Electronic Supporting Information (ESI)

Visible light promoted tandem dehydrogenation-deaminative cyclocondensation under aerobic condition for the synthesis of 2-aryl benzimidazoles/quinoxalines from *ortho*-phenylenediamines and arylmethyl/ethyl amines

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SECTION 1. EXPERIMENTAL PROCEDURES AND SPECTRAL DATA

Experimental Procedures:

S1.1. General. The chemicals required for the study were obtained from Sigma-Aldrich Company and were used as such without further purification unless otherwise mentioned. Thin Layer Chromatography (TLC) performed on silica gel aluminium plates monitored the progress of the reaction and visualization was done by UV chamber. ^{1}H NMR and ^{13}C NMR spectra were recorded at 400 MHz and 100 MHz instrument respectively, with TMS as an internal standard. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$, 7.26 ppm; CD_3OD, 3.31 ppm; DMSO-d_6 2.51 ppm). Chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent ($CDCl_3$, 77.16 ppm; CD_3OD, 49.0; DMSO-d_6 39.51 ppm). Coupling constants (*J*) were reported in hertz (Hz). The abbreviations used to characterize the signals are as follows: s = singlet, m = multiplet, d = doublet, br. s. = broad singlet, dd = doublet of doublet, t = triplet. ESI-MS spectra were recorded on Agilent 1100 LC-Q-TOF. IR spectra were recorded on Perkin-Elmer IR spectrophotometer.

Typical procedure for the synthesis of 2-phenyl-1*H*-benzo[*d*]imidazole: To the magnetically stirred mixture of the *o*-phenylenediamine **1a** (108.1 mg, 1 mmol) and benzylamine **2a** (128.5 mg, 1.2 mmol, 131.07 µL) in DMSO (4 mL) was added aq. HCl (0.864 mg, 0.24 mmol, 24 mol%: 20 µL of aq. 12 N HCl) and the mixture was irradiated with visible light (White CFL, 32 W) for 30 h. After completion of the reaction (TLC), the mixture was diluted with water (5 mL) and extracted with EtOAc (3 × 5 mL). The combined EtOAcextracts were dried (anh Na_2SO_4), filtered,the filtrate concentarted under rotary vacuum evaporation, and the residue was charged on to chromatography (100-200 mesh silica gel) column and eluted with 12% EtOAc-hexaneto afford pure **3a** (151.4 mg, 78%). All the remaining reactions were performed on 1 mmol scale following this general procedure and. The spectral data of the synthesised compounds are provided below.

Experimental procedure for the synthesis of 2-aryl quinoxalines: To the magnetically stirred mixture of the *o*-phenylenediamine **1a** (108.1 mg, 1 mmol) and phenethylamine **4a** (145.4 mg, 150.8 µL, 1.2 mmol) in DMSO (4 mL) was added HCl (0.864 mg, 0.24 mmol, 24 mol%: 20 µL of aq. 12 N HCl) and irradiated under visible light (White CFL, 32 W) for 30 h. After completion of

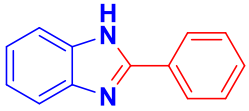
the reaction (TLC), the mixture was diluted with water (5 mL) and extracted with EtOAc (3 × 5 mL). The combined EtOAc extracts were dried (anh Na_2SO_4), filtered, the filtrate was concentarted under rotary vacuum evaporation, the residue was charged on to chromatography (100-200 mesh silica gel) column and eluted with 10% EtOAc-hexane to afford pure **5a** (154.6 mg, 75%). All the remaining reactions were performed following this general procedure and on 1 mmol scale. The spectral data of the synthesised compounds are provided below.

Separation of the regioisomeric mixtures of 5m & 5m^1 and of 5n & 5n^1 by column chromatography: The separation of regioisomeric products was achieved by adsorbing the crude reaction mixture on silica gel (60-120 mesh size) and charged on the column chromatography of silica gel (230-400 mesh size) and eluting with hexane-EtOAc (98:2) to obtain the pure regioisomers. In case of separation of the regioisomeric mixture of **5m** and **5m^1**, the compound **5m** eluted first (67 mg, 30% yield) followed by the compound **5m^1** (89 mg, 40% yield). In case of separation of the regioisomeric mixture of **5n** and **5n^1**, the compound **5n** eluted first (60 mg, 25% yield) followed by the compound **5n^1** (103 mg, 43% yield).

Spectral Data:

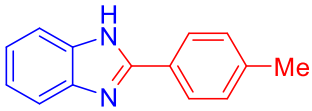
(**Note:** In general, in a ^{1}H NMR spectrum recorded in $CDCl_3$, a peak at around δ 1.6 refers to moisture in the solvent/sample and a peak at δ 1.2 refers to oil/grease present in the sample. Similarly, in ^{1}H NMR spectrum recorded in DMSO, a peak at around δ 3.3 refers to moisture in the solvent/sample.

2-Phenyl-1*H*-benzo[*d*]imidazole (3a)[1]



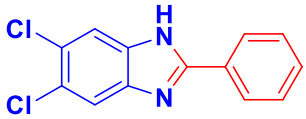
White solid; 151.4 mg, 78%, m.p 294-297 °C (295-298 °C)[2]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.93 [s, 1H (NH)], 8.21 (d, J = 8 Hz, 2H), 7.69 (d, J = 8 Hz, 1H), 7.58-7.48 (m, 4H), 7.23 (t, J = 8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 144.3, 135.5, 130.6, 130.3, 129.4, 126.9, 122.9, 122.1, 119.3, 111.8; IR ($CHCl_3$): ν_{max} 2955.1, 2920.8, 2870.4, 1713.2, 1458.4, 1377.9, 1275, 1260.7, 1187.8, 1081.5, 1019 cm^{-1}; ESI-MS (m/z): 195.20 $[M+H]^+$.

2-(4-Methylphenyl)-1*H*-benzo[d]imidazole (3b)[2]



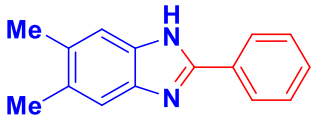
Off white solid; 145.7 mg, 70%, m.p 266-268 ℃ (267-269 ℃)[2]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.82 [s, 1H (NH)], 8.08 (d, *J* = 8 Hz, 2H), 7.65-7.51 (m, 2H), 7.37 (d, *J* = 8 Hz, 2H), 7.22-7.17 (m, 2H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.8, 144.3, 140, 135.4, 129.9, 129.4, 127.9, 126.8, 122.8, 122, 119.2, 111.6, 21.4; IR ($CHCl_3$): ν_{max}3405.9, 2924.7, 2255, 1657.4, 1457.1, 1378.3, 1275.6, 1260.9, 1023.5, 999.1 cm^{-1}; ESI-MS (*m*/*z*): 209.06 $[M+H]^+$.

5,6-Dichloro-2-phenyl-1*H*-benzo[*d*]imidazole (3i)[1]



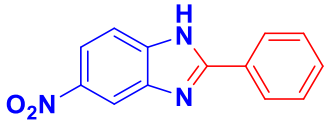
White solid; 188.6 mg, 72%, m.p 225-227 ℃ (226-227 ℃)[5]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.3 [s, 1H (NH)], 8.19 (d, *J* = 8 Hz, 2H), 7.95 (s, 1H), 7.91 (d, *J* = 8 Hz, 1H), 7.77 (s, 1H), 7.59-7.54 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.6, 143.8, 135.3, 131, 129.7, 128.7, 127.7, 127.1, 120.2, 113.4; IR ($CHCl_3$): ν_{max} 2954.9, 2922.9, 2854.2, 1711.9, 1457.5, 1378, 1275.5, 1260.8, 1189, 1081.4, 1027.9 cm^{-1}; ESI-MS (*m*/*z*): 340.99 $[M+H]^+$.

5,6-Dimethyl-2-phenyl-1*H*-benzo[*d*]imidazole (3j)[3]



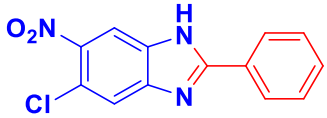
White solid; 151.0 mg, 68%, m.p 245-248 ℃ (246-248 ℃)[5]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.65 [s, 1H (NH)], 8.16 (d, *J* = 8 Hz, 2H), 7.55 (t, *J* = 8Hz, 2H), 7.48 (t, *J* = 8 Hz, 2H), 7.30 (s, 1H), 2.34 (s, 3H), 2.32 (s, 3H); ^{13} C NMR (100 MHz, DMSO-d_6) δ 150.8, 142.9, 133.9, 131.6, 130.4, 130.8, 129.9, 129.3, 126.6, 119.4, 111.8, 20.5 IR ($CHCl_3$): ν_{max} 3434.9, 2251.8, 2125.6, 1770.3, 1658.4, 1451, 1376.3, 1240.2, 1031 cm^{-1}; ESI-MS (*m*/*z*): 223.11 $[M+H]^+$.

5-Nitro-2-phenyl-1*H*-benzo[*d*]imidazole (3g)[3]



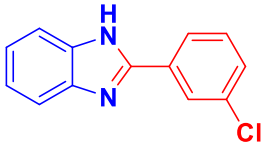
White solid; 181.7 mg, 76%, m.p 207-209 °C (208-209 °C)[5]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.44 (s, 1H), 8.21 (d, *J* = 8Hz, 2H), 8.11 (d, *J* = 8 Hz, 1H), 7.74 (d, *J* = 8 Hz, 1H), 7.59-7.57 (m, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 156.2, 144.3, 143.1, 139.5, 137.4, 131.4, 129.6, 127.4, 118.4, 116.3, 111.5; IR ($CHCl_3$): ν_{max}3428.9, 2253.2, 2126.4, 1658.6, 1275.8, 1260.9, 1051.2, 1023.4, 1003.6 cm^{-1}; ESI-MS (*m*/*z*): 240.06 $[M+H]^+$.

5-Chloro-6-nitro-2-phenyl-1*H*-benzo[*d*]imidazole (3k)



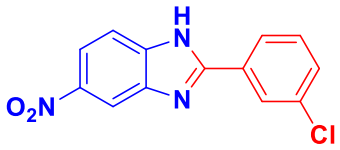
Off white low melting solid; 188.4 mg, 69%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.34 (s, 1H), 8.21 (d, *J* = 8Hz, 2H), 7.88 (s, 1H), 7.60-7.58 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.8, 143.1, 142.3, 138.2, 131.5, 129.6, 129.2, 127.5, 119.2, 117.1, 113.9; IR ($CHCl_3$): ν_{max} 3440.1, 3049.4, 2299.9, 1646.5, 1275.1, 1052.7, 1026.3, 1007.4 cm^{-1}; ESI-MS (*m*/*z*)): 274.03 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{13}H_9ClN_3O_2$ 274.0378; Found 274.0375.

2-(3-Chlorophenyl)-1*H*-benzo[*d*]imidazole (3c)[2]



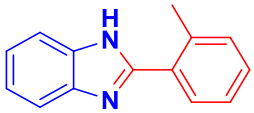
White solid; 175.6 mg, 77%, m.p 239-241 °C (238-240 °C)[2]; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.07 (s, 1H), 8.24 (s, 1H), 8.16 (d, *J* = 4Hz, 1H), 7.70 (d, *J* = 4Hz, 1H), 7.61-7.55 (m, 3H), 7.26 (t, *J* = 8Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150, 143.9, 135.5, 134.6, 132.7, 131.4, 129.9, 126.8, 125.6, 123.4, 122.8, 119.6, 111.9; IR ($CHCl_3$): ν_{max}3434.9, 2252.6, 2126.3, 1658.2, 1441.4, 1275.9, 1027.1 cm^{-1}; ESI-MS (*m*/*z*): 229.04 $[M+H]^+$.

2-(3-Chlorophenyl)-5-nitro-1*H*-benzo[*d*]imidazole (3h)[4]



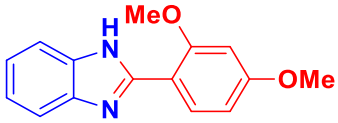
Off white solid; 218 mg, 80%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.50 (s, 1H), 8.25 (s, 1H), 8.19-8.14 (m, 2H), 7.80 (d, *J* = 8Hz, 1H), 7.65-7.64 (m, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 154.5, 142.8, 138.2, 133.9, 131.1, 131, 126.5, 125.9; IR ($CHCl_3$): ν_{max} 3434.9, 2253, 2126.7, 1658.6, 1344.8, 1241.1, 1027, 1007 cm^{-1}; ESI-MS (*m*/*z*): 273.98 $[M+H]^+$.

2-(2-Methylphenyl)-1*H*-benzo[*d*]imidazole (3d)[5]



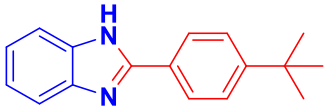
Off white solid; 145.6 mg, 70%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.76 (d, *J* = 4Hz, 1H), 7.63-7.61 (m, 2H), 7.43-7.35 (m, 3H), 7.24-7.20 (m, 2H), 2.62 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 152.4, 137.5, 131.7, 130.5, 129.9, 129.8, 126.4, 122.4, 21.5; IR ($CHCl_3$): ν_{max} 2923.4, 2853.9, 1733.9, 1457.1, 1378.2, 1260.3, 1025.2 cm^{-1}; ESI-MS (*m*/*z*): 208.95 $[M+H]^+$.

2-(2,4-Dimethoxyphenyl)-1*H*-benzo[*d*]imidazole (3e)[6]



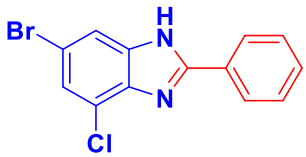
Off white solid; 157.5 mg, 62%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 8.27 (d, *J* = 8Hz, 1H), 7.60-7.57 (m, 2H), 7.17-7.15 (m, 2H), 6.77-6.71 (m, 2H), 4.03 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 158.5, 149.6, 131.3, 121.9, 111.4, 106.7, 99, 56.3, 55.9; IR ($CHCl_3$): ν_{max} 3420.2, 3051.9, 1646.6, 1275.1, 1050.2, 1024.4, 1004.5 cm^{-1}; ESI-MS: 255.15 $[M+H]^+$.

2-(4-*tert*-Butylphenyl)-1*H*-benzo[*d*]imidazole (3f)[5]



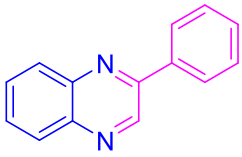
Off white solid; 180 mg, 72%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 12.87 (s, 1H), 8.13 (d, *J* = 8Hz, 2H), 7.67 (d, *J* = 8Hz, 1H), 7.58 (d, *J* = 8Hz, 2H), 7.54 (d, *J* = 8Hz, 1H), 7.23 (t, *J* = 8Hz, 2H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 153, 1517, 144.1, 135.3, 127.9, 126.7, 126.2, 122.8, 122.1, 119.2, 111.7, 35, 31.5; IR ($CHCl_3$): ν_{max} 3399, 1675.4, 1275.6, 1023.1, 996.4 cm^{-1}; ESI-MS (*m*/*z*): 251.67 $[M+H]^+$

6-Bromo-4-chloro-2-phenyl-1*H*-benzo[*d*]imidazole (3l)



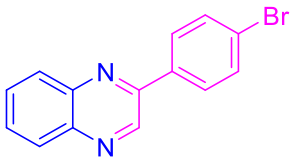
Off white solid; 214 mg, 70%; ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.40 (s, 1H), 8.29-8.19 (m, 2H), 7.68 (s, 1H), 7.57 (t, *J* = 8Hz, 3H), 7.46)s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 153.4, 140.6, 137.4, 131, 129.6, 129.5, 127.3, 124.4, 124.2, 114.6, 113.7; ESI-MS (*m*/*z*): 306.95 $[M+H]^+$.

2-Phenylquinoxaline (5a)[7]



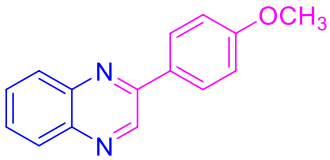
Off white solid; 154.6 mg, 75%, m.p 72-72 ^{0}C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.35 (s, 1H), 8.23-8.13 (m, 4H), 7.82-7.74 (m, 2H), 7.60-7.52 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.8, 143.4, 142.3, 141.6, 136.8, 130.3, 130.2, 129.6, 129.5, 129.1, 127.6 cm^{-1}; ESI-MS (*m*/*z*): 207 $[M+H]^+$HRMS (ESI-TOF) m/z: $[M+ H]^+$calcd for $C_{14}H_{11}N_2$ 207.0917; Found 207.0923.

2-(4-Bromophenyl)quinoxaline (5b)[7]



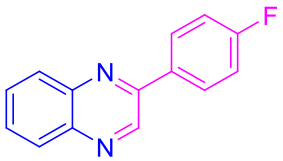
Light brown solid; 215.8 mg, 76%; m.p 138-140℃ (138 ℃)[10]; ^{1}H NMR (400 MHz, MeOD): δ 9.42 (s, 1H), 8.24 (d, *J* = 8 Hz, 2H), 8.17 (d, *J* = 8 Hz, 2H), 8.13 (d, *J* = 8 Hz, 2H), 7.90-7.83 (m, 2H), 7.78 (d, *J* = 12 Hz, 2H); ^{13}CNMR (100 MHz, MeOD): δ 150.8, 142.8, 142, 141.2, 135.5, 132, 130.5, 129.9, 129.1, 128.9, 128.3, 124.6 cm^{-1}; ESI-MS (*m*/*z*): 285 $[M+2H]^{+}$; HRMS (ESI-TOF) m/z: $[M+H]^{+}$calcd for $C_{14}H_{10}BrN_2$ 285.0022; Found 285.0026.

2-(4-Methoxyphenyl)quinoxaline (5c)[7]



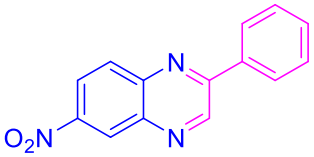
Off white solid; 153.5 mg, 65%; m.p 96-98 ℃ (97-98 ℃)[10]; ^{1}H NMR (400 MHz, MeOD): δ 9.33 (s, 1H), 8.22 (d, *J* = 8Hz, 2H), 8.10-8.04 (m, 2H), 7.82-7.76 (m, 2H), 7.12 (d, *J* = 2H), 3.90 (s, 3H); ^{13}C NMR (100 MHz, MeOD): δ 161.9, 151.7, 142.8, 142.1, 140.5, 130.3, 129.1, 128.8, 128.7, 128.1, 114.2, 54.5; ESI-MS (*m*/*z*): 237 $[M+H]^{+}$.

2-(4-Fluorophenyl)quinoxaline (5d)[8]



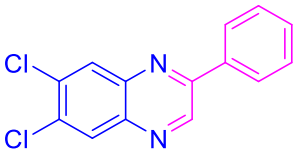
Off white solid; 172.5 mg, 77%, m.p 128-131; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.21-8.18 (m, 2H), 8.14-8.11 (m, 2H), 7.79-7.74 (m, 2H), 7.27-7.23 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.5 (J_{CF1} = 249 Hz), 150.7, 142.9, 142.2, 141.5, 132.9 ($^{4}J_{CF}$ = 3Hz), 130.4, 129.6, 129.5, 129.4, 129.1, 116.3 ($^{2}J_{CF}$ = 21 Hz); ESI-MS (*m*/*z*): 225 $[M+H]^{+}$.

6-Nitro-2-phenylquinoxaline (5e)[9]



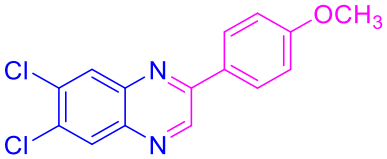
Off white solid; 163.2 mg, 65%, m.p 199-202; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.53 (s, 1H), 9.06 (s, 1H), 8.60 (d, *J* = 1H), 8.33-8.28 (m, 3H), 7.65-7.63 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.5, 140.1, 131.1, 129.4, 127.9, 125.6, 123.8; ESI-MS (*m*/*z*): 252 $[M+H]^+$.

6,7-Dichloro-2-phenylquinoxaline (5f)[8]



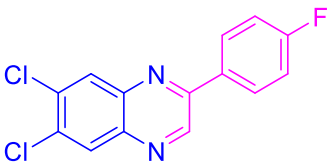
White solid; 186 mg, 68%, m.p 158-161; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.34 (s, 1H), 8.30 (s, 1H), 8.26 (s, 1H), 8.22 (d, *J* = 8 Hz, 2H), 7.61-7.59 (m, 3H); ^{13}CNMR (100 MHz, $CDCl_3$): δ 152.6, 144.3, 141.1, 140.3, 136, 134.9, 134, 130.8, 130.2, 129.8, 129.3, 127.6; ESI-MS (*m*/*z*): 275 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+H]^+$calcd for $C_{14}H_9Cl_2N_2$ 275.0137; Found 275.0144.

6,7-Dichloro-2-(4-methoxyphenyl)quinoxaline (5g)



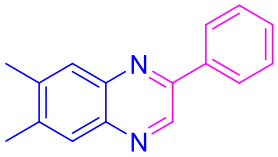
Off white solid; 185 mg, 61%, m.p 203-205; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.29 (s, 1H), 8.24-8.17 (m, 4H), 7.11-7.09 (m, 2H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.9, 152.2, 143.9, 141.1, 139.6, 134.7, 133.3, 129.9, 129.7, 129.1, 128.4, 114.7, 55.5; ESI-MS (*m*/*z*): 305 $[M+H]^+$.

6,7-Dichloro-2-(4-fluorophenyl)quinoxaline (5h)



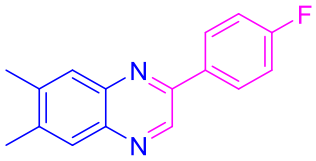
Off white solid; 207 mg, 71%, ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.31 (s, 1H), 8.28 (d, *J* = 12 Hz, 1H), 8.24-8.19 (m, 2H), 7.31-7.25 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.8 (J_{CF1} = 249 Hz), 151.5, 143.8, 140.9, 140.2, 135.1, 134.1, 132.1, 130.1, 129.8, 129.7, 116.5 (J_{CF2} = 22 Hz); ESI-MS (*m/z*): 292 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+H]^+$calcd for $C_{14}H_8Cl_2FN_2$ 293.0043; Found 293.0035.

6,7-Dimethyl-2-phenylquinoxaline (5i)[8]



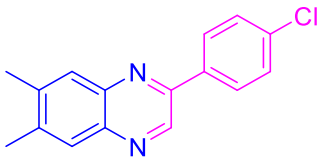
Off white solid; 170.9 mg, 73%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.47 (s, 1H), 8.32-8.30 (m, 2H), 7.92 (s, 1H), 7.89 (s, 1H), 7.62-7.56 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 150.5, 143.1, 141.4, 140.8, 140.7, 136.8, 130.6, 129.6, 128.6, 128.2, 127.7, 20.3; ESI-MS (*m/z*): 235 $[M+H]^+$.

2-(4-Fluorophenyl)-6,7-dimethylquinoxaline (5j)[10]



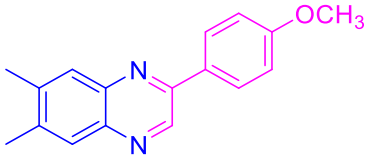
Off white solid; 191.6 mg, 76%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.17 (s, 1H), 8.18-8.14 (m, 2H), 7.86 (d, *J* = 8Hz, 2H), 7.25 (t, *J* = 8Hz, 2H), 2.50 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 165.25 (J_{CF1} = 248 Hz), 149.8, 141.9, 141.1, 140.9, 140.2, 129.3, 129.2, 128.5, 128.1, 116.2 (J_{CF2} = 21 Hz), 20.4, 20.3; ESI-MS (*m/z*): 253 $[M+H]^+$. HRMS (ESI-TOF) m/z: $[M+H]^+$calcd for $C_{16}H_{14}FN_2$ 253.1136; Found 253.1146.

2-(4-Chlorophenyl)-6,7-dimethylquinoxaline (5k)[10]



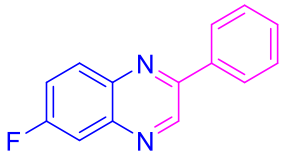
Off white solid; 195.6 mg, 73%, ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.19 (s, 1H), 8.14 (d, *J* = 8 Hz, 2H), 7.89 (d, *J* = 12 Hz, 2H), 7.54 (d, *J* = 2H), 2.53 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.7, 141.9, 141.1, 140.6, 140.5, 135.5, 129.3, 128.6, 128.1, 20.4, 20.3; ESI-MS (*m*/*z*): 269 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+ H]^+$calcd for $C_{16}H_{14}ClN_2$ 269.0840; Found 269.0838.

2-(4-Methoxyphenyl)-6,7-dimethylquinoxaline (5l)[8]



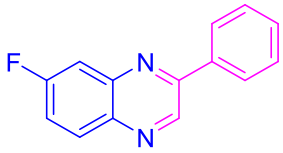
Off white solid; 163.7 mg, 62%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.19 (s, 1H), 8.16 (d, *J* = 8 Hz, 2H), 7.88 (s, 1H), 7.84 (s, 1H), 7.12 (d, *J* = 8 Hz, 2H), 3.91 (s, 3H), 2.51 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.2, 150.7, 142.1, 140.7, 140.1, 139.6, 129.6, 128.8, 128.5, 128.1, 114.5, 55.4, 20.4, 20.3; ESI-MS (*m*/*z*): 265 $[M+H]^+$.

6-Fluoro-2-phenylquinoxaline (5m)[8]



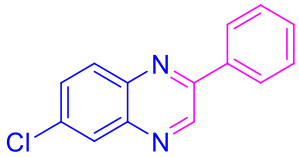
Off white solid; 67 mg, 30%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.35 (s, 1H), 8.22-8.17 (m, 2H), 7.79 (d, *J* = 8Hz, 1H), 7.63-7.56 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 163.76 (J_{CF1} = 250 Hz), 151.4, 144.1, 142.1, 139.5, 131.7, 130.3, 129.2, 122.4, 120.8, 120.6, 112.8 (J_{CF2} = 22 Hz); ESI-MS (*m*/*z*): 225 $[M+H]^+$HRMS (ESI-TOF) m/z: $[M+ H]^+$ calcd for $C_{14}H_{10}FN_2$ 225.0823; Found 225.0829.

7-Fluoro-2-phenylquinoxaline (5m[1])[8]



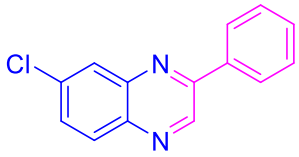
Off white solid; 89 mg, 40%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.27 (s, 1H), 8.18 (d,*J* =8Hz, 2H), 8.11 (dd, *J* = 4, 8 Hz, 1H), 7.76-7.74 (m, 1H); 7.57-7.48 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.1 (J_{CF1} = 201 Hz), 152.6, 144.1, 143.3, 142.7 (J_{CF4}=3 Hz),138.9, 136.5, 131.3 (J_{CF3} = 8 Hz), 130.6, 129.3, 127.7, 120.1, 113.2 ESI-MS (*m*/*z*): 225 $[M+H]^+$.

6-Chloro-2-phenylquinoxaline (5n)[7]



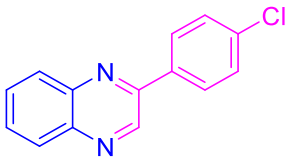
Off white solid; 60 mg, 25%, ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.36 (s, 1H), 8.23-8.21 (m, 2H), 8.15 (m, 2H), 7.77 (dd, *J* = 4, 8 Hz, 1H), 7.63-7.56 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.9, 144.2, 141.8, 140.8, 136.3, 135.2, 131.3, 130.8, 130.4, 129.4, 128.0, 127.5, ESI-MS (*m*/*z*): 241 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+H]^+$ calcd for $C_{14}H_{10}ClN_2$ 241.0527; Found 241.0538.

7-Chloro-2-phenylquinoxaline (5n[1])[7]



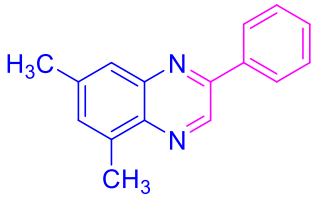
Off white solid; 103 mg, 43%; m.p 104-106 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.33 (s, 1H), 8.22-8.20 (m, 2H), 8.18 (d, *J* = 4 Hz, 1H), 8.08 (d, *J* = 8 Hz, 1H), 7.72 (dd, *J* = 4, 8 Hz, 1H), 7.62-7.55 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 143.4, 142.7, 140.0, 136.3, 136.1, 130.6, 130.5, 130.3, 129.2, 128.5, 127.6; ESI-MS (*m*/*z*): 241 $[M+H]^+$.

2-(4-Chlorophenyl)quinoxaline (5o)[7]



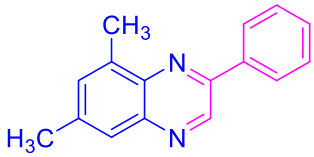
Off white solid; 180 mg, 75%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.30 (s, 1H), 8.17-8.12 (m, 4H), 7.83-7.75 (m, 2H), 7.56 (d, *J* = 12 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.5, 141.8, 141.1, 140.6, 135.5, 134.1, 129.4, 128.7, 128.5, 128.3, 128.1, 127.7; ESI-MS (*m*/*z*): 241 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+ H]^+$calcd for $C_{14}H_{10}ClN_2$ 241.0527; Found 241.0536.

5,7-Dimethyl-2-phenylquinoxaline (5p)



Off white solid; 75 mg, 32%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.28 (s, 1H), 8.21 (d, *J* = 8 Hz, 2H), 7.79 (s, 1H), 7.60-7.51 (m, 3H), 7.44 (s, 1H), 2.81 (s, 3H), 2.58 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 151.3, 142.6, 141.1, 140.4, 139.3, 137.1, 136.7, 132, 129.9, 129.1, 127.5, 126.4, 21.9, 17.2; ESI-MS (*m*/*z*): 235 $[M+H]^+$; HRMS (ESI-TOF) m/z: $[M+ H]^+$ calcd for $C_{16}H_{15}N_2$ 235.1230; Found 235.1236.

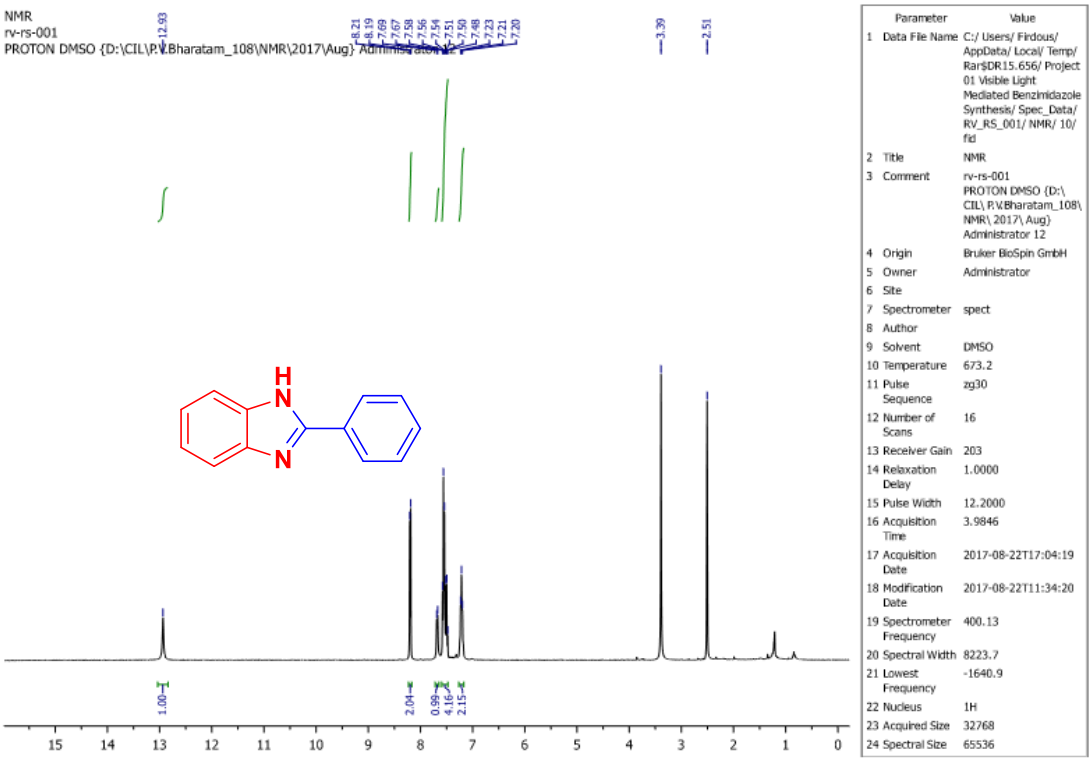
6,8-Dimethyl-2-phenylquinoxaline (5p[1])



Off white solid; 82 mg, 35%; ^{1}H NMR (400 MHz, $CDCl_3$): δ 9.29 (s, 1H), 8.27 (d, *J* = 8 Hz, 2H), 7.73 (s, 1H), 7.59-7.49 (m, 3H), 7.46 (s, 1H), 2.85 (s, 3H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): 149.4, 142.5, 141.8, 139.8, 139.7, 137.3, 137.2, 132.5, 129.8, 129.0, 127.3, 125.7, 21.9, 16.9; ESI-MS (*m*/*z*): 235 $[M+H]^+$.

Section 2. Scanned ^{1}H NMR, ^{13}C NMR, and HRMS Spectra

^{1}H NMR of 2-phenyl-1H-benzo[d]imidazole (3a)



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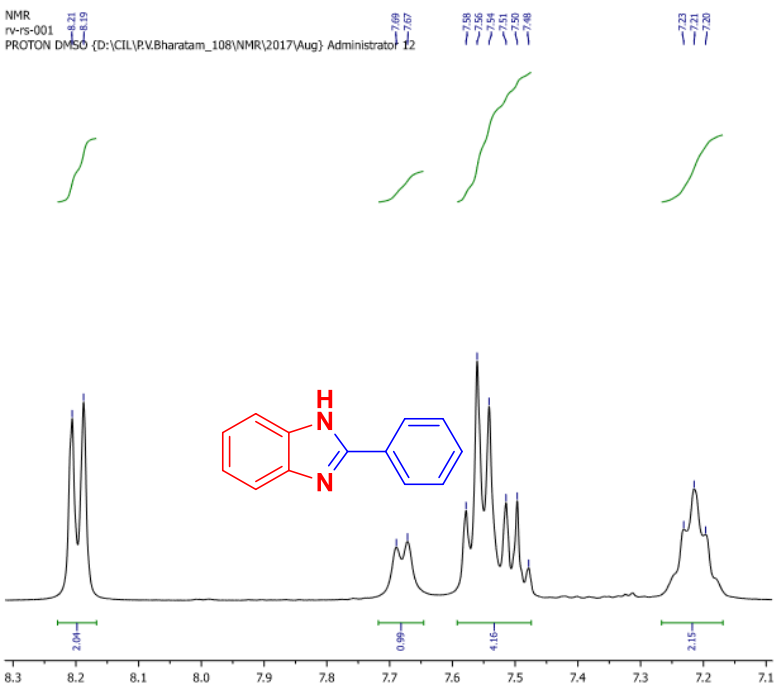
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR15.656/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV_RS_001/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-001 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Aug} Administrator 12
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-08-22T17:04:19
18	Modification Date	2017-08-22T11:34:20
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of aromatic region of ^{1}H NMR of 2-phenyl-1H-benzo[d]imidazole (3a)



	Parameter	Value
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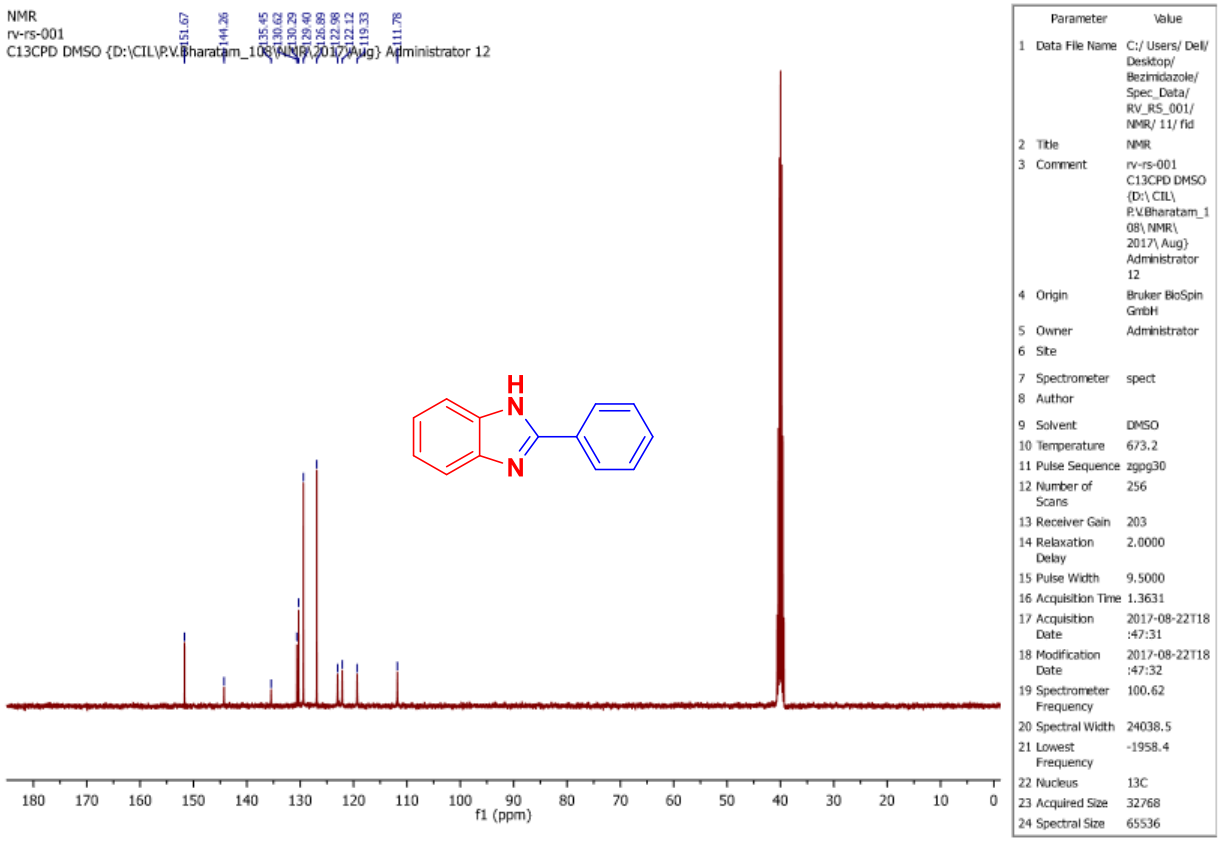
2	Title	NMR
3	Comment	rv-rs-001 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Aug} Administrator 12
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-08-22T17:04:19
18	Modification Date	2017-08-22T11:34:20
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-phenyl-1H-benzo[d]imidazole (3a)



	Parameter	Value
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2	Title	NMR
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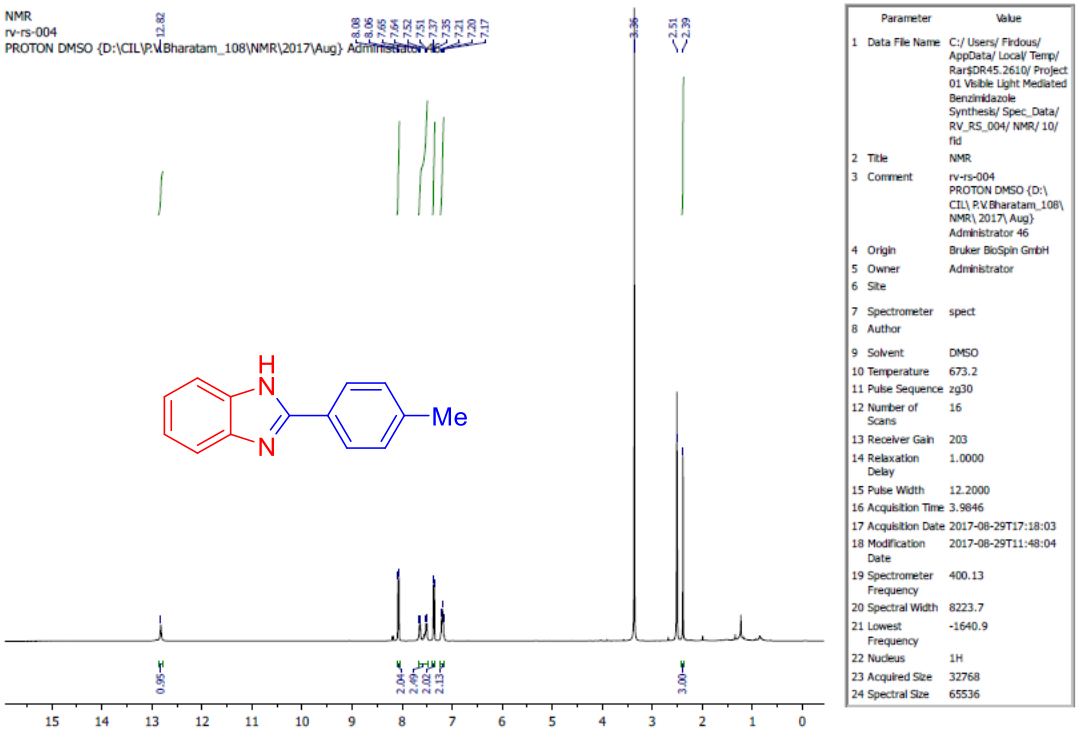
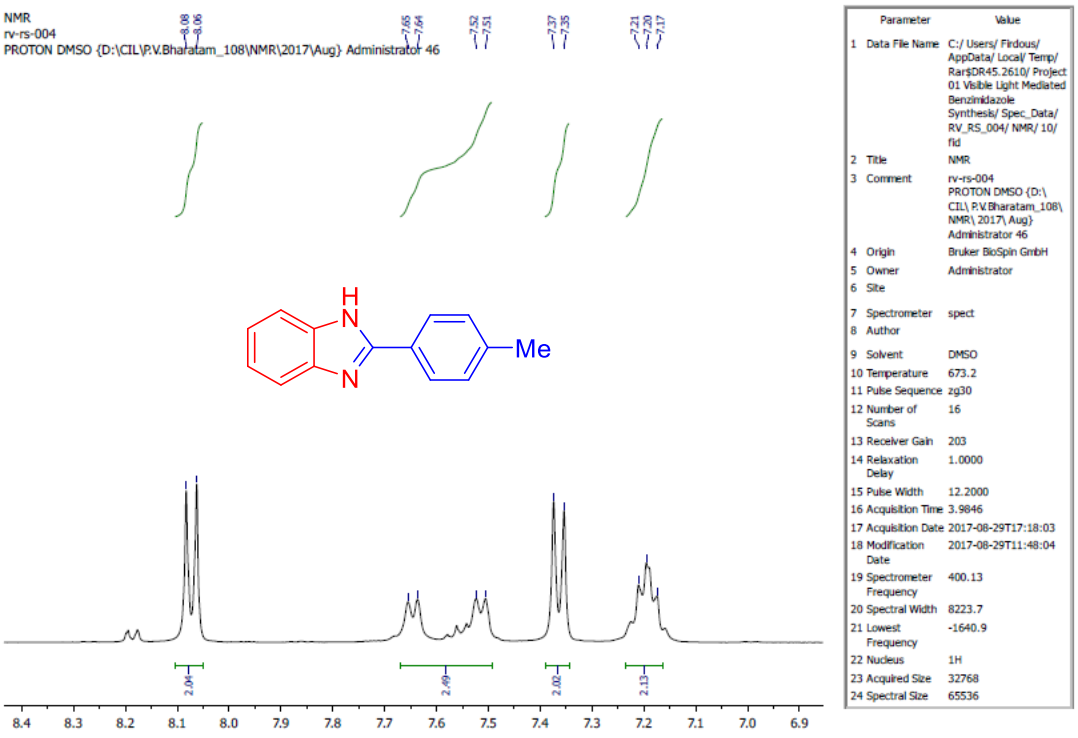
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2017-08-22T18 :47:31
18	Modification Date	2017-08-22T18 :47:32
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(4-methylphenyl)-1H-benzo[d]imidazole (3b)



	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR45.2610/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV_RS_004/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-004 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Aug} Administrator 46
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-08-29T17:18:03
18	Modification Date	2017-08-29T11:48:04
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of aromatic region of ^{1}H NMR of 2-(4-methylphenyl)-1H-benzo[d]imidazole (3b)



	Parameter	Value
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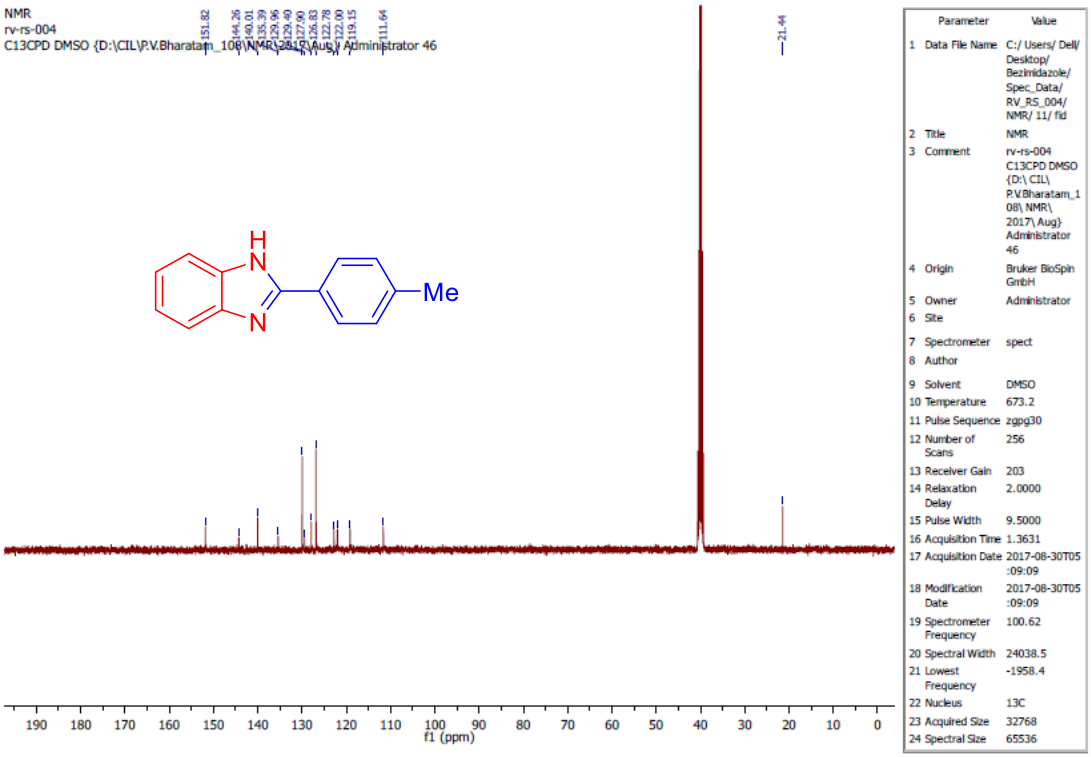
2	Title	NMR
3	Comment	rv-rs-004 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Aug} Administrator 46
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-08-29T17:18:03
18	Modification Date	2017-08-29T11:48:04
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-methylphenyl)-1H-benzo[d]imidazole (3b)



	Parameter	Value
1	Data File Name	C:/ Users/ Dell/ Desktop/ Bezimidazole/ Spec_Data/ RV_RS_004/ NMR/ 11/ fid
2	Title	NMR
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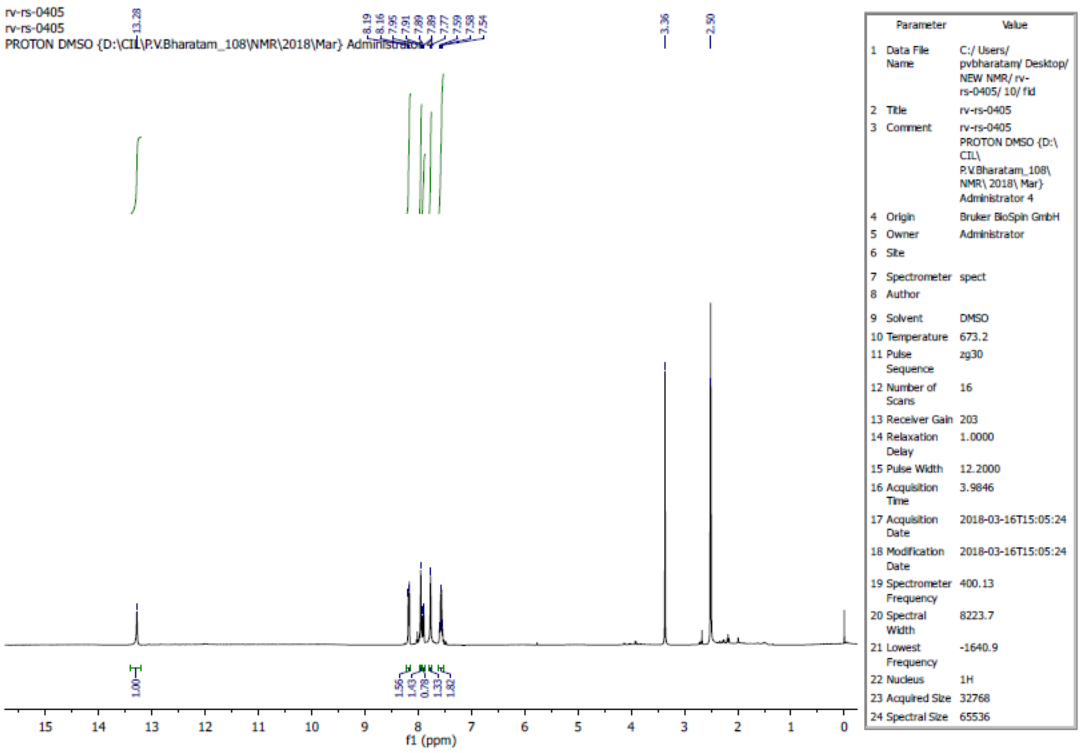
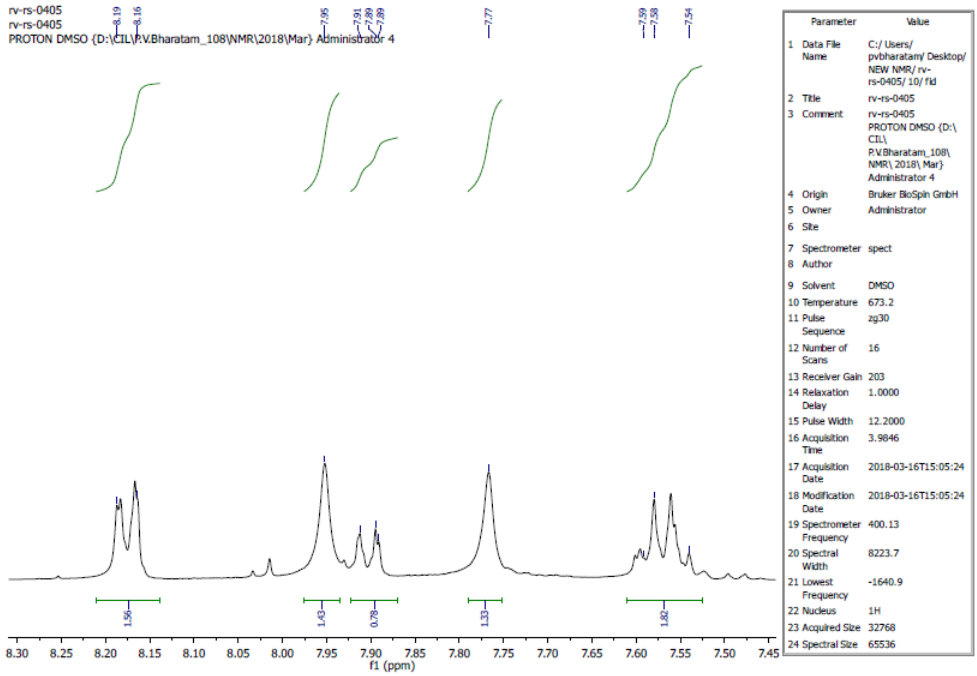
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2017-08-30T05:09:09
18	Modification Date	2017-08-30T05:09:09
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

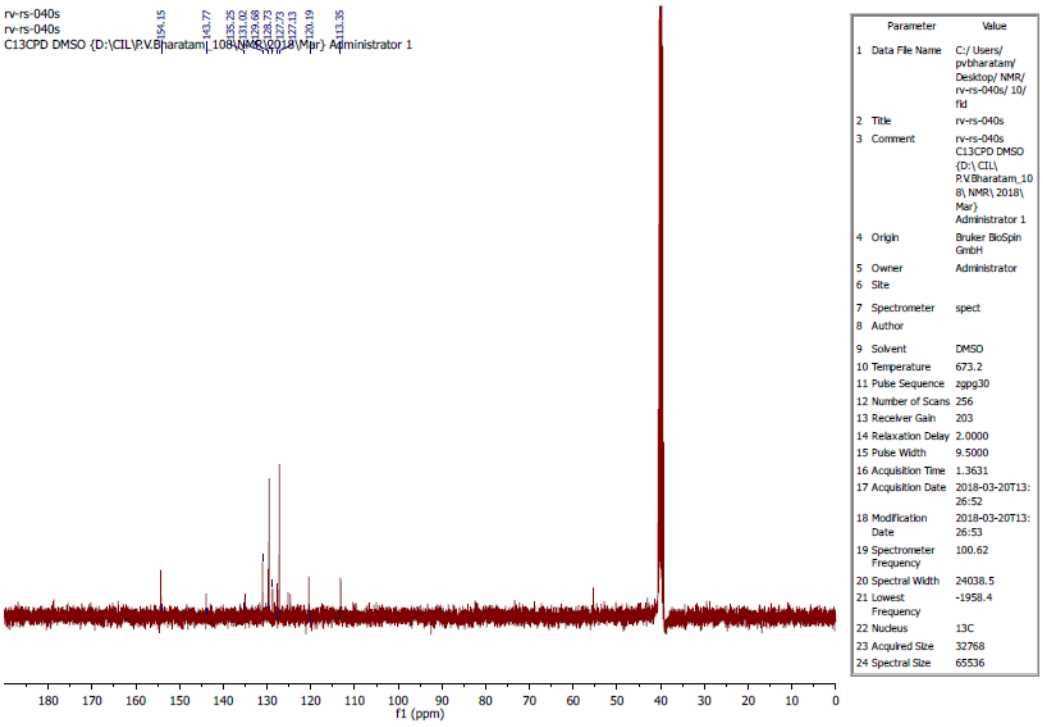
^{1}H NMR of 5, 6-dichloro-2-phenyl-1H-benzo[d]imidazole (3i)



Expansion of the aromatic region of the ^{1}H NMR of 5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (3i)



^{13}C NMR of 5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (3i)



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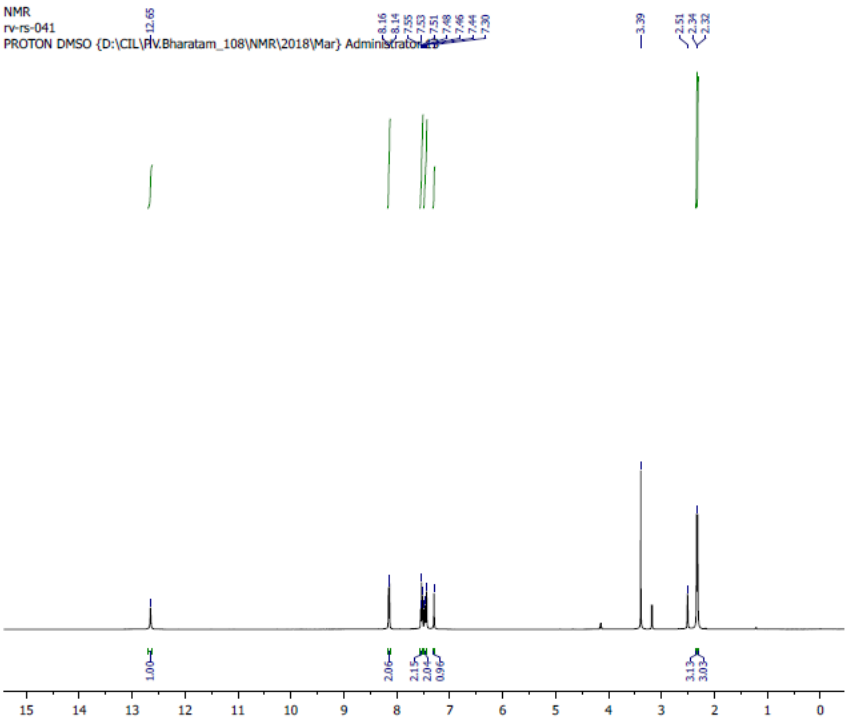
3	Comment	rv-rs-040s C13CPD DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 1
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-20T13:26:52
18	Modification Date	2018-03-20T13:26:53
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 5,6-dimethyl-2-phenyl-1H-benzo[d]imidazole (3j)



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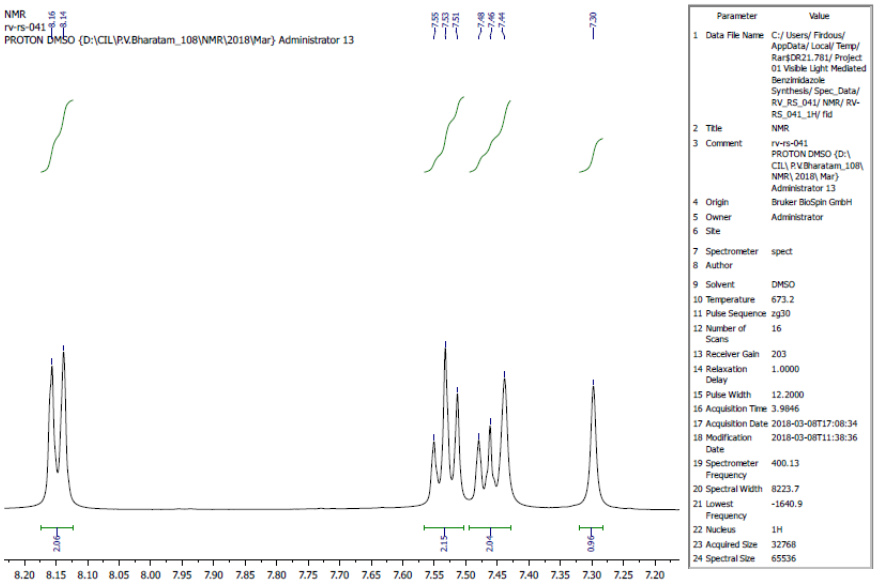
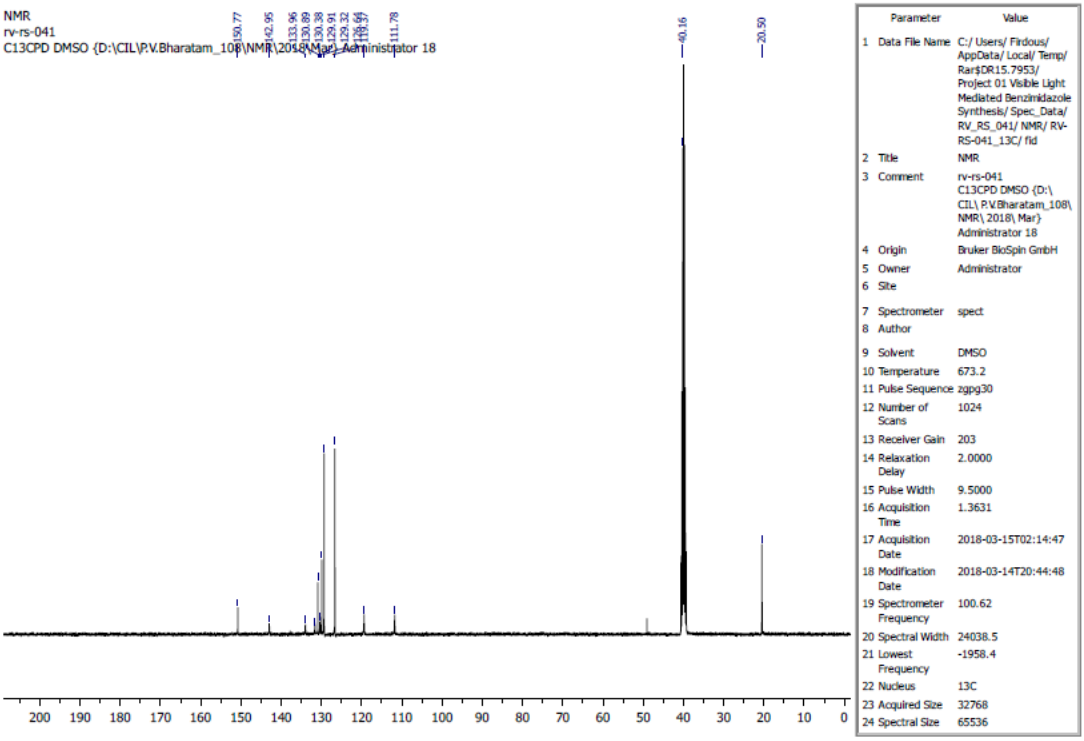
2	Title	NMR
3	Comment	rv-rs-041 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 13
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-08T17:08:34
18	Modification Date	2018-03-08T11:38:36
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

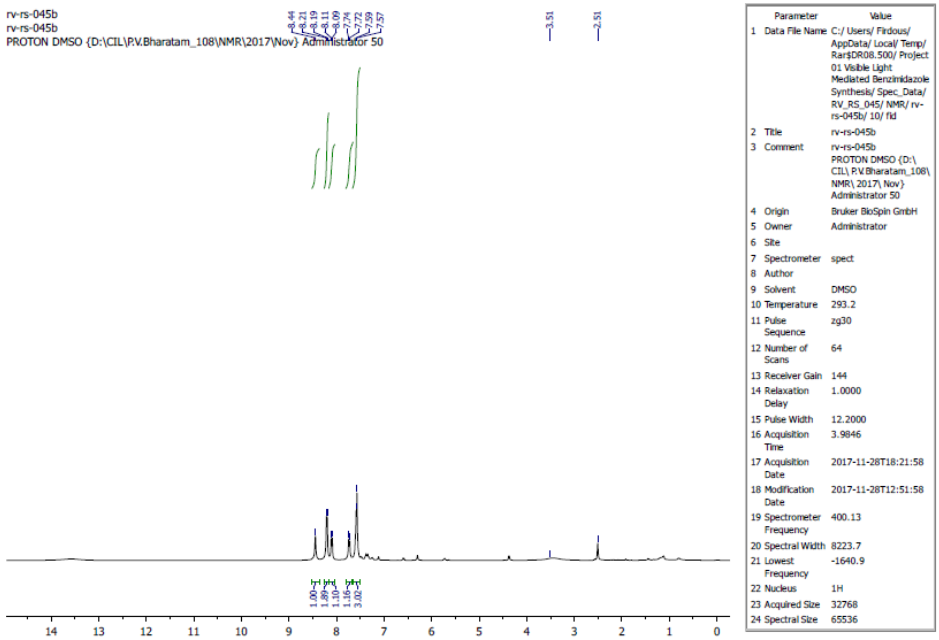
Expansion of the aromatic region of the ^{1}H NMR of 5, 6-dimethyl-2-phenyl-1H-benzo[d]imidazole (3j)



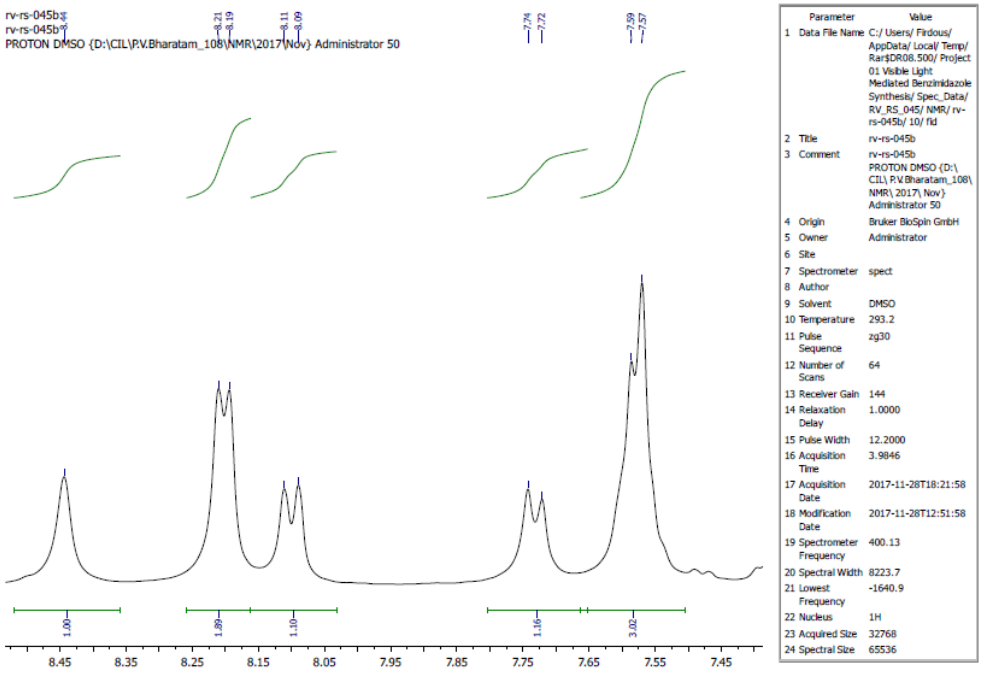
^{13}C NMR of 5,6-dimethyl-2-phenyl-1H-benzo[d]imidazole (3j)



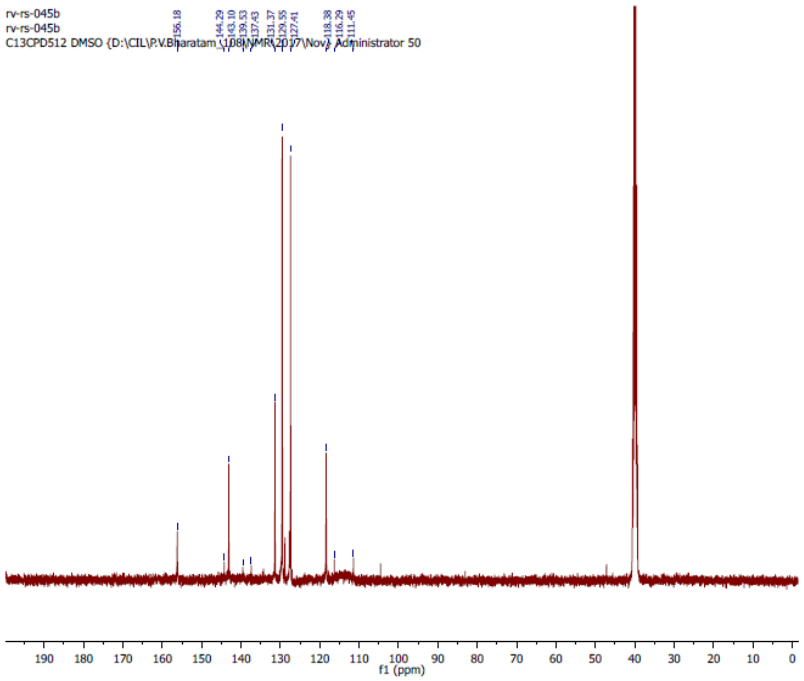
^{1}H NMR of 5-nitro-2-phenyl-1H-benzo[d]imidazole (3g)



Expansion of the aromatic region of the ^{1}H NMR of 5-nitro-2-phenyl-1H-benzo[d]imidazole (3g)



^{13}C NMR of 5-nitro-2-phenyl-1H-benzo[d]imidazole (3g)



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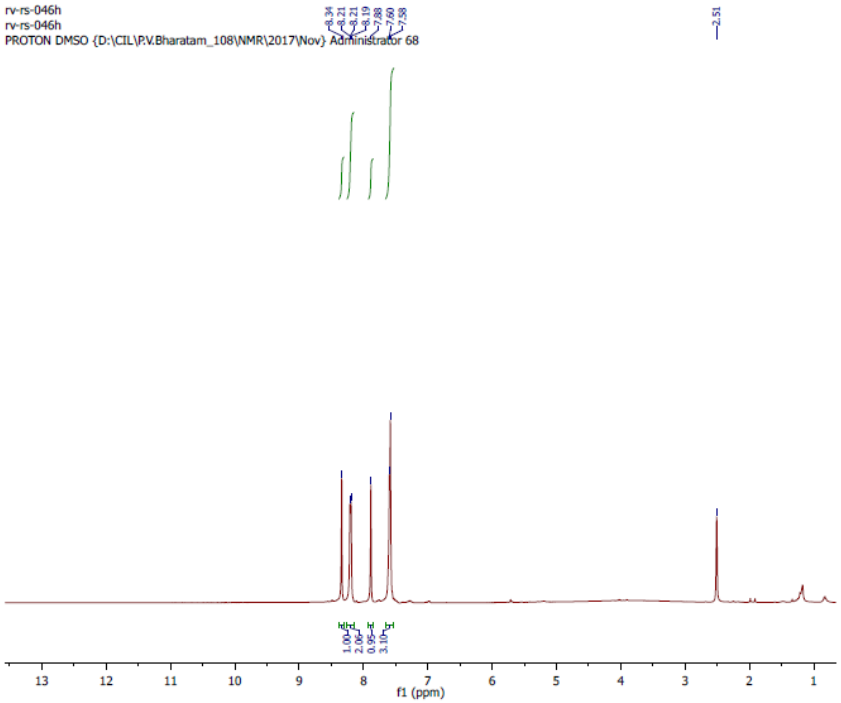
3	Comment	rv-rs-045b C13CPD512 DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Nov} Administrator 50
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	295.0
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2017-11-29T12:13:47
18	Modification Date	2017-11-29T12:26:37
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of 5-chloro-6-nitro-2-phenyl-1H-benzo[d]imidazole (3k)



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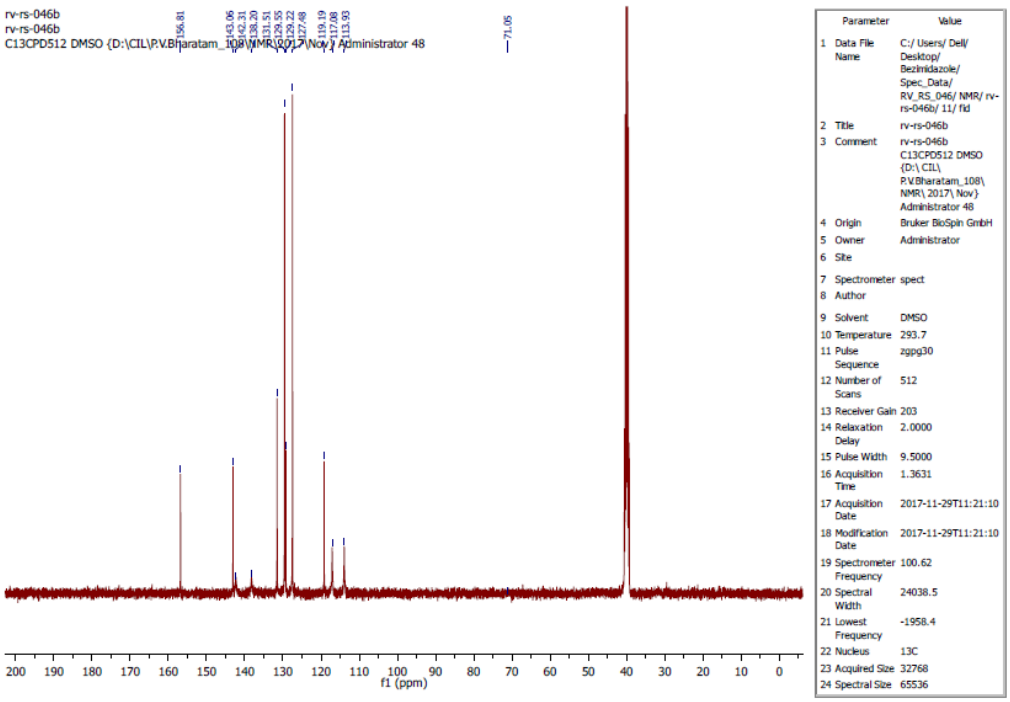
3	Comment	rv-rs-046h PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2017\ Nov} Administrator 68
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.0
11	Pulse Sequence	zg30
12	Number of Scans	32
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-11-29T16:28:26
18	Modification Date	2017-11-29T21:58:26
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 5-chloro-6-nitro-2-phenyl-1H-benzo[d]imidazole (3k)



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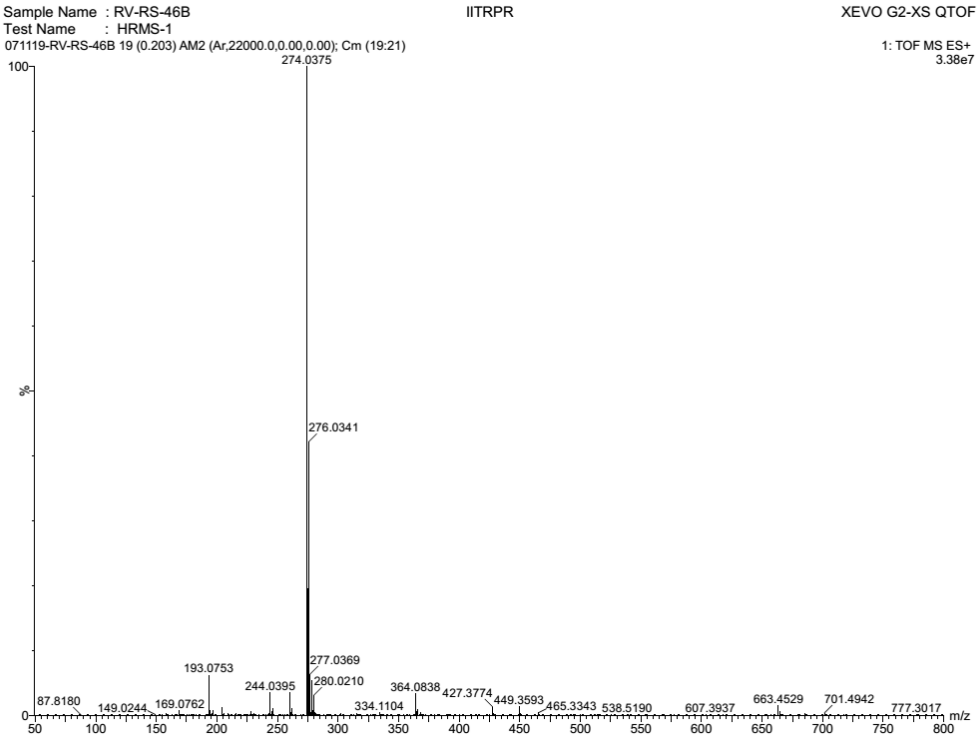
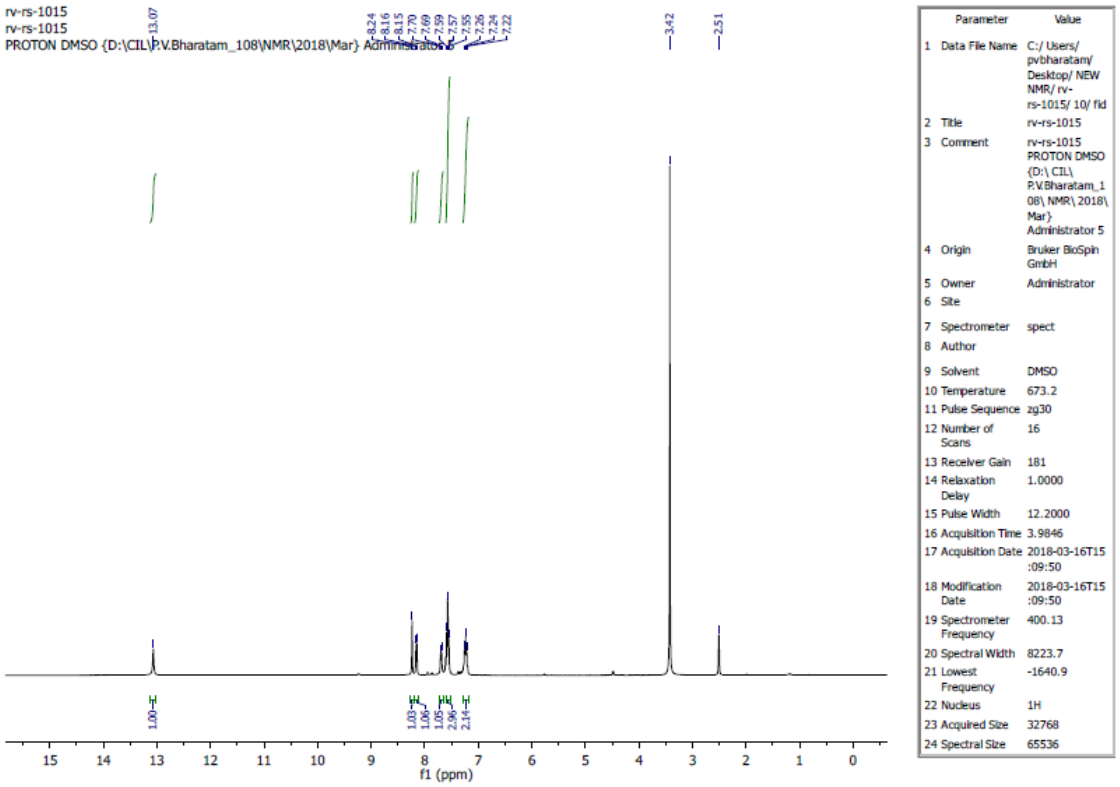
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.7
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2017-11-29T11:21:10
18	Modification Date	2017-11-29T11:21:10
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

HRMS of 5-chloro-6-nitro-2-phenyl-1H-benzo[d]imidazole (3k)



^{1}H NMR of 2-(3-chlorophenyl)-1H-benzo[d]imidazole (3c)



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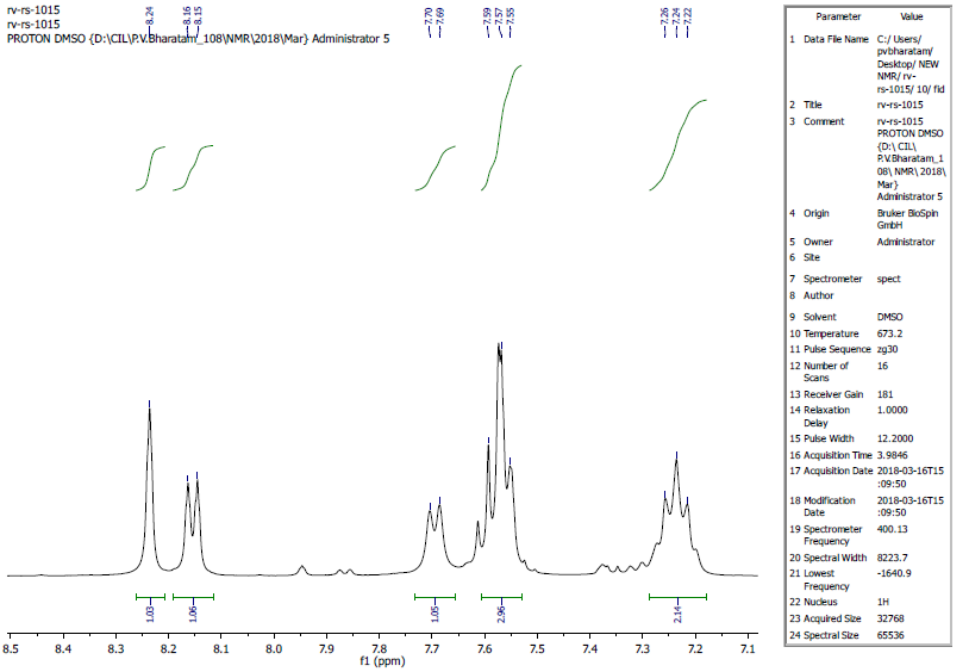
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-16T15 :09:50
18	Modification Date	2018-03-16T15 :09:50
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(3-chlorophenyl)-1H-benzo[d]imidazole (3c)



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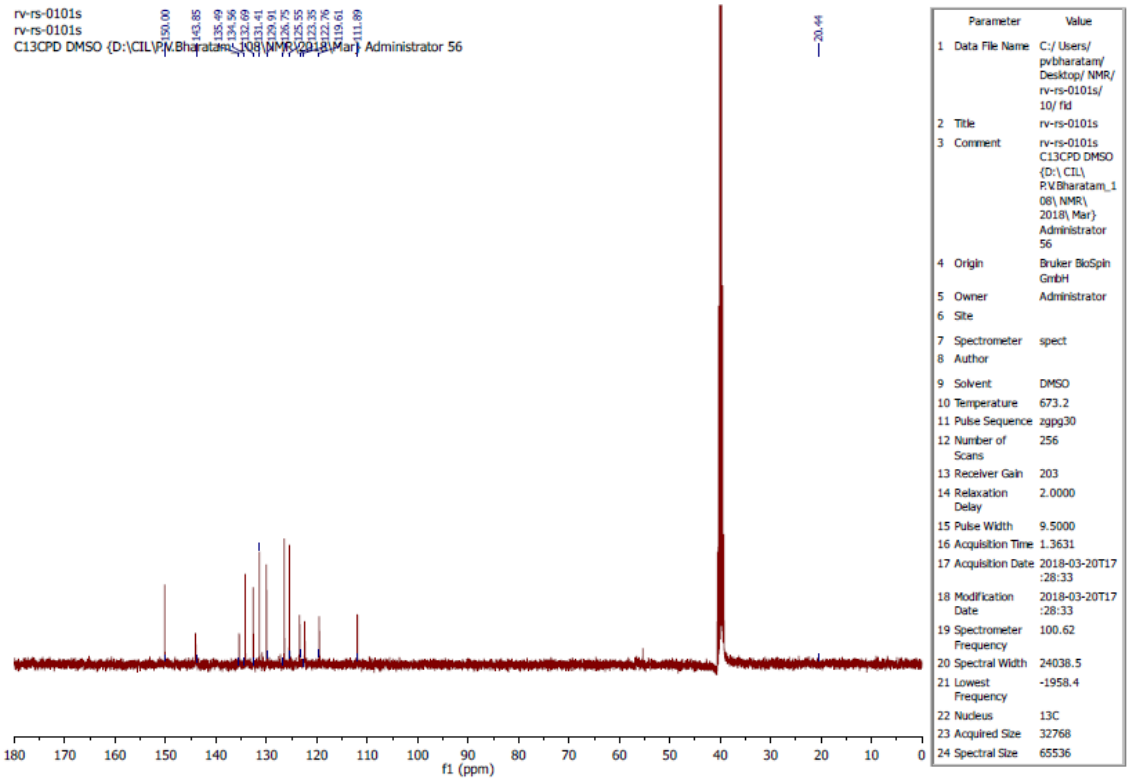
3	Comment	rv-rs-1015 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 5
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-16T15 :09:50
18	Modification Date	2018-03-16T15 :09:50
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(3-chlorophenyl)-1H-benzo[d]imidazole (3c)



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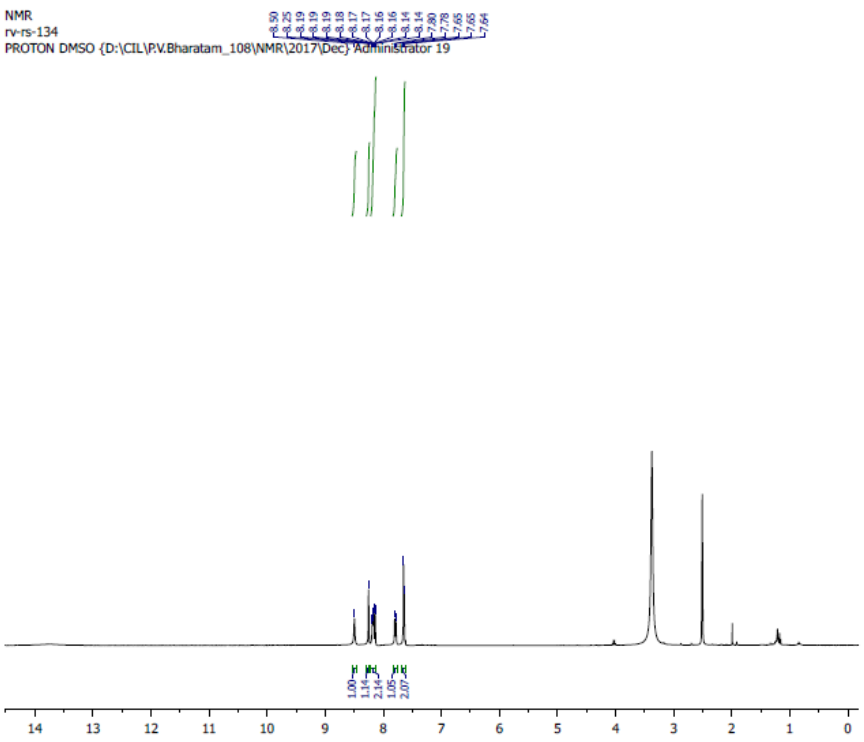
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-20T17 :28:33
18	Modification Date	2018-03-20T17 :28:33
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(3-chlorophenyl)-5-nitro-1H-benzo[d]imidazole (3h)



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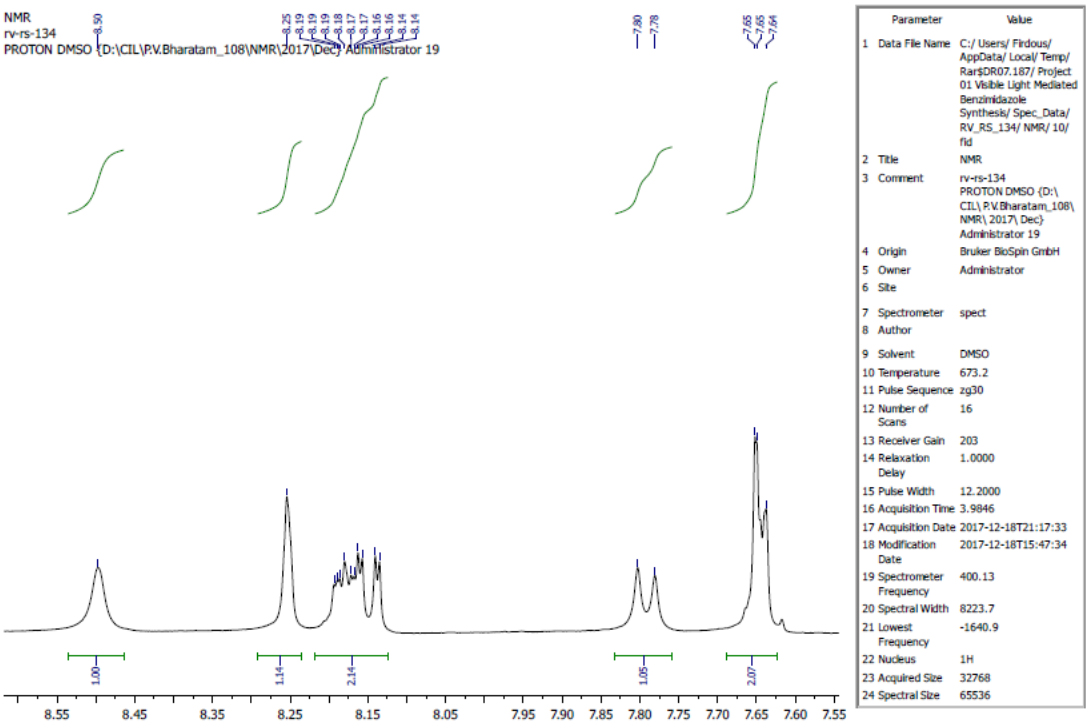
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-12-18T21:17:33
18	Modification Date	2017-12-18T15:47:34
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(3-chlorophenyl)-5-nitro-1H-benzo[d]imidazole (3h)



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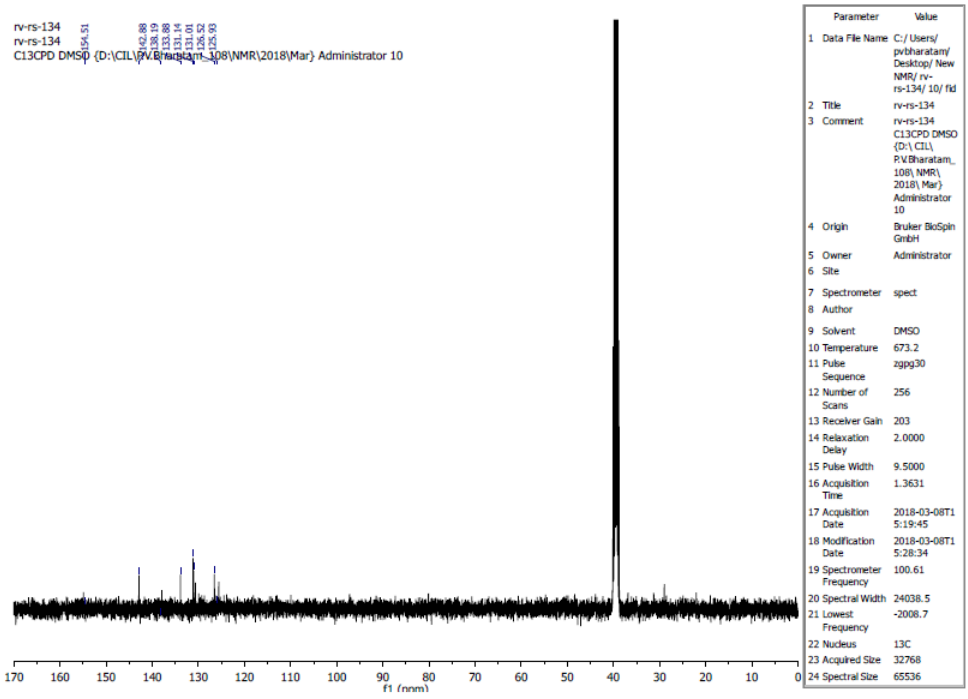
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-12-18T21:17:33
18	Modification Date	2017-12-18T15:47:34
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(3-chlorophenyl)-5-nitro-1H-benzo[d]imidazole (3h)



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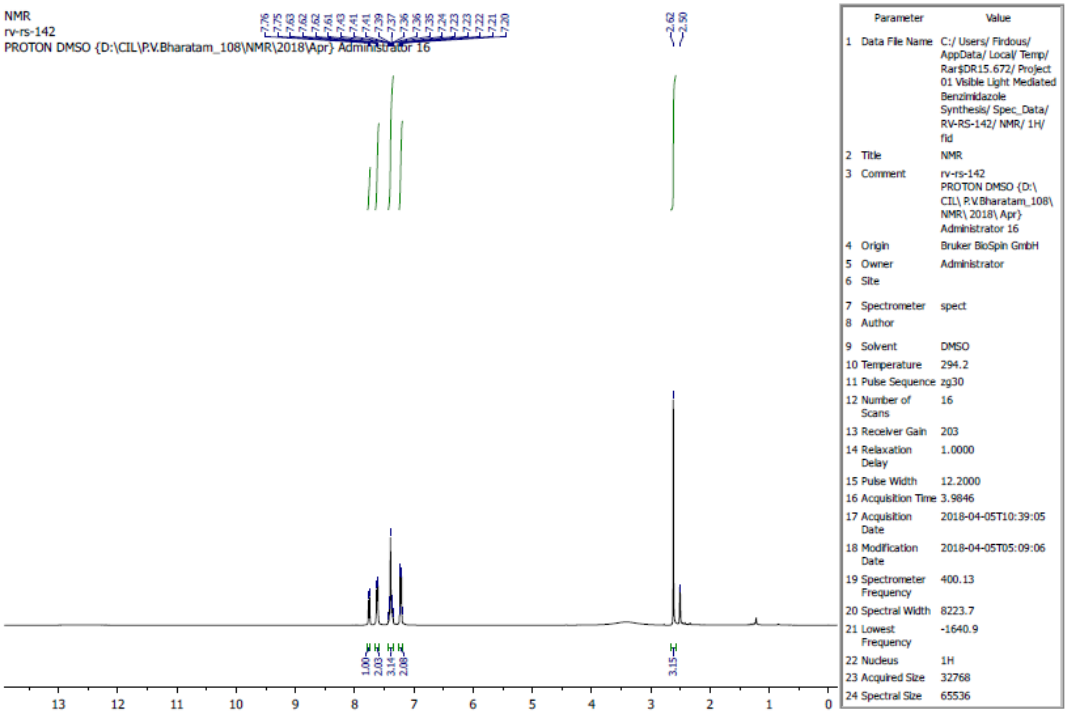
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-08T1 5:19:45
18	Modification Date	2018-03-08T1 5:28:34
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-2008.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(2-methylphenyl)-1H-benzo[d]imidazole (3d)



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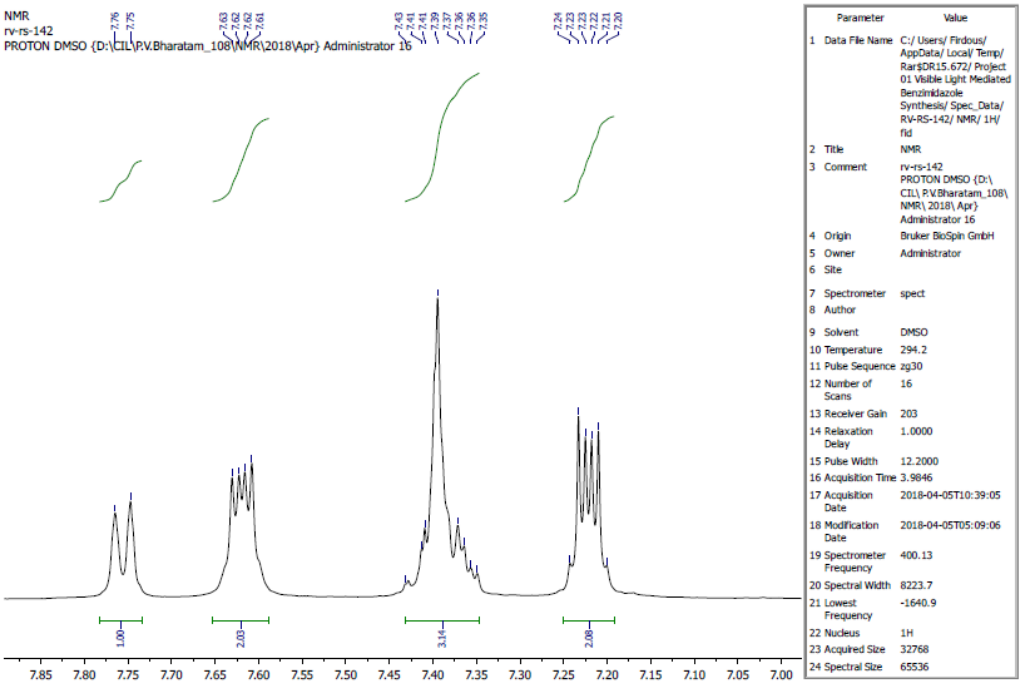
2	Title	NMR
3	Comment	rv-rs-142 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 16
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-05T10:39:05
18	Modification Date	2018-04-05T05:09:06
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(2-methylphenyl)-1H-benzo[d]imidazole (3d)



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2	Title	NMR
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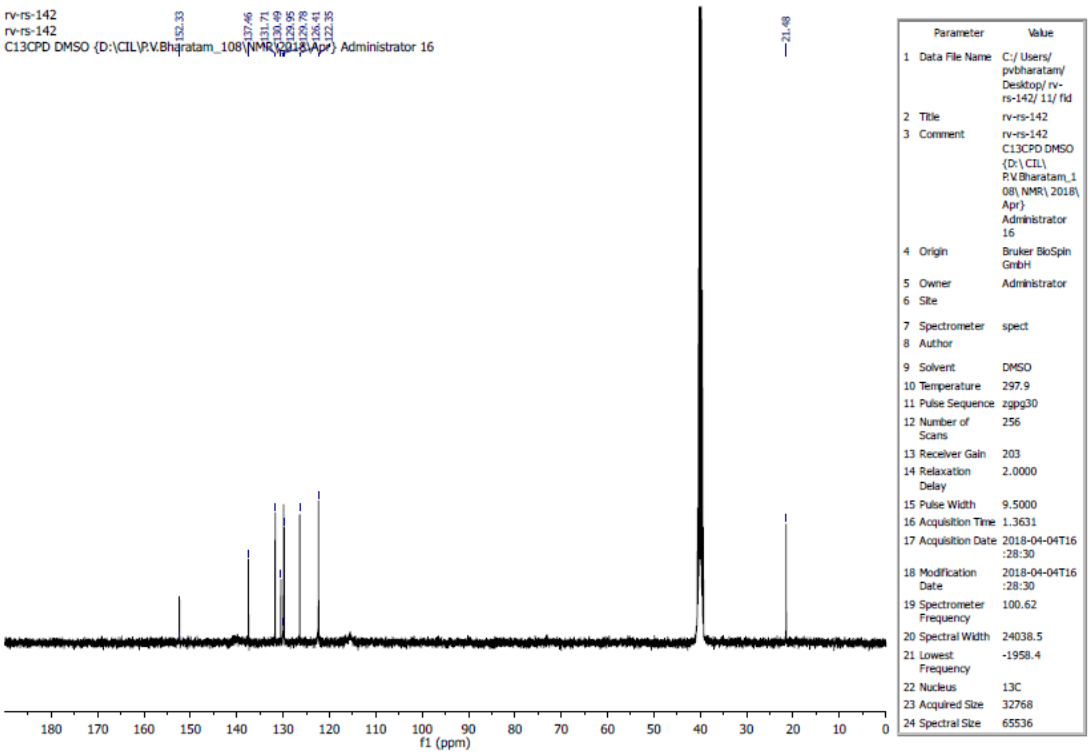
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-05T10:39:05
18	Modification Date	2018-04-05T05:09:06
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(2-methylphenyl)-1H-benzo[d]imidazole (3d)



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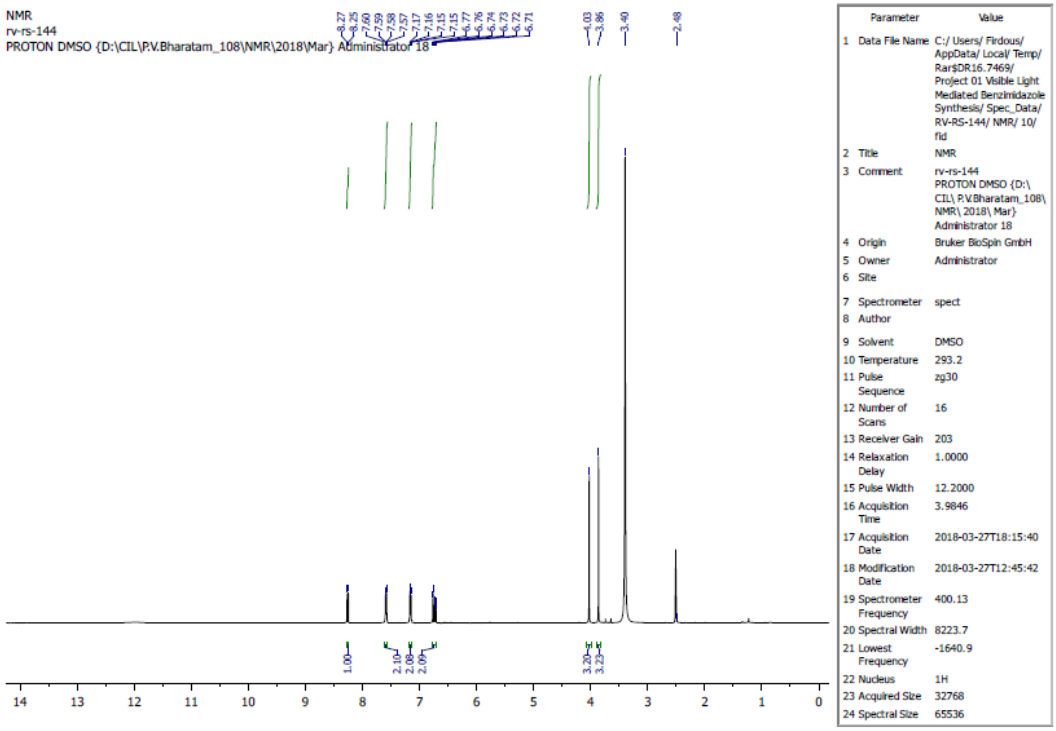
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	297.9
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-04-04T16:28:30
18	Modification Date	2018-04-04T16:28:30
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(2,4-dimethoxyphenyl)-1H-benzo[d]imidazole (3e)



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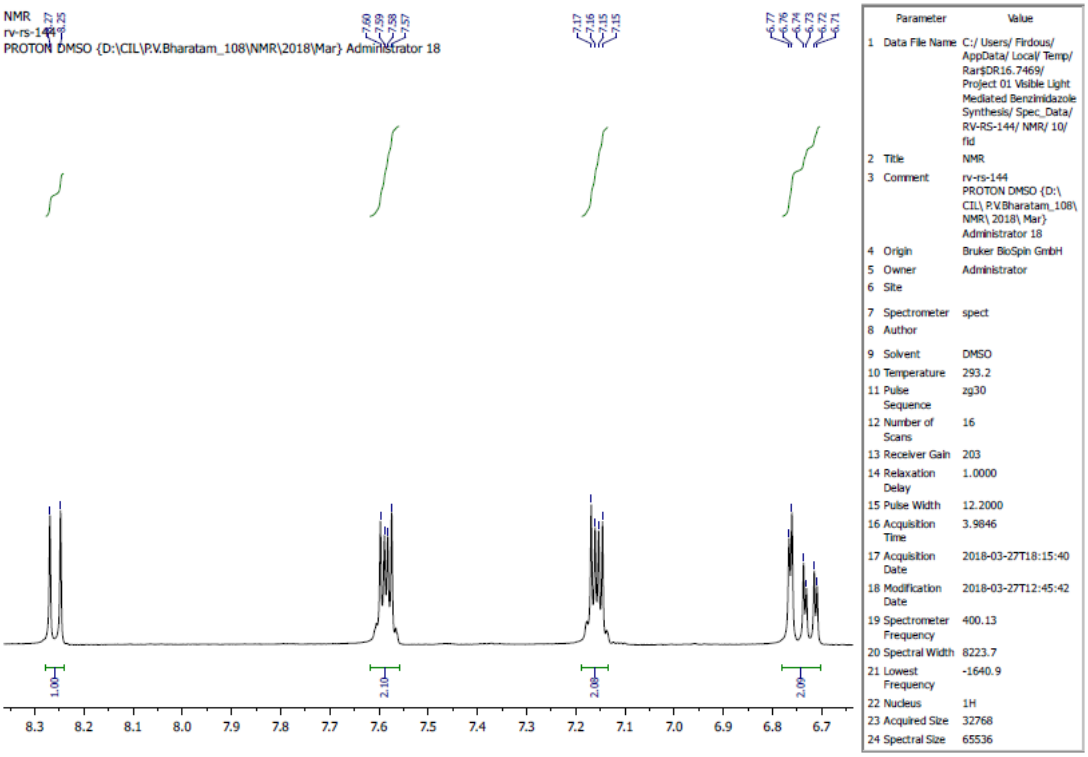
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR16.7469/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-144/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-144 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 18
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-27T18:15:40
18	Modification Date	2018-03-27T12:45:42
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(2,4-dimethoxyphenyl)-1H-benzo[*d*]imidazole (3e)



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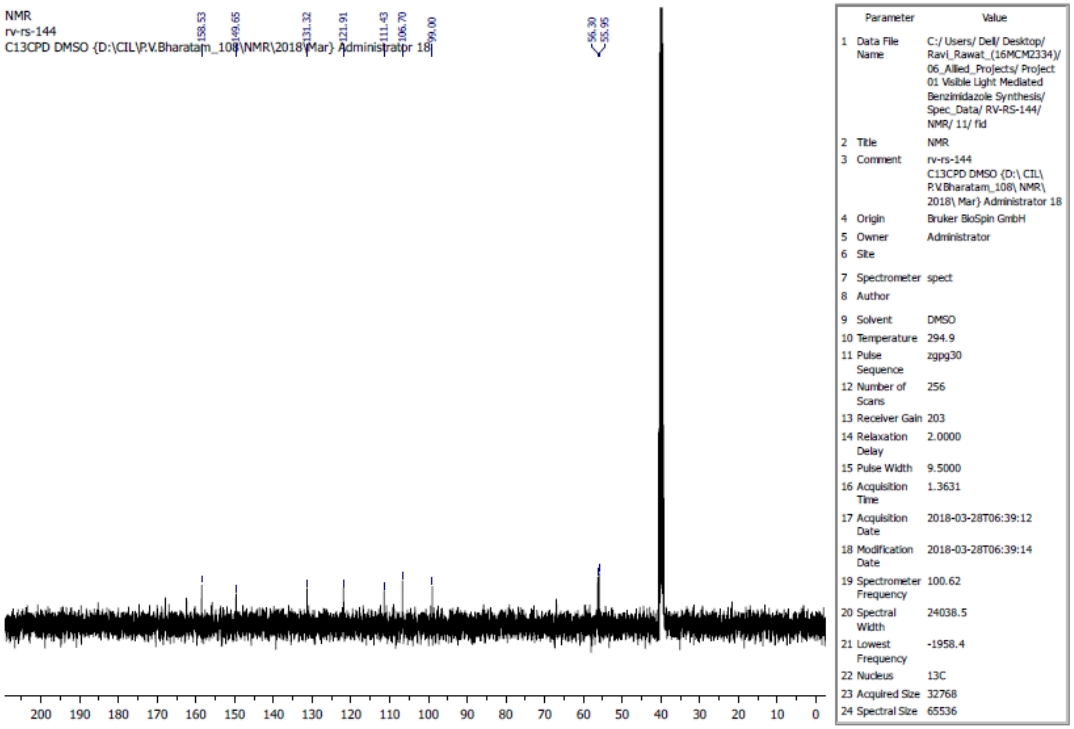
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR16.7469/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-144/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-144 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 18
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-27T18:15:40
18	Modification Date	2018-03-27T12:45:42
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(2,4-dimethoxyphenyl)-1*H*-benzo[*d*]imidazole (3e)



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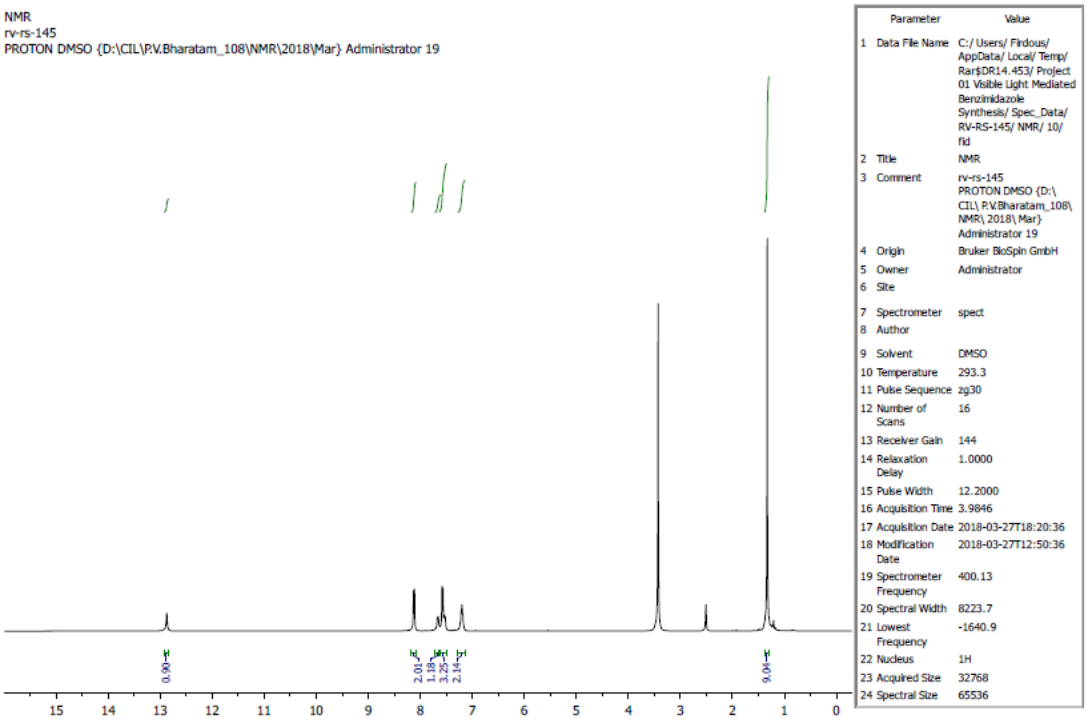
2	Title	NMR
3	Comment	rv-rs-144 C13CPD DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 18
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.9
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-28T06:39:12
18	Modification Date	2018-03-28T06:39:14
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(4-(tert-butyl)phenyl)-1H-benzo[d]imidazole (3f)



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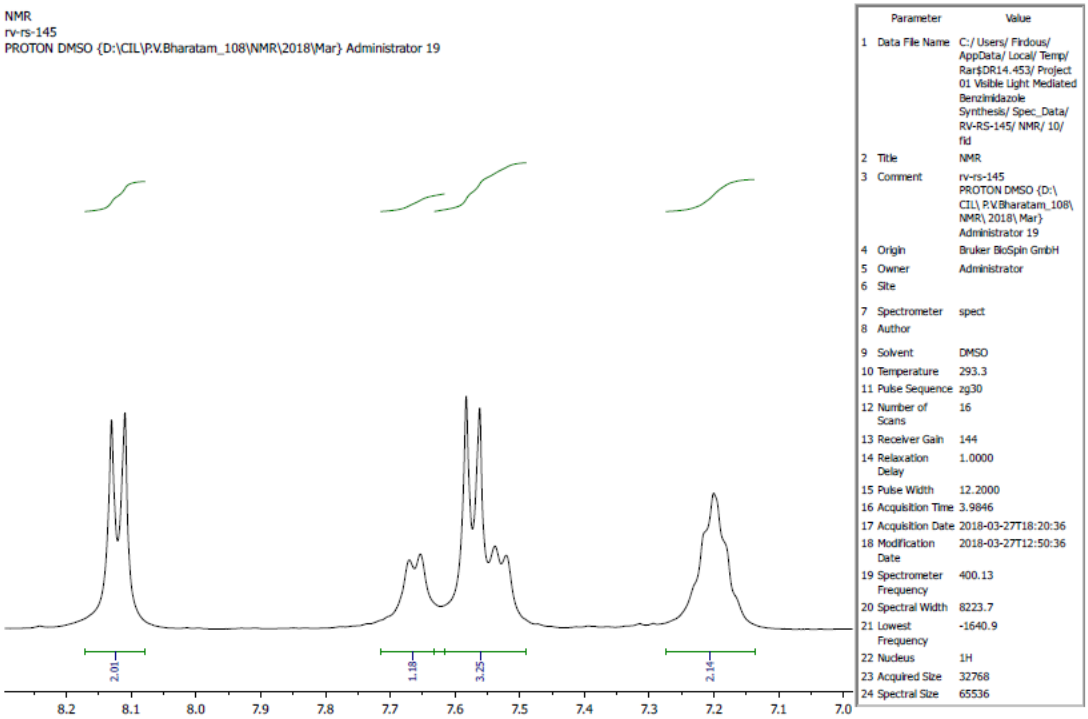
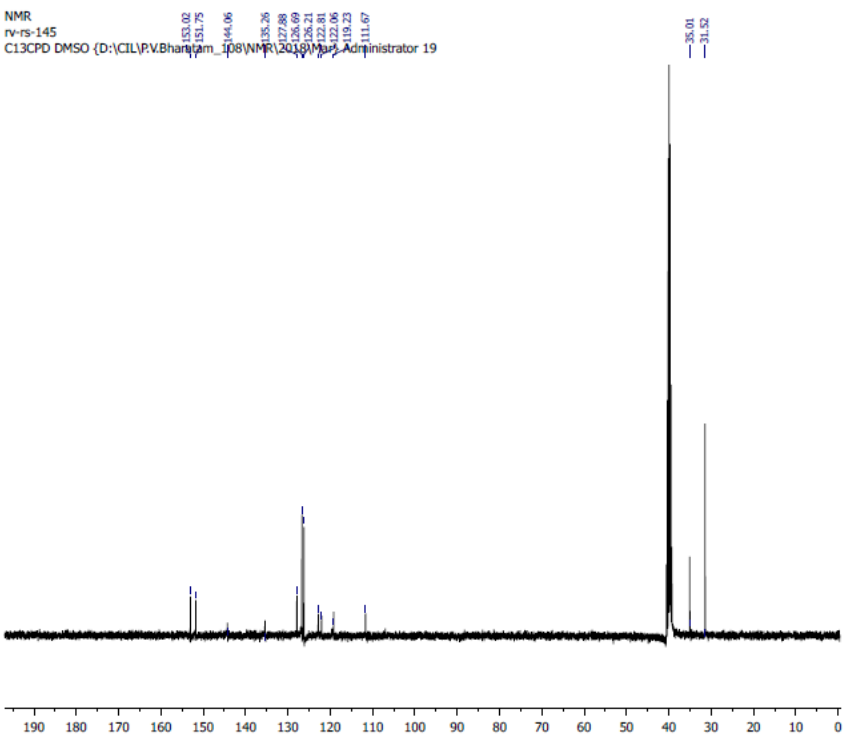
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR14.453/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-145/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-145 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 19
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-27T18:20:36
18	Modification Date	2018-03-27T12:50:36
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(4-(*tert*-butyl)phenyl)-1H-benzo[d]imidazole (3f)



	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR14.453/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-145/ NMR/ 10/ fid
2	Title	NMR
3	Comment	rv-rs-145 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 19
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-27T18:20:36
18	Modification Date	2018-03-27T12:50:36
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-(*tert*-butyl)phenyl)-1*H*-benzo[*d*]imidazole (3f)



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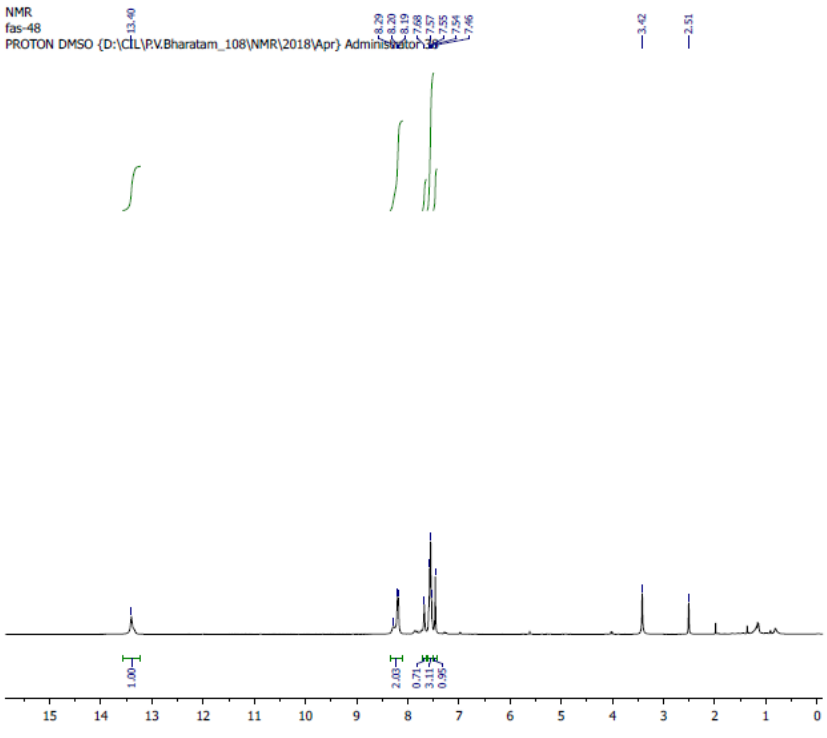
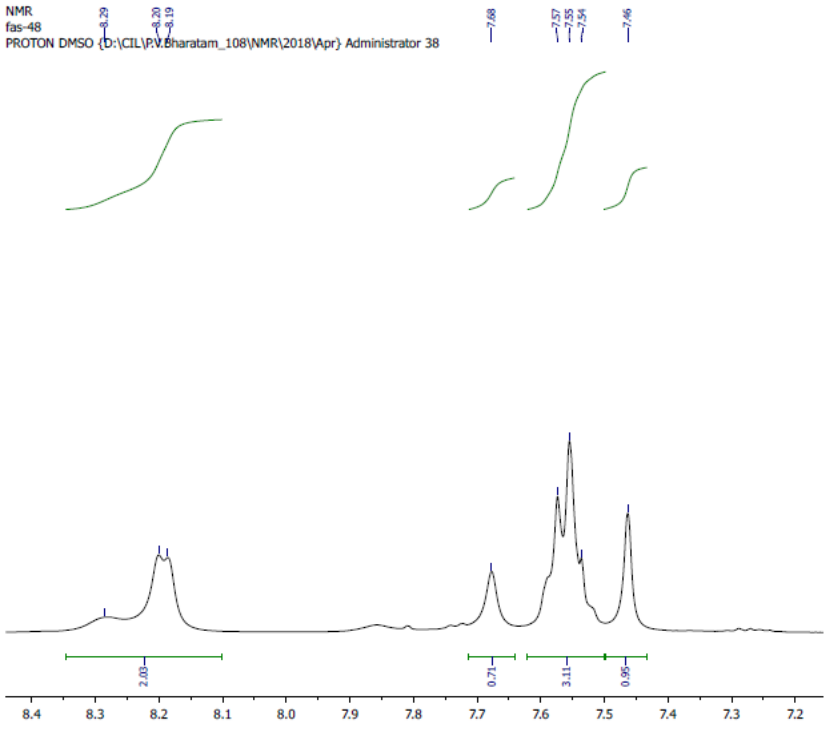
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR69.297/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-145/ NMR/ 11/ fid
2	Title	NMR
3	Comment	rv-rs-145 C13CPD DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 19
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	294.6
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-28T06:57:00
18	Modification Date	2018-03-28T01:27:02
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 6-bromo-4-chloro-2-phenyl-1H-benzo[d]imidazole (3l)



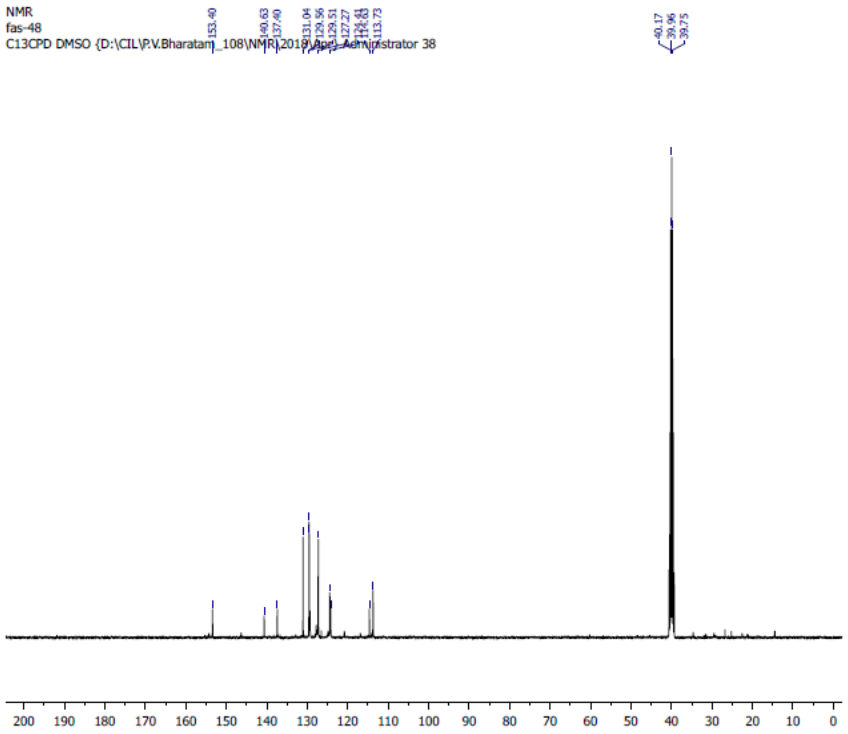
	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR90.828/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-148/ NMR/ 10/ fid
2	Title	NMR
3	Comment	fas-48 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 38
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-13T18:15:44
18	Modification Date	2018-04-13T12:45:46
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 6-bromo-4-chloro-2-phenyl-1H-benzo[d]imidazole (3l)



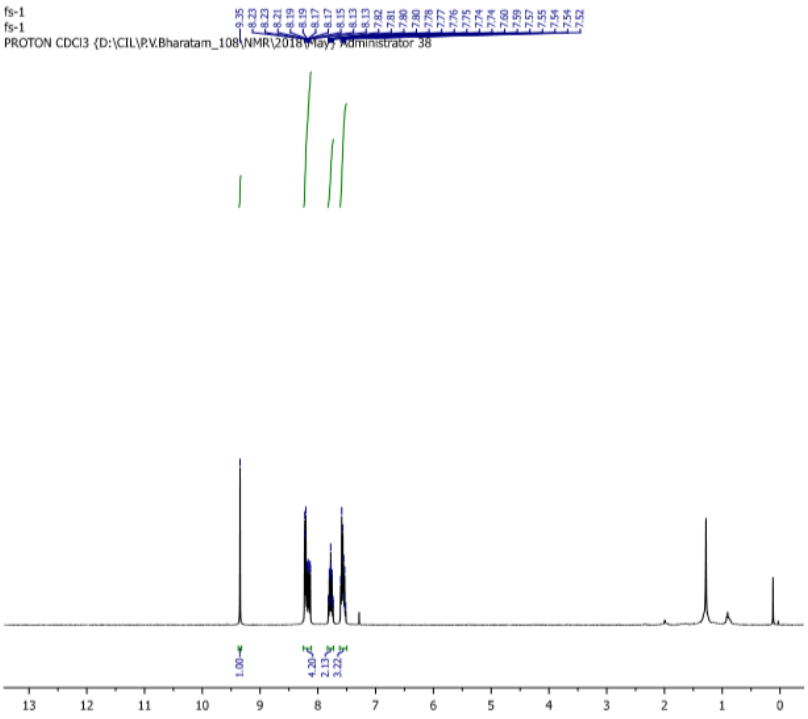
	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR90.828/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-148/ NMR/ 10/ fid
2	Title	NMR
3	Comment	fas-48 PROTON DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 38
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-13T18:15:44
18	Modification Date	2018-04-13T12:45:46
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 6-bromo-4-chloro-2-phenyl-1H-benzo[d]imidazole (3l)



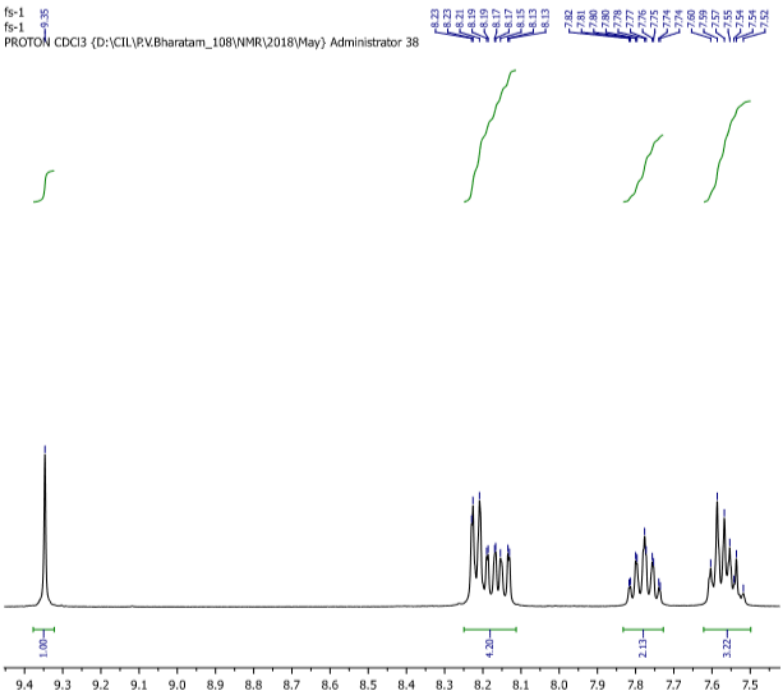
	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ AppData/ Local/ Temp/ Rar$DR17.4484/ Project 01 Visible Light Mediated Benzimidazole Synthesis/ Spec_Data/ RV-RS-148/ NMR/ 12/ fid
2	Title	NMR
3	Comment	fas-48 C13CPD DMSO {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 38
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	293.8
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-04-14T12:04:47
18	Modification Date	2018-04-14T06:34:48
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-Phenylquinoxaline (5a)



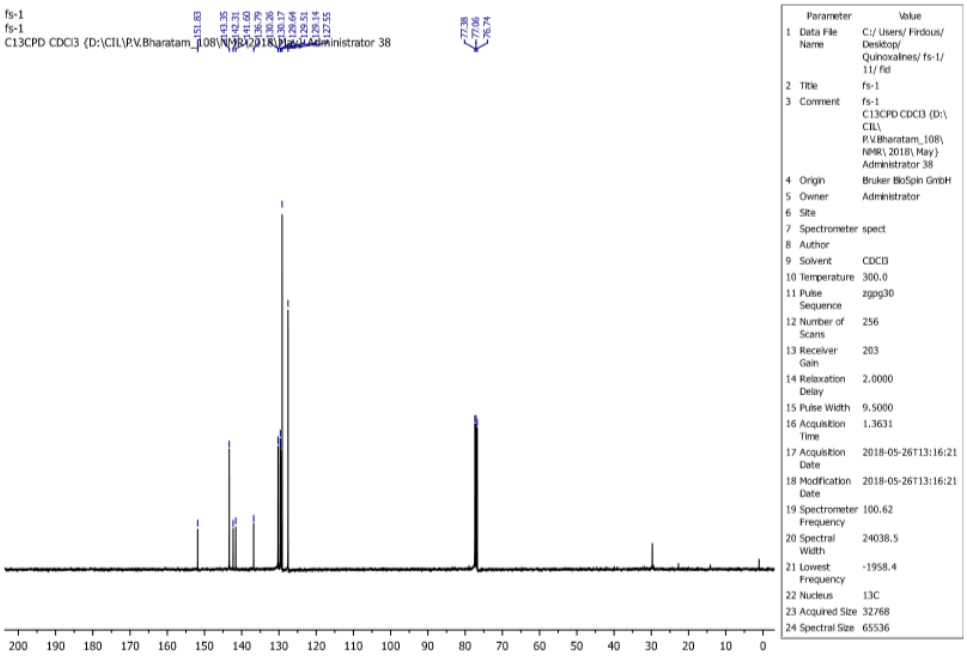
	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ Desktop/ Quinoxalines/ fs-1/ 10/ fid
2	Title	fs-1
3	Comment	fs-1 PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ May} Administrator 38
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	299.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-25T18: 42:14
18	Modification Date	2018-05-25T18: 42:14
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-Phenylquinoxaline (5a)



	Parameter	Value
1	Data File Name	C:/ Users/ Firdous/ Desktop/ Quinoxalines/ fs-1/ 10/ fid
2	Title	fs-1
3	Comment	fs-1 PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ May} Administrator 38
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	299.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-25T18: 42:14
18	Modification Date	2018-05-25T18: 42:14
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-Phenylquinoxaline (5a)



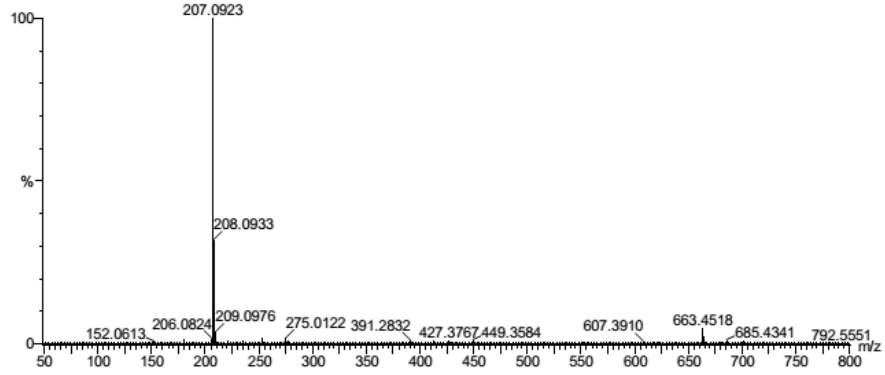
HRMS of 2-Phenylquinoxaline (5a)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

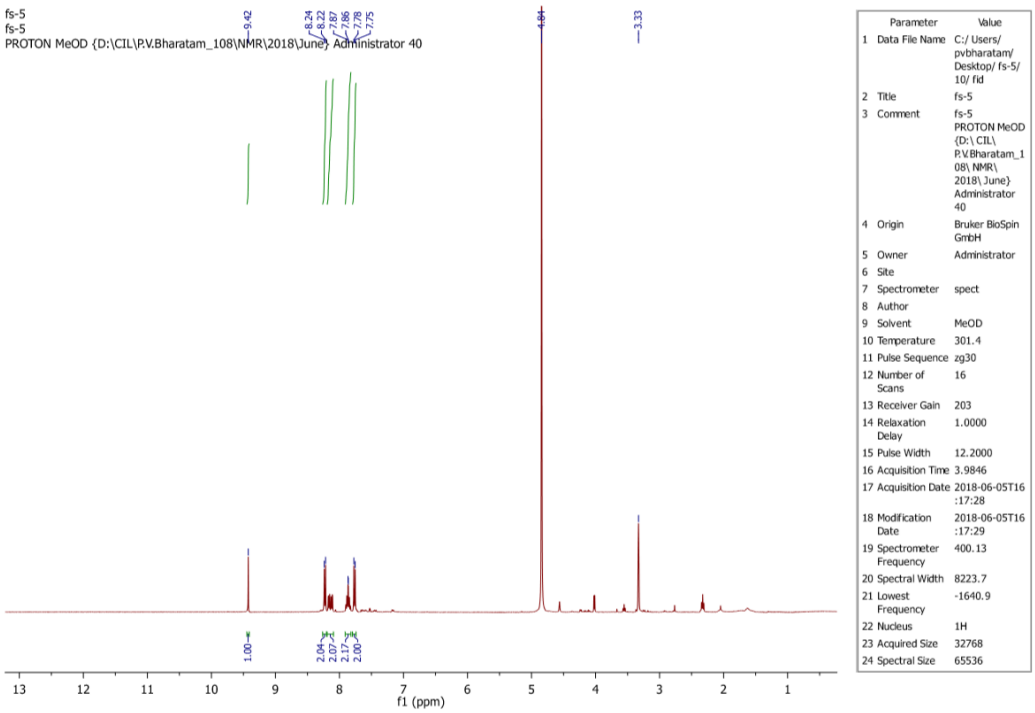
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 F: 0-3

Sample Name : FS-1 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-1 20 (0.211) AM2 (Ar,22000.0,0.00,0.00); Cm (20:26) 1: TOF MS ES+ 1.04e+008



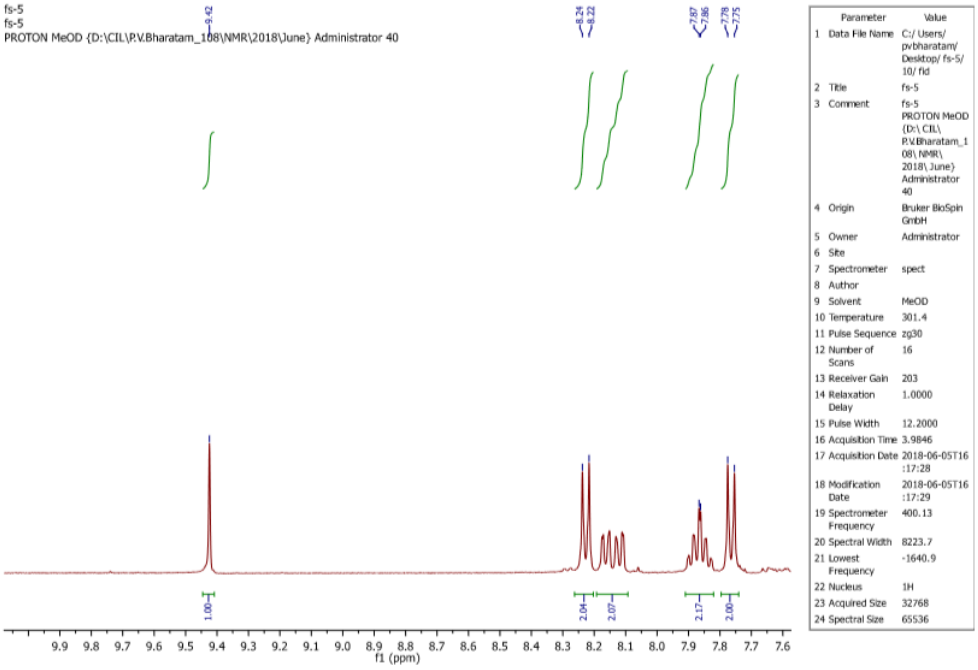
Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
207.0923	207.0922	0.1	0.5	10.5	1352.3	n/a	n/a	C14 H11 N2

^{1}H NMR of 2-(4-Bromophenyl)quinoxaline (5b)



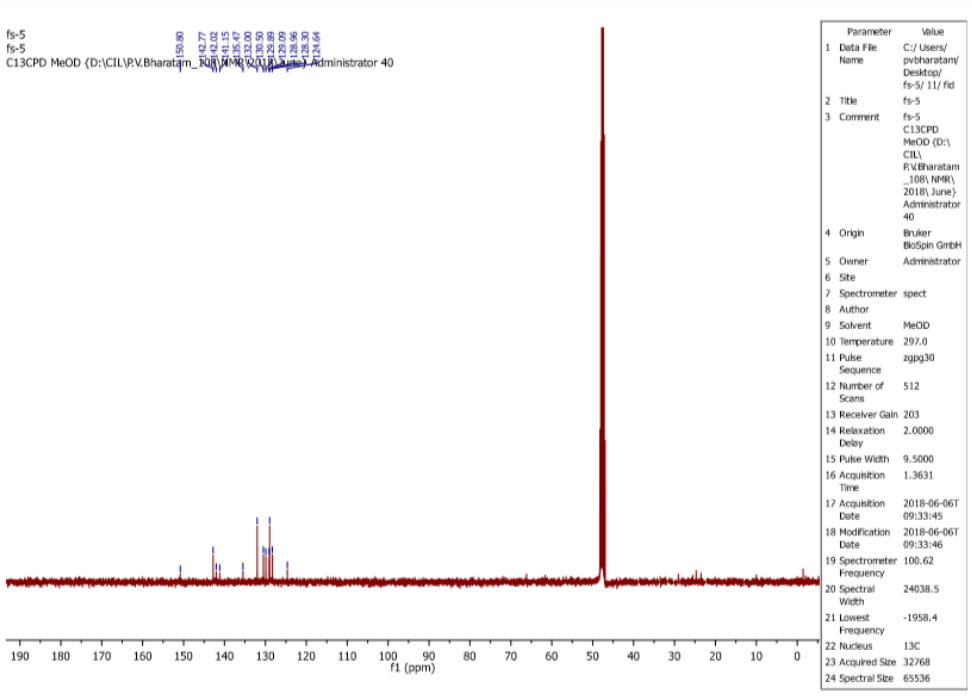
	Parameter	Value
1	Data File Name	C:/ Users/ pvbharatam/ Desktop/ fs-5/ 10/ fid
2	Title	fs-5
3	Comment	fs-5 PROTON MeOD {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ June} Administrator 40
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	301.4
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-06-05T16 :17:28
18	Modification Date	2018-06-05T16 :17:29
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(4-Bromophenyl)quinoxaline (5b)



	Parameter	Value
1	Data File Name	C:/ Users/ pvbharatam/ Desktop/ fs-5/ 10/ fid
2	Title	fs-5
3	Comment	fs-5 PROTON MeOD {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ June} Administrator 40
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	301.4
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-06-05T16 :17:28
18	Modification Date	2018-06-05T16 :17:29
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-Bromophenyl)quinoxaline (5b)



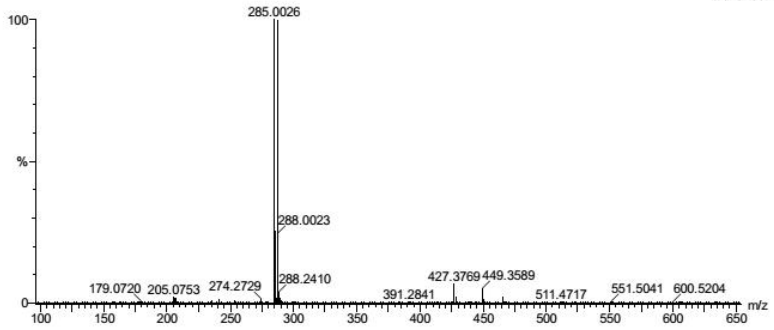
HRMS of 2-(4-Bromophenyl)quinoxaline (5b)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

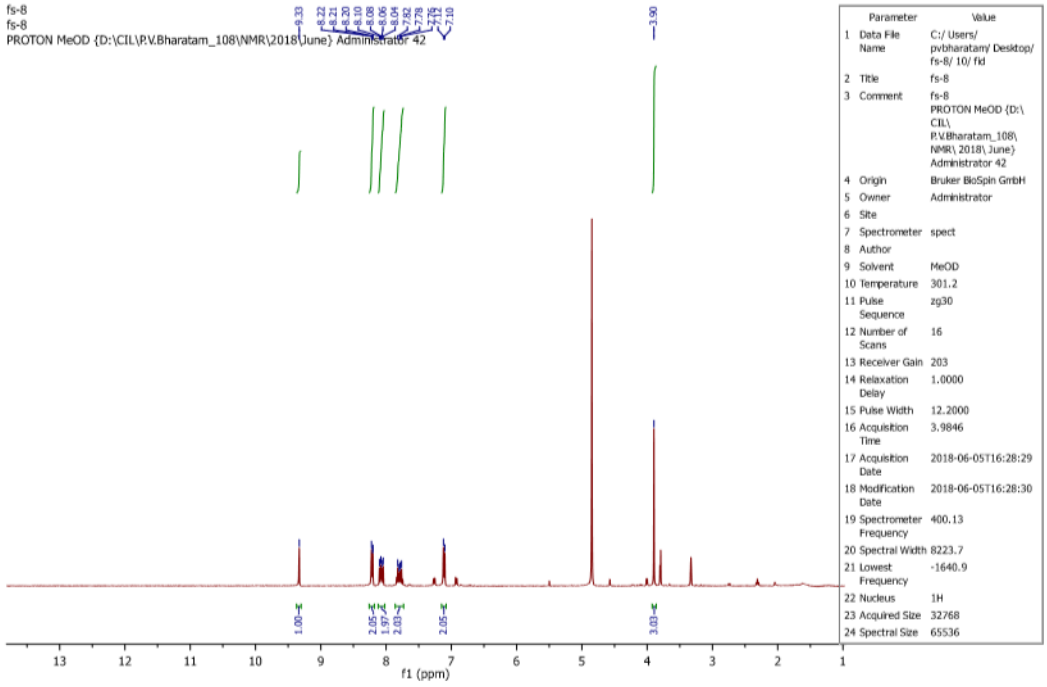
Monoisotopic Mass, Even Electron Ions
23 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-3 Br: 0-2

Sample Name : FS-5 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-5 21 (0.220) AM2 (Ar,22000.0,0.00,0.00); Cm (21:25) 1: TOF MS ES+
6.87e+007

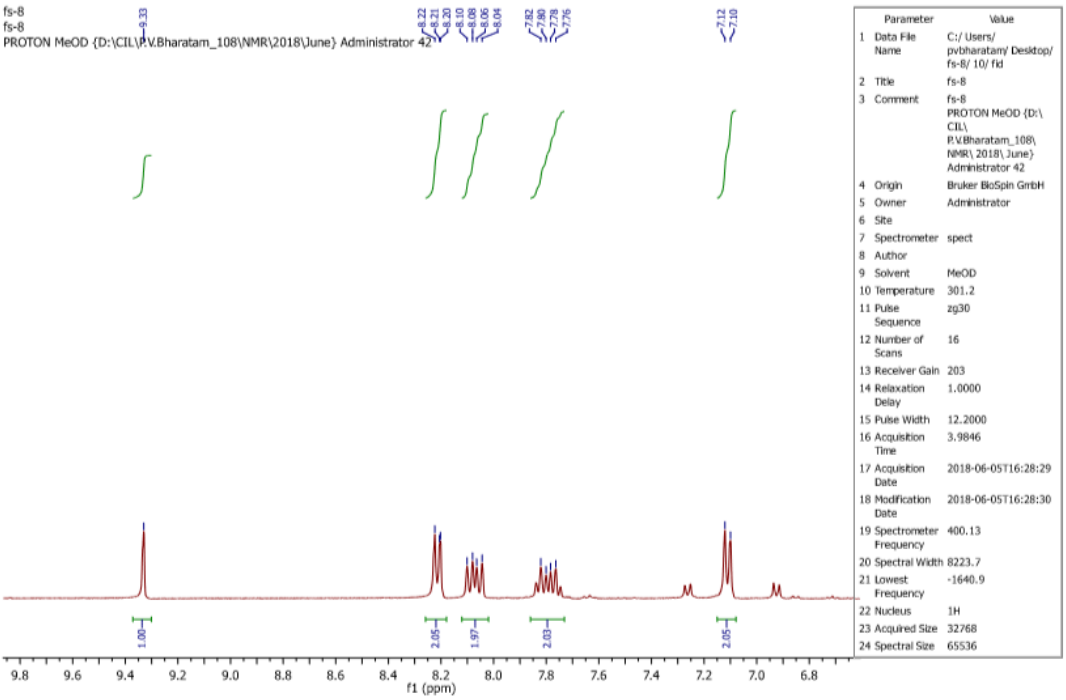


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
285.0026	285.0027	-0.1	-0.4	10.5	1202.4	n/a	n/a	C14 H10 N2 Br

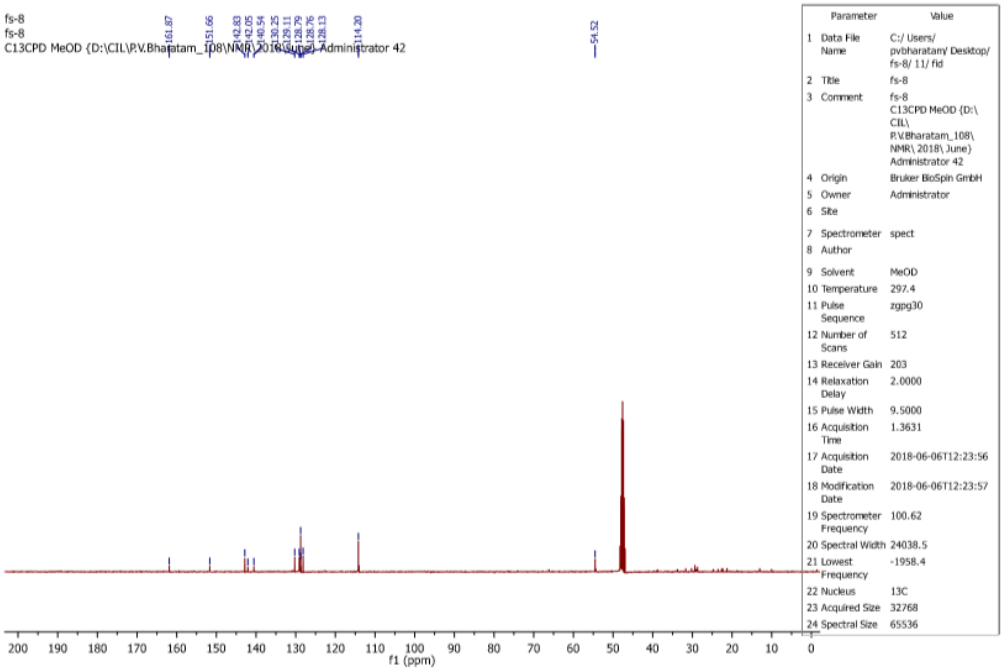
^{1}H NMR of 2-(4-methoxyphenyl)quinoxaline (5c)



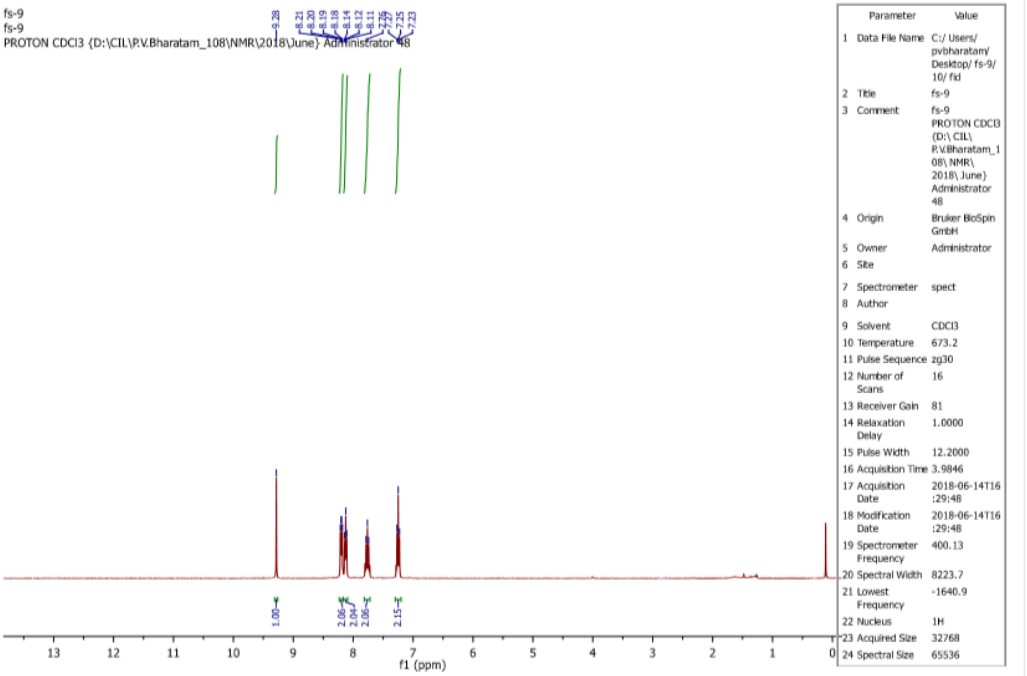
Expansion of the aromatic region of the ^{1}H NMR of 2-(4-methoxyphenyl)quinoxaline (5c)



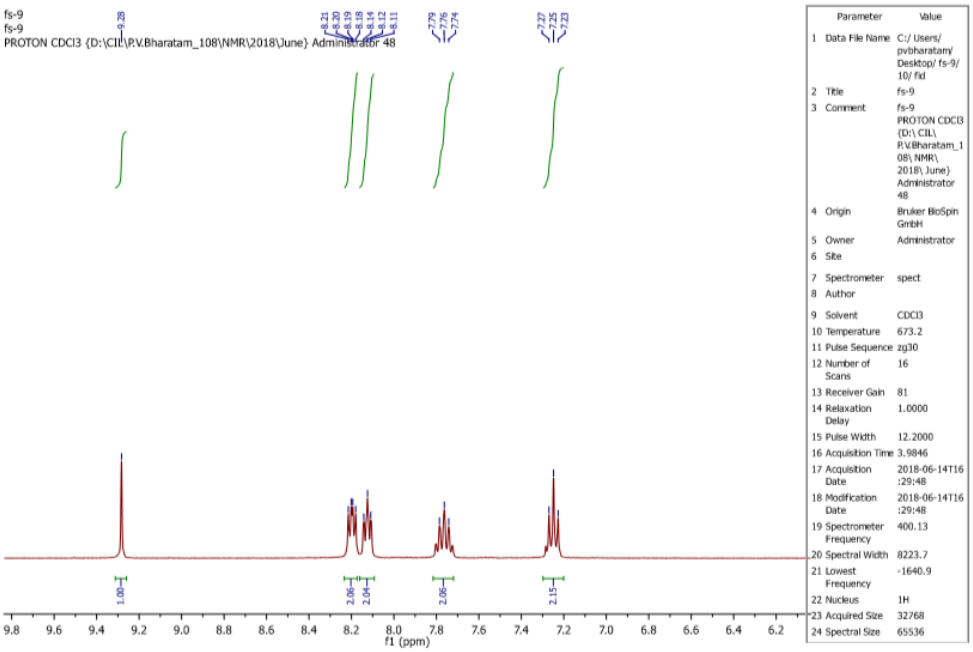
^{13}C NMR of 2-(4-methoxyphenyl)quinoxaline (5c)



^{1}H NMR of 2-(4-fluorophenyl)quinoxaline (5d)



Expansion of the aromatic region of ^{1}H NMR of 2-(4-fluorophenyl)quinoxaline (5d)



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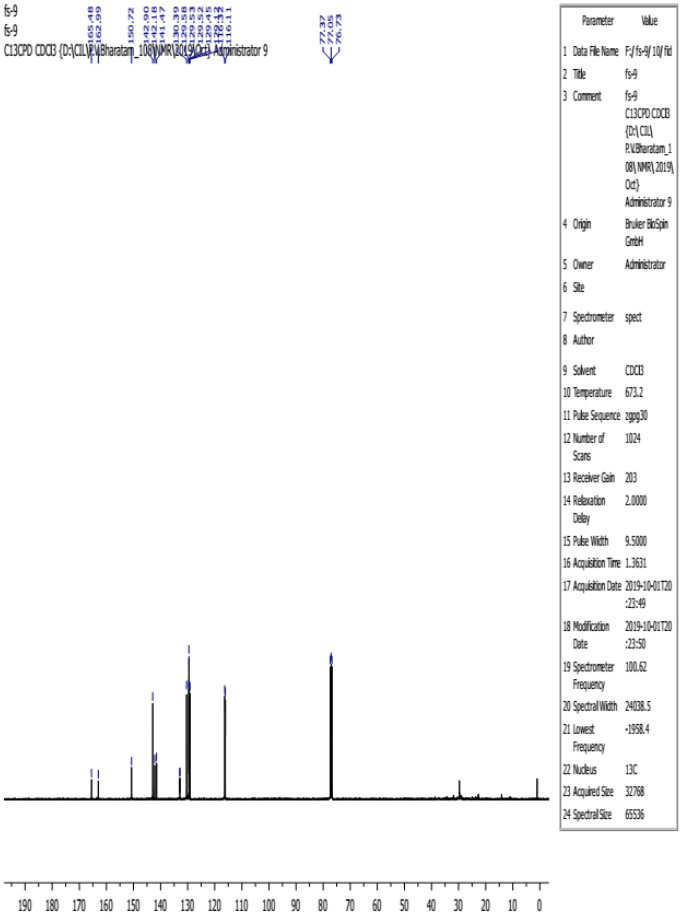
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	81
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-06-14T16 :29:48
18	Modification Date	2018-06-14T16 :29:48
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-fluorophenyl)quinoxaline (5d)



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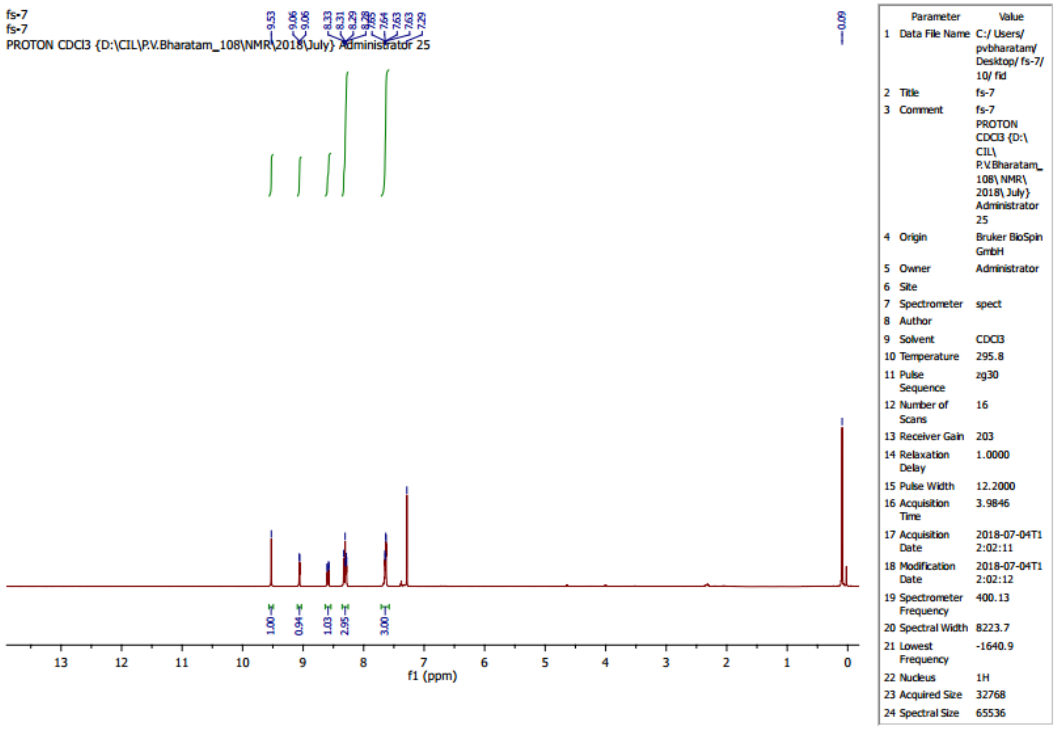
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2019-10-01T20 :23:49
18	Modification Date	2019-10-01T20 :23:50
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 6-nitro-2-phenylquinoxaline (5e)



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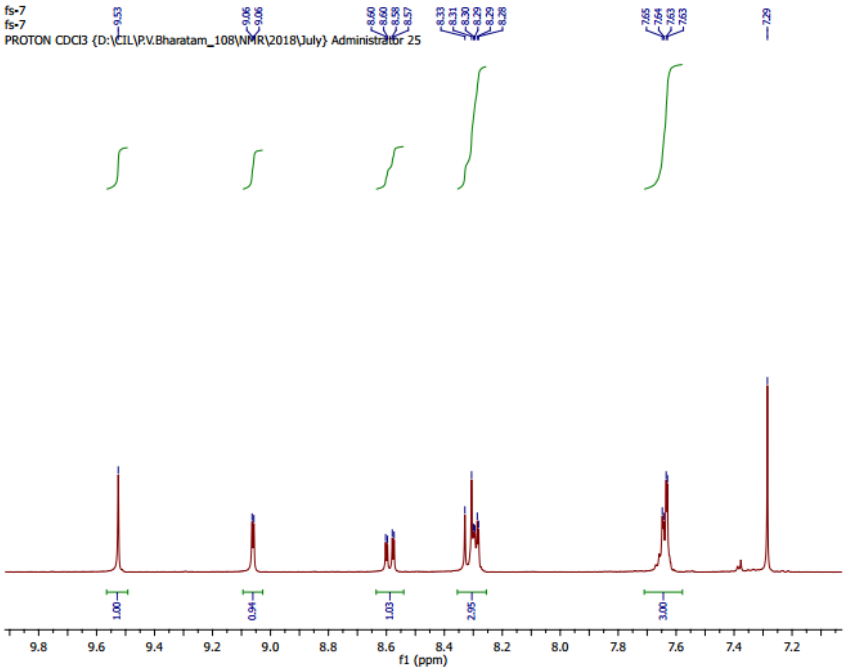
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-04T1 2:02:11
18	Modification Date	2018-07-04T1 2:02:12
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 6-nitro-2-phenylquinoxaline (5e)



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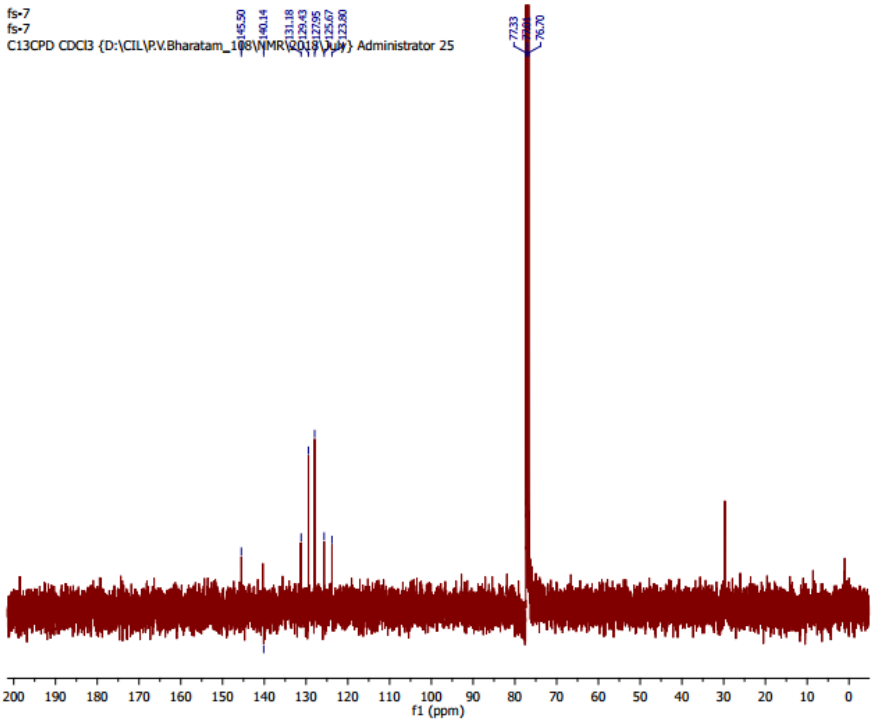
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.8
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-04T1 2:02:11
18	Modification Date	2018-07-04T1 2:02:12
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 6-nitro-2-phenylquinoxaline (5e)



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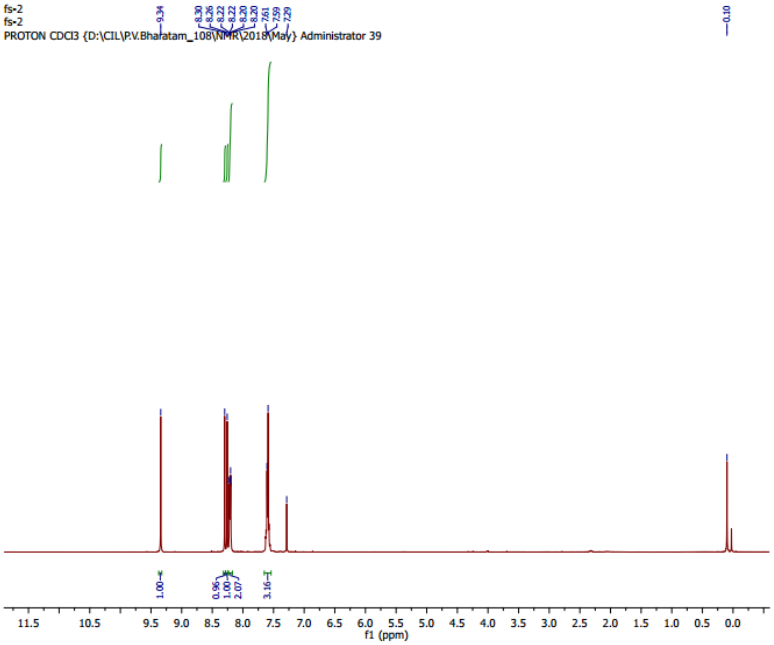
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.4
11	Pulse Sequence	zgpg30
12	Number of Scans	202
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-07-04T12:14:21
18	Modification Date	2018-07-04T12:14:21
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 6,7-dichloro-2-phenylquinoxaline (5f)



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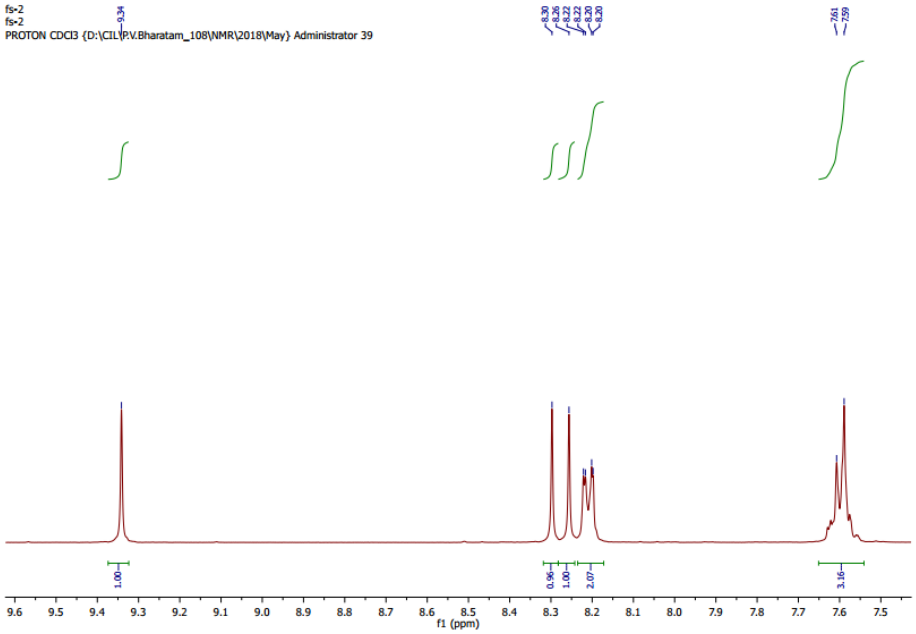
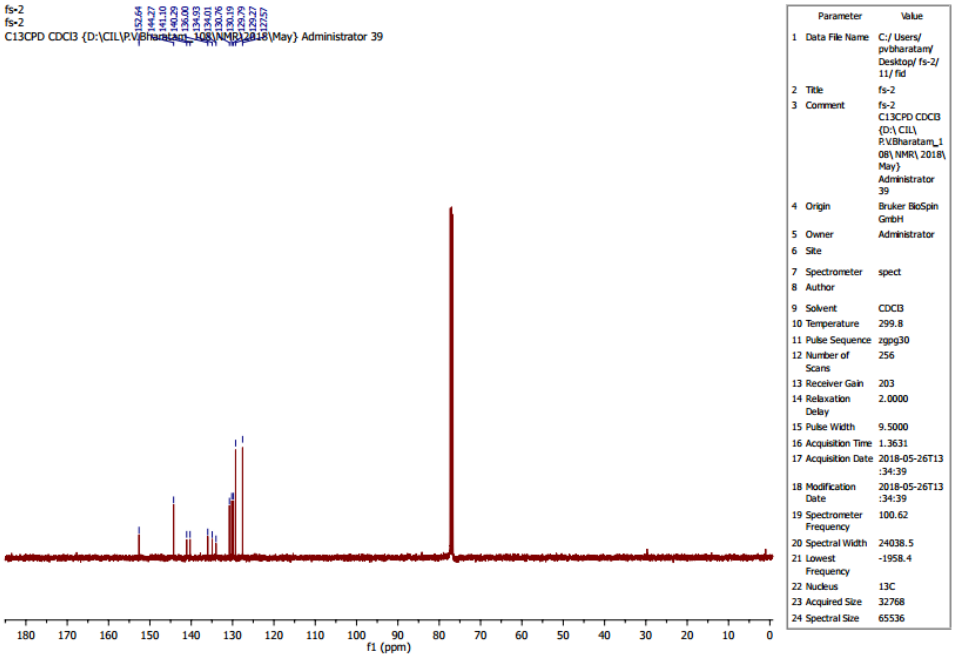
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.9
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-25T18 :48:19
18	Modification Date	2018-05-25T18 :48:19
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR spectra of 6,7-dichloro-2-phenylquinoxaline (5f)



^{13}C NMR of 6,7-dichloro-2-phenylquinoxaline (5f)



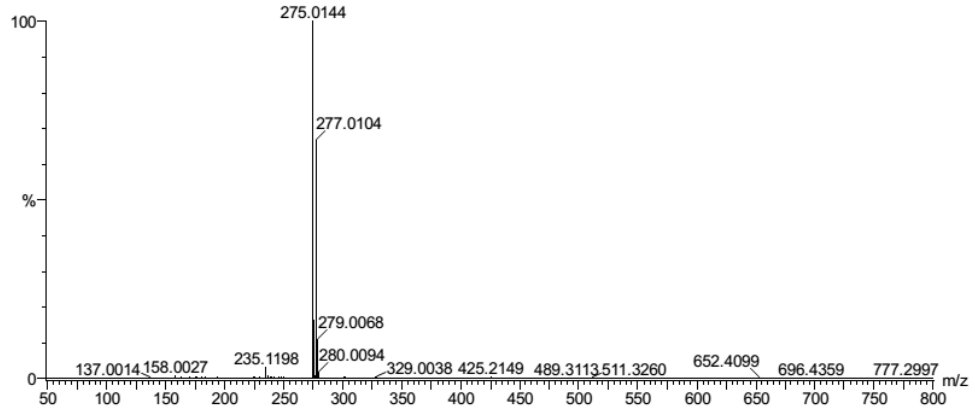
HRMS of 6,7-dichloro-2-phenylquinoxaline (5f)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

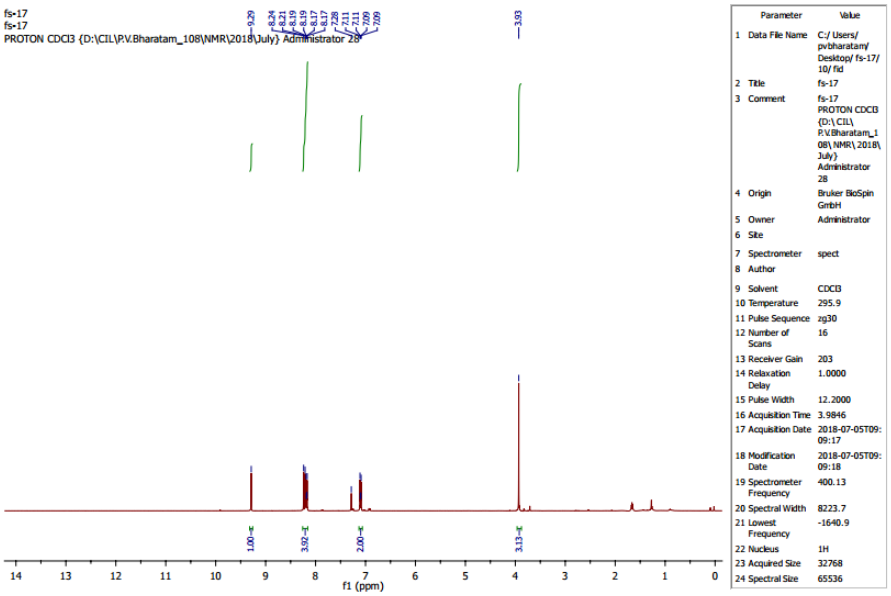
Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 Cl: 0-2

Sample Name : FS-2 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-2 76 (0.726) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (76:88) 1: TOF MS ES+
1.12e+008



Minimum:				-1.5				
Maximum:		5.0	50.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
275.0144	275.0143	0.1	0.4	10.5	1280.3	n/a	n/a	C14 H9 N2 Cl2

^{1}H NMR of 6,7-dichloro-2-(4-methoxyphenyl)quinoxaline (5g)



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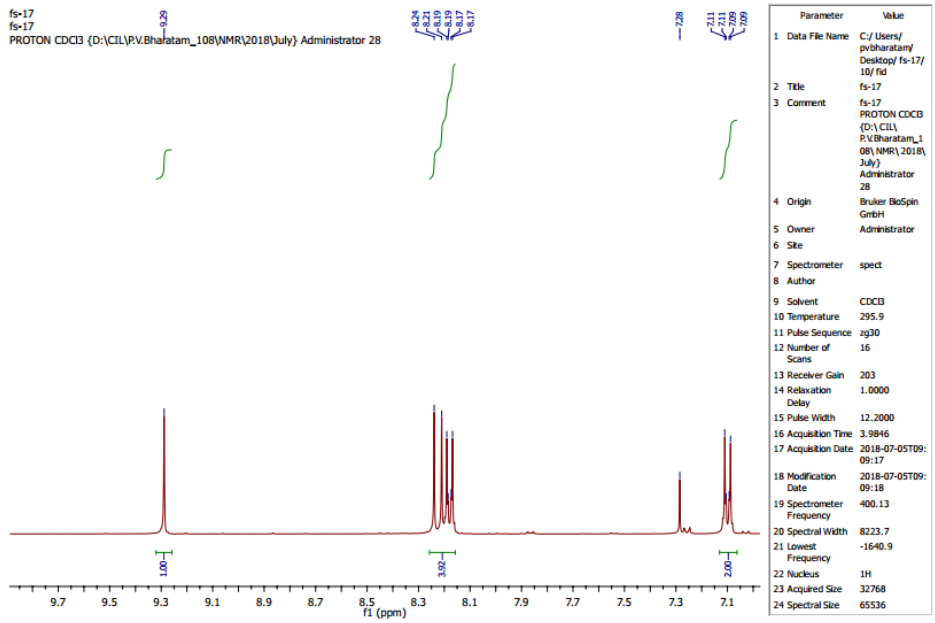
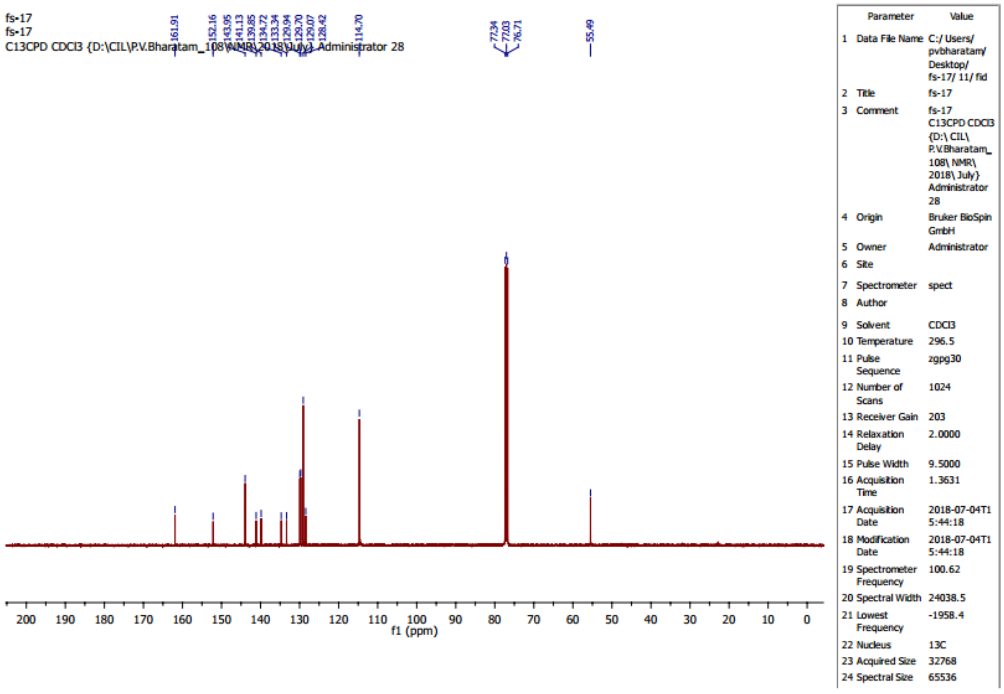
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.9
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-05T09: 09:17
18	Modification Date	2018-07-05T09: 09:18
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

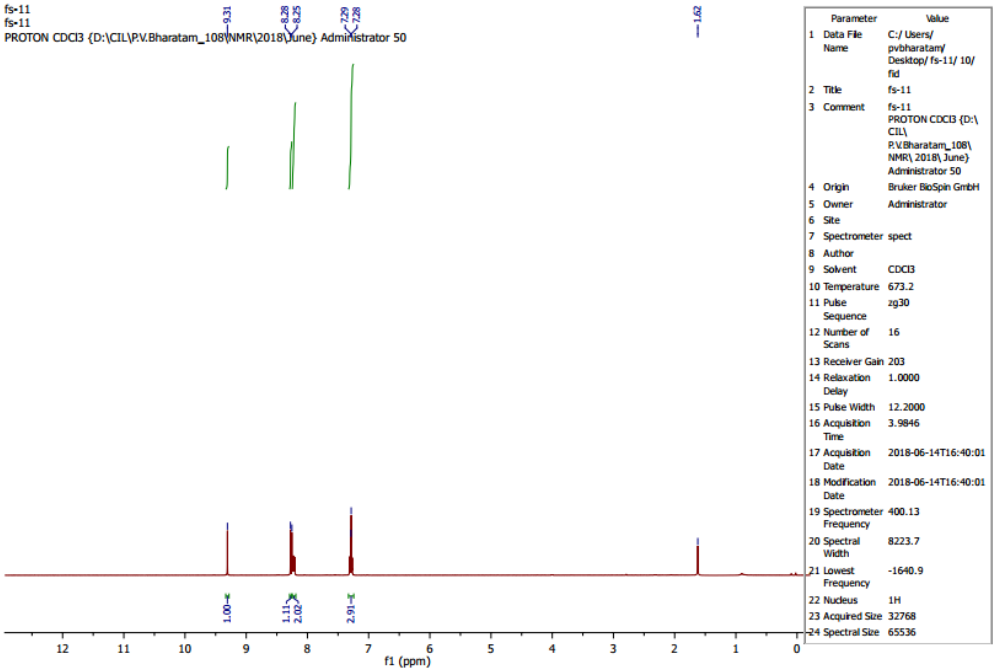
Expansion of the aromatic region of the ^{1}H NMR of 6,7-dichloro-2-(4-methoxyphenyl)quinoxaline (5g)



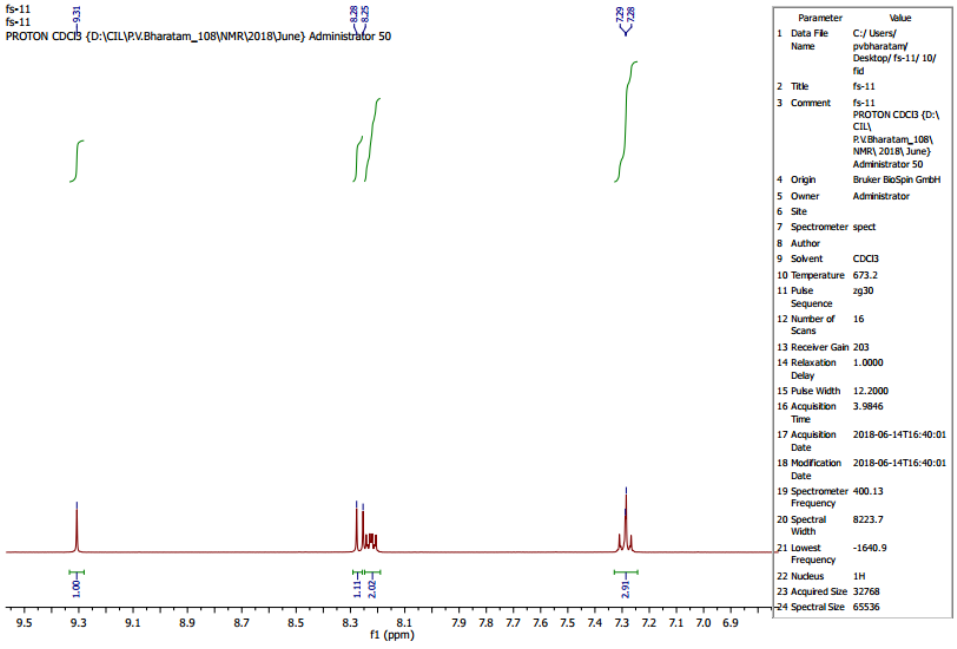
^{13}C NMR of 6,7-dichloro-2-(4-methoxyphenyl)quinoxaline (5g)



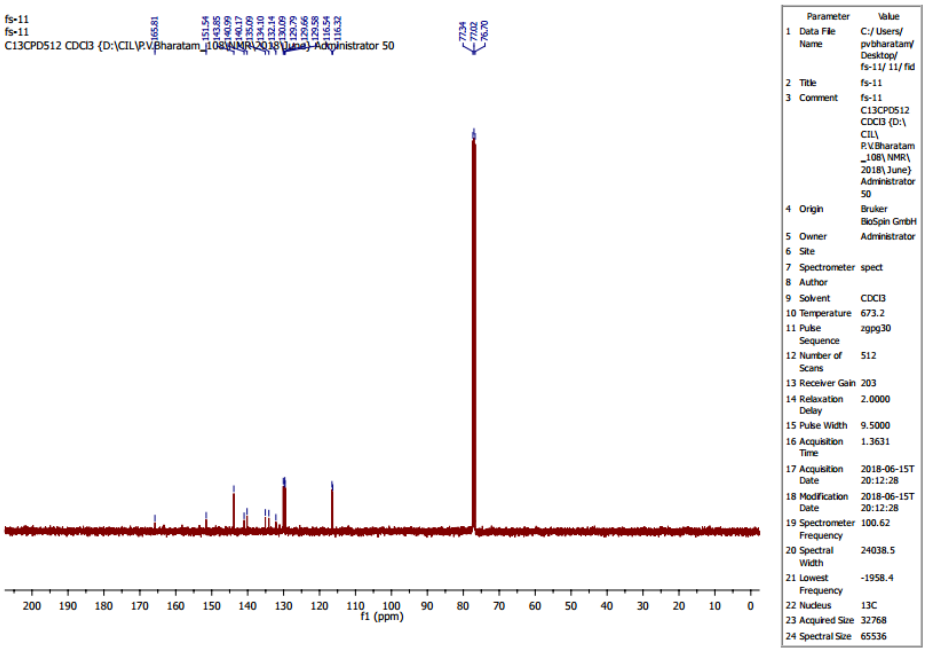
^{1}H NMR of 6,7-dichloro-2-(4-fluorophenyl)quinoxaline (5h)



Expansion of the aromatic region of the ^{1}H NMR of 6,7-dichloro-2-(4-fluorophenyl)quinoxaline (5h)



^{13}C NMR of 6,7-dichloro-2-(4-fluorophenyl)quinoxaline (5h)



HRMS of 6,7-dichloro-2-(4-fluorophenyl)quinoxaline (5h)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
152 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 F: 0-3 Cl: 0-2

Sample Name : FS-11 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
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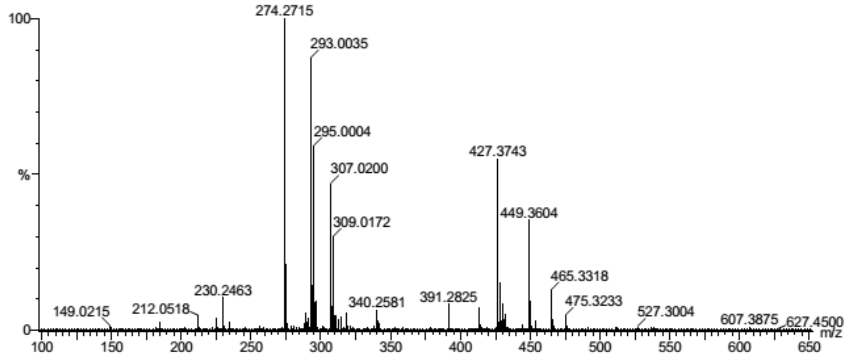
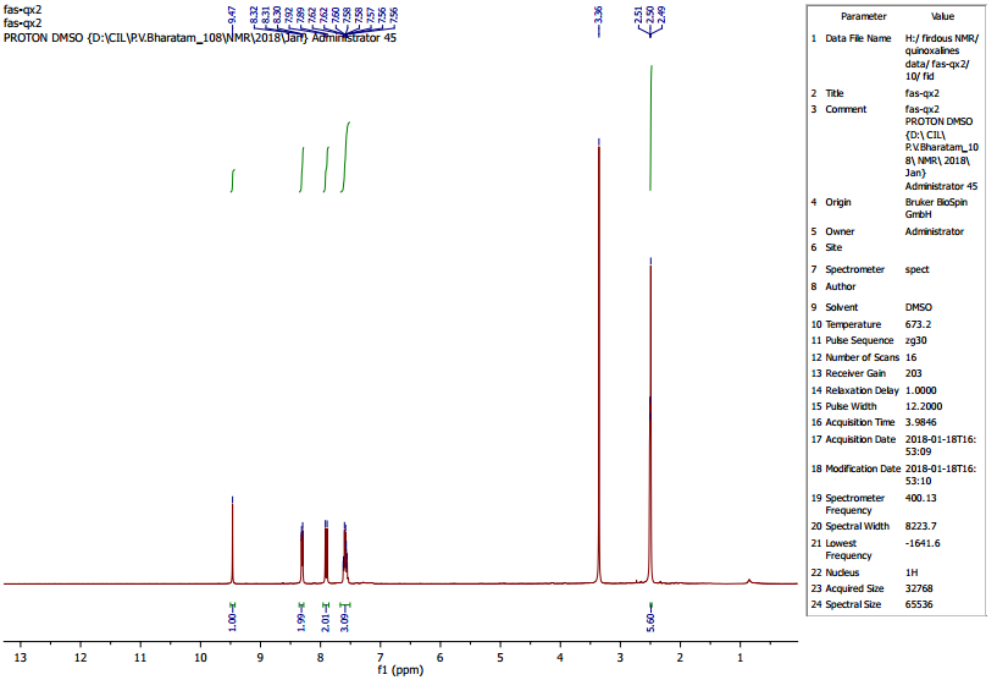
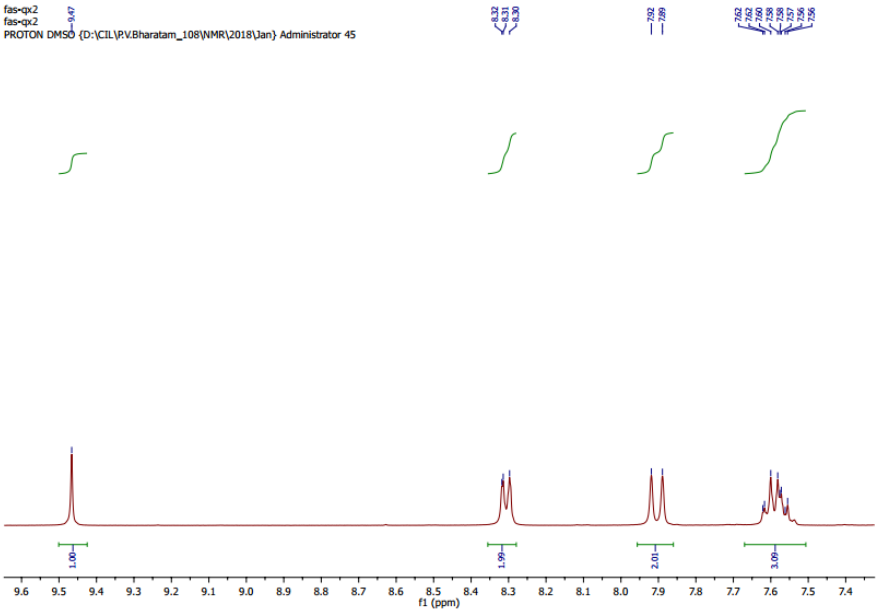


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
293.0035	293.0049	-1.4	-4.8	10.5	1209.7	n/a	n/a	C14 H8 N2 F Cl2

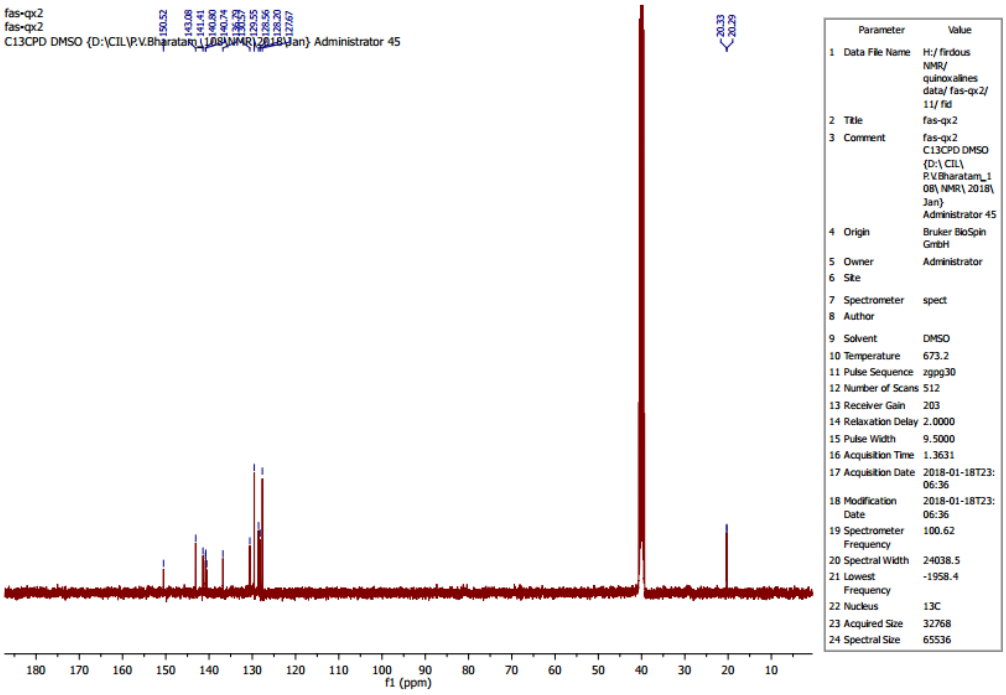
^{1}H NMR of 6,7-dimethyl-2-phenylquinoxaline (5i)



Expansion of the aromatic region of the ^{1}H NMR of 6,7-dimethyl-2-phenylquinoxaline (5i)



^{13}C NMR of 6,7-dimethyl-2-phenylquinoxaline (5i)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
10	Temperature	673.2
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12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-01-18T23: 06:36
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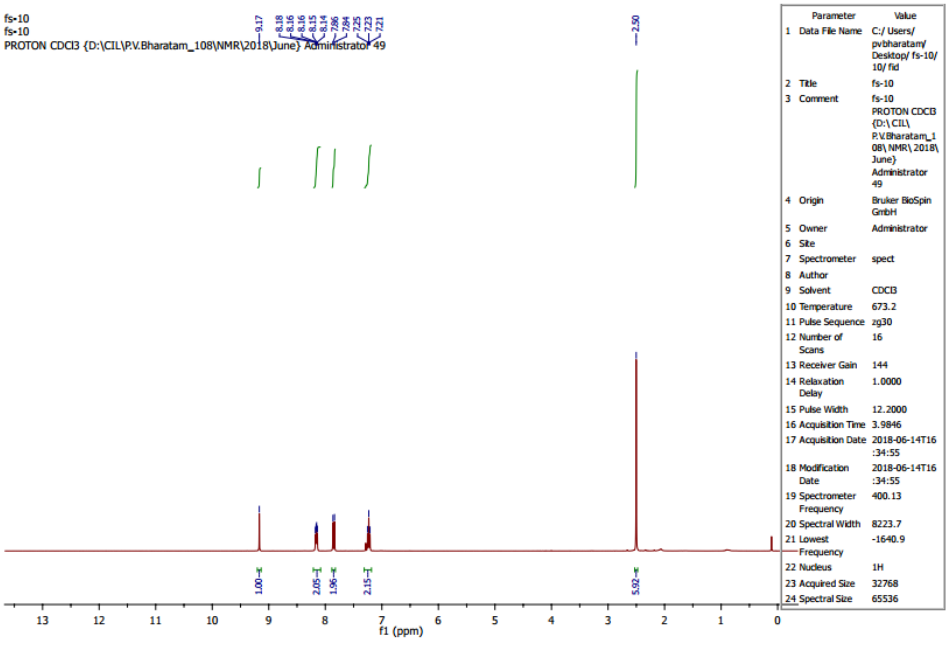
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(4-fluorophenyl)-6,7-dimethylquinoxaline (5j)



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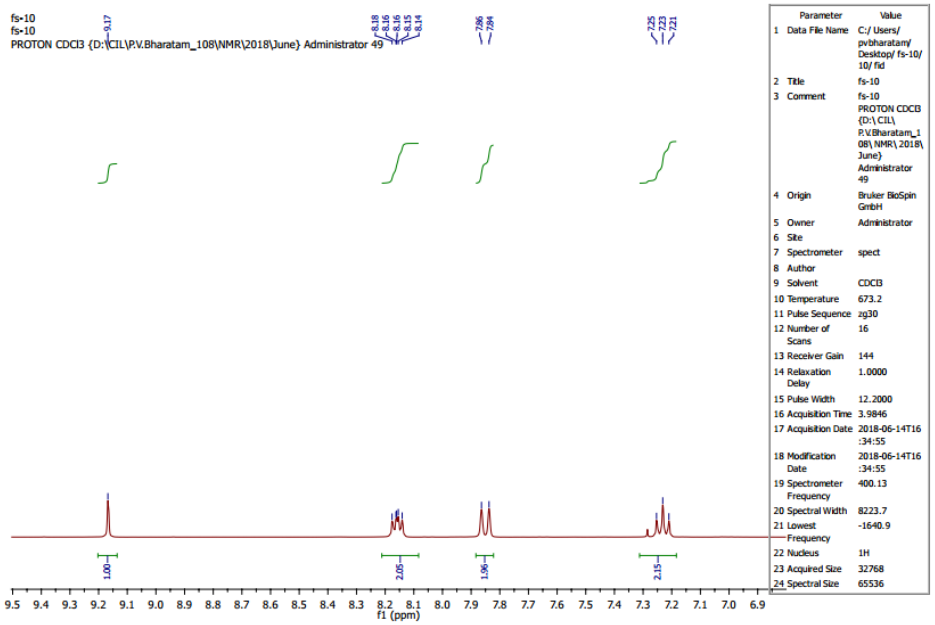
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-06-14T16 :34:55
18	Modification Date	2018-06-14T16 :34:55
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of2-(4-fluorophenyl)-6,7-dimethylquinoxaline (5j)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-06-14T16 :34:55
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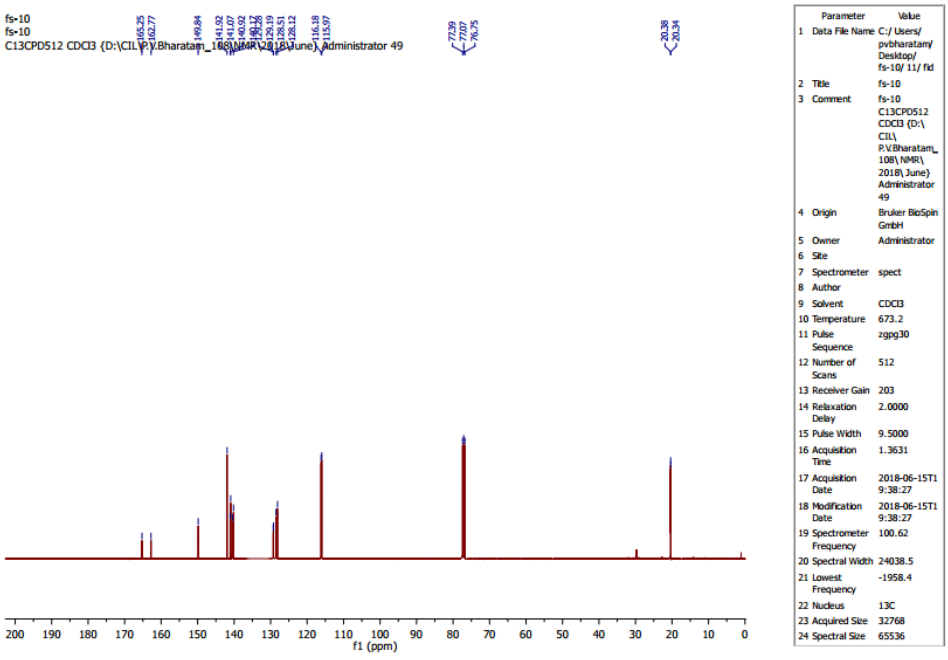
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-fluorophenyl)-6,7-dimethylquinoxaline (5j)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-06-15T1 9:38:27
18	Modification Date	2018-06-15T1 9:38:27
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

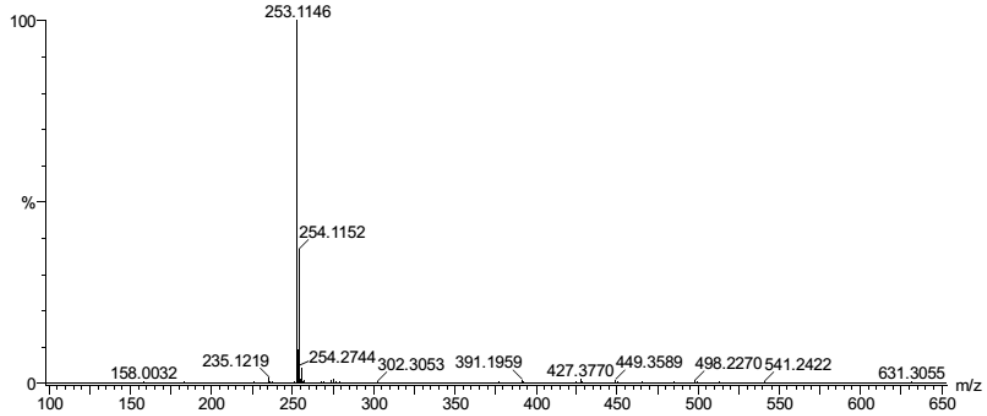
HRMS of 2-(4-fluorophenyl)-6,7-dimethylquinoxaline (5j)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

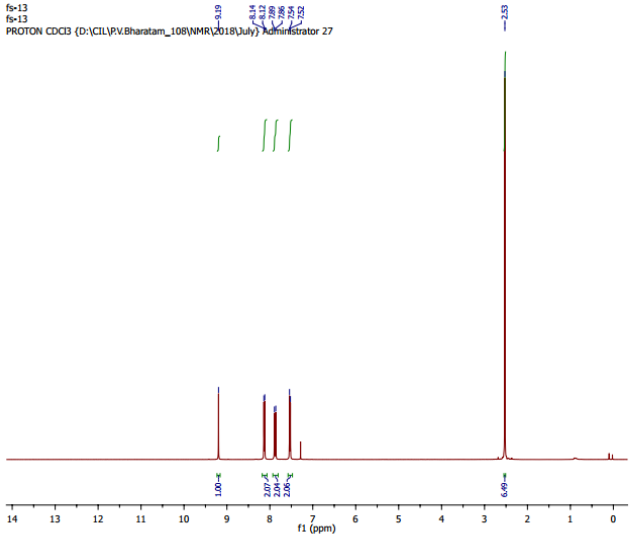
Monoisotopic Mass, Even Electron Ions
52 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 F: 0-3

Sample Name : FS-10 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-10 24 (0.245) AM2 (Ar,22000.0,0.00,0.00); Cm (24:27) 1: TOF MS ES+
6.21e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
253.1146	253.1141	0.5	2.0	10.5	1142.1	n/a	n/a	C16 H14 N2 F

^{1}H NMR of 2-(4-chlorophenyl)-6,7-dimethylquinoxaline (5k)



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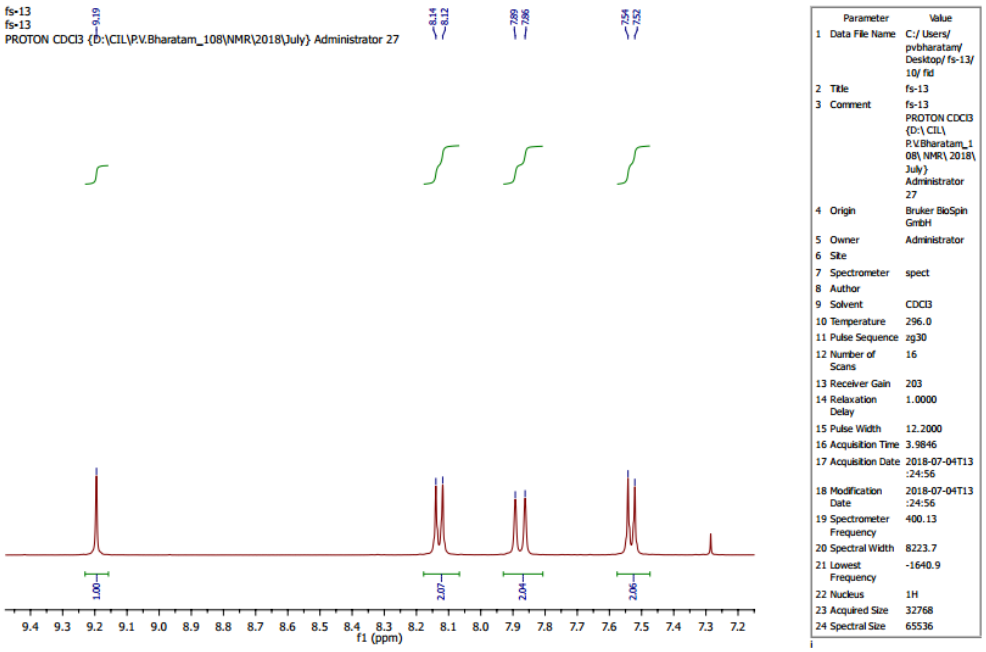
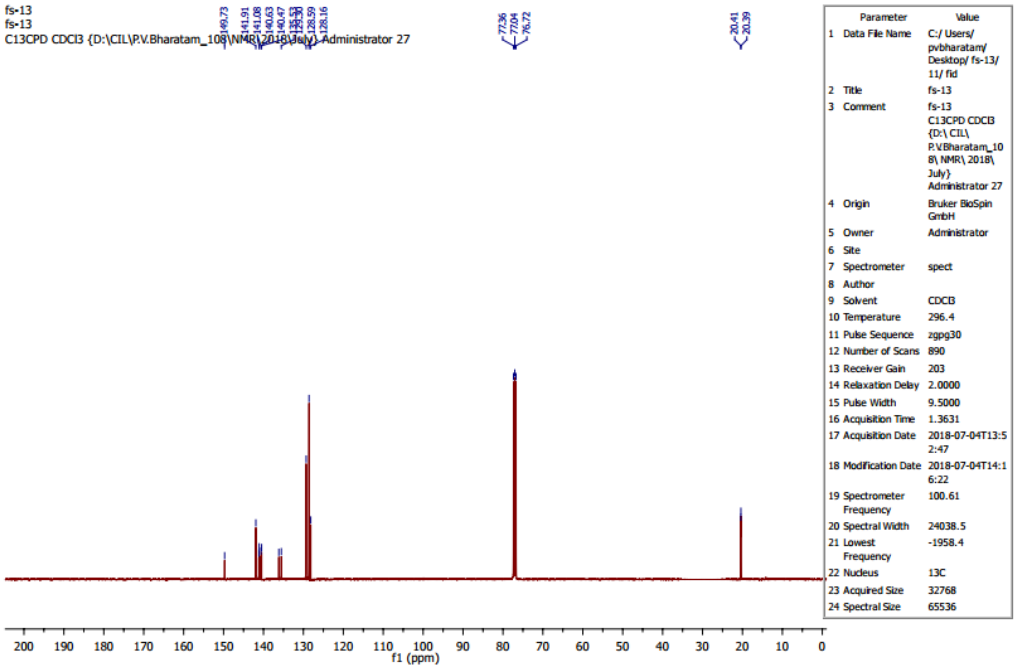
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-04T13 :24:56
18	Modification Date	2018-07-04T13 :24:56
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR spectra of 2-(4-chlorophenyl)-6,7-dimethylquinoxaline (5k)



^{13}C NMR of 2-(4-chlorophenyl)-6,7-dimethylquinoxaline (5k)



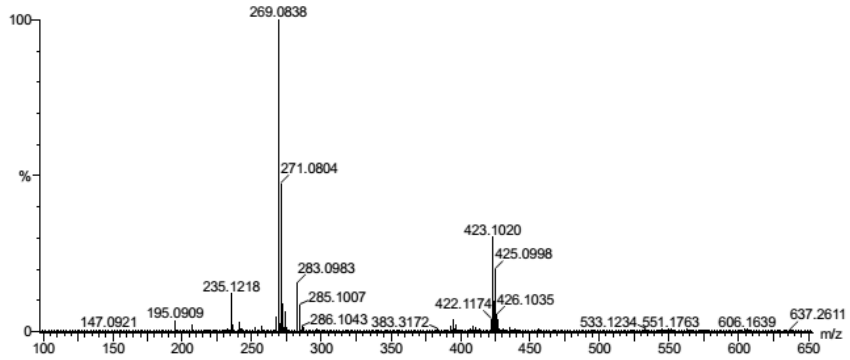
HRMS of 2-(4-chlorophenyl)-6,7-dimethylquinoxaline (5k)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

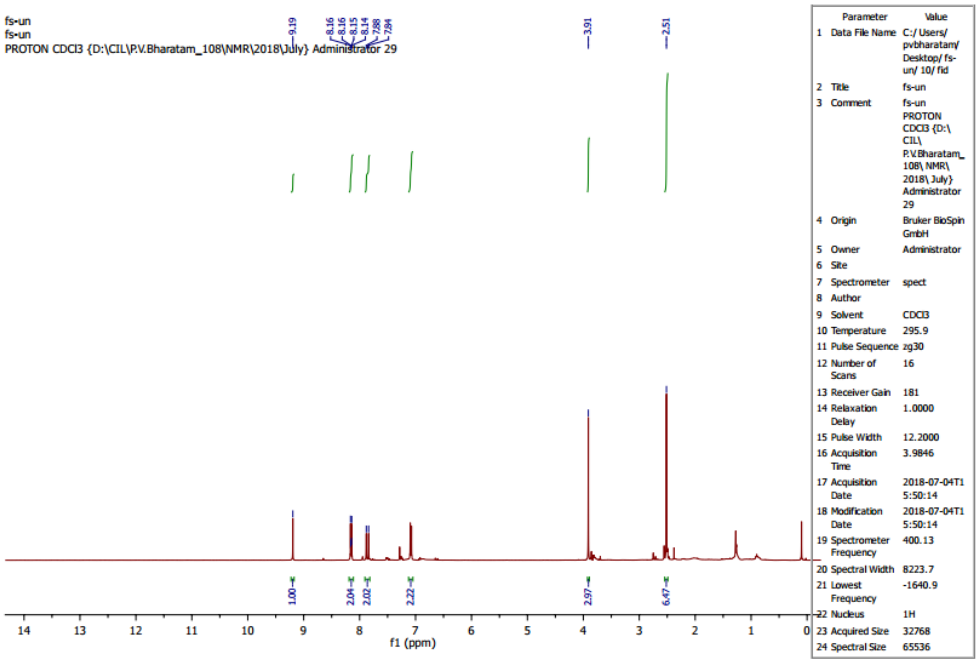
Monoisotopic Mass, Even Electron Ions
26 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-3 Cl: 0-2

Sample Name : FS-13 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-13 18 (0.183) AM2 (Ar,22000.0,0.00,0.00); Cm (18:21) 1: TOF MS ES+ 4.41e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
269.0838	269.0846	-0.8	-3.0	10.5	1107.9	n/a	n/a	C16 H14 N2 Cl

^{1}H NMR of 2-(4-Methoxyphenyl)-6,7-dimethylquinoxaline (5l)



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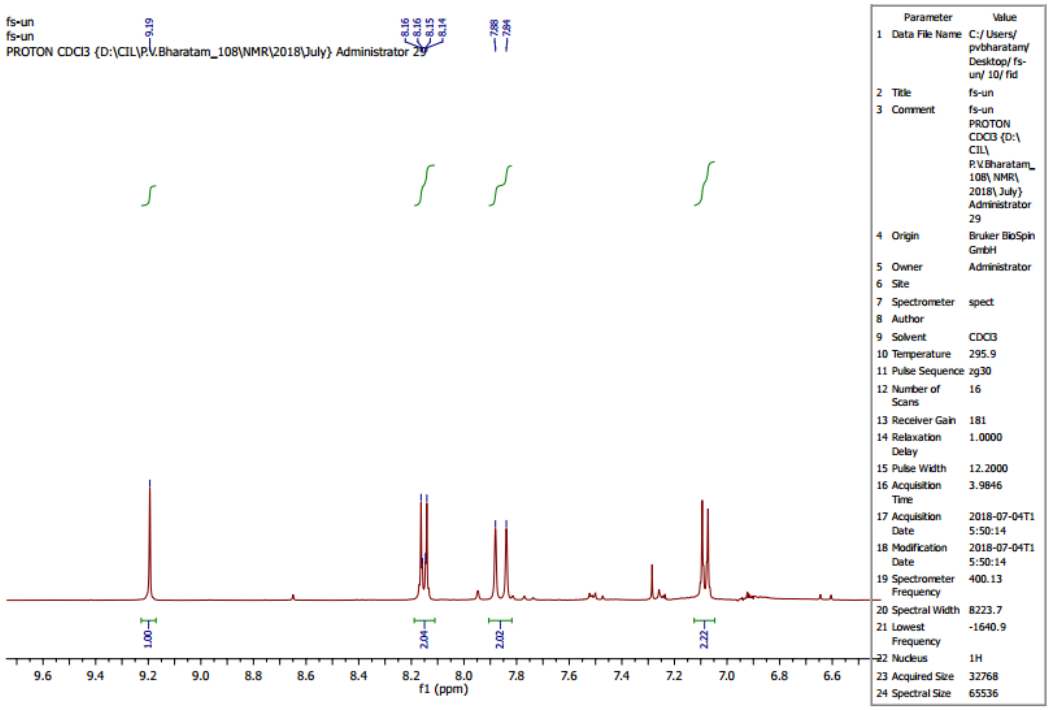
3	Comment	fs-un PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_ 108\ NMR\ 2018\ July} Administrator 29
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.9
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-04T1 5:50:14
18	Modification Date	2018-07-04T1 5:50:14
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR spectra of 2-(4-Methoxyphenyl)-6,7-dimethylquinoxaline (5l)



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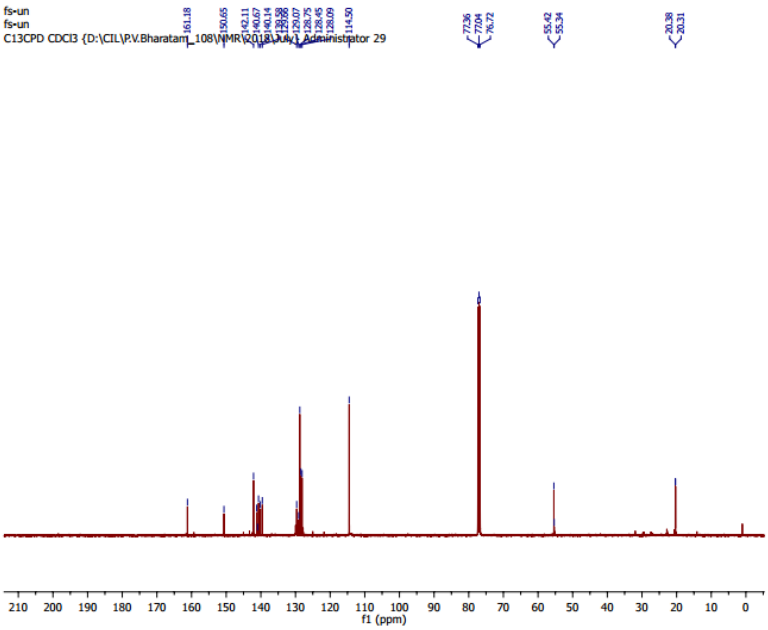
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.9
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-07-04T15:50:14
18	Modification Date	2018-07-04T15:50:14
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-Methoxyphenyl)-6,7-dimethylquinoxaline (5l)



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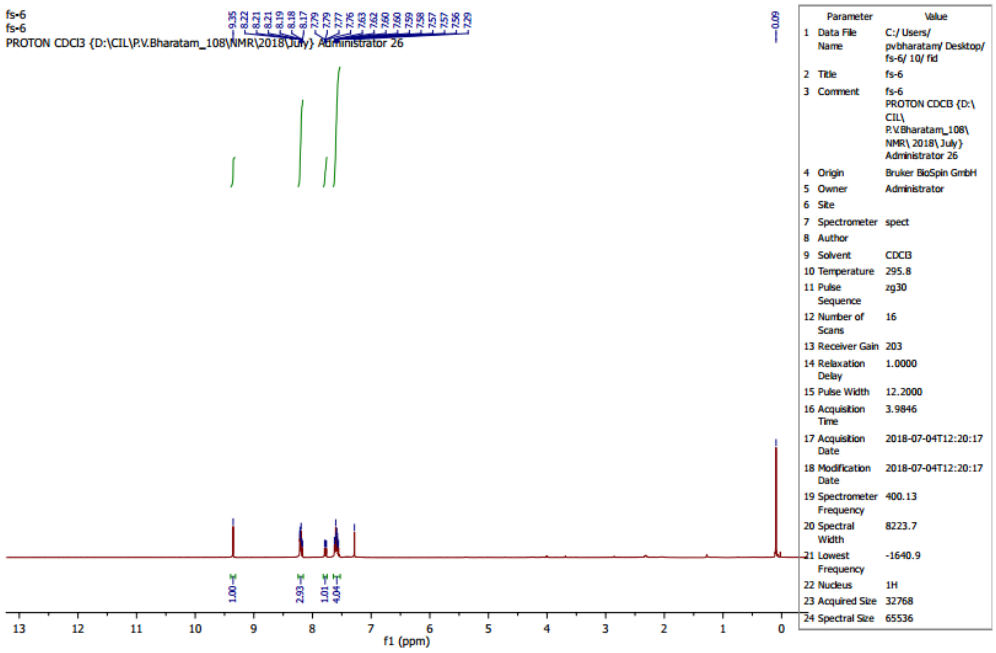
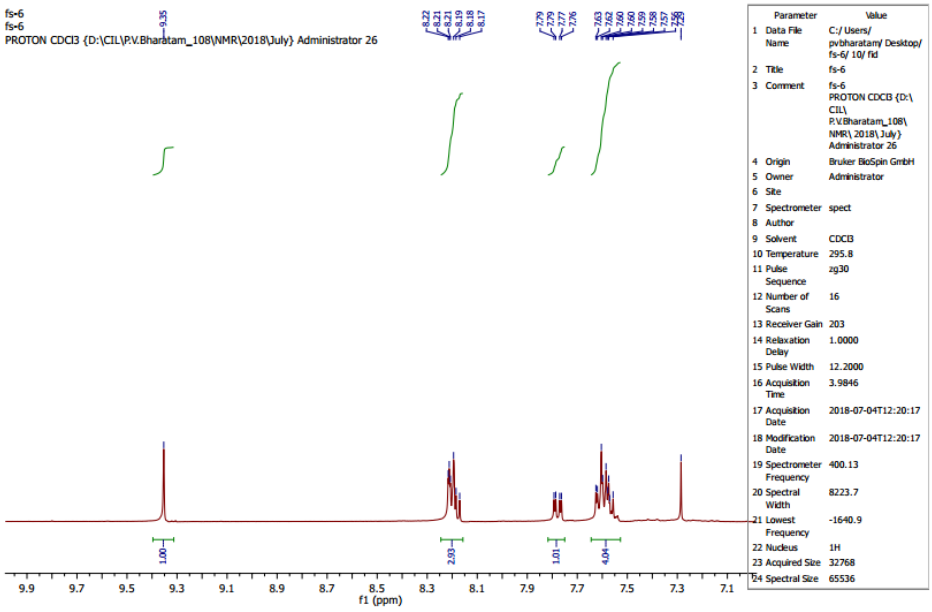
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.4
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-07-04T16:49:18
18	Modification Date	2018-07-04T16:49:18
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

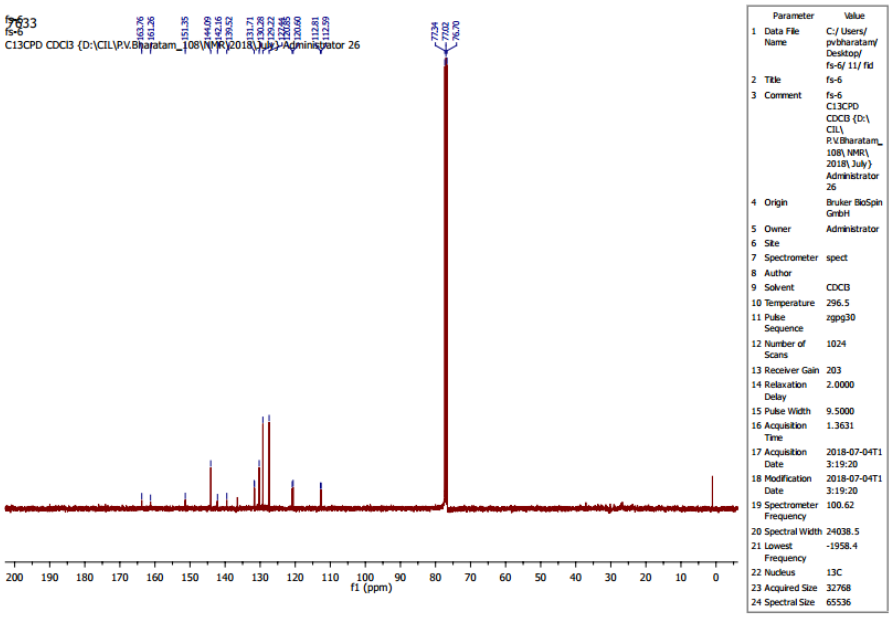
^{1}H NMR of 6-fluoro-2-phenylquinoxaline (5m)



Expansion of the aromatic region of the ^{1}H NMR of 6-fluoro-2-phenylquinoxaline (5m)



^{13}C NMR of 6-fluoro-2-phenylquinoxaline (5m)



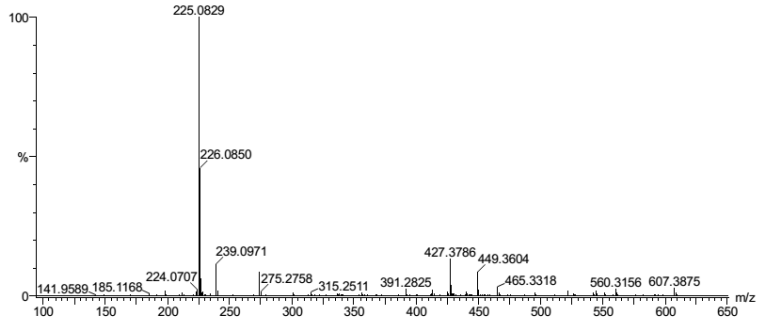
HRMS of 6-fluoro-2-phenylquinoxaline (5m)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

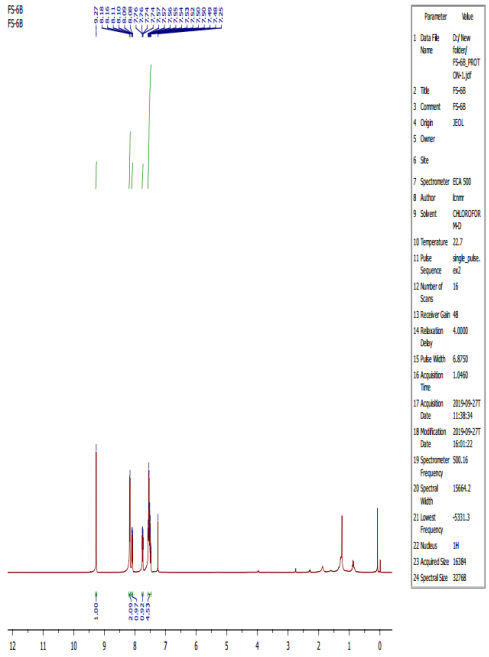
Monoisotopic Mass, Even Electron Ions
41 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 F: 0-3

Sample Name : FS-6a IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-6a 17 (0.174) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (17:19) 1: TOF MS ES+ 5.68e+007

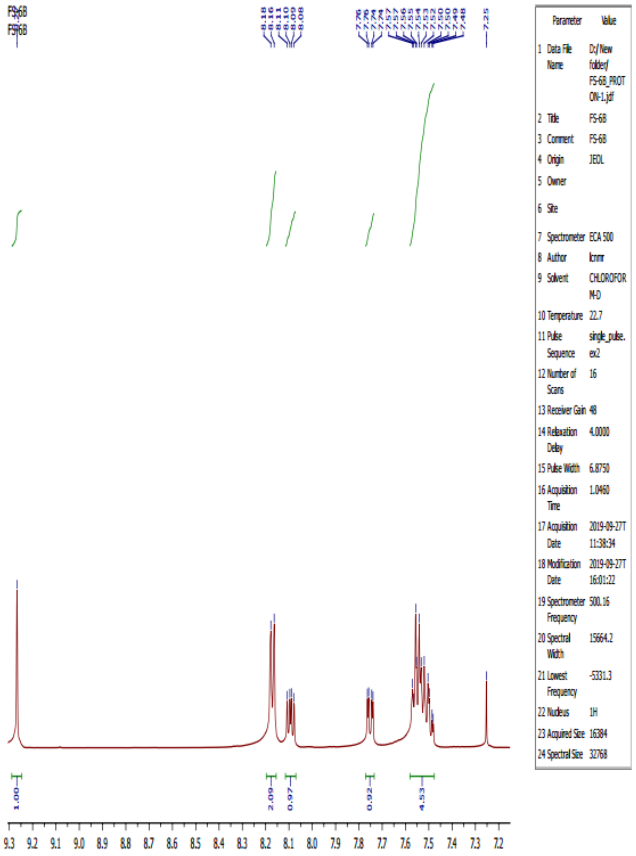


Minimum:				-1.5			
Maximum:		5.0	5.0	50.0			
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Norm**	**Conf(%)**	**Formula**
225.0829	225.0828	0.1	0.4	10.5	1402.8	n/a	n/a	C14 H10 N2 F

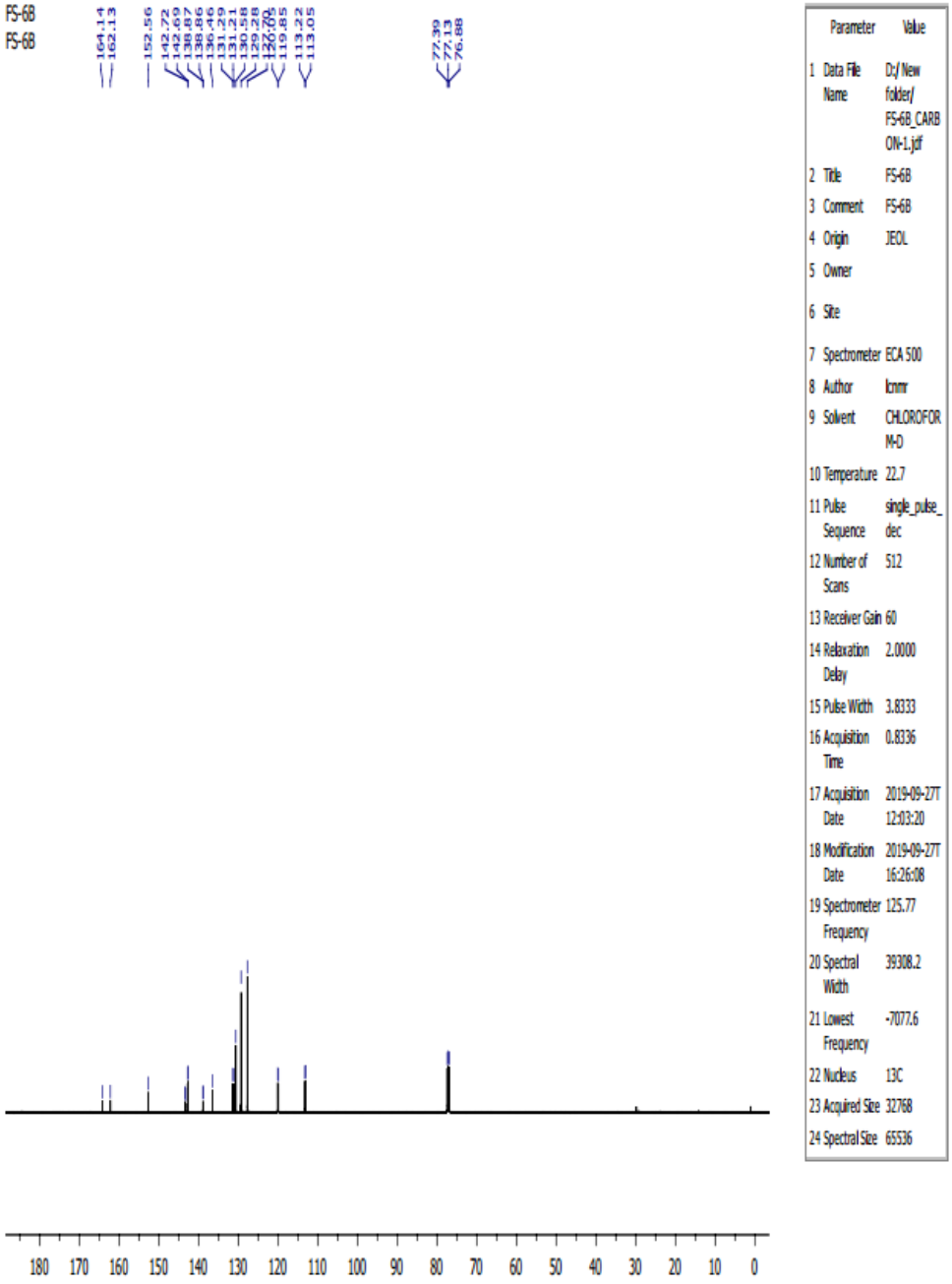
^{1}H NMR of 7-fluoro-2-phenylquinoxaline (5m^{1})



Expansion of the aromatic region of the ^{1}H NMR of 7-fluoro-2-phenylquinoxaline (5m^{1})



^{13}C NMR of 7-fluoro-2-phenylquinoxaline (5m[1])



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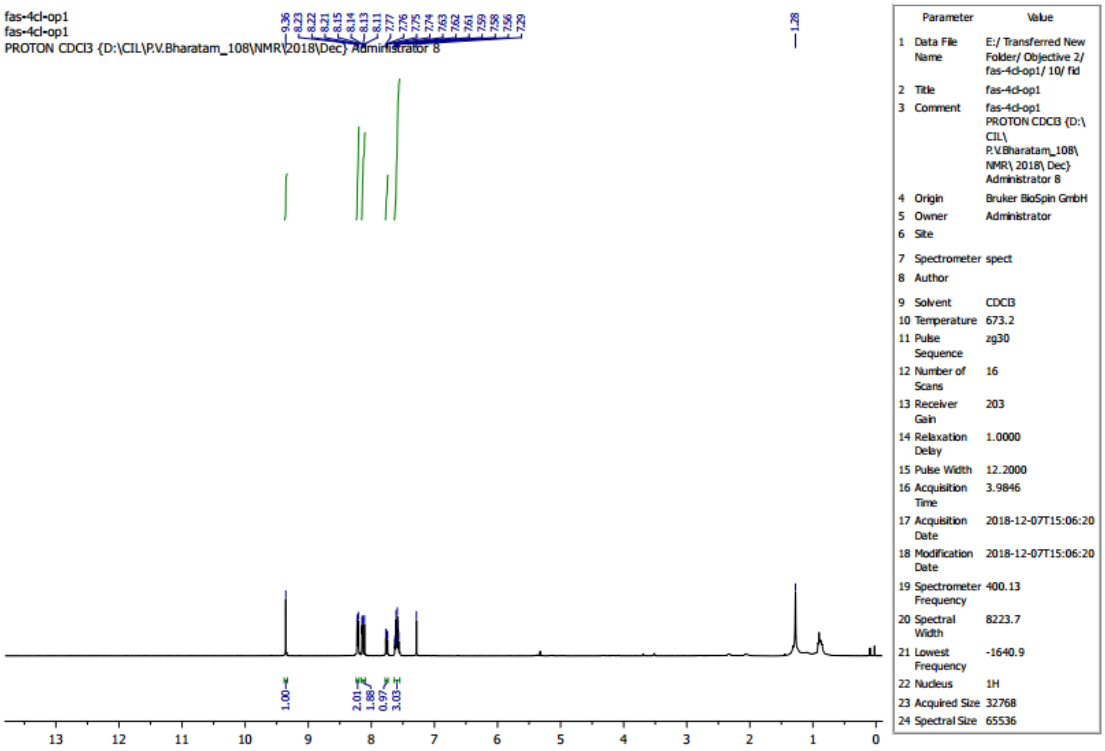
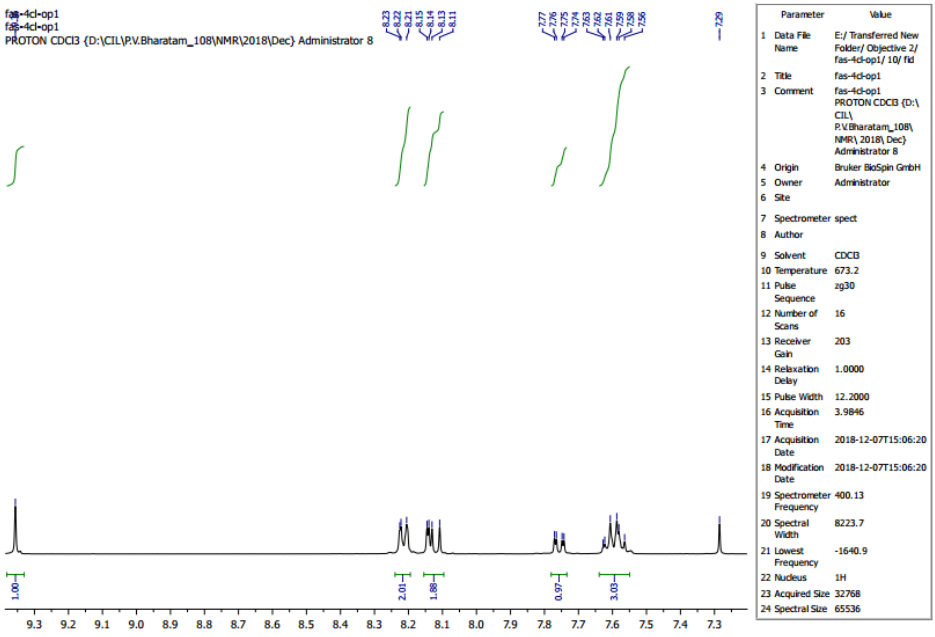
6	Site	
7	Spectrometer	ECA 500
8	Author	lcnmr
9	Solvent	CHLOROFORM-D
10	Temperature	22.7
11	Pulse Sequence	single_pulse_dec
12	Number of Scans	512
13	Receiver Gain	60
14	Relaxation Delay	2.0000
15	Pulse Width	3.8333
16	Acquisition Time	0.8336
17	Acquisition Date	2019-09-27T 12:03:20
18	Modification Date	2019-09-27T 16:26:08
19	Spectrometer Frequency	125.77
20	Spectral Width	39308.2
21	Lowest Frequency	-7077.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

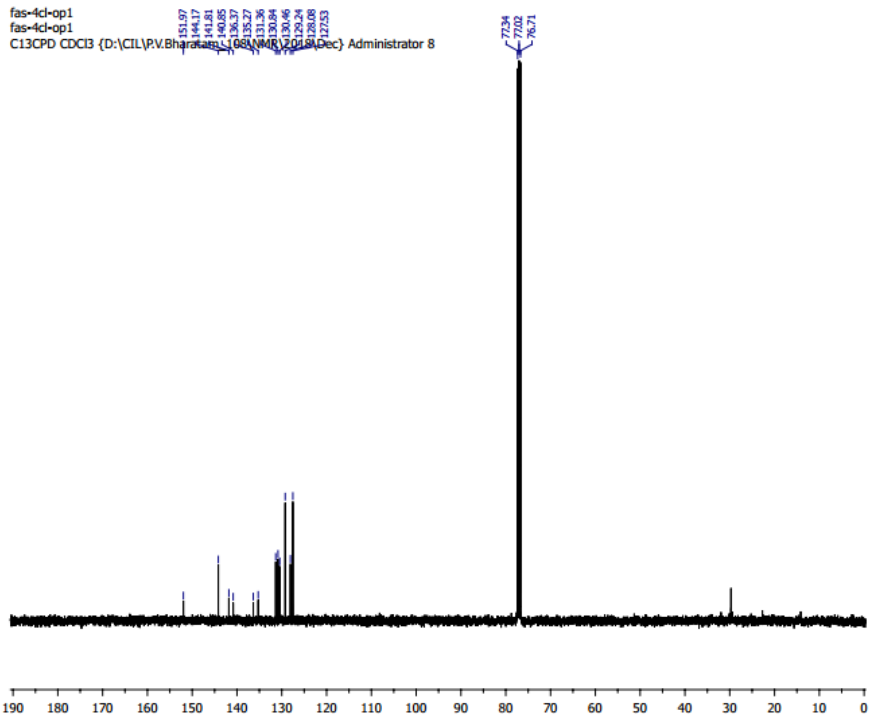
^{1}H NMR of 6-Chloro-2-phenylquinoxaline (5n)



Expansion of the aromatic region of the ^{1}H NMR of 6-Chloro-2-phenylquinoxaline (5n)



^{13}C NMR of 6-Chloro-2-phenylquinoxaline (5n)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-12-07T15: 21:32
18	Modification Date	2018-12-07T15: 21:32
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

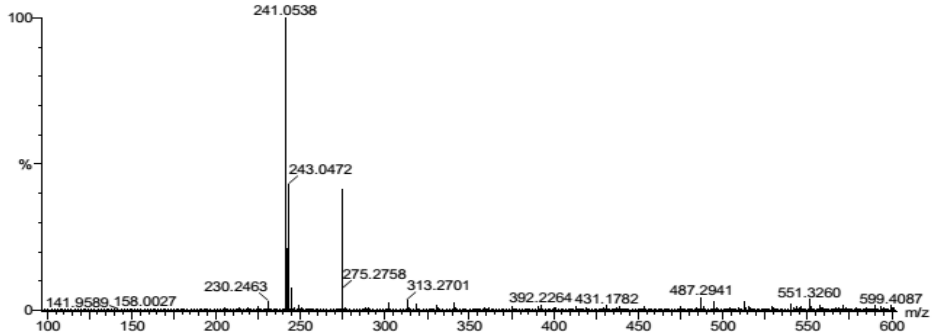
HRMS of 6-Chloro-2-phenylquinoxaline (5n)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

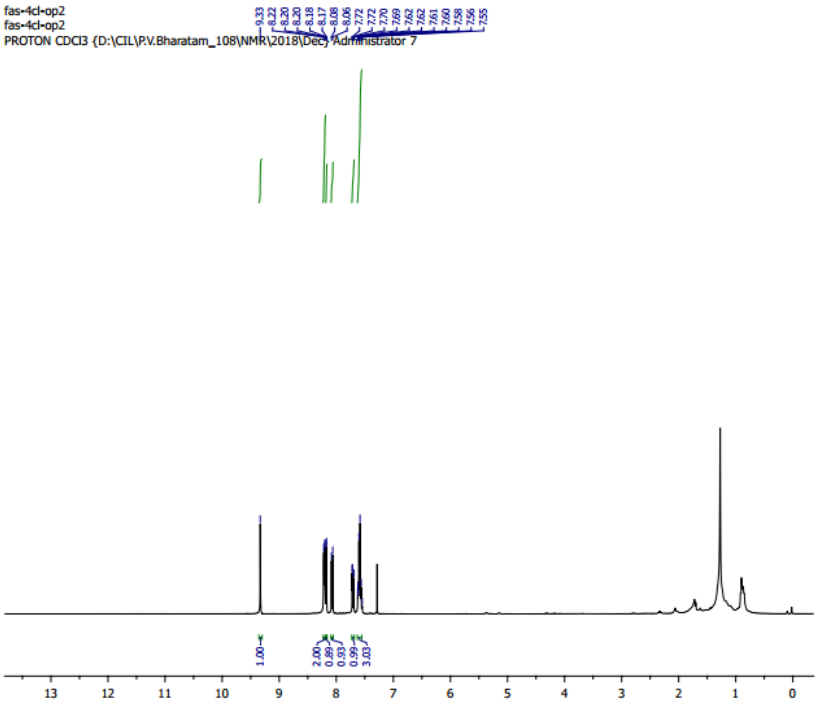
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 Cl: 0-2

Sample Name : FAS-OP1 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FAS-OP1 16 (0.165) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (16:19) 1: TOF MS ES+ 3.19e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
241.0538	241.0533	0.5	2.1	10.5	1195.8	n/a	n/a	C14 H10 N2 Cl

^{1}H NMR of 7-Chloro-2-phenylquinoxaline (5n^{1})



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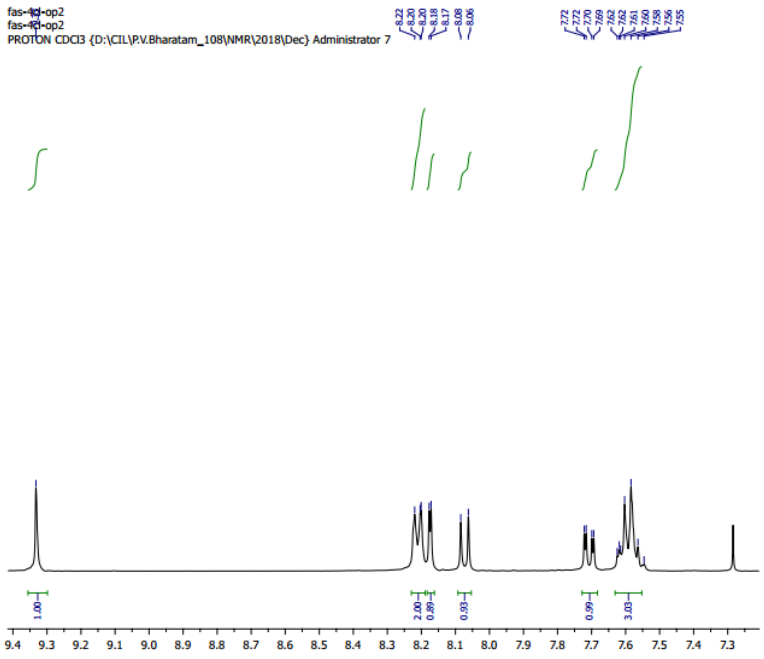
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-12-07T14:43:23
18	Modification Date	2018-12-07T14:43:24
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the^{1}H NMR of 7-Chloro-2-phenylquinoxaline (5n^{1})



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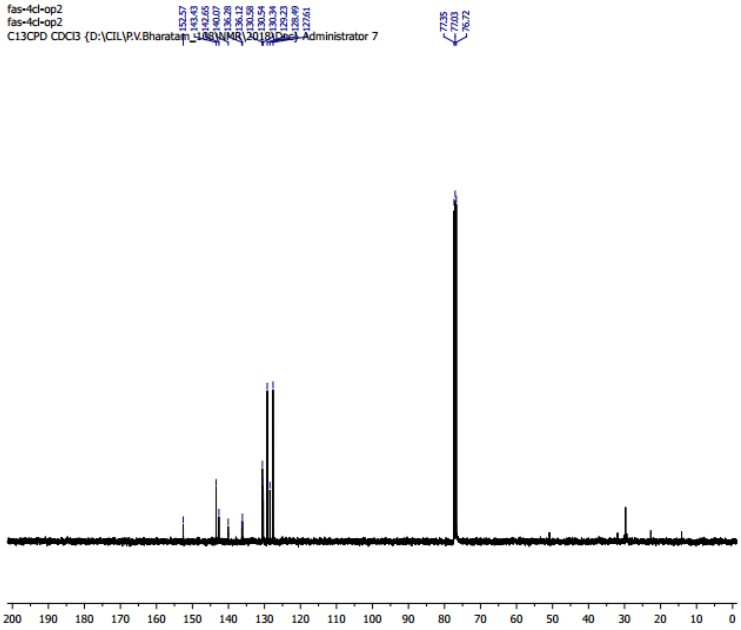
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-12-07T14:43:23
18	Modification Date	2018-12-07T14:43:24
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 7-Chloro-2-phenylquinoxaline (5n[1])



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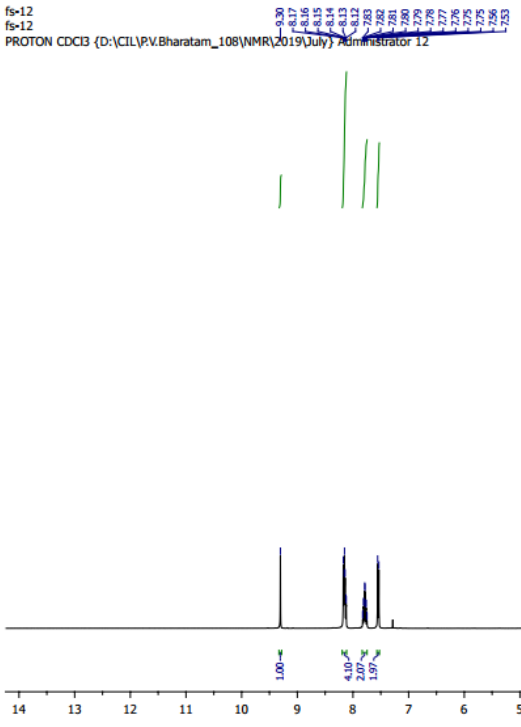
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	256
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-12-07T14:59:05
18	Modification Date	2018-12-07T14:59:06
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR of 2-(4-Chlorophenyl)quinoxaline (5o)



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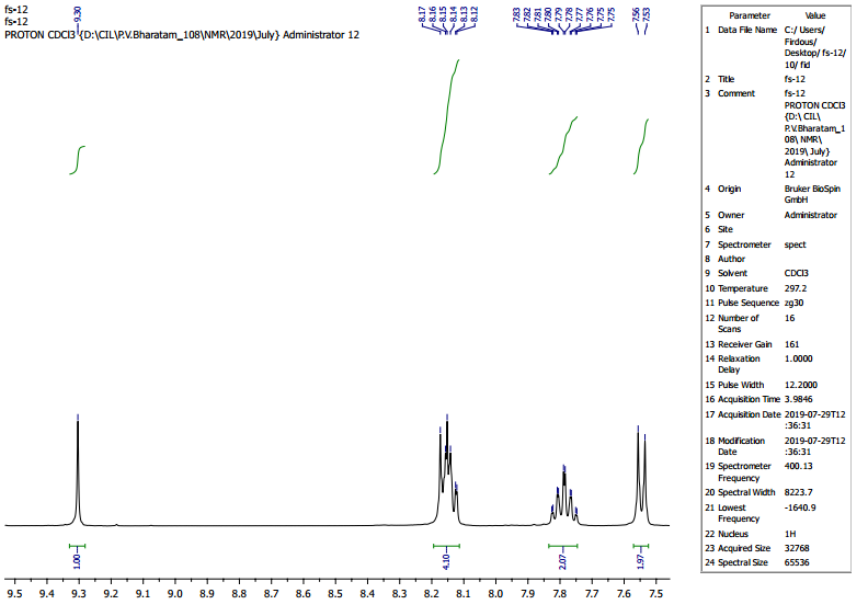
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2019-07-29T12:36:31
18	Modification Date	2019-07-29T12:36:31
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Expansion of the aromatic region of the ^{1}H NMR of 2-(4-Chlorophenyl)quinoxaline (5o)



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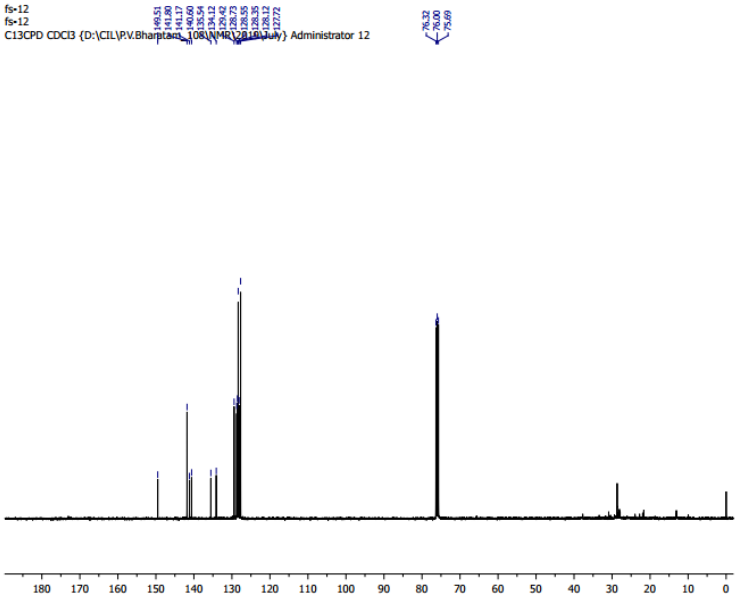
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2019-07-29T12 :36:31
18	Modification Date	2019-07-29T12 :36:31
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{13}C NMR of 2-(4-Chlorophenyl)quinoxaline (5o)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2019-07-29T15:2 7:53
18	Modification Date	2019-07-29T15:2 7:54
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-2063.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

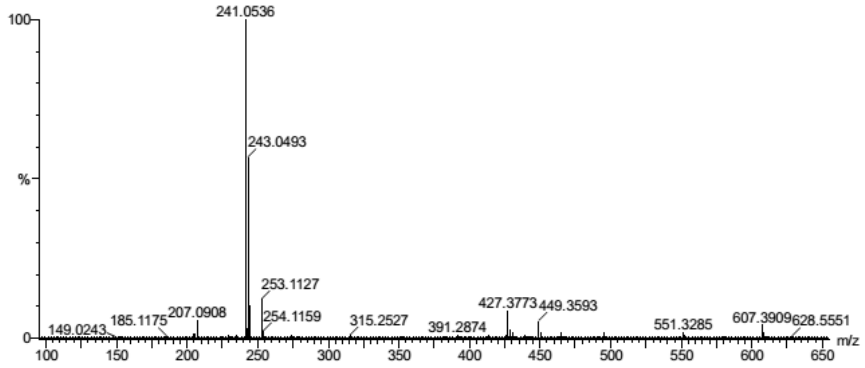
HRMS of 2-(4-Chlorophenyl)quinoxaline (5o)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

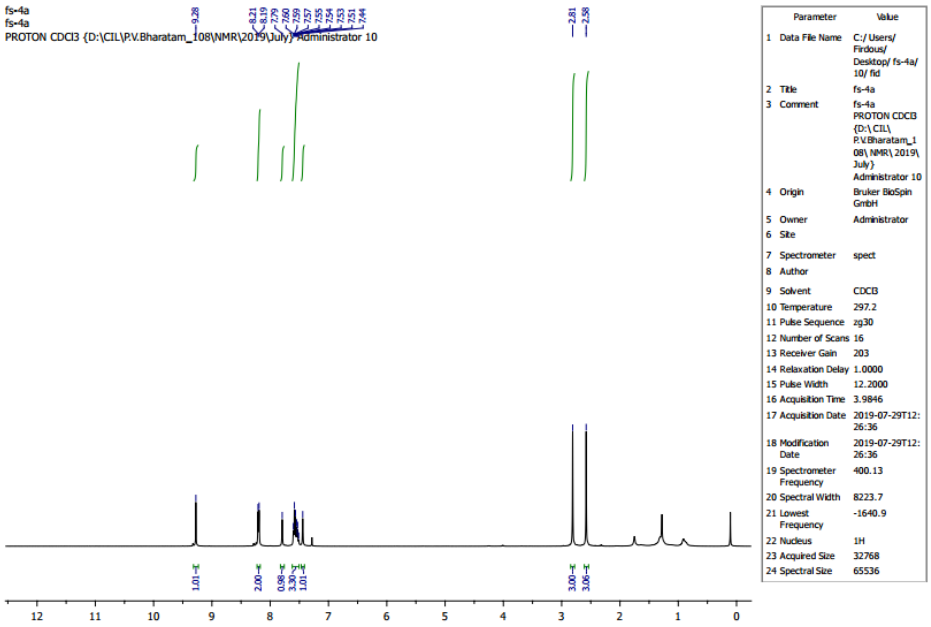
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 Cl: 0-2

Sample Name : FS-12 IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-12 24 (0.245) AM2 (Ar,22000.0,0.00,0.00); Cm (24:29) 1: TOF MS ES+
8.60e+007

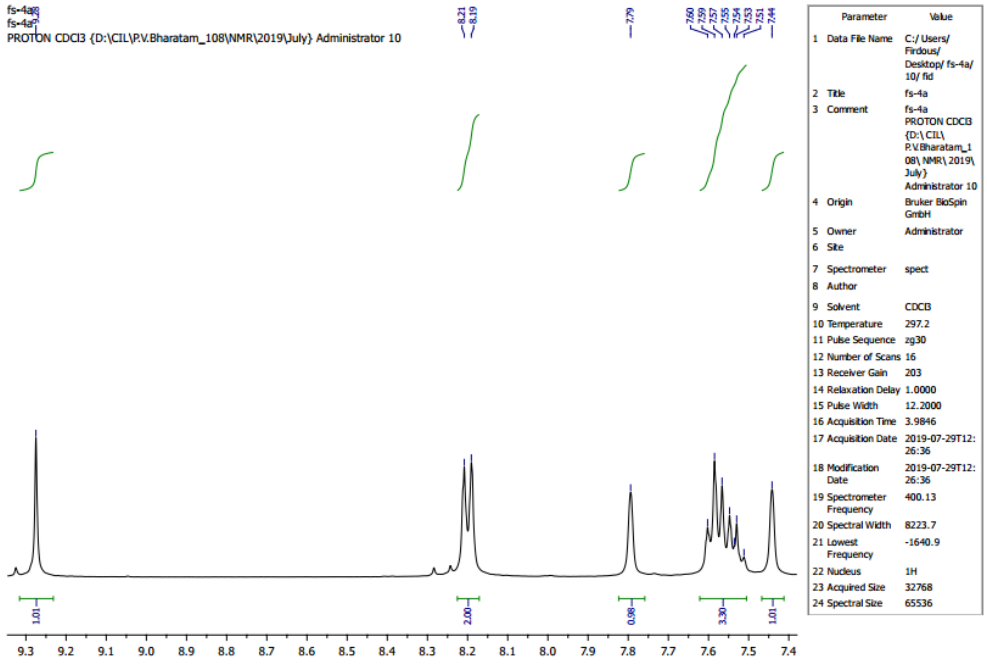


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
241.0536	241.0533	0.3	1.2	10.5	1271.1	n/a	n/a	C14 H10 N2 Cl

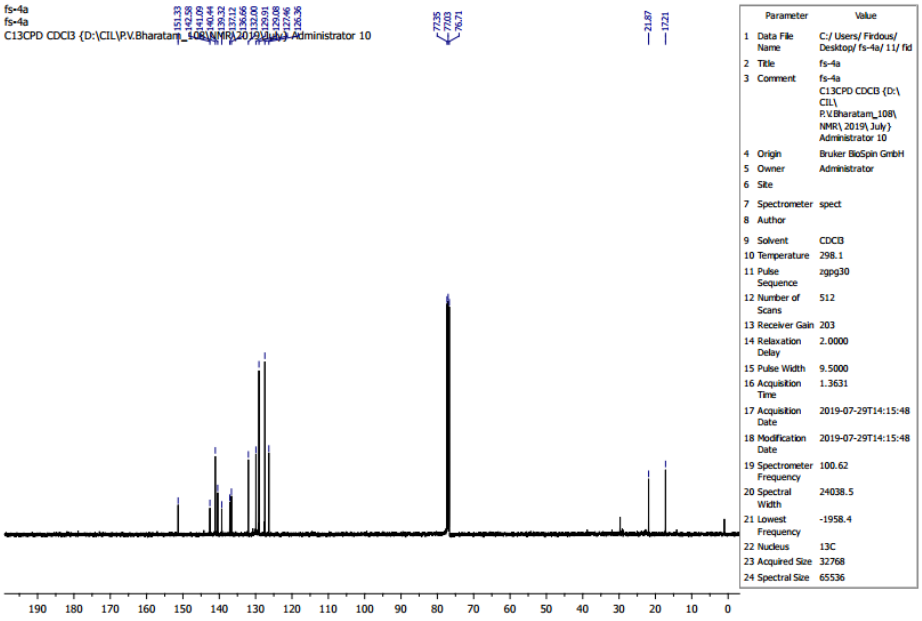
^{1}H NMR of 5,7-Dimethyl-2-phenylquinoxaline (5p)



Expansion of the aromatic region of the ^{1}H NMR of 5,7-Dimethyl-2-phenylquinoxaline (5p)



^{13}C NMR of 5,7-Dimethyl-2-phenylquinoxaline (5p)



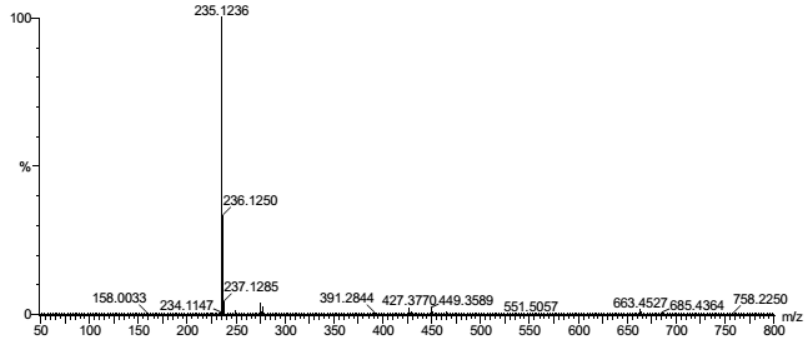
HRMS of 5,7-Dimethyl-2-phenylquinoxaline (5p)

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

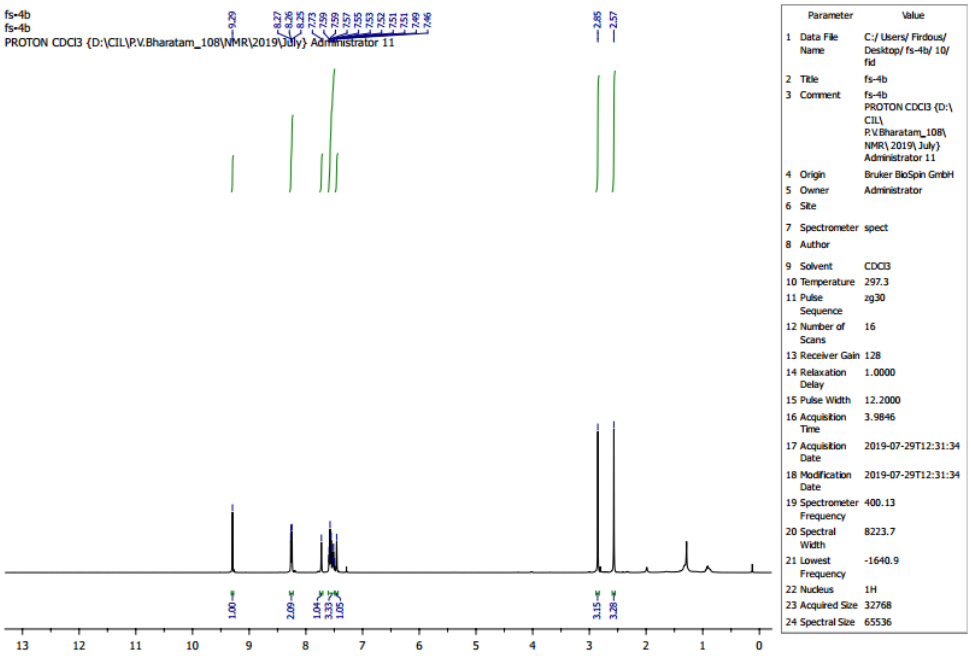
Monoisotopic Mass, Even Electron Ions
33 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 11-30 H: 7-35 N: 0-5 Cl: 0-2

Sample Name : FS-4A IITRPR XEVO G2-XS QTOF
Test Name : HRMS-1
071119-FS-4A 24 (0.245) AM2 (Ar,22000.0,0.00,0.00); Cm (24:26) 1: TOF MS ES+ 4.41e+007

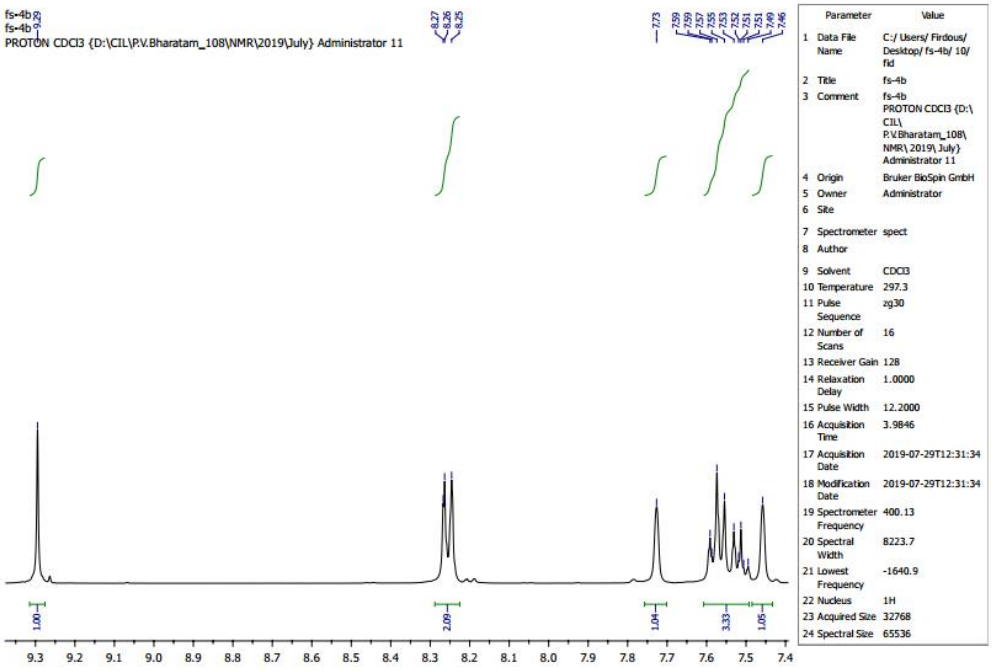


Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
235.1236	235.1235	0.1	0.4	10.5	1153.9	n/a	n/a	C16 H15 N2

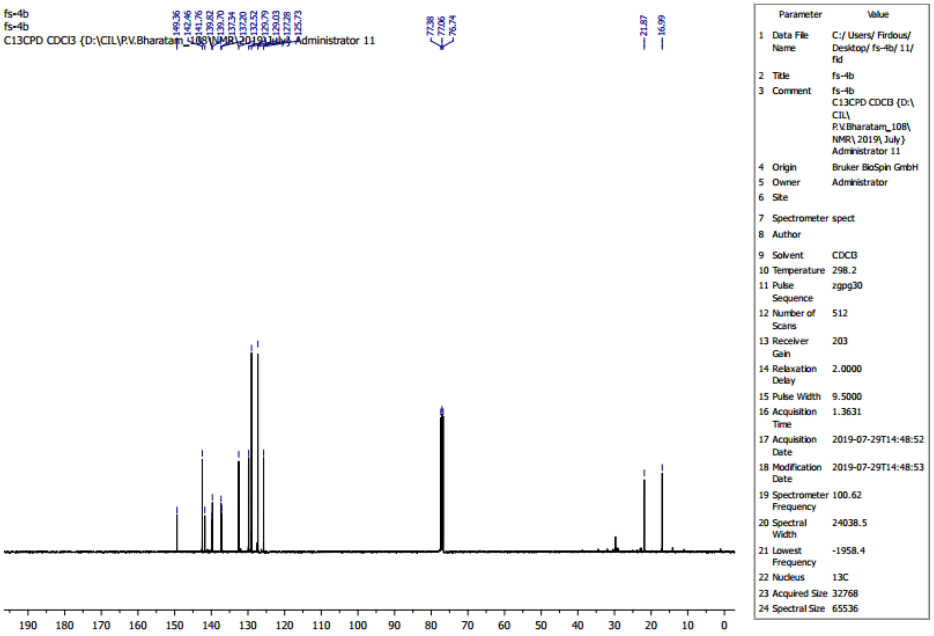
^{1}H NMR of 6,8-Dimethyl-2-phenylquinoxaline (5p^{1})



Expansion of the aromatic region of the ^{1}H NMR of 6,8-Dimethyl-2-phenylquinoxaline (5p1)



^{13}C NMR of 6,8-Dimethyl-2-phenylquinoxaline (5p[1])



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2019-07-29T14:48:52
18	Modification Date	2019-07-29T14:48:53
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

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