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Supporting Information

A highly efficient one-pot synthesis of indenopyridine-fused spirocyclic systems

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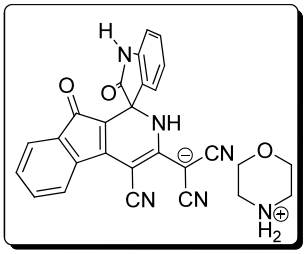
Materials and Methods. Melting points were determined with a melting point Thermo Scientific 9100 apparatus and are uncorrected. IR spectra were taken with a Bomem FT-IR MB spectrometer. NMR spectra were recorded with 300 and 400 MHz Bruker DRX Avance spectrometers. MS spectra were recorded with a Finnigan LCQ mass spectrometer in negative ion mode.

All chemicals were purchased from Merck or Aldrich and were used without further purification. 1,1-dicyanomethylene-3-indanone,[1] isatylidenemalononitrile[2] and indeno[1,2-*b*]quinoxalin-11-ones[3] were prepared by reported procedures.

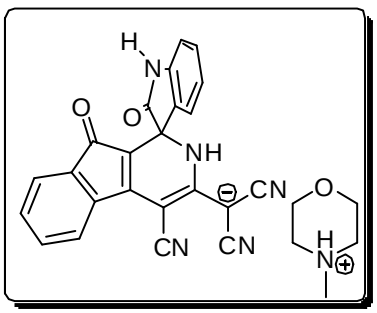
General procedure for synthesis of 4 or 10. To a stirred solution of 1,1-dicyanomethylene-3-indanone **1** or indeno[1,2-b]quinoxalin-11-ones **12** (1 mmol) and amine (1 mmol) in ethanol at room temperature, isatin **2** (1mmol), malononitrile **3** (1mmol) were added and continued stirring for about 12 hours. The completion of the reaction was indicated by the disappearance of the starting materials in thin layer chromatography. After completion of the reaction, the solvent was evaporated and the crude product was with cold ether to obtain the corresponding salt product **4** or **10**.

General procedure for synthesis of 6. Corresponding dicyano(4-cyano-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-c]pyridine-1,3'-indolin]-3-yl)methanide salt **4** (1mmol) was dissolved in ethanol and the aqueous solution of hydrochloric acid was slowly added until the amine is completely neutralized. After an hour, the precipitated solids were collected by filtration, washed thoroughly with water and dried to afford product **6**.

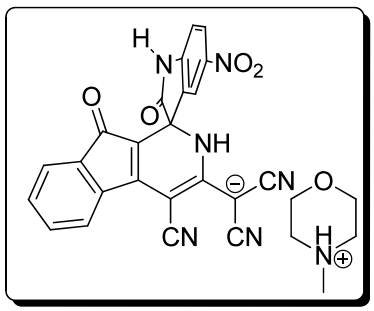
X-ray crystallography. The X-ray diffraction measurements were made with a STOE IPDS-II diffractometer with graphite-monochromated MoKa radiation. Cell constants and an orientation matrix for data collection were obtained by least-squares refinement of diffraction data from 4998 unique reflections for **4f** and **6d**. Data were collected at a temperature of 298(2) K to a maximum 2q value of 51.988 and in a series of w scans in 18 oscillations and integrated using the Stoe X-AREA[4]software package. The data were corrected for Lorentz and Polarizing effects. The structures were solved by direct methods and refined on F2 by full-matrix least-squares procedure. All hydrogen atoms were added at ideal positions and constrained to ride on their parent atoms, with Uiso(H)= 1.2Ueq. All refinements were performed by using the X-STEP32 crystallographic software package.[5] Complete crystallographic data for compound **4f** and **6d** has been deposited with the Cambridge Crystallographic Data Centre as supplementary publication No. CCDC-1437636 and CCDC-1437637, respectively. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Morpholin-4-ium dicyano(4-cyano-2',9-dioxo-2,9-dihydro spiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl)methanide (4a). Purple powder (yield 92%); m.p. 222-224 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3479, 3279, 2200, 2170, 1717, 1648. ESI: 338 [M- $C_4H_{10}NO^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 3.05 (4H, bs, $2CH_2$), 3.70 (4H, bs, $2CH_2$), 6.76 (1H, d, $^3J_{HH}$=7.5 Hz, H-Ar), 6.85 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7-06-7.16 (2H, m, H-Ar), 7.16 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.27 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.36 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.85 (1H, s, H-Ar), 8.10 (1H, s, NH), 10.30 (1H, s, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm) 43.4, 62.5, 63.9, 64.4, 108.3, 109.8, 119.2, 119.3, 120.0, 120.7, 122.1, 124.4, 129.4, 130.0, 131.3, 133.9, 135.8, 138.9, 142.3, 153.3, 159.8, 176.8, 184.9. Anal. Calcd for $C_{27}H_{20}N_6O_3$: C, 68.06; H, 4.23; N, 17.64%. Found: C, 67.85; H, 4.11; N, 17.82

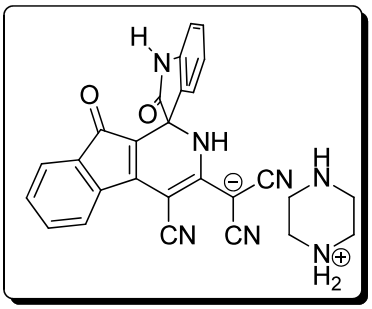


4-Methylmorpholin-4-ium dicyano(4-cyano-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl) methanide (4b). Purple powder (yield 88%); m.p. 246-248 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3276, 2205, 2177, 1720, 1620. ESI: 338 [M- $C_5H_{12}NO^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 2.68 (3H, s,NCH_3), 3.03 (4H, bs, $2CH_2$), 3.72 (4H, bs, $2CH_2$), 6.76 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 6.85(1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7-06-7.09 (2H, m, H-Ar), 7.16 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.27 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.36 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.87 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar), 8.07 (1H, s, NH),10.29 (1H, s, NH).^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 43.5, 53.5, 62.9, 64.3, 64.9, 108.8, 110.2, 119.5, 119.7, 120.3, 121.1, 122.5, 124.8, 129.8, 130.4, 131.6, 134.3, 136.3, 139.4, 142.8, 153.7, 160.2, 177.1, 185.2. .Anal. Calcd for $C_{28}H_{22}N_6O_3$: C, 68.56; H, 4.52; N, 17.13%. Found: C, 68.37; H, 4.64; N, 17.26.

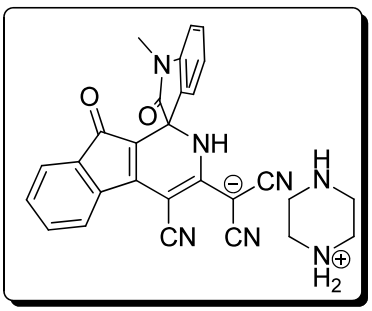


4-Methylmorpholin-4-ium dicyano(4-cyano-5'-nitro-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl)methanide (4c).Purple powder (yield 90%); m.p 175-177 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3362, 3223, 3096,

2837, 1726, 1650. ESI: 433 [M- $C_5H_{12}NO^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 2.70 (3H, s,NCH_3), 3.06 (4H, bs, $2CH_2$), 3.73 (4H, bs, $2CH_2$), 6.99 (1H, d, $^3J_{HH}$=8.7 Hz, H-Ar), 7.11 (1H, d,J_{HH} = 6.9 Hz, H-Ar), 7.30 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.40 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.90-7.93 (2H, m, H-Ar), 8.16-8.20 (2H, m, H-Ar and NH),11.06 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 43.6, 53.6, 62.6, 64.7, 64.8, 107.1, 110.3, 119.2, 120.1, 120.5, 121.5, 123.4, 127.1, 130.6, 131.7, 133.3, 135.1, 136.2, 139.1, 143.1, 149.6, 154.2, 160.3, 178.0, 184.6. Anal. Calcd for $C_{28}H_{21}N_7O_5$: C, 62.80; H, 3.95; N, 18.31%. Found: C, 62.72; H, 3.88; N, 18.25.

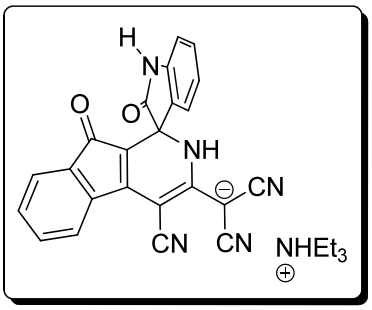


Piperazin-1-ium dicyano(4-cyano-2',9-dioxo-2,9-dihydro spiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl)methanide (4d). Purple powder (yield 91%); m.p. 265 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3487, 3257, 2211, 2181, 1734, 1574. ESI: 338 [M- $C_4H_{11}N_2^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)2.88 (8H, s, $4CH_2$), 6.77 (1H, d, $^3J_{HH}$=7.5 Hz, H-Ar), 6.86(1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7-07-7.10 (2H, m, H-Ar), 7.17 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.28 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.37 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.88 (1H, m, H-Ar), 8.07 (1H, s, NH),10.30 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 44.0, 62.9, 64.9, 108.8, 110.2, 119.6, 119.7, 120.3, 121.2, 122.5, 124.8, 129.8, 130.4, 131.6, 134.3, 136.3, 139.4, 142.8, 153.7, 160.2, 177.1, 185.2. .Anal. Calcd for $C_{27}H_{21}N_7O_2$: C, 68.20; H, 4.45; N, 20.62%. Found: C, 68.31; H, 4.52; N, 20.53.



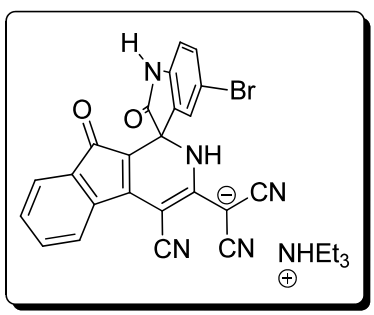
Piperazin-1-ium dicyano(4-cyano-1'-methyl-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3-yl) methanide (4e).Purple powder (yield 88%); m.p. 251 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3469, 3296, 2211, 2197, 1720, 1636. ESI: 402 [M-$C_4H_{11}N_2^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)2.86 (8H, s, $4CH_2$), 3.08 (3H, s, NCH_3), 6.96 (2H, bs, H-Ar), 7.05-7.11 (2H, m, H-Ar), 7.26-7.34 (3H, m, H-Ar), 7.87-7.96(2H, m, H-Ar and NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 27.1, 43.8, 62.5, 64.8, 108.5, 108.9, 119.5, 120.3, 121.2, 123.2, 124.3, 129.9, 130.4, 131.6, 133.7, 136.2, 139.3, 144.2,

153.7, 160.2, 175.6, 185.1..Anal. Calcd for $C_{28}H_{23}N_7O_2$: C, 68.70; H, 4.74; N, 20.03%. Found: C, 68.65; H, 4.61; N, 20.18.



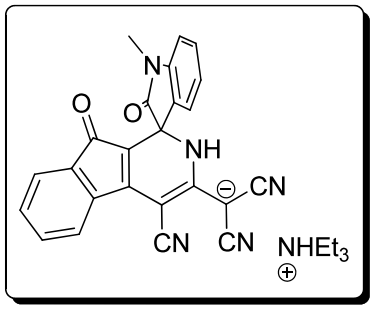
Triethylammonium dicyano(4-cyano-2',9-dioxo-2,9-dihydro spiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl)methanide (4f).Purplepowder (yield 94%); m.p. 266-268 ˚C.IR (KBr) ν_{max}(KBr) (ν_{max} /cm^{-1}): 3447, 3288, 2201, 2181, 2168, 1731, 1696. ESI: 338 [M- $C_6H_{16}N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)1.15 (9H, t, $^3J_{HH}$=7.2 Hz, 3CH_3), 3.05 (6H, q, $^3J_{HH}$=7.2 Hz 3CH_2), 6.76 (1H, d, $^3J_{HH}$=7.8 Hz, H-Ar), 6.86 (1H, t, $^3J_{HH}$=7.5 Hz,H-Ar), 7.07-7.09 (2H, m, H-Ar), 7.17 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.27 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.37 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.87 (1H, d, $^3J_{HH}$=7.5 Hz,H-Ar), 8.08 (1H, s, NH),10.30 (1H, s, NH).^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm)9.0, 46.2, 62.5, 64.4, 108.3, 109.8, 119.2, 119.3, 120.0, 120.7, 122.1, 124.4, 129.4, 130.0, 131.3, 133.9, 135.8, 138.9, 142.3, 153.3, 159.8, 176.7, 184.9..Anal. Calcd for $C_{29}H_{26}N_6O_2$: C, 71.00; H, 5.34; N, 17.13%. Found: C, 71.07; H, 5.40; N, 17.05.

X-Ray data for 4f: $C_{29}H_{26}N_6O_2$, M= 490.56 g/mol, triclinic system, space group P$\bar{1}$, a = 8.898(4), b = 11.774(6), c = 12.676(7) ?, α=80.45(4)^o, β=81.87(4)^o, γ=89.64(4)^o, V= 1296.2(12) ?^{3}, Z= 2, Dc=1.257 g.cm^{-3}, μ(Mo-Kα)= 0.71073 ?, crystal dimension of 0.15 x 0.20 x 0.35 mm. The structure was solved by using SHELXS. The structure refinement and data reduction was carried out with SHELXL of the X-Step32 suite of programs. The non-hydrogen atoms were refined anisotropically by full matrix least-squares on F^2 values to final R_1=0.1464, wR_2= 0.3138 and S=1.109 with 334 parameters using 6944 independent reflection (θ range = 2.20– 29.32^o). Hydrogen atoms were located from expected geometry and were not refined.

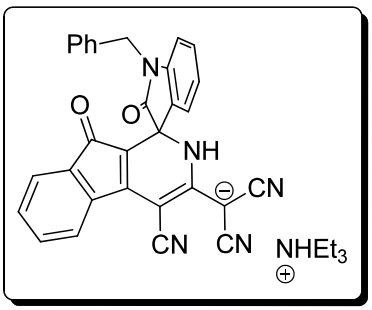


Triethylammonium (5'-bromo-4-cyano-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl) di cyanomethanide (4g). Purple powder (yield 91%); m.p. 203-205 ˚C. IR (KBr) (ν_{max} /cm^{-1}): 3424, 3300, 2201, 2169, 1718, 1677. ESI: 467 [M- $C_6H_{16}N^+$]$^-$, 469 [M+2- $C_6H_{16}N^+$]$^-$

.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)1.18 (9H, bs, $3CH_3$), 3.07-309 (6H, m, $3CH_2$), 6.73 (1H, d, $^{3}J_{HH}$=7.2 Hz, H-Ar), 7.10 (1H, d, $^{3}J_{HH}$=5.7 Hz, H-Ar), 7.21 (1H, s, H-Ar), 7.29-7.36 (3H, m, H-Ar), 7.89 (1H, d, $^{3}J_{HH}$=6.3 Hz, H-Ar), 8.12 (1H, s, NH), 8.89 (1H, bs, NH), 10.45 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 9.7, 46.7, 63.0, 65.1, 107.8, 112.1, 113.9, 119.4, 120.4, 121.3, 127.5,130.5, 131.7, 132.4, 136.3, 136.5, 139.3, 142.3, 154.0, 160.3, 176.9, 185.1. .Anal. Calcd for $C_{29}H_{25}BrN_6O_2$: C, 61.17; H, 4.43; N, 14.76;%. Found: C, 61.22; H, 4.35; N, 14.82.

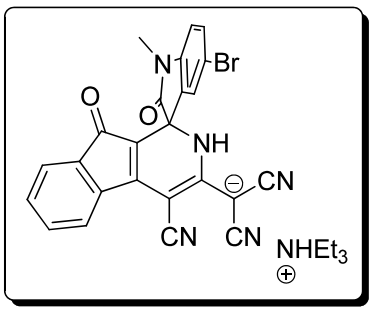


Triethylammonium dicyano(4-cyano-1'-methyl-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl) methanide (4h).Purple powder (yield 89%); m.p. 192-194 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3438, 3258, 2203, 2173, 1715, 1653. ESI: 402 [M- $C_6H_{16}N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)1.15 (9H, bs,CH_3), 3.08 (9H, bs, $3CH_2$ and NCH_3), 6.96 (2H, bs, H-Ar), 7.07-7.12(2H, m, H-Ar), 7.27-7.36 (3H, m, H-Ar), 7.88-7.97(2H, m, H-Ar and NH), 8.84(1H, bs, NH).^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 9.5, 27.1, 46.7, 62.5, 64.8, 108.6, 108.9, 119.4, 119.5, 120.3, 121.2, 123.2, 124.3, 129.9, 130.4, 131.6, 133.8, 136.2, 139.4, 144.2, 153.7, 160.2, 175.6, 185.2..Anal. Calcd for $C_{30}H_{28}N_6O_2$: C, 71.41; H, 5.59; N, 16.66%. Found: C, 71.49; H, 5.52; N, 16.60.

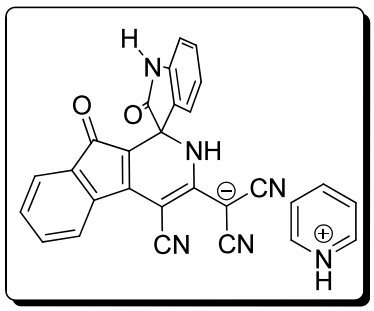


Triethylammonium (1'-benzyl-4-cyano-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl) dicyanomethanide (4i).Purple powder (yield 79%); m.p. 200-201 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3436, 3256, 2198, 1718, 1680.ESI: 478 [M- $C_6H_{16}N^+$]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 1.14 (9H, bs,CH_3), 3.04-3.06 (6H, m, $3CH_2$), 4.41, 5.29 (2H, ABq, J_{AB}=16.2 Hz), 6.63 (1H, d, $^{3}J_{HH}$=7.5 Hz, H-Ar), 6.96 (1H, t, $^{3}J_{HH}$=7.2 Hz, H-Ar), 7.16 (3H, m, H-Ar), 7.31-7.35 (5H, m, H-Ar),7.60 (2H, d, $^{3}J_{HH}$=7.2 Hz, H-Ar), 7.92 (1H, d, $^{3}J_{HH}$=7.2 Hz, H-Ar),8.15 (1H, s, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm) 9.0, 44.3, 46.1, 62.2, 64.6, 107.9, 109.4, 119.1, 119.2, 120.2, 120.9, 123.0, 124.2, 127.3, 127.5, 127.7, 128.8, 129.0, 129.5, 130.2, 131.4, 133.3, 135.8, 136.5,

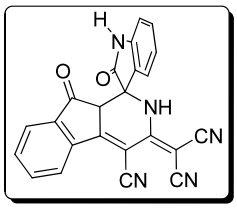
138.9, 143.1, 153.6, 159.7, 175.6, 185.0.Anal. Calcd for $C_{36}H_{32}N_6O_2$: C, 74.46; H, 5.55; N, 14.47%. Found: C, 74.62; H, 5.42; N, 14.32.



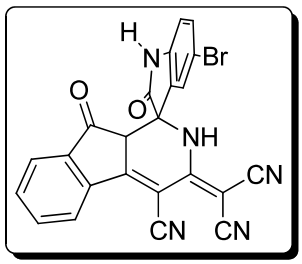
Triethylammonium (5'-bromo-4-cyano-1'-methyl-2',9-dioxo-2,9-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl) dicyanomethanide (4j). Purple powder (yield 85%); m.p. 174-176 ˚C. IR (KBr) (v_{max} /cm^{-1}): 3417, 2200, 2170, 1731, 1655. ESI: 480 [M-$C_6H_{16}N^+$]$^-$, 482 [M+2-$C_6H_{16}N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)1.14 (9H, bs,CH_3), 3.08 (9H, bs, CH_2 and NCH_3), 6.97 (1H, d, $^3J_{HH}$=6.0 Hz, H-Ar), 7.06 (1H, bs, H-Ar), 7.27 (2H, bs, H-Ar), 7-32-7.38 (1H, m, H-Ar), 7-43-7.45 (1H, m, H-Ar), 7.89-7.90 (1H, m, H-Ar).^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 9.4, 27.2, 46.8, 62.5, 65.2, 107.6, 111.3, 114.9, 119.4, 120.7, 121.4, 126.9, 130.9, 131.9, 132.8, 135.6, 136.0, 138.9, 143.6, 154.2, 160.2, 175.4, 185.4.Anal. Calcd for $C_{30}H_{27}BrN_6O_2$: C, 61.75; H, 4.66; N, 14.40%. Found: C, 61.67; H, 4.61; N, 14.49.



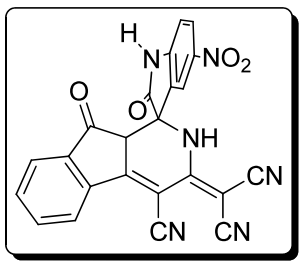
Pyridiniumdicyano(4-cyano-2',9-dioxo-2,9-dihydro spiro[indeno[2,1-*c*]pyridine-1,3'-indoline]-3-yl)methanide (4k). Purple powder (yield 79%); m.p. 259 ˚C dec. IR (KBr) (v_{max} /cm^{-1}): 3228, 2199, 2171, 1733, 1617.ESI: 338 [M-$C_5H_6N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 6.76 (1H, d, $^3J_{HH}$=7.5 Hz, H-Ar), 6.86(1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7-06-7.09 (2H, m, H-Ar), 7.17 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.27 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.36 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.75 (1H, t, $^3J_{HH}$=6.3 Hz, H-py), 7.87 (1H, m, H-Ar),8.08(1H, s, NH), 8.21 (1H, t, $^3J_{HH}$=6.3 Hz, H-py), 8.75-8.76(2H, m, H-py), 10.31 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 6.9, 64.9, 108.8, 110.2, 119.6, 119.7, 120.4, 121.2, 122.5, 123.3, 124.8, 126.8, 129.8, 130.4, 131.6, 132.5, 134.3, 136.3, 139.4, 142.8, 143.3, 145.8, 153.8, 160.2, 177.1, 185.2.Anal. Calcd for $C_{28}H_{16}N_6O_2$: C, 71.79; H, 3.44; N, 17.94%. Found: C, 71.80; H, 3.51; N, 17.81.



2-(4-Cyano-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene)malononitrile(6a).Olive powder (yield 93%); m.p. 215 ˚C dec IR (KBr) (v_{max} /cm^{-1}): 3250, 2219, 2197, 1733, 1617. ESI: 389 $[M]^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)6.74 (1H, bs, H-Ar), 6.83-6.85 (1H, m, H-Ar), 7.06-7.16 (4H, m, H-Ar), 7.25-7.33 (2H, m, H-Ar), 7.85 (1H, s, H-Ar), 8.10 (1H, s, NH),10.30 (1H, s, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm)62.4, 64.9, 108.2, 109.8, 119.0, 119.1, 119.2, 120.0, 120.9, 122.1, 124.4, 129.4, 130.0, 131.3, 133.8, 135.8, 138.7, 142.4, 153.3, 159.8, 176.6, 184.8.Anal. Calcd for $C_{23}H_{11}N_5O_2$: C, 70.95; H, 2.85; N, 17.99%. Found: C, 71.04; H, 2.79; N, 17.89.

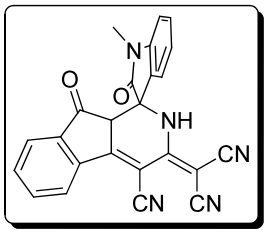


2-(-5'-Bromo-4-cyano-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene)malononitrile (6b). Olive powder (yield 90%); m.p 210 ˚C dec IR (KBr) (v_{max} /cm^{-1}): 3444, 2212, 1735, 1616.468 $[M]^-$, 470 [M+2]. ^{1}H NMR (400 MHz, DMSO-d_6): δ_H (ppm) 6.74 (1H, d, $^3J_{HH}$=8 Hz, H-Ar), 7.12 (1H, d, $^3J_{HH}$=6.8 Hz, H-Ar), 7.23 (1H, d, $^4J_{HH}$=1.6 Hz, H-Ar), 7.30 (1H, t,$^3J_{HH}$=7.6 Hz, H-Ar), 7.35-7.40 (2H, m, H-Ar), 7.90 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 8.15 (1H, s, NH), 10.46 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 62.5, 65.2, 107.2, 111.8, 113.6, 118.9, 119.1, 120.1, 121.0, 127.1, 130.2, 131.3, 132.1, 135.8, 136.0, 138.6, 141.9, 153.6, 159.7, 176.5, 184.2. Anal. Calcd for $C_{23}H_{10}BrN_5O_2$: C, 58.99; H, 2.15; N, 14.96%. Found: C, 58.93; H, 2.19; N, 14.89.



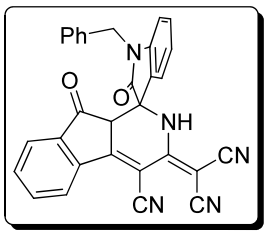
2-(4-Cyano-5'-nitro-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene)malononitrile(6c).Olive powder (yield 85%); m.p. 208 ˚C dec. IR (KBr) (v_{max} /cm^{-1}): 3444, 2202, 1727, 1627. ESI: 434 $[M]^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 6.98 (1H, d, $^3J_{HH}$=8.4 Hz, H-Ar), 7.11 (1H, d,J_{HH}=7.2 Hz, H-Ar), 7.27-7.41 (3H, m, H-Ar), 7.30 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.89-7.92 (2H, m, H-Ar), 8.16-8.18 (2H, m, H-Ar and NH), 11.05 (1H, s, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm) 61.8, 64.4, 106.0, 109.5, 118.4, 119.3, 119.7, 120.6, 126.3, 129.8,

130.9, 134.3, 135.3, 138.2, 142.2, 148.8, 153.3, 159.4, 177.2, 184.1.Anal. Calcd for $C_{23}H_{10}N_6O_4$: C, 63.60; H, 2.32; N, 19.35%. Found: C, 63.46; H, 2.42; N, 19.42.



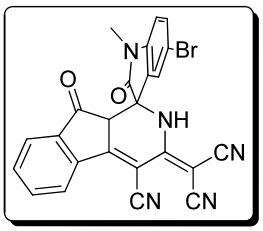
2-(4-Cyano-1'-methyl-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene)malononitrile (6d).Olive powder (yield 88%); m.p. 212 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3449, 2214, 1729, 1617. ESI: 403 [M]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 3.10 (3H, s, CH_3), 6.92-6.99 (2H, m, H-Ar), 7.07 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar), 7.14 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 7.28 (2H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.38 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.89 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 7.99 (1H, s, NH). ^{13}C NMR (100 MHz, DMSO-d_6): δ_C (ppm) 26.3, 61.5, 65.8, 107.6, 108.1, 118.5, 119.5, 120.3, 121.5, 122.3, 129.1, 130.1, 130.8, 132.8, 135.3, 138.3, 143.3, 152.8, 159.2, 174.7, 183.9.Anal. Calcd for $C_{24}H_{13}N_5O_2$: C, 71.46; H, 3.25; N, 17.36%. Found: C, 71.39; H, 3.18; N, 17.30.

X-Ray data for 6d: $C_{24}H_{13}N_5O_2(CH_3CN)$, M= 444.45 g/mol, triclinic system, space group Pī, a = 8.0008(11), b = 11.6372(18), c = 12.3753(18) ?, α=87.946(12)^o,β=72.447(11)^o, γ=85.708(12)^o, V= 1095.4(3) ?^{3}, Z= 2, Dc=1.347 g.cm^{-3}, μ(Mo-Kα)= 0.090 ?, crystal dimension of 0.16 x 0.15 x 0.13 mm. The structure was solved by using SHELXS. The structure refinement and data reduction was carried out with SHELXL of the X-Step32 suite of programs. The non-hydrogen atoms were refined anisotropically by full matrix least-squares on F^2 values to final R_1= 0.0955, wR_2= 0.1727 and S= 1.038 with 319 parameters using 5821 independent reflection (θ range = 1.73 – 29.28^o). Hydrogen atoms were located from expected geometry and were not refined.



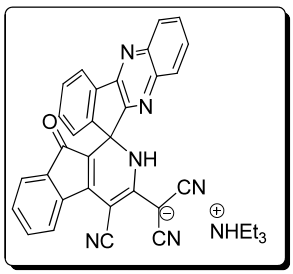
2-(1'-Benzyl-4-cyano-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene)malononitrile (6e).Olive powder (yield 87%); m.p. 227 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3225, 2222, 1741, 1612.ESI: 479 [M]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 4.40, 5.28 (2H, ABq, J_{AB}=16.2 Hz), 6.65 (1H, d, $^3J_{HH}$=7.8 Hz, H-Ar), 6.93 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.15-7.19 (3H, m, H-Ar), 7.24-7.42 (5H, m, H-Ar), 7.60 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar),7.91 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar), 8.14 (1H, s, NH). ^{13}C

NMR (100 MHz, DMSO-d_6): δ_C (ppm) 44.3, 62.2, 65.2, 107.8, 109.3, 119.0, 119.1, 120.2, 121.0, 123.0, 124.2, 127.3, 127.5, 127.7, 128.8, 129.0, 129.5, 130.2, 131.4, 133.3, 135.8, 136.5, 138.9, 143.1, 153.6, 159.7, 175.6, 185.0.Anal. Calcd for $C_{30}H_{17}N_5O_2$: C, 75.23; H, 3.53; N, 14.69%. Found: C, 75.15; H, 3.57; N, 14.61.

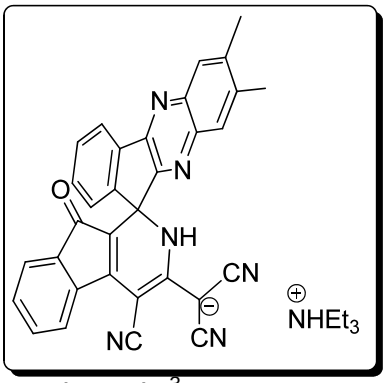


2-(-5'-Bromo-4-cyano-1'-methyl-2',9-dioxo-9,9a-dihydrospiro[indeno[2,1-*c*]pyridine-1,3'-indolin]-3(2*H*)-ylidene) malononitrile(6f).Olive powder (yield 92%); m.p. 207 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3308, 2213, 1739, 1625.ESI: 481 [M]$^-$, 483 [M+2]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm)3.09 (3H,s,CH_3), 6.94 (1H, d, $^3J_{HH}$=8.4 Hz, H-Ar), 7.08 (1H, d, $^3J_{HH}$=6.6 Hz, H-Ar), 7.28-7.32 (2H, m, H-Ar), 7.36-7.48 (3H, m, H-Ar), 7.90 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 8.00 (1H, s, NH). ^{13}C NMR (75 MHz, DMSO-d_6): δ_C (ppm) 26.4, 61.6, 64.0, 106.6, 110.2, 113.9, 118.4, 119.6, 120.5, 126.2, 129.7, 130.1, 130.9, 131.4, 135.0, 135.3, 138.3, 142.9, 159.3, 174.5, 184.0. Anal. Calcd for $C_{24}H_{12}BrN_5O_2$: C, 59.77; H, 2.51; N, 14.52%. Found: C, 59.67; H, 2.44; N, 14.61.

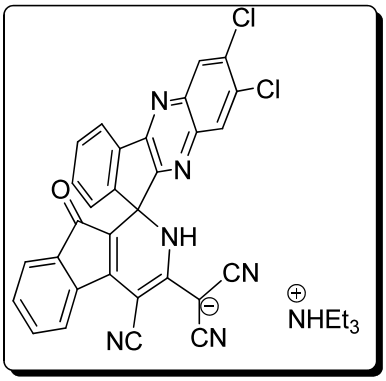
Due to very low solubility of the products **10a-f**, we cannot report the ^{13}C NMR data for these products.



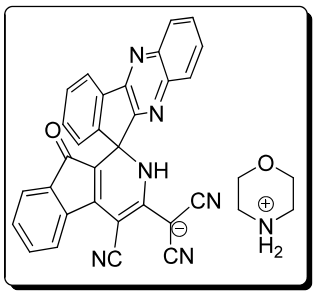
Triethylammonium dicyano(4'-cyano-9'-oxo-2',9'-dihydrospiro[indeno[1,2-*b*]quinoxaline-11,1'-indeno[2,1-*c*]pyridin]-3'-yl)methanide(10 a).Purple powder (yield 81%); m.p. 201 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3397, 2198, 1675.ESI: 473 [M- $C_6H_{16}N^+$]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 1.16 (9H, t, $^3J_{HH}$ = 7.2 Hz, 3CH_3), 3.07-3.09 (6H, q, $^3J_{HH}$ = 7.2 Hz, 3CH_2), 6.94 (1H, t, $^3J_{HH}$ = 7.2 Hz, H-Ar), 7.25 (1H, t, $^3J_{HH}$ = 7.5 Hz, H-Ar), 7.39 (1H, t, $^3J_{HH}$ = 7.5 Hz, H-Ar), 7.60 (3H, m, H-Ar), 7.75 (1H, t, $^3J_{HH}$ = 7.5 Hz, H-Ar), 7.88-7.94 (3H, m, H-Ar), 8.03-8.12 (3H, s, H-Ar and NH), 8.54 (1H, s, NH). Anal. Calcd for $C_{36}H_{29}N_7O$: C, 75.11; H, 5.08; N, 17.03%. Found: C, 75.18; H, 5.04; N, 16.94.



Triethylammonium dicyano(4'-cyano-7,8-dimethyl-9'-oxo-2',9'-dihydrospiro[indeno[1,2-*b*]quinoxaline-11,1'-indeno [2,1-*c*]pyridin]-3'-yl)methanide(10b).Purple powder (yield 79%); m.p. 214 ˚C dec.IR (KBr) (v_{max} /cm^{-1}): 3443, 22196, 1630. ESI: 501 [M- $C_6H_{16}N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 1.16 (9H, t, $^3J_{HH}$=7.2 Hz,3CH_3), 2.43 (3H, bs, CH_3), 3.08 (6H, q, $^3J_{HH}$=7.2 Hz,3CH_2), 6.93(1H, d, $^3J_{HH}$=6.6 Hz,H-Ar), 7.24 (1H, d, $^3J_{HH}$=7.5 Hz,H-Ar), 7.38 (1H, d, $^3J_{HH}$=7.5 Hz,H-Ar), 7.54 (3H, bs, H-Ar), 7.81 (1H, m, H-Ar), 7.91-7.95 (2H, m, H-Ar), 7.98-8.00 (1H, m, H-Ar), 8.12 (1H, s, NH), 8.91 (1H, bs, NH). Anal. Calcd for $C_{38}H_{33}N_7O$: C, 75.60; H, 5.51; N, 16.24%. Found: C, 75.70; H, 5.42; N, 16.39.

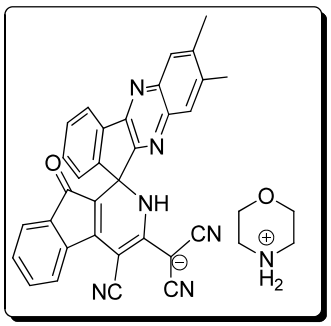


Triethylammonium dicyano(7,8-dichloro-4'-cyano-9'-oxo-2',9'-dihydrospiro[indeno[1,2-*b*]quinoxaline-11,1'-indeno[2,1-*c*]pyridin]-3'-yl)methanide (10c).Purple powder (yield 89%); m.p. 234 ˚C dec. IR (KBr) (v_{max} /cm^{-1}): 3436, 2197, 1653.ESI: 541 [M- $C_6H_{16}N^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 1.15 (9H, bs, 3CH_3), 3.07 (6H, bs, 3CH_2), 6.94 (1H, bs, H-Ar), 7.24 (1H, bs, H-Ar), 7.37 (1H, bs, H-Ar), 7.59(3H, bs, H-Ar), 7.93 (1H, m, H-Ar), 8.03-8.11 (2H, m, H-Ar and NH), 8.44 (2H, bs, H-Ar), 8.81-8.90 (1H, bs, NH).Anal. Calcd for $C_{36}H_{27}Cl_2N_7O$: C, 67.08; H, 4.22; N, 15.21%. Found: C, 66.96; H, 4.13; N, 15.10.

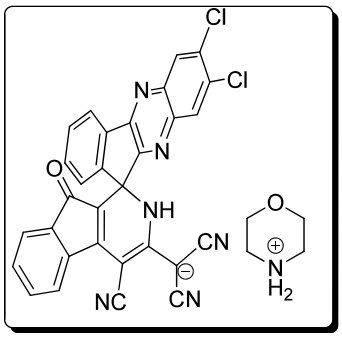


Morpholin-4-ium dicyano(4'-cyano-9'-oxo-2',9'-dihydrospiro [indeno[1,2-b]quinoxaline-11,1'-indeno[2,1-c]pyridin]-3'-yl)methanide(10d). Purple powder (yield 85%); m.p. 254 ˚C dec. IR (KBr) (v_{max} /cm^{-1}): 3436, 2193, 1642. ESI: 473 [M- $C_4H_{10}NO^+$]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 3.09 (4H, bs, 2CH_2), 3.74 (4H, bs, 2CH_2), 6.92 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar),7.23 (1H,

t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.38 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.56 (3H, bs, H-Ar),7.73-7.80 (3H, bs, H-Ar)8.12 (s, 3H), 7.93 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar), 8.03 (1H, bs, H-Ar), 8.12 (1H, s, NH), 8.67(2H, bs, NH_2). Anal. Calcd for $C_{34}H_{23}N_7O_2$: C, 72.72; H, 4.13; N, 17.46%. Found: C, 72.79; H, 4.18; N, 17.39.



Morpholin-4-ium dicyano(4'-cyano-7,8-dimethyl-9'-oxo-2',9'-dihydrospiro[indeno[1,2-*b*]quinoxaline-11,1'-indeno[2,1-*c*]pyridin]-3'-yl)methanide(10e).Purple powder (yield 83%); m.p. 268 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3456, 2201, 2174, 1651. ESI: 501 [M-$C_4H_{10}NO^+$]$^-$. ^{1}H NMR (300 MHz, DMSO-d_6): 2.42 (3H, s, CH_3), 3.09 (4H, bs, $2CH_2$), 3.74 (4H, bs, $2CH_2$), 6.92 (1H, d, $^3J_{HH}$=6.3 Hz, H-Ar), 7.26 (1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.37(1H, t, $^3J_{HH}$=6.9 Hz, H-Ar), 7.52(3H, m, H-Ar), 7.81 (1H, bs, H-Ar), 7.91-7.98 (3H, m, H-Ar), 8.12 (1H, s, NH), 8.63(2H, bs, NH_2). ^{1}H NMR (400 MHz, MeOH-d_4): 2.48 (3H, s, CH_3), 2.53 (3H, s, CH_3), 3.20 (4H, t, $^3J_{HH}$ = 4.8 Hz, $2CH_2$), 3.85 (4H, t, $^3J_{HH}$ = 4.8 Hz, $2CH_2$), 7.02 (1H, d, $^3J_{HH}$=6.8 Hz, H-Ar), 7.21(1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.32 (1H, t, $^3J_{HH}$=7.2 Hz, H-Ar), 7.53-7.64 (3H, m, H-Ar), 7.82 (1H, s, H-Ar), 7.88 (1H, s, H-Ar), 8.01 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 8.12 (1H, t, $^3J_{HH}$=6.8 Hz, H-Ar).Anal. Calcd for $C_{36}H_{27}N_7O_2$: C, 73.33; H, 4.62; N, 16.63%. Found: C, 73.22; H, 4.70; N, 16.55.



Morpholin-4-ium dicyano(7,8-dichloro-4'-cyano-9'-oxo-2',9'-dihydrospiro[indeno[1,2-*b*]quinoxaline-11,1'-indeno[2,1-*c*]pyridin]-3'-yl)methanide(10f).Purple powder (yield 91%); m.p. 243 ˚C dec. IR (KBr) (ν_{max} /cm^{-1}): 3397, 2198, 1655. ESI: 541 [M- $C_4H_{10}NO^+$]$^-$.^{1}H NMR (300 MHz, DMSO-d_6): δ_H (ppm) 3.09 (4H, t, $^3J_{HH}$ = 4.5 Hz, $2CH_2$), 3.74 (4H, t, $^3J_{HH}$ = 4.5 Hz, $2CH_2$), 6.94 (1H, d, $^3J_{HH}$=6.9 Hz, H-Ar), 7.25 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar), 7.38 (1H, t, $^3J_{HH}$=7.5 Hz, H-Ar),7.59 (3H, bs, H-Ar), 7.93 (1H, d, $^3J_{HH}$=7.2 Hz, H-Ar), 8.03-8.05 (1H,m, H-Ar), 8.12 (1H,s, NH), 8.45 (2H, s, H-Ar).Anal. Calcd for $C_{34}H_{21}Cl_2N_7O_2$: C, 64.77; H, 3.36; N, 15.55%. Found: C, 64.65; H, 3.30; N, 15.63.

References:

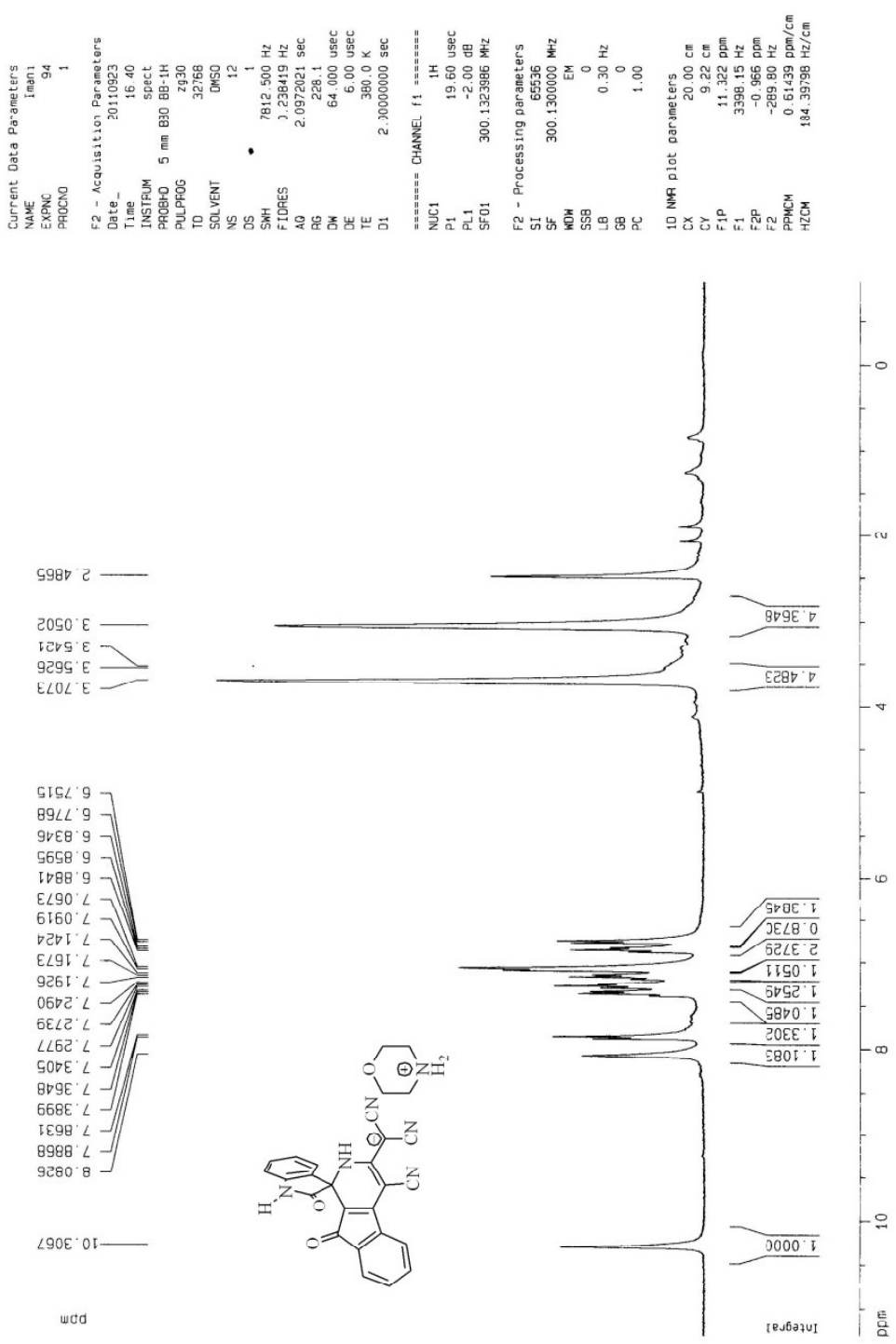
1 K. A. Bello, L. Cheng and J. Griffiths, *J.Chem. Soc. Perkin Trans. 2.,* 1987, 815.

2 D. V. Demchuk, M. N. Elinson and G. I. Nikishin, *Mendeleev Commun.*, 2011, **21**, 224

3 M.T. Maghsoodlou, S.M. Habibi-Khorassani, A. Moradi, N. Hazeri, A. Davodi and S.S. Sajadikhah, *Tetrahedron,* 2011, **67,** 8492.

4 Stoe&Cie, X-AREA, Version 1.30, Program for the acquisition andanalysis of data, Stoe&Cie GmbH, Darmstadt, Germany, 2005.

5 Stoe&Cie, X-STEP32, Version 1.07b, Crystallographic package,Stoe&Cie GmbH, Darmstadt, Germany, 2000.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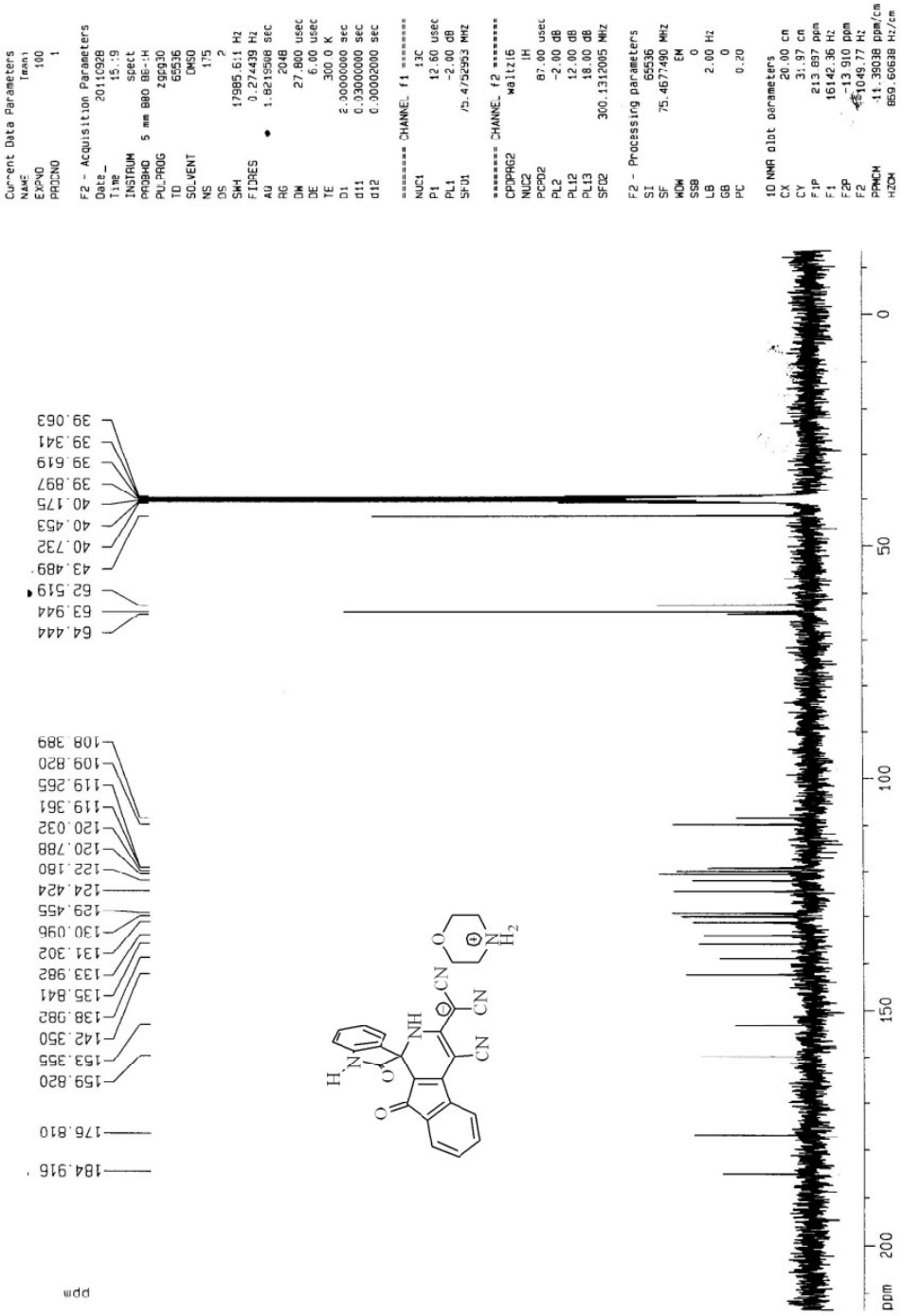
NAME iman1
EXPNO 94
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110923
Time 16.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 12
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.22 cm
F1P 11.322 ppm
F1 3398.15 Hz
F2P -0.966 ppm
F2 -289.80 Hz
PPMCM 0.61439 ppm/cm
HZCM 184.39798 Hz/cm
2.4865
3.0502
3.5421
3.5626
3.7073
6.7515
6.7768
6.8346
6.8595
6.8841
7.0673
7.0919
7.1424
7.1673
7.1926
7.2490
7.2739
7.2977
7.3405
7.3648
7.3899
7.8631
7.8868
8.0826
10.3067
4.3648
4.4823
1.3845
0.8736
2.3729
1.0511
1.2549
1.0485
1.3302
1.1083
1.0000
Integral
ppm


Current Data Parameters
NAME Imani
EXPNO 100
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110928
Time 15.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 175
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.60 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.20
1D NMR plot parameters
CX 20.00 cm
CY 31.97 cm
F1P 213.897 ppm
F1 16142.36 Hz
F2P -13.910 ppm
F2 -1049.77 Hz
PPMCM 11.39038 ppm/cm
HZCM 859.60638 Hz/cm
64.444
63.944
62.519
43.489
40.732
40.453
40.175
39.897
39.619
39.341
39.063
184.916
176.810
159.820
153.355
142.350
138.082
135.841
133.982
131.302
130.096
129.455
124.424
122.180
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119.265
109.820
108.389
ppm
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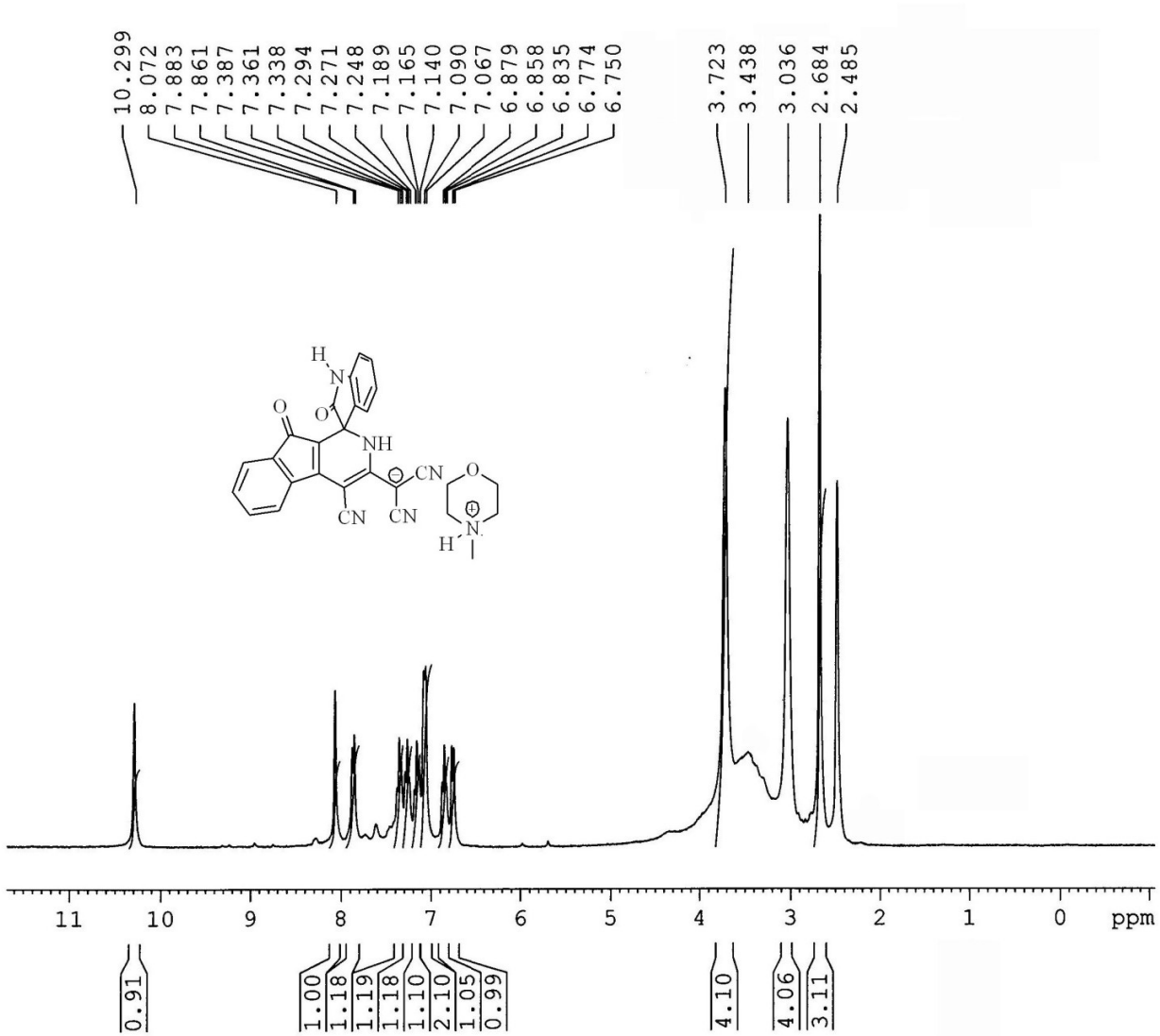
50
100
150
200
ppm

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Current Data Parameters
NAME                  Imani
EXPNO                   108
PROCNO                    1

F2 - Acquisition Parameters
Date_              20111102
Time                  13.55
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                        12
DS                         1
SWH                7812.500 Hz
FIDRES            0.238419 Hz
AQ                2.0972021 sec
RG                    228.1
DW                   64.000 usec
DE                    6.00 usec
TE                   380.0 K
D1                2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    19.60 usec
PL1                   -2.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF             300.1300000 MHz
WDW                       EM
SSB                        0
LB                     0.30 Hz
GB                         0
PC                      1.00
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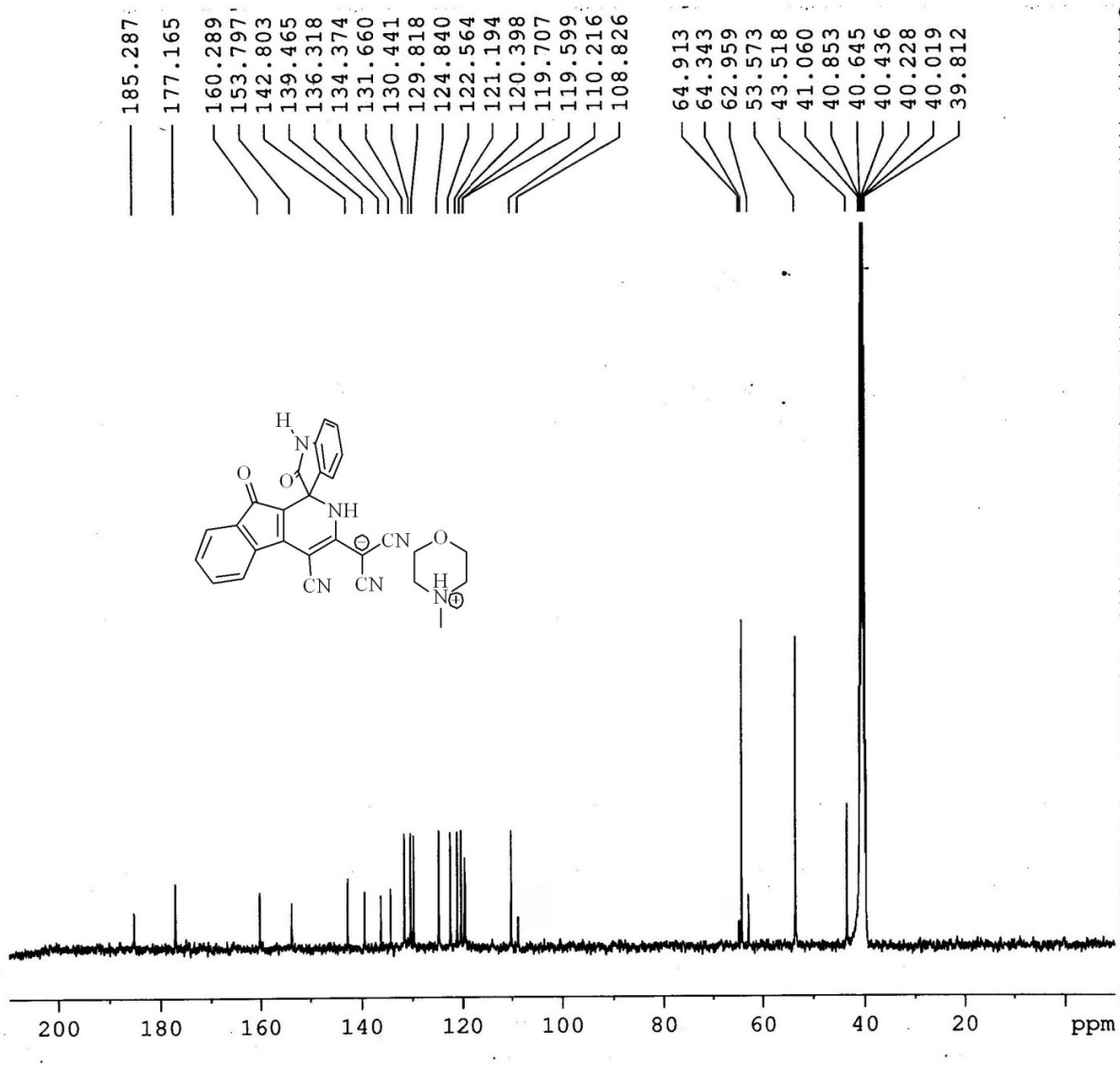


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Current Data Parameters
NAME                  gh-2
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130203
Time                 13.37
INSTRUM              spect
PROBHD    5 mm BBO BB-1H
PULPROG               zgdc
TD                   32768
SOLVENT               DMSO
NS                    1076
DS                       0
SWH           22075.055 Hz
FIDRES         0.673677 Hz
AQ             0.7422452 sec
RG                    2048
DW               22.650 usec
DE                6.00 usec
TE                297.2 K
D1           5.00000000 sec
d11          0.03000000 sec
MCREST       0.00000000 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                 13C
P1                6.30 usec
PL1               -2.00 dB
SFO1        100.6227903 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2               18.00 dB
PL12              18.00 dB
SFO2        400.1324008 MHz

F2 - Processing parameters
SI                 131072
SF          100.6127290 MHz
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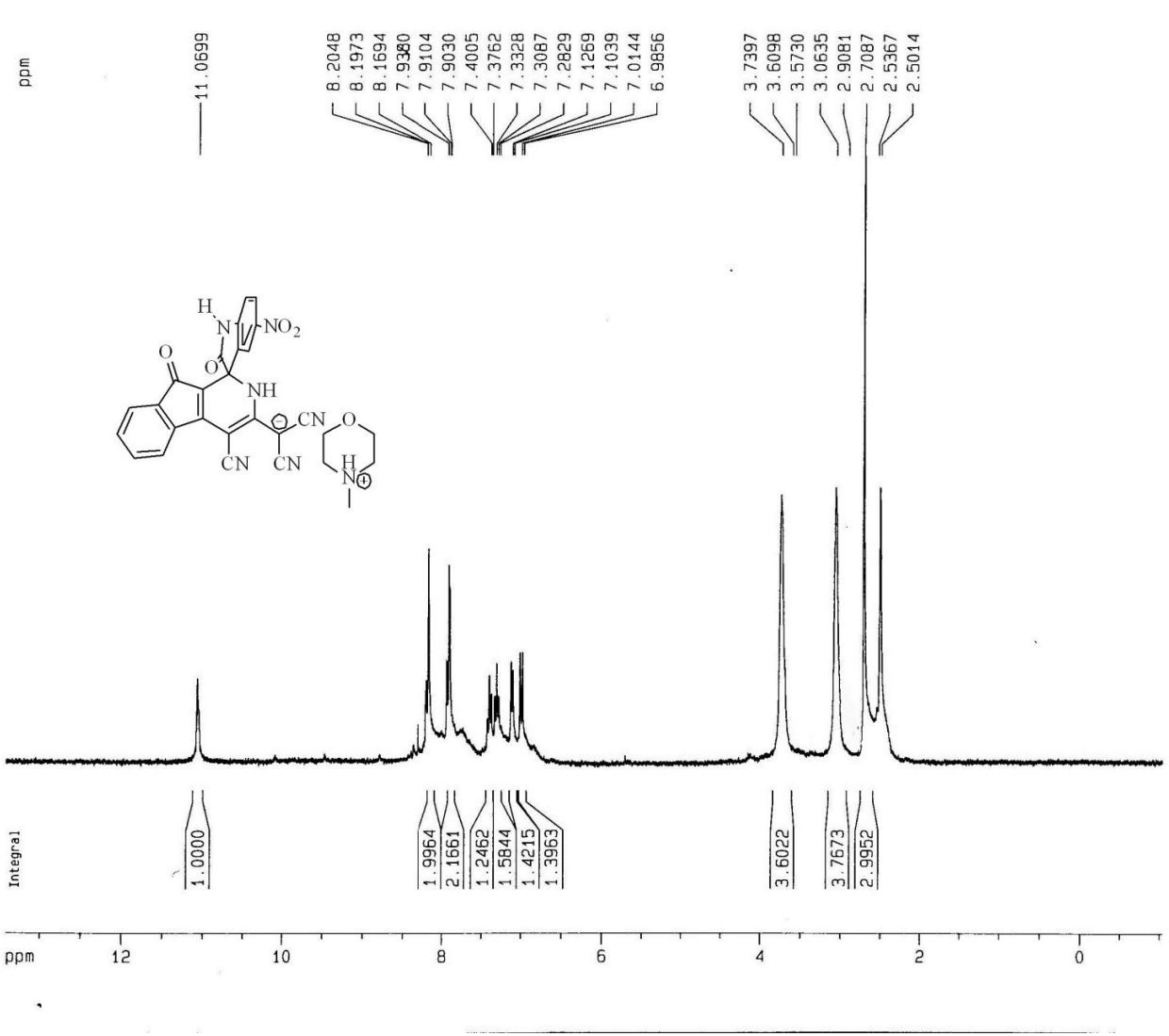
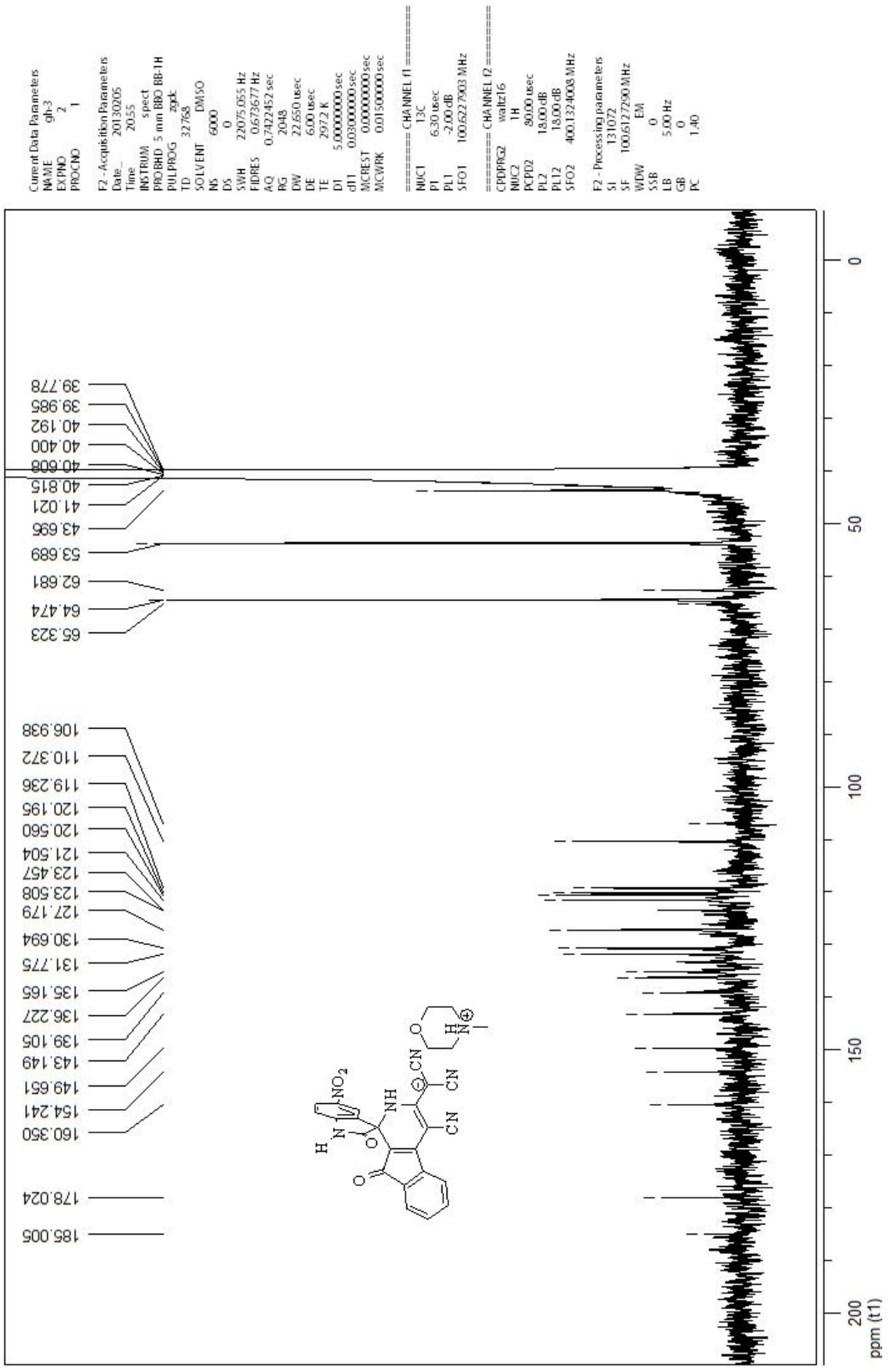
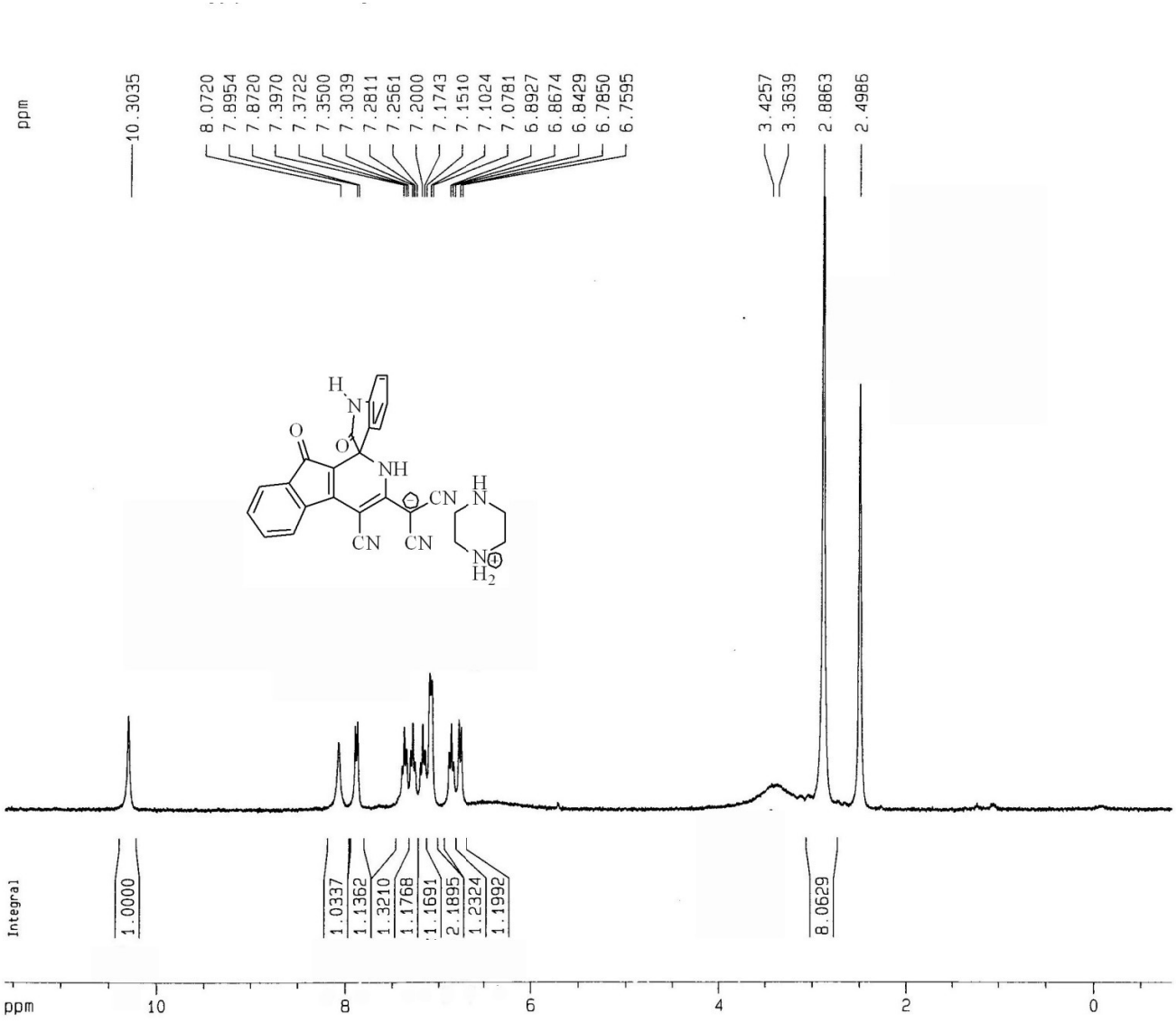



```
Current Data Parameters
NAME                  Imani
EXPNO                   123
PROCNO                    1

F2 - Acquisition Parameters
Date_              20111119
Time                  15.47
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       14
DS                        1
SWH               7812.500 Hz
FIDRES            0.238419 Hz
AQ                2.0972021 sec
RG                    228.1
DW                 64.000 usec
DE                  6.00 usec
TE                  380.0 K
D1               2.00000000 sec

======== CHANNEL f1 ========
NUC1                    1H
P1                  19.60 usec
PL1                 -2.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                    65536
SF             300.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00

1D NMR plot parameters
CX                    20.00 cm
CY                    10.91 cm
F1P                  13.428 ppm
F1                  4030.05 Hz
F2P                  -1.042 ppm
F2                  -312.78 Hz
PPMCM              0.72349 ppm/cm
HZCM             217.14156 Hz/cm
```


Current Data Parameters
NAME gh-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130205
Time 20.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpk
TD 32768
SOLVENT DMSO
NS 6000
DS 0
SWH 22075.055 Hz
FIDRES 0.673677 Hz
AQ 0.7422452 sec
RG 2048
DW 22.650 usec
DE 6.00 usec
TE 297.2 K
D1 5.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 usec
PL1 -2.00 dB
SFO1 100.6227003 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 18.00 dB
PL12 18.00 dB
SFO2 400.1324008 MHz
F2 - Processing parameters
SI 131072
SF 100.6127290 MHz
WDW EM
SSB 0
LB 5.00 Hz
GB 0
PC 1.40
39.778
39.985
40.192
40.400
40.608
40.815
41.021
43.695
53.689
62.681
64.474
65.323
106.938
110.372
119.236
120.195
120.560
121.504
123.457
123.508
127.179
130.694
131.775
135.165
136.227
139.105
143.149
149.651
154.241
160.350
178.024
185.005
200
150
100
50
0
ppm (t1)



Current Data Parameters

NAME	Imani
EXPNO	125
PROCNO	1

F2 - Acquisition Parameters

Date_	20111121
Time	15.45
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 sec
RG	228.1
DW	64.000 usec
DE	6.00 usec
TE	380.0 K
D1	2.00000000 sec

======== CHANNEL f1 ========

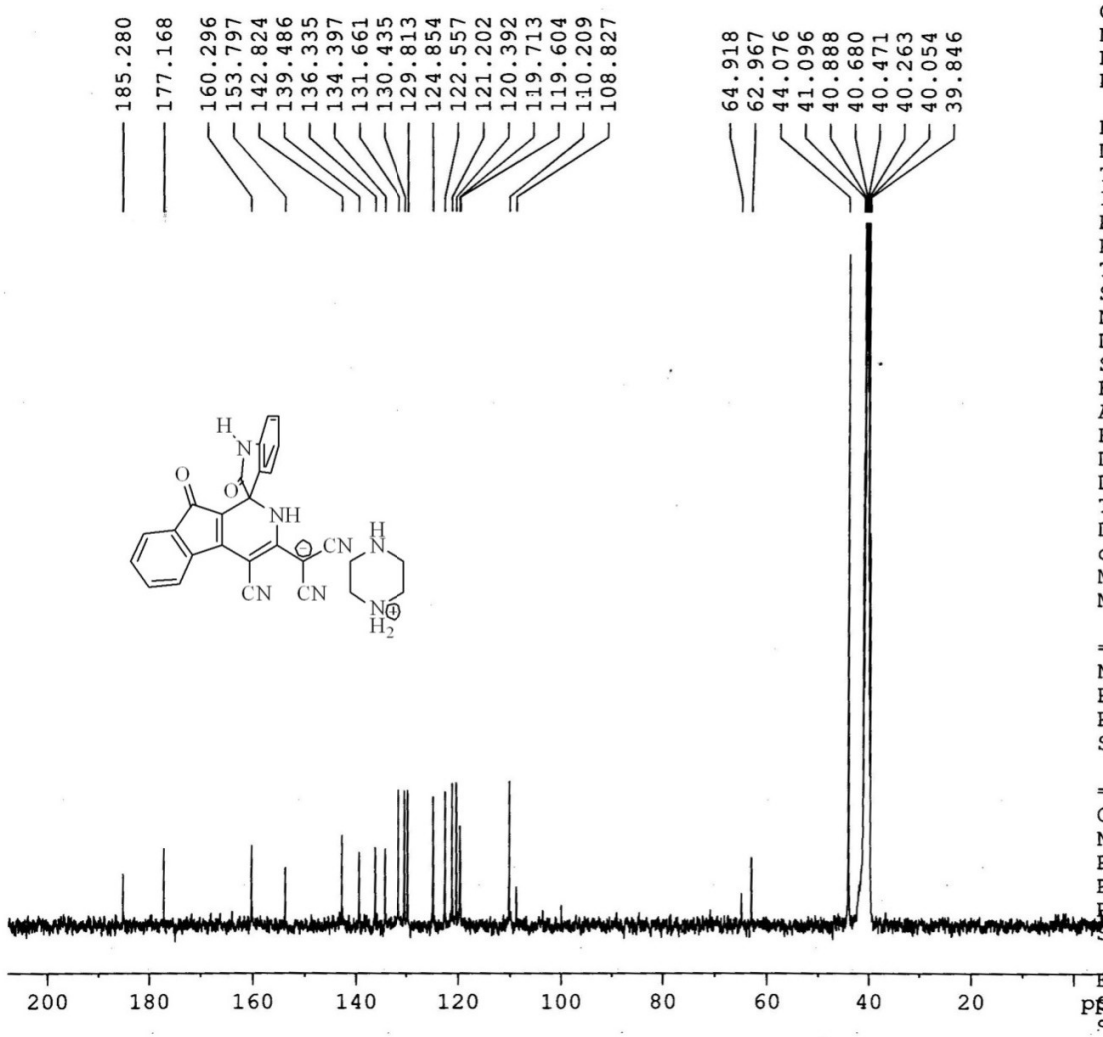
NUC1	1H
P1	19.60 usec
PL1	-2.00 dB
SFO1	300.1323986 MHz

F2 - Processing parameters

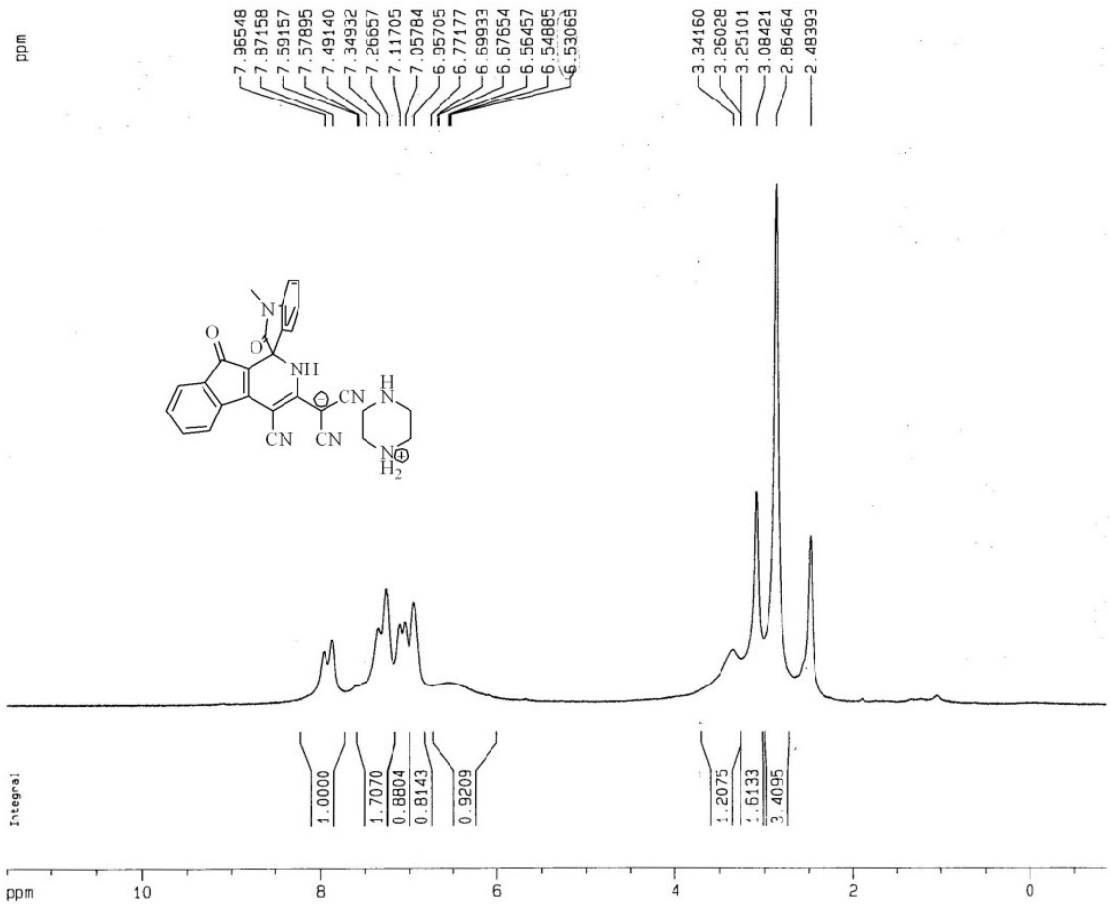
SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

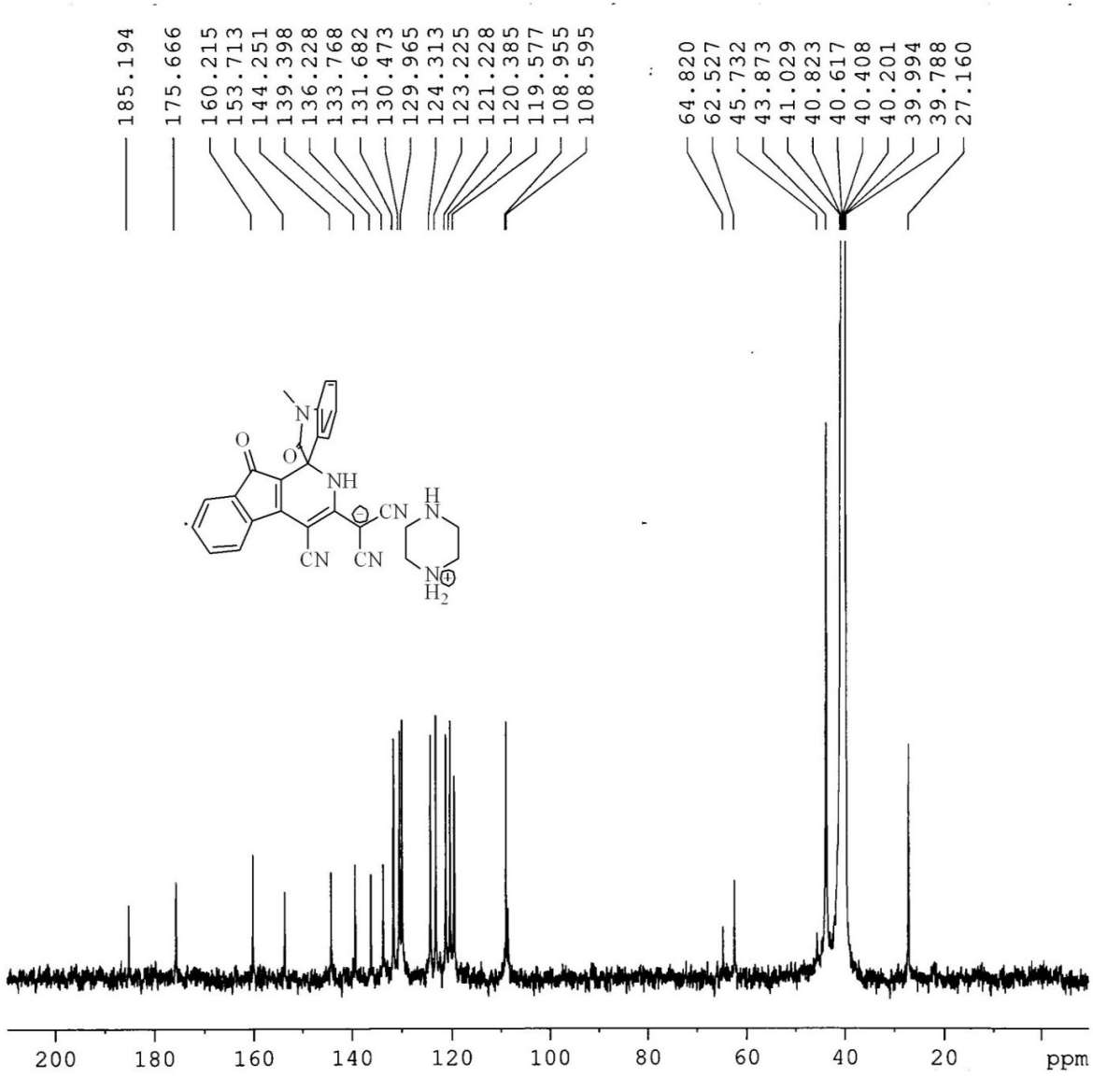
CX	20.00 cm
CY	19.92 cm
F1P	11.594 ppm
F1	3479.81 Hz
F2P	-0.840 ppm
F2	-252.06 Hz
PPMCM	0.62171 ppm/cm
HZCM	186.59322 Hz/cm



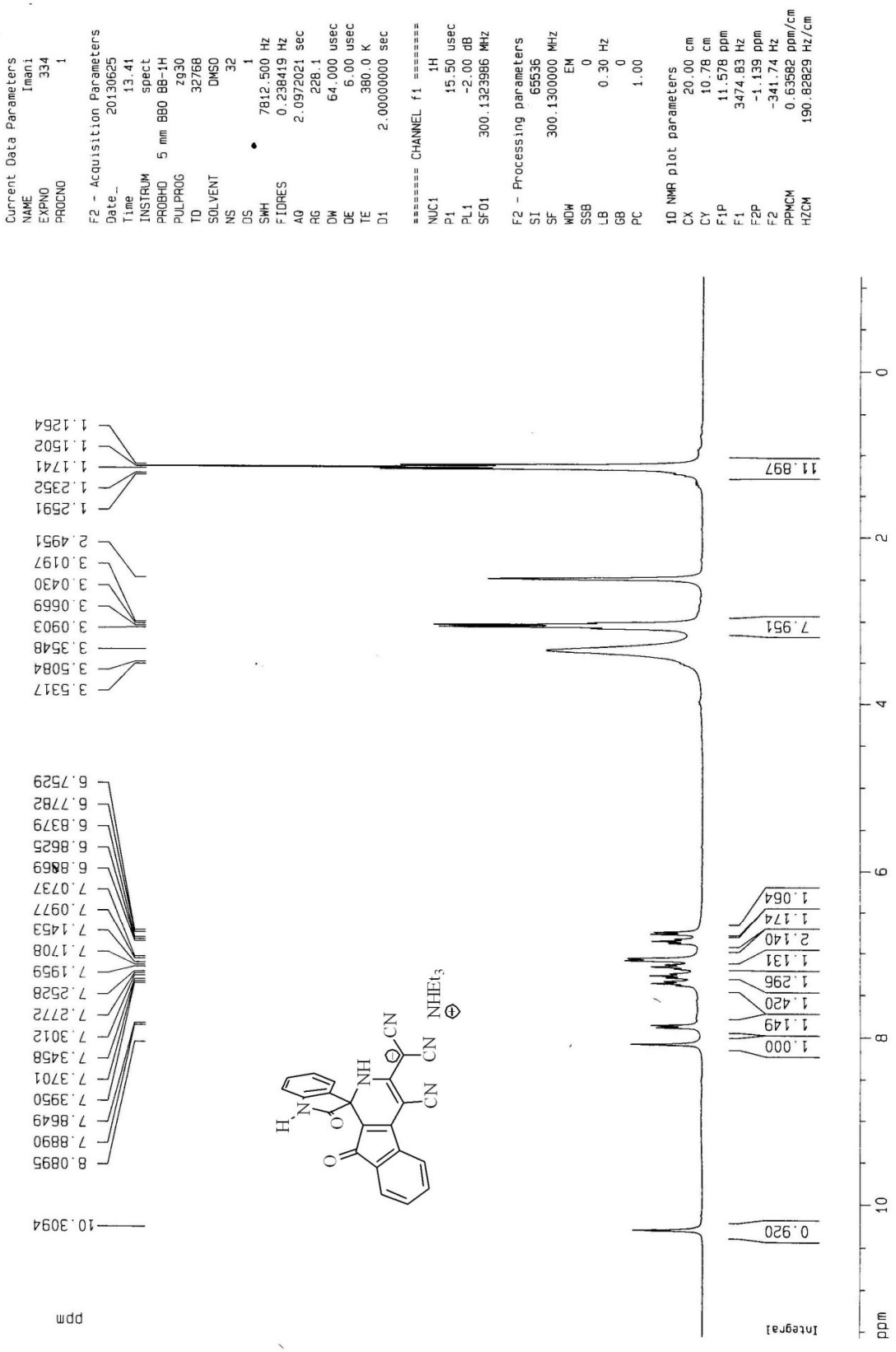

```
Current Data Parameters
NAME                  gh-22
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130421
Time                  19.12
INSTRUM               spect
PROBHD    5 mm BBO BB-1H
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                     1200
DS                        0
SWH              22075.055 Hz
FIDRES            0.673677 Hz
AQ                0.7422452 sec
RG                     2048
DW                  22.650 usec
DE                   6.00 usec
TE                  298.2 K
D1                5.00000000 sec
d11               0.03000000 sec
MCREST            0.00000000 sec
MCWRK             0.01500000 sec

======== CHANNEL f1 ========
NUC1                    13C
P1                   6.30 usec
PL1                 -2.00 dB
SFO1          100.6227903 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                    1H
PCPD2               80.00 usec
PL2                 18.00 dB
PL12                18.00 dB
SFO2          400.1324008 MHz

F2 - Processing parameters
SI                    131072
SF                100.6127290 MHz
```




```
Current Data Parameters
NAME                  Imani
EXPNO                   165
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120306
Time                  16.23
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       32
DS                        1
SWH                7812.500 Hz
FIDRES             0.238419 Hz
AQ                 2.0972021 sec
RG                      35.9
DW                 64.000 usec
DE                  6.00 usec
TE                  380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                 15.50 usec
PL1                 -2.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF             300.1300000 MHz
WDW                       EM
SSB                        0
LB                  0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   9.45 cm
F1P                 11.511 ppm
F1                3454.66 Hz
F2P                 -0.861 ppm
F2                 -258.54 Hz
PPMCM             0.61860 ppm/cm
HZCM            185.66043 Hz/cm
```




```
Current Data Parameters
NAME                  gh-6
EXPNO                    1
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130205
Time                 19.20
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG               zgdc
TD                   32768
SOLVENT               DMSO
NS                     872
DS                       0
SWH             22075.055 Hz
FIDRES           0.673677 Hz
AQ               0.7422452 sec
RG                    2048
DW                  22.650 usec
DE                   6.00 usec
TE                  297.2 K
D1              5.00000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                   6.30 usec
PL1                 -2.00 dB
SFO1         100.6227903 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 18.00 dB
PL12                18.00 dB
SFO2         400.1324008 MHz

F2 - Processing parameters
SI                   131072
```


Current Data Parameters
NAME Imani
EXPNO 334
PROCNO 1
F2 - Acquisition Parameters
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Time 13.41
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.78 cm
F1P 11.578 ppm
F1 3474.83 Hz
F2P -1.139 ppm
F2 -341.74 Hz
PPMCM 0.63582 ppm/cm
HZCM 190.82829 Hz/cm
1.1264
1.1502
1.1741
1.2352
1.2591
2.4951
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3.0430
3.0669
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3.3548
3.5084
3.5317
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6.8379
6.8625
6.8869
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7.1453
7.1708
7.1959
7.2528
7.2772
7.3012
7.3458
7.3701
7.3950
7.8649
7.8890
8.0895
10.3094
11.897
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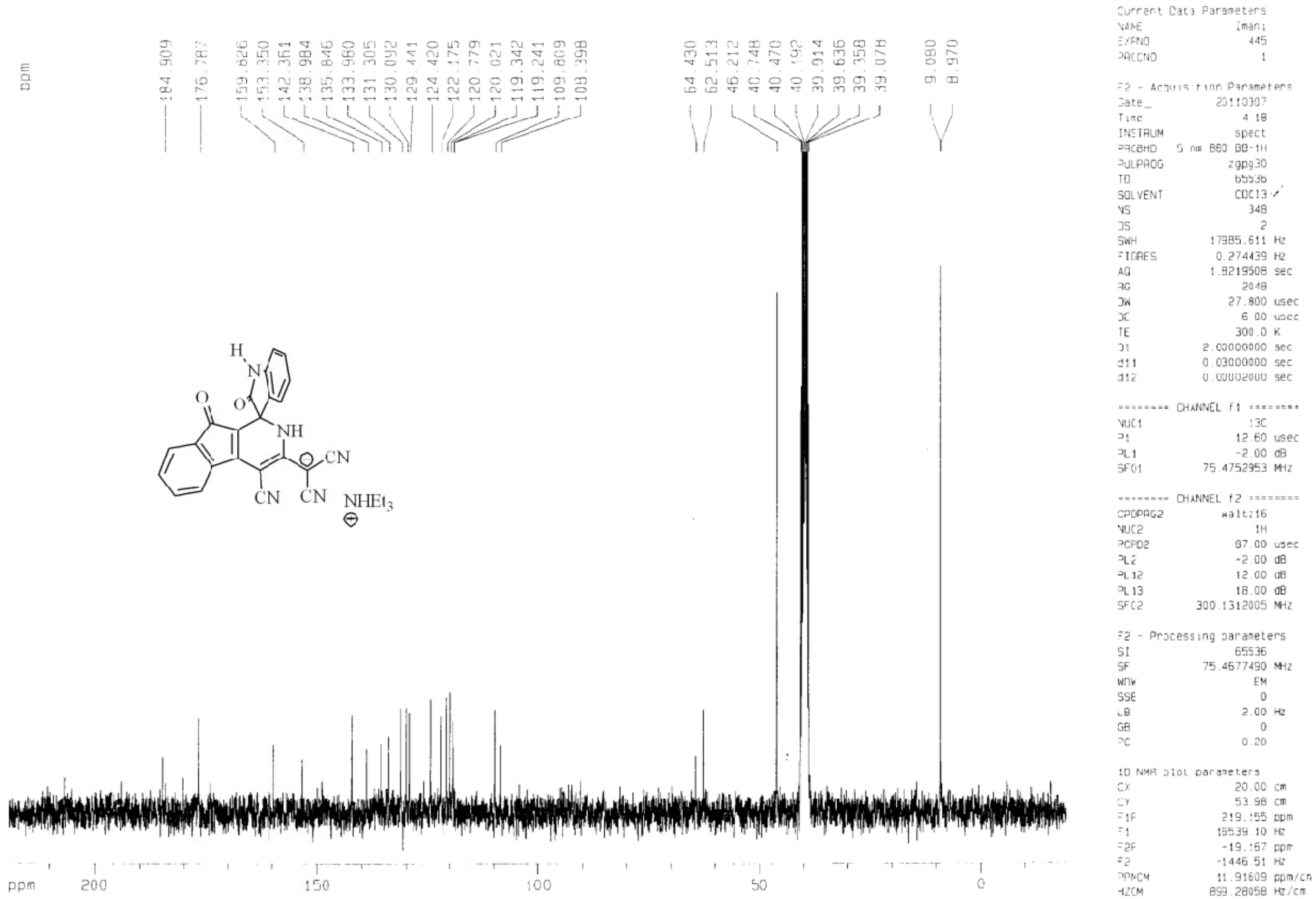
NHEt3
ppm
Integral



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159.826
153.350
142.361
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133.960
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122.175
120.779
120.021
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40.470
40.192
39.914
39.636
39.358
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9.080
8.970
ppm
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CN
CN
CN
NHEt3
ppm 200 150 100 50 0
Current Data Parameters
NAME Imani
EXPNO 445
PROCNO 1
F2 - Acquisition Parameters
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Time 4.18
INSTRUM spect
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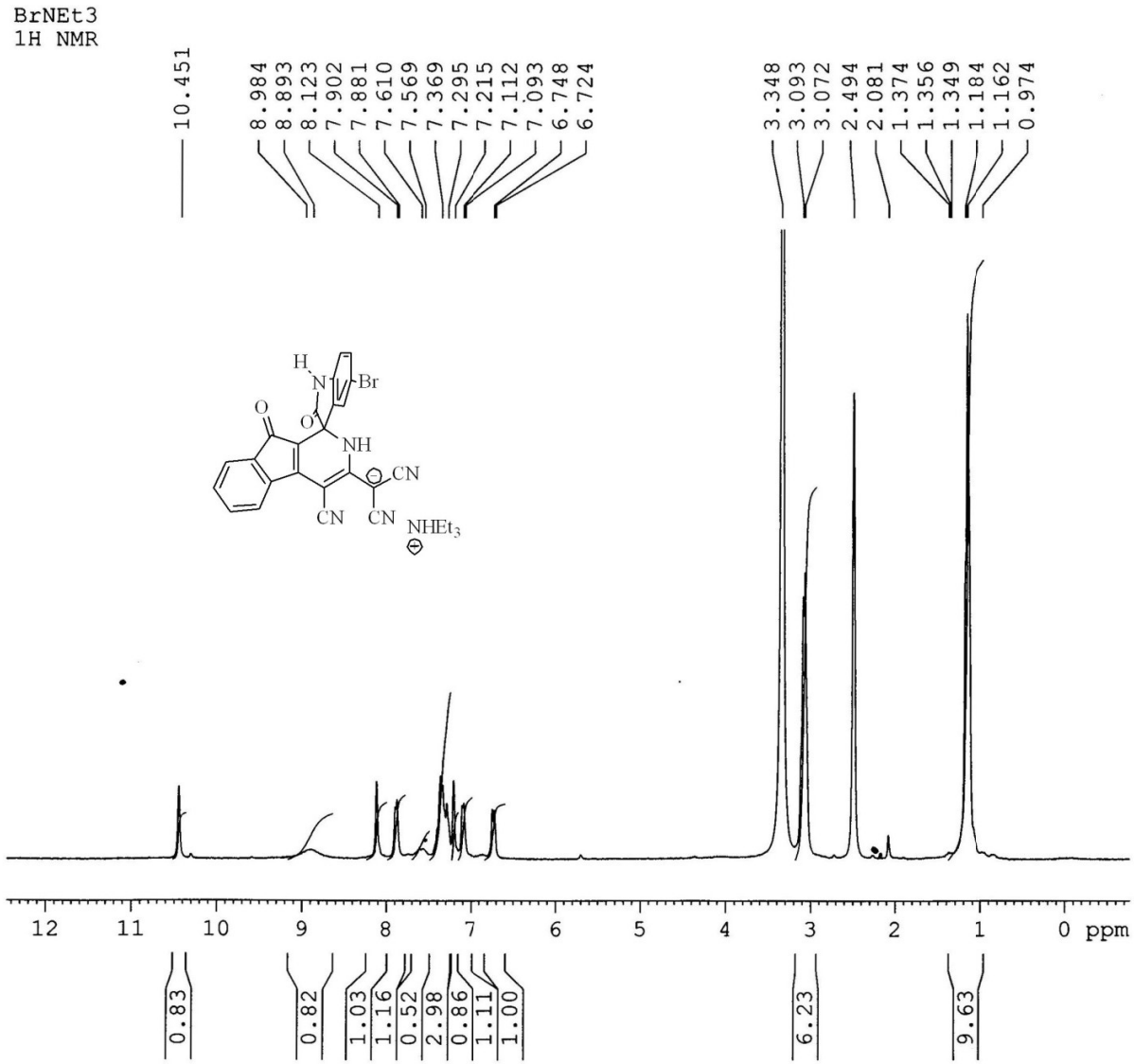
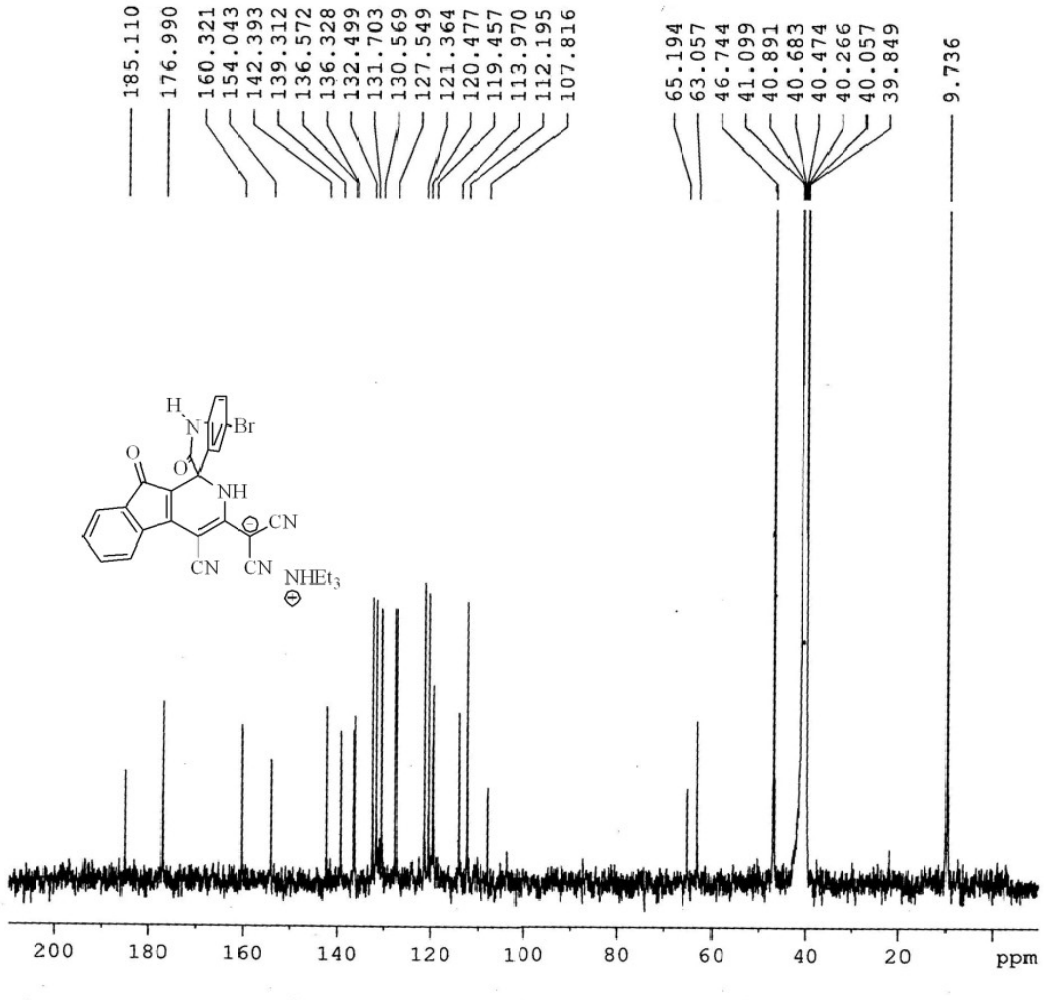
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 348
DS 2
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2048
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
d12 0.00002000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 12.60 usec
PL1 -2.00 dB
SFO1 75.4752953 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 87.00 usec
PL2 -2.00 dB
PL12 12.00 dB
PL13 18.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 65536
SF 75.4677490 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 0.20
1D NMR plot parameters
CX 20.00 cm
CY 53.98 cm
F1P 219.155 ppm
F1 16539.10 Hz
F2P -19.167 ppm
F2 -1446.51 Hz
PPMCM 11.91609 ppm/cm
HZCM 899.28058 Hz/cm

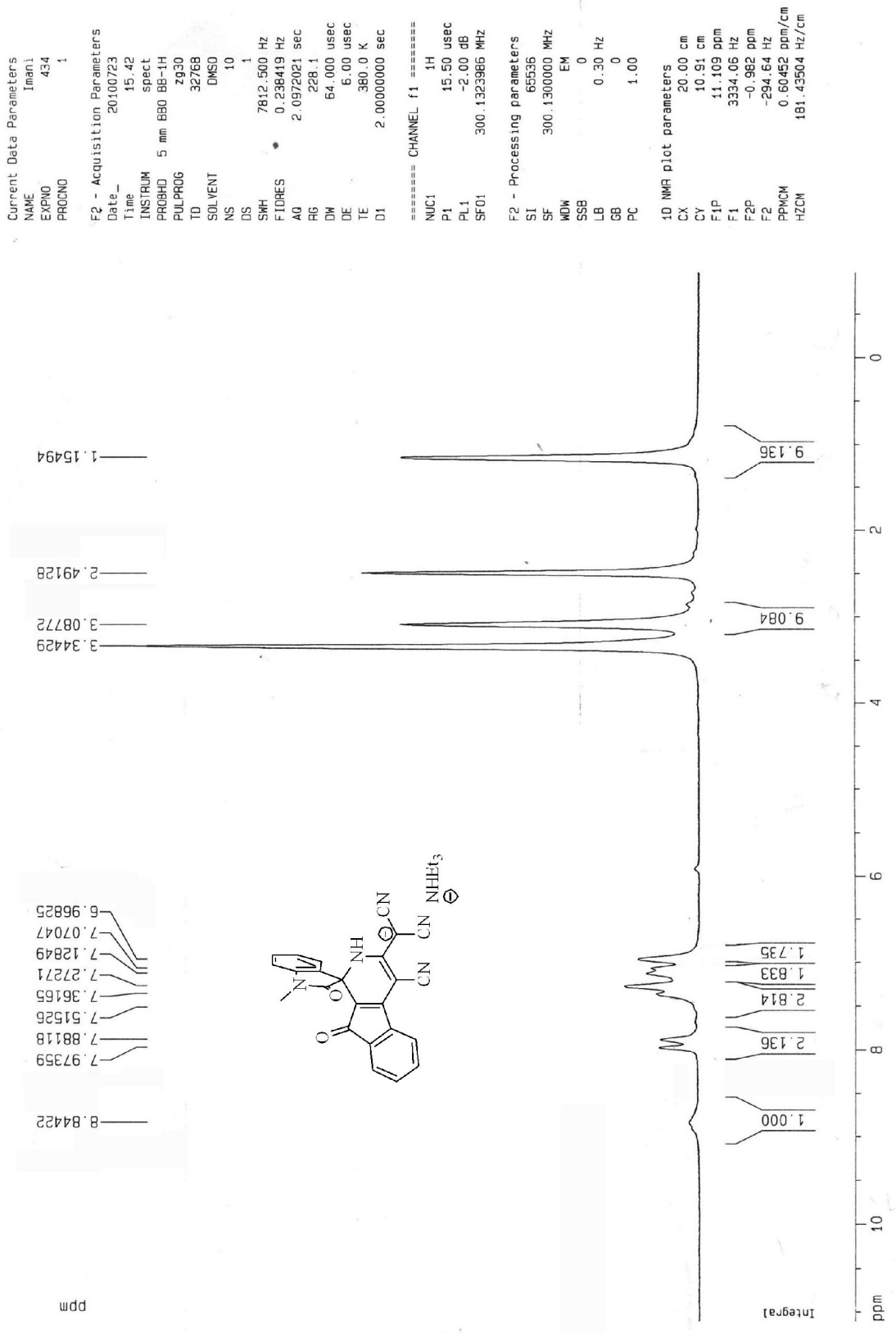
BrNEt3
1H NMR

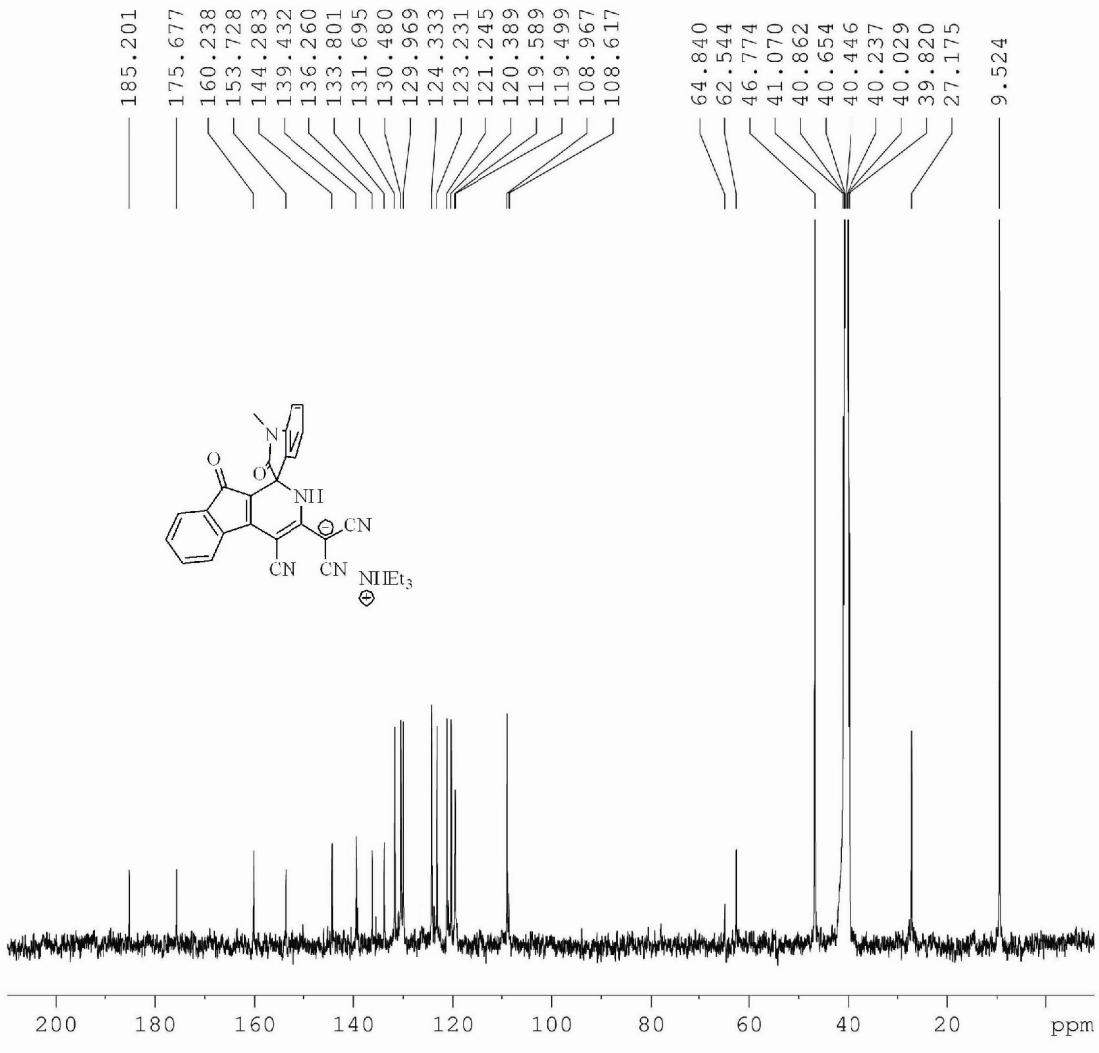



```
Current Data Parameters
NAME                  Imani
EXPNO                   336
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130701
Time                  14.16
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       32
DS                        1
SWH               7812.500 Hz
FIDRES            0.238419 Hz
AQ                2.0972021 sec
RG                    228.1
DW                 64.000 usec
DE                  6.00 usec
TE                  380.0 K
D1                2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                 15.50 usec
PL1                 -2.00 dB
SFO1          300.1323986 MHz

F2 - Processing parameters
SI                    65536
SF            300.1300000 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```




```
Current Data Parameters
NAME                  gh-19
EXPNO                     1
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130421
Time                  10.46
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zgdc
TD                    32768
SOLVENT                DMSO
NS                     1200
DS                        0
SWH              22075.055 Hz
FIDRES            0.673677 Hz
AQ                0.7422452 sec
RG                     2048
DW                  22.650 usec
DE                   6.00 usec
TE                   296.2 K
D1              5.00000000 sec
d11             0.03000000 sec
MCREST          0.00000000 sec
MCWRK           0.01500000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                   6.30 usec
PL1                 -2.00 dB
SFO1          100.6227903 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                 18.00 dB
PL12                18.00 dB
SFO2          400.1324008 MHz

F2 - Processing parameters
SI                   131072
```


Current Data Parameters
NAME Imani
EXPNO 434
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100723
Time 15.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 10.91 cm
F1P 11.109 ppm
F1 3334.06 Hz
F2P -0.982 ppm
F2 -294.64 Hz
PPMCM 0.60452 ppm/cm
HZCM 181.43504 Hz/cm
1.15494
2.49128
3.08772
3.34429
8.84422
7.97359
7.88118
7.51526
7.36165
7.27271
7.12849
7.07047
6.96825
9.136
9.084
1.735
1.833
2.814
2.136
1.000
NH
CN
CN
CN
NHEt3
O
O
N
ppm
Integral



Current Data Parameters

NAME	gh-1
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20130129
Time	17.24
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgdc
TD	32768
SOLVENT	DMSO
NS	992
DS	0
SWH	22075.055 Hz
FIDRES	0.673677 Hz
AQ	0.7422452 sec
RG	1625.5
DW	22.650 usec
DE	6.00 usec
TE	297.2 K
D1	5.00000000 sec
d11	0.03000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

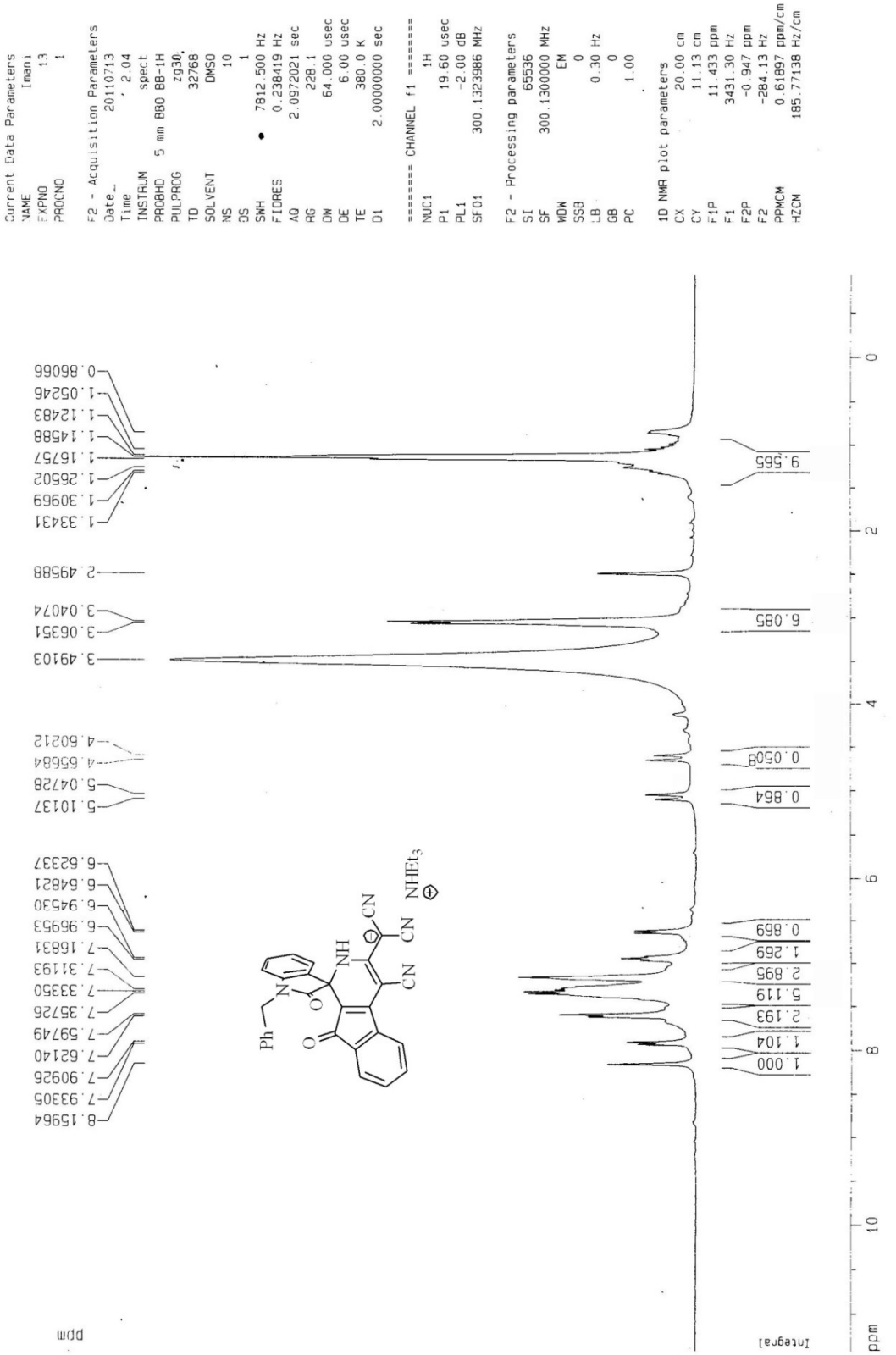
NUC1	13C
P1	6.30 usec
PL1	-2.00 dB
SFO1	100.6227903 MHz

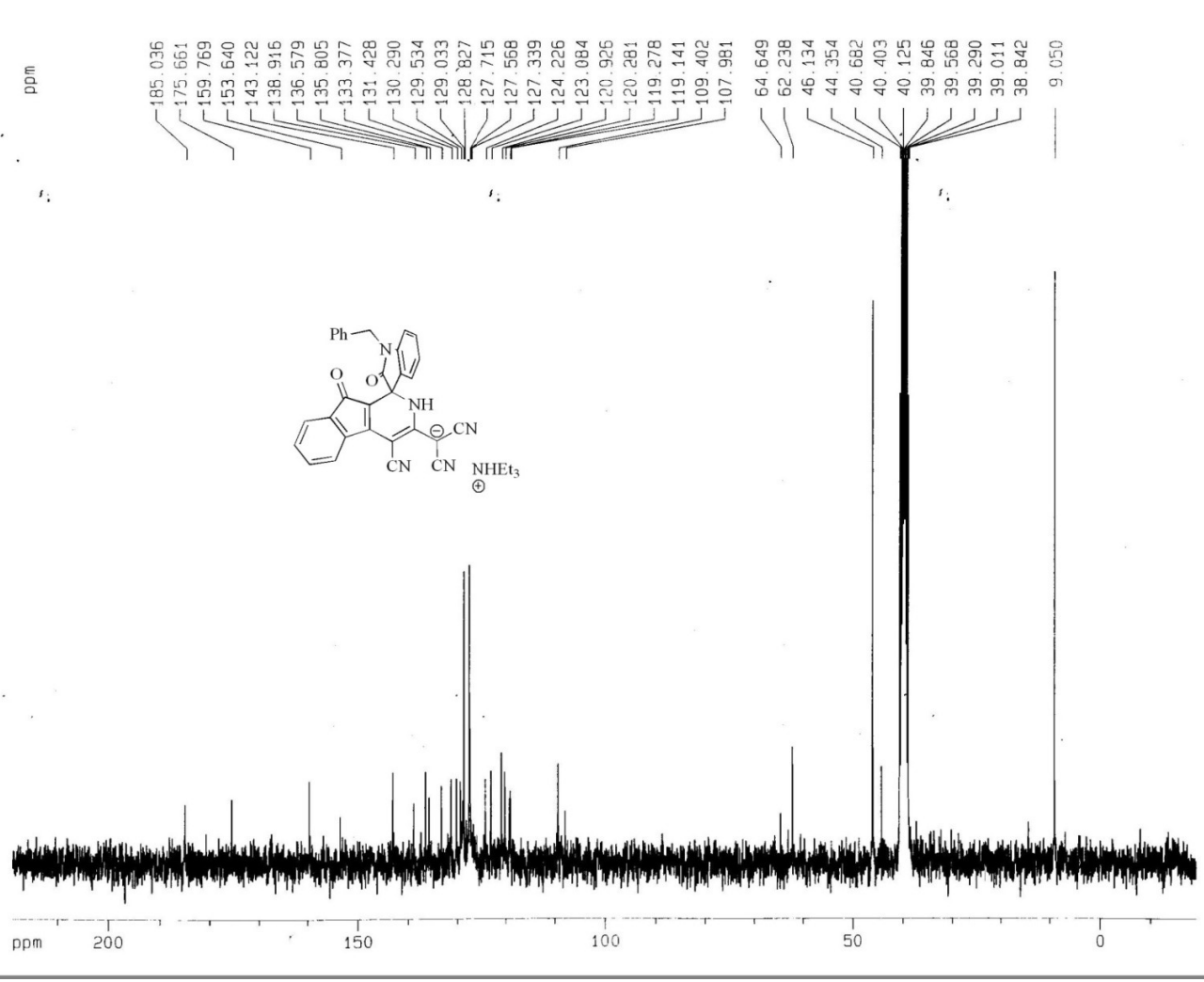
======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	18.00 dB
PL12	18.00 dB
SFO2	400.1324008 MHz

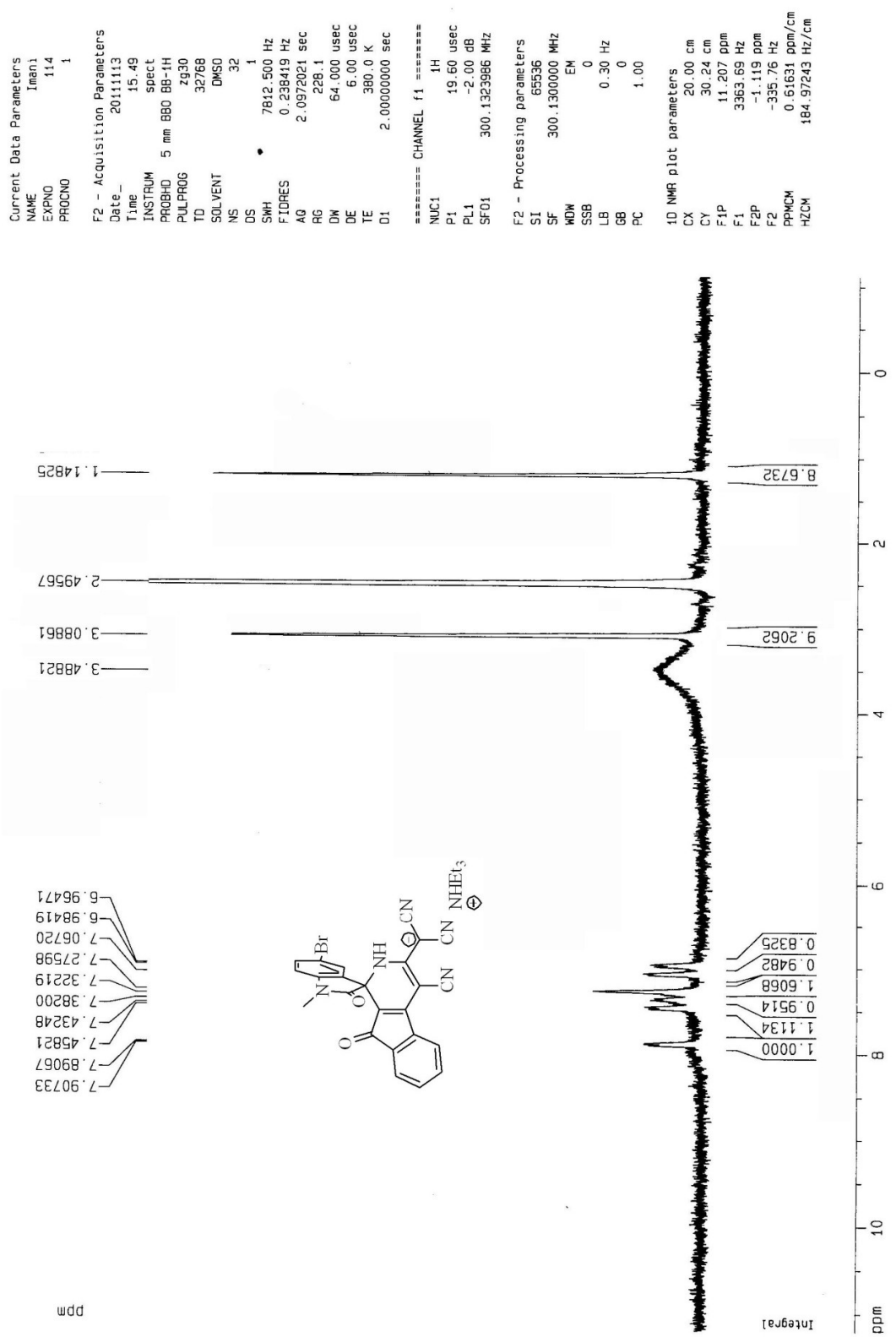
F2 - Processing parameters

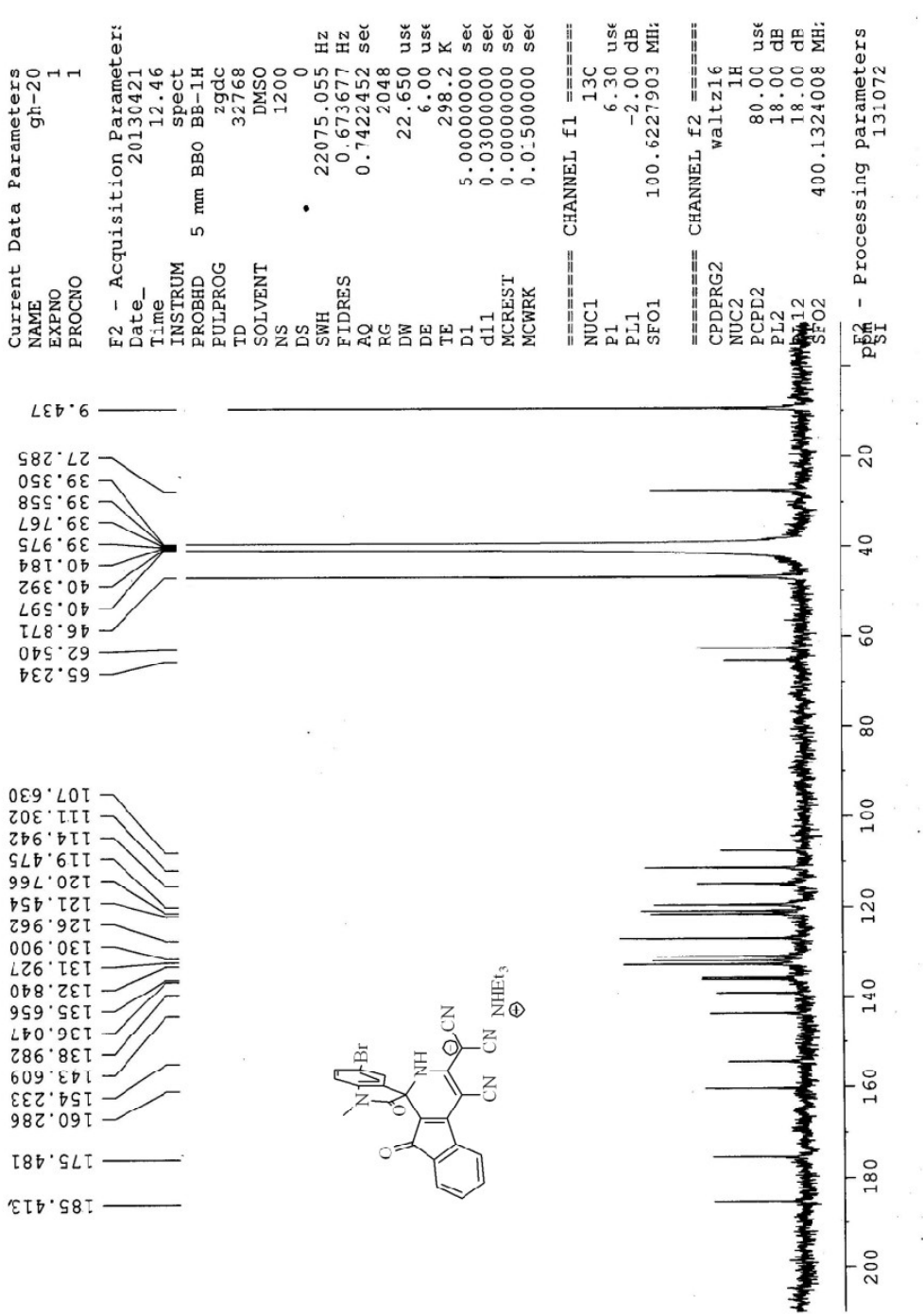
SI	131072
SF	100.6127290 MHz

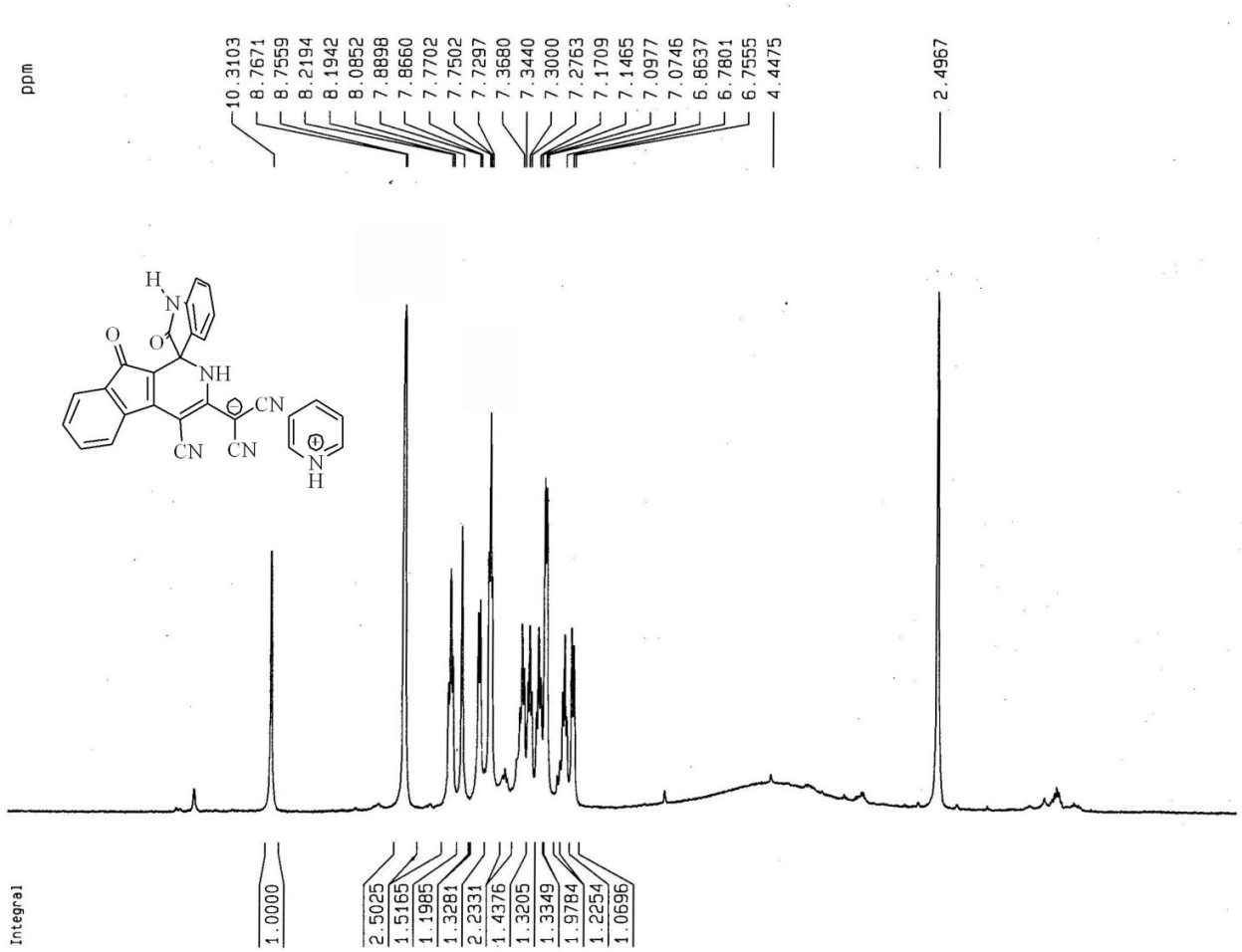

Current Data Parameters
NAME Imani
EXPNO 13
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110713
Time 2.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 10
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 11.13 cm
F1P 11.433 ppm
F1 3431.30 Hz
F2P -0.947 ppm
F2 -284.13 Hz
PPMCM 0.61897 ppm/cm
HZCM 185.77138 Hz/cm
8.15964
7.93305
7.90926
7.62140
7.59749
7.35726
7.33350
7.31193
7.16831
6.96953
6.94530
6.64821
6.62337
5.10137
5.04728
4.65584
4.60212
3.49103
3.06351
3.04074
2.49588
1.33431
1.30969
1.26502
1.16757
1.14588
1.12483
1.05246
0.86066
9.565
6.085
0.508
0.864
0.869
1.269
2.895
5.119
2.193
1.104
1.000
Ph
N
O
O
NH
CN
CN
CN
NHEt3
ppm
Integral



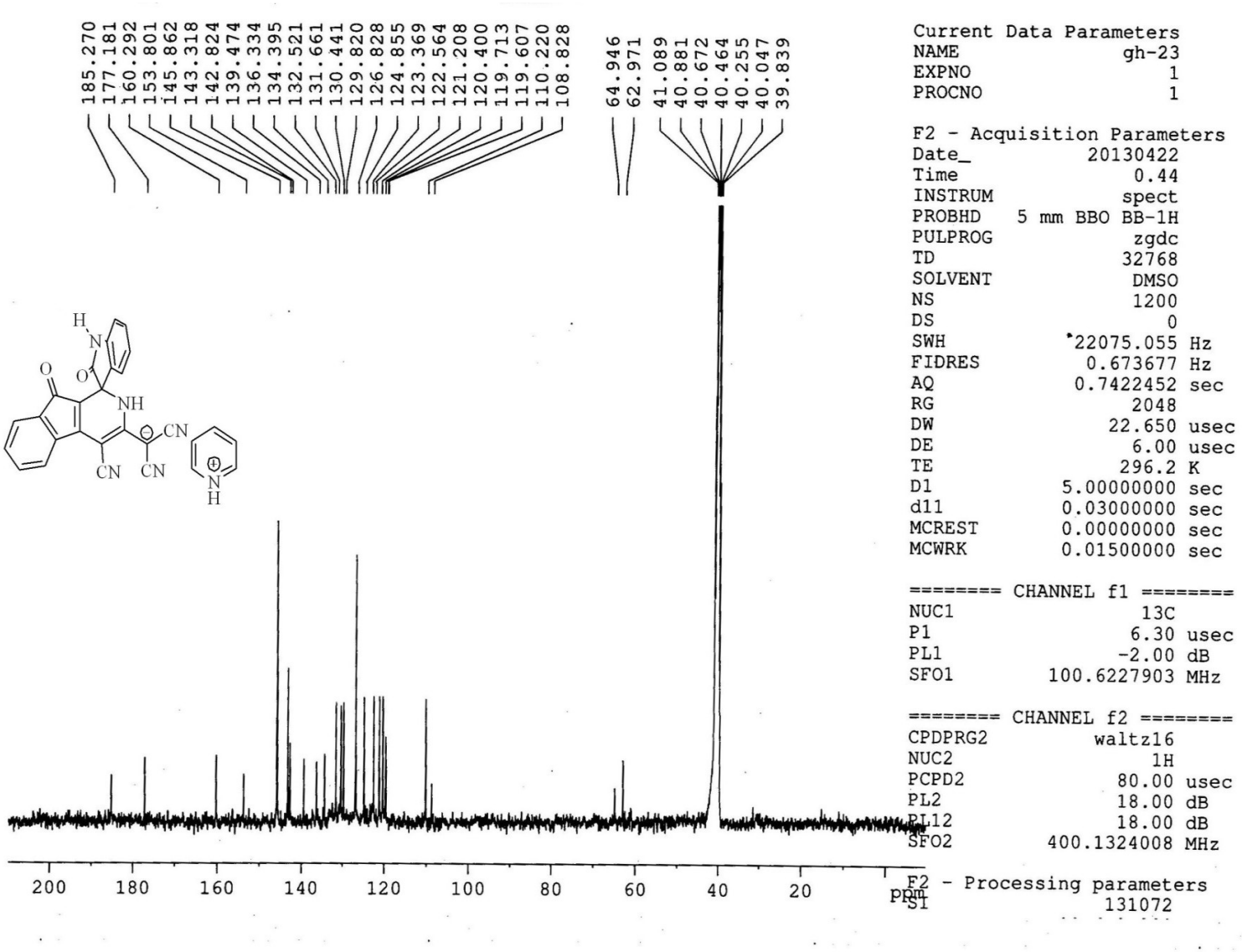

```
Current Data Parameters
NAME                  Imani
EXPNO                    12
PROCNO                    1

F2 - Acquisition Parameters
Date_              20110713
Time                   2.02
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      250
DS                        2
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                     2048
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1                2.00000000 sec
d11               0.03000000 sec
d12               0.00002000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   12.60 usec
PL1                   -2.00 dB
SF01              75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                87.00 usec
PL2                   -2.00 dB
PL12                  12.00 dB
PL13                  18.00 dB
SF02             300.1312005 MHz

F2 - Processing parameters
SI                    65536
SF                75.4677490 MHz
WDW                      EM
SSB                       0
LB                     2.00 Hz
GB                        0
PC                     0.20

1D NMR plot parameters
CX                    20.00 cm
CY                    57.15 cm
F1P                  219.155 ppm
F1                 16539.11 Hz
F2P                 -19.167 ppm
F2                 -1446.51 Hz
PPMCM              11.91609 ppm/cm
HZCM              899.28058 Hz/cm
```


Current Data Parameters
NAME Imani
EXPNO 114
PROCNO 1
F2 - Acquisition Parameters
Date_ 20111113
Time 15.49
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 19.60 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 30.24 cm
F1P 11.207 ppm
F1 3363.69 Hz
F2P -1.119 ppm
F2 -335.76 Hz
PPMCM 0.61631 ppm/cm
HZCM 184.97243 Hz/cm
1.14825
2.49567
3.08861
3.48821
7.90733
7.89067
7.45821
7.43248
7.38200
7.32219
7.27598
7.06720
6.98419
6.96471
8.6732
9.2062
1.0000
1.1134
0.9514
1.6068
0.9482
0.8325
Br
NH
CN
CN
CN
NHEt3
O
O
N
ppm
Integral


Current Data Parameters
NAME gh-20
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130421
Time 12.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgdc
TD 32768
SOLVENT DMSO
NS 1200
DS 0
SWH 22075.055 Hz
FIDRES 0.673677 Hz
AQ 0.7422452 sec
RG 2048
DW 22.650 use
DE 6.00 use
TE 298.2 K
D1 5.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 6.30 use
PL1 -2.00 dB
SFO1 100.6227903 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 use
PL2 18.00 dB
PL12 18.00 dB
SFO2 400.1324008 MHz
F2 - Processing parameters
SI 131072
9.437
27.285
39.350
39.558
39.767
39.975
40.184
40.392
40.597
46.871
62.540
65.234
107.630
111.302
114.942
119.475
120.766
121.454
126.962
130.900
131.927
132.840
135.656
136.047
138.982
143.609
154.233
160.286
175.481
185.413
Br
NH
CN
CN
CN
NHEt3
O
O
N
ppm
200
180
160
140
120
100
80
60
40
20




```
Current Data Parameters
NAME                  Imani
EXPNO                   163
PROCNO                    1

F2 - Acquisition Parameters
Date_              20120303
Time                  14.41
INSTRUM               spect
PROBHD   5 mm BBO BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       24
DS                        1
SWH          •     7812.500 Hz
FIDRES           0.238419 Hz
AQ               2.0972021 sec
RG                     35.9
DW                64.000 usec
DE                 6.00 usec
TE                 380.0 K
D1              2.00000000 sec

======== CHANNEL f1 ========
NUC1                   1H
P1                 15.50 usec
PL1                -2.00 dB
SFO1          300.1323986 MHz

F2 - Processing parameters
SI                    65536
SF          300.1300000 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                   1.00

1D NMR plot parameters
CX                  20.00 cm
CY                   9.42 cm
F1P                13.364 ppm
F1                4011.08 Hz
F2P                -1.013 ppm
F2                -303.97 Hz
PPMCM            0.71886 ppm/cm
HZCM           215.75218 Hz/cm
```



Current Data Parameters

NAME	gh-23
EXPNO	1
PROCNO	1

F2 - Acquisition Parameters

Date_	20130422
Time	0.44
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zgdc
TD	32768
SOLVENT	DMSO
NS	1200
DS	0
SWH	22075.055 Hz
FIDRES	0.673677 Hz
AQ	0.7422452 sec
RG	2048
DW	22.650 usec
DE	6.00 usec
TE	296.2 K
D1	5.00000000 sec
d11	0.03000000 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec

======== CHANNEL f1 ========

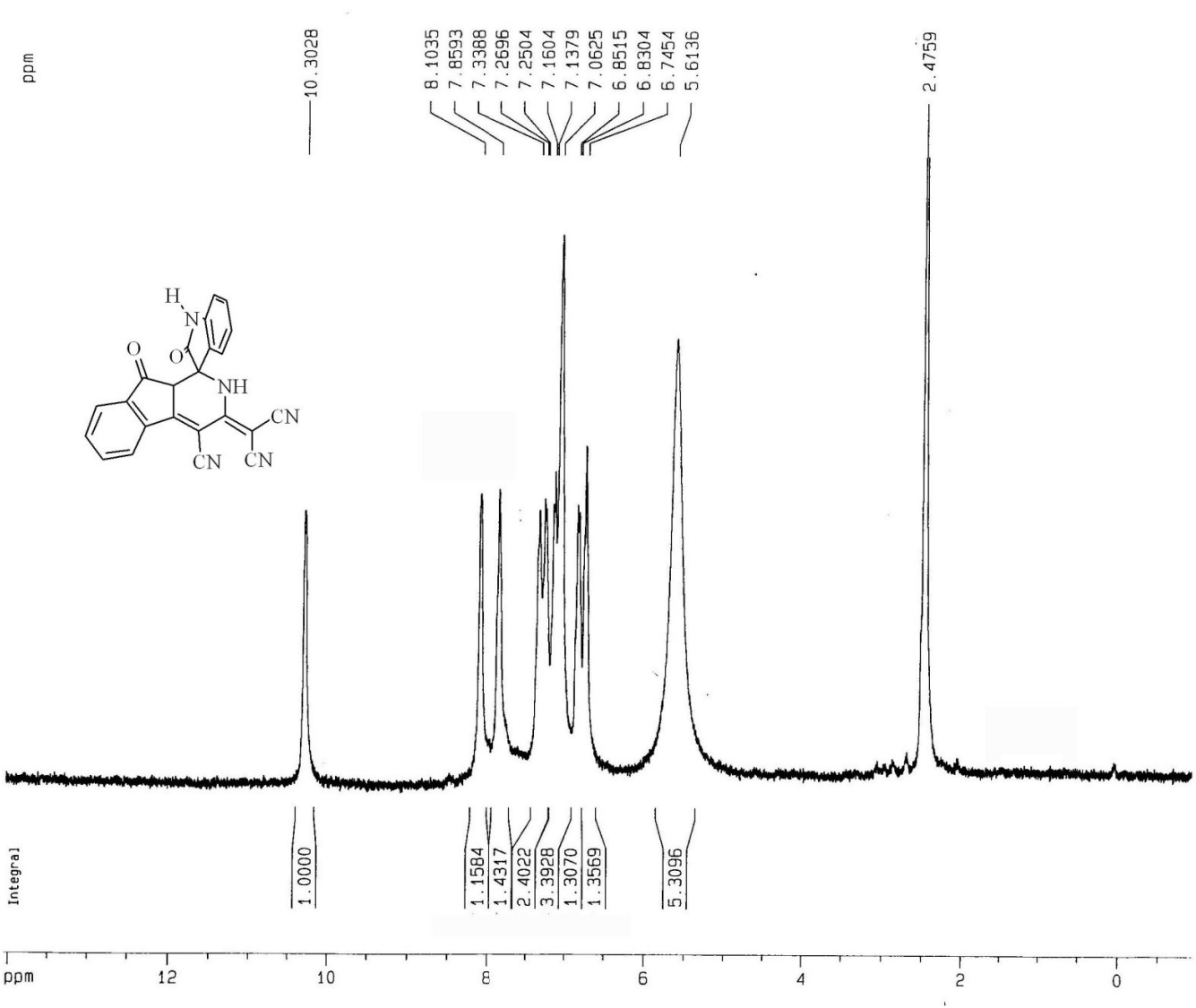
NUC1	13C
P1	6.30 usec
PL1	-2.00 dB
SFO1	100.6227903 MHz

======== CHANNEL f2 ========

CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	18.00 dB
PL12	18.00 dB
SFO2	400.1324008 MHz

F2 - Processing parameters

SI	131072



Current Data Parameters

NAME	Imani
EXPNO	88
PROCNO	1

F2 - Acquisition Parameters

Date_	20110918
Time	16.13
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	10
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 sec
RG	228.1
DW	64.000 usec
DE	6.00 usec
TE	380.0 K
D1	2.00000000 sec

======== CHANNEL f1 ========

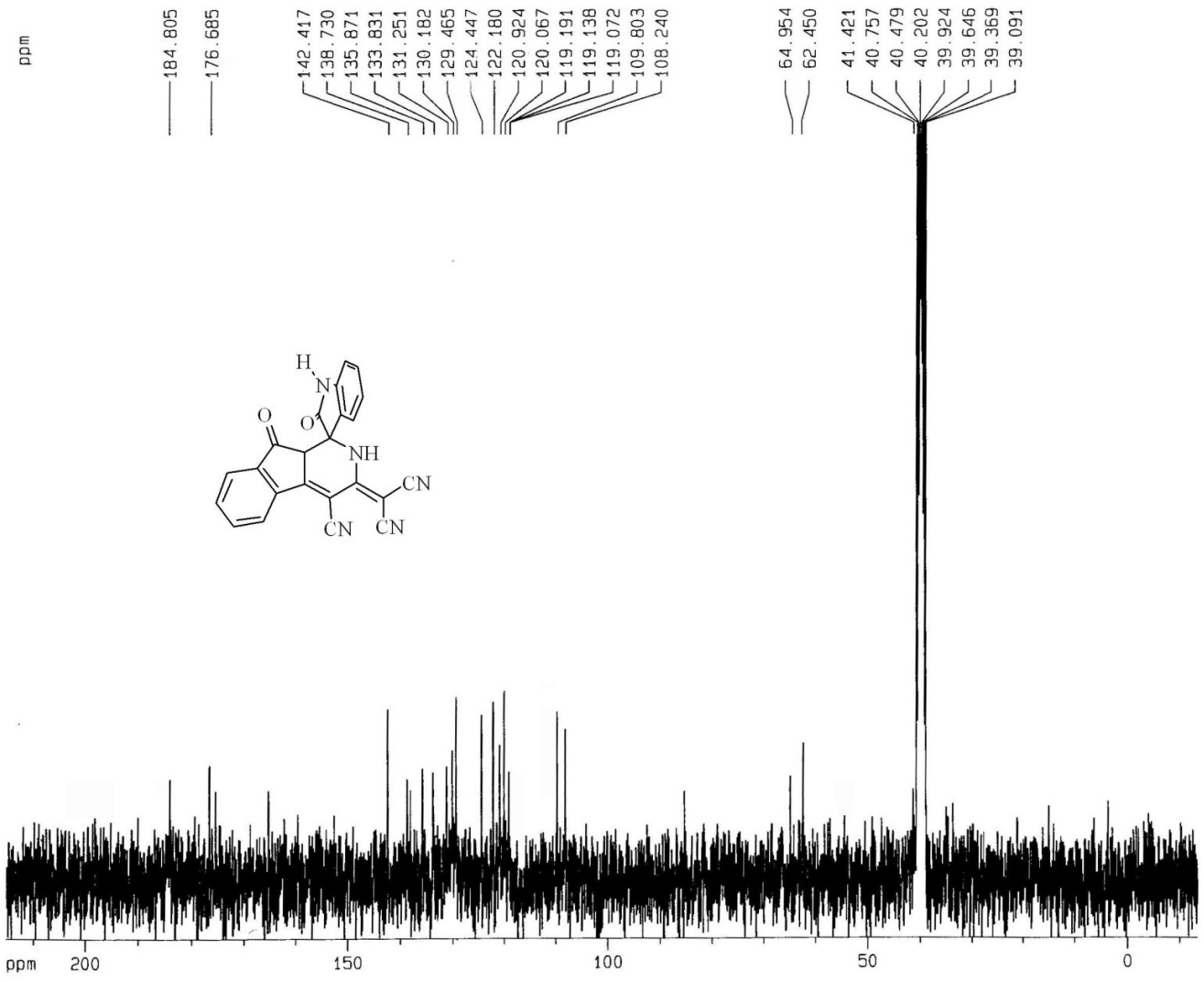
NUC1	1H
P1	19.60 usec
PL1	-2.00 dB
SF01	300.1323986 MHz

F2 - Processing parameters

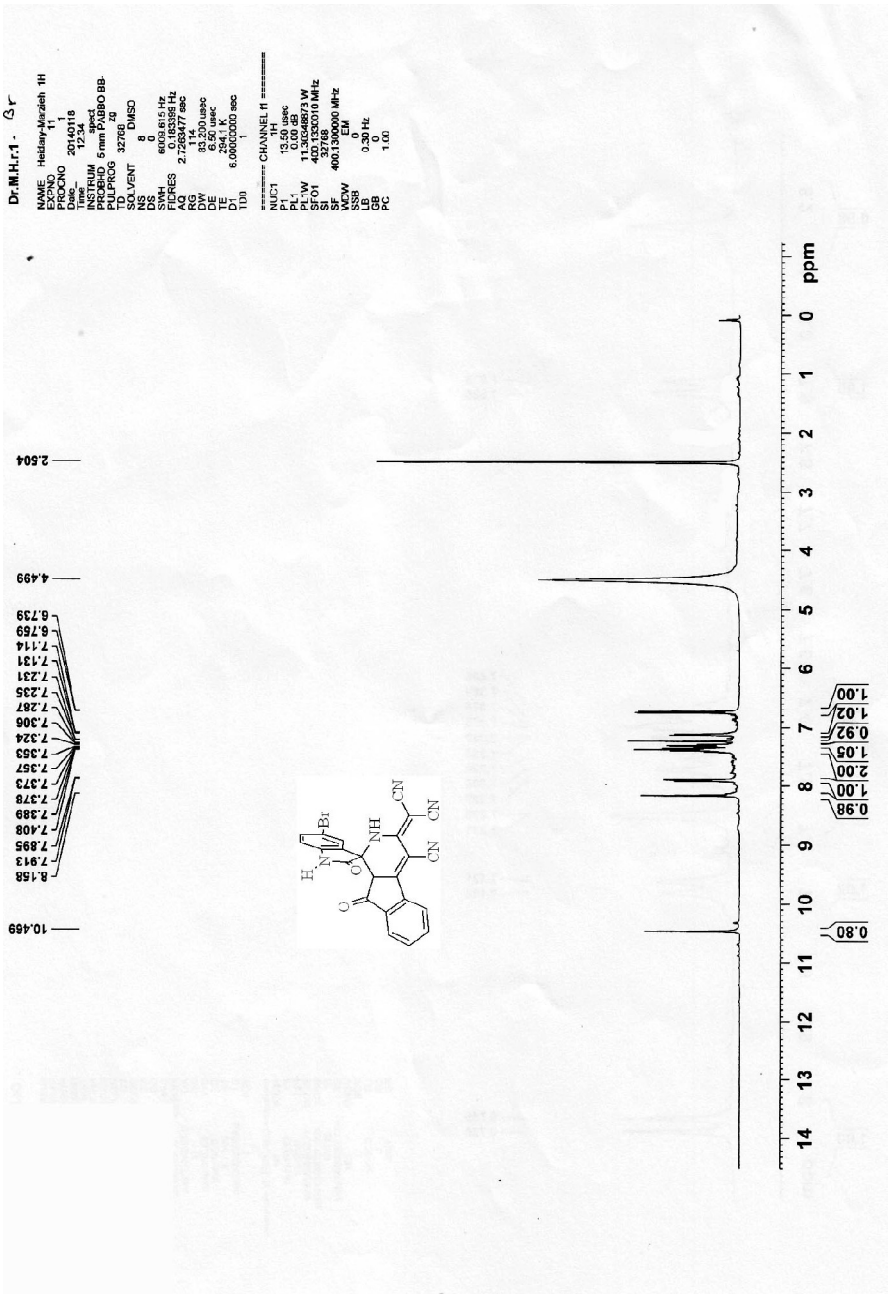
SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

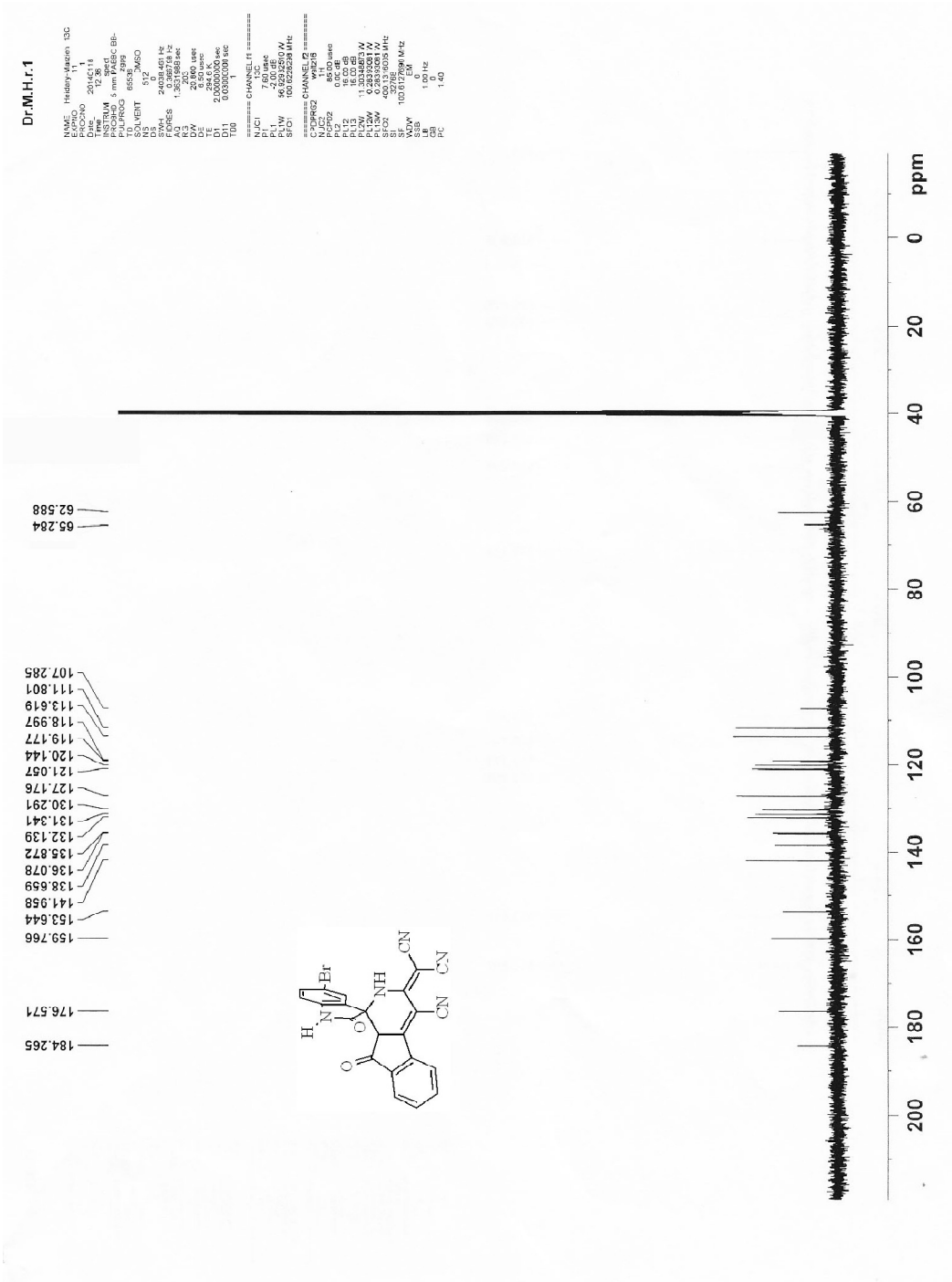
1D NMR plot parameters

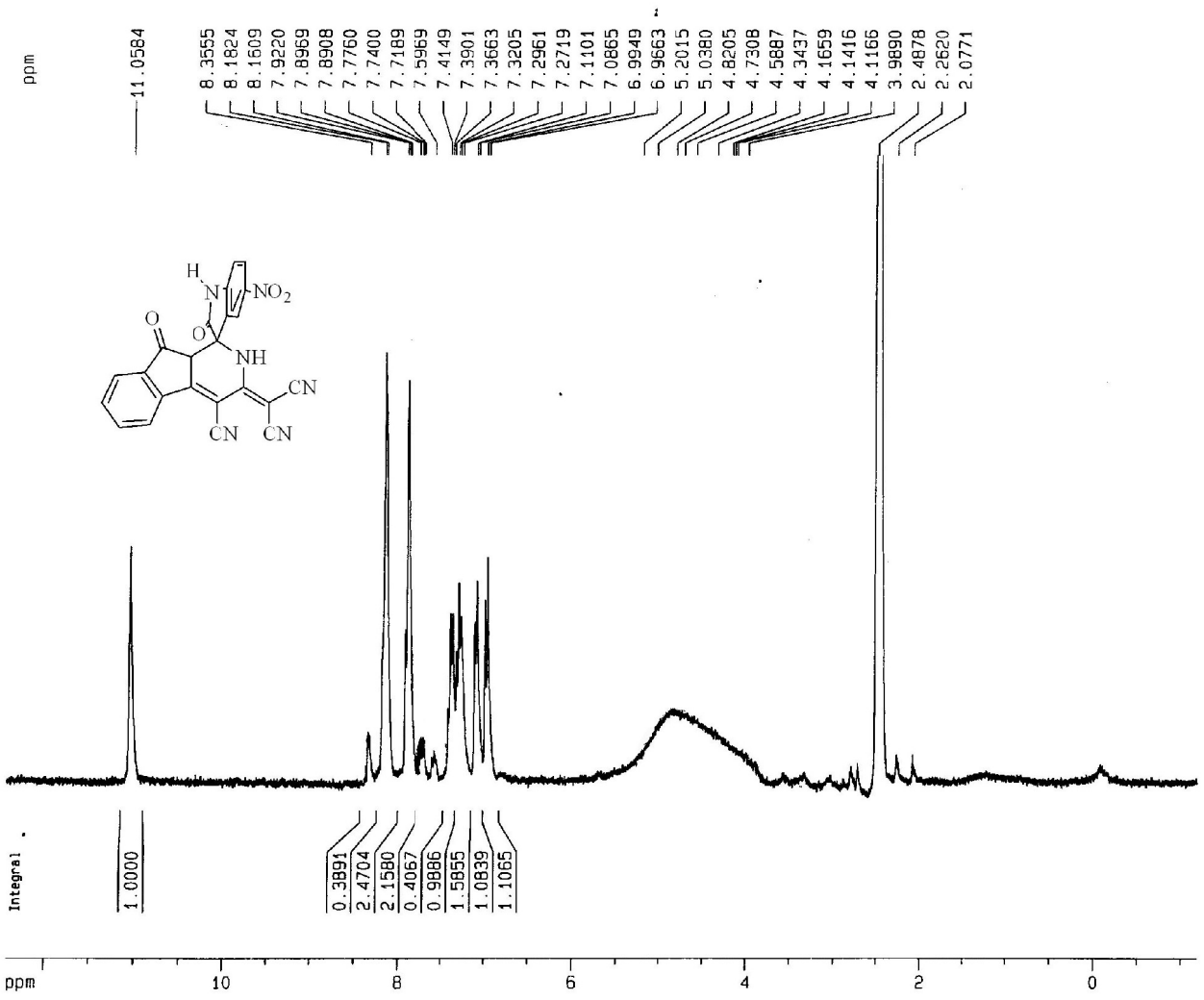
CX	20.00 cm
CY	12.24 cm
F1P	14.040 ppm
F1	4213.87 Hz
F2P	-0.927 ppm
F2	-278.32 Hz
PPMCM	0.74837 ppm/cm
HZCM	224.60938 Hz/cm



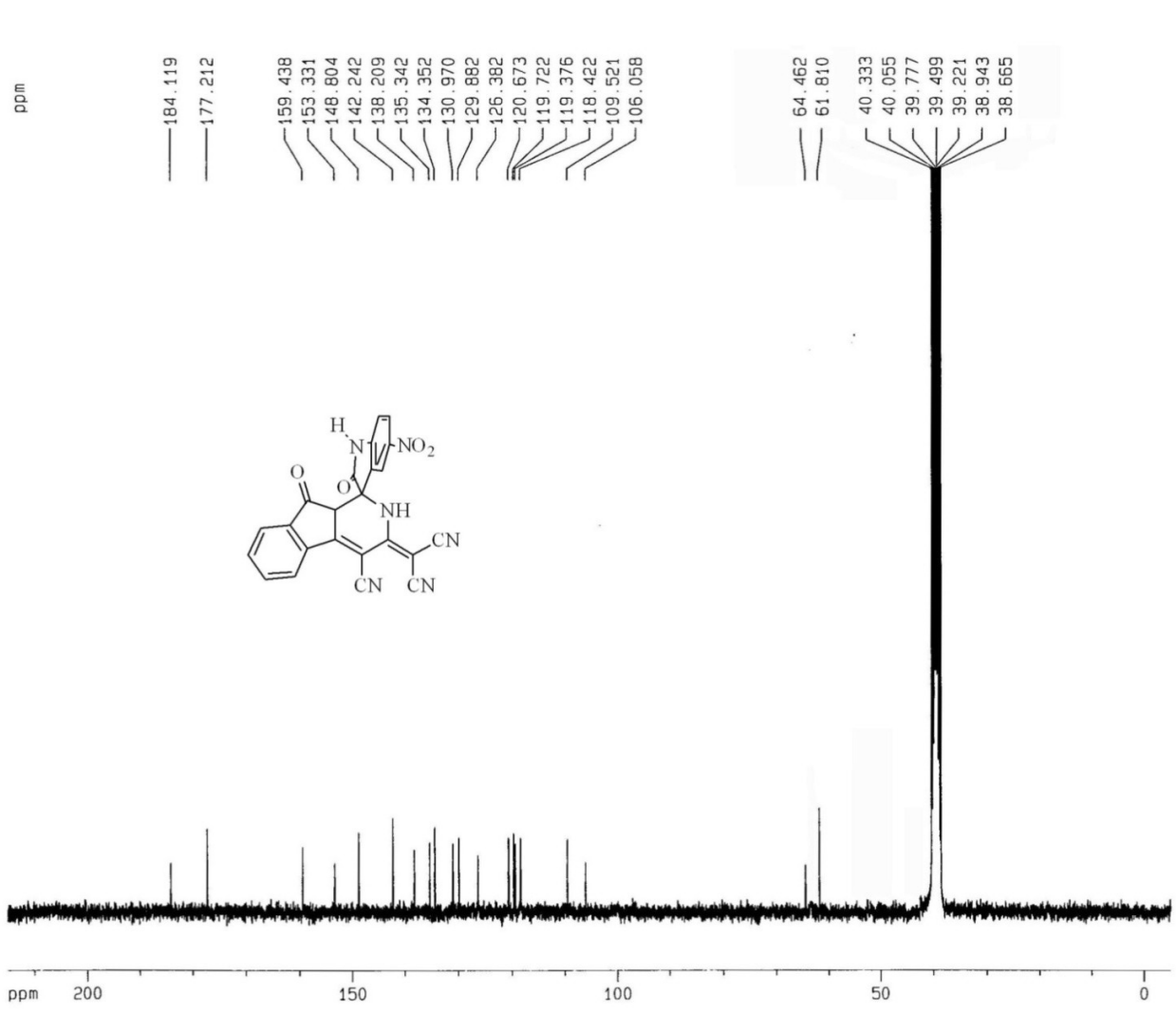

```
Current Data Parameters
NAME                   Imani
EXPNO                    113
PROCNO                     1

F2 - Acquisition Parameters
Date_               20111106
Time                   14.24
INSTRUM                spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgpg30
TD                     65536
SOLVENT                DMSO
NS                       294
DS                         2
SWH               17985.611 Hz
FIDRES            0.274439 Hz
AQ                1.8219508 sec
RG                      2048
DW                  27.800 usec
DE                   6.00 usec
TE                   300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                     13C
P1                   12.60 usec
PL1                  -2.00 dB
SFO1            75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                     1H
PCPD2                87.00 usec
PL2                  -2.00 dB
PL12                 12.00 dB
PL13                 18.00 dB
SFO2           300.1312005 MHz

F2 - Processing parameters
SI                     65536
SF              75.4677490 MHz
WDW                       EM
SSB                        0
LB                    2.00 Hz
GB                         0
PC                      0.20

1D NMR plot parameters
CX                   20.00 cm
CY                   89.74 cm
F1P                215.253 ppm
F1                 16244.70 Hz
F2P                -13.493 ppm
F2                 -1018.28 Hz
PPMCM              11.43732 ppm/cm
HZCM              863.14880 Hz/cm
```


Dr.M.H.r1 - 3r
NAME Heiday-Marzieh 1H
EXPNO 11
PROCNO 1
Date_ 20140118
Time 12:34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg
TD 32768
SOLVENT DMSO
NS 8
DS 0
SWH 6009.615 Hz
FIDRES 0.183350 Hz
AQ 2.7268477 sec
RG 114
DW 83.200 usec
DE 6.50 usec
TE 294.1 K
D1 6.00000000 sec
1 1
======== CHANNEL f1 ========
NUC1 1H
P1 13.60 usec
PL1 0.00 dB
PL1W 11.30348873 W
SFO1 400.1320010 MHz
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
2.504
4.499
10.459
8.158
7.913
7.895
7.408
7.389
7.378
7.373
7.357
7.353
7.324
7.306
7.287
7.235
7.231
7.131
7.114
6.769
6.739
0.80
0.98
1.00
2.00
1.03
0.92
1.02
1.00
ppm

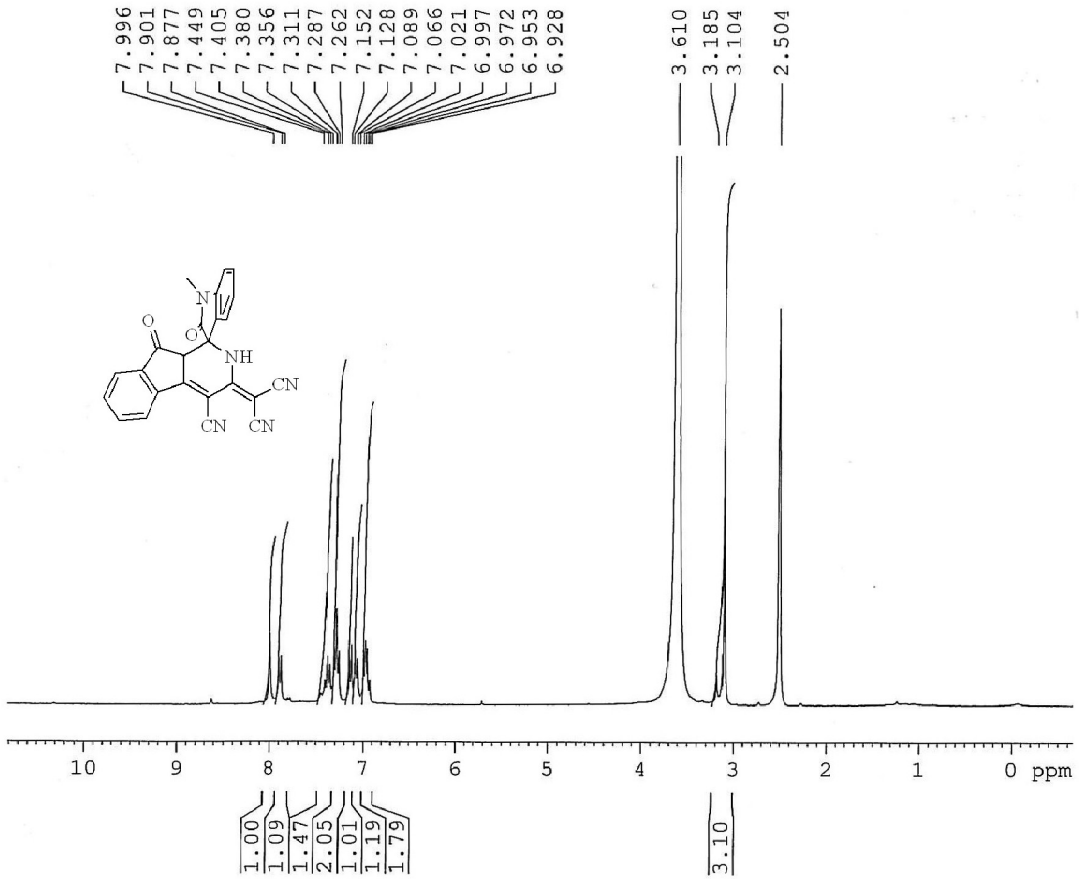

Dr.M.H.r.1
62.588
65.284
107.285
111.801
113.619
118.997
119.177
120.144
121.057
127.176
130.291
131.341
132.139
135.872
136.078
138.659
141.958
153.644
159.766
176.571
184.265
ppm
0
20
40
60
80
100
120
140
160
180
200



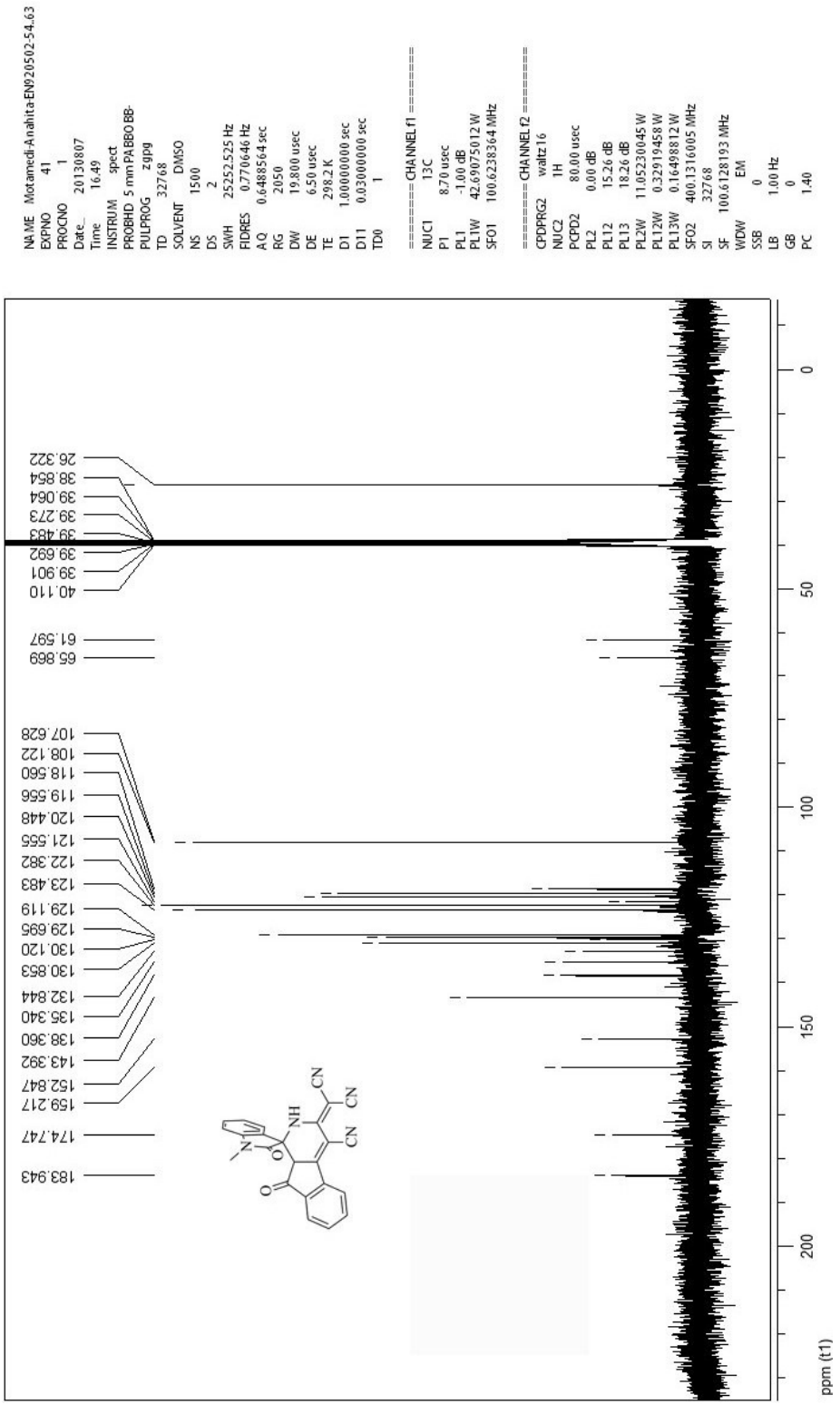

```
Current Data Parameters
NAME                  Imani
EXPNO                   137
PROCNO                    1

F2 - Acquisition Parameters
Date_              20111213
Time                  17.46
INSTRUM               spect
PROBHD   5 mm 880 BB-1H
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       32
DS                        1
SWH                7812.500 Hz
FIDRES             0.238419 Hz
AQ                 2.0972021 sec
RG                     228.1
DW                    64.000 usec
DE                     6.00 usec
TE                    380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                     85.00 usec
PL1                    -2.00 dB
SFO1             300.1323986 MHz

F2 - Processing parameters
SI                        65536
SF               300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00

1D NMR plot parameters
CX                     20.00 cm
CY                     58.02 cm
F1P                   12.432 ppm
F1                  3731.33 Hz
F2P                   -1.195 ppm
F2                  -358.74 Hz
PPMCM               0.68138 ppm/cm
HZCM              204.50368 Hz/cm
```

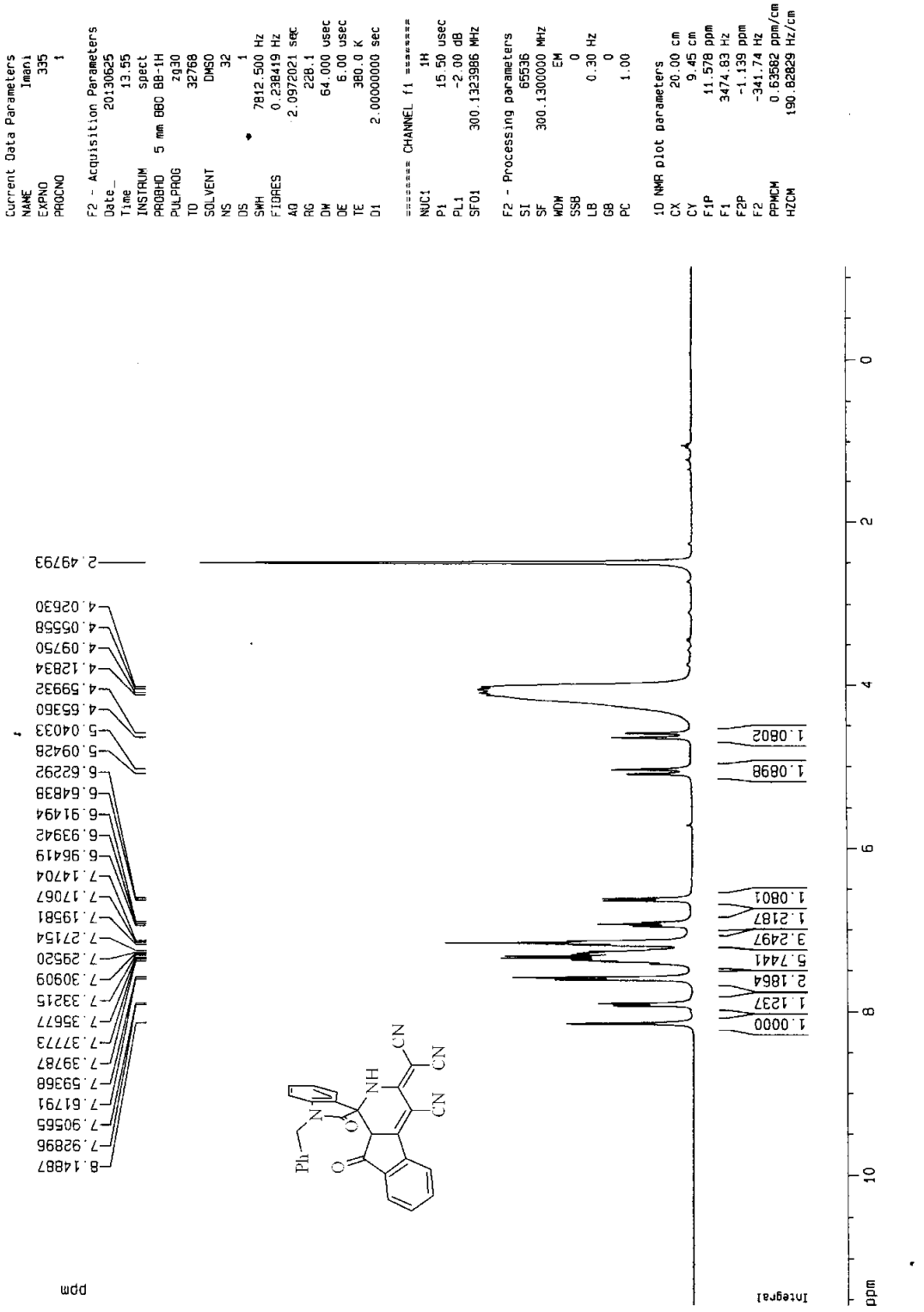


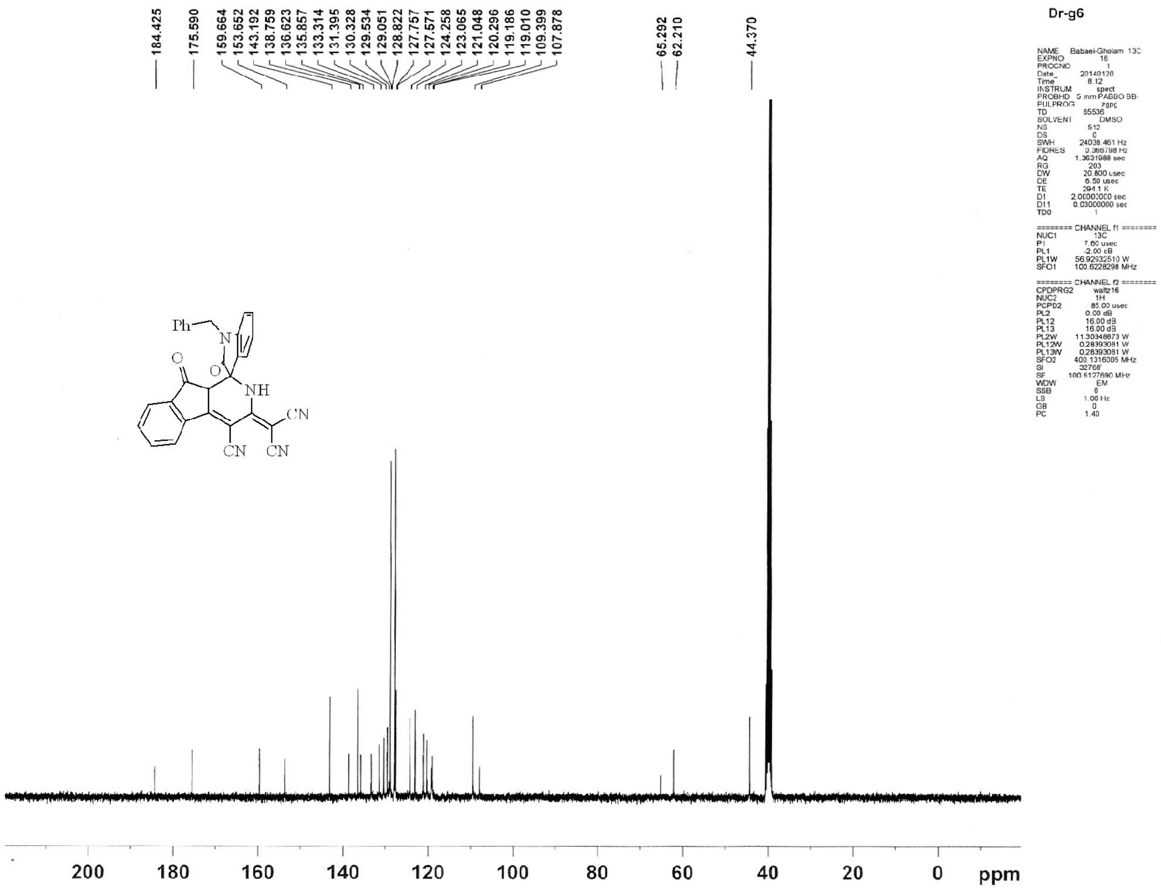

```
Current Data Parameters
NAME                  azad
EXPNO                  698
PROCNO                   1

F2 - Acquisition Parameters
Date_              20130710
Time                  3.02
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG             zgpg30
TD                   32768
SOLVENT                DMSO
NS                   10240
DS                       0
SWH              17985.611 Hz
FIDRES           0.548877 Hz
AQ               0.9110004 sec
RG                   16384
DW                27.800 usec
DE                 6.00 usec
TE                 300.0 K
D1              2.00000000 sec
d11             0.03000000 sec
d12             0.00002000 sec

======== CHANNEL f1 ========
NUC1                   13C
P1                  7.00 usec
PL1                -4.00 dB
SF01           75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               21.00 dB
PL13               21.00 dB
SF02          300.1312005 MHz

F2 - Processing parameters
SI                   65536
SF             75.4677844 MHz
WDW                    EM
SSB                     0
LB                  1.00 Hz
GB                      0
PC                   1.40

1D NMR plot parameters
CX                 20.00 cm
CY                100.00 cm
F1P              215.000 ppm
F1              16225.57 Hz
F2P               -5.000 ppm
F2               -377.34 Hz
PPMCM          11.00000 ppm/cm
HZCM           830.14557 Hz/cm
```

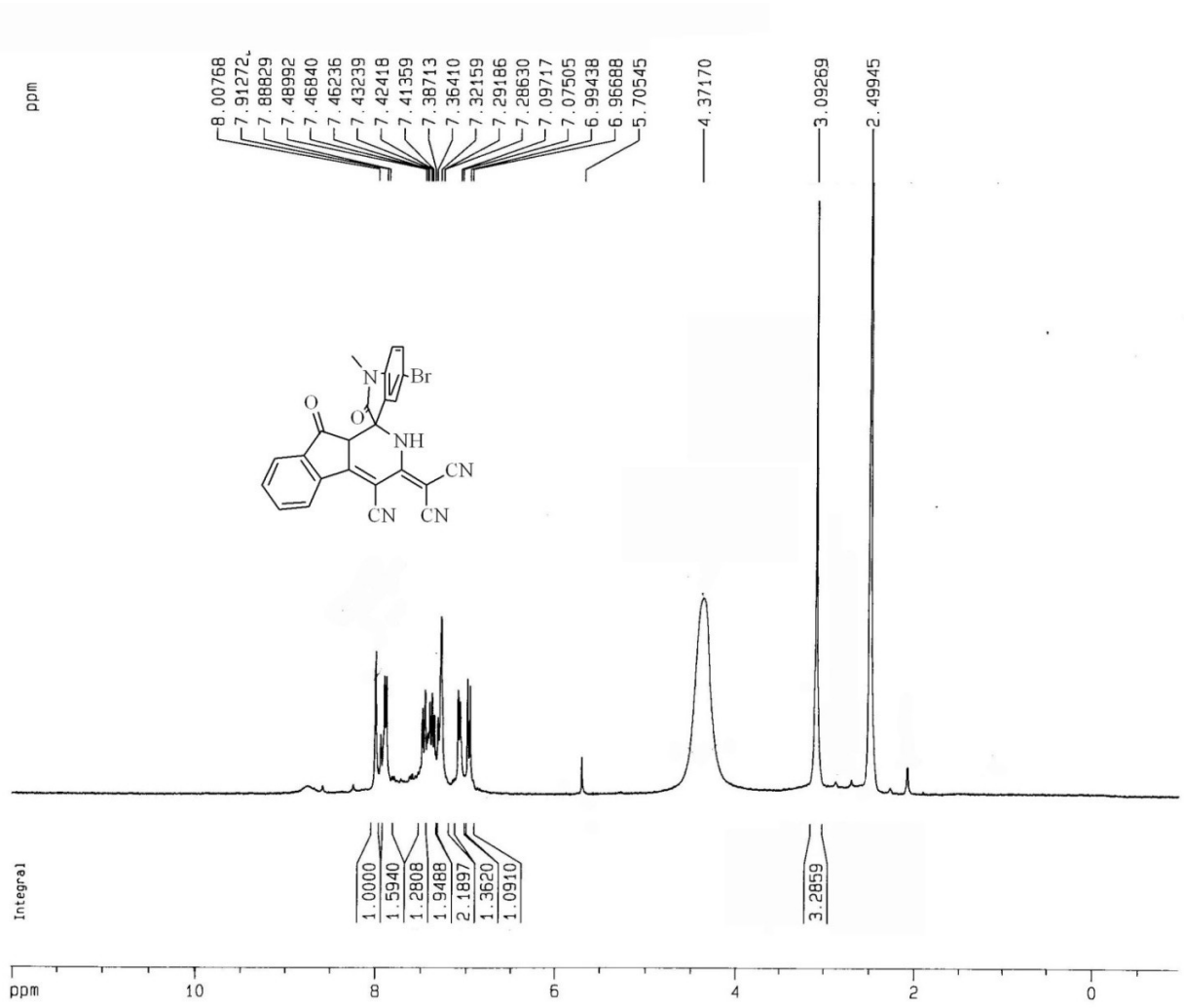



```
Current Data Parameters
NAME                  Imani
EXPNO                   340
PROCNO                    1

F2 - Acquisition Parameters
Date_              20130721
Time                  16.19
INSTRUM               spect
PROBHD      5 mm BBO BB-
PULPROG               zg30
TD                   32768
SOLVENT               DMSO
NS                       32
DS                        1
SWH                7812.500 Hz
FIDRES                0.238419 Hz
AQ                 2.0972021 sec
RG                     228.1
DW                    64.000 usec
DE                     6.00 usec
TE                    380.0 K
D1                 2.00000000 sec

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.50 usec
PL1                   -2.00 dB
SFO1           300.1323986 MHz

F2 - Processing parameters
SI                    65536
SF             300.1300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```


NAME Motamedi-Anahita-EN9210502-54.63
EXPNO 41
PROCNO 1
Date_ 20130807
Time 16.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 32768
SOLVENT DMSO
NS 1500
DS 2
SWH 25252.525 Hz
FIDRES 0.770646 Hz
AQ 0.6488564 sec
RG 2050
DW 19.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 8.70 usec
PL1 -1.00 dB
PL1W 42.69075012 W
SFO1 100.6238364 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.26 dB
PL13 18.26 dB
PL2W 11.05230045 W
PL12W 0.32919458 W
PL13W 0.16498812 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
26.322
38.854
39.064
39.273
39.483
39.692
39.901
40.110
61.597
65.869
107.628
108.122
118.560
119.556
120.448
121.555
122.382
123.483
129.119
129.695
130.120
130.853
132.844
135.340
138.360
143.392
152.847
159.217
174.747
183.943
CN
CN
CN
NH
N
O
O
0
50
100
150
200
ppm (t1)


Current Data Parameters
NAME Imani
EXPNO 335
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130625
Time 13.55
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 9.45 cm
F1P 11.578 ppm
F1 3474.83 Hz
F2P -1.139 ppm
F2 -341.74 Hz
PPMCM 0.63582 ppm/cm
HZCM 190.82829 Hz/cm
2.49793
4.02530
4.05558
4.09750
4.12834
4.59932
4.65360
5.04033
5.09428
6.62292
6.64838
6.91494
6.93942
6.96419
7.14704
7.17067
7.19581
7.27154
7.29520
7.30909
7.33215
7.35677
7.37773
7.39787
7.59368
7.61791
7.90565
7.92896
8.14887
1.0000
1.1237
2.1864
5.7441
3.2497
1.2187
1.0801
1.0898
1.0802
Integral
ppm
Ph
N
O
NH
CN
CN
CN
O


184.425
175.590
159.664
153.652
143.192
138.759
136.623
135.857
133.314
131.395
130.328
129.534
129.051
128.822
127.757
127.571
124.258
123.065
121.048
120.296
119.186
119.010
109.399
107.878
65.292
62.210
44.370
Ph
N
O
O
NH
CN
CN
CN
200
180
160
140
120
100
80
60
40
20
0
ppm
Dr-g6
NAME Babaei-Gholam 13C
EXPNO 16
PROCNO 1
Date_ 20140120
Time 8.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg
TD 65536
SOLVENT DMSO
NS 512
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 7.60 usec
PL1 -2.00 dB
PL1W 56.92932510 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 85.00 usec
PL2 0.00 dB
PL12 16.00 dB
PL13 16.00 dB
PL2W 11.30348873 W
PL12W 0.28393081 W
PL13W 0.28393081 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



Current Data Parameters

NAME	Imani
EXPNO	189
PROCNO	1

F2 - Acquisition Parameters

Date_	20120620
Time	9.38
INSTRUM	spect
PROBHD	5 mm BBO BB-1H
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	32
DS	1
SWH	7812.500 Hz
FIDRES	0.238419 Hz
AQ	2.0972021 sec
RG	35.9
DW	64.000 usec
DE	6.00 usec
TE	380.0 K
D1	2.00000000 sec

======== CHANNEL f1 ========

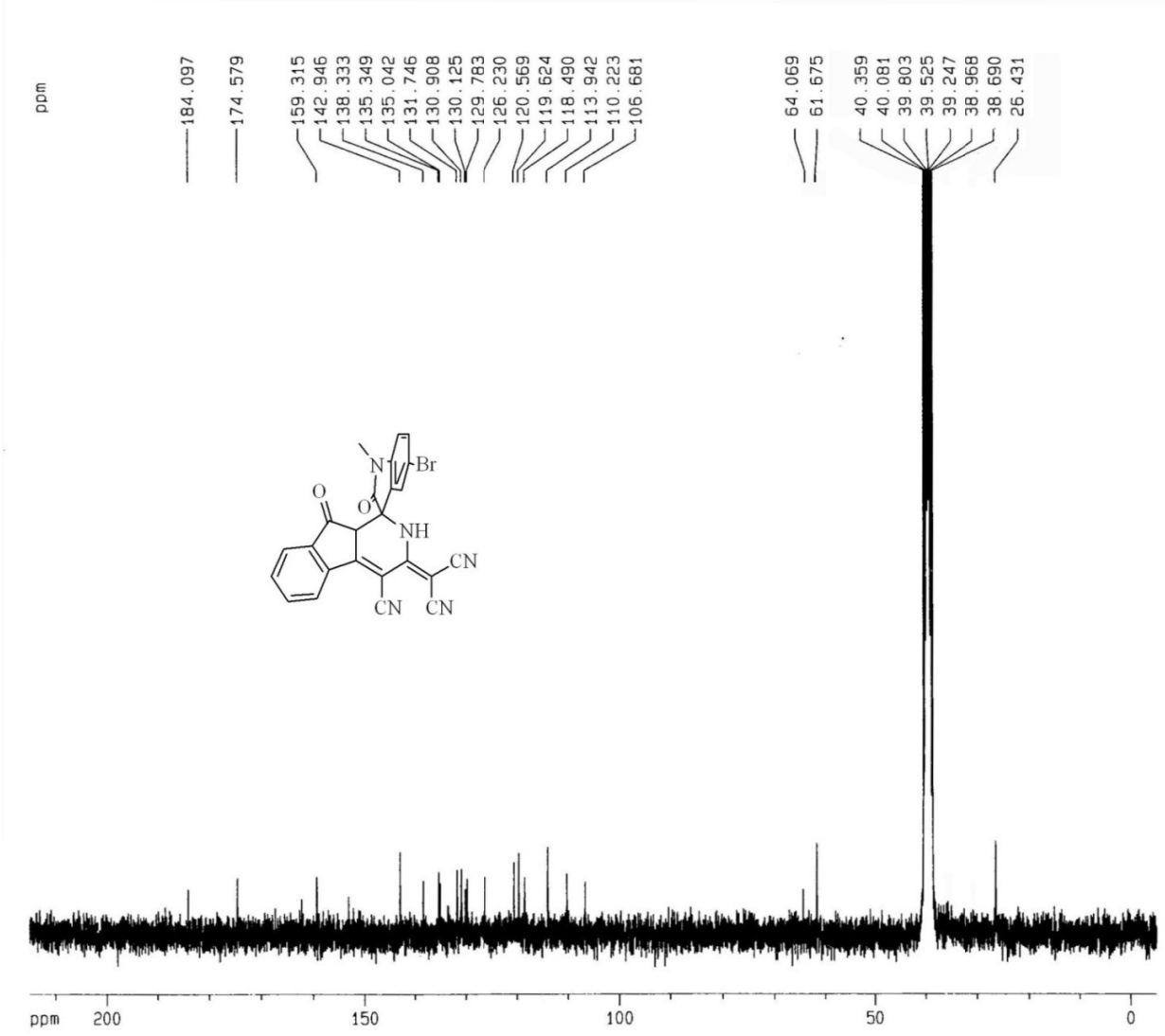
NUC1	1H
P1	15.50 usec
PL1	-2.00 dB
SFO1	300.1323986 MHz

F2 - Processing parameters

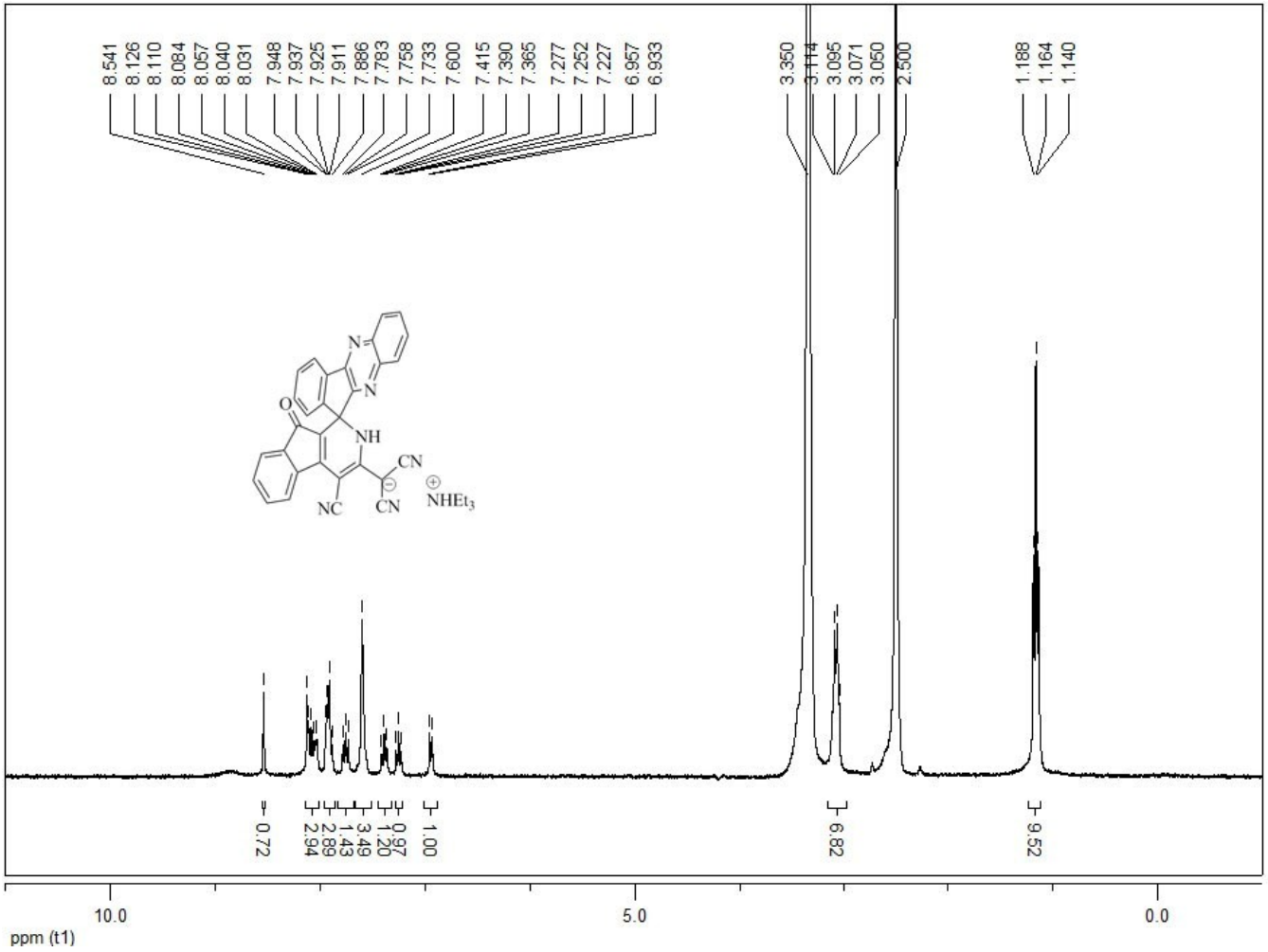
SI	65536
SF	300.1300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

1D NMR plot parameters

CX	20.00 cm
CY	11.68 cm
F1P	12.024 ppm
F1	3608.70 Hz
F2P	-0.956 ppm
F2	-286.93 Hz
PPMCM	0.64899 ppm/cm
HZCM	194.78177 Hz/cm




```
Current Data Parameters
NAME                 azad
EXPNO                 697
PROCNO                  1

F2 - Acquisition Parameters
Date_             20130614
Time                  2.51
INSTRUM              spect
PROBHD   5 mm Multinucl
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                  10240
DS                      0
SWH           17985.611 Hz
FIDRES        0.548877 Hz
AQ            0.9110004 sec
RG                 2580.3
DW                27.800 usec
DE                 6.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
d12          0.00002000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 7.00 usec
PL1               -4.00 dB
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              21.00 dB
PL13              21.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 65536
SF           75.4677844 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY               200.00 cm
F1P             215.000 ppm
F1             16225.57 Hz
F2P             -5.000 ppm
F2              -377.34 Hz
PPMCM          11.00000 ppm/cm
HZCM          830.14557 Hz/cm
```

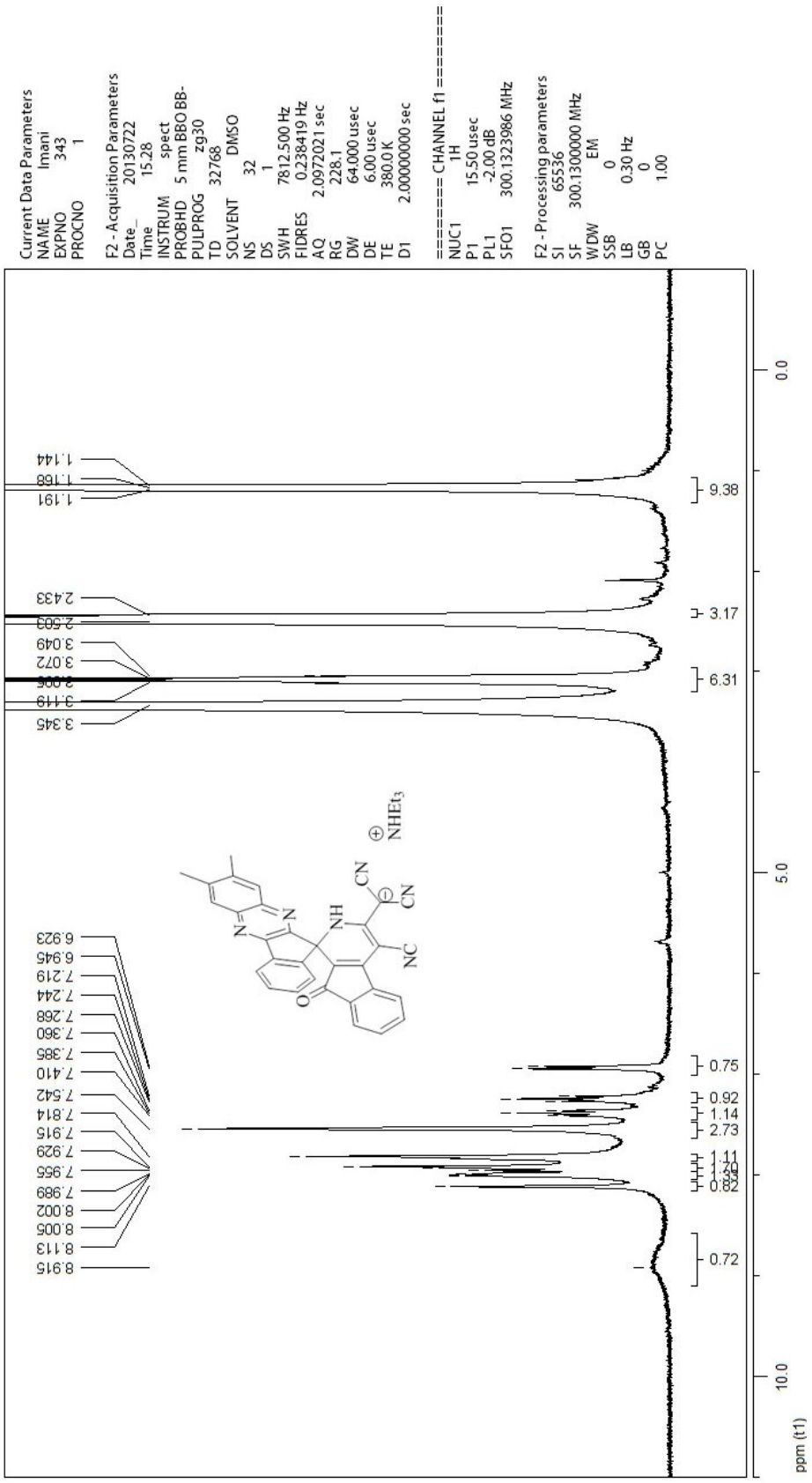


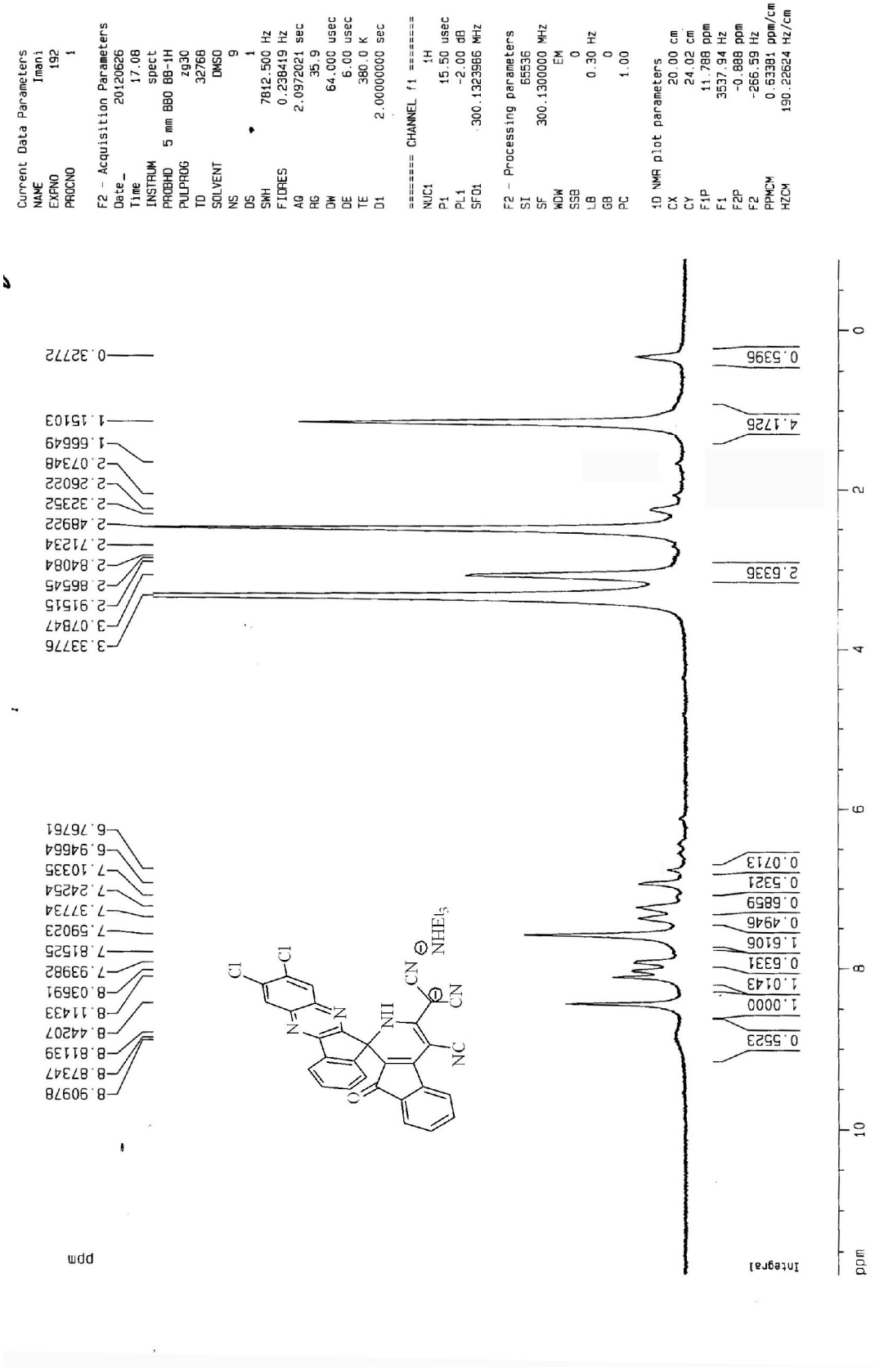
Current Data Parameters
NAME Imani
EXPNO 188
PROCNO 1

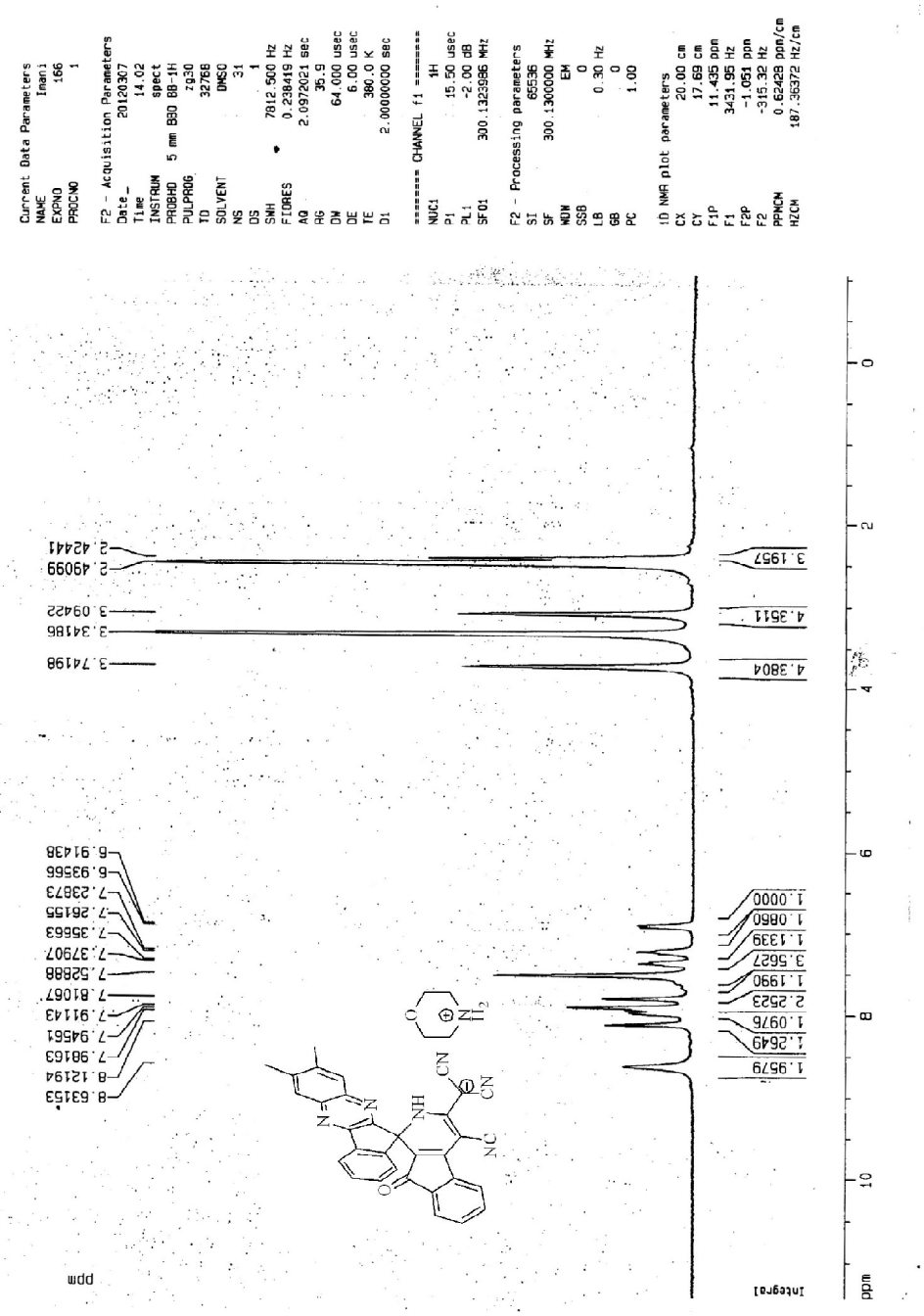
F2 - Acquisition Parameters
Date_ 20120617
Time 13.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 35.9
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

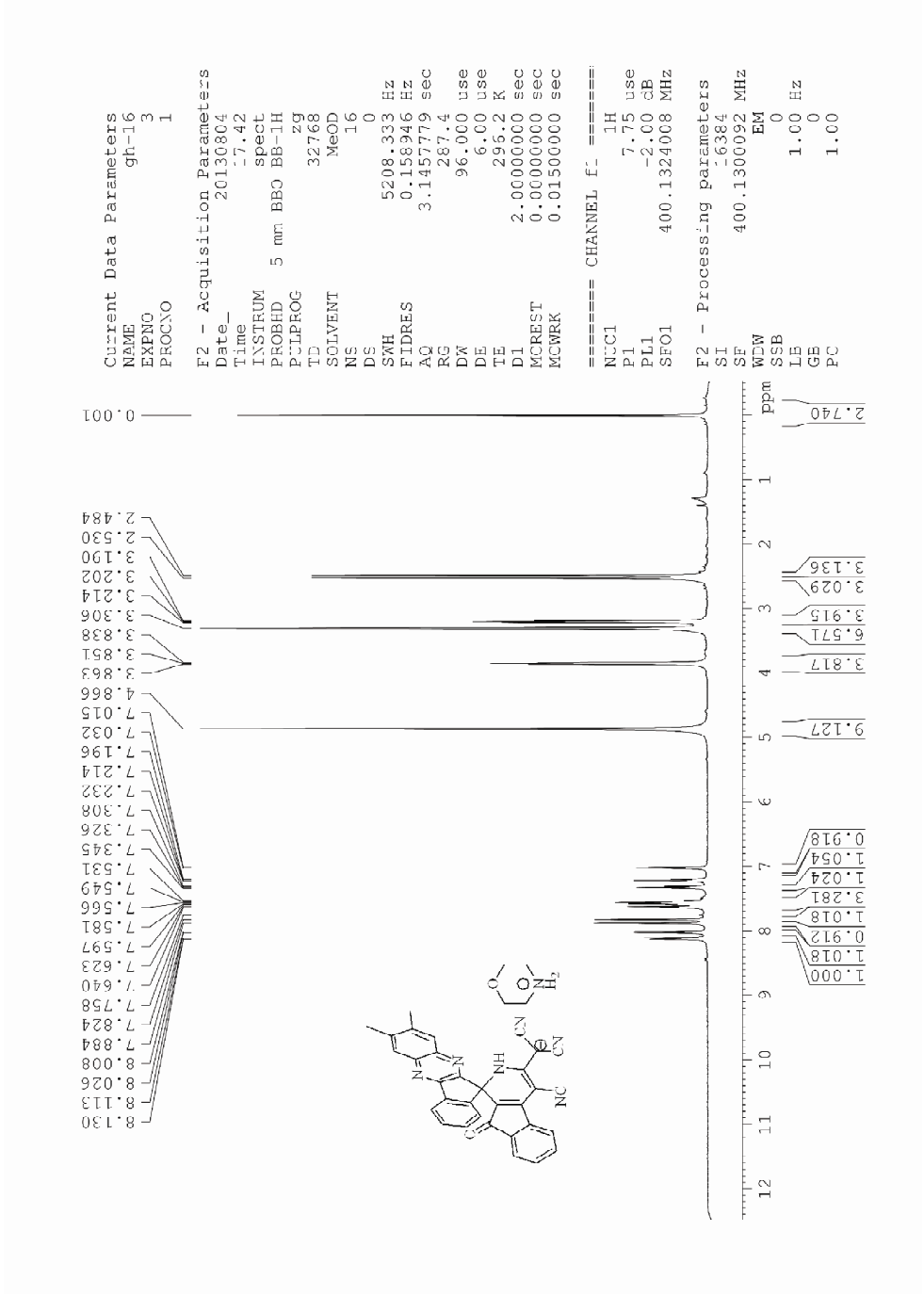
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

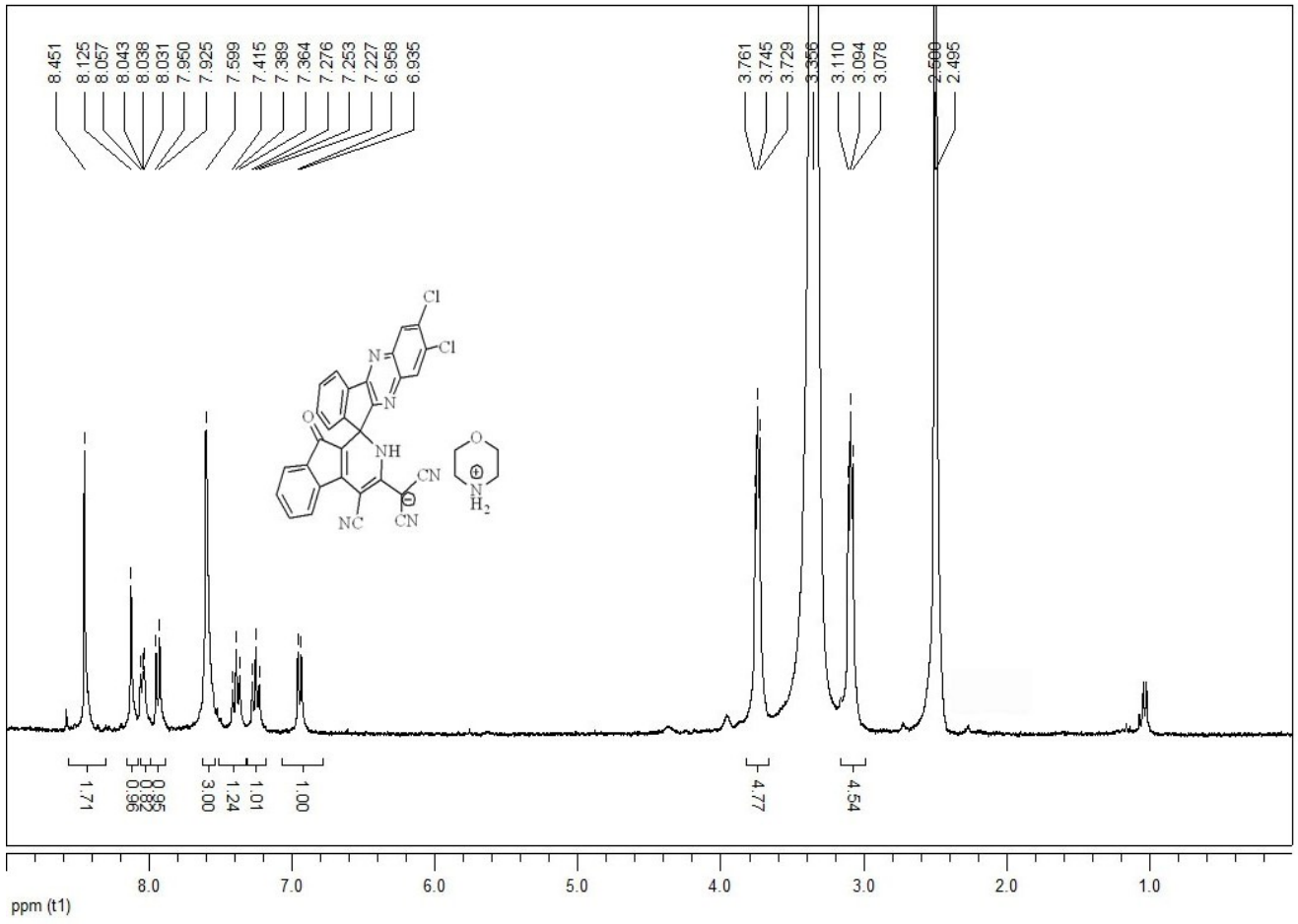

Current Data Parameters
NAME Imani
EXPNO 343
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130722
Time 15.28
INSTRUM spect
PROBHD 5 mm BBO BB-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 32
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 228.1
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.144
1.168
1.191
2.433
2.503
3.049
3.072
3.095
3.119
3.345
6.923
6.945
7.219
7.244
7.268
7.360
7.385
7.410
7.542
7.814
7.915
7.929
7.955
7.989
8.002
8.005
8.113
8.915
9.38
3.17
6.31
0.75
0.92
1.14
2.73
1.11
1.20
1.33
0.82
0.72
NHEt3
CN
CN
NC
NH
N
N
O
10.0
5.0
0.0
ppm (t1)


Current Data Parameters
NAME Imani
EXPNO 192
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120626
Time 17.08
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 9
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 35.9
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 24.02 cm
F1P 11.788 ppm
F1 3537.94 Hz
F2P -0.888 ppm
F2 -266.59 Hz
PPMCM 0.63381 ppm/cm
HZCM 190.22624 Hz/cm
0.32772
1.15103
1.66649
2.07348
2.26022
2.32352
2.48922
2.71234
2.84084
2.86545
2.91515
3.07847
3.33776
6.76761
6.94664
7.10335
7.24254
7.37734
7.59023
7.81525
7.93982
8.03691
8.11433
8.44207
8.81139
8.87347
8.90978
0.5396
4.1726
2.6336
0.0713
0.5321
0.6859
0.4946
1.6106
0.6331
1.0143
1.0000
0.5523
Cl
Cl
N
N
NH
CN
CN
NC
O
NHEt3
ppm
Integral


Current Data Parameters
NAME Inan1
EXPNO 166
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120307
Time 14.02
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 31
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.09720021 sec
RG 36.9
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SF01 300.1323986 MHz
F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 17.69 cm
F1P 11.435 ppm
F1 3431.95 Hz
F2P -1.051 ppm
F2 -315.32 Hz
PPMCM 0.62428 ppm/cm
HZCM 187.36572 Hz/cm
2.42441
2.49099
3.09422
3.34186
3.74198
3.19
4.35
4.38
1.00
1.09
1.26
1.96
6.91438
6.93566
7.23873
7.26155
7.35563
7.37907
7.52688
7.81067
7.91143
7.94561
7.98163
8.12194
8.63153
Integral
ppm


Current Data Parameters
NAME gh-16
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130804
Time -7.42
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg
TD 32768
SOLVENT MeOD
NS 16
DS 0
SWH 5208.333 Hz
FIDRES 0.158946 Hz
AQ 3.1457779 sec
RG 287.4
DW 96.000 use
DE 6.00 use
TE 296.2 K
D1 2.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 7.75 use
PL1 -2.00 dB
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 16384
SF 400.1300092 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
ppm
2.740
9.127
3.817
6.571
3.915
3.029
3.136
1.000
1.018
0.912
1.018
3.281
1.024
1.054
0.918
7.130
8.113
8.026
8.008
7.884
7.824
7.758
7.640
7.623
7.597
7.581
7.566
7.549
7.531
7.345
7.326
7.308
7.232
7.214
7.196
7.032
7.015
4.866
3.863
3.851
3.838
3.306
3.214
3.202
3.190
2.530
2.484
0.001

S53



Current Data Parameters
NAME Imani
EXPNO 193
PROCNO 1

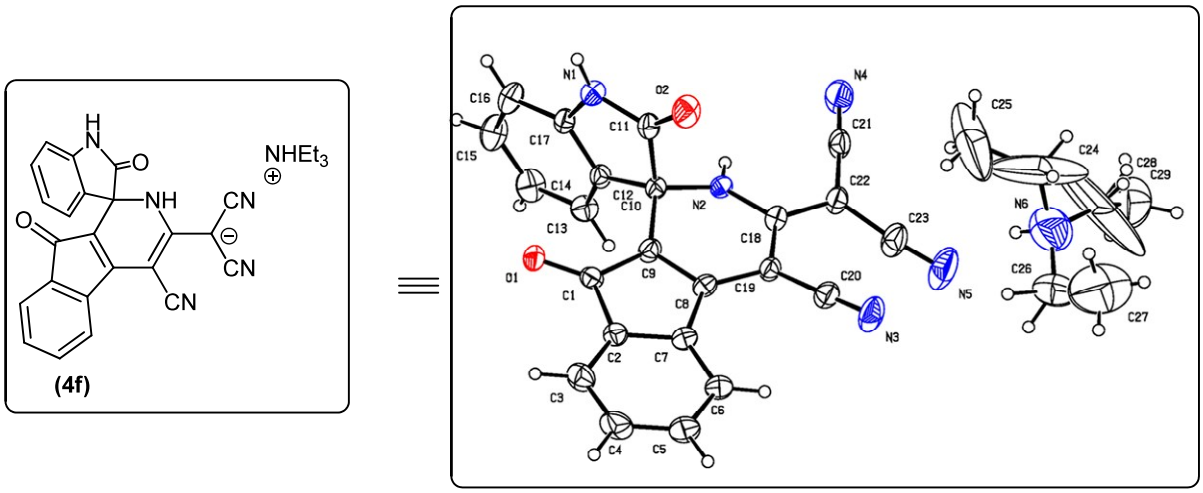
F2 - Acquisition Parameters
Date_ 20120701
Time 16.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 21
DS 1
SWH 7812.500 Hz
FIDRES 0.238419 Hz
AQ 2.0972021 sec
RG 35.9
DW 64.000 usec
DE 6.00 usec
TE 380.0 K
D1 2.00000000 sec

======== CHANNEL f1 ========
NUC1 1H
P1 15.50 usec
PL1 -2.00 dB
SFO1 300.1323986 MHz

F2 - Processing parameters
SI 65536
SF 300.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

1D NMR plot parameters
CX 20.00 cm
CY 91.65 cm
F1P 3.856 ppm
F1 1157.28 Hz
F2P 2.952 ppm
F2 886.07 Hz
PPMCM 0.04518 ppm/cm
HZCM 13.56047 Hz/cm

X-ray crystal structure of 4f.



X-ray crystal structure of 6d.