Electronic Supporting Information (ESI)

Bimetallic Cu-Mn B spinel oxide catalyzed oxidative synthesis of 1,2-disubstituted benzimidazoles from benzyl bromides

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TABLE OF CONTENTS

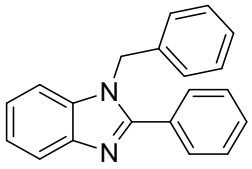
S1. EXPERIMENTAL PROCEDURES

S1.1. Chemistry protocols

General. All chemicals were obtained from Sigma-Aldrich Company and used as received. ^{1}H, ^{13}C and DEPT NMR spectra were recorded on Brucker-Avance DPX FT-NMR 500 and 400 MHz instruments. 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). The carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 100 MHz: 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). ESI-MS spectra were recorded on Agilent 1100 LC-Q-TOF. IR spectra were recorded on Perkin-Elmer IR spectrophotometer.

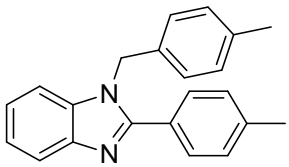
Procedure for synthesis of substituted 2-aryl-N benzyl benzimidazoles and 2-aryl benzimidazoles: To a solution of substituted *o*-phenylenediamine **1** (1 equiv.) in 3 mL of DMSO was added 10% w/w of Cu-Mn B, 2.5 equiv of K_2CO_3 and 2 equiv. of benzyl bromide **2** (2 equiv.) and heated at 100 ^{o}C for 12h. After completion of reaction monitored by TLC, reaction mixture was filtered to recover the catalyst. Water and ethyl acetate work up was done, organic layer was separated, dried over anhydrous sodium sulphate and finally concentrated to get crude product. The residue was subjected to purification by 100-200 silica gel column using EtOAc/hexane as eluent to get the desired products **3(a-q)** in 48-72% and **4(a-q)** in 12-22 % yield**.**

1-benzyl-2-phenyl-1H-benzo[d]imidazole (3a)[1]



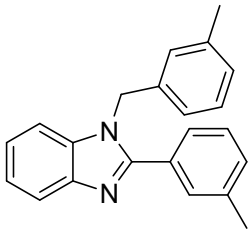
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8Hz, 1H), 7.73-7.71 (m, 2H), 7.51-7.47 (m, 3H), 7.38-7.32 (m, 4H), 7.28-7.23 (m, 2H), 7.14 (d, *J* = 8Hz, 2H), 5.48 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.2, 143.2, 136.4, 136.1, 129.3, 129.1, 128.8, 125.9, 123.1, 122.7, 119.9, 110.5, 48.4; ESI-MS (LTQ): 285.21 $[M+H]^+$

1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole (3b)[2]



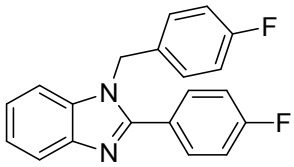
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8Hz, 1H), 7.88 (d, *J* = 8Hz, 1H), 7.61 (d, *J* = 8Hz, 2H), 7.33-7.30 (m, 2H), 7.27-7.24 (m, 2H), 7.17 (d, *J* = 8Hz, 2H), 7.03 (d, *J* = 8Hz, 2H), 5.44 (s, 2H), 2.41 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.5, 140.2, 137.5, 133.3, 129.7, 129.5, 129.1, 126.7, 125.9, 125.7, 122.9, 122.7, 119.7, 110.6, 48.2, 21.4, 21.1; IR ($CHCl_3$): ν_{max} 3410, 2919, 1621, 1429, 1274, 1083, 963 cm^{-1}; ESI-MS (LTQ): 313.14 $[M+H]^+$

1-(3-methylbenzyl)-2-(m-tolyl)-1H-benzo[d]imidazole (3c)[3]



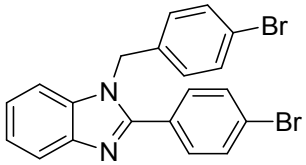
^{1} HNMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8Hz, 1H), 7.61 (s, 1H), 7.46 (d, *J* = 8Hz, 1H), 7.34-7.22 (m, 6H), 7.14 (d, *J* = 8Hz, 1H), 6.96-6.92 (m, 2H), 5.44 (s, 2H), 2.40 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 143.1, 138.8, 138.7, 136.5, 130.7, 128.9, 128.5,128.5, 126.7, 123.1, 122.9, 110.6, 48.5, 21.5, 21.4; ESI-MS (LTQ): 313.17 $[M+H]^+$

1-(4-fluorobenzyl)-2-(4-fluorophenyl)-1H-benzo[d]imidazole (3d)[4]



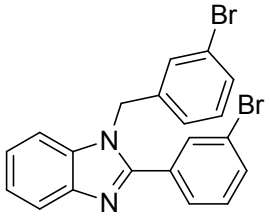
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8Hz, 1H), 7.66-7.63 (m, 2H), 7.34-7.30 (m, 1H), 7.27-7.19 (m, 2H), 7.16 (t, *J* = 8Hz, 2H), 7.04-7.00 (m, 4H), 5.37 (s, 2H); IR ($CHCl_3$): ν_{max} 2956, 2924, 1711, 1607, 1509, 1482, 1458, 1414, 1381, 1226, 1157 cm^{-1}; ESI-MS (LTQ): 321.51 $[M+H]^+$

1-(4-bromobenzyl)-2-(4-bromophenyl)-1H-benzo[d]imidazole (3e)[5]



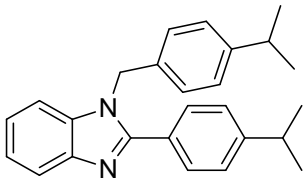
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8Hz, 1H), 7.65 (t, *J* = 8Hz, 2H), 7.55 (d, *J* = 8Hz, 2H), 7.51 (d, *J* = 8Hz, 2H), 7.39-7.30 (m, 2H), 7.23 (d, *J* = 8Hz, 1H), 7.00 (d, *J* = 8Hz, 2H), 5.40 (s, 2H); ^{13}C NMR (100 MHz, CDCl3) δ 152.3, 142, 139.4, 135.1, 132.4, 132.1, 130.6, 129.3, 128, 123.6, 123.1, 122, 120.1, 111.6, 110.3, 47.9; IR ($CHCl_3$): ν_{max} 2925, 1733, 1455, 1260, 1012 cm^{-1}; ESI-MS (LTQ): 341. 40$[M+2H]^+$

1-(3-bromobenzyl)-2-(3-bromophenyl)-1H-benzo[d]imidazole (3f)[4]



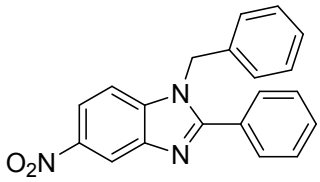
^{1} HNMR (400 MHz, $CDCl_3$) δ 7.91-786 (m, 1H), 7.62 (d, *J* = 8Hz, 1H), 7.54 (d, *J* = 8Hz, 1H), 7.48 (d, *J* = 8Hz, 1H), 7.39-7.26 (m, 6H), 7.24 (t, *J* = 8Hz, 1H), 5.42 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 142.8, 138.3, 133.2, 132.3, 131.3, 130.8, 130.3, 129.2, 127.5, 126, 125, 124.6, 123.8, 123.3, 123.2, 123, 120.2, 110.4, 47.9; IR ($CHCl_3$): ν_{max} 2957, 2923, 2870, 1713, 1597, 1571, 1456, 1379, 1248, 1190, 1160, 1072 cm^{-1}; ESI-MS (LTQ): 341.97 $[M+H]^+$

1-(4-isopropylbenzyl)-2-(4-isopropylphenyl)-1H-benzo[d]imidazole (3g)[6]



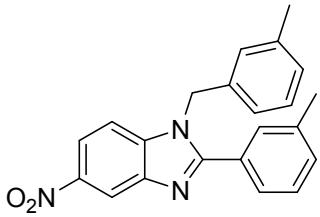
^{1} HNMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8Hz, 1H), 7.68 (d, *J* = 12 Hz, 2H), 7.35-7.30 (m, 4H), 7.25-7.20 (m, 5H), 7.08 (d, *J* = 8Hz, 2H), 5.47 (s, 2H), 1.30 (s, 3H), 1.29 (s, 3H), 1.27 (s, 3H), 1.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4, 150.9, 148.4, 143.2, 136.1, 133.8, 129.3, 127.5, 127.1, 126.9, 125.9, 122.8, 122.5, 119.8, 110.6, 48.2, 34.1, 33.8, 23.9, 23.8; IR ($CHCl_3$): ν_{max} 2959, 2904, 1613, 1513, 1458, 1417, 1383, 1361, 1329, 1276, 1254, 1161, 1054, 1018 cm$^{-1;}$ ESI-MS (LTQ): 369.21 $[M+H]^+$

1-benzyl-5-nitro-2-phenyl-1H-benzo[d]imidazole (3h)[7]



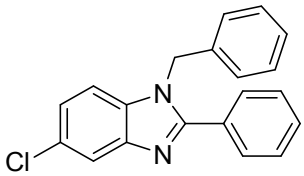
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.79 (s, 1H), 8.22 (dd, *J* = 8, 12 Hz, 1H), 7.33 (d, *J* = 8Hz, 2H), 7.62-7.51 (m, 3H), 7.41-7.36 (m, 2H), 7.30 (d, *J* = 8Hz, 2H), 7.11 (d, *J* = 8Hz, 2H), 5.54 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.1, 144.1, 142.5, 140.2, 135.2, 130.8, 129.4, 129.3, 129.1, 128.3, 125.9, 118.8, 116.6, 110.5, 48.8; ESI-MS (LTQ): 330.08 $[M+H]^+$

1-(3-methylbenzyl)-5-nitro-2-(m-tolyl)-1H-benzo[d]imidazole (3i)



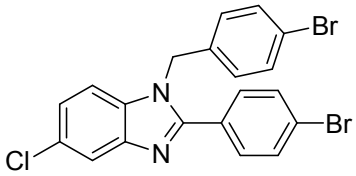
Yellow semi solid; ^{1} HNMR (400 MHz, $CDCl_3$) δ 8.77 (s, 1H), 8.20 (dd, *J* = 8, 12 Hz, 1H), 7.60 (s, 1H), 7.47 (d, *J* = 8Hz, 1H), 7.39 (d, *J* = 8Hz, 2H), 7.30-7.24 (m, 2H), 7.17 (d, *J* = 8Hz, 1H), 6.91 (t, *J* = 8Hz, 2H), 5.49 (s, 2H), 2.42 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 144, 142.5, 139.1, 139, 135.3, 131.6, 130.2, 129.2, 129, 128.8, 126.6, 126, 122.9, 118.8, 116.5, 110.5, 48.9, 21.5, 21.4; IR ($CHCl_3$): ν_{max} 3430, 2923, 1634, 1522, 1454, 1341 cm^{-1}; ESI-MS (LTQ): 358.16 $[M+H]^+$; HRMS (ESI): m/z 358.1540 calcd for $C_{22}H_{19}N_3O_2+H^+$ (358.1550).

1-benzyl-5-chloro-2-phenyl-1H-benzo[d]imidazole (3j)[1]



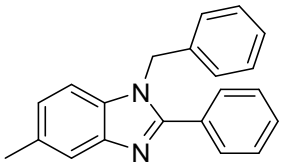
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.86 (d, *J* = 1.8Hz, 1H), 7.71 (t, *J* = 8Hz, 2H), 7.53-7.47 (m, 3H), 7.39-7.33 (m, 3H), 7.23-7.20 (m, 1H), 7.13-7.08 (m, 3H), 5.46 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.4, 144, 136, 135, 130.2, 129.3, 129.2, 129.2, 128.9, 128.8, 128, 126, 123.5, 120, 111.3, 48.6; IR ($CHCl_3$): ν_{max} 2956, 2924, 1714, 1604, 1454, 1379, 1078 cm^{-1}; ESI-MS (LTQ): 319.01 $[M+H]^+$

1-(4-bromobenzyl)-2-(4-bromophenyl)-5-chloro-1H-benzo[d]imidazole (3k)



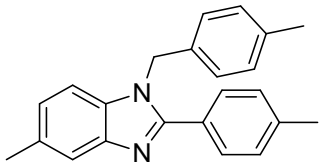
Yellow Semisolid; ^{1}HNMR (400 MHz, $CDCl_3$+MeOD) δ 7.79 (d, *J* =8Hz, 1H), 7.63 (d, *J* = 8Hz, 2H), 7.53 (d, *J* = 8Hz, 3H), 7.33 (d, *J* = 8Hz, 1H), 7.27 (d, *J* = 8Hz, 1H), 7.21 (s, 1H), 6.97 (d, *J* = 8Hz, 2H), 5.36 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.6, 139.8, 134.5, 132.5, 132.2, 131.6, 130.5, 129.3, 128.6, 127.4, 125, 123.9, 122.2, 121, 110.4, 47.9; IR ($CHCl_3$): ν_{max} 2957, 2924, 1709, 1596, 1465, 1400, 1378, 1072, 1011 cm^{-1}; ESI-MS (LTQ): 475.52 $[M+2H]^+$; HRMS (ESI): m/z 474.9214 calcd for $C_{20}H_{13}Br_2ClN_2+H^+$ (474.9207).

1-benzyl-5-methyl-2-phenyl-1H-benzo[d]imidazole (3l)[8]



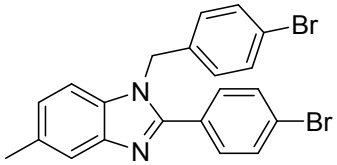
^{1} HNMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8Hz, 1H), 7.71-7.68 (m, 2H), 7.48-7.45 (m, 3H), 7.39-7.33 (m, 3H), 7.17-7.03 (m, 4H), 5.45 (s, 2H), 2.46 (s, 3H)IR ($CHCl_3$): ν_{max} 3031, 2956, 2924, 2854, 1715, 1606, 1454, 1386, 1357, 1329, 1260, 1170, 1076, 1029 cm^{-1}ESI-MS (LTQ): 299.12 $[M+H]^+$

5-methyl-1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole (3m)[9]



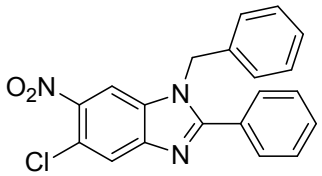
^{1}HNMR (400 MHz, $CDCl_3$) δ 7.76 (d, *J* = 8Hz, 1H), 7.60-7.57 (m, 2H), 7.28-7.25 (m, 3H), 7.18 (t, *J* = 8Hz, 2H), 7.09-7.00 (m, 3H), 5.39 (s, 2H), 2.45 (s, 3H), 2.42 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.9, 139.9, 137.4, 133.6, 132.8, 129.7, 129.6, 129.4, 129.1, 129.0, 125.9, 125.8, 124.3, 124.2, 119.3, 110.3, 110, 48.1, 21.9, 21.4, 21.1; IR ($CHCl_3$): ν_{max} 2956, 2923, 1712, 1459, 1378, 1275 cm^{-1}; ESI-MS (LTQ): 327.69 $[M+H]^+$

1-(4-bromobenzyl)-2-(4-bromophenyl)-5-methyl-1H-benzo[d]imidazole (3n)



White semisolid; ^{1}HNMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8Hz, 1H), 7.54-7.43 (m, 5H), 7.19-7.10 (m, 2H), 7.00-7.96 (m, 3H), 5.36 (s, 2H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 143.3, 135.3, 133.7, 132.9, 132.3, 132.1, 130.6, 128.9, 127.5, 124.8, 121.8, 110.1, 47.7, 21.9; IR ($CHCl_3$): ν_{max} 2956, 2924, 2854, 1713, 1594, 1488, 1461, 1404, 1378, 1251, 1073, 1011 cm^{-1}; ESI-MS (LTQ): 455.55 $[M+2H]^+$; HRMS (ESI): m/z 454.9763 calcd for $C_{21}H_{16}Br_2N_2+H^+$ (454.9753).

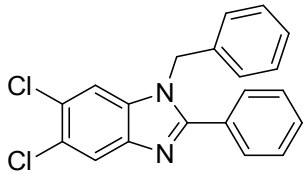
1-benzyl-5-chloro-6-nitro-2-phenyl-1H-benzo[d]imidazole (3o)



White semisolid; ^{1}HNMR (400 MHz, $CDCl_3$) δ 8.41 (s, 1H), 7.97 (s, 1H), 7.74 (t, *J* = 8Hz, 2H), 7.55-7.52 (m, 3H), 7.41-7.33 (m, 3H), 7.09 (d, *J* = 4HZ, 2H), 5.53 (d, *J* = 16Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 145.9, 141, 138.6, 134.8, 133.8, 131.1, 129.5, 129.3, 129.1, 125.8, 122.4, 117.9, 112.9, 48.9; IR ($CHCl_3$): ν_{max} 2957, 2924, 1732, 1616, 1585, 1528, 1445, 1379,

1327, 1260, 1150, 1079, 1028, 1006 cm^{-1}; ESI-MS (LTQ): 364. 43 $[M+H]^+$; HRMS (ESI): *m/z* 364.0847 calcd for $C_{20}H_{14}N_3O_2Cl+H^+$ (364.0847).

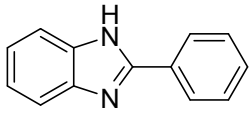
1-benzyl-5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (3p)[10]



[1] HNMR (400 MHz, $CDCl_3$) δ 7.95 (s, 1H), 7.70 (d, *J* = 8Hz, 2H), 7.55-7.47 (m, 3H), 7.41-7.35 (m, 3H), 7.31 (s, 1H), 7.10 (d, *J* = 8Hz, 2H), 5.44 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.1, 142.5, 135.4, 130.5, 129.3, 129.2, 129.1, 128.9, 128.2, 126.9, 125.8, 121.1, 111.8, 48.6; ESI-MS (LTQ): 353.01 $[M+H]^+$

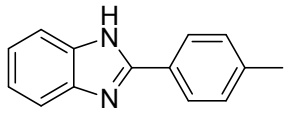
<u>Monosubstituted Benzimidazole</u>

2-phenyl-1H-benzo[d]imidazole (4a)[11]



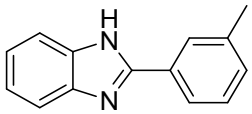
[1] HNMR (400 MHz, $CDCl_3$) δ 12.93 (s, 1H (NH)), 8.21 (d, *J* = 8 Hz, 2H), 7.69 (d, *J* = 8 Hz, 1H), 7.58-7.48 (m, 4H), 7.23 (t, *J* = 8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 144.3, 135.5, 130.6, 130.3, 129.4, 126.9, 122.9, 122.1, 119.3, 111.8; IR ($CHCl_3$): ν_{max} 2955.1, 2920.8, 2870.4, 1713.2, 1458.4, 1377.9, 1275, 1260.7, 1187.8, 1081.5, 1019 cm^{-1}; ESI-MS (LTQ): 195.20 $[M+H]^+$

2-(p-tolyl)-1H-benzo[d]imidazole (4b)[12]



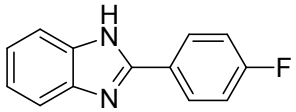
[1] HNMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8Hz, 2H), 7.66 (s, 2H), 7.34 (d, *J* = 8Hz, 2H), 7.30-7.28 (m, 2H), 2.44 (s, 3H); IR ($CHCl_3$): ν_{max} 3410, 2919, 1621, 1429, 1274, 1083 cm^{-1}; ESI-MS (LTQ): 209.05 $[M+H]^+$

2-(m-tolyl)-1H-benzo[d]imidazole (4c)[13]



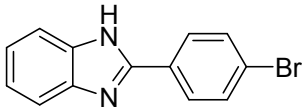
^{1} HNMR (400 MHz, $CDCl_3$+MeOD) δ 7.98-7.89 (m, 2H), 7.65 (m, 2H), 7.33-7.28 (m, 4H), 2.30 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$+MeOD) δ 156.1, 142.6, 134.7, 133.6, 132.7, 131.2, 127.6, 126.50, 25.1; IR ($CHCl_3$): ν_{max} 3418, 2957, 2923, 1633, 1455, 1378, 1309 cm^{-1}; ESI-MS (LTQ): 209.04 $[M+H]^+$

2-(4-fluorophenyl)-1H-benzo[d]imidazole (4d)[14]



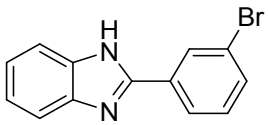
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.10-8.07 (m, 2H), 7.67-7.65 (m, 2H), 7.31-7.27 (m, 2H), 7.20 (t, *J* = 8Hz, 2H); IR ($CHCl_3$): ν_{max} 2918, 1600, 1496, 1429, 1395, 1275, 1227, 1083 cm^{-1}; ESI-MS (LTQ): 212.98 $[M+H]^+$

2-(4-bromophenyl)-1H-benzo[d]imidazole (4e)[15]



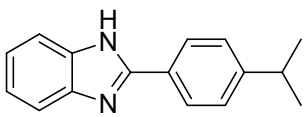
^{1} HNMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8Hz, 2H), 7.68 (d, *J* = 8Hz, 4H), 7.34-7.31 (m, 2H); IR ($CHCl_3$): ν_{max} 2923, 1427, 1275, 749 cm^{-1}; ESI-MS (LTQ): 272.95 $[M+H]^+$

2-(3-bromophenyl)-1H-benzo[d]imidazole (4f)



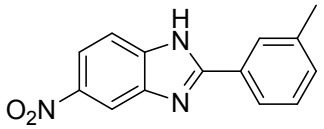
Yellow oil; ^{1} HNMR (400 MHz, $CDCl_3$+MeOD) δ 8.18 (s, 1H), 7.98 (d, *J* = 8Hz, 1H), 7.51 (d, *J* = 8Hz, 1H), 7.31-7.27 (m, 2H), 7.21-7.19 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$+MeOD) δ 150.3, 132.7, 131.9, 130.4, 129.5, 125.2, 122.9; IR ($CHCl_3$): ν_{max} 2955, 2917, 1709, 1589, 1436, 1399, 1119 cm^{-1}; ESI-MS (LTQ): 273.05 $[M+2H]^+$

2-(4-isopropylphenyl)-1H-benzo[d]imidazole (4g)[16]



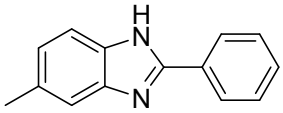
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8Hz, 2H), 7.66-7.64 (m, 2H), 7.36 (d, *J* = 2H), 7.29-7.27 (m, 3H), 1.31 (s, 3H), 1.29 (s, 3H); IR ($CHCl_3$): ν_{max} 2956, 2920, 1590, 1434, 1400, 1275, 1111, 969 cm^{-1}; ESI-MS (LTQ): 237.06 $[M+H]^+$

5-nitro-2-(m-tolyl)-1H-benzo[d]imidazole (4i)[17]



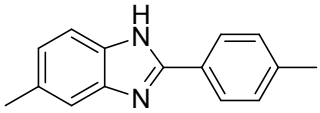
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.31 (d, *J* = 8Hz, 1H), 7.65 (s, 1H), 7.57 (d, *J* = 8Hz, 1H), 7.49-7.46 (m, 2H), 7.42 (d, *J* = 8Hz, 1H), 2.49 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 143.9, 142.2, 140.6, 139, 131.4, 130.2, 128.9, 128.8, 126.3, 118.6, 116.5, 109.5, 21.5; IR ($CHCl_3$): ν_{max} 2924, 1520, 1464, 1320, 1276, 1053 cm^{-1}; ESI-MS (LTQ): 254.04 $[M+H]^+$

5-methyl-2-phenyl-1H-benzo[d]imidazole (4l)[18]



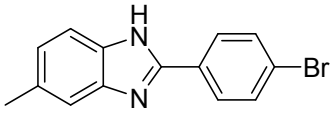
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.09 (s, 2H), 7.55 (d, *J* = 12 Hz, 1H), 7.44-7.42 (m, 3H), 7.39 (s, 1H), 7.10 (d, *J* = 8Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 132.9, 130, 129.8, 129, 126.6, 124.5, 21.7; IR ($CHCl_3$): ν_{max} 2924, 1629, 1455, 1276, 1026 cm^{-1}; ESI-MS (LTQ): 209.02 $[M+H]^+$

5-methyl-2-(p-tolyl)-1H-benzo[d]imidazole (4m)[19]



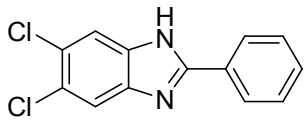
^{1} HNMR (400 MHz, $CDCl_3$) δ 8.02 (d, *J* = 8Hz, 2H), 7.51 (d, *J* = 8Hz, 1H), 7.36 (s, 1H), 7.20 (d, *J* = 8Hz, 2H), 7.07 (d, *J* = 8Hz, 1H), 2.44 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.9, 140.2, 138.7, 137.7, 132.7, 129.7, 127.1, 126.6, 124.3, 115, 114.4, 21.7, 21.4; IR ($CHCl_3$): ν_{max} 3418, 2957, 2923, 1633, 1455, 1378, 1309 cm^{-1}; ESI-MS (LTQ): 223.32 $[M+H]^+$

2-(4-bromophenyl)-5-methyl-1H-benzo[d]imidazole (4n)[20]



^{1} HNMR (400 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8Hz, 2H), 7.60 (d, *J* = 8Hz, 2H), 7.55 (d, *J* = 8Hz, 1H), 7.40 (s, 1H), 7.13 (d, *J* = 8Hz, 1H), 2.49 (s, 3H); IR ($CHCl_3$): ν_{max} 3424, 2953, 2916, 1633, 1427, 1377, 1271, 1071, 1009 cm^{-1}; ESI-MS (LTQ): 288.17 $[M+2H]^+$

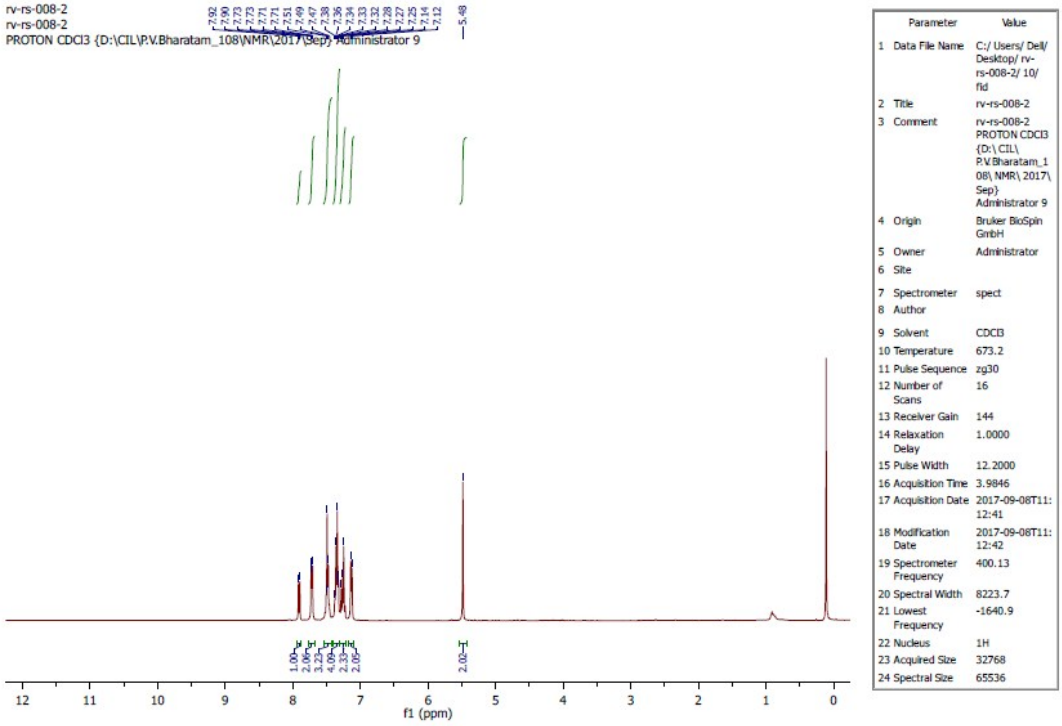
5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (4p)[21]

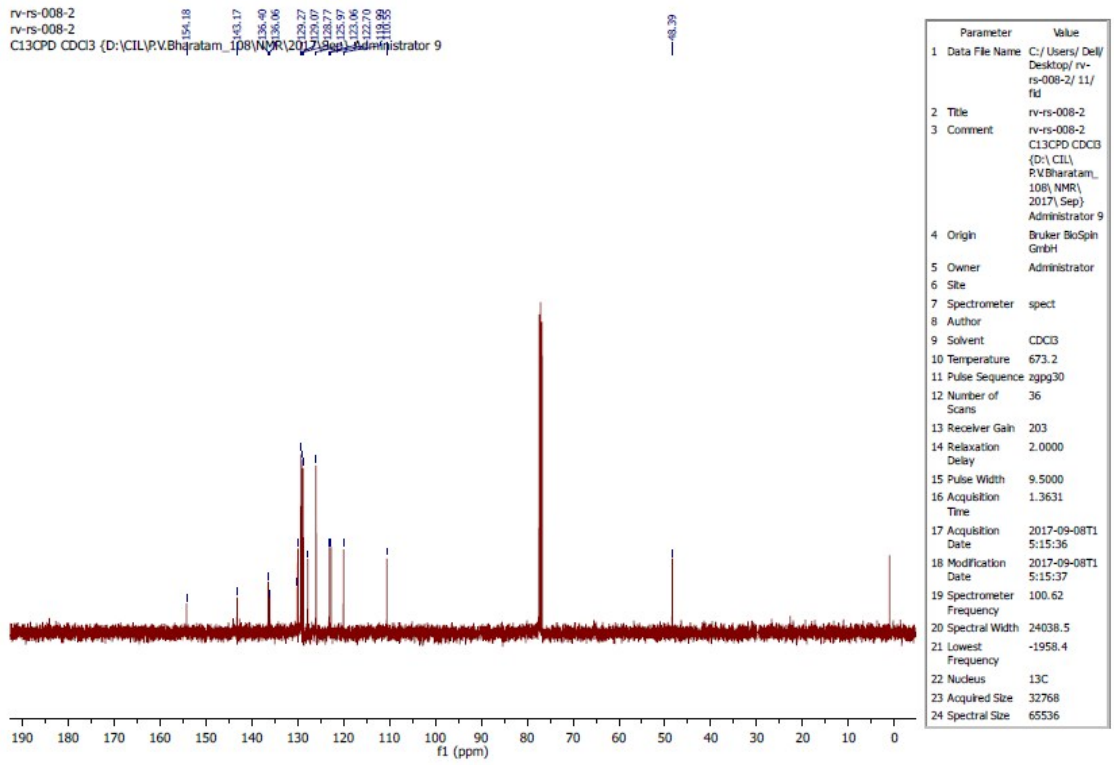


^{1} HNMR (400 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.77-7.75 (m, 2H), 7.57-7.55 (m, 3H), 7.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.9, 142.1, 130.3, 129.6, 129.4, 128.9, 128.8, 120.9, 111.1; IR ($CHCl_3$): ν_{max} 2924, 1629, 1455, 1276, 1026 cm^{-1}; ESI-MS (LTQ): 263.10 $[M+H]^+$

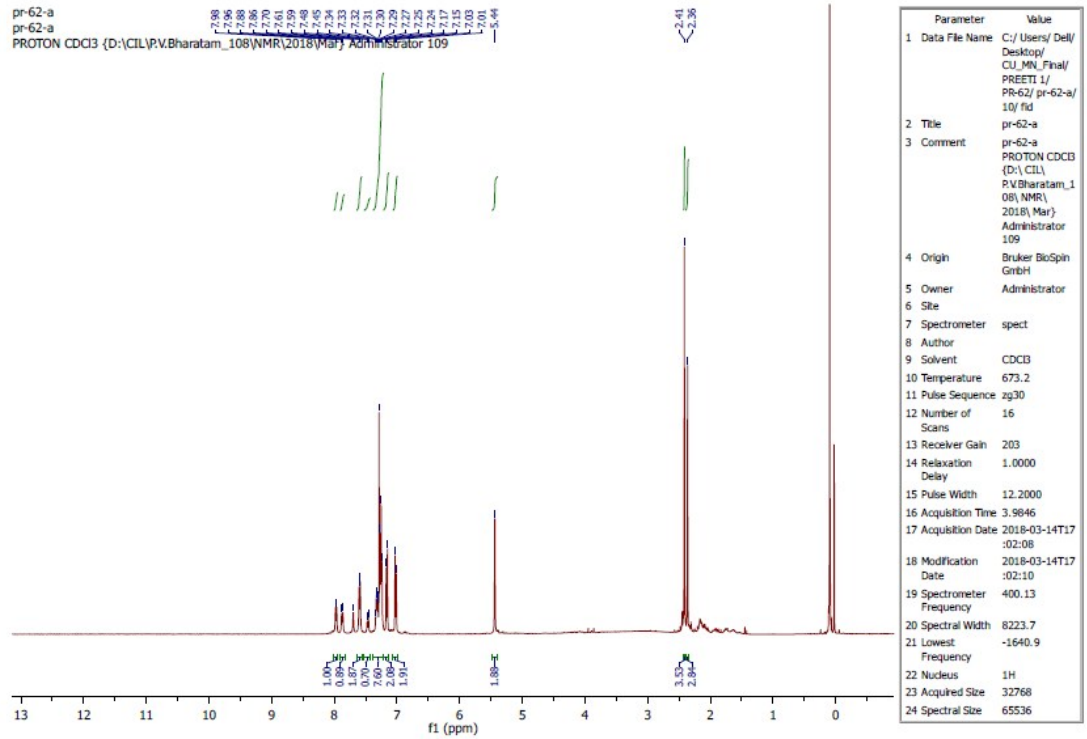
S2. Scanned copies of ^{1}H , ^{13}C NMR and HRMS spectra of compounds.

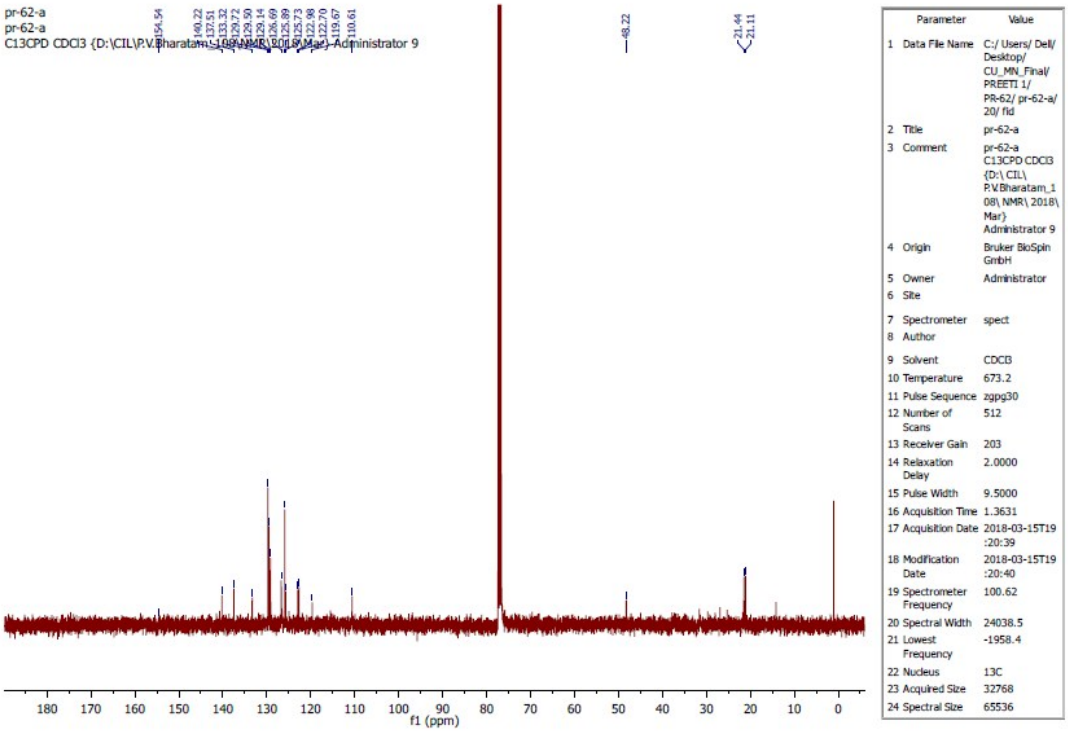
^{1}H and ^{13}C NMR spectra's of 1-benzyl-2-phenyl-1H-benzo[d]imidazole (3a).





^{1}H and ^{13}C NMR spectra of 1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole (3b).





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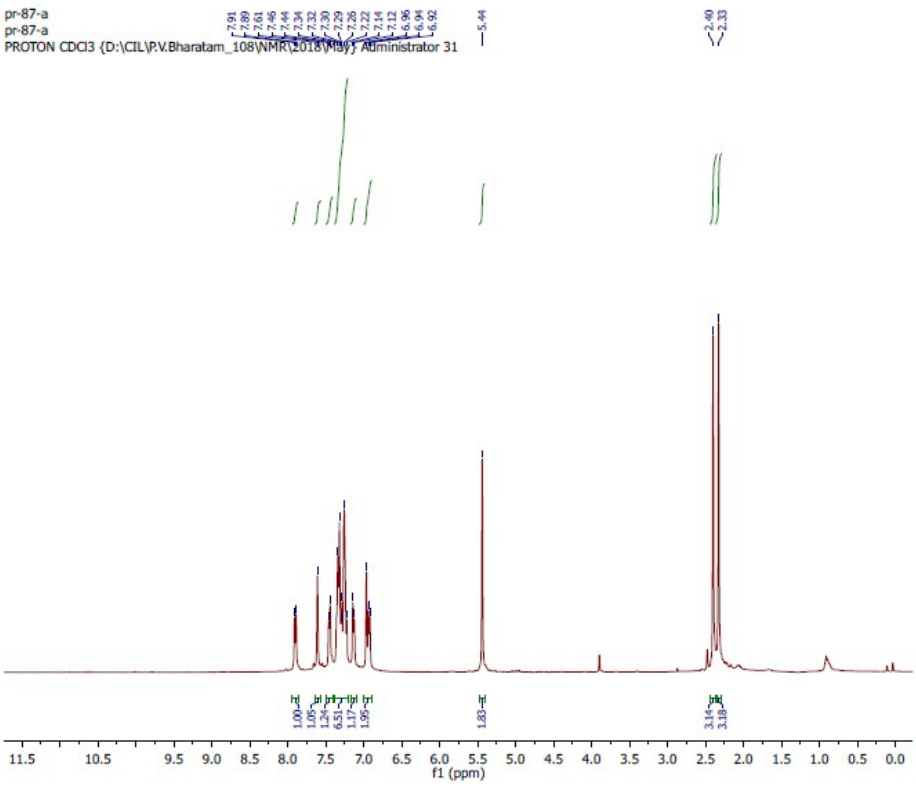
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-03-15T19:20:39
18	Modification Date	2018-03-15T19:20:40
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 and ^{13}C NMR spectra of 1-(3-methylbenzyl)-2-(m-tolyl)-1H-benzo[d]imidazole (3c).



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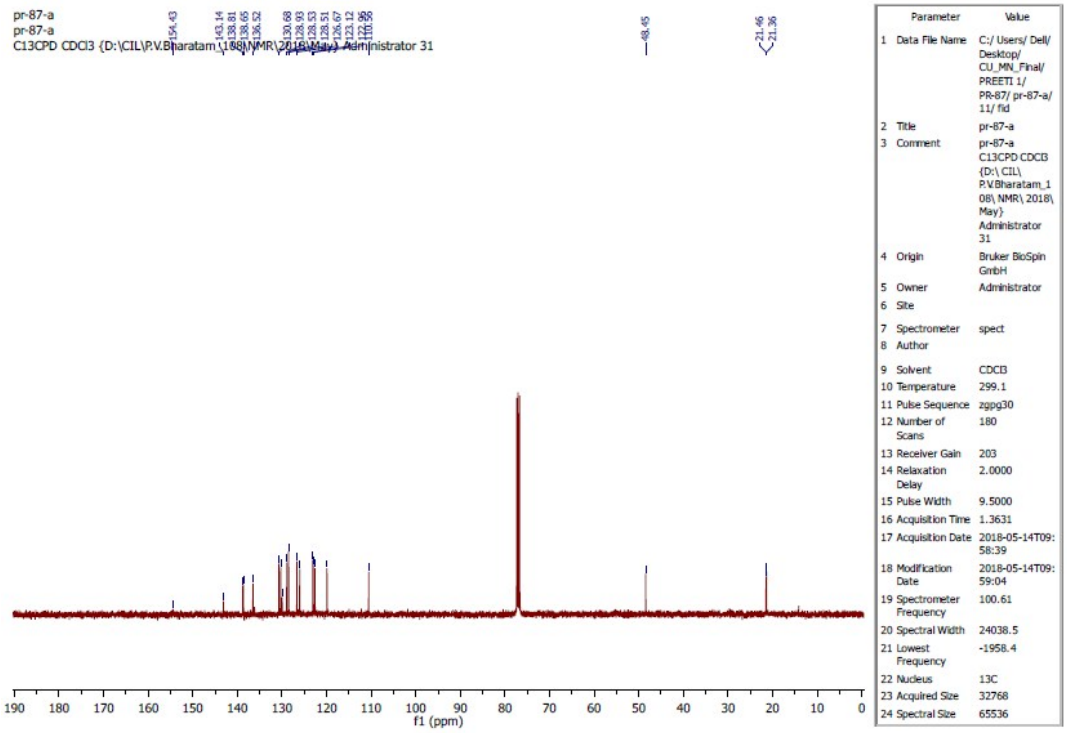
3	Comment	pr-87-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ May} Administrator 31
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-14T09:38:47
18	Modification Date	2018-05-14T09:38:48
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



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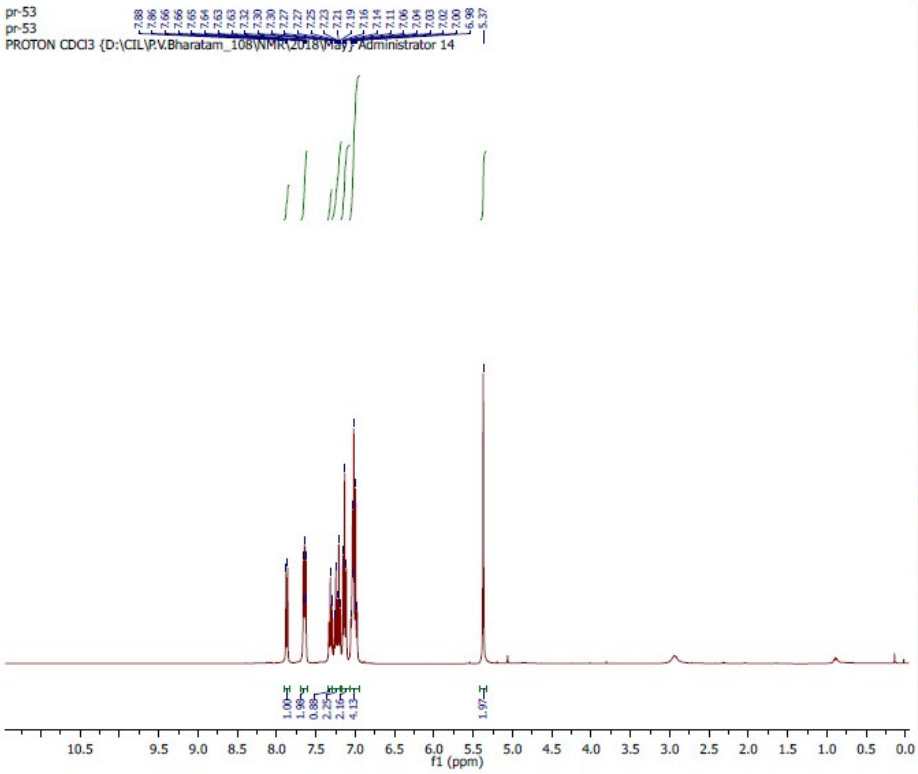
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	299.1
11	Pulse Sequence	zgpg30
12	Number of Scans	180
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-05-14T09:58:39
18	Modification Date	2018-05-14T09:59:04
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra's of 1-(4-fluorobenzyl)-2-(4-fluorophenyl)-1H-benzo[d]imidazole (3d).



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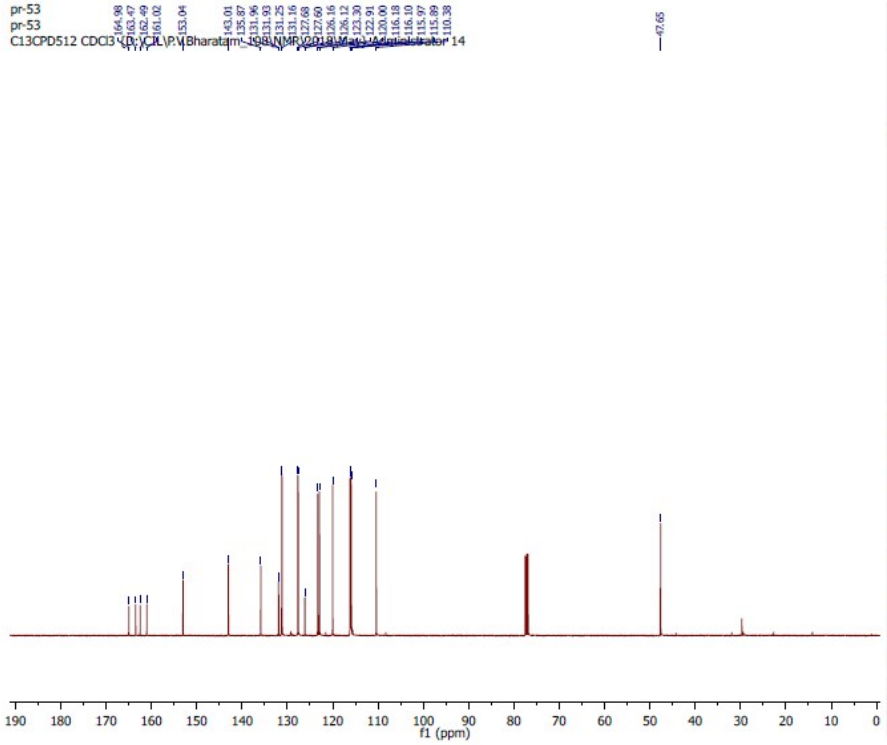
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.1
11	Pulse Sequence	zg30
12	Number of Scans	64
13	Receiver Gain	45
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-10T10:54:27
18	Modification Date	2018-05-10T10:54:28
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



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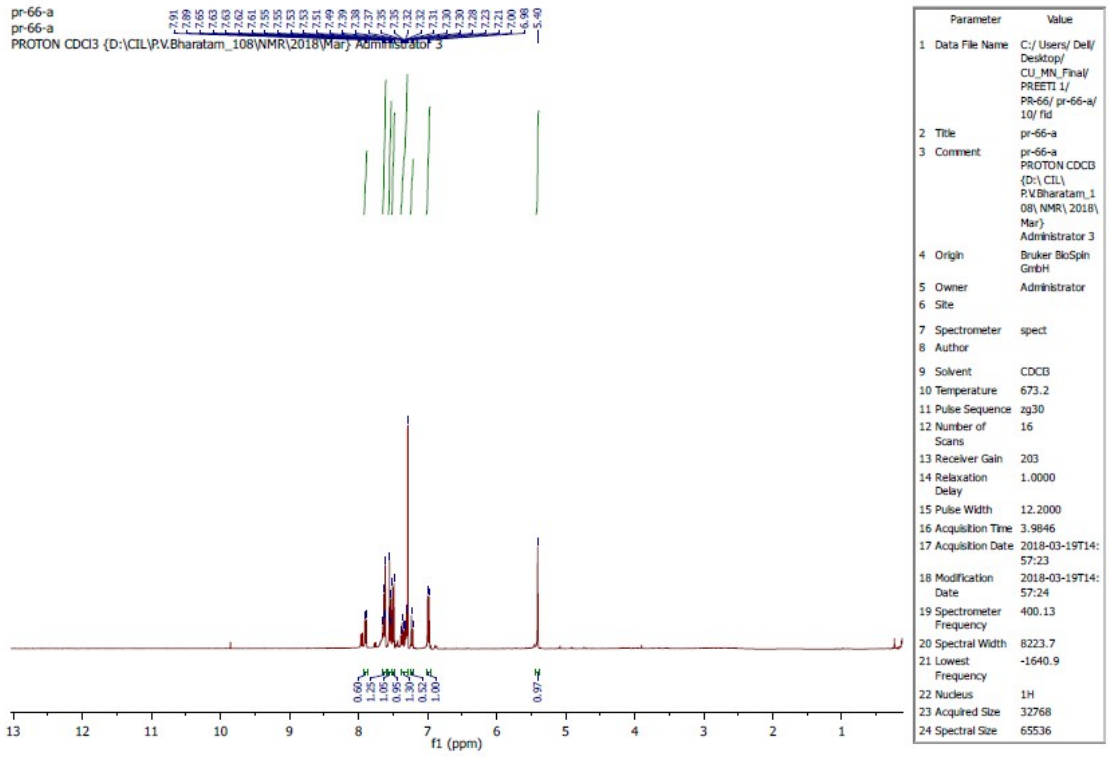
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-05-11T04:41:57
18	Modification Date	2018-05-11T04:41:58
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 and ^{13}C NMR spectra of 1-(4-bromobenzyl)-2-(4-bromophenyl)-1H-benzo[d]imidazole (3e).



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2	Title	pr-66-a
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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
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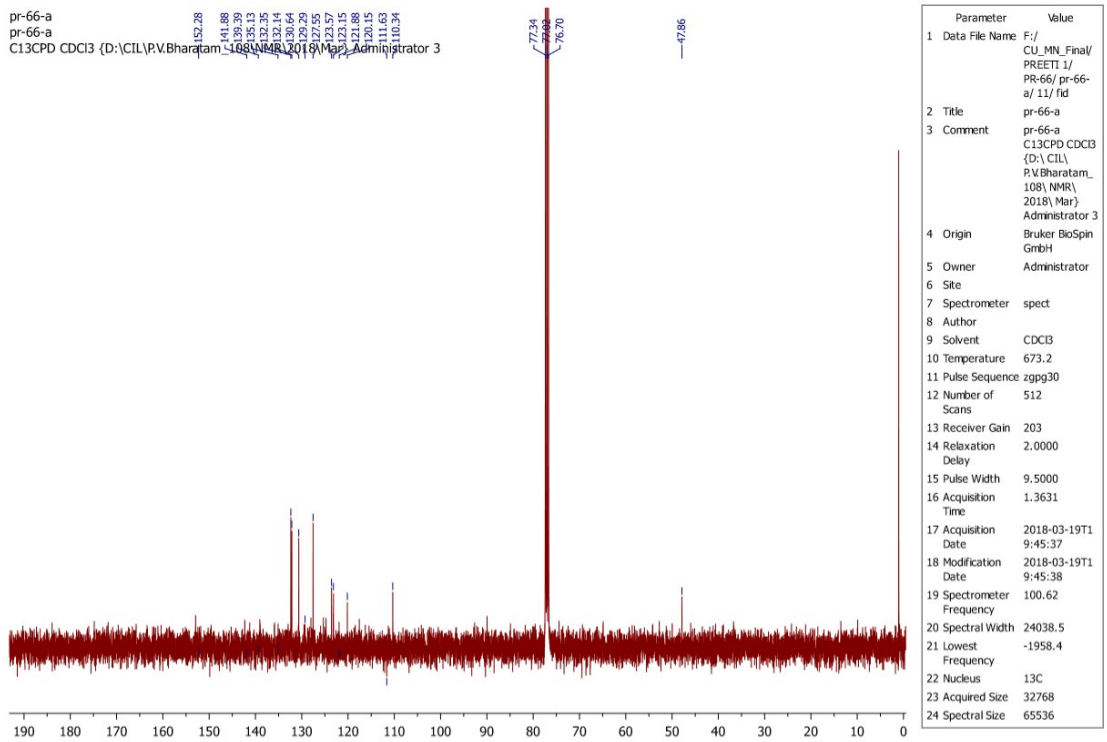
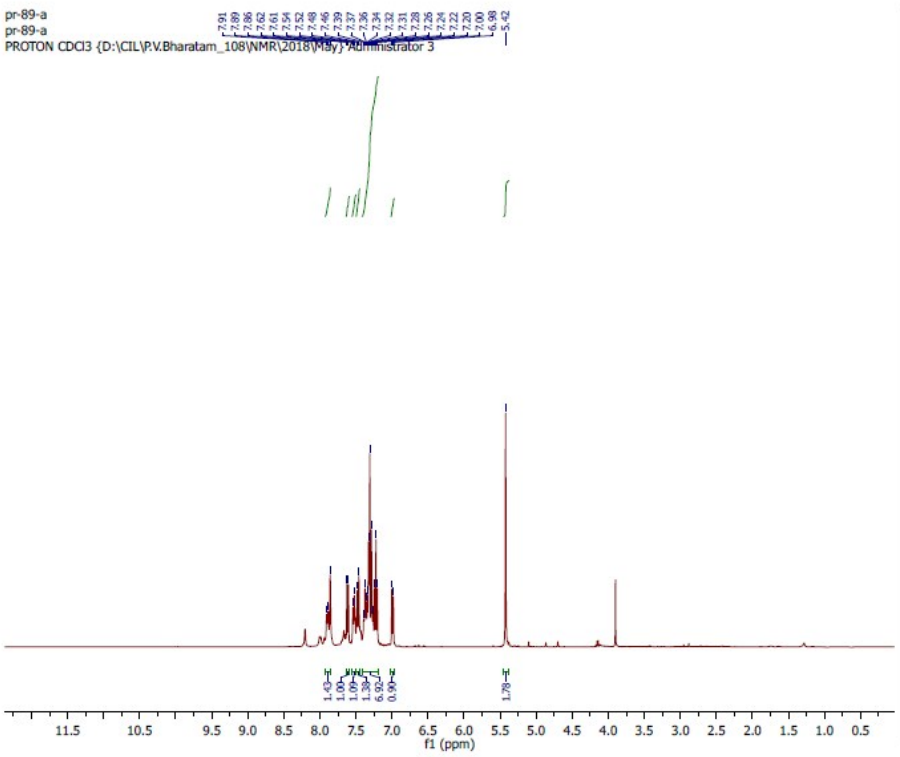
17	Acquisition Date	2018-03-19T14:57:23
18	Modification Date	2018-03-19T14:57:24
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



^{1}H and ^{13}C NMR spectra of 1-(3-bromobenzyl)-2-(3-bromophenyl)-1H-benzo[d]imidazole (3f).



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
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	2018-05-14T14:42:21
18	Modification Date	2018-05-14T14:42:22
19	Spectrometer Frequency	400.13
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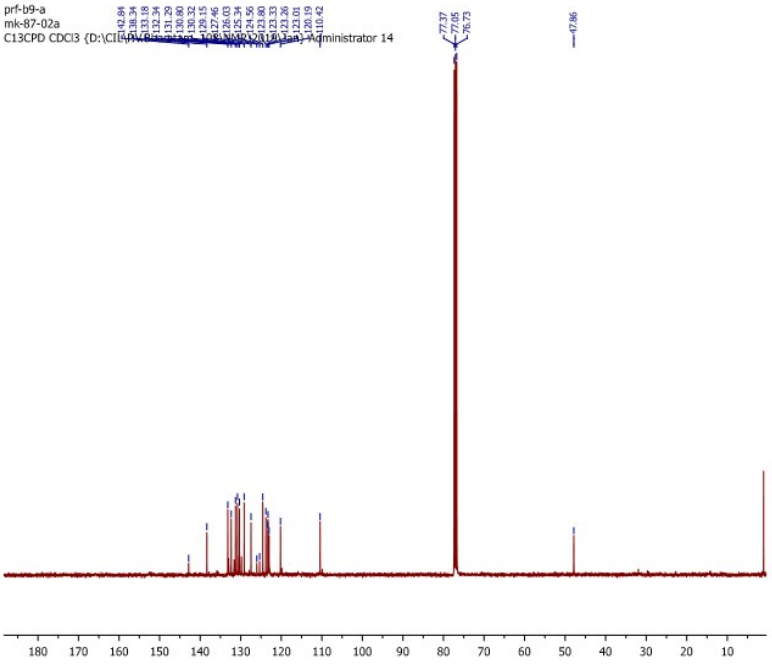
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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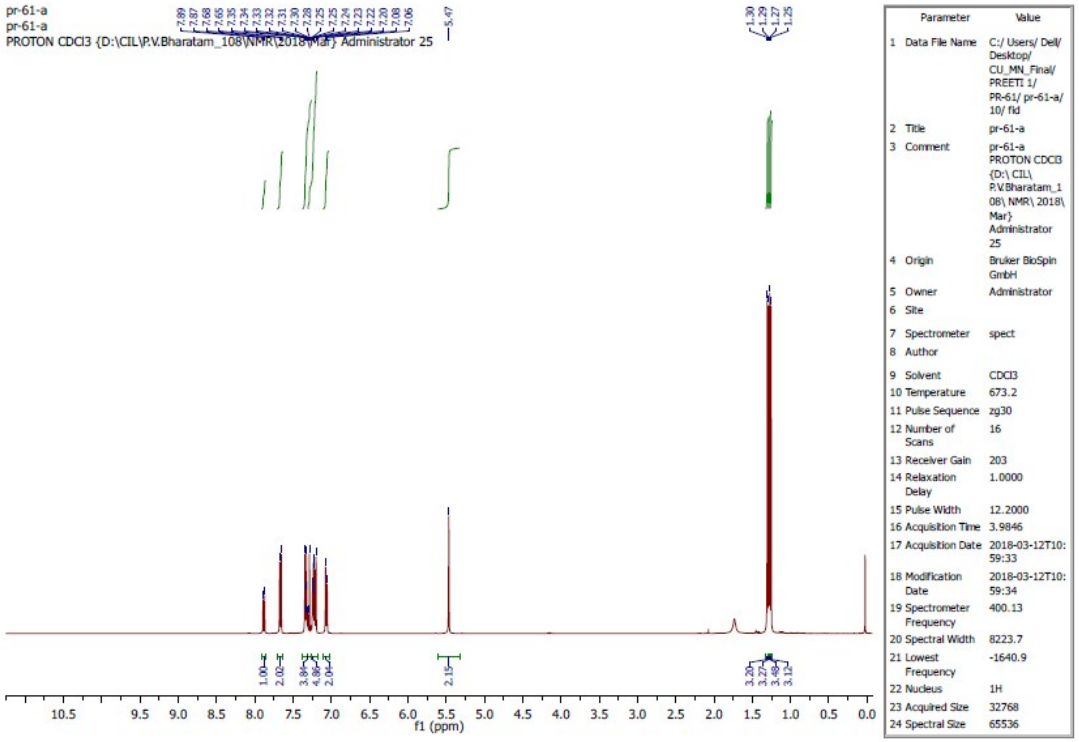
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	1024
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2019-01-28T13:37:59
18	Modification Date	2019-01-28T13:37:59
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 and ^{13}C NMR spectra of 1-(4-isopropylbenzyl)-2-(4-isopropylphenyl)-1H-benzo[d]imidazole (3g).



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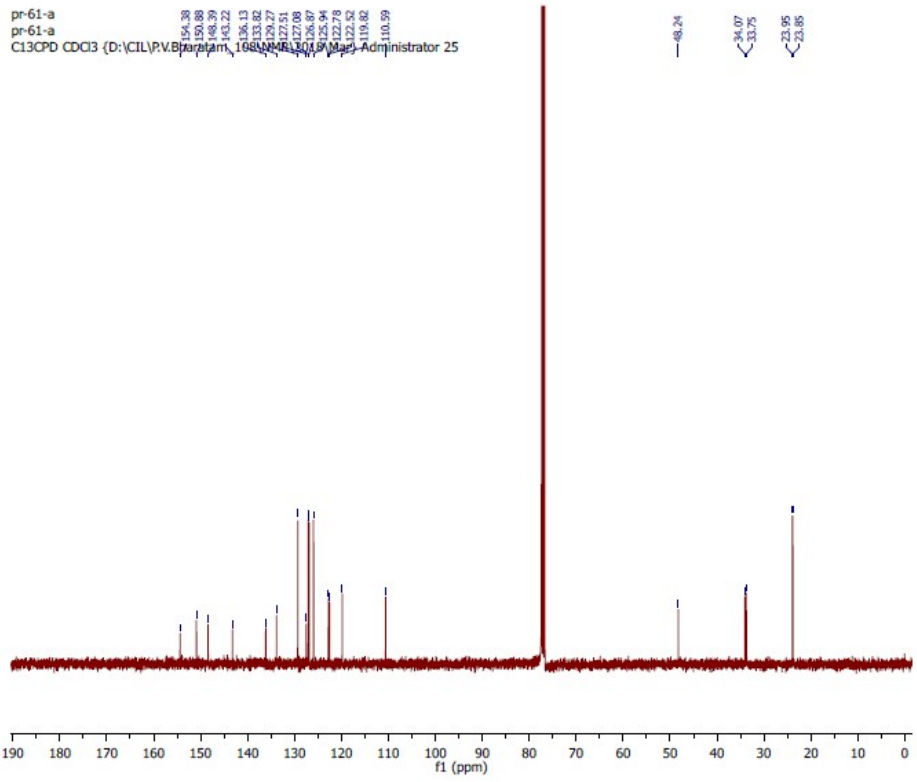
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-03-12T10:59:33
18	Modification Date	2018-03-12T10:59:34
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



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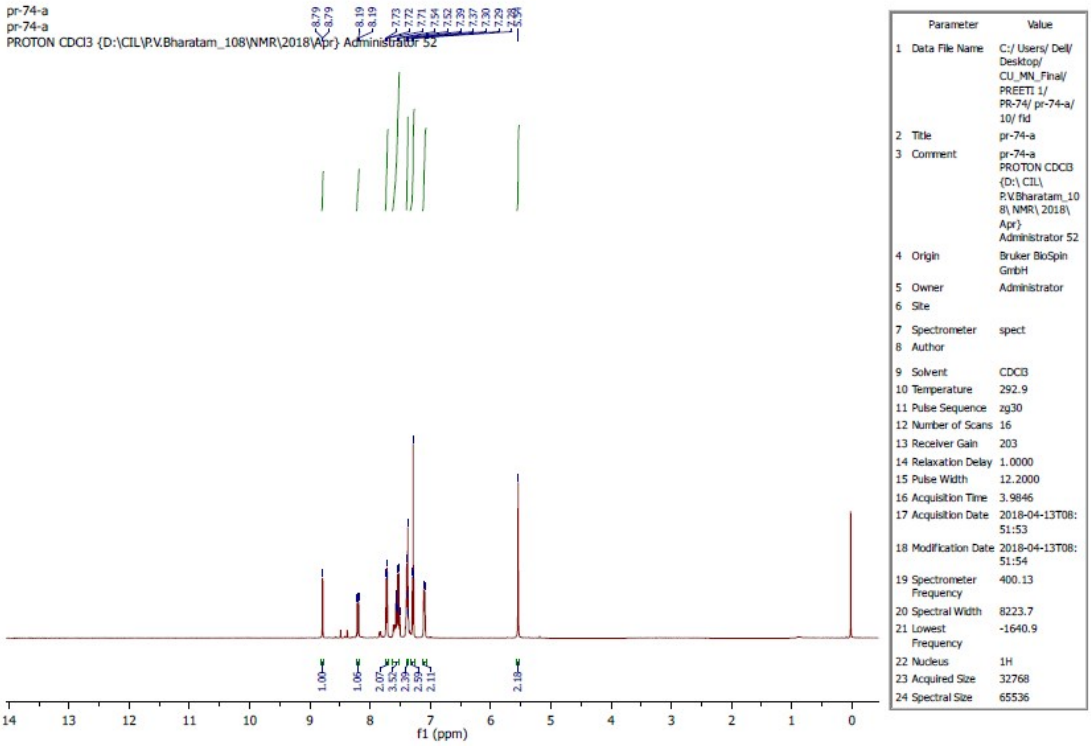
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-61/ pr-61-a/ 11/ fid
2	Title	pr-61-a
3	Comment	pr-61-a C13CPD CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Mar} Administrator 25
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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	2018-03-12T11:59:57
18	Modification Date	2018-03-12T12:27:48
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra of 1-benzyl-5-nitro-2-phenyl-1H-benzo[d]imidazole (3h).



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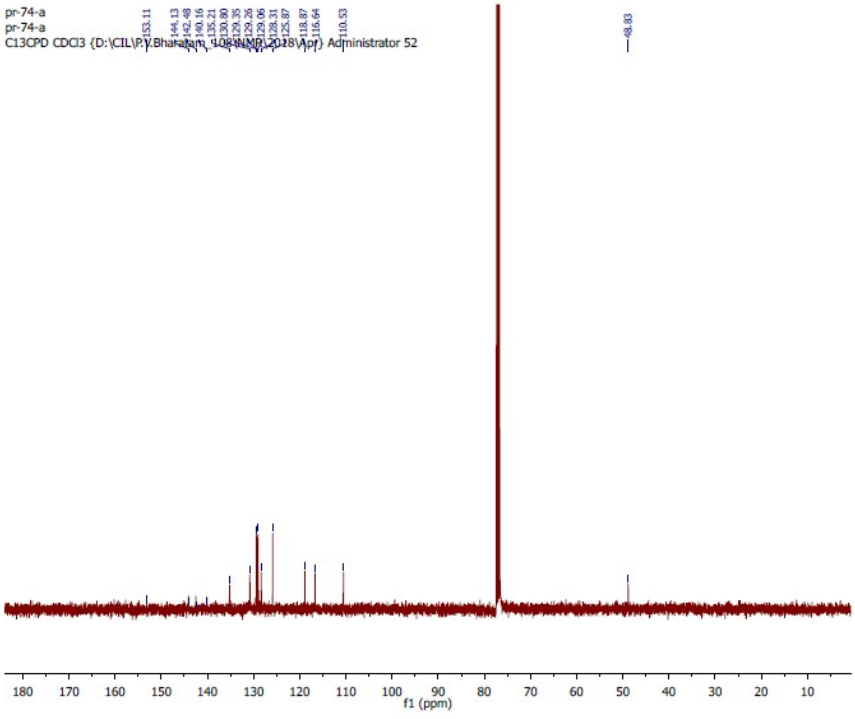
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-74/ pr-74-a/ 10/ fid
2	Title	pr-74-a
3	Comment	pr-74-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 52
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.9
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	2018-04-13T08:51:53
18	Modification Date	2018-04-13T08:51:54
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



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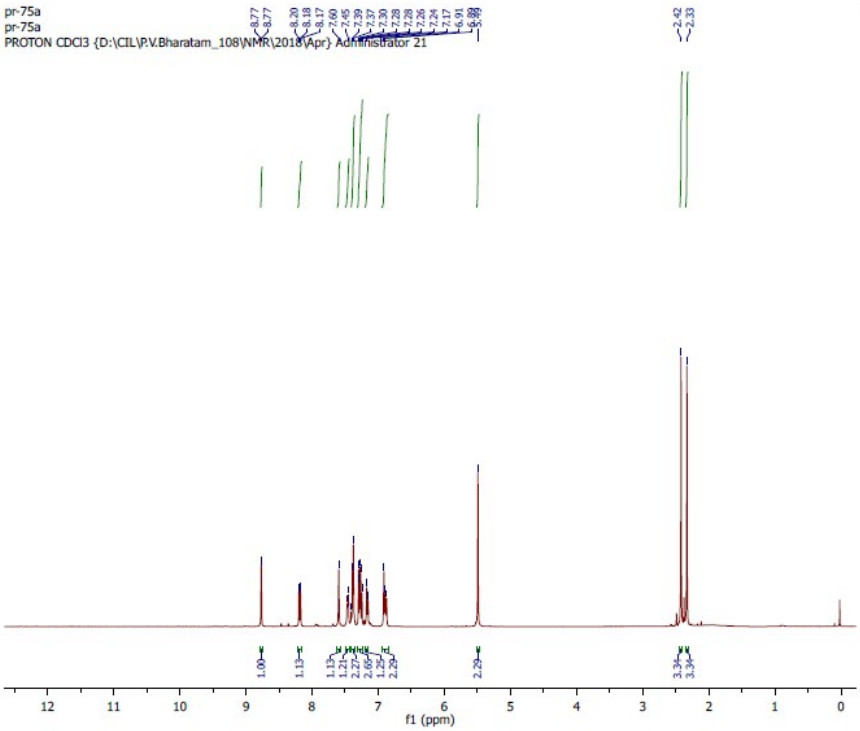
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-74/ pr-74-a/ 11/ fid
2	Title	pr-74-a
3	Comment	pr-74-a C13CPD CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 52
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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	2018-04-13T10:46:07
18	Modification Date	2018-04-13T10:46:08
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, ^{13}C NMR and HRMS spectra of 1-(3-methylbenzyl)-5-nitro-2-(m-tolyl)-1H-benzo[d]imidazole (3i).



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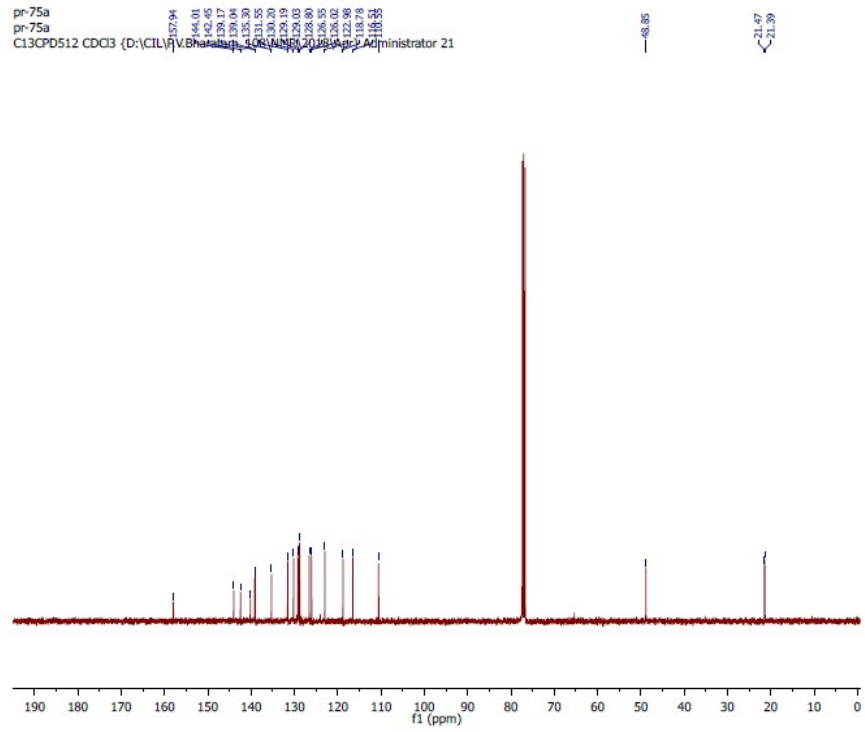
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-75 dl-only repeat/ pr-75a/ 10/ fid
2	Title	pr-75a
3	Comment	pr-75a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 21
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	292.7
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	2018-04-11T15:05:21
18	Modification Date	2018-04-11T15:05:22
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



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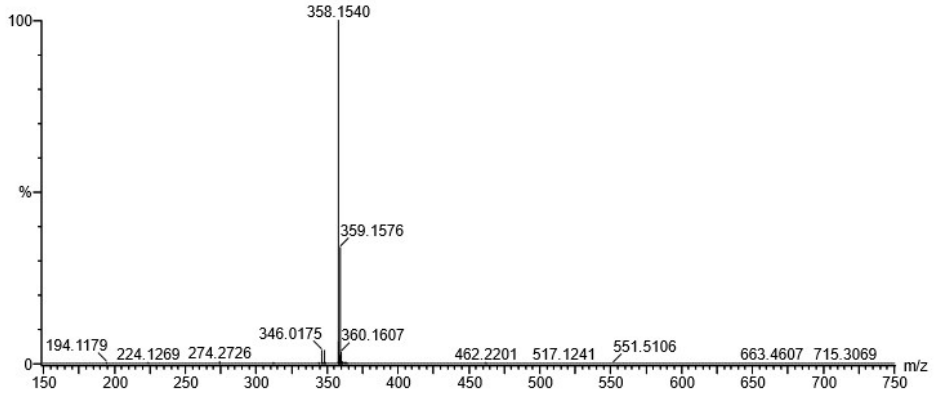
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-75 dl-only repeat/ pr-75a/ 11/ fid
2	Title	pr-75a
3	Comment	pr-75a C13CPD512 CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 21
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.8
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	2018-04-12T03:03:19
18	Modification Date	2018-04-12T03:03:20
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

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

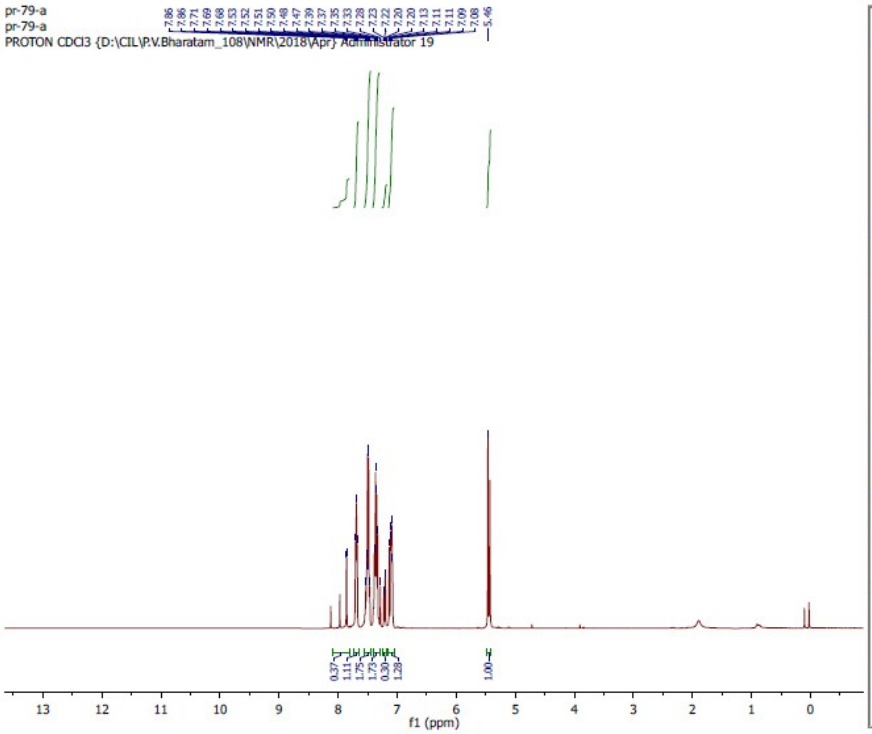
Monoisotopic Mass, Even Electron Ions
76 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-4 O: 0-4 Cl: 0-1

Sample Name : PR-75-A I.I.T.ROPAR XEVO G2-XS QTOF
Test Name : HRMS-1
280119-PR-75-A 18 (0.183) AM2 (Ar,19000.0,0.00,0.00); Cm (18:26) 1: TOF MS ES+
1.24e+008



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
358.1540	358.1556	-1.6	-4.5	14.5	766.8	n/a	n/a	C22 H20 N3 O2

^{1}H and ^{13}C NMR spectra of 1-benzyl-5-chloro-2-phenyl-1H-benzo[d]imidazole (3j).



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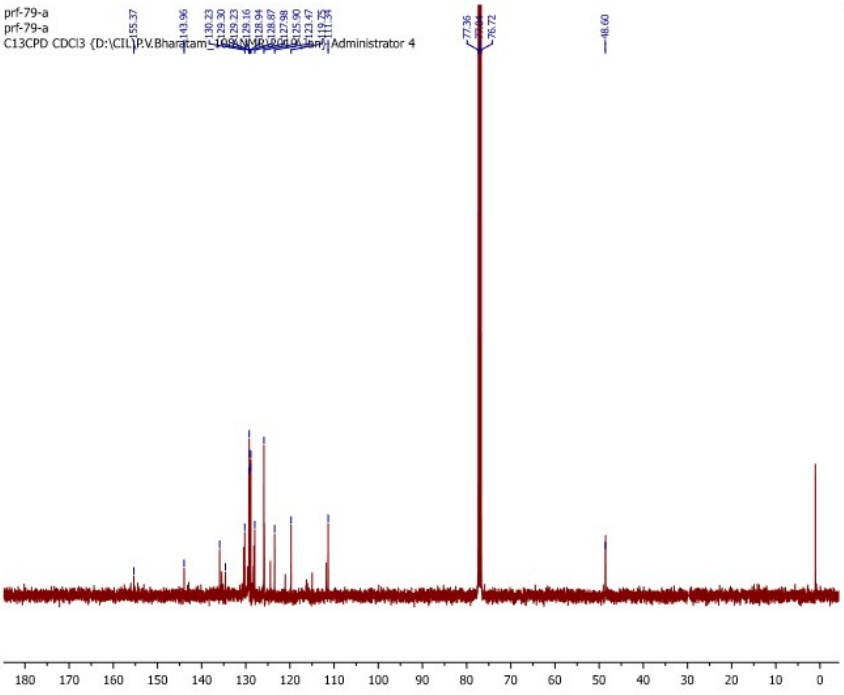
2	Title	pr-79-a
3	Comment	pr-79-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 19
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.9
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-20T16:31:48
18	Modification Date	2018-04-20T16:31:48
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



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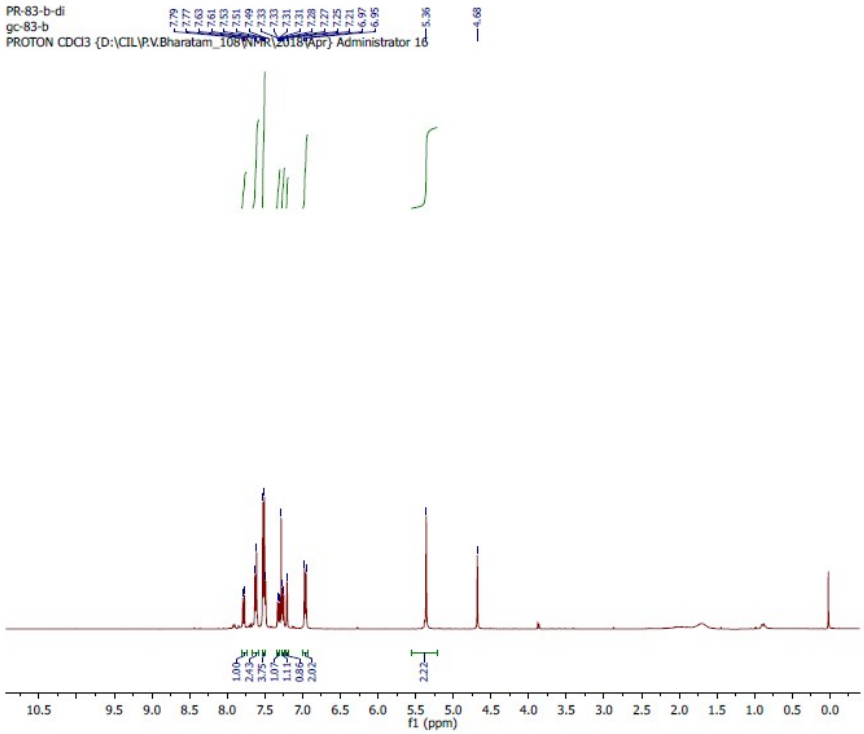
3	Comment	prf-79-a C13CPD CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2019\ Jan} Administrator 4
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	673.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2019-01-28T11:13:22
18	Modification Date	2019-01-28T11:13:23
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 , ^{13}C NMR and HRMS spectra of 1-(4-bromobenzyl)-2-(4-bromophenyl)-5-chloro-1H-benzo[d]imidazole (3k).



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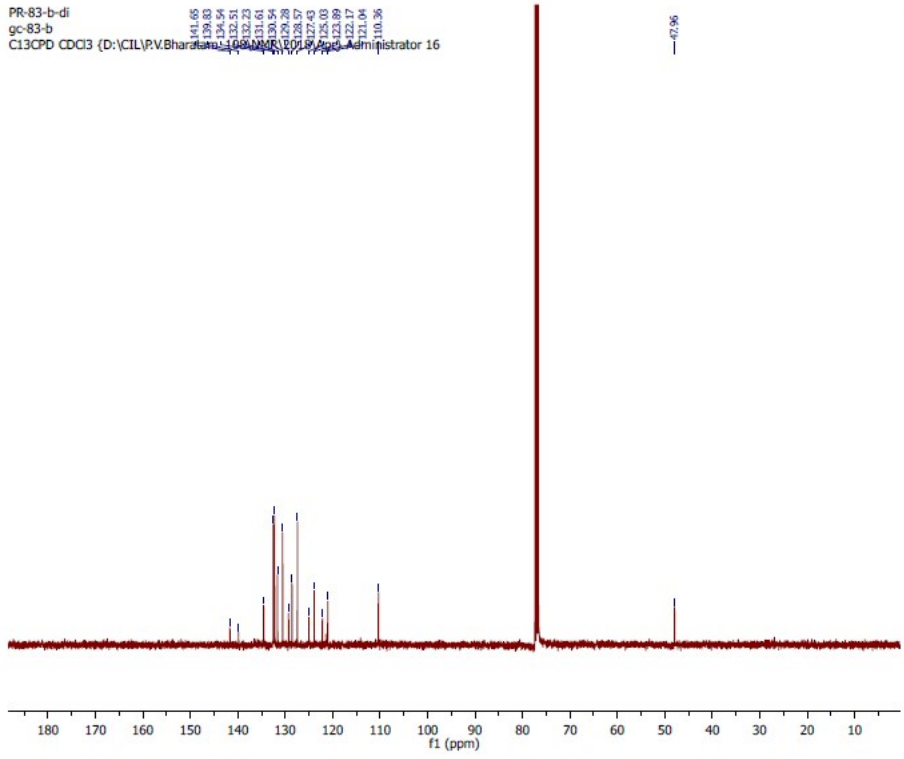
2	Title	PR-83-b-di
3	Comment	gc-83-b PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 16
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-26T13 :57:48
18	Modification Date	2018-04-26T13 :57:50
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



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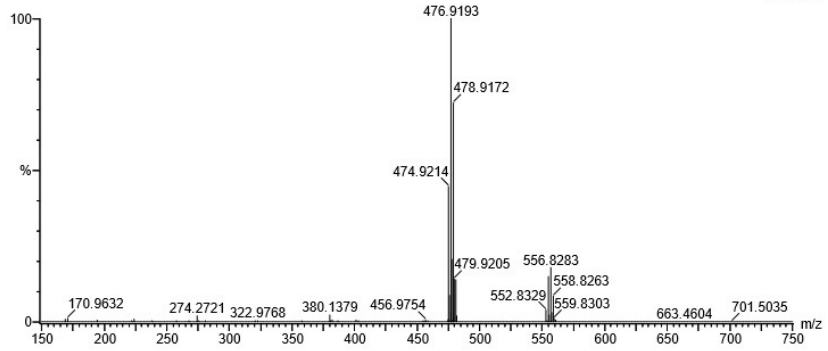
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-83/ PR-83-b-di/ 11/ fid
2	Title	PR-83-b-di
3	Comment	gc-83-b C13CPD CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 16
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.9
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	2018-04-27T01 :28:30
18	Modification Date	2018-04-27T01 :28:32
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

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

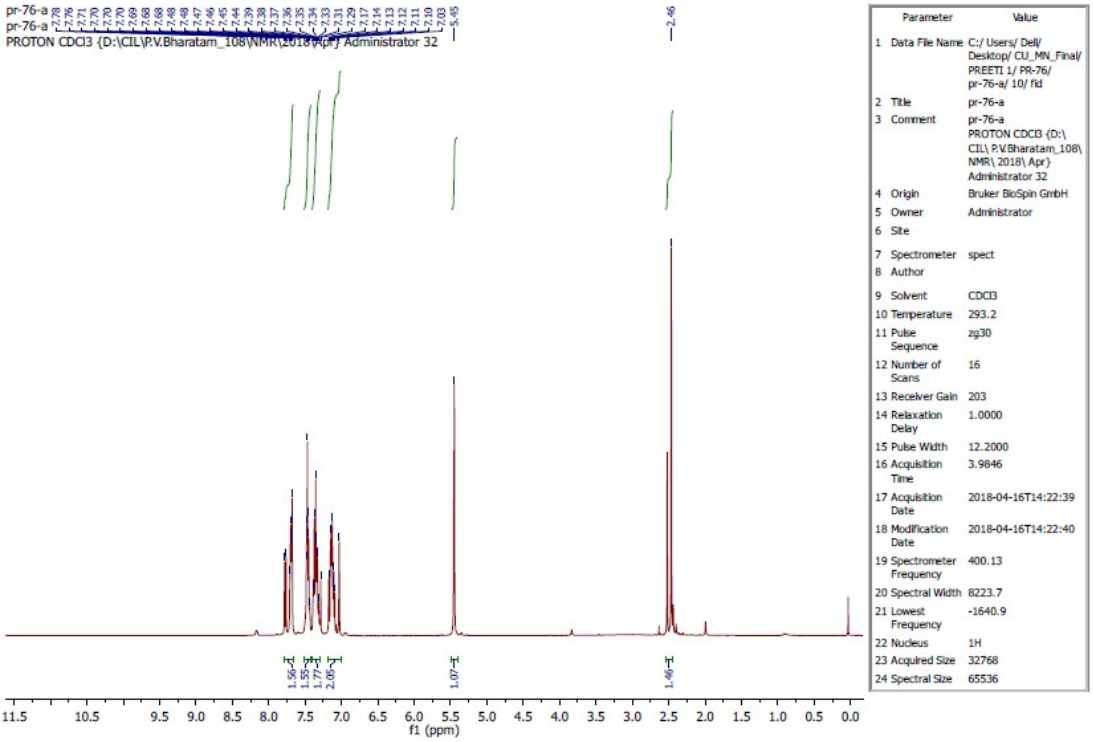
Monoisotopic Mass, Even Electron Ions
28 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-3 Cl: 0-1 Br: 0-2

Sample Name : PR-83-A I.I.T.ROPAR XEVO G2-XS QTOF
Test Name : HRMS-1
280119-PR-83-A 18 (0.183) AM2 (Ar,19000.0,0.00,0.00); Cm (18:24) 1: TOF MS ES+
4.51e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
474.9214	474.9212	0.2	0.4	13.5	485.7	n/a	n/a	C20 H14 N2 Cl Br2

^{1}H NMR spectra of 1-benzyl-5-methyl-2-phenyl-1H-benzo[d]imidazole (3l).



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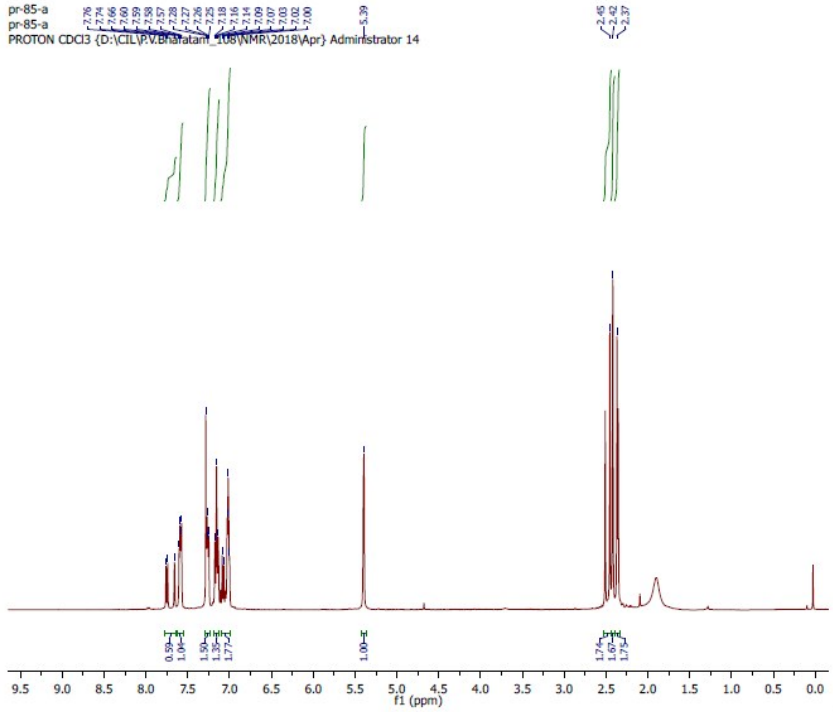
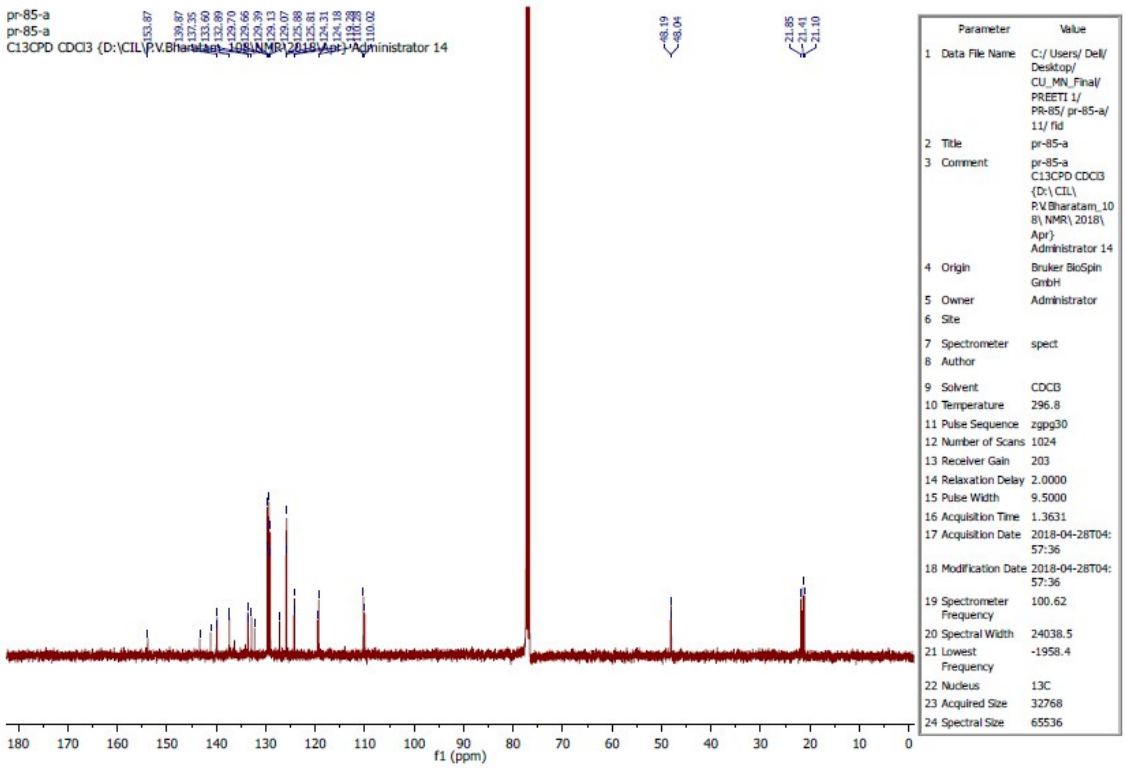
2	Title	pr-76-a
3	Comment	pr-76-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 32
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-16T14:22:39
18	Modification Date	2018-04-16T14:22:40
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

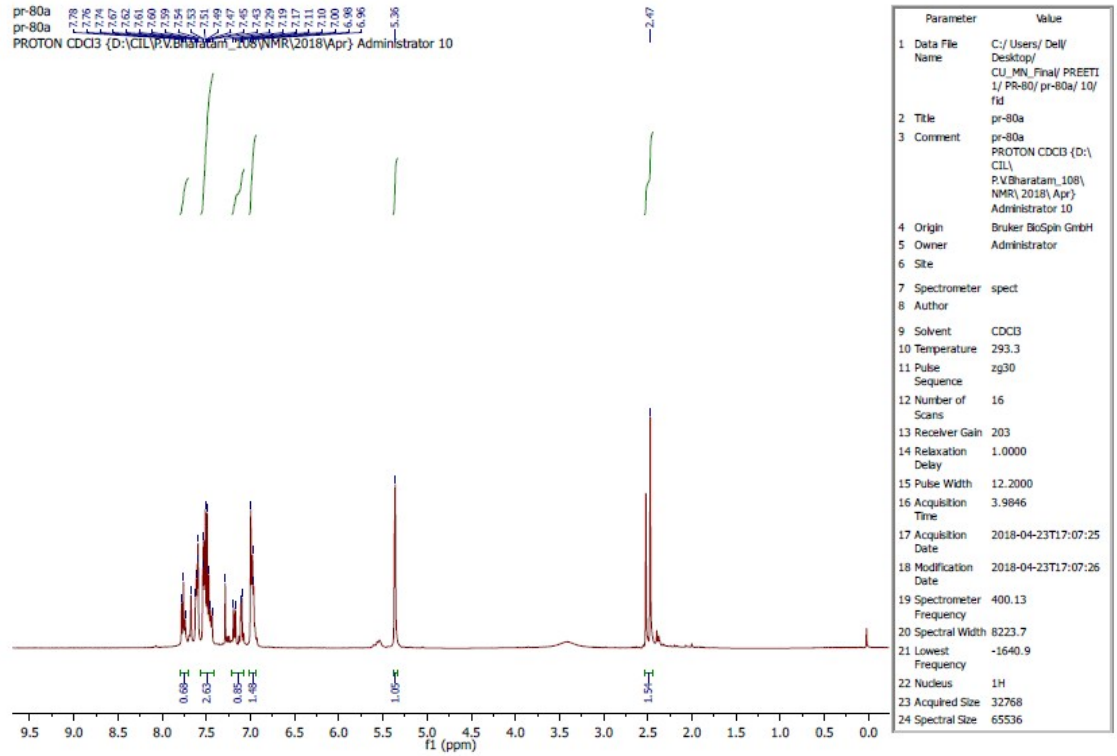
^{1}H and ^{13}C NMR spectra of 5-methyl-1-(4-methylbenzyl)-2-(p-tolyl)-1H-benzo[d]imidazole (3m)

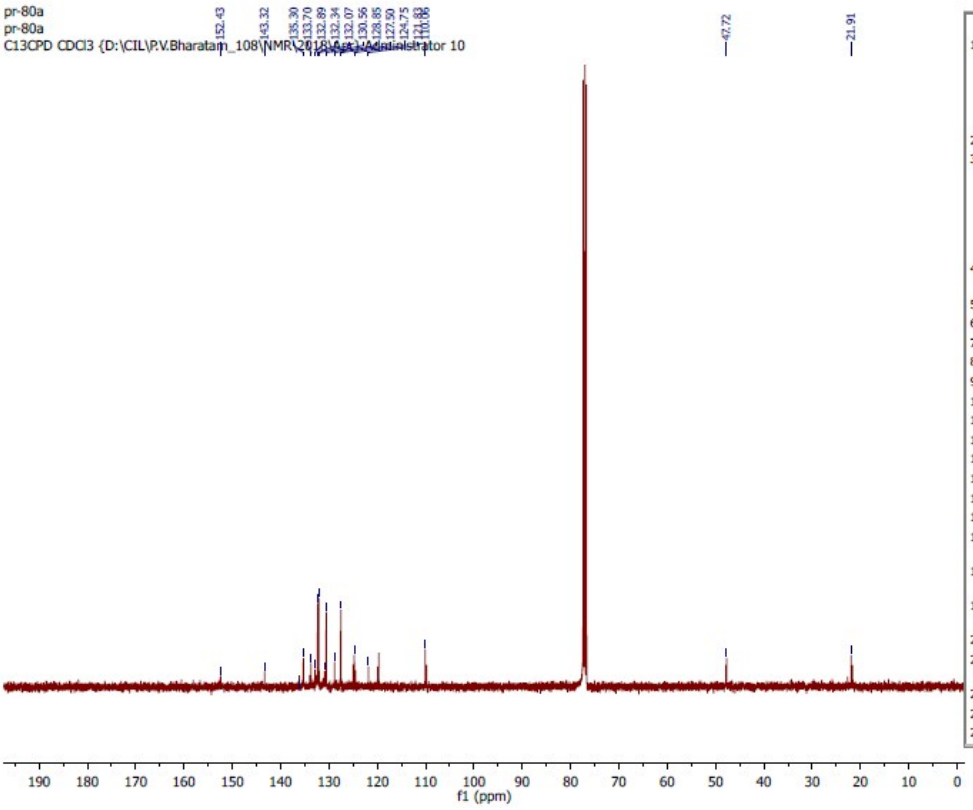


	Parameter	Value
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-85/ pr-85-a/ 10/ fid
2	Title	pr-85-a
3	Comment	pr-85-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 14
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.4
11	Pulse Sequence	zg30
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-27T16:14:53
18	Modification Date	2018-04-27T16:14:54
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



^{1}H, ^{13}C NMR and HRMS spectra of 1-(4-bromobenzyl)-2-(4-bromophenyl)-5-methyl-1H-benzo[d]imidazole (3n).





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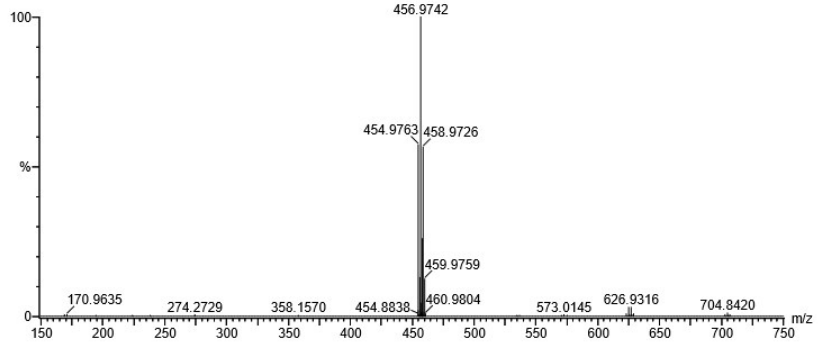
1	Data File Name	C:/ Users/ Dell/ Desktop/ CU_MN_Final/ PREETI 1/ PR-80/ pr-80a/ 11/ fid
2	Title	pr-80a
3	Comment	pr-80a C13CPD CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 10
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.2
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	2018-04-23T21:19:37
18	Modification Date	2018-04-23T21:19:38
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

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

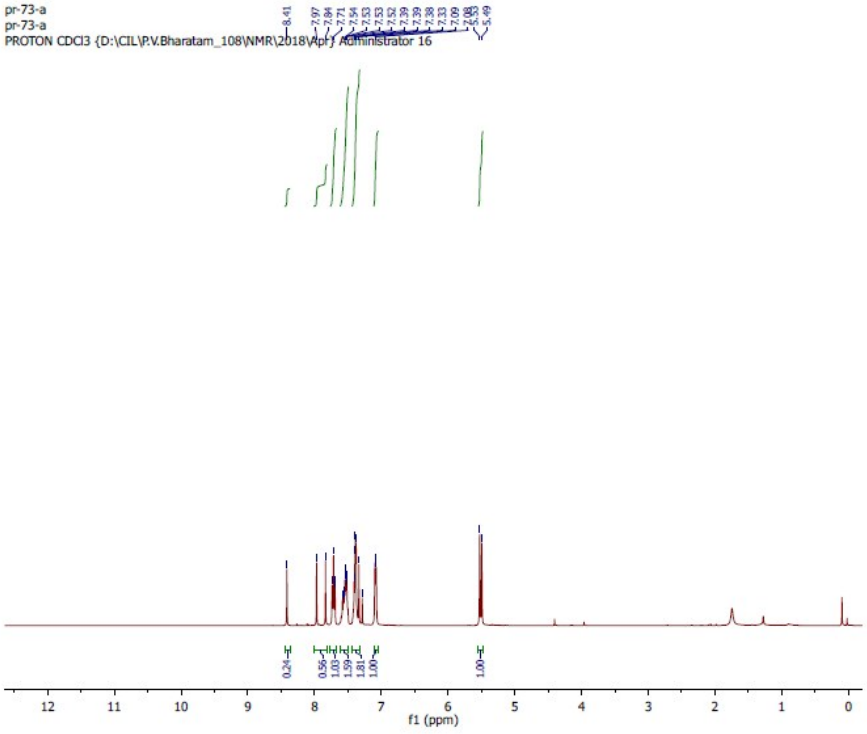
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-4 Br: 0-2

Sample Name : PR-80-A I.I.T.ROPAR XEVO G2-XS QTOF
Test Name : HRMS-1
280119-PR-80-A 18 (0.183) AM2 (Ar,19000.0,0.00,0.00); Cm (18:26) 1: TOF MS ES+
9.62e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
454.9763	454.9758	0.5	1.1	13.5	637.9	n/a	n/a	C21 H17 N2 Br2

^{1}H ,^{13}C NMR and HRMS spectra of 1-benzyl-5-chloro-6-nitro-2-phenyl-1H-benzo[d]imidazole (3o).



	Parameter	Value
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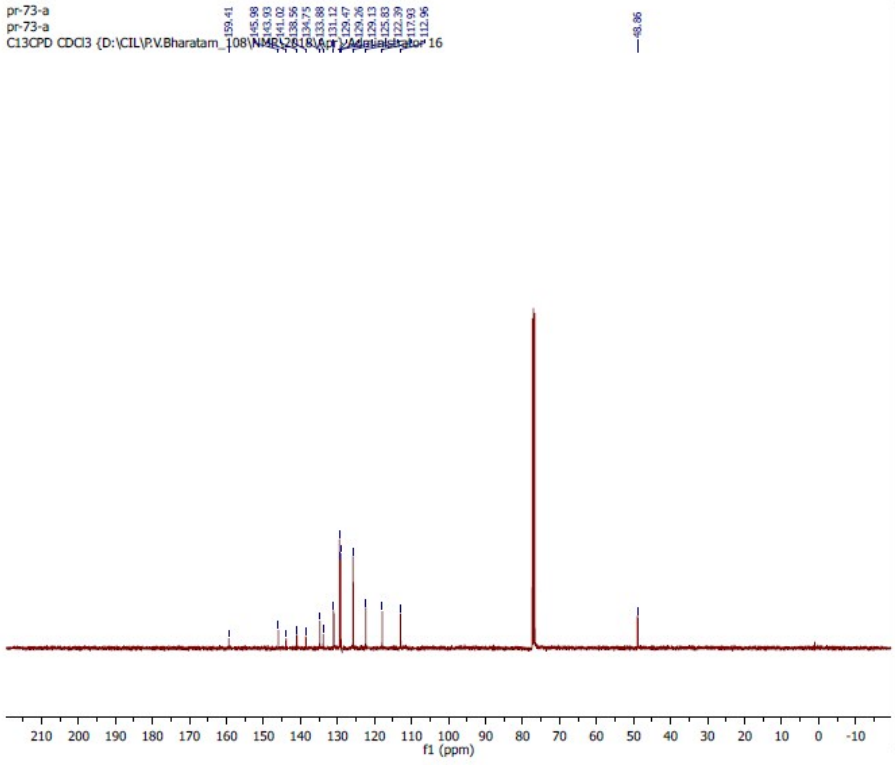
2	Title	pr-73-a
3	Comment	pr-73-a PROTON CDCl3 {D:\ CIL\ P.V.Bharatam_108\ NMR\ 2018\ Apr} Administrator 16
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	296.7
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-09T13:57:26
18	Modification Date	2018-04-09T13:57:28
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



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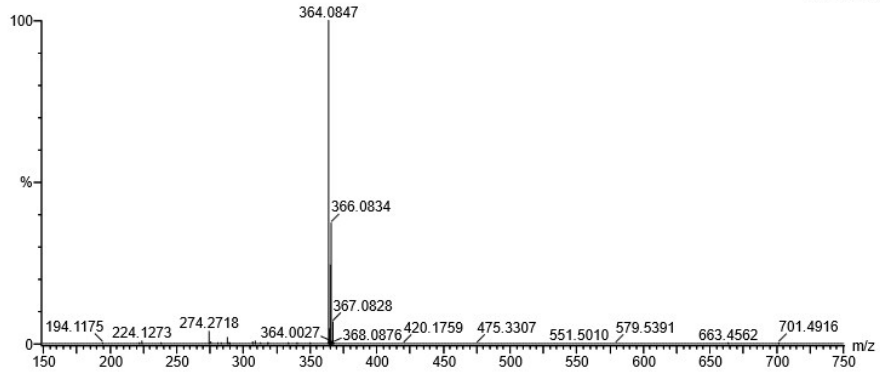
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	295.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-04-09T15:14:42
18	Modification Date	2018-04-09T15:14:42
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

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

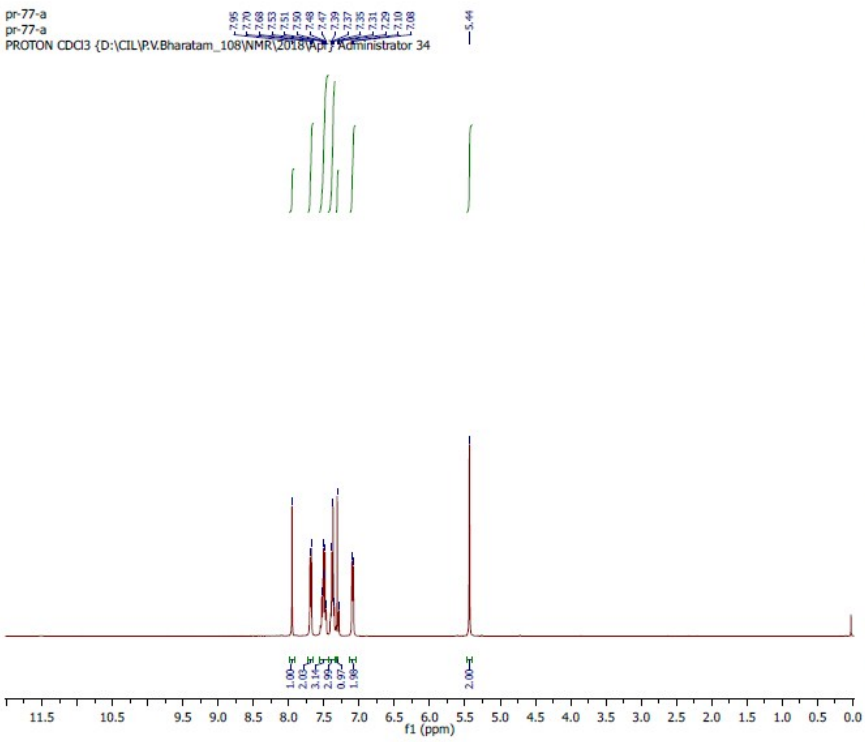
Monoisotopic Mass, Even Electron Ions
73 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-20 N: 0-4 O: 0-4 Cl: 0-1

Sample Name : PR-73-A I.I.T.ROPAR XEVO G2-XS QTOF
Test Name : HRMS-1
280119-PR-73-A 18 (0.183) AM (Top,4, Ar,10000.0,0.00,0.00); Cm (18:21) 1: TOF MS ES+
3.67e+007



Minimum:				-1.5				
Maximum:		5.0	5.0	50.0				
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
364.0847	364.0853	-0.6	-1.6	14.5	930.0	n/a	n/a	C20 H15 N3 O2 Cl

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



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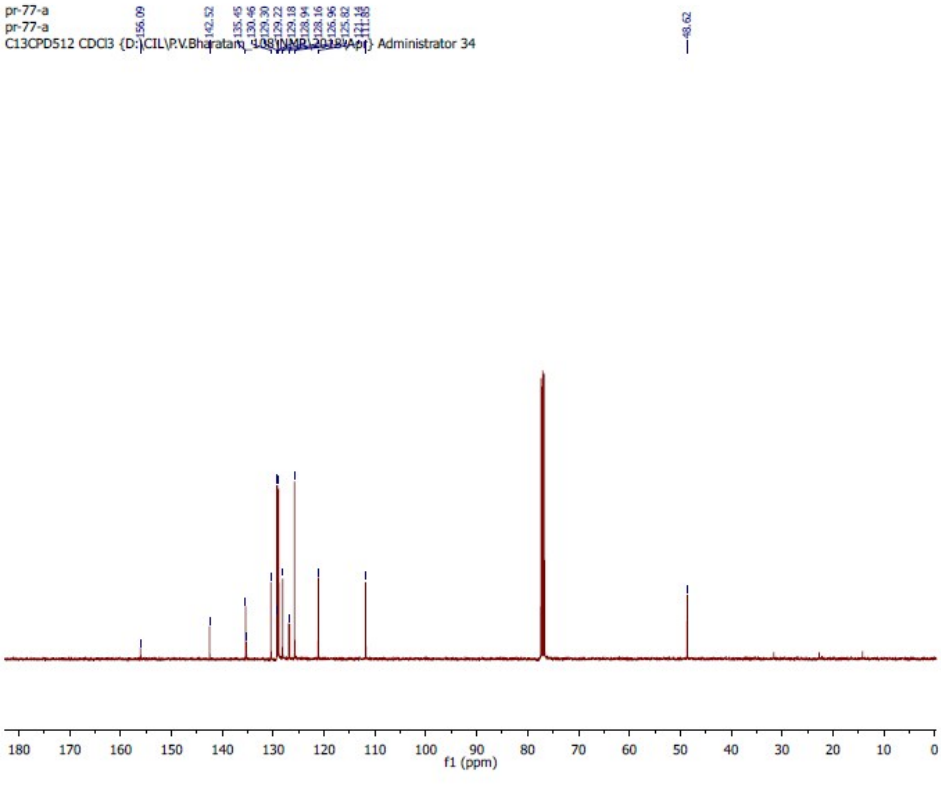
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-04-16T14:33:59
18	Modification Date	2018-04-16T14:34:00
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



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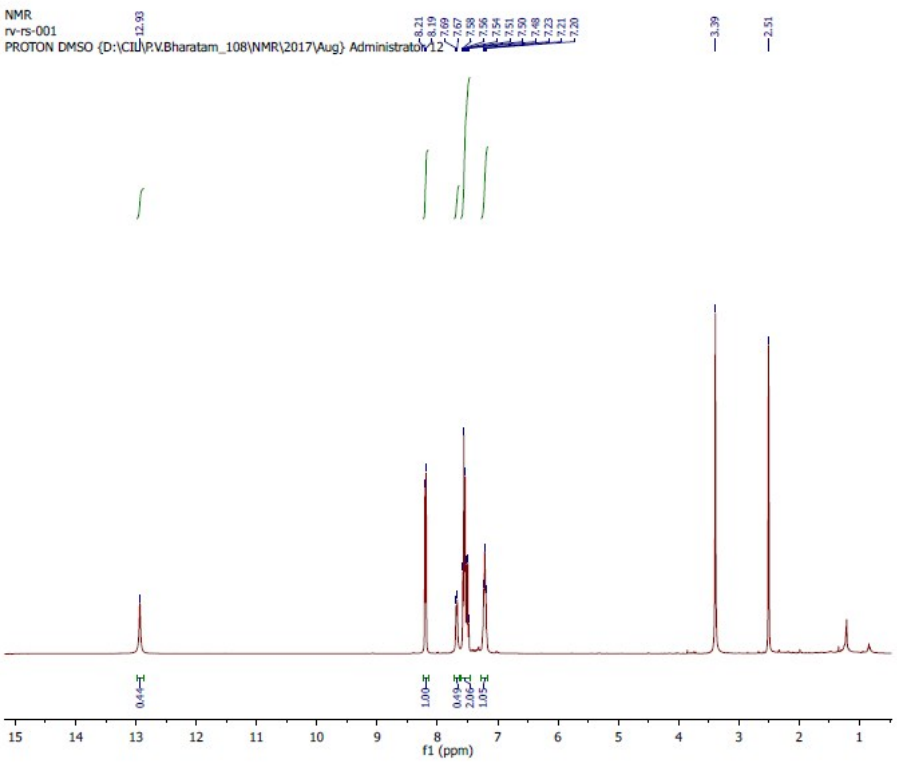
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.3
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-04-16T23:45:16
18	Modification Date	2018-04-16T23:45:16
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 and ^{13}C NMR spectra of 2-phenyl-1H-benzo[d]imidazole (4a).



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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
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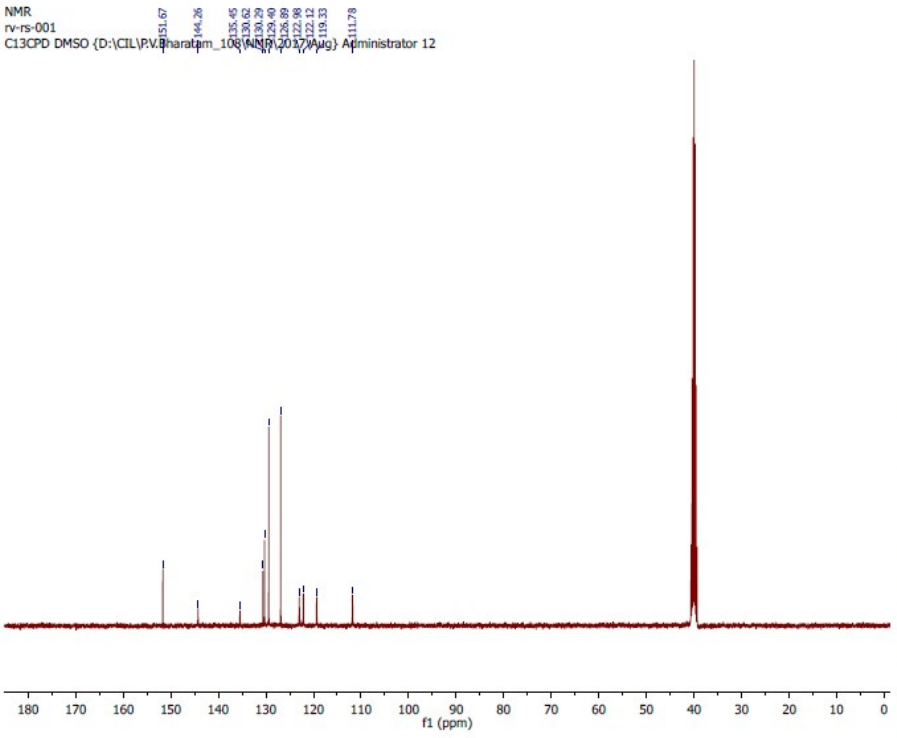
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2017-08-22T17 :04:19
18	Modification Date	2017-08-22T17 :04:19
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
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11	Pulse Sequence	zgpg30
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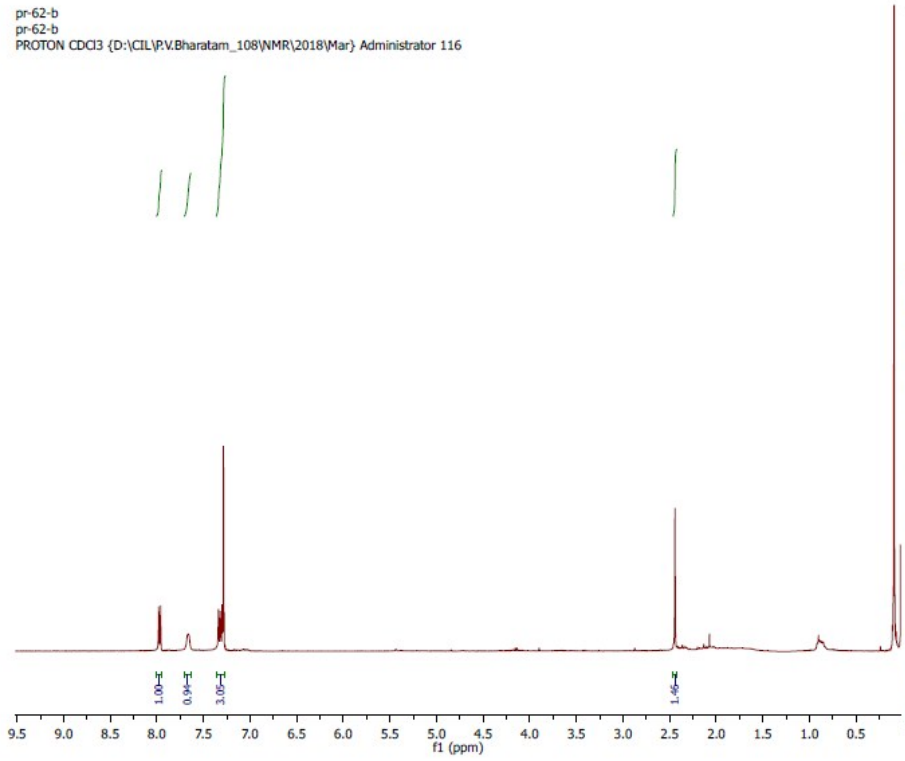
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2017-08-22T18 :47:31
18	Modification Date	2017-08-22T18 :47:32
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of 2-(p-tolyl)-1H-benzo[d]imidazole (4b).



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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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14	Relaxation Delay	1.0000
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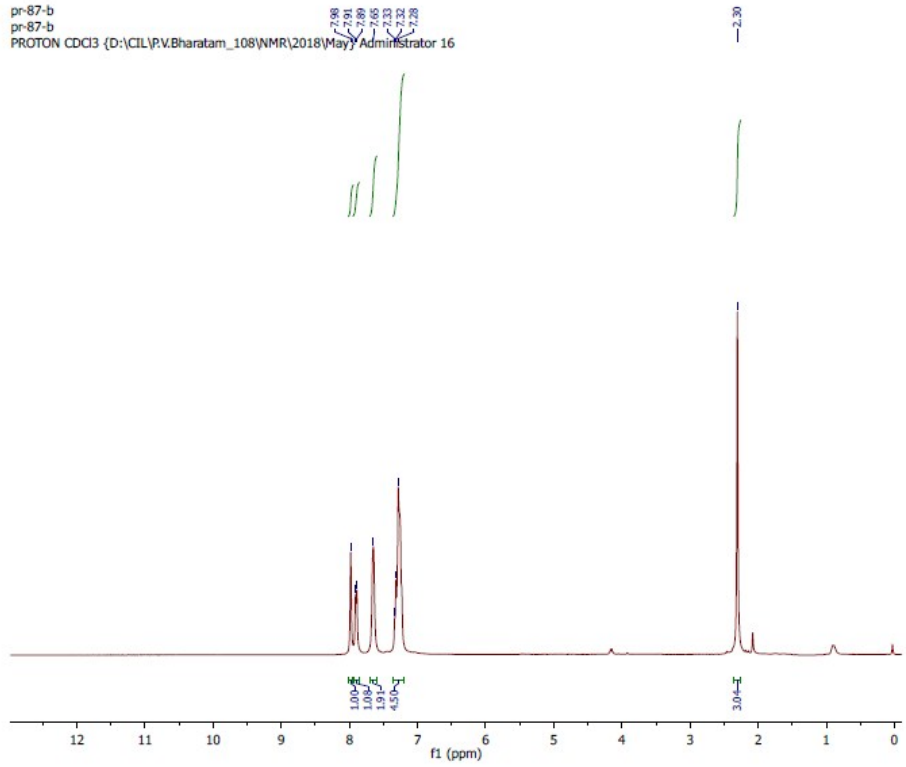
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra of 2-(m-tolyl)-1H-benzo[d]imidazole (4c).



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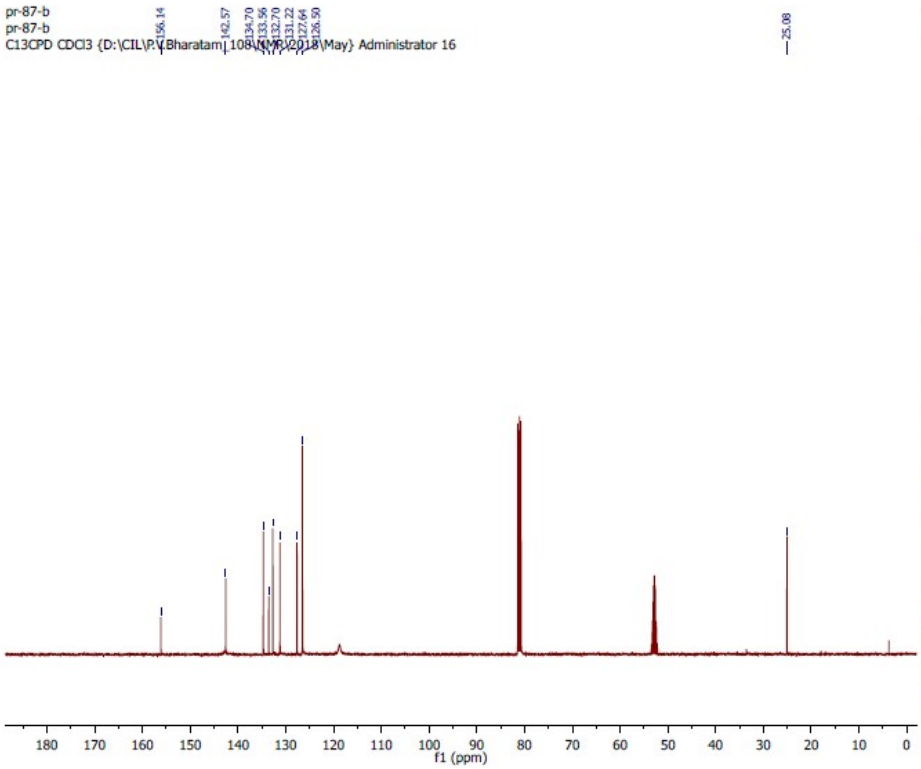
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	297.4
11	Pulse Sequence	zg30
12	Number of Scans	64
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	12.2000
16	Acquisition Time	3.9846
17	Acquisition Date	2018-05-14T15:29:01
18	Modification Date	2018-05-14T15:29:02
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



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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	1024
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
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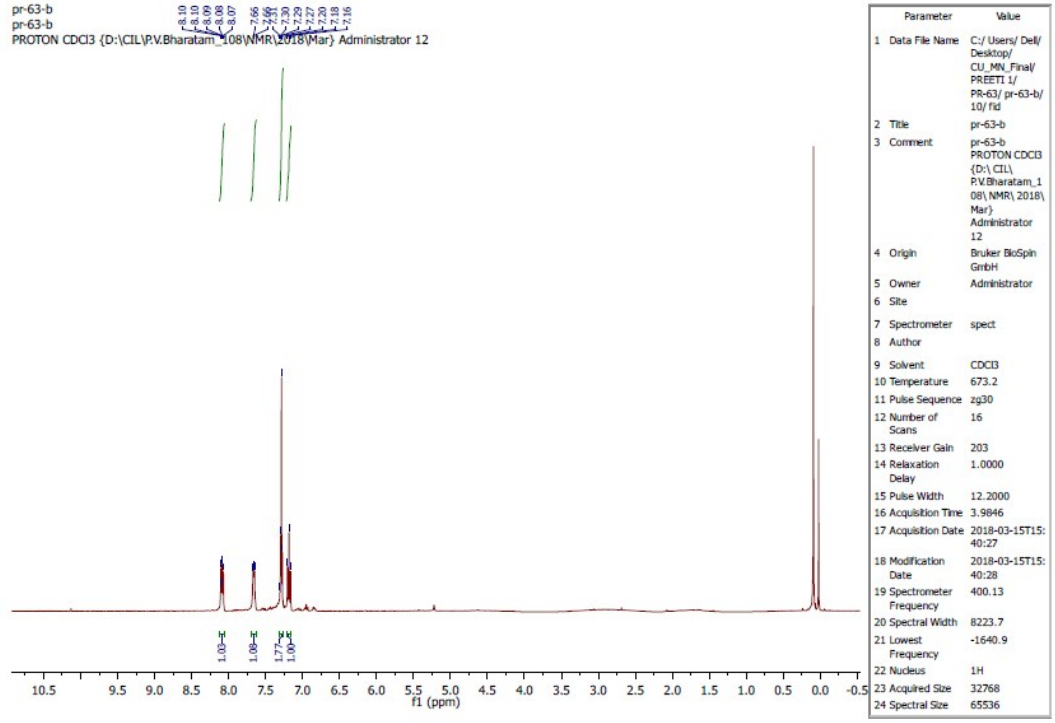
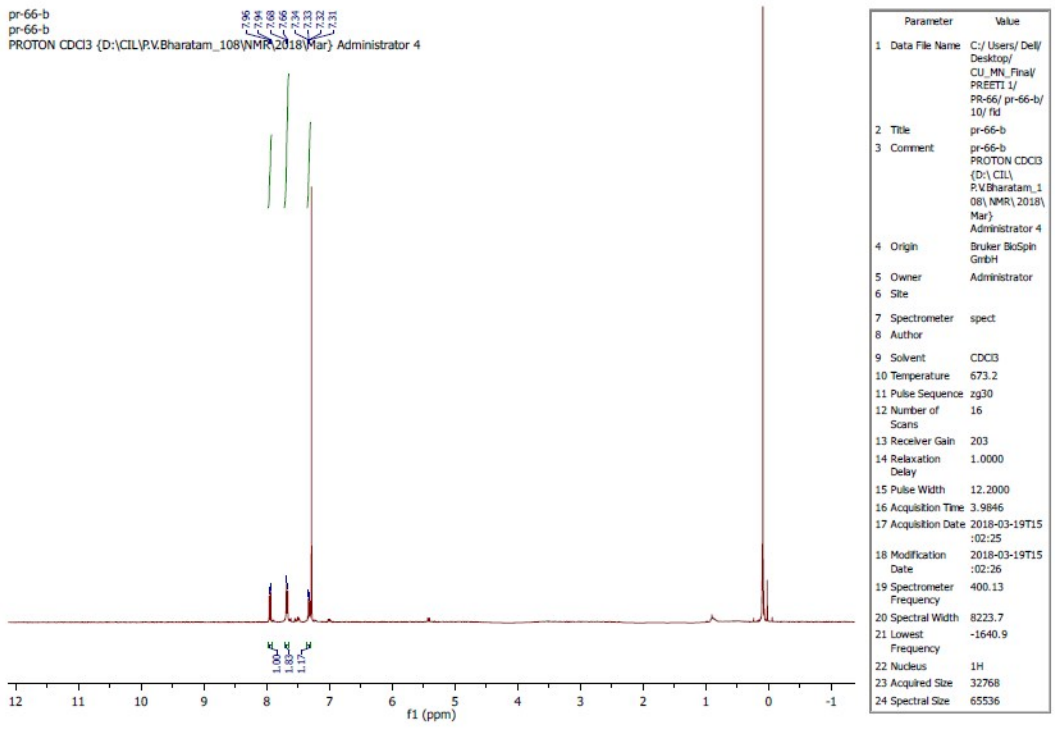
19	Spectrometer Frequency	100.62
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

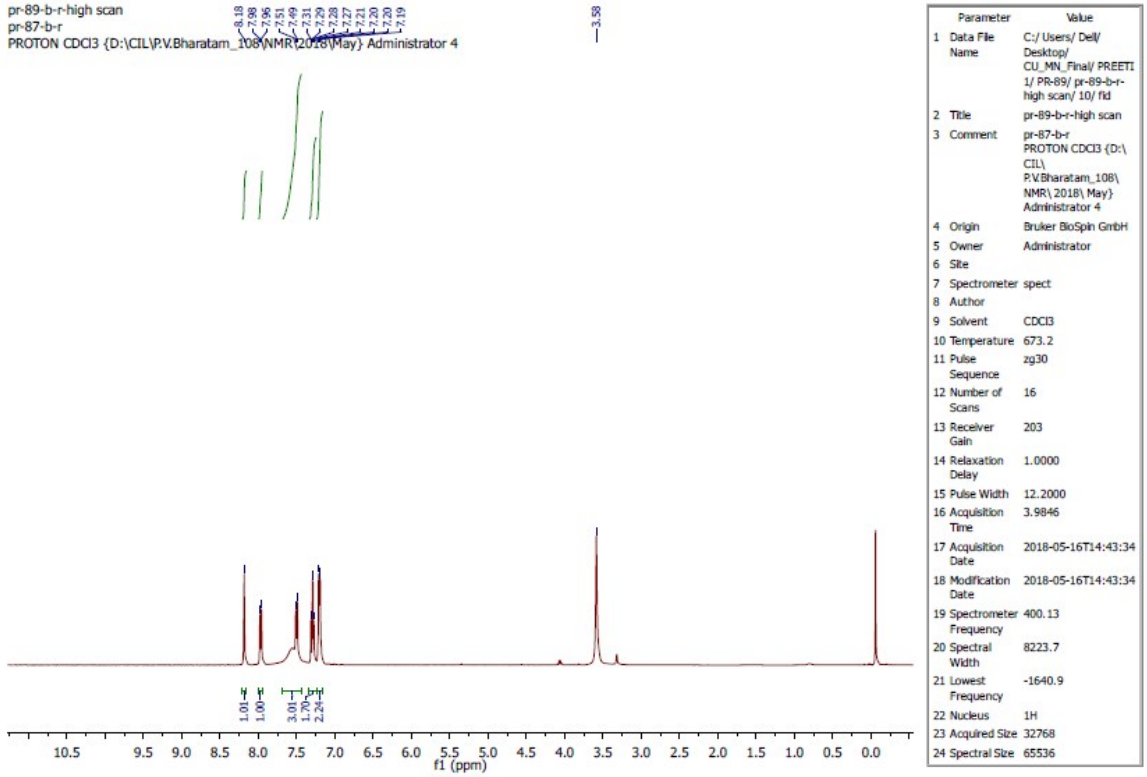
^{1}H NMR spectra of 2-(4-fluorophenyl)-1H-benzo[d]imidazole (4d).



^{1}H NMR spectra of 2-(4-bromophenyl)-1H-benzo[d]imidazole (4e).



^{1}H and ^{13}C NMR spectra of 2-(3-bromophenyl)-1H-benzo[d]imidazole (4f)



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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
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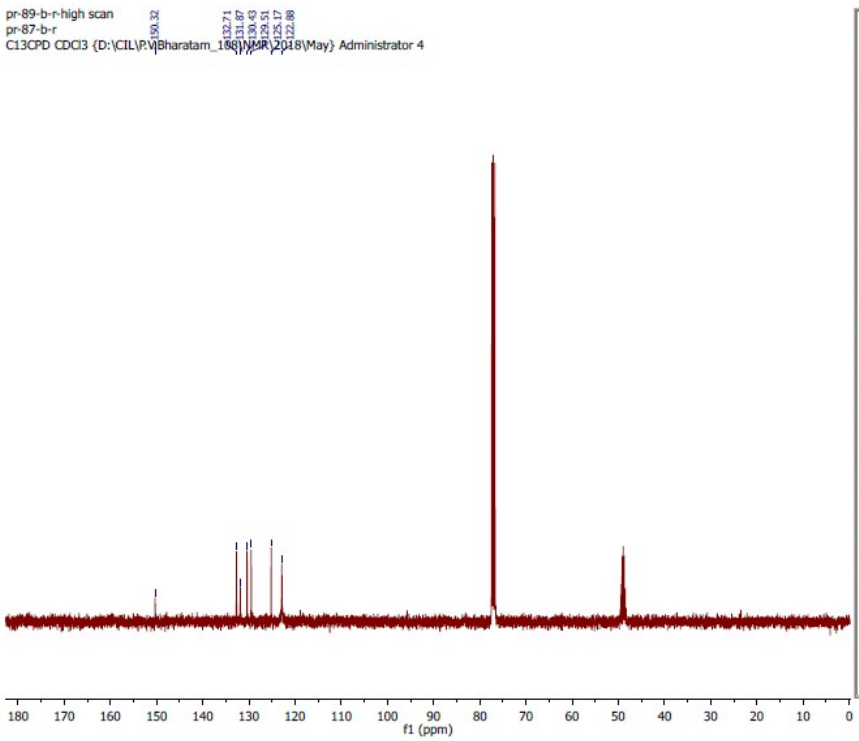
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	301.2
11	Pulse Sequence	zgpg30
12	Number of Scans	512
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14	Relaxation Delay	2.0000
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20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
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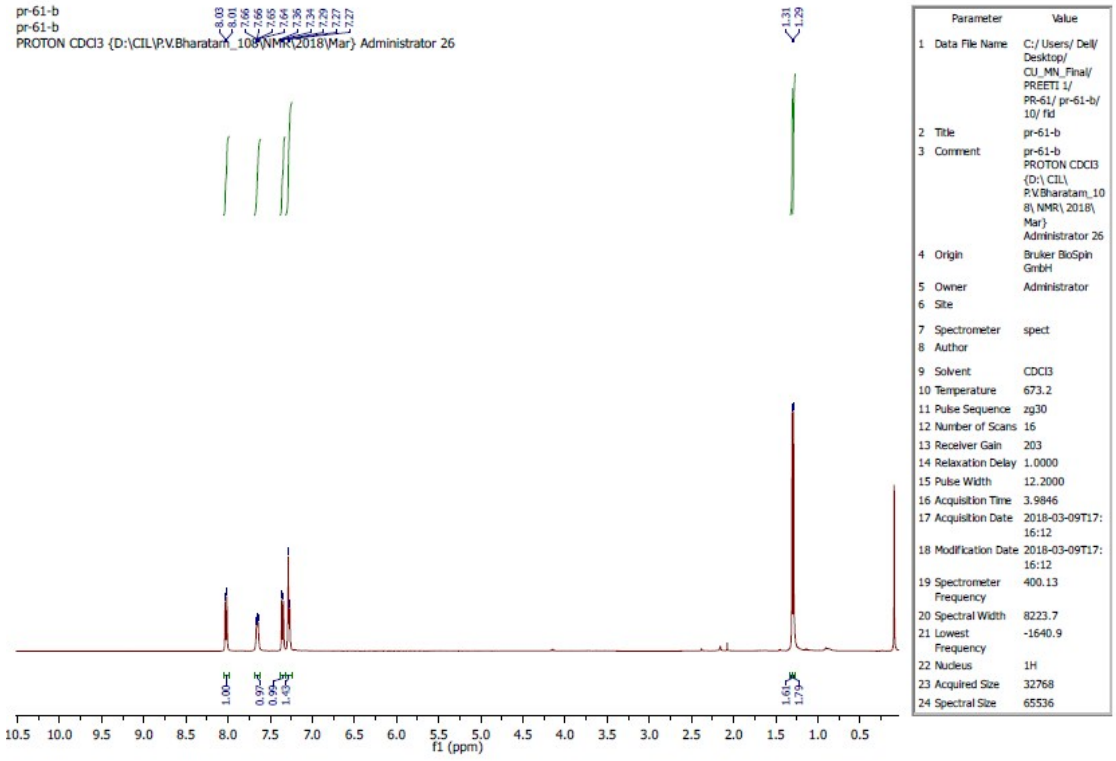
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H NMR spectra of 2-(4-isopropylphenyl)-1H-benzo[d]imidazole (4g).



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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
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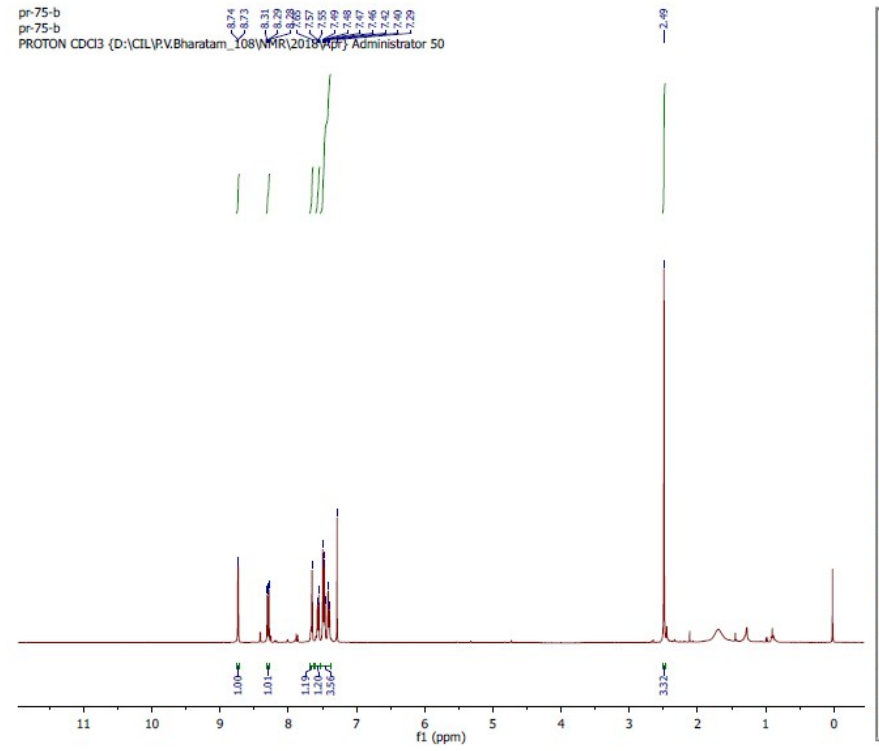
18	Modification Date	2018-03-09T17:16:12
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra of 5-nitro-2-(m-tolyl)-1H-benzo[d]imidazole (4i)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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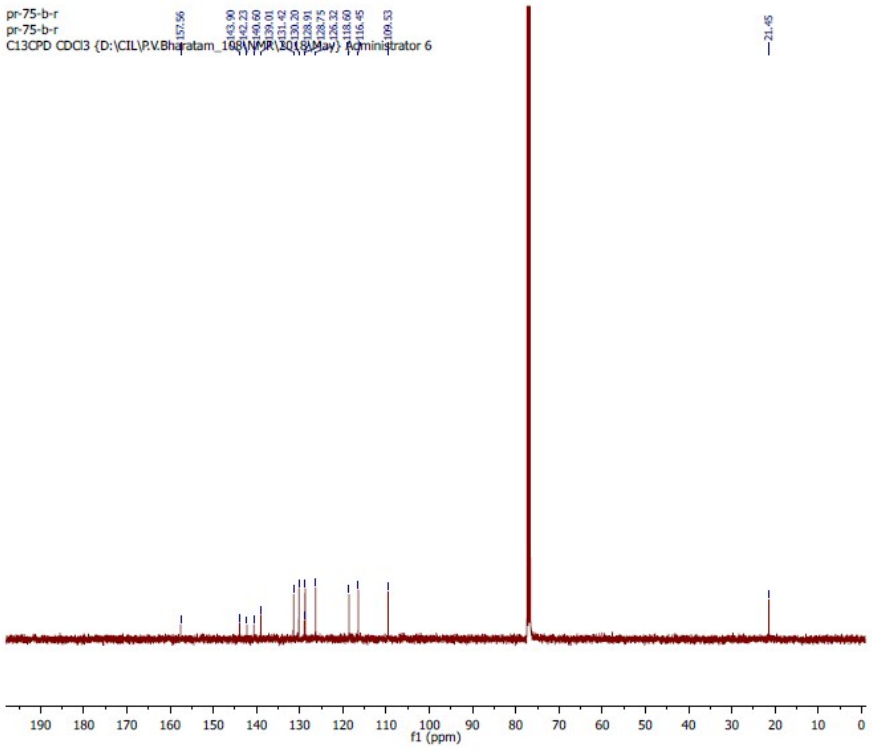
24	Spectral Size	65536



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zgpg30
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14	Relaxation Delay	2.0000
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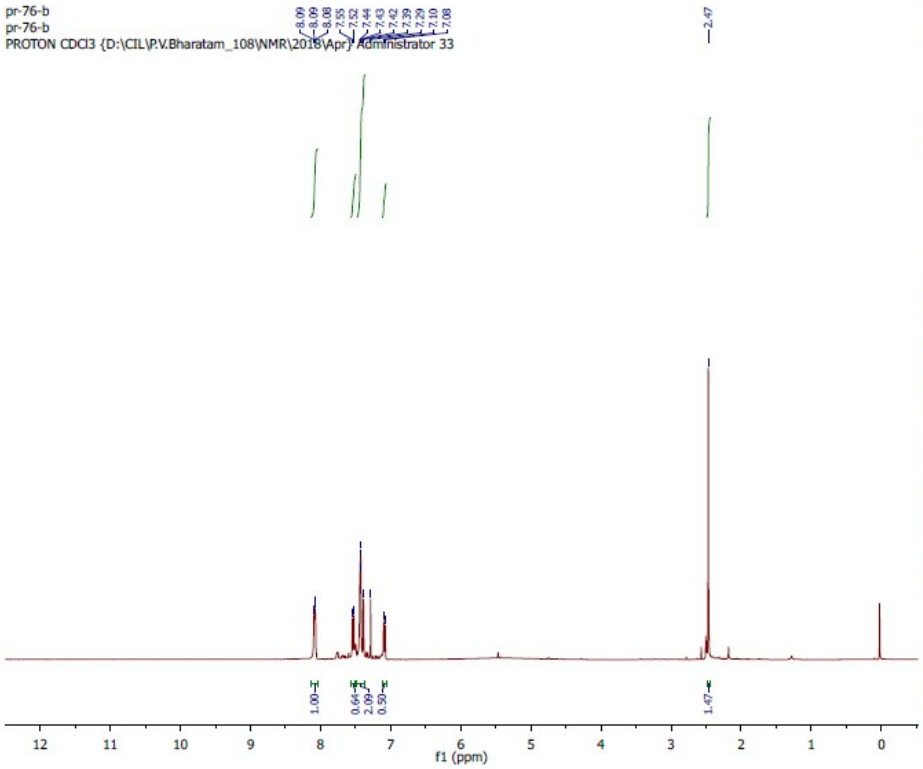
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra of 5-methyl-2-phenyl-1H-benzo[d]imidazole (4l)



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4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.1
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12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
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19	Spectrometer Frequency	400.13
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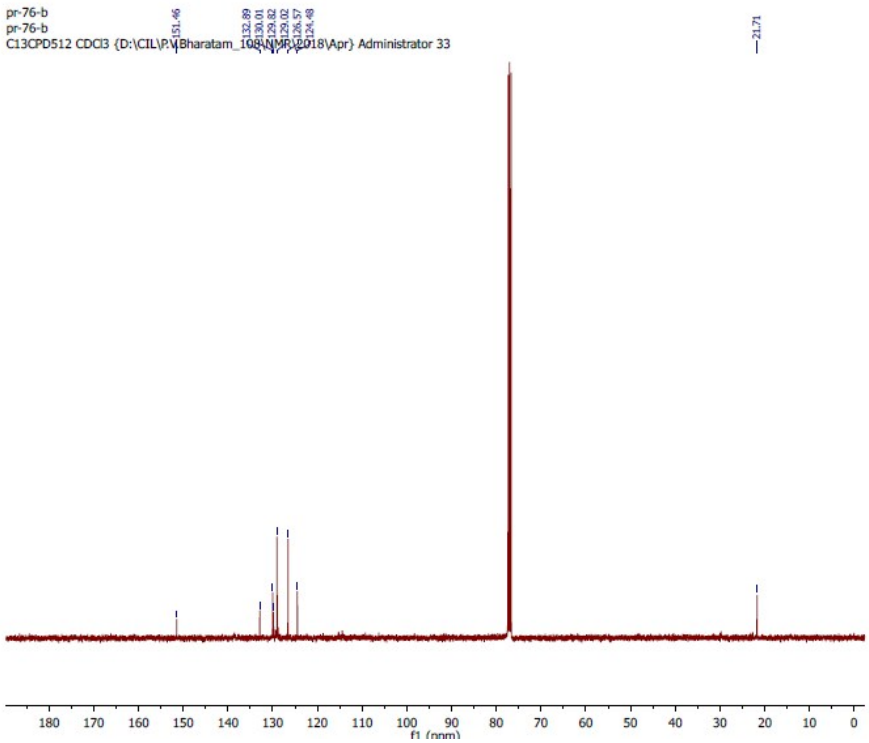
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
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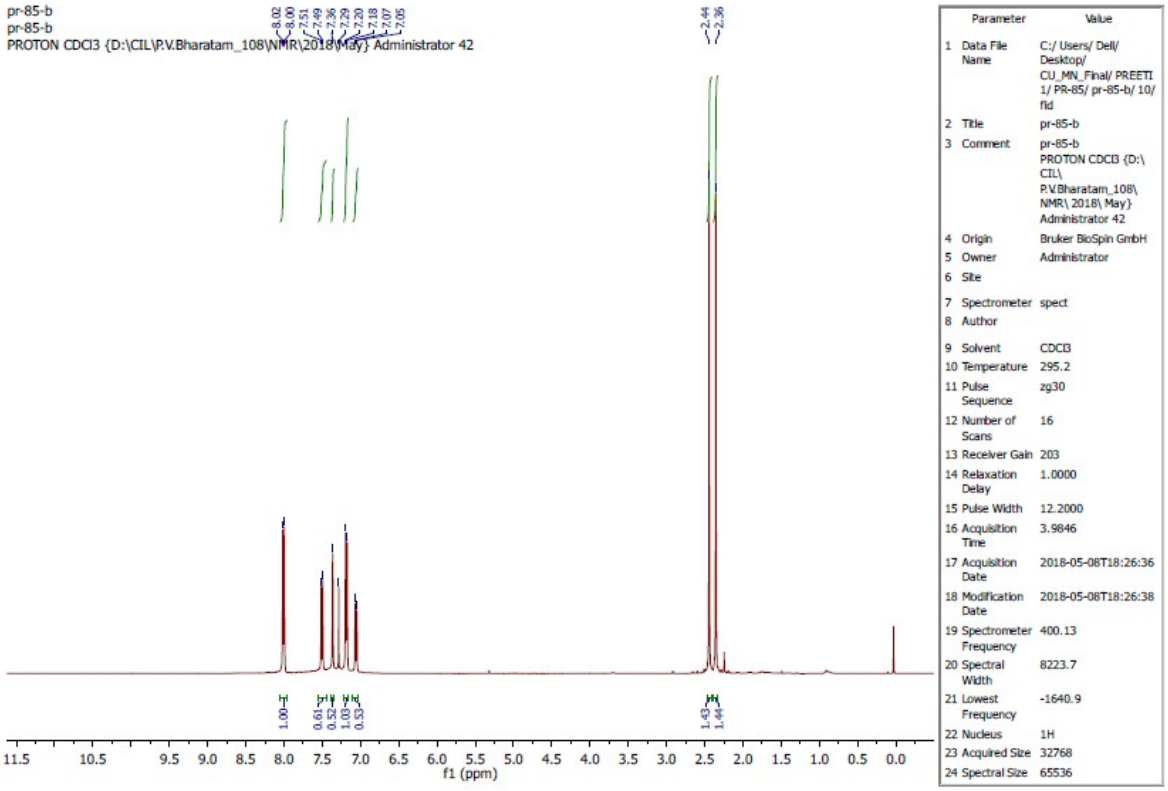
4	Origin	Bruker BioSpin GmbH
5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.3
11	Pulse Sequence	zgpg30
12	Number of Scans	512
13	Receiver Gain	203
14	Relaxation Delay	2.0000
15	Pulse Width	9.5000
16	Acquisition Time	1.3631
17	Acquisition Date	2018-04-16T23:11:59
18	Modification Date	2018-04-16T23:12:00
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 and ^{13}C NMR spectra of 5-methyl-2-(p-tolyl)-1H-benzo[d]imidazole (4m).



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7	Spectrometer	spect
8	Author	
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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	2018-05-08T18:26:36
18	Modification Date	2018-05-08T18:26:38
19	Spectrometer Frequency	400.13
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21	Lowest Frequency	-1640.9
22	Nucleus	1H
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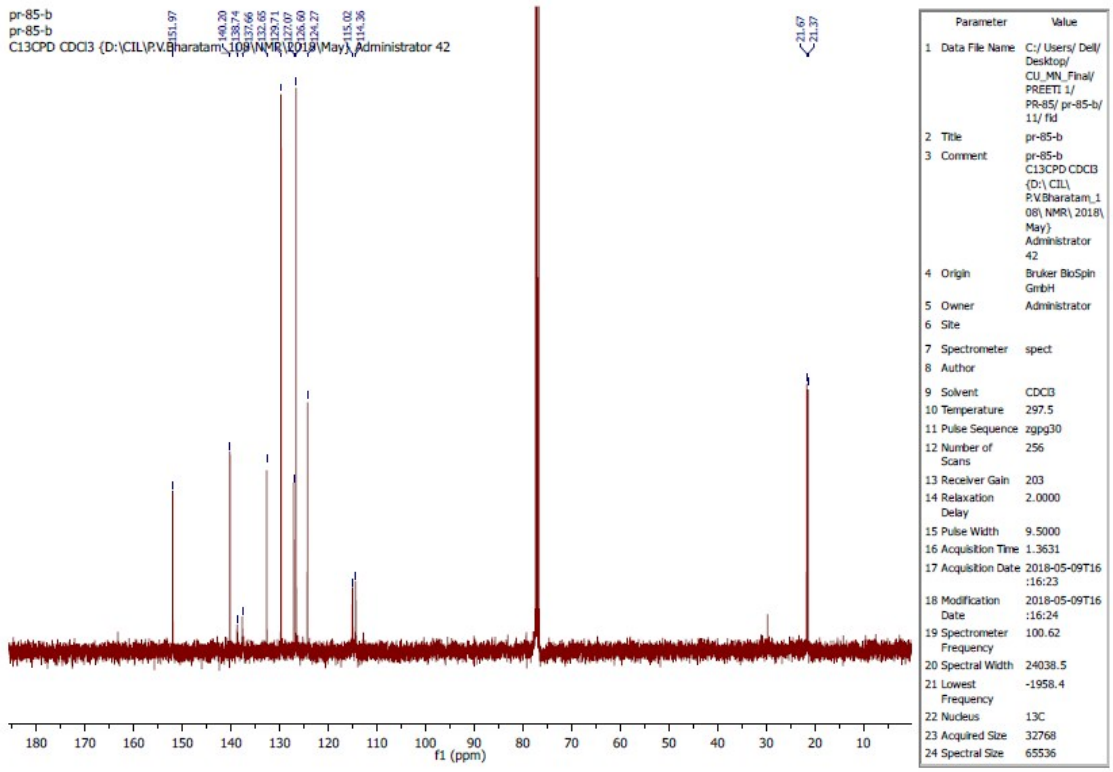

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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
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14	Relaxation Delay	2.0000
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20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
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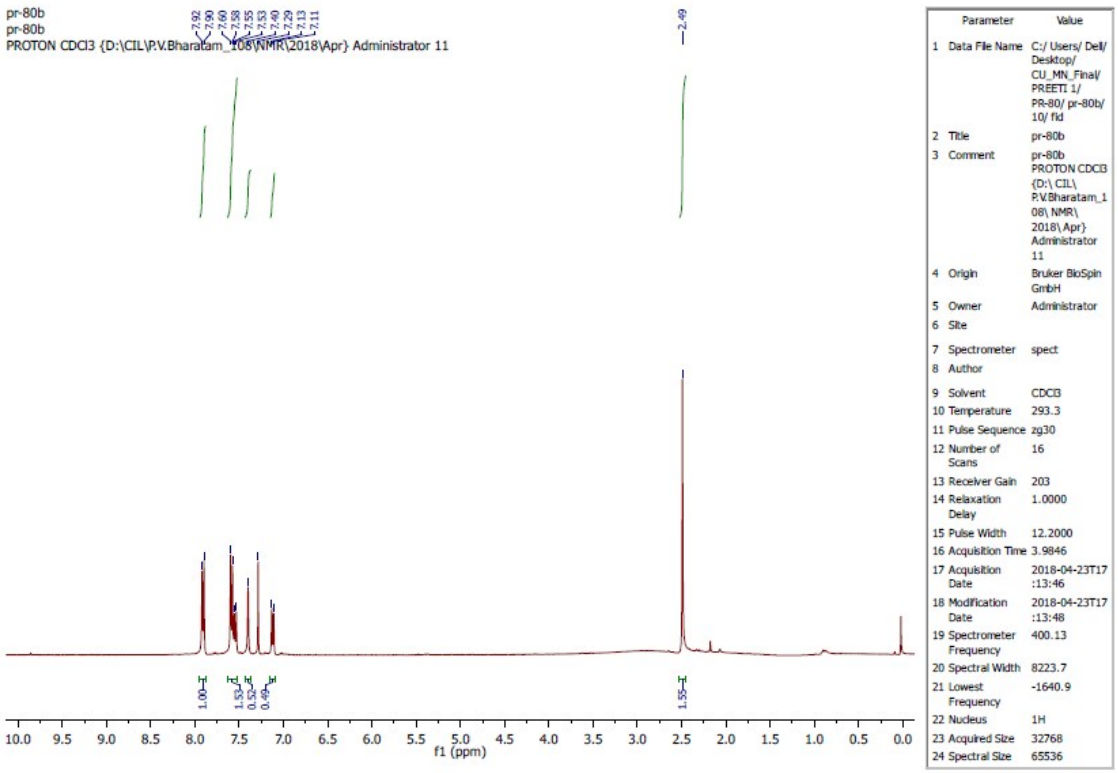
24	Spectral Size	65536

[1]H NMR spectra of 2-(4-bromophenyl)-5-methyl-1H-benzo[d]imidazole (4n).



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5	Owner	Administrator
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	293.3
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
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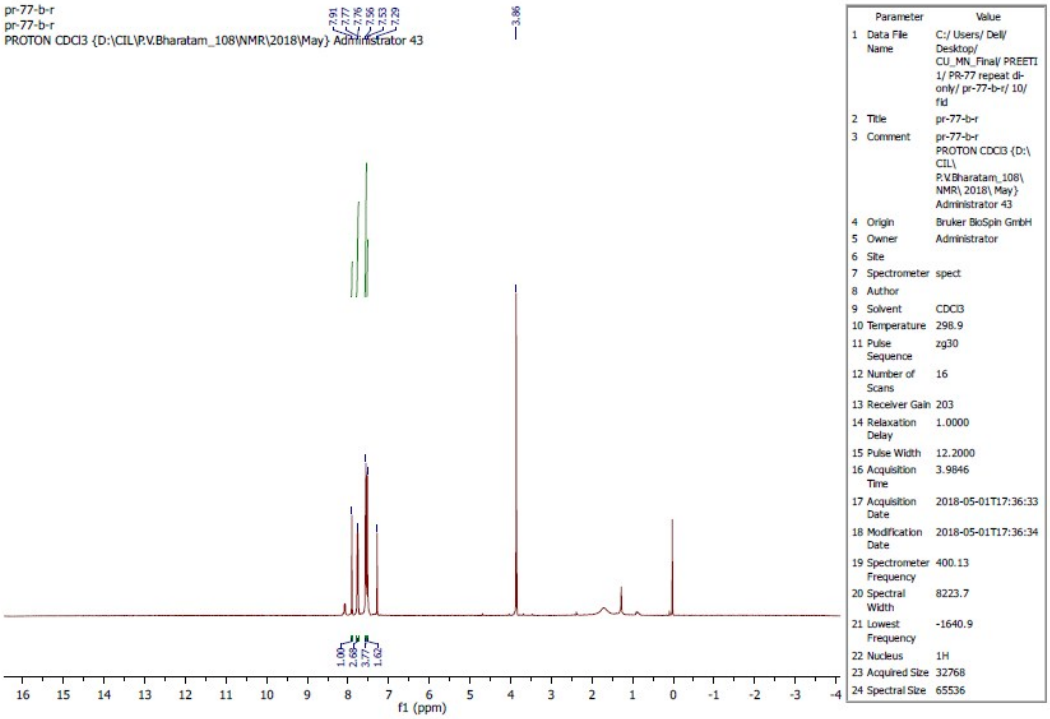
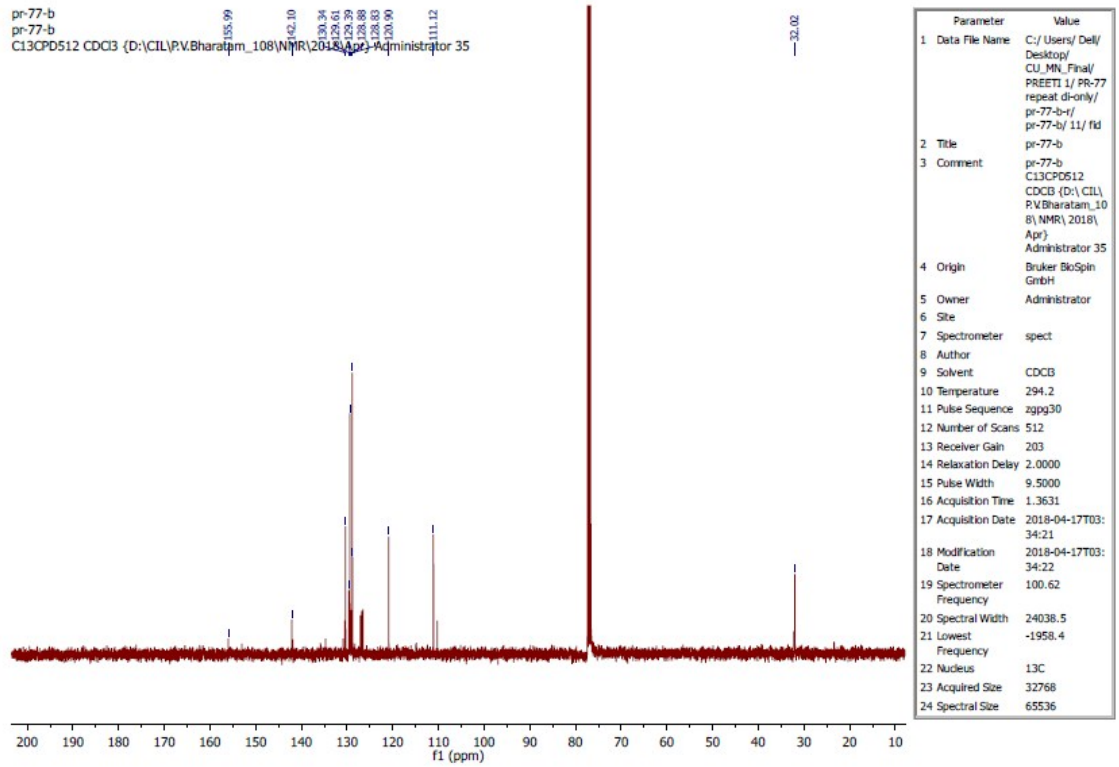
20	Spectral Width	8223.7
21	Lowest Frequency	-1640.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

^{1}H and ^{13}C NMR spectra of 5,6-dichloro-2-phenyl-1H-benzo[d]imidazole (4p).





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