Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION:

Synthesis of Novel Benoxaborinin-4-one and Their Application in Suzuki-Miyaura Coupling Reaction to 2-Oxindole Derivatives

Kannan Murugan, Murugan Chinnapattu, Fazlur Rahman Nawaz Khan*, Pravin S. Iyer*

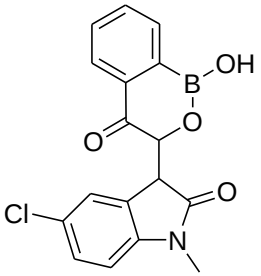
Experimental procedures and Data for all new compounds S2-S11

Experimental Section:

All reactions were carried out under nitrogen atmosphere using a Pre-assembled screw top, 7 ml/15ml supelco vials purchased from sigma Aldrich. All anhydrous solvents, reagent grade solvents for chromatography and starting materials were purchased from either Sigma Aldrich Chemical Co., Alfa aesar, Combi-Blocks or Fisher Scientific. Water was distilled and purified through a Milli-Q water system (Millipore Corp., Bedford, MA). General methods of purification of compounds involved the use of silica cartridges purchased from Grace Purification systems. The reactions were monitored by TLC on pre-coated Merck 60 F254 silica gel plates and visualized using UV light (254 nm). All compounds were analyzed for purity by HPLC and characterized by LCMS, ^{1}H NMR using Bruker 300 MHz NMR and/or Bruker 400 MHz NMR and/or Bruker 500 MHz NMR spectrometers. Chemical shifts are reported in ppm (δ) relative to the residual solvent peak in the corresponding spectra; chloroform δ 7.26, DMSO-d*6* δ 3.33 and coupling constants (J) are reported in hertz (Hz) (where s = singlet, bs = broad singlet, d = doublet, dd = double doublet, bd = broad doublet, ddd = double doublet of doublet, t = triplet, tt – triple triplet, q = quartet, m = multiplet) and analyzed using ACD NMR data processing software. 11B NMR spectra were recorded on a Bruker 300 MHz spectrometer at ambient temperature. Mass spectra values are reported as m/z. All reactions were conducted under Nitrogen and monitored using LCMS unless otherwise noted. Solvents were removed *in vacuo* on a rotary evaporator.

General produce I: A substituted isatin (1 mmol) and 2-acetyl boronic acid (1.1 mmol) was taken in supelco vial with screw cap and ethanol (5 ml). The vial was heated in thermal block at 120 °C for 16 h. After completion of the reaction, the solvent was evaporated under pressure and the crude was absorbed on silica gel and purified by CombiFlash RF purification system using Hexane:Ethyl acetate as a elutent. The isolated product was triturated with acetonitrile solvent to get diastereoisomeric mixture and one major diastereoisomer products.

5-chloro-3-(1-hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1-methyl-1,3-dihydro-indol-2-one (**1a**)



1a

5-chloro-1-methylindoline-2,3-dione (200 mg, 1.03 mmol) was treated with 2-acetyl phenyl boronic acid (185 mg, 1.13 mmol) in ethanol (5 ml) as described in the general procedure I to give **1a** diastereoisomeric mixture as a colourless solid (220 mg, 60%), single diastereoisomer **1aa** (26 mg, 7%) and **1ab** (24 mg, 6.8%).

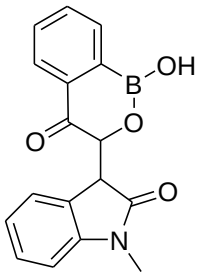
Mixture of diastereoisomers (**1a**): ^{1}H NMR (300MHz, DMSO-d_6): δ = 9.00 (s, 1H) (single isomer), 8.95 (s, 1H) (single isomer), 8.05-7.70 (m, 8H) (mixture of isomers), 7.57 (s, 1H)

(single isomer), 7.40- 7.25 (m, 2H) (mixture of isomers), 7.05-7.02 (m, 2H) (mixture of isomers), 6.48 (s, 1H) (single isomer), 5.59 (d, *J* = 2.2 Hz, 1H) (single isomer), 5.50 (d, *J* = 2.5 Hz, 1 H) (single isomer), 4.47 (s, 1H) (single isomer), 4.29 (s, 1H) (single isomer), 3.16 (s, 3H) (single isomer), 3.06 (s, 3H) (single isomer); LCMS (m/z) = 342 [M+1].

Single diastereisomers **1aa:** White solid; m.p. 204-205 °C; ^{1}H NMR (500MHz, DMSO-d_6): δ = 9.01 (bs, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 7.90 (d, *J* = 6.9 Hz, 1H), 7.70-7.81 (m, 2H), 7.42 (d, *J* = 6.0 Hz, 1H), 7.12-7.20 (m, 1H), 7.01 (dd, *J* = 8.7, 4.3 Hz, 1H), 5.57 (d, *J* = 2.2 Hz, 1H), 4.46 (s, 1H), 3.06 (s, 3H); ^{1}H NMR (DMSO-d_6, 125 MHz): δ = 196.3, 173.3, 144.0, 138.1, 134.0, 133.2, 132.6, 132.0, 128.7, 128.0, 126.2, 125.2, 123.8, 109.8, 78.5, 50.9, 26.1. ^{11}B NMR (96 MHz, DMSO-d6): = δ 26.6; HR-MS (ESI): Calcd. $C_{17}H_{13}BClNO_4$, $[M+H]^+$ m/z: 342.06985, found: 342.06988.

Single diastereisomers **1ab:** White solid; m.p. 228-230°C; ^{1}H NMR (500MHz, DMSO-d_6): δ = 8.96 (s, 1H), 8.05 - 8.09 (m, 1H), 7.76 - 7.87 (m, 3H), 7.31 (dd, *J* = 8.5, 1.9 Hz, 1H), 7.05 (d, *J* = 8.2 Hz, 1H), 6.48 (s, 1H), 5.50 (d, *J* = 2.5 Hz, 1H), 4.30 (d, *J* = 2.2 Hz, 1H), 3.16 (s, 3H). ^{1}H NMR (125 MHz, DMSO-d_6): δ = 197.1, 174.3, 144.0, 137.9, 134.6, 133.3, 133.0, 132.3, 128.2, 126.1, 125.6, 125.4, 123.5, 110.0, 78.7, 50.0, 26.3; ^{11}B NMR (96 MHz, DMSO-d6): = δ 26.7. HR-MS (ESI): Calcd. $C_{17}H_{13}BClNO_4$, $[M+H]^+$ m/z: 342.06985, found: 342.06976.

3-(1-Hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1-methyl-1,3-dihydro-indol-2-one (**1b**).



1b

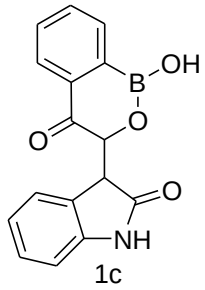
N-Methylindoline-2,3-dione (200 mg, 1.24 mmol) was treated with 2-acetyl phenyl boronic acid (223 mg, 1.36 mmol) in ethanol (5 ml) as described in the general procedure I to give **1** diastereoisomeric mixture as a colourless solid (213 mg, 56%) and single diastereoisomer 2a (26 mg, 7%)

Mixture of diastereoisomers (**1b**): ^{1}H NMR (500MHz, DMSO-d_6): δ = 9.03 (bs, 1H) (single isomer), 8.88 (bs, 1H) (single isomer), 8.03 - 8.12 (m, 1H) (single isomer), 7.95 (d, *J* = 7.6 Hz, 1H) (single isomer), 7.90 (d, *J* = 7.3 Hz, 1H) (single isomer), 7.69 - 7.84 (m, 6H) (mixture of isomers), 7.44 (d, *J* = 7.3 Hz, 1H) (single isomer), 7.30 (t, *J* = 7.9 Hz, 1H) (single isomer), 7.22 (t, *J* = 7.7 Hz, 1H) (single isomer), 6.97 - 7.07 (m, 2H) (mixture of isomers), 6.75 (t, *J* = 7.4 Hz, 1H) (single isomer), 6.49 (d, *J* = 7.3 Hz, 1H) (single isomer), 5.54 (s, 1H) (single isomer), 5.49 (d, *J* = 2.2 Hz, 1H) (single isomer), 4.39 (s, 1H) (single isomer), 4.26 (s, 1H) (single isomer), 3.17 (s, 3H) (single isomer), 3.08 (s, 3H) (single isomer). LCMS (m/z) = 308 [M+1].

Major diastereoisomers (**1ba**): White solid, m.p. 208-210 °C; ^{1}H NMR (500MHz, DMSO-d_6): δ = 8.88 (s, 1H), 8.05-8.11 (m, 1H), 7.74-7.84 (m, 3H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 7.6 Hz, 1H), 6.75 (t, *J* = 7.6 Hz, 1H), 6.49 (d, *J* = 7.6 Hz, 1H), 5.48 (d, *J* = 2.5 Hz, 1H),

4.26 (s, 1H), 3.17 (s, 3H); ^{1}H NMR (125 MHz, DMSO-d_6): δ = 197.3, 174.5, 144.9, 137.8, 134.4, 133.1, 132.9, 132.1, 128.3, 125.2, 123.7, 123.1, 121.6, 108.5, 78.7, 49.9, 26.1; HR-MS (ESI): Calcd. $C_{17}H_{14}BNO_4$, $[M+H]^+$ m/z: 308.10885, found: 308.10889.

3-(1-Hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1,3-dihydro-indol-2-one (**1c**).



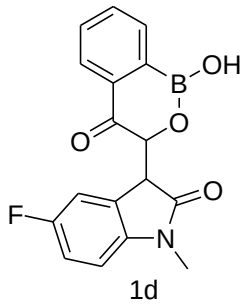
1c

Isatine (200 mg, 1.36 mmol) was treated with 2-acetyl phenyl boronic acid (245 mg, 1.49 mmol) in ethanol (5 ml) as described in the general procedure I to give **1** diastereoisomeric mixture as a colourless solid (167 mg, 42%) and single diastereoisomer **1ca** (32 mg, 8%).

Mixture of diastereoisomers (**1c**): ^{1}H NMR (300 MHz, DMSO-d_6): δ = 10.52 (s, 1H) (single isomer), 10.41 (s, 1H) (single isomer), 9.01 (s, 1H) (single isomer), 8.89 (s, 1H) (single isomer), 7.63 - 8.14 (m, 8H) (mixture of isomers), 7.39 (d, J = 7.2 Hz, 1H) (single isomer), 7.04 - 7.24 (m, 2H) (mixture of isomers), 6.96 (t, J = 7.4 Hz, 1H) (single isomer), 6.82 (d, J = 7.5 Hz, 2H) (single isomer), 6.66 (t, J = 7.5 Hz, 1H) (single isomer), 6.43 (d, J = 7.5 Hz, 1H) (single isomer), 5.49 (d, J = 2.1 Hz, 1H) (single isomer), 5.43 (d, J = 2.3 Hz, 1H) (single isomer), 4.33 (s, 1H) (single isomer), 4.16 (s, 1H) (single isomer). LCMS (m/z) = 294 [M+1].

Major diastereoisomers (**1ca**): ^{1}H NMR (500 MHz, DMSO-d_6): δ = 10.54 (s, 1H), 8.91 (s, 1H), 8.03 - 8.15 (m, 1H), 7.72 - 7.90 (m, 3H), 7.11 (t, J = 7.7 Hz, 1H), 6.82 (d, J = 7.8 Hz, 1H), 6.66 (t, J = 7.6 Hz, 1H), 6.43 (d, J = 7.3 Hz, 1H), 5.43 (d, J = 2.2 Hz, 1H), 4.17 (s, 1H). ^{1}H NMR (125 MHz, DMSO-d_6): δ = 197.5, 176.4, 143.6, 137.9, 134.5, 133.3, 133.0, 132.2, 128.2, 125.3, 124.6, 123.6, 121.0, 109.5, 78.93, 50.59. HR-MS (ESI): Calcd. $C_{16}H_{12}BNO_4$, $[M+H]^+$ m/z: 294.09315, found: 294.09323.

5-Fluoro-3-(1-hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1-methyl-1,3-dihydro-indol-2-one (**1d**).



1d

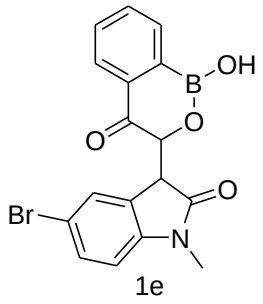
5-Fluoro-1-methylindoline-2,3-dione (200 mg, 1.12 mmol) was treated with 2-acetyl phenyl boronic acid (202 mg, 1.23 mmol) in ethanol (5 ml) as described in the general procedure I to

give **1d** diastereoisomeric mixture as a colourless solid (254 mg, 70%), single diastereoisomer **1da** (32 mg, 9 %).

Mixture of diastereoisomers (**1d**): ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.00 (s, 1H) (single isomer), 8.93 (s, 1H) (single isomer), 8.02 - 8.12 (m, 1H) (single isomer), 7.67 - 8.02 (m, 7 H) (mixture of isomers), 7.41 (d, J = 8.3 Hz, 1H) (single isomer), 6.95 - 7.20 (m, 4H) (mixture of isomers), 6.31 (d, J = 6.6 Hz, 1H) (single isomer), 5.56 (d, J = 2.3 Hz, 1H) (single isomer), 5.49 (d, J = 2.3 Hz, 1H) (single isomer), 4.45 (s, 1H) (single isomer), 4.28 (s, 1H) (single isomer), 3.16 (s, 3H) (single isomer), 3.06 (s, 3H) (single isomer). LCMS (m/z) = 326 [M+1].

Major diastereoisomers (**1da**): ^{1}H NMR (500MHz, DMSO-d_6): δ = 9.01 (bs, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.90 (d, J = 6.9 Hz, 1H), 7.70-7.81 (m, 2H), 7.42 (d, J = 6.0 Hz, 1H), 7.12-7.20 (m, 1H), 7.01 (dd, J = 8.7, 4.3 Hz, 1H), 5.57 (d, J = 2.2 Hz, 1H), 4.46 (s, 1H), 3.06 (s, 3H). ^{1}H NMR (125 MHz, DMSO-d_6): δ = 196.3, 173.3, 158.4 (d, J = 235 Hz), 141.3, 138.1, 134.0, 133.2, 132.7, 132.0, 128.4 (d, J = 8.7 Hz), 125.2, 114.2 (d, J = 22 Hz), 111.6 (d, J = 25 Hz), 109.1 (d, J = 8.7 Hz), 78.5, 51.2, 26.1. HR-MS (ESI): Calcd. $C_{17}H_{13}BFNO_4$, $[M+H]^+$ m/z: 326.09945, found: 326.09953.

5-Bromo-3-(1-hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1-methyl-1,3-dihydro-indol-2-one (**1e**).



1e

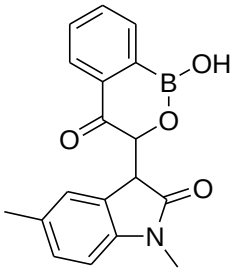
5-Bromo-1-methylindoline-2,3-dione (200 mg, 0.84 mmol) was treated with 2-acetyl phenyl boronic acid (151 mg, 0.92 mmol) in ethanol (5 ml) as described in the general procedure I to give **1e** diastereoisomeric mixture as a colourless solid (168 mg, 52%), single diastereoisomer **1ea** (28 mg, 8.6 %).

Mixture of diastereoisomers (**1e**): ^{1}H NMR (300 MHz, DMSO-d_6): δ = 9.00 (s, 1H) (single isomer), 8.95 (s, 1H) (single isomer), 8.02 - 8.11 (m, 1H) (single isomer), 7.97 (d, J = 7.4 Hz, 1H) (single isomer), 7.65 - 7.93 (m, 7H) (mixture of isomers), 7.37 - 7.54 (m, 2H) (single isomer), 6.99 (d, J = 8.3 Hz, 2H) (single isomer), 6.59 (s, 1H) (single isomer), 5.58 (d, J = 2.3 Hz, 1H) (single isomer), 5.49 (d, J = 2.5 Hz, 1H) (single isomer) 4.48 (s, 1H) (single isomer), 4.29 (s, 1H) (single isomer), 3.15 (s, 3H) (single isomer), 3.06 (s, 3H) (single isomer). LCMS (m/z) = 386 [M+1].

Major diastereoisomers (**1ea**): ^{1}H NMR (500 MHz, DMSO-d_6): δ = 9.01 (s, 1H), 7.97 (d, J = 7.6 Hz, 1H), 7.89 (d, J = 7.2 Hz, 1H), 7.68 - 7.81 (m, 3H), 7.50 (d, J = 8.2 Hz, 1H), 6.99 (d, J = 8.2 Hz, 1H), 5.59 (d, J = 1.9 Hz, 1H), 4.49 (s, 1H), 3.06 (s, 3H). ^{1}H NMR (125 MHz, DMSO-d_6): δ = 196.3, 173.2, 144.4, 138.1, 134.0, 133.2, 132.6, 132.0, 130.8, 129.0, 126.4,

125.2, 113.9, 110.3, 78.45, 50.9, 26.0. HR-MS (ESI): Calcd. $C_{17}H_{13}BBrNO_4$, $[M+H]^+$ m/z: 386.01935, found: 386.01901.

3-(1-Hydroxy-3, 4-dihydro-1H-benzo[c][1,2]oxaborinin-3-yl)-1, 5-dimethyl-1,3-dihydro-indol-2-one (**1f**).



1f

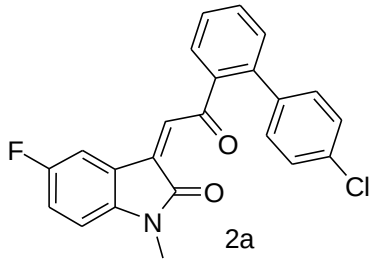
5-Methyl-1-methylindoline-2,3-dione (200 mg, 1.14 mmol) was treated with 2-acetyl phenyl boronic acid (206 mg, 1.25 mmol) in ethanol (5 ml) as described in the general procedure I to give **1f** diastereoisomeric mixture as a colourless solid (165 mg, 45%), single diastereoisomer **1fa** (21 mg, 5.7 %).

Mixture of diastereoisomers (**1f**): ^{1}H NMR (300 MHz, DMSO-d_6): δ = 8.98 (s, 1H) (single isomer), 8.86 (s, 1H) (single isomer), 7.67 - 8.13 (m, 8H) (mixture of isomers), 7.27 (s, 1H) (single isomer), 7.10 (d, J = 7.9 Hz, 1H) (single isomer), 7.02 (d, J = 7.9 Hz, 1H) (single isomer), 6.89 (s, 1H) (single isomer), 6.87 (s, 1H) (single isomer), 6.27 (s, 1H) (single isomer), 5.50 (d, J = 2.1 Hz, 1H) (single isomer), 5.45 (d, J = 2.3 Hz, 1H) (single isomer), 4.35 (s, 1H) (single isomer), 4.18 (s, 1H) (single isomer), 3.14 (s, 3H) (single isomer), 3.04 (s, 3H) (single isomer), 2.27 (s, 3H) (single isomer), 1.95 (s, 3H). LCMS (m/z) = 322 [M+1].

Major diastereoisomers (**1fa**): ^{1}H NMR (500 MHz, DMSO-d_6): δ = 8.88 (s, 1H), 8.04 - 8.14 (m, 1H), 7.74 - 7.87 (m, 3H), 7.05 (d, J = 7.9 Hz, 1H), 6.88 (d, J = 7.9 Hz, 1H), 6.27 (s, 1H), 5.45 (d, J = 2.5 Hz, 1H), 4.19 (s, 1H), 3.14 (s, 3H), 1.95 (s, 3H). ^{1}H NMR (125 MHz, DMSO-d_6): δ = 197.3, 174.3, 142.6, 137.9, 134.3, 133.1, 133.0, 132.1, 130.2, 128.4, 125.2, 124.2, 123.6, 108.1, 78.7, 49.9, 26.1, 20.3. HR-MS (ESI): Calcd. $C_{18}H_{16}BNO_4$, $[M+H]^+$ m/z: 322.12445, found: 322.12474.

General produce for Suzuki-Miyaura reaction: Substituted submitted benzoxaborinin-4-one (1 mmol), Ar/Het halide (1.3 mmol) and $NaHCO_3$ (1.5 mmol) were taken in supelco vial with screw cap and followed by addition of DME:Water (6 mL, 5:1 ratio). The reaction mixture was degassed for 5 min in nitrogen gas. Then Tetrakis(triphenylphosphine)palladium(0) (10 % mol) was added and heated in thermal block at 100 °C for 5 min. The reaction mixture was diluted with ethyl acetate (50 mL) and washed with water, brine solution and dried over sodium sulphate. The organic layer was evaporated under pressure. The resultant crude was absorbed on silica gel and purified by CombiFlash RF purification system using Hexane:Ethyl acetate as a elutent to afford pure product.

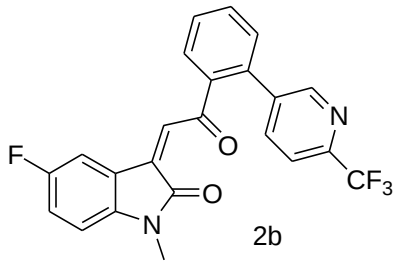
3-[2-(4'-Chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-5-fluoro-1-methyl-1,3-dihydro-indol-2-one (2a)



2a

Compound **1d** (50 mg, 0.15 mmol) was treated with 1-chloro-4-iodobenzene (47 mg, 0.2 mmol), $NaHCO_3$ (19 mg, 0.225 mmol) and Tetrakis(triphenylphosphine)palladium(0) (17 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2a** as a light red colour solid (40 mg, 65 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16 (dd, *J* = 9.3, 2.8 Hz, 1H), 7.77 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.59 - 7.65 (m, 1H), 7.50 - 7.56 (m, 1H), 7.42 - 7.46 (m, 1H), 7.17 - 7.26 (m, 4H), 7.11 (td, *J* = 8.7, 2.8 Hz, 1H), 6.92 (s, 1H), 6.70 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.16 (s, 3H). ^{1}H NMR (125 MHz, $CDCl_3$): δ = 195.2, 167.3, 158.8 (d, *J* = 238 Hz), 140.9 (d, *J* = 1 Hz), 140.5, 139.8, 128.6, 134.4, 134.2 (d, *J* = 3 Hz), 131.9, 130.4, 130.3, 130.0, 128.8, 128.7, 128.0, 120.9 (d, *J* = 9 Hz), 118.7 (d, *J* = 24 Hz), 115.0 (d, *J* = 27 Hz), 108.4, 26.2. HR-MS (ESI): Calcd. $C_{23}H_{15}ClFNO_2$, $[M+H]^+$ m/z: 392.08475, found: 392.08436.

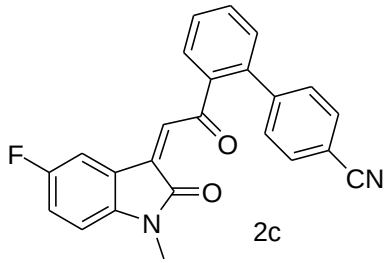
5-Fluoro-1-methyl-3-[2-oxo-2-[2-(6-trifluoromethyl-pyridin-3yl)-phenyl]-eth-(Z)-ylidene]-1,3-dihydro-indol-2-one (2b)



2b

Compound **1d** (50 mg, 0.15 mmol) was treated with 5-bromo-2-(trifluoromethyl)pyridine (45 mg, 0.2 mmol), $NaHCO_3$ (19 mg, 0.22 mmol) and Tetrakis(triphenylphosphine)palladium(0) (17 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2b** as a light red colour solid (37 mg, 57 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.60 (d, *J* = 2.0 Hz, 1H), 8.07 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.85 - 7.93 (m, 2H), 7.59 - 7.73 (m, 3H), 7.45 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.21 (s, 1H), 7.11 (td, *J* = 8.6, 2.8 Hz, 1H), 6.70 (dd, *J* = 8.5, 4.5 Hz, 1H), 3.17 (s, 3H). ^{1}H NMR (125 MHz, $CDCl_3$): δ = 193.3, 167.1, 158.8 (d, *J* = 238 Hz), 149.7, 147.2 (q, *J* = 33 Hz), 142.3, 139.2, 137.4, 135.9 (d, *J* = 4 Hz), 132.4, 130.9, 129.4, 129.1, 128.8, 121.4 (q, *J* = 271 Hz), 120.6, 120.5, 120.1 (d, *J* = 4 Hz), 119.5, 119.3, 115.4 (d, *J* = 26 Hz), 108, 26.2. HR-MS (ESI): Calcd. $C_{23}H_{14}F_4N_2O_2$, $[M+H]^+$ m/z: 427.10635, found: 427.10617.

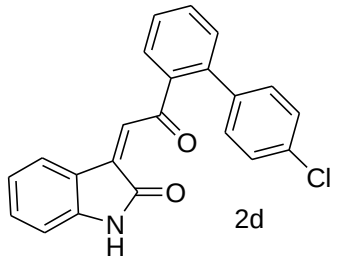
2'-{2-[5-Fluoro-1-methyl-2-oxo-1,2-dihydro-indol-(3Z)-ylidene]-acetyl}-biphenyl-4-carbonitrile (2c):



2c

Compound **1d** (50 mg, 0.15 mmol) was treated with 4-bromobenzonitrile (36 mg, 0.2 mmol), $NaHCO_3$ (19 mg, 0.22 mmol) and Tetrakis(triphenylphosphine)palladium(0) (17 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2c** as a light red colour solid (27 mg, 46 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.16 (dd, *J* = 9.0, 2.5 Hz, 1H), 7.81 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.63 - 7.69 (m, 1H), 7.54 - 7.61 (m, 3H), 7.38 - 7.48 (m, 3H), 7.13 (td, *J* = 8.6, 2.8 Hz, 1H), 7.00 (s, 1H), 6.72 (dd, *J* = 8.5, 4.0 Hz, 1H), 3.18 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 194.4, 167.2, 158.8 (d, *J* = 238 Hz), 145.0, 142.2, 139.8, 139.6, 135.1 (d, *J* = 2 Hz), 132.2, 132.1, 130.1, 129.8, 129.5, 129.1, 128.8, 120.7 (d, *J* = 10 Hz), 119.2 (d, *J* = 24 Hz), 118.4, 115.2 (d, *J* = 27 Hz), 111.8, 108.6 (d, *J* = 8 Hz), 26.3. HR-MS (ESI): Calcd. $C_{24}H_{15}FN_2O_2$, $[M+H]^+$ m/z: 383.11905, found: 383.11839.

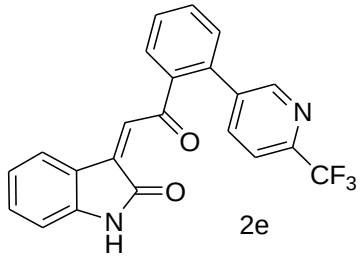
3-[2-(4'-Chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-1,3-dihydro-indol-2-one (2d)



2d

Compound **1c** (50 mg, 0.17 mmol) was treated with 1-chloro-4-iodobenzene (52 mg, 0.22 mmol), $NaHCO_3$ (21 mg, 0.255 mmol) and Tetrakis(triphenylphosphine)palladium(0) (19 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2d** as a light red colour solid (38 mg, 62 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* =7.5 Hz, 1H), 7.83 (bs, 1H), 7.78 (dd, *J* =7.5, 1.0 Hz, 1H), 7.58 - 7.64 (m, 1H), 7.50 - 7.55 (m, 1H), 7.44 (d, *J* =7.0 Hz, 1H), 7.34 (td, *J* =7.8, 1.0 Hz, 1H), 7.20 - 7.26 (m, 4H), 7.00 - 7.07 (m, 1H), 6.90 (s, 1H), 6.82 (d, *J* =7.5 Hz, 1H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 195.2, 168.8, 143.1, 140.5, 139.9, 138.7, 134.9, 134.4, 132.8, 131.8, 130.4, 130.1, 129.2, 128.8, 128.7, 128.0, 127.9, 122.8, 120.9, 109.9. HR-MS (ESI): Calcd. $C_{22}H_{14}ClNO_2$, $[M+H]^+$ m/z: 360.07855, found: 360.07799.

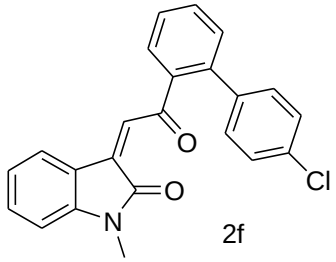
3-[2-Oxo-2-[2-(6-trifluoromethyl-pyridin-3-yl)-phenyl]-eth-(Z)-ylidene]-1,3-dihydro-indol-2-one (2e)



2e

Compound **1c** (50 mg, 0.17 mmol) was treated with 5-bromo-2-(trifluoromethyl)pyridine (42 mg, 0.22 mmol), $NaHCO_3$ (21 mg, 0.255 mmol) and Tetrakis(triphenylphosphine)palladium(0) (19 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2e** as a light red colour solid (23 mg, 35 %). 1H NMR (500 MHz, DMSO-d_6): δ = 10.71 (s, 1H), 8.71 (d, *J* = 1.6 Hz, 1H), 8.10 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 2H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.76 - 7.81 (m, 1H), 7.68 - 7.74 (m, 1H), 7.59 - 7.64 (m, 1H), 7.31 - 7.39 (m, 1H), 7.09 (s, 1H), 6.92 (t, *J* = 7.7 Hz, 1H), 6.85 (d, *J* =7.9 Hz, 1H). ^{1}H NMR (125 MHz, $CDCl_3$): δ = 193.6, 167.9, 149.6, 145.2 (d, *J* = 34 Hz), 145.1, 139.5, 138.7, 138.2, 136.4, 136.0, 133.3, 132.5, 131.2, 129.4, 129.2, 127.6, 126.9, 121.72, 121.6 (d, *J* = 272 Hz), 120.2, 119.6, 54.9. HR-MS (ESI): Calcd. $C_{22}H_{13}F_3N_2O_2$, $[M+H]^+$ m/z: 395.10015, found: 395.1006.

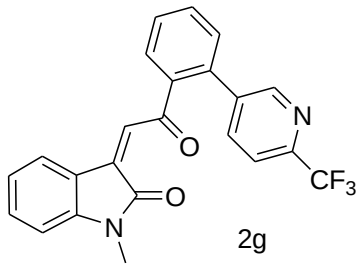
3-[2-(4'-Chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-1-methyl-1,3-dihydro-indol-2-one (2f)



2f

Compound **1b** (50 mg, 0.16 mmol) was treated with 1-chloro-4-iodobenzene (50 mg, 0.21 mmol), $NaHCO_3$ (20 mg, 0.24 mmol) and Tetrakis(triphenylphosphine)palladium(0) (19 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2f** as a light red colour solid (39 mg, 65 %). 1H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* =7.5 Hz, 1H), 7.77 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.57 - 7.64 (m, 1H), 7.48 - 7.54 (m, 1H), 7.36 - 7.46 (m, 2H), 7.16 - 7.25 (m, 4H), 7.01 - 7.08 (m, 1H), 6.93 (s, 1H), 6.78 (d, *J* = 7.5 Hz, 1H), 3.17 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 195.4, 167.6, 145.9, 140.5, 140.0, 138.7, 134.7, 134.3, 132.6, 131.7, 130.4, 130.0, 129.2, 128.8, 128.7, 127.9, 127.4, 122.6, 120.1, 108.1, 26.1. HR-MS (ESI): Calcd. $C_{23}H_{16}ClNO_2$, $[M+H]^+$ m/z: 374.09425, found: 374.09408.

1-Methyl-3-[2-oxo-2-[2-(6-trifluoromethyl-pyridin-3-yl)-phenyl]-eth-(Z)-ylidene]-1,3-dihydro-indol-2-one (2g)

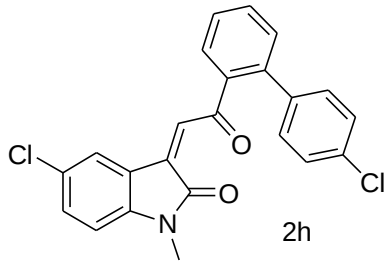


2g

Compound **1b** (50 mg, 0.16 mmol) was treated with 5-bromo-2-(trifluoromethyl)pyridine (47 mg, 0.21 mmol), $NaHCO_3$ (20 mg, 0.24 mmol) and Tetrakis(triphenylphosphine)palladium(0) (19 mg, 10 % mol) as described in the general procedure Suzuki-Miyaura reaction to afford compound **2g** as a light red colour solid (28 mg, 43 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.62 (d, *J* = 2.0 Hz, 1H) 8.25 (d, *J* = 7.5 Hz, 1H) 7.91 (dd, *J* = 7.5, 1.0 Hz, 1H) 7.85 (dd, *J* = 8.0, 1.5 Hz, 1H) 7.59 - 7.71 (m, 3H) 7.36 - 7.47 (m, 2H) 7.23 (s, 1H) 6.97 - 7.04 (m, 1H) 6.78

(d, *J* = 8.0 Hz, 1H) 3.19 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 193.5, 167.5, 149.7, 147.1 (q, *J* = 35 Hz), 146.2, 139.4, 139.3, 137.4, 136.8, 136.4, 133.3, 132.2, 130.9, 129.4, 129.1, 127.8, 127.6, 122.8, 121.5 (q, *J* = 272 Hz), 119.9 (d, *J* = 3 Hz), 119.7, 108.2, 26.1. HR-MS (ESI): Calcd. $C_{23}H_{15}F_3N_2O_2$, $[M+H]^+$ m/z: 409.11585, found: 409.11576.

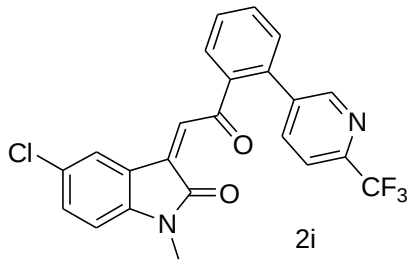
5-Chloro-3-[2-(4'-chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-1-methyl-1,3-dihydro-indol-2-one (2h)



2h

Compound **1a** (50 mg, 0.14 mmol) was treated with 1-chloro-4-iodobenzene (45 mg, 0.19 mmol), $NaHCO_3$ (18 mg, 0.21 mmol) and Tetrakis(triphenylphosphine)palladium(0) (16 mg, 10 % mol) as described in the general procedure for Suzuki-Miyaura reaction to afford compound **2h** as a light red colour solid (32 mg, 55 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.35 (d, *J* = 2.0 Hz, 1H), 7.77 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.59 - 7.65 (m, 1H), 7.50 - 7.55 (m, 1H), 7.43 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.36 (dd, *J* = 8.3, 2.3 Hz, 1H), 7.18 - 7.26 (m, 4H), 6.90 (s, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 3.15 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 195.2, 167.1, 144.2, 140.5, 139.7, 138.6, 134.5, 133.5, 132.1, 131.9, 130.6, 130.5, 130.0, 128.8, 128.7, 128.1, 128.0, 127.3, 121.1, 108.9, 26.7. HR-MS (ESI): Calcd. $C_{23}H_{15}Cl_2NO_2$, $[M+H]^+$ m/z: 408.05525, found: 408.05417.

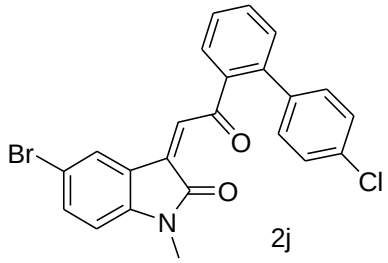
5-Chloro-1-methyl-3-[2-oxo-2-[2-(6-trifluoromethyl-pyridin-3-yl)-phenyl]-eth-(Z)-ylidene]-1,3-dihydro-indol-2-one (2i)



2i

Compound **1a** (50 mg, 0.14 mmol) was treated with 5-bromo-2-(trifluoromethyl)pyridine (43 mg, 0.19 mmol), $NaHCO_3$ (19 mg, 0.21 mmol) and Tetrakis(triphenylphosphine)palladium(0) (16 mg, 10 % mol) as described in the general procedure for Suzuki-Miyaura reaction to afford compound 2i as a light red colour solid (27 mg, 41 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.61 (d, *J* = 2.0 Hz, 1 H), 8.27 (d, *J* = 2.0 Hz, 1H), 7.89 (ddd, *J* = 14.2, 7.9, 1.5 Hz, 2H), 7.60 - 7.73 (m, 3H), 7.44 - 7.48 (m, 1H), 7.37 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.19 (s, 1H), 6.72 (d, *J* = 8.0 Hz, 1H), 3.17 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 193.4, 167.0, 149.7, 147.2 (q, *J* = 27 Hz), 144.5, 139.1, 137.4, 136.8, 135.2, 132.7, 132.5, 130.9, 129.5, 129.2, 129.1, 128.2, 127.7, 121.4 (q, *J* = 218), 120.8, 120.14, 120.12, 109.1, 26.2. HR-MS (ESI): Calcd. $C_{23}H_{14}ClF_3N_2O_2$, $[M+H]^+$ m/z: 443.07685, found: 443.0769.

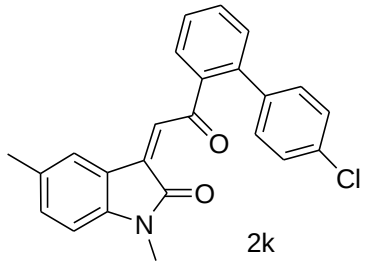
5-Bromo-3-[2-(4'-chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-1-methyl-1,3-dihydro-indol-2-one (2j)



2j

Compound **1e** (50 mg, 0.130 mmol) was treated with 1-chloro-4-iodobenzene (40 mg, 0.17 mmol), $NaHCO_3$ (16 mg, 0.195 mmol) and Tetrakis(triphenylphosphine)palladium(0) (15 mg, 10 % mol) as described in the general procedure for Suzuki-Miyaura reaction to afford compound 16 as a light red colour solid (24 mg, 42 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.48 (d, J = 2.0 Hz, 1H), 7.77 (dd, J = 7.5, 1.0 Hz, 1H), 7.59 - 7.66 (m, 1H), 7.49 - 7.56 (m, 2H), 7.42 - 7.46 (m, 1H), 7.17 - 7.25 (m, 4H), 6.90 (s, 1H), 6.67 (d, J = 8.0 Hz, 1H), 3.16 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 195.1, 167.0, 144.6, 140.5, 139.7, 138.6, 135.0, 134.5, 133.3, 132.0, 130.6, 130.4, 130.05, 130.02, 128.8, 128.7, 128.0, 121.6, 115.3, 109.4, 26.2. HR-MS (ESI): Calcd. $C_{23}H_{15}BrClNO_2$, $[M+H]^+$ m/z: 452.00475, found: 452.00447.

3-[2-(4'-Chloro-biphenyl-2-yl)-2-oxo-eth-(Z)-ylidene]-1,5-dimethyl-1,3-dihydro-indol-2-one (2k):



2k

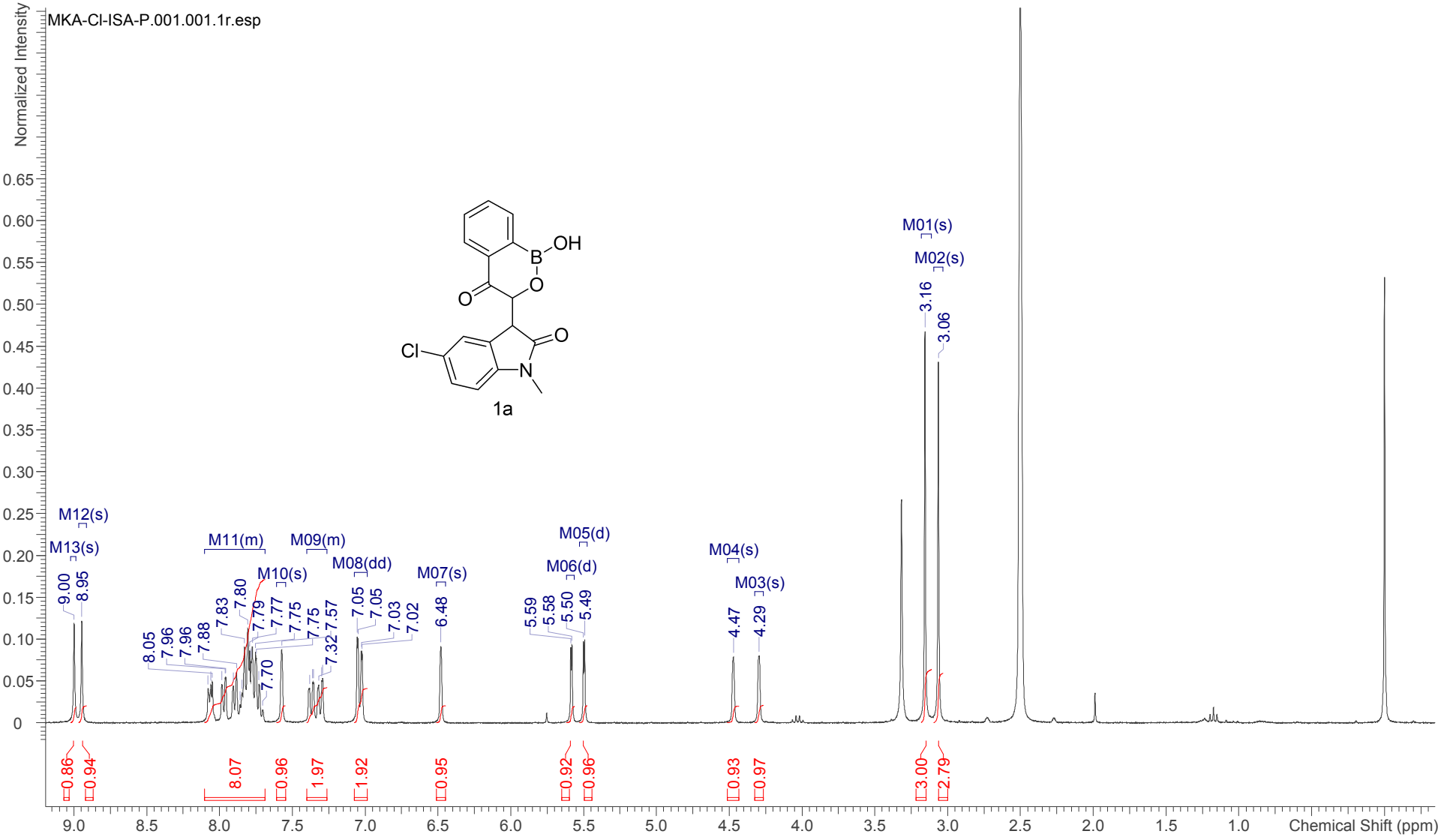
Compound **1f** (50 mg, 0.155 mmol) was treated with 1-chloro-4-iodobenzene (48 mg, 0.20 mmol), $NaHCO_3$ (20 mg, 0.233 mmol) and Tetrakis(triphenylphosphine)palladium(0) (18 mg, 10 % mol) as described in the general procedure for Suzuki-Miyaura reaction to afford compound 16 as a light red colour solid (32 mg, 51 %). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.14 (s, 1H), 7.77 (dd, J = 7.8, 1.3 Hz, 1H), 7.57 - 7.63 (m, 1H), 7.48 - 7.55 (m, 1H), 7.43 (dd, J = 7.5, 1.0 Hz, 1H), 7.17 - 7.25 (m, 5H), 6.91 (s, 1H), 6.67 (d, J = 8.0 Hz, 1H), 3.15 (s, 3H), 2.35 (s, 3H). ^{1}H NMR (100 MHz, $CDCl_3$): δ = 195.5, 167.6, 143.7, 140.4, 140.0, 138.7, 135.1, 134.2, 133.0, 132.1, 131.6, 130.4, 130.0, 128.9, 128.7, 128.6, 128.0, 127.9, 120.0, 107.8, 26.1, 21.0. HR-MS (ESI): Calcd. $C_{24}H_{18}ClNO_2$, $[M+H]^+$ m/z: 388.10985, found: 388.11021.

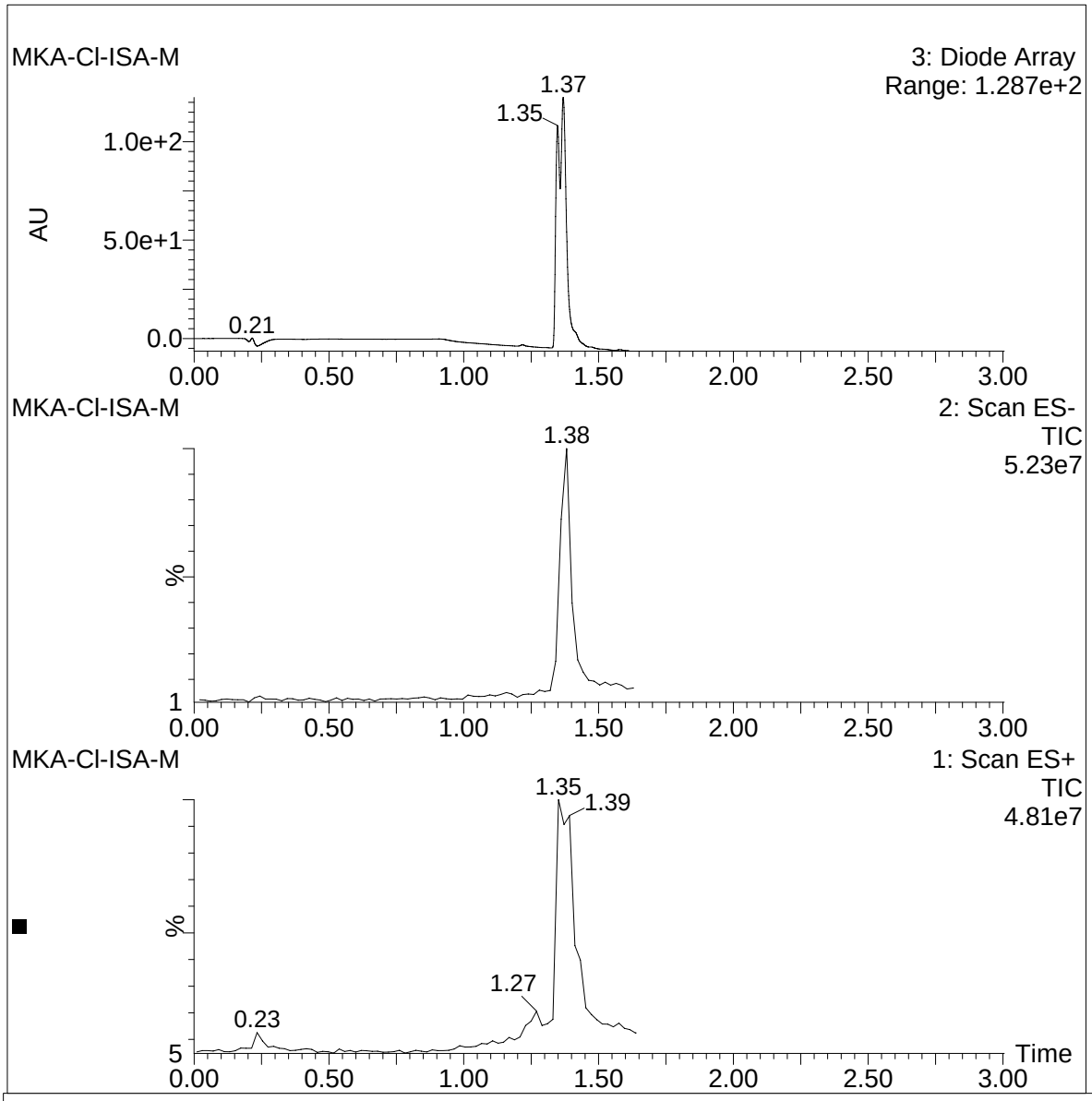
MKA-Cl-ISA-M

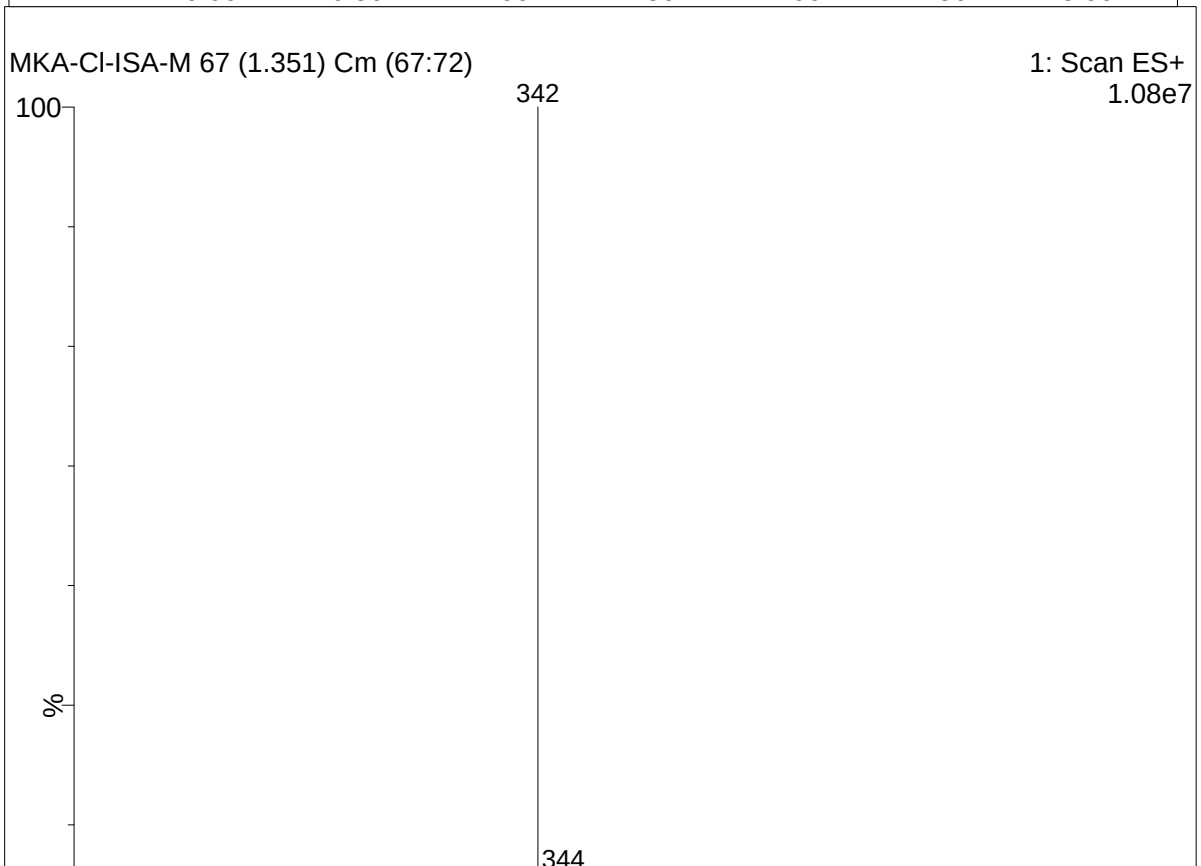
16/05/2014 14:32:16

OriginalDateForRelativeTime	2014-04-03T22:09:12	***Multiplets Integrals Sum***	25.25	***Number of Nuclei***	26 H's

Acquisition Time (sec)	5.3084	***Comment***	MKA-Cl-ISA-P/DMSO			***Date***	03 Apr 2014 22:09:12
Date Stamp	03 Apr 2014 22:09:12			***File Name***	C:\Users\kkth216\Desktop\NMR-300\MKA-Cl-ISA-P\1\PDATA\1\1r		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	126	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1625.50	***SW(cyclical) (Hz)***	6172.84	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1853.3636
Spectrum Type	STANDARD	***Sweep Width (Hz)***	6172.65	***Temperature (degree C)***	25.000		




MKA-Cl-ISA-M
3: Diode Array
Range: 1.287e+2
1.37
1.35
1.0e+2
AU
5.0e+1
0.21
0.0
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-Cl-ISA-M
2: Scan ES-
TIC
5.23e7
1.38
%
1
MKA-Cl-ISA-M
1: Scan ES+
TIC
4.81e7
1.35
1.39
%
1.27
0.23
5
Time

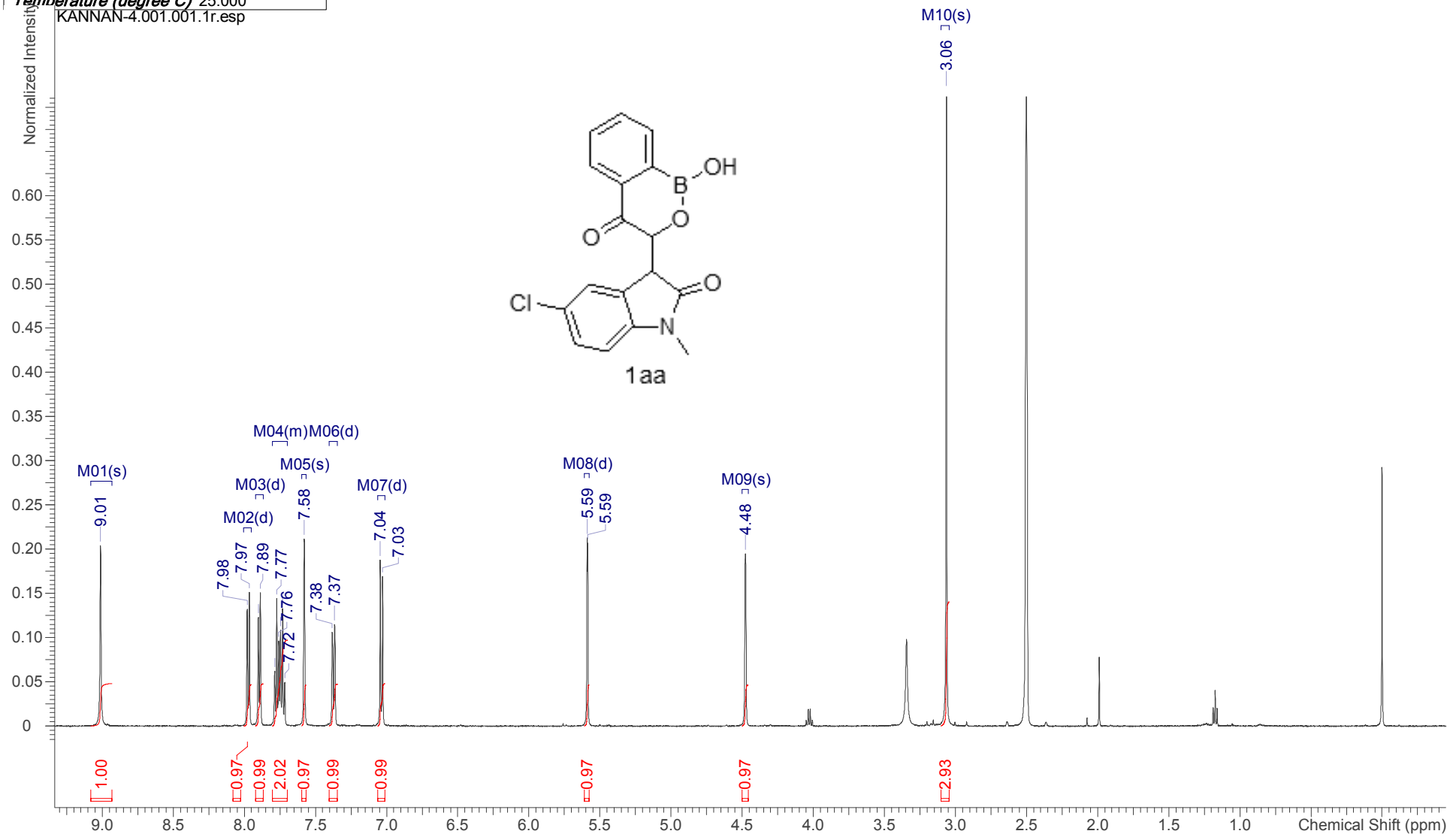

MKA-Cl-ISA-M 67 (1.351) Cm (67:72)
1: Scan ES+
1.08e7
100
342
%
344

MKA-Cl-ISA-P1

15/05/2014 17:06:39

OriginalDateForRelativeTime 2014-05-10T16:27:52			***Multiplets Integrals Sum*** 12.81		***Number of Nuclei*** 13 H's

Acquisition Time (sec)	3.1719	***Comment***	MKA-Cl-ISA-01P PROTON DMSO {F:\ecm\DATA\2014-05} bionmr 44				
Date	10 May 2014 16:27:52			***Date Stamp***	10 May 2014 16:27:52		
File Name	\\inbgrdsfp01\elndata\MKA\KANNAN-4\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	administrator
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00	***SW(cyclical) (Hz)***	10330.58
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3091.9285	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10330.26
Temperature (degree C) 25.000							

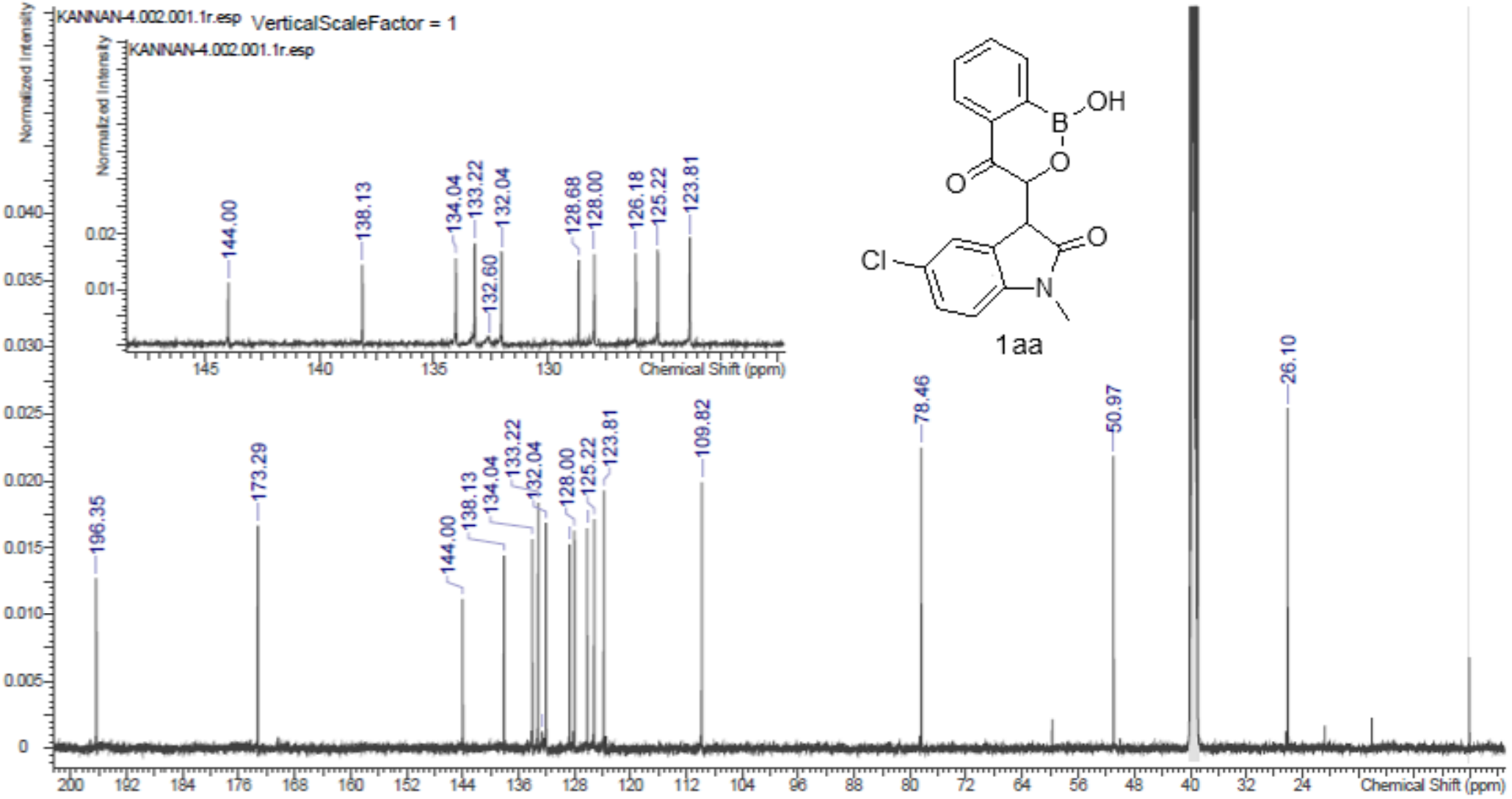


MKA-CI-ISA-P2

21/06/2014 12:24:01

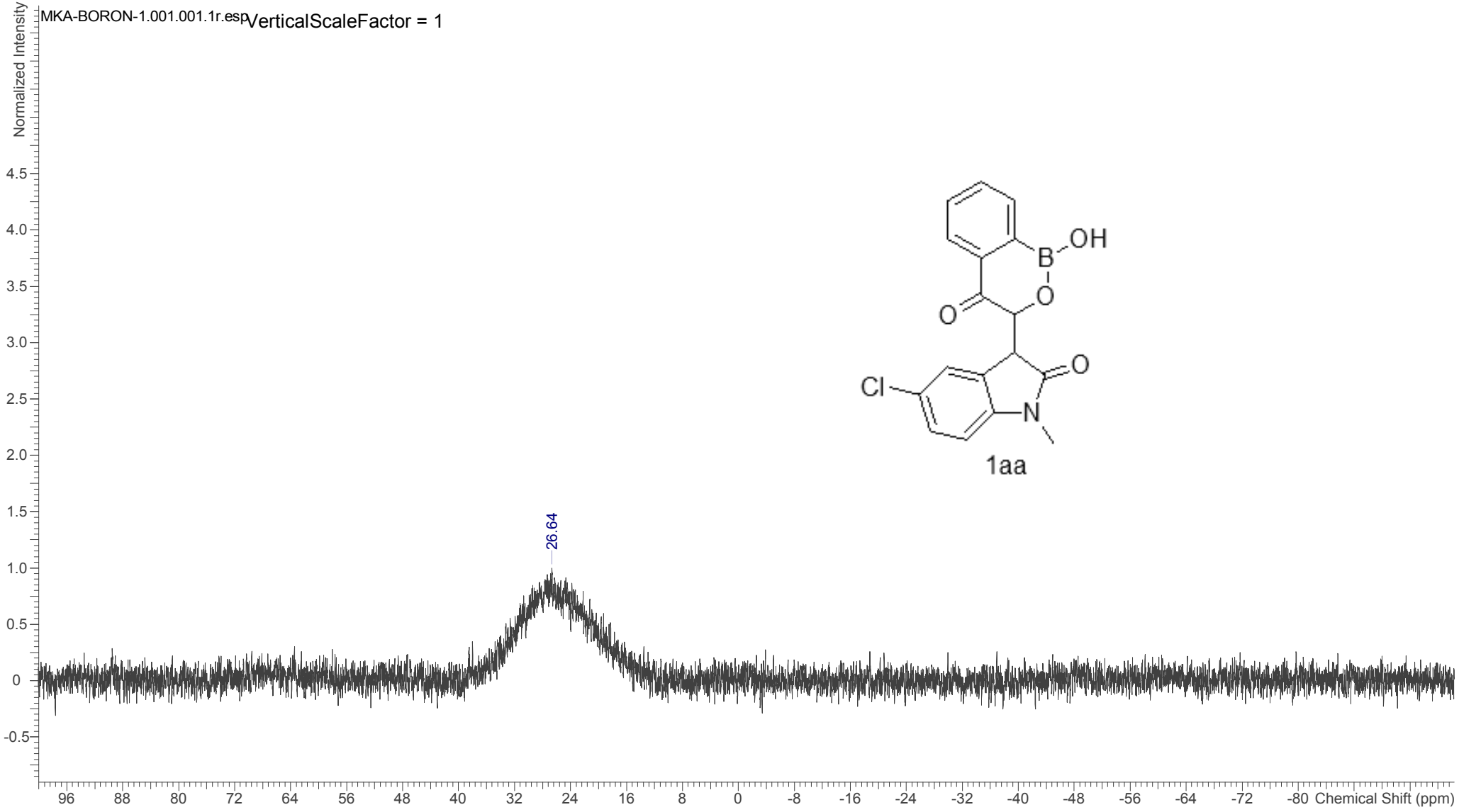
OriginalDateForRelativeTime 2014-05-10T21:45:44	*Multiplets Integrals Sum* 0.00	*Number of Nuclei* 0 C's

Acquisition Time (sec)	1.0912	*Comment*	C13CPD DMSO (F:\ecm\DATA\2014-05) bionmr 44			*Date*	10 May 2014 21:45:44
Date Stamp	10 May 2014 21:45:44			*File Name*	\\inbgrdsfp01\elndata\MKA\KANNAN-4\2\PDATA\1\1r		
Frequency (MHz)	125.77	*Nucleus*	13C	*Number of Transients*	6000	*Origin*	spect
Original Points Count	32768	*Owner*	administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	32768.00	*SW(cyclical) (Hz)*	30030.03	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	12518.3926
Spectrum Type	STANDARD	*Sweep Width (Hz)*	30029.11	*Temperature (degree C)*	25.000		



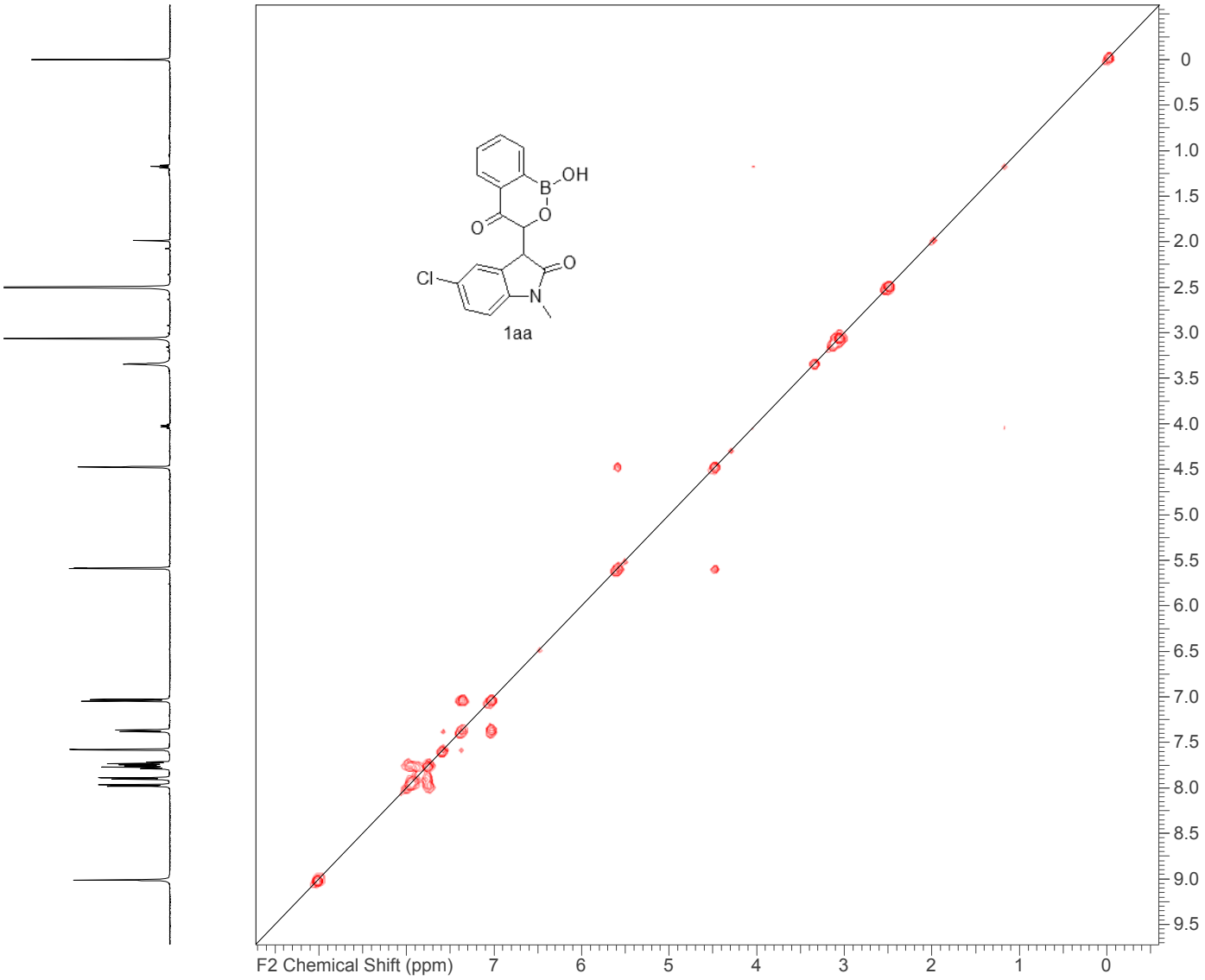
OriginalDateForRelativeTime 2014-05-13T12:37:28	***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 B's

Acquisition Time (sec)	0.8503	***Comment***	MKA-BORON-1			***Date***	13 May 2014 12:37:28
Date Stamp	13 May 2014 12:37:28			***File Name***	\\inbglab176164\ECM_2014\MKA\data\iMED\nmr\MKA-BORON-1\1\PDATA\1\1r		
Frequency (MHz)	96.29	***Nucleus***	11B	***Number of Transients***	1024	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg
Receiver Gain	5160.60	***SW(cyclical) (Hz)***	38535.64	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	0.0038
Spectrum Type	STANDARD	***Sweep Width (Hz)***	38534.47	***Temperature (degree C)***	25.000		

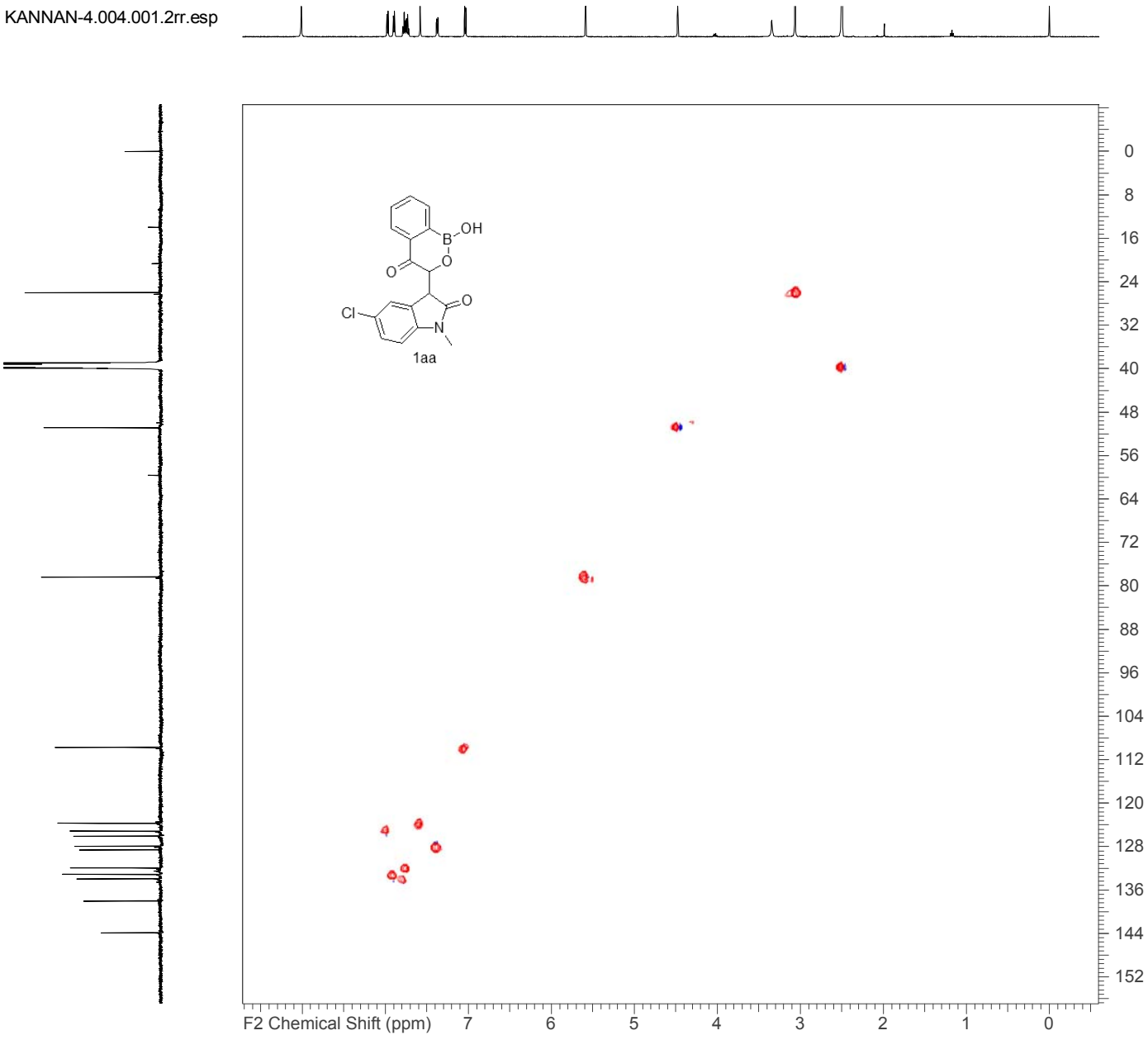


1aa

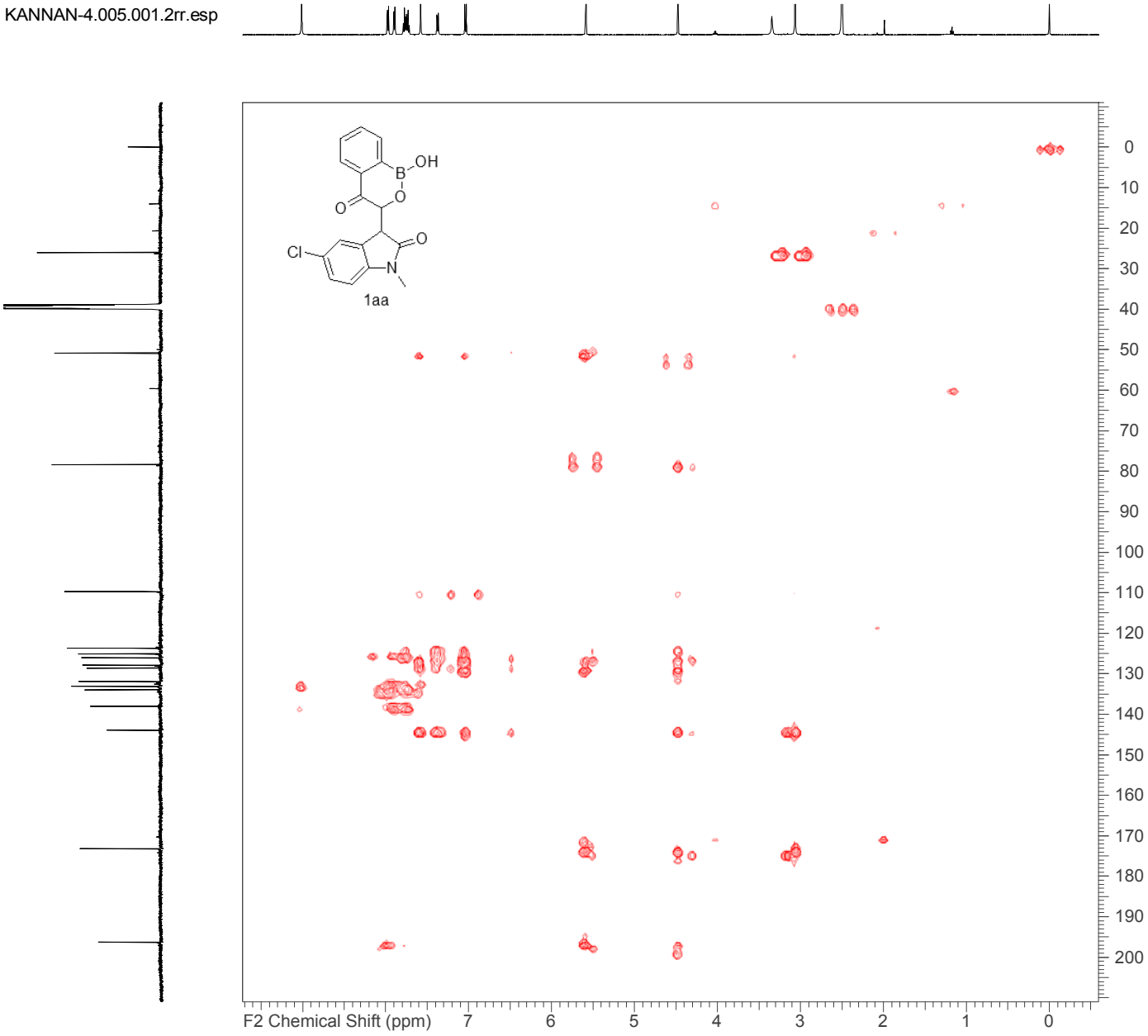
KANNAN-4.003.001.2rr.esp



KANNAN-4.004.001.2rr.esp



KANNAN-4.005.001.2rr.esp

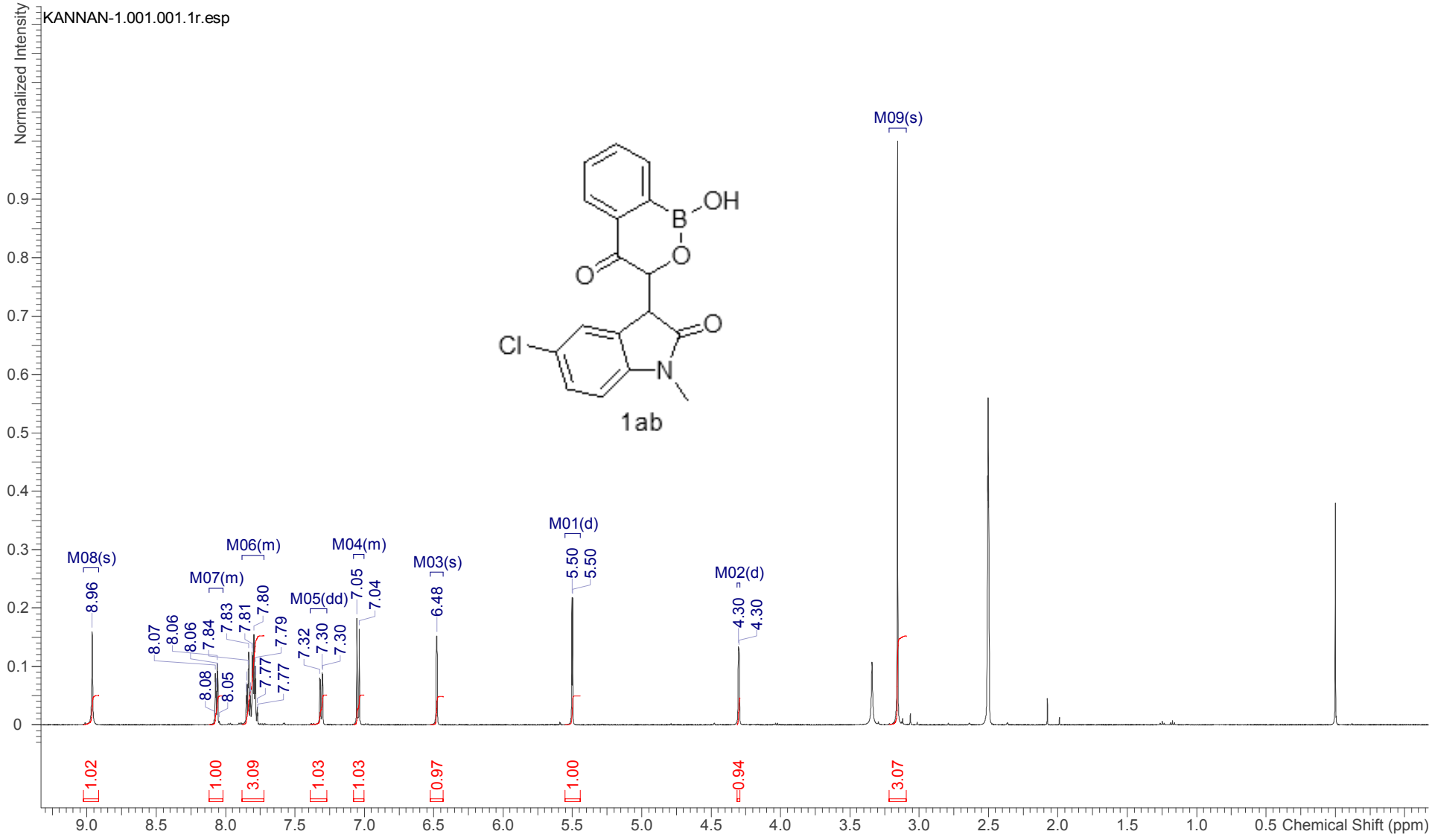


MKA-Cl-ISA-P2

15/05/2014 12:59:34

OriginalDateForRelativeTime 2014-05-05T09:48:56	***Multiplets Integrals Sum*** 13.16	***Number of Nuclei*** 13 H's

Acquisition Time (sec)	3.1719	***Comment***	PROTON DMSO {F:\ecm\DATA\2014-05} bionmr 41			***Date***	05 May 2014 09:48:56
Date Stamp	05 May 2014 09:48:56			***File Name***	\\inbgrdsfp01\elndata\MKA\KANNAN-1\1\PDATA\1\1r		
Frequency (MHz)	500.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	4.00	***SW(cyclical) (Hz)***	10330.58	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3090.4678
Spectrum Type	STANDARD	***Sweep Width (Hz)***	10330.26	***Temperature (degree C)***	25.000		

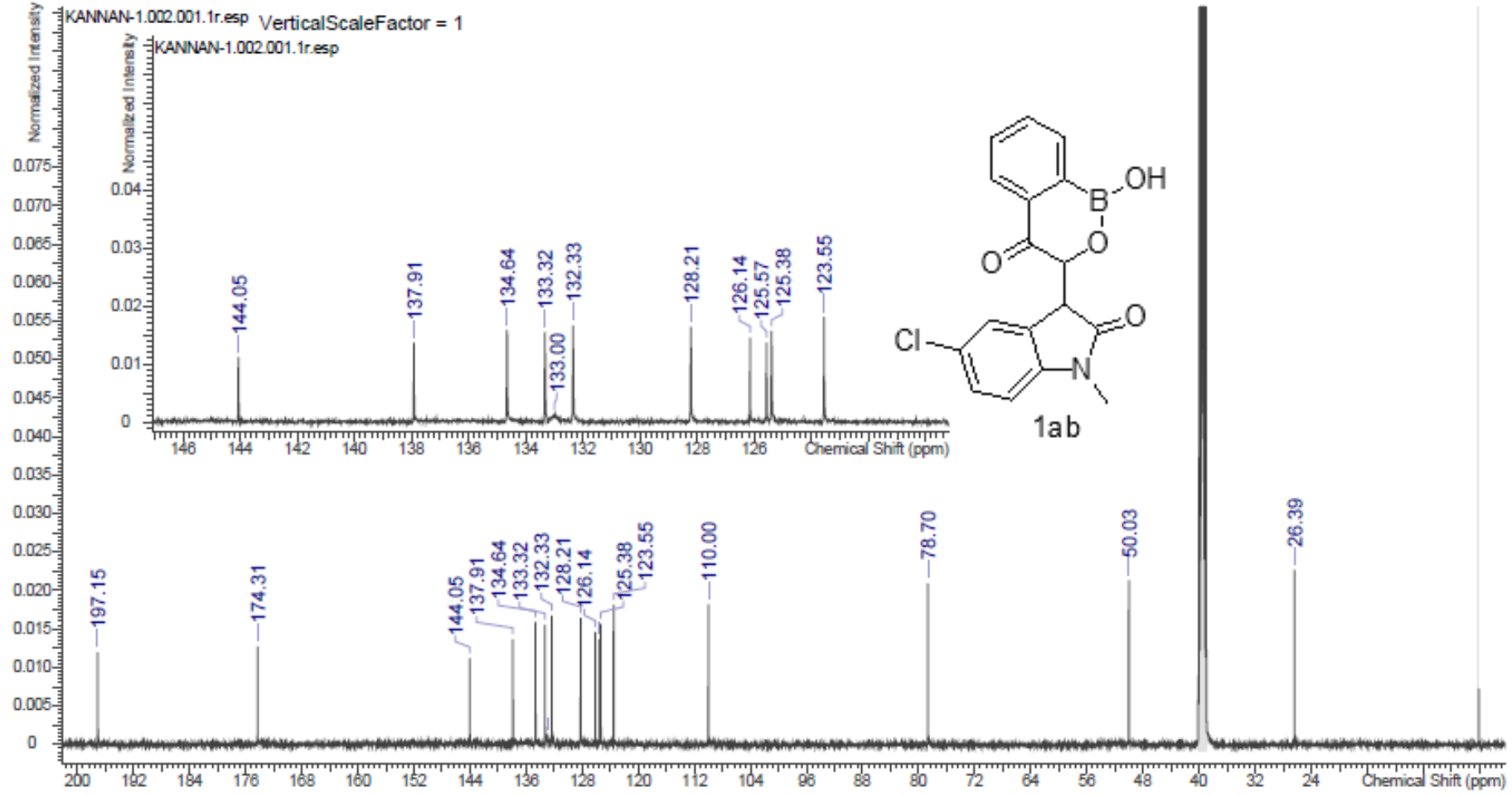


MKA-CI-ISA-P1

21/06/2014 12:12:57

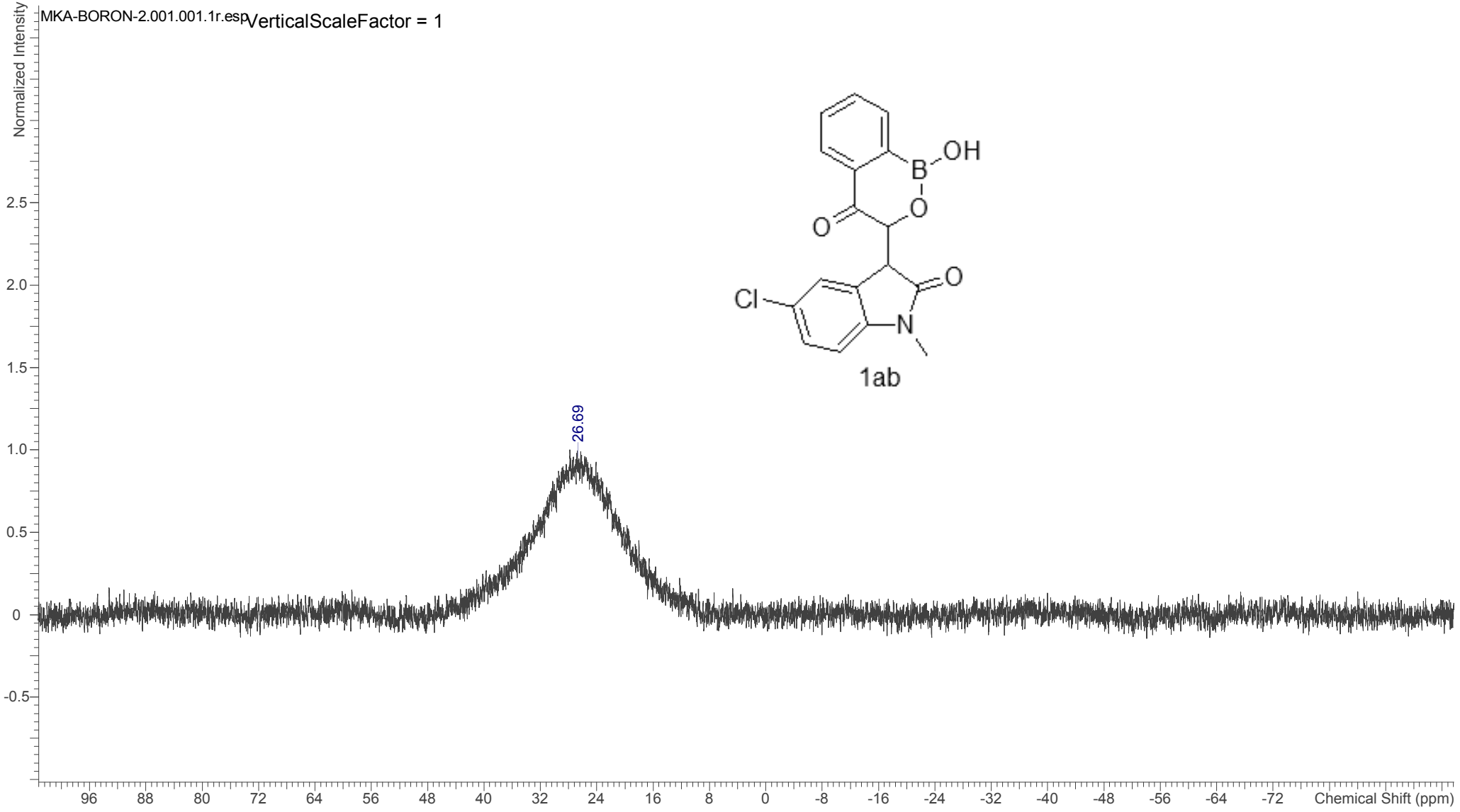
OriginalDateForRelativeTime	2014-05-05T16:59:52	*Multiplets Integrals Sum*	0.00	*Number of Nuclei*	0 C's

Acquisition Time (sec)	1.0912	*Comment*	C13CPD DMSO {F:\ecm\DATA\2014-05} bionmr 41			*Date*	05 May 2014 16:59:52
Date Stamp	05 May 2014 16:59:52			*File Name*	\\inbgrdsfp01\eln\data\MKA\KANNAN-1\2\PDATA\1\1r		
Frequency (MHz)	125.77	*Nucleus*	13C	*Number of Transients*	8192	*Origin*	spect
Original Points Count	32768	*Owner*	administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30
Receiver Gain	32768.00	*SW(cyclical) (Hz)*	30030.03	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	12518.3926
Spectrum Type	STANDARD	*Sweep Width (Hz)*	30029.11	*Temperature (degree C)*	25.000		



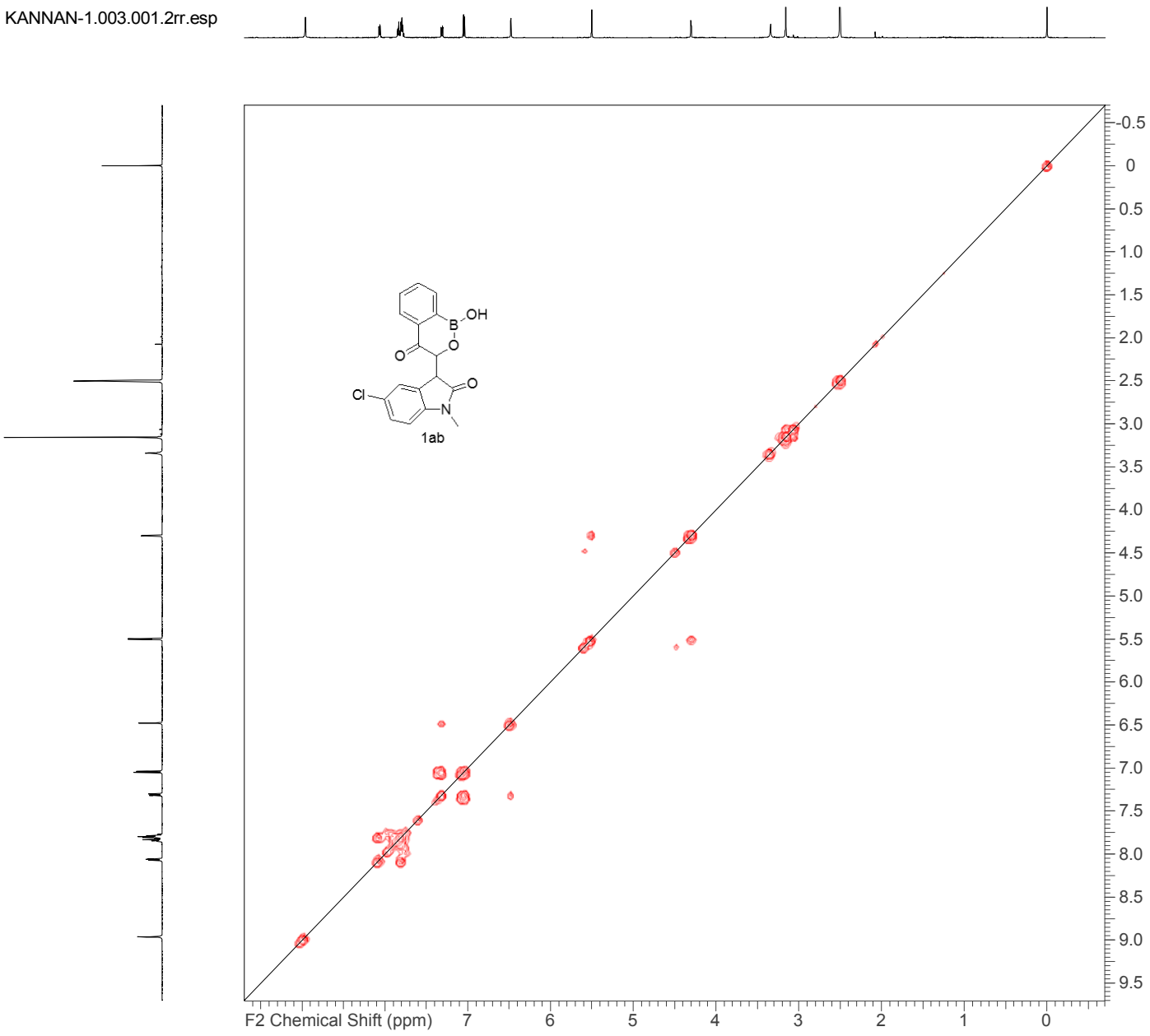
OriginalDateForRelativeTime 2014-05-13T14:00:40	***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 B's

Acquisition Time (sec)	0.8503	***Comment***	MKA-BORON-2			***Date***	13 May 2014 14:00:40
Date Stamp	13 May 2014 14:00:40			***File Name***	\\inbglab176164\ECM_2014\MKA\data\iMED\nmr\MKA-BORON-2\1\PDATA\1\1r		
Frequency (MHz)	96.29	***Nucleus***	11B	***Number of Transients***	1024	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg
Receiver Gain	5160.60	***SW(cyclical) (Hz)***	38535.64	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	0.0038
Spectrum Type	STANDARD	***Sweep Width (Hz)***	38534.47	***Temperature (degree C)***	25.000		

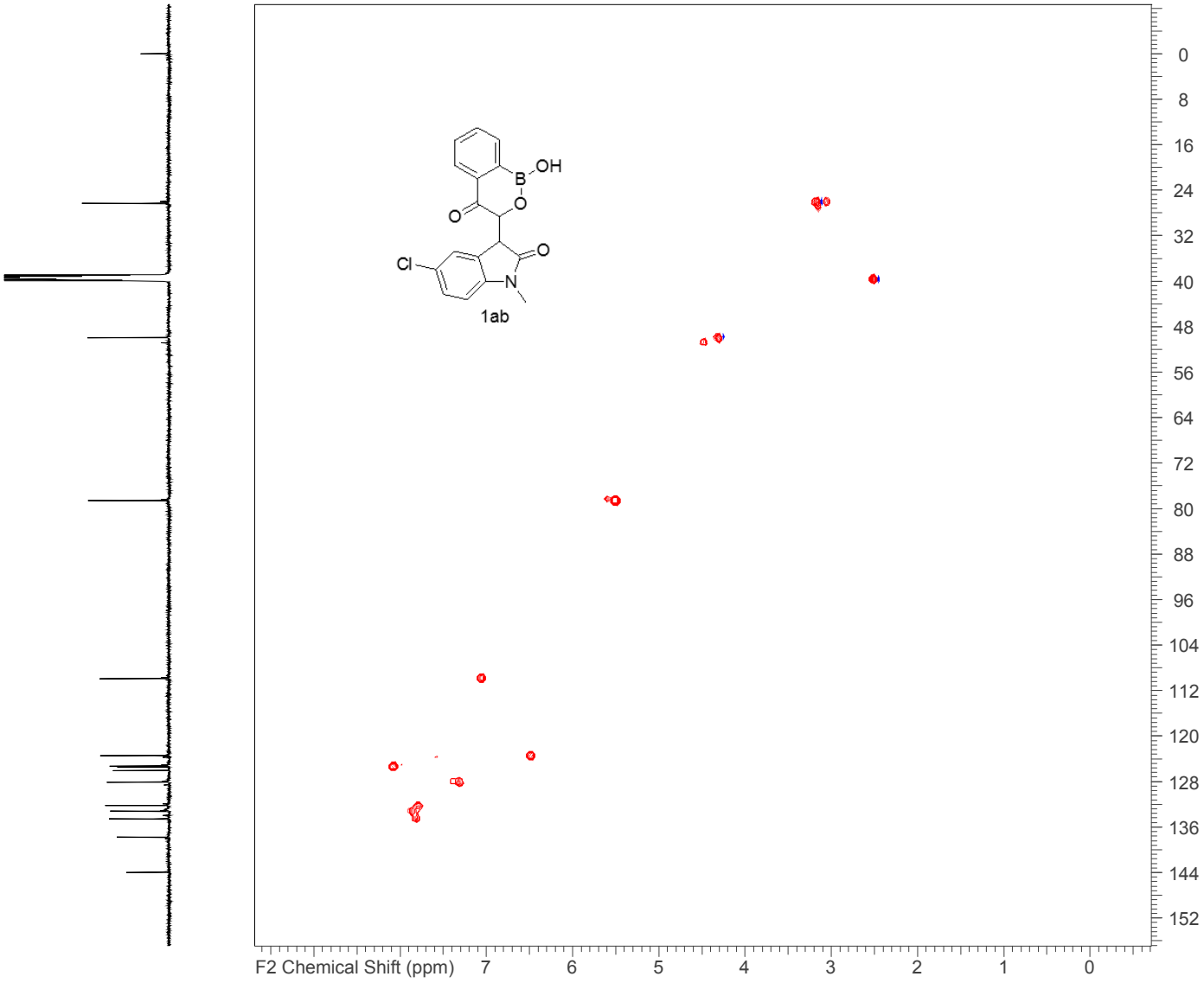


1ab

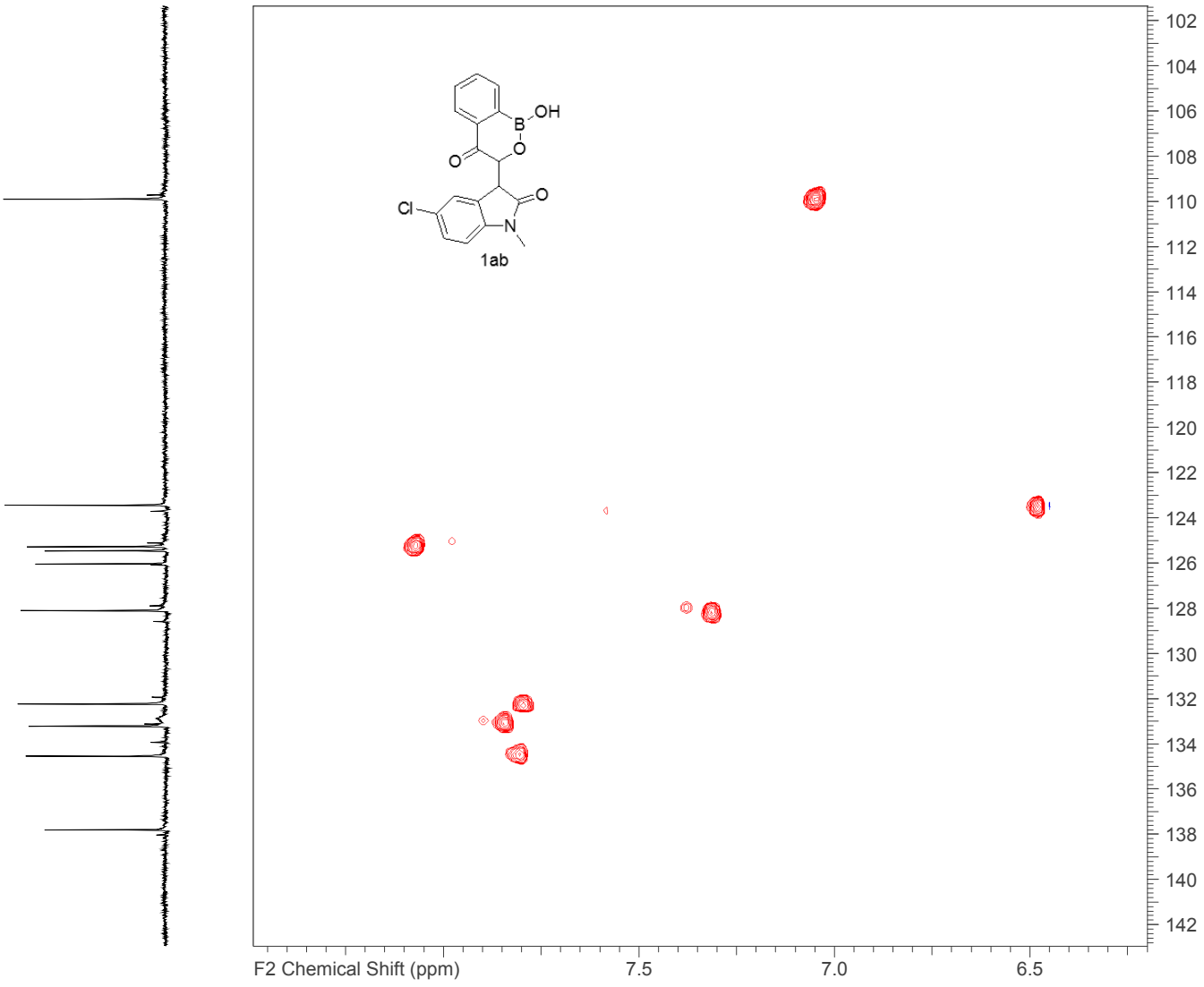
KANNAN-1.003.001.2rr.esp



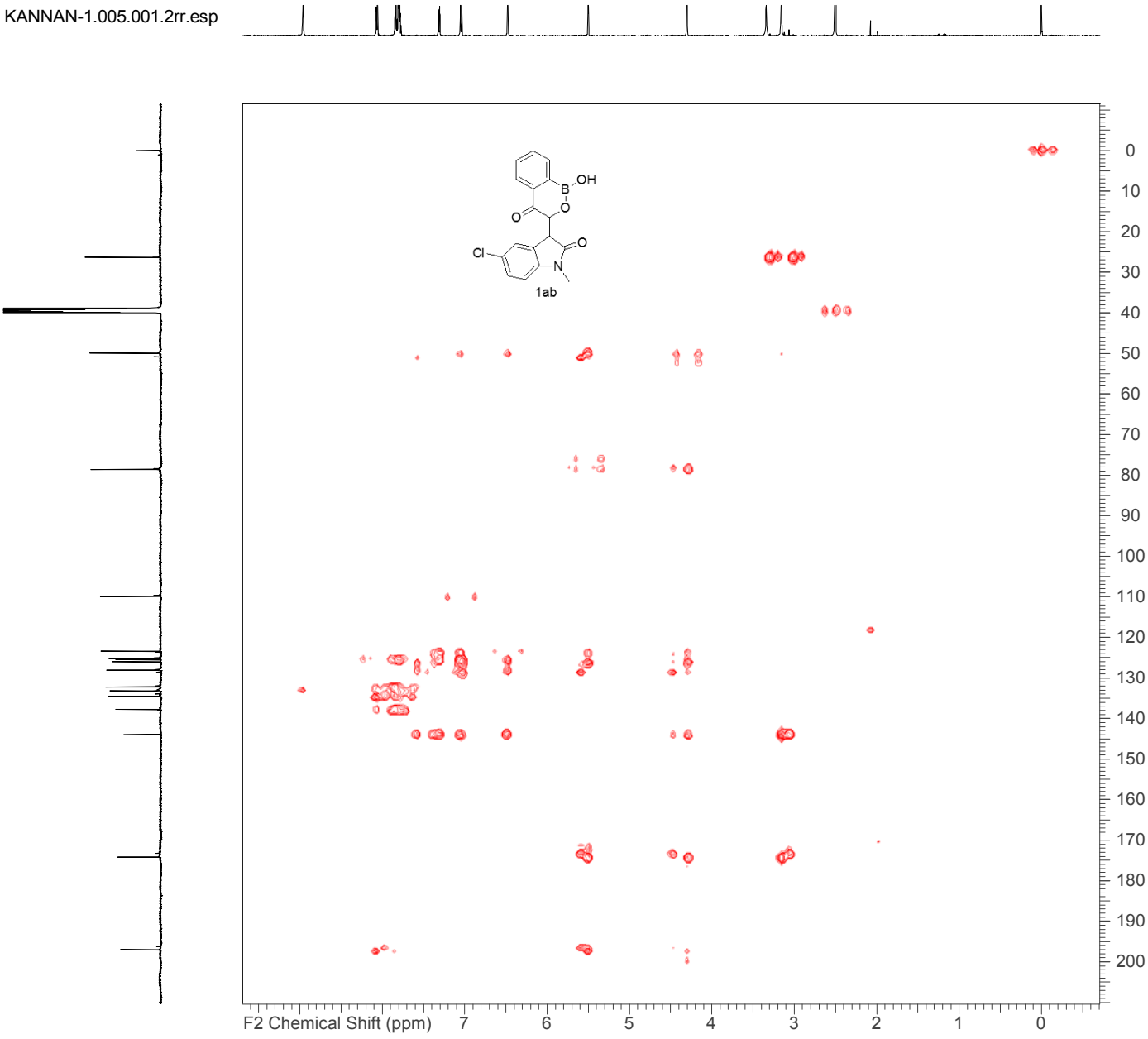
KANNAN-1.004.001.2rr.esp



KANNAN-1.004.001.2rr.esp



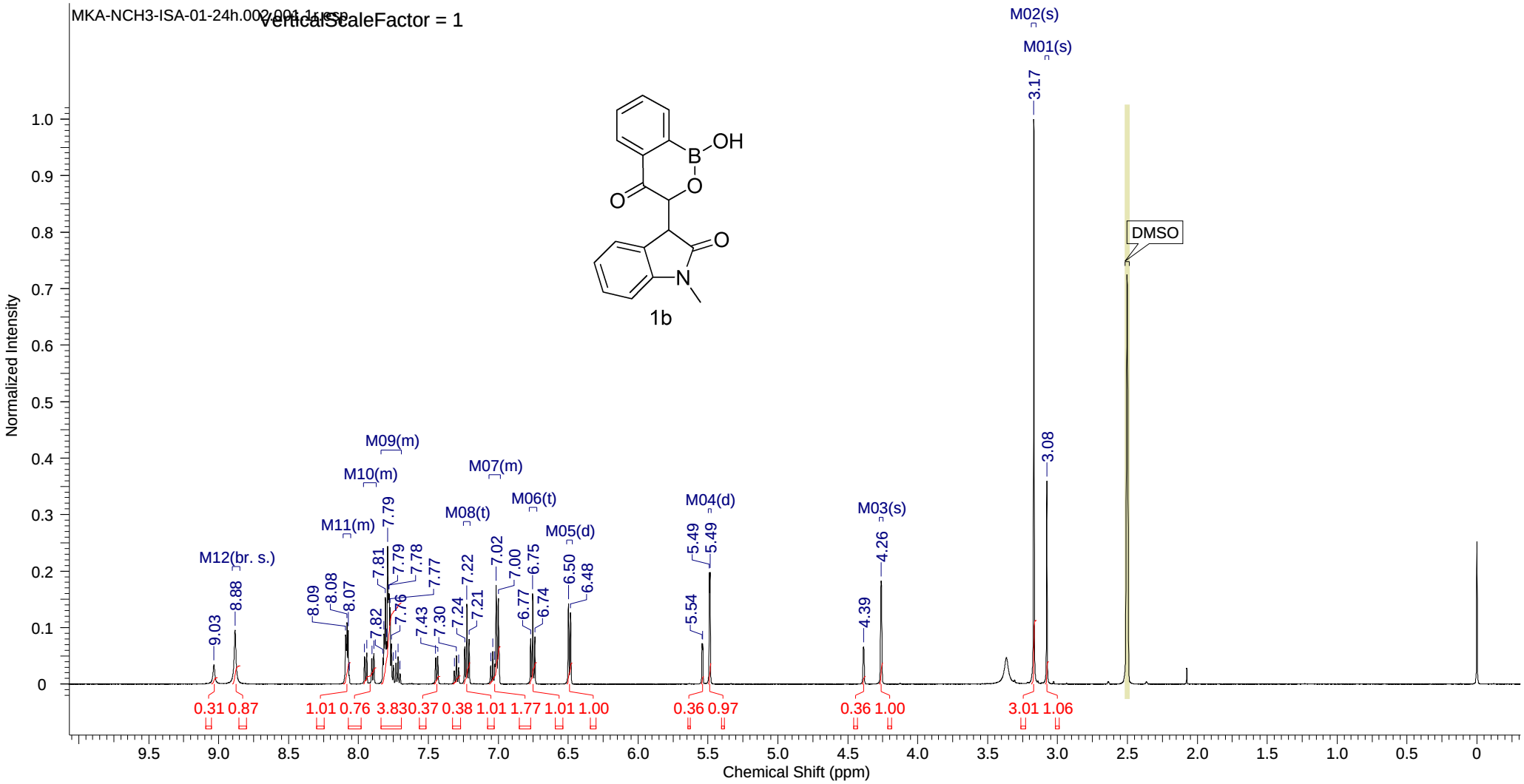
KANNAN-1.005.001.2rr.esp

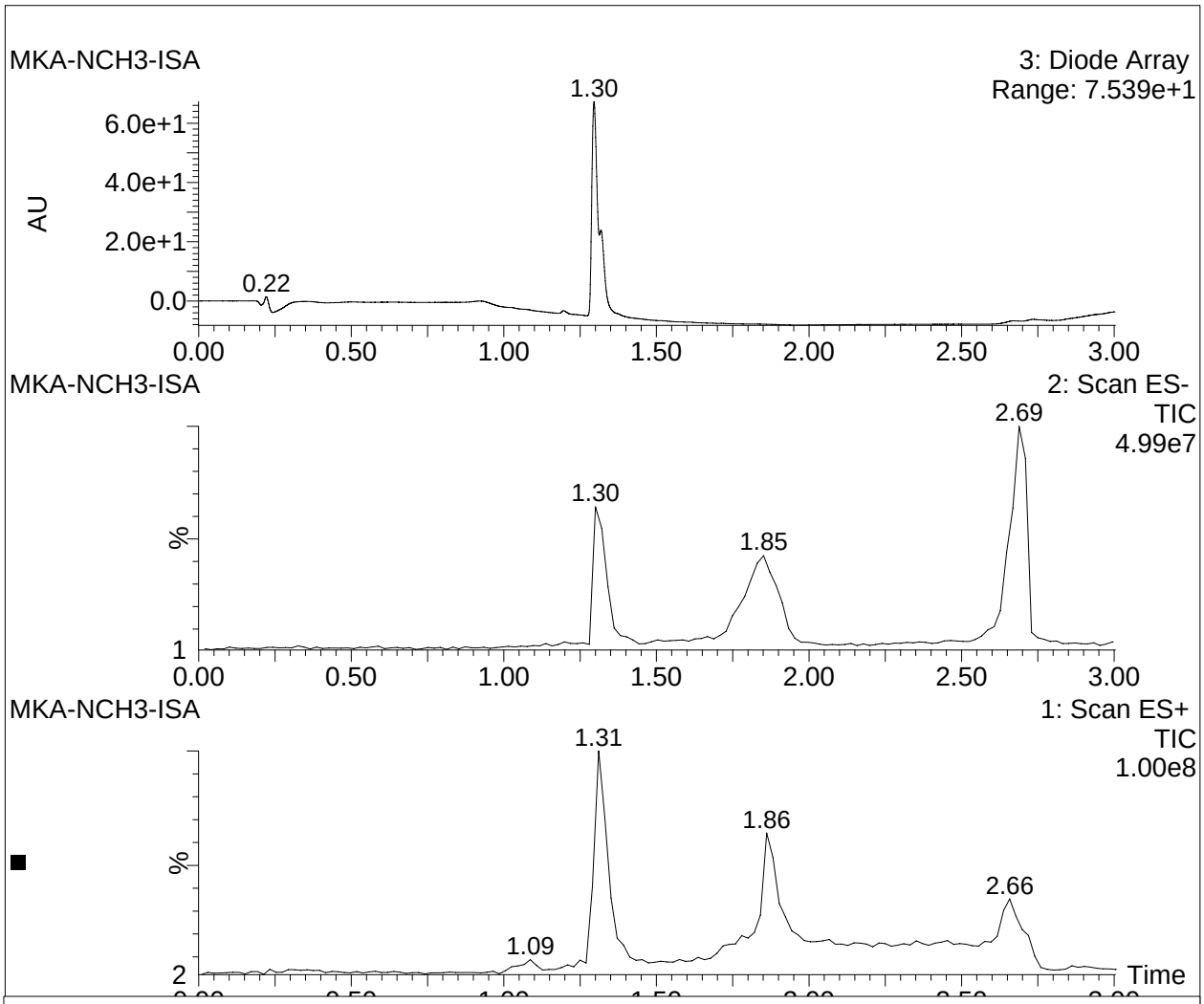


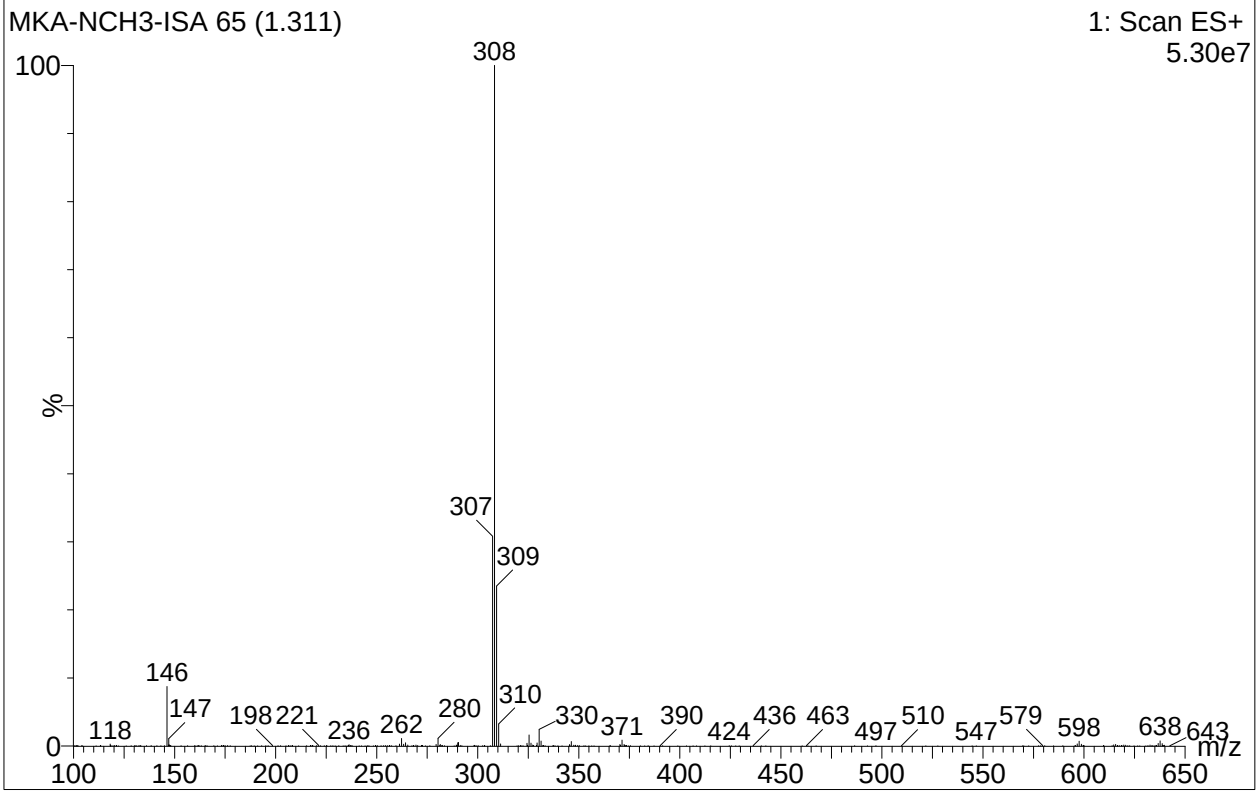
MKA-NCH3-ISA-M

11-01-2015 12:57:16

Acquisition Time (sec)	3.1719	**Comment**	MKA-NCH3-ISA-01-24h/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 24				
Date	12 May 2014 00:32:08			**Date Stamp**	12 May 2014 00:32:08		
File Name	D:\New folder\Pandrive 1\Transcend\ECM final\MKA-NCH3-ISA-01-24h\2\PDATA\1\1r					**Frequency (MHz)**	500.13
Nucleus	1H	**Number of Transients**	16	**Origin**	spect	**Original Points Count**	32768
Owner	administrator	**Points Count**	32768	**Pulse Sequence**	zg30	**Receiver Gain**	4.00
SW(cyclical) (Hz)	10330.58	**Solvent**	DMSO-d6	**Spectrum Offset (Hz)**	3091.6387	**Spectrum Type**	STANDARD
Sweep Width (Hz)	10330.26	**Temperature (degree C)**	25.000				




MKA-NCH3-ISA
3: Diode Array
Range: 7.539e+1
1.30
6.0e+1
4.0e+1
2.0e+1
0.0
AU
0.22
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-NCH3-ISA
2: Scan ES-
TIC
4.99e7
2.69
1.30
1.85
%
1
MKA-NCH3-ISA
1: Scan ES+
TIC
1.00e8
1.31
1.86
2.66
1.09
%
2
Time

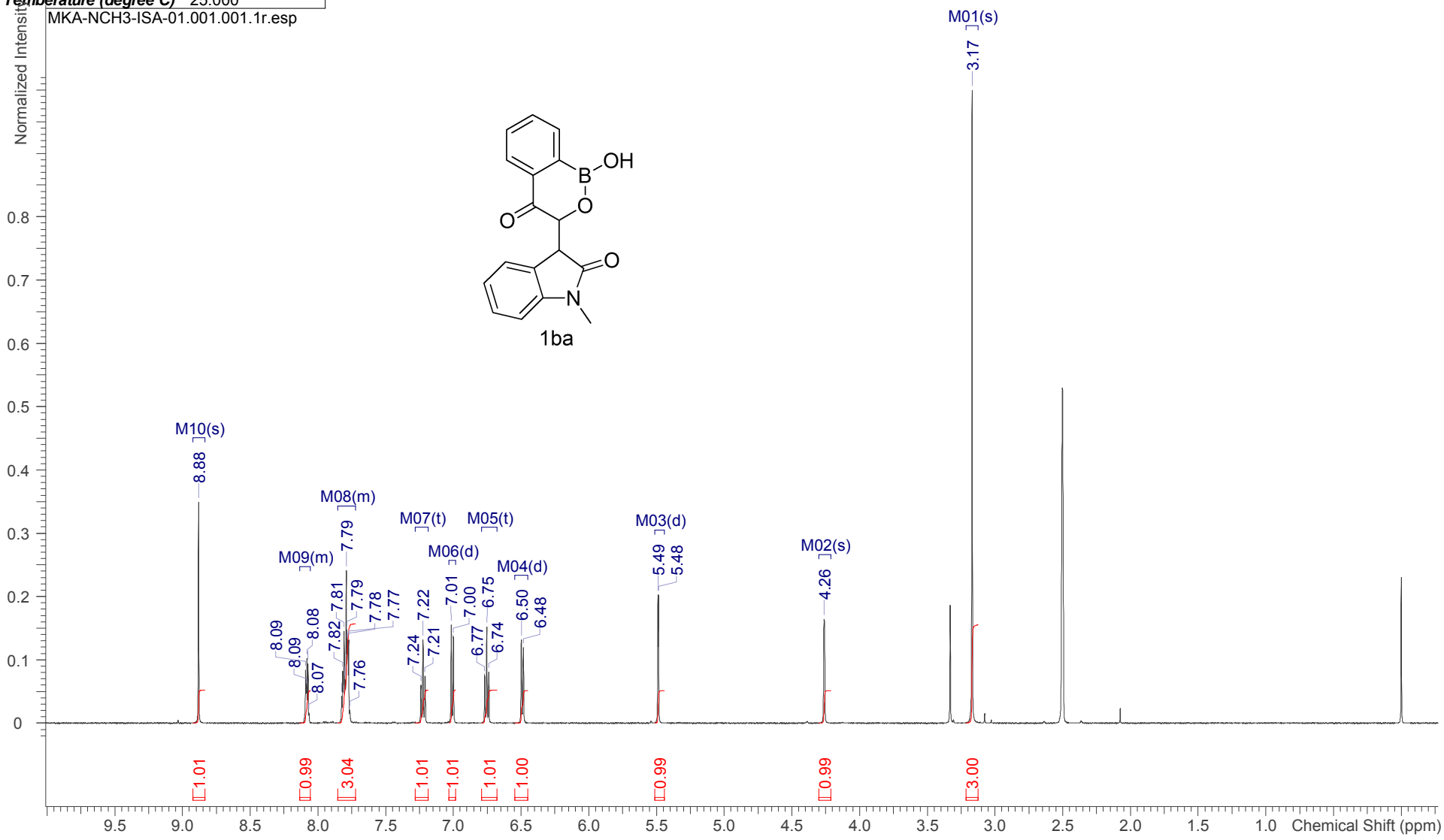

MKA-NCH3-ISA 65 (1.311)
1: Scan ES+
5.30e7
100
%
0
308
307
309
146
147
118
198
221
236
262
280
310
330
371
390
424
436
463
497
510
547
579
598
638
643
m/z
100
150
200
250
300
350
400
450
500
550
600
650

MKA-Cl-ISA-P1

16/05/2014 11:08:55

OriginalDateForRelativeTime	2014-05-09T15:04:40	***Multiplets Integrals Sum***	14.04	***Number of Nuclei***	14 H's

Acquisition Time (sec)	3.1719	***Comment***	MKA-NCH3-ISA-01/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 24				
Date	09 May 2014 15:04:40			***Date Stamp***	09 May 2014 15:04:40		
File Name	\\inbgrdsfp01\elndata\MKA\MKA-NCH3-ISA-01\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	administrator
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00	***SW(cyclical) (Hz)***	10330.58
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3090.5376	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10330.26
Temperature (degree C)	25.000						

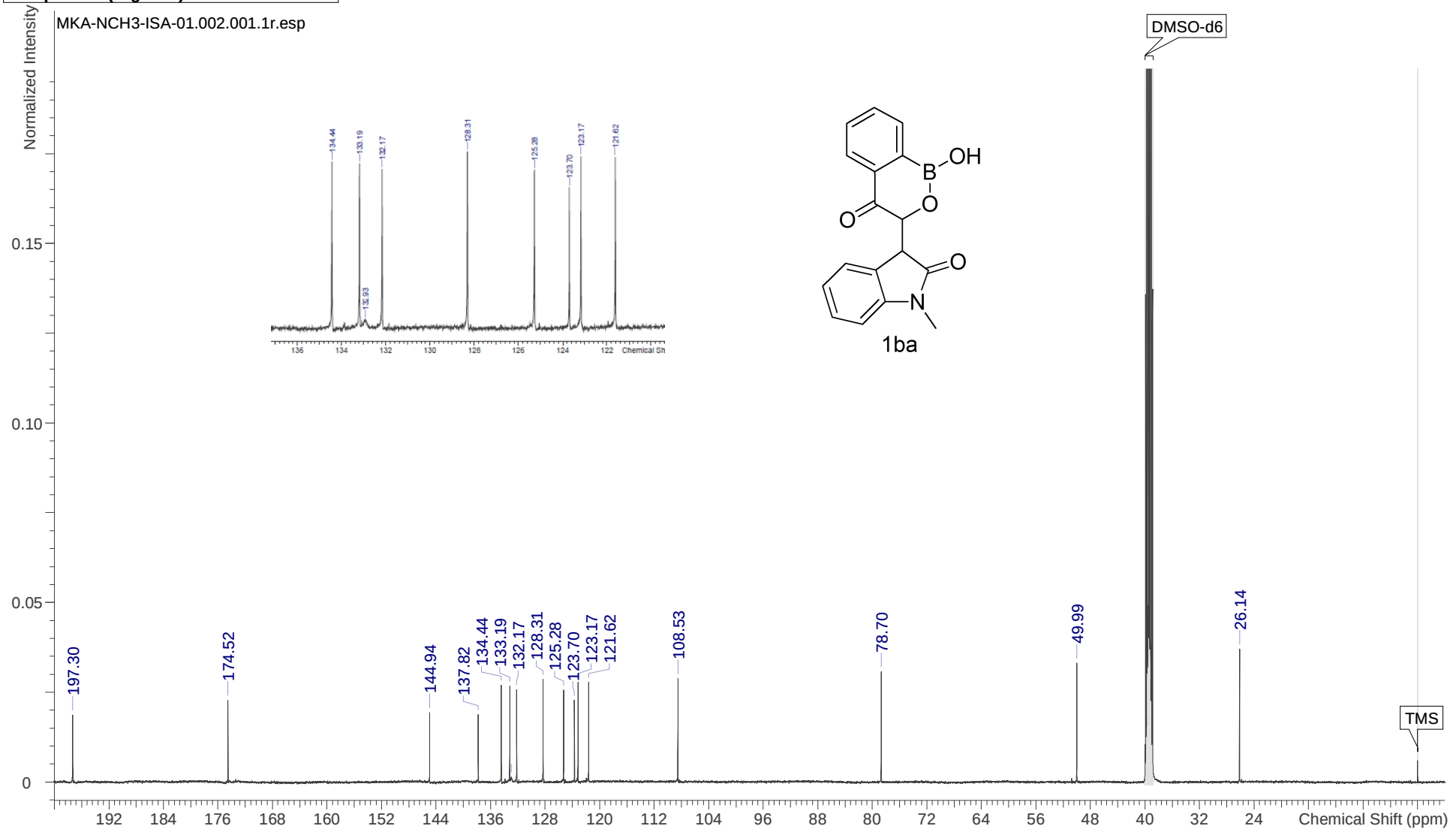


MKA-NCH3-ISA-P1

16/05/2014 13:31:49

OriginalDateForRelativeTime	2014-05-09T20:20:24	**Multiplets Integrals Sum**	0.00	**Number of Nuclei**	0 C's

Acquisition Time (sec)	1.0912	**Comment**	MKA-NCH3-ISA-01/DMSO C13CPD DMSO {F:\ecm\DATA\2014-04} bionmr 24				
Date	09 May 2014 20:20:24			**Date Stamp**	09 May 2014 20:20:24		
File Name	\\inbgrdsfp01\elndata\MKA\MKA-NCH3-ISA-01\2\PDATA\1\1r			**Frequency (MHz)**	125.77	**Nucleus**	13C
Number of Transients	6000	**Origin**	spect	**Original Points Count**	32768	**Owner**	administrator
Points Count	32768	**Pulse Sequence**	zgpg30	**Receiver Gain**	32768.00	**SW(cyclical) (Hz)**	30030.03
Solvent	DMSO-d6	**Spectrum Offset (Hz)**	12504.4170	**Spectrum Type**	STANDARD	**Sweep Width (Hz)**	30029.11
Temperature (degree C)	25.000						

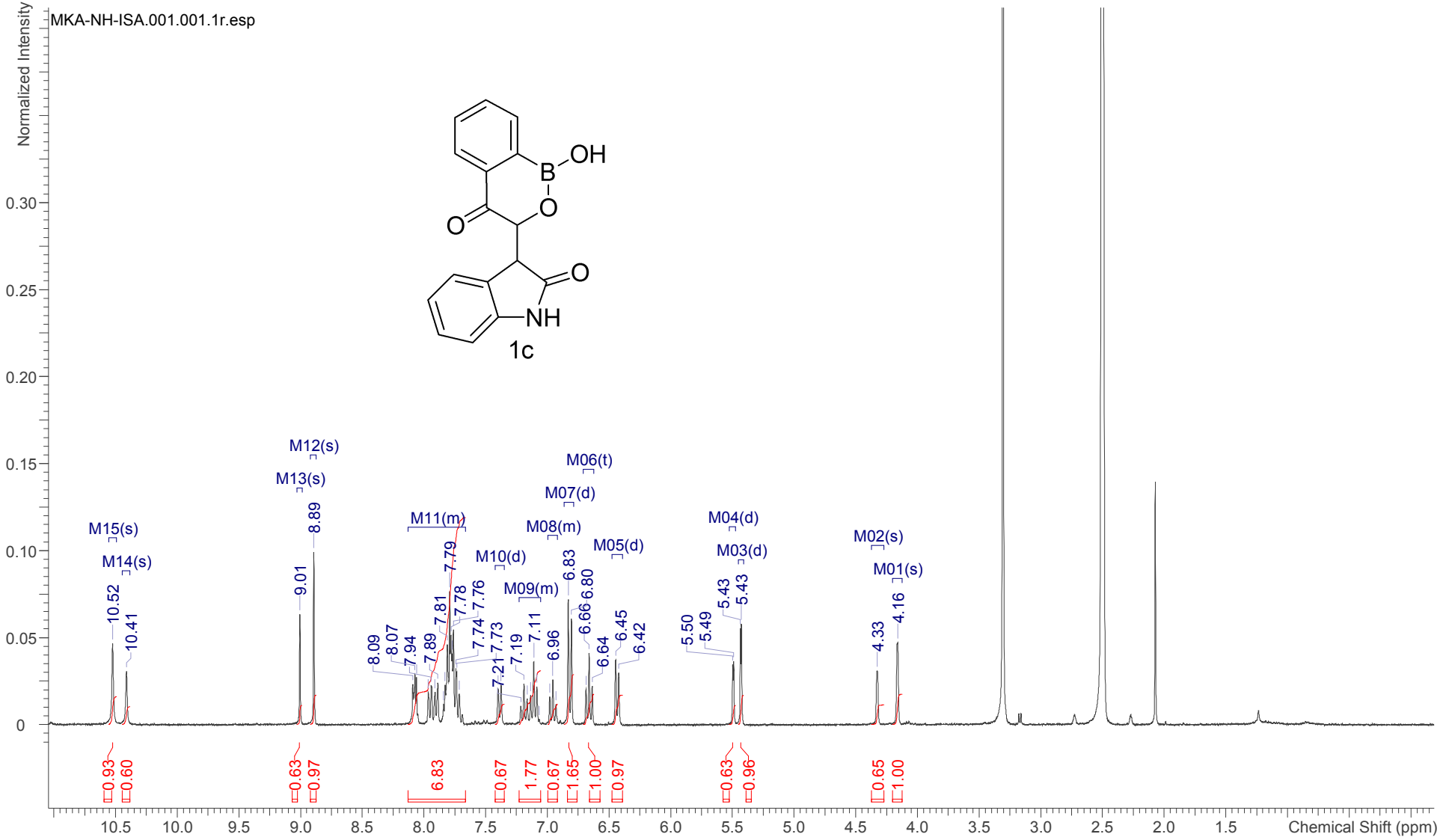


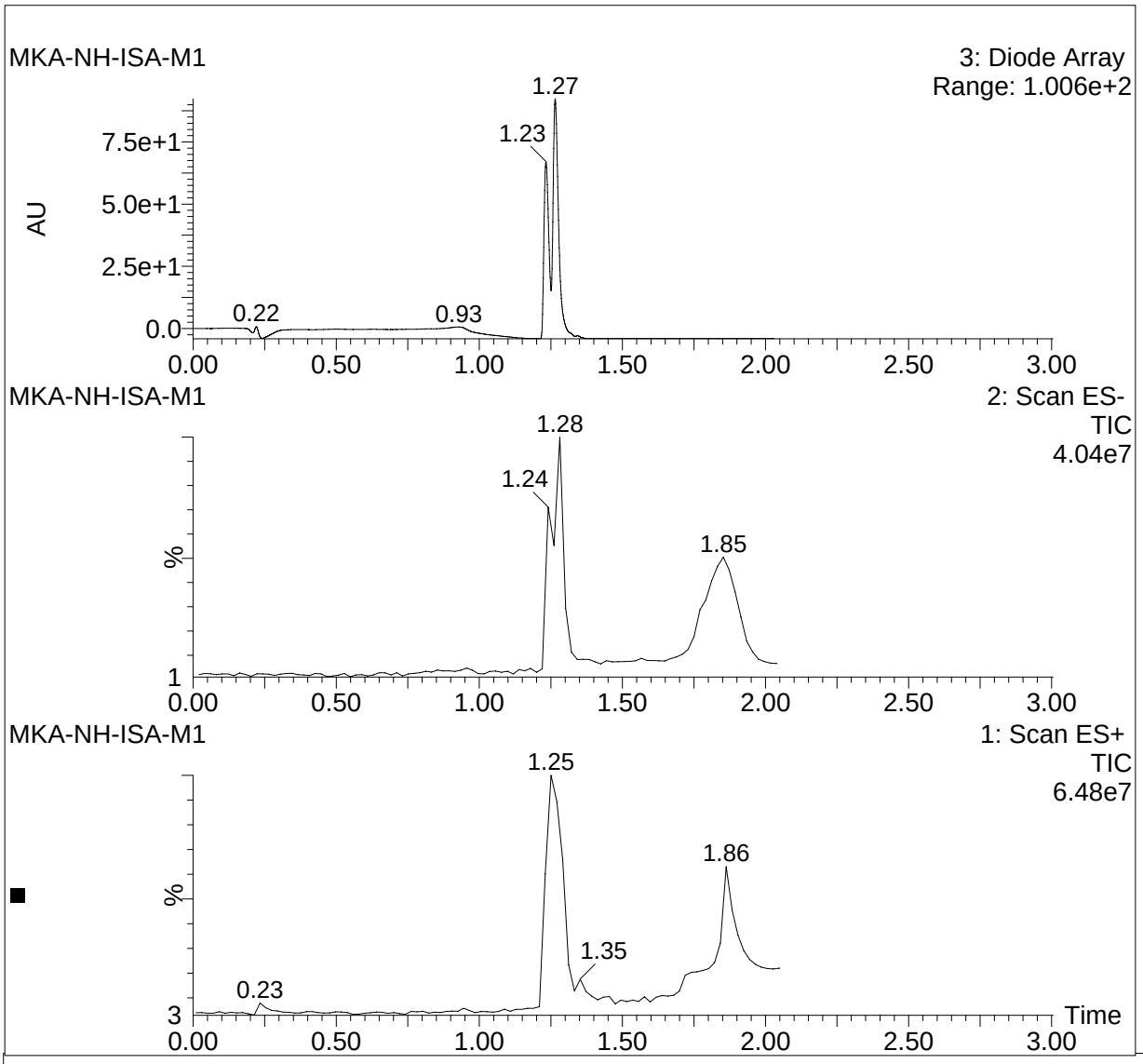
MKA-NH-ISA-M

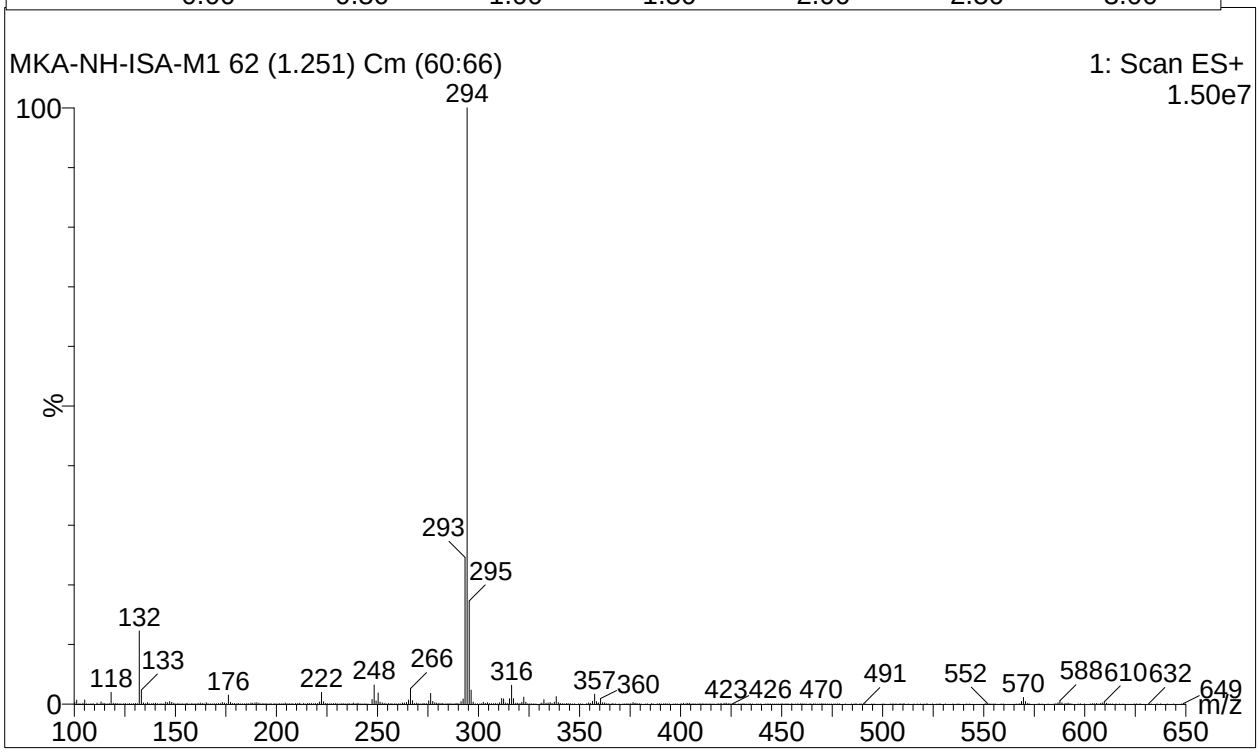
16/05/2014 14:18:28

OriginalDateForRelativeTime	2014-04-11T20:16:08	***Multiplets Integrals Sum***	19.93	***Number of Nuclei***	23 H's

Acquisition Time (sec)	5.3084	***Comment***	MKA-NH-ISA/DMSO			***Date***	11 Apr 2014 20:16:08
Date Stamp	11 Apr 2014 20:16:08			***File Name***	C:\Users\kkth216\Desktop\NMR-300\MKA-NH-ISA\1\PDATA\1\1r		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	126	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1625.50	***SW(cyclical) (Hz)***	6172.84	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1853.4569
Spectrum Type	STANDARD	***Sweep Width (Hz)***	6172.65	***Temperature (degree C)***	25.000		




MKA-NH-ISA-M1
3: Diode Array
Range: 1.006e+2
1.27
1.23
7.5e+1
5.0e+1
2.5e+1
0.0
AU
0.22
0.93
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-NH-ISA-M1
2: Scan ES-
TIC
4.04e7
1.28
1.24
1.85
%
1
MKA-NH-ISA-M1
1: Scan ES+
TIC
6.48e7
1.25
1.86
1.35
0.23
3
Time

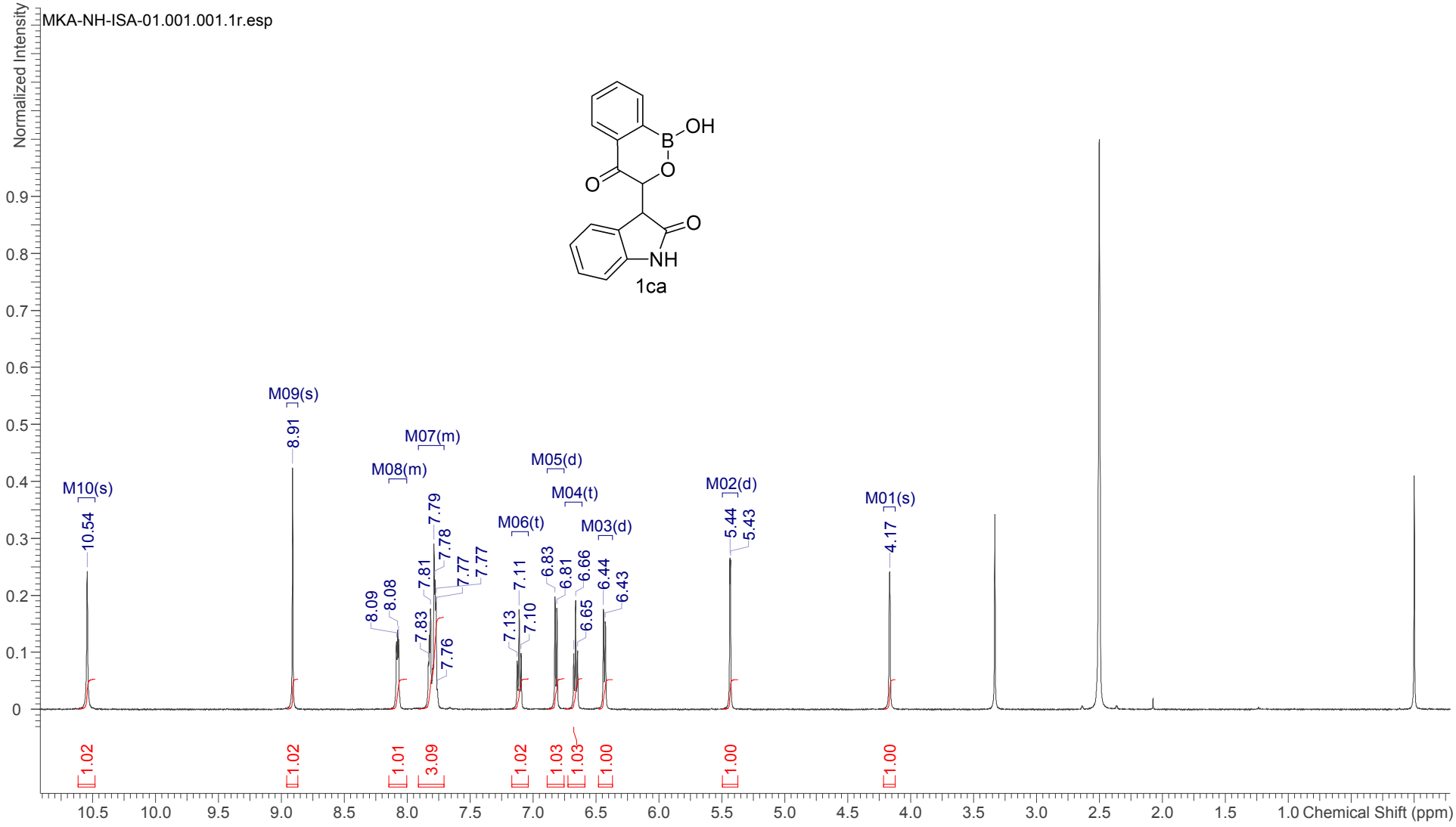

MKA-NH-ISA-M1 62 (1.251) Cm (60:66)
1: Scan ES+
1.50e7
100
294
%
293
295
132
133
118
176
222
248
266
316
357
360
423
426
470
491
552
570
588
610
632
649
0
m/z
100
150
200
250
300
350
400
450
500
550
600
650

MKA-NH-ISA-P1

16/05/2014 13:34:23

OriginalDateForRelativeTime	2014-05-09T09:36:08	***Multiplets Integrals Sum***	12.22	***Number of Nuclei***	12 H's

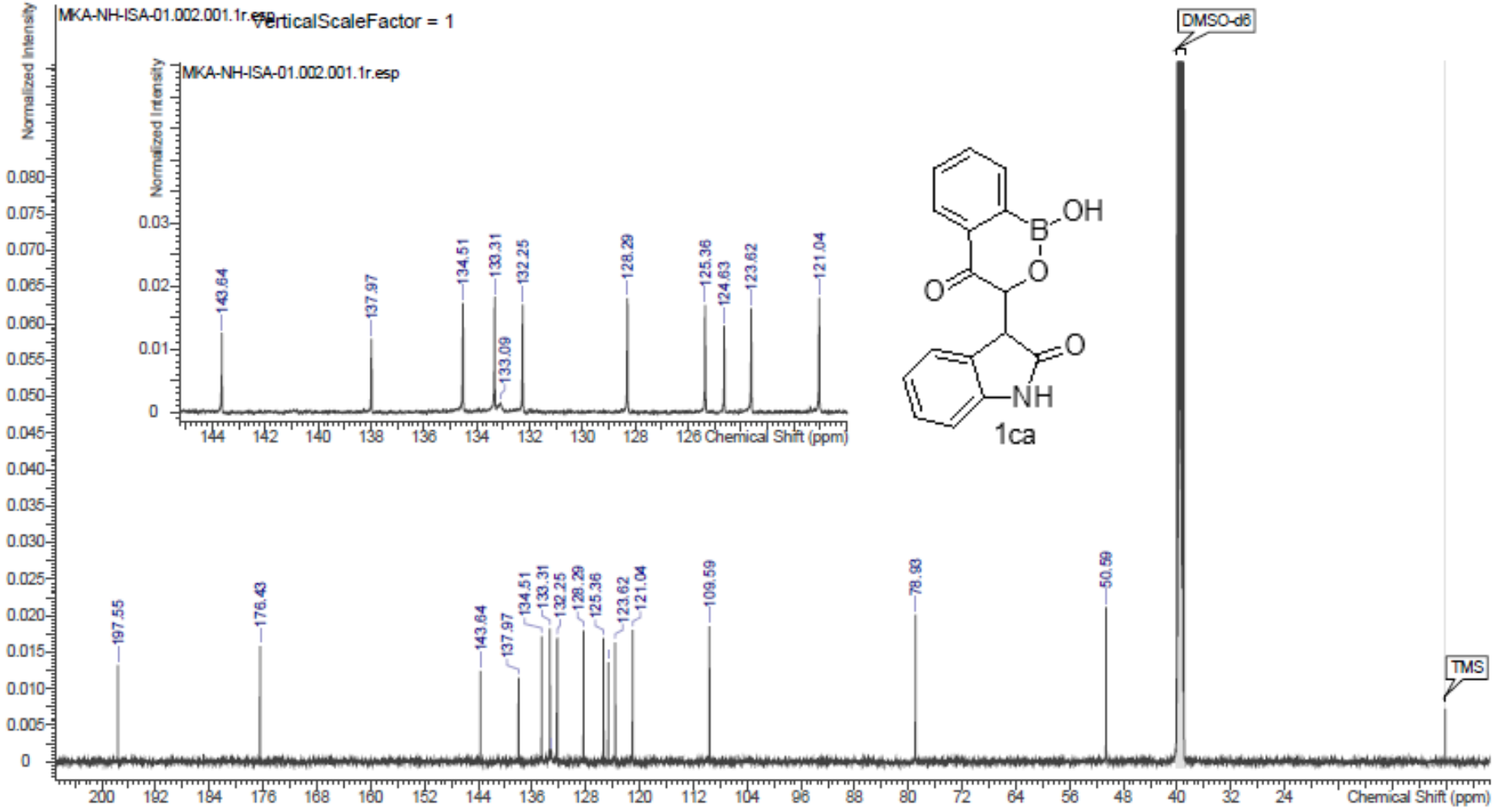
Acquisition Time (sec)	3.1719	***Comment***	MKA-NH-ISA-01/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 23				
Date	09 May 2014 09:36:08			***Date Stamp***	09 May 2014 09:36:08		
File Name	\\inbgrdsfp01\elndata\MKA\MKA-NH-ISA-01\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	administrator
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00	***SW(cyclical) (Hz)***	10330.58
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3094.0537	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10330.26
Temperature (degree C)	25.000						



24/06/2014 07:19:10

OriginalDateForRelativeTime 2014-05-09T14:51:52			*Multiplets Integrals Sum*	0.00	*Number of Nuclei* 0 C's

Acquisition Time (sec)	1.0912	*Comment*	MKA-NH-ISA-01/DMSO C13CPD DMSO (F:\ecm\DATA\2014-04) bionmr 23				
Date	09 May 2014 14:51:52			*Date Stamp*	09 May 2014 14:51:52		
File Name	\\inbgrdsfp01\elndata\MKA\07052014\MKA-NH-ISA-01\2\PDATA\1\1r					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	6000	*Origin*	spect	*Original Points Count*	32768
Owner	administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	32768.00
SW(cyclical) (Hz)	30030.03	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	12519.3086	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				

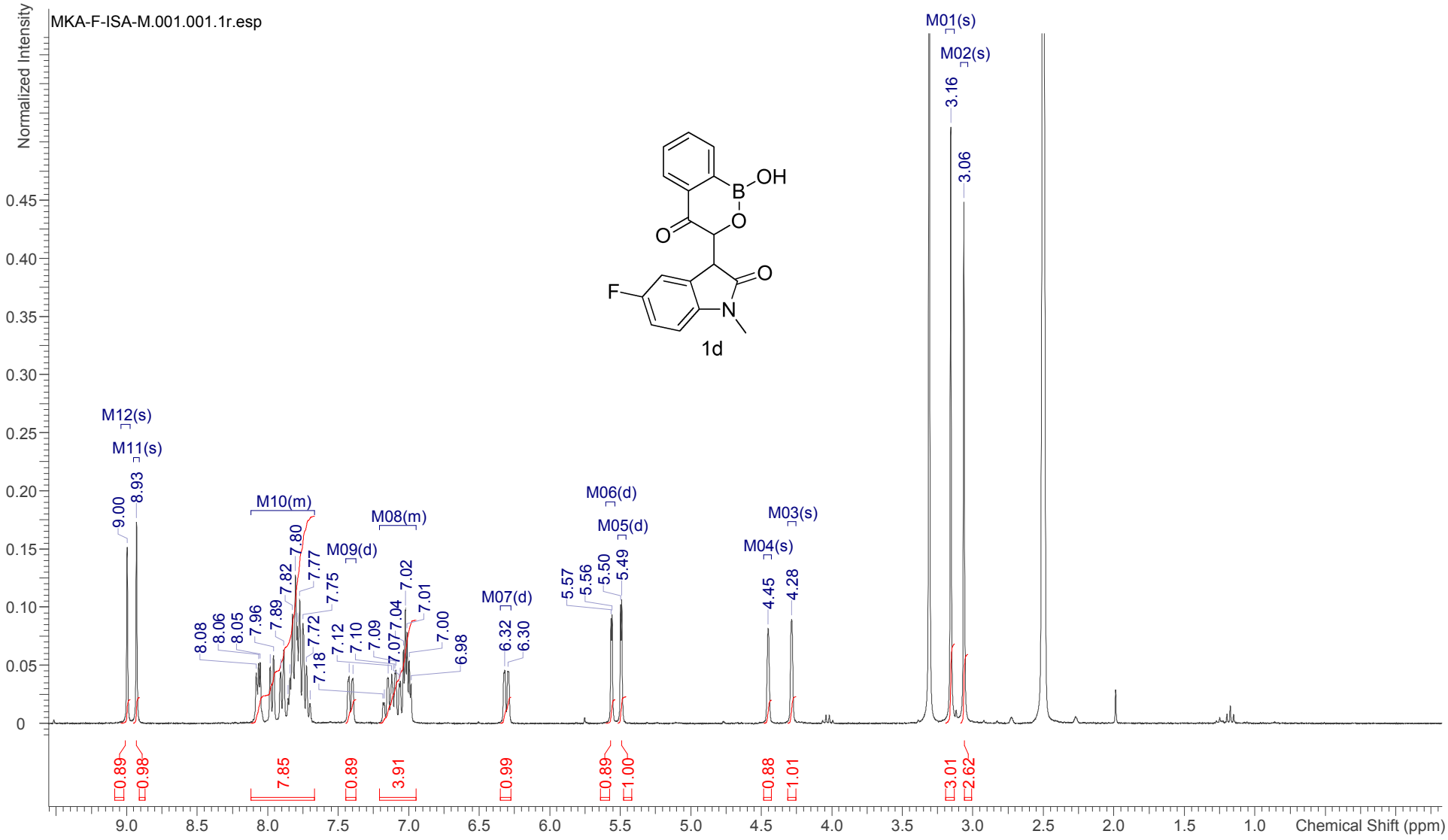


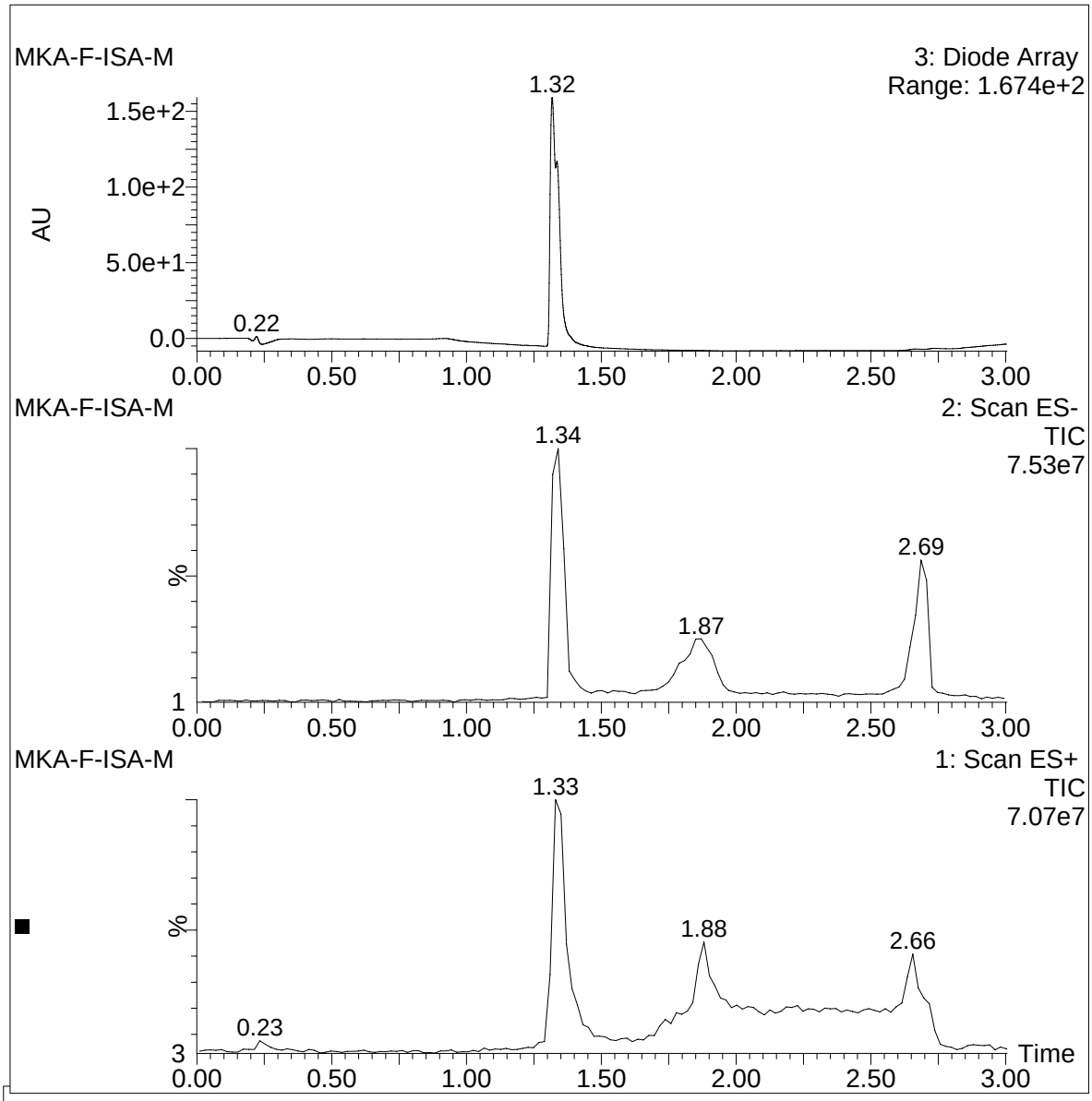
MKA-F-ISA-M

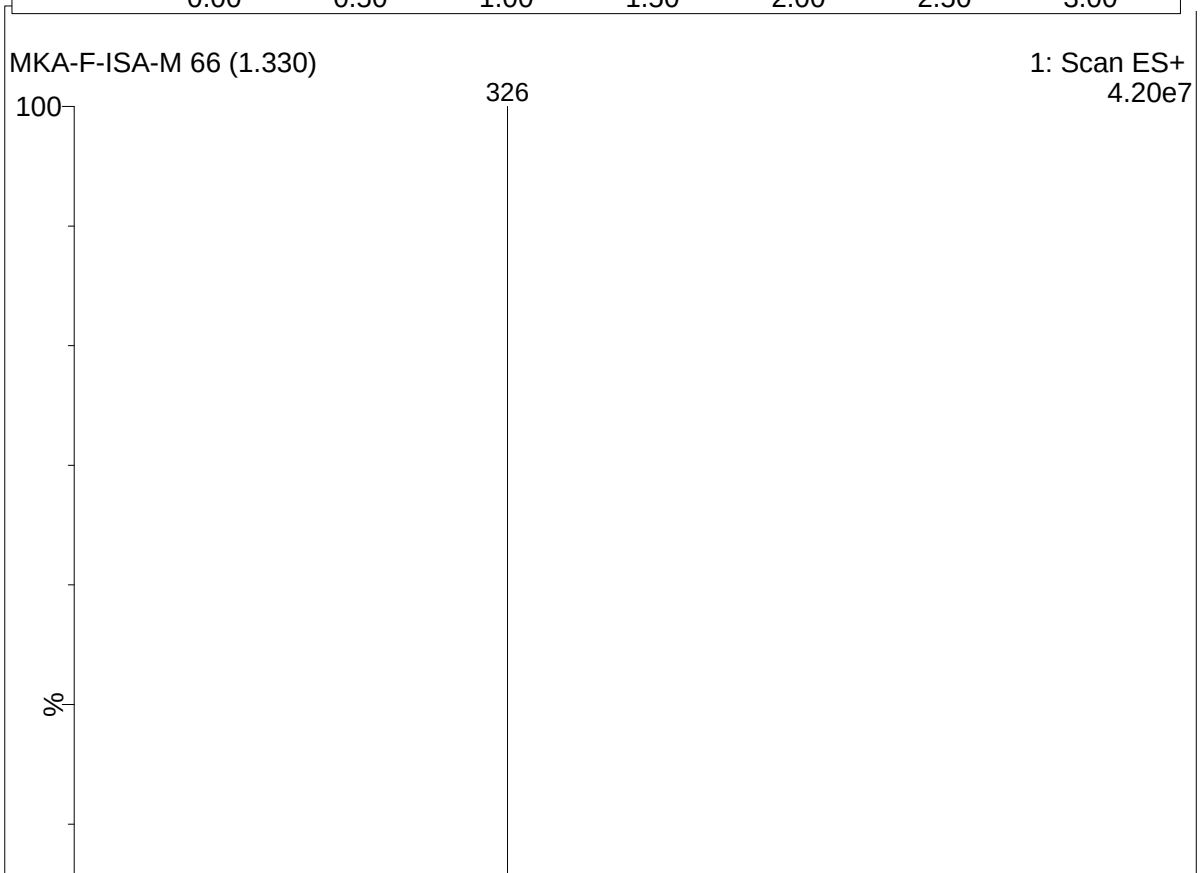
16/05/2014 14:21:59

OriginalDateForRelativeTime	2014-04-12T11:27:04	***Multiplets Integrals Sum***	24.92	***Number of Nuclei***	26 H's

Acquisition Time (sec)	5.3084	***Comment***	MKA-F-ISA-M/DMSO			***Date***	12 Apr 2014 11:27:04
Date Stamp	12 Apr 2014 11:27:04			***File Name***	C:\Users\kkth216\Desktop\NMR-300\MKA-F-ISA-M\1\PDATA\1\1r		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	126	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1625.50	***SW(cyclical) (Hz)***	6172.84	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1853.4569
Spectrum Type	STANDARD	***Sweep Width (Hz)***	6172.65	***Temperature (degree C)***	24.500		




MKA-F-ISA-M
3: Diode Array
Range: 1.674e+2
1.32
1.5e+2
1.0e+2
5.0e+1
0.0
AU
0.22
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-F-ISA-M
2: Scan ES-
TIC
7.53e7
1.34
2.69
1.87
%
1
MKA-F-ISA-M
1: Scan ES+
TIC
7.07e7
1.33
1.88
2.66
0.23
3
Time

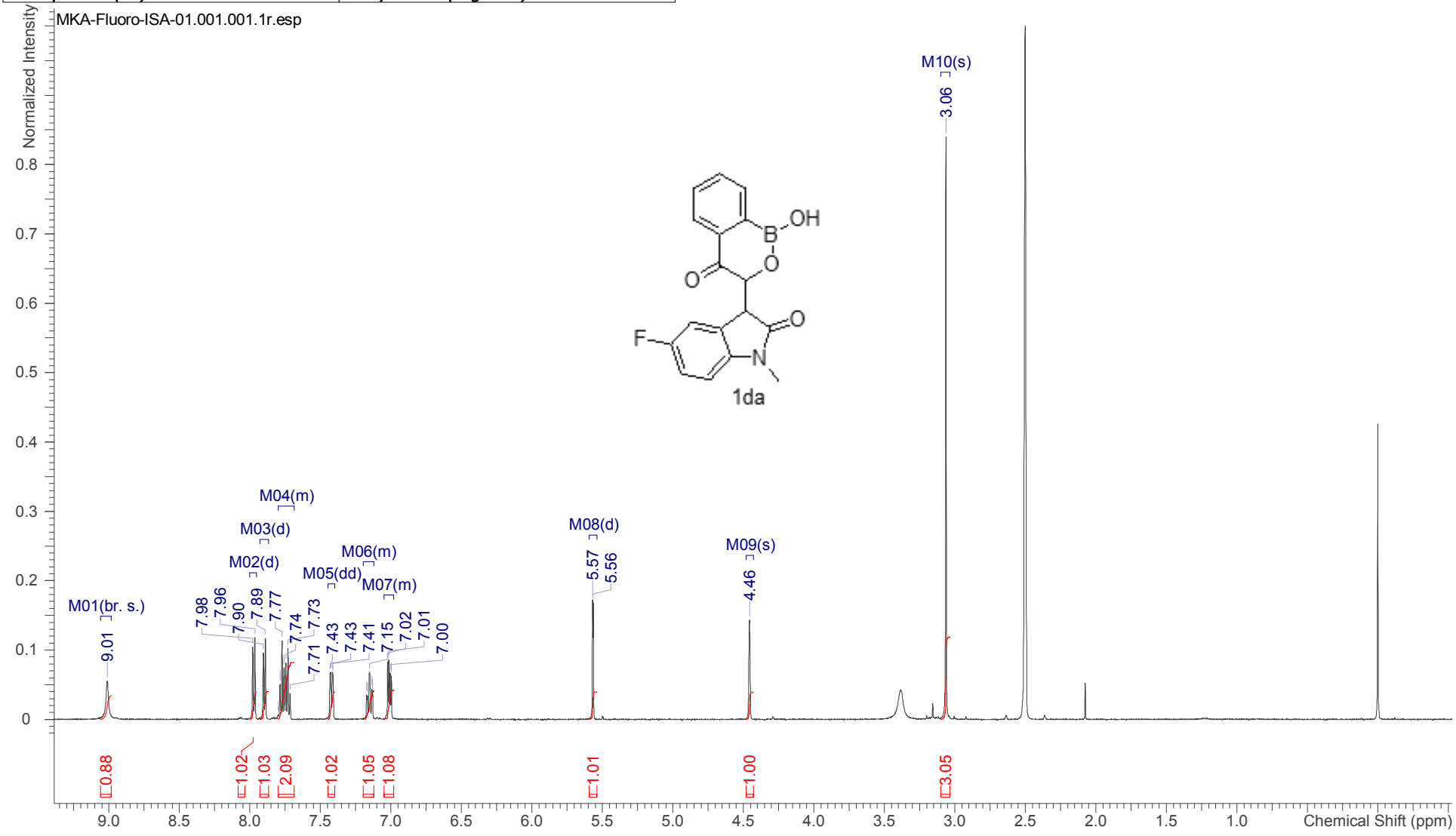

MKA-F-ISA-M 66 (1.330)
1: Scan ES+
4.20e7
326
100
%

MKA-F-ISA-P1

15/05/2014 12:17:55

OriginalDateForRelativeTime 2014-05-09T20:26:48			***Multiplets Integrals Sum*** 13.24	***Number of Nuclei***	13 H's

Acquisition Time (sec)	3.1719	***Comment***	MKA-Fluoro-ISA-01/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 25				
Date	09 May 2014 20:26:48			***Date Stamp***	09 May 2014 20:26:48		
File Name	\\inbgrdsfp01\elndata\MKA\07052014\MKA-Fluoro-ISA-01\1\PDATA\1\1r					***Frequency (MHz)***	500.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	administrator	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00
SW(cyclical) (Hz)	10330.58	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3091.0784	***Spectrum Type***	STANDARD
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	25.000				

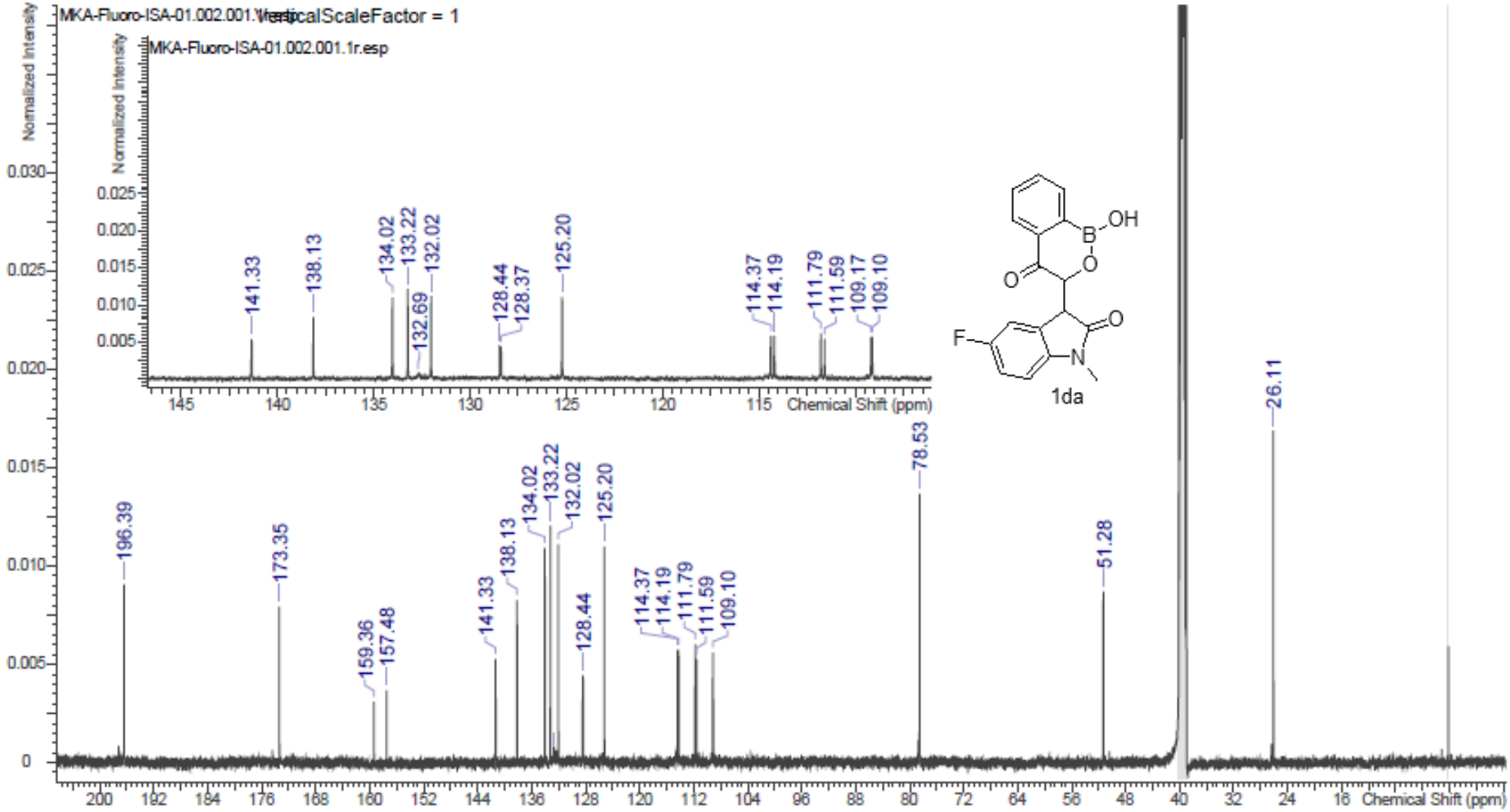


1da

21/08/2014 11:07:14

OriginalDateForRelativeTime 2014-05-10T01:42:32	*Multiplets Integrals Sum* 0.00	*Number of Nuclei* 0 C's

Acquisition Time (sec)	1.0912	*Comment*	MKA-Fluoro-ISA-01/DMSO C13CPD DMSO {F:\ecm\DATA\2014-04} bionmr 25				
Date	10 May 2014 01:42:32			*Date Stamp*	10 May 2014 01:42:32		
File Name	\\inbgrdsfp01\eindata\MKA\07052014\MKA-Fluoro-ISA-01\2\PDATA\1\1r					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	6000	*Origin*	spect	*Original Points Count*	32768
Owner	administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	32768.00
SW(cyclical) (Hz)	30030.03	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	12518.3926	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				

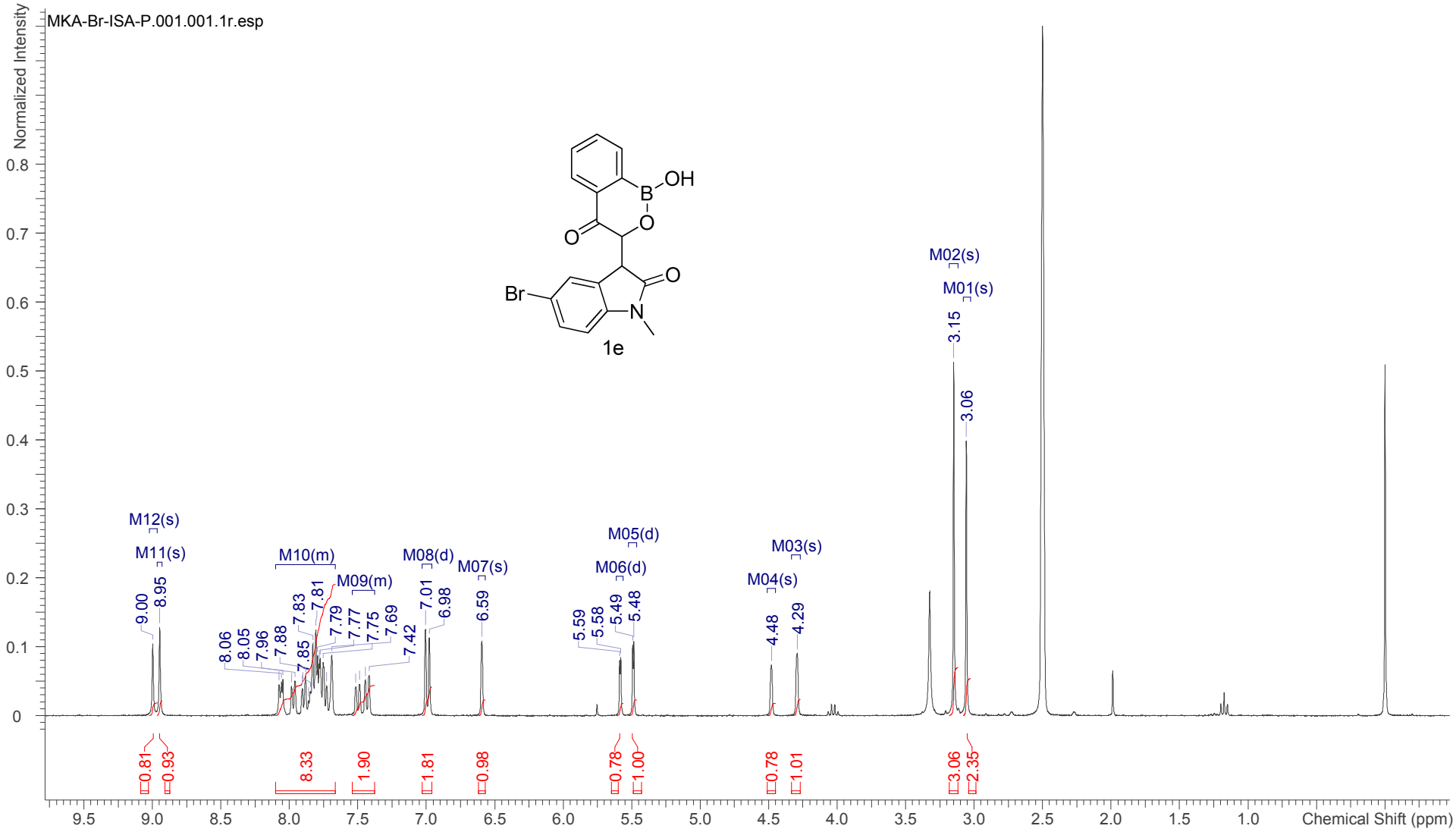


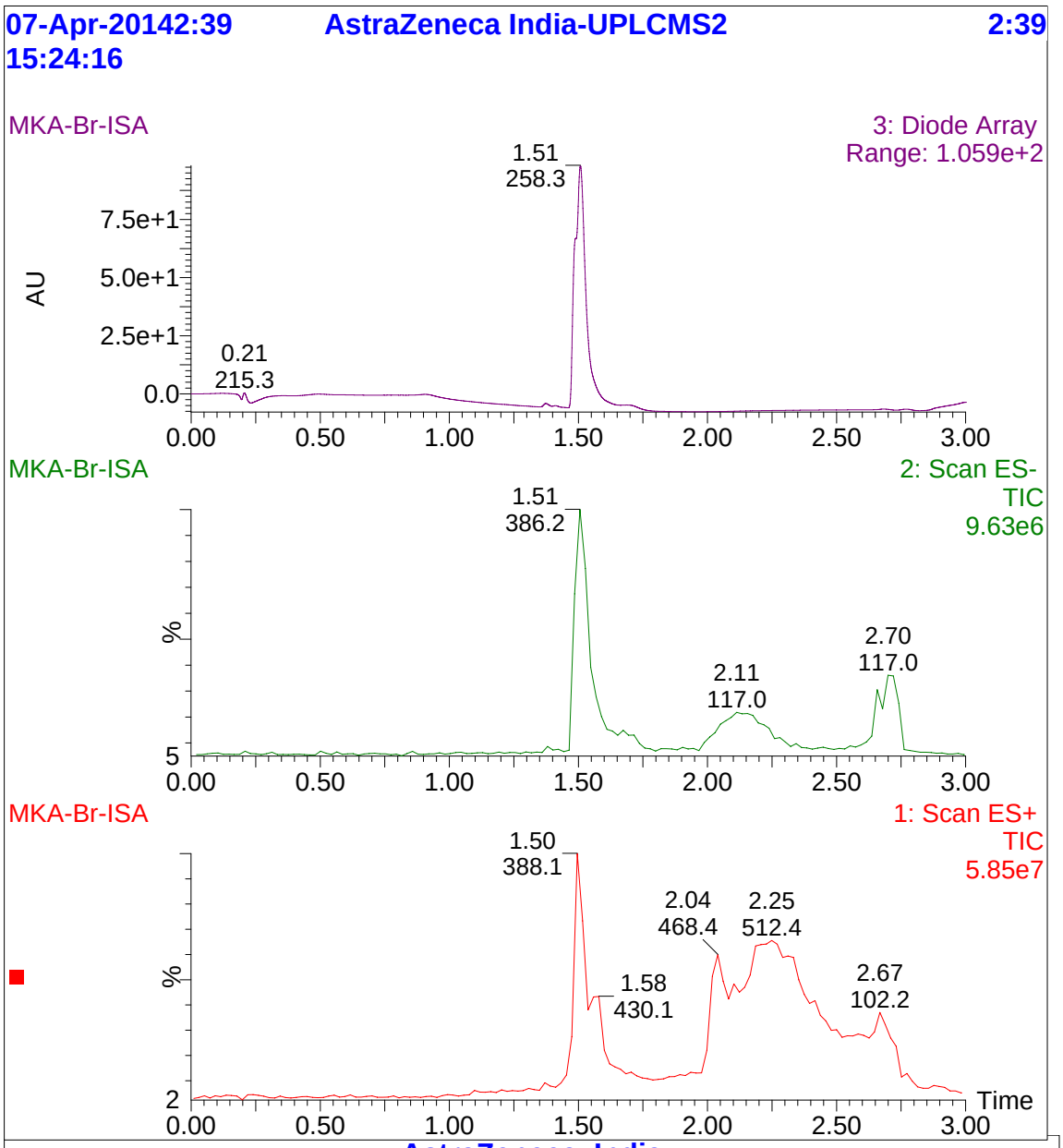
MKA-Br-ISA-M

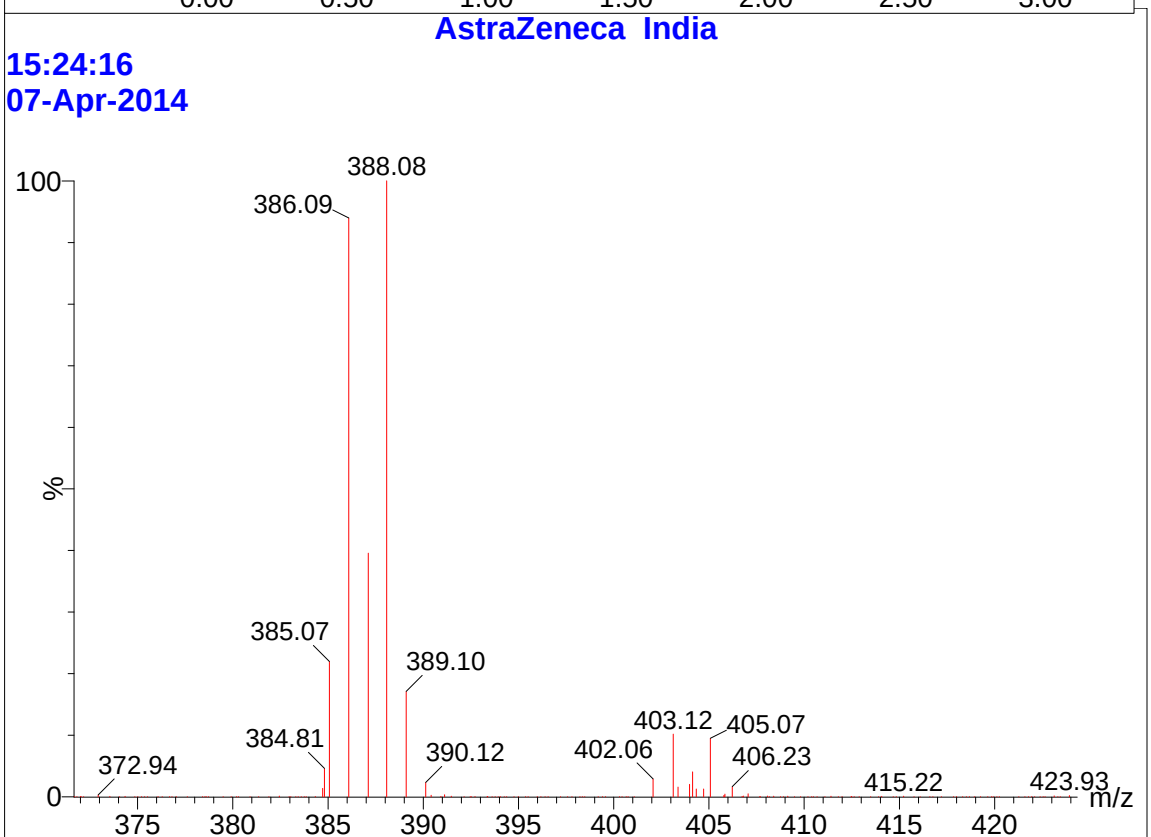
16/05/2014 14:37:41

OriginalDateForRelativeTime	2014-04-03T21:50:00	***Multiplets Integrals Sum***	23.75	***Number of Nuclei***	24 H's

Acquisition Time (sec)	5.3084	***Comment***	MKA-Br-ISA-P/DMSO			***Date***	03 Apr 2014 21:50:00
Date Stamp	03 Apr 2014 21:50:00			***File Name***	C:\Users\kkth216\Desktop\NMR-300\MKA-Br-ISA-P\1\PDATA\1\1r		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	126	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1625.50	***SW(cyclical) (Hz)***	6172.84	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1853.2285
Spectrum Type	STANDARD	***Sweep Width (Hz)***	6172.65	***Temperature (degree C)***	25.000		




07-Apr-20142:39
AstraZeneca India-UPLCMS2
2:39
15:24:16
MKA-Br-ISA
3: Diode Array
Range: 1.059e+2
1.51
258.3
7.5e+1
5.0e+1
2.5e+1
0.0
AU
0.21
215.3
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-Br-ISA
2: Scan ES-
TIC
9.63e6
1.51
386.2
%
2.70
117.0
2.11
117.0
5
MKA-Br-ISA
1: Scan ES+
TIC
5.85e7
1.50
388.1
2.04
468.4
2.25
512.4
%
1.58
430.1
2.67
102.2
2
Time

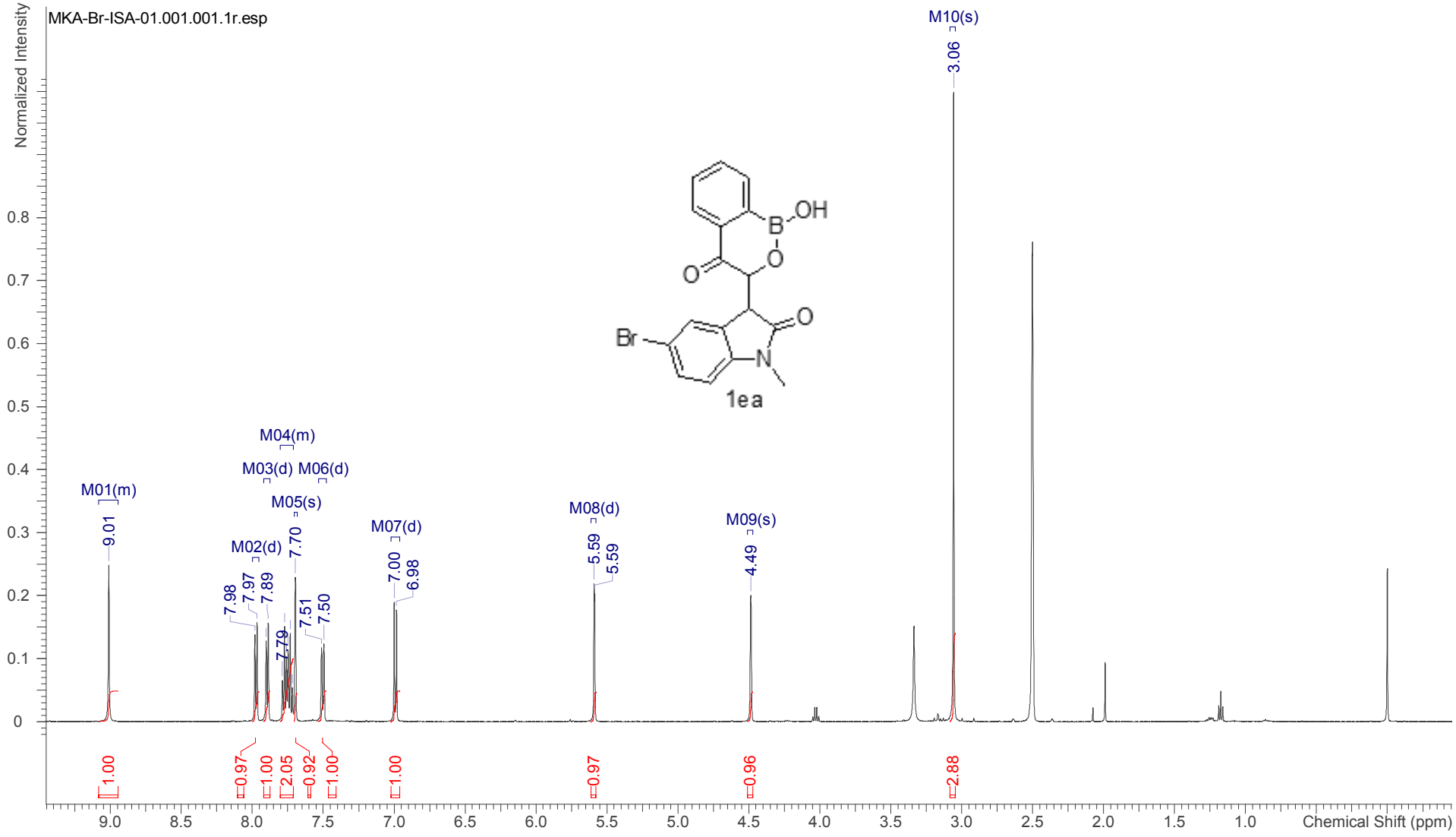

AstraZeneca India
15:24:16
07-Apr-2014
100
388.08
386.09
%
385.07
389.10
384.81
403.12
405.07
372.94
390.12
402.06
406.23
415.22
423.93
0
m/z
375
380
385
390
395
400
405
410
415
420

MKA-Br-ISA-P1

15/05/2014 17:22:24

OriginalDateForRelativeTime 2014-05-10T10:42:16			***Multiplets Integrals Sum*** 12.76	***Number of Nuclei*** 13 H's	

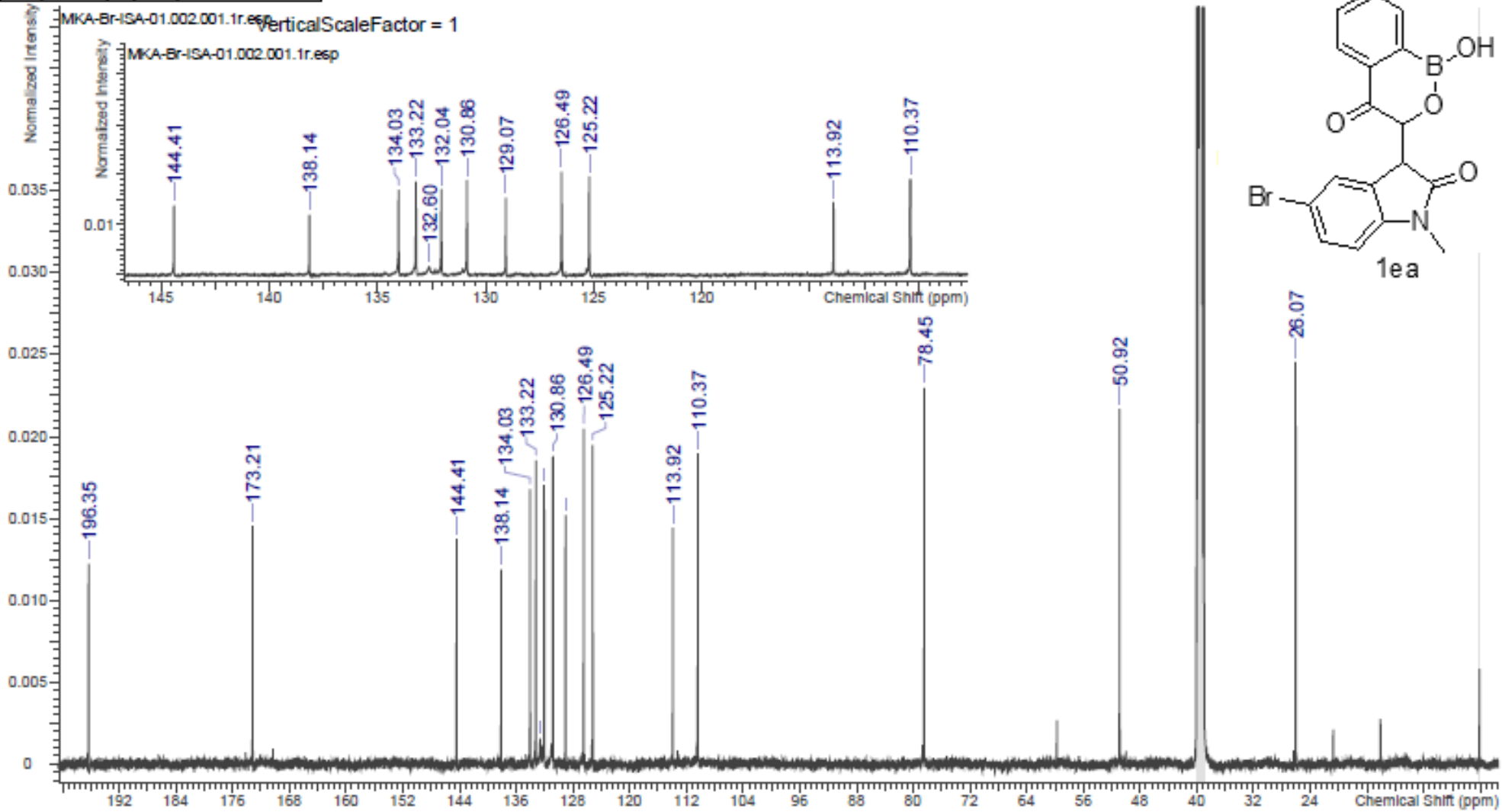
Acquisition Time (sec)	3.1719	***Comment***	MKA-Br-ISA-01/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 26				
Date	10 May 2014 10:42:16			***Date Stamp***	10 May 2014 10:42:16		
File Name	\\inbgrdsfp01\elndata\MKA\MKA-Br-ISA-01\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	administrator
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00	***SW(cyclical) (Hz)***	10330.58
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3092.0627	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10330.26
Temperature (degree C)	25.000						



21/06/2014 11:22:04

OriginalDateForRelativeTime	2014-05-10T15:58:00	Multipliers Integrals Sum	0.00	Number of Nuclei	0 C's

Acquisition Time (sec)	1.0912	Comment	MKA-Br-ISA-01/DMSO C13CPD DMSO {F:\ecm\DATA\2014-04} bionmr 26				
Date	10 May 2014 15:58:00			Date Stamp	10 May 2014 15:58:00		
File Name	\\nbgrdsfp01\eln\data\MKA\MKA-Br-ISA-01\2\PDATA\1\1r			Frequency (MHz)	125.77	Nucleus	13C
Number of Transients	6000	Origin	spect	Original Points Count	32768	Owner	administrator
Points Count	32768	Pulse Sequence	zgpg30	Receiver Gain	32768.00	SW(cyclical) (Hz)	30030.03
Solvent	DMSO-d6	Spectrum Offset (Hz)	12519.3086	Spectrum Type	STANDARD	Sweep Width (Hz)	30029.11
Temperature (degree C)	25.000						

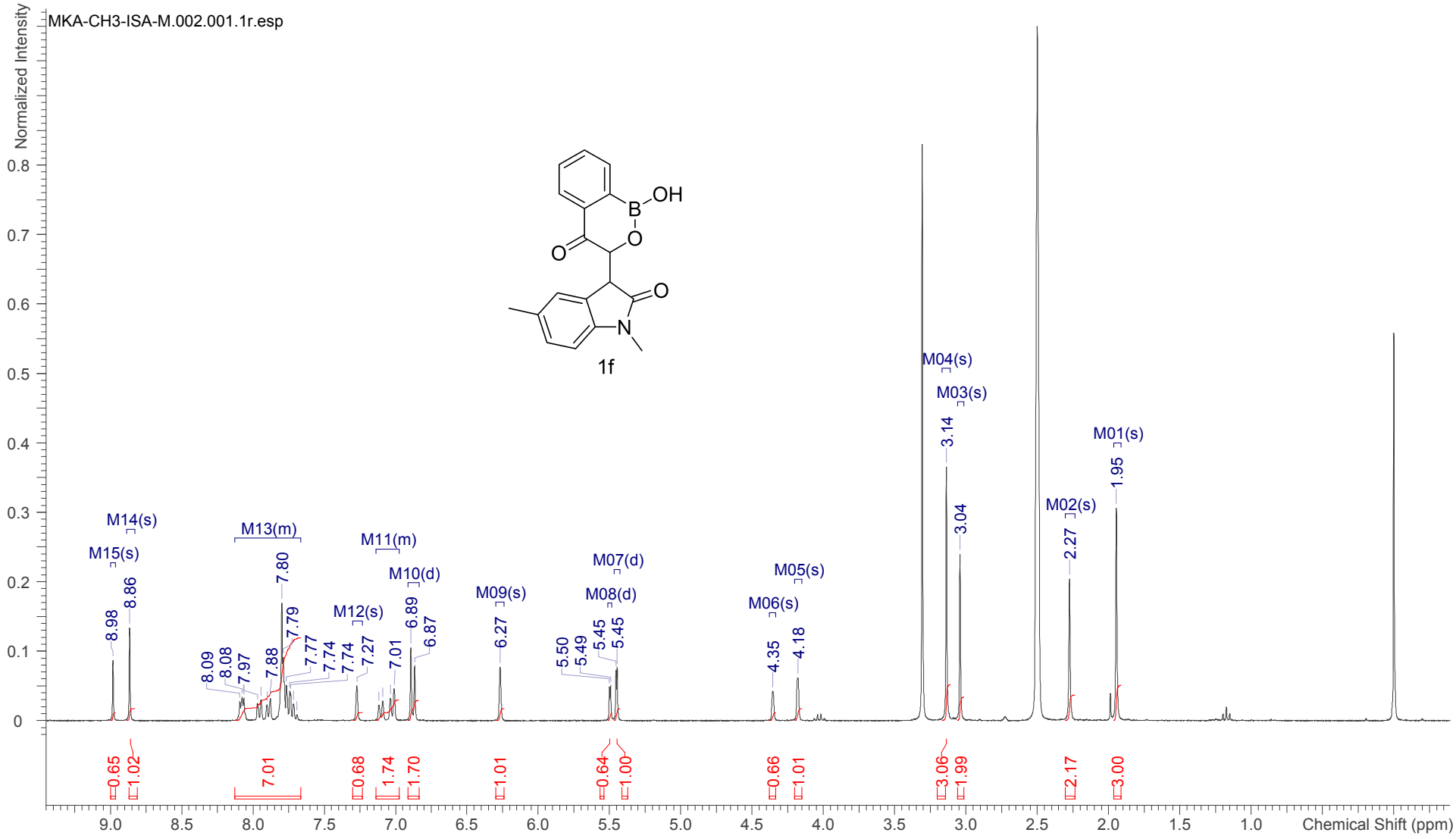


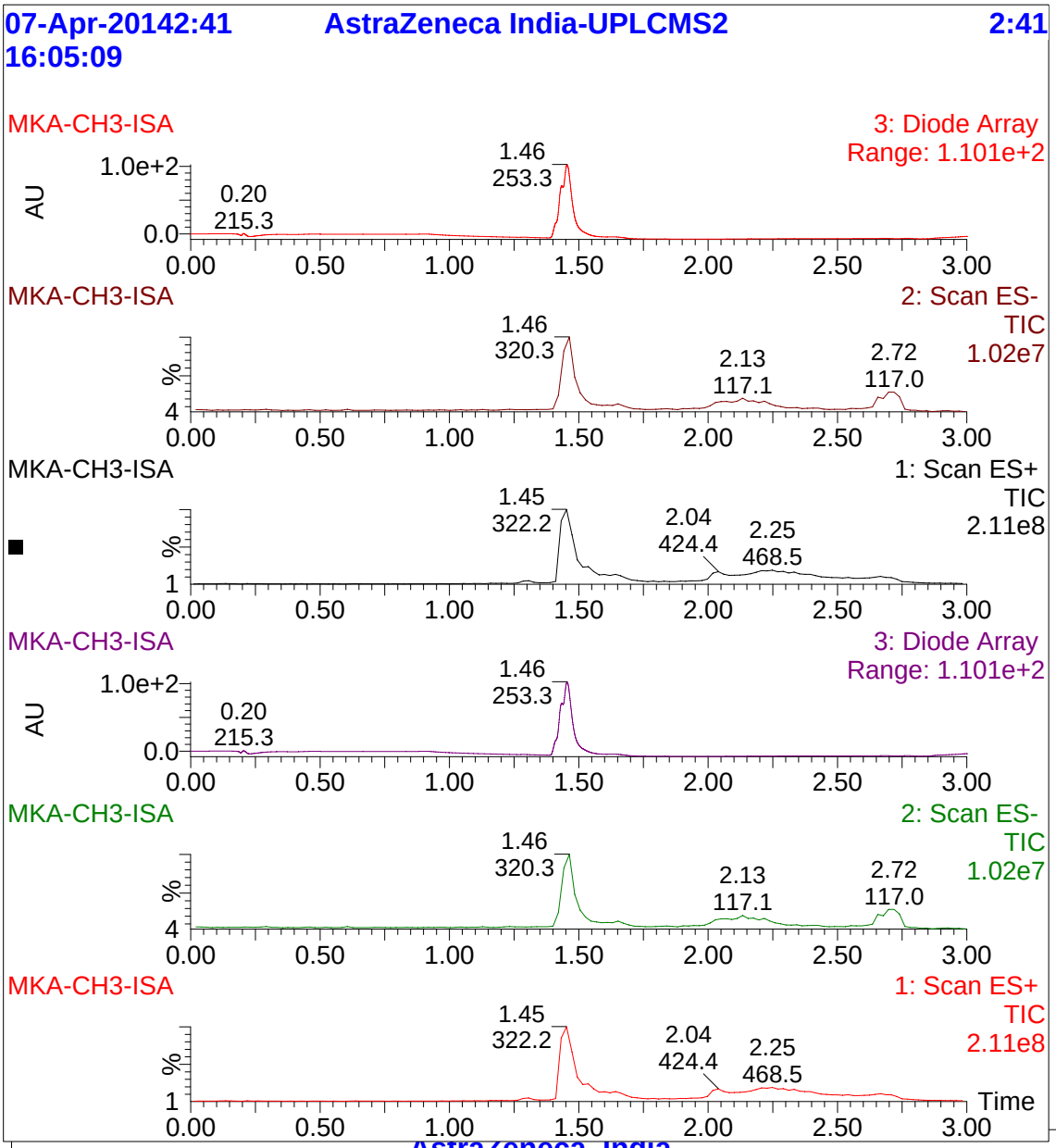
MKA-CH3-ISA-M

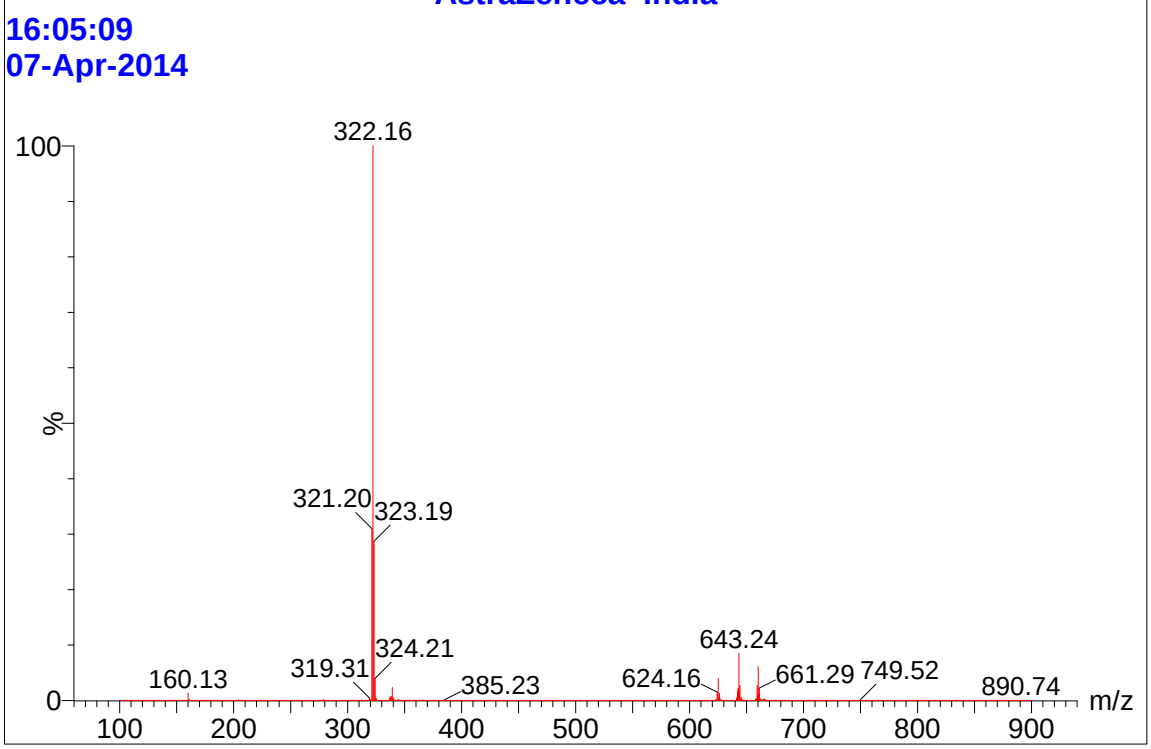
16/05/2014 14:35:13

OriginalDateForRelativeTime	2014-04-12T12:46:00	***Multiplets Integrals Sum***	27.36	***Number of Nuclei***	29 H's

Acquisition Time (sec)	5.3084	***Comment***	MKA-CH3-ISA-M/DMSO			***Date***	12 Apr 2014 12:46:00
Date Stamp	12 Apr 2014 12:46:00			***File Name***	C:\Users\kkth216\Desktop\NMR-300\MKA-CH3-ISA-M\2\PDATA\1\1r		
Frequency (MHz)	300.13	***Nucleus***	1H	***Number of Transients***	126	***Origin***	av300
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zg30
Receiver Gain	1625.50	***SW(cyclical) (Hz)***	6172.84	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	1853.3098
Spectrum Type	STANDARD	***Sweep Width (Hz)***	6172.65	***Temperature (degree C)***	25.000		




07-Apr-20142:41
AstraZeneca India-UPLCMS2
2:41
16:05:09
MKA-CH3-ISA
3: Diode Array
Range: 1.101e+2
1.0e+2
AU
0.0
0.20
215.3
1.46
253.3
0.00
0.50
1.00
1.50
2.00
2.50
3.00
MKA-CH3-ISA
2: Scan ES-
TIC
1.02e7
%
4
1.46
320.3
2.13
117.1
2.72
117.0
MKA-CH3-ISA
1: Scan ES+
TIC
2.11e8
1
1.45
322.2
2.04
424.4
2.25
468.5
MKA-CH3-ISA
3: Diode Array
Range: 1.101e+2
MKA-CH3-ISA
2: Scan ES-
TIC
1.02e7
MKA-CH3-ISA
1: Scan ES+
TIC
2.11e8
Time

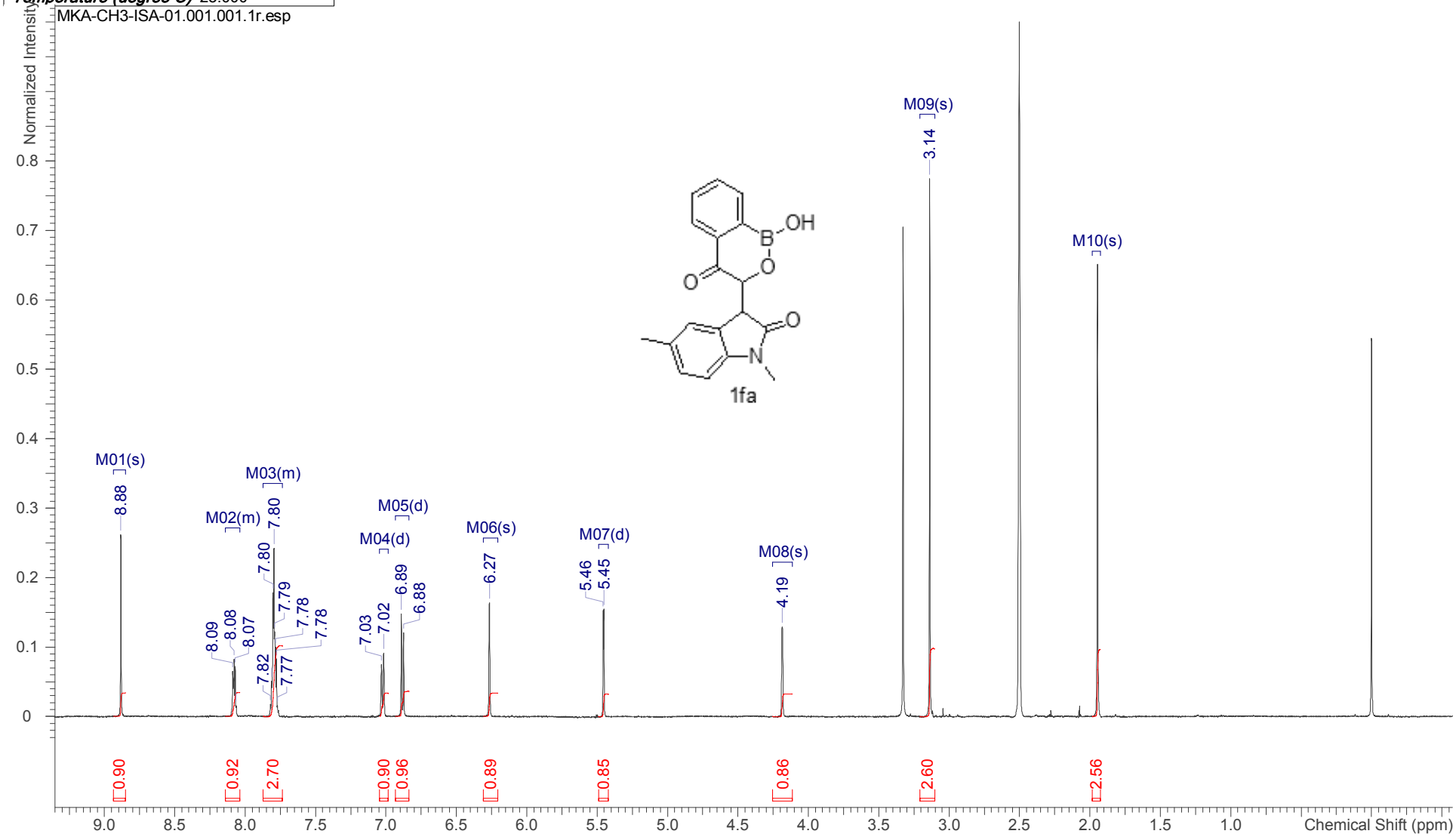

AstraZeneca India
16:05:09
07-Apr-2014
100
%
0
322.16
321.20
323.19
319.31
324.21
160.13
385.23
624.16
643.24
661.29
749.52
890.74
m/z
100
200
300
400
500
600
700
800
900

MKA-CH3-ISA-P1

15/05/2014 17:58:03

OriginalDateForRelativeTime 2014-05-08T14:41:12			***Multiplets Integrals Sum*** 14.16	***Number of Nuclei*** 16 H's	

Acquisition Time (sec)	3.1719	***Comment***	MKA-CH3-ISA-01/DMSO PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 22				
Date	08 May 2014 14:41:12			***Date Stamp***	08 May 2014 14:41:12		
File Name	\\inbgrdsfp01\elndata\MKA\MKA-CH3-ISA-01\1\PDATA\1\1r			***Frequency (MHz)***	500.13	***Nucleus***	1H
Number of Transients	16	***Origin***	spect	***Original Points Count***	32768	***Owner***	administrator
Points Count	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00	***SW(cyclical) (Hz)***	10330.58
Solvent	DMSO-d6	***Spectrum Offset (Hz)***	3090.3782	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	10330.26
Temperature (degree C)	25.000						

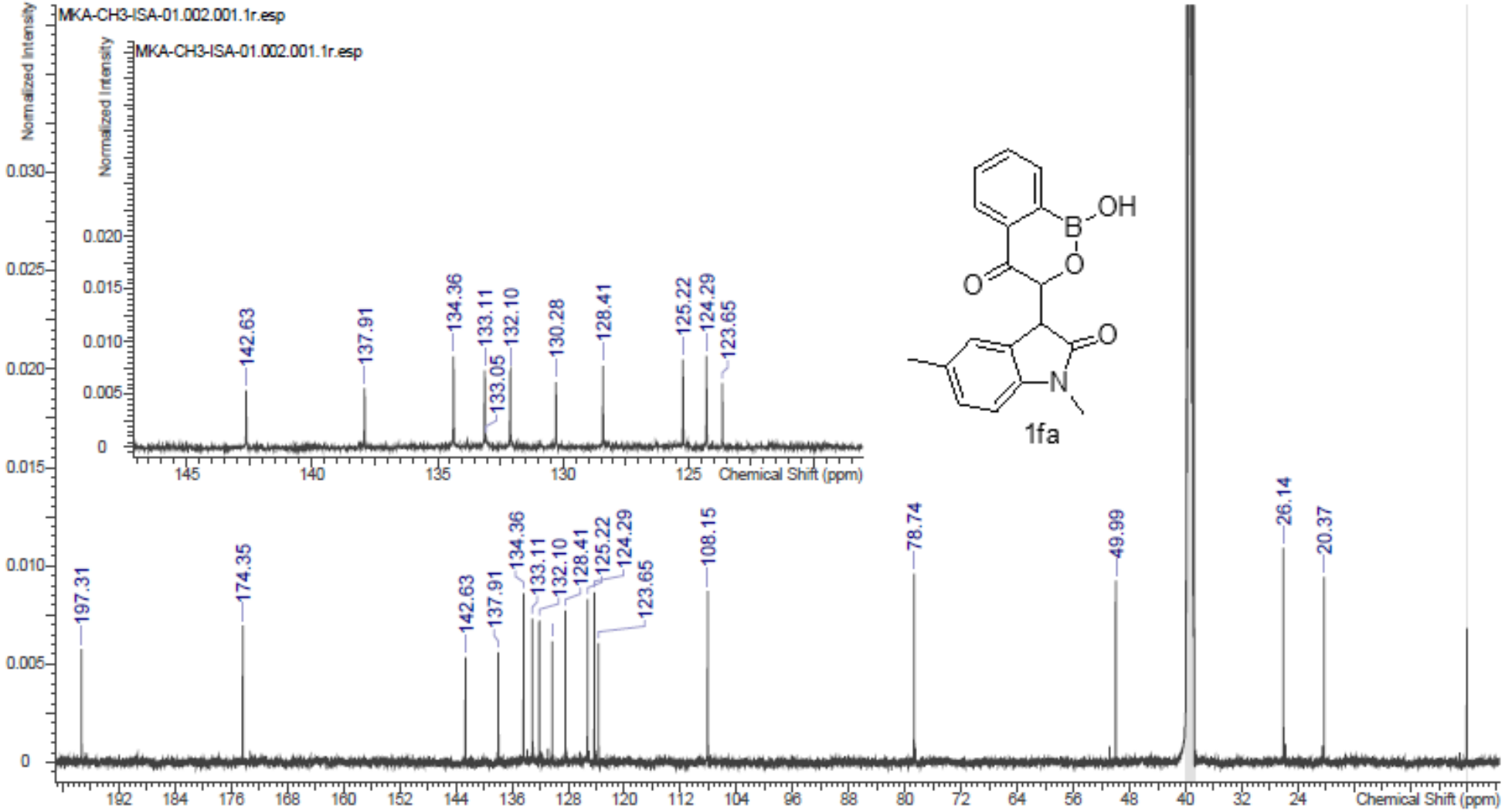


1fa

21/06/2014 12:44:58

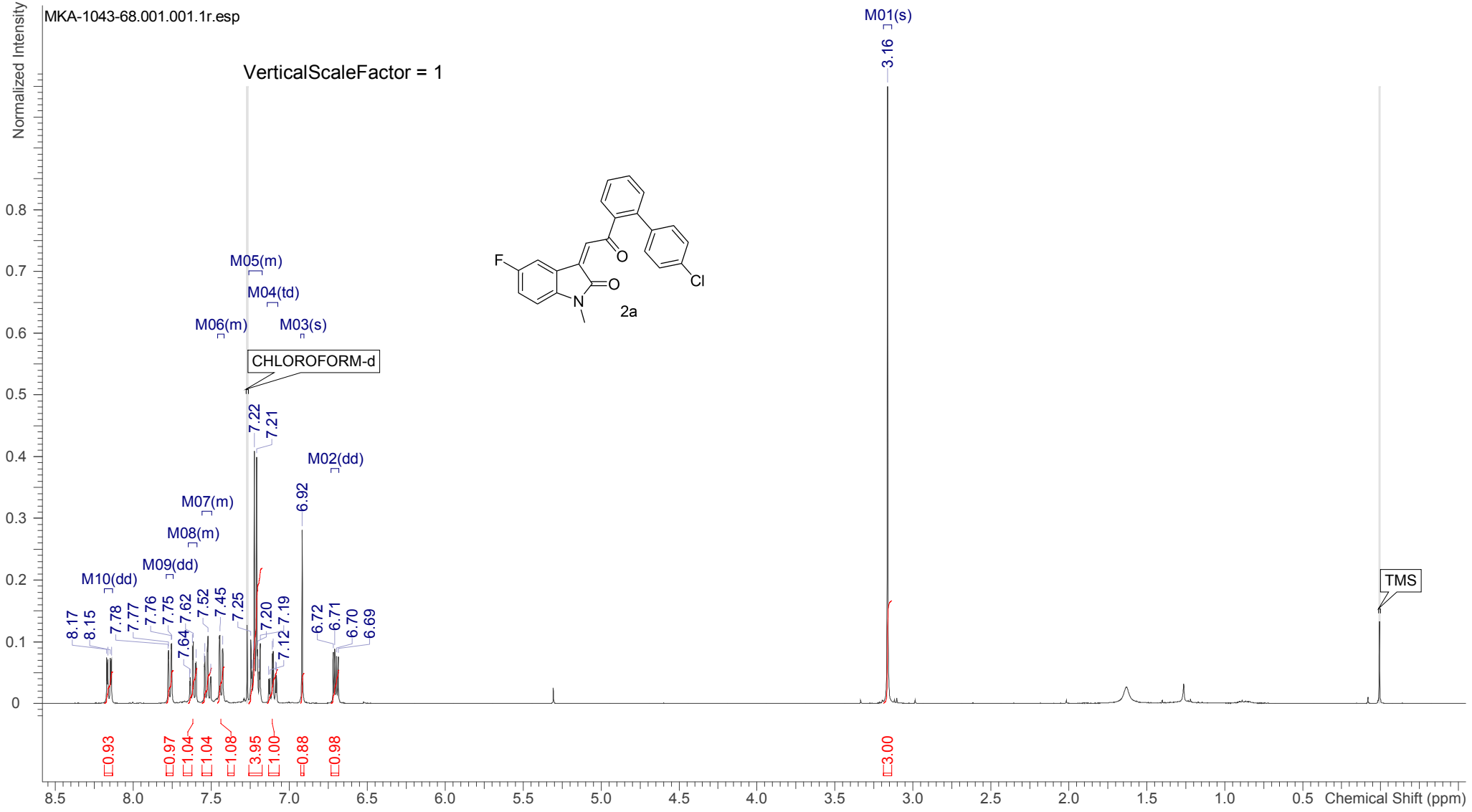
OriginalDateForRelativeTime 2014-05-08T23:28:08	*Multiplets Integrals Sum* 0.00	*Number of Nuclei* 0 C's

Acquisition Time (sec)	1.0912	*Comment*	MKA-CH3-ISA-01/DMSO C13CPD DMSO {F:\ecmlDATA\2014-04} bionmr 22				
Date	08 May 2014 23:28:08			*Date Stamp*	08 May 2014 23:28:08		
File Name	\\inbgrdsfp01\eindata\MKA\07052014\MKA-CH3-ISA-01\2\PDATA\1\1r					*Frequency (MHz)*	125.77
Nucleus	13C	*Number of Transients*	10000	*Origin*	spect	*Original Points Count*	32768
Owner	administrator	*Points Count*	32768	*Pulse Sequence*	zgpg30	*Receiver Gain*	32768.00
SW(cyclical) (Hz)	30030.03	*Solvent*	DMSO-d6	*Spectrum Offset (Hz)*	12503.5010	*Spectrum Type*	STANDARD
Sweep Width (Hz)	30029.11	*Temperature (degree C)*	25.000				



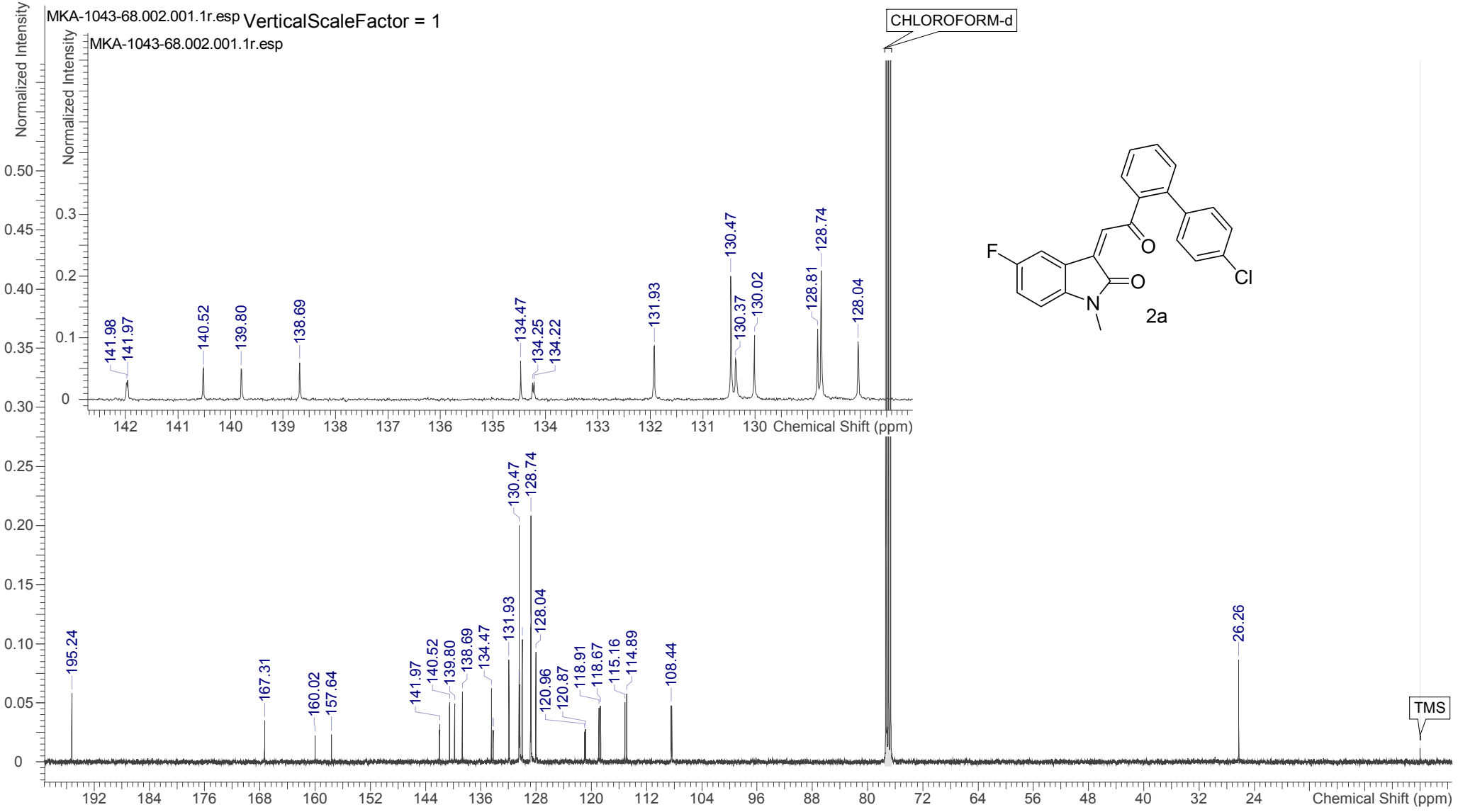
OriginalDateForRelativeTime 2014-04-18T09:34:00	***Multiplets Integrals Sum*** 14.85	***Number of Nuclei*** 15 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-68 PROTON CDCl3 {D:\RA} SamTrack 43			***Date***	18 Apr 2014 09:34:00
Date Stamp	18 Apr 2014 09:34:00			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-68\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	161.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



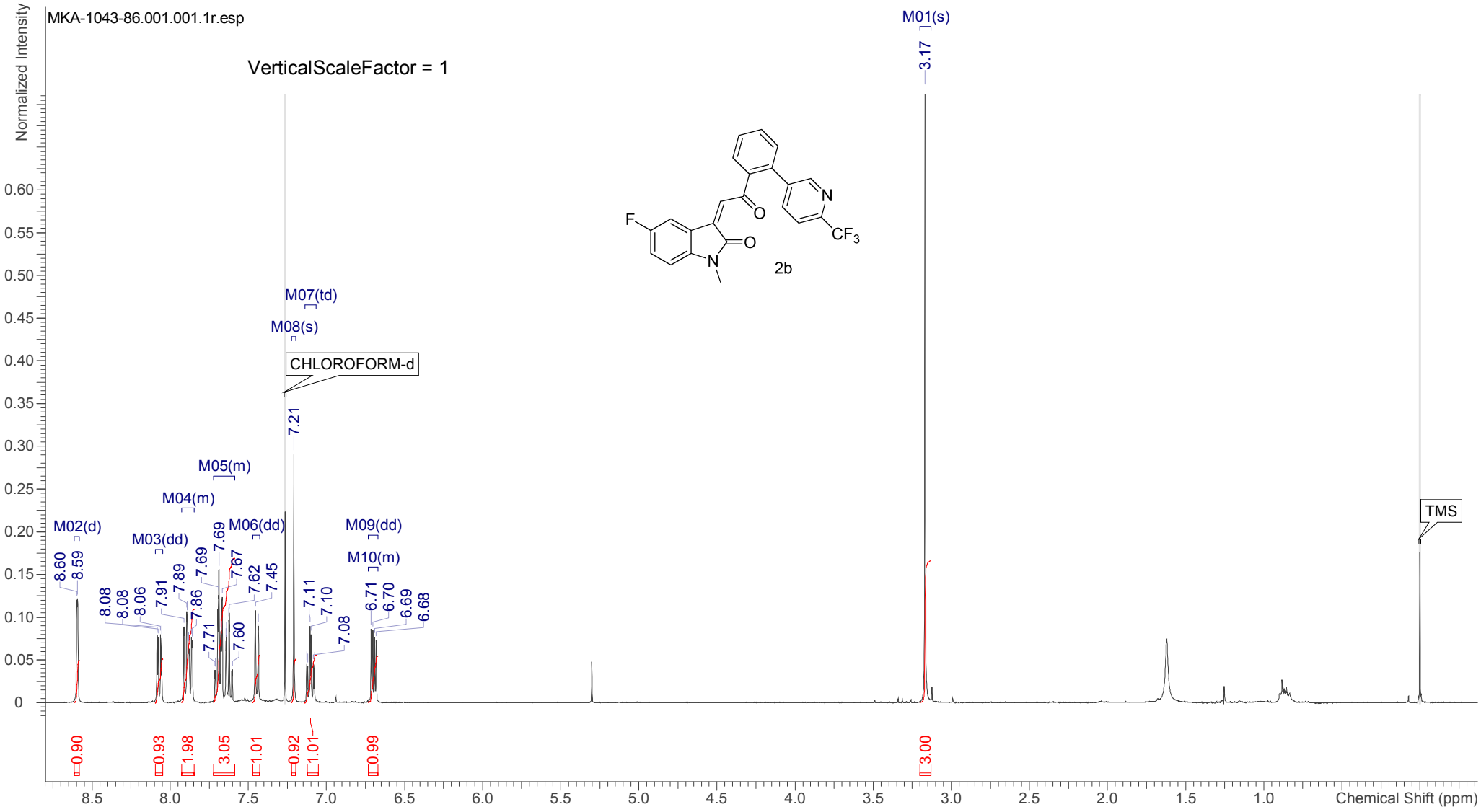
OriginalDateForRelativeTime 2014-04-18T12:24:40			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-68 C13CPD CDCl3 {D:\RA} SamTrack 43	***Date***	18 Apr 2014 12:24:40
Date Stamp	18 Apr 2014 12:24:40		***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-68\2\PDATA\1\1r	
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	3000	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	406.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10059.1504	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.000



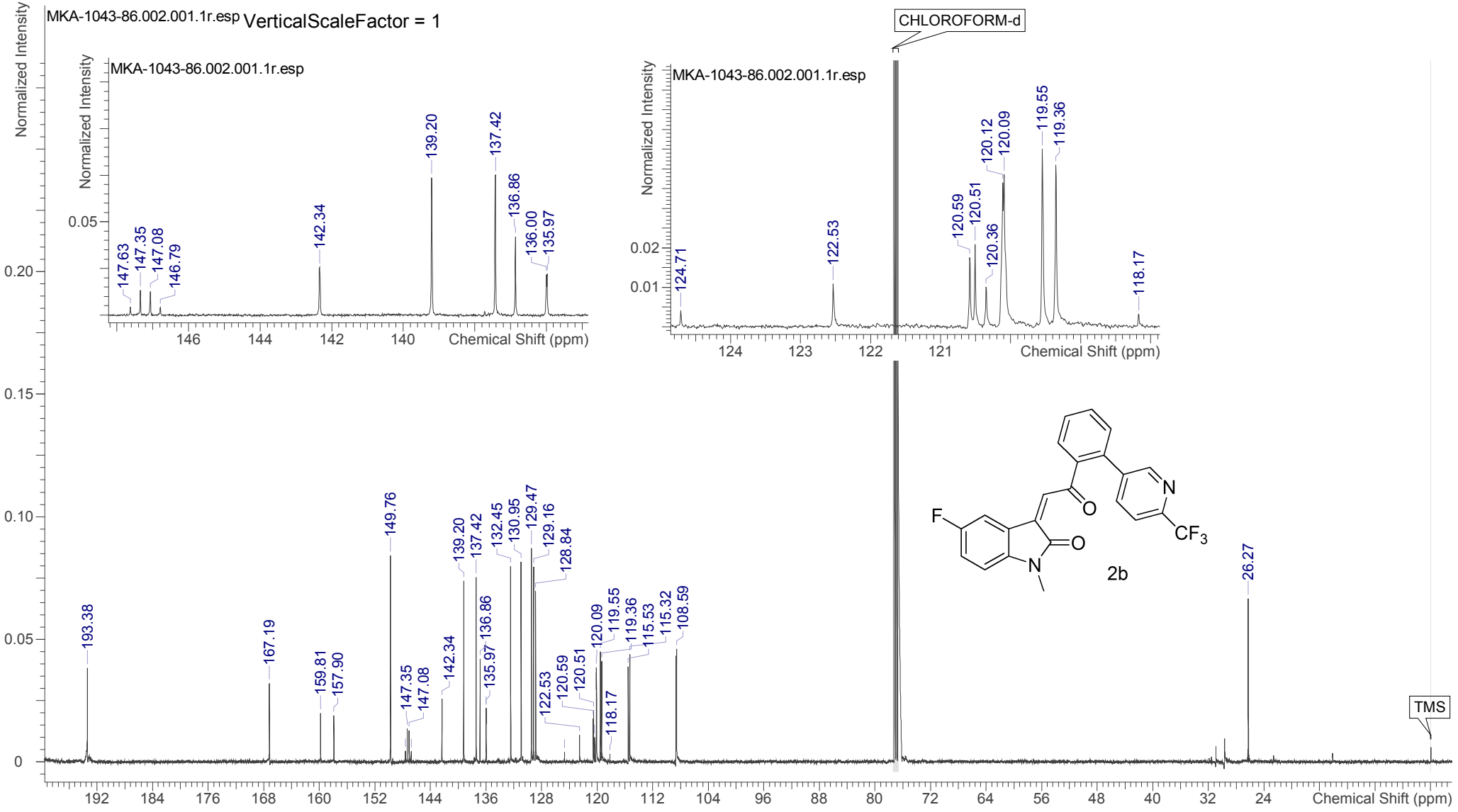
OriginalDateForRelativeTime 2014-04-18T12:28:56	***Multiplets Integrals Sum*** 13.76	***Number of Nuclei*** 15 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-86 PROTON CDCl3 {D:\RA} SamTrack 44			***Date***	18 Apr 2014 12:28:56
Date Stamp	18 Apr 2014 12:28:56			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-86\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	203.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2463.2405	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



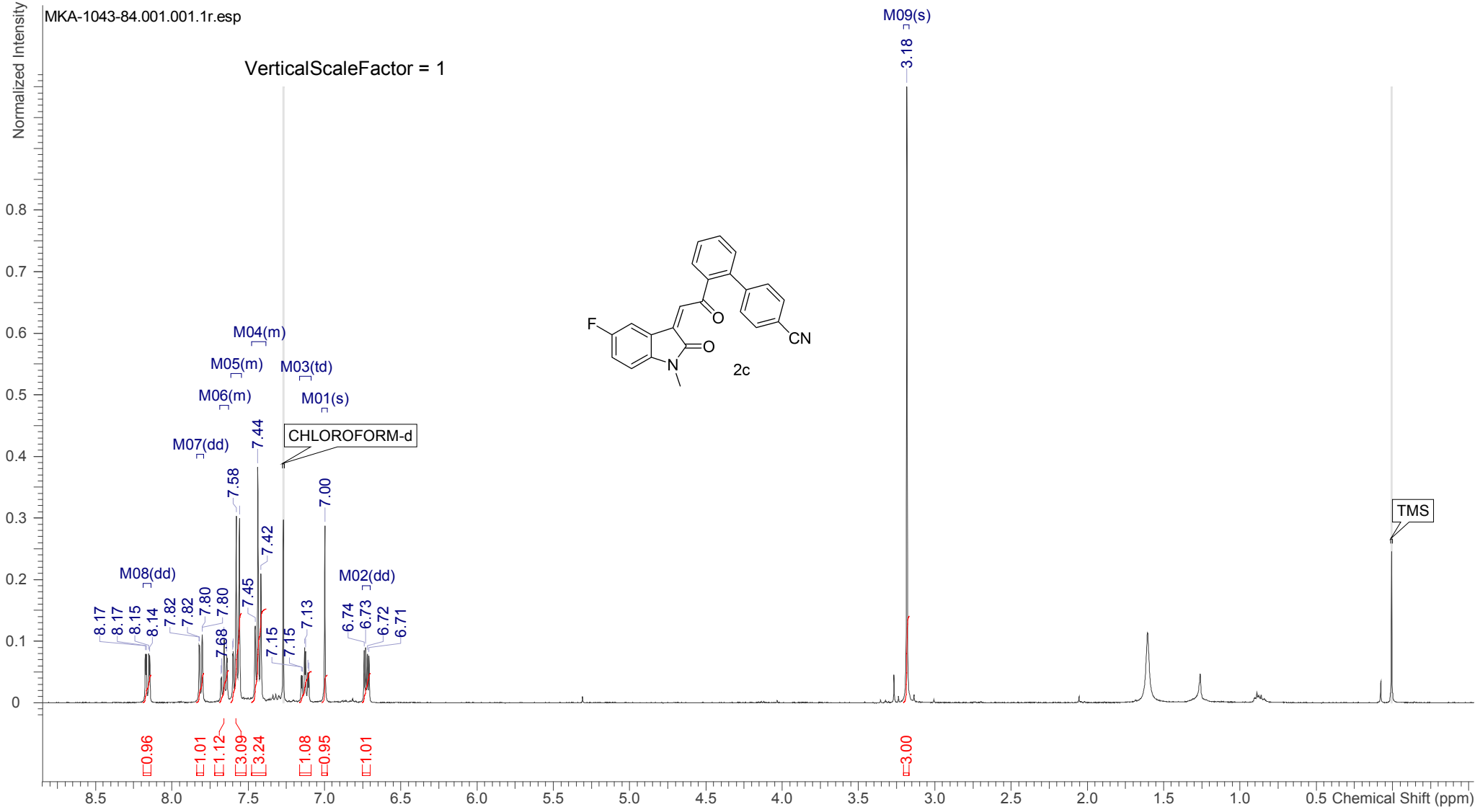
OriginalDateForRelativeTime 2014-05-02T23:40:56			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.0912	***Comment***	MKA-1043-86 C13CPD CDCl3 {F:\ecm\DATA\2014-04} bionmr 14			***Date***	02 May 2014 23:40:56
Date Stamp	02 May 2014 23:40:56			***File Name***	\\inbgrdsfp01\elndata\MKA\07052014\MKA-1043-86\2\PDATA\1\1r		
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	10000	***Origin***	spect
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	30030.03	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12574.3232
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30029.11	***Temperature (degree C)***	25.000		



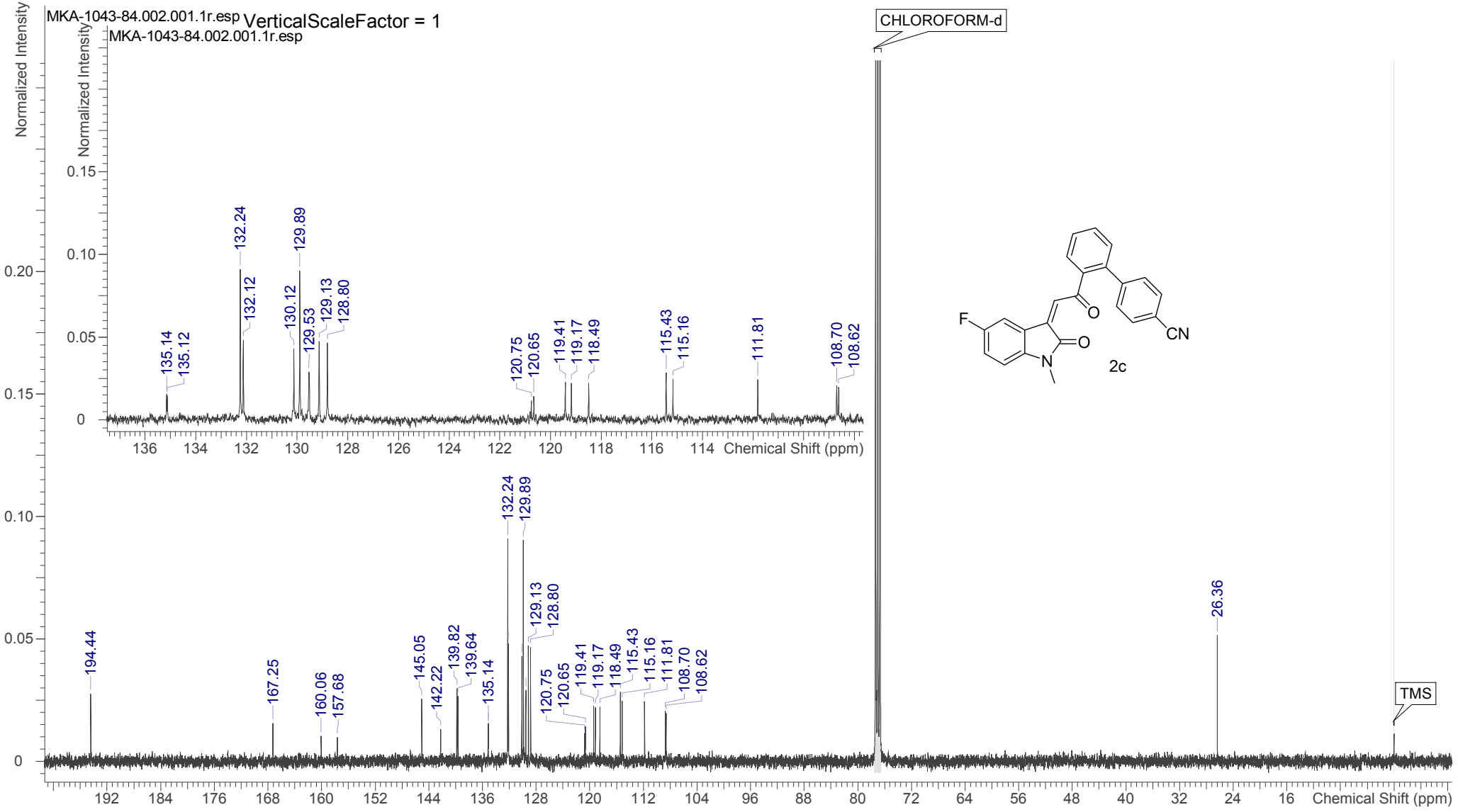
OriginalDateForRelativeTime 2014-04-16T18:12:24	***Multiplets Integrals Sum*** 15.46	***Number of Nuclei*** 15 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-84/CDCl3 PROTON CDCl3 {D:\RA} astra 1			***Date***	16 Apr 2014 18:12:24
Date Stamp	16 Apr 2014 18:12:24			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-84\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	203.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



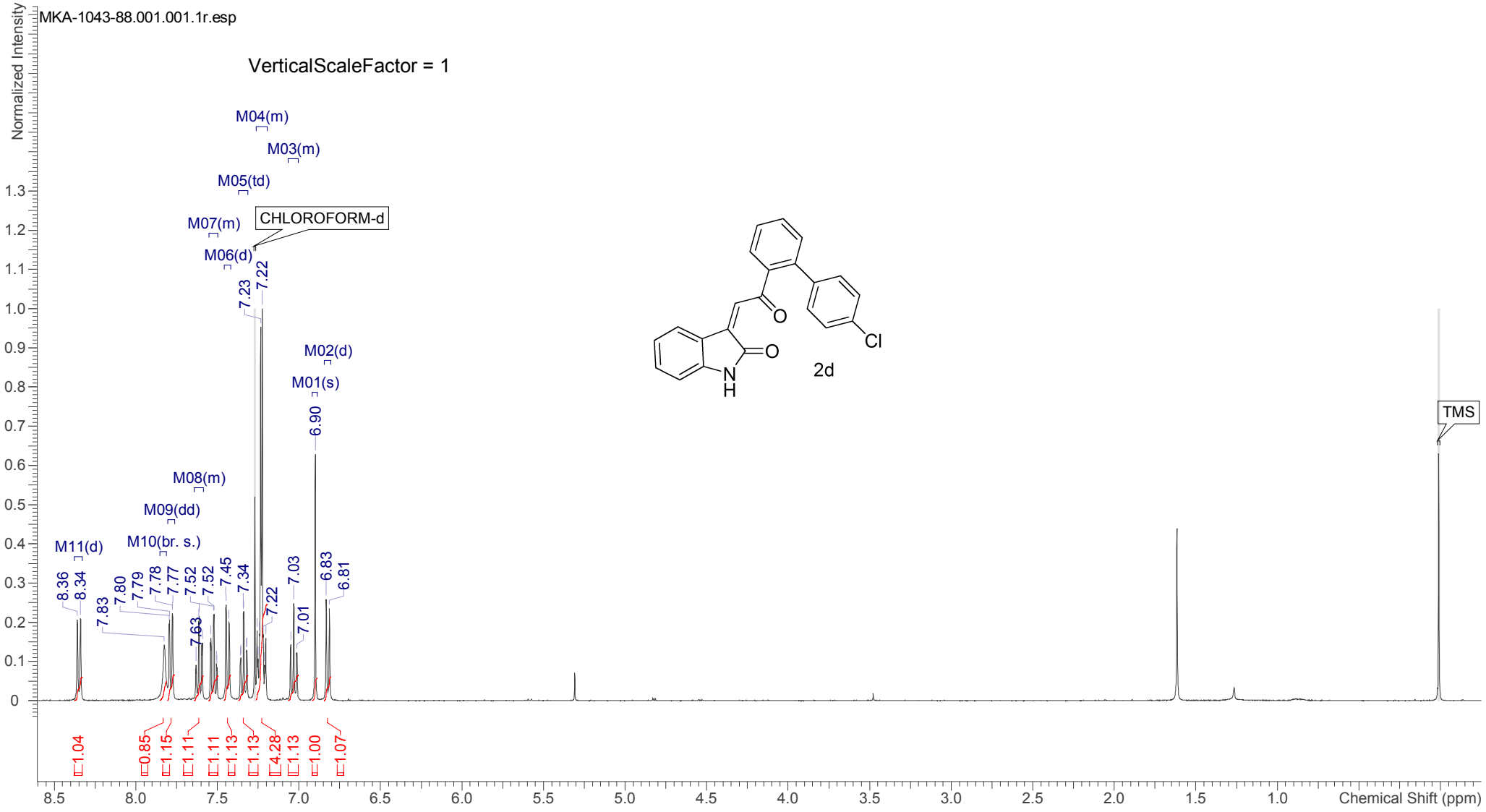
OriginalDateForRelativeTime 2014-04-16T20:07:36			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-84-13C/CDCl3 C13CPD CDCl3 {D:\RA} astra 1	***Date***	16 Apr 2014 20:07:36
Date Stamp	16 Apr 2014 20:07:36		***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-84\2\PDATA\1\1r	
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	2000	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	322.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10061.6299	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.000



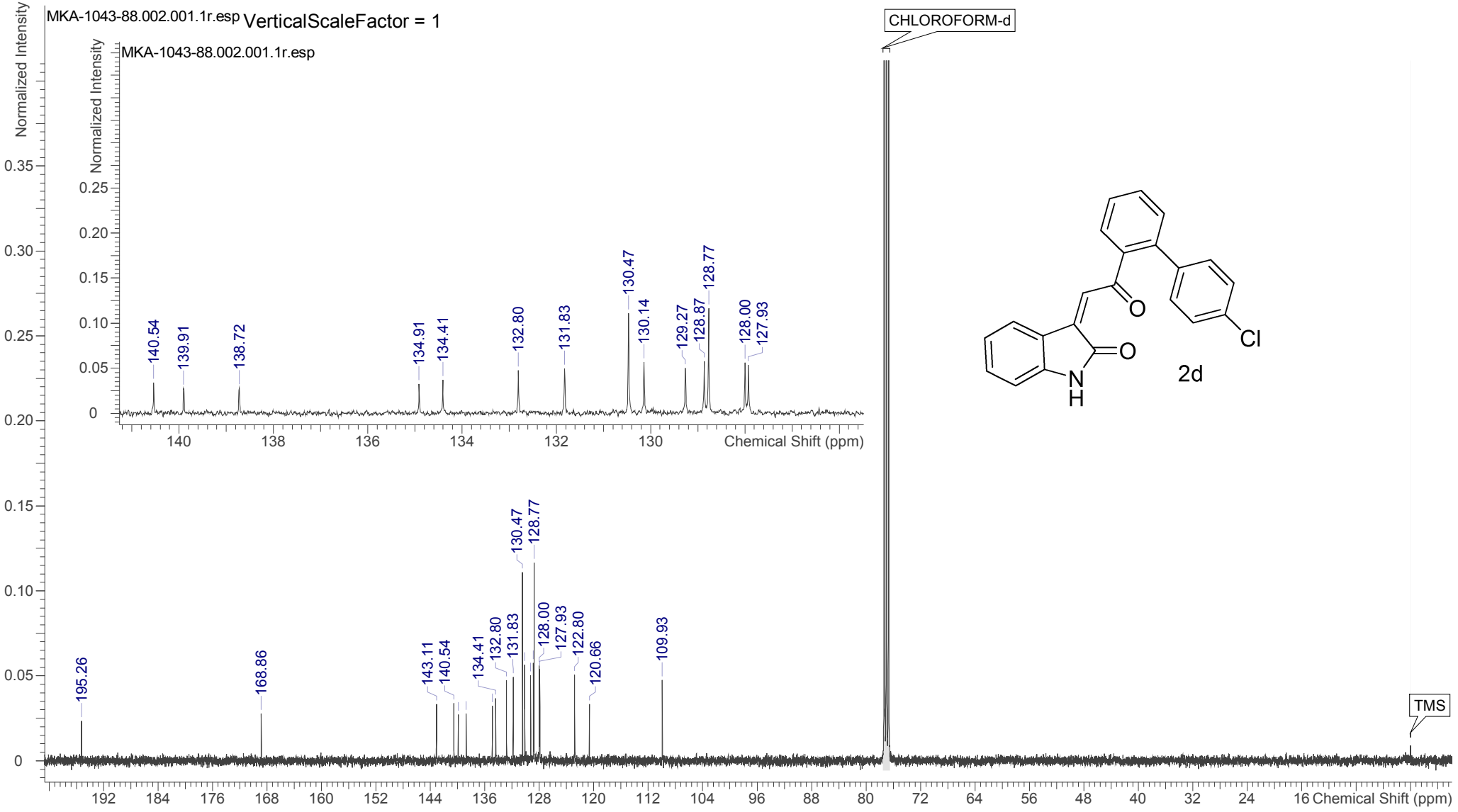
OriginalDateForRelativeTime 2014-04-17T14:17:44	***Multiplets Integrals Sum*** 15.02	***Number of Nuclei*** 14 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-88 PROTON CDCl3 {D:\RA} SamTrack 4			***Date***	17 Apr 2014 14:17:44
Date Stamp	17 Apr 2014 14:17:44			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-88\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	228.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



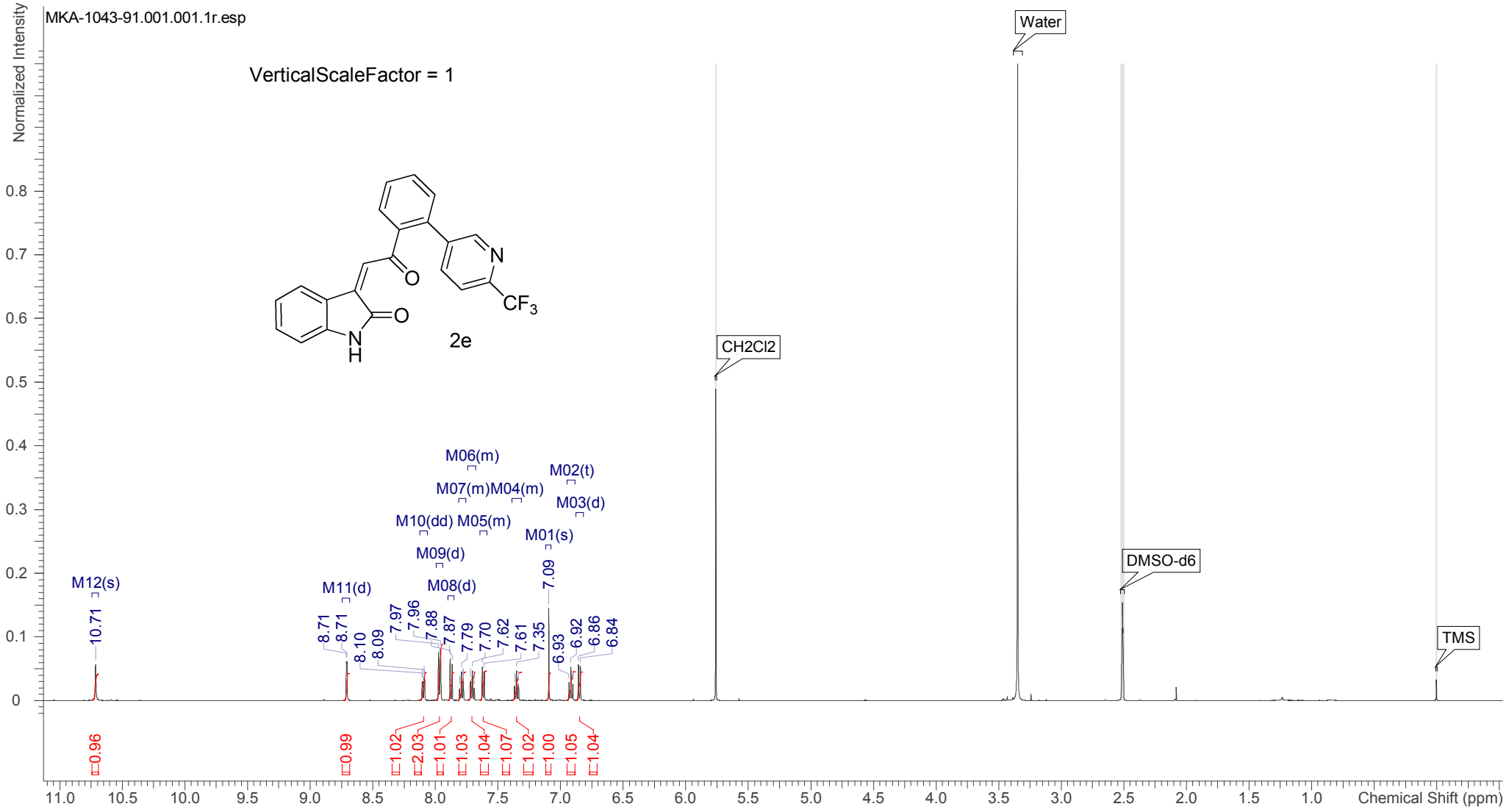
OriginalDateForRelativeTime 2014-04-17T15:45:12			***Multiplets Integrals Sum*** 0.00		***Number of Nuclei*** 0 C's

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-88 C13CPD CDCl3 {D:\RA} SamTrack 4			***Date***	17 Apr 2014 15:45:12
Date Stamp	17 Apr 2014 15:45:12			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-88\2\PDATA\1\1r		
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	1500	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	406.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10061.6299	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.000



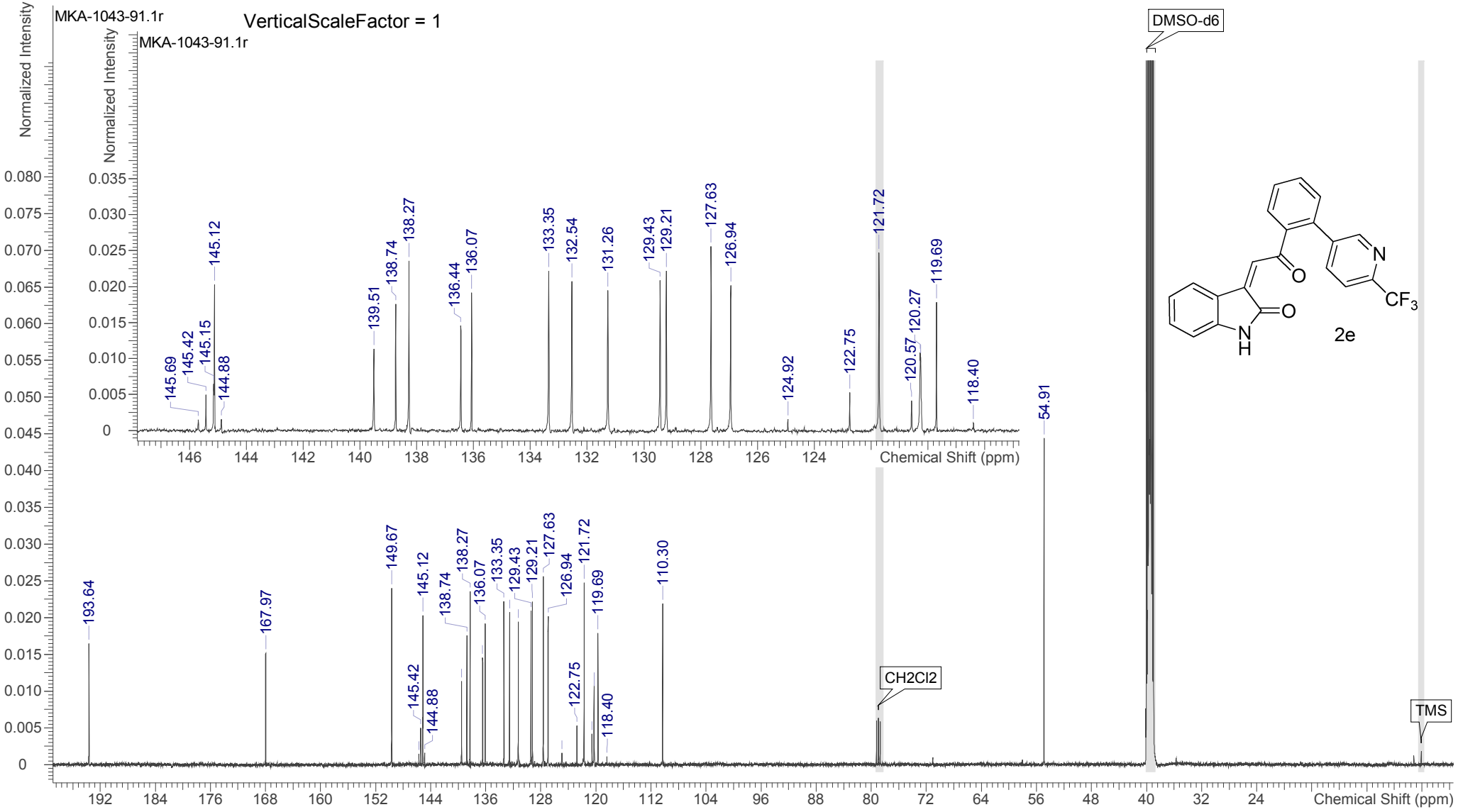
OriginalDateForRelativeTime 2014-05-04T02:23:04	***Multiplets Integrals Sum*** 13.26	***Number of Nuclei*** 13 H's

Acquisition Time (sec)	3.1719	***Comment***	MKA-1043-91 PROTON DMSO {F:\ecm\DATA\2014-04} bionmr 18				
Date	04 May 2014 02:23:04			***Date Stamp***	04 May 2014 02:23:04		
File Name	\\inbgrdsfp01\elndata\MKA\07052014\MKA-1043-91\1\PDATA\1\1r					***Frequency (MHz)***	500.13
Nucleus	1H	***Number of Transients***	16	***Origin***	spect	***Original Points Count***	32768
Owner	administrator	***Points Count***	32768	***Pulse Sequence***	zg30	***Receiver Gain***	4.00
SW(cyclical) (Hz)	10330.58	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	3092.7820	***Spectrum Type***	STANDARD
Sweep Width (Hz)	10330.26	***Temperature (degree C)***	25.000				



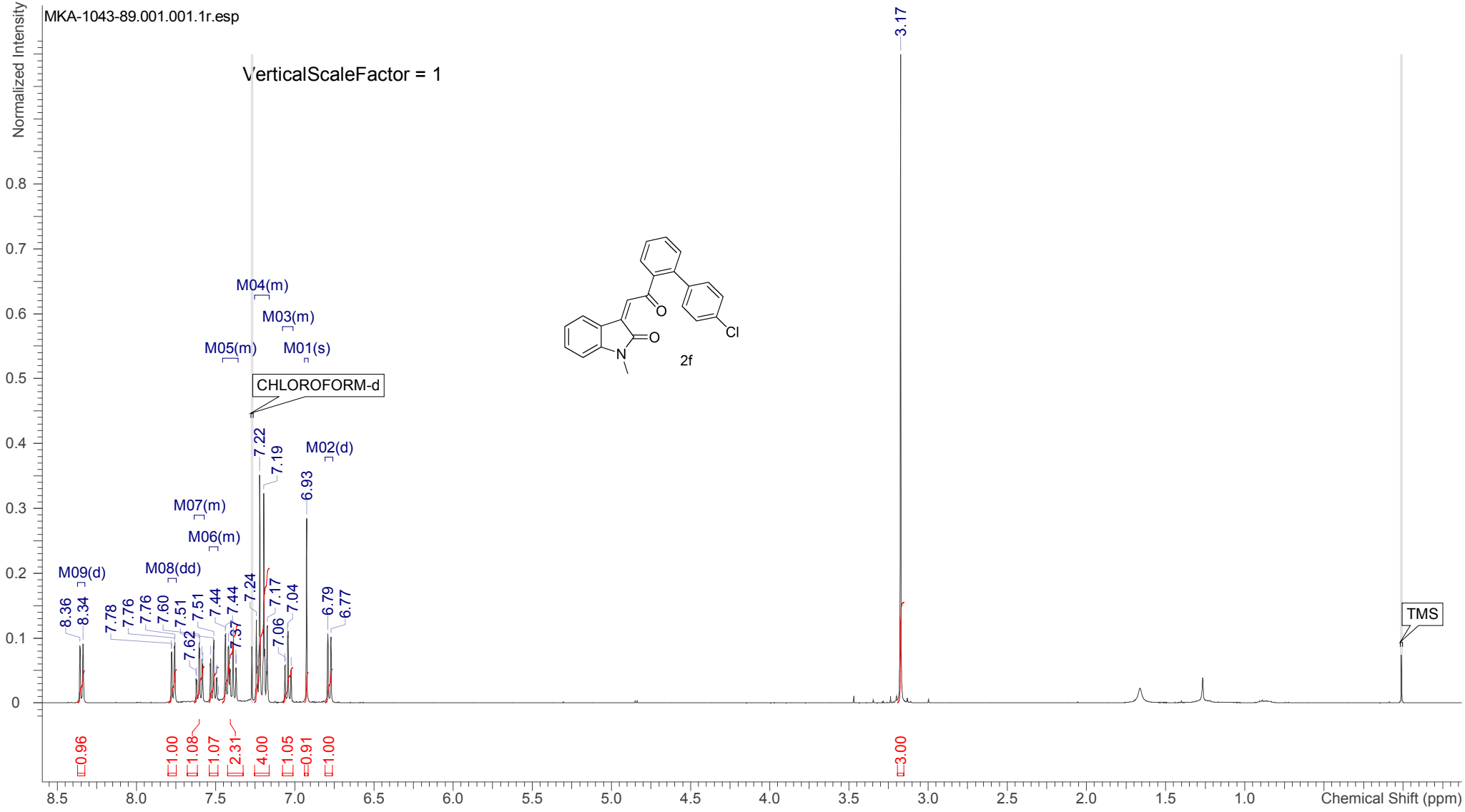
OriginalDateForRelativeTime 2014-05-04T11:10:00			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei***	0 C's

Acquisition Time (sec)	1.0912	***Comment***	MKA-1043-91 C13CPD DMSO {F:\ecm\DATA\2014-04} bionmr 18			***Date***	04 May 2014 11:10:00
Date Stamp	04 May 2014 11:10:00			***File Name***	\\inbgrdsfp01\elndata\MKA\07052014\MKA-1043-91\2\PDATA\1\1r		
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	10000	***Origin***	spect
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	30030.03	***Solvent***	DMSO-d6	***Spectrum Offset (Hz)***	12518.3926
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30029.11	***Temperature (degree C)***	25.000		



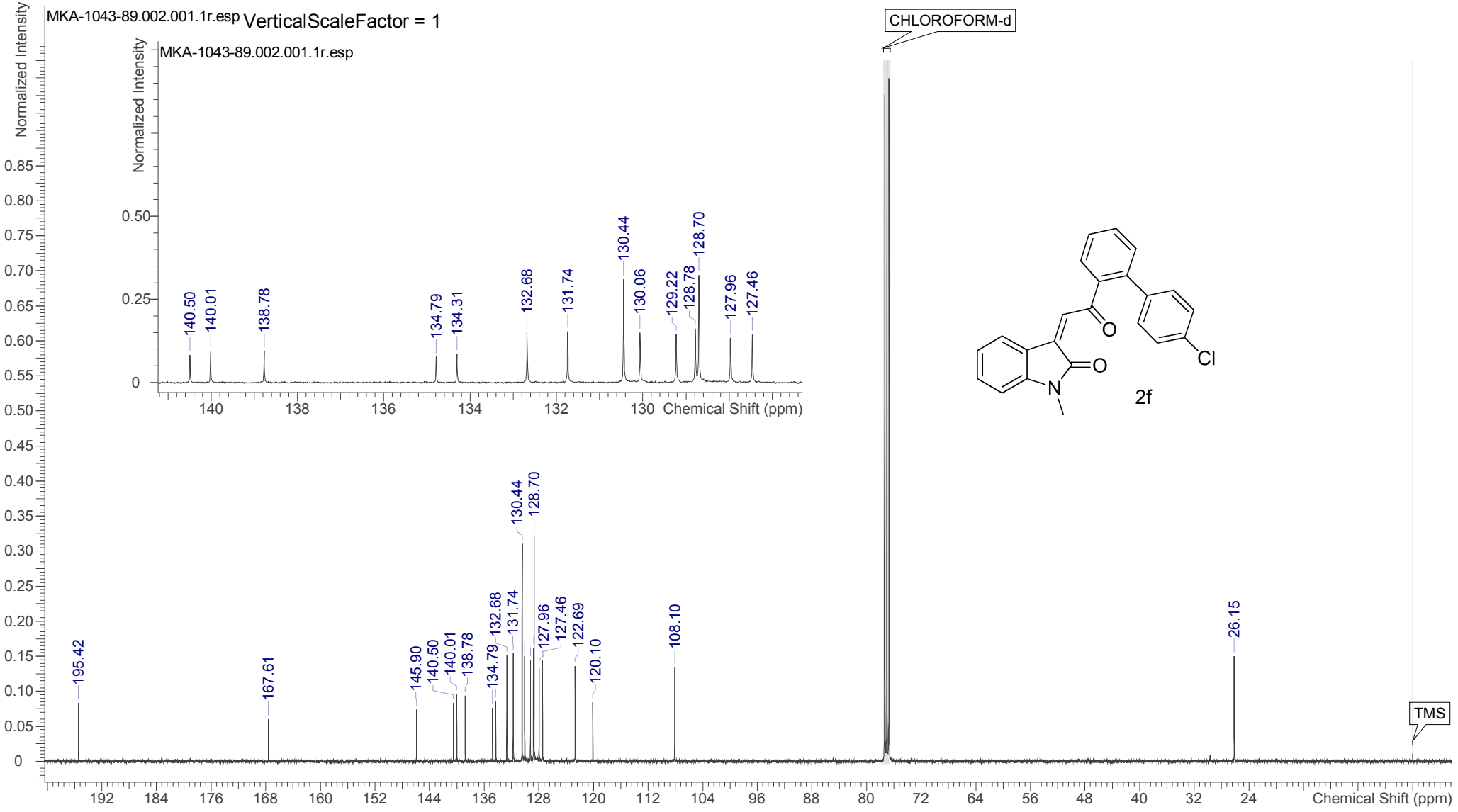
OriginalDateForRelativeTime 2014-04-18T06:34:48	***Multiplets Integrals Sum*** 16.38	***Number of Nuclei*** 16 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-89 PROTON CDCl3 {D:\RA} SamTrack 42			***Date***	18 Apr 2014 06:34:48
Date Stamp	18 Apr 2014 06:34:48			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-89\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	144.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



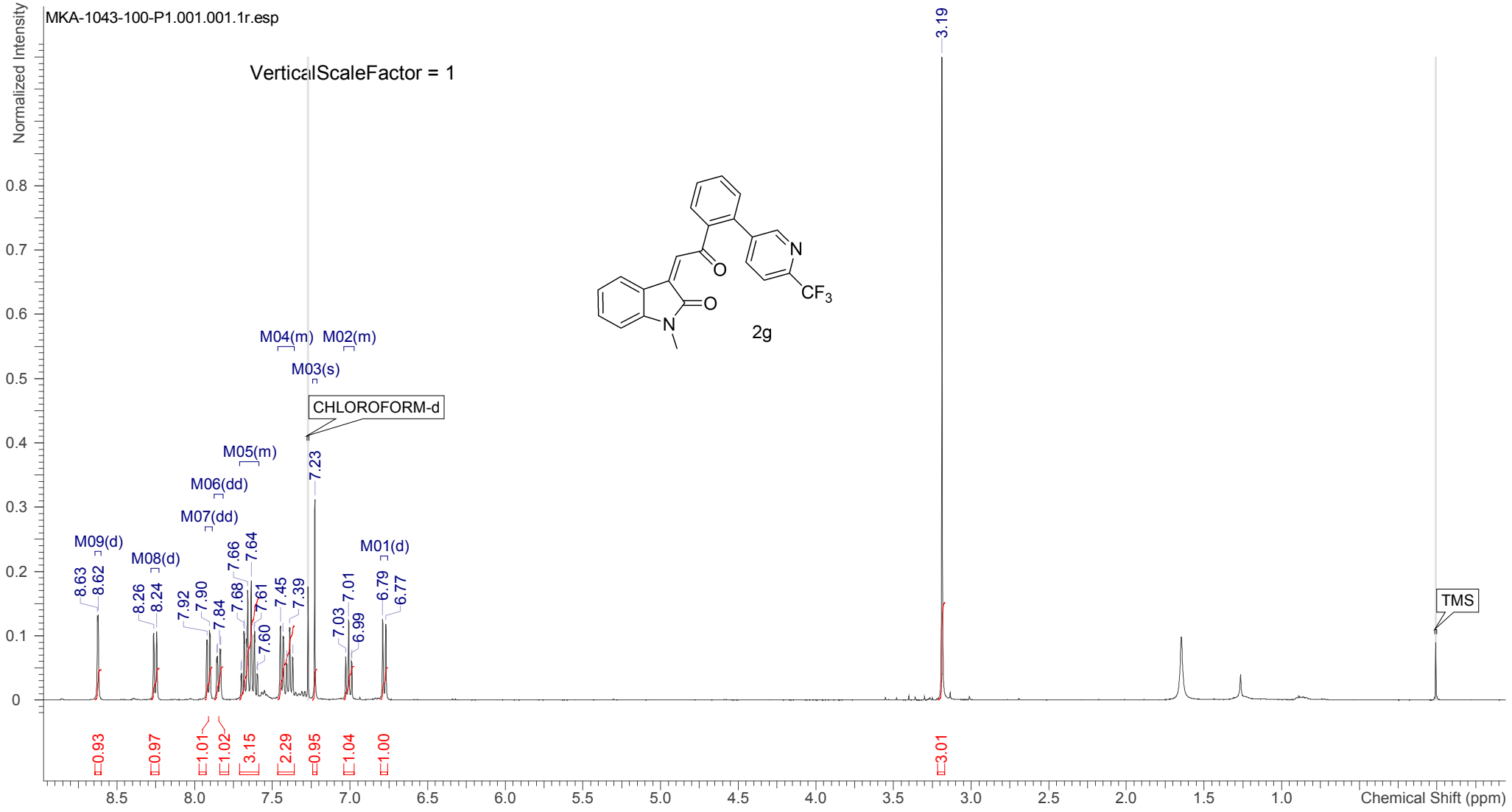
OriginalDateForRelativeTime 2014-04-18T09:27:36			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-89 C13CPD CDCl3 {D:\RA} SamTrack 42			***Date***	18 Apr 2014 09:27:36
Date Stamp	18 Apr 2014 09:27:36			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-89\2\PDATA\1\1r		
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	3000	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	362.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10060.1631	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.000



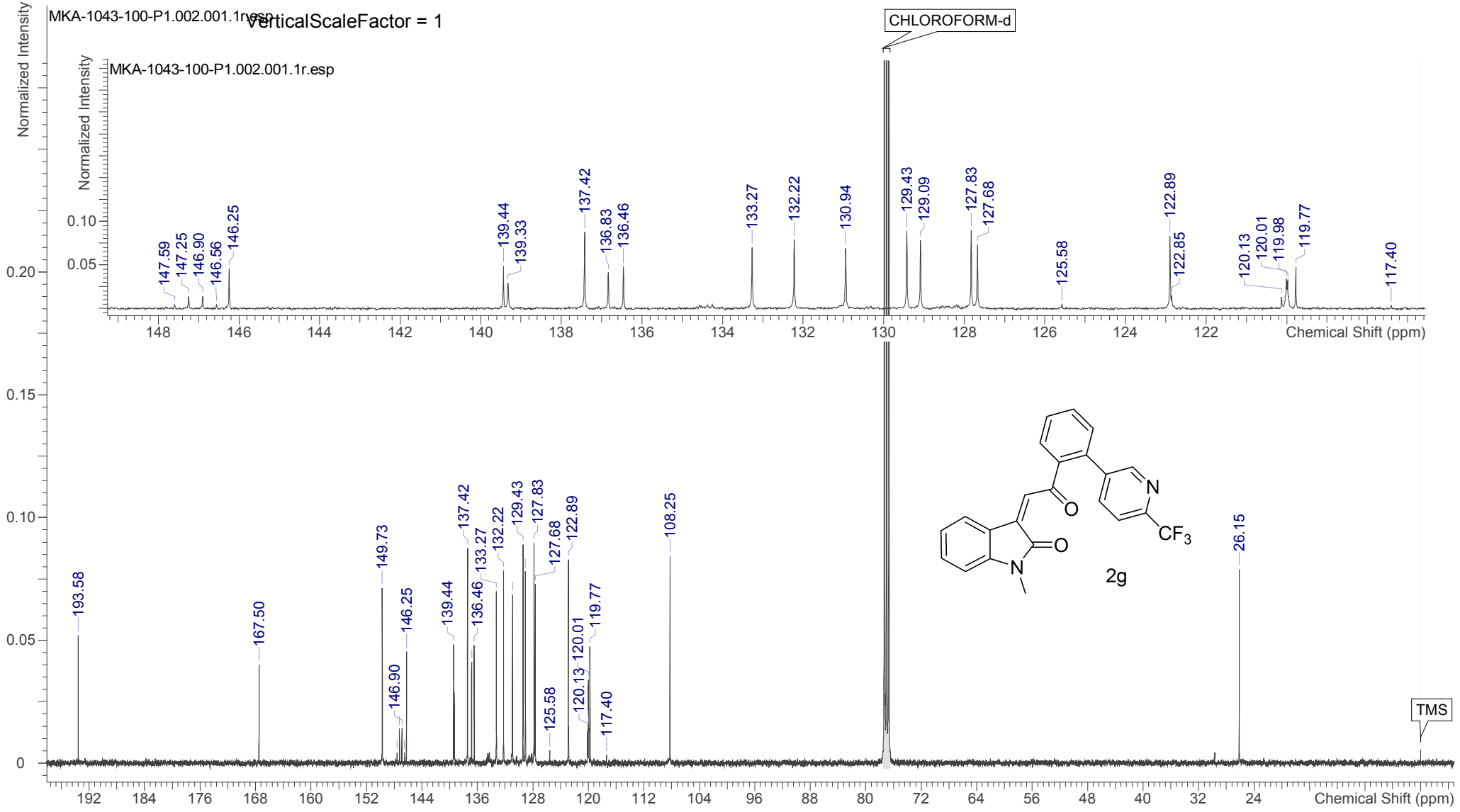
OriginalDateForRelativeTime 2014-05-18T09:38:16			***Multiplets Integrals Sum*** 15.37	***Number of Nuclei*** 15 H's	

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-100-P1/CDCL3 PROTON CDCl3 {D:\RA} SamTrack 7		
Date	18 May 2014 09:38:16		***Date Stamp***	18 May 2014 09:38:16	
File Name	\\inbgrdsfp01\elndata\MKA\NEW\MKA-1043-100-P1\1\PDATA\1\1r			***Frequency (MHz)***	400.13
Nucleus	1H	***Number of Transients***	16	***Origin*** spect	***Original Points Count*** 16384
Owner	nmrsu	***Points Count***	16384	***Pulse Sequence*** zg30	***Receiver Gain*** 203.00
SW(cyclical) (Hz)	8223.68	***Solvent***	CHLOROFORM-d		***Spectrum Offset (Hz)*** 2465.5046
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)*** 27.000	



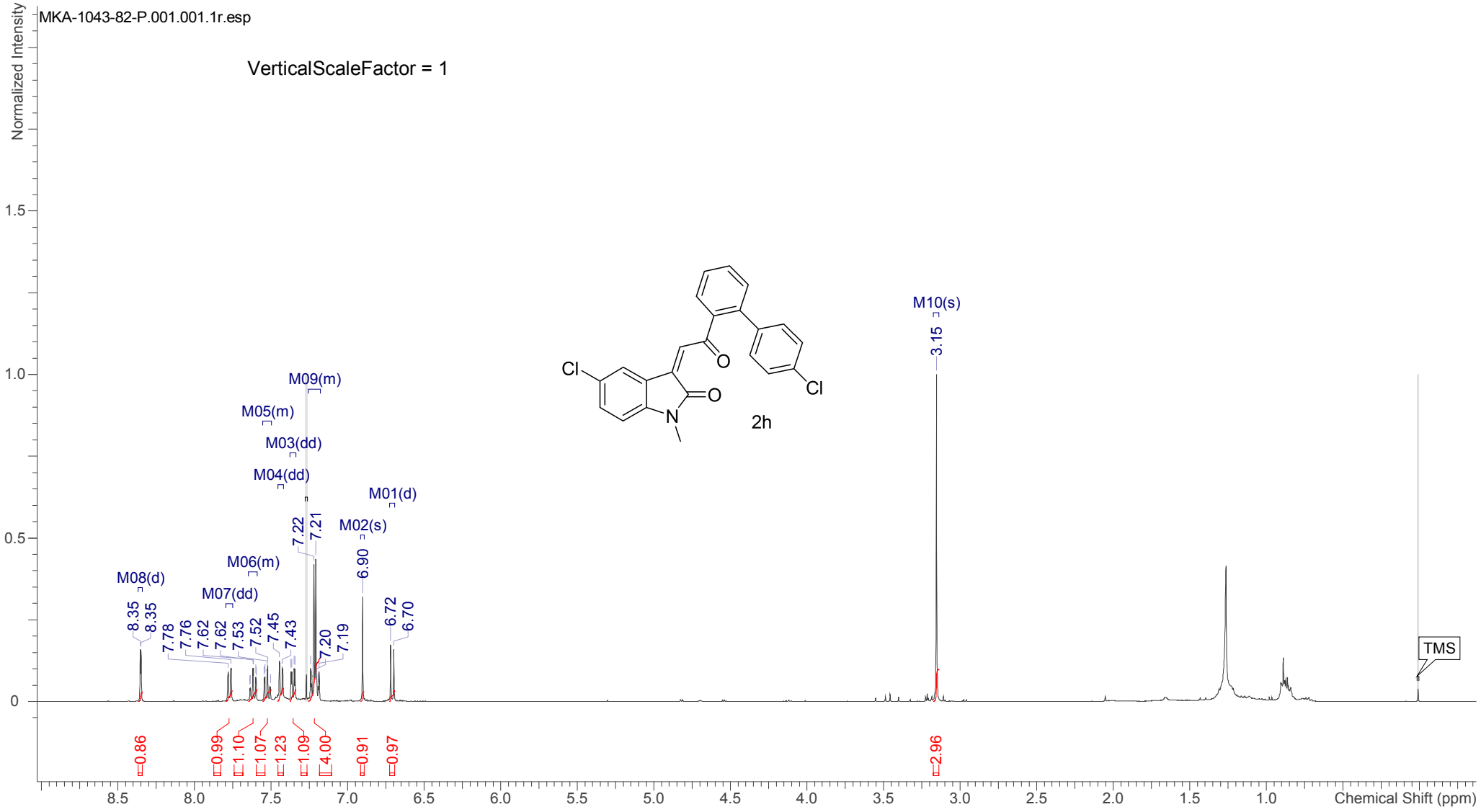
OriginalDateForRelativeTime 2014-05-18T19:10:00			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-100-P1/CDCL3 C13CPD CDCl3 {D:\RA} SamTrack 7			***Date***	18 May 2014 19:10:00
Date Stamp	18 May 2014 19:10:00			***File Name***	\\inbgrdsfp01\elndata\MKA\NEW\MKA-1043-100-P1\2\PDATA\1\1r		
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients***	10000	***Origin***	spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	456.00	***SW(cyclical) (Hz)***	24038.46	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	10059.8848	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	24037.73	***Temperature (degree C)***	27.000

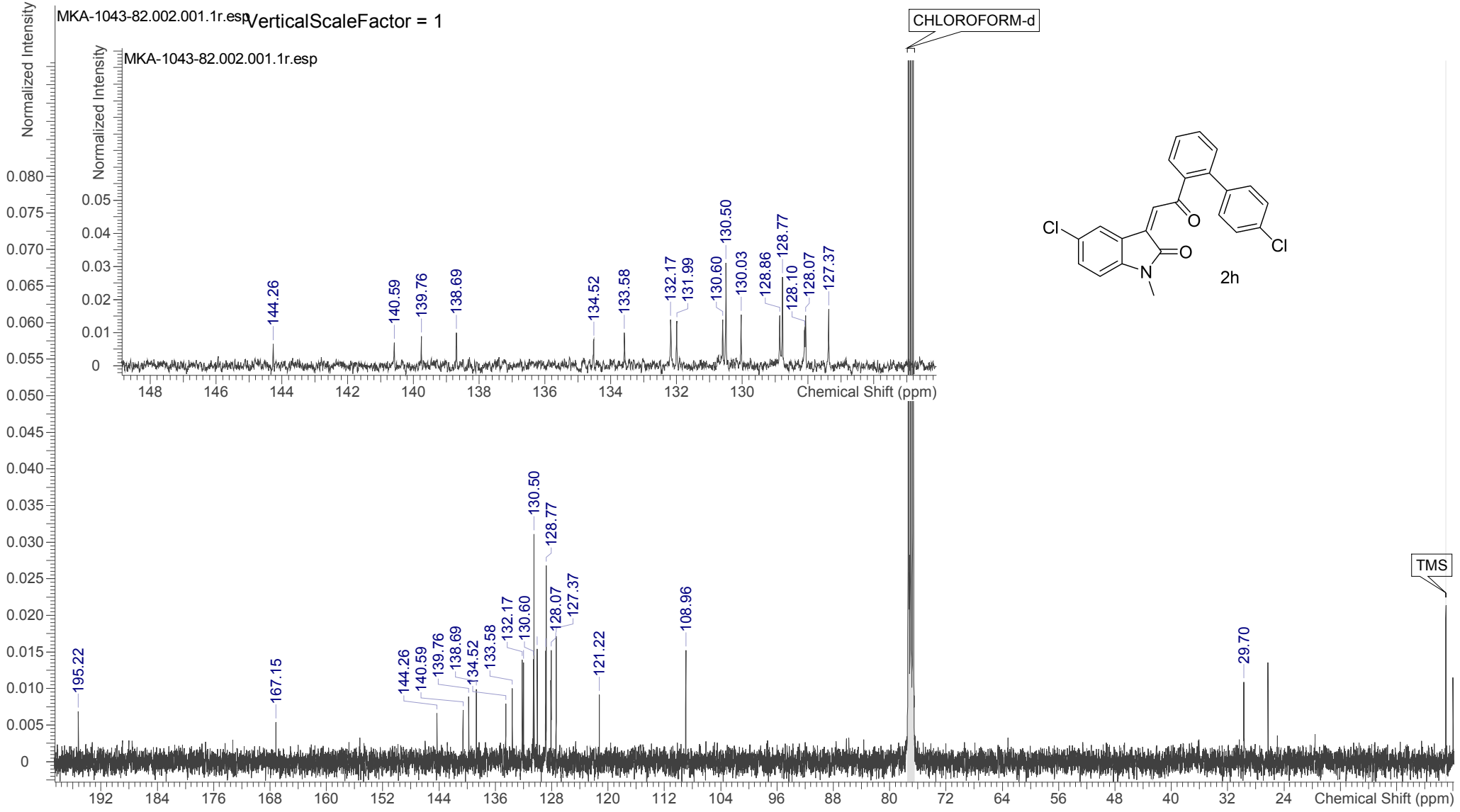


OriginalDateForRelativeTime 2014-04-21T01:16:56	***Multiplets Integrals Sum*** 15.17	***Number of Nuclei*** 15 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-82-P PROTON CDCl3 {D:\RA} SamTrack 60	***Date***	21 Apr 2014 01:16:56
Date Stamp	21 Apr 2014 01:16:56			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-82-P\1\PDATA\1\1r
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16
Origin	spect	***Original Points Count***	16384	***Owner***	nmrsu
Points Count	16384	***Pulse Sequence***	zg30	***Receiver Gain***	80.60
SW(cyclical) (Hz)	8223.68	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	2465.5046
Spectrum Type	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000

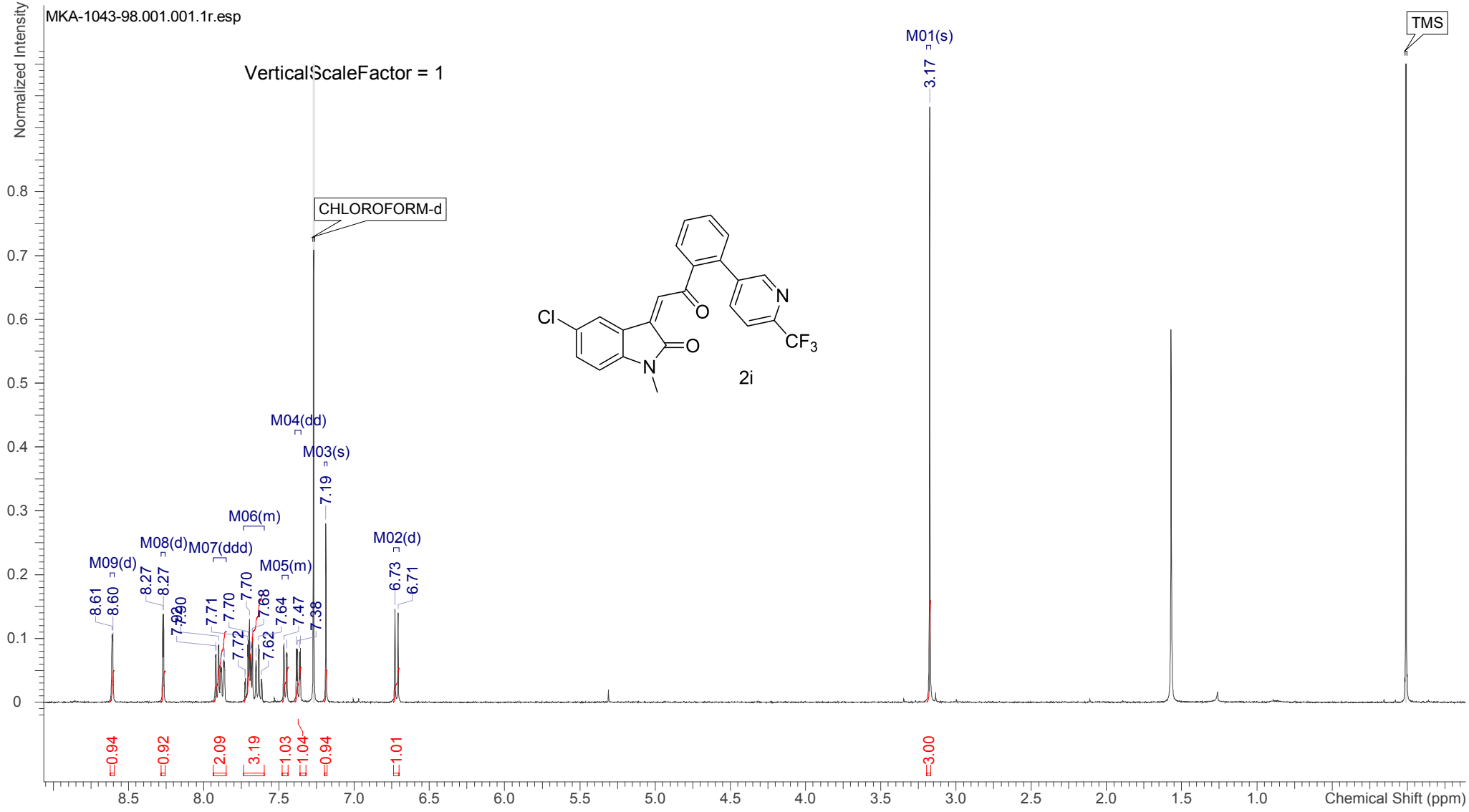


OriginalDateForRelativeTime 2014-04-18T21:15:52			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	
Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-82 C13CPD CDCl3 {D:\RA} SamTrack 46	***Date***	18 Apr 2014 21:15:52
Date Stamp	18 Apr 2014 21:15:52		***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-82\2\PDATA\1\1r	
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients*** 3000	***Origin*** spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count*** 32768	***Pulse Sequence*** zgpg30
Receiver Gain	362.00	***SW(cyclical) (Hz)***	24038.46	***Solvent*** CHLOROFORM-d	
Spectrum Offset (Hz)	10060.6182	***Spectrum Type***	STANDARD	***Sweep Width (Hz)*** 24037.73	***Temperature (degree C)*** 27.000



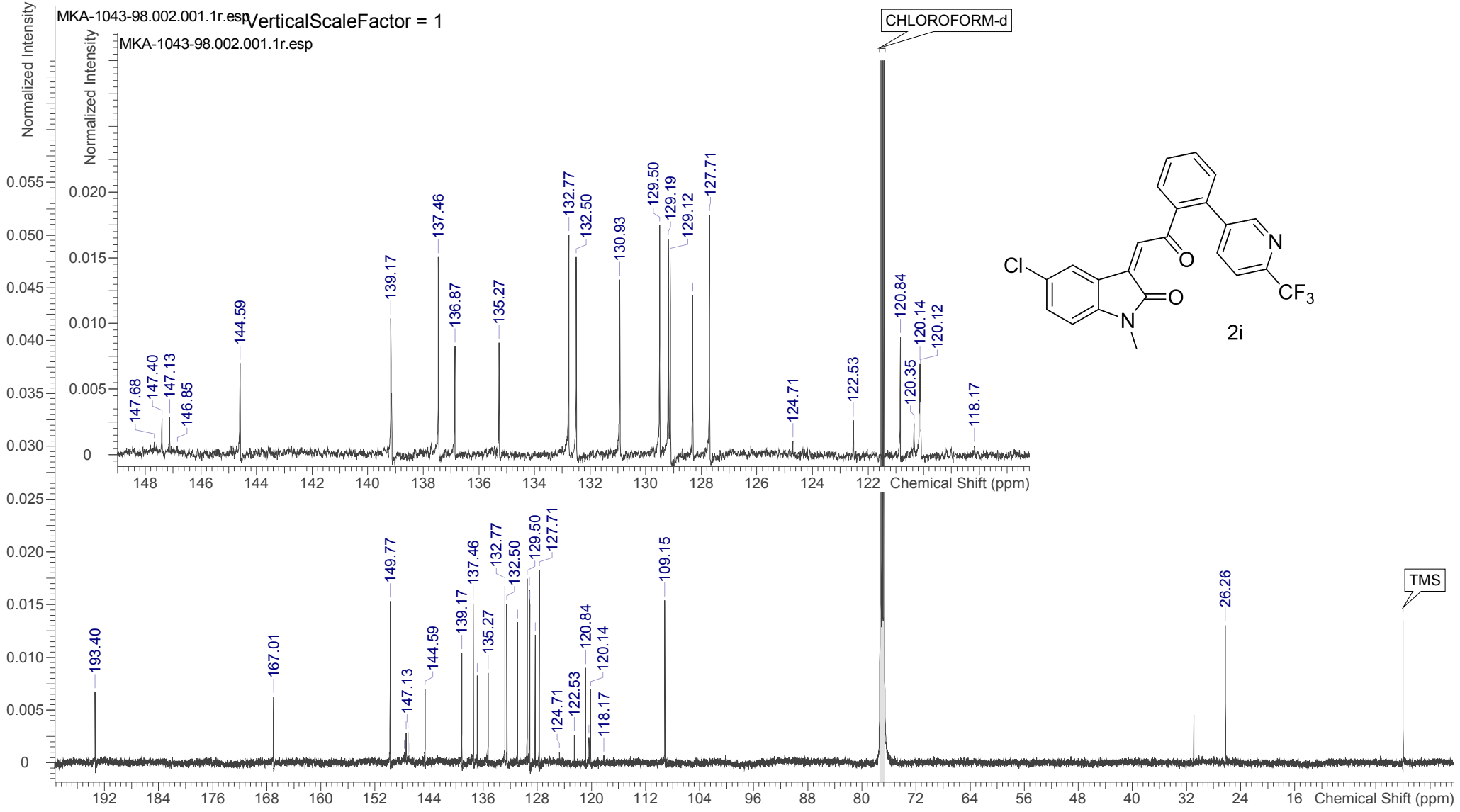
OriginalDateForRelativeTime 2014-04-16T22:22:00	***Multiplets Integrals Sum*** 14.15	***Number of Nuclei*** 14 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-98/CDCl3 PROTON CDCl3 {D:\RA} astra 36			***Date***	16 Apr 2014 22:22:00
Date Stamp	16 Apr 2014 22:22:00			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-98\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	287.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



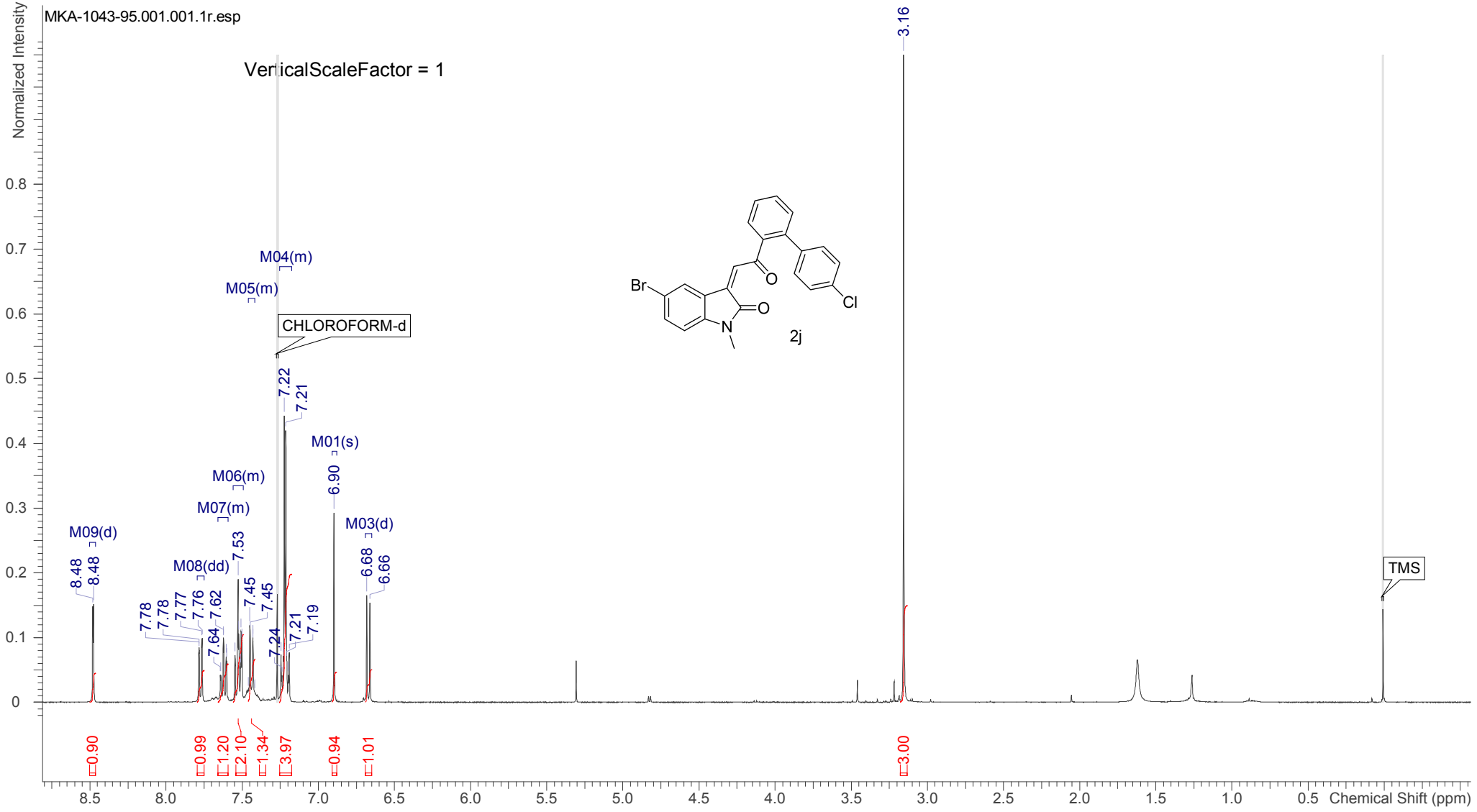
OriginalDateForRelativeTime 2014-05-03T08:34:16			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.0912	***Comment***	MKA-1043-98 C13CPD CDCl3 {F:\ecm\DATA\2014-04} bionmr 15	***Date***	03 May 2014 08:34:16
Date Stamp	03 May 2014 08:34:16		***File Name***	\\inbgrdsfp01\elndata\MKA\07052014\MKA-1043-98\2\PDATA\1\1r	
Frequency (MHz)	125.77	***Nucleus***	13C	***Number of Transients***	10000	***Origin***	spect
Original Points Count	32768	***Owner***	administrator	***Points Count***	32768	***Pulse Sequence***	zgpg30
Receiver Gain	32768.00	***SW(cyclical) (Hz)***	30030.03	***Solvent***	CHLOROFORM-d	***Spectrum Offset (Hz)***	12573.4072
Spectrum Type	STANDARD	***Sweep Width (Hz)***	30029.11	***Temperature (degree C)***	25.000		



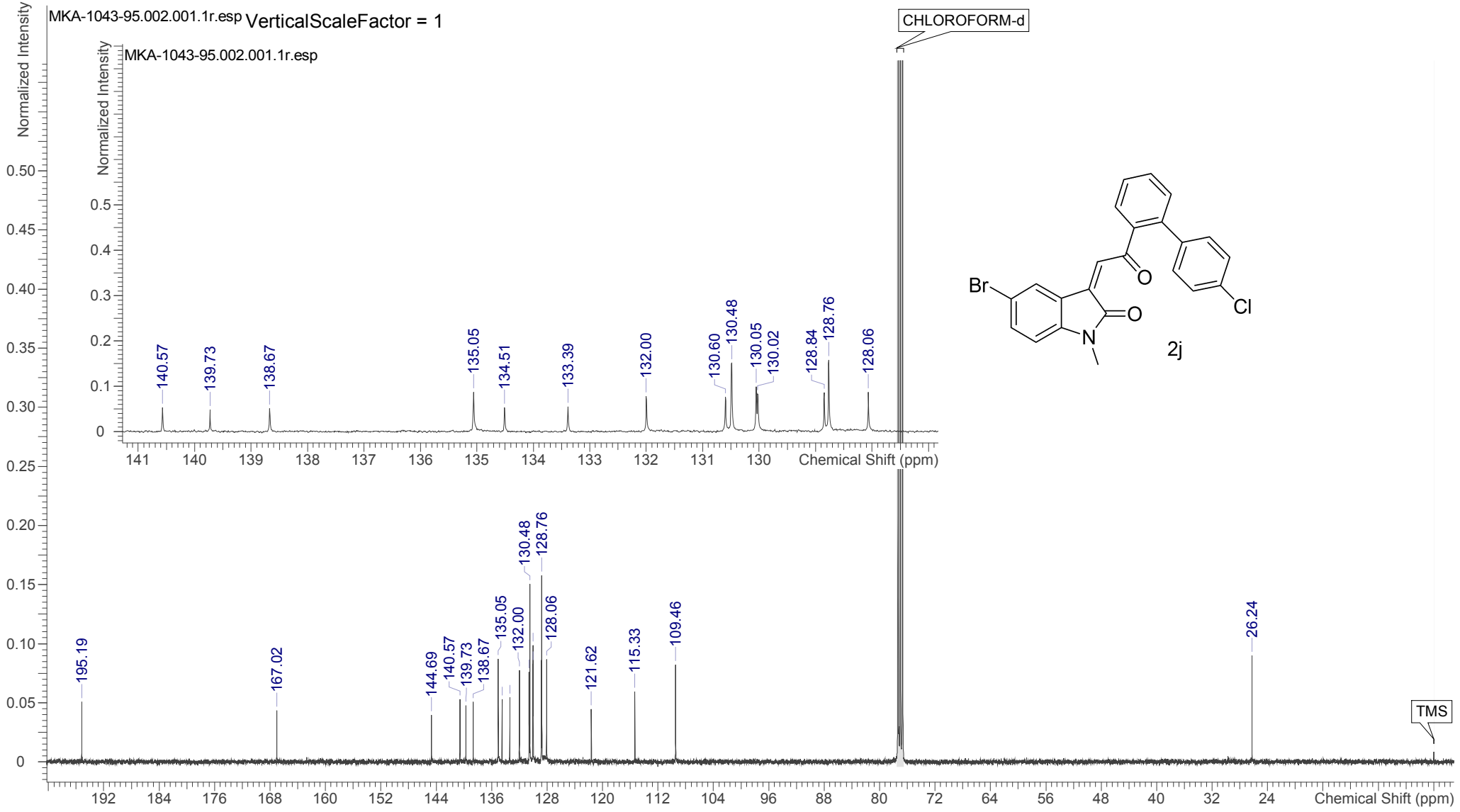
OriginalDateForRelativeTime 2014-04-18T15:26:00	***Multiplets Integrals Sum*** 15.44	***Number of Nuclei*** 15 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-95 PROTON CDCl3 {D:\RA} SamTrack 45			***Date***	18 Apr 2014 15:26:00
Date Stamp	18 Apr 2014 15:26:00			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-95\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	181.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



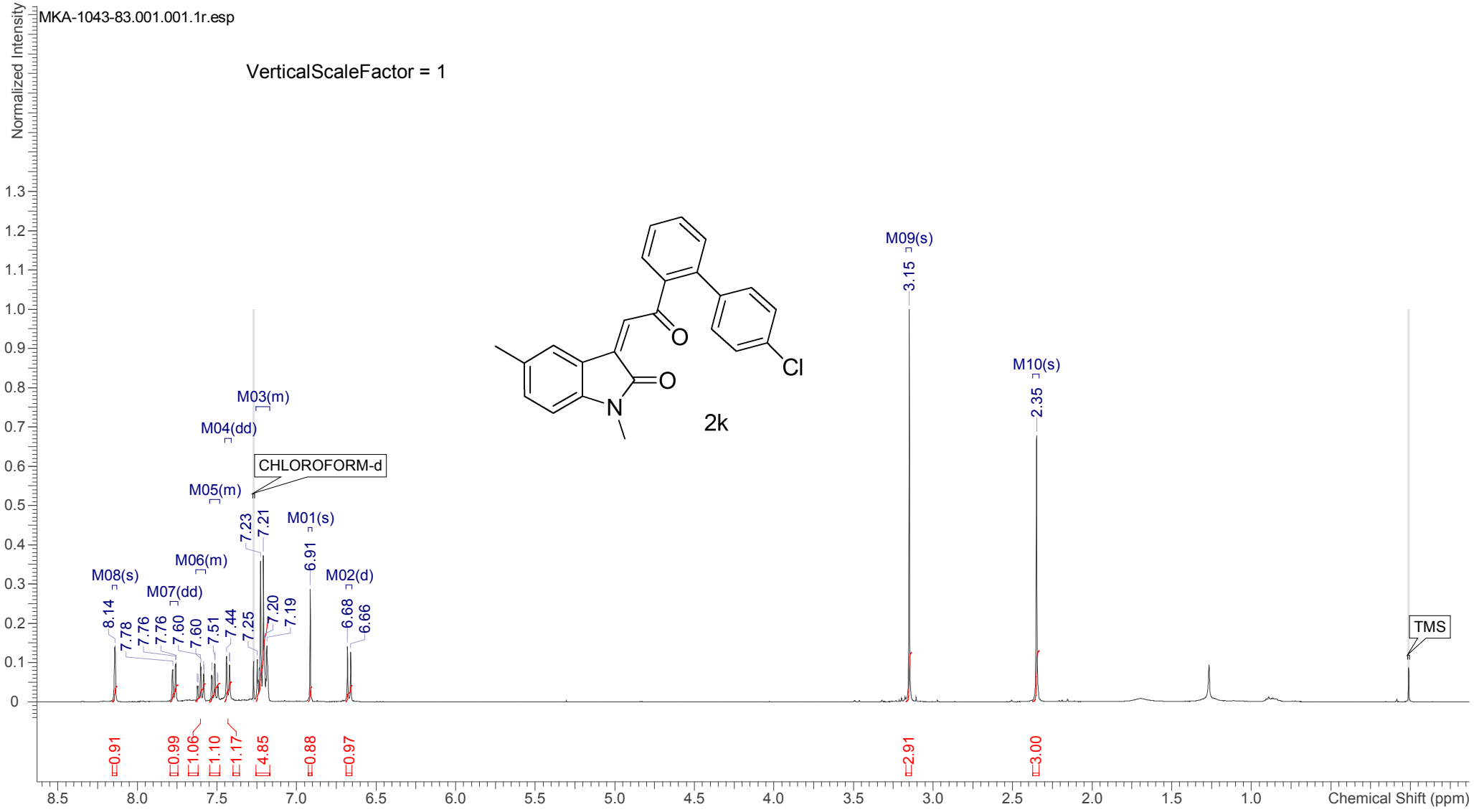
OriginalDateForRelativeTime 2014-04-18T18:18:48			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-95 C13CPD CDCl3 {D:\RA} SamTrack 45	***Date***	18 Apr 2014 18:18:48
Date Stamp	18 Apr 2014 18:18:48		***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-95\2\PDATA\1\1r	
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients*** 3000	***Origin*** spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count*** 32768	***Pulse Sequence*** zgpg30
Receiver Gain	456.00	***SW(cyclical) (Hz)***	24038.46	***Solvent*** CHLOROFORM-d	
Spectrum Offset (Hz)	10059.1504	***Spectrum Type***	STANDARD	***Sweep Width (Hz)*** 24037.73	***Temperature (degree C)*** 27.000



OriginalDateForRelativeTime 2014-04-18T00:42:48	***Multiplets Integrals Sum*** 17.84	***Number of Nuclei*** 18 H's

Acquisition Time (sec)	1.9923	***Comment***	MKA-1043-83 PROTON CDCl3 {D:\RA} SamTrack 40			***Date***	18 Apr 2014 00:42:48
Date Stamp	18 Apr 2014 00:42:48			***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-83\1\PDATA\1\1r		
Frequency (MHz)	400.13	***Nucleus***	1H	***Number of Transients***	16	***Origin***	spect
Original Points Count	16384	***Owner***	nmrsu	***Points Count***	16384	***Pulse Sequence***	zg30
Receiver Gain	128.00	***SW(cyclical) (Hz)***	8223.68	***Solvent***	CHLOROFORM-d		
Spectrum Offset (Hz)	2465.5046	***Spectrum Type***	STANDARD	***Sweep Width (Hz)***	8223.18	***Temperature (degree C)***	27.000



OriginalDateForRelativeTime 2014-04-18T03:33:28			***Multiplets Integrals Sum*** 0.00	***Number of Nuclei*** 0 C's	

Acquisition Time (sec)	1.3631	***Comment***	MKA-1043-83 C13CPD CDCl3 {D:\RA} SamTrack 40	***Date***	18 Apr 2014 03:33:28
Date Stamp	18 Apr 2014 03:33:28		***File Name***	\\inbgrdsfp01\elndata\MKA\MKA-1043-83\2\PDATA\1\1r	
Frequency (MHz)	100.62	***Nucleus***	13C	***Number of Transients*** 3000	***Origin*** spect
Original Points Count	32768	***Owner***	nmrsu	***Points Count*** 32768	***Pulse Sequence*** zgpg30
Receiver Gain	456.00	***SW(cyclical) (Hz)***	24038.46	***Solvent*** CHLOROFORM-d	
Spectrum Offset (Hz)	10058.4170	***Spectrum Type***	STANDARD	***Sweep Width (Hz)*** 24037.73	***Temperature (degree C)*** 27.000