Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

2-Aroylindoles from *o*-bromochalcones via Cu (I)-catalyzed S_NAr with azide and intramolecular nitrene C–H insertion

Yogesh Goriya and Chepuri V. Ramana*

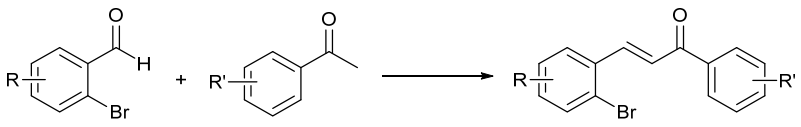
CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road,
Pune – 411 008 (India).

Email: vr.chepuri@ncl.res.in

General Remarks

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). ^{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 Chloroform-d (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 spectrometer or UPLC coupled Mass Spectrometer (Waters). HRMS mass spectra were recorded on a Thermo Scientific Q-Exactive, Accela 1250 pump.

General Procedure for Preparation of chalcone:

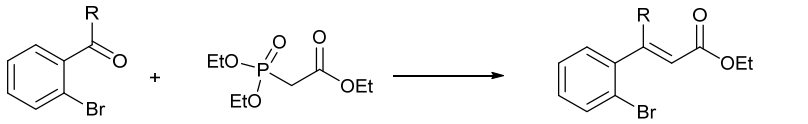


Compounds **1a–1t** was prepared according to literature procedure.[1] Aqueous NaOH (2.5 N, 1 mL) was added drop-wise to a mixture of 2-bromobenzaldehyde (2.7 mmol), acetophenone (2.7 mmol) in ethanol (4 mL) at ambient temperature. After stirring overnight, the reaction mixture was poured into brine solution (20 mL) and extracted with CH_2Cl_2 (20 mL). The extract was washed with water (2 × 30 mL), dried over Na_2SO_4, and evaporated under

[1] M. Shen, B. E. Leslie and T. G. Driver, *Angew. Chem. Int. Ed.*, 2008, **47**, 5056.

reduced pressure. The crude was purified over silica gel (ethyl acetate and pet ether as eluent) to give the product. Yields were not optimized.

General Scheme for Preparation of 4c–4e:[2]

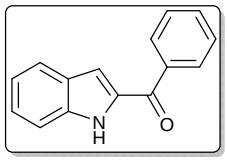


4c, R = -CH_3; **4d**, R = -C_4H_9; **4e**, R = -Ph

General procedure for Cu(I)-catalyzed synthesis of 2-aroyl indole:

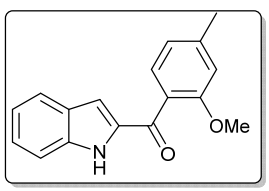
To a solution of *o*-bromochalcone (1.0 mmol) in NMP (1 mL), were added L-proline (0.2 mmol), K_2CO_3 (4.0 mmol), CuI (0.2 mmol), and NaN_3 (1.2 mmol). The mixture was stirred at 110 °C. After 15h the reaction mixture was cooled and diluted with 30 mL of water and extracted with ethyl acetate (3 X 30 mL). Combined organic layer was dried (Na_2SO_4) and evaporated under reduced pressure. The crude was purified over silica gel (ethyl acetate and pet ether as eluent) provided 2-aroyl indole in moderate to good yields.

(1*H*-Indol-2-yl)(phenyl)methanone (**2a**)[3]:-



Light yellow solid; 76% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 7.16 (s, 1H), 7.16 (dt, J = 1.0, 7.0 Hz, 1H), 7.37 (ddd, J = 1.0, 6.8, 8.4 Hz, 1H), 7.45–7.62 (m, 4H), 7.71 (d, J = 8.0 Hz, 1H), 7.96–8.01 (m, 2H), 9.27 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.2 (d), 112.9 (d), 121.0 (d), 123.2 (d), 126.5 (d), 127.7 (s), 128.5 (d, 2C), 129.2 (d, 2C), 132.4 (d), 134.3 (s), 137.5 (s), 138.0 (s), 187.2 (s) ppm.

(1*H*-Indol-2-yl)(2-methoxy-4-methylphenyl) methanone (**2b**):-

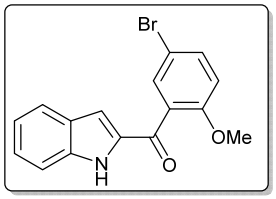


Brown solid; 59% Yield; R_f 0.2 (10% ethyl acetate/pet. ether); mp: 112–113 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.82 (s, 3H),

[2] M. Gallant, M. Belley, M.-C. Carriere, A. Chateauneuf, D. Denis, N. Lachance, S. Lamontagne, K. M. Metters, N. Sawyer, D. Slipetz, J. F. Truchon and M. Labelle, *Bioorg. Med. Chem. Lett.*, 2003, **13**, 3813
[3] W.-C. Gao, S. Jiang, R.-L. Wang and C. Zhang, *Chem. Commun.*, 2013, **49**, 4890.

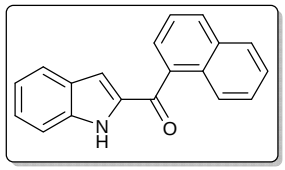
6.84 (s, 1H), 6.86 (d, J = 6.8 Hz, 1H), 6.93 (d, J = 1.8 Hz, 1H), 7.12 (ddd, J = 0.9, 6.9, 7.9 Hz, 1H), 7.29–7.37 (m, 1H), 7.42–7.48 (m, 2H), 7.64 (d, J = 8.0 Hz, 1H), 9.43 (s, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 21.9 (q), 55.7 (q), 112.2 (d), 112.5 (d), 112.8 (d), 120.7 (d), 120.8 (d), 123.1 (d), 125.4 (s), 126.3 (d), 127.6 (s), 130.0 (d), 135.9 (s), 137.7 (s), 142.8 (s), 157.6 (s), 187.1 (s) ppm; HRMS (ESI+): calcd. for $C_{17}H_{15}O_2NNa$ = 288.0995, found 288.0995**.**

(5-Bromo-2-methoxyphenyl)(1*H*-Indol-2-yl)methanone (**2c**)[4]:



Brown solid; 67% Yield; R_f 0.5 (15% ethyl acetate/pet. ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.80 (s, 3H), 6.91 (m, 2H), 7.14 (ddd, J = 1.1, 6.8, 8.0 Hz, 1H), 7.36 (ddd, J = 1.0, 6.8, 7.9 Hz, 1H), 7.44–7.48 (m, 1H), 7.55–7.60 (m, 2H), 7.66 (br d, J = 8.2 Hz, 1H), 9.37 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 56.0 (q), 112.7 (2C, s and d), 113.4 (d), 113.6 (d), 121.1 (d), 123.3 (d), 126.8 (d), 127.5 (s), 129.8 (s), 132.0 (d), 134.5 (d), 135.2 (s), 137.9 (s), 156.5 (s), 185.4 (s) ppm.

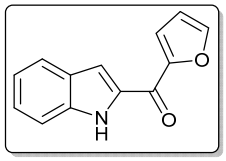
(1*H*-Indol-2-yl)(naphthalen-1-yl)methanone (**2d**):-



Yellow solid; 77% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); mp: 150–151 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.97 (d, J = 1.0 Hz, 1H), 7.15 (t, J = 6.0 Hz, 1H), 7.38 (ddd, J = 0.8, 7.0, 8.0 Hz, 1H), 7.50–7.59 (m, 4H), 7.65 (d, J = 8.0 Hz, 1H), 7.88–7.95 (m, 2H), 8.04 (d, J = 8.3 Hz, 1H), 8.28–8.30 (m, 1H), 9.62 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.3 (d), 113.7 (d), 121.1 (d), 123.3 (d), 124.3 (d), 125.5 (d), 126.5 (d), 126.8 (d), 127.3 (d), 127.6 (s), 127.8 (d), 128.4 (d), 130.8 (s), 131.5 (d), 133.8 (s), 135.6 (s), 136.0 (s), 137.9 (s), 188.8 (s) ppm; HRMS (ESI+): calcd. for $C_{19}H_{13}ONNa$ = 294.0889, found 294.0890**.**

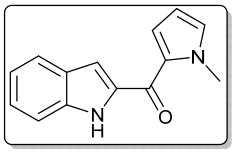
[4] Y. Miki, Y. Tsuzaki, C. Kai and H. Hachiken, *Heterocycles*, 2002, **57**, 1635

Furan-2-yl(1*H*-Indol-2-yl)methanone (**2e**)[3]:



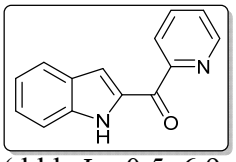
Brown solid; 76% Yield; R_f 0.5 (10% ethyl acetate/pet. ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 6.63–6.64 (m, 1H), 7.71 (t, J = 7.6 Hz, 3H), 7.37 (t, J = 7.7 Hz, 1H), 7.45–7.47 (m, 2H), 7.72 (br d, J = 8.6 Hz, 2H), 7.76 (d, J = 1.0 Hz, 1H), 9.44 (s, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 111.5 (d), 112.1 (d), 112.5 (d), 118.6 (d), 121.0 (d), 123.3 (d), 126.5 (d), 128.0 (s), 133.4 (s), 137.2 (s), 146.5 (d), 152.7 (s), 172.6 (s) ppm.

(1*H*-Indol-2-yl)(1-methyl-1H-pyrrol-2-yl) methanone (**2f**):-



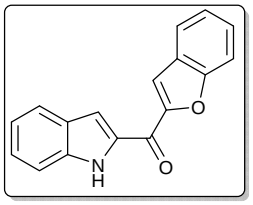
Brown solid; 49% Yield; R_f 0.2 (10% ethyl acetate/pet. ether); mp: 100–101 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 4.02 (s, 3H), 6.23 (dd, J = 2.7, 3.8 Hz, 1H), 6.94 (br s, 1H), 7.16 (t, J = 7.6 Hz, 1H), 7.20 (dd, J = 1.4, 3.9 Hz, 1H), 7.23 (s, 1H), 7.33 (t, J = 7.6 Hz, 1H), 7.45 (d, J = 8.3 Hz, 1H), 7.72 (d, J = 8.0 Hz, 1H), 9.37 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 37.0 (q), 108.5 (d), 109.7 (d), 111.9 (d), 120.7 (d, 2C), 122.9 (d), 125.5 (d), 127.8 (s), 130.3 (s), 131.2 (d), 135.6 (s), 136.9 (s), 176.3 (s) ppm; HRMS (ESI+): calcd. for $C_{14}H_{12}ON_2H^+$ = 225.1022, found 225.1021**.**

(1*H*-Indol-2-yl)(pyridin-2-yl)methanone (**2g**):-



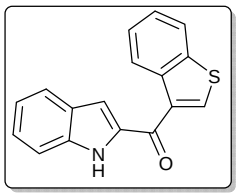
Yellow solid; 57% Yield; R_f 0.2 (10% ethyl acetate/pet. ether); mp: 130–131 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.15 (t, J = 7.5 Hz, 1H), 7.36 (ddd, J = 0.5, 6.9, 7.9 Hz, 1H), 7.48–7.55 (m, 2H), 7.75 (d, J = 8.0 Hz, 1H), 7.84 (s, 1H), 7.93 (dt, J = 1.5, 7.8 Hz, 1H), 8.28 (d, J = 8.0 Hz, 1H), 8.81 (d, J = 4.3 Hz, 1H), 10.84 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 112.4 (d), 113.3 (d), 120.8 (d), 123.3 (d), 124.2 (d), 126.3 (d), 126.7 (d), 127.4 (s), 135.0 (s), 137.4 (d), 137.7 (s), 148.5 (d), 155.0 (s), 181.2 (s) ppm; HRMS (ESI+): calcd. for $C_{14}H_{10}ON_2Na$ = 245.0685, found 245.0688**.**

Benzofuran-2-yl(1*H*-Indol-2-yl)methanone (2h)[5]:



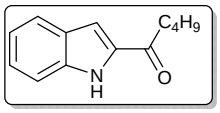
Yellow solid; 78% Yield; R_f 0.4 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.20 (t, J = 7.5 Hz, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.40 (t, J = 7.6 Hz, 1H), 7.48 (d, J = 8.2 Hz, 1H), 7.53 (t, J = 7.8 Hz, 1H), 7.69 (d, J = 8.4 Hz, 1H), 7.77 (d, J = 7.9 Hz, 1H), 7.78 (s, 1H), 7.81 (d, J = 8.1 Hz, 1H), 7.88 (br s, 1H), 9.33 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 112.1 (d), 112.3 (d), 112.4 (d), 114.3 (d), 121.2 (d), 123.2 (d), 123.6 (d), 124.0 (d), 126.9 (d), 127.1 (s), 128.0 (s), 128.2 (d), 133.7 (s), 137.5 (s), 152.9 (s), 155.9 (s), 174.0 (s) ppm.

Benzo[b]thiophen-3-yl(1*H*-Indol-2-yl)methanone (**2i**):-



Light brown solid; 69% Yield; R_f 0.4 (10% ethyl acetate/pet. ether); mp: 187–188 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.18 (t, J = 6.7 Hz, 1H), 7.25 (s, 1H), 7.38 (t, J = 6.6 Hz, 1H), 7.45–7.51 (m, 3H), 7.74 (d, J = 7.3, 1H), 7.93 (d, J = 7.3 Hz, 1H), 8.36 (s, 1H), 8.50 (d, J = 7.3 Hz, 1H), 9.52 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 111.6 (d), 112.2 (d), 121.1 (d), 122.4 (d), 123.2 (d), 124.7 (d), 125.5 (d), 125.6 (d), 126.5 (d), 127.7 (s), 134.7 (s), 135.5 (2C, s and d), 137.2 (s), 137.6 (s), 140.0 (s), 181.2 (s) ppm; HRMS (ESI+): calcd. for $C_{17}H_{11}ONSH^+$ = 278.0634, found 278.0634.

1-(1*H*-Indol-2-yl)pentan-1-one (**2j**)[6]**:**

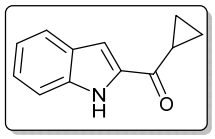


Brown solid; 47% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.96 (t, J = 7.4 Hz, 3H), 1.39–1.46 (m, 2H), 1.73–1.79 (m, 2H), 2.94 (t, J = 7.6 Hz, 2H), 7.15 (t, J = 7.5 Hz, 1H), 7.20 (s, 1H), 7.34 (t, J = 7.6 Hz, 1H), 7.42 (d, J = 8.3 Hz, 1H), 7.70 (d, J = 8.1 Hz, 1H), 9.09 (s, 1H); ^{13}C NMR (125

[5] S. Mahboobi, A. Uecker, C. Cenac, A. Sellmer, E. Eichhorn, S. Elz, F.-D. Bohmer and S. Dove, *Bioorg. Med. Chem.*, 2007, **15**, 2187.
[6] P. C. Too, S. H. Chua, S. H. Wong and S. Chiba, *J. Org. Chem.*, 2011, **76**, 6159.

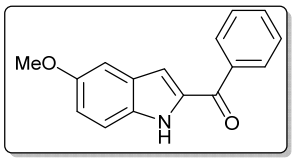
MHz, $CDCl_3$): δ 13.9 (q), 22.5 (t), 27.3 (t), 38.1 (t), 109.0 (d), 112.1 (d), 120.9 (d), 123.0 (d), 126.2 (d), 127.6 (s), 135.2 (s), 137.2 (s), 193.6 (s) ppm.

Cyclopropyl (1*H*-Indol-2-yl) methanone (**2k**):-



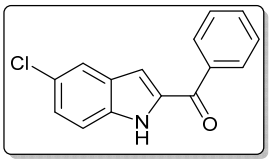
Brown solid; 46% Yield; R_f 0.5 (10% ethyl acetate/pet. ether); mp: 143–145 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.02–1.11 (m, 2H), 1.25–1.32 (m, 2H), 2.59–2.71 (m, 1H), 7.11–7.19 (m, 1H), 7.30–7.45 (m, 3H), 7.73 (dd, J = 0.5, 8.1 Hz, 1H), 9.24 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 11.4 (t, 2C), 17.5 (d), 109.1 (d), 112.2 (d), 120.8 (d), 122.9 (d), 126.1 (d), 127.6 (s), 135.8 (s), 137.3 (s), 192.9 (s) ppm; HRMS (ESI+): calcd. for $C_{12}H_{11}ONH^+$ = 186.0913, found 186.0916.

(5-Methoxy-1*H*-Indol-2-yl)(phenyl)methanone (**2l**)[7]:-



Yellow solid; 74% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.84 (s, 3H), 7.02–7.08 (m, 3H), 7.37–7.41 (m, 1H), 7.49–7.63 (m, 3H), 7.69–8.01 (m, 2H), 9.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6 (q), 102.6 (d), 112.5 (d), 113.3 (d), 118.4 (d), 127.9 (s), 128.4 (d, 2C), 129.2 (d, 2C), 132.2 (d), 133.3 (s), 134.7 (s), 138.1 (s), 154.7 (s), 187.1 (s) ppm.

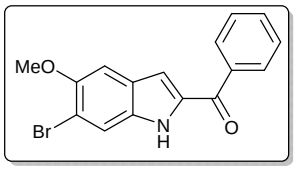
(5-Chloro-1*H*-Indol-2-yl)(phenyl)methanone (**2m**)**:-**



Light yellow solid; 74% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); mp: 198–200 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.08–7.09 (m, 1H), 7.32 (dd, J = 1.9, 8.8 Hz, 1H), 7.42 (d, J = 8.8 Hz, 1H), 7.52–7.56 (m, 2H), 7.61–7.65 (m, 1H), 7.68 (br s, 1H), 7.97–7.99 (m, 2H), 9.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 111.7 (d), 113.3 (d), 122.3 (d), 126.6 (s), 127.0 (d), 128.6 (d, 2C and s, 1C), 129.2 (d, 2C), 132.6 (d), 135.3 (s), 135.7 (s), 137.6 (s), 187.0 (s) ppm; HRMS (ESI+): calcd. for $C_{15}H_{10}ONClH^+$ = 256.0524, found 256.0522.

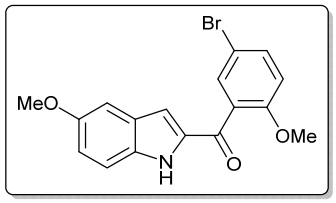
[7] S. Mahboobi, S. Teller, H. Pongratz, H. Hufsky, A. Sellmer, A. Botzki, A. Uecker, T. Beckers, S. Baasner, C. Schachtele, F. Uberall, M. U. Kassack, S. Dove and F.-D. Bohmer, *J. Med. Chem.*, 2002, **45**, 1002.

(6-Bromo-5-methoxy-1*H*-Indol-2-yl)(phenyl)methanone (2n):-



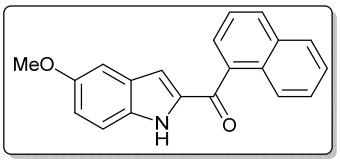
Yellow solid; 59% Yield; R_f 0.2 (10% ethyl acetate/pet. ether); mp: 177–178 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.92 (s, 3H), 7.06 (s, 1H), 7.11 (s, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 7.7 Hz, 1H), 7.63 (t, J = 7.3 Hz, 1H), 7.71 (s, 1H), 7.96 (s, 1H), 7.98 (s, 1H), 9.42 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 56.6 (q), 103.3 (d), 112.1 (d), 113.3 (s), 116.8 (d), 127.3 (s), 128.5 (d, 2C), 129.2 (d, 2C), 132.5 (d), 133.0 (s), 135.1 (s), 137.8 (s), 151.0 (s), 186.9 (s) ppm; HRMS (ESI+): calcd. for $C_{16}H_{12}O_2NBrH^+$ = 330.0124, found 330.0132.

(5-Bromo-2-methoxyphenyl)(5-methoxy-1*H*-Indol-2-yl)methanone (2o):-



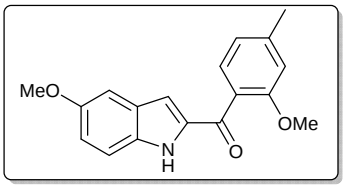
Yellow solid; 68% Yield; R_f 0.4 (15% ethyl acetate/pet. ether); mp: 168–170 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 3.80 (s, 3H), 3.82 (s, 3H), 6.84 (s, 1H), 6.91 (d, J = 8.7 Hz, 1H), 7.03–7.05 (m, 2H), 7.35 (d, J = 8.8 Hz, 1H), 7.56–7.59 (m, 2H), 9.20 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 55.6 (q), 56.1 (q), 102.8 (d), 112.3 (s), 113.0 (d), 113.2 (d), 113.4 (d), 118.9 (d), 127.9 (s), 129.9 (s), 132.1 (d), 133.4 (s), 134.4 (d), 135.6 (s), 154.8 (s), 156.5 (s), 185.0 (s) ppm; HRMS (ESI+): calcd. for $C_{17}H_{14}O_3NBrH^+$ = 360.0230, found 360.0234.

(5-Methoxy-1*H*-Indol-2-yl)(naphthalen-1-yl)methanone (2p)[7]:-



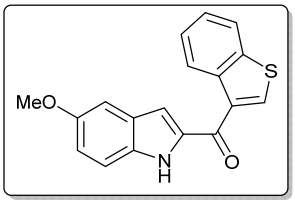
Brown solid; 73% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.82 (s, 3H), 6.87 (s, 1H), 7.01 (s, 1H), 7.06 (dd, J = 1.9, 8.9 Hz, 1H), 7.40 (d, J = 9.0 Hz, 1H), 7.52–7.57 (m, 3H), 7.87 (d, J = 7.1 Hz, 1H), 7.92–7.94 (m, 1H), 8.04 (d, J = 8.3 Hz, 1H), 8.27–8.28 (m, 1H), 9.54 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 55.6 (q), 102.8 (d), 113.2 (d), 113.3 (d), 118.7 (d), 124.3 (d), 125.5 (d), 126.5 (d), 127.3 (d), 127.7 (d), 127.9 (s), 128.4 (d), 130.8 (s), 131.5 (d), 133.5 (s), 133.8 (s), 135.7 (s), 136.4 (s), 154.8 (s), 188.5 (s) ppm.

(5-Methoxy-1*H*-Indol-2-yl)(2-methoxy-4-methylphenyl)methanone (2q):-



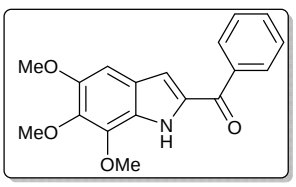
Grey solid; 64% Yield; R_f 0.3 (15% ethyl acetate/pet. ether); mp: 94–95 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.43 (s, 3H), 3.82 (s, 6H), 6.83–6.85 (m, 3H), 7.01–7.03 (m, 2H), 7.34 (d, J = 9.7 Hz, 1H), 7.42 (d, J = 7.5 Hz, 1H), 9.17 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 21.9 (q), 55.7 (q), 55.8 (q), 102.8 (d), 112.2 (d), 112.5 (d), 113.1 (d), 118.1 (d), 120.6 (d), 125.4 (s), 128.0 (s), 130.0 (d), 133.1 (s), 136.4 (s), 142.8 (s), 154.7 (s), 157.6 (s), 186.8 (s) ppm; HRMS (ESI+): calcd. for $C_{18}H_{17}O_3NNa$ = 318.1101, found 318.1101.

Benzo[b]thiophen-3-yl(5-methoxy-1*H*-Indol-2-yl)methanone (2r):-



Light yellow solid; 52% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); mp: 198–199 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.85 (s, 3H), 7.06 (dd, J = 2.4, 8.9 Hz, 1H), 7.10 (br d, J = 1.8 Hz, 1H), 7.15 (br d, J = 1.3 Hz, 1H), 7.39 (d, J = 8.9 Hz, 1H), 7.46 (br t, J = 7.5 Hz, 1H), 7.51(br t, J = 7.6 Hz, 1H), 7.93 (d, J = 7.9 Hz, 1H), 8.33 (s, 1H), 8.47 (d, J = 8.1 Hz, 1H), 9.27 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 55.7 (q), 102.8 (d), 111.1 (d), 113.1 (d), 118.3 (d), 122.4 (d), 124.7 (d), 125.5 (d), 125.6 (d), 128.0 (s), 133.0 (s), 134.7 (s), 135.2 (d), 135.9 (s), 137.3 (s), 140.0 (s), 154.9 (s), 180.0 (s) ppm; HRMS (ESI+): calcd. for $C_{18}H_{13}O_2NSH^+$ = 308.0740, found 308.0741.

Phenyl(5,6,7-trimethoxy-1*H*-Indol-2-yl)methanone (2s)[8]**:-**

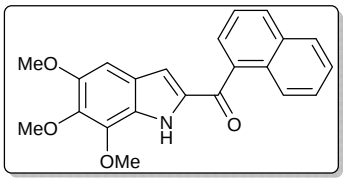


Light yellow solid; 72% Yield; R_f 0.3 (15% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 3.89 (s, 3H), 3.94 (s, 3H), 4.08 (s, 3H), 6.82 (s, 1H), 7.03 (d, J = 2.1 Hz, 1H), 7.50 (d, J = 7.5 Hz, 1H), 7.52 (d, J = 7.7 Hz, 1H), 7.58–7.61 (m, 1H), 7.94 (d, J = 7.4 Hz, 2H), 9.29 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 56.2 (q), 61.1 (q), 61.5 (q), 98.0 (d), 112.8 (d), 123.4 (s), 127.6 (s),

[8] M. Arthuis, R. Pontikis, G. G. Chabot, L. Quentin, D. Scherman and J.-C. Florent, *Eur. J. Med. Chem.*, 2011, **46**, 95.

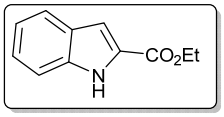
128.4 (d, 2C), 129.1 (d, 2C), 132.1 (d), 134.2 (s), 138.2 (s), 138.9 (s), 141.6 (s), 150.4 (s), 186.4 (s) ppm.

Naphthalen-1-yl(5,6,7-trimethoxy-1*H*-Indol-2-yl)methanone (2t):-



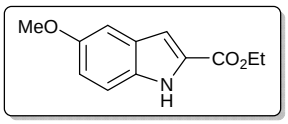
Yellow solid; 79% Yield; R_f 0.4 (20% ethyl acetate/pet. ether); mp: 148–149 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 3.85 (s, 3H), 3.95 (s, 3H), 4.10 (s, 3H), 6.75 (s, 1H), 6.82 (d, J = 2.2 Hz, 1H), 7.52–7.56 (m, 3H), 7.83 (br d, J = 7.1 Hz, 1H), 7.91–7.93 (m, 1H), 8.02 (d, J = 8.2 Hz, 1H), 8.23–8.26 (m, 1H), 9.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 56.2 (q), 61.2 (q), 61.5 (q), 98.0 (d), 113.7 (d), 123.2 (s), 124.3 (d), 125.5 (d), 126.5 (d), 127.2 (d), 127.5 (d), 128.0 (s), 128.3 (d), 130.8 (s), 131.3 (d), 133.7 (s), 135.8 (s, 2C), 138.9 (s), 141.7 (s), 150.4 (s), 187.9 (s) ppm; HRMS (ESI+): calcd. for $C_{22}H_{19}O_4NH^+$ = 362.1387, found 362.1390.

Ethyl 1*H*-Indole-2-carboxylate (5a)[9]:



Brown solid; 57% Yield, R_f 0.4 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.42 (t, J = 7.1 Hz, 3H), 4.41 (q, J = 7.0 Hz, 2H), 7.15 (t, J = 7.5 Hz, 1H), 7.23 (s, 1H), 7.32 (t, J = 7.7 Hz, 1H), 7.42 (d, J = 8.3 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 9.0 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 14.4 (q), 61.0 (t), 108.6 (d), 111.8 (d), 120.8 (d), 122.6 (d), 125.3 (d), 127.5 (s, 2C), 136.8 (s), 162.0 (s) ppm.

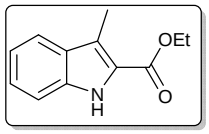
Ethyl 5-methoxy-1*H*-Indole-2-carboxylate (5b):-



Brown solid; 67% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.41 (t, J = 7.1 Hz, 3H), 3.84 (s, 3H), 4.40 (q, J = 7.1 Hz, 2H), 6.99 (dd, J = 2.3, 9.0 Hz, 1H), 7.07 (d, J = 1.5 Hz, 1H), 7.14 (s, 1H), 7.31 (d, J = 9.0 Hz, 1H), 8.90 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 14.4 (q), 55.7 (q), 61.0 (t), 102.5 (d), 108.2 (d), 112.7 (d), 116.9 (d), 127.8 (s), 127.9 (s), 132.1 (s), 154.7 (s), 161.9 (s) ppm; HRMS (ESI+): calcd. for $C_{12}H_{13}O_3NNa$ = 242.0788, found 242.0788.

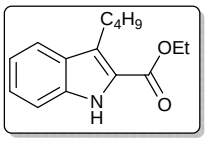
[9] Q. Cai, Z. Li, J. Wei, C. Ha, D. Pei and K. Ding, *Chem. Commun.*, 2009, 7581.

Ethyl 3-methyl-1*H*-Indole-2-carboxylate (5c)[9]:-



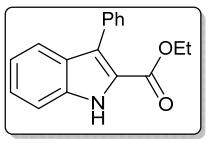
Light yellow solid; 74% Yield; R_f 0.3 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.43 (t, J = 7.1 Hz, 3H), 2.61 (s, 3H), 4.42 (q, J = 7.1 Hz, 2H), 7.14 (t, J = 7.4 Hz, 1H), 7.32 (t, J = 7.5 Hz, 1H), 7.36 (d, J = 8.2 Hz, 1H), 7.66 (d, J = 8.1 Hz, 1H), 8.72 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 9.9 (q), 14.5 (q), 60.7 (t), 111.6 (d), 119.9 (d), 120.2 (s), 120.8 (d), 123.4 (s), 125.5 (d), 128.5 (s), 135.8 (s), 162.7 (s) ppm.

Ethyl 3-butyl-1*H*-Indole-2-carboxylate (5d):-



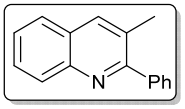
Off white solid; 59% Yield; R_f 0.4 (15% ethyl acetate/pet. ether); mp: 71–74 °C; ^{1}H NMR (500 MHz, $CDCl_3$): δ 0.94 (t, J = 7.3 Hz, 3H), 1.39–1.44 (m, 5H), 1.63–1.69 (m, 2H), 3.10 (t, J = 7.7 Hz, 2H), 4.41 (q, J = 7.1 Hz, 2H), 7.13 (t, J = 7.5 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.37 (d, J = 8.24 Hz, 1H), 7.68 (d, J = 8.24 Hz, 1H), 8.73 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 14.0 (q), 14.4 (q), 22.8 (t), 24.5 (t), 33.2 (t), 60.6 (t), 111.7 (d), 119.8 (d), 120.9 (d), 123.0 (s), 125.4 (d and s), 128.1 (s), 135.9 (s), 162.5 (s) ppm; HRMS (ESI+): calcd. for $C_{15}H_{19}O_2NH^+$ = 246.1489, found 246.1491.

Ethyl 3-phenyl-1*H*-Indole-2-carboxylate (5e):-



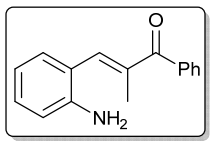
Yellow solid; 61% Yield; R_f 0.4 (15% ethyl acetate/pet. ether); mp: 137–139 °C; ^{1}H NMR (200 MHz, $CDCl_3$): δ 1.23 (t, J = 7.1 Hz, 3H), 4.29 (q, J = 7.1 Hz, 2H), 7.11–7.18 (m, 1H), 7.32–7.49 (m, 5H), 7.52–7.58 (m, 2H), 7.63 (d, J = 8.3 Hz, 1H), 9.01 (s, 1H); ^{13}C NMR (50 MHz, $CDCl_3$): δ 14.0 (q), 60.9 (t), 111.7 (d), 120.9 (d), 121.8 (d), 122.8 (s), 124.3 (s), 125.8 (d), 127.2 (d), 127.7 (d, 2C), 127.9 (s), 130.6 (d, 2C), 133.5 (s), 135.7 (s), 162.0 (s) ppm; HRMS (ESI+): calcd. for $C_{17}H_{15}O_2NNa$ = 288.0995, found 288.0997.

3-Methyl-2-phenylquinoline (3u)[10]:-



Colorless oil; 29% Yield; R_f 0.4 (10% ethyl acetate/pet. ether); ^{1}H NMR (500 MHz, $CDCl_3$): δ 2.46 (s, 3H), 7.41–7.53 (m, 4H), 7.58–7.60 (m, 2H), 7.63–7.68 (m, 1H), 7.77 (d, J = 8.2 Hz, 1H), 8.01 (s, 1H), 8.13 (d, J = 8.5 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 20.6 (q), 126.4 (d), 126.7 (d), 127.6 (s), 128.2 (d), 128.3 (d, 2C), 128.7 (d), 128.8 (d, 2C), 129.2 (s), 129.3 (d), 136.7 (d), 140.8 (s), 146.6 (s), 160.5 (s) ppm.

(*E*)-3-(2-Aminophenyl)-2-methyl-1-phenylprop-2-en-1-one (7):-

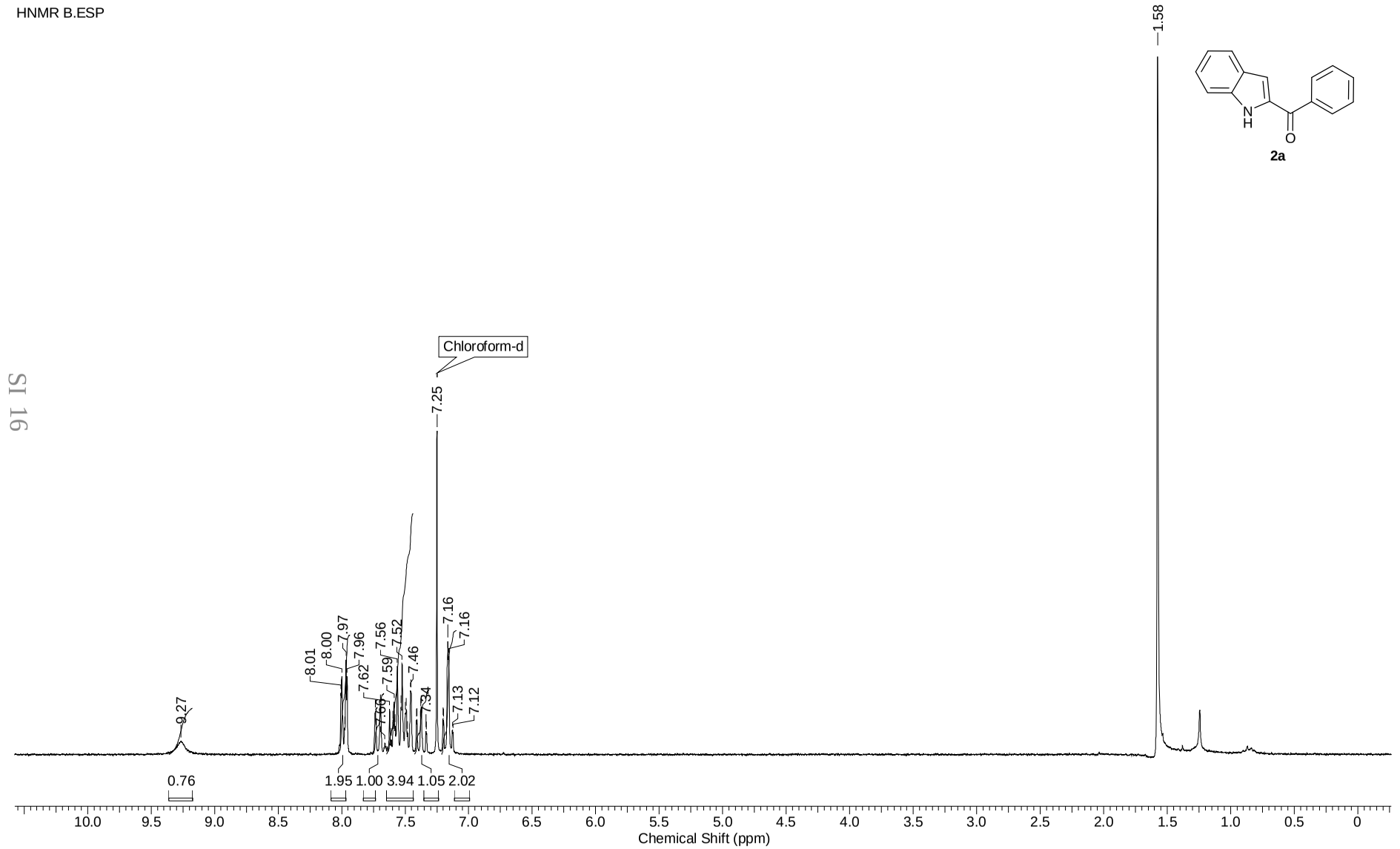


Yellow Liquid; 42% Yield; R_f 0.2 (15% ethyl acetate/pet. ether); ^{1}H NMR (200 MHz, $CDCl_3$): δ 2.16 (d, J = 1.4 Hz, 3H), 3.63 (s, 2H), 6.71 (dd, J = 0.9, 8.1 Hz, 1H), 6.81 (dt, J = 0.9, 7.6 Hz, 1H), 7.09–7.25 (m, 3H), 7.40–7.54 (m, 3H), 7.73–7.77 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 14.4 (q), 115.7 (d), 118.3 (d), 121.2 (s), 128.2 (d, 2C), 129.4 (d, 2C), 129.6 (d), 129.7 (d), 131.8 (d), 138.1 (s), 138.2 (d), 138.5 (s), 144.3 (s), 199.2 (s) ppm.

[10] I. Hyodo, M. Tobisu and N. Chatani, *Chem. Asian J.*, 2012, **7**, 1357.

Acquisition Time (sec)	7.9167	***Comment***	yogesh	***Date***	18/06/2013 05:27:24		
File Name	F:\yogesh\Indole metho\NMR\ym-936\HNMR B.ESP			***Frequency (MHz)***	200.13	***Nucleus*** 1H	***Original Points Count*** 32768
Points Count	32768	***Spectrum Offset (Hz)***	1225.1484	***Sweep Width (Hz)***	4139.07	***Temperature (degree C)*** 0.000	

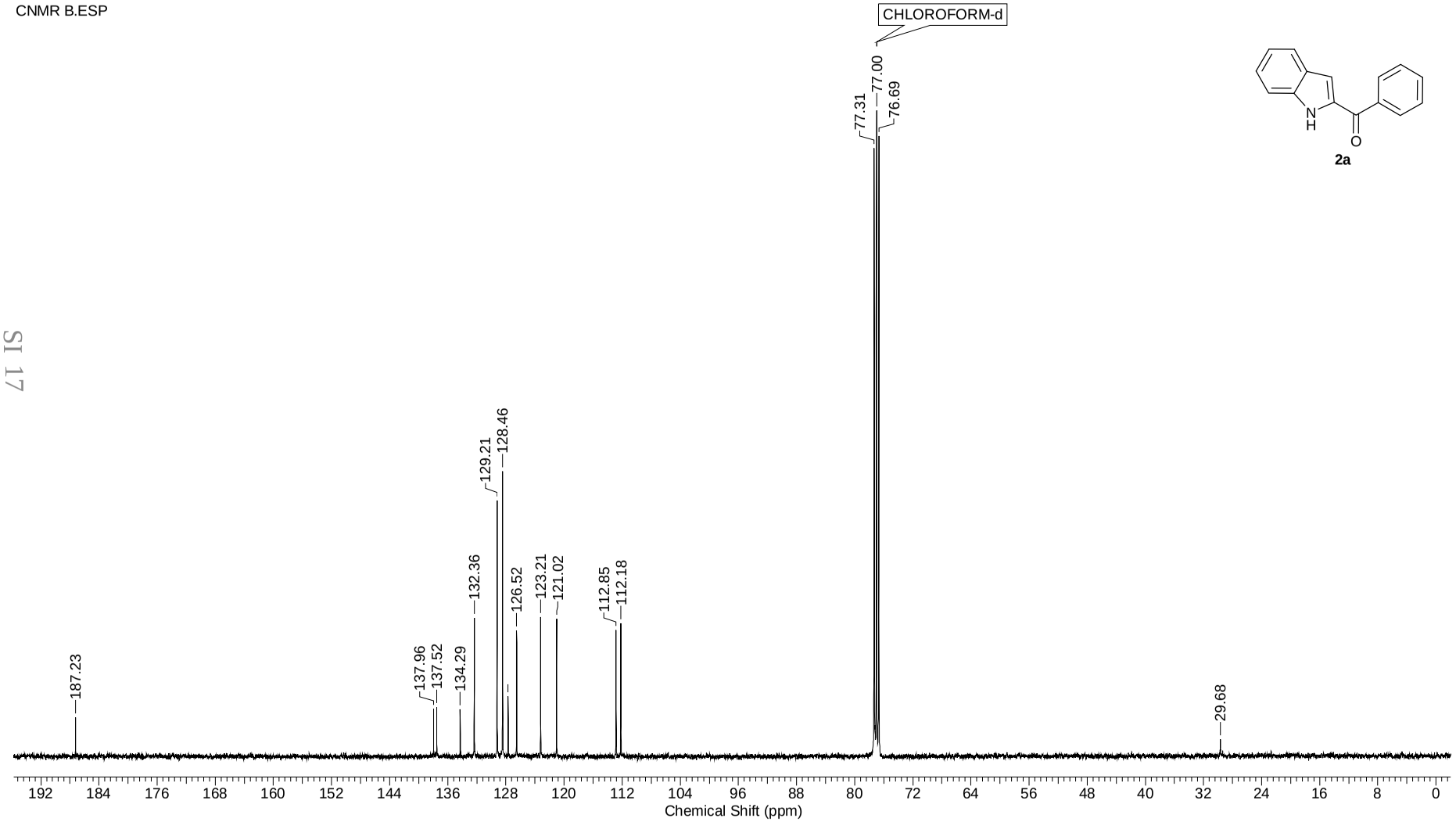
HNMR B.ESP



2a

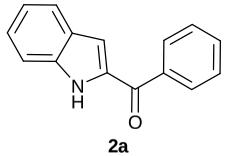
Acquisition Time (sec)	1.0434	***Comment***	yogesh	***Date***	20 Jun 2013 02:58:30		
Date Stamp	20 Jun 2013 02:05:46			***File Name***	\\agni\nmr_data\JEOL_400\2013\June 2013\Wed4ECX400#053_CARBON-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	1200	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	single_pulse_dec
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10040.2900
Spectrum Type	STANDARD	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	19.200		

CNMR B.ESP



Acquisition Time (sec)	1.0434	***Comment***	yogesh	***Date***	20 Jun 2013 02:58:30		
Date Stamp	20 Jun 2013 02:37:03			***File Name***	\\agni\nmr_data\JEOL_400\2013\June 2013\Wed4ECX400#053_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	800	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	dept.ex2 (selection_angle=135)
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10040.0273
Spectrum Type	DEPT135	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	19.100		

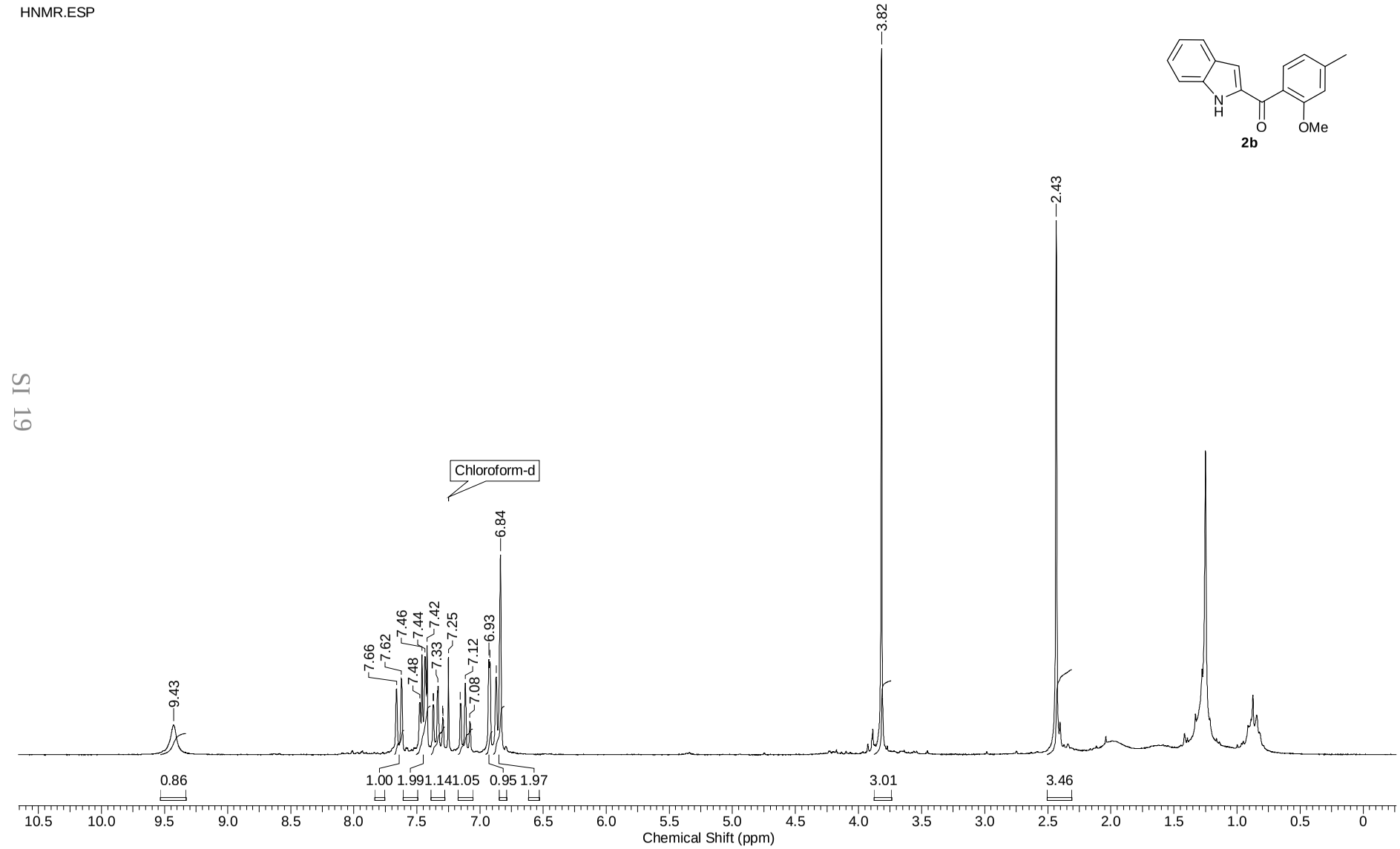
DEPT B.ESP



2a

Acquisition Time (sec)	7.9167	***Comment***	Yogesh	***Date***	12/07/2013 22:57:18		
File Name	F:\yogesh\Indole metho\NMR\ym-953\HNMR.ESP			***Frequency (MHz)***	200.13	***Nucleus*** 1H	***Original Points Count*** 32768
Points Count	32768	***Spectrum Offset (Hz)***	1225.4011	***Sweep Width (Hz)***	4139.07	***Temperature (degree C)*** 0.000	

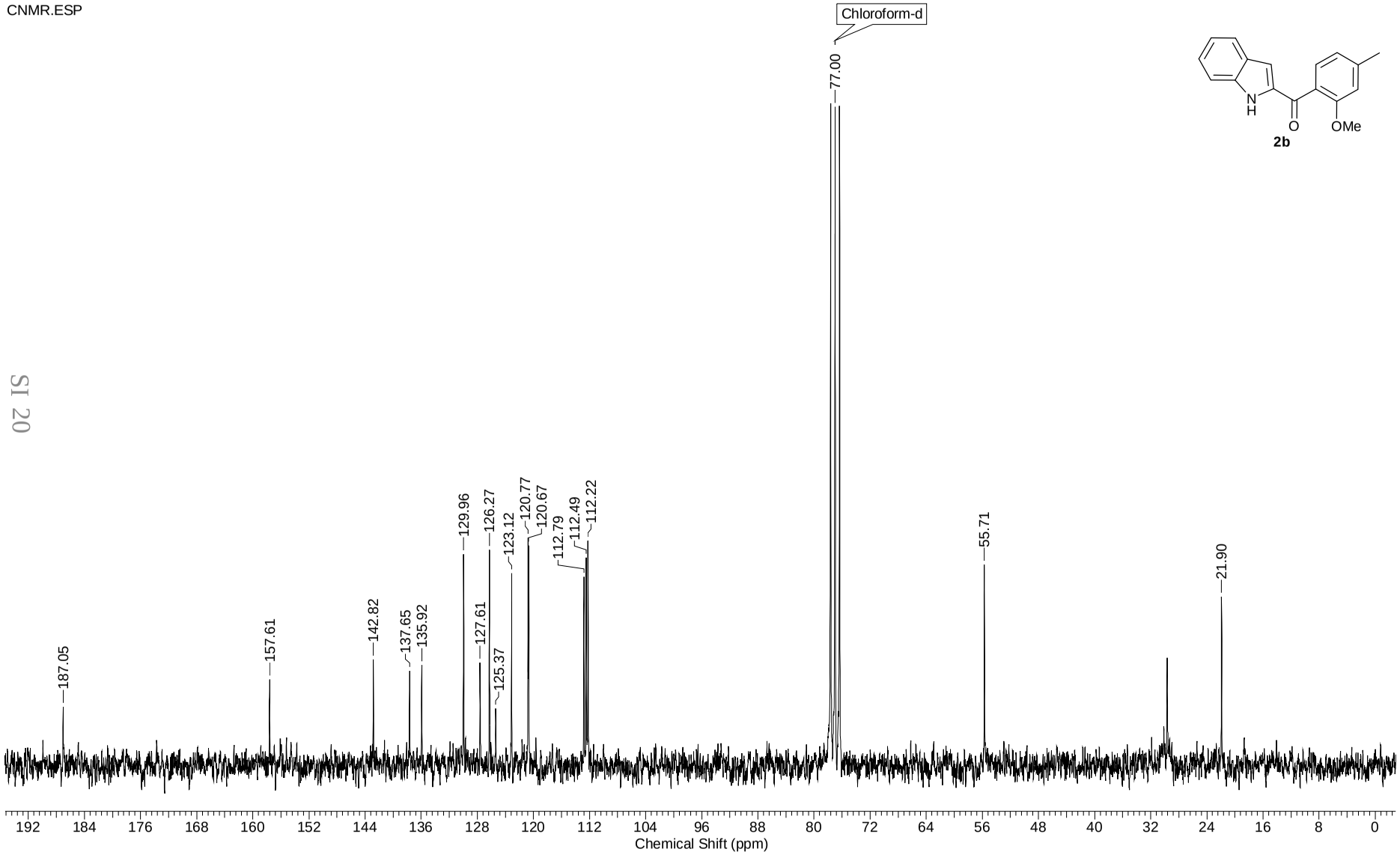
HNMR.ESP



2b

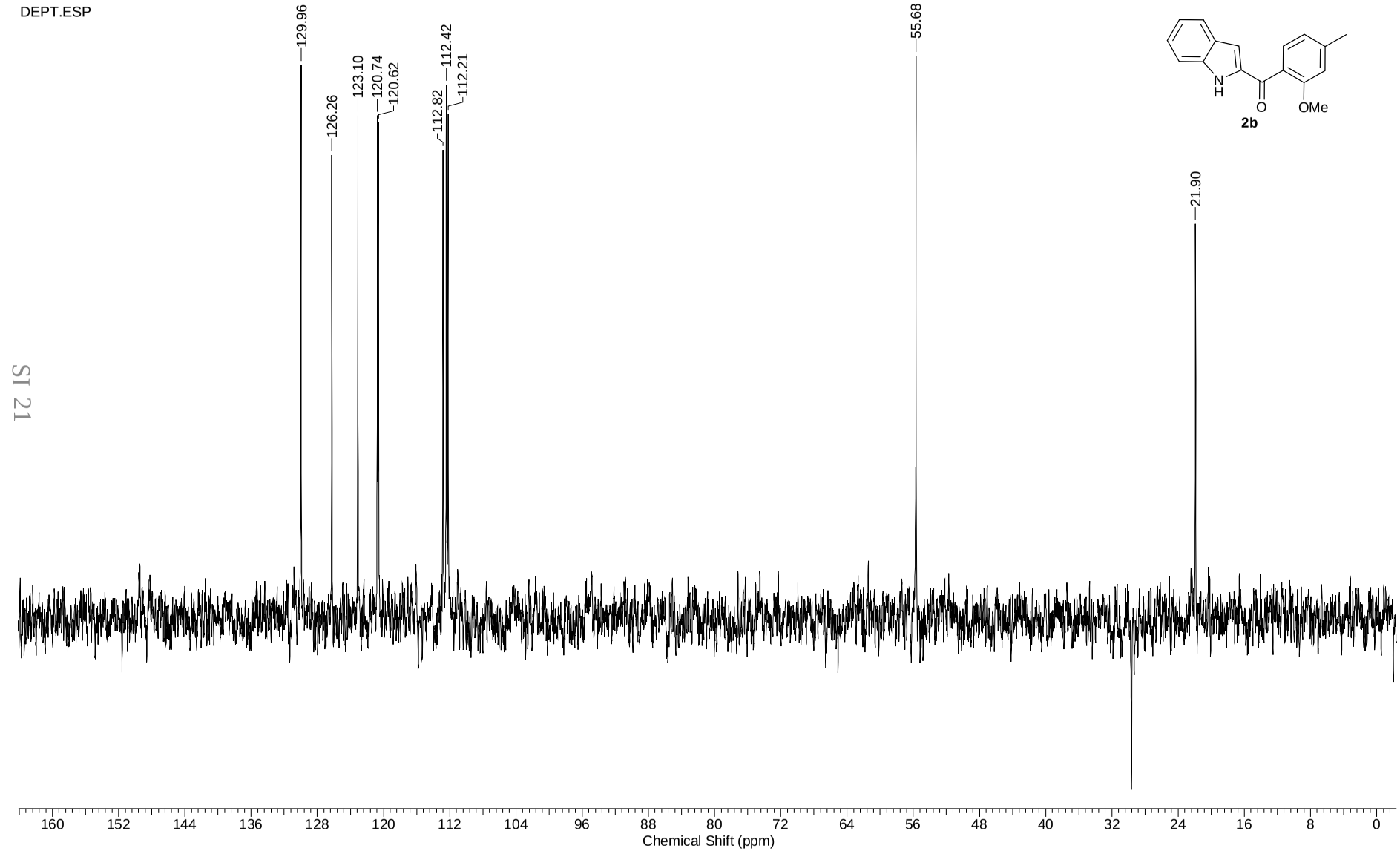
Acquisition Time (sec)	2.7329	***Comment***	yogesh	***Date***	25/07/2013 07:52:42				
File Name	F:\yogesh\Indole metho\NMR\ym-953\CNMR.ESP			***Frequency (MHz)***	50.32	***Nucleus***	13C	***Original Points Count***	32768
Points Count	32768	***Spectrum Offset (Hz)***	5028.8081	***Sweep Width (Hz)***	11990.41	***Temperature (degree C)***	0.000		

CNMR.ESP



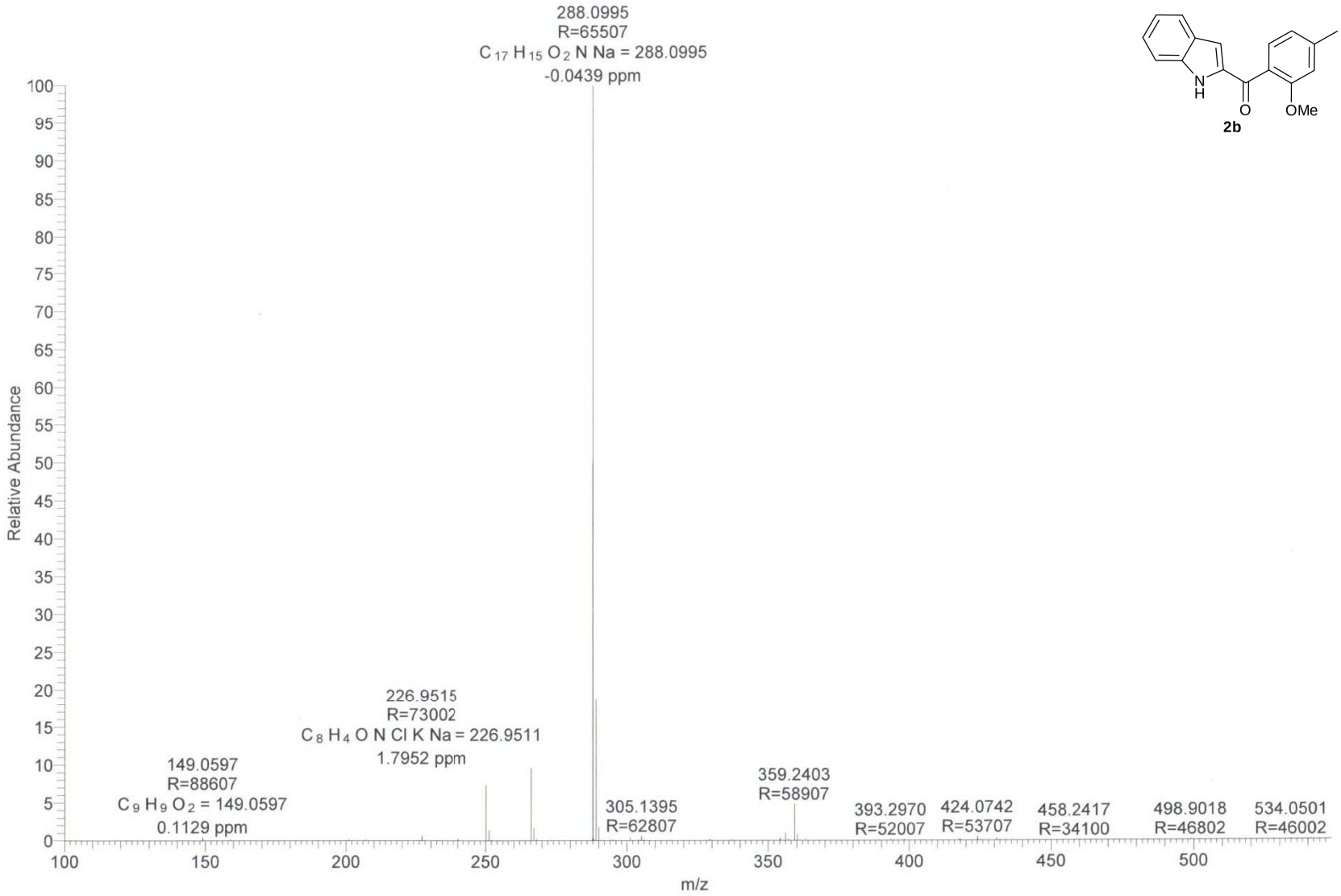
Acquisition Time (sec)	2.7329	***Comment***	yogesh	***Date***	25/07/2013 07:14:56		
File Name	F:\yogesh\Indole metho\NMR\ym-953\DEPT.ESP			***Frequency (MHz)***	50.32	***Nucleus*** 13C	***Original Points Count*** 32768
Points Count	32768	***Spectrum Offset (Hz)***	5027.2090	***Sweep Width (Hz)***	11990.41	***Temperature (degree C)*** 0.000	

DEPT.ESP

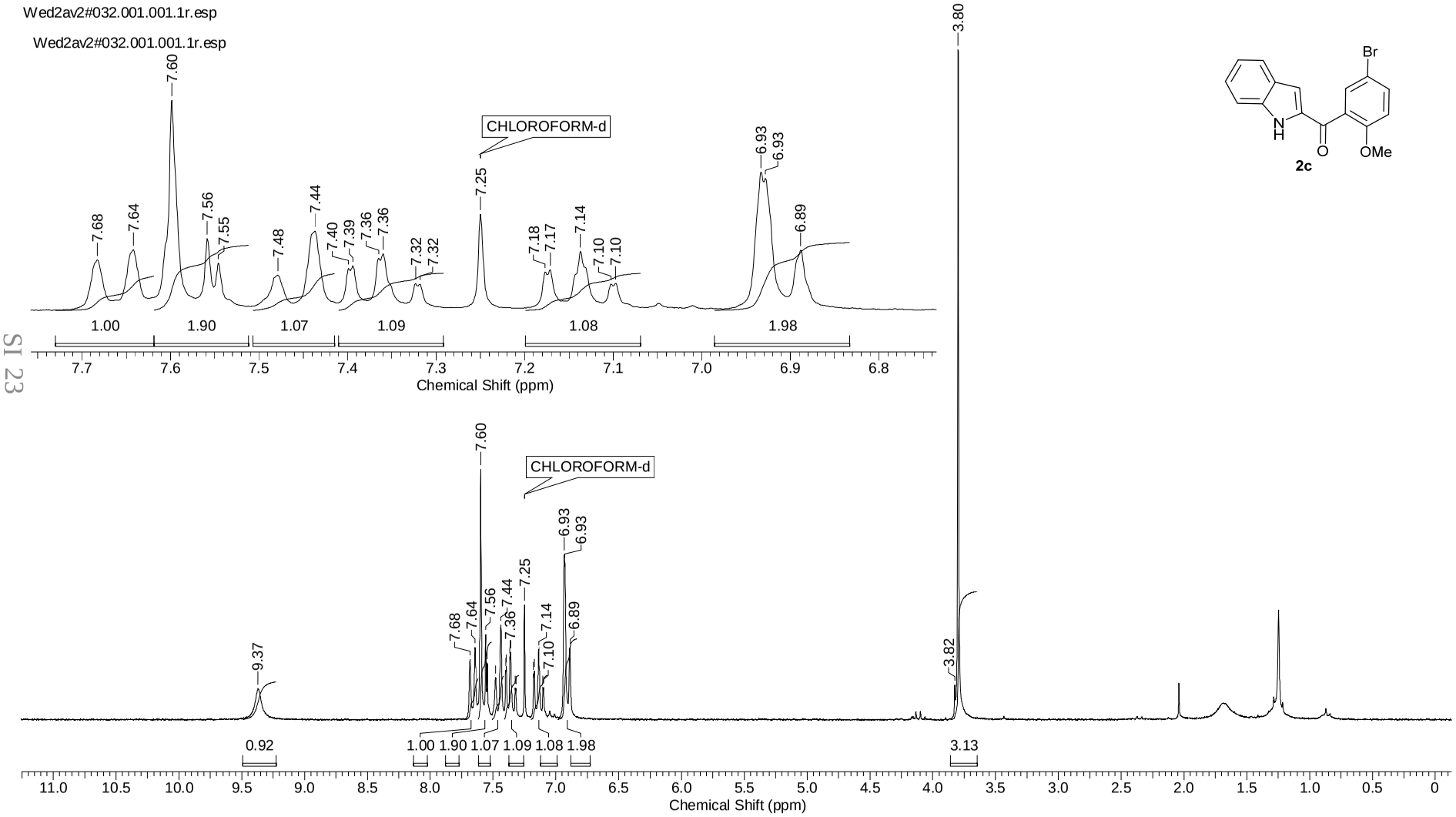


D:\Data\YM-953 9/13/2013 11:07:41 AM

YM-953 #1077 RT: 4.80 AV: 1 NL: 2.36E9
T: FTMS + p ESI Full ms [100.00-700.00]

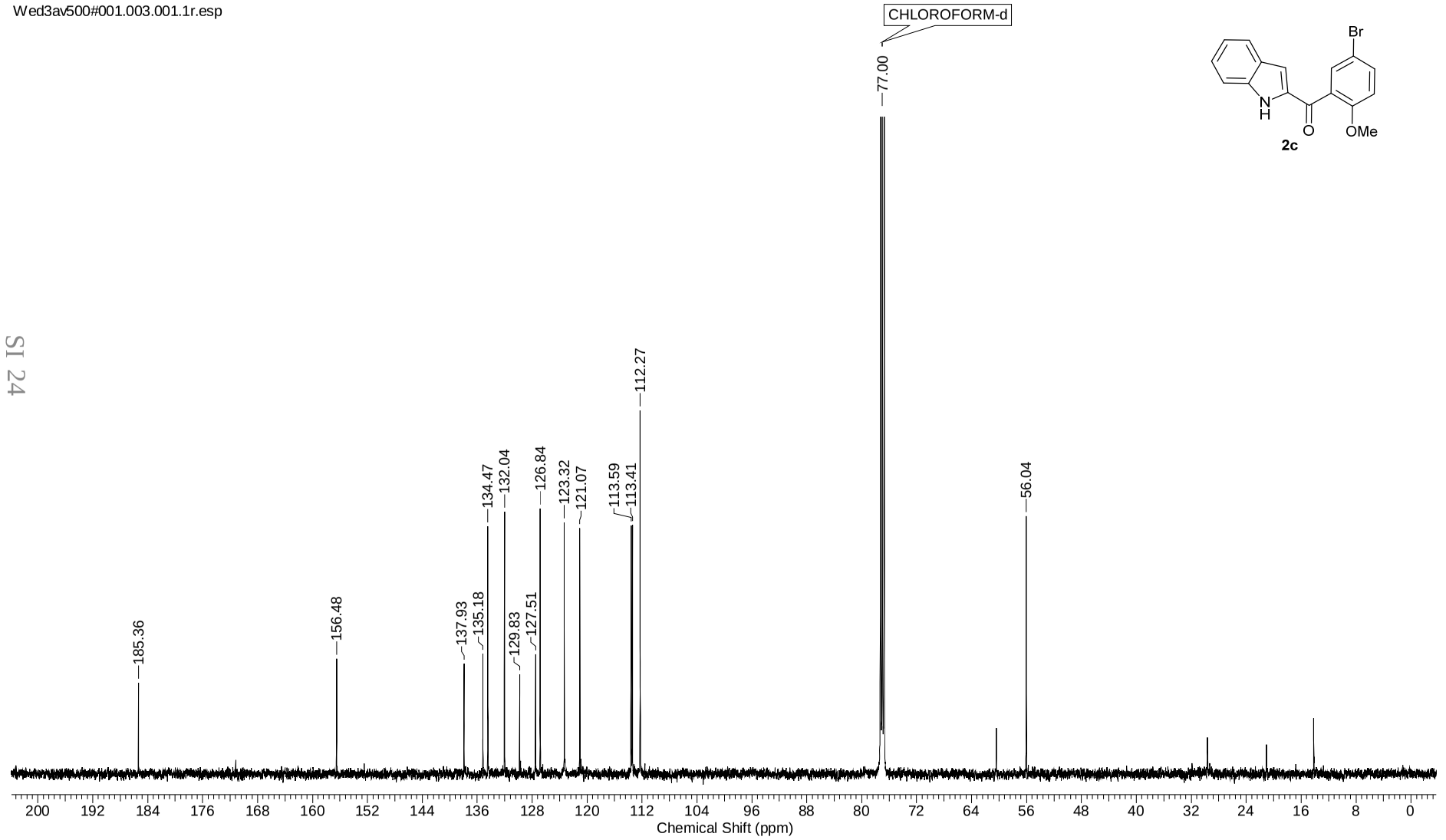


Acquisition Time (sec)	3.9584	***Comment***	yogesh	***Date***	07 Aug 2013 15:26:00		
Date Stamp	07 Aug 2013 15:26:00			***File Name***	\\agni\nmr_data\AV200\AUG_13#AV200\data\Administrator\nmr\Wed2av2#032\1\PDATA\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	av200
Original Points Count	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1149.40	***SW(cyclical) (Hz)***	4139.07	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1225.6606	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4138.95	***Temperature (degree C)***	27.000



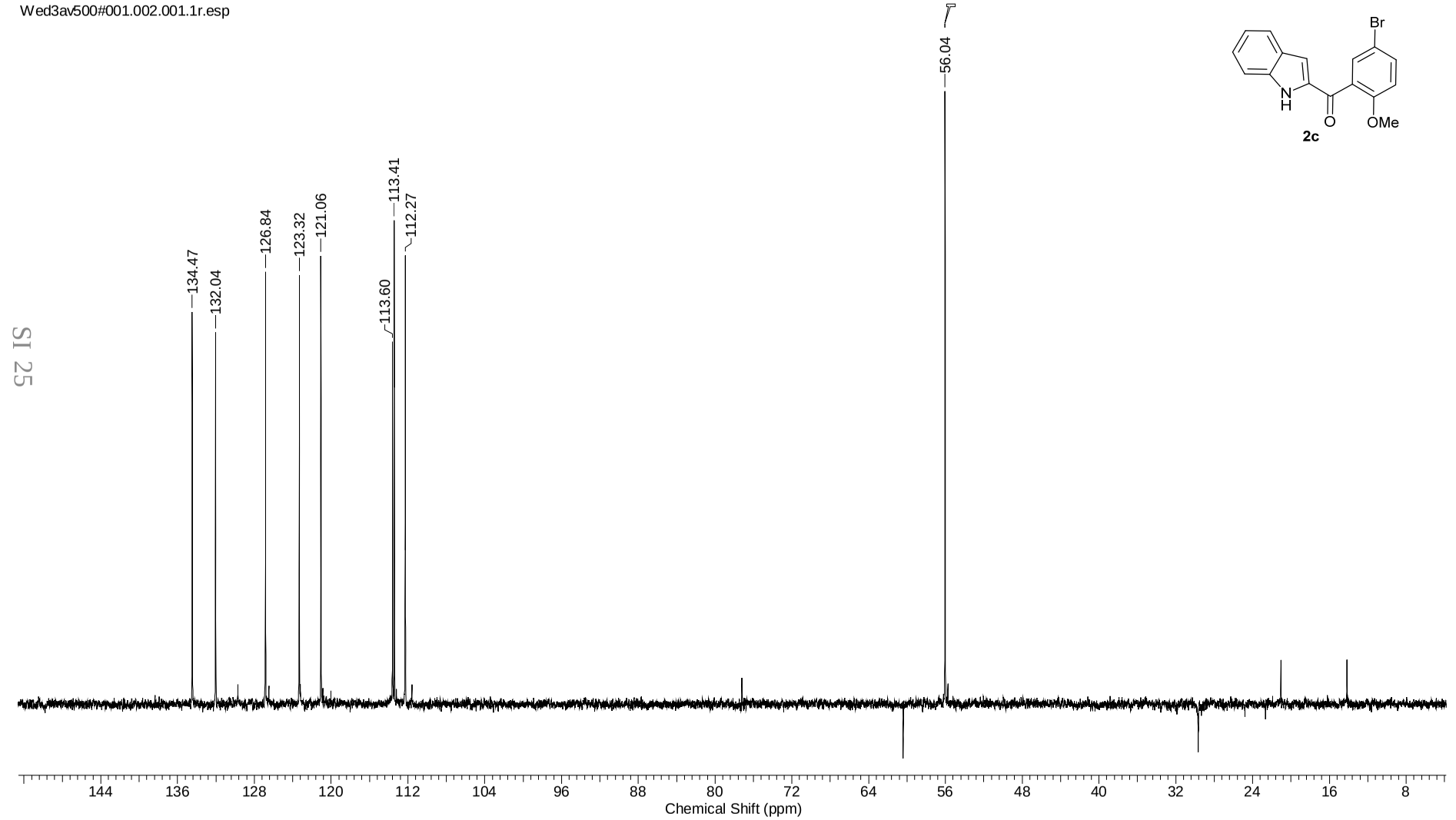
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	14 Aug 2013 10:49:04			***Date Stamp***	14 Aug 2013 10:49:04
File Name	H:\New folder\Wed3av500#001 ym-967\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	635
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11979.3203
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	22.500				

Wed3av500#001.003.001.1r.esp



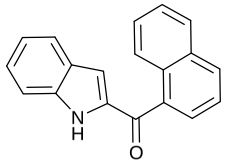
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	14 Aug 2013 10:27:44			***Date Stamp***	14 Aug 2013 10:27:44
File Name	H:\New folder\Wed3av500#001 ym-967\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1000
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12568.3320
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.000				

Wed3av500#001.002.001.1r.esp



Acquisition Time (sec)	1.9923	***Comment***	Yogesh 1H	***Date***	31 Jul 2013 21:45:44				
Date Stamp	31 Jul 2013 21:45:44			***File Name***	\\agni\nmr_data\AV400\July_13_400\Wed5av400#019\1\PDATA\1\1r				
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	456.00	***SW(cyclical) (Hz)***	8223.68
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2456.8567	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43
Temperature (degree C)	23.100								

Wed5av400#019.001.HNMR.1r.esp

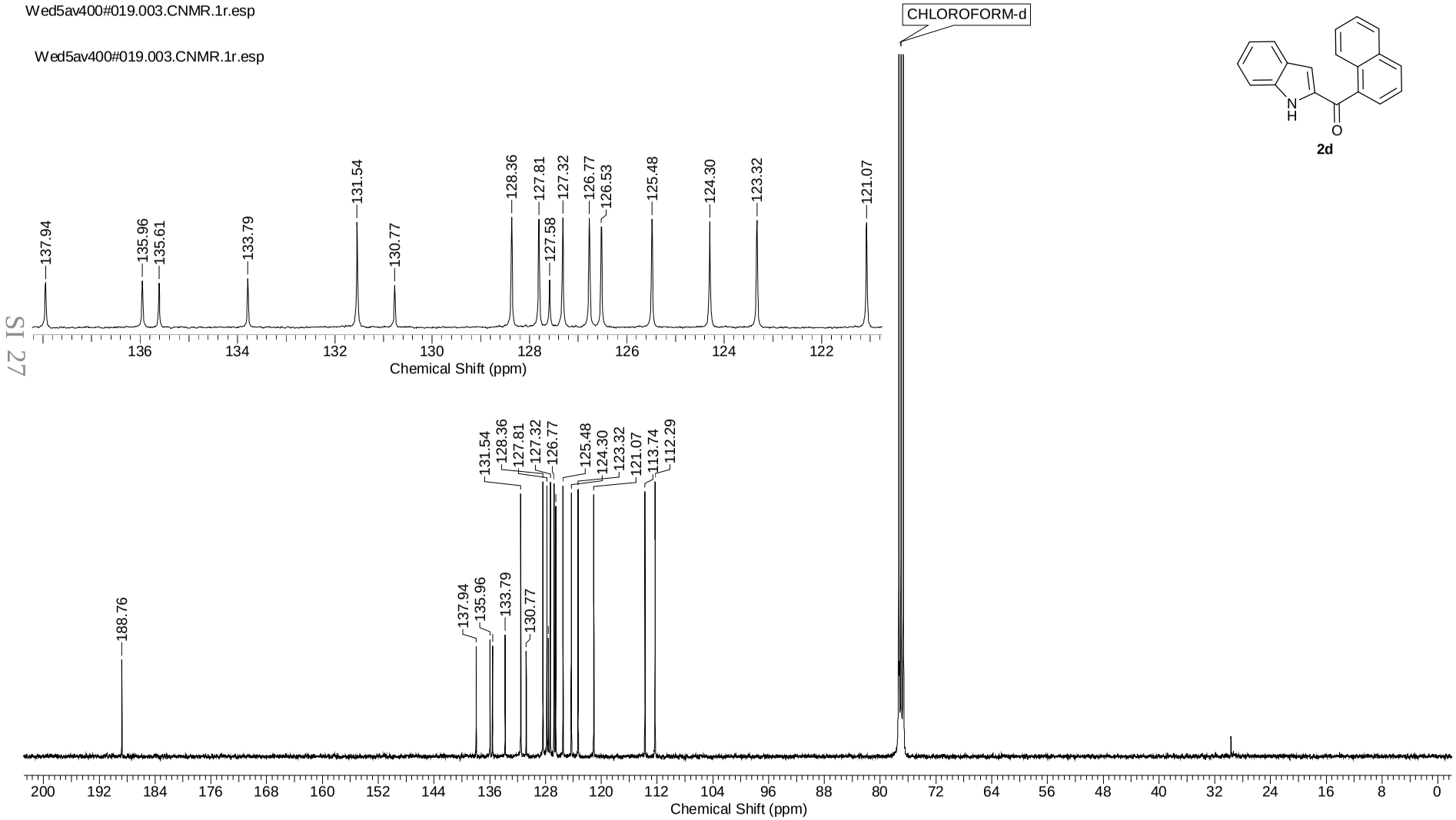


2d

Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	01 Aug 2013 08:55:36				
Date Stamp	01 Aug 2013 08:55:36			***File Name***	\\agni\nmr_data\AV400\July_13_400\Wed5av400#019\3\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	10855	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	9553.9619	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	23.300								

Wed5av400#019.003.CNMR.1r.esp

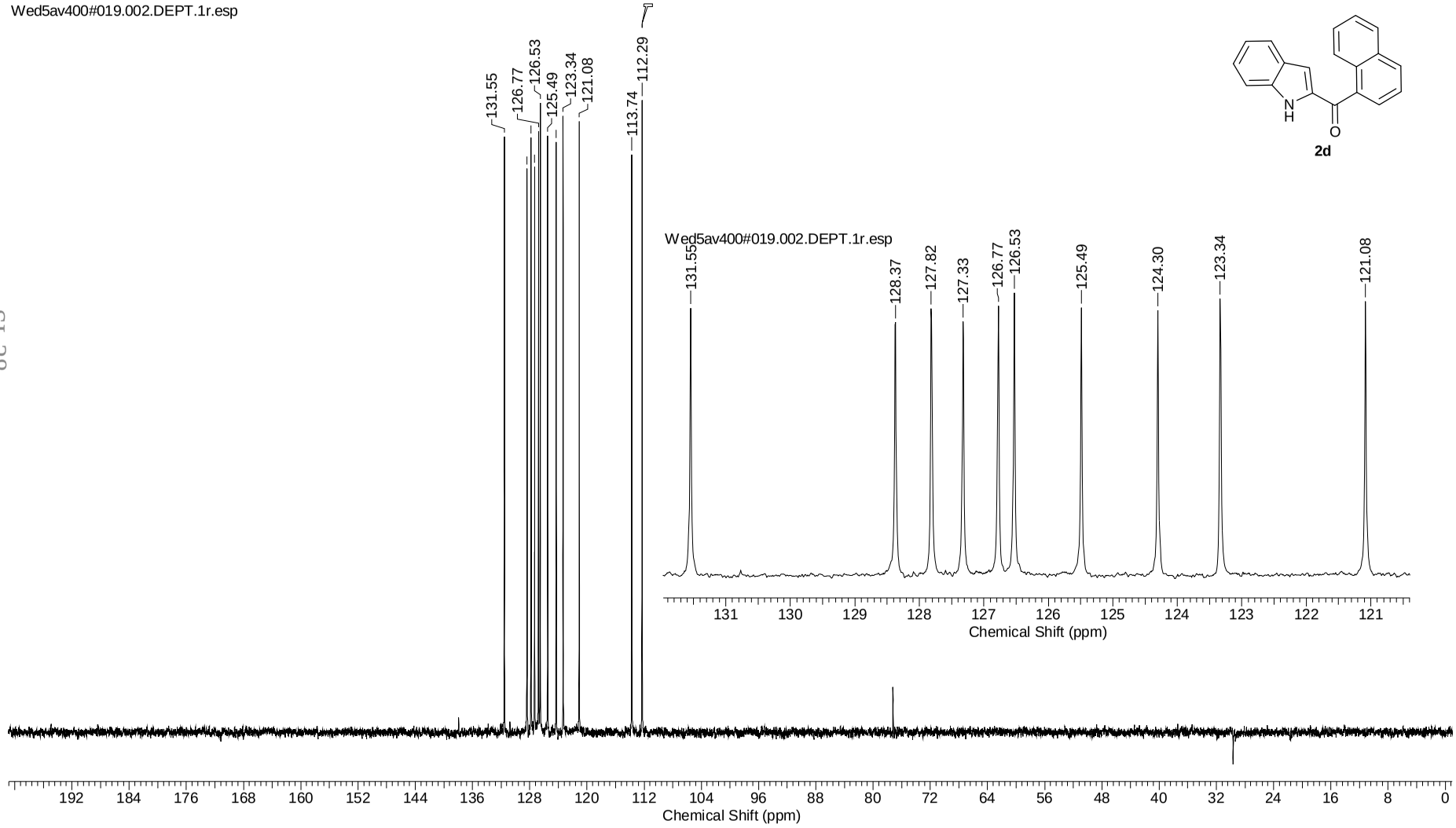
Wed5av400#019.003.CNMR.1r.esp



2d

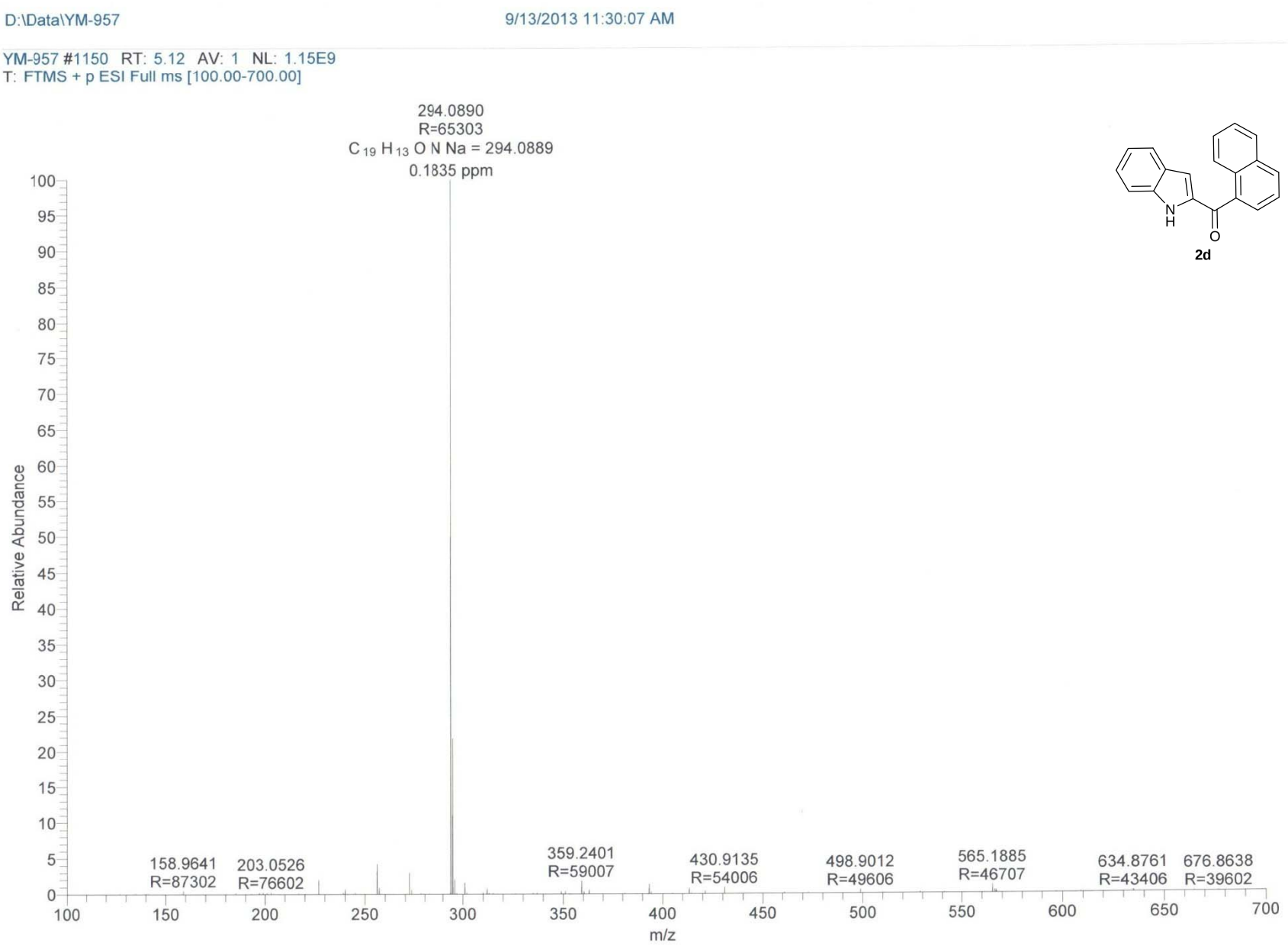
Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	01 Aug 2013 00:44:56				
Date Stamp	01 Aug 2013 00:44:56			***File Name***	\\agni\nmr_data\AV400\July_13_400\Wed5av400#019\2\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	4000	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	16384.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	10056.6826	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	23.200								

Wed5av400#019.002.DEPT.1r.esp

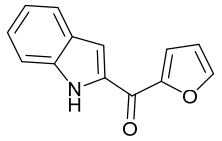


2d

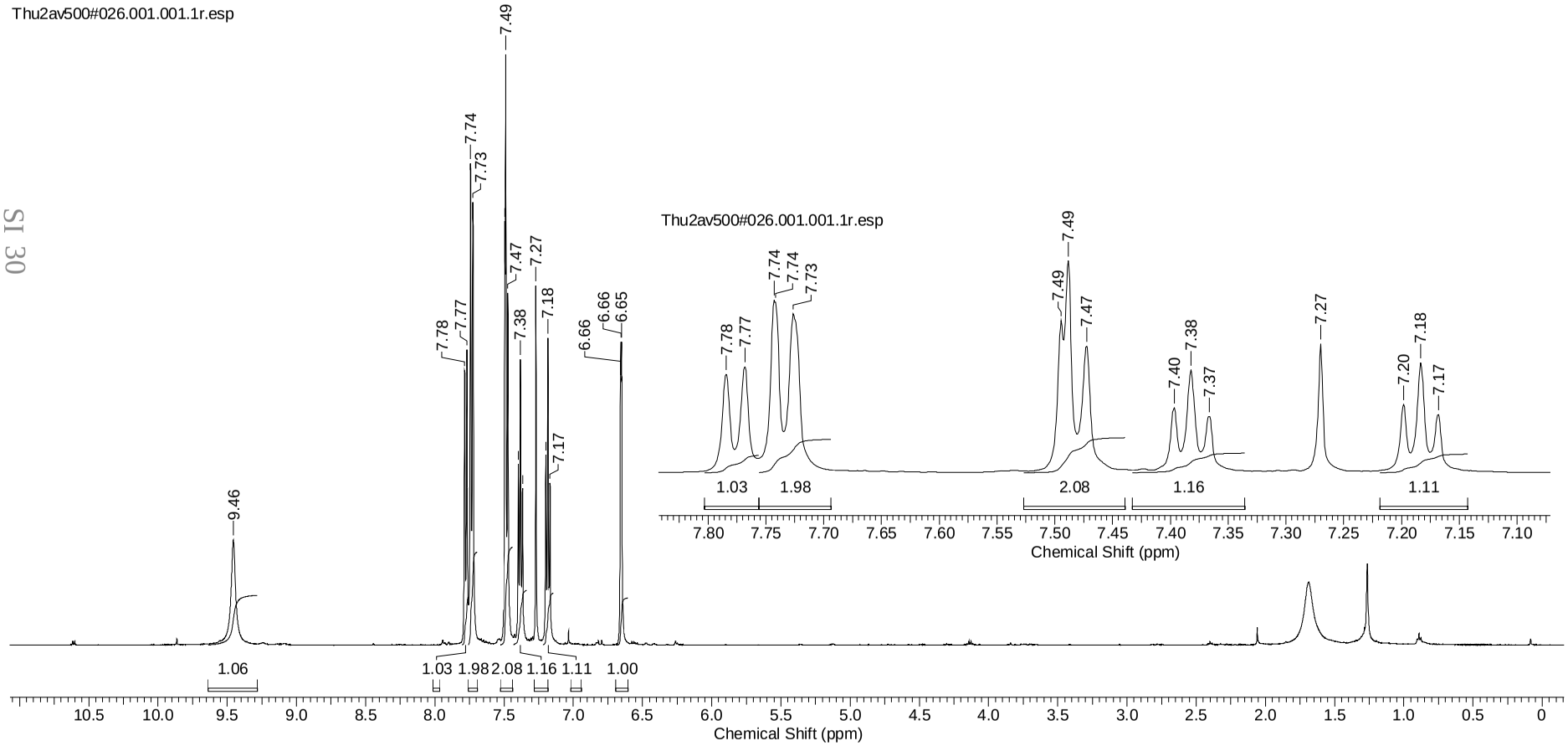
Wed5av400#019.002.DEPT.1r.esp


D:\Data\YM-957
9/13/2013 11:30:07 AM
YM-957 #1150 RT: 5.12 AV: 1 NL: 1.15E9
T: FTMS + p ESI Full ms [100.00-700.00]
294.0890
R=65303
C 19 H 13 O N Na = 294.0889
0.1835 ppm
Relative Abundance
m/z
158.9641 R=87302
203.0526 R=76602
359.2401 R=59007
430.9135 R=54006
498.9012 R=49606
565.1885 R=46707
634.8761 R=43406
676.8638 R=39602
N H
O
2d

Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	08 Aug 2013 23:09:20			***Date Stamp***	08 Aug 2013 23:09:20
File Name	H:\New folder\Thu2av500#026\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	20031	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	256.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.70	***Temperature (degree C)***	21.900				

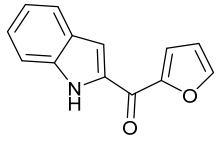


2e



Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	09 Aug 2013 09:40:48			***Date Stamp***	09 Aug 2013 09:40:48
File Name	H:\New folder\Thu2av500#026\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	9471
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	22.400				

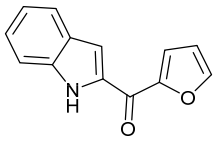
Thu2av500#026.003.001.1r.esp



2e

Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	09 Aug 2013 01:30:08			***Date Stamp***	09 Aug 2013 01:30:08
File Name	H:\New folder\Thu2av500#026\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	3200
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.5576
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.100				

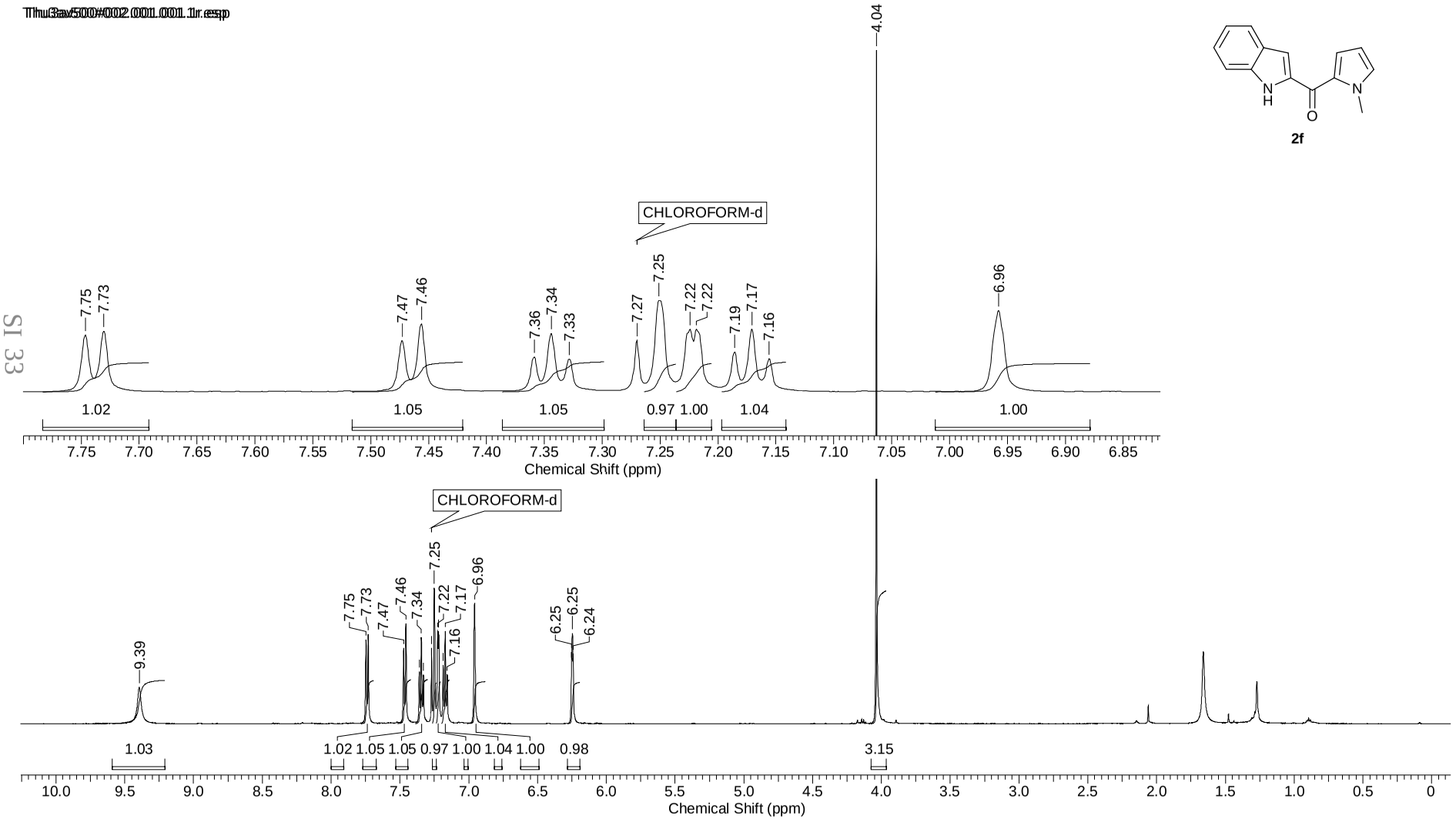
Thu2av500#026.002.001.1r.esp



2e

Acquisition Time (sec)	2.0031	***Comment***	yogesh 1H	***Date***	19 Sep 2013 12:44:16				
Date Stamp	19 Sep 2013 12:44:16			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Thu3av500#002\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	287.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	23.000								

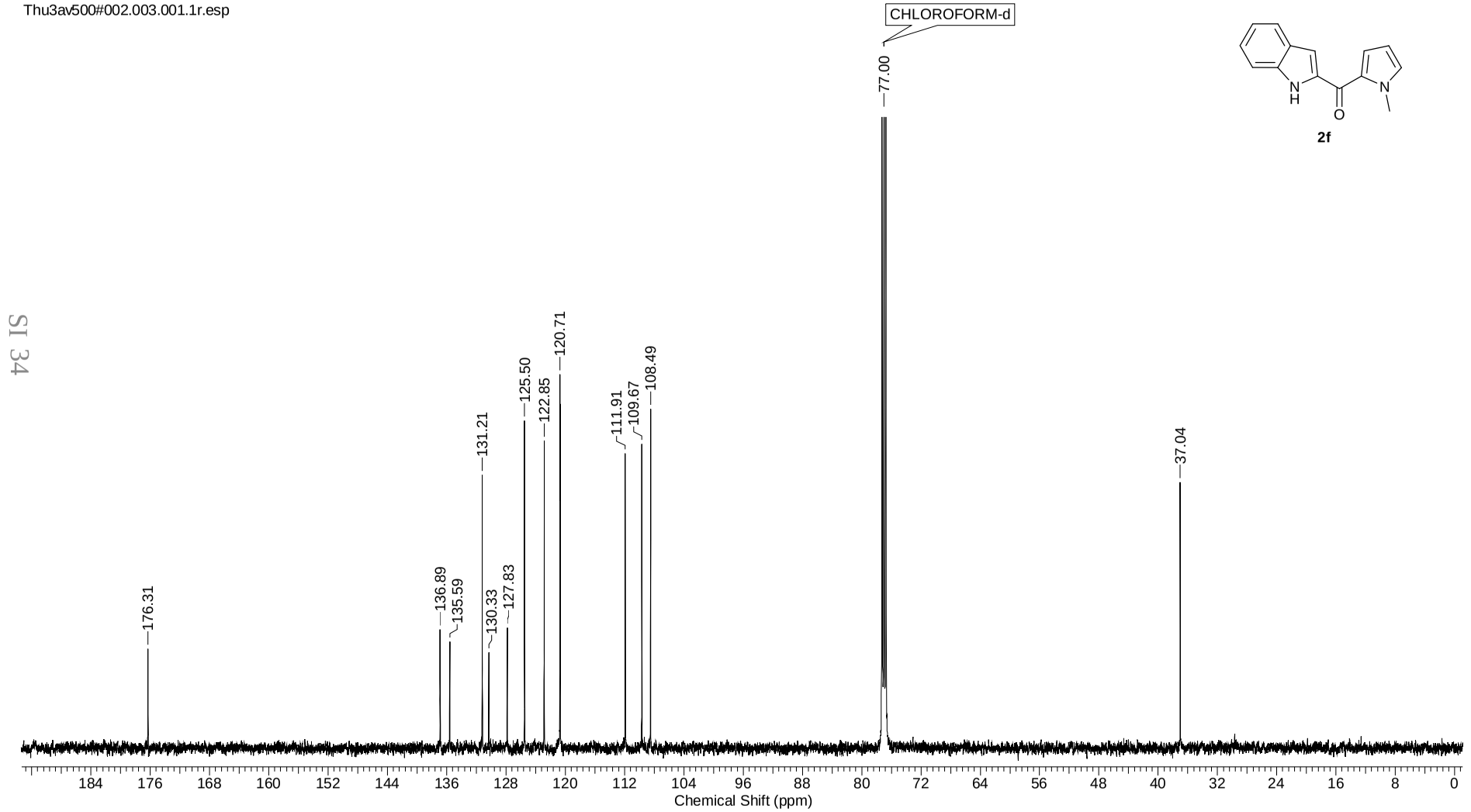
Thu3av500#002 001.001.1r.esp



2f

Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	19 Sep 2013 13:39:44				
Date Stamp	19 Sep 2013 13:39:44			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Thu3av500#002\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1175	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	23.900								

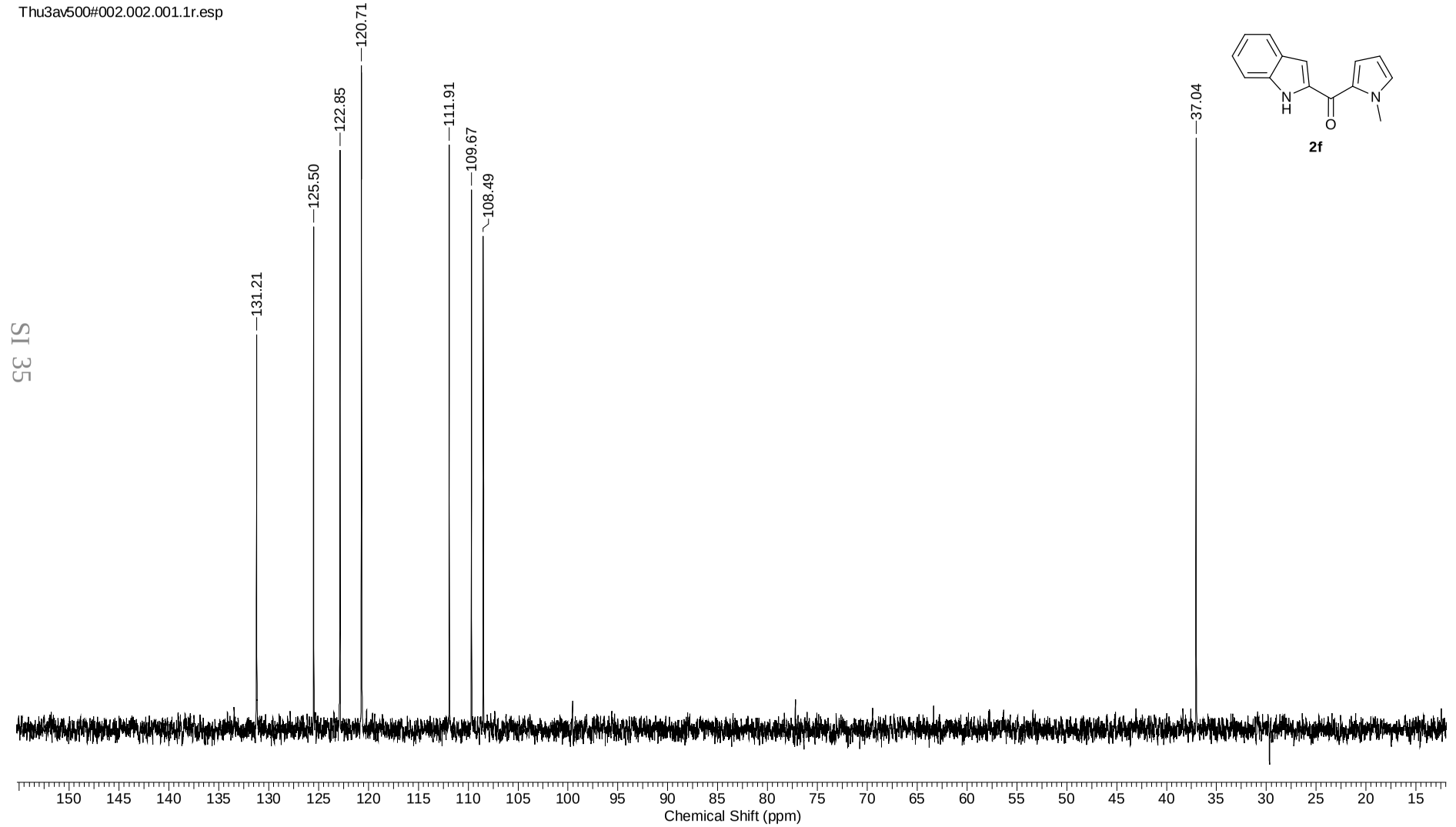
Thu3av500#002.003.001.1r.esp

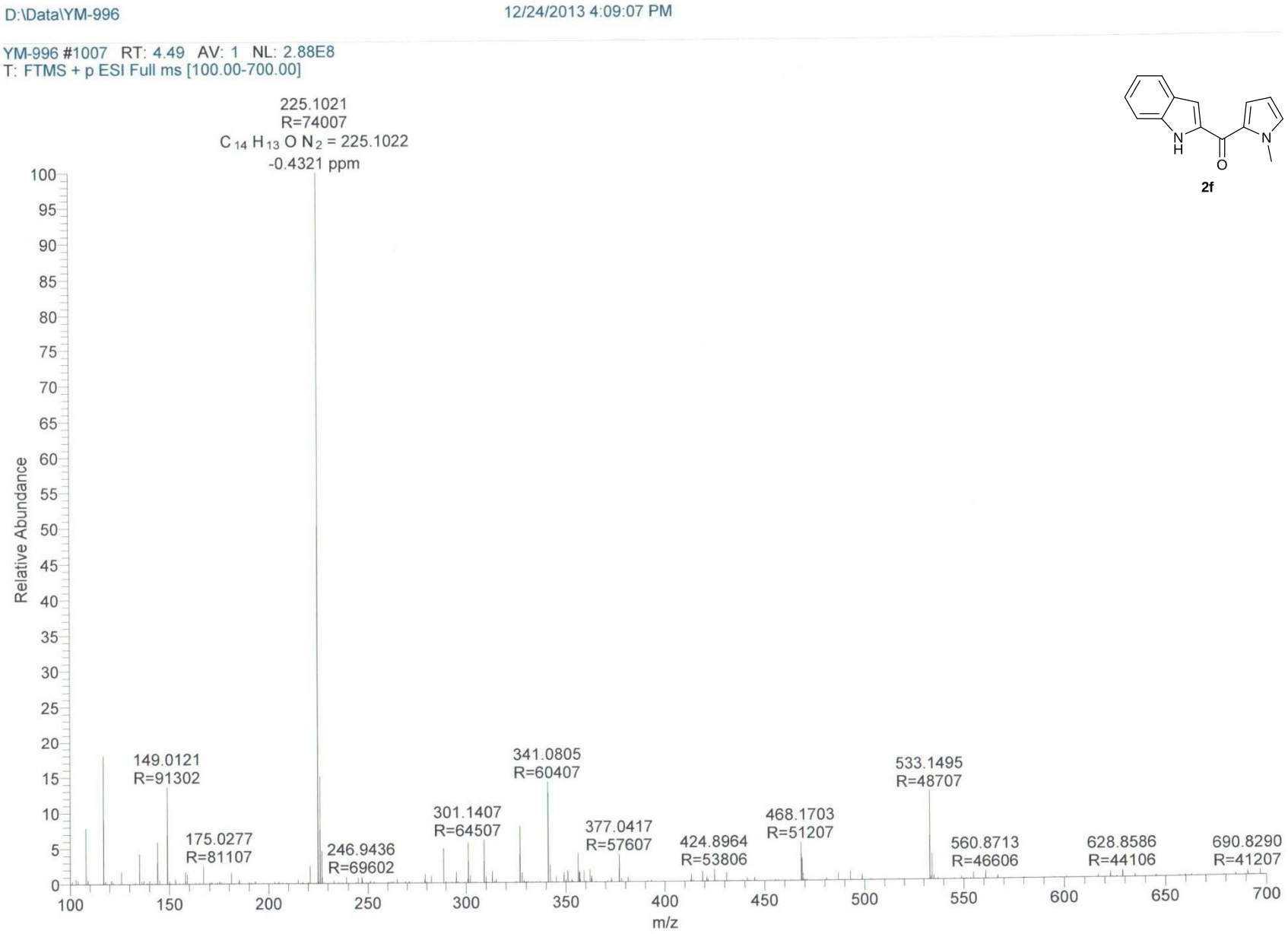


2f

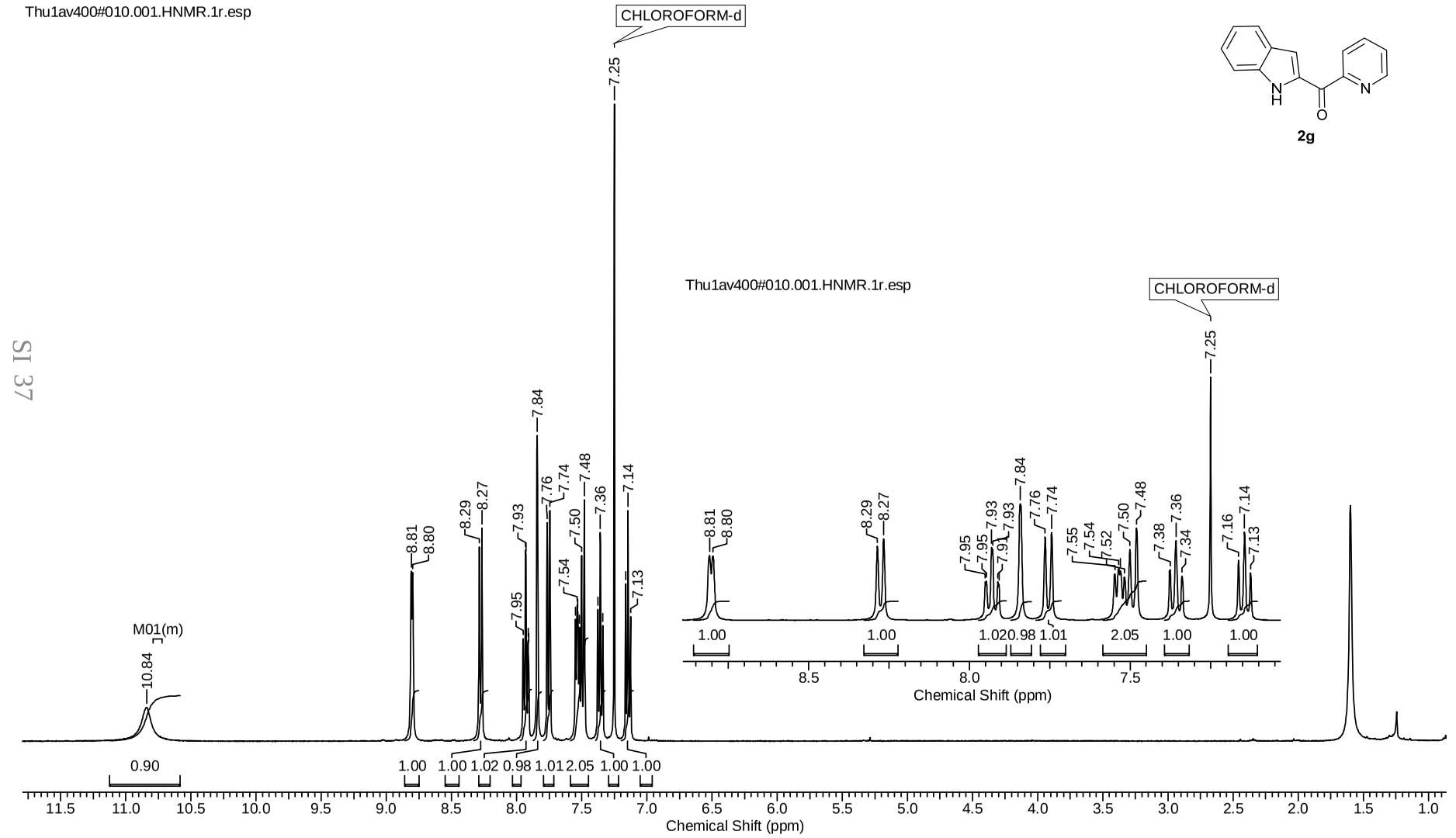
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	19 Sep 2013 12:50:40				
Date Stamp	19 Sep 2013 12:50:40			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Thu3av500#002\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	600	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.3867	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	23.300								

Thu3av500#002.002.001.1r.esp




D:\Data\YM-996
12/24/2013 4:09:07 PM
YM-996 #1007 RT: 4.49 AV: 1 NL: 2.88E8
T: FTMS + p ESI Full ms [100.00-700.00]
225.1021
R=74007
C 14 H 13 O N 2 = 225.1022
-0.4321 ppm
Relative Abundance
m/z
149.0121
R=91302
175.0277
R=81107
246.9436
R=69602
301.1407
R=64507
341.0805
R=60407
377.0417
R=57607
424.8964
R=53806
468.1703
R=51207
533.1495
R=48707
560.8713
R=46606
628.8586
R=44106
690.8290
R=41207
2f

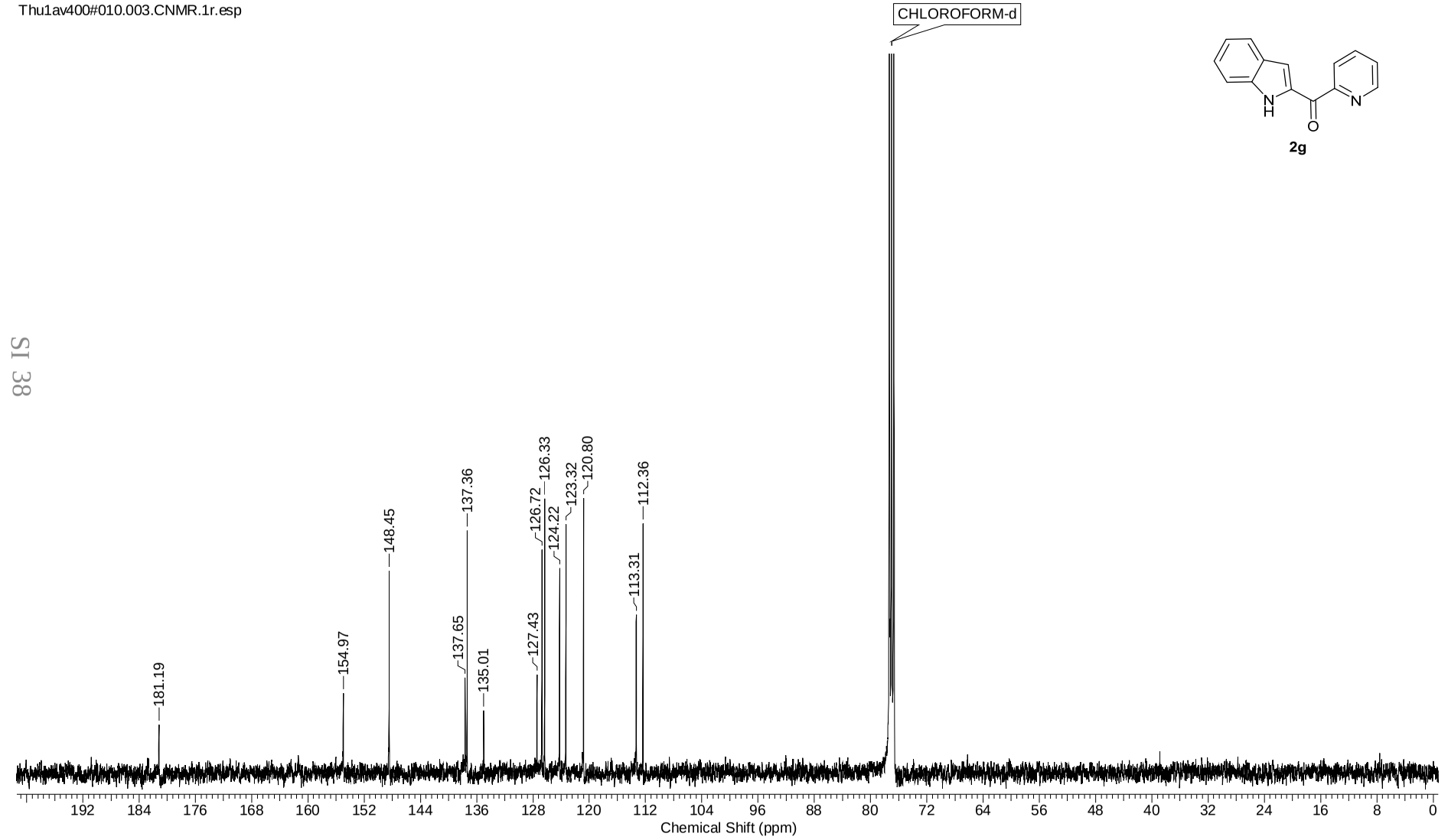
Acquisition Time (sec)	1.9923	***Comment***	Yogesh 1H	***Date***	01 Aug 2013 21:45:44			***Date Stamp***	01 Aug 2013 21:45:44
File Name	E:\New folder\Thu1av400#010\1\PDATA\1\1r			***Frequency (MHz)***	400.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	645.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2464.8591
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.43	***Temperature (degree C)***	23.700				



2g

Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	01 Aug 2013 23:47:20			***Date Stamp***	01 Aug 2013 23:47:20
File Name	E:\New folder\Thu1av400#010\3\PDATA\1\1r			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	1086
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	25252.53	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	9554.7334
Spectrum Type	STANDARD	***Sweep Width (Hz)***	25251.75	***Temperature (degree C)***	23.600				

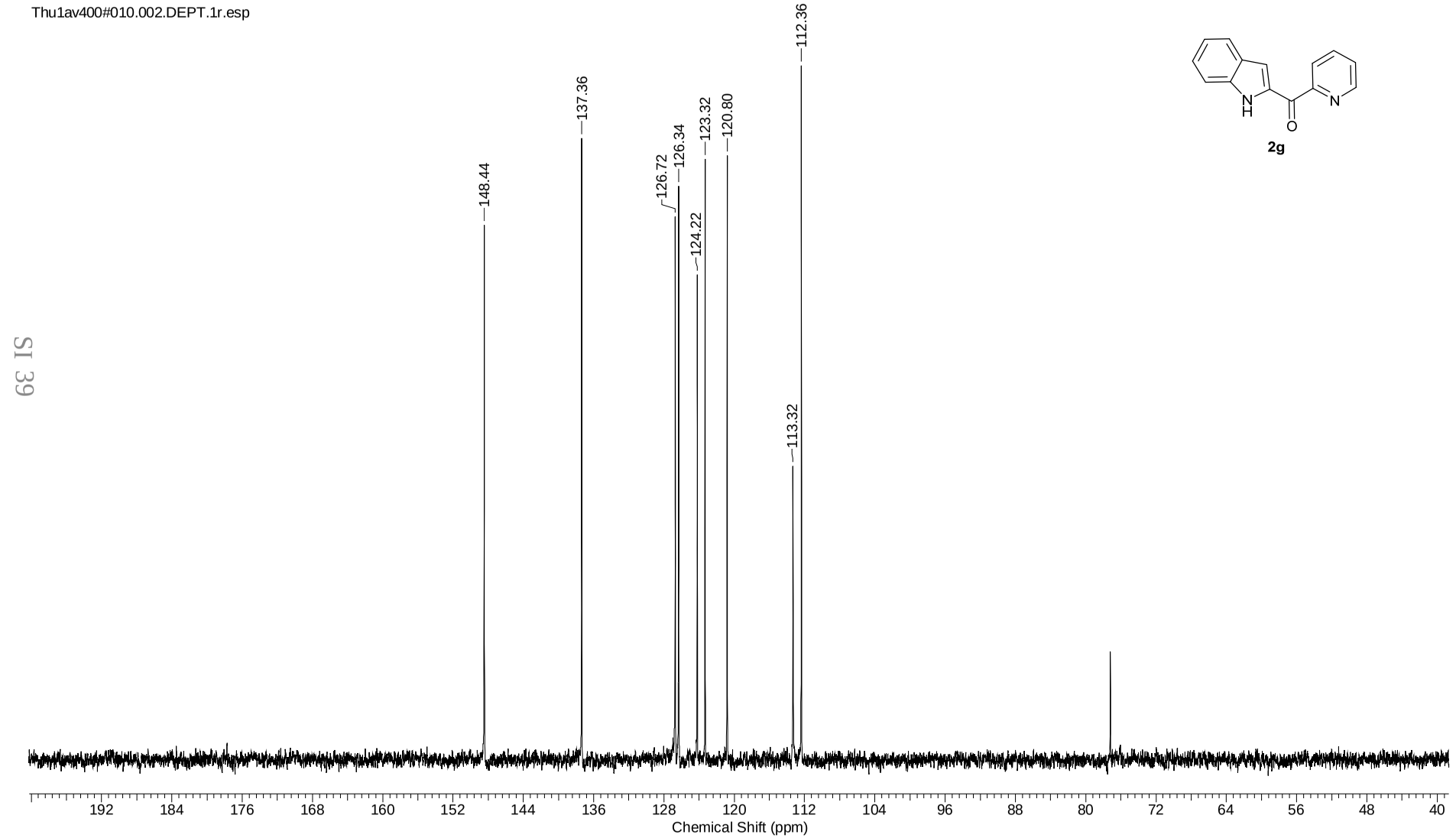
Thu1av400#010.003.CNMR.1r.esp



2g

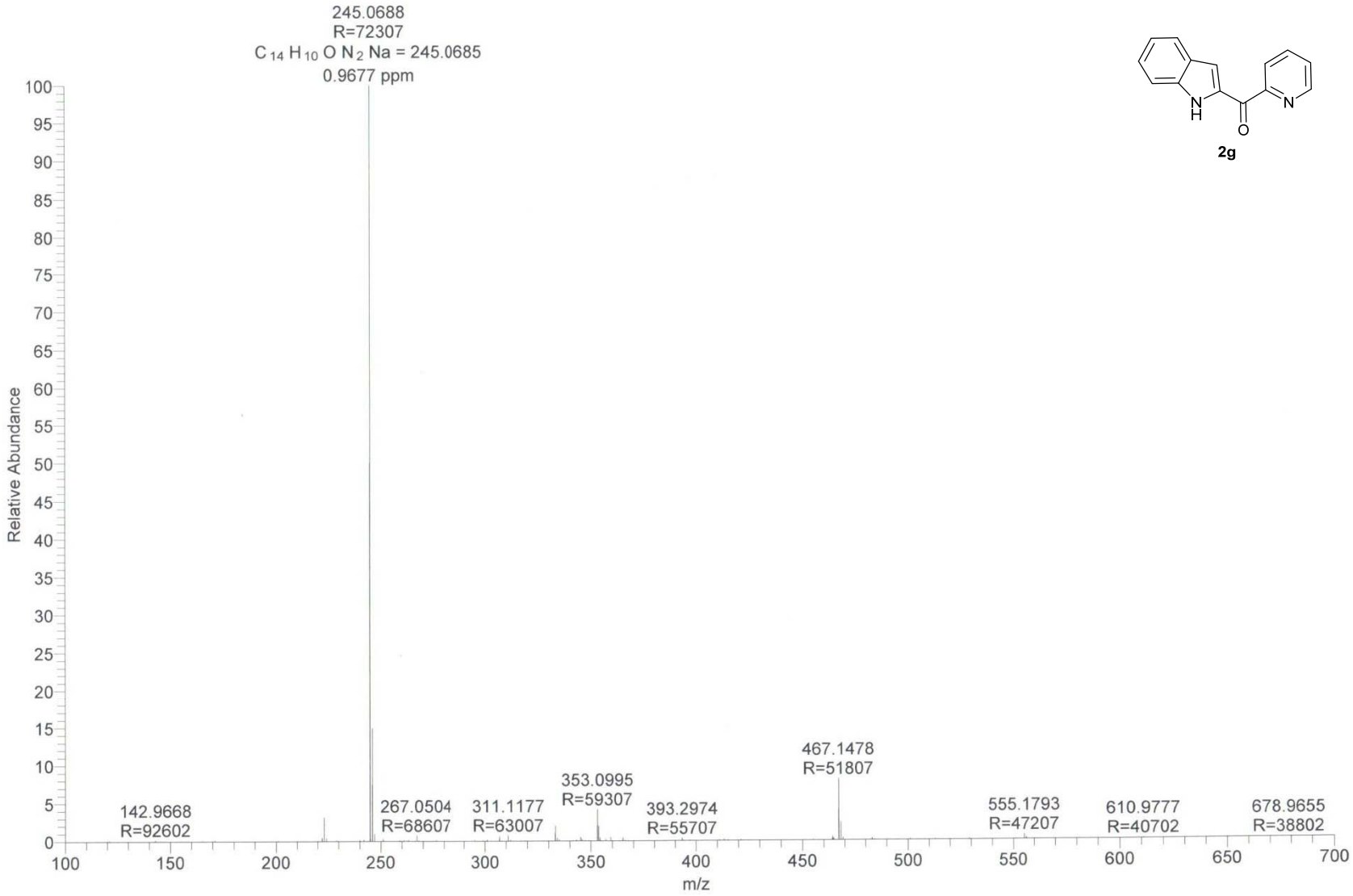
Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	01 Aug 2013 21:52:08			***Date Stamp***	01 Aug 2013 21:52:08
File Name	E:\New folder\Thu1av400#010\2\PDATA\1\1r			***Frequency (MHz)***	100.61	***Nucleus***	13C	***Number of Transients***	2685
Origin	spect	***Original Points Count***	16384	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	16384.00	***SW(cyclical) (Hz)***	25252.53	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10056.7900
Spectrum Type	DEPT135	***Sweep Width (Hz)***	25251.75	***Temperature (degree C)***	23.800				

Thu1av400#010.002.DEPT.1r.esp



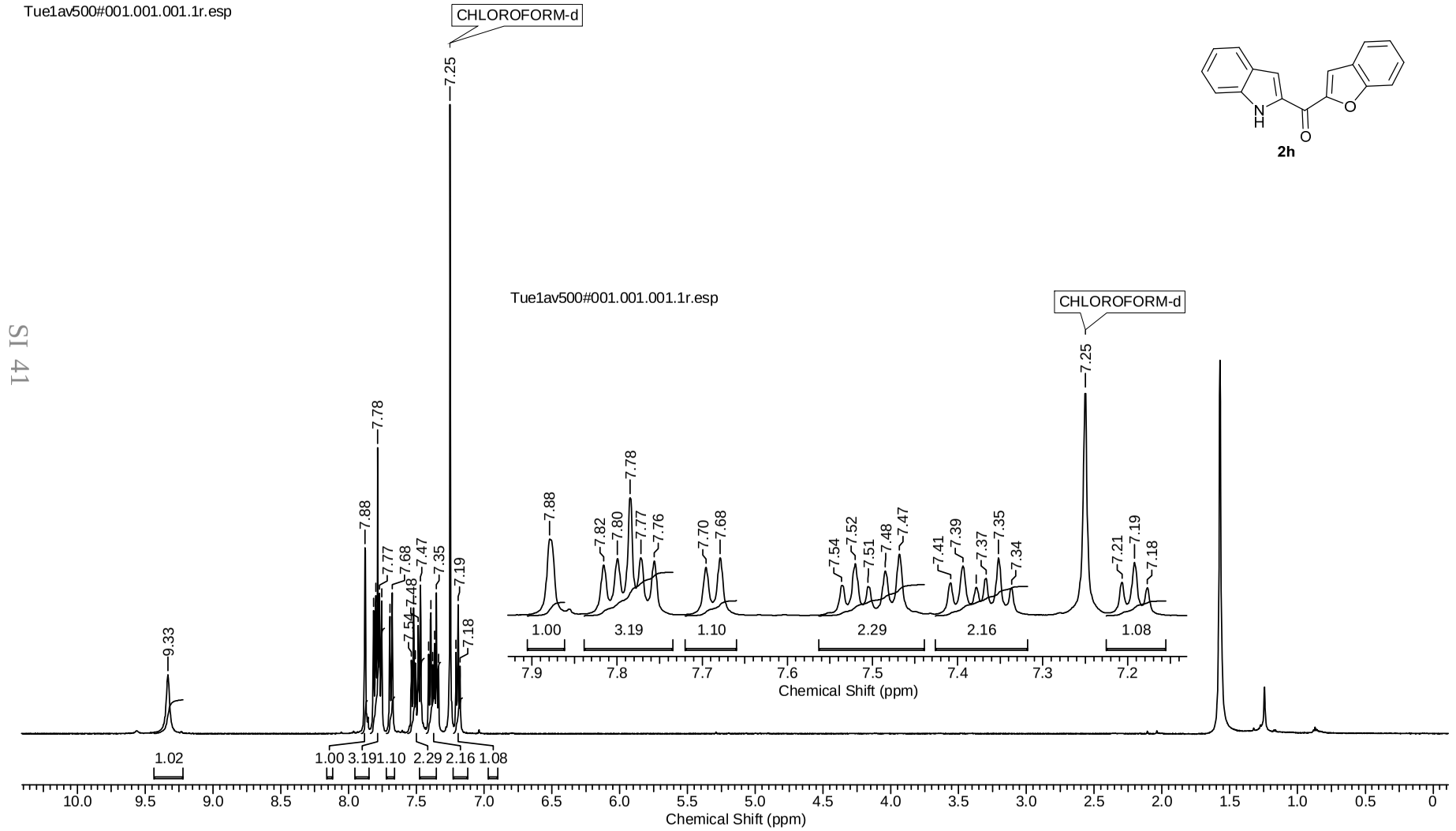
D:\Data\YM-958 9/13/2013 12:03:44 PM

YM-958 #956 RT: 4.26 AV: 1 NL: 3.92E9
T: FTMS + p ESI Full ms [100.00-700.00]



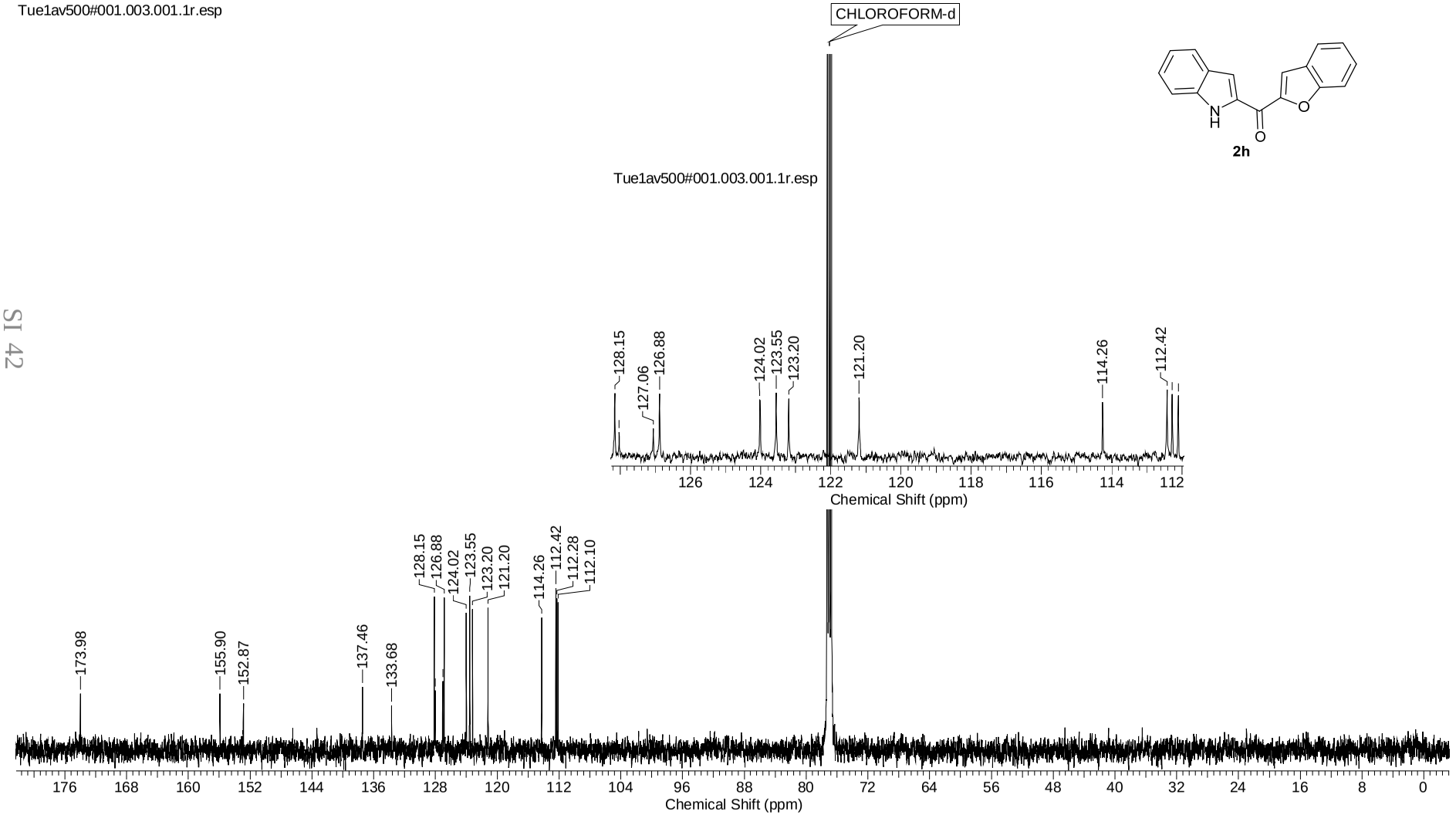
2g

Acquisition Time (sec)	2.0031	***Comment***	Anand 1H	***Date***	03 Sep 2013 09:17:20				
Date Stamp	03 Sep 2013 09:17:20			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue1av500#001\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.400								



Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	03 Sep 2013 10:23:28				
Date Stamp	03 Sep 2013 10:23:28			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue1av500#001\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	808	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11983.1357	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	23.000								

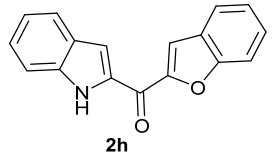
Tue1av500#001.003.001.1r.esp



2h

Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	03 Sep 2013 09:51:28				
Date Stamp	03 Sep 2013 09:51:28			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue1av500#001\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	800	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12572.0234	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	22.500								

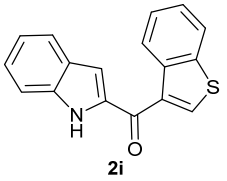
Tue1av500#001.002.001.1r.esp



2h

Acquisition Time (sec)	2.0031	***Comment***	YOGESH 1H	***Date***	15 Aug 2013 15:13:36			***Date Stamp***	15 Aug 2013 15:13:36
File Name	E:\New folder\Thu3av500#003 ym-960\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	20031	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	362.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2175.4456
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.70	***Temperature (degree C)***	22.400				

Thu3av500#003 ym-960.001.001.1r.esp

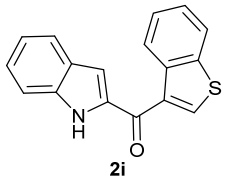


2i

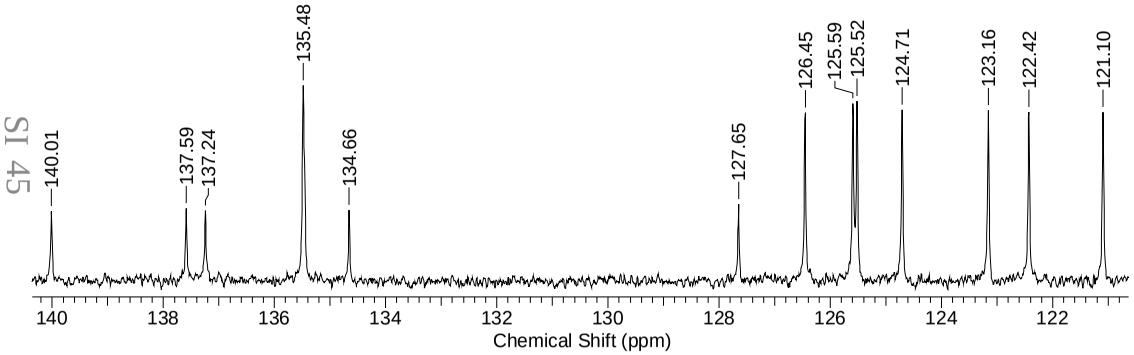
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	15 Aug 2013 17:00:16			***Date Stamp***	15 Aug 2013 17:00:16
File Name	E:\New folder\Thu3av500#003 ym-960\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1342
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11980.2744
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	23.200				

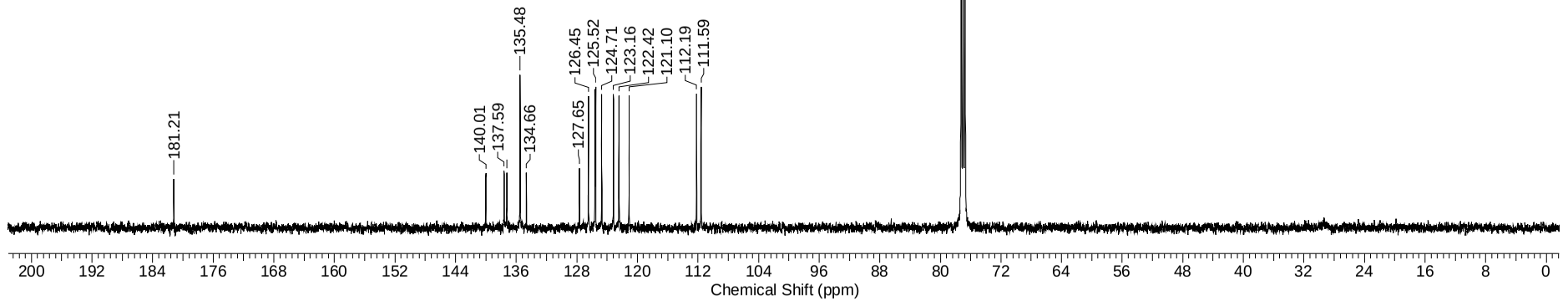
Thu3av500#003 ym-960.003.001.1r.esp

Thu3av500#003 ym-960.003.001.1r.esp



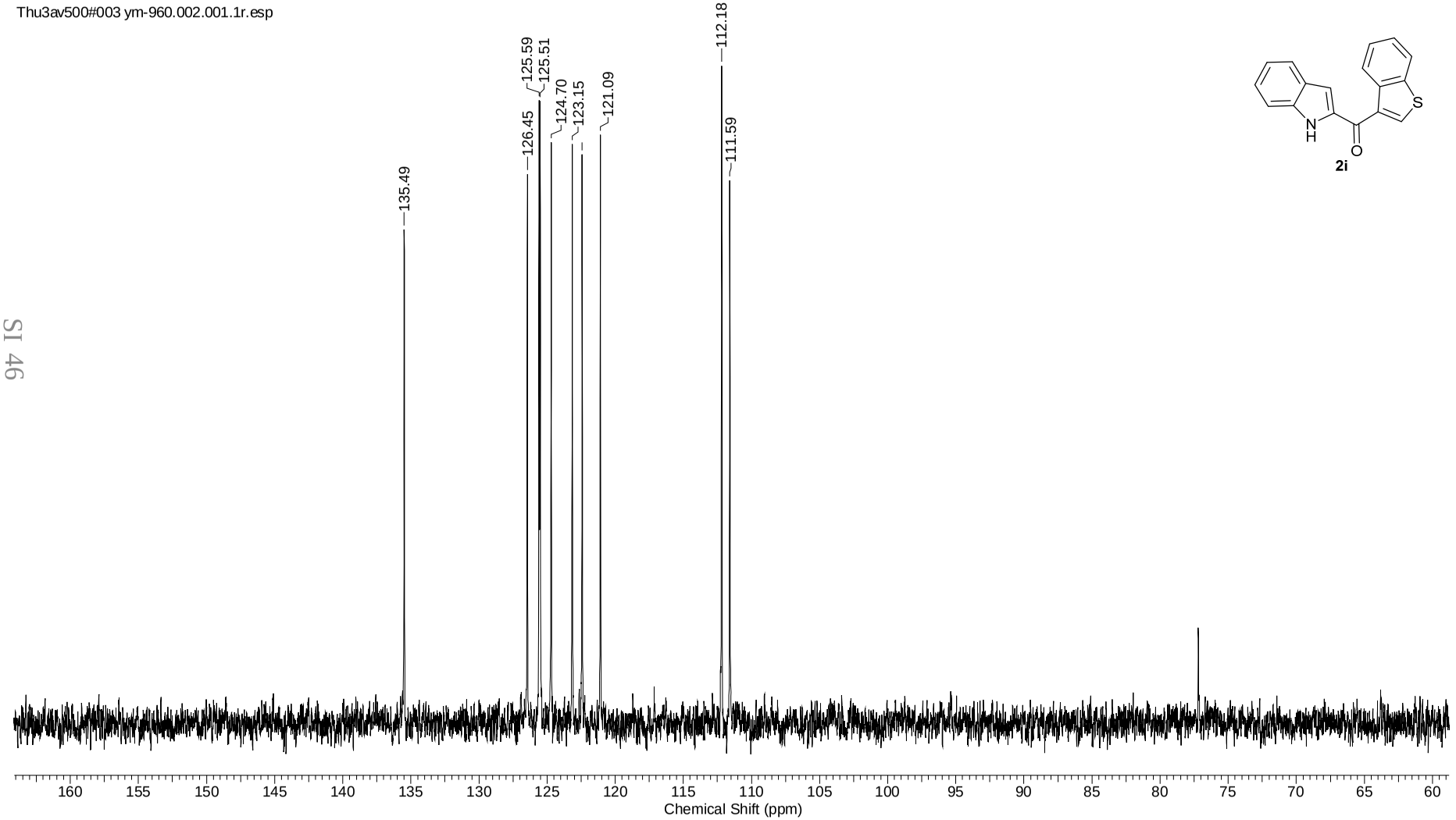
2i





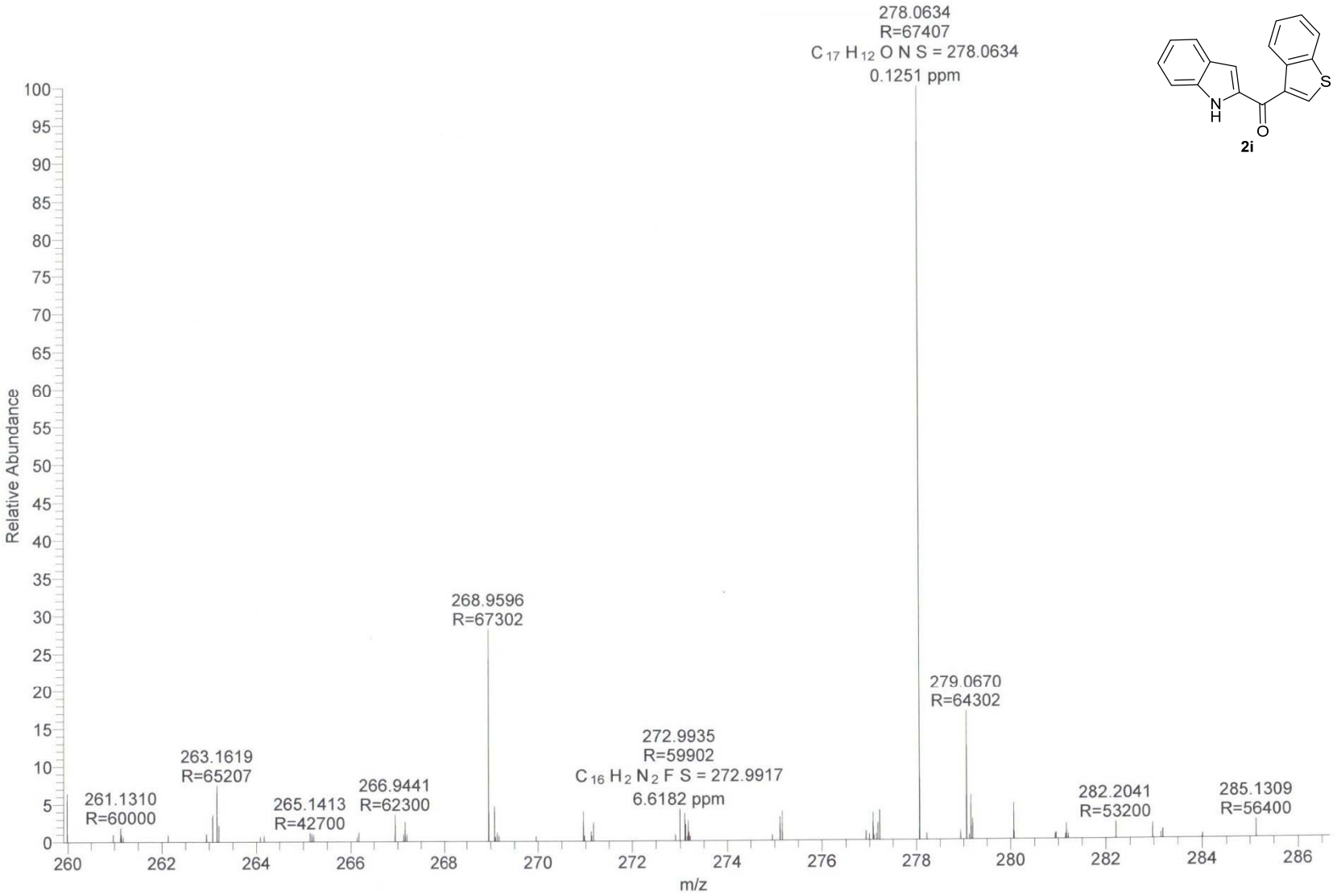
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	15 Aug 2013 15:39:12			***Date Stamp***	15 Aug 2013 15:39:12
File Name	E:\New folder\Thu3av500#003 ym-960\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	800
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12568.7402
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.700				

Thu3av500#003 ym-960.002.001.1r.esp



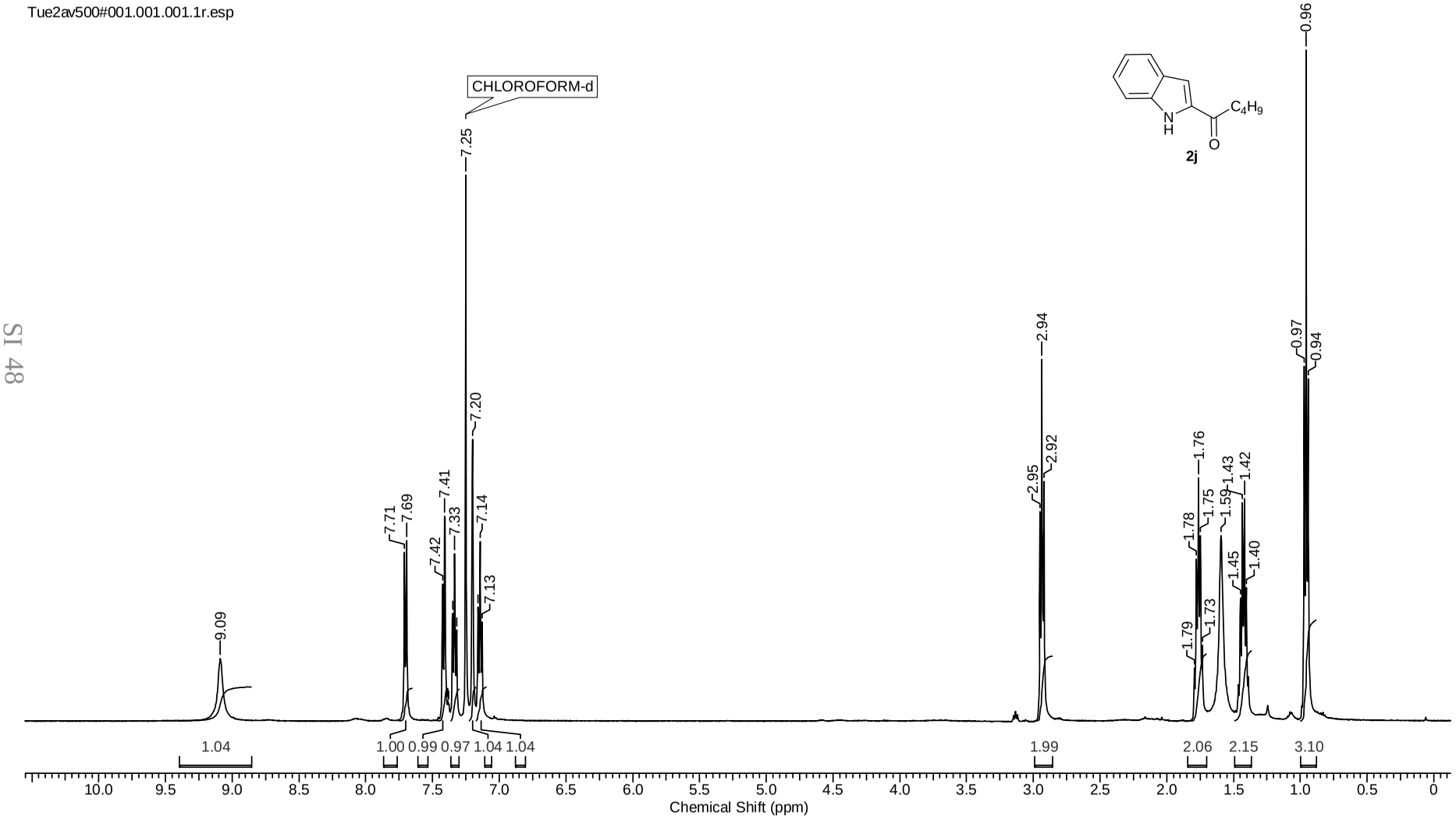
D:\Data\YM-960 9/13/2013 11:52:33 AM

YM-960 #1163 RT: 5.18 AV: 1 NL: 4.32E6
T: FTMS + p ESI Full ms [100.00-700.00]



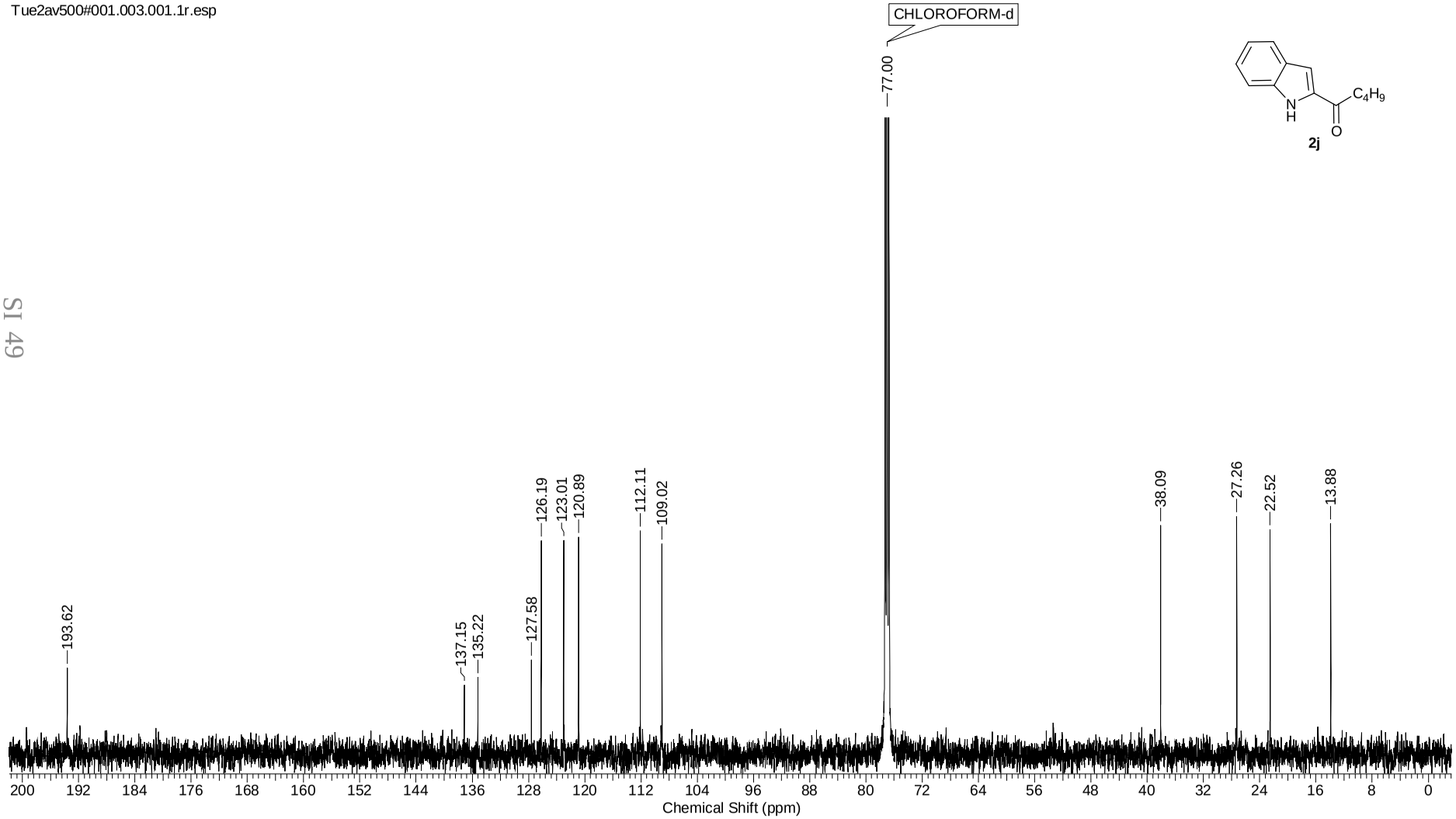
Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	10 Sep 2013 09:57:52				
Date Stamp	10 Sep 2013 09:57:52			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue2av500#001\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	23.200								

Tue2av500#001.001.001.1r.esp



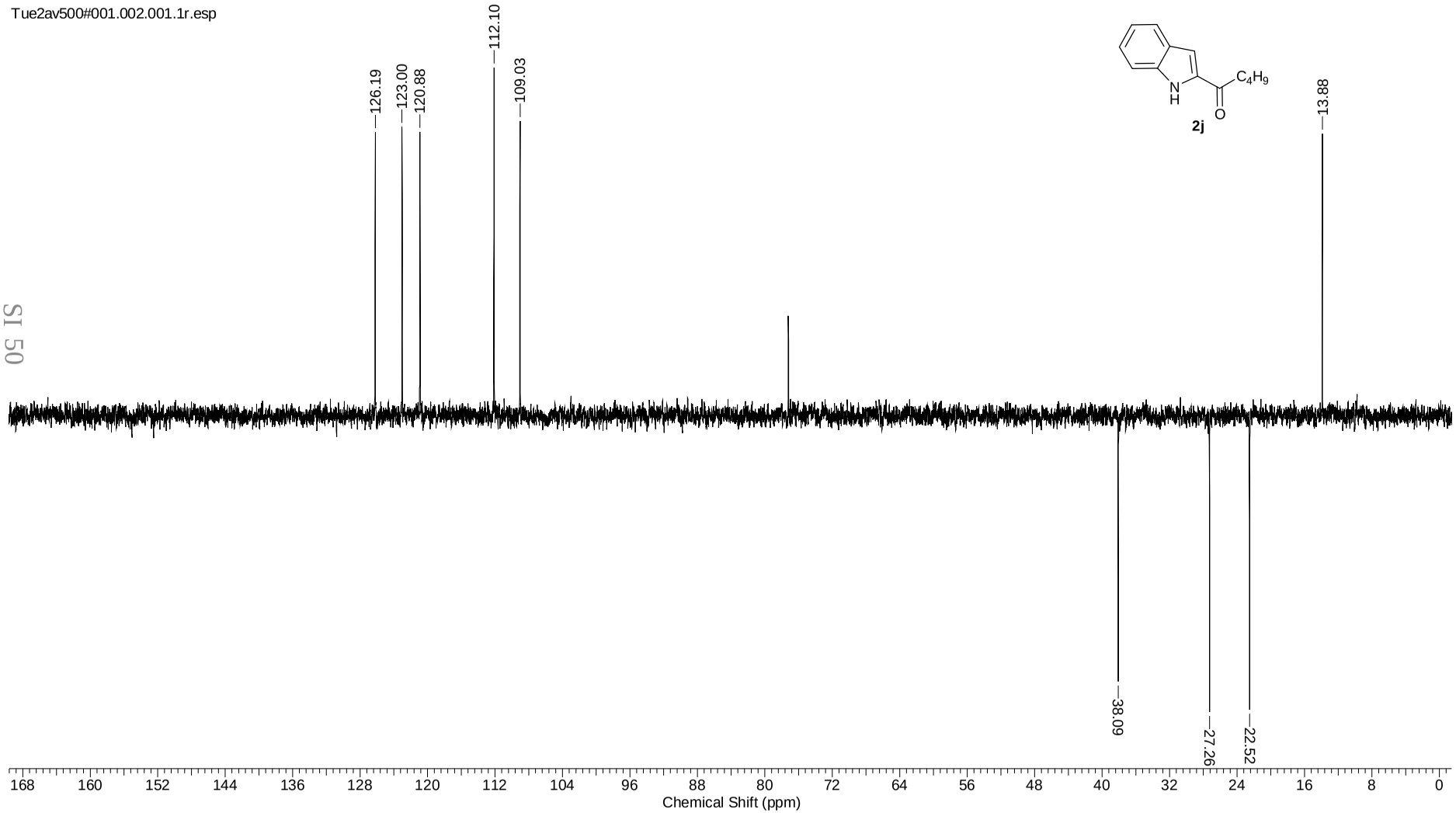
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	10 Sep 2013 10:46:56				
Date Stamp	10 Sep 2013 10:46:56			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue2av500#001\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	522	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11982.1826	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	24.100								

Tue2av500#001.003.001.1r.esp



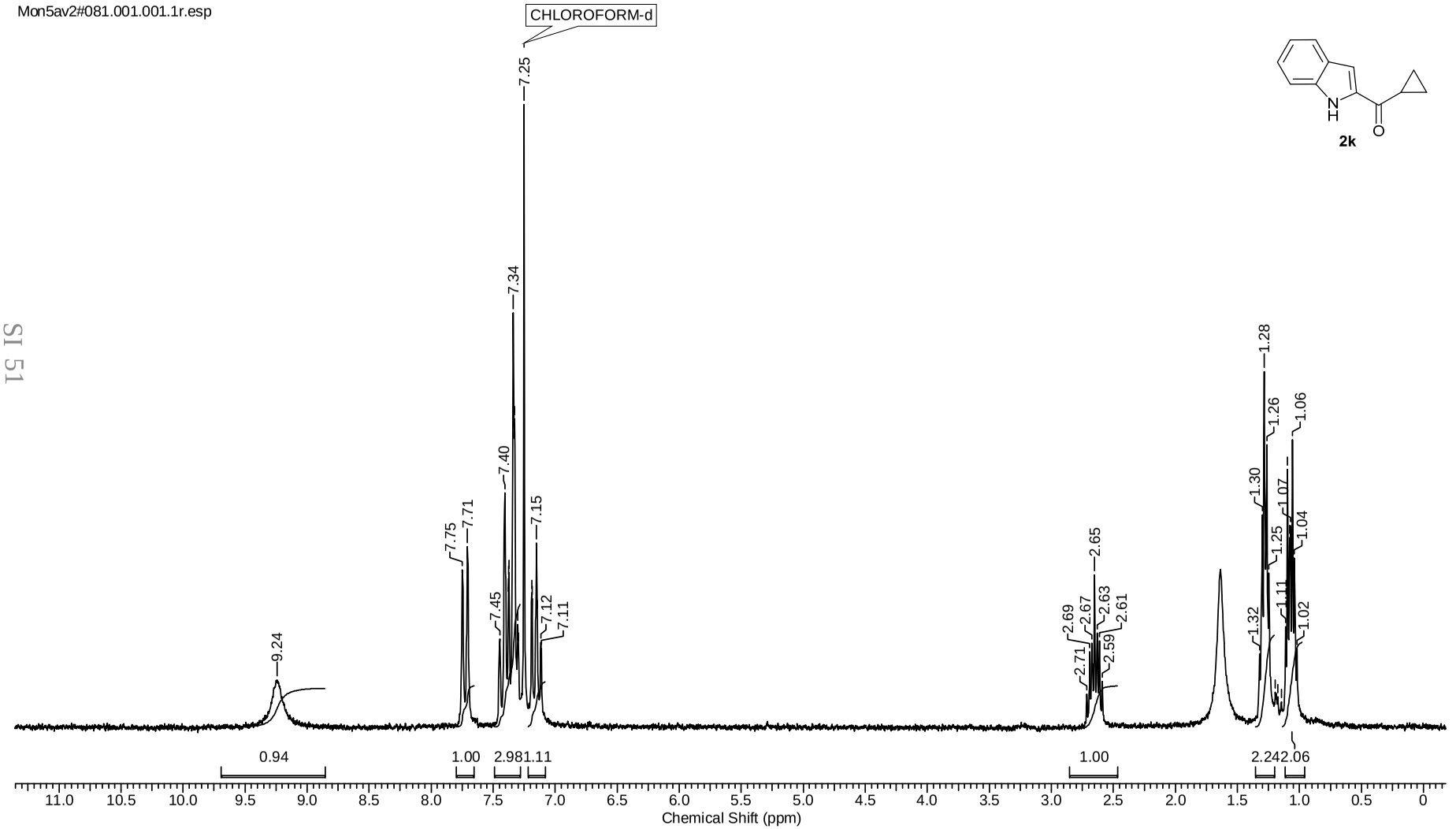
2j

Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	10 Sep 2013 10:21:20				
Date Stamp	10 Sep 2013 10:21:20			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Tue2av500#001\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.6299	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	23.500								



Acquisition Time (sec)	3.9584	***Comment***	Yogesh	***Date***	26 Aug 2013 23:17:28		
Date Stamp	26 Aug 2013 23:17:28			***File Name***	\\agni\nmr_data\AV200\AUG_13#AV200\data\Administrator\nmr\Mon5av2#081\1\PDATA\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	av200
Original Points Count	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1149.40	***SW(cyclical) (Hz)***	4139.07	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1229.5370	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4138.95	***Temperature (degree C)***	27.000

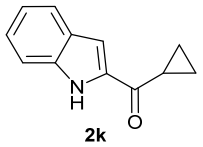
Mon5av2#081.001.001.1r.esp



2k

Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	14 Aug 2013 20:46:24			***Date Stamp***	14 Aug 2013 20:46:24
File Name	H:\New folder\Wed3av500#016 ym-962\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	2043
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11980.2744
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	22.800				

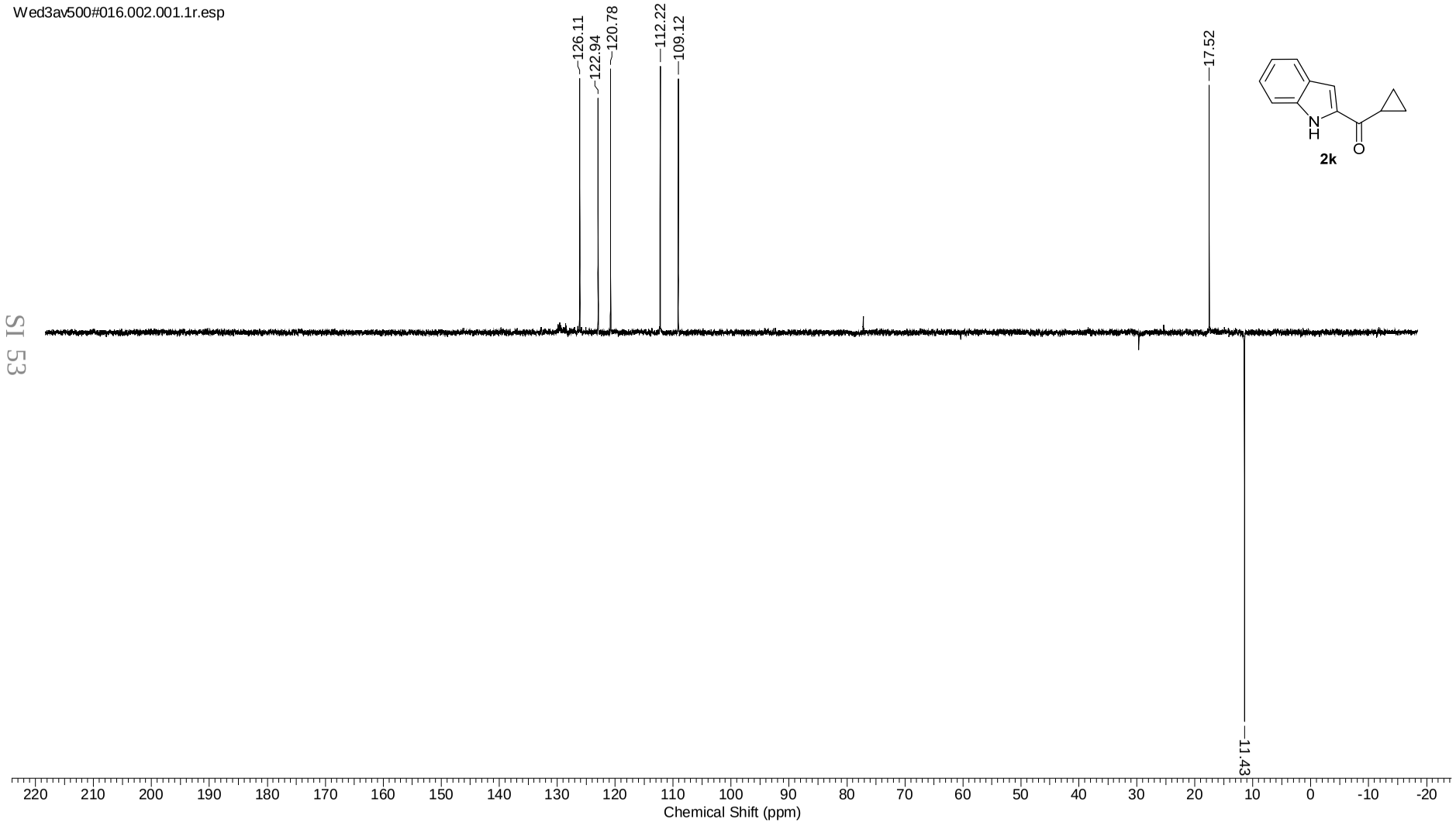
Wed3av500#016.003.001.1r.esp

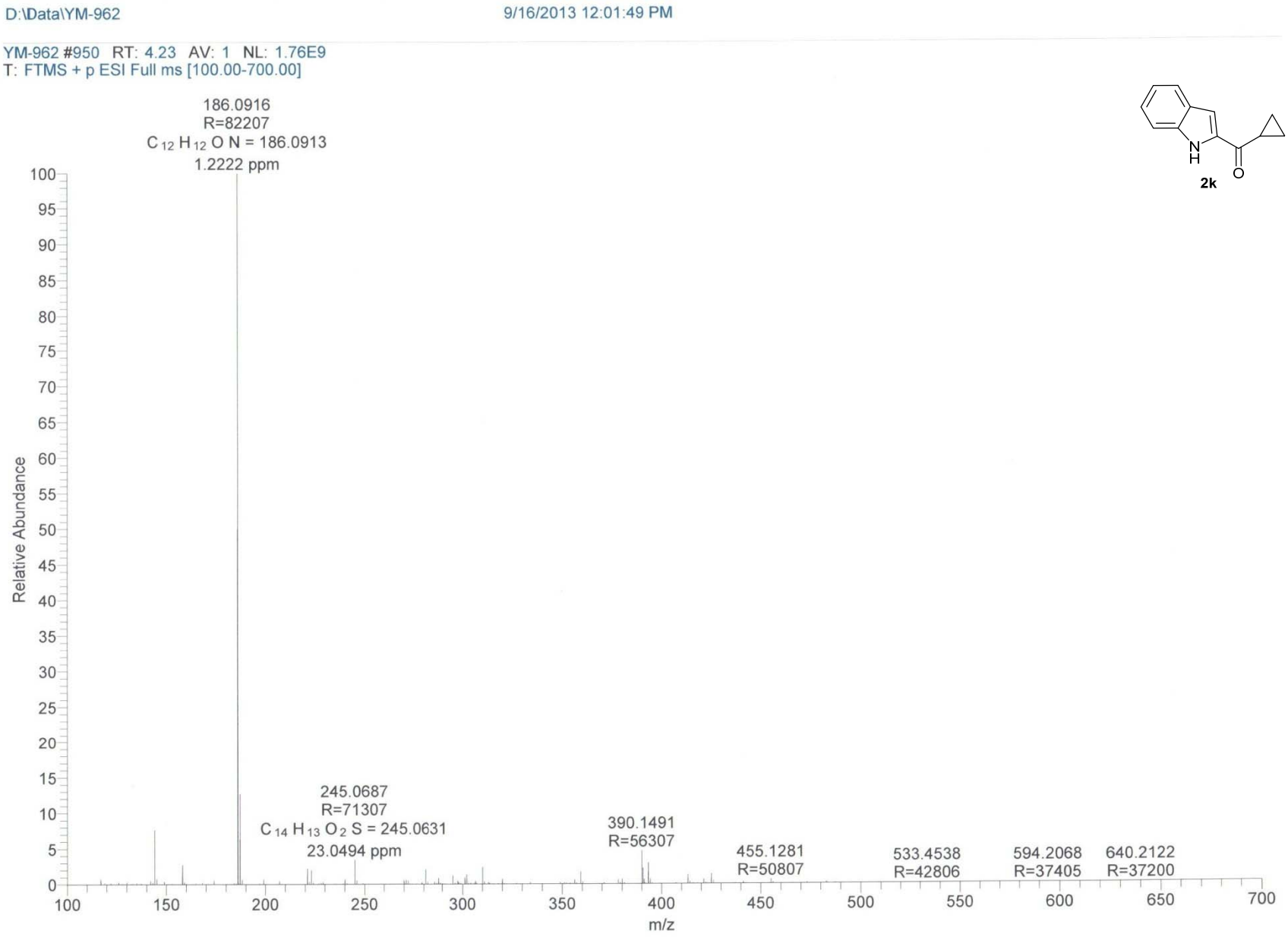


2k

Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	14 Aug 2013 19:04:00			***Date Stamp***	14 Aug 2013 19:04:00
File Name	H:\New folder\Wed3av500#016 ym-962\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1200
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12569.5156
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.400				

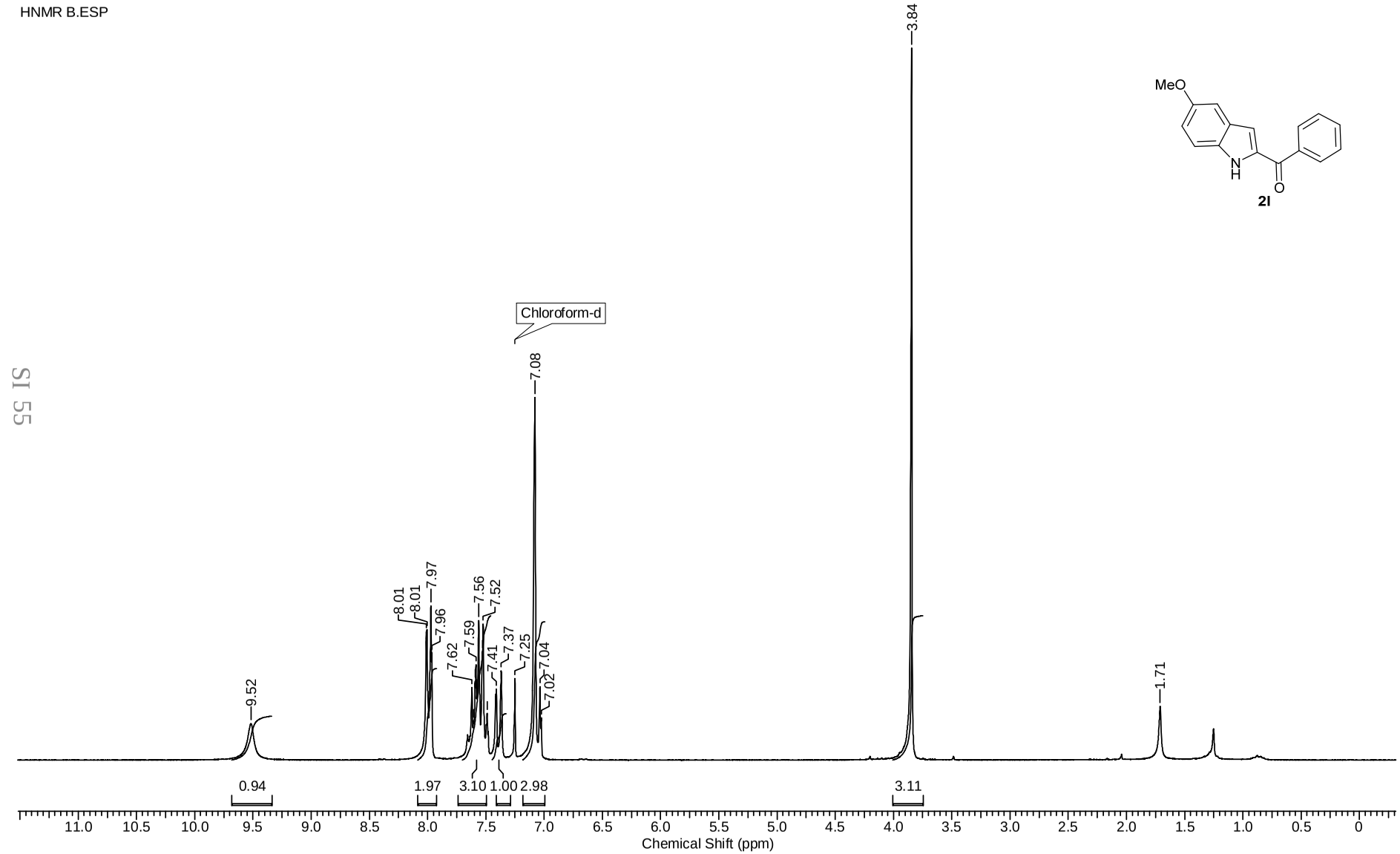
Wed3av500#016.002.001.1r.esp




D:\Data\YM-962
9/16/2013 12:01:49 PM
YM-962 #950 RT: 4.23 AV: 1 NL: 1.76E9
T: FTMS + p ESI Full ms [100.00-700.00]
186.0916
R=82207
C 12 H 12 O N = 186.0913
1.2222 ppm
245.0687
R=71307
C 14 H 13 O 2 S = 245.0631
23.0494 ppm
390.1491
R=56307
455.1281
R=50807
533.4538
R=42806
594.2068
R=37405
640.2122
R=37200
Relative Abundance
m/z
2k

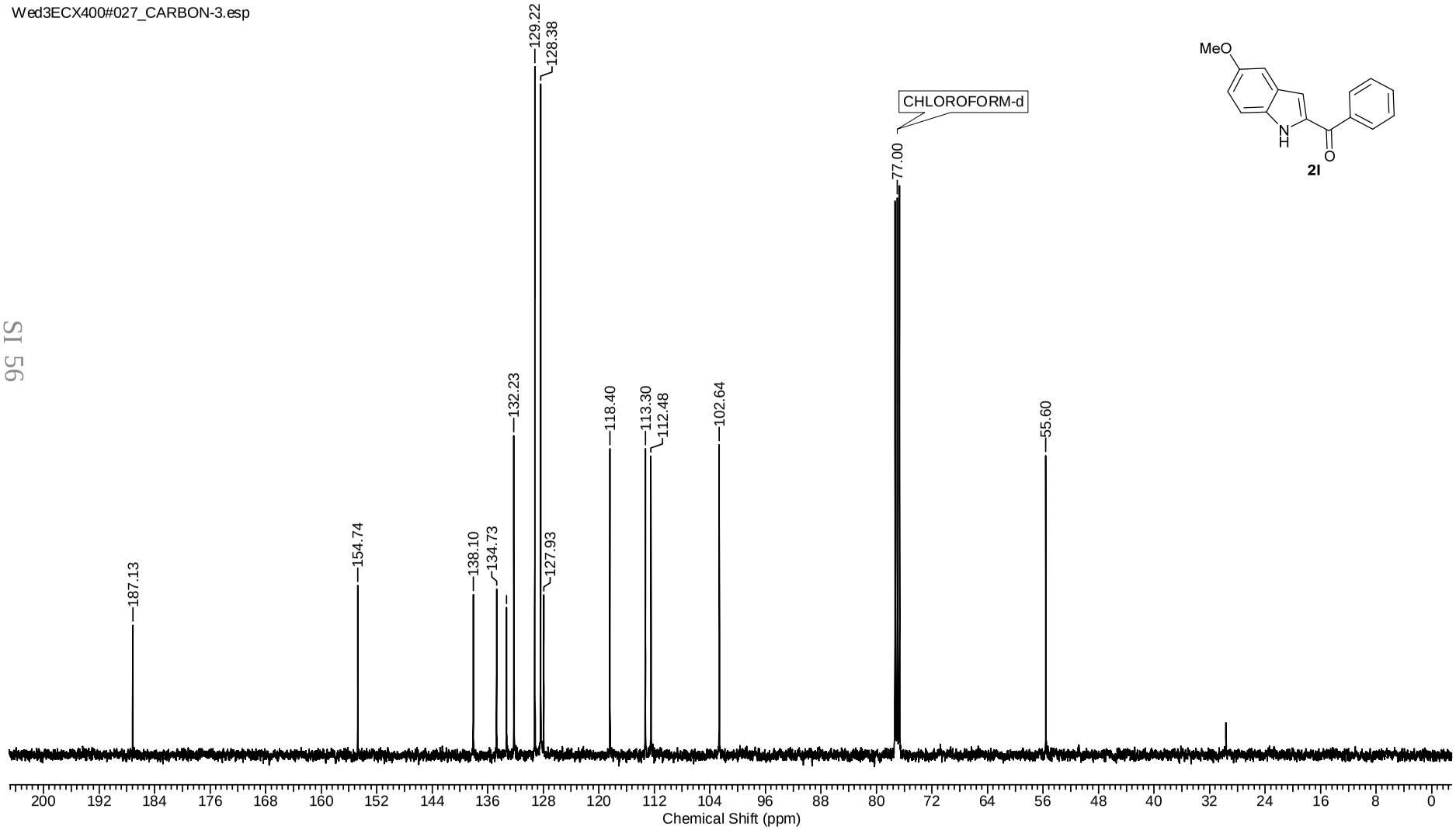
Acquisition Time (sec)	7.9167	***Comment***	yogesh	***Date***	25/06/2013 15:30:18		
File Name	F:\yogesh\Indole metho\NMR\ym-942\HNMR B.ESP			***Frequency (MHz)***	200.13	***Nucleus*** 1H	***Original Points Count*** 32768
Points Count	32768	***Spectrum Offset (Hz)***	1225.4011	***Sweep Width (Hz)***	4139.07	***Temperature (degree C)*** 0.000	

HNMR B.ESP



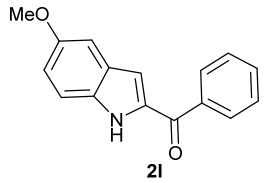
Acquisition Time (sec)	1.0434	***Comment***	yogesh	***Date***	19 Sep 2013 07:56:04		
Date Stamp	19 Sep 2013 07:28:11			***File Name***	\\agni\nmr_data\JEOL_400\2013\Sep 2013 Liquid\Wed3ECX400#027_CARBON-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	101	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	single_pulse_dec
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10036.4561
Spectrum Type	STANDARD	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	22.500		

Wed3ECX400#027_CARBON-3.esp



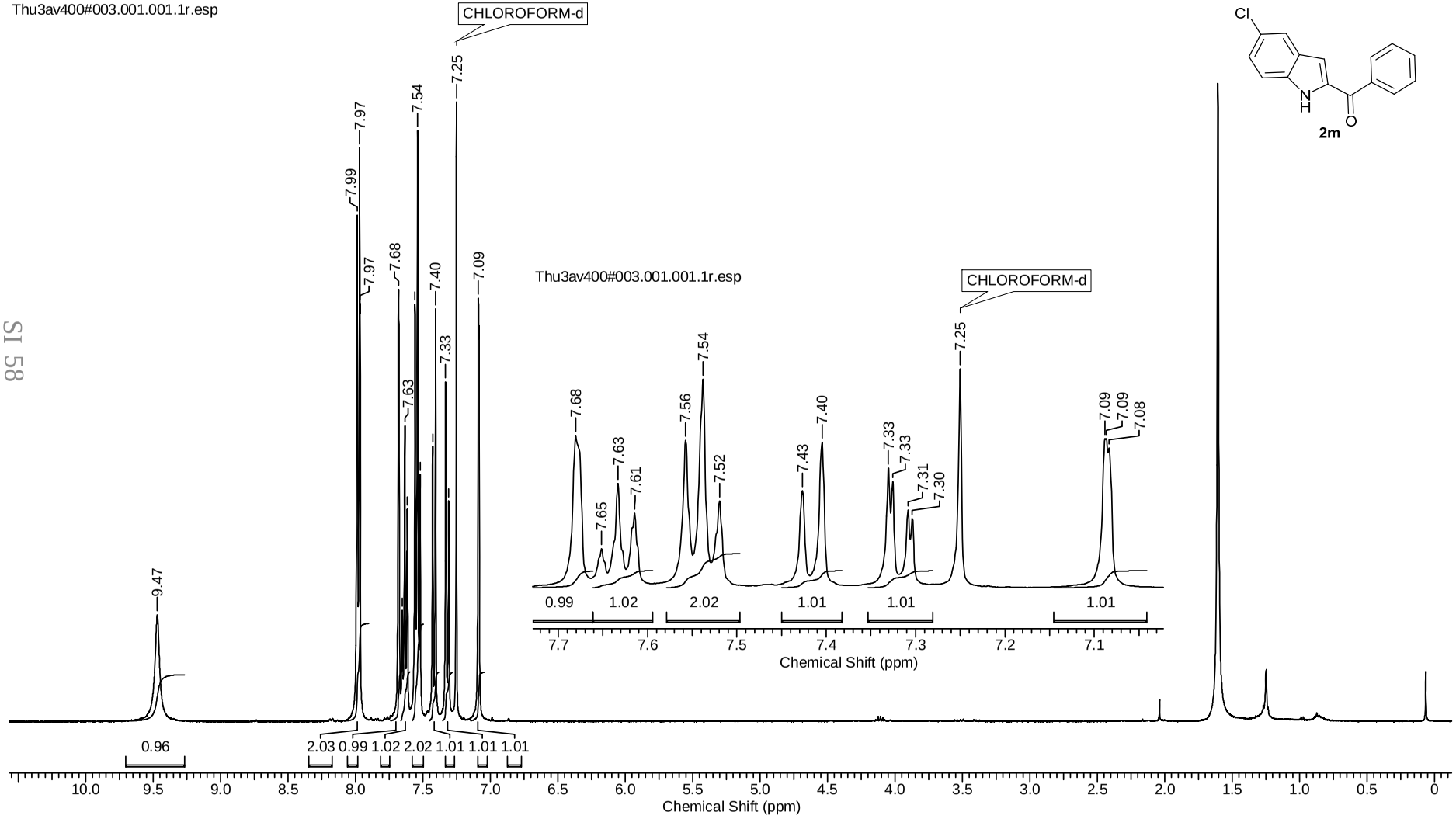
Acquisition Time (sec)	1.0434	***Comment***	yogesh	***Date***	19 Sep 2013 07:56:04		
Date Stamp	19 Sep 2013 07:30:24			***File Name***	\\agni\nmr_data\JEOL_400\2013\Sep 2013 Liquid\Wed3ECX400#027_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	47	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	dept.ex2 (selection_angle=135)
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10036.0127
Spectrum Type	DEPT135	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	22.600		

Wed3ECX400#027_DEPT135-3.esp



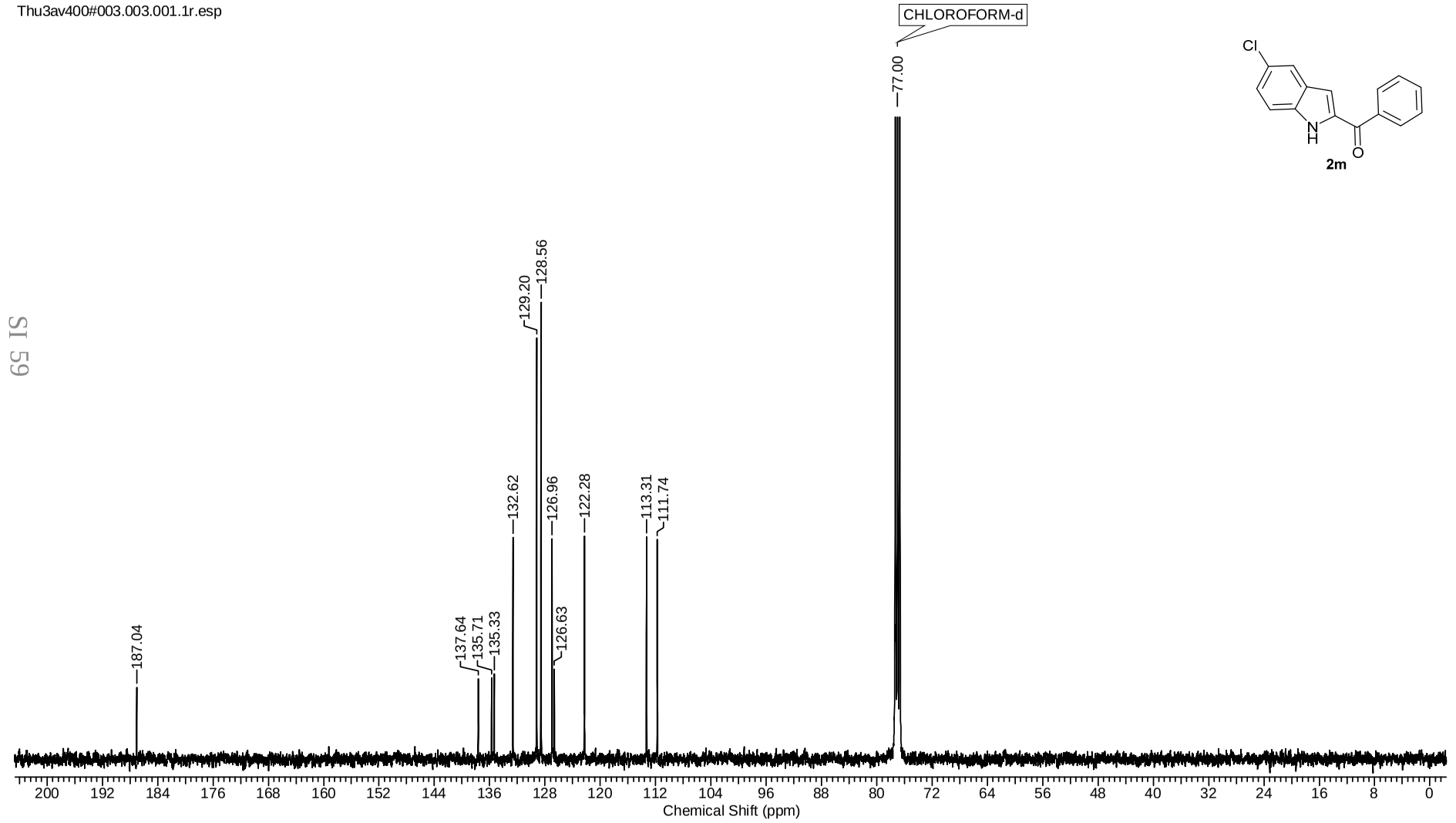
2l

Acquisition Time (sec)	2.0447	***Comment***	Yogesh 1H	***Date***	19 Sep 2013 17:29:44				
Date Stamp	19 Sep 2013 17:29:44			***File Name***	\\agni\nmr_data\AV400\Sep_13_400\Thu3av400#003\1\PDATA\1\1r				
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	724.00	***SW(cyclical) (Hz)***	8012.82
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2257.9458	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8012.58
Temperature (degree C)	25.100								



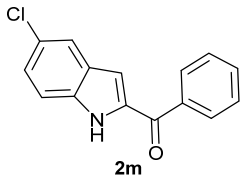
Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	19 Sep 2013 19:48:24				
Date Stamp	19 Sep 2013 19:48:24			***File Name***	\\agni\nmr_data\AV400\Sep_13_400\Thu3av400#003\3\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	2063	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	9634.8799	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	24.800								

Thu3av400#003.003.001.1r.esp



Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	19 Sep 2013 18:16:40				
Date Stamp	19 Sep 2013 18:16:40			***File Name***	\\agni\nmr_data\AV400\Sep_13_400\Thu3av400#003\2\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	16384.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	7608.4902	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	24.700								

Thu3av400#003.002.001.1r.esp

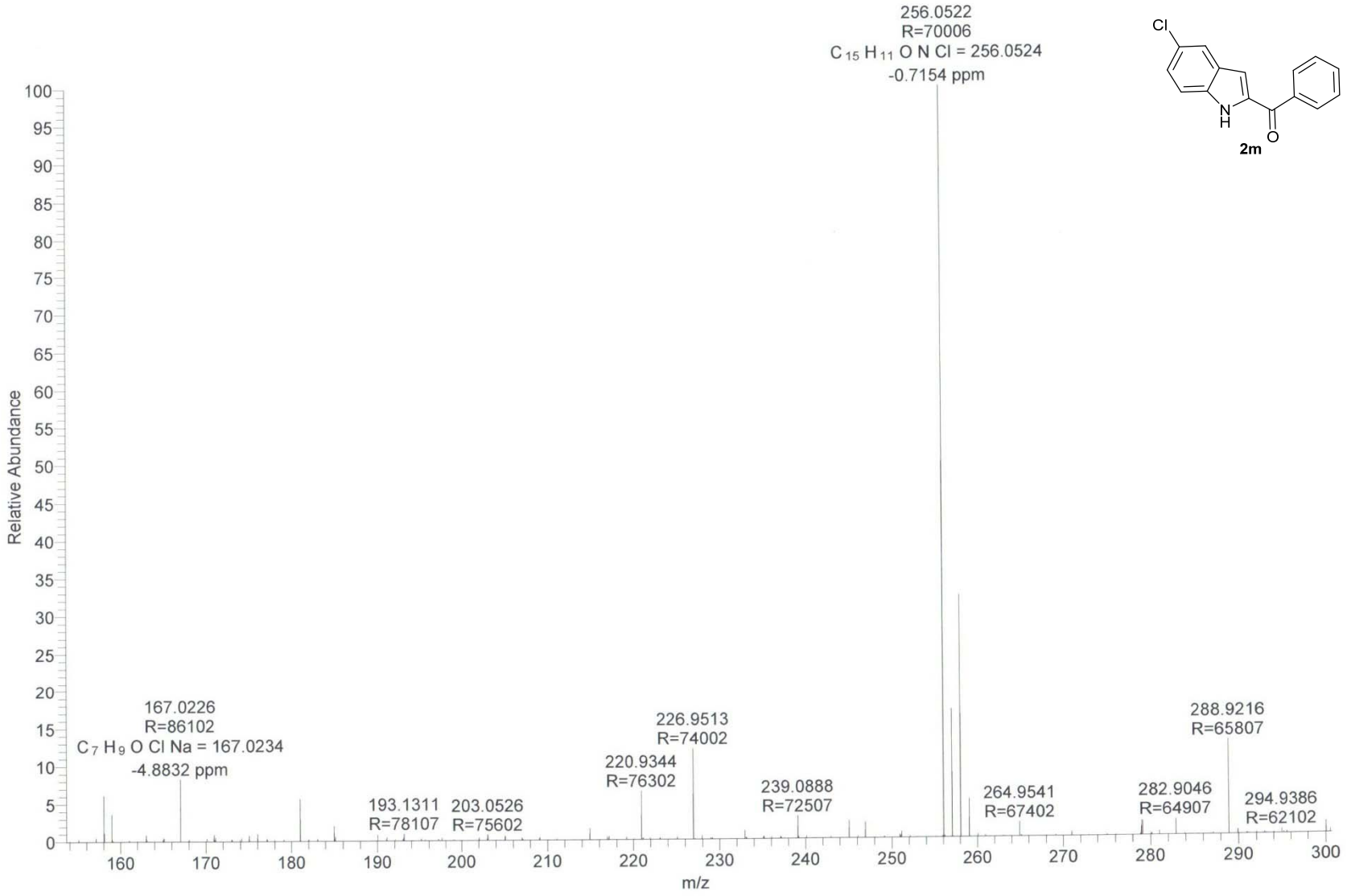


2m

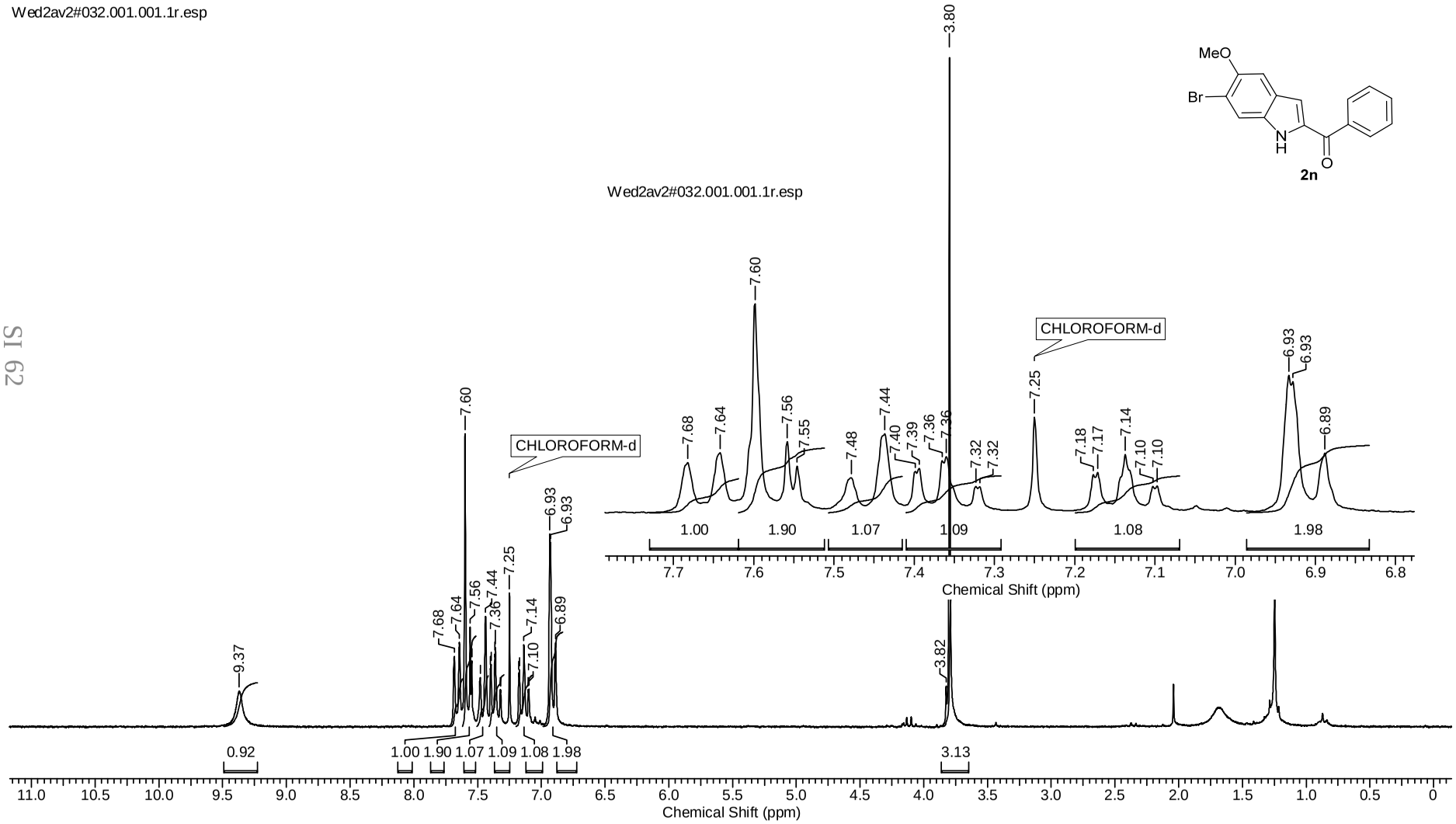
09 IS

D:\Data\YM-997 12/24/2013 3:54:41 PM

YM-997 #1166 RT: 5.20 AV: 1 NL: 1.09E8
T: FTMS + p ESI Full ms [100.00-700.00]

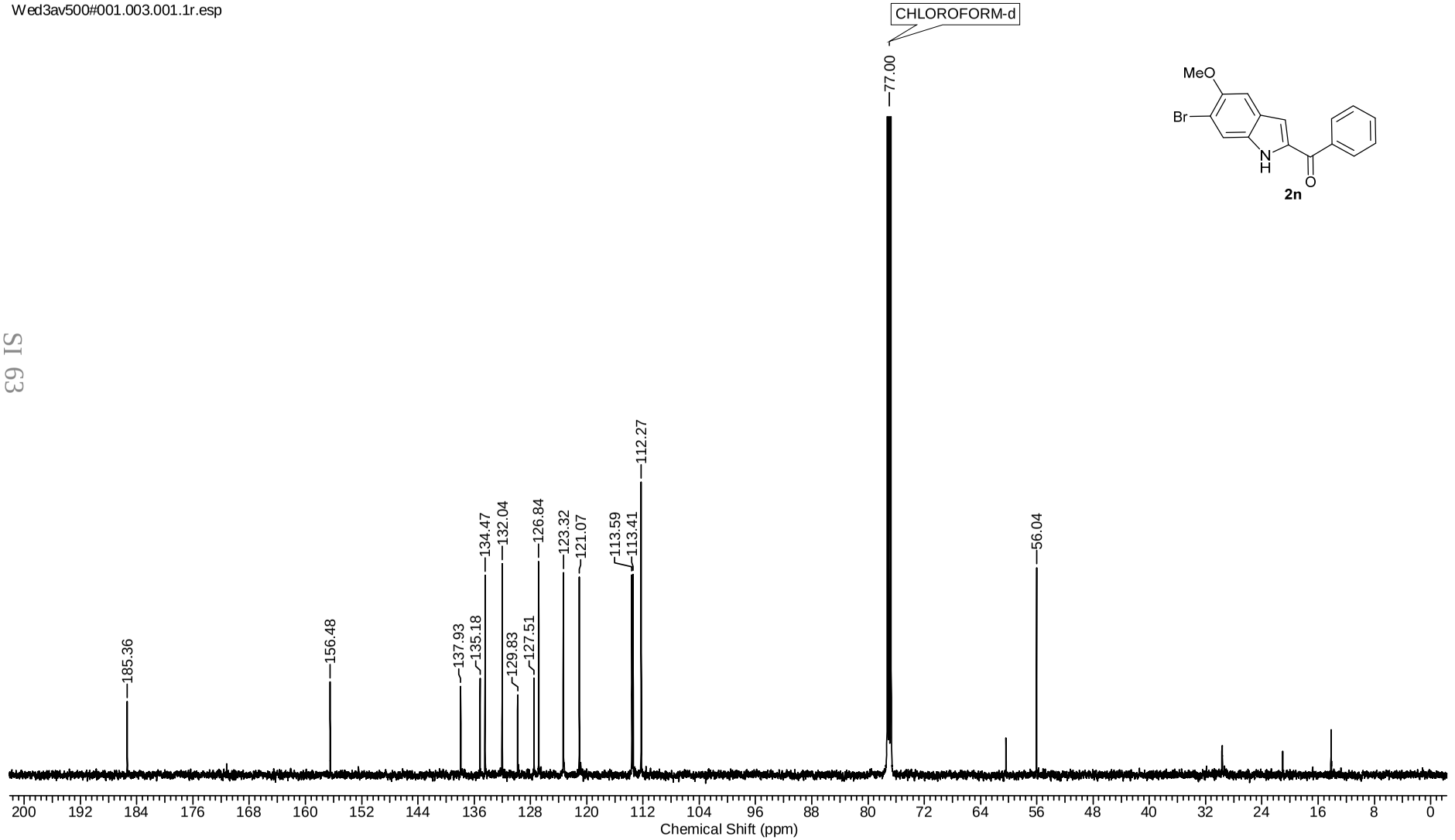


Acquisition Time (sec)	3.9584	***Comment***	yogesh	***Date***	07 Aug 2013 15:26:00		
Date Stamp	07 Aug 2013 15:26:00			***File Name***	\\agni\nmr_data\AV200\AUG_13#AV200\data\Administrator\nmr\Wed2av2#032\1\PDATA\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	av200
Original Points Count	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1149.40	***SW(cyclical) (Hz)***	4139.07	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1225.6606	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4138.95	***Temperature (degree C)***	27.000



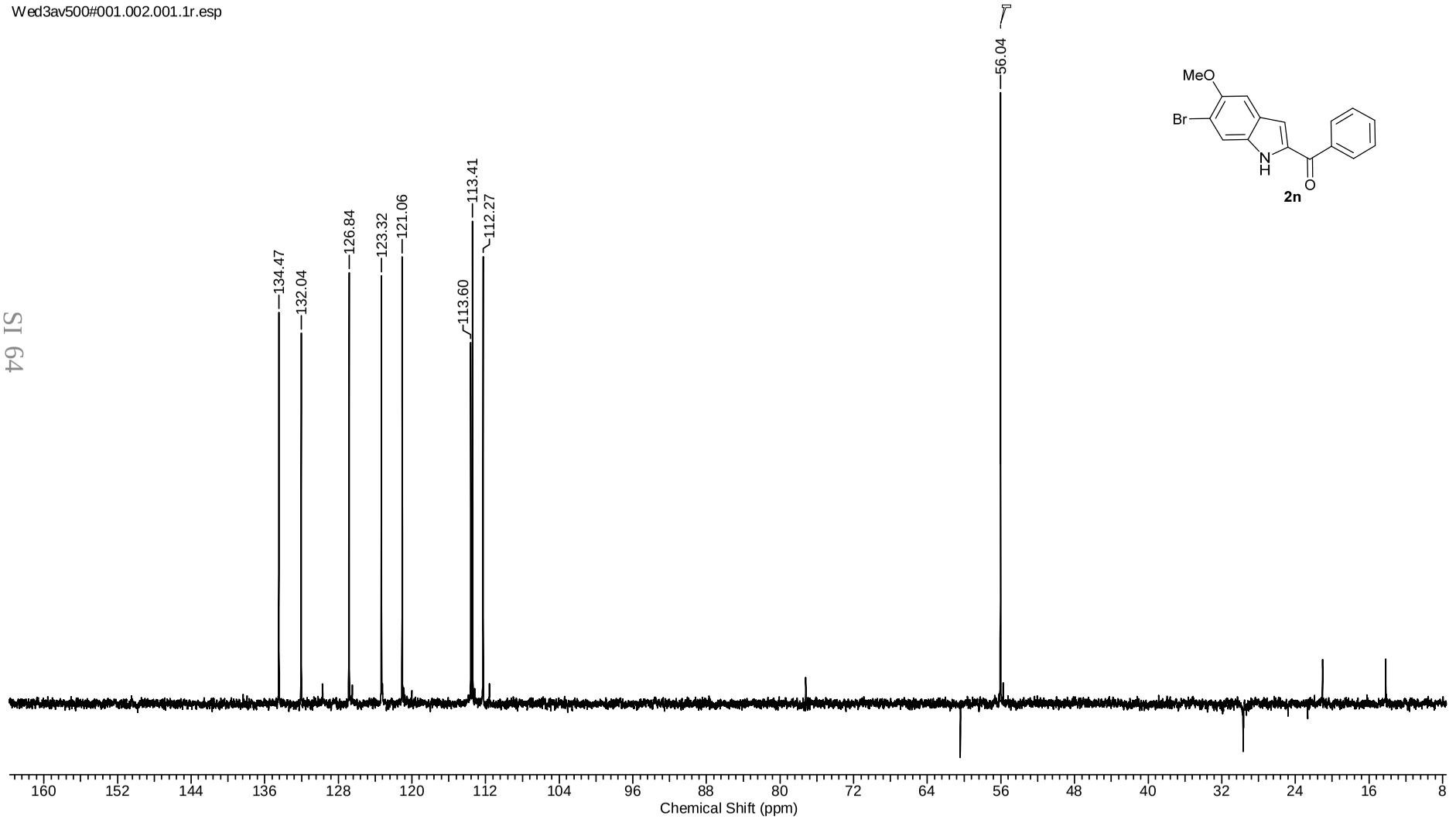
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	14 Aug 2013 10:49:04			***Date Stamp***	14 Aug 2013 10:49:04
File Name	H:\New folder\Wed3av500#001 ym-967\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	635
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11979.3203
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	22.500				

Wed3av500#001.003.001.1r.esp



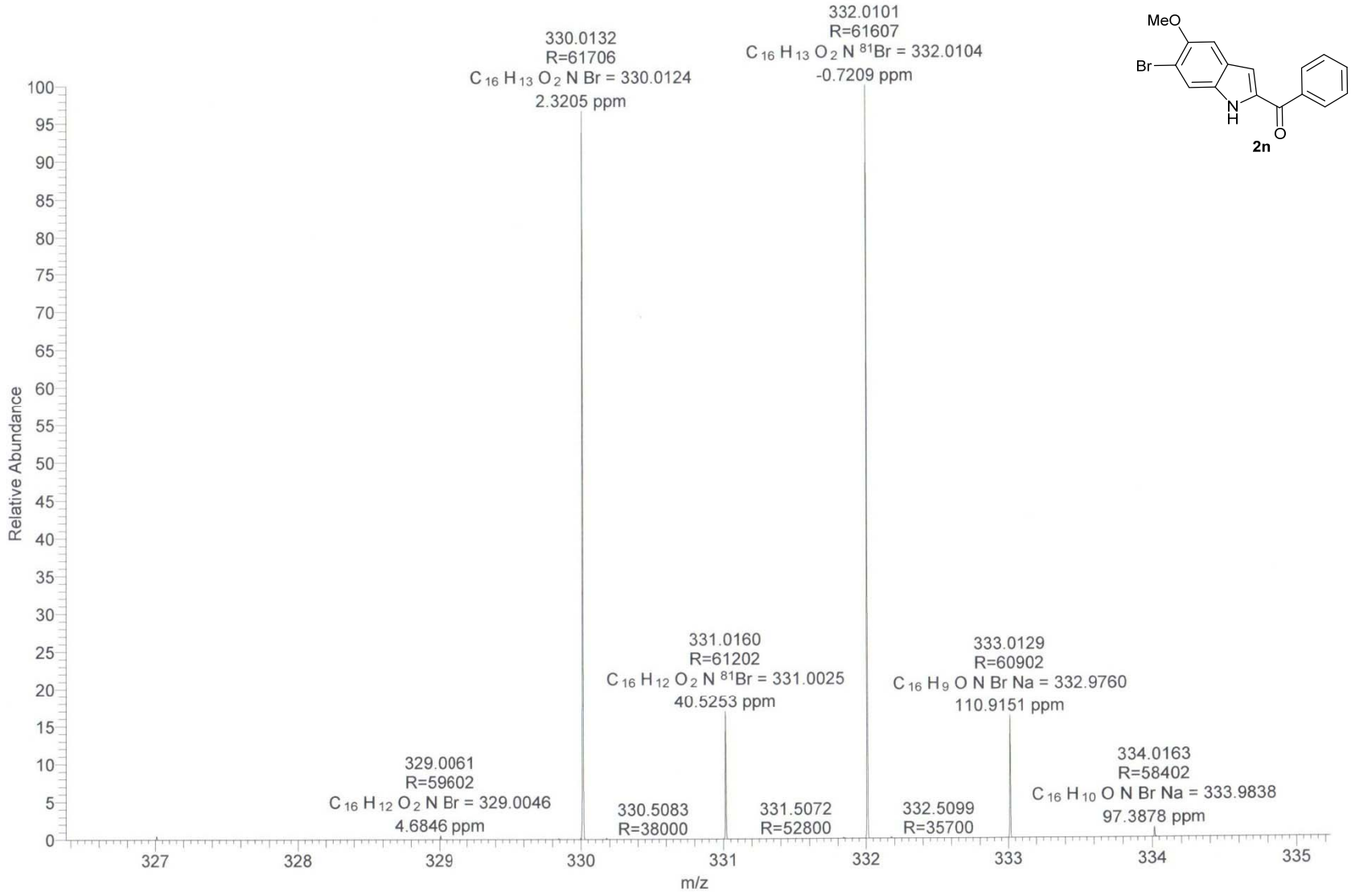
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	14 Aug 2013 10:27:44			***Date Stamp***	14 Aug 2013 10:27:44
File Name	H:\New folder\Wed3av500#001 ym-967\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1000
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12568.3320
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.000				

Wed3av500#001.002.001.1r.esp



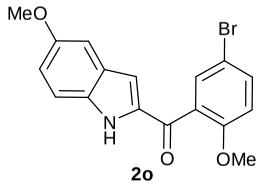
D:\Data\YM-990 9/16/2013 12:35:21 PM

YM-990 #1030 RT: 4.59 AV: 1 NL: 3.99E8
T: FTMS + p ESI Full ms [100.00-700.00]



Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	19 Aug 2013 17:25:52				
Date Stamp	19 Aug 2013 17:25:52			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Mon4av500#013\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	322.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.200								

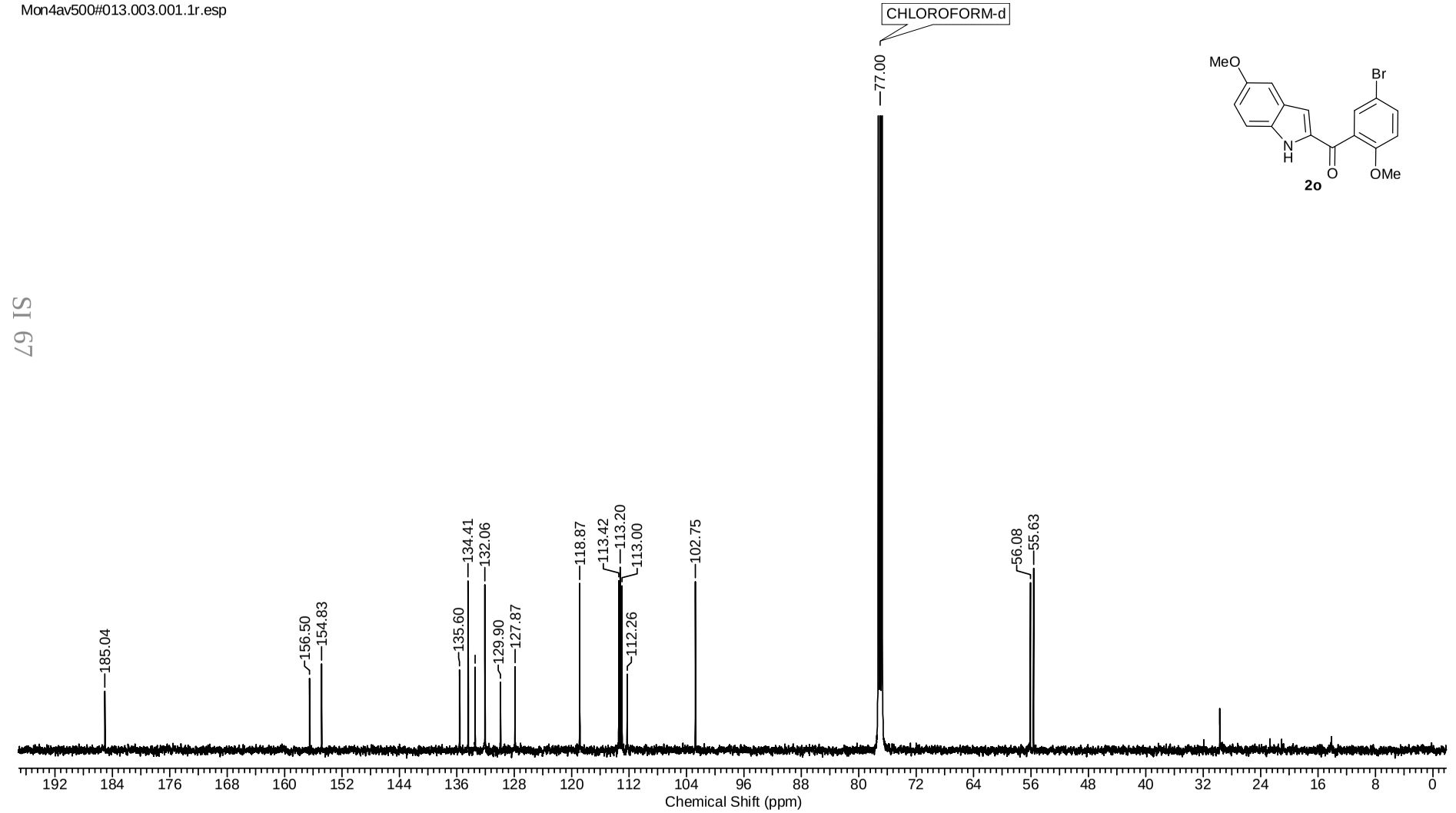
Mon4av500#013.001.001.1r.esp



2o

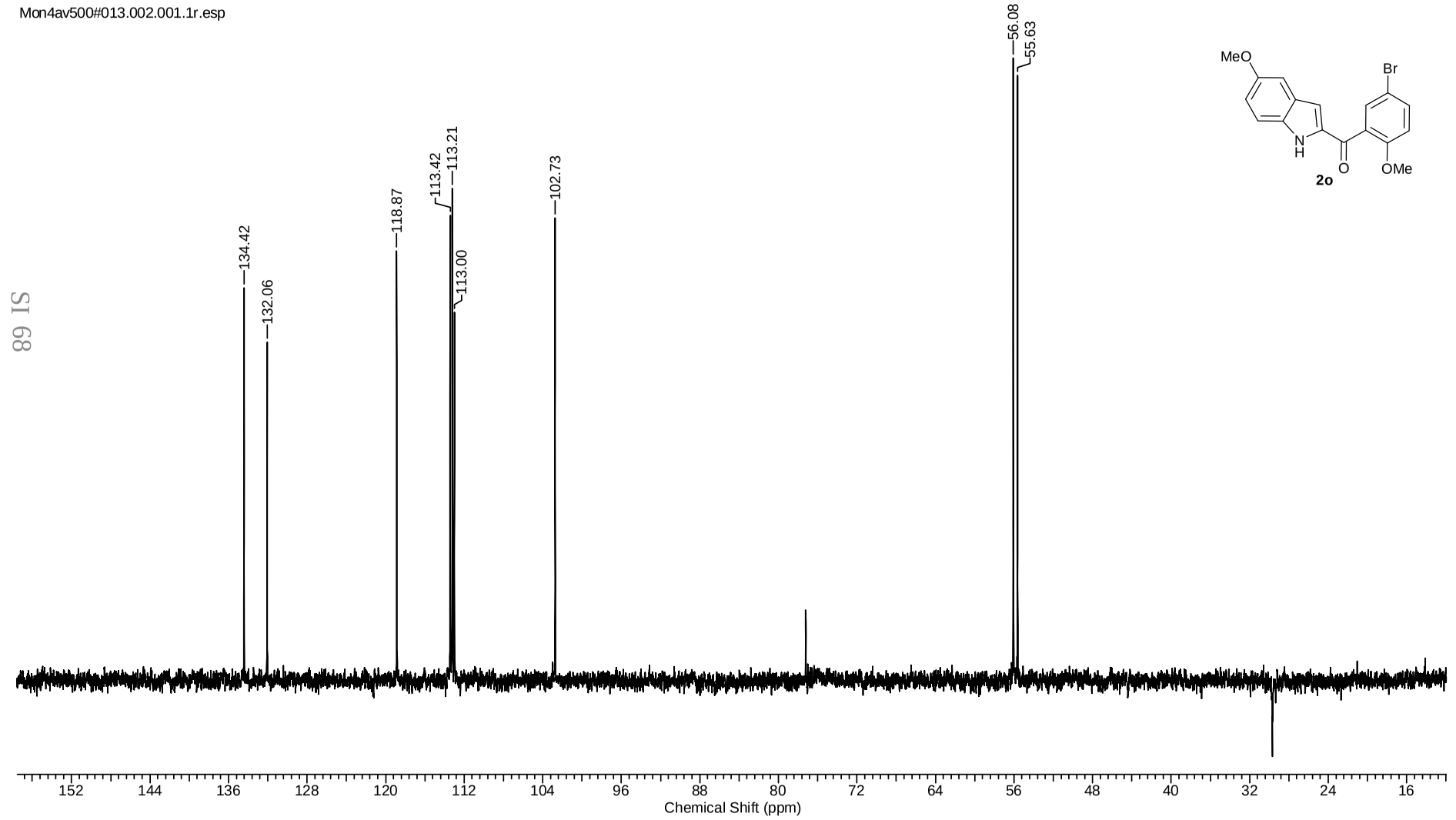
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	19 Aug 2013 20:08:00				
Date Stamp	19 Aug 2013 20:08:00			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Mon4av500#013\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	2102	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11982.1816	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	22.800								

Mon4av500#013.003.001.1r.esp



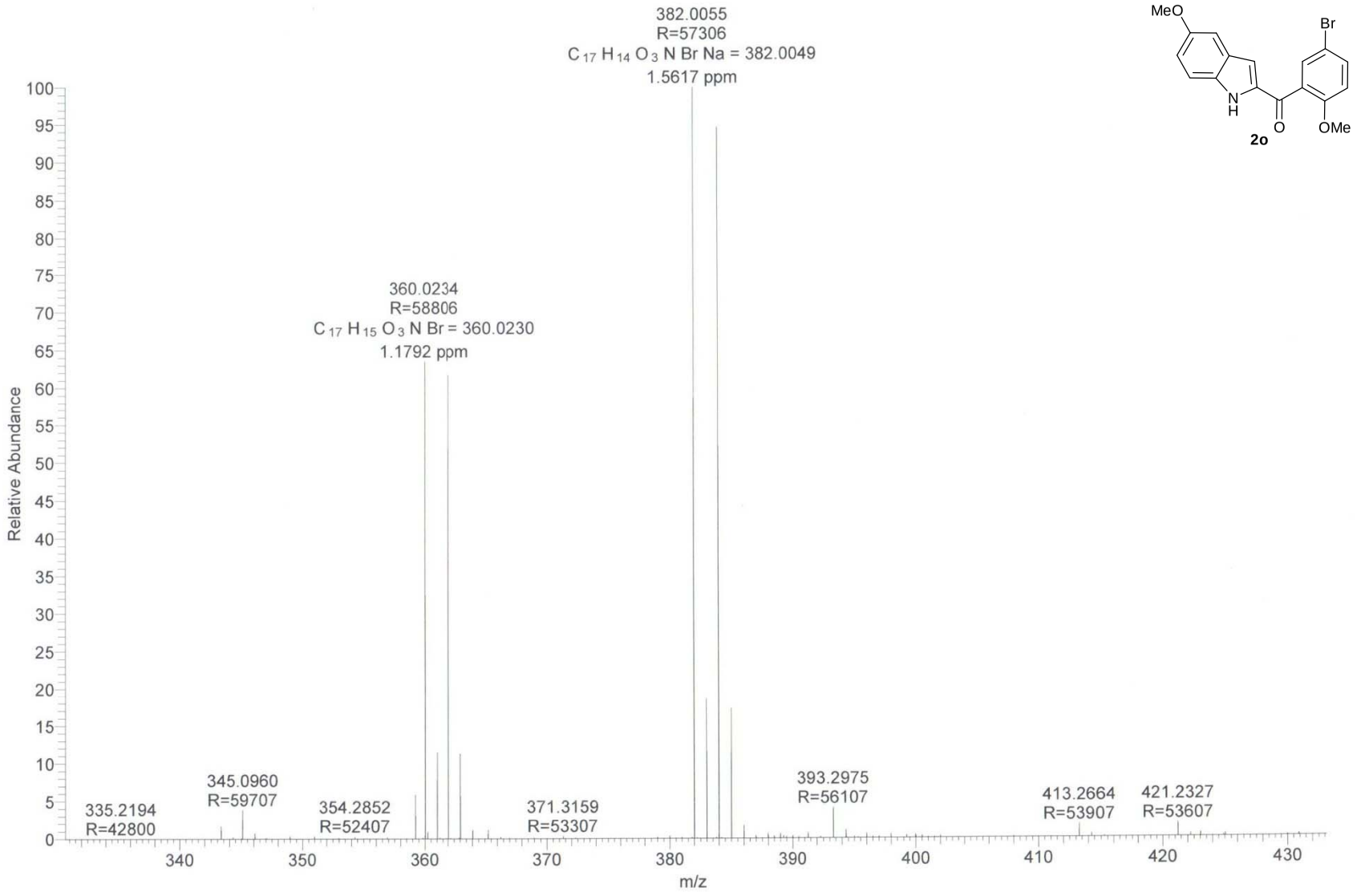
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	19 Aug 2013 18:19:12				
Date Stamp	19 Aug 2013 18:19:12			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Mon4av500#013\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1200	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12571.2676	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	22.500								

Mon4av500#013.002.001.1r.esp



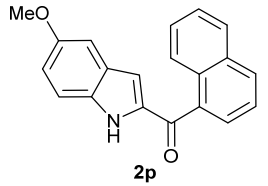
D:\Data\YM-976 9/16/2013 12:13:01 PM

YM-976 #1015 RT: 4.52 AV: 1 NL: 4.79E8
T: FTMS + p ESI Full ms [100.00-700.00]



Acquisition Time (sec)	2.0031	***Comment***	yogesh 1H	***Date***	16 Aug 2013 13:29:04			***Date Stamp***	16 Aug 2013 13:29:04
File Name	H:\New folder\Fri3av500#010\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	20031	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	322.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7742
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.70	***Temperature (degree C)***	22.400				

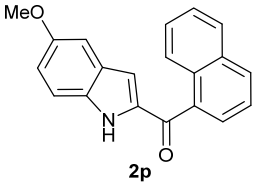
Fri3av500#010.001.001.1r.esp



2p

Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	16 Aug 2013 15:00:48			***Date Stamp***	16 Aug 2013 15:00:48
File Name	H:\New folder\Fri3av500#010\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1172
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	23.400				

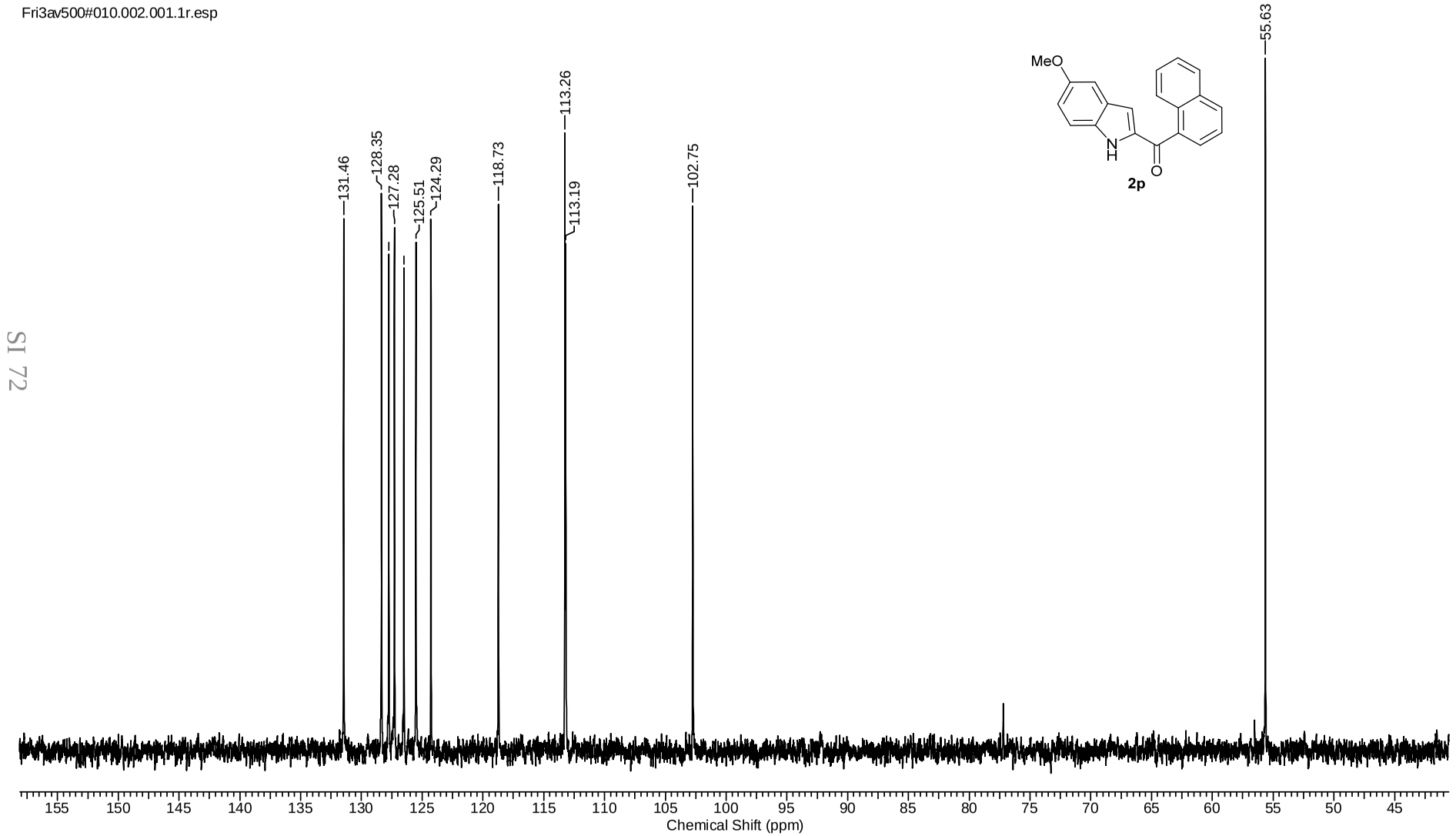
Fri3av500#010.003.001.1r.esp



2p

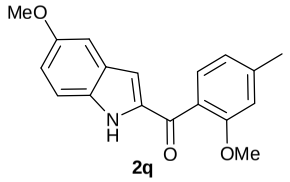
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	16 Aug 2013 13:44:00			***Date Stamp***	16 Aug 2013 13:44:00
File Name	H:\New folder\Fri3av500#010\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	700
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.3594
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.800				

Fri3av500#010.002.001.1r.esp



Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	17 Aug 2013 15:02:56			***Date Stamp***	17 Aug 2013 15:02:56
File Name	E:\New folder\Sat3av500#014\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	9
Origin	spect	***Original Points Count***	20031	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	322.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7742
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.70	***Temperature (degree C)***	22.700				

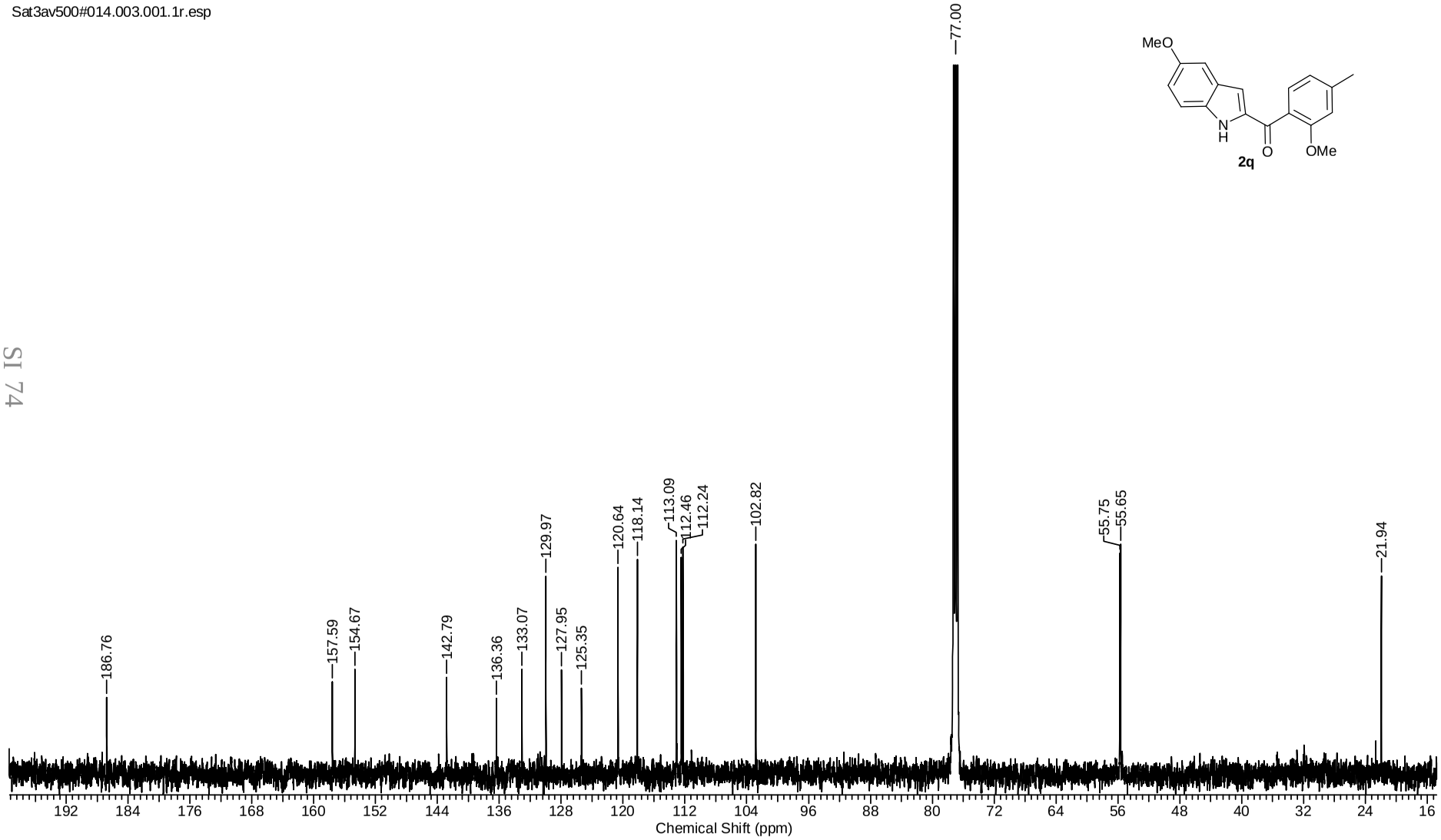
Sat3av500#014.001.001.1r.esp



2q

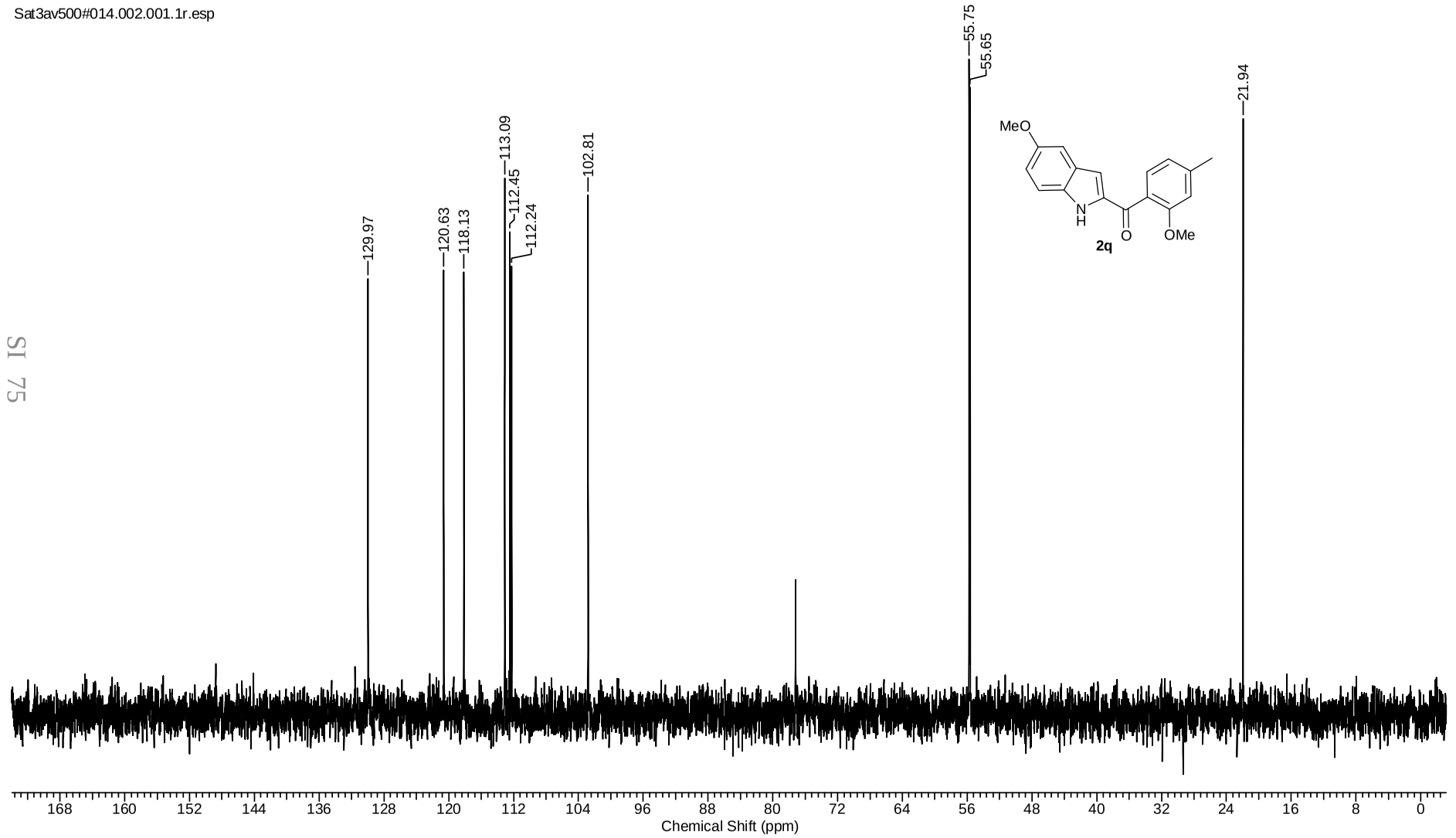
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	17 Aug 2013 15:43:28			***Date Stamp***	17 Aug 2013 15:43:28
File Name	E:\New folder\Sat3av500#014\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	959
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11982.1826
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	23.500				

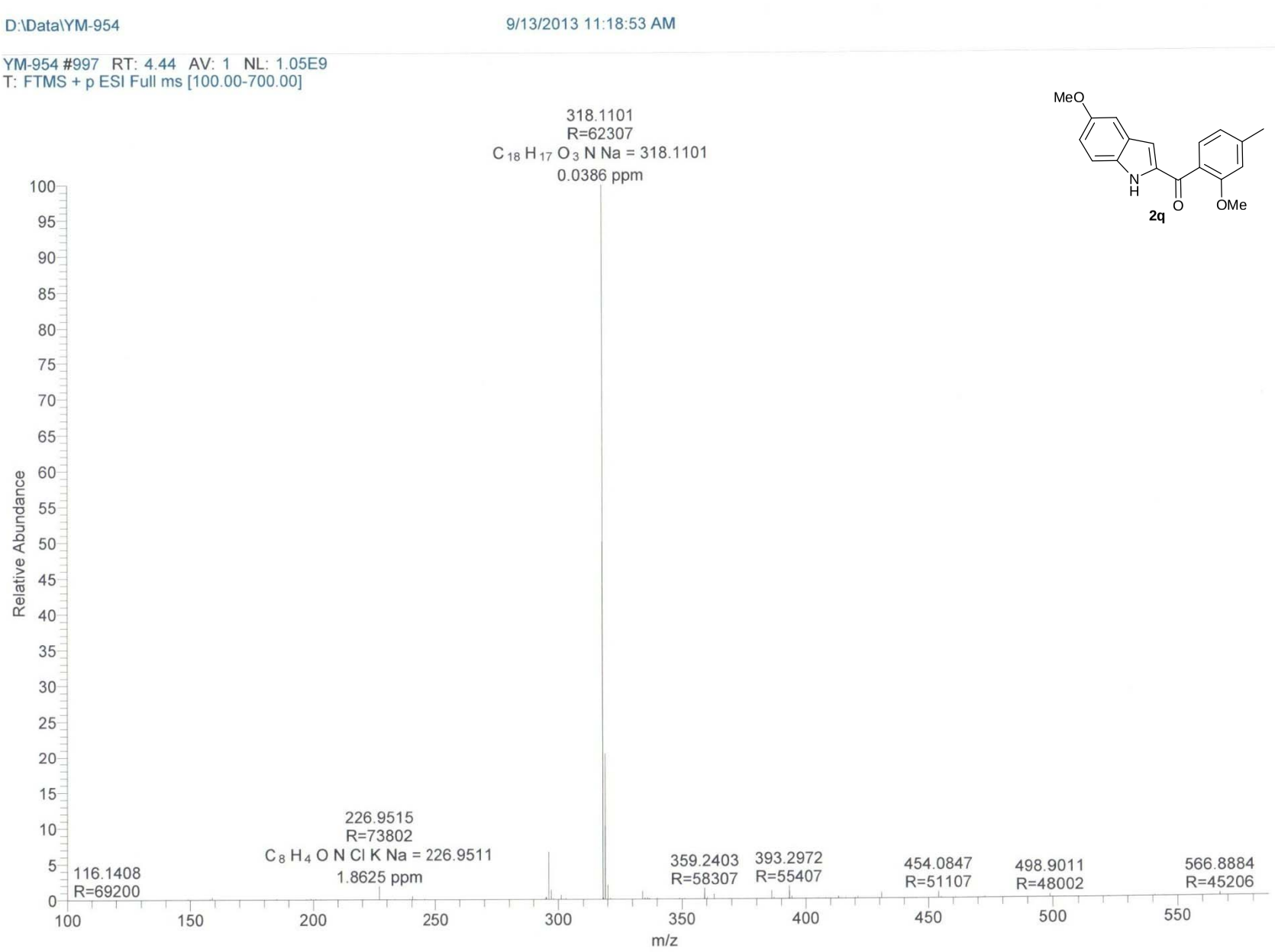
Sat3av500#014.003.001.1r.esp



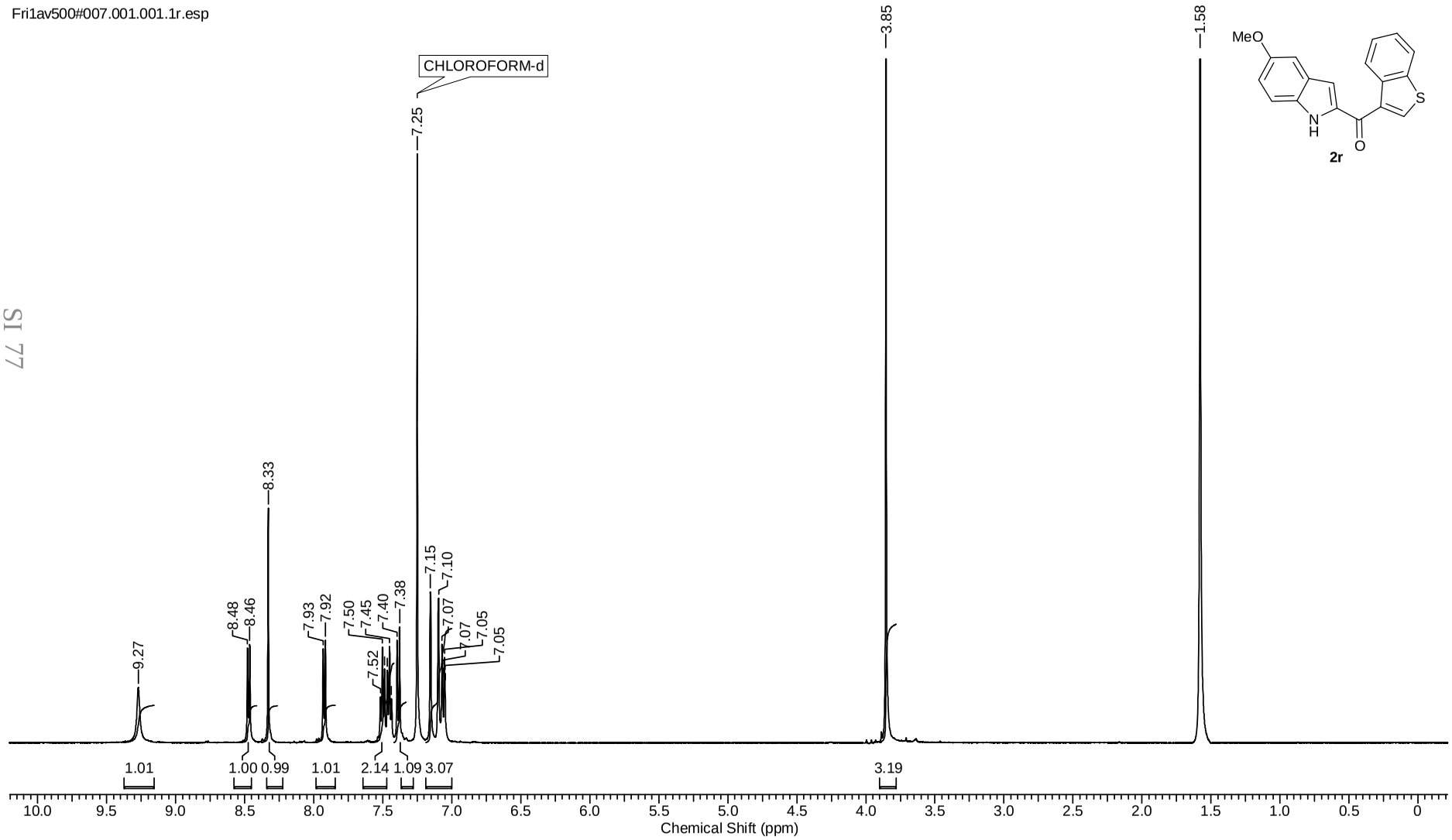
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	17 Aug 2013 15:02:56			***Date Stamp***	17 Aug 2013 15:02:56
File Name	E:\New folder\Sat3av500#014\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	600
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.6182
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.900				

Sat3av500#014.002.001.1r.esp



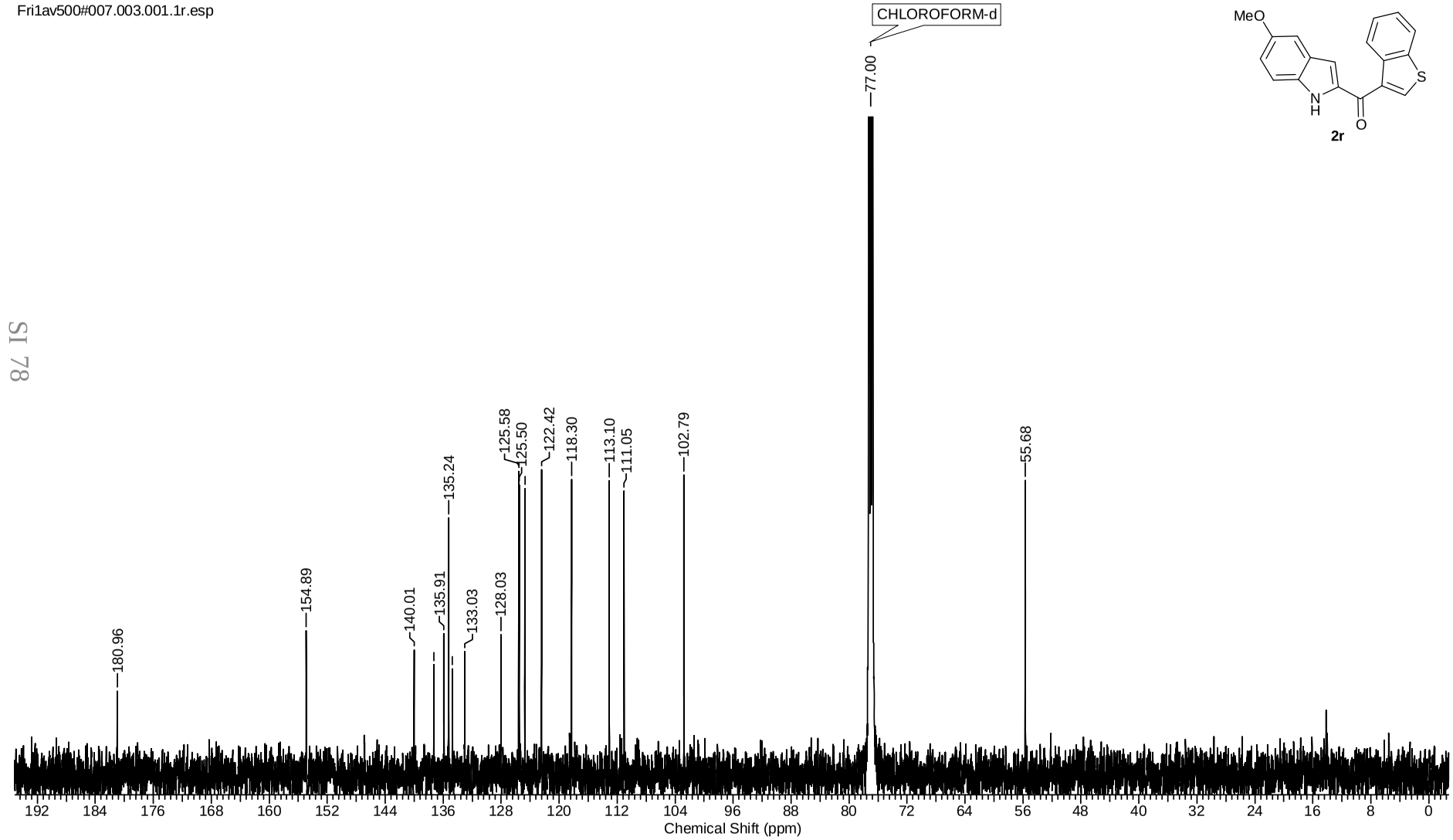

D:\Data\YM-954
9/13/2013 11:18:53 AM
YM-954 #997 RT: 4.44 AV: 1 NL: 1.05E9
T: FTMS + p ESI Full ms [100.00-700.00]
318.1101
R=62307
C 18 H 17 O 3 N Na = 318.1101
0.0386 ppm
MeO
N
H
O
OMe
2q
Relative Abundance
m/z
226.9515
R=73802
C 8 H 4 O N Cl K Na = 226.9511
1.8625 ppm
116.1408
R=69200
359.2403
R=58307
393.2972
R=55407
454.0847
R=51107
498.9011
R=48002
566.8884
R=45206

Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	02 Aug 2013 14:11:44			***Date Stamp***	02 Aug 2013 14:11:44
File Name	H:\New folder\Fri1av500#007\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H	***Number of Transients***	64
Origin	spect	***Original Points Count***	20031	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	512.00	***SW(cyclical) (Hz)***	10000.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7742
Spectrum Type	STANDARD	***Sweep Width (Hz)***	9999.70	***Temperature (degree C)***	22.300				



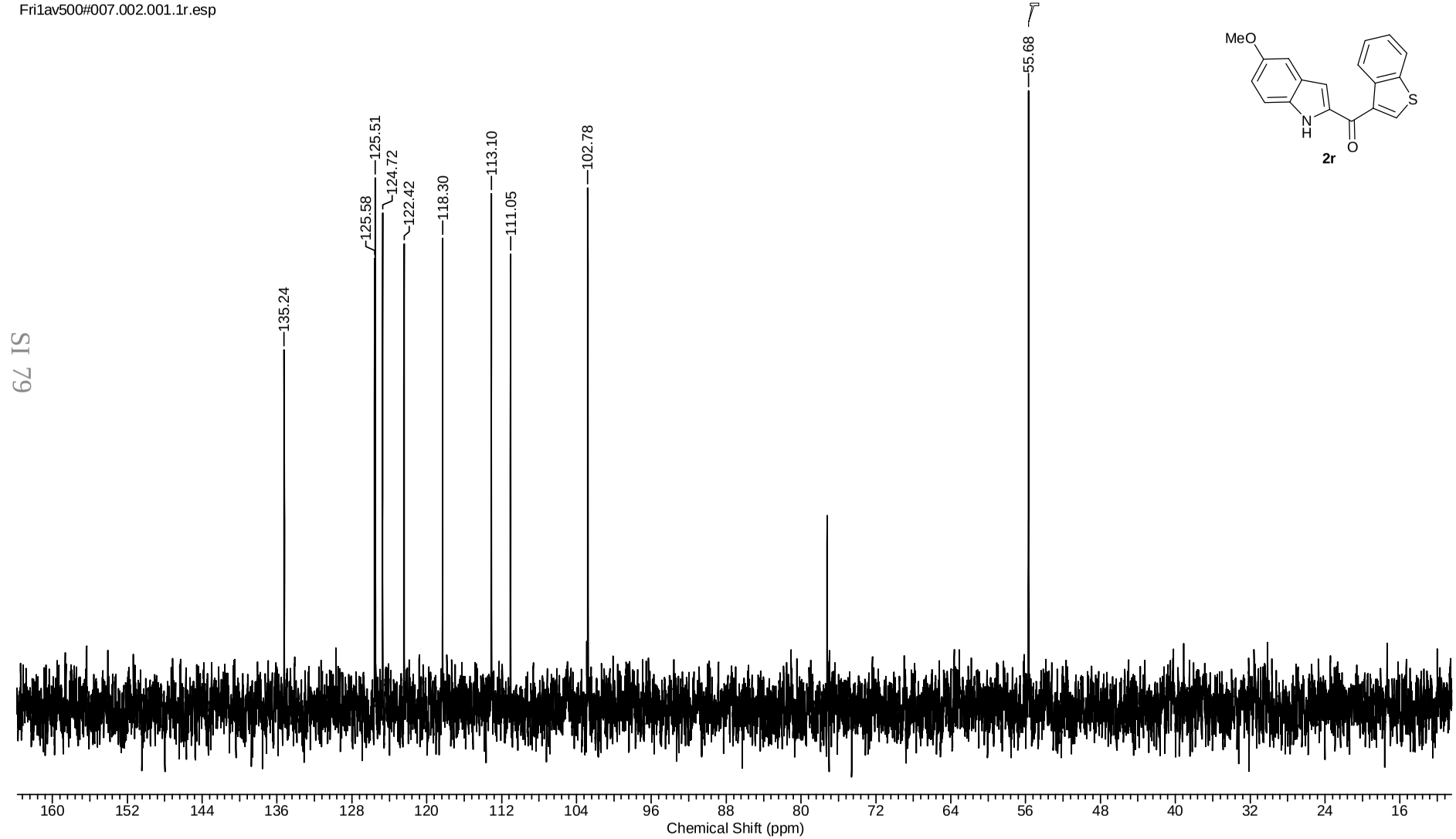
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	02 Aug 2013 14:52:16			***Date Stamp***	02 Aug 2013 14:52:16
File Name	H:\New folder\Fri1av500#007\3\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	1223
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	575.00	***SW(cyclical) (Hz)***	31250.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	11983.1357
Spectrum Type	STANDARD	***Sweep Width (Hz)***	31249.05	***Temperature (degree C)***	23.000				

Fri1av500#007.003.001.1r.esp



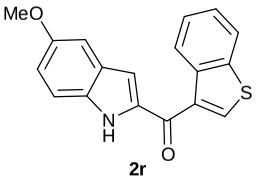
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	02 Aug 2013 14:35:12			***Date Stamp***	02 Aug 2013 14:35:12
File Name	H:\New folder\Fri1av500#007\2\PDATA\1\1r			***Frequency (MHz)***	125.76	***Nucleus***	13C	***Number of Transients***	800
Origin	spect	***Original Points Count***	32768	***Owner***	nmr	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	29761.90	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	12572.1055
Spectrum Type	DEPT135	***Sweep Width (Hz)***	29761.00	***Temperature (degree C)***	22.600				

Fri1av500#007.002.001.1r.esp



D:\Data\YM-961 9/16/2013 11:50:39 AM

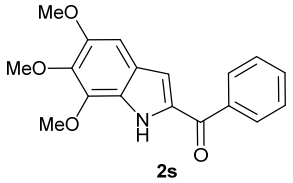
YM-961 #1053 RT: 4.69 AV: 1 NL: 1.90E8
T: FTMS + p ESI Full ms [100.00-700.00]



2r

Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	08 Sep 2013 12:05:52				
Date Stamp	08 Sep 2013 12:05:52			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sun2av500#001\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	362.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7742	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	24.800								

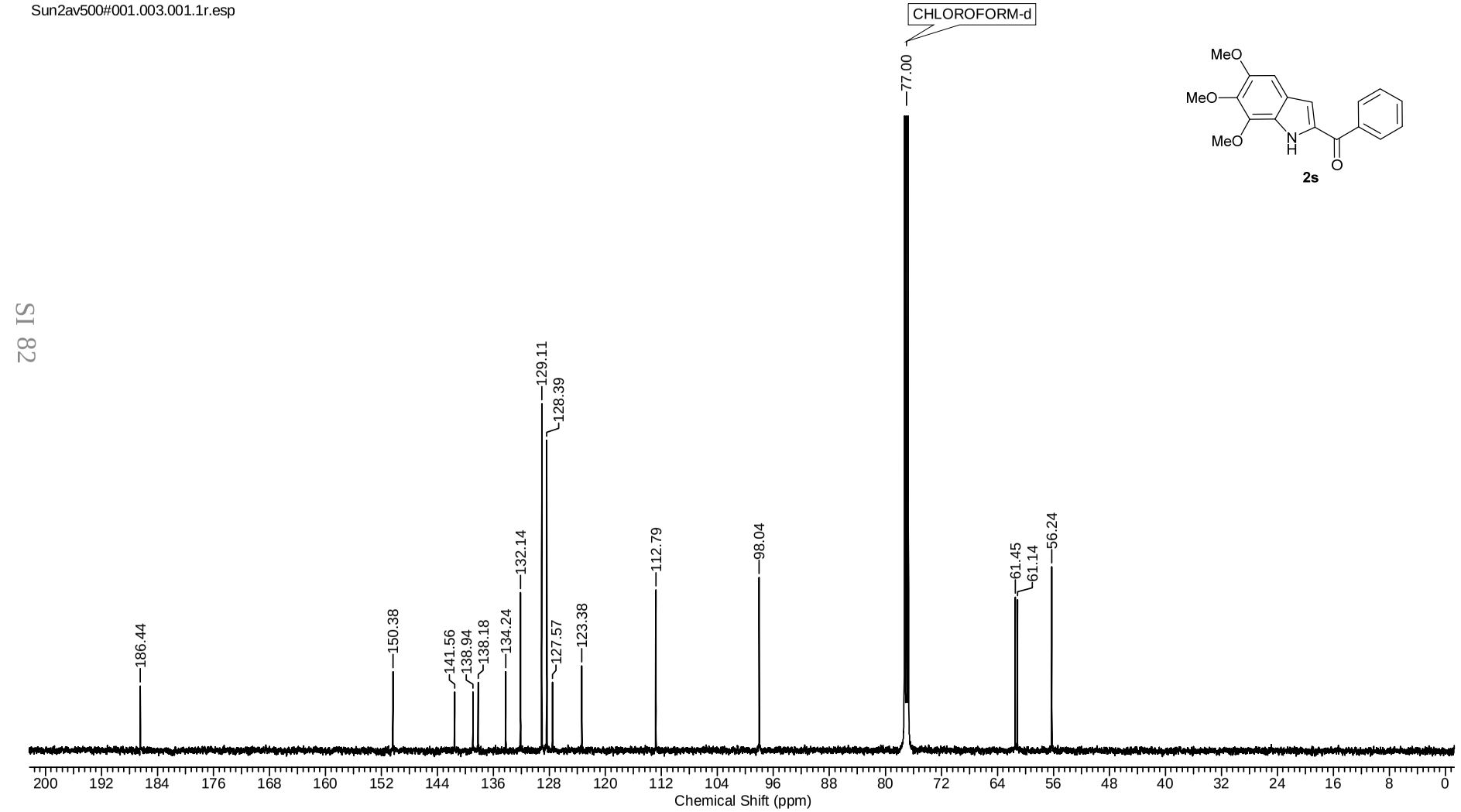
Sun2av500#001.001.001.1r.esp



2s

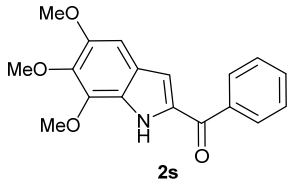
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	08 Sep 2013 13:50:24				
Date Stamp	08 Sep 2013 13:50:24			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sun2av500#001\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1862	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11982.1826	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	25.700								

Sun2av500#001.003.001.1r.esp



Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	08 Sep 2013 12:12:16				
Date Stamp	08 Sep 2013 12:12:16			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sun2av500#001\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	183	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12572.5947	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	25.100								

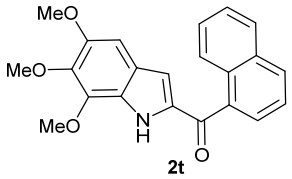
Sun2av500#001.002.001.1r.esp



2s

Acquisition Time (sec)	1.9923	***Comment***	Yogesh 1H	***Date***	15 Aug 2013 17:31:52				
Date Stamp	15 Aug 2013 17:31:52			***File Name***	\\agni\nmr_data\AV400\Aug_13_400\Thu3av400#004\1\PDATA\1\1r				
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	16384
Owner	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	256.00	***SW(cyclical) (Hz)***	8223.68
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2456.8564	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.43
Temperature (degree C)	22.200								

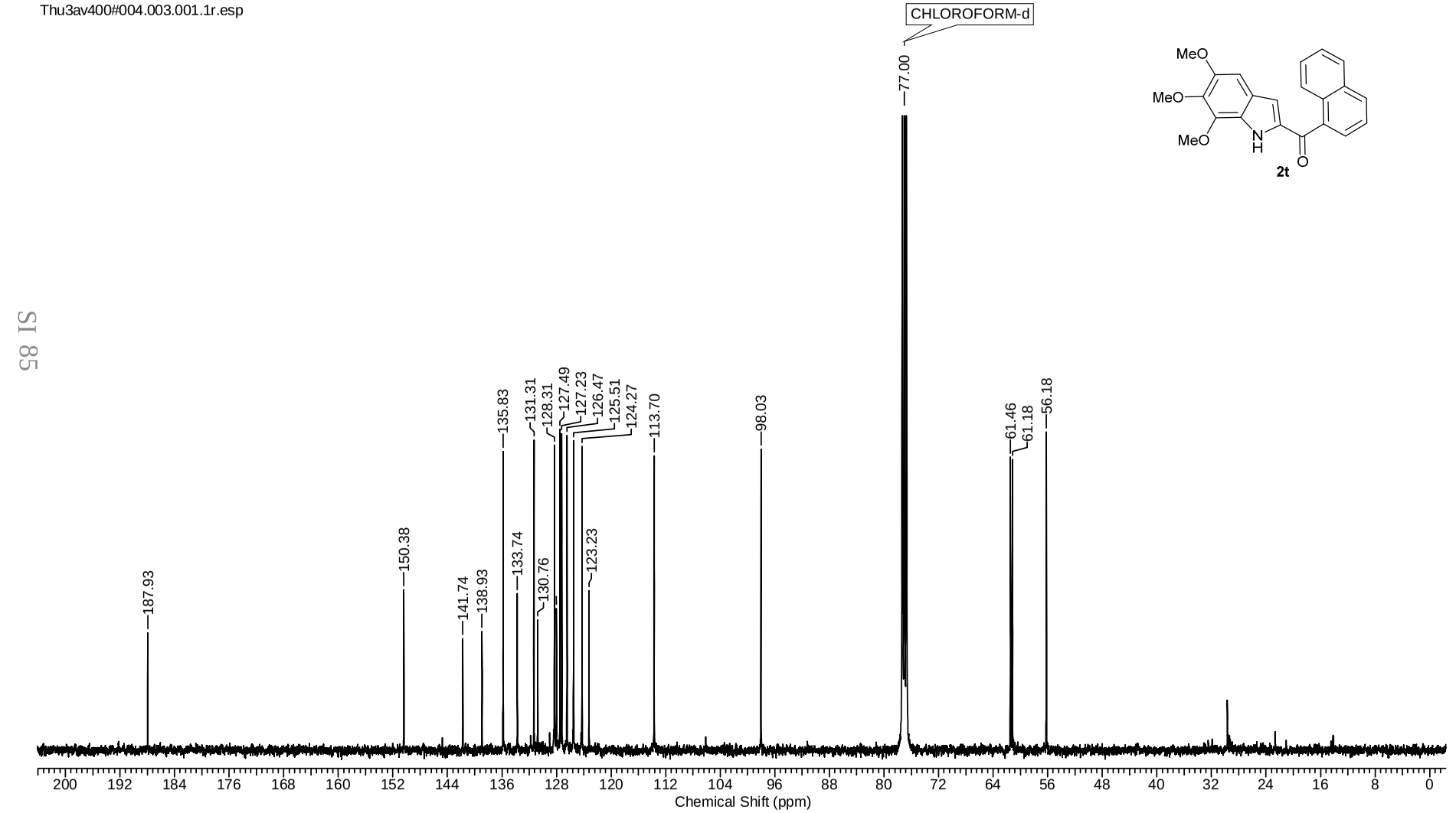
Thu3av400#004.001.001.1r.esp



2t

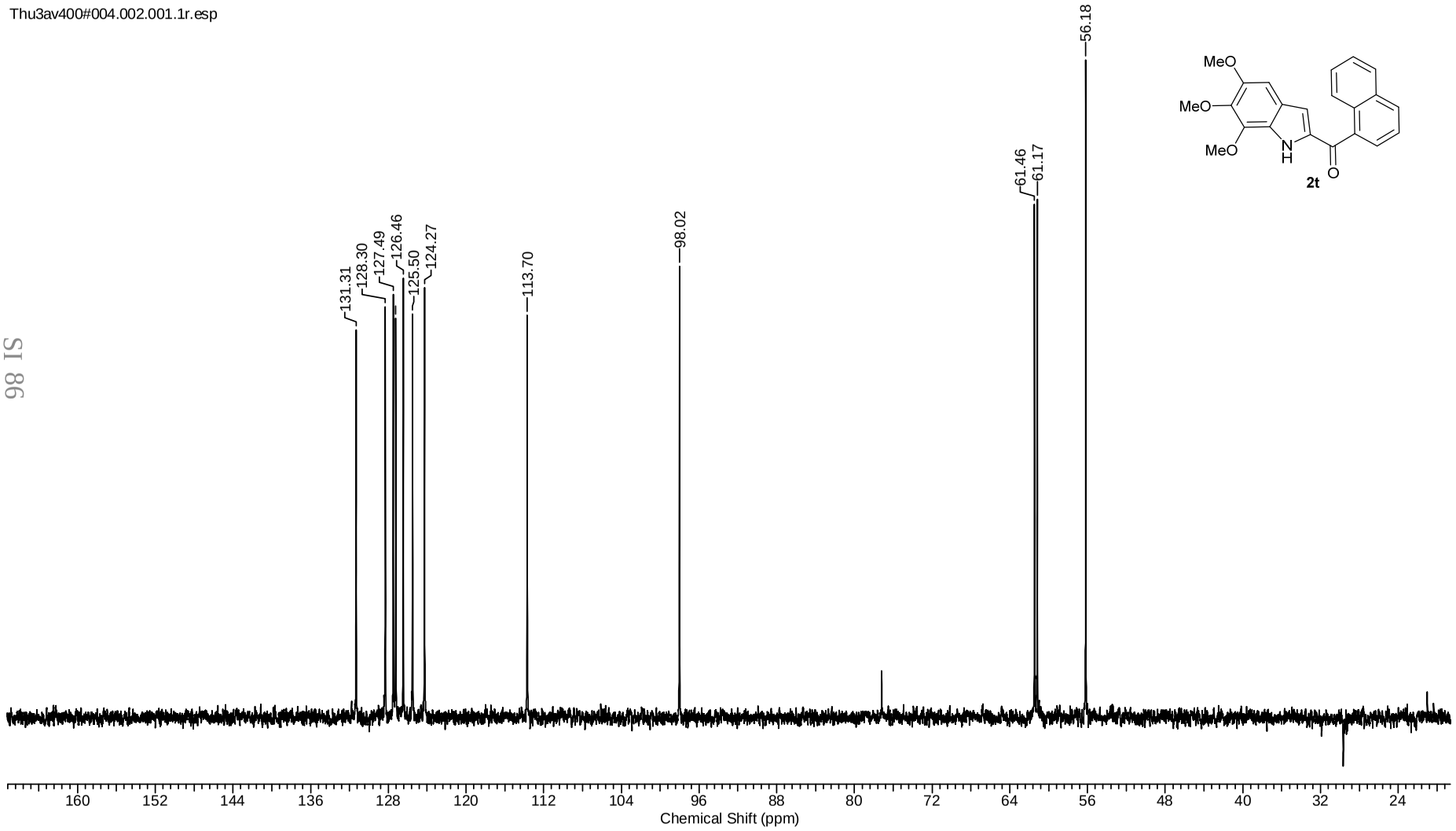
Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	15 Aug 2013 21:20:08				
Date Stamp	15 Aug 2013 21:20:08			***File Name***	\\agni\nmr_data\AV400\Aug_13_400\Thu3av400#004\3\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	4000	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	9553.9619	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	22.300								

Thu3av400#004.003.001.1r.esp



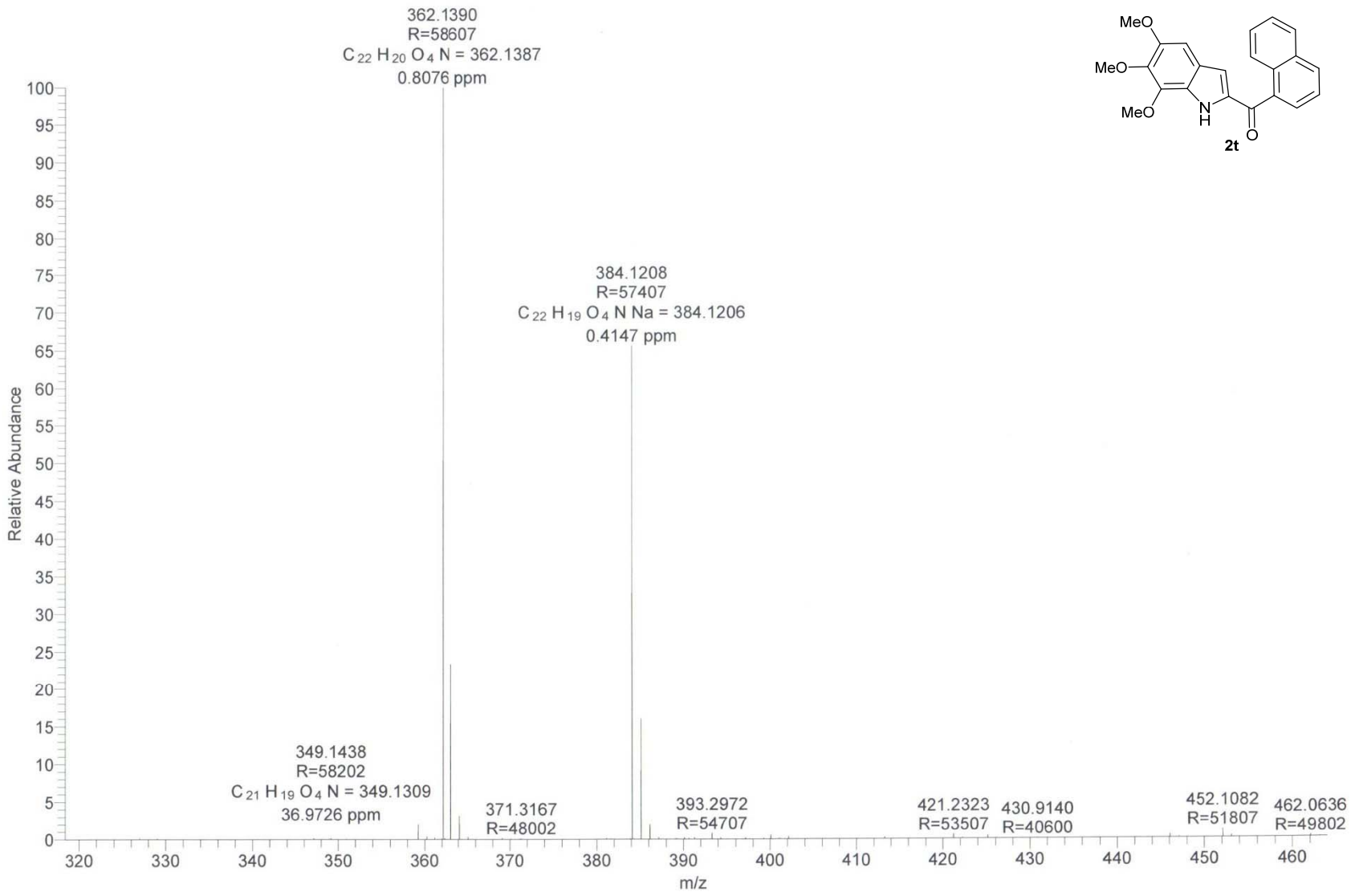
Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	15 Aug 2013 18:18:48				
Date Stamp	15 Aug 2013 18:18:48			***File Name***	\\agni\nmr_data\AV400\Aug_13_400\Thu3av400#004\2\PDATA\1\1r				
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1000	***Origin***	spect	***Original Points Count***	16384
Owner	root	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	16384.00	***SW(cyclical) (Hz)***	25252.53
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	10055.5107	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	25251.75
Temperature (degree C)	22.300								

Thu3av400#004.002.001.1r.esp



D:\Data\YM-977 9/16/2013 12:24:11 PM

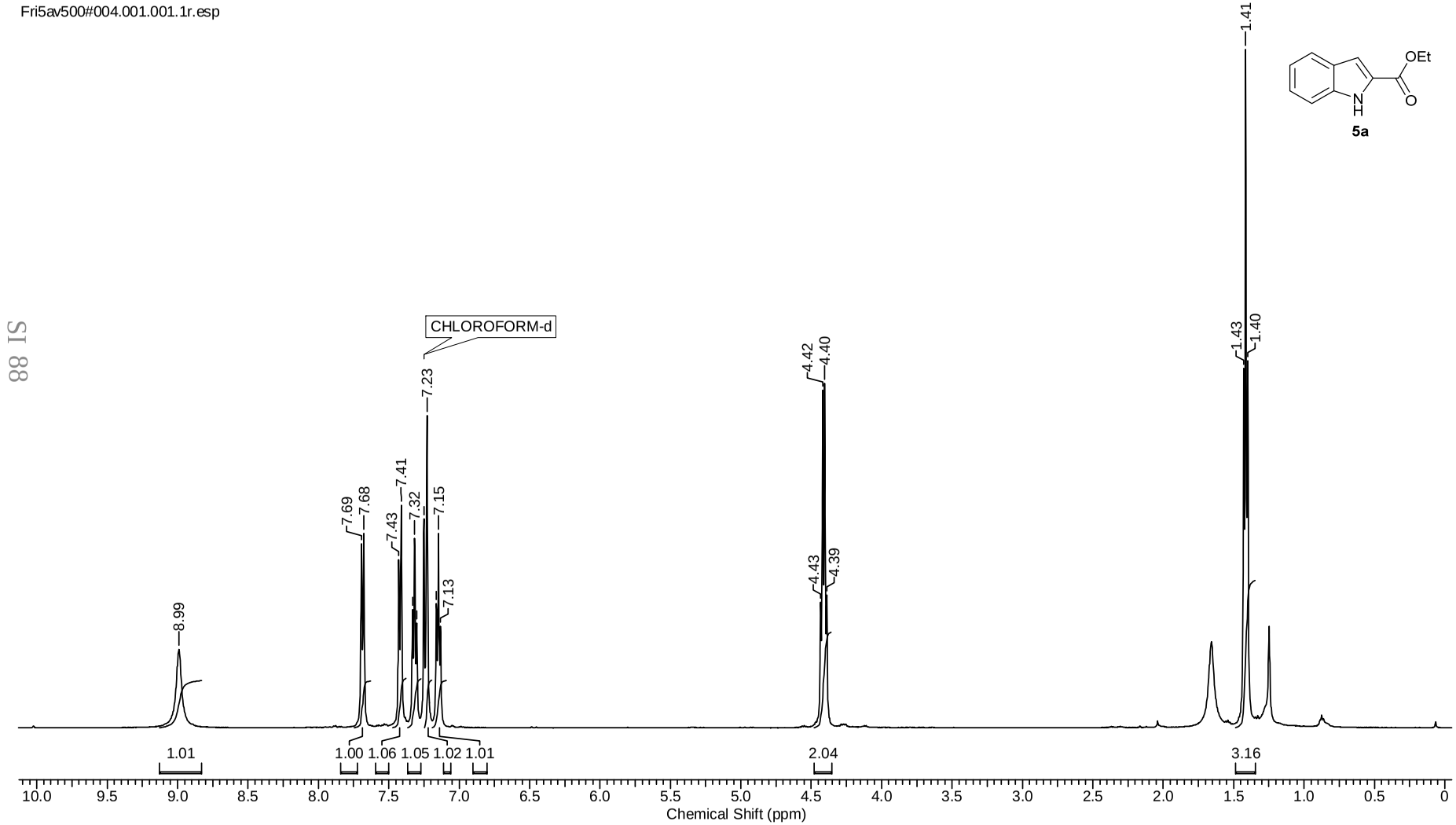
YM-977 #1048 RT: 4.67 AV: 1 NL: 1.36E9
T: FTMS + p ESI Full ms [100.00-700.00]



2t

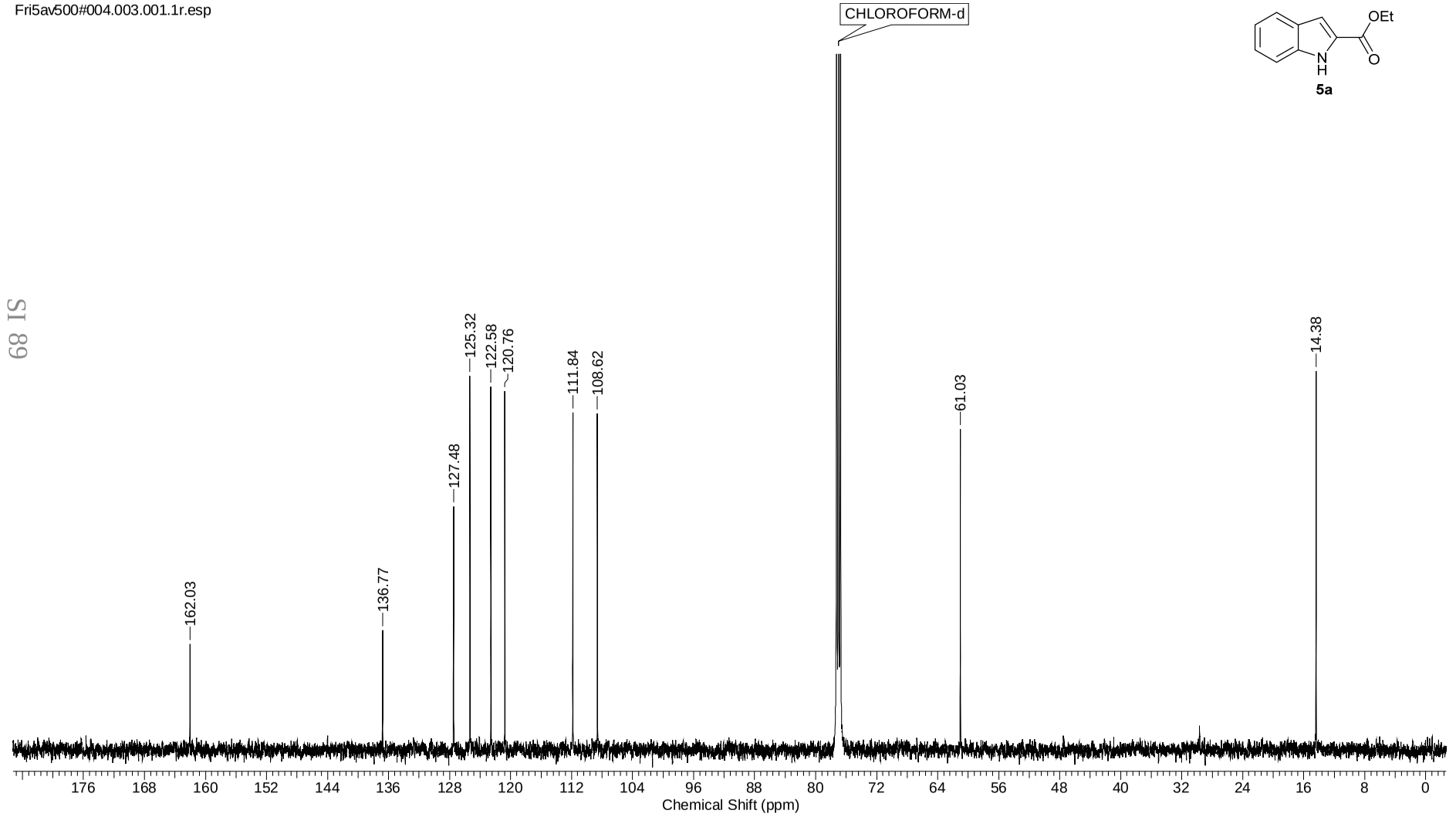
Acquisition Time (sec)	2.0031	***Comment***	yogesh 1H	***Date***	30 Aug 2013 11:12:32				
Date Stamp	30 Aug 2013 11:12:32			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Fri5av500#004\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	322.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2219.7769	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.100								

Fri5av500#004.001.001.1r.esp



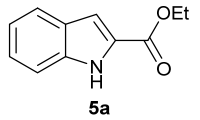
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	30 Aug 2013 12:14:24				
Date Stamp	30 Aug 2013 12:14:24			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Fri5av500#004\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	674	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	22.900								

Fri5av500#004.003.001.1r.esp



Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	30 Aug 2013 11:33:52				
Date Stamp	30 Aug 2013 11:33:52			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Fri5av500#004\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	600	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12569.9307	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	22.400								

Fri5av500#004.002.001.1r.esp



5a

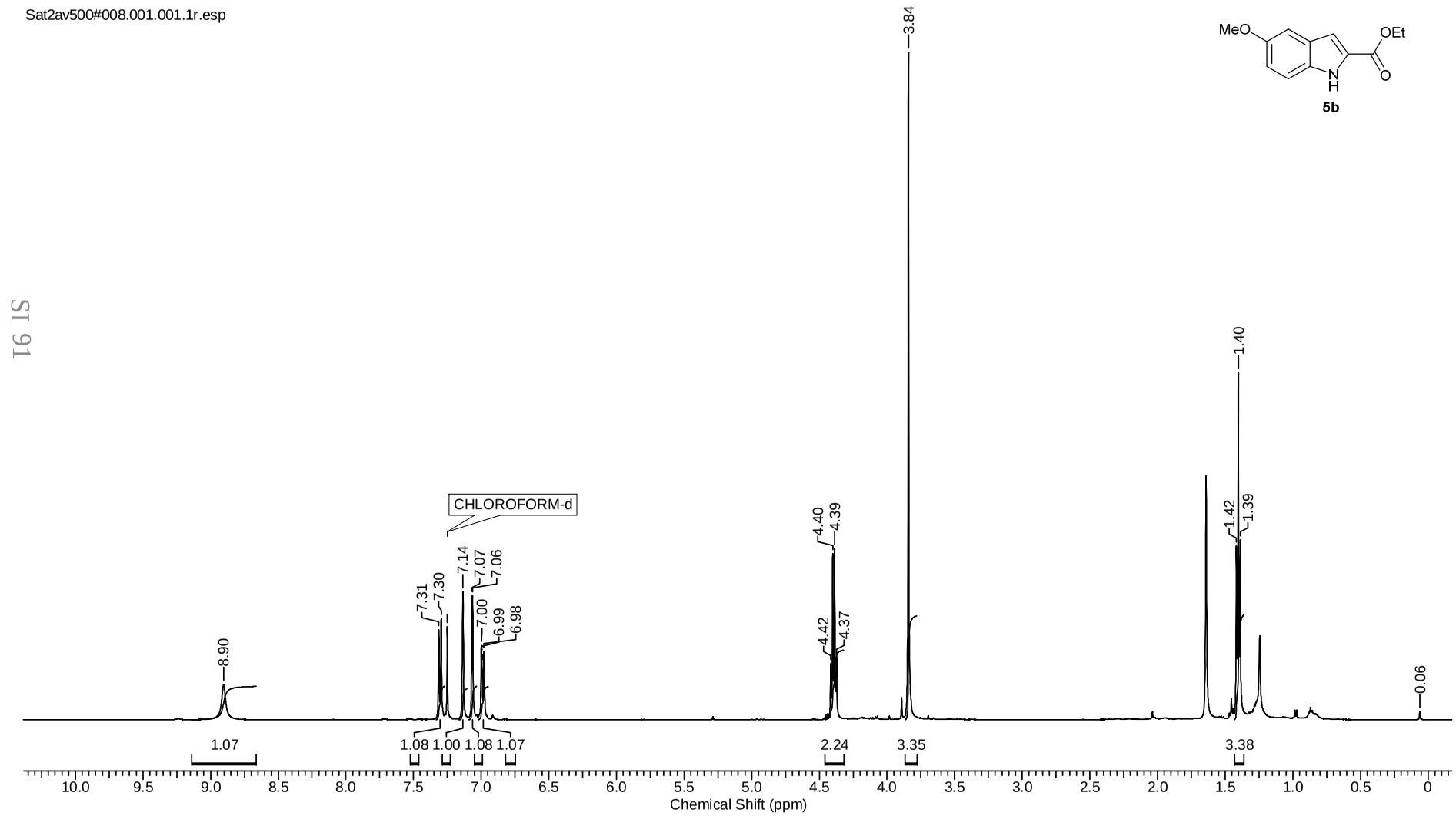
125.31
122.58
120.76
111.83
108.62
14.38
61.02

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)

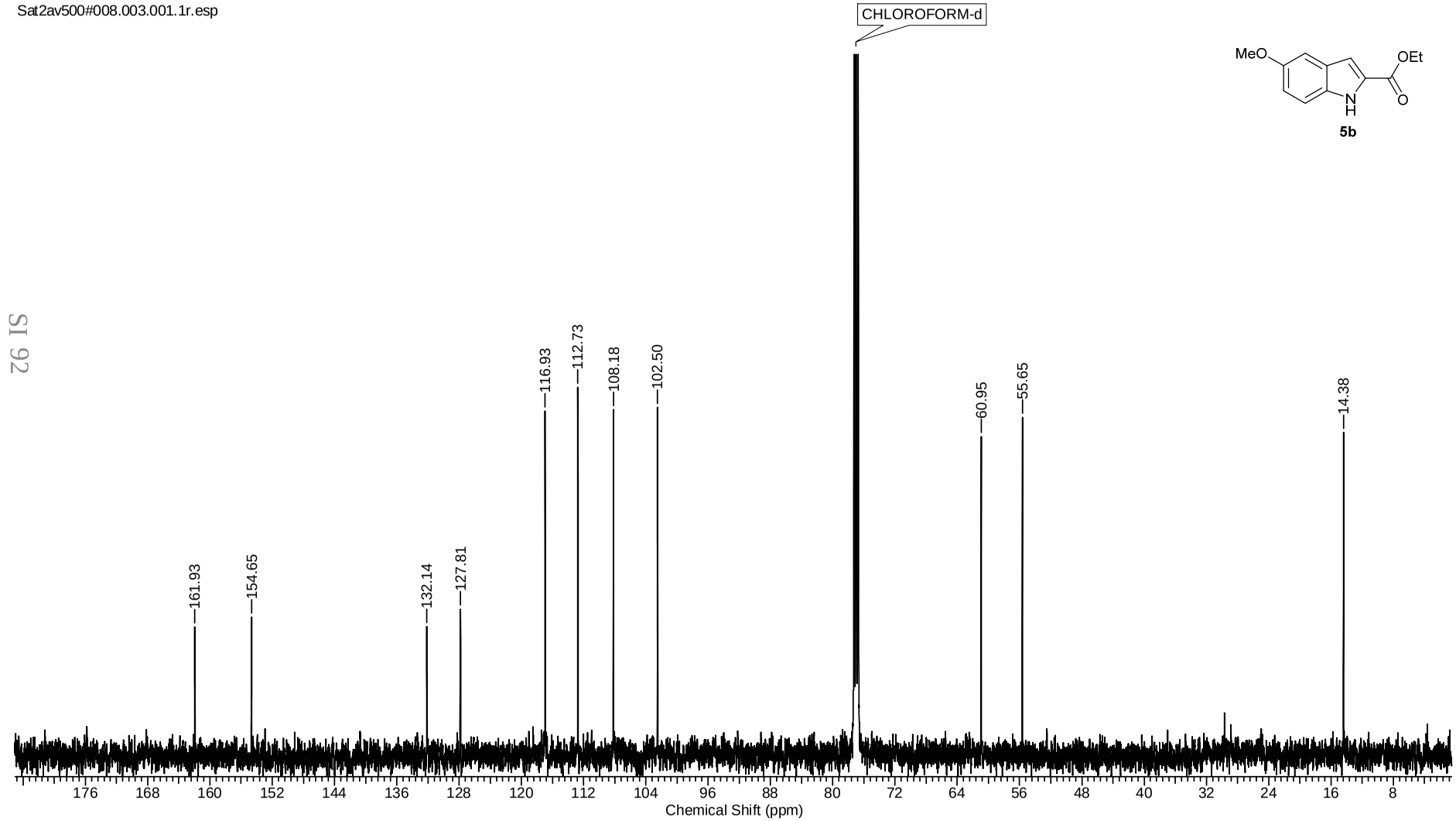
Acquisition Time (sec)	2.0031	***Comment***	yogesh 1H	***Date***	14 Sep 2013 13:22:40				
Date Stamp	14 Sep 2013 13:22:40			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sat2av500#008\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	287.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7742	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.100								

Sat2av500#008.001.001.1r.esp



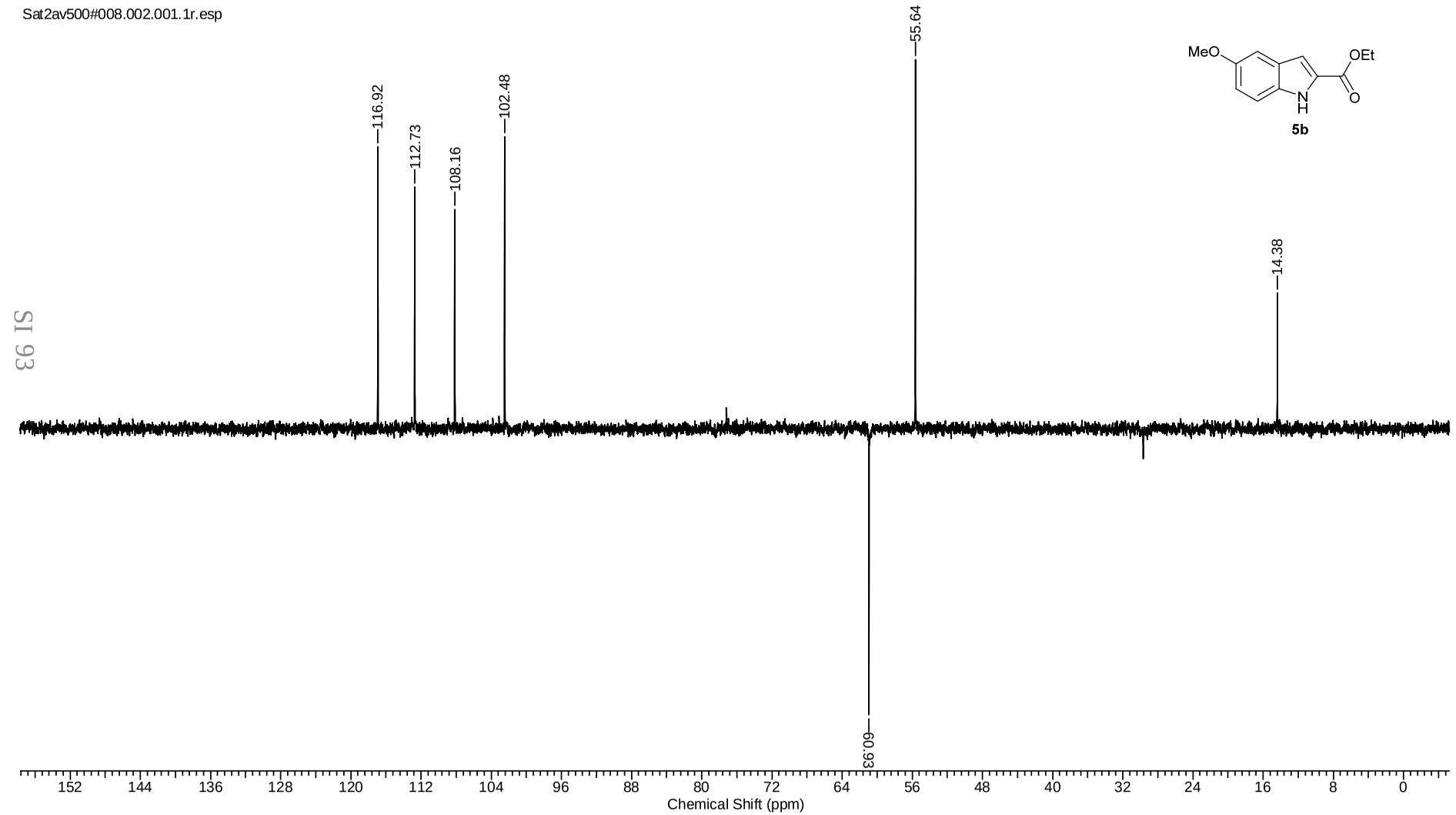
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	14 Sep 2013 13:58:56				
Date Stamp	14 Sep 2013 13:58:56			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sat2av500#008\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	223	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	23.000								

Sat2av500#008.003.001.1r.esp



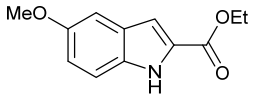
Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	14 Sep 2013 13:48:16				
Date Stamp	14 Sep 2013 13:48:16			***File Name***	\\agni\nmr_data\AV_500\Sep_13_500\Sat2av500#008\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	600	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12569.0225	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	22.500								

Sat2av500#008.002.001.1r.esp

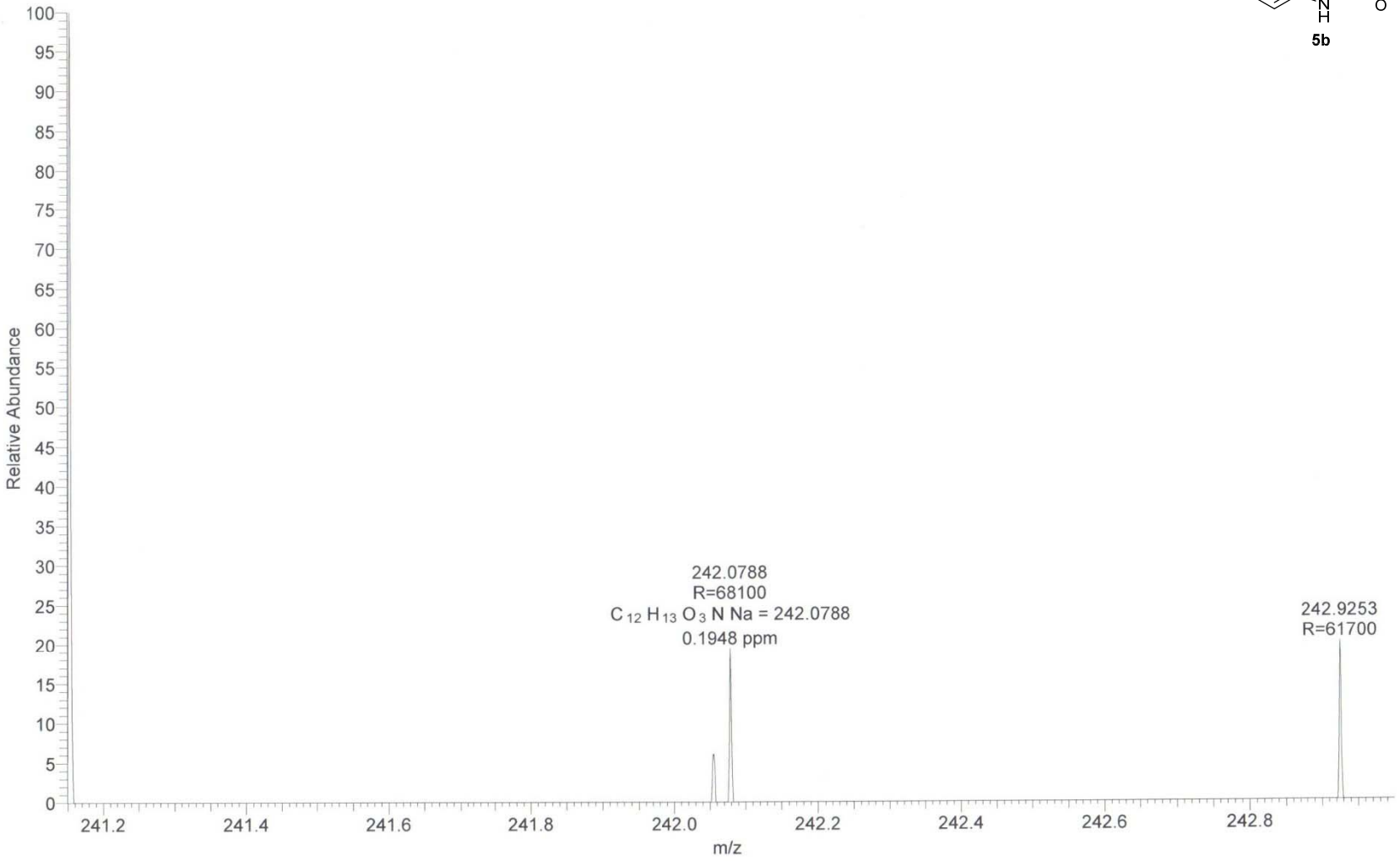


D:\Data\YM-988 9/13/2013 11:41:18 AM

YM-988 #894 RT: 3.98 AV: 1 NL: 1.12E6
T: FTMS + p ESI Full ms [100.00-700.00]

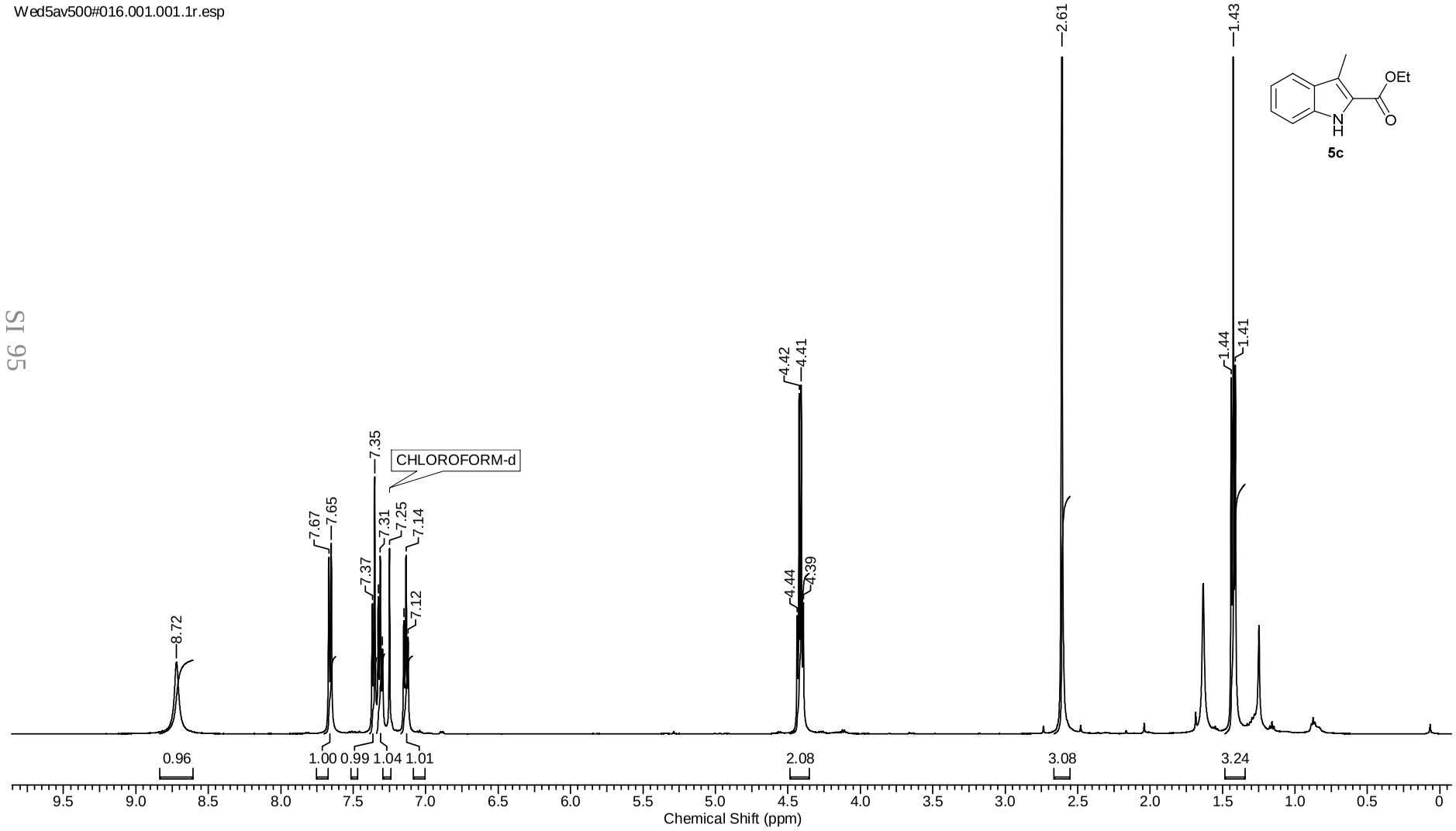


5b



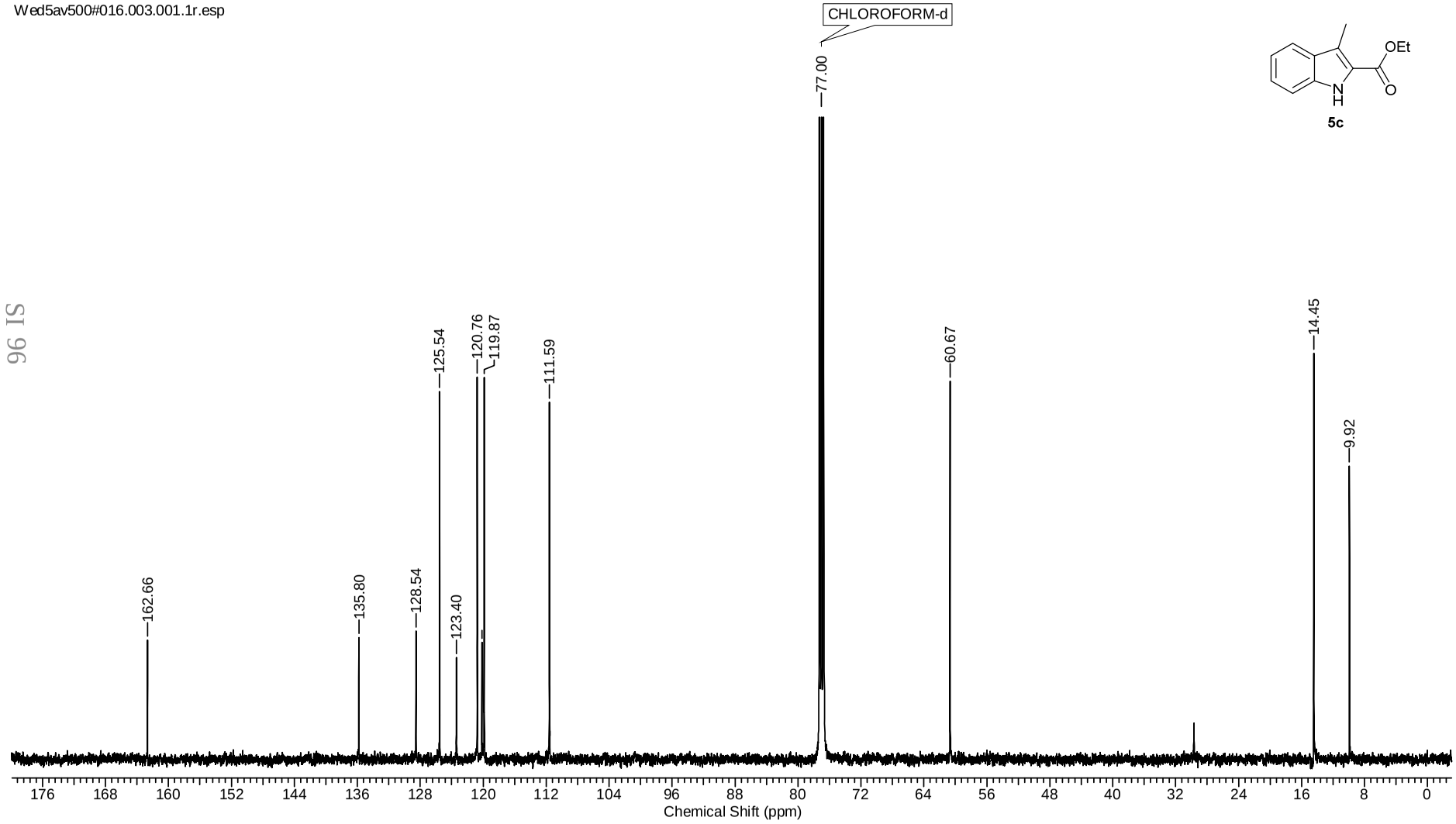
Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	28 Aug 2013 16:04:48				
Date Stamp	28 Aug 2013 16:04:48			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Wed5av500#016\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	64	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	256.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.4690	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.200								

Wed5av500#016.001.001.1r.esp



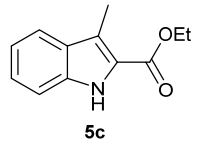
Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	28 Aug 2013 18:17:04				
Date Stamp	28 Aug 2013 18:17:04			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Wed5av500#016\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1525	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	11981.2275	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	23.000								

Wed5av500#016.003.001.1r.esp



Acquisition Time (sec)	1.1010	***Comment***	DEPT;	***Date***	28 Aug 2013 16:58:08				
Date Stamp	28 Aug 2013 16:58:08			***File Name***	\\agni\nmr_data\AV_500\Aug_13_500\Wed5av500#016\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	1200	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	29761.90
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.3564	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	29761.00
Temperature (degree C)	22.500								

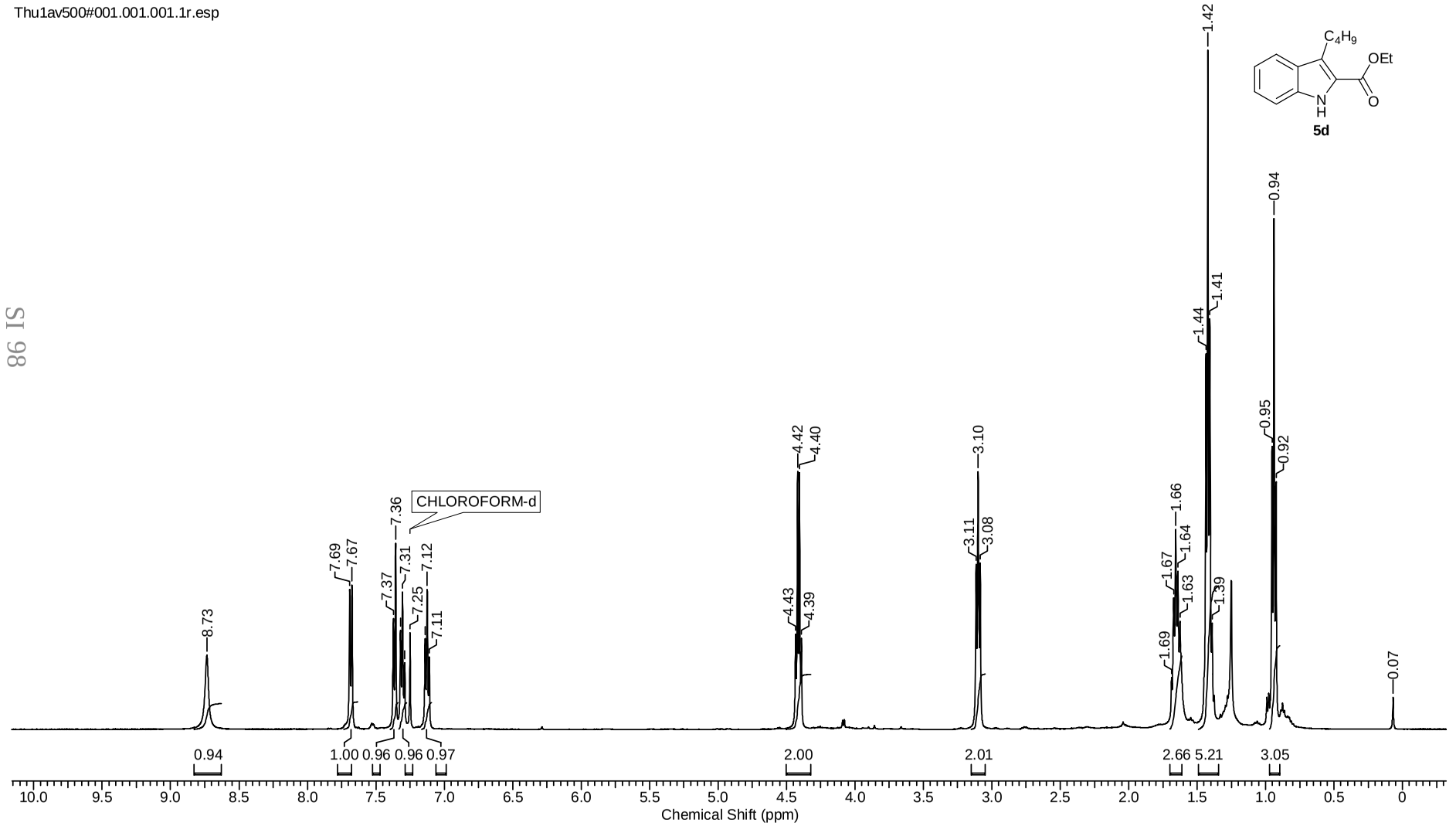
Wed5av500#016.002.001.1r.esp



5c

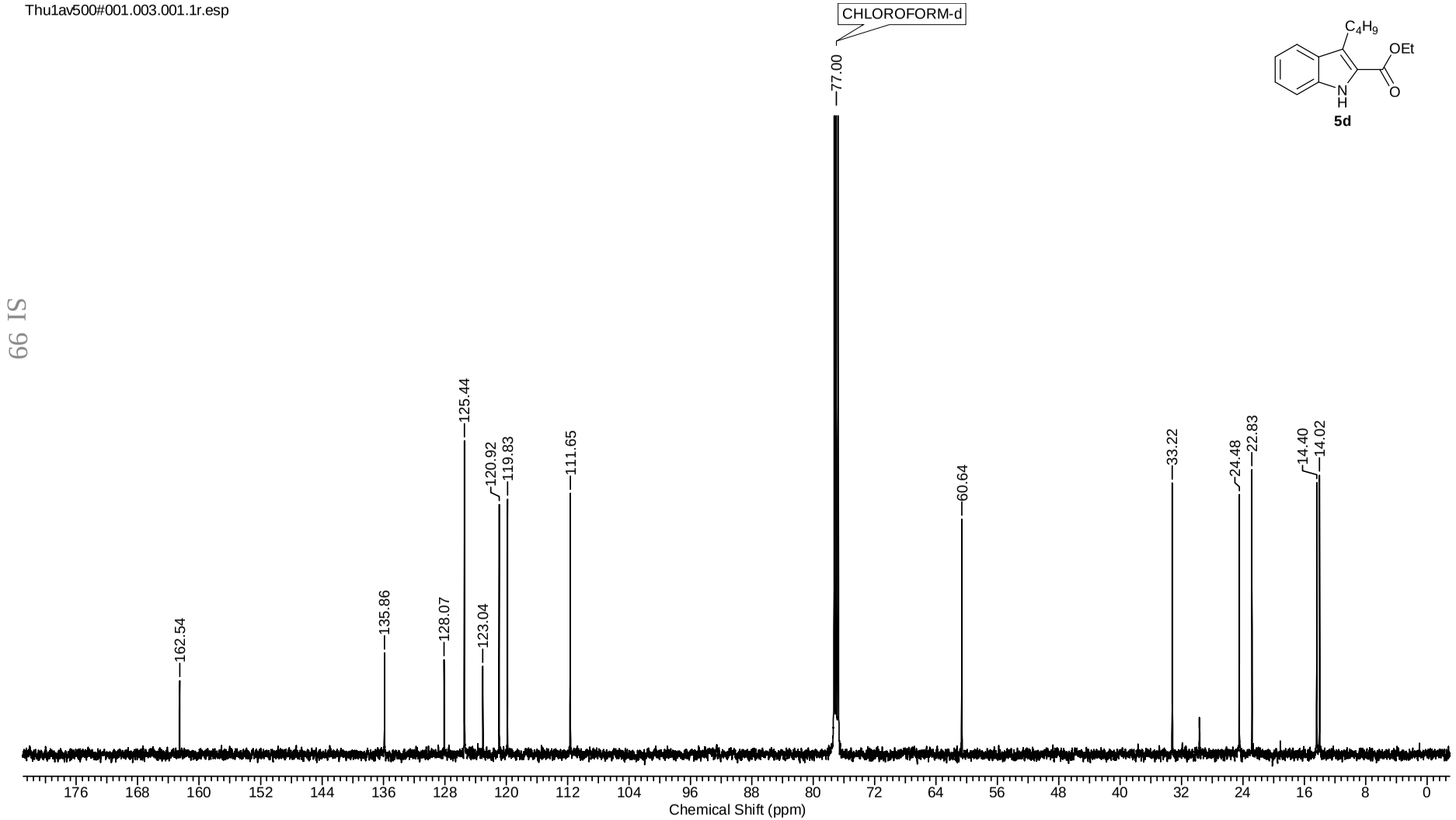
Acquisition Time (sec)	2.0031	***Comment***	Yogesh 1H	***Date***	03 Oct 2013 11:21:04				
Date Stamp	03 Oct 2013 11:21:04			***File Name***	\\agni\nmr_data\AV_500\Oct_13_500\Thu1av500#001\1\PDATA\1\1r				
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	37	***Origin***	spect	***Original Points Count***	20031
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	203.00	***SW(cyclical) (Hz)***	10000.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	2209.7744	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	9999.70
Temperature (degree C)	22.700								

Thu1av500#001.001.001.1r.esp

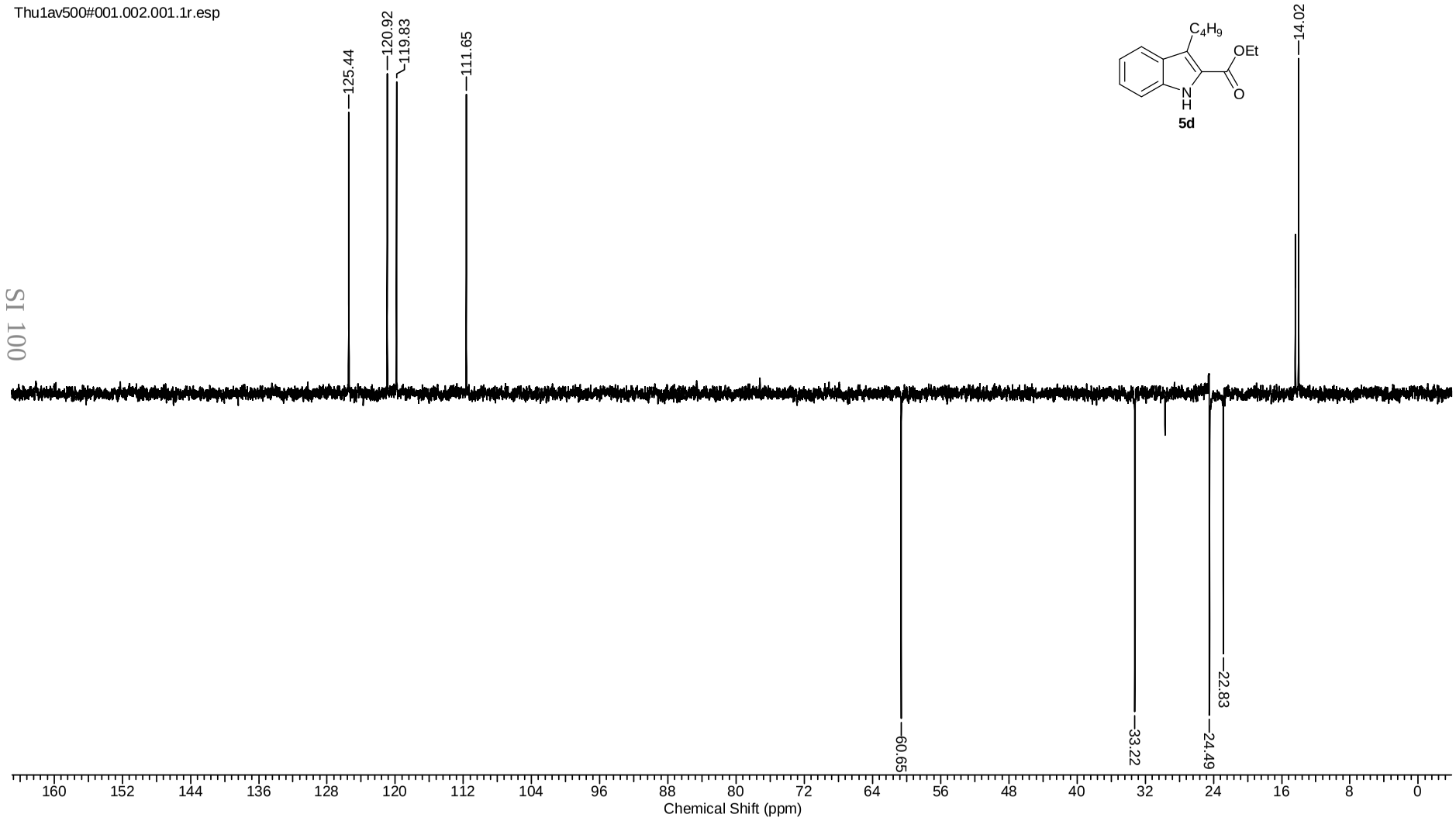


Acquisition Time (sec)	1.0486	***Comment***	13C	***Date***	03 Oct 2013 11:50:56				
Date Stamp	03 Oct 2013 11:50:56			***File Name***	\\agni\nmr_data\AV_500\Oct_13_500\Thu1av500#001\3\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	512	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	zgpg30	***Receiver Gain***	575.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.5986	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	23.600								

Thu1av500#001.003.001.1r.esp

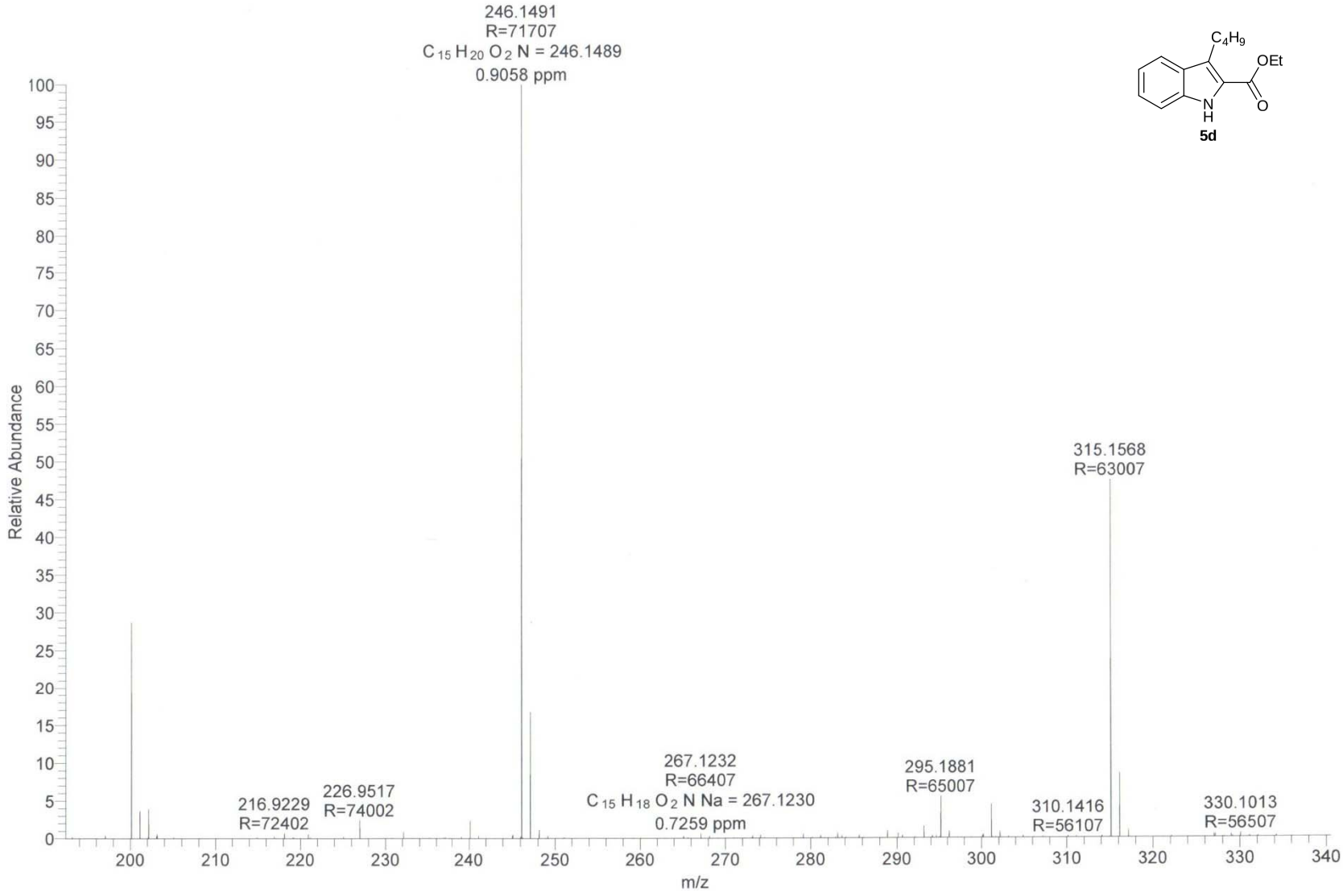


Acquisition Time (sec)	1.0486	***Comment***	DEPT;	***Date***	03 Oct 2013 11:23:12				
Date Stamp	03 Oct 2013 11:23:12			***File Name***	\\agni\nmr_data\AV_500\Oct_13_500\Thu1av500#001\2\PDATA\1\1r				
Frequency (MHz)	125.76	***Nucleus***	13C	***Number of Transients***	300	***Origin***	spect	***Original Points Count***	32768
Owner	nmr	***Points Count***	32768	***Pulse Sequence***	dept135	***Receiver Gain***	2050.00	***SW(cyclical) (Hz)***	31250.00
Solvent	CHLOROFORM-d			***Spectrum Offset (Hz)***	12570.6387	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	31249.05
Temperature (degree C)	22.900								



D:\Data\YM-993 9/16/2013 12:46:33 PM

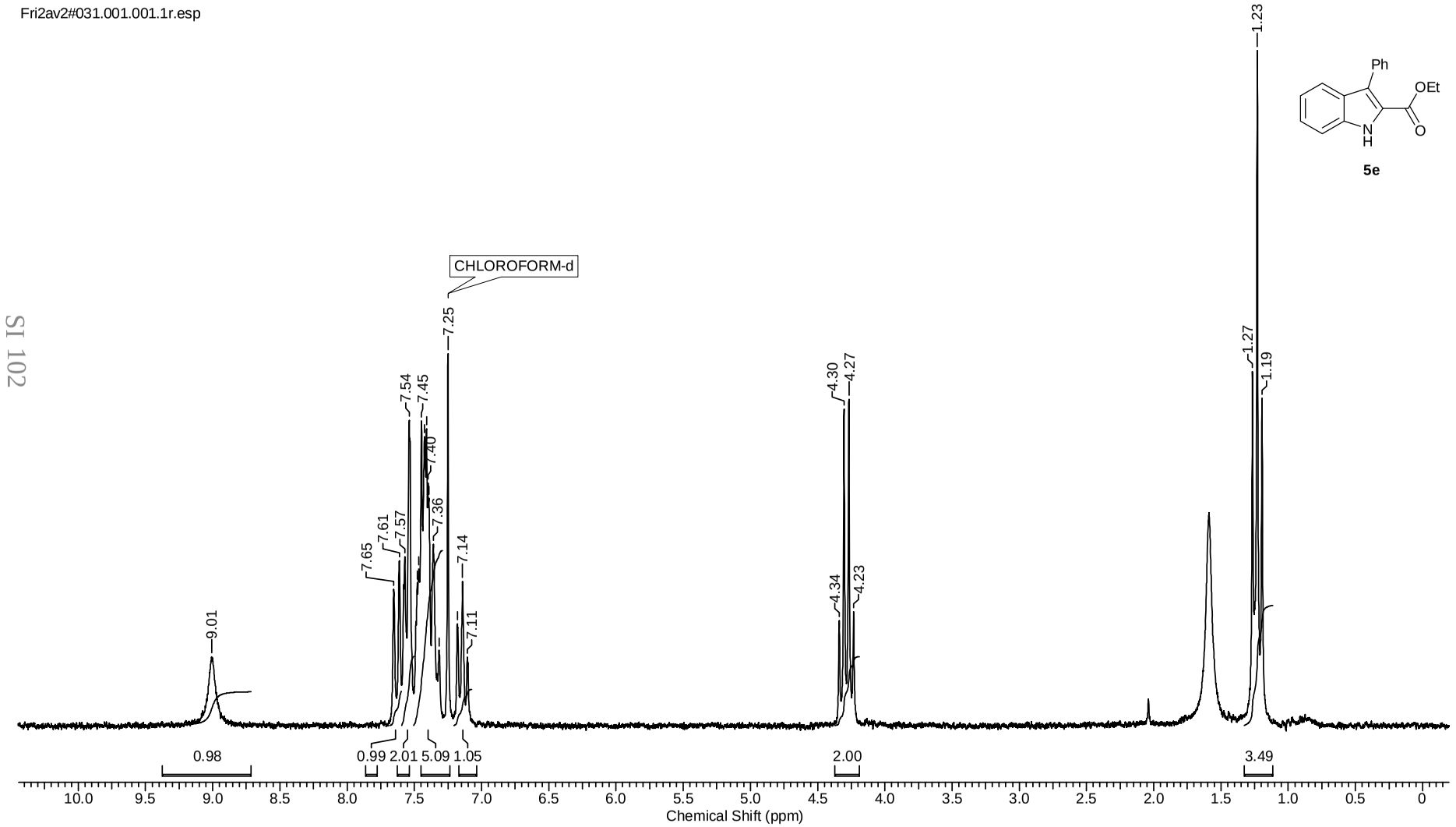
YM-993 #1267 RT: 5.64 AV: 1 NL: 5.19E8
T: FTMS + p ESI Full ms [100.00-700.00]



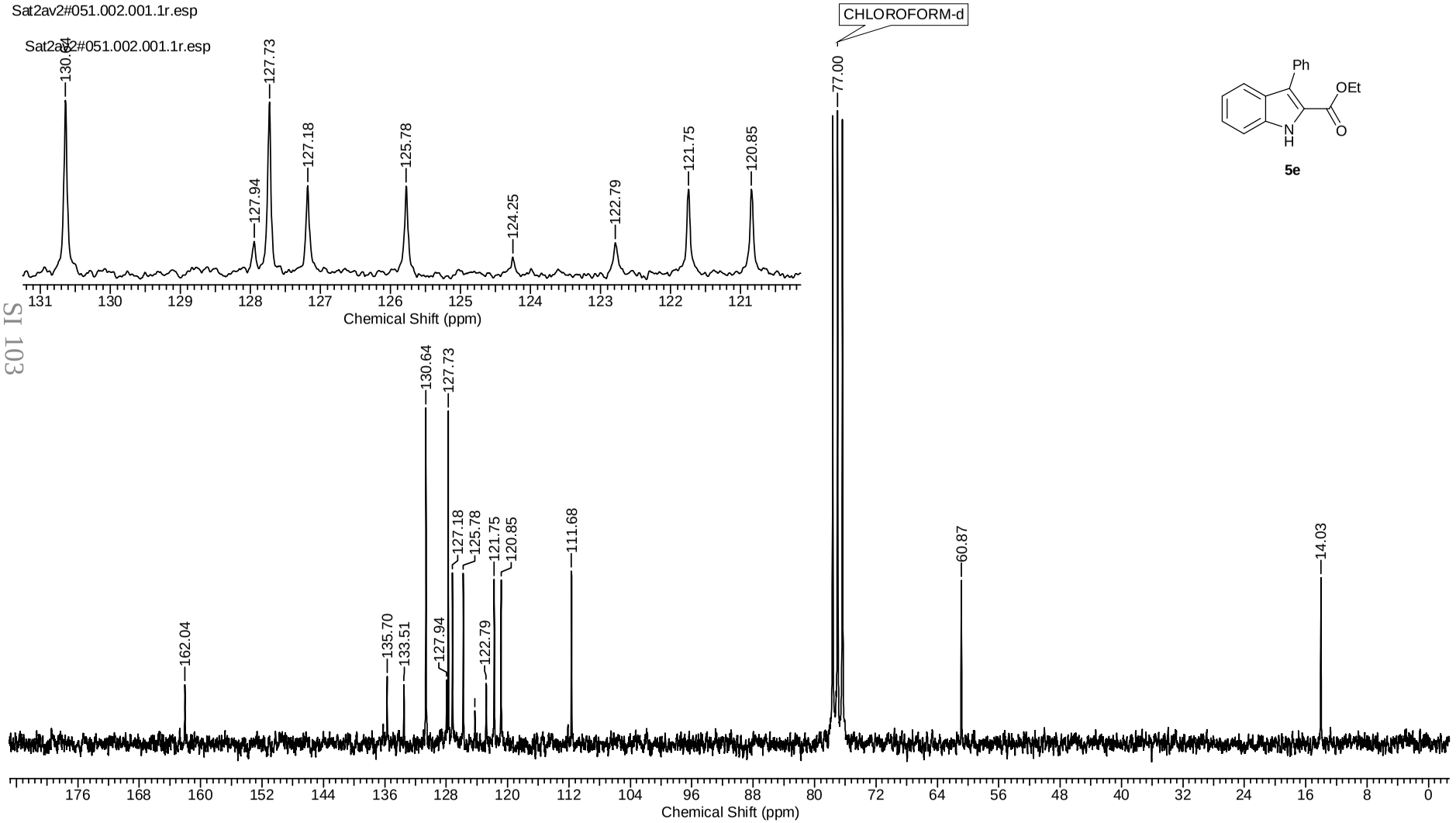
5d

Acquisition Time (sec)	3.9584	***Comment***	Yogesh	***Date***	13 Sep 2013 15:04:40		
Date Stamp	13 Sep 2013 15:04:40			***File Name***	\\agni\nmr_data\AV200\SEPT_13#AV200\data\Administrator\nmr\Fri2av2#031\1\PDATA\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	av200
Original Points Count	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1149.40	***SW(cyclical) (Hz)***	4139.07	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	1225.5343	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	4138.95	***Temperature (degree C)***	27.000

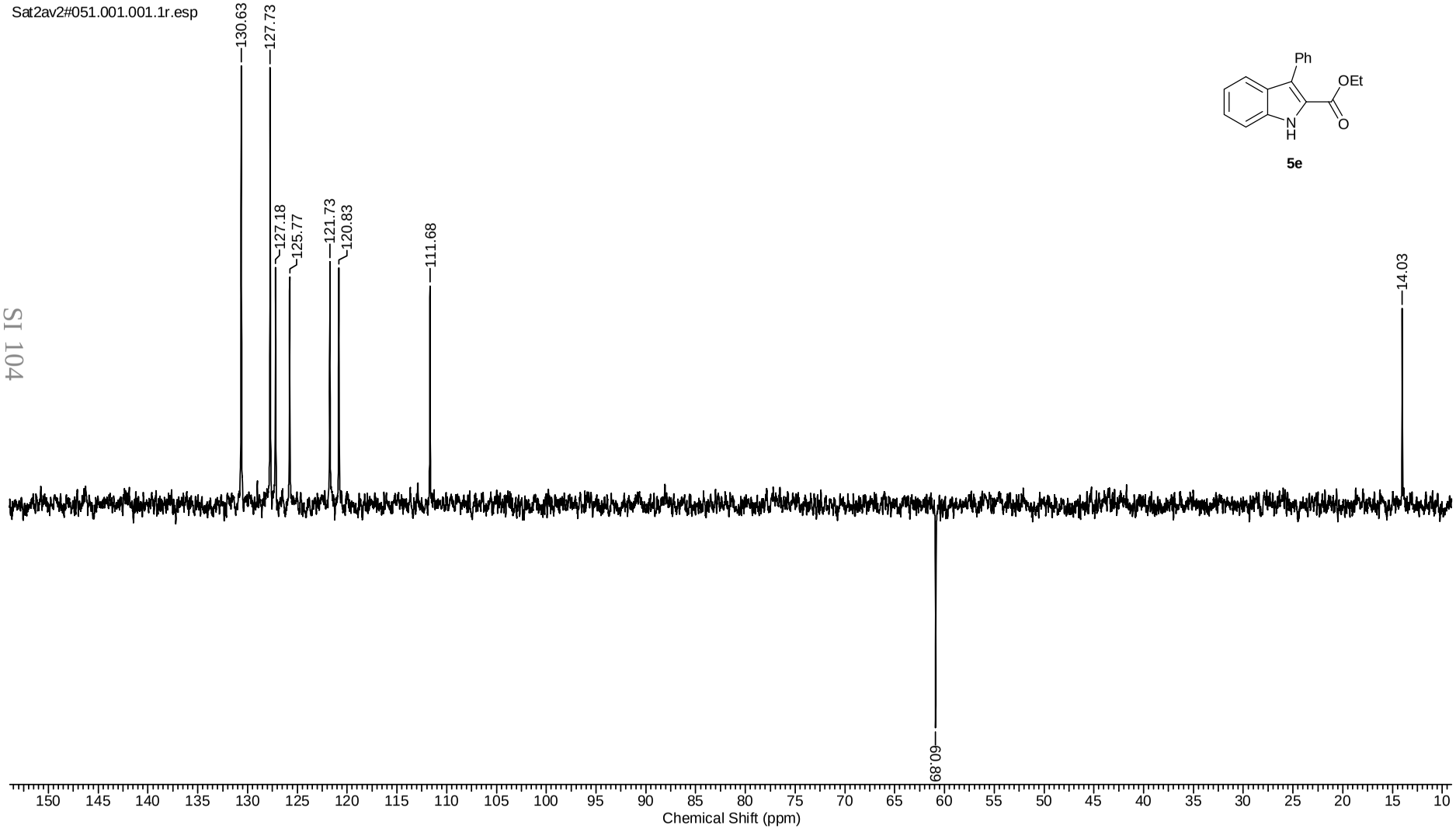
Fri2av2#031.001.001.1r.esp



Acquisition Time (sec)	0.6832	***Comment***	yogesh	***Date***	14 Sep 2013 21:39:20		
Date Stamp	14 Sep 2013 21:39:20			***File Name***	\\agni\nmr_data\AV200\SEPT_13#AV200\data\Administrator\nmr\Sat2av2#051\2\PDATA\1\1r		
Frequency (MHz)	50.32	***Nucleus***	13C	***Number of Transients***	1600	***Origin***	av200
Original Points Count	8192	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	812.70	***SW(cyclical) (Hz)***	11990.41	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	5029.8706	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	11990.04	***Temperature (degree C)***	27.000

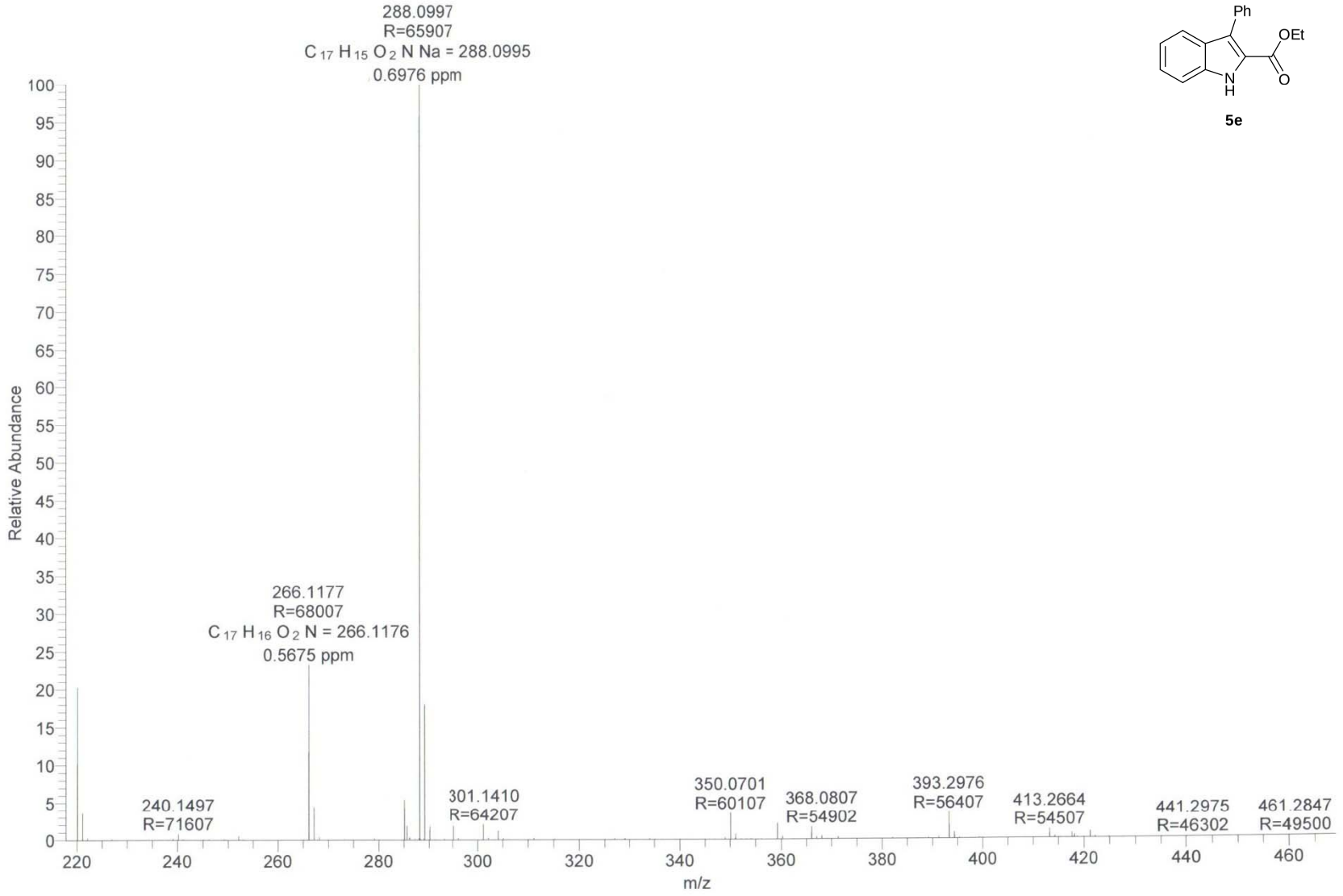


Acquisition Time (sec)	0.6832	***Comment***	yogesh	***Date***	14 Sep 2013 20:24:40		
Date Stamp	14 Sep 2013 20:24:40			***File Name***	\\agni\nmr_data\AV200\SEPT_13#AV200\data\Administrator\nmr\Sat2av2#051\1\PDATA\1\1r		
Frequency (MHz)	50.32	***Nucleus***	13C	***Number of Transients***	800	***Origin***	av200
Original Points Count	8192	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	16384.00	***SW(cyclical) (Hz)***	11990.41	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	5029.1680	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	11990.04	***Temperature (degree C)***	27.000



D:\Data\YM-995 9/16/2013 12:57:42 PM

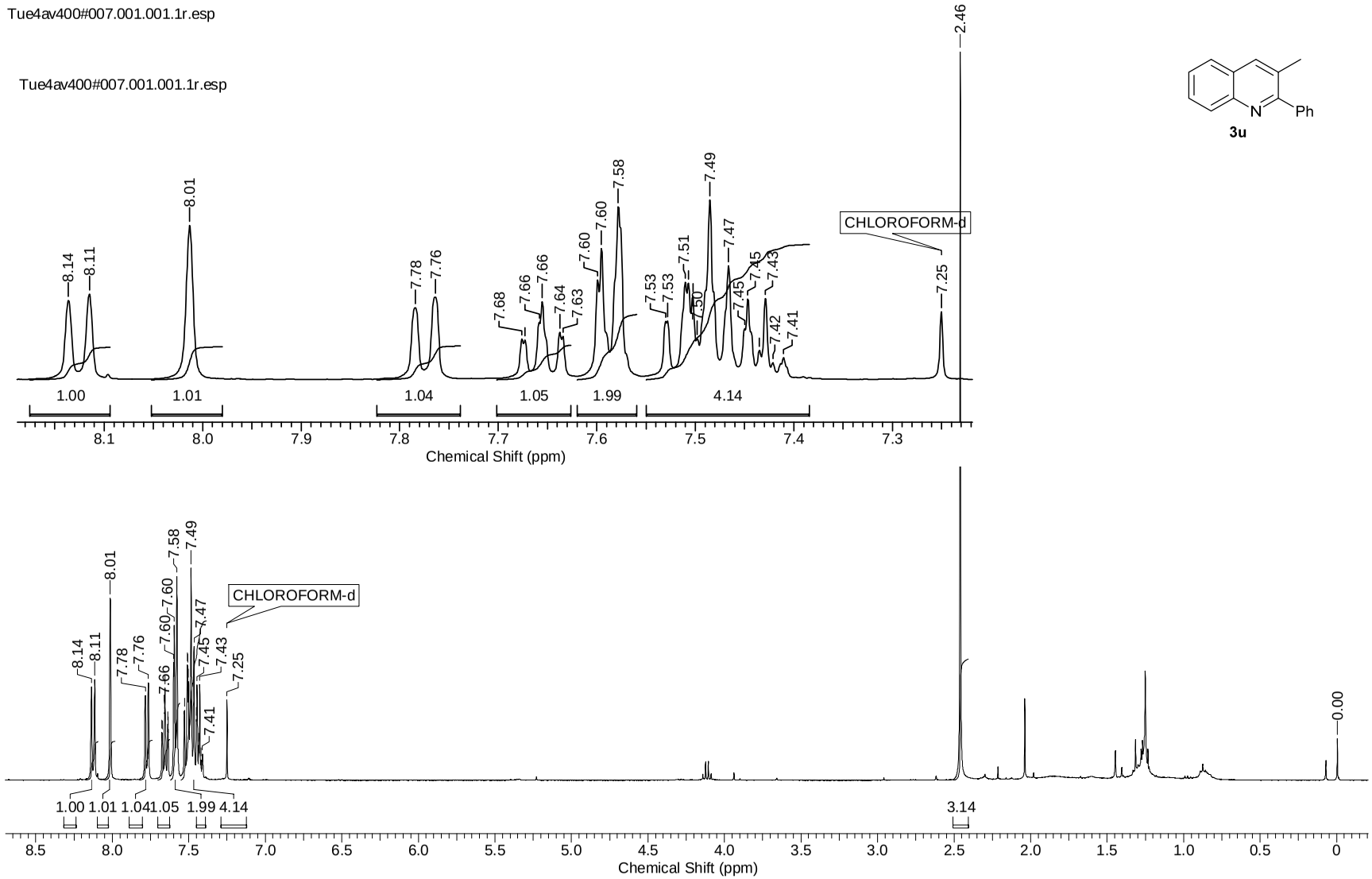
YM-995 #1109 RT: 4.94 AV: 1 NL: 1.51E9
T: FTMS + p ESI Full ms [100.00-700.00]



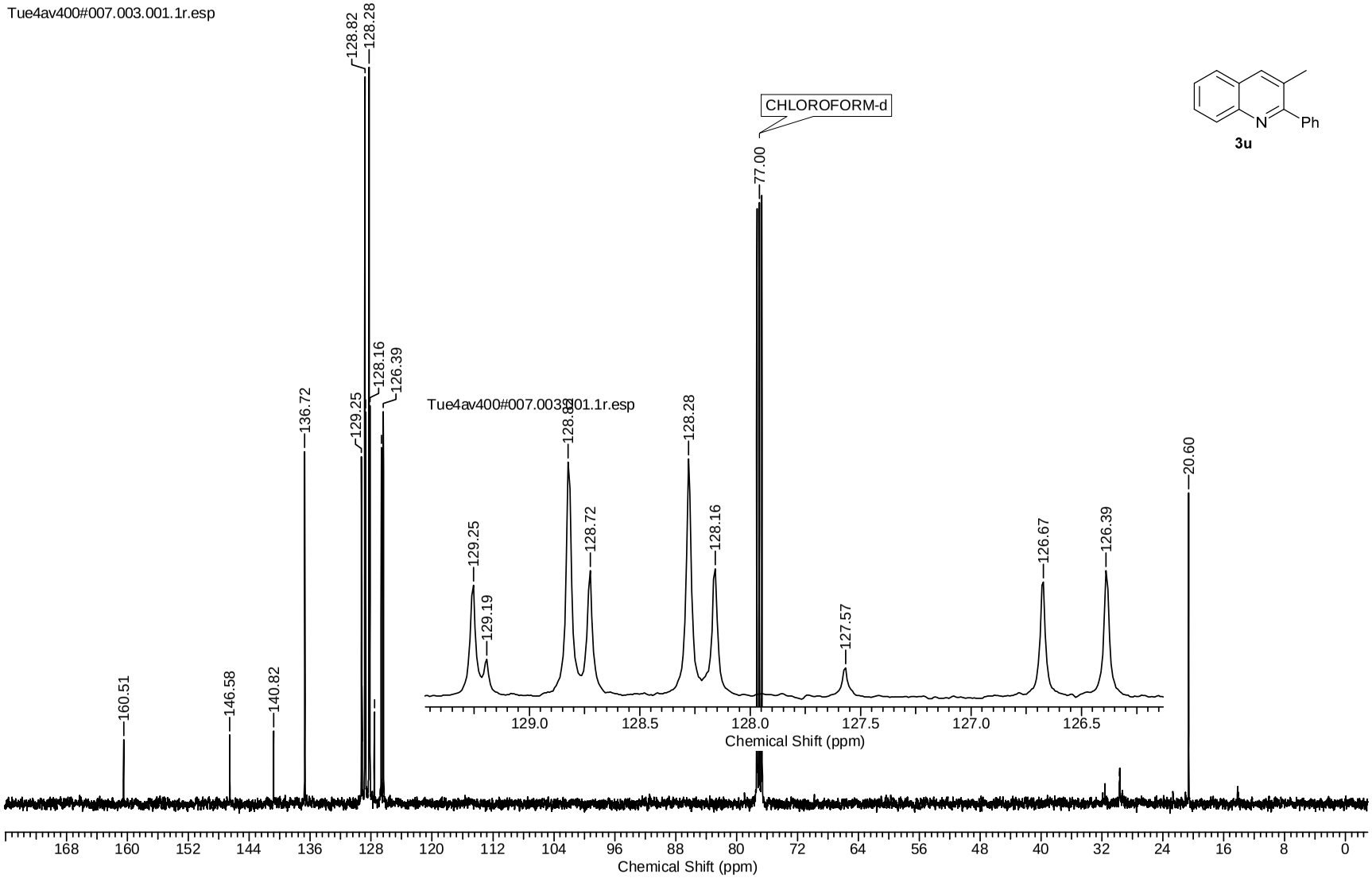
5e

Acquisition Time (sec)	2.0447	***Comment***	Yogesh 1H	***Date***	18 Feb 2014 15:58:00		
Date Stamp	18 Feb 2014 15:58:00			***File Name***	\\agni\nmr_data\AV400\Feb_14_400\Tue4av400#007\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	32	***Origin***	spect
Original Points Count	16384	***Owner***	Administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	287.00	***SW(cyclical) (Hz)***	8012.82	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2787.6018	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8012.58	***Temperature (degree C)***	22.200

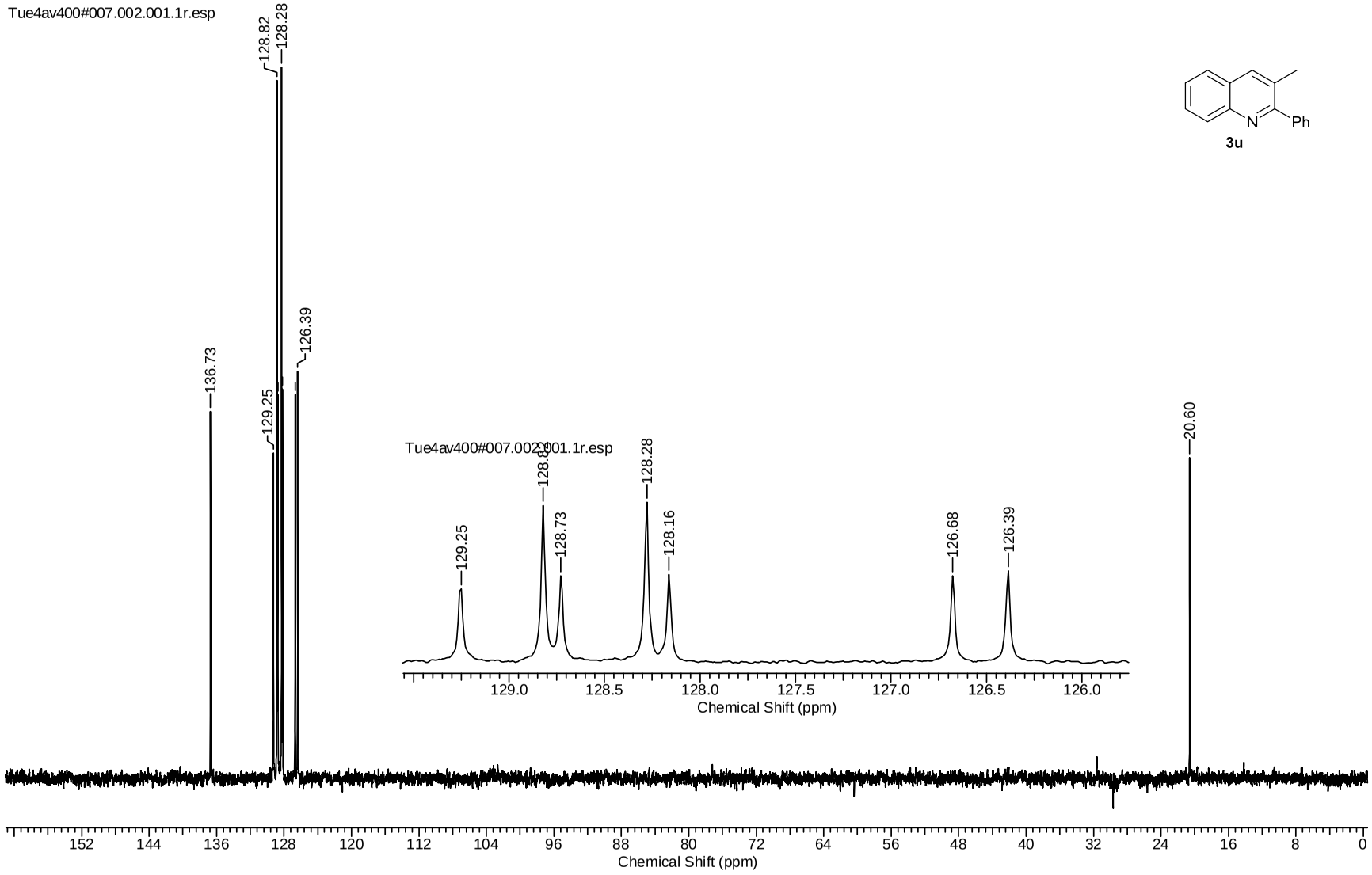
Tue4av400#007.001.001.1r.esp



Acquisition Time (sec)	0.6488	***Comment***	13C	***Date***	18 Feb 2014 16:49:12		
Date Stamp	18 Feb 2014 16:49:12			***File Name***	\\agni\nmr_data\AV400\Feb_14_400\Tue4av400#007\3\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	1046	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	zgpg
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	25252.53	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	9632.5684	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	25251.75	***Temperature (degree C)***	22.700

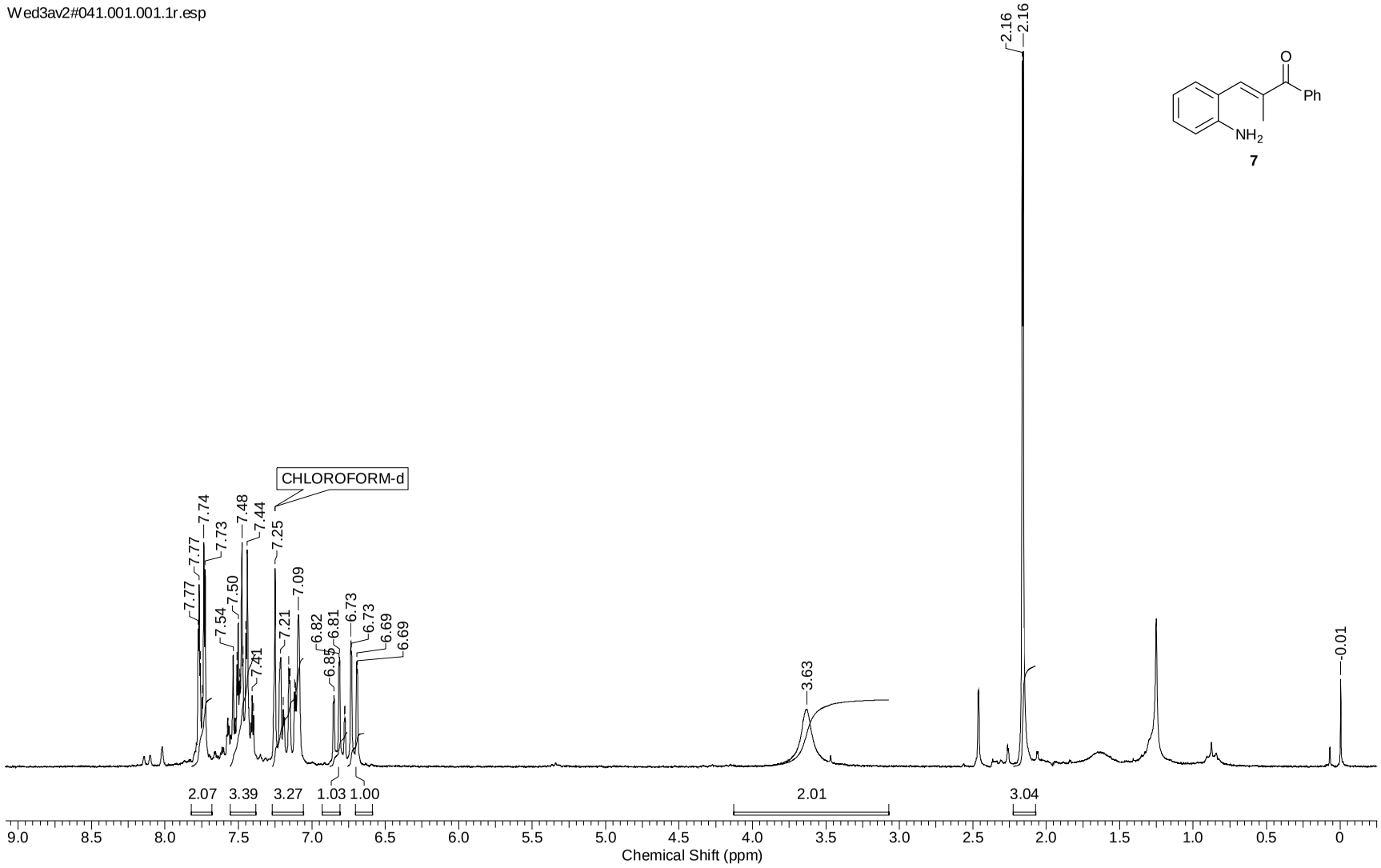


Acquisition Time (sec)	0.6488	***Comment***	DEPT	***Date***	18 Feb 2014 16:21:28		
Date Stamp	18 Feb 2014 16:21:28			***File Name***	\\agni\nmr_data\AV400\Feb_14_400\Tue4av400#007\2\PDATA\1\1r		
Frequency (MHz)	100.61	***Nucleus***	13C	***Number of Transients***	782	***Origin***	spect
Original Points Count	16384	***Owner***	root	***Points Count***	32768	***Pulse Sequence***	dept135
Receiver Gain	2050.00	***SW(cyclical) (Hz)***	25252.53	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10056.9004	***Spectrum Type***	DEPT135	***Sweep Width (Hz)***	25251.75	***Temperature (degree C)***	22.600



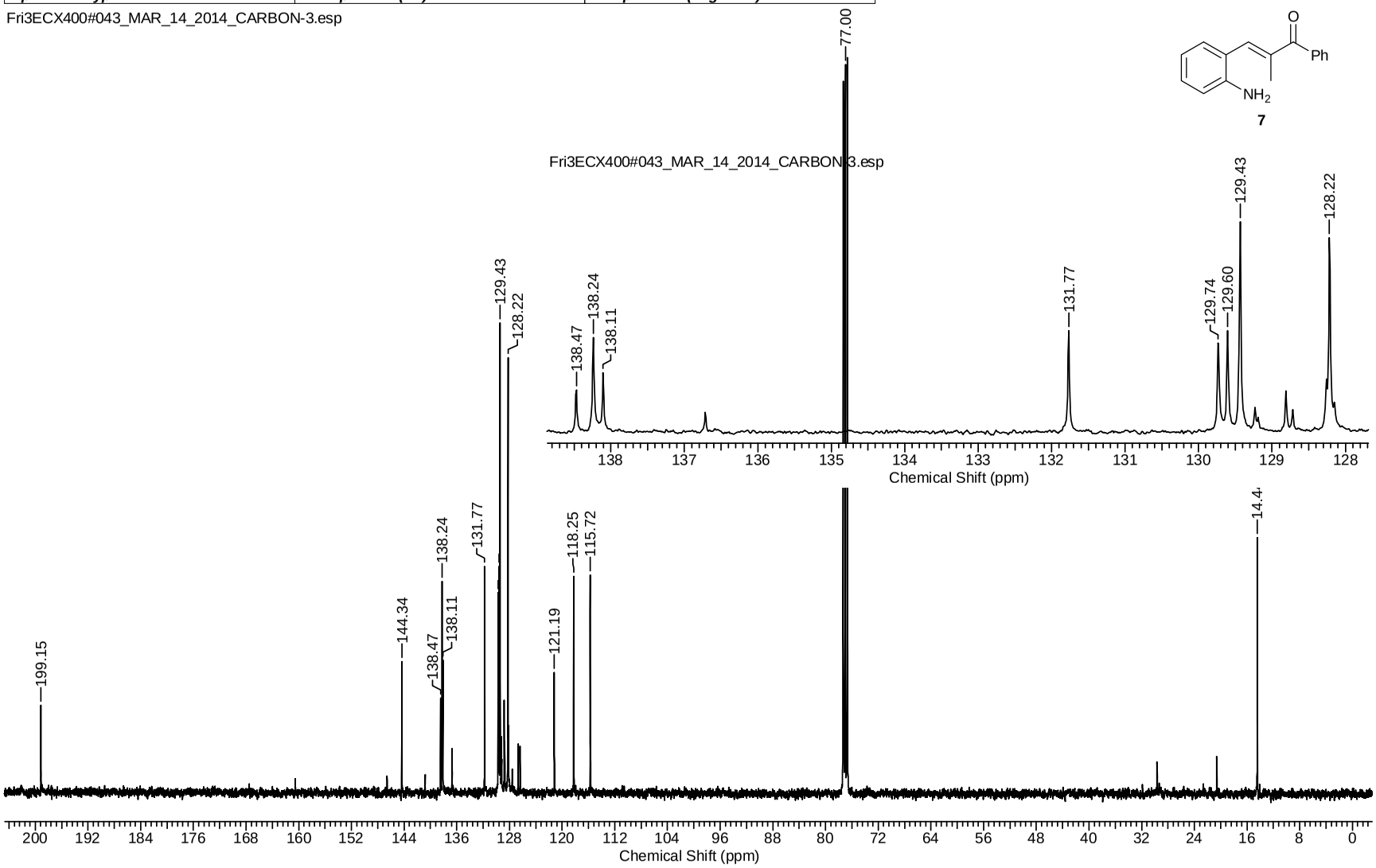
Acquisition Time (sec)	3.9584	***Comment***	Yogesh	***Date***	12 Mar 2014 17:23:20		
Date Stamp	12 Mar 2014 17:23:20			***File Name***	K:\Wed3av2#041\1\PDATA\1\1r		
Frequency (MHz)	200.13	***Nucleus***	1H	***Number of Transients***	8	***Origin***	av200
Original Points Count	16384	***Owner***	Administrator			***Points Count***	32768
Pulse Sequence	zg30	***Receiver Gain***	724.10	***SW(cyclical) (Hz)***	4139.07	***Solvent***	CHLOROFORM-d
Spectrum Offset (Hz)	1225.6606	***Spectrum Type***	STANDARD			***Sweep Width (Hz)***	4138.95
Temperature (degree C)	27.000						

Wed3av2#041.001.001.1r.esp



Acquisition Time (sec)	1.0434	***Comment***	yogesh goria	***Date***	16 Mar 2014 01:25:29		
Date Stamp	16 Mar 2014 00:36:06			***File Name***	K:\Fri3ECX400#043_MAR_14_2014_CARBON-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	600	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	single_pulse_dec
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10039.3311
Spectrum Type	STANDARD	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	22.900		

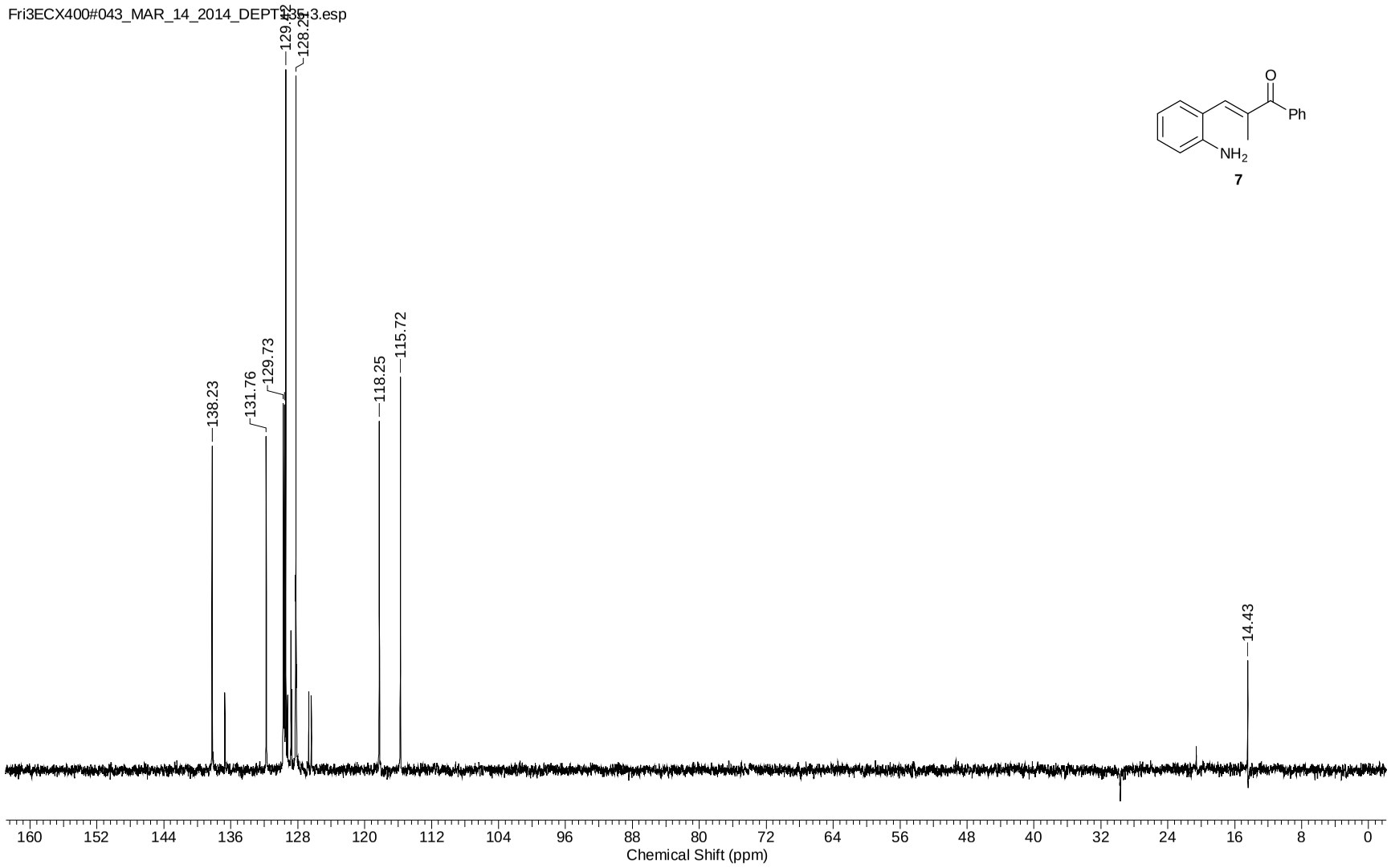
Fri3ECX400#043_MAR_14_2014_CARBON-3.esp



E:\Yogesh\2-Aroyl Indole\Indole metho\NMR\Propionate B\Fri3ECX400#043_MAR_14_2014_CARBON-3.esp

Acquisition Time (sec)	1.0434	***Comment***	yogesh goria	***Date***	16 Mar 2014 01:25:29		
Date Stamp	16 Mar 2014 00:48:10			***File Name***	K:\Fri3ECX400#043_MAR_14_2014_DEPT135-3.jdf		
Frequency (MHz)	100.53	***Nucleus***	13C	***Number of Transients***	300	***Origin***	ECX 400
Original Points Count	26214	***Owner***	delta	***Points Count***	26214	***Pulse Sequence***	dept.ex2 (selection_angle=135)
Receiver Gain	60.00	***Solvent***	CHLOROFORM-d			***Spectrum Offset (Hz)***	10038.3789
Spectrum Type	DEPT135	***Sweep Width (Hz)***	25124.29	***Temperature (degree C)***	22.800		

Fri3ECX400#043_MAR_14_2014_DEPT135-3.esp



7

E:\Yogesh\2-Aroyl Indole\Indole metho\NMR\Propionate B\Fri3ECX400#043_MAR_14_2014_DEPT135-3.esp