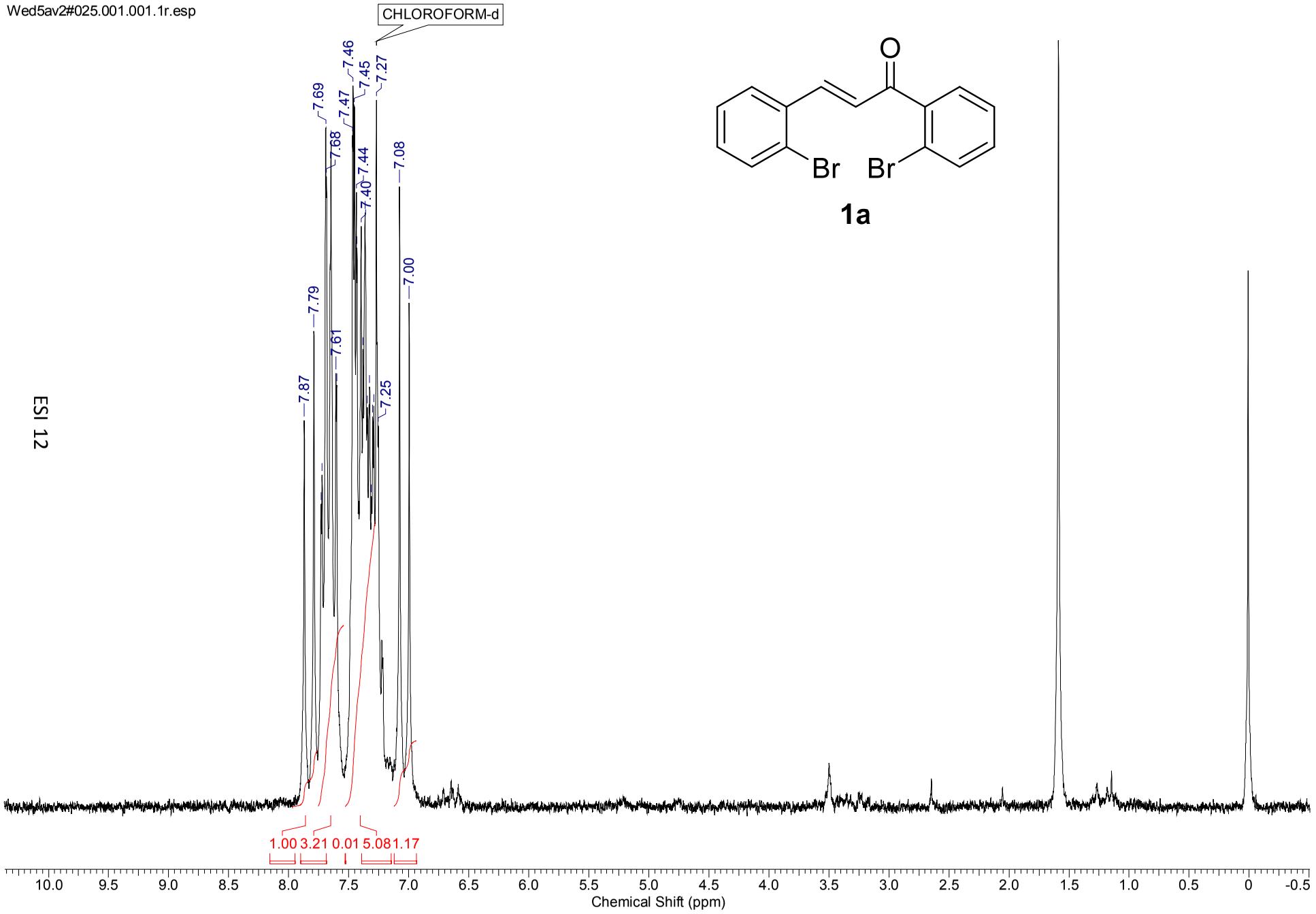
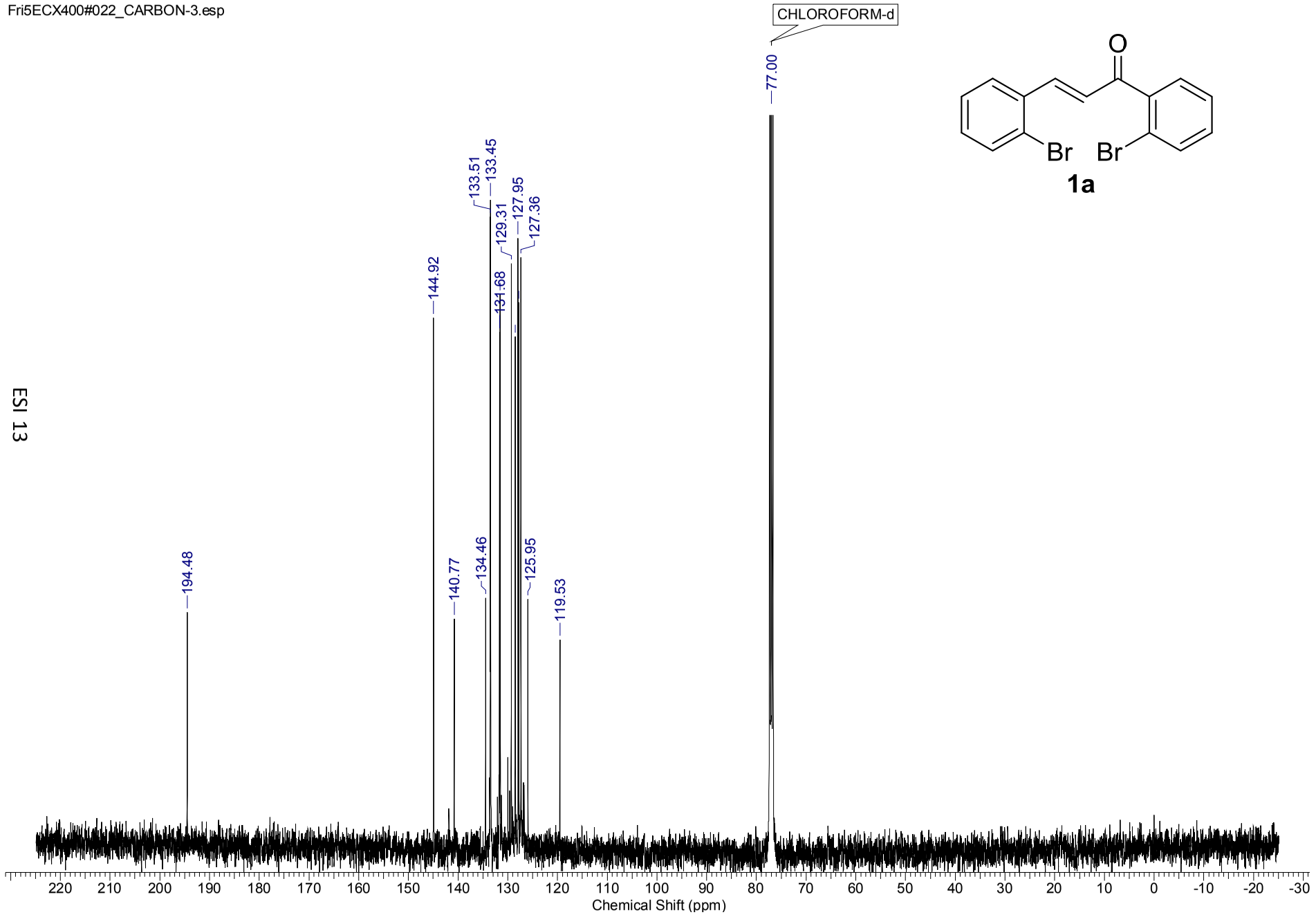


1a

Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	31 May 2014 05:36:17		
Date Stamp	31 May 2014 04:23:45			***File Name***	\\agni\nmr_data\JEOL_400\2014\May 2014\Fri5ECX400#022_CARBON-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1200	***Origin***	ECX 400

Fri5ECX400#022_CARBON-3.esp



ESI 13

Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	31 May 2014 05:36:17		
Date Stamp	31 May 2014 04:55:13			***Solvent***	CHLOROFORM-d		
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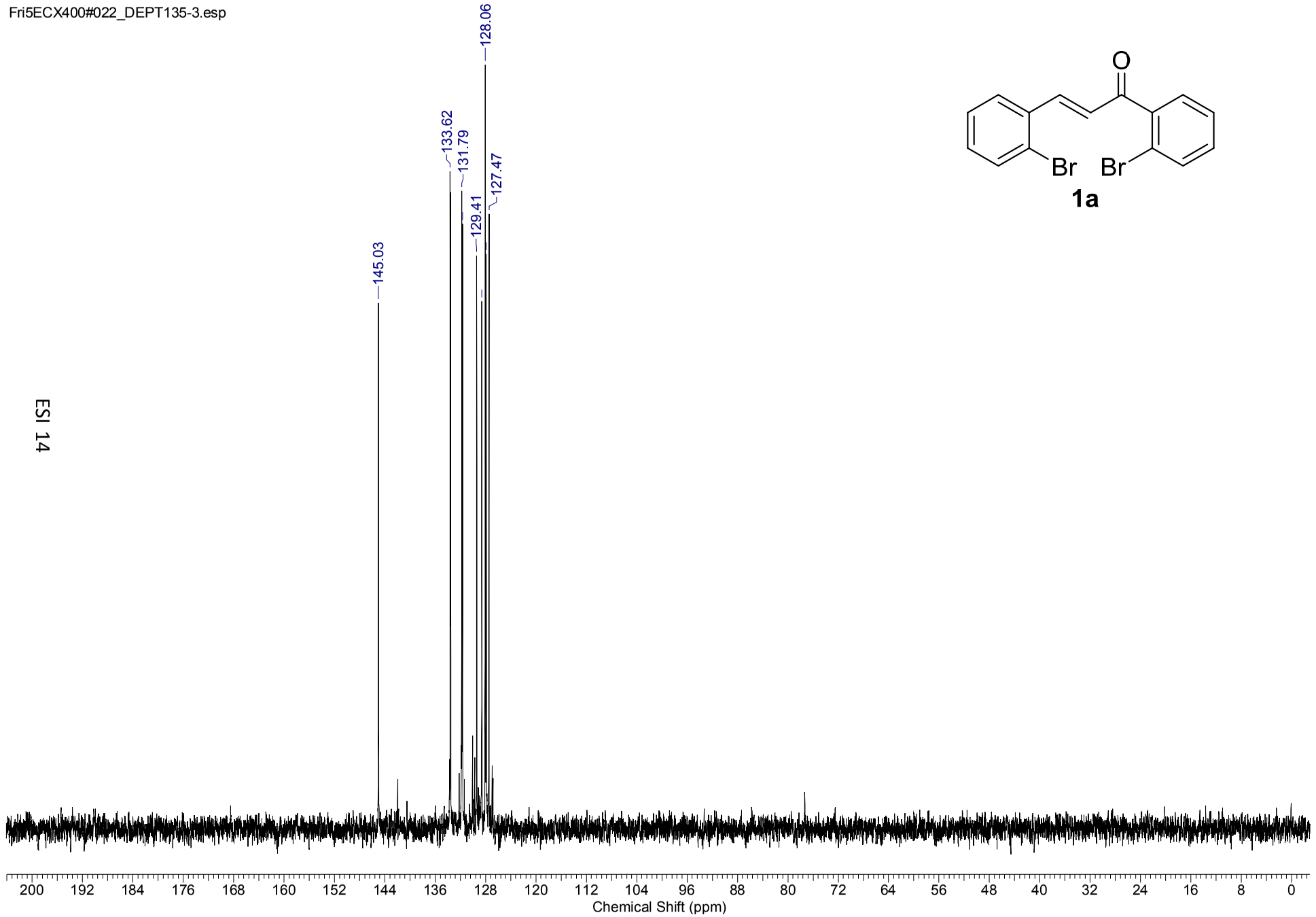

ESI 14

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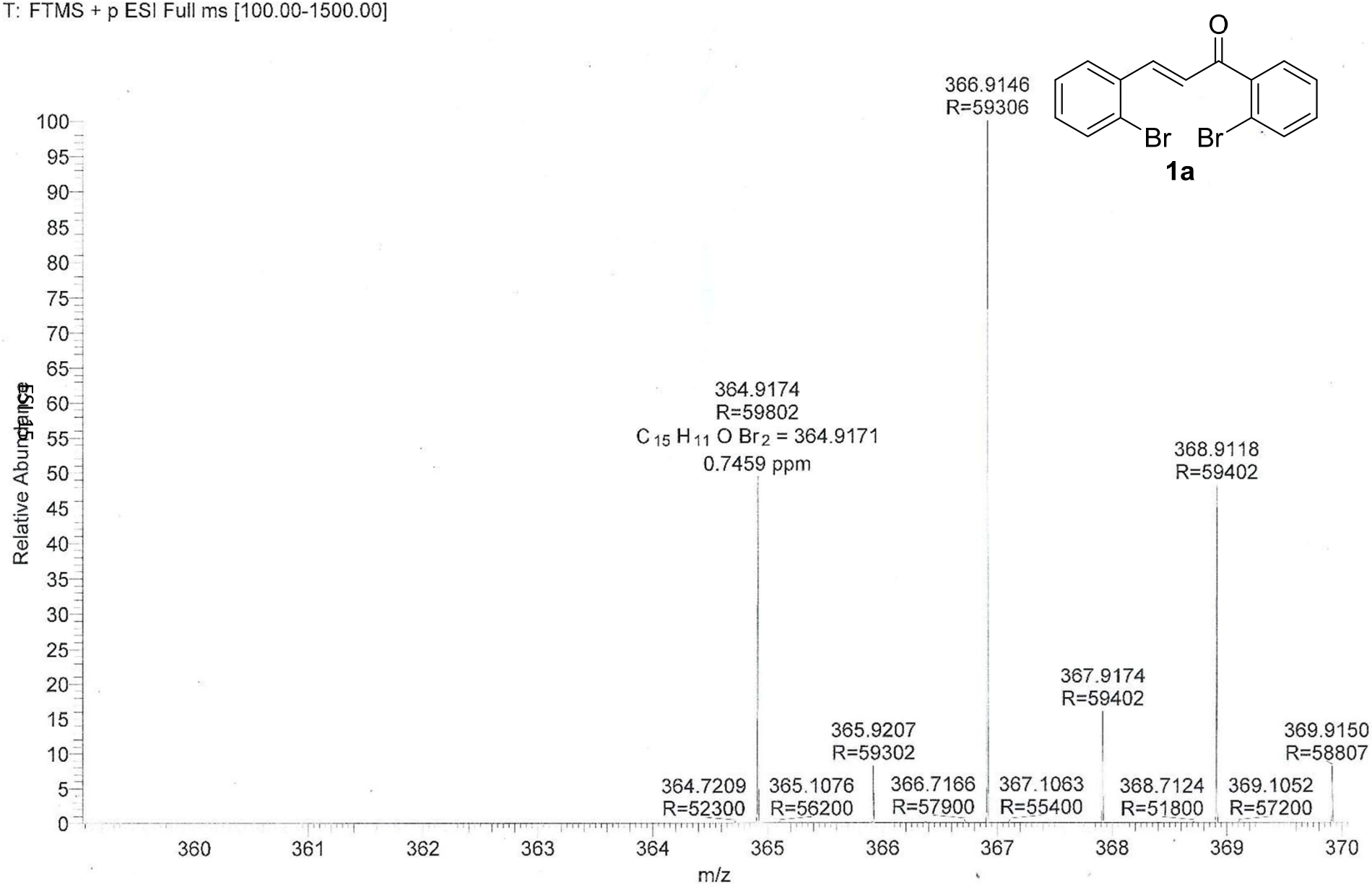

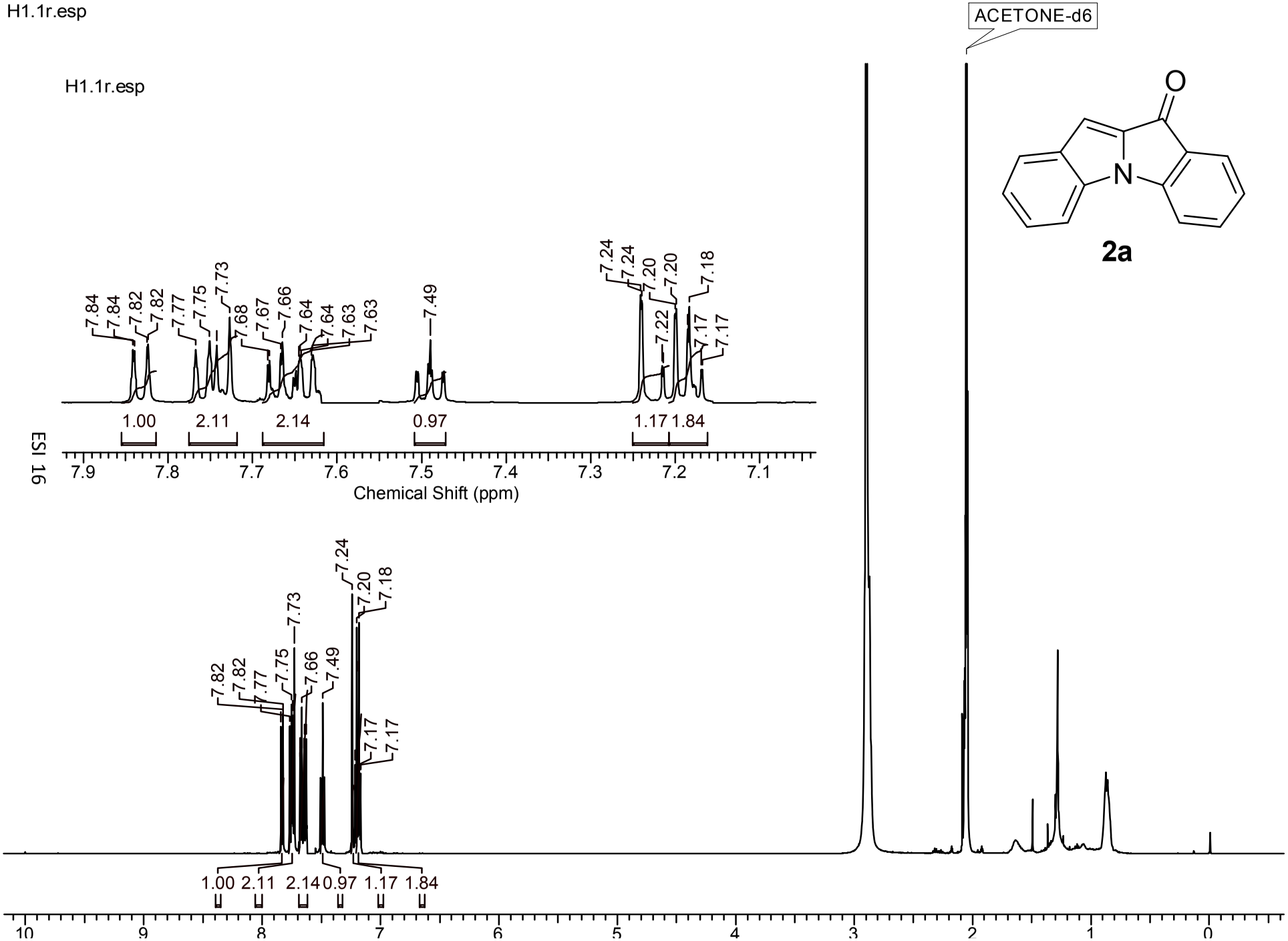
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0

Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	04 Nov 2014 19:22:56		
Date Stamp	04 Nov 2014 19:22:56			***Solvent***	Acetone		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	4207	***Origin***	spect

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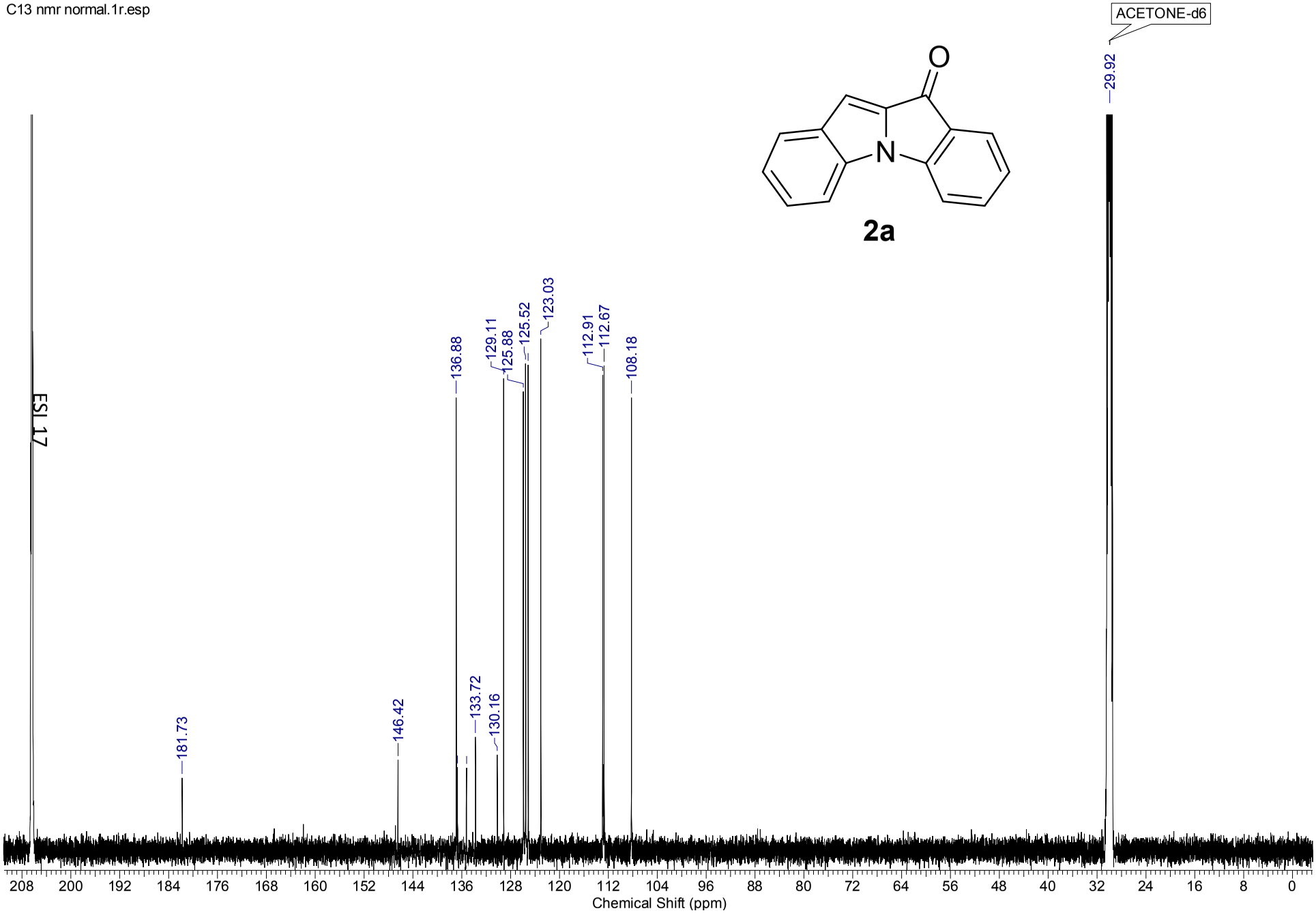

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Date Stamp	04 Nov 2014 17:23:28			***Solvent***	Acetone		
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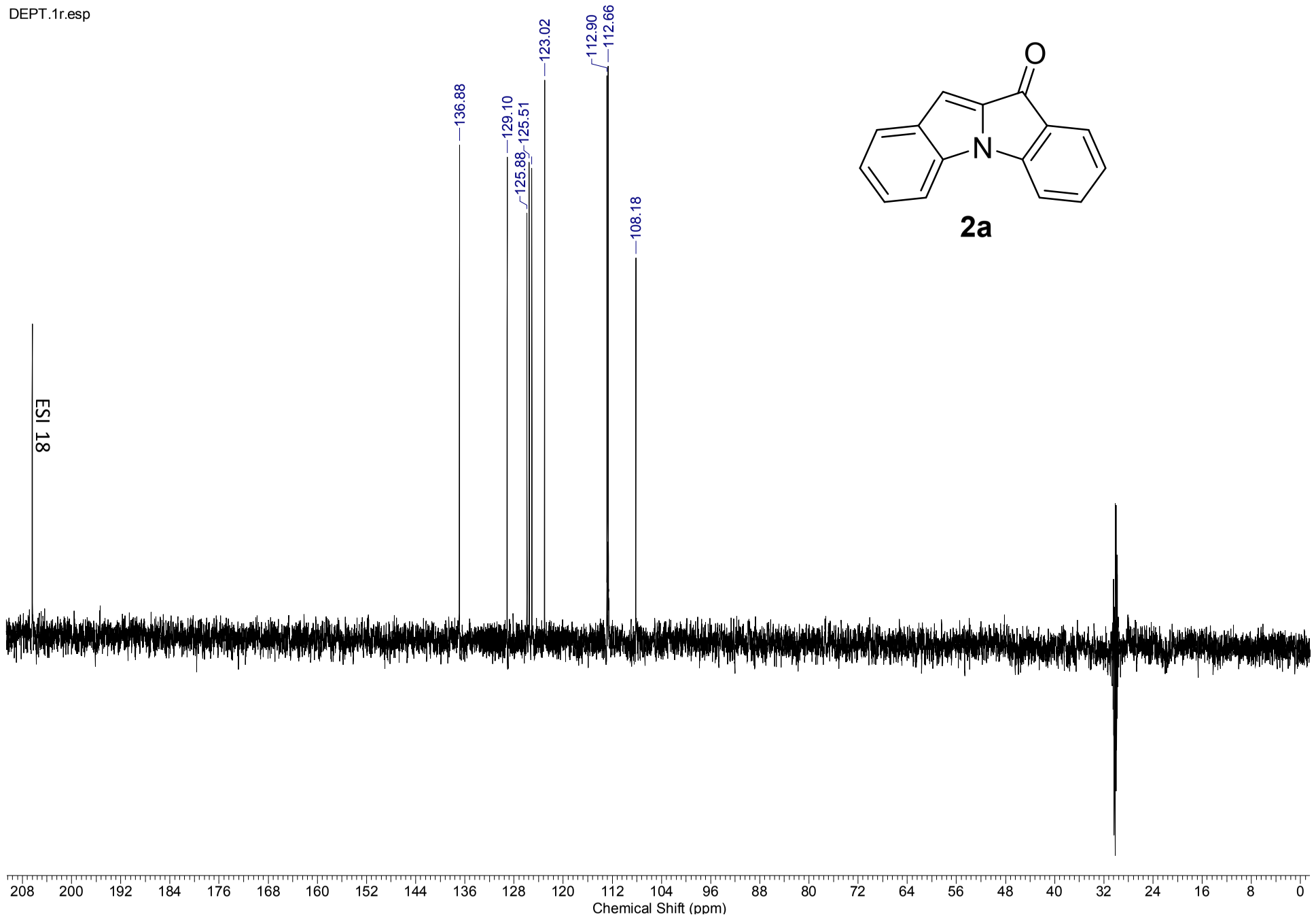
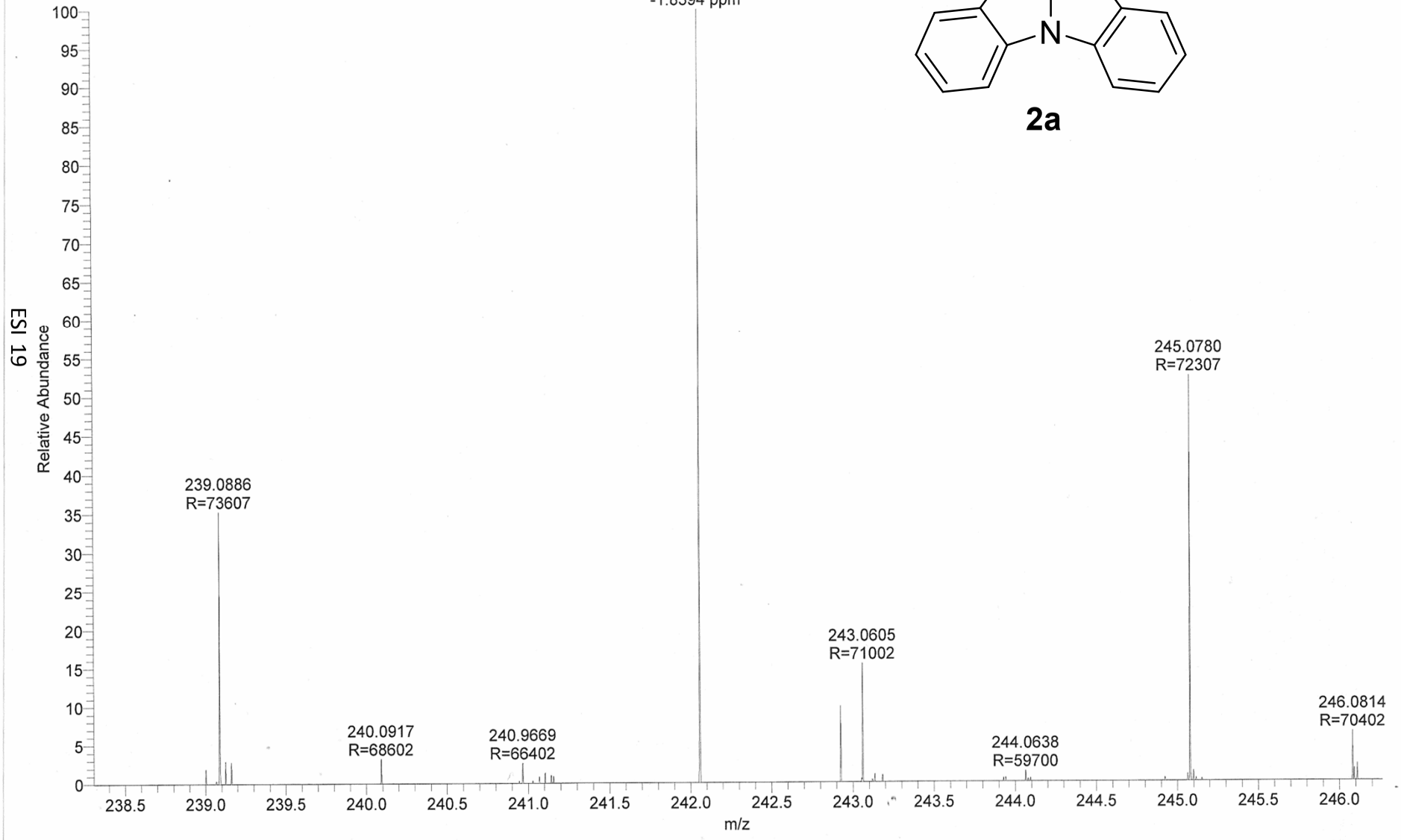
DEPT.1r.esp



D:\Data\11 normal

12/30/2014 2:13:21 PM

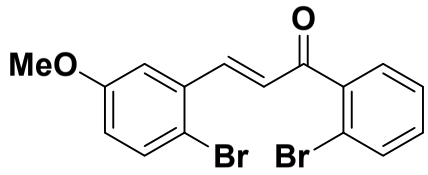
11 #1170 RT: 5.21 AV: 1 NL: 7.08E6
T: FTMS + p ESI Full ms [66.70-1000.00]



2a

Acquisition Time (sec)	3.9584	***Comment***	anand	***Solvent***	CHLOROFORM-d		
Date Stamp	07 Apr 2014 15:36:40						
File Name	\\agni\nmr_data\AV200\APR_14#AV200\data\Administrator\nmr\Mon2av2#040\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Mon2av2#040.001.001.1r.esp

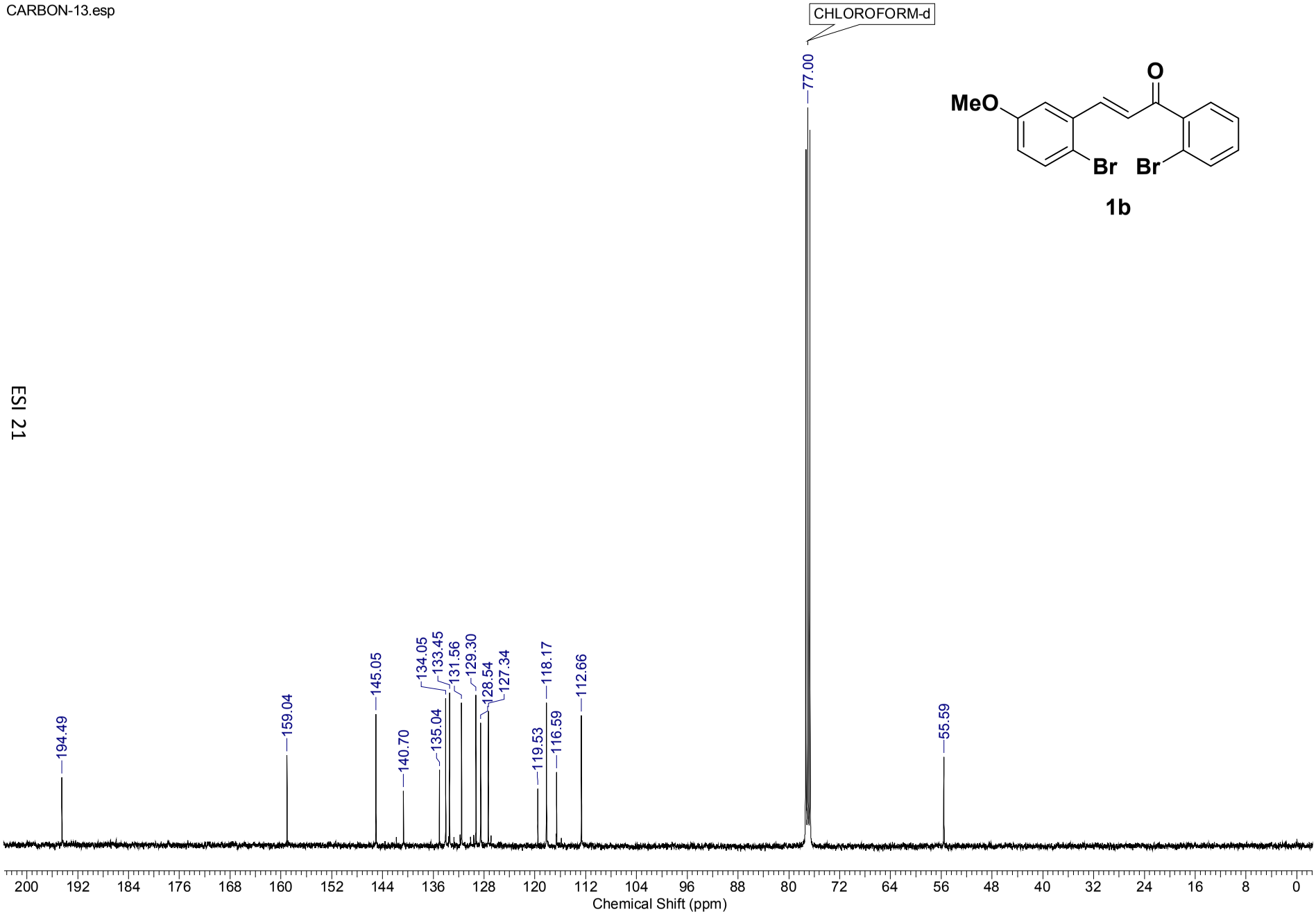


1b

ESI 20

Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	29 Apr 2014 06:33:55		
Date Stamp	29 Apr 2014 05:24:14			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1200	***Origin***	ECX 400

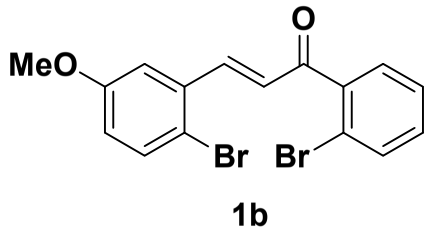
CARBON-13.esp



ESI 21

Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	29 Apr 2014 06:33:55		
Date Stamp	29 Apr 2014 05:55:36			***File Name***	\\agni\nmr_data\JEOL_400\2014\April 2014\Mon5ECX400#022_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	800	***Origin***	ECX 400

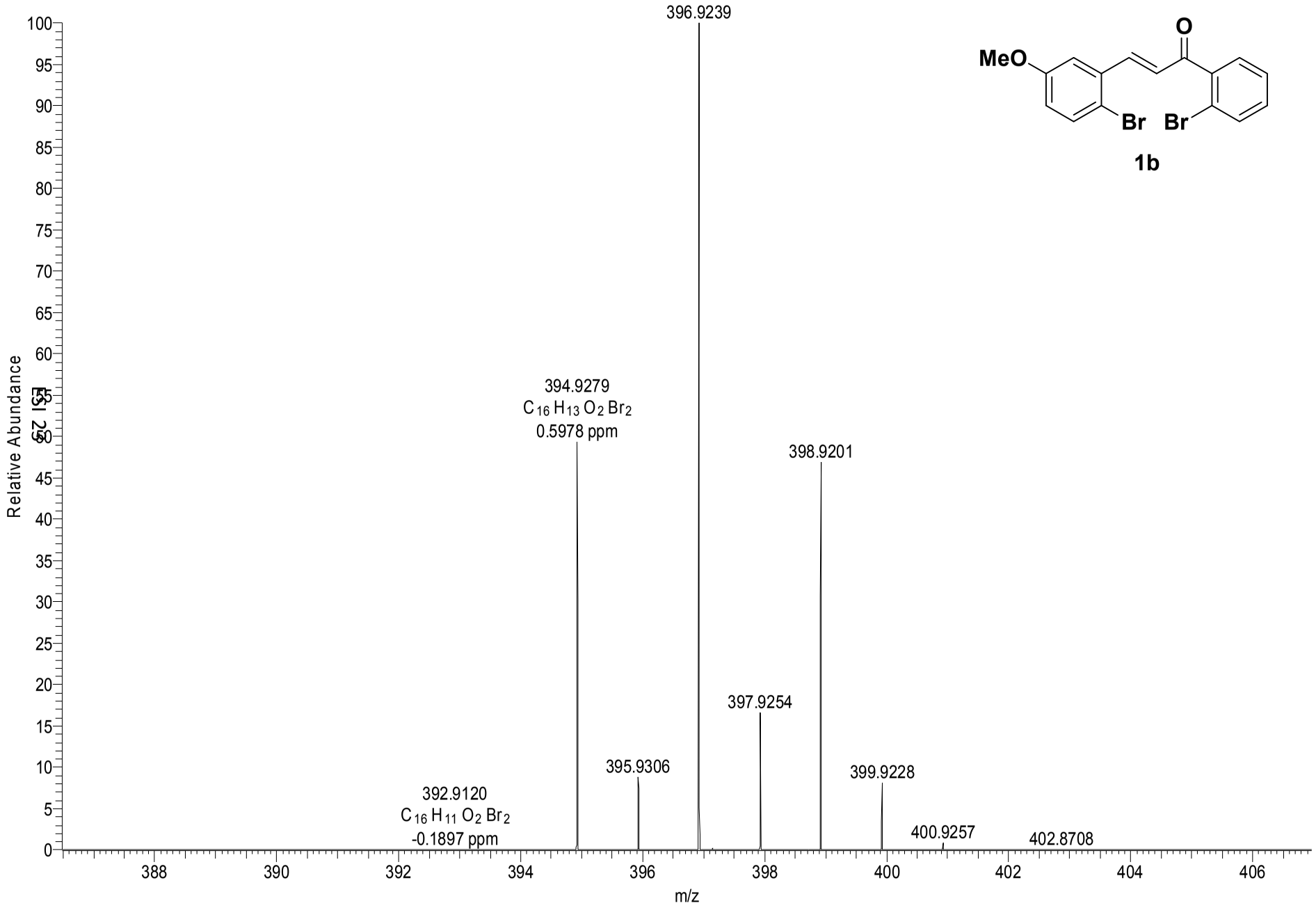
Mon5ECX400#022_DEPT135-3.esp



1b

ESI 22

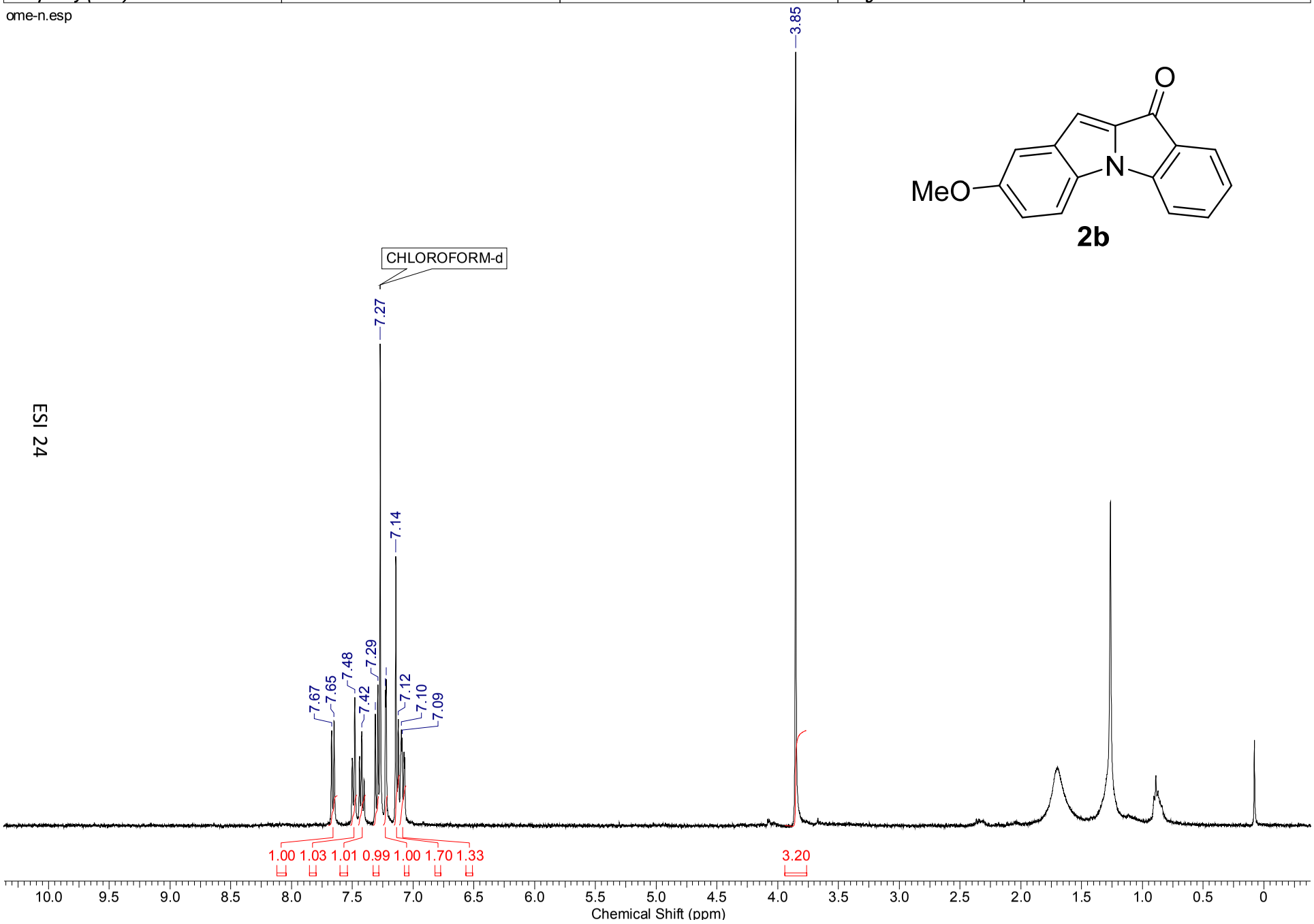
AKC-5 #109 RT: 0.58 AV: 1 NL: 2.36E9
T: FTMS + p ESI Full ms [100.00-1500.00]



1b

Acquisition Time (sec)	2.0447	***Comment***	anadaa 1H	***Date***	14 Dec 2013 12:52:24		
Date Stamp	14 Dec 2013 12:52:24			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	spect

ome-n.esp

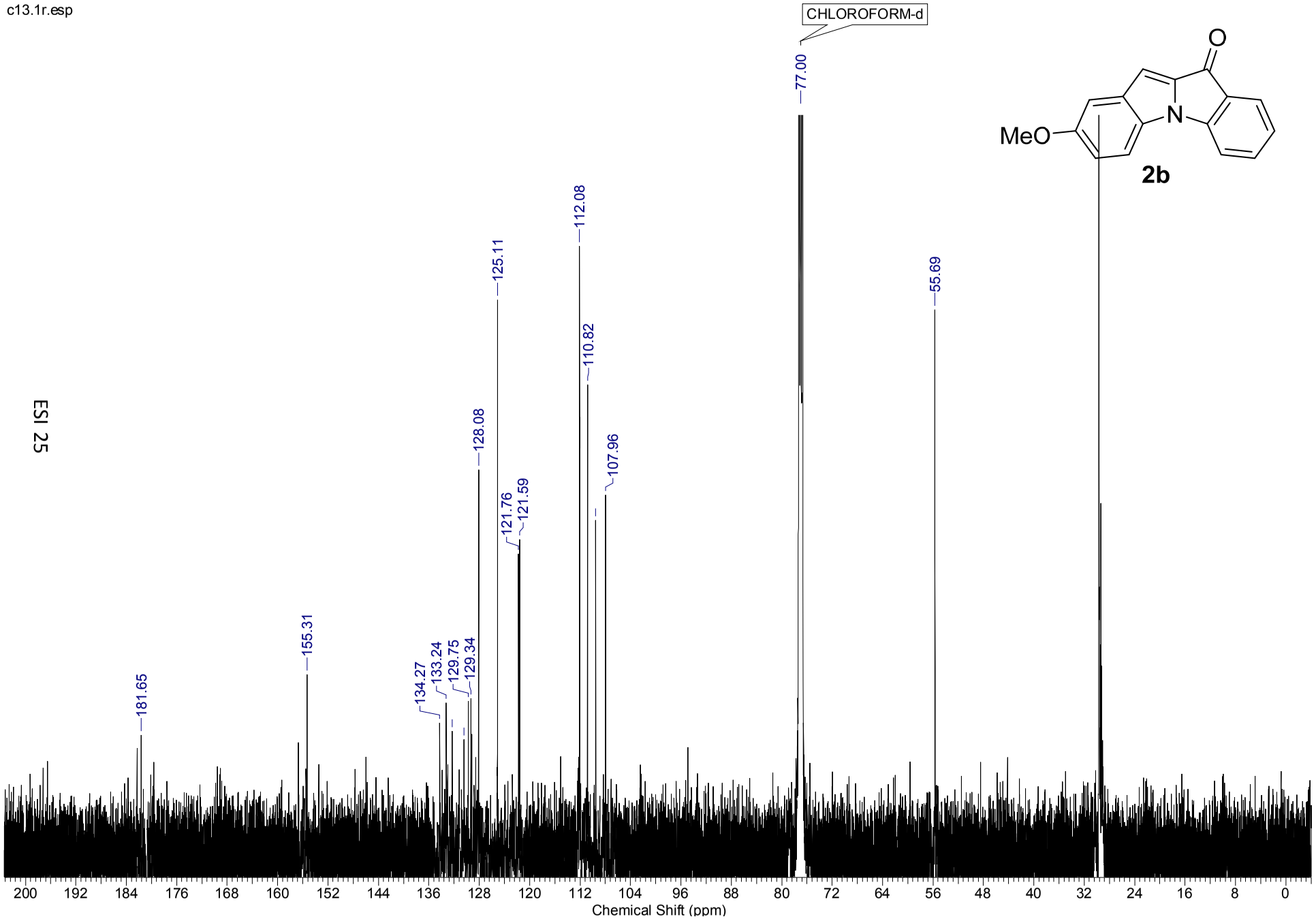


2b

ESI 24

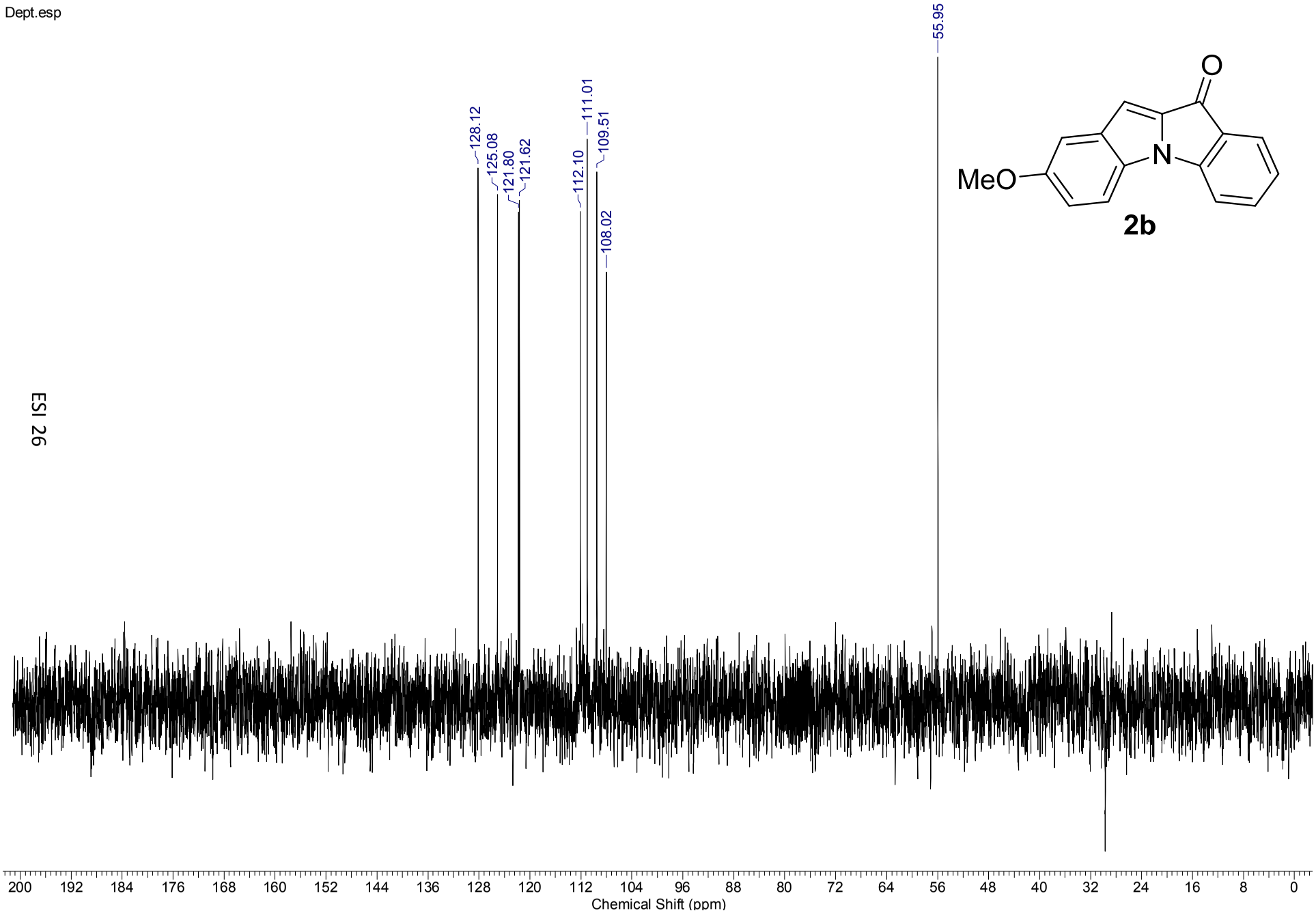
Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	18 Dec 2014 14:43:28		
Date Stamp	18 Dec 2014 14:43:28			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1236	***Origin***	spect

c13.1r.esp



Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	14 Dec 2013 13:39:20		
Date Stamp	14 Dec 2013 13:39:20			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect

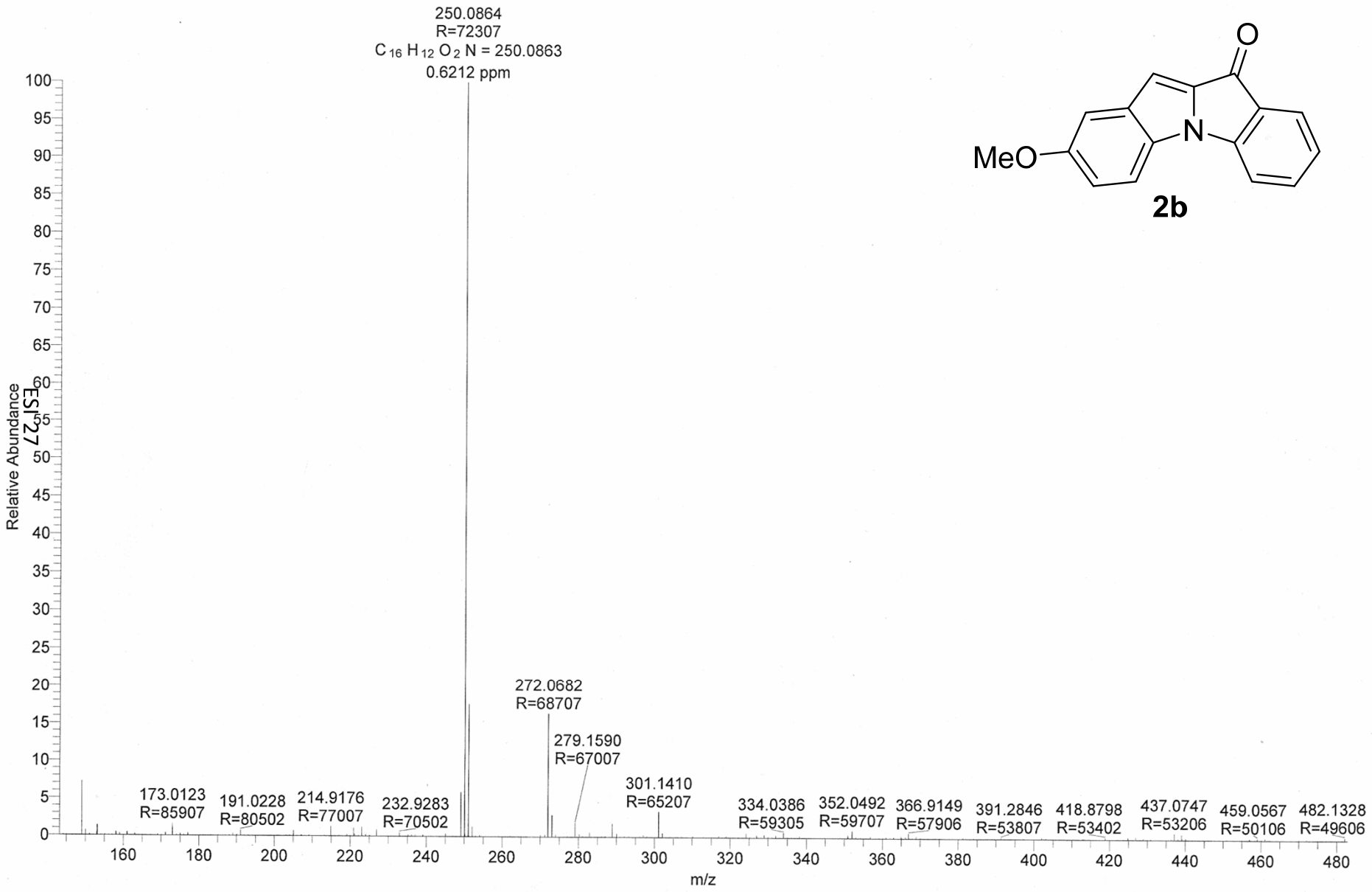
Dept.esp



D:\Data\OME-N

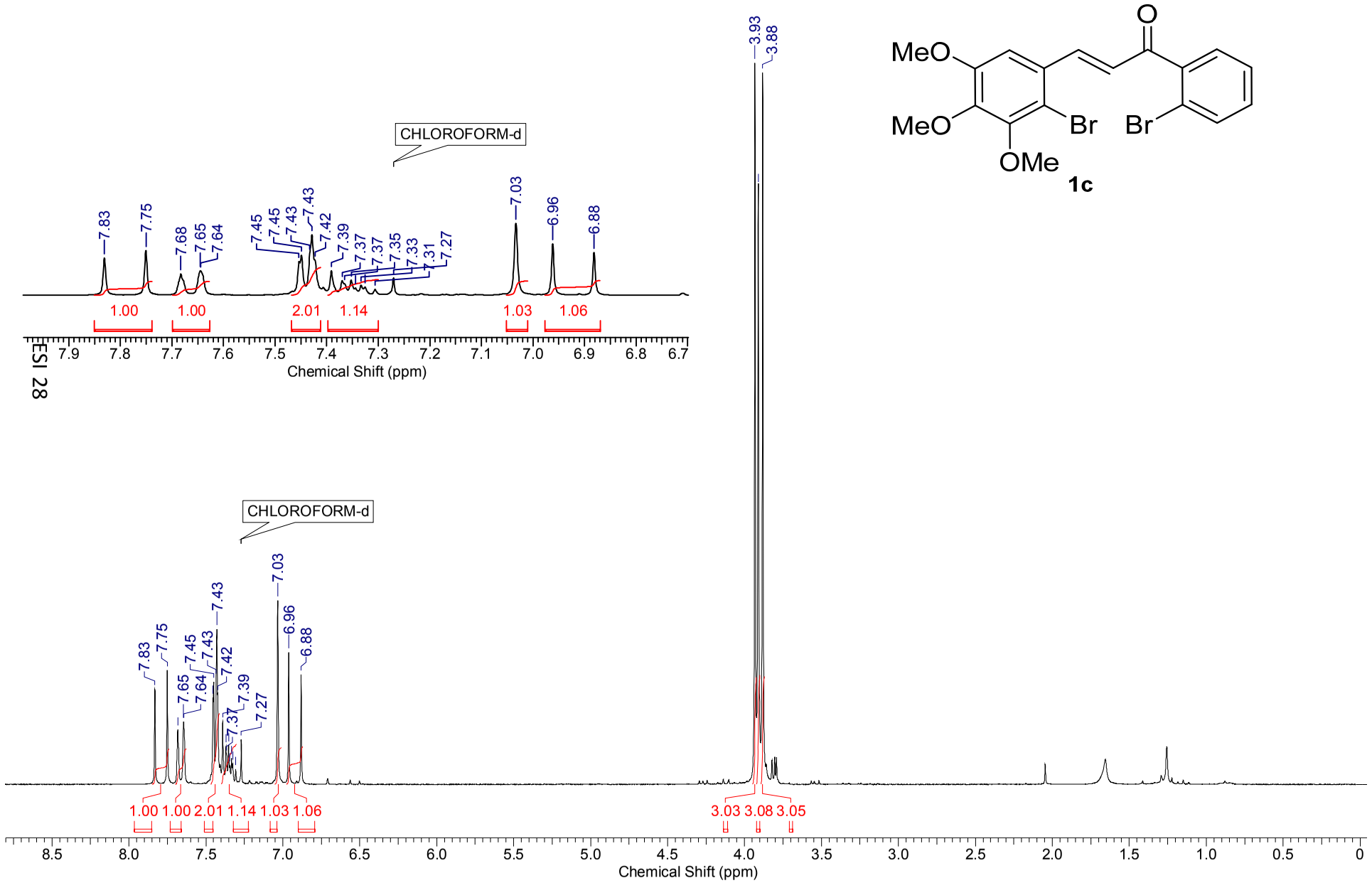
3/20/2015 12:12:07 PM

OME-N #144 RT: 0.64 AV: 1 NL: 2.09E8
T: FTMS + p ESI Full ms [85.40-1000.00]



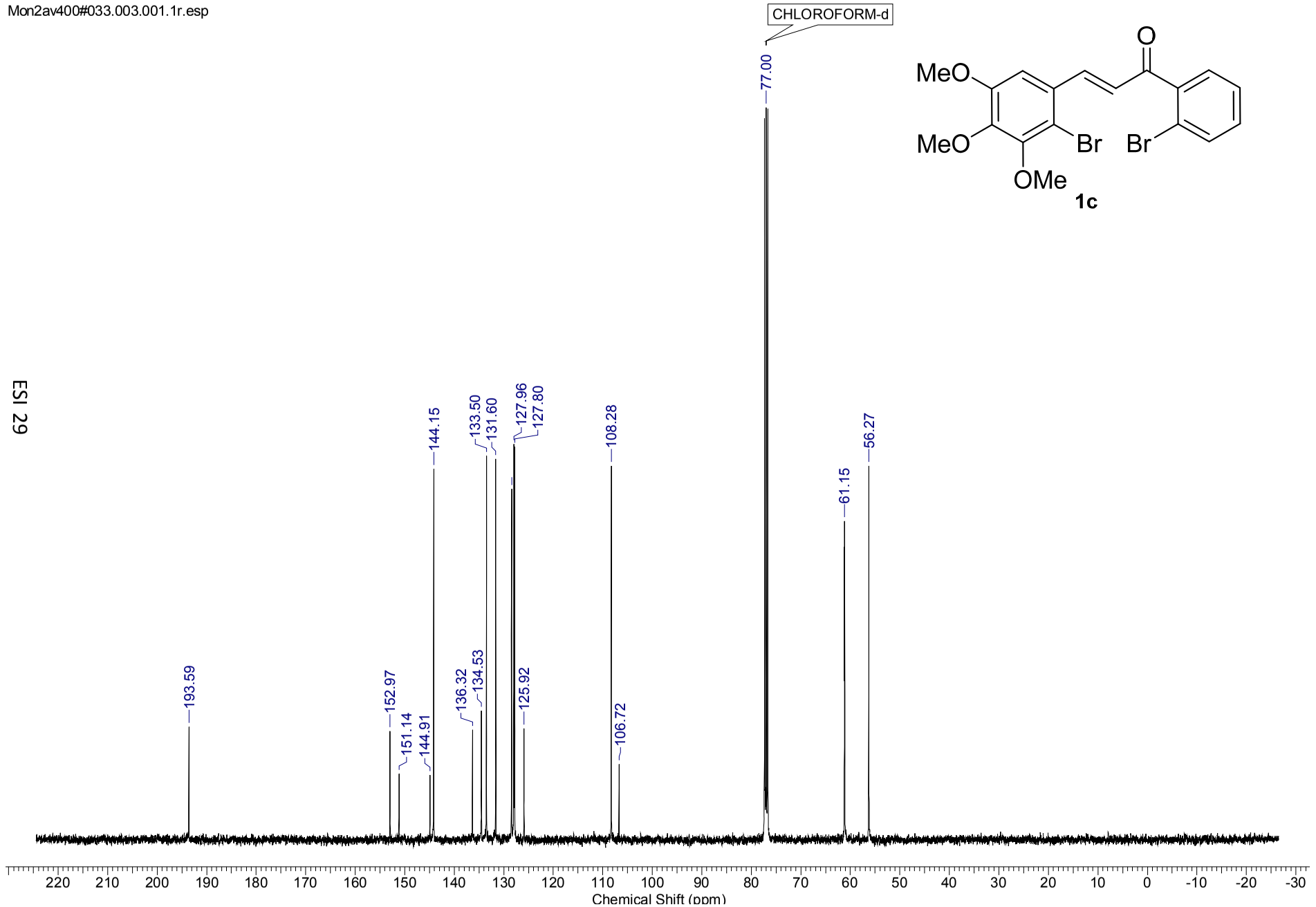
2b

Acquisition Time (sec)	3.9584	***Comment***	Srinivas	***Date***	16 Oct 2015 17:25:28		
Date Stamp	16 Oct 2015 17:25:28			***File Name***	\\agni\nmr_data\AV200\OCT_15#AV200\data\Administrator\nmr\Fri3av2#111\1\pdata\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	4	***Origin***	av200



Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	06 Jul 2015 16:55:36		
Date Stamp	06 Jul 2015 16:55:36			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	2184	***Origin***	spect

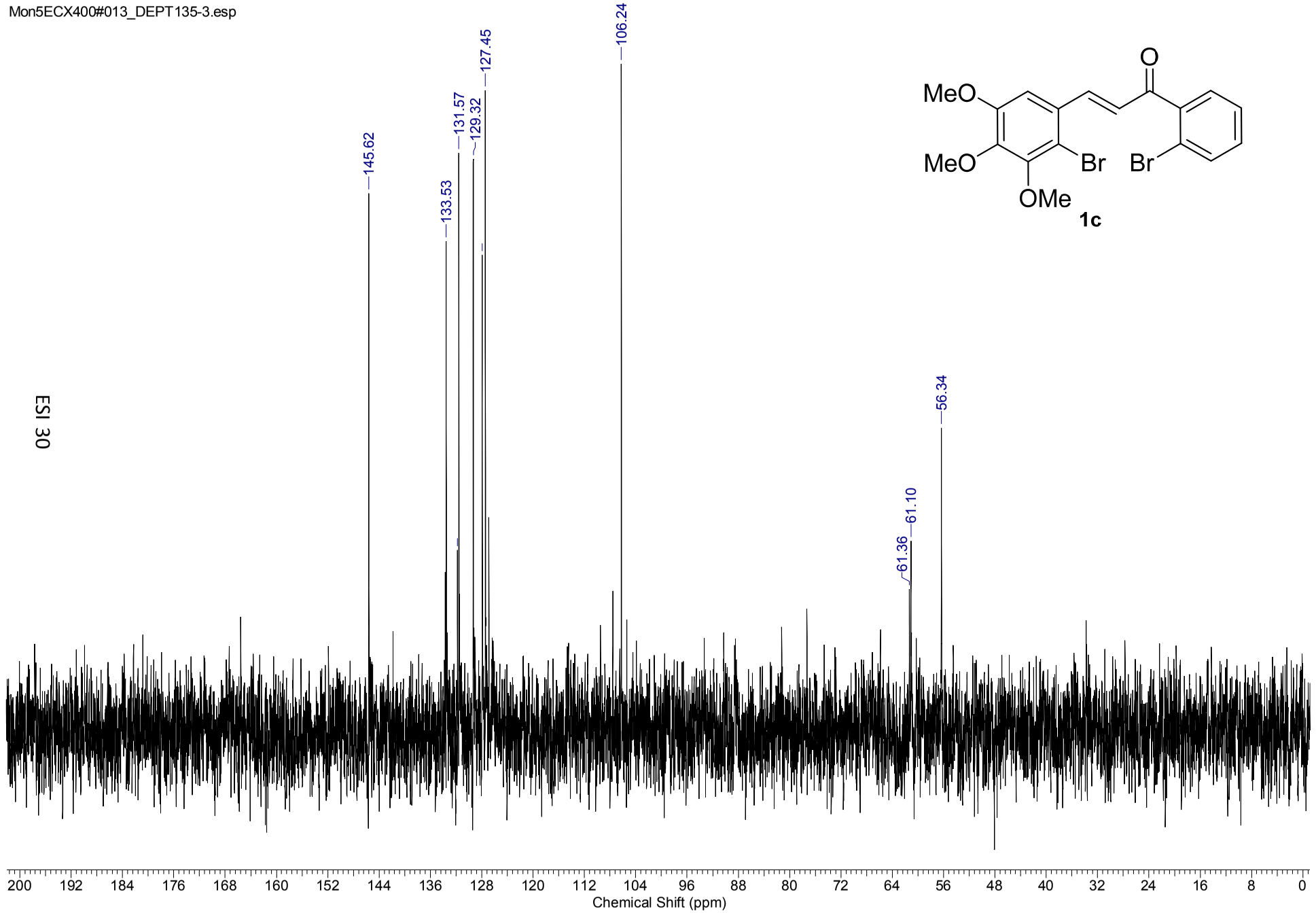
Mon2av400#033.003.001.1r.esp



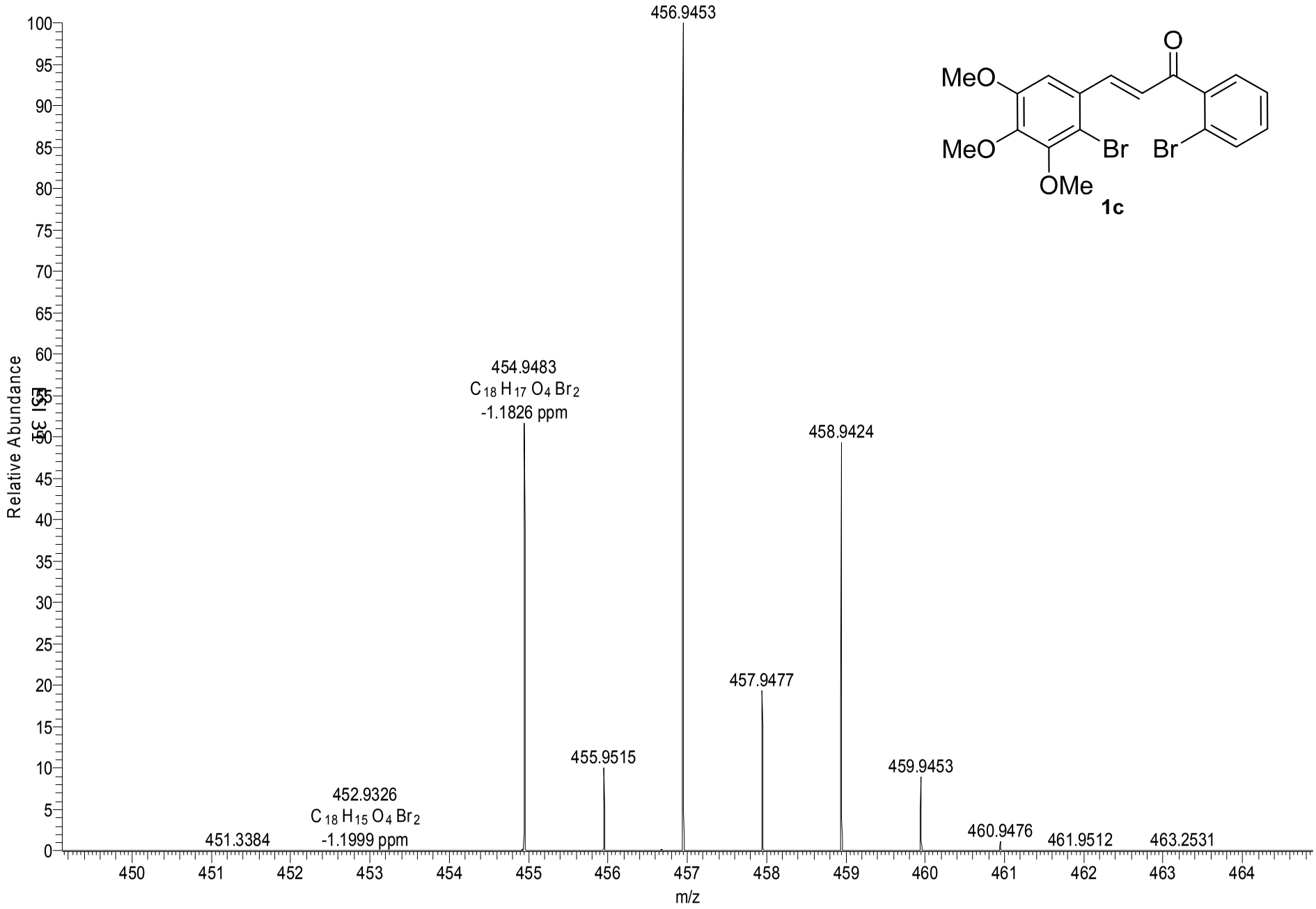
1c

Acquisition Time (sec)	1.0434	***Comment***	ananda	***Solvent***	CHLOROFORM-d		
Date Stamp	27 May 2014 02:35:15			***File Name***	\\agni\nmr_data\JEOL_400\2014\May 2014\Mon5ECX400#013_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	800	***Origin***	ECX 400

Mon5ECX400#013_DEPT135-3.esp

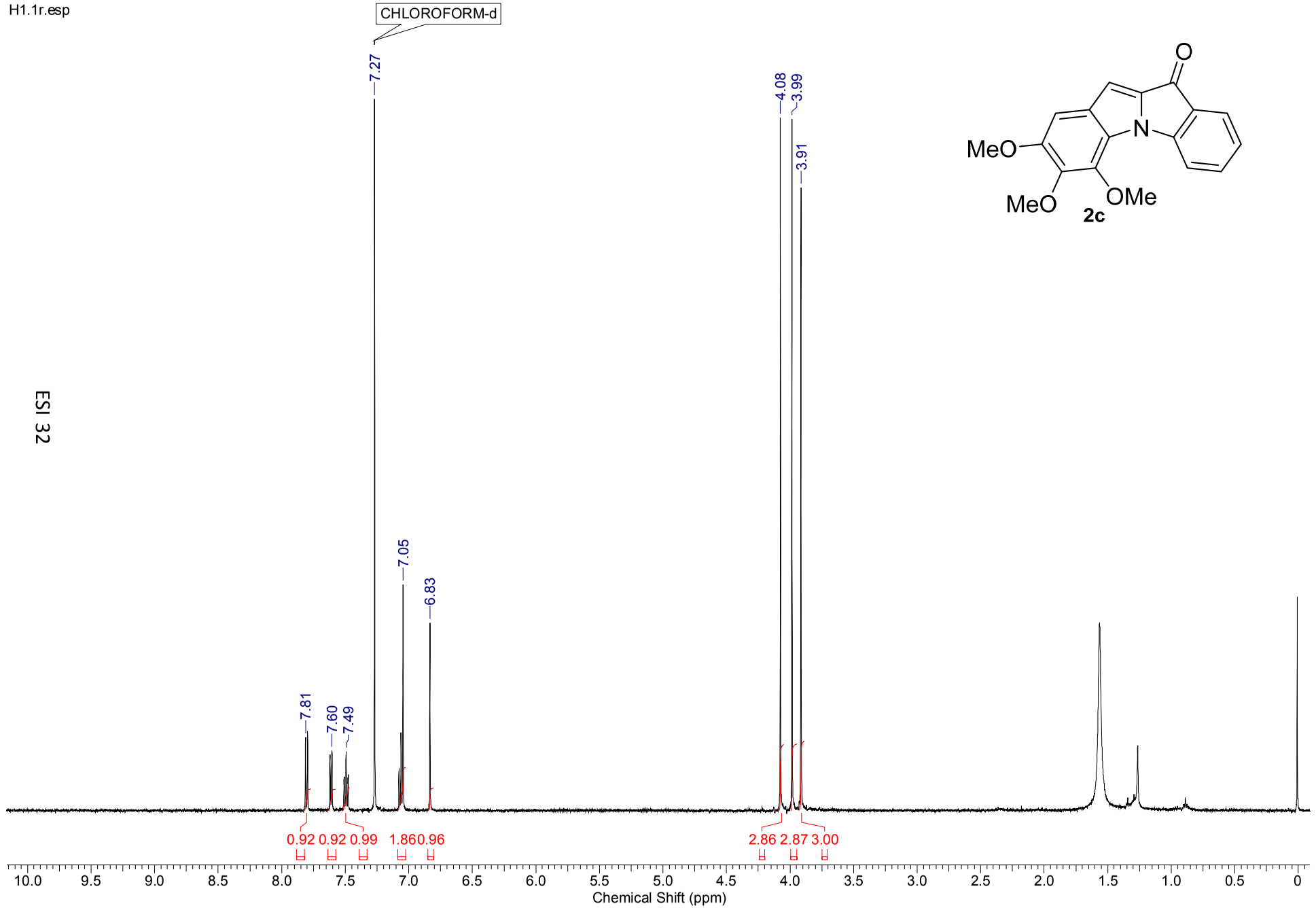


AKC-9 #100 RT: 0.53 AV: 1 NL: 3.89E8
T: FTMS + p ESI Full ms [100.00-1500.00]



Acquisition Time (sec)	1.6000	***Comment***	anand	***Date***	31 Dec 2014 13:37:20		
Date Stamp	31 Dec 2014 13:37:20			***File Name***	\\agni\nmr_data\AV_500\Dec-14_500\Wed5av500#022\1\PDATA\1\1r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect

H1.1r.esp

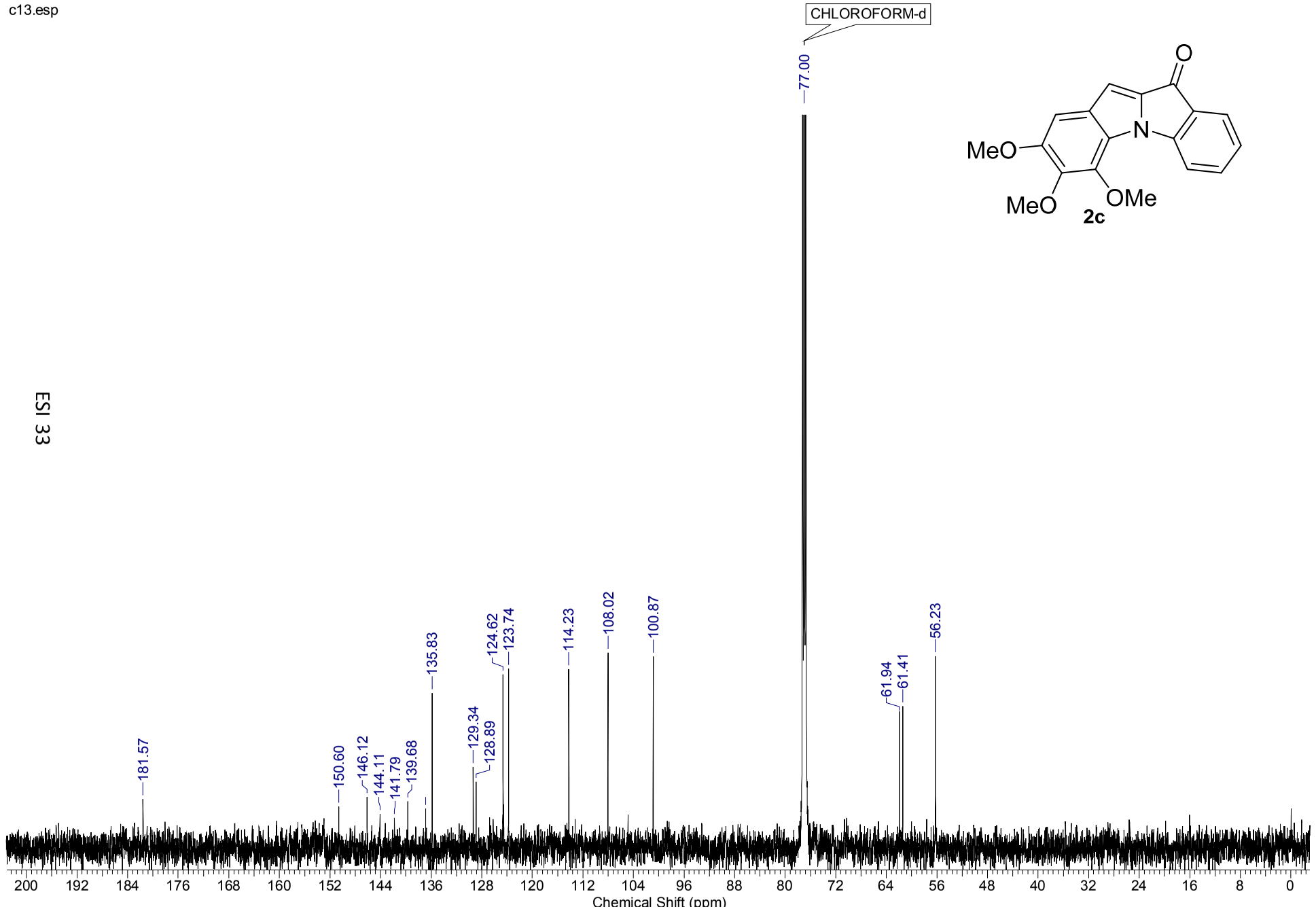


2c

ESI 32

Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	31 Dec 2014 14:37:04		
Date Stamp	31 Dec 2014 14:37:04			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	4243	***Origin***	spect

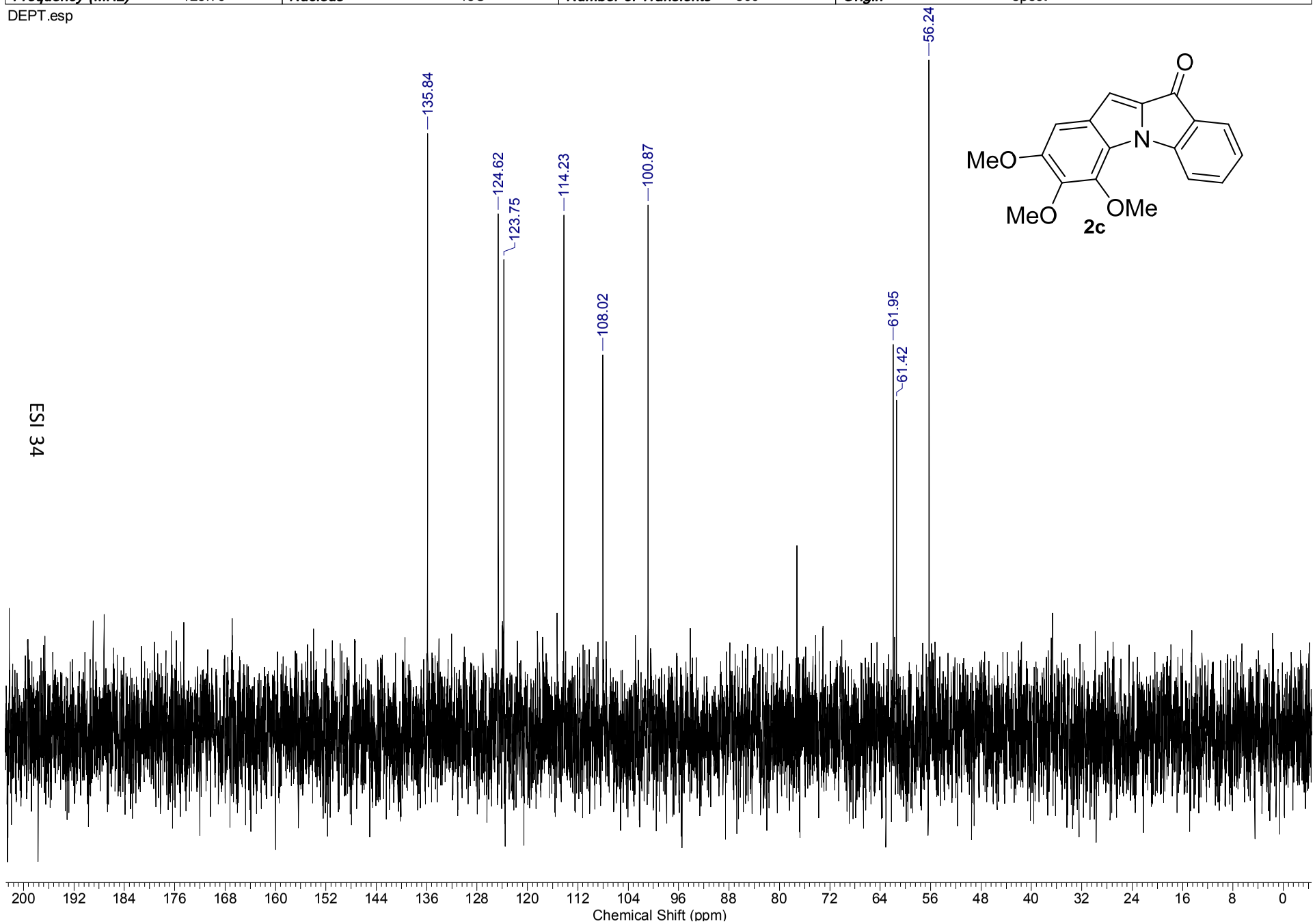
c13.esp



ESI 33

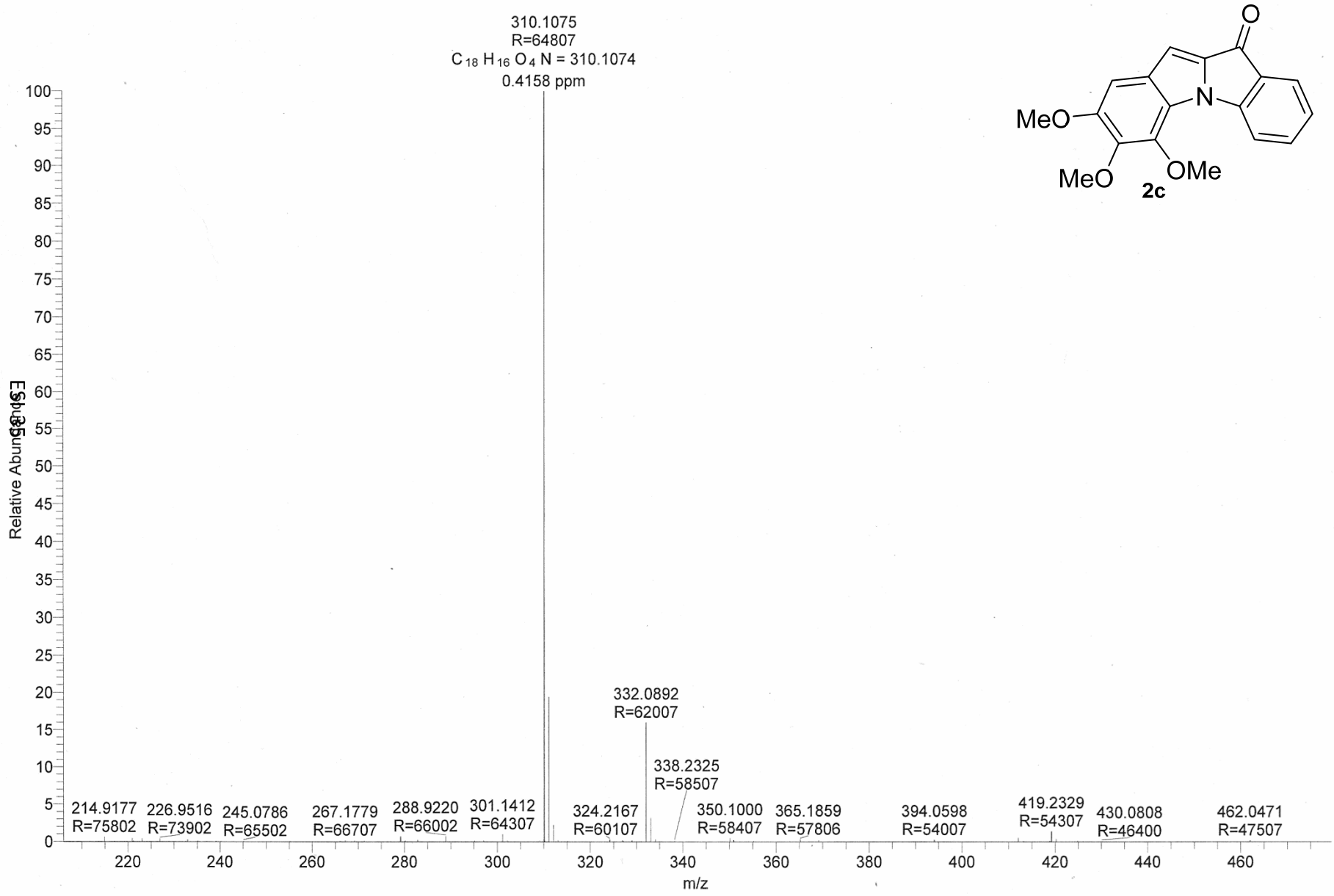
Acquisition Time (sec)	0.6554	***Comment***	DEPT	***Date***	31 Dec 2014 14:17:52		
Date Stamp	31 Dec 2014 14:17:52			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	800	***Origin***	spect

DEPT.esp



D:\Data\TME-N 3/20/2015 12:06:55 PM

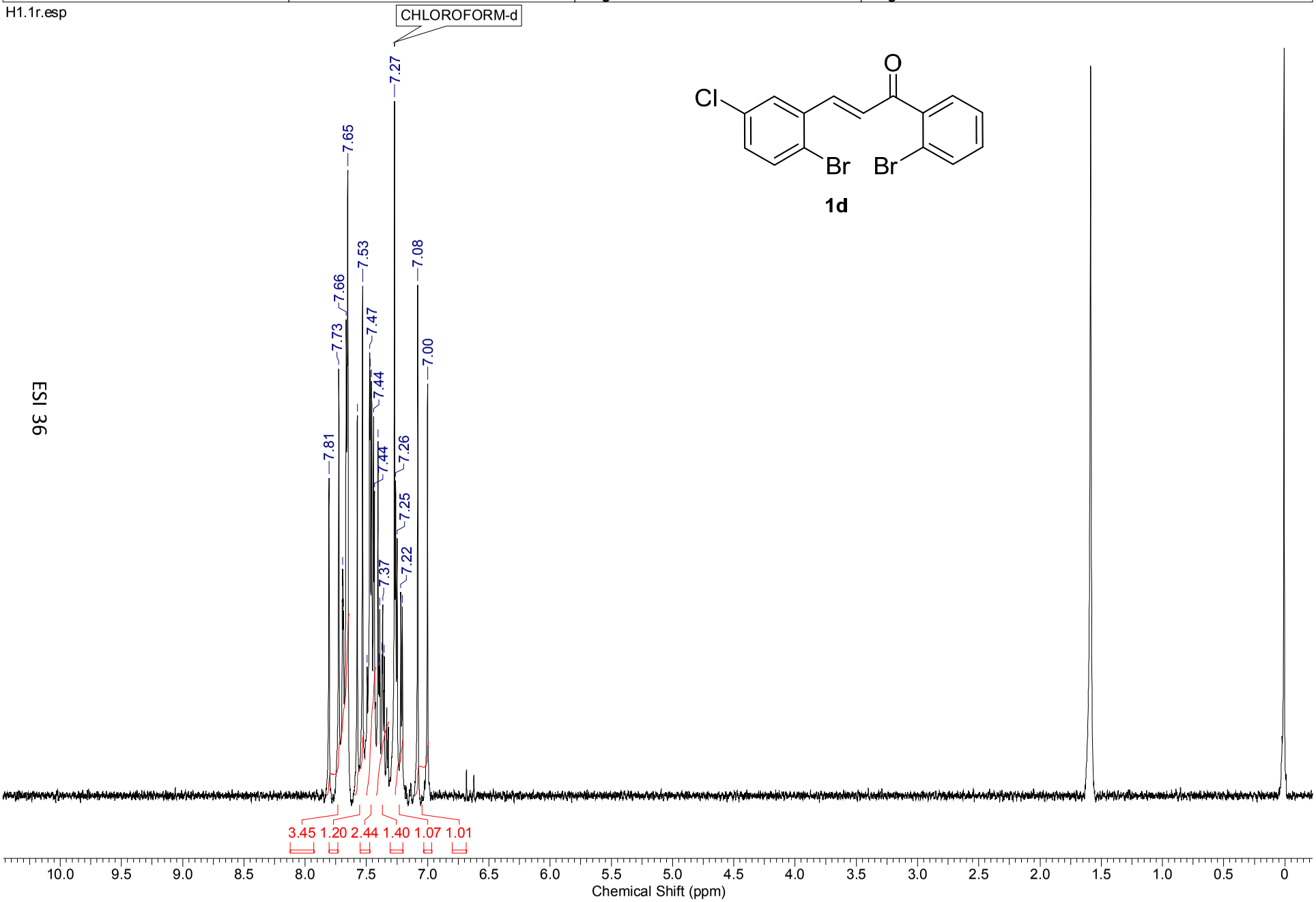
TME-N #147 RT: 0.66 AV: 1 NL: 4.49E8
T: FTMS + p ESI Full ms [85.40-1000.00]



2c

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	02 Jul 2014 01:12:40						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Tue1av2#093\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

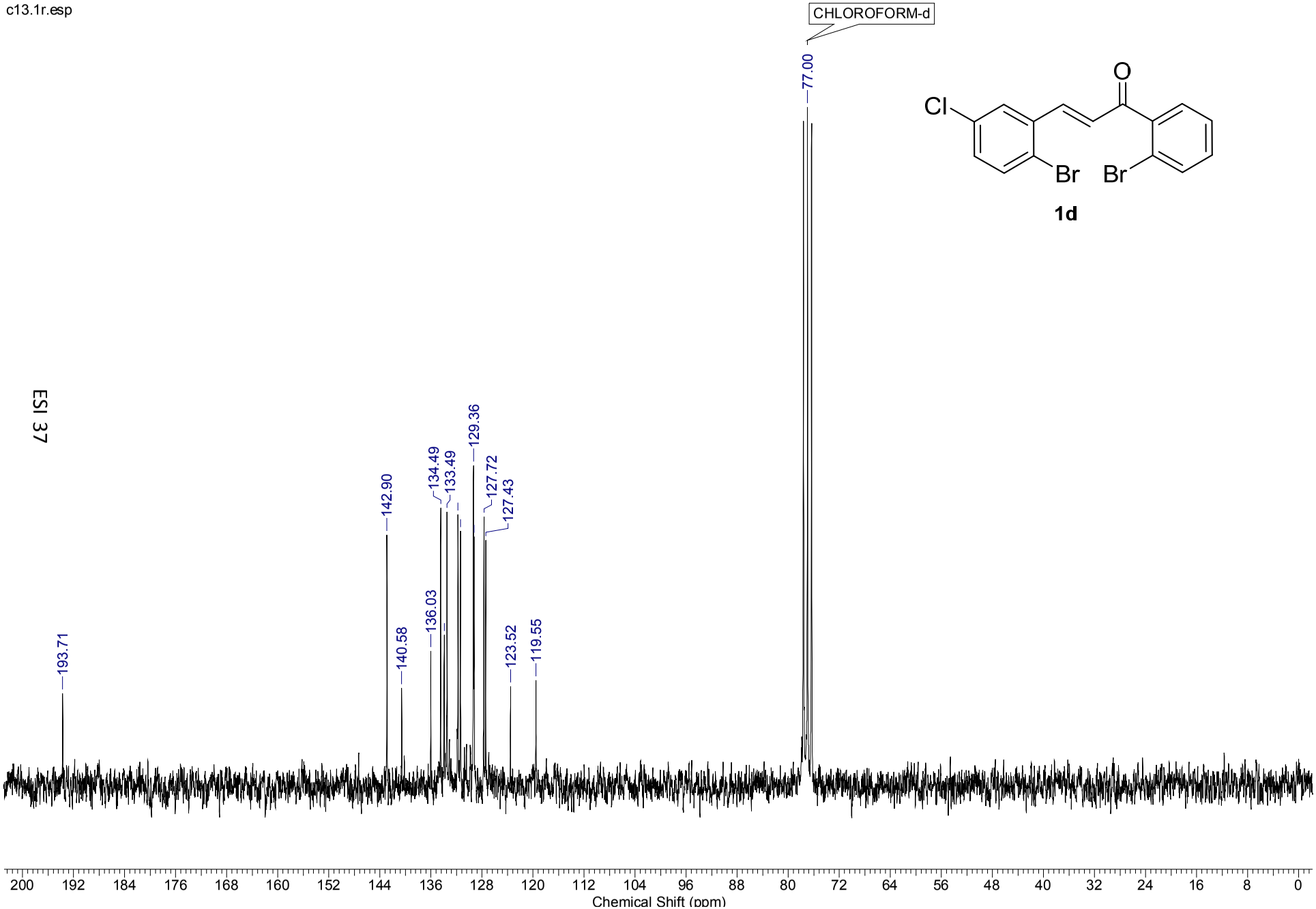
H1.1r.esp



1d

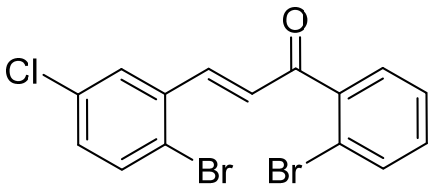
Acquisition Time (sec)	0.6832	***Comment***	Anand	***Date***	27 Jul 2014 02:20:56
Date Stamp	27 Jul 2014 02:20:56			***Solvent***	CHLOROFORM-d
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat4av2#056\2\pdata\1\1r			***Frequency (MHz)***	50.32

c13.1r.esp



Acquisition Time (sec)	0.6832	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	27 Jul 2014 02:01:44						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat4av2#056\1\PDATA\1\1r					***Frequency (MHz)***	50.32
Nucleus	13C	***Number of Transients***	200	***Origin***	av200	***Original Points Count***	8192

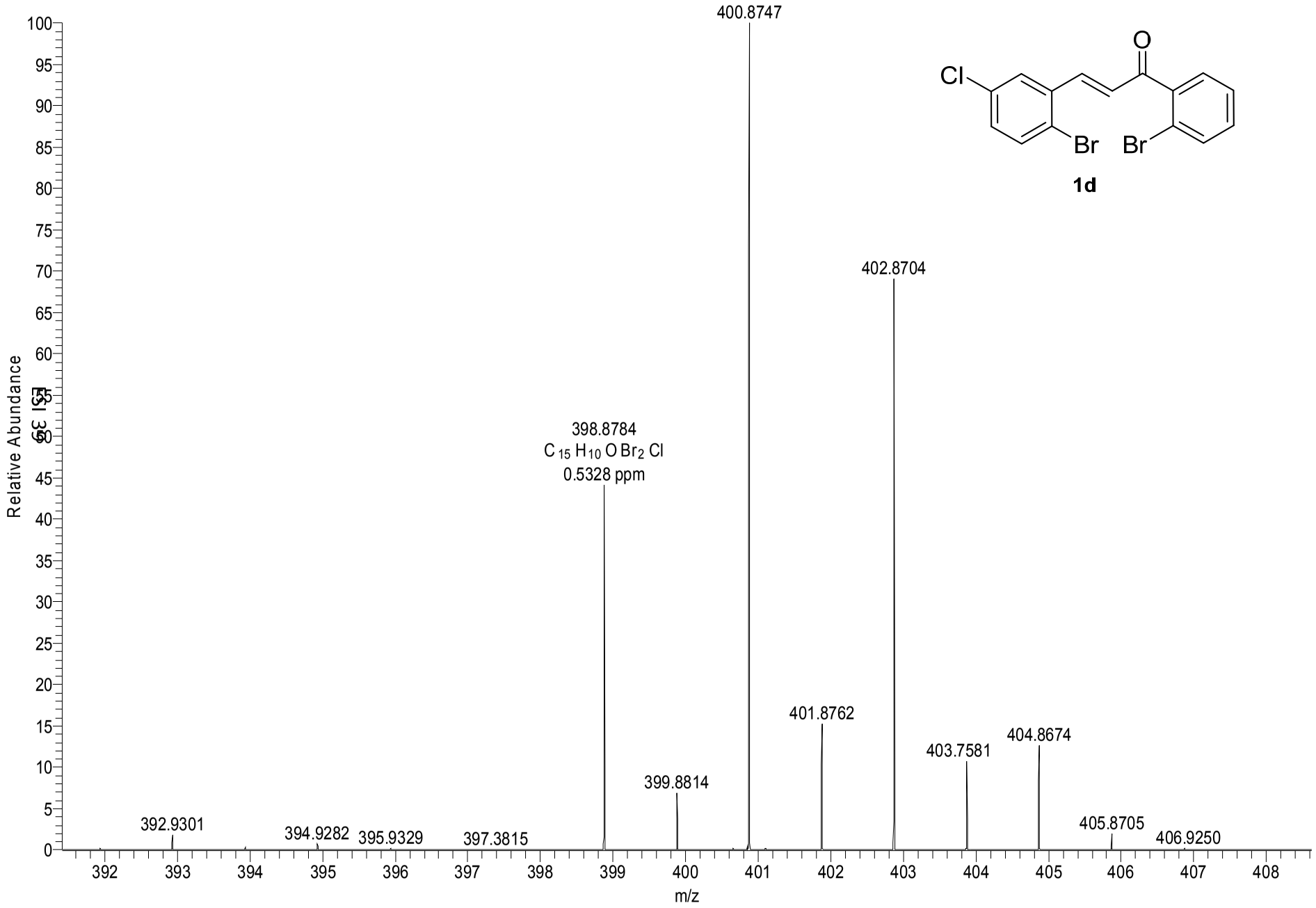
Sat4av2#056.001.001.1r.esp



1d

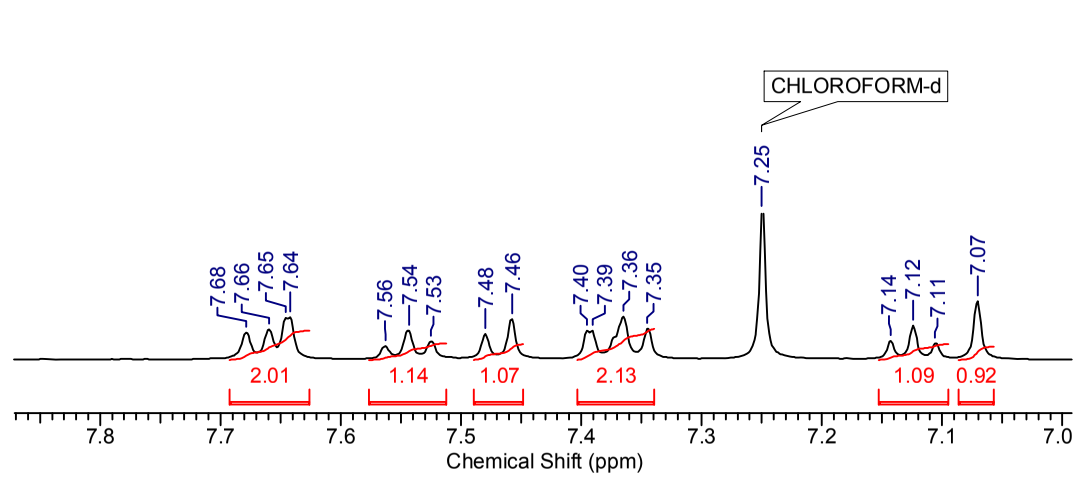
ESI 38

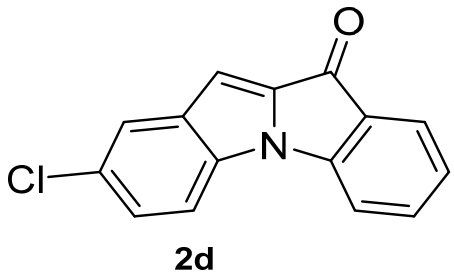
AKC-4 #117 RT: 0.62 AV: 1 NL: 1.27E9
T: FTMS + p ESI Full ms [100.00-1500.00]



1d

Acquisition Time (sec)	2.0447	***Comment***	Aanand 1H	***Date***	28 Oct 2015 14:47:36		
Date Stamp	28 Oct 2015 14:47:36			***File Name***	\\agni\nmr_data\AV400\Oct_15_400\Wed5av400#018\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	40	***Origin***	spect

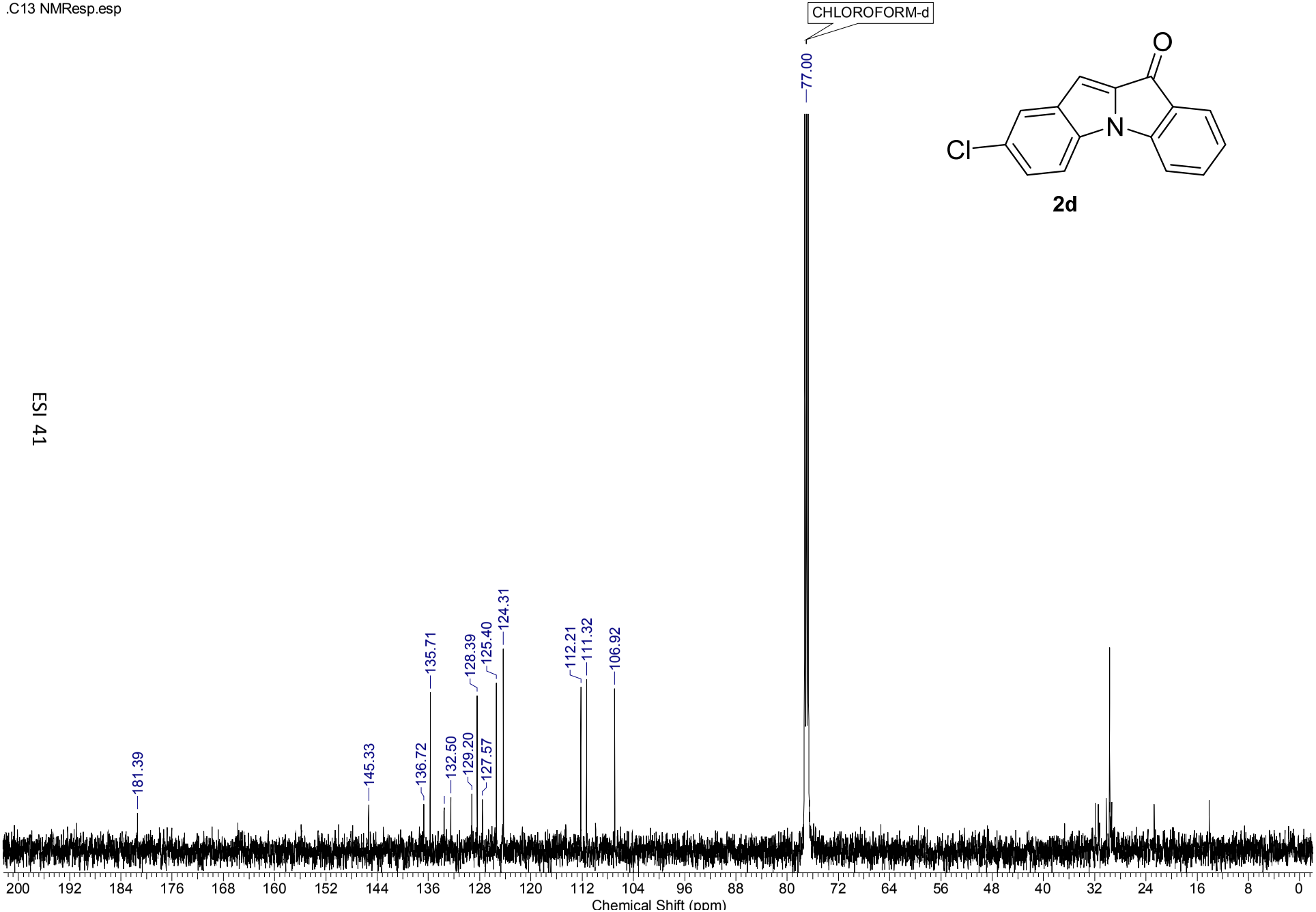




2d

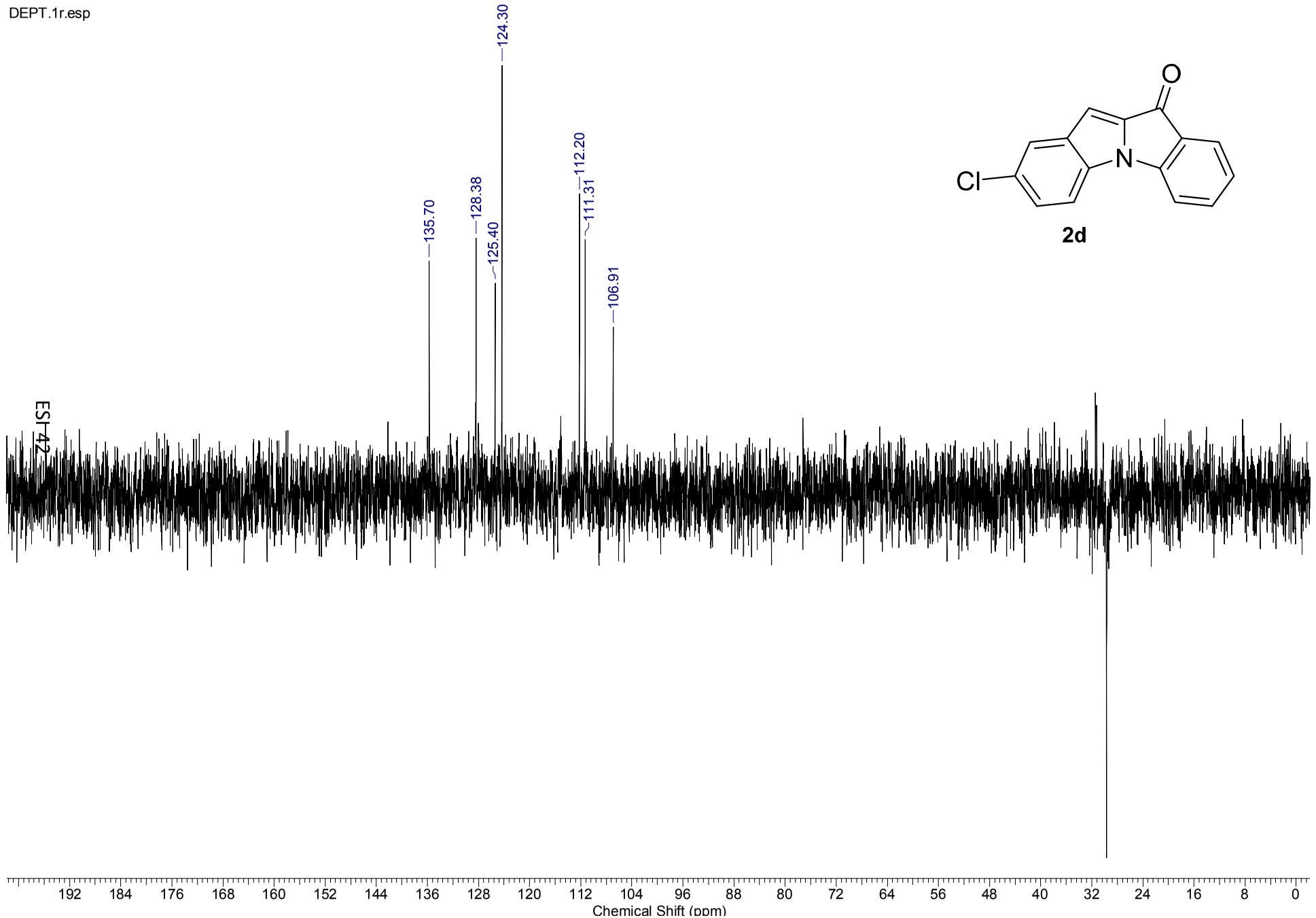
Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	17 Dec 2014 15:51:44		
Date Stamp	17 Dec 2014 15:51:44			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	2297	***Origin***	spect

.C13 NMResp.esp



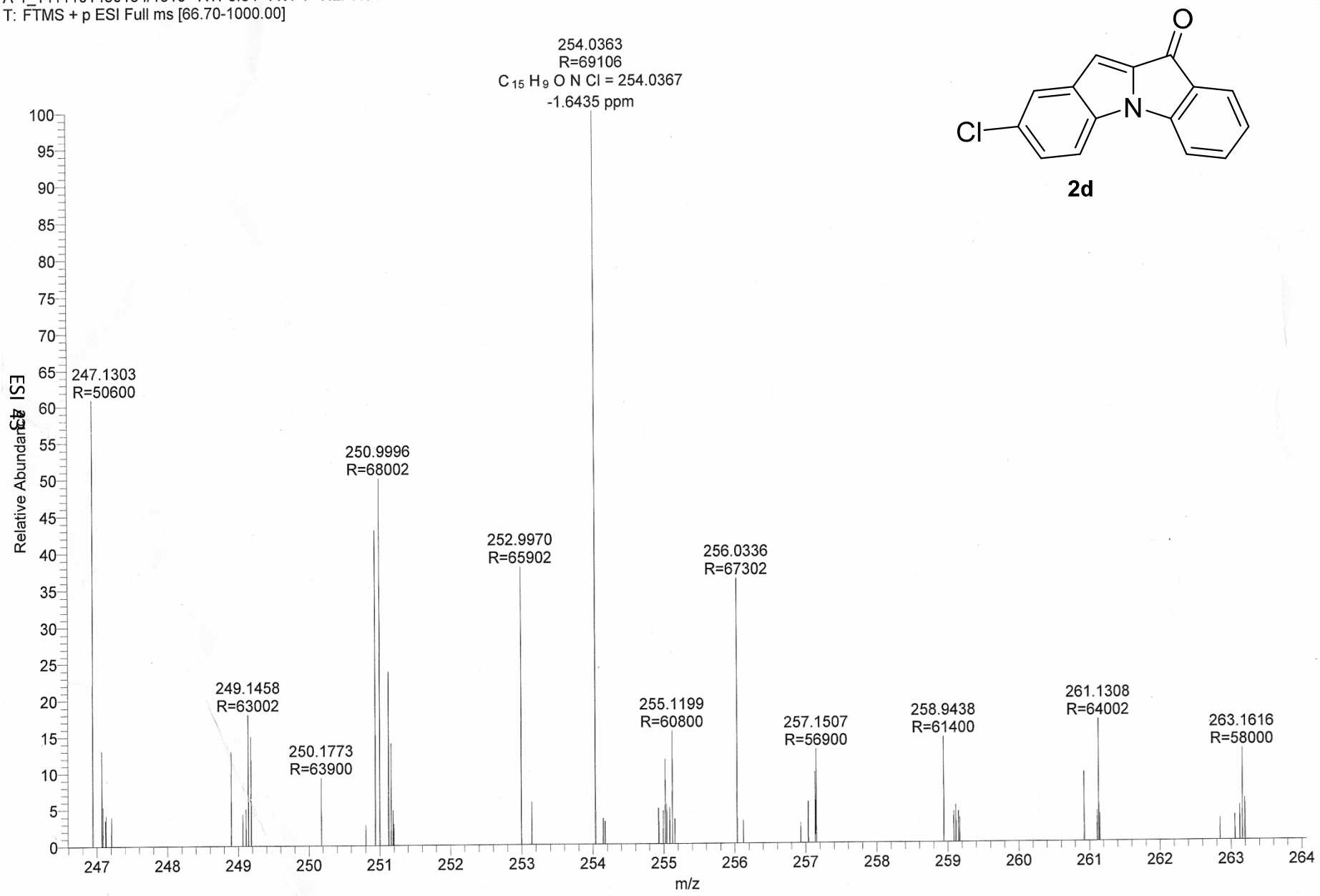
Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	05 Dec 2014 13:07:20		
Date Stamp	05 Dec 2014 13:07:20			***Solvent***	CHLOROFORM		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1645	***Origin***	spect

DEPT.1r.esp



D:\Data\A-1_141110145016 11/10/2014 2:50:16 PM

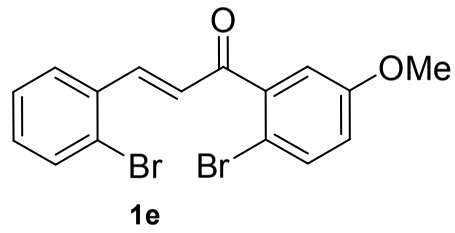
A-1_141110145016 #1310 RT: 5.84 AV: 1 NL: 7.81E5
T: FTMS + p ESI Full ms [66.70-1000.00]



2d

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	19 Jul 2014 09:38:16						
File Name						***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Fri3av2#131.001.001.1r.esp

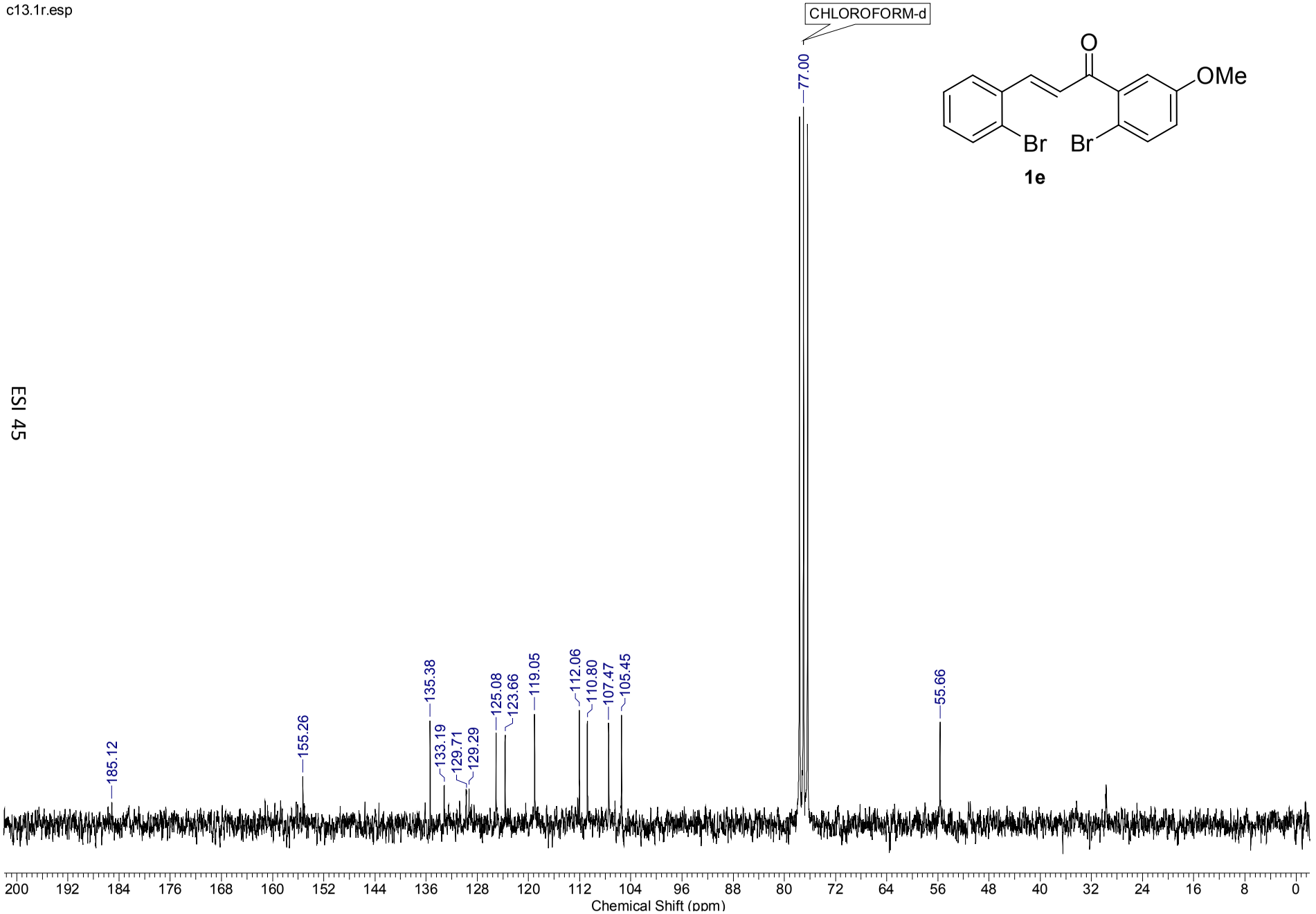


1e

ESI 44

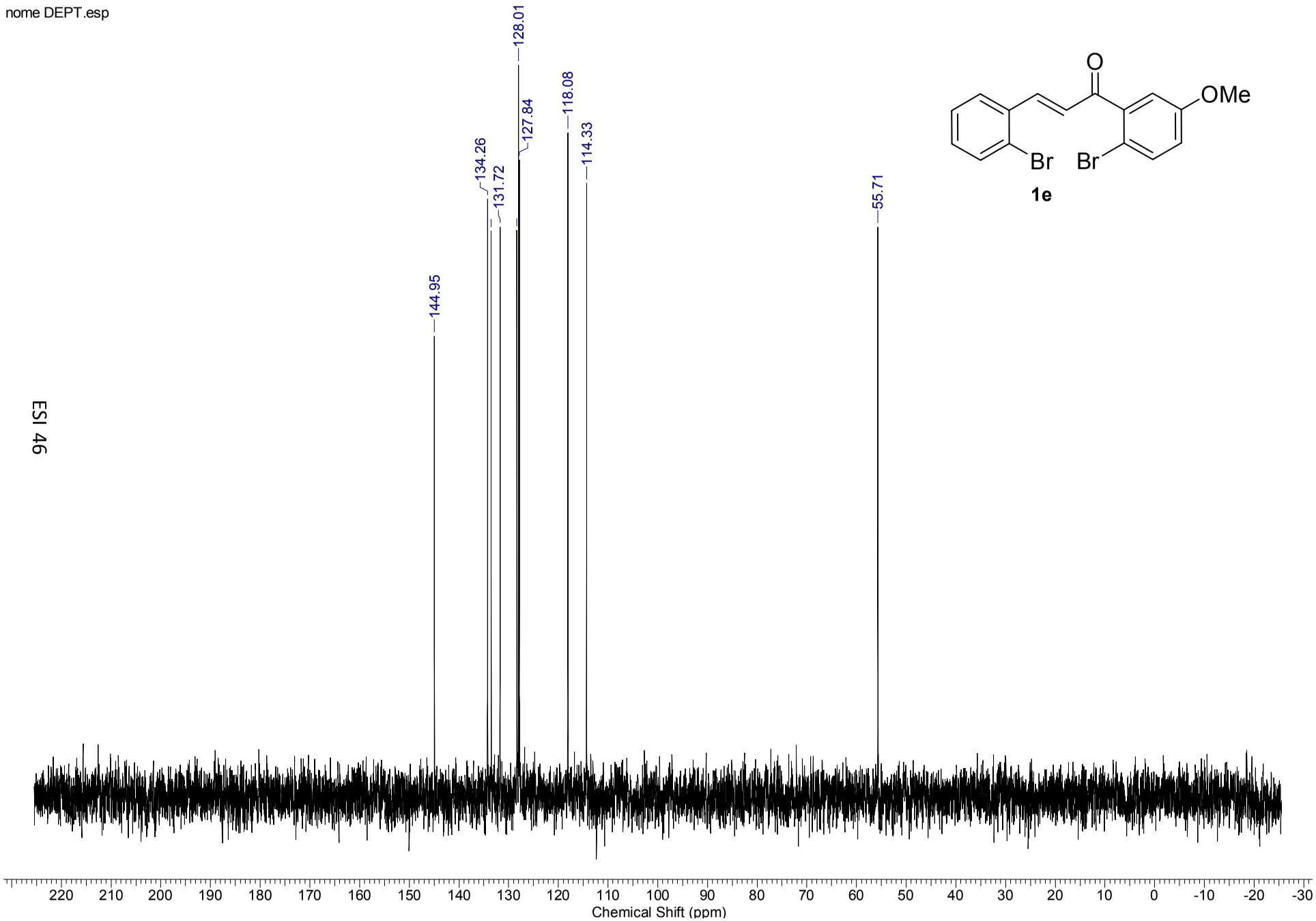
Acquisition Time (sec)	0.6832	***Comment***	anand	***Date***	03 May 2015 18:29:28
Date Stamp	03 May 2015 18:29:28				
File Name	\\agni\nmr_data\AV200\APR_15#AV200\data\Administrator\nmr\Sat5av2#255\2\PDATA\1\1r			***Frequency (MHz)***	50.32

c13.1r.esp

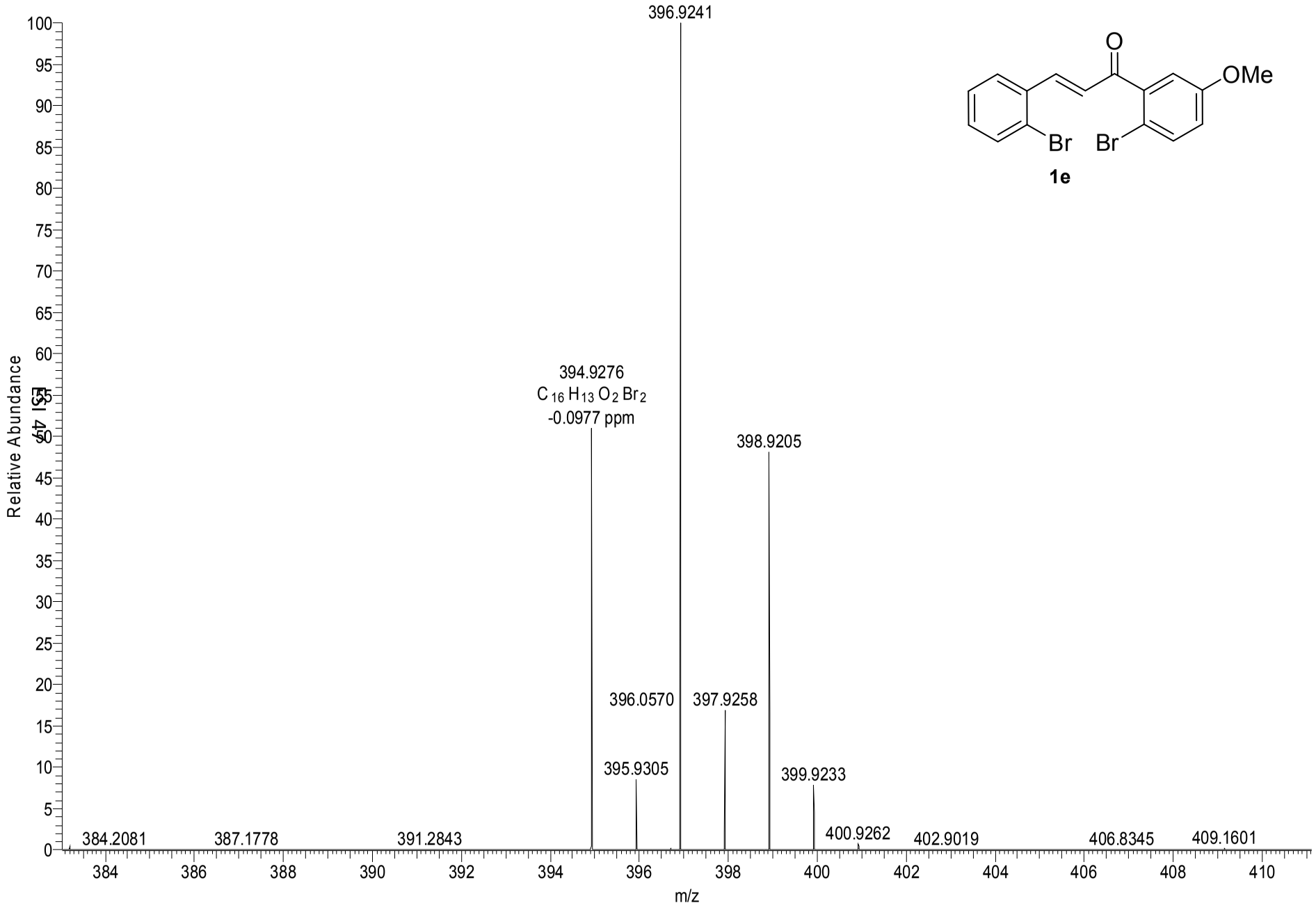


Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	02 Jul 2015 11:01:28		
Date Stamp	02 Jul 2015 11:01:28			***File Name***	\\agni\nmr_data\AV400\July_15_400\Thu1av400#006\2\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	200	***Origin***	spect

nome DEPT.esp

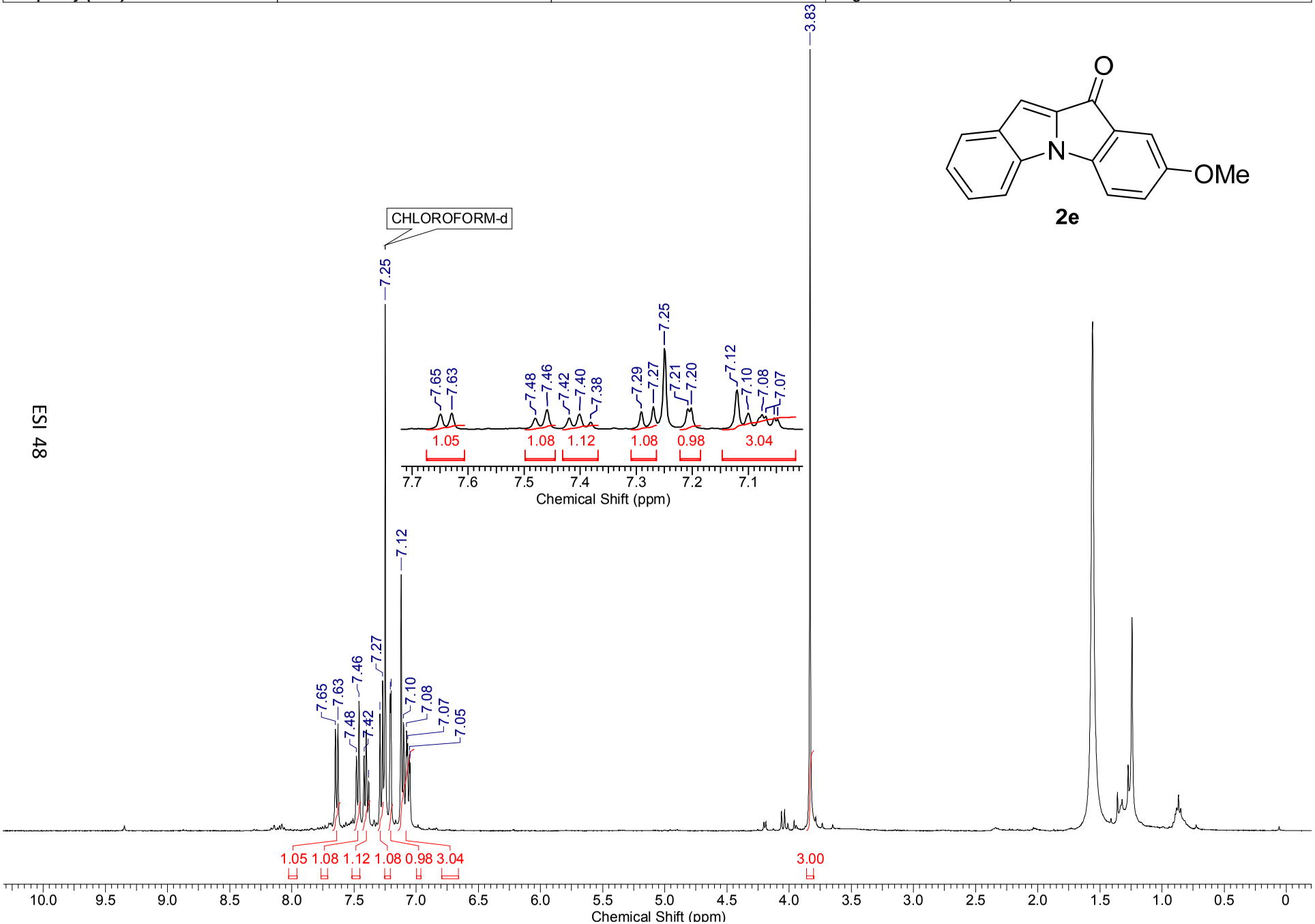


AKC-8 #103 RT: 0.55 AV: 1 NL: 8.51E8
T: FTMS + p ESI Full ms [100.00-1500.00]



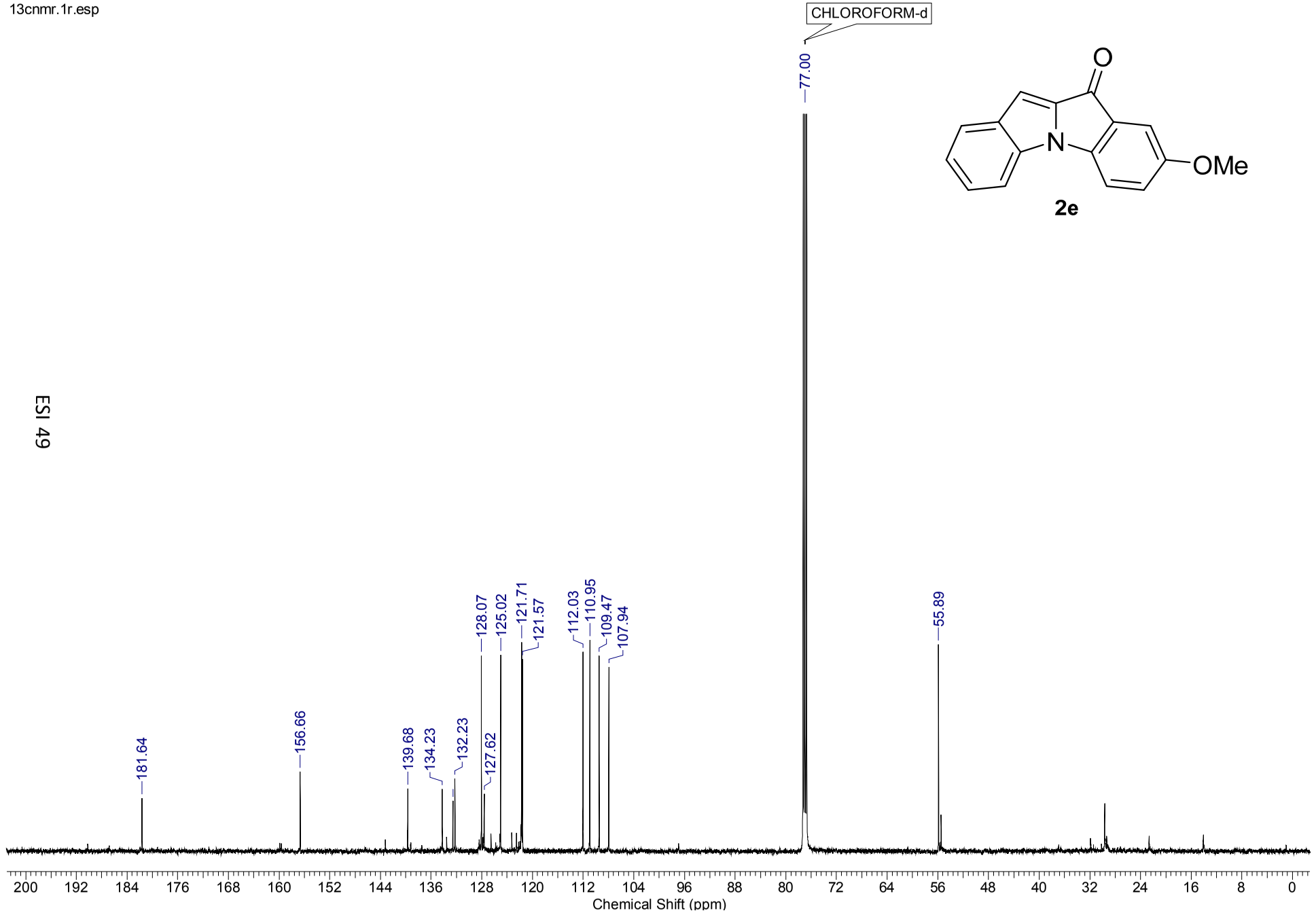
1e

Acquisition Time (sec)	2.0447	***Comment***	Anand 1H	***Date***	29 Oct 2015 12:52:24		
Date Stamp	29 Oct 2015 12:52:24			***File Name***	\\agni\nmr_data\AV400\Oct_15_400\Thu5av400#008\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	128	***Origin***	spect



Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	07 Dec 2014 16:45:04		
Date Stamp	07 Dec 2014 16:45:04			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	7648	***Origin***	spect

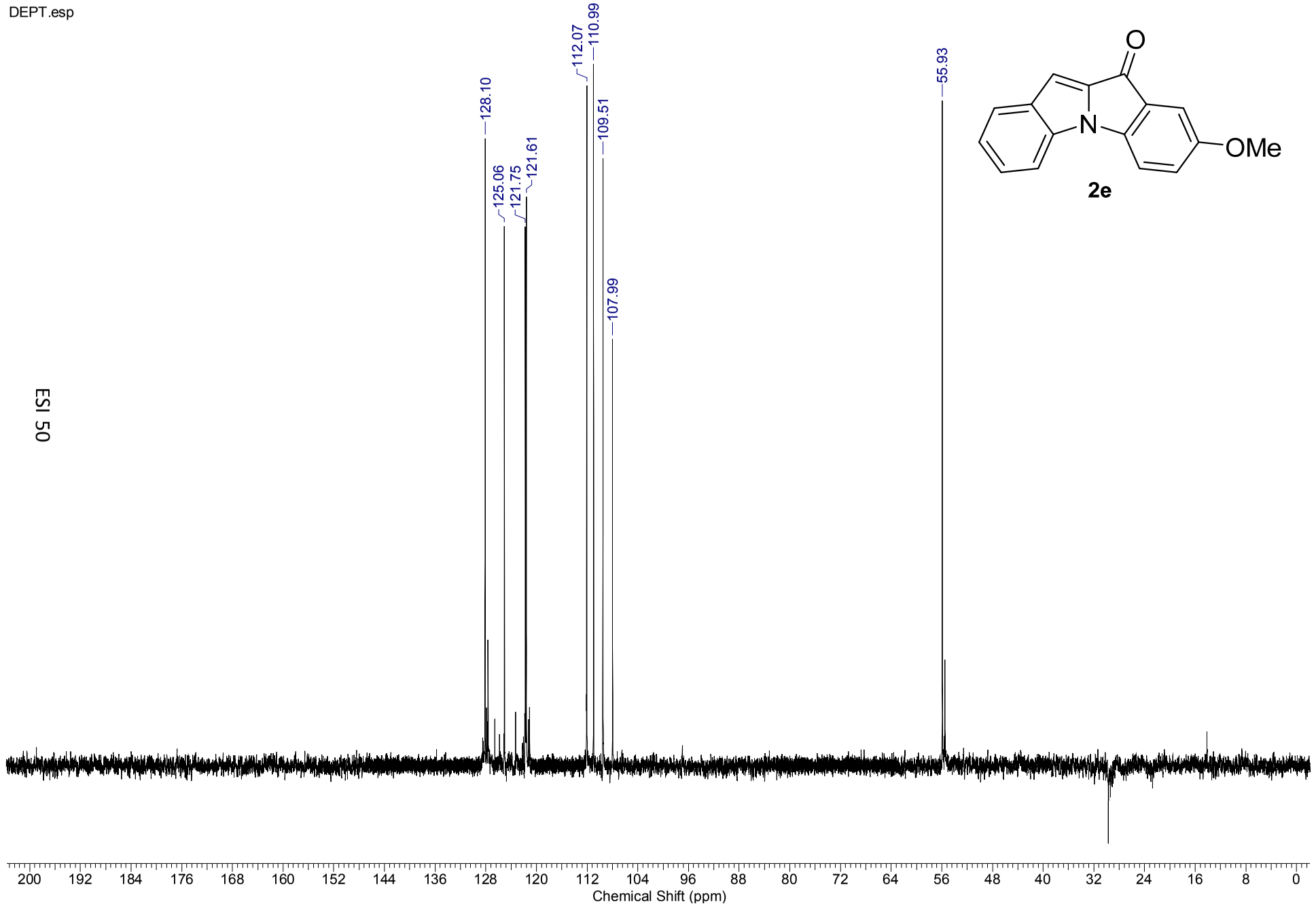
13cnmr.1r.esp



ESI 49

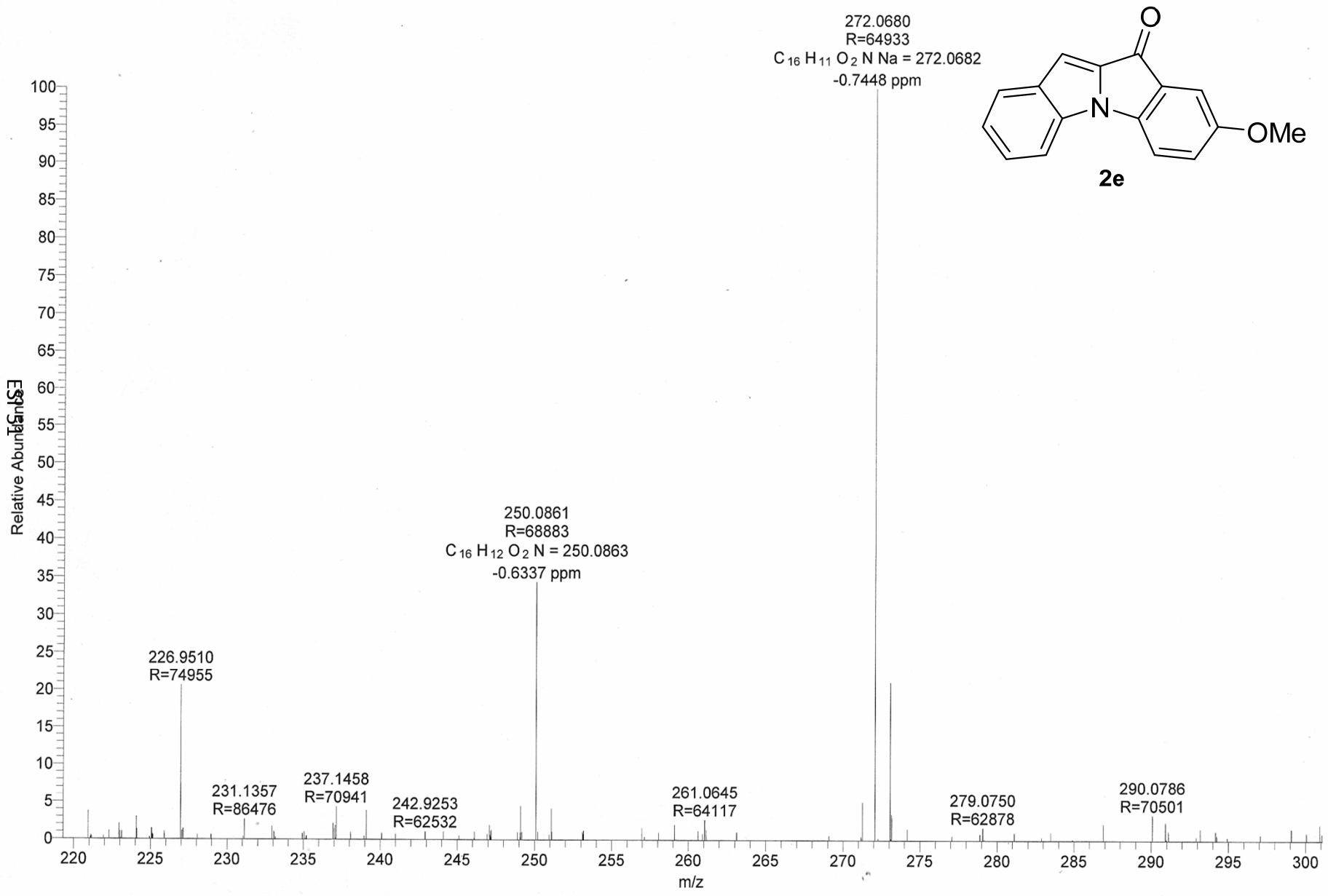
Acquisition Time (sec)	0.6554	***Comment***	DEPT	***Date***	07 Dec 2014 12:26:56		
Date Stamp	07 Dec 2014 12:26:56			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect

DEPT.esp



D:\Data\Br-OMe (10) 9/22/2014 5:39:54 PM

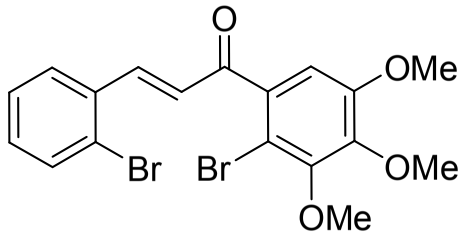
Br-OMe #1185 RT: 5.28 AV: 1 SB: 233 3.78-4.35 , 5.99-6.45 NL: 2.60E6
T: FTMS + p ESI Full ms [66.70-1000.00]



2e

Acquisition Time (sec)	2.0447	***Comment***	Anand 1H	***Date***	06 Jul 2015 15:45:12		
Date Stamp	06 Jul 2015 15:45:12			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect

Mon2av400#033.001.001.1r.esp

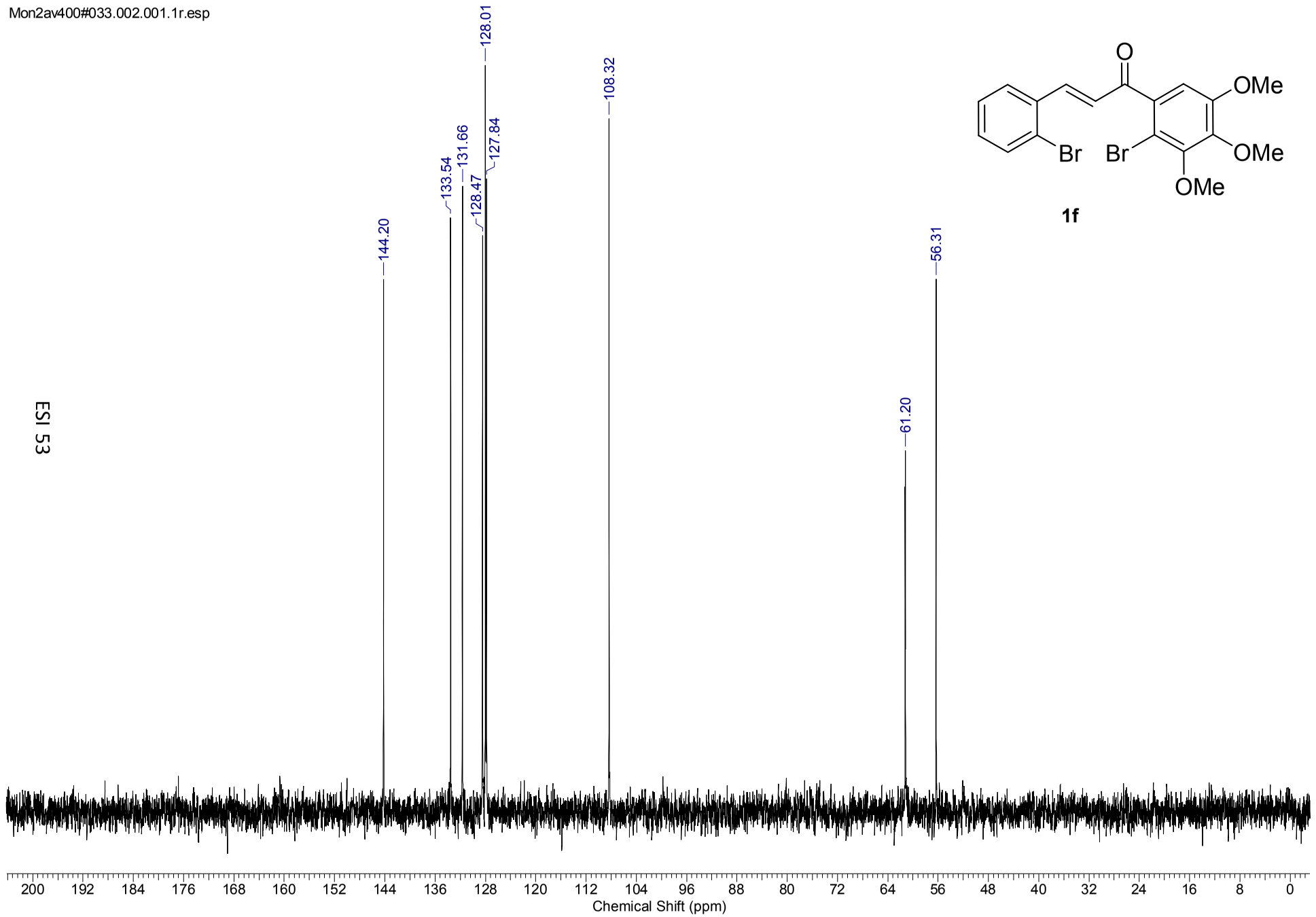


1f

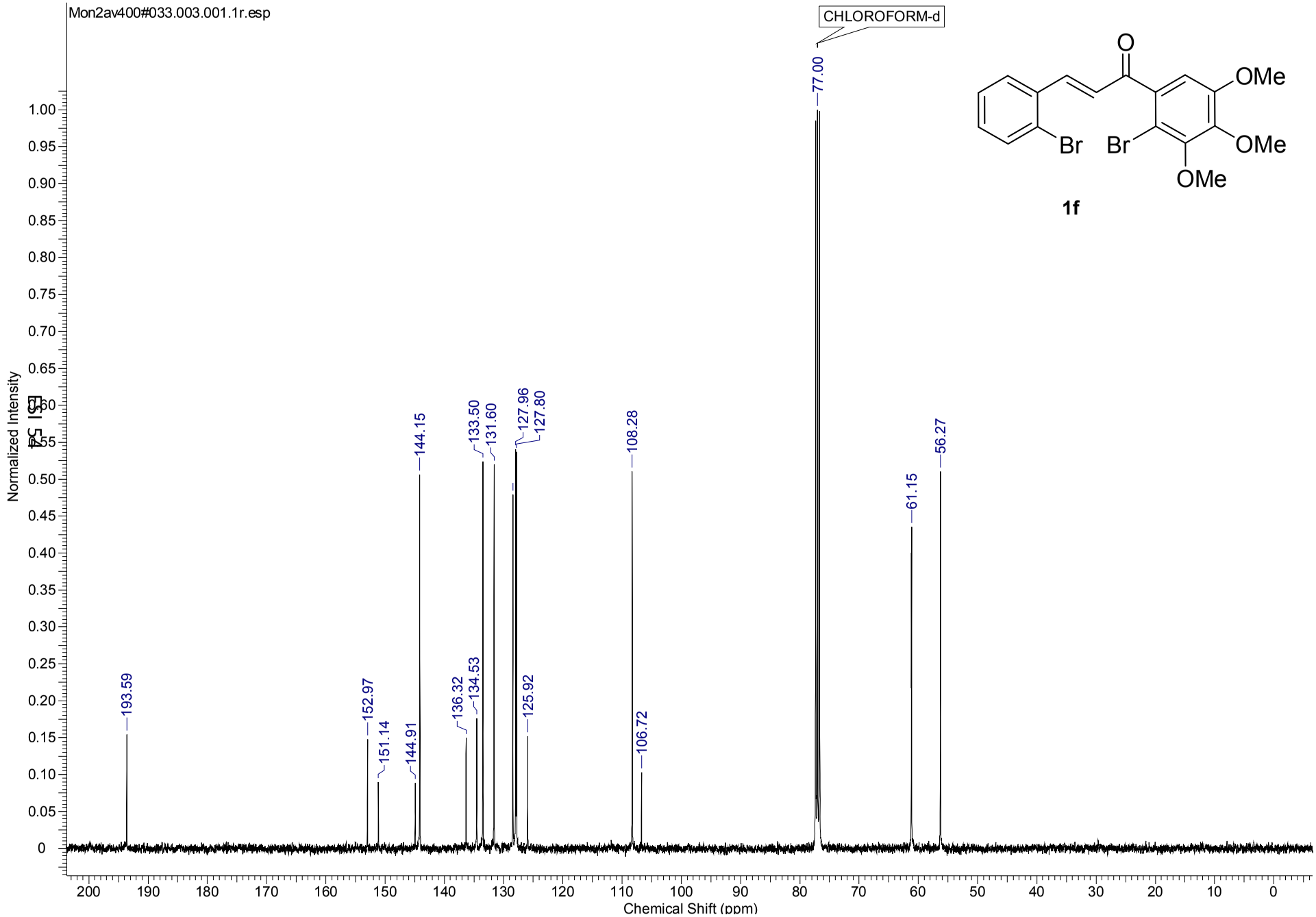
ESI 52

Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	06 Jul 2015 15:53:44				
Date Stamp	06 Jul 2015 15:53:44			***Solvent***	CHLOROFORM-d			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	257	***Origin***	spect	***Original Points Count***	16384	***Owner***	root

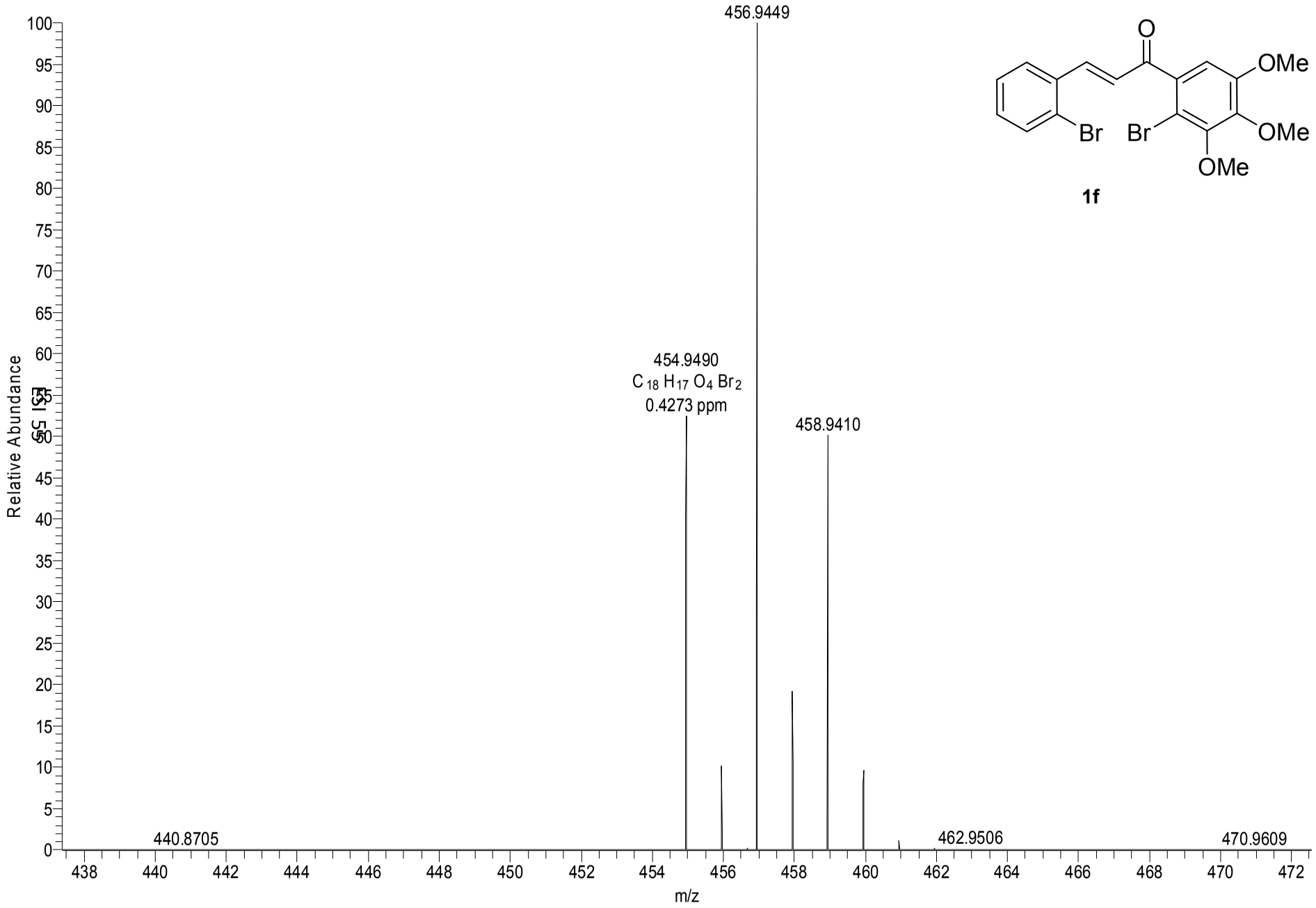
Mon2av400#033.002.001.1r.esp



Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	06 Jul 2015 16:55:36				
Date Stamp	06 Jul 2015 16:55:36			***Solvent***	CHLOROFORM-d			***Frequency (MHz)***	100.61
Nucleus	13C	***Number of Transients***	2184	***Origin***	spect	***Original Points Count***	16384	***Owner***	root

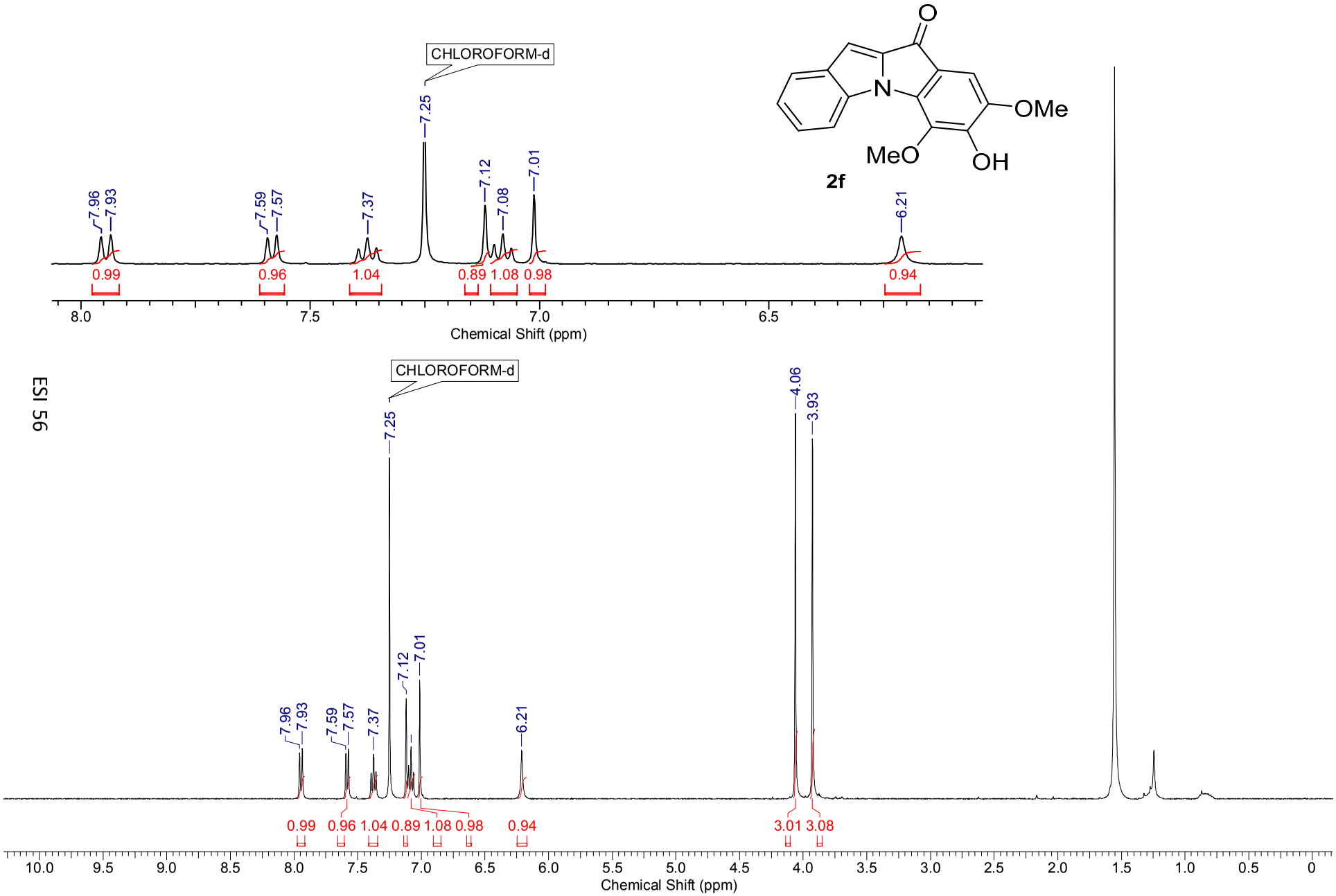


AKC-6 #101 RT: 0.53 AV: 1 NL: 2.30E9
T: FTMS + p ESI Full ms [100.00-1500.00]



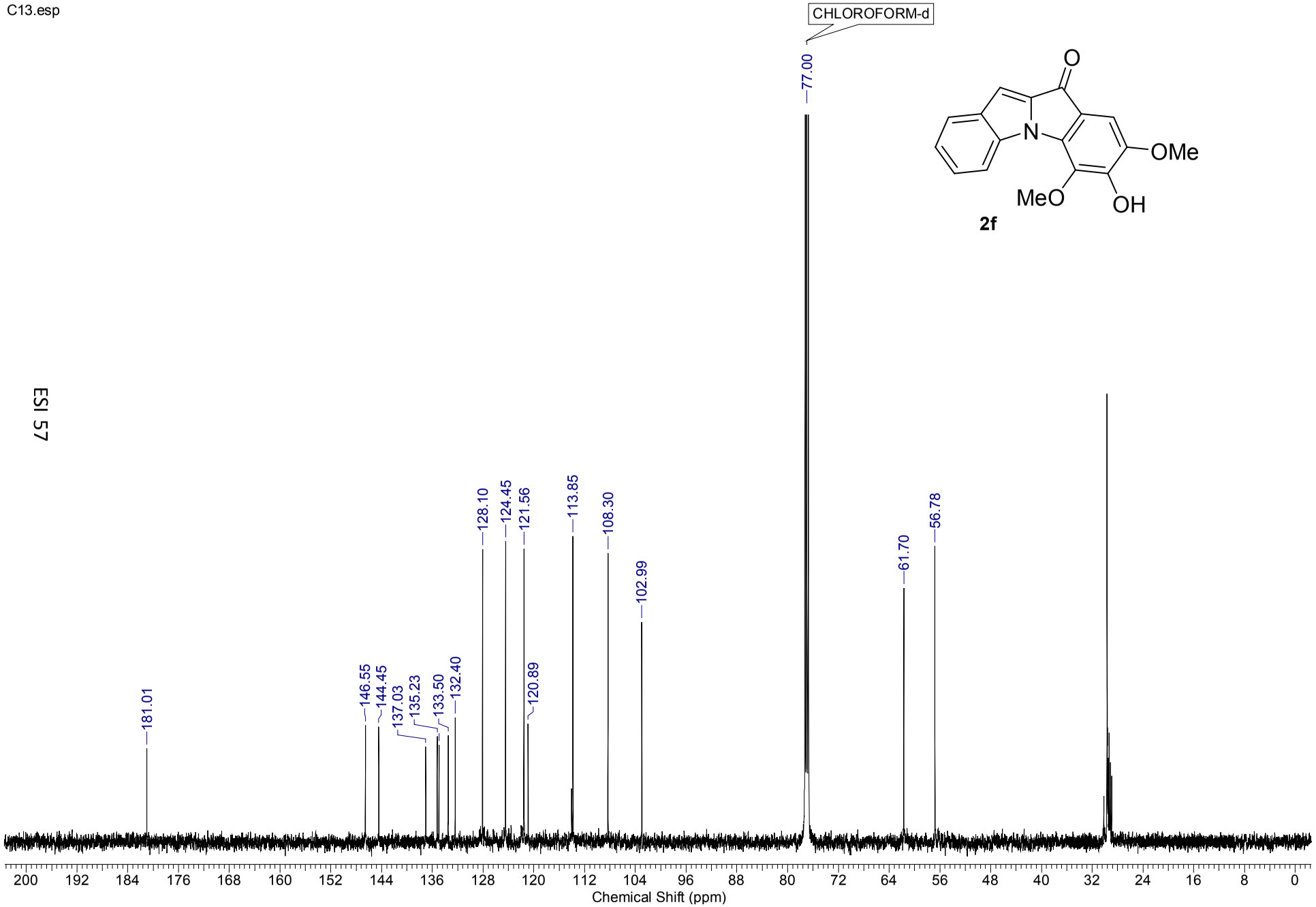
1f

Acquisition Time (sec)	2.0447	***Comment***	Aanand 1H	***Date***	28 Oct 2015 14:43:20		
Date Stamp	28 Oct 2015 14:43:20			***File Name***	\\agni\nmr_data\AV400\Oct_15_400\Wed5av400#017\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	36	***Origin***	spect



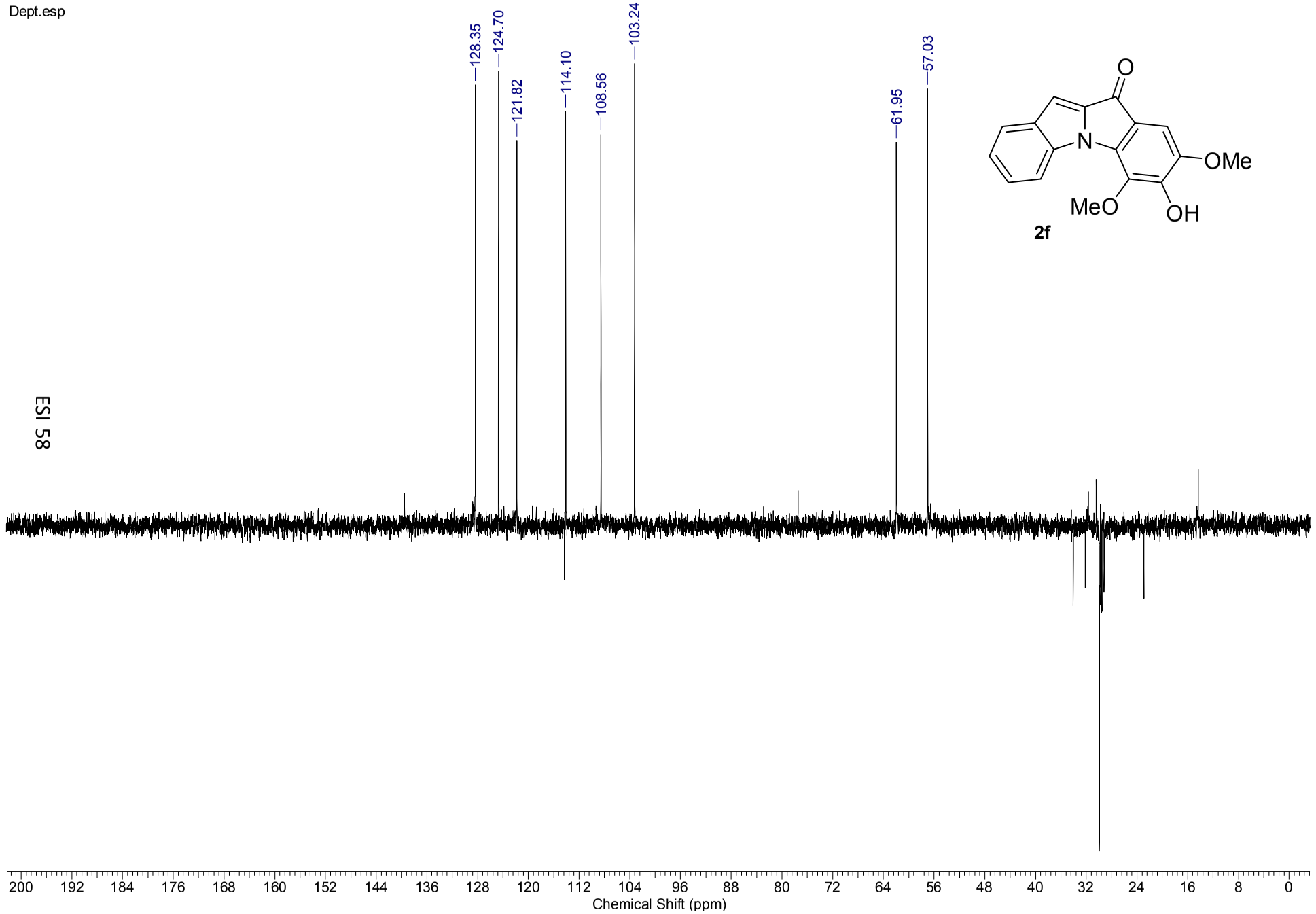
Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	06 Dec 2014 15:28:16		
Date Stamp	06 Dec 2014 15:28:16			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	3135	***Origin***	spect

C13.esp



Acquisition Time (sec)	0.6554	***Comment***	DEPT	***Date***	06 Dec 2014 13:58:40		
Date Stamp	06 Dec 2014 13:58:40			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect

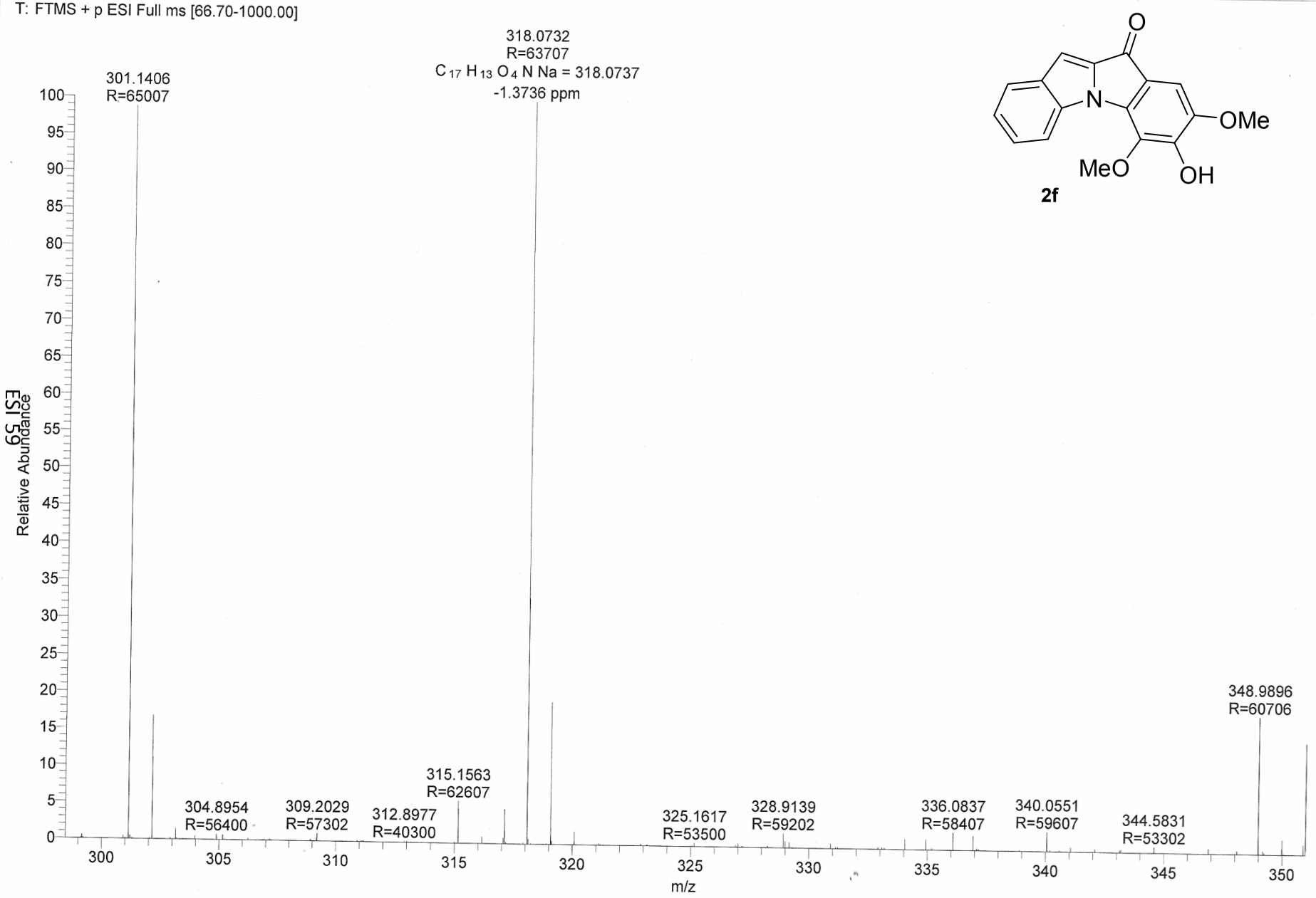
Dept.esp



D:\Data\7 Normal – TMS

12/30/2014 1:51:02 PM

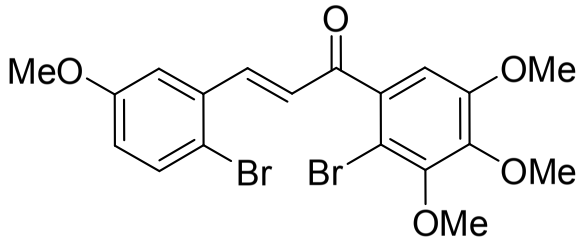
7 #1158 RT: 5.16 AV: 1 NL: 1.35E7
T: FTMS + p ESI Full ms [66.70-1000.00]



2f

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	15 May 2014 17:08:24						
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Thu3av2#108\1\pdata\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Thu3av2#108.001.001.1r.esp

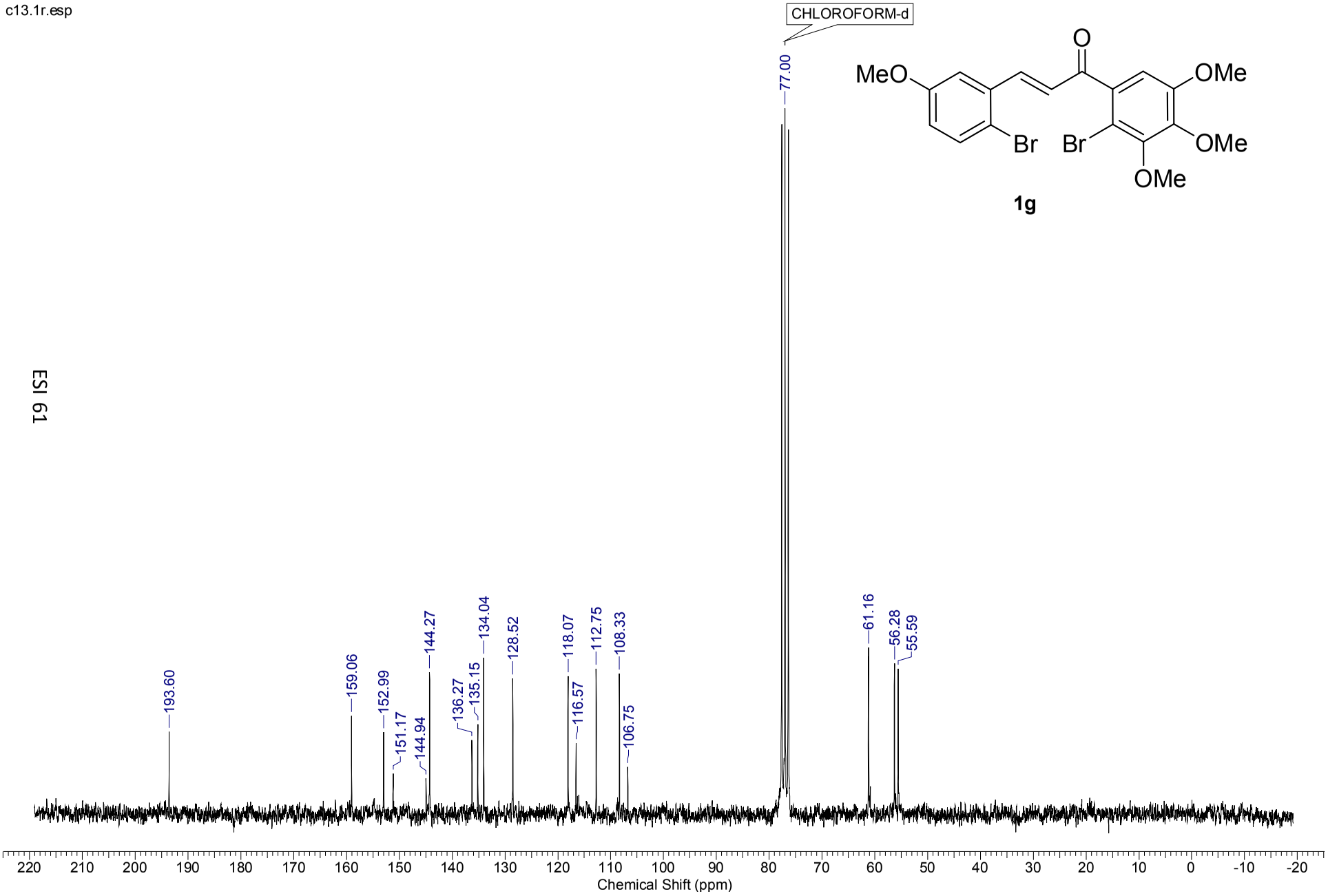


1g

ESI 60

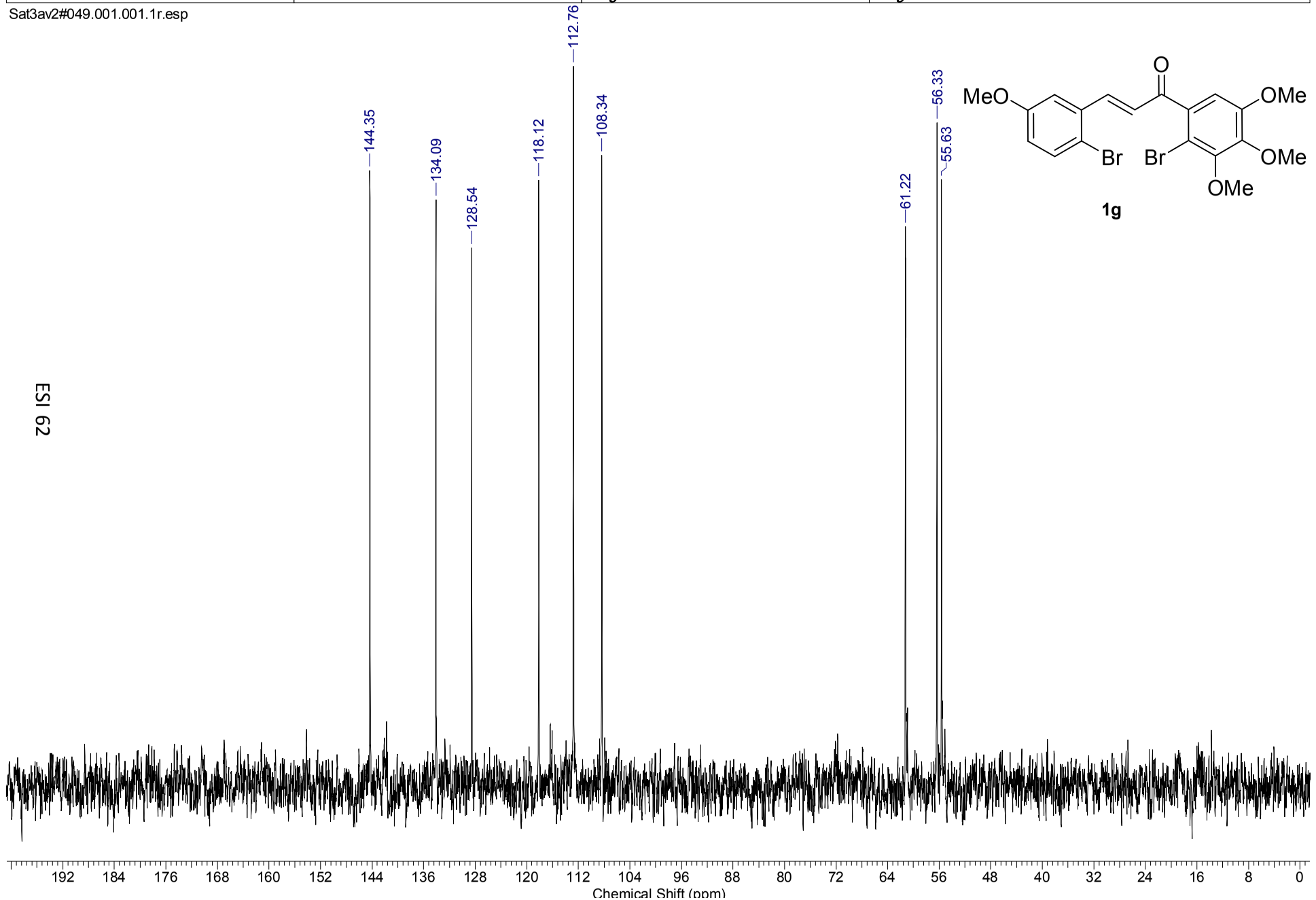
Acquisition Time (sec)	0.6832	***Comment***	Anand	***Date***	19 May 2014 07:04:40
Date Stamp	19 May 2014 07:04:40			***Solvent***	CHLOROFORM-d
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Sat3av2#049\2\pdata\1\1r			***Frequency (MHz)***	50.32

c13.1r.esp

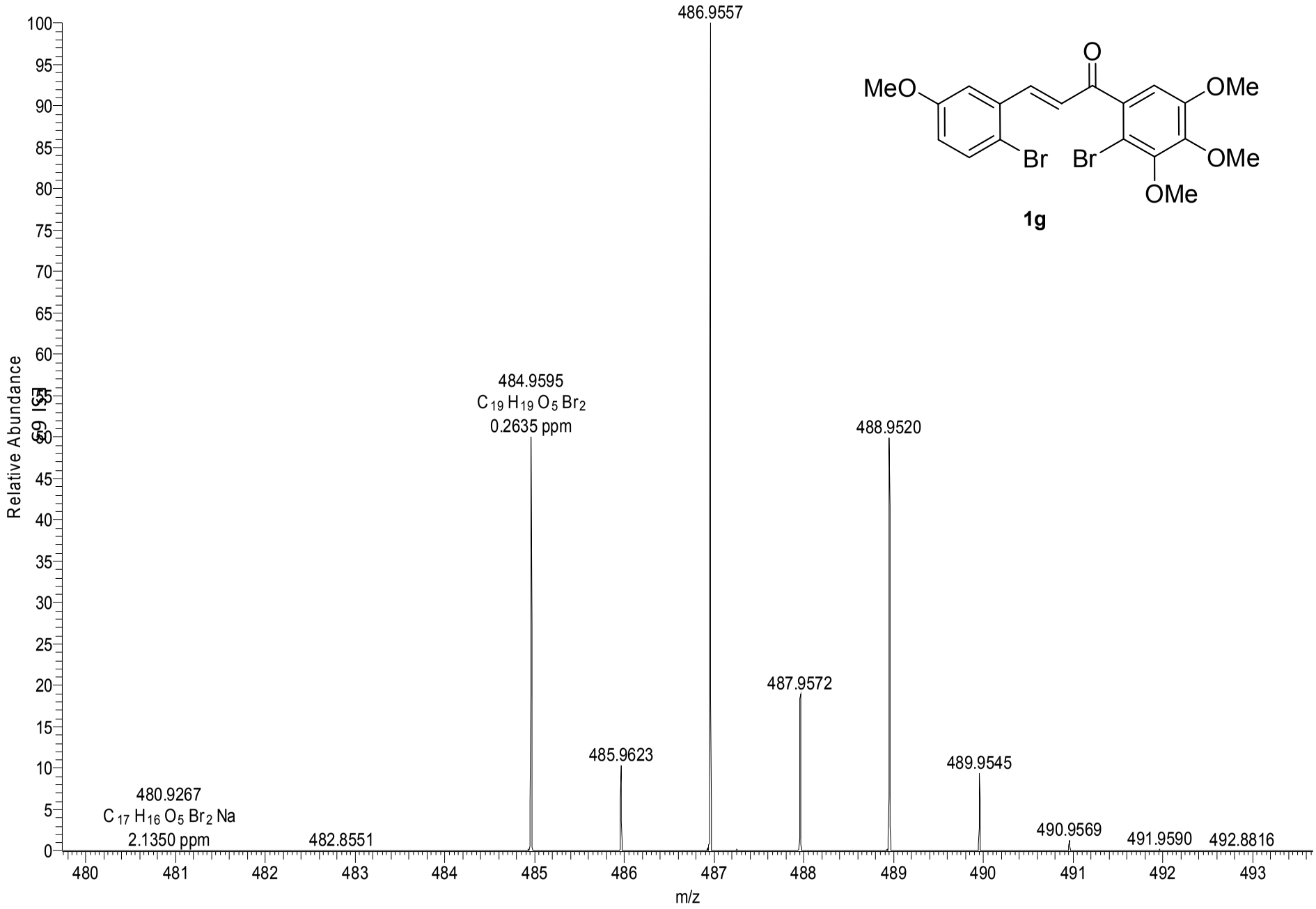


Acquisition Time (sec)	0.6832	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	19 May 2014 05:13:44						
File Name						***Frequency (MHz)***	50.32
Nucleus	13C	***Number of Transients***	1200	***Origin***	av200	***Original Points Count***	8192

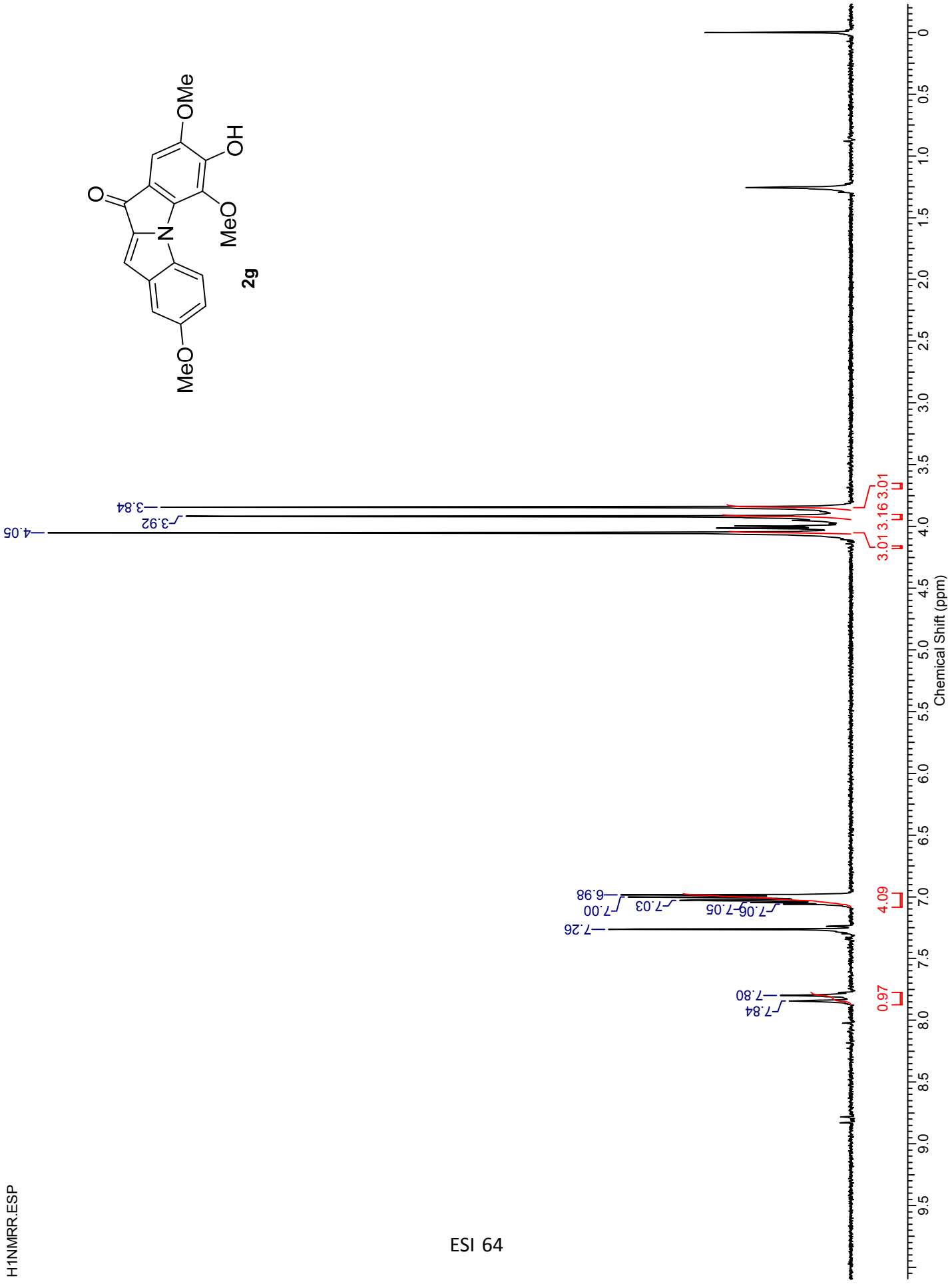
Sat3av2#049.001.001.1r.esp



AKC-3 #102 RT: 0.54 AV: 1 NL: 1.11E9
T: FTMS + p ESI Full ms [100.00-1500.00]



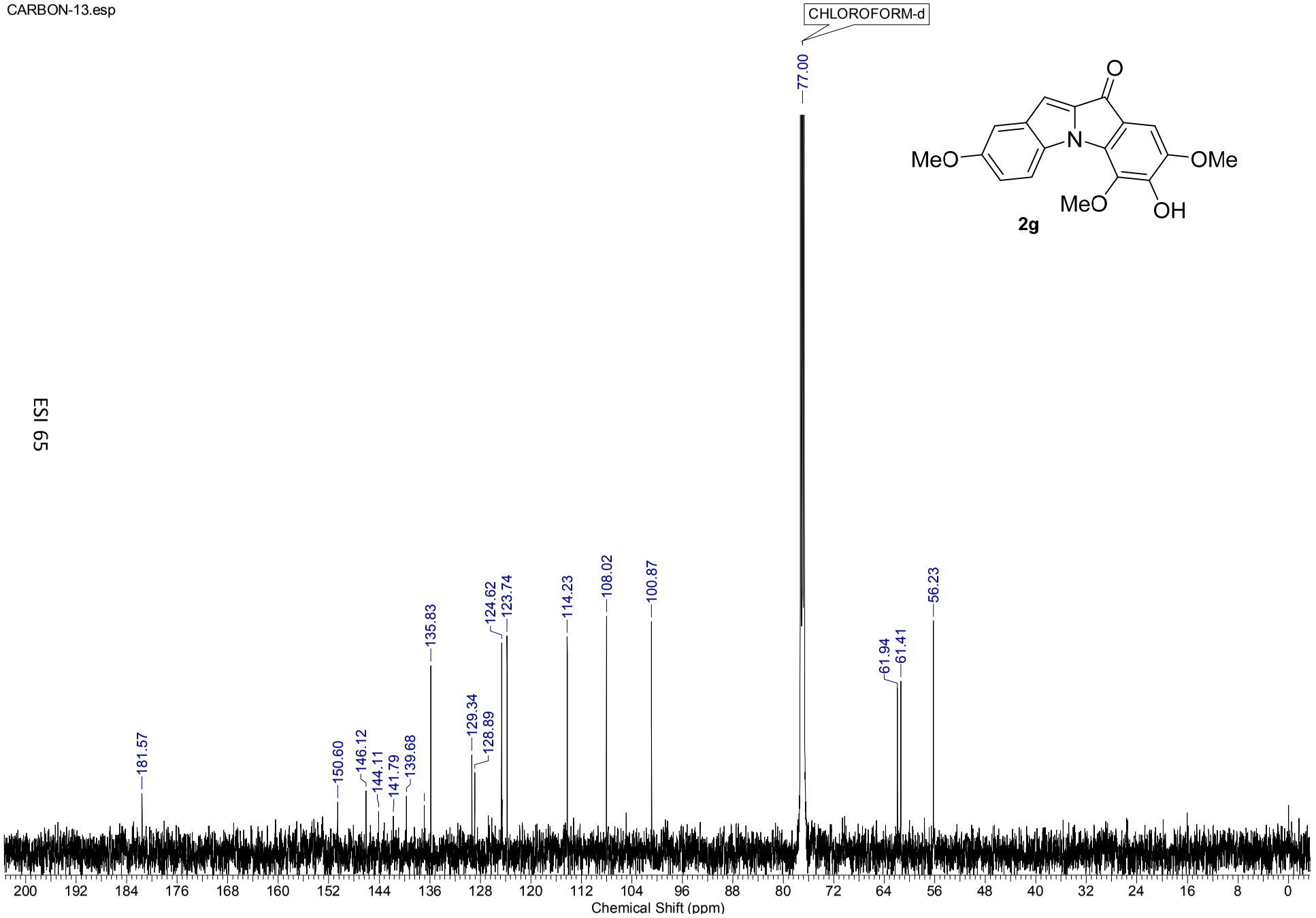
1g


OMe
OH
MeO
MeO
O
N
2g
4.05
3.92
3.84
3.01
3.16
3.01
7.84
7.80
0.97
7.26
7.06-7.05
7.03
7.00
6.98
4.09
Chemical Shift (ppm)
H1NMRR.ESP

Acquisition Time (sec)	0.6554	***Comment***	13C	***Date***	31 Dec 2014 14:37:04		
Date Stamp	31 Dec 2014 14:37:04			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	4243	***Origin***	spect

CARBON-13.esp

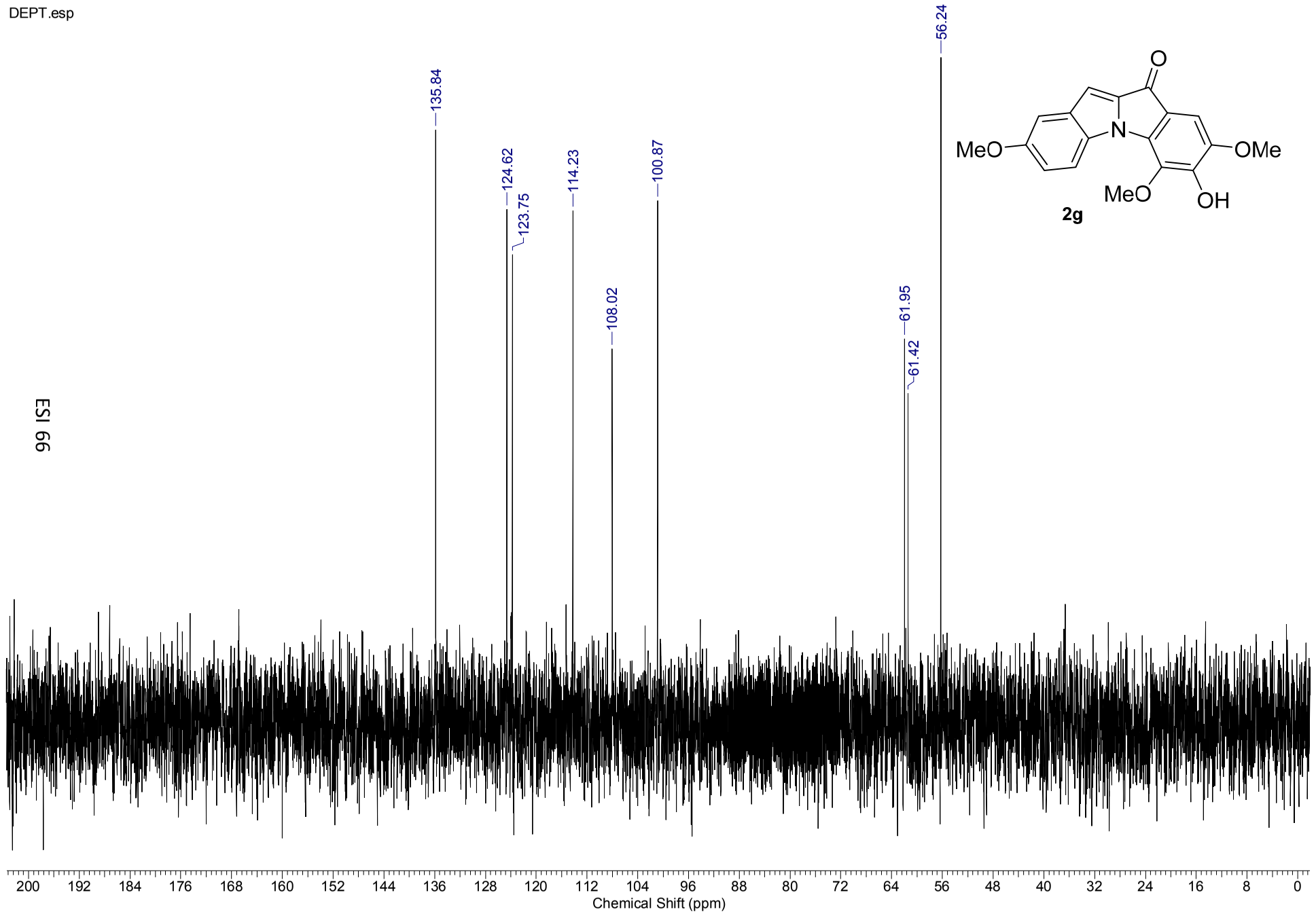
ESI 65



2g

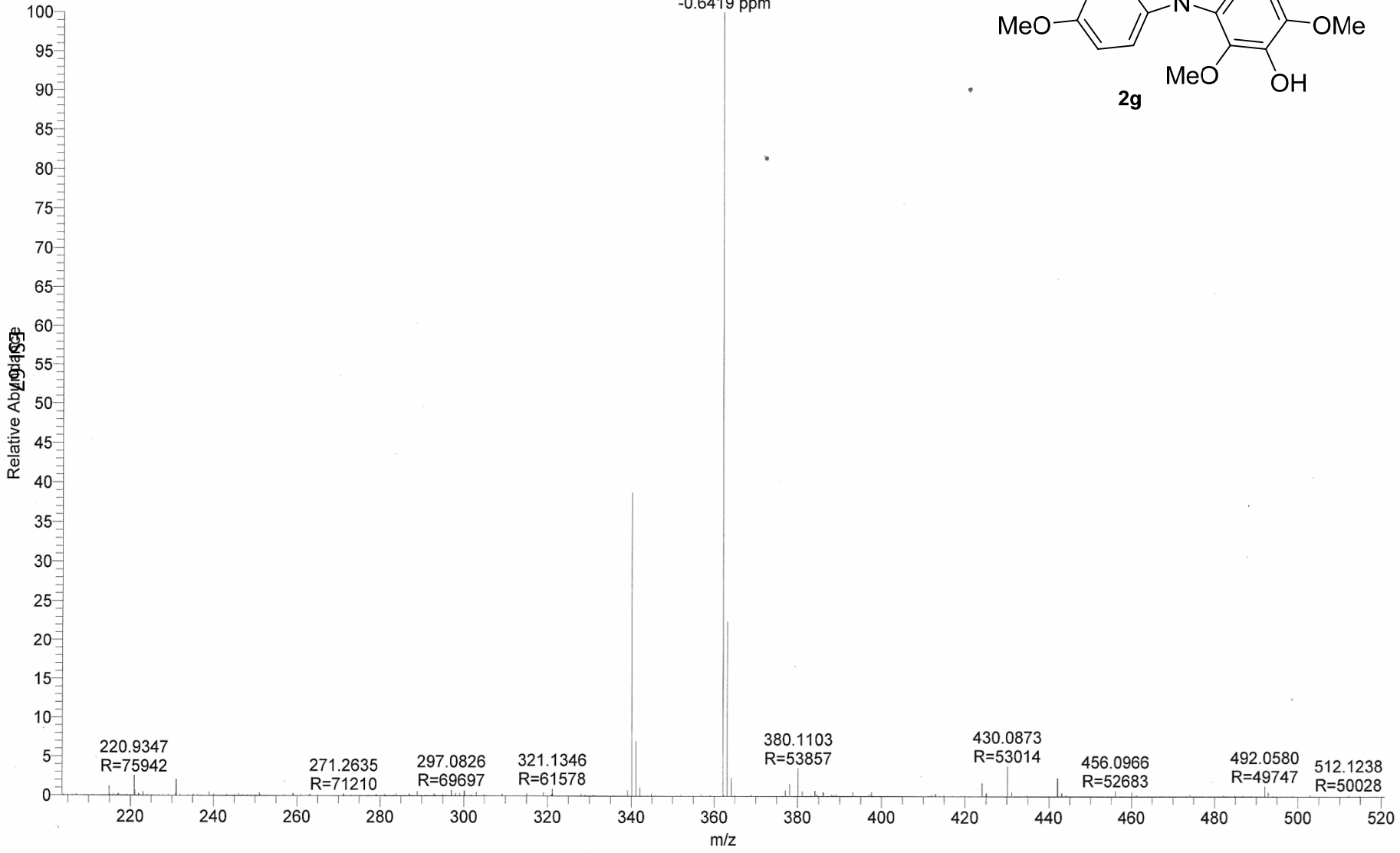
Acquisition Time (sec)	0.6554	*Comment*	DEPT	*Date*	31 Dec 2014 14:17:52		
Date Stamp	31 Dec 2014 14:17:52			*Solvent*	CHLOROFORM-d		
Frequency (MHz)	125.76	*Nucleus*	13C	*Number of Transients*	800	*Origin*	spect

DEPT.esp



D:\Data\Me-TME (6) 9/22/2014 5:06:25 PM

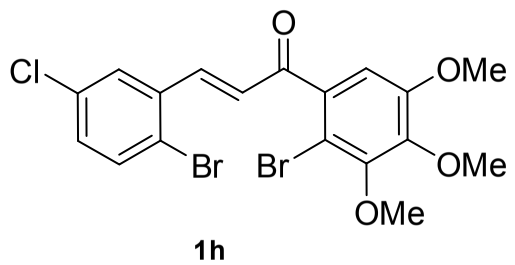
Me-TME #1224 RT: 5.46 AV: 1 SB: 220 3.80-4.22 , 6.13-6.69 NL: 2.24E7
T: FTMS + p ESI Full ms [66.70-1000.00]



2g

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	02 Jul 2014 21:32:56						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Wed1av2#127\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Wed1av2#127.001.001.1r.esp

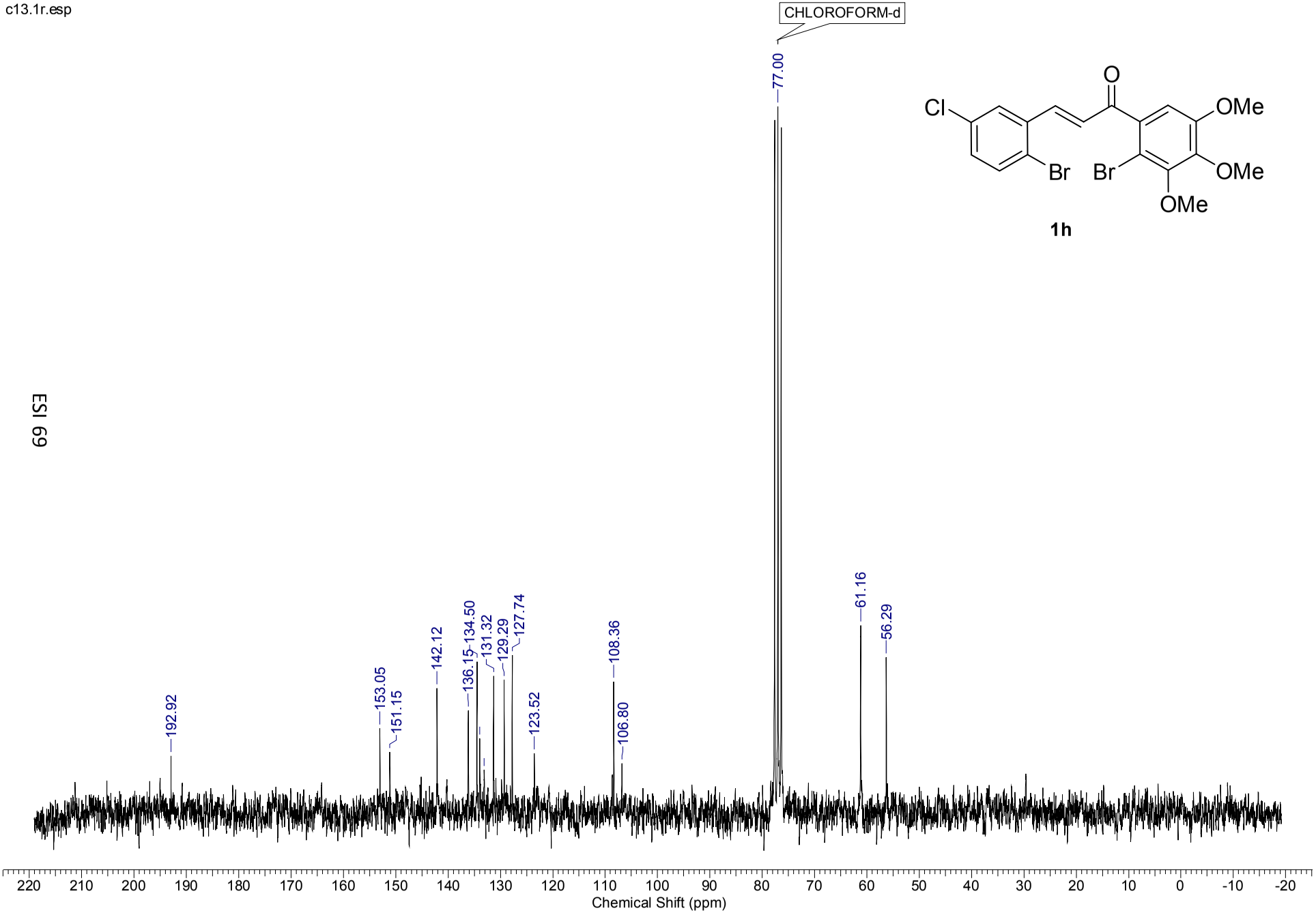


1h

ESI 68

Acquisition Time (sec)	0.6832	***Comment***	Anand	***Date***	06 Jul 2014 15:36:40
Date Stamp	06 Jul 2014 15:36:40			***Solvent***	CHLOROFORM-d
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat1av2#054\2\pdata\1\1r			***Frequency (MHz)***	50.32

c13.1r.esp

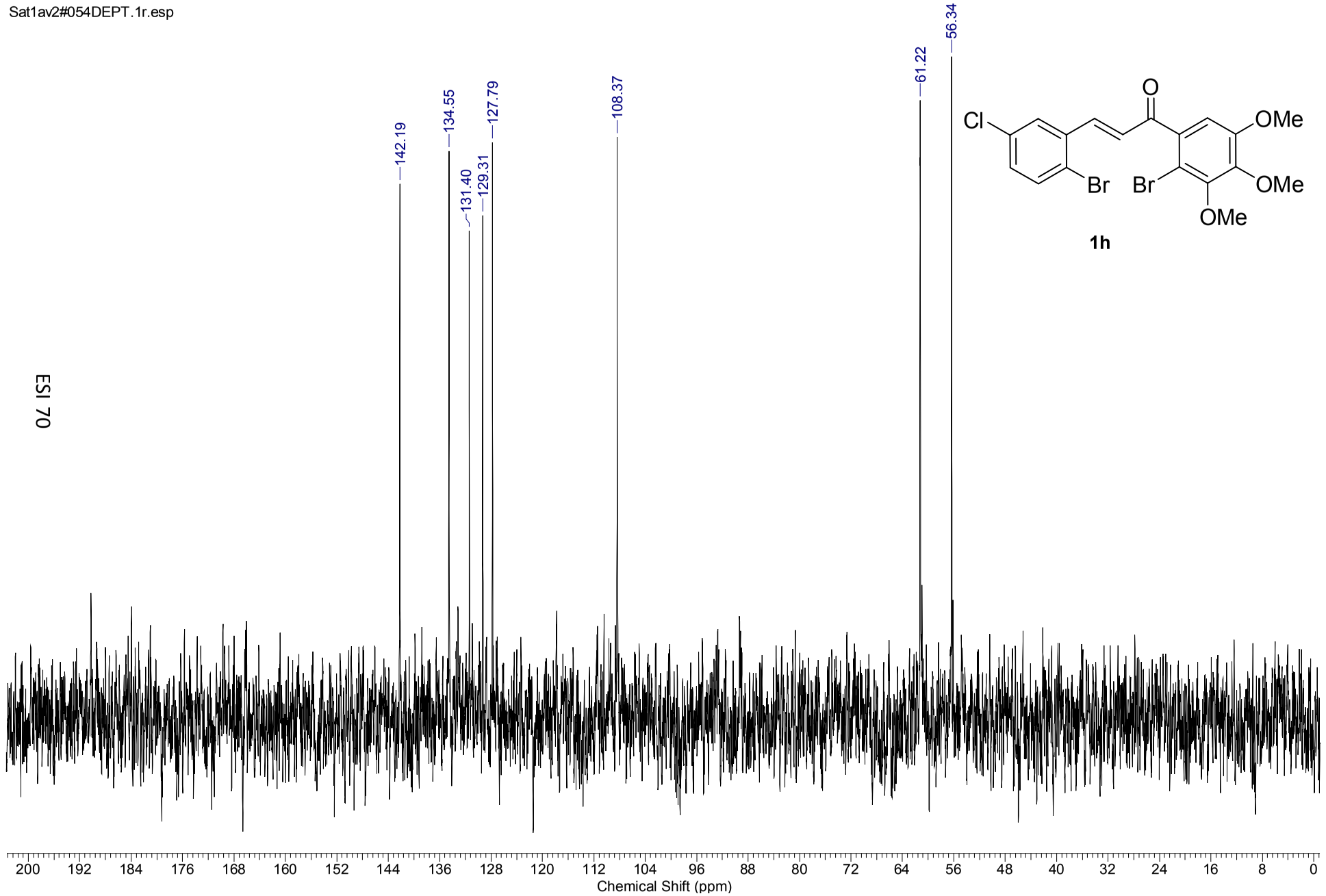


1h

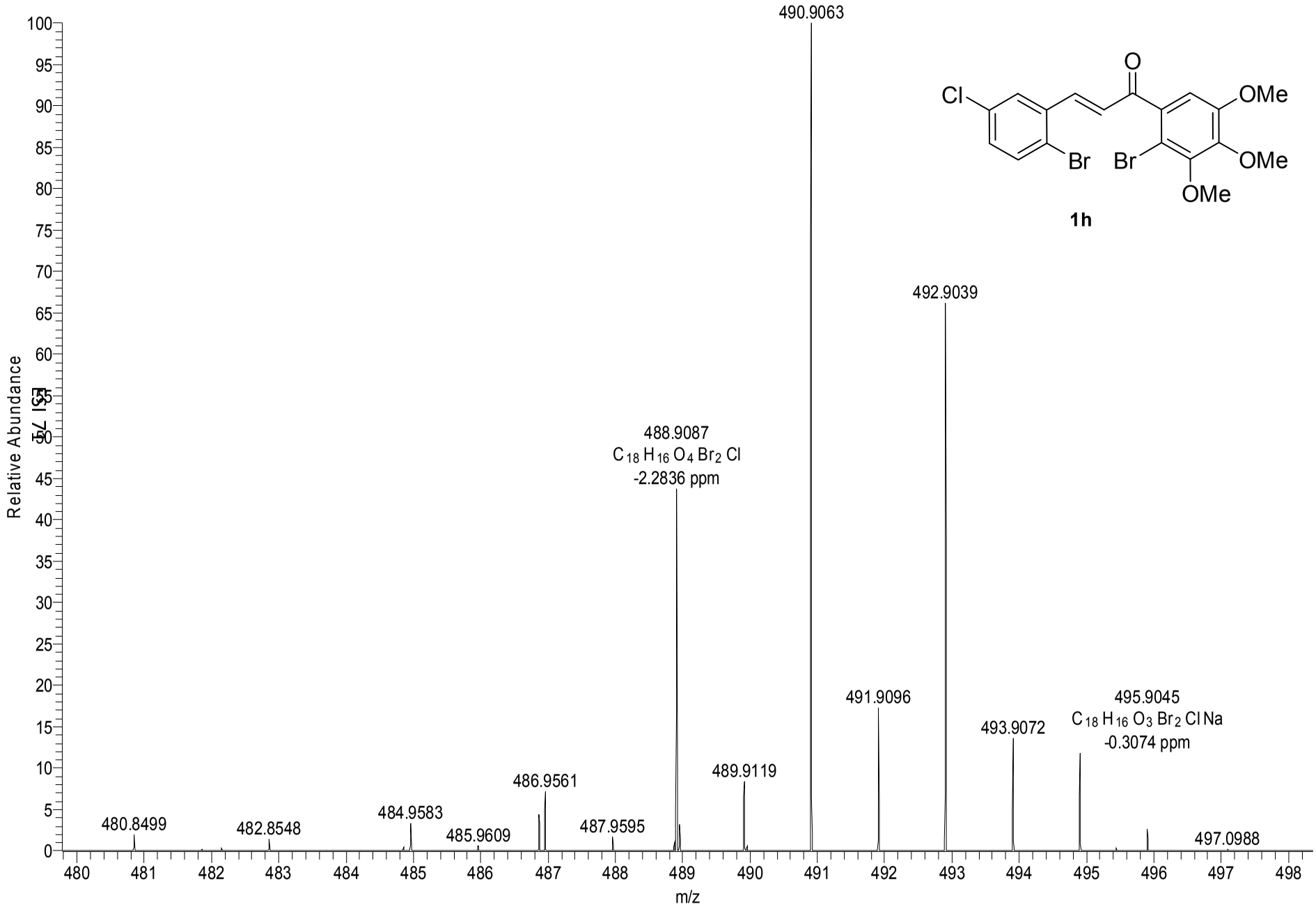
ESI 69

Acquisition Time (sec)	0.6832	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	06 Jul 2014 15:08:56						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat1av2#054\1\pdata\1\1r					***Frequency (MHz)***	50.32
Nucleus	13C	***Number of Transients***	300	***Origin***	av200	***Original Points Count***	8192

Sat1av2#054DEPT.1r.esp

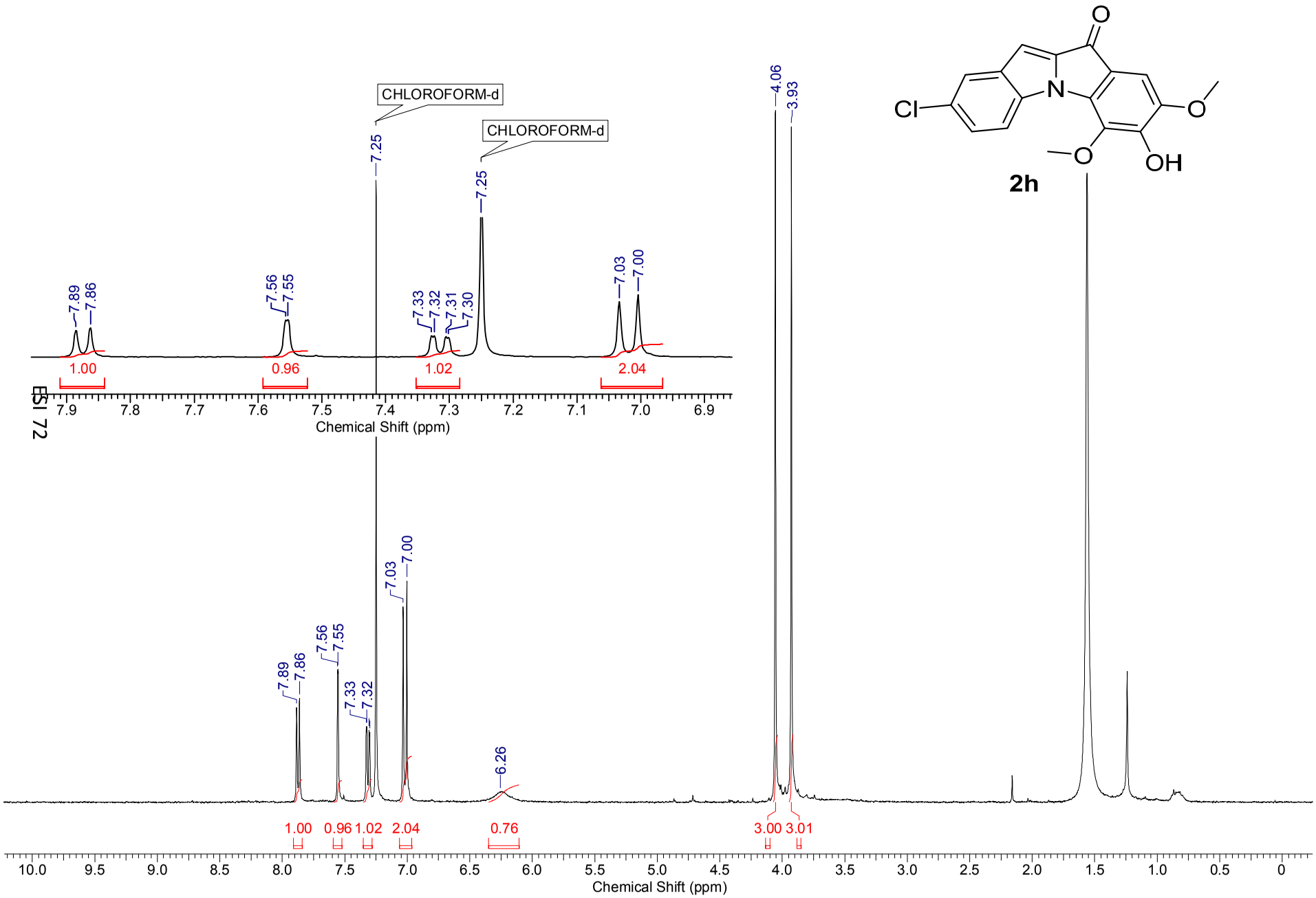


AKC-1 #133 RT: 0.70 AV: 1 NL: 3.15E7
T: FTMS + p ESI Full ms [100.00-1500.00]



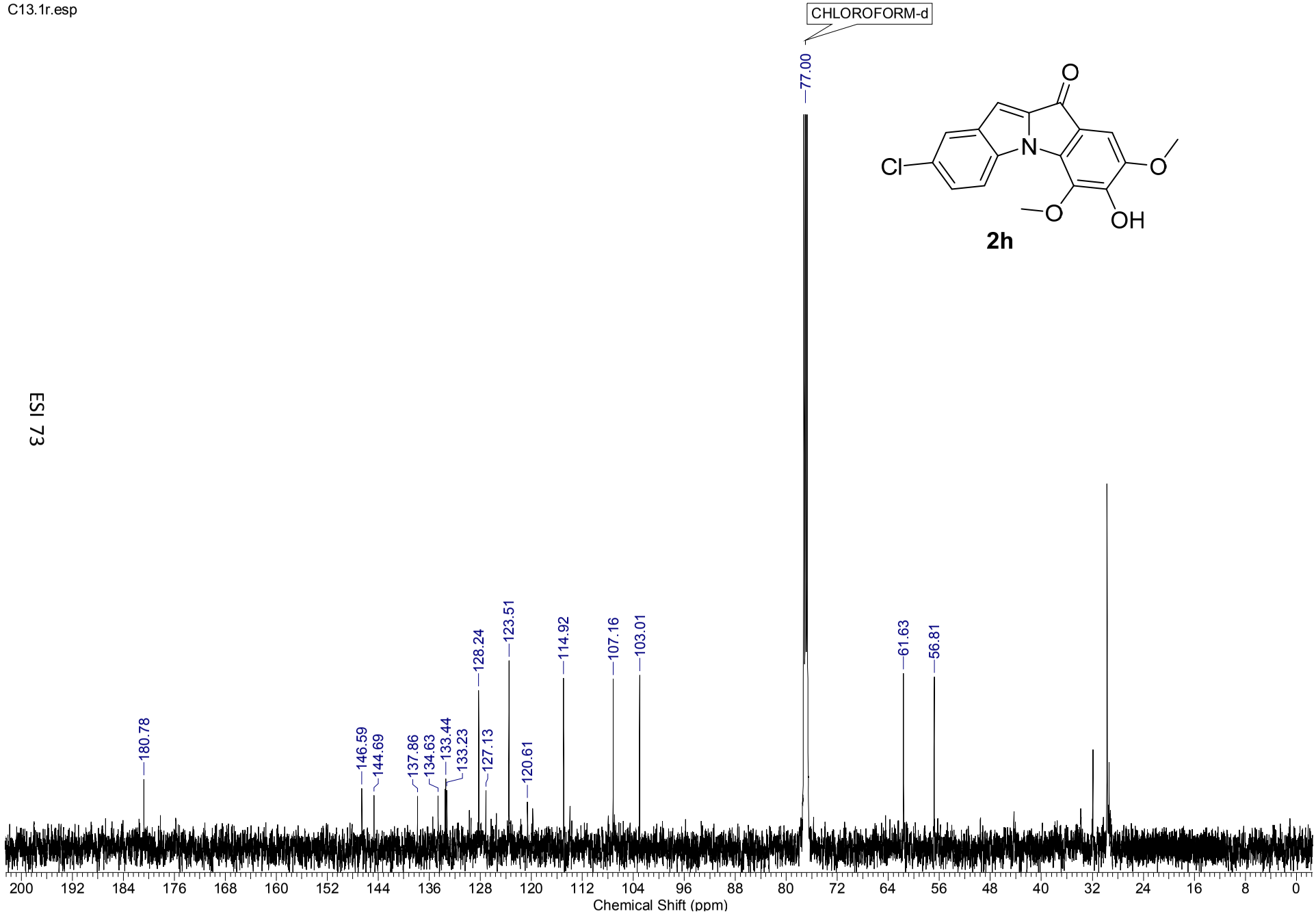
1h

Acquisition Time (sec)	2.0447	***Comment***	Anand 1H	***Date***	29 Oct 2015 12:43:52		
Date Stamp	29 Oct 2015 12:43:52			***File Name***	\\agni\nmr_data\AV400\Oct_15_400\Thu5av400#006\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	23	***Origin***	spect



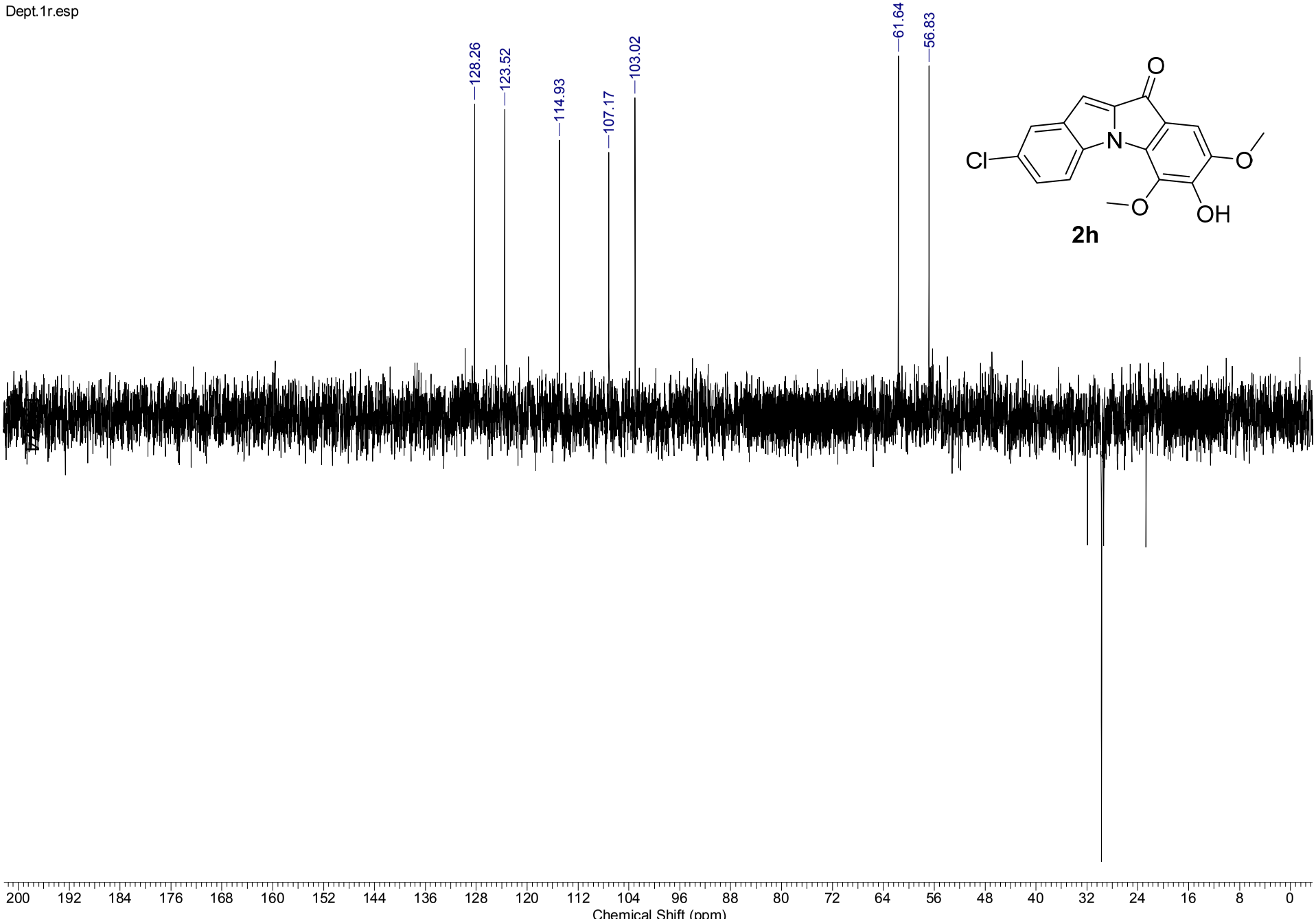
Acquisition Time (sec)	0.6881	***Comment***	13C	***Date***	14 Aug 2014 17:42:56		
Date Stamp	14 Aug 2014 17:42:56			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1697	***Origin***	spect

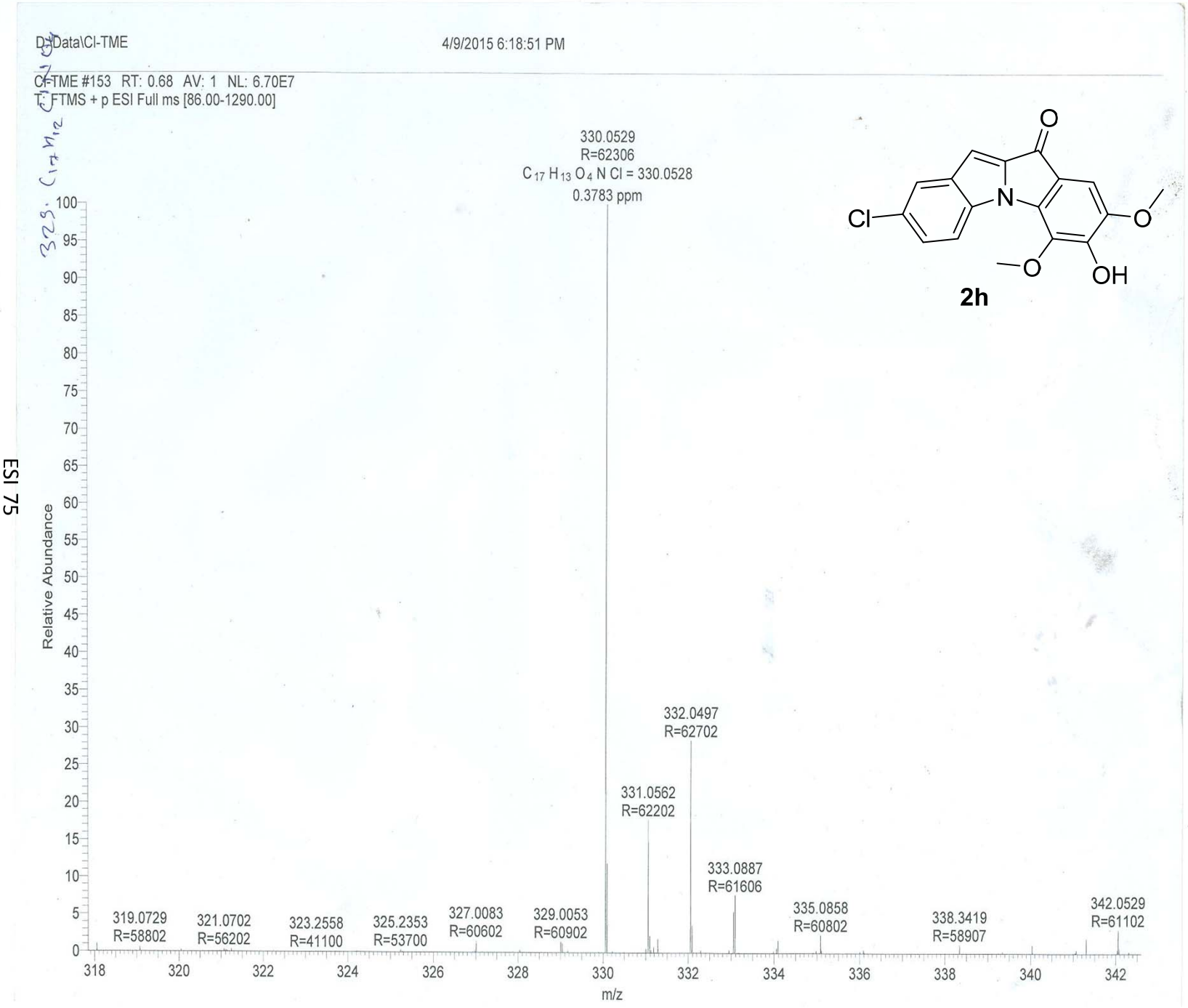
C13.1r.esp



Acquisition Time (sec)	0.6881	***Comment***	DEPT	***Date***	14 Aug 2014 17:40:48		
Date Stamp	14 Aug 2014 17:40:48			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	600	***Origin***	spect

Dept.1r.esp

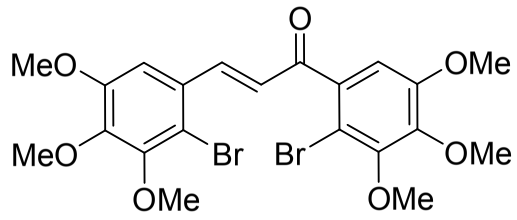



D:\Data\Cl-TME
4/9/2015 6:18:51 PM
Cl-TME #153 RT: 0.68 AV: 1 NL: 6.70E7
T: FTMS + p ESI Full ms [86.00-1290.00]
330.0529
R=62306
C 17 H 13 O 4 N Cl = 330.0528
0.3783 ppm
Relative Abundance
m/z
319.0729 R=58802
321.0702 R=56202
323.2558 R=41100
325.2353 R=53700
327.0083 R=60602
329.0053 R=60902
331.0562 R=62202
332.0497 R=62702
333.0887 R=61606
335.0858 R=60802
338.3419 R=58907
342.0529 R=61102
Cl
N
O
O
O
OH
2h

ESI 75

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	07 May 2014 00:12:56						
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Tue2av2#150\1\pdata\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Tue2av2#150.001.001.1r.esp

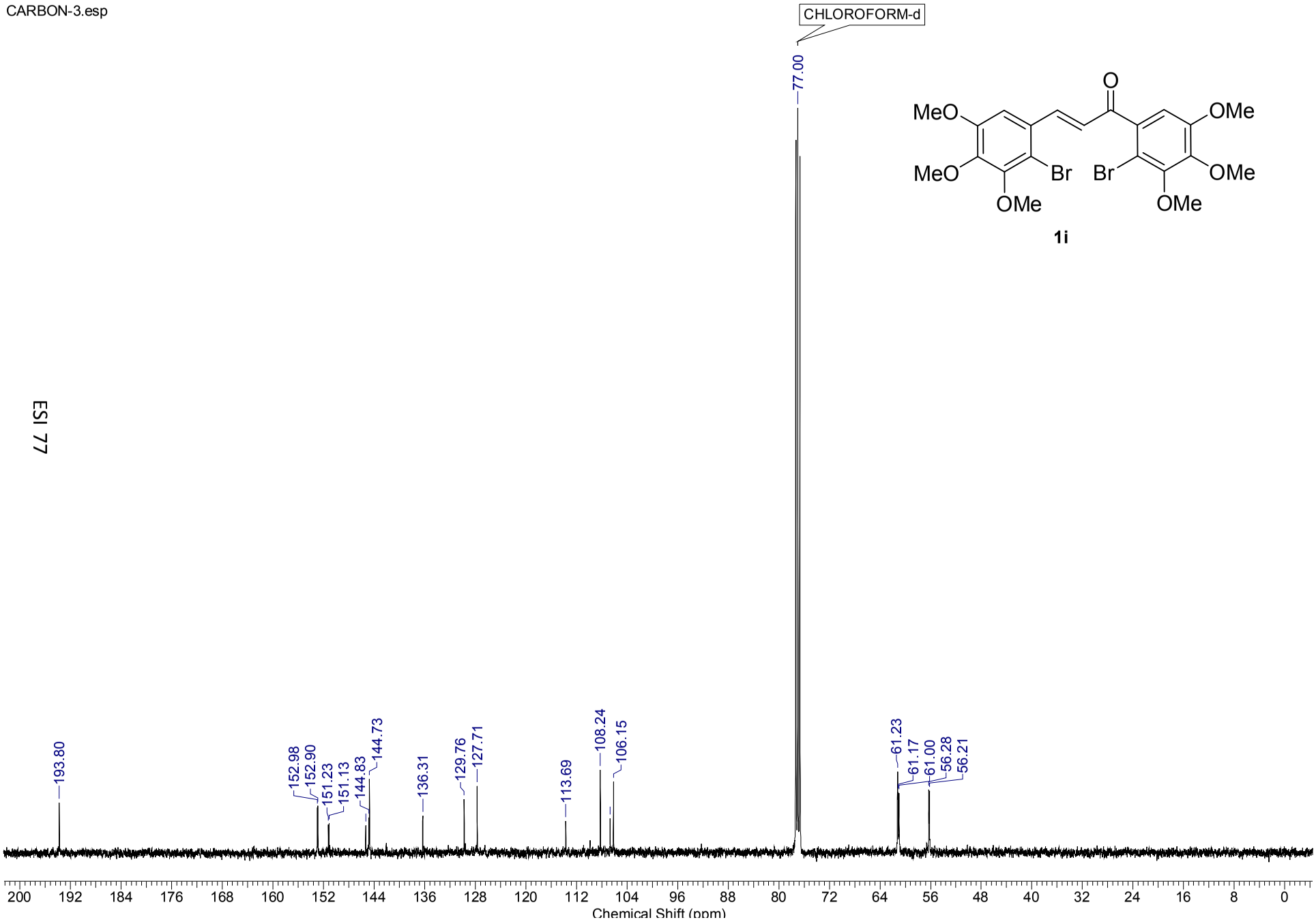


1i

ESI 76

Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	10 May 2014 08:16:29		
Date Stamp	10 May 2014 07:04:34			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	546	***Origin***	ECX 400

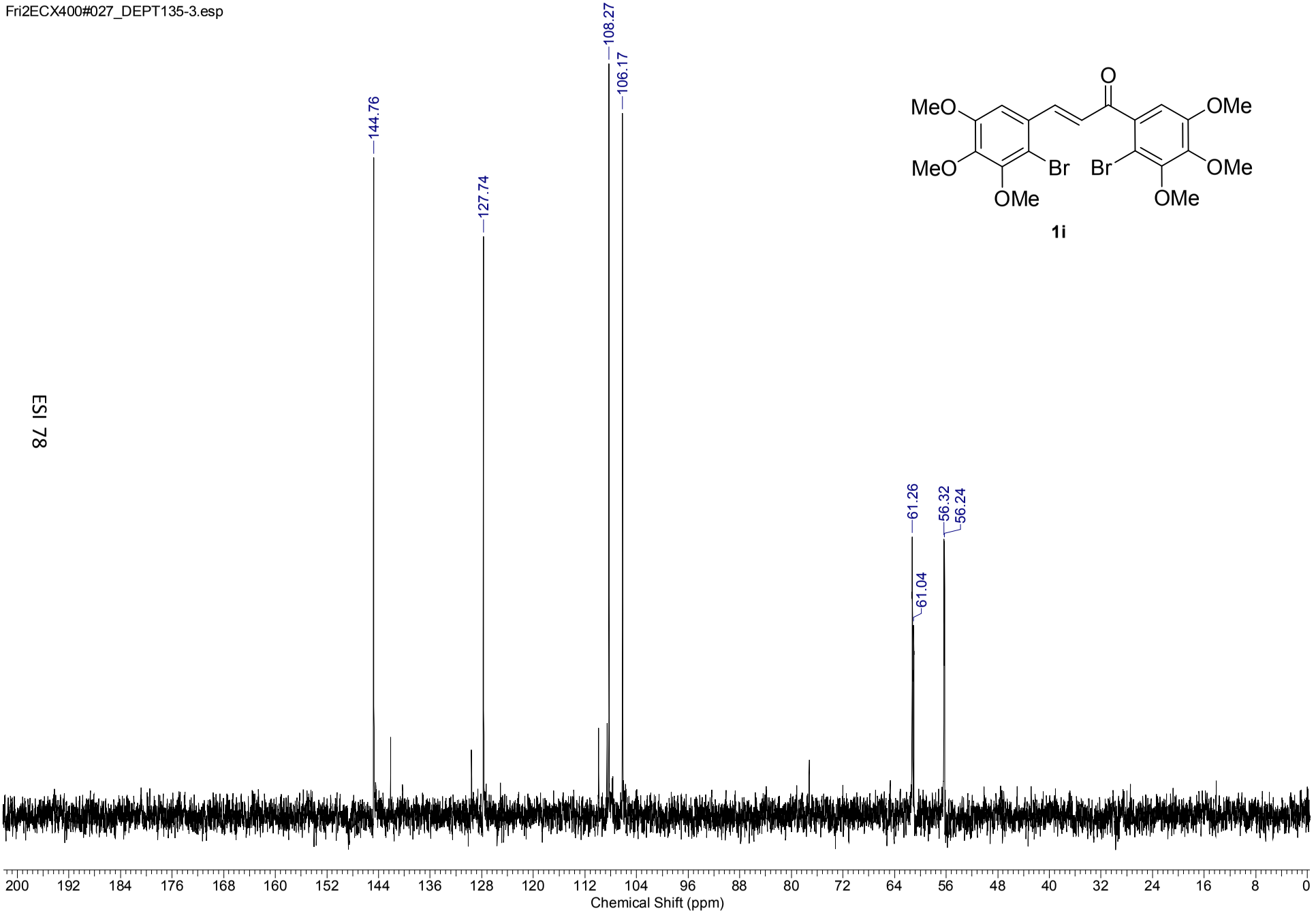
CARBON-3.esp



1i

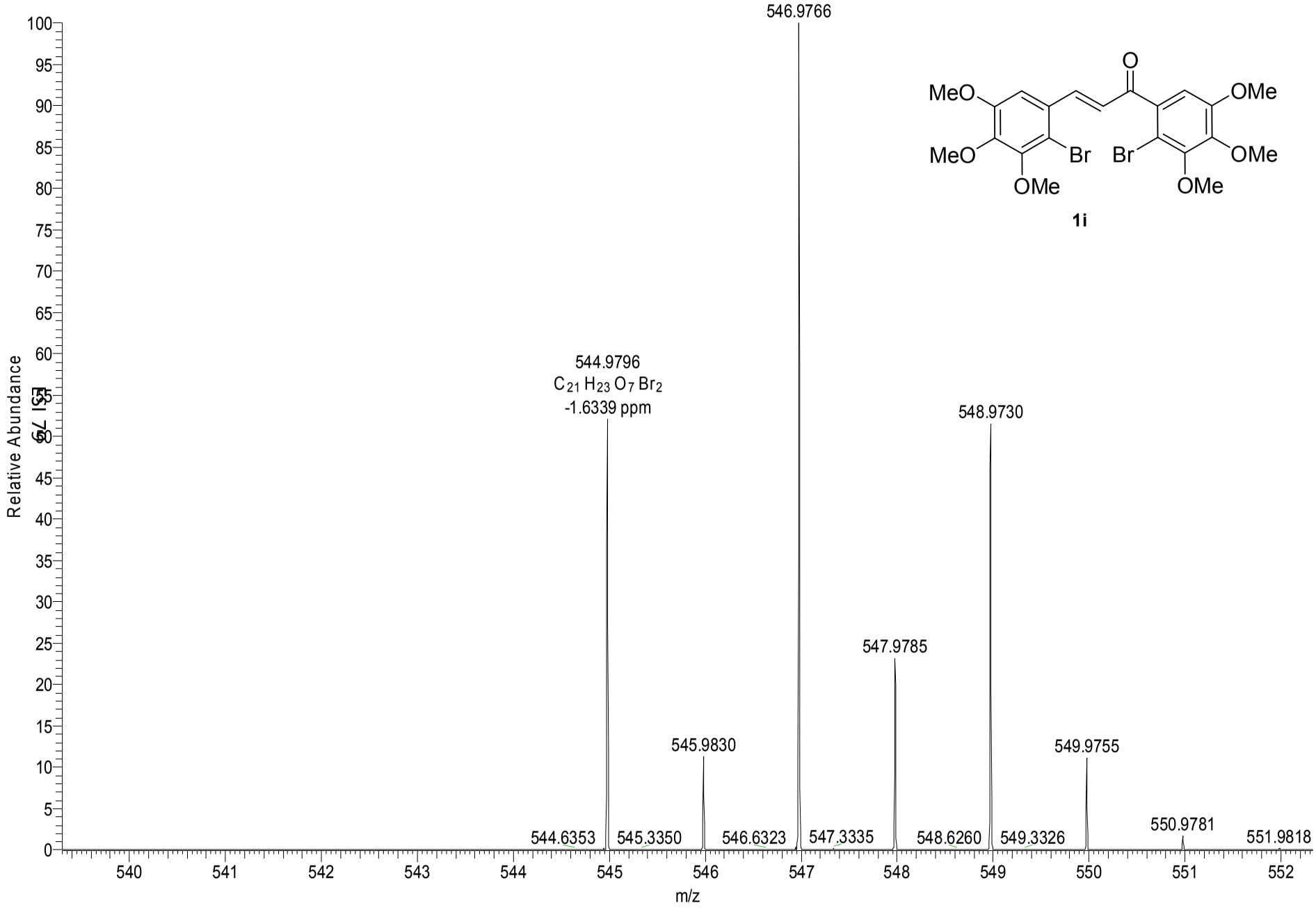
Acquisition Time (sec)	1.0434	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	10 May 2014 07:35:57			***File Name***	\\agni\nmr_data\JEOL_400\2014\May 2014\Fri2ECX400#027_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	800	***Origin***	ECX 400

Fri2ECX400#027_DEPT135-3.esp



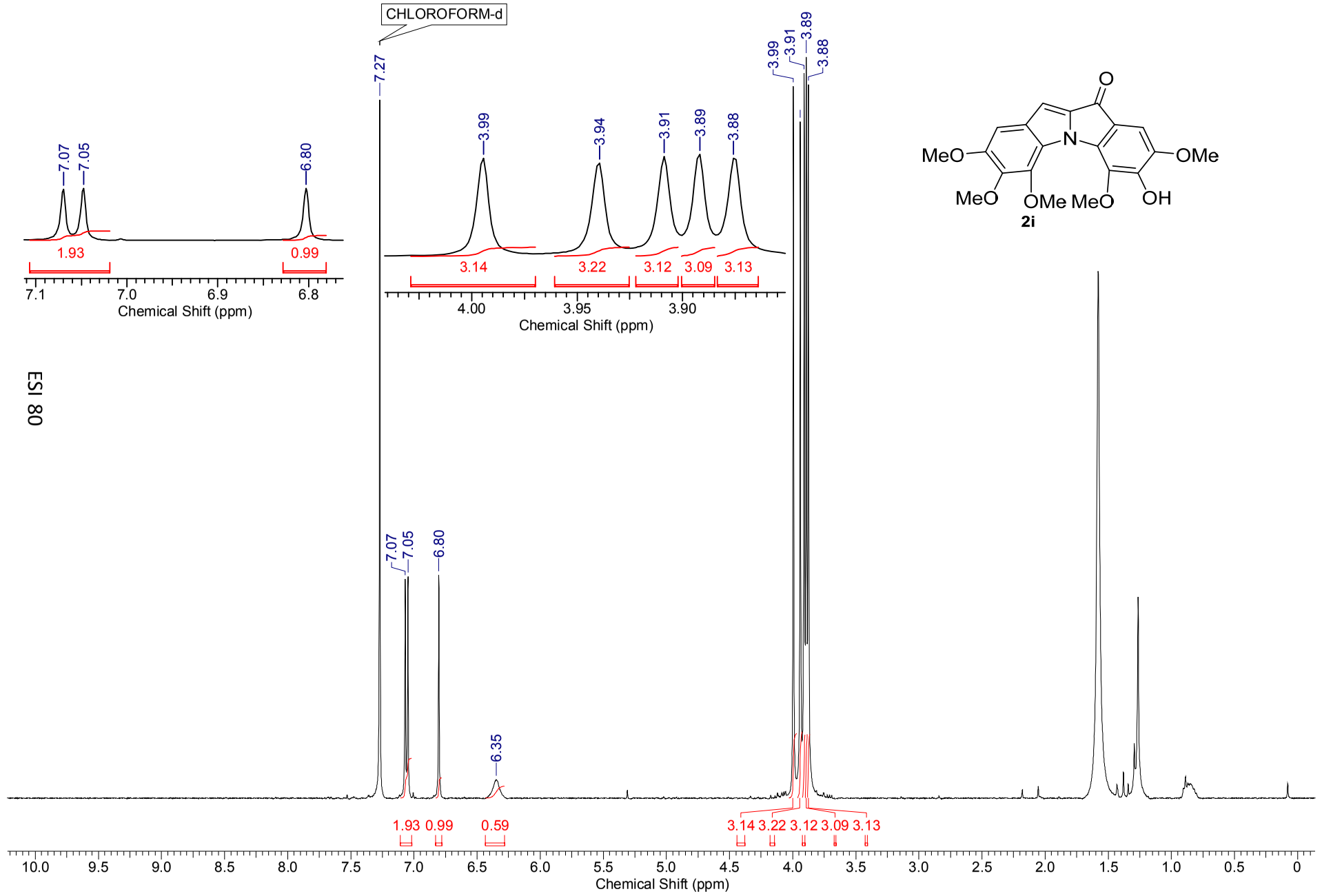
1i

AKC-11 #97 RT: 0.51 AV: 1 NL: 6.84E8
T: FTMS + p ESI Full ms [100.00-1500.00]



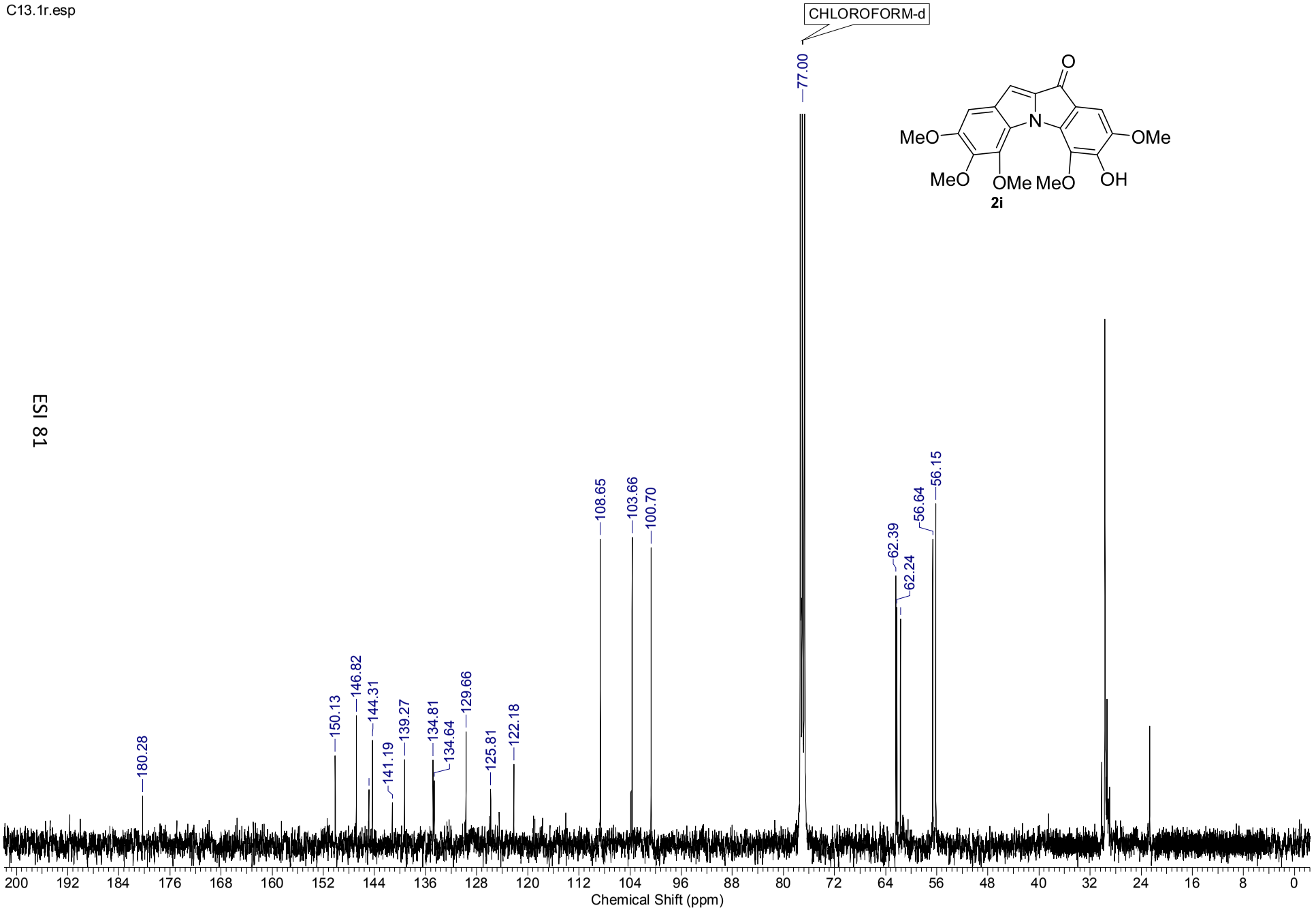
1i

Acquisition Time (sec)	2.0447	***Comment***	Anand 1H	***Date***	29 Oct 2015 19:27:04		
Date Stamp	29 Oct 2015 19:27:04			***File Name***	\\agni\nmr_data\AV400\Oct_15_400\Thu5av400#021\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	56	***Origin***	spect



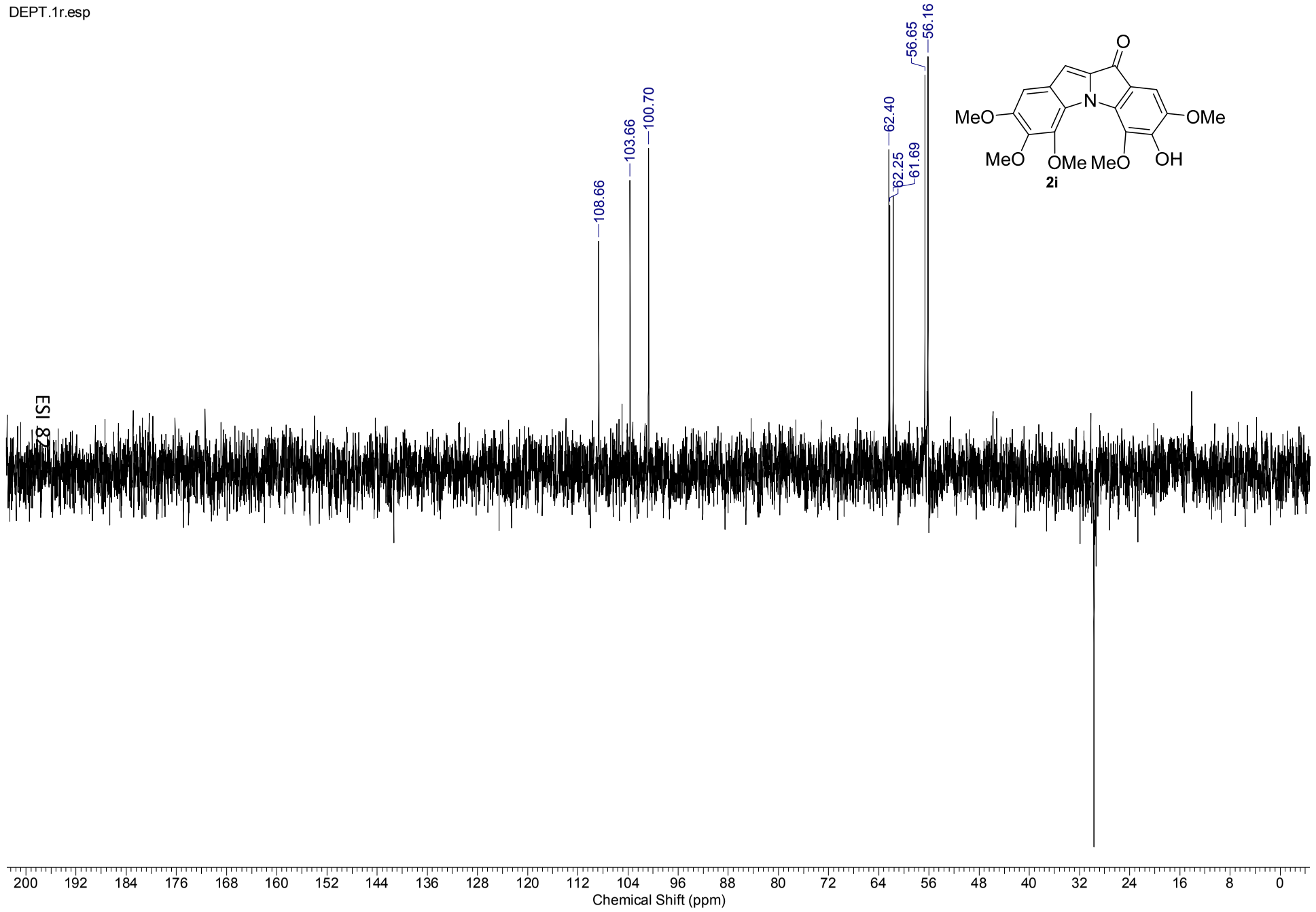
Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	05 Dec 2014 21:35:04		
Date Stamp	05 Dec 2014 21:35:04			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	6599	***Origin***	spect

C13.1r.esp



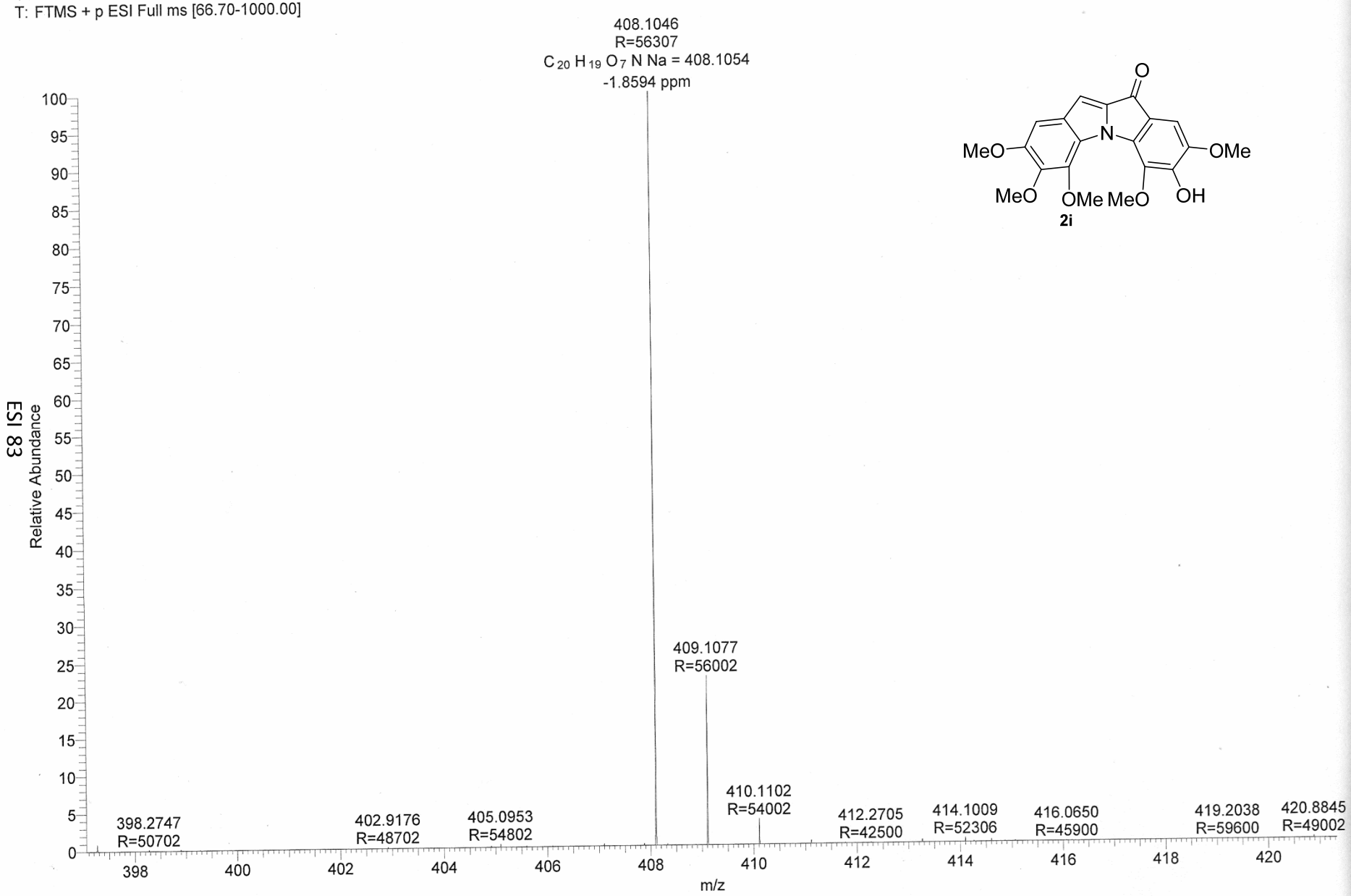
Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	05 Dec 2014 18:27:20		
Date Stamp	05 Dec 2014 18:27:20			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect

DEPT.1r.esp



D:\Data\14 TME-TME 12/30/2014 2:35:37 PM

14 #1019 RT: 4.54 AV: 1 NL: 1.28E8
T: FTMS + p ESI Full ms [66.70-1000.00]

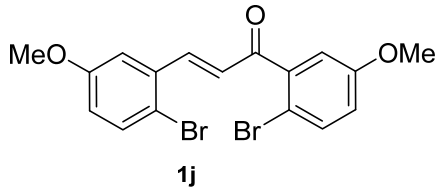


2i

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	20 May 2014 12:48:08						
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Tue4av2#013\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

Tue4av2#013.001.001.1r.esp

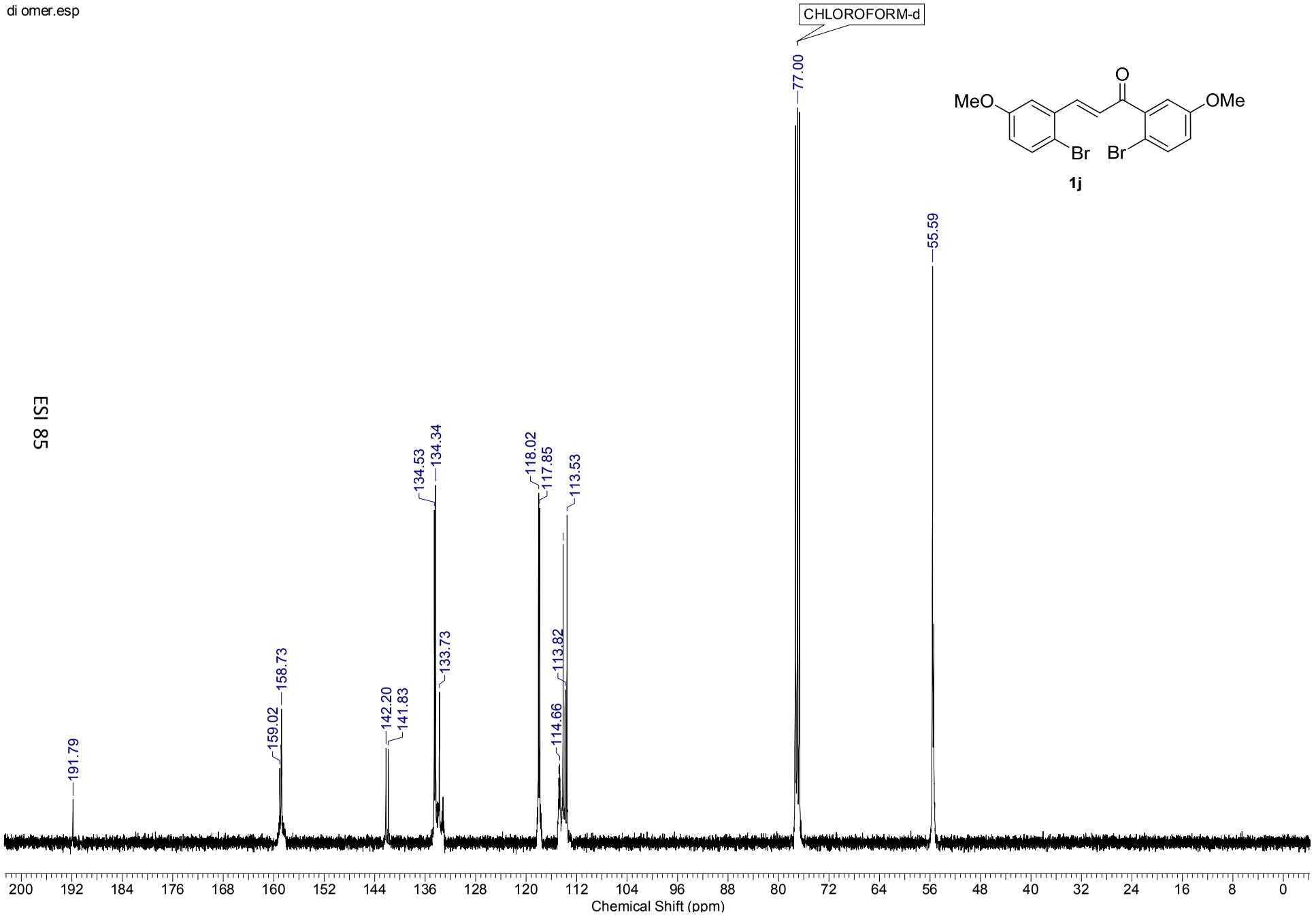
ESI 84



1j

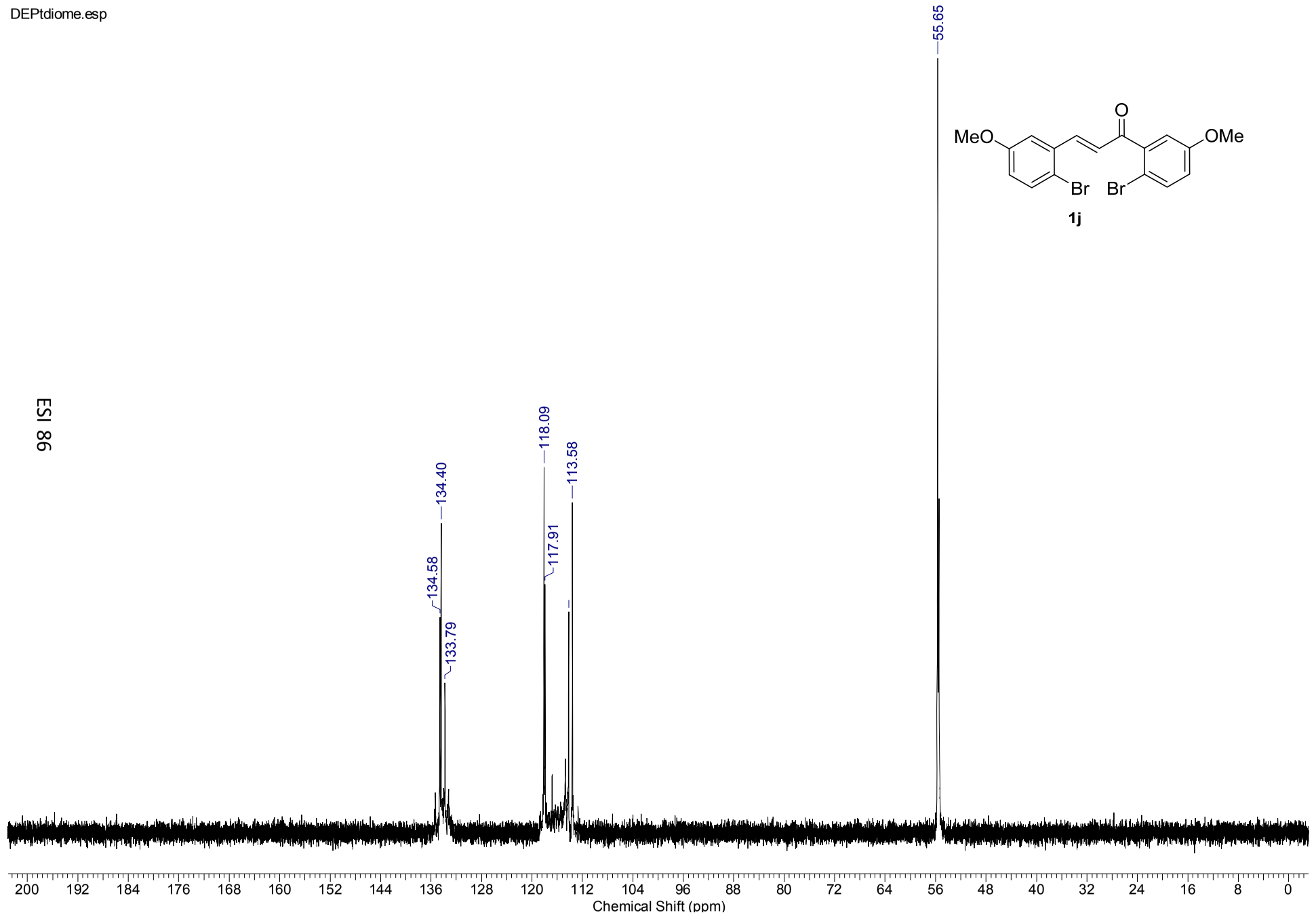
Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	01 Jul 2015 13:37:12		
Date Stamp	01 Jul 2015 13:37:12			***File Name***	\\agni\nmr_data\AV400\July_15_400\Wed1av400#013\3\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1627	***Origin***	spect

di omer.esp



Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	01 Jul 2015 13:30:48		
Date Stamp	01 Jul 2015 13:30:48			***File Name***	\\agni\nmr_data\AV400\July_15_400\Wed1av400#013\2\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	600	***Origin***	spect

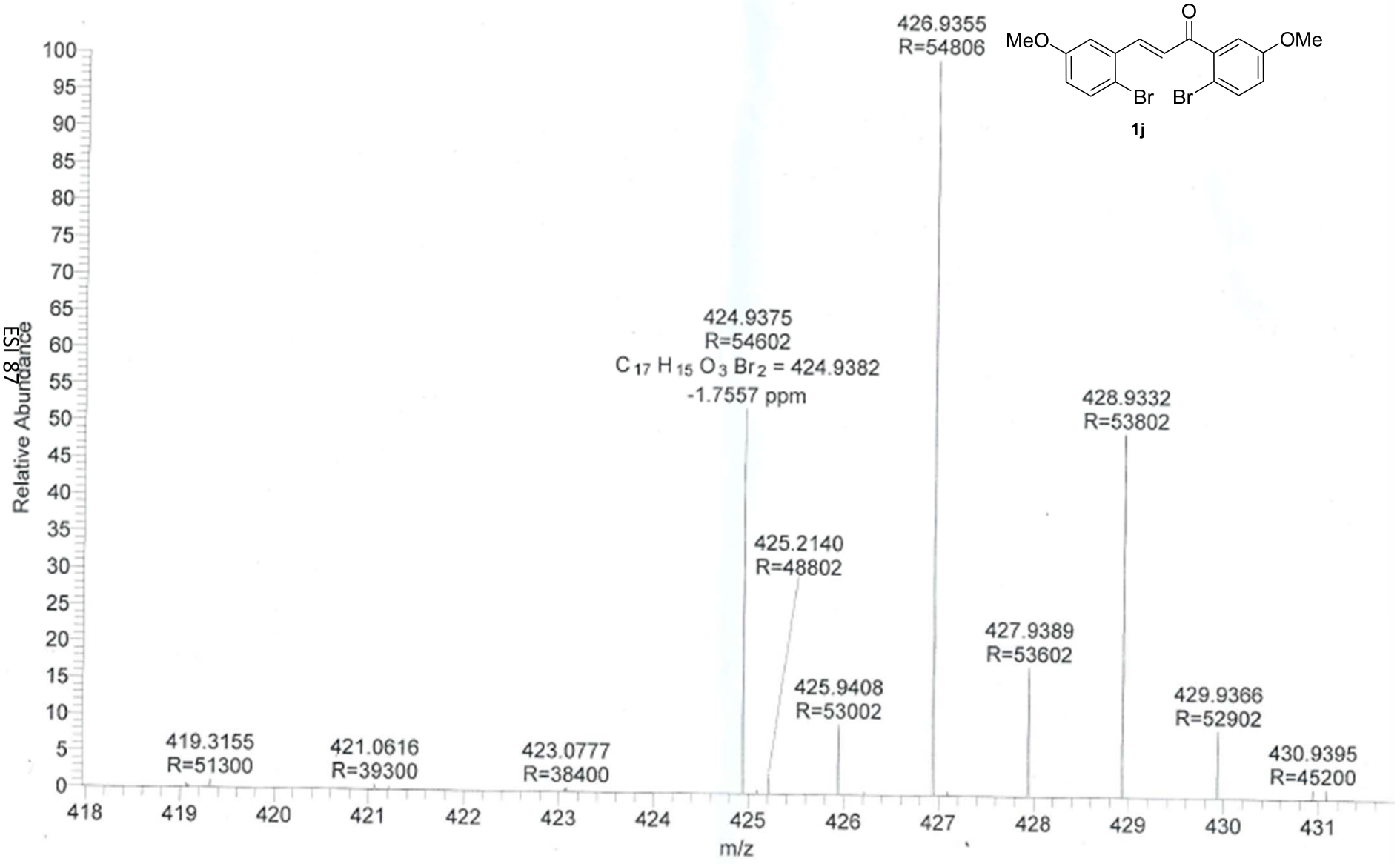
DEPtdiome.esp



D:\Data\AKC-7

07/06/15 11:15:36

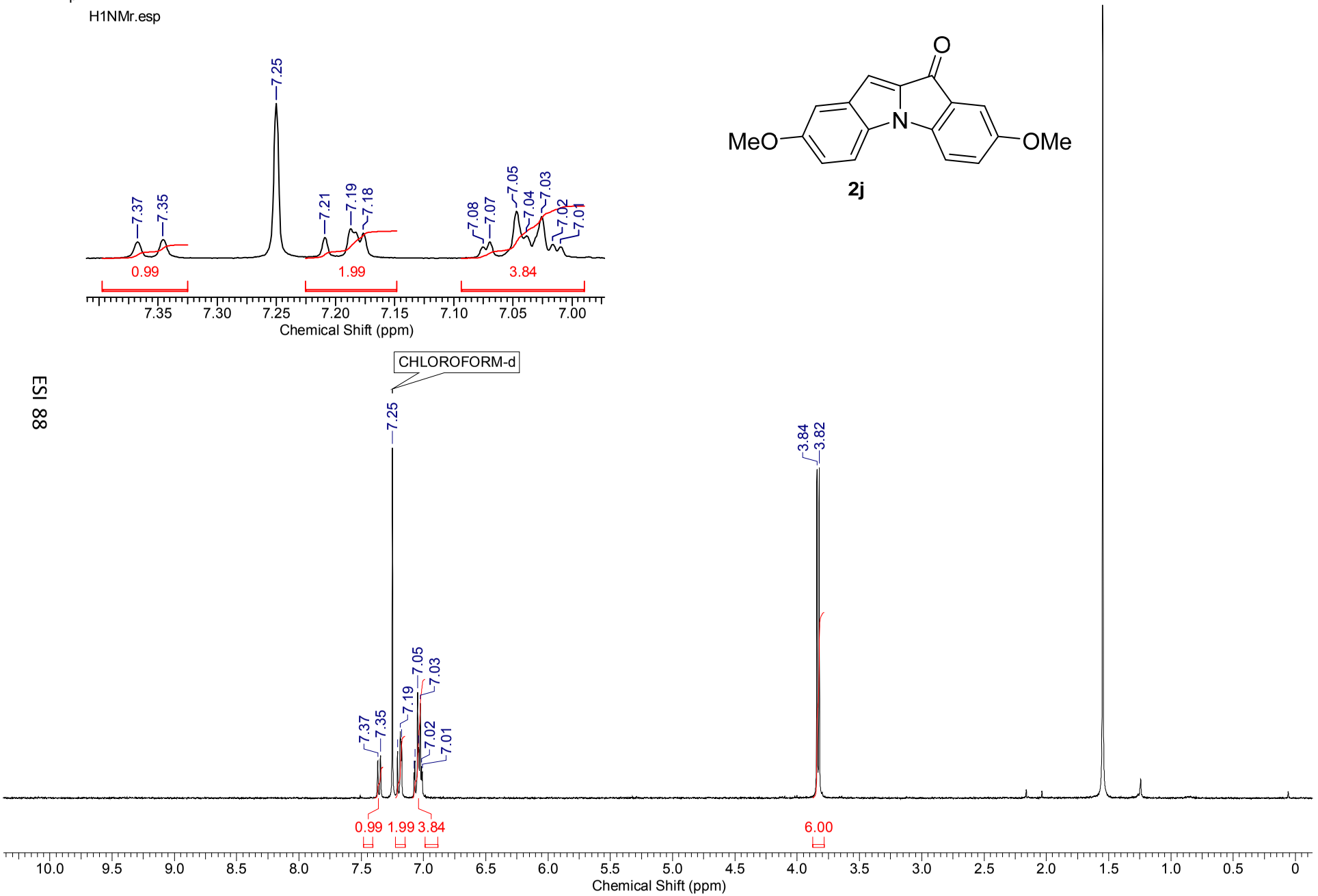
AKC-7 #150 RT: 0.67 AV: 1 NL: 3.18E7
T: FTMS + p ESI Full ms [100.00-1500.00]



1j

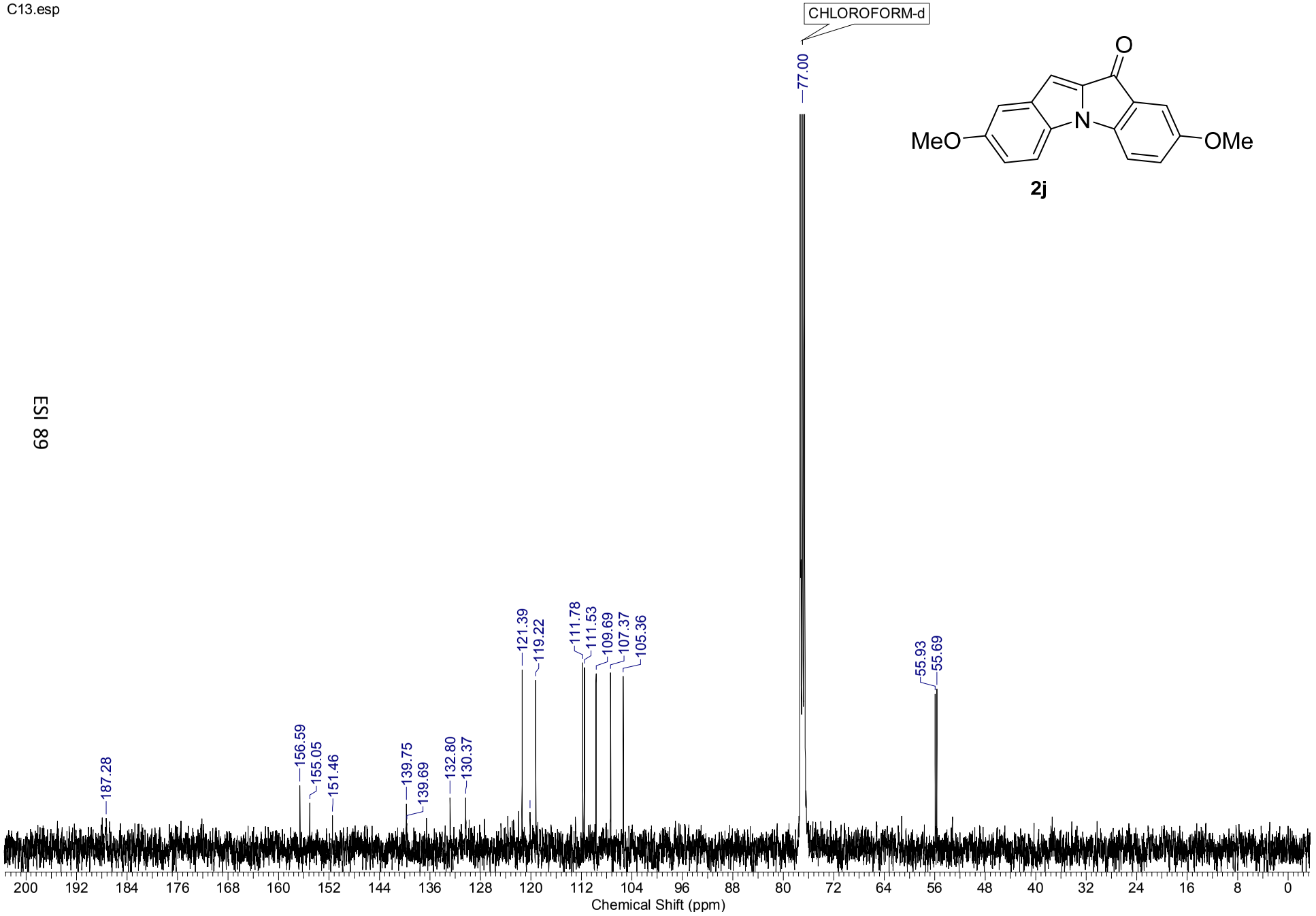
Acquisition Time (sec)	2.0447	***Comment***	anand 1H	***Date***	16 Dec 2014 12:28:56		
Date Stamp	16 Dec 2014 12:28:56			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	10	***Origin***	spect

H1NMr.esp



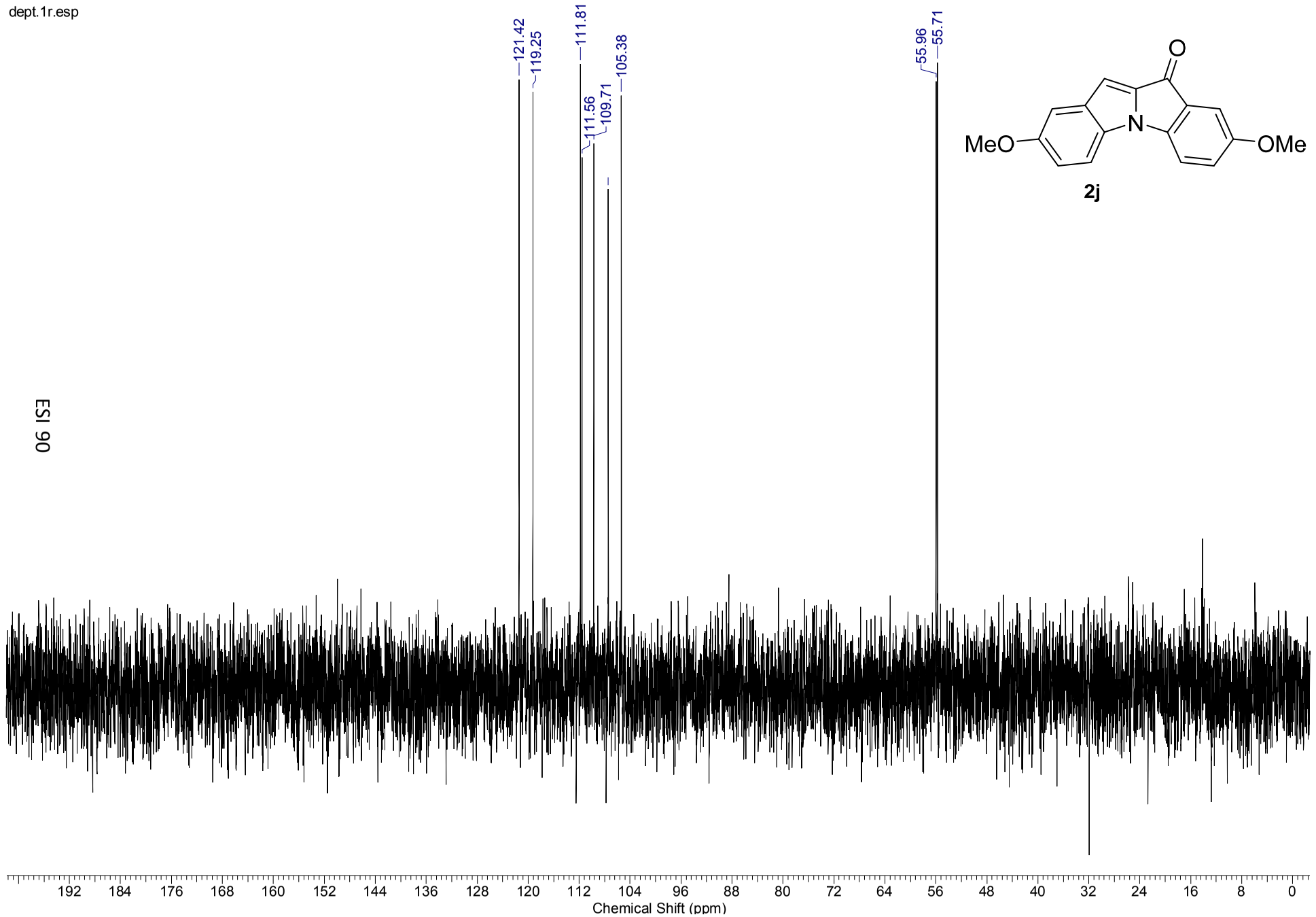
Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	16 Dec 2014 14:04:56		
Date Stamp	16 Dec 2014 14:04:56			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	3957	***Origin***	spect

C13.esp



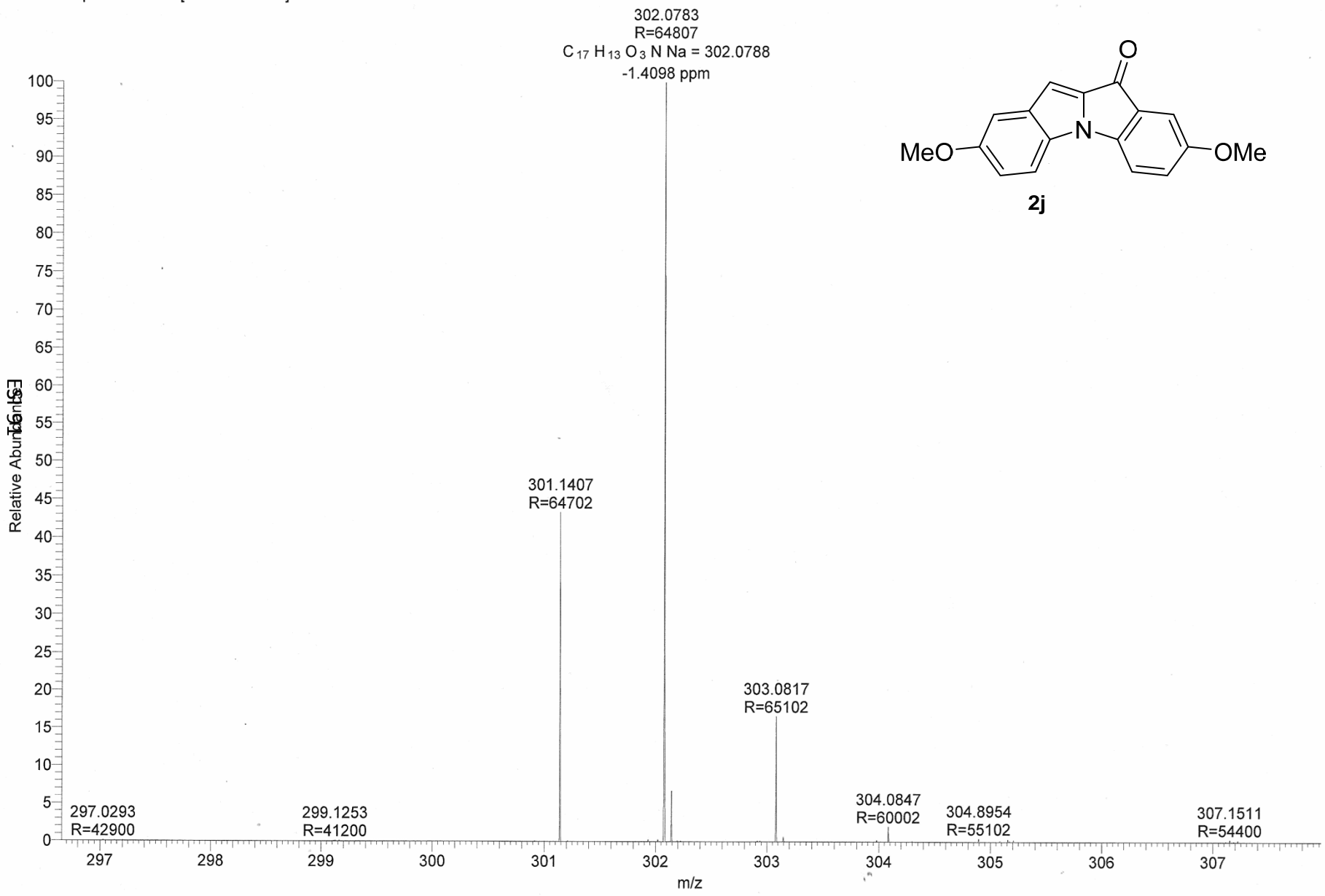
Acquisition Time (sec)	0.6554	***Comment***	DEPT				
Date Stamp	01 May 2015 14:43:44			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	800	***Origin***	spect

dept.1r.esp



D:\Data\9 Ome-ome. 12/30/2014 2:02:13 PM

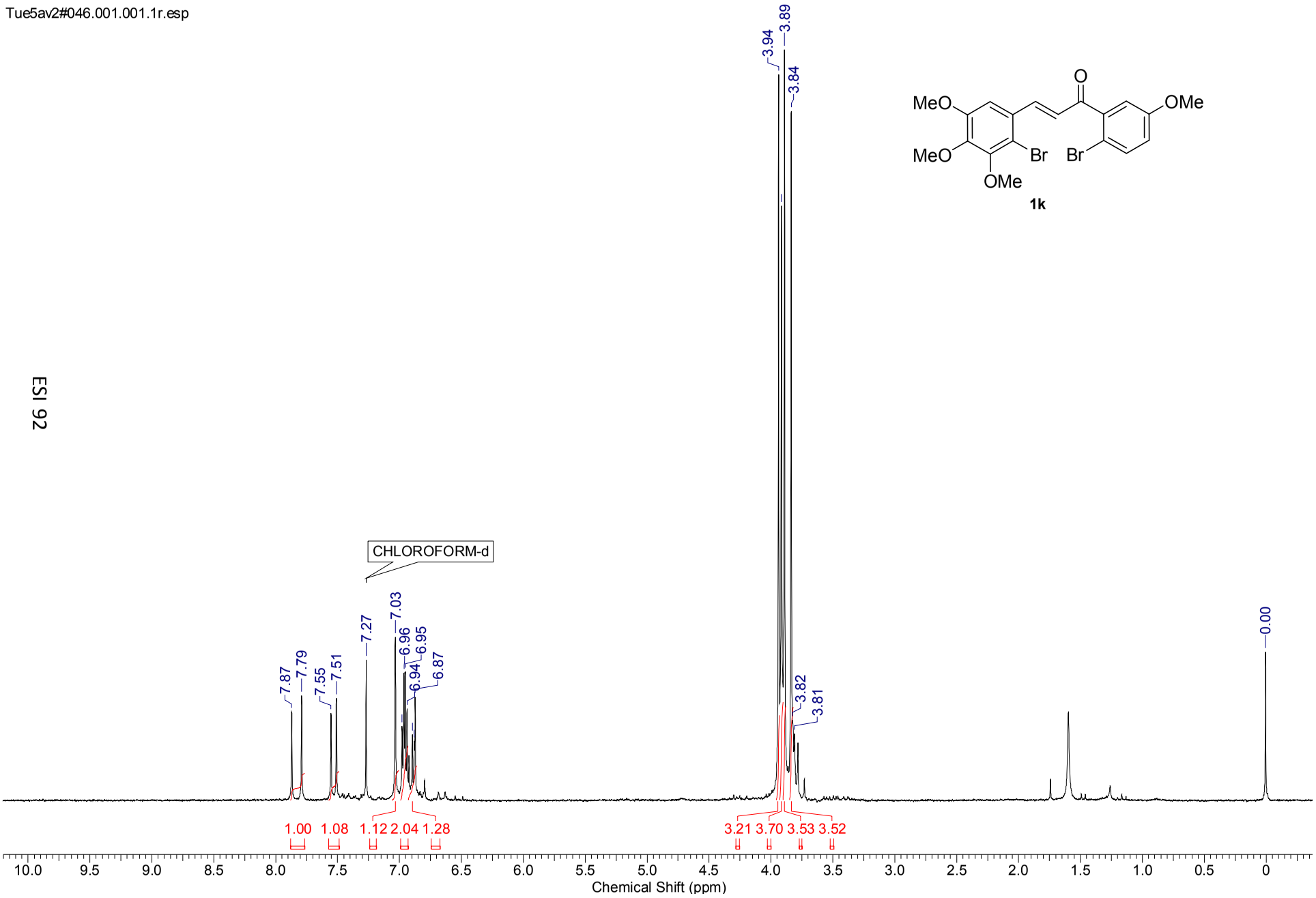
9 #1233 RT: 5.50 AV: 1 NL: 2.41E7
T: FTMS + p ESI Full ms [66.70-1000.00]



2j

Acquisition Time (sec)	3.9584	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	27 May 2014 15:55:52						
File Name	\\agni\nmr_data\AV200\MAY_14#AV200\data\Administrator\nmr\Tue5av2#046\1\pdata\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

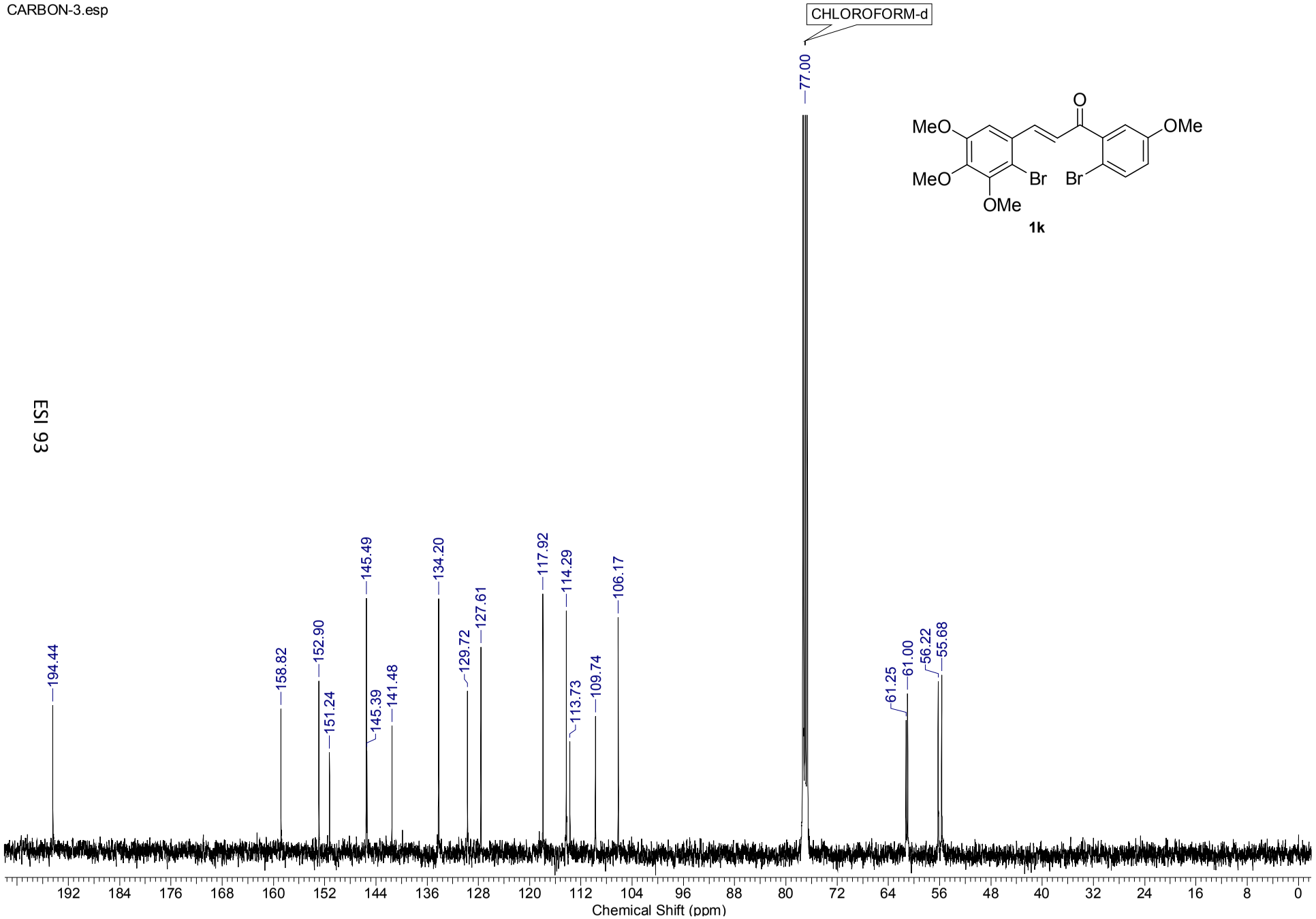
Tue5av2#046.001.001.1r.esp



ESI 92

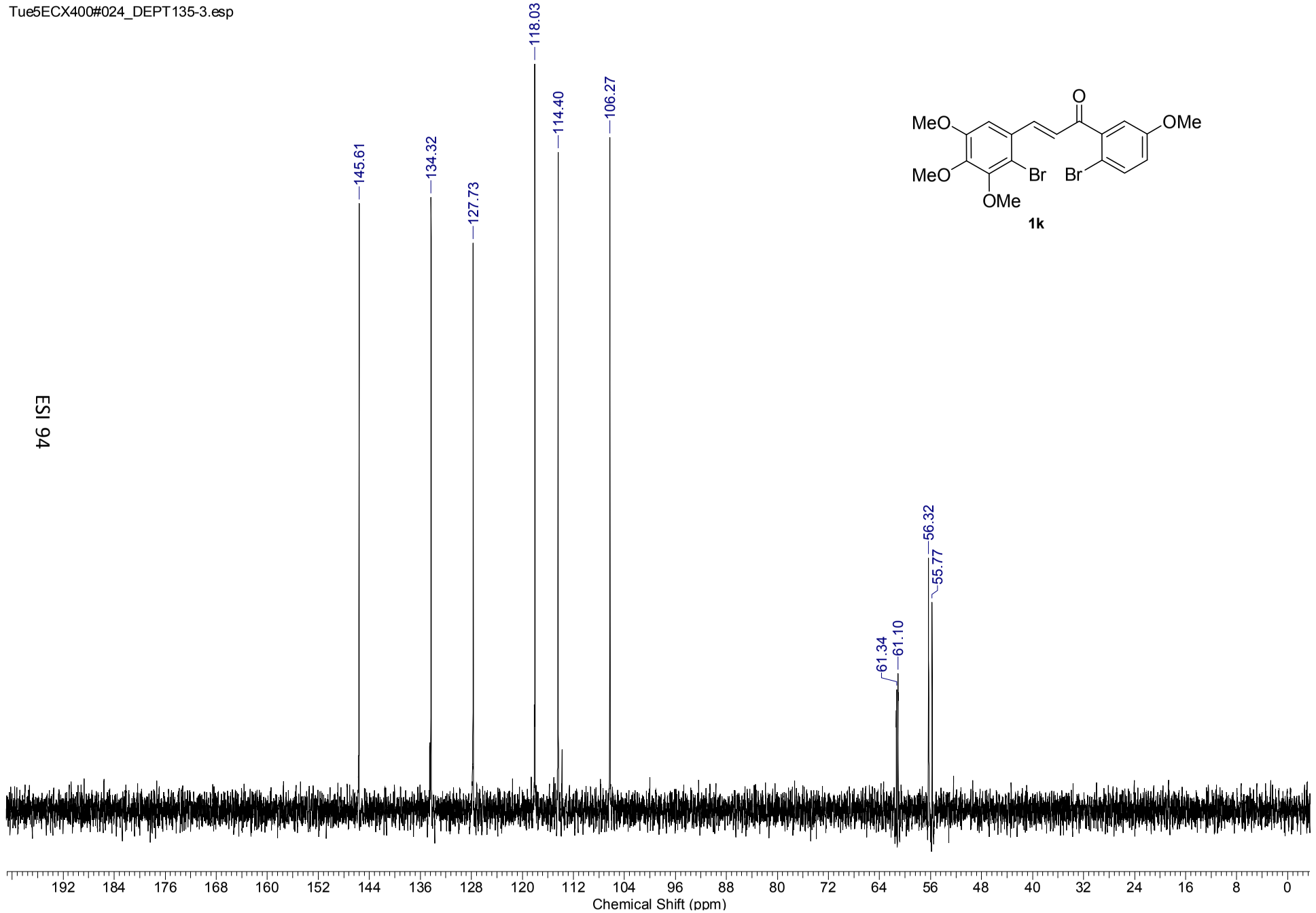
Acquisition Time (sec)	1.0434	***Comment***	Aanad	***Date***	28 May 2014 08:59:39		
Date Stamp	28 May 2014 07:54:52			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	ECX 400

CARBON-3.esp

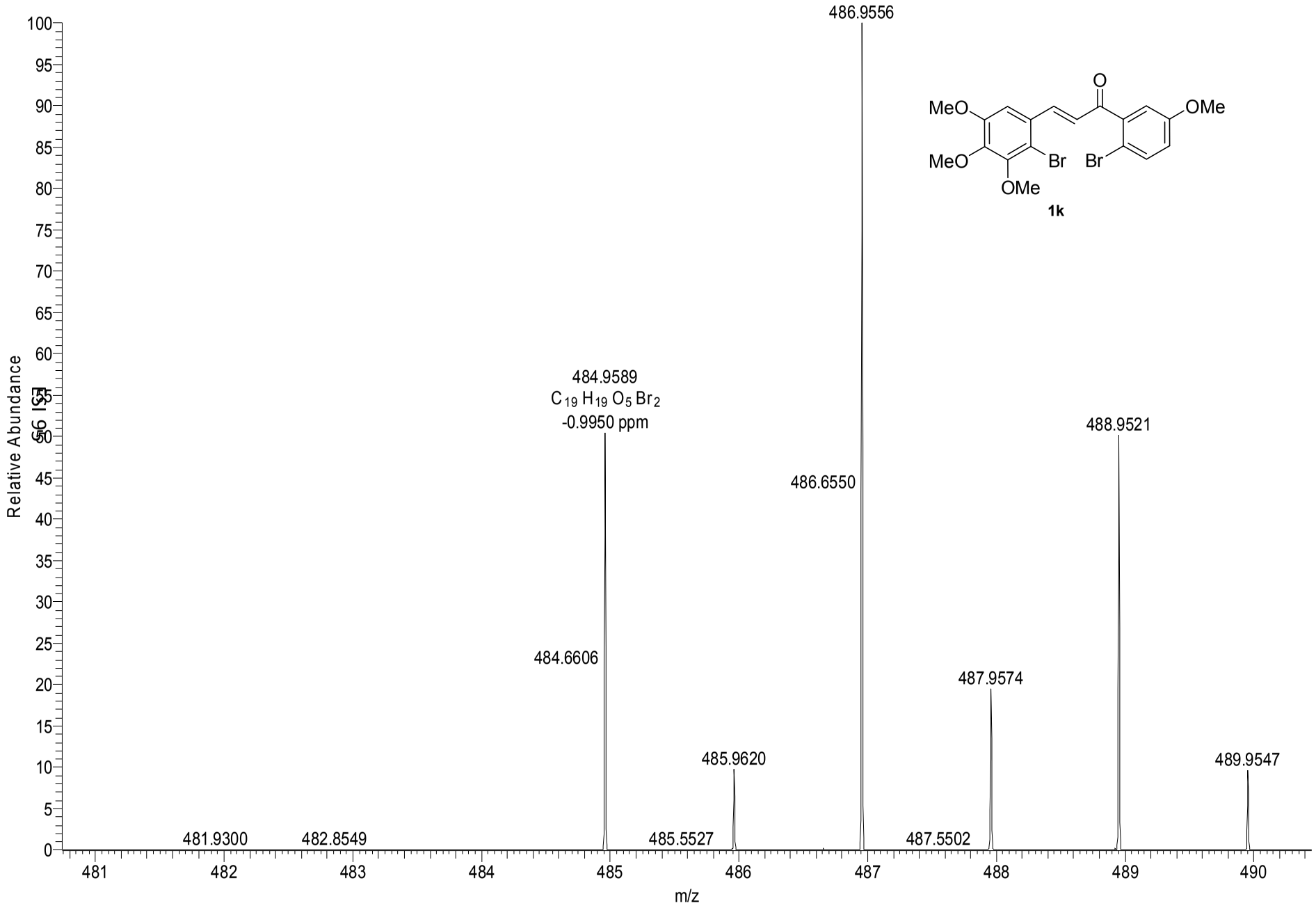


Acquisition Time (sec)	1.0434	***Comment***	Aanad	***Solvent***	CHLOROFORM-d		
Date Stamp	28 May 2014 08:18:33			***File Name***	\\agni\nmr_data\JEOL_400\2014\May 2014\Tue5ECX400#024_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	600	***Origin***	ECX 400

Tue5ECX400#024_DEPT135-3.esp



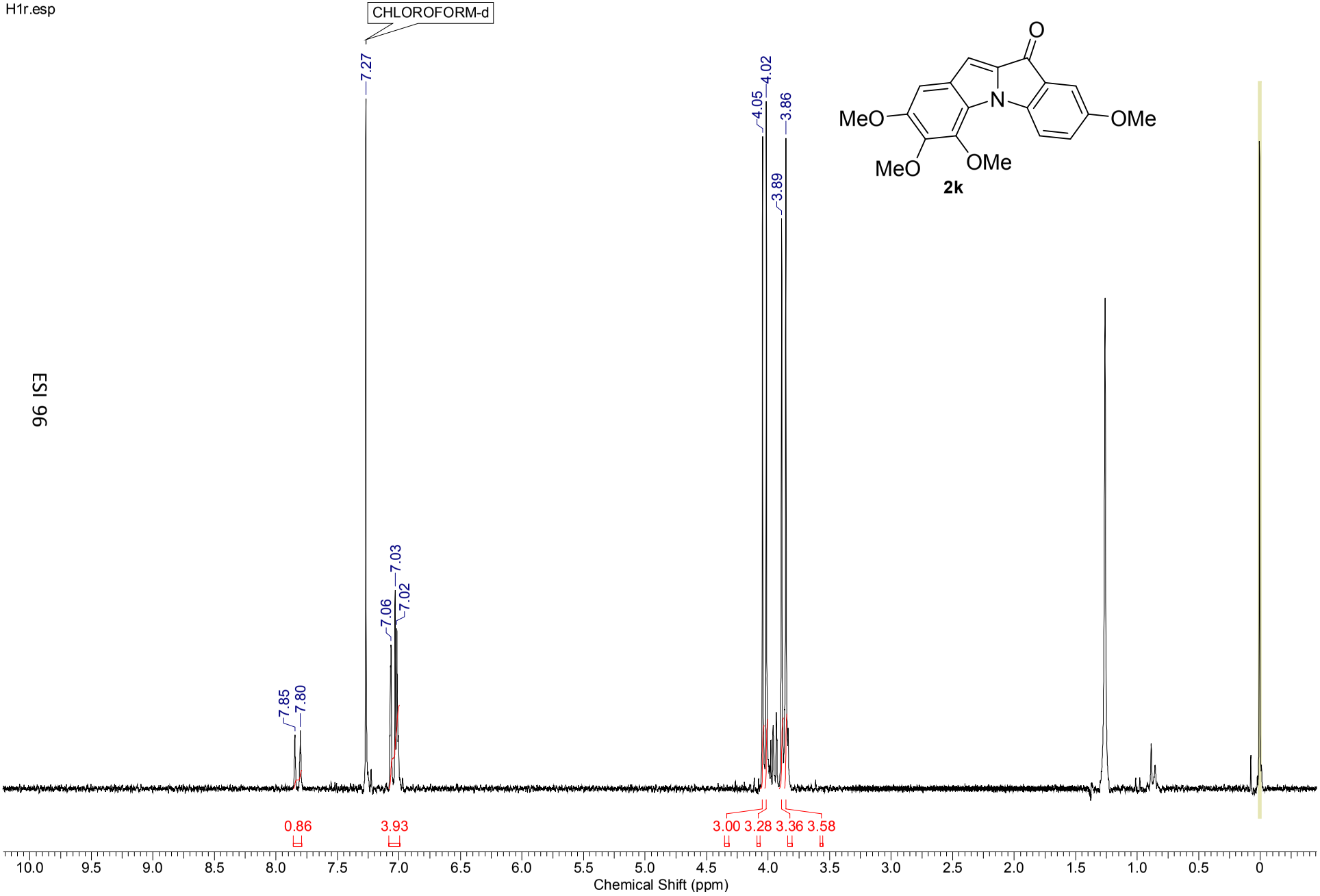
AKC-10 #103 RT: 0.54 AV: 1 NL: 6.74E8
T: FTMS + p ESI Full ms [100.00-1500.00]



Acquisition Time (sec)	3.9584	***Comment***	Anand	***Date***	24 Jun 2014 20:31:04		
Date Stamp	24 Jun 2014 20:31:04			***Solvent***	CHLOROFORM-d		
File Name	\\agni\nmr_data\AV200\JUNE_14#AV200\data\Administrator\nmr\Tue4av2#135\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

H1r.esp

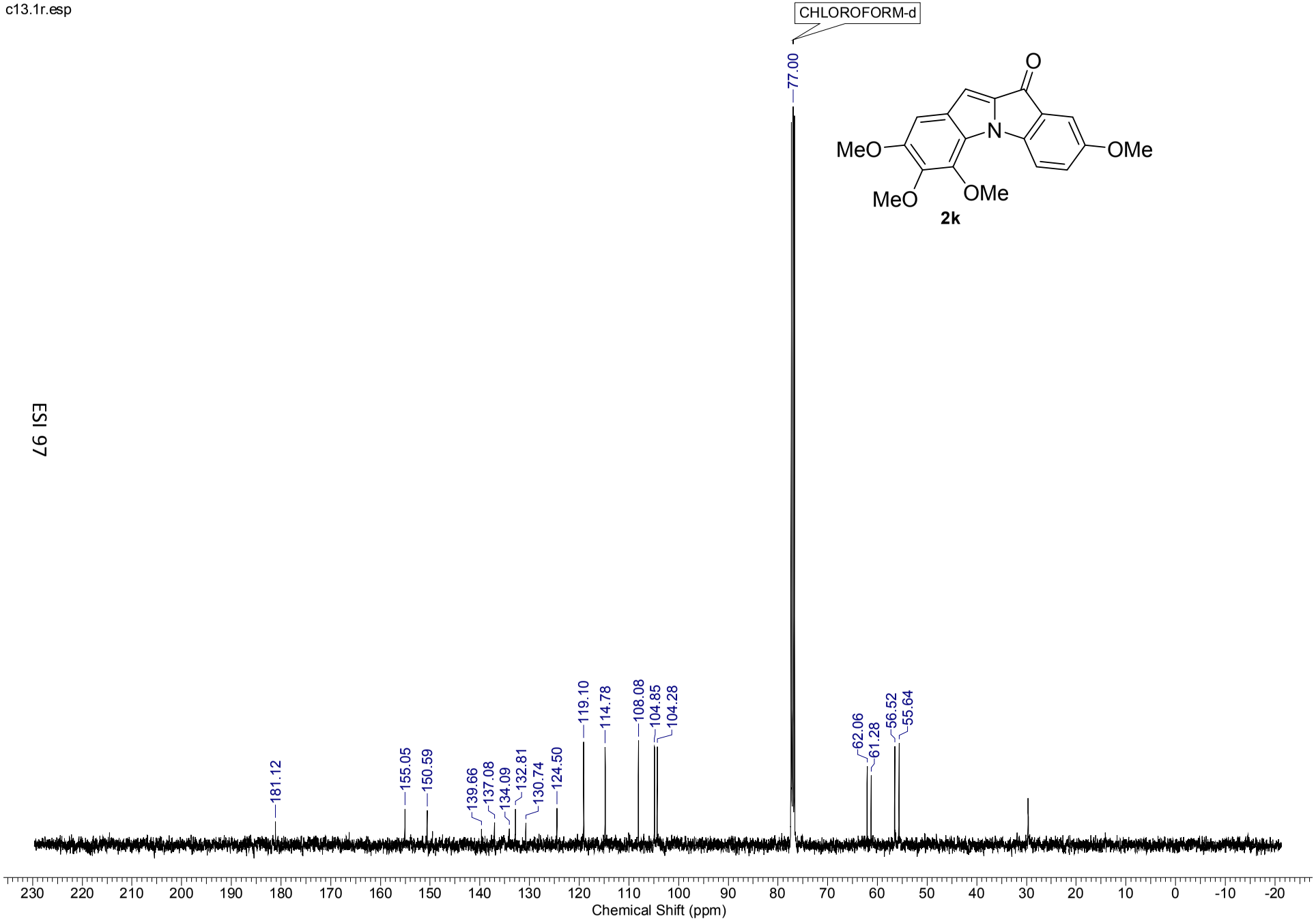
ESI 96



2k

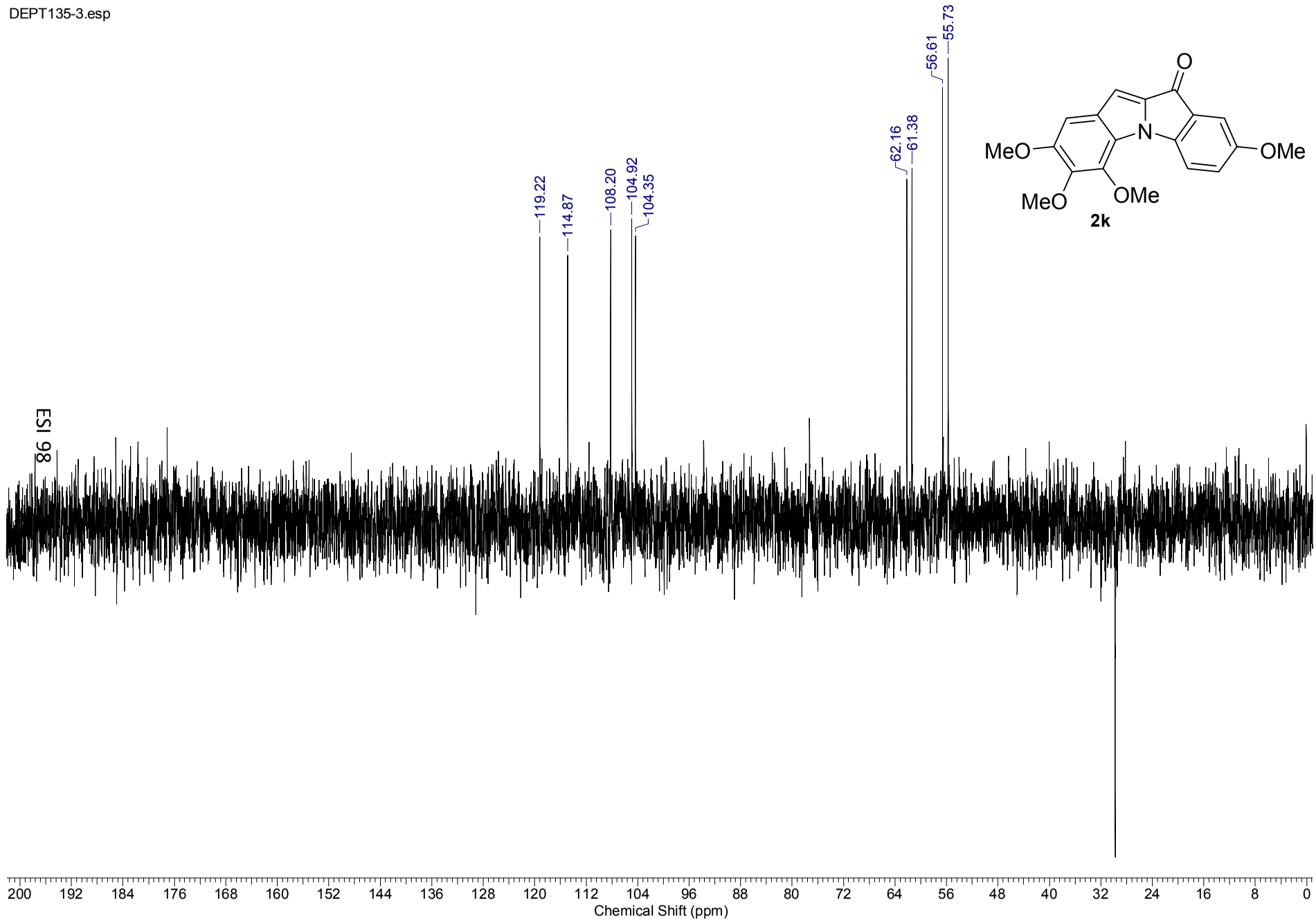
Acquisition Time (sec)	0.6488	***Comment***	13C				
Date Stamp	03 Nov 2014 16:23:36			***Solvent***			
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1408	***Origin***	spect

c13.1r.esp



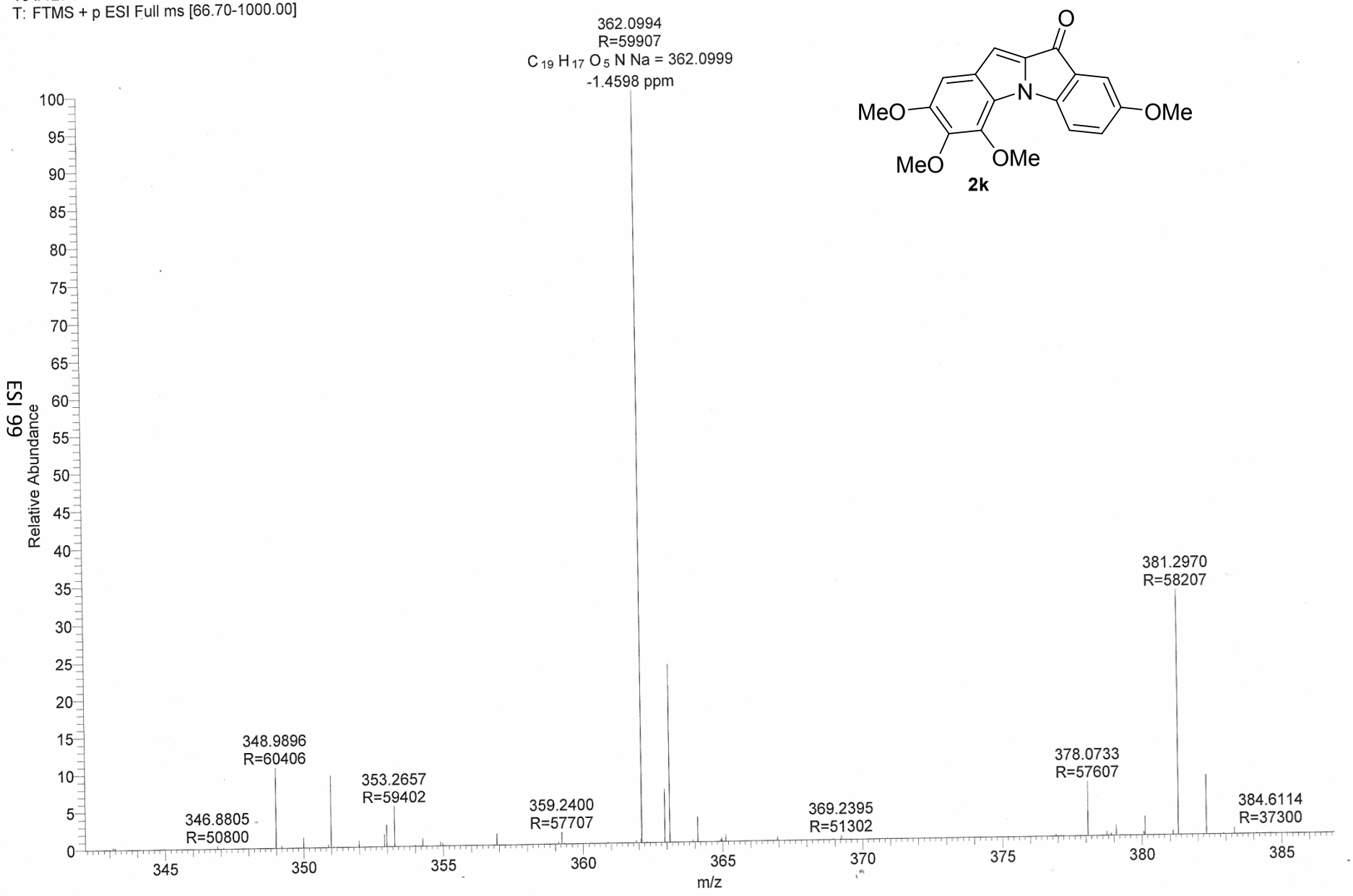
Acquisition Time (sec)	1.0434	***Comment***	Anand	***Date***	26 Jun 2014 12:08:50		
Date Stamp	26 Jun 2014 02:36:04			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	600	***Origin***	ECX 400

DEPT135-3.esp



D:\Data\13 TME-OME 12/30/2014 2:24:29 PM

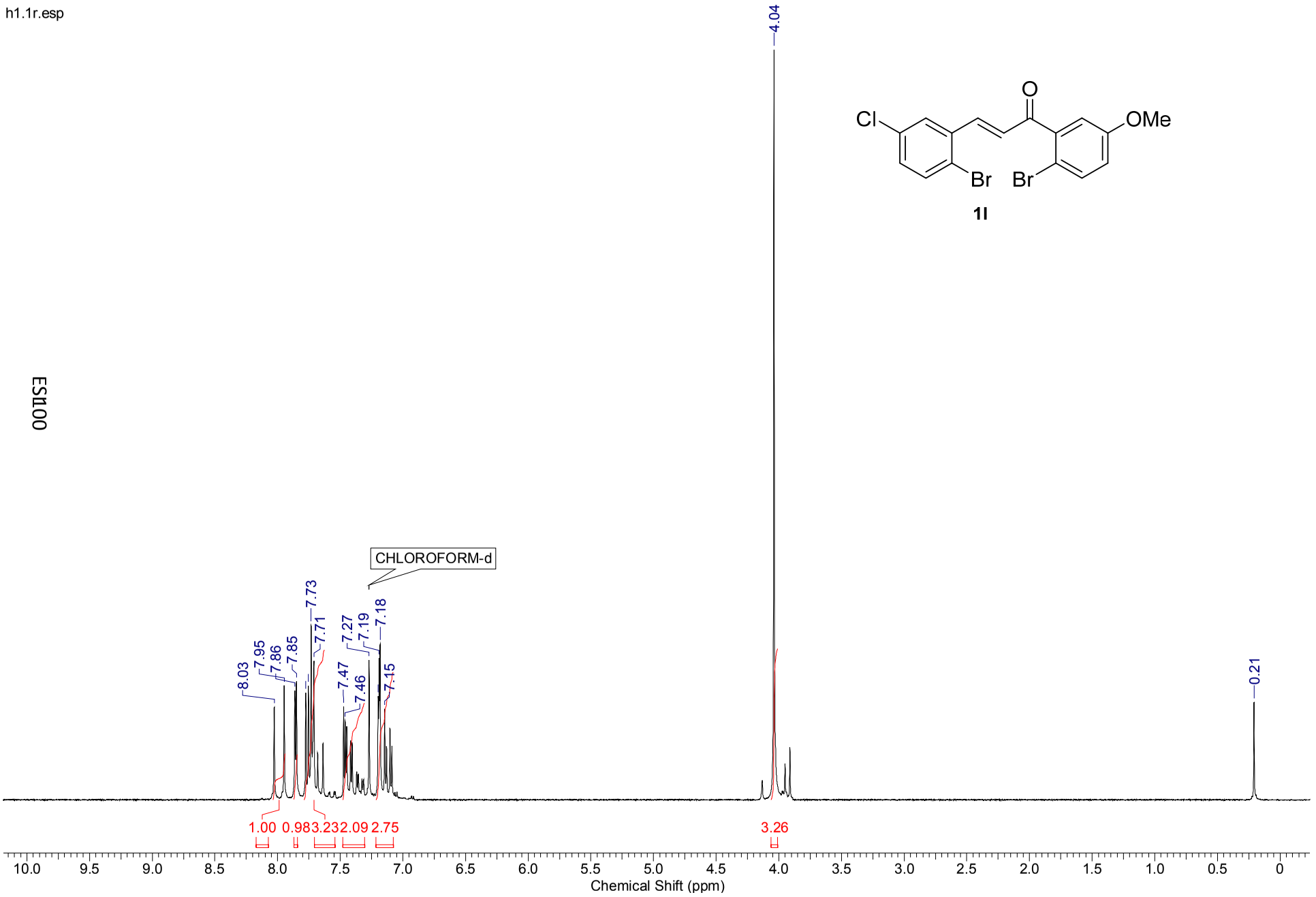
13 #1274 RT: 5.68 AV: 1 NL: 2.36E7
T: FTMS + p ESI Full ms [66.70-1000.00]



2k

Acquisition Time (sec)	3.9584	***Comment***	anand	CHLOROFORM-d			
Date Stamp	22 Jul 2014 00:53:28						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Mon4av2#128\1\PDATA\1\1r					***Frequency (MHz)***	200.13
Nucleus	1H	***Number of Transients***	8	***Origin***	av200	***Original Points Count***	16384

h1.1r.esp

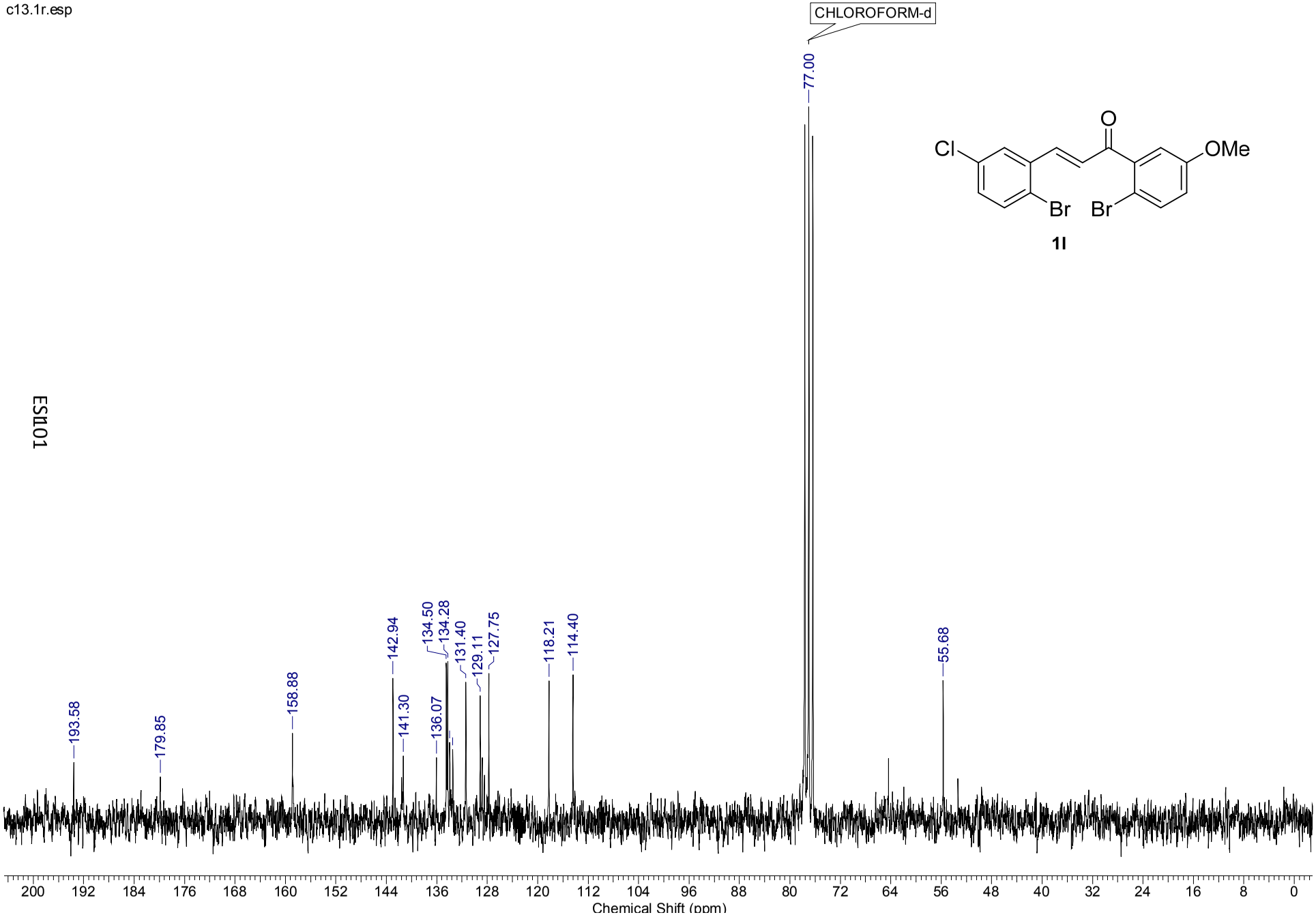


1l

ES100

Acquisition Time (sec)	0.6832	***Comment***	Anand	***Date***	27 Jul 2014 04:09:44
Date Stamp	27 Jul 2014 04:09:44			***Solvent***	CHLOROFORM-d
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat4av2#059\2\pdata\1\1r			***Frequency (MHz)***	50.32

c13.1r.esp



1l

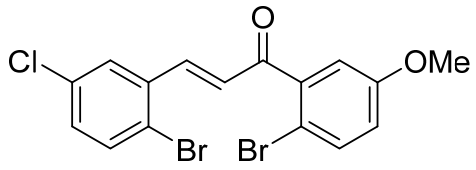
ES101

Acquisition Time (sec)	0.6832	***Comment***	Anand	***Solvent***	CHLOROFORM-d		
Date Stamp	27 Jul 2014 03:50:32						
File Name	\\agni\nmr_data\AV200\JUL_14#AV200\data\Administrator\nmr\Sat4av2#059\1\PDATA\1\1r					***Frequency (MHz)***	50.32
Nucleus	13C	***Number of Transients***	200	***Origin***	av200	***Original Points Count***	8192

Sat4av2#059.001.001.1r.esp

ES102

55.73
118.27
127.80
129.14
134.55
134.33
131.47
114.43
143.02
133.51

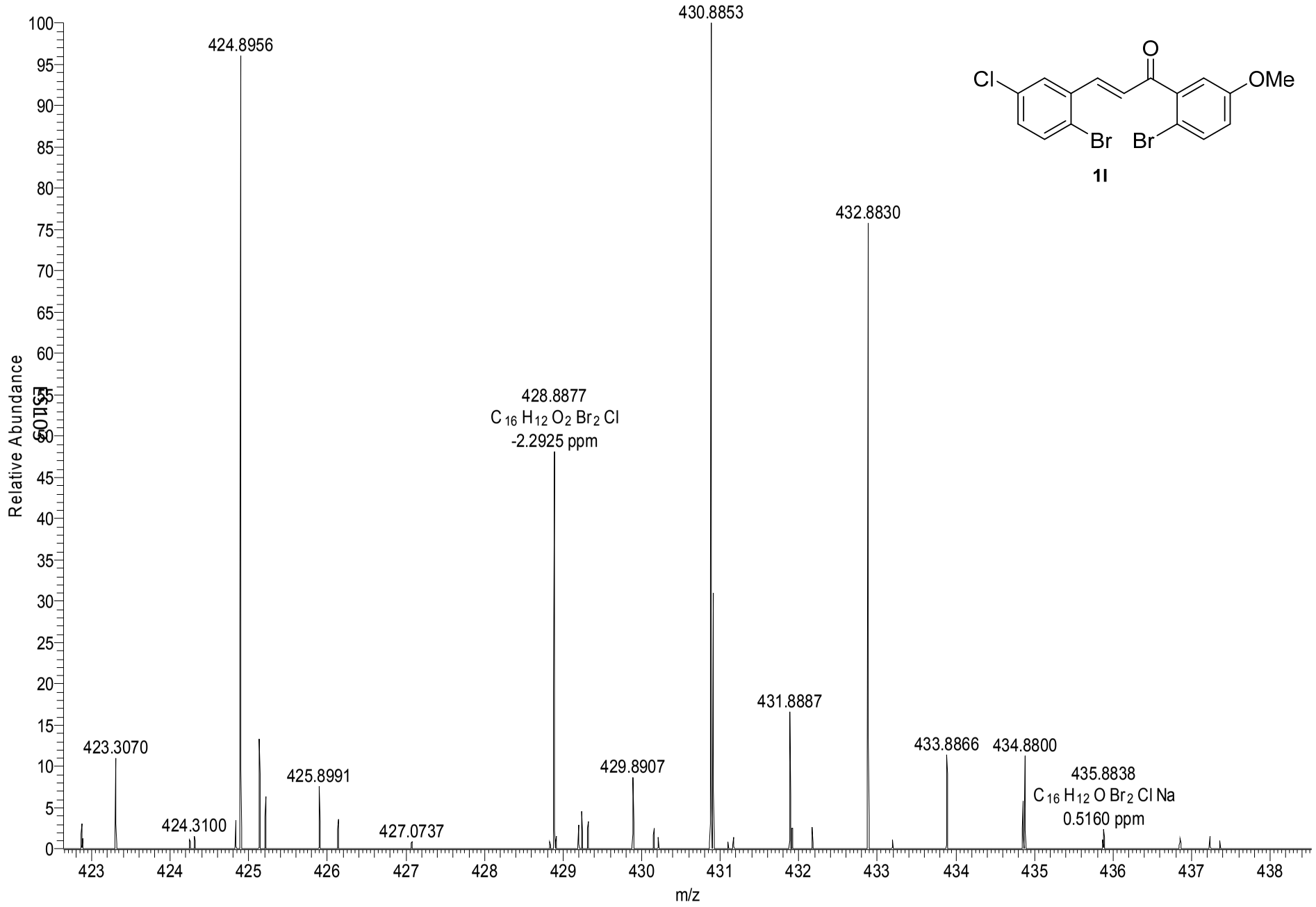


1l

200 192 184 176 168 160 152 144 136 128 120 112 104 96 88 80 72 64 56 48 40 32 24 16 8 0

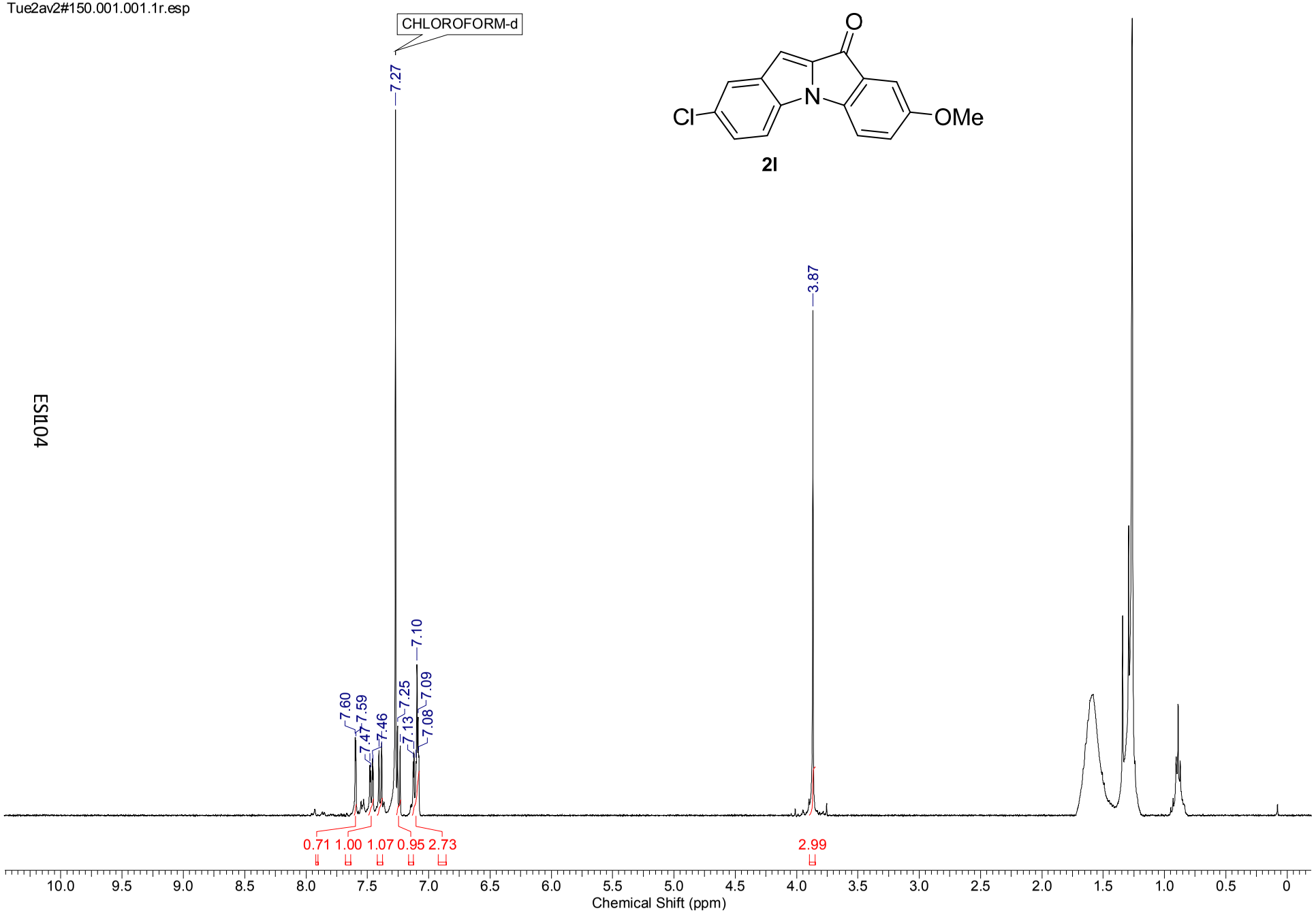
Chemical Shift (ppm)

AKC-2 #161 RT: 0.85 AV: 1 NL: 2.89E6
T: FTMS + p ESI Full ms [100.00-1500.00]



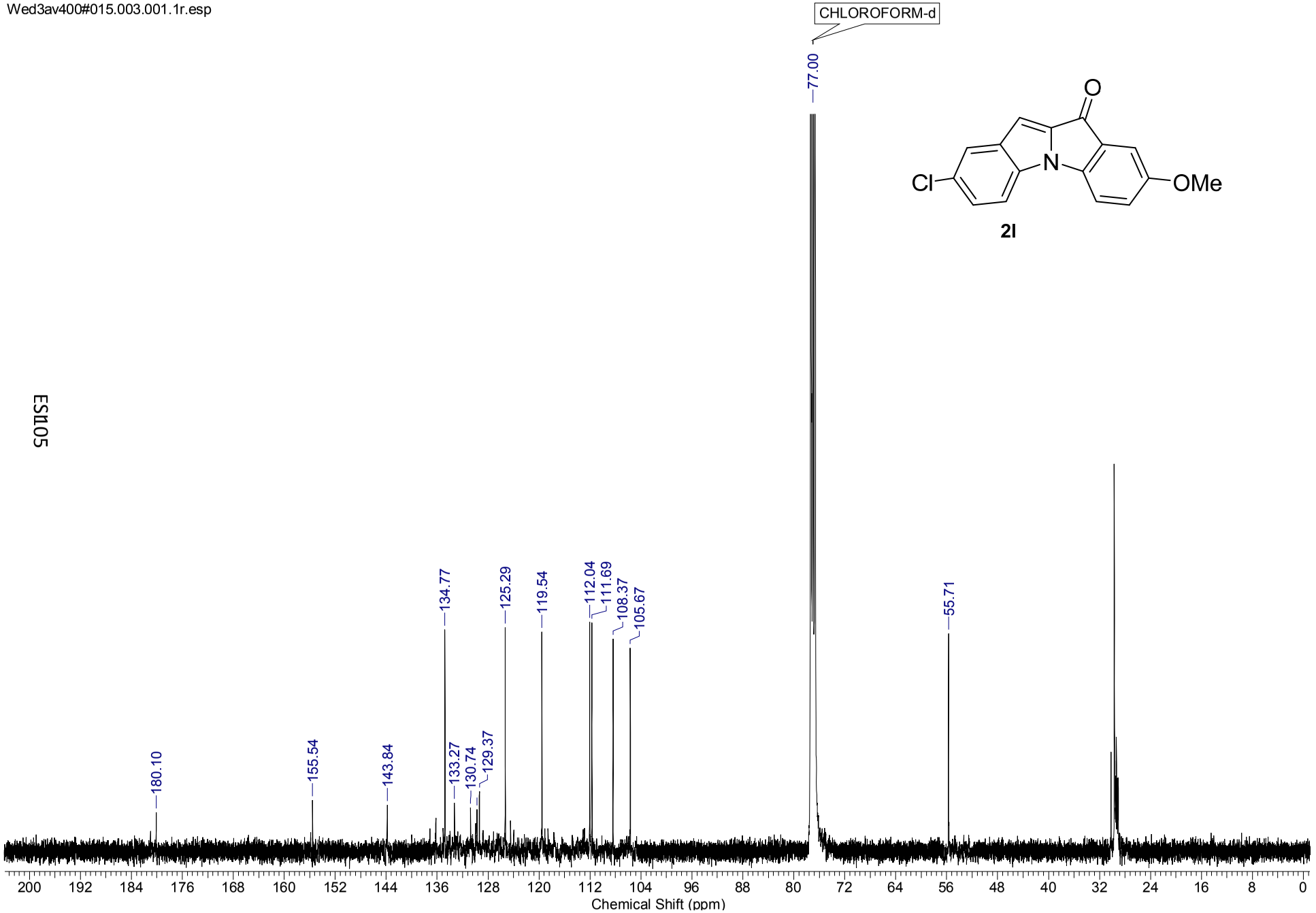
Acquisition Time (sec)	2.0447	***Comment***	Anand 1H	***Date***	12 Nov 2014 18:18:48		
Date Stamp	12 Nov 2014 18:18:48			***File Name***	\\agni\nmr_data\AV400\Nov_14_400\Wed3av400#015\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	128	***Origin***	spect

Tue2av2#150.001.001.1r.esp



Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	13 Nov 2014 09:21:12		
Date Stamp	13 Nov 2014 09:21:12			***Solvent***	CHLOROFORM-d		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	27671	***Origin***	spect

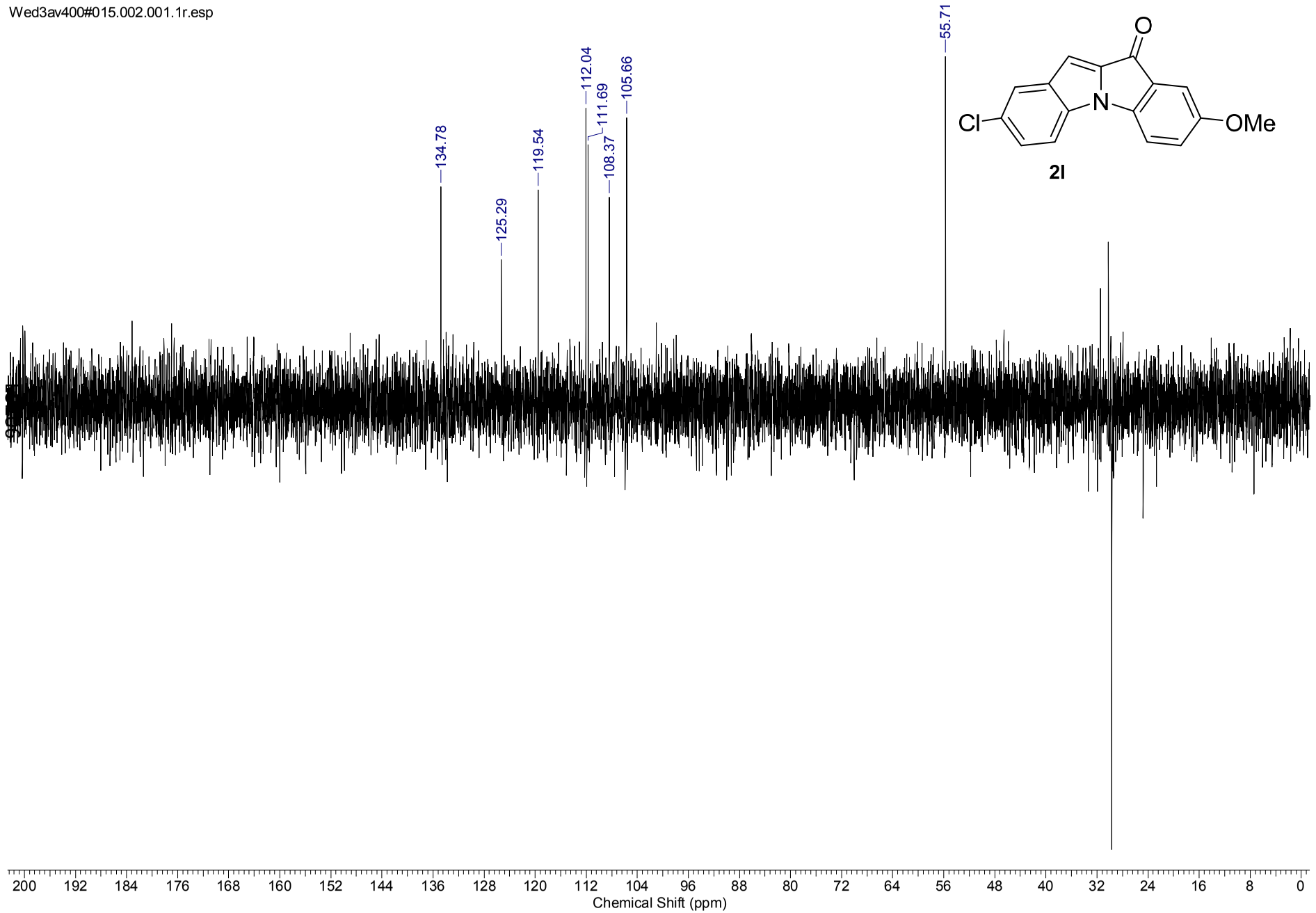
Wed3av400#015.003.001.1r.esp



2l

Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	12 Nov 2014 20:11:52		
Date Stamp	12 Nov 2014 20:11:52			***File Name***	\\agni\nmr_data\AV400\Nov_14_400\Wed3av400#015\2\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	4000	***Origin***	spect

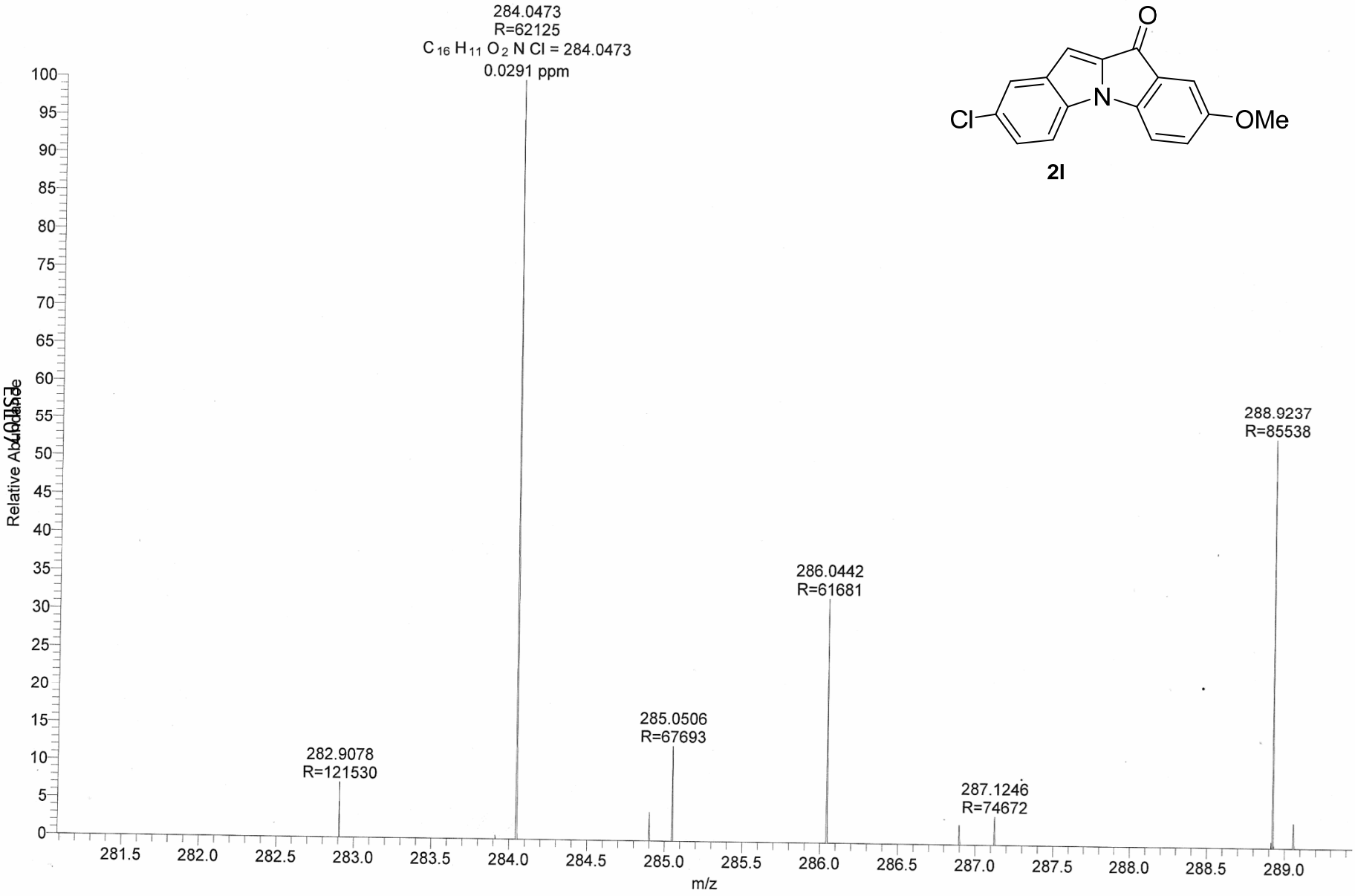
Wed3av400#015.002.001.1r.esp



D:\Data\Cl-OMe (3)

9/22/2014 4:55:17 PM

Cl-OMe #1331 RT: 5.93 AV: 1 SB: 331 4.49-4.94 , 6.50-7.51 NL: 9.75E5
T: FTMS + p ESI Full ms [66.70-1000.00]



2l