Supplementary Data:

A new NBS/Oxone promoted one pot cascade synthesis of 2-aminobenzimidazoles/2-aminobenzoxazoles: a facile approach

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Contents:

General procedure for the Synthesis of substituted 2-aminobenzazoles

Cyclohexanone (1 mmol, 1 equivalent) was treated with PTSA (1.7 mmol) in a 100 mL RB flask. After five minutes of magnetic stirring NBS (1.3 mmol) was added dropwise by using 6:4 v/v acetonitrile/water as solvent. Later after five minutes oxone as external oxidant (1.3 mmol) was added. This speeds up the reaction and avoids by-product formation. Stirring was continued at room temperature. The progress of reaction was monitored by TLC taking benzene and ethyl acetate as solvent systems in ratio 3:2. After the *in situ* generation, of 2-bromocyclohexanone (**III**) reactant second (1 mmol, 1 equivalent) was added. Stirring was further continued maintaining temperature at 50 °C and progress of reaction was monitored by TLC. After completion of the reaction as indicated by chromatographic technique work-up procedure was started. On completion of the reaction as monitored by TLC, the reaction mixture was cooled to room temperature and treated with ethyl acetate (3 x 10 mL). The organic layer so obtained was dried with sodium sulfate and filtered to obtain the product.

Spectral findings for all the synthesized 2-amino substituted benzimidazole derivatives are given below:

1*H*-benzo[*d*]imidazol-2-amine [3a]

Prepared by reacting *in situ* generated **III** with Guanidine (1 mmol, 0.05g); Beige solid, yield: 95%; m.p.135-137 °C; IR (KBr, ν, cm^{-1}); 3376, 3054, 1663, 1563, 1480, 1157. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 6.98 (t, 2H, J = 7.4 Hz, Ar-H), 7.27 (d, 2H, J = 7.4 Hz, Ar-H), 10.25 (s, 1H, NH), 11.03 (s, 2H, NH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 111.5, 117.3, 126.7, 130.9, 138.3, 142.9, 156.5. ESI–MS: 134 $[M+H]^+$; Anal. Calcd. For $C_7H_7N_3$: C, 63.14; H, 5.30; N, 31.56%. Found: C, 63.15; H, 5.28; N, 31.59%.

***N*-phenyl-1*H*-benzo[*d*]imidazol-2-amine [3b]**

Prepared by reacting *in situ* generated **III** with 1-Phenylguanidine (1 mmol, 0.13 g); Beige solid, Yield: 93%, mp 123–125 °C; IR (KBr, ν, cm^{-1}); 3362, 3025, 1629, 1597, 1521, 1134; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.02 (t, 2H, J = 7.6, Ar-H), 7.32 (d, 2H, J = 7.6 Hz, Ar-H), 7.46 (t, 1H, J = 7.8 Hz, Ar-H), 7.58 (d, 2H, J = 8.0 Hz, Ar-H), 7.73 (t, 2H, J = 8.0 Hz, Ar-H), 10.34 (s, 1H, NH), 11.12 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 115.7, 116.2, 121.6, 123.4, 128.8, 129.3, 130.6, 141.2, 144.8, 148.1, 157.6; ESI–MS: 210 $[M+H]^+$; Anal. Calcd. For $C_{13}H_{11}N_3$: C, 74.62; H, 5.30; N, 20.08%. Found: C, 74.65; H, 5.33; N, 20.06%.

4-(1*H*-benzo[*d*]imidazol-2-ylamino)-2-aminobutanoic acid [3c]

Prepared by reacting *in situ* generated **III** with (*S*)-2-amino-5-guanidinopentanoic acid (1 mmol, 0.17g); Beige solid, Yield: 90%; mp 130–132 °C; IR (KBr, ν, cm^{-1}); 3462, 3029, 1720, 1615, 1465, 1403, 1134, 723; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 1.87 (t, 2H, J = 6.1 Hz, CH_2), 2.74 (m, 2H, CH_2), 3.28 (t, 2H, J = 5.8 Hz, CH), 5.82 (br s, 1H, OH), 7.03 (d, 2H, J = 7.8 Hz, Ar-H), 7.14 (t, 2H, J = 7.8 Hz, Ar-H), 9.87 (s, 2H, NH), 10.57 (s, 1H, NH_2); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 28.6, 36.2, 54.7, 115.3, 116.8, 121.8, 123.5, 128.2, 135.9, 142.7, 172.4; ESI–MS: 235 $[M+H]^+$; Anal. Calcd. For $C_{11}H_{14}N_4O_2$: C, 56.40; H, 6.02; N, 23.92%. Found: C, 56.43; H, 5.99; N, 23.96%.

***N*-(4-chlorophenyl)-1*H*-benzo[*d*]imidazol-2-amine [3d]**

Prepared by reacting *in situ* generated **III** with 1-(4-chlorophenyl)guanidine (1 mmol, 0.16g); Beige solid, Yield: 91%; mp 142–144 °C; IR (KBr, ν, cm^{-1}); 3450, 3036, 1557, 1495, 1414, 1148, 735; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.08 (t, 2H, J = 7.6 Hz, Ar-H), 7.32 (d, 2H, J = 7.6 Hz, Ar-H), 7.56 (d, 2H, J = 8.0 Hz, Ar-H), 7.93 (d, 2H, J = 8.0 Hz, Ar-H), 10.36 (s, 1H, NH), 11.55 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 115.9, 117.6, 122.6, 123.4, 127.1, 127.87, 129.3, 137.5, 140.9, 155.4, 160.3; ESI–MS: 245

[M+H]$^+$; Anal. Calcd. For $C_{13}H_{10}ClN_3$: C, 64.07; H, 4.14; N, 17.24%. Found: C, 64.09; H, 4.12; N, 17.22%.

***N*-(4-bromophenyl)-1*H*-benzo[*d*]imidazol-2-amine [3e]**

Prepared by reacting *in situ* generated **III** with 1-(4-bromophenyl)guanidine (1 mmol, 0.21g); Pale yellow solid, Yield: 90%; mp 128–130 °C; IR (KBr, ν, cm^{-1}); 3442, 2997, 1672, 1629, 1537, 1140, 656; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.12 (t, 2H, J = 7.8 Hz, Ar-H), 7.28 (d, 2H, J = 7.8 Hz, Ar-H), 7.34 (d, 2H, J = 8.2 Hz, Ar-H), 7.58 (d, 2H, J = 8.5 Hz, Ar-H), 10.07 (s, 1H, NH), 11.63 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 115.3, 116.5, 119.2, 121.5, 122.6, 126.9, 128.3, 138.6, 142.1, 145.3, 158.7; ESI–MS: 289 [M+H]$^+$; Anal. Calcd. For $C_{13}H_{10}BrN_3$: C, 54.19; H, 3.50; N, 27.73%. Found: C, 54.16; H, 3.48; N, 27.75%.

***N*-(4-nitrophenyl)-1*H*-benzo[*d*]imidazol-2-amine [3f]**

Prepared by reacting *in situ* generated **III** with 1-(4-nitrophenyl)guanidine (1 mmol, 0.18g); Golden yellow solid, Yield: 84%; mp 131–133 °C; IR (KBr, ν, cm^{-1}); 3448, 3104, 1631, 1535, 1485, 1430, 1359, 1137; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.08 (t, 2H, J = 7.7 Hz, Ar-H), 7.37 (d, 2H, J = 7.7 Hz, Ar-H), 8.02 (d, 2H, J = 8.2 Hz, Ar-H), 8.28 (d, 2H, J = 8.0 Hz, Ar-H), 9.80 (s, 1H, NH), 11.52 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 115.8, 117.5, 118.9, 121.5, 123.2, 127.6, 136.7, 139.7, 144.8, 155.13, 157.8; ESI–MS: 255 [M+H]$^+$; Anal. Calcd. For $C_{13}H_{10}N_4O_2$: C, 61.41; H, 3.96; N, 22.04%. Found: C, 61.23; H, 3.55; N, 16.44%.

***N*-(3-chlorophenyl)-1*H*-benzo[*d*]imidazol-2-amine [3g]**

Prepared by reacting *in situ* generated **III** with 1-(3-chlorophenyl)guanidine (1 mmol, 0.16g); Beige solid, Yield: 88%; mp 140–142 °C; IR (KBr, ν, cm^{-1}); 3457, 3029, 1575, 1474, 1413, 1136, 730; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 6.95 (t, 2H, J = 7.6 Hz, Ar-H), 7.22 (d, 2H, J = 7.6 Hz, Ar-H), 7.36 (s, 1H, Ar-H), 7.52 (d, 1H, J = 8.2 Hz, Ar-H), 7.56 (t, 1H, J = 8.4 Hz, Ar-H), 8.06 (d, 1H, J = 8.2 Hz, Ar-H), 10.12 (s, 1H, NH), 11.57 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 115.4, 116.9, 119.1, 121.4, 124.0, 127.2, 128.4, 129.8, 135.54, 137.8, 142.4, 152.3, 16.8; ESI–MS: 245 [M+H]$^+$; Anal. Calcd. For $C_{13}H_{10}ClN_3$: C, 64.07; H, 4.14; N, 17.24%. Found: C, 64.05; H, 4.16; N, 17.25%.

***N*-(3-nitrophenyl)-1*H*-benzo[*d*]imidazol-2-amine [3h]**

Prepared by reacting *in situ* generated **III** with 1-(3-nitrophenyl)guanidine (1 mmol, 0.18g); Golden yellow solid, Yield: 84%; mp 130–132 °C; IR (KBr, ν, cm^{-1}); 3452, 3034, 1625, 1590, 1532, 1415, 1365, 1147; ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.02 (t, 2H, J = 7.6 Hz, Ar-H), 7.26 (d, 2H, J = 7.6 Hz, Ar-H),

7.64 (s, 1H, Ar-H), 7.76 (d, 1H, *J* = 8.0 Hz, Ar-H), 7.95-7.98 (t, 1H, *J* = 8.2 Hz, Ar-H), 8.40 (d, 1H, *J* = 8.0 Hz, Ar-H), 11.12 (s, 1H, NH), 11.64 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 113.2, 115.4, 116.5, 117.9, 121.2, 122.1, 127.3, 129.51, 136.48, 142.6, 146.8, 157.73, 162.3; ESI–MS: 255 $[M+H]^+$; Anal. Calcd. For $C_{13}H_{10}N_4O_2$: C, 61.41; H, 3.96; N, 22.04%. Found: C, 61.43; H, 3.94; N, 22.06%.

Spectral findings for all the synthesized 2-amino substituted benzoxazole derivatives are given below:

Benzo[*d*]oxazol-2-amine [3a']

Prepared by reacting *in situ* generated **III** with Urea (1 mmol, 0.06g); Off white solid, yield: 93%; m.p.128-131 °C; IR (KBr, ν, cm^{-1}); 3440, 3021, 1665, 1613, 1557, 1140, 1050. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.16 (t, 2H, *J* = 8.0 Hz, Ar-H), 7.36 (d, 2H, *J* = 8.0 Hz, Ar-H), 9.56 (s, 2H, NH_2). ^{13}C NMR (100 MHz, DMSO-d_6) δ: 110.3, 115.5, 124.3, 125.9, 138.7, 146.9, 158.3. ESI–MS: 135 $[M+H]^+$; Anal. Calcd. For $C_7H_6N_2O$: C, 62.68; H, 4.51; N, 20.88%. Found: C, 62.66; H, 4.53; N, 20.86%.

***N*-phenylbenzo[*d*]oxazol-2-amine [3b']**

Prepared by reacting *in situ* generated **III** with 1-Phenylurea (1 mmol, 0.13g); Off white solid, Yield: 91%; mp 122–125 °C; IR (KBr, ν, cm^{-1}); 3442, 3025, 1559, 1489, 1411, 1140, 1048. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.06 (t, 2H, *J* = 7.8 Hz, Ar-H), 7.19 (d, 2H, *J* = 7.8 Hz, Ar-H), 7.27–7.33 (m, 2H, Ar-H), 7.39–7.44 (m, 1H, Ar-H), 7.70 (d, 2H, *J* = 8.0 Hz, Ar-H), 10.12 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 107.3, 116.8, 118.0, 121.2, 121.7, 124.5, 130.3, 140.5, 143.7, 147.4, 156.2; ESI–MS: 211 $[M+H]^+$; Anal. Calcd. For $C_{13}H_{10}N_2O$: C, 74.27; H, 4.79; N, 13.33%. Found: C, 74.23; H, 4.83; N, 13.34%.

***N*-(4-methoxyphenyl)benzo[*d*]oxazol-2-amine [3c']**

Prepared by reacting *in situ* generated **III** with 1-(4-methoxyphenyl)urea (1 mmol, 0.16g); Off white solid, Yield: 90%; mp 125–127 °C; IR (KBr, ν, cm^{-1}); 3445, 2993, 1664, 1593, 1549, 1136, 1053. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.26 (s, 3H, CH_3), 7.10 (t, 2H, *J* = 7.6 Hz, Ar-H), 7.22 (d, 2H, *J* = 7.6 Hz, Ar-H), 7.33 (d, 2H, *J* = 8.3 Hz, Ar-H), 7.54 (d, 2H, *J* = 8.3 Hz, Ar-H), 10.17 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 21.6, 109.2, 115.4, 117.1, 118.5, 122.8, 124.9, 127.2, 130.4, 131.5, 136.8, 143.6, 147.9, 159.2; ESI–MS: 241 $[M+H]^+$; Anal. Calcd. For $C_{14}H_{12}N_2O_2$: C, 69.99; H, 5.03; N, 11.66%. Found: C, 70.03; H, 5.01; N, 11.64%.

***N*-(4-chlorophenyl)benzo[*d*]oxazol-2-amine [3d']**

Prepared by reacting *in situ* generated **III** with 1-(4-chlorophenyl)urea (1 mmol, 0.17g); Off white solid, Yield: 89%,; mp 125–127 °C; IR (KBr, ν, cm^{-1}); 3442, 3016, 1650, 1585, 1520, 1141, 1056, 725. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.11 (t, 2H, J = 7.7 Hz, Ar-H), 7.29 (d, 2H, J = 7.5 Hz, Ar-H), 7.46 (d, 2H, J = 8.3 Hz, Ar-H), 7.65 (d, 2H, J = 8.3 Hz, Ar-H), 10.36 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 118.5, 119.2, 121.4, 123.6, 126.7, 126.7, 128.0, 130.4, 139.8, 153.3, 164.8; ESI–MS: 246 $[M+H]^+$; Anal. Calcd. For $C_{13}H_9ClN_2O$: C, 63.81; H, 3.71; N, 11.45%. Found: C, 63.83; H, 3.69; N, 11.46%.

***N*-(4-bromophenyl)benzo[*d*]oxazol-2-amine [3e']**

Prepared by reacting *in situ* generated **III** with 1-(4-bromophenyl)urea (1 mmol, 0.21g); Off white solid, Yield: 86%,; mp 125–127 °C; IR (KBr, ν, cm^{-1}); 3450, 3119, 1629, 1553, 1401, 1145, 1047, 660. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.09 (t, 2H, J = 7.5 Hz, Ar-H), 7.16 (d, 2H, J = 7.5 Hz, Ar-H), 7.56 (d, 2H, J = 8.1 Hz, Ar-H), 7.74 (d, 2H, J = 8.1 Hz, Ar-H), 10.24 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 108.2, 116.7, 116.0, 119.9, 122.7, 124.4, 131.4, 138.3, 143.4, 146.7, 157.8; ESI–MS: 290 $[M+H]^+$; Anal. Calcd. For $C_{13}H_9BrN_2O$: C, 54.00; H, 3.14; N, 9.69%. Found: C, 53.97; H, 3.16; N, 9.70%.

***N*-(4-nitrophenyl)benzo[*d*]oxazol-2-amine [3f']**

Prepared by reacting *in situ* generated **III** with 1-(4-nitrophenyl)urea (1 mmol, 0.18g); Golden yellow solid, Yield: 79%,; mp 122–125 °C; IR (KBr, ν, cm^{-1}); 3442, 3005, 1630, 1552, 1436, 1348, 1140, 1048. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.05 (t, 2H, J = 7.8 Hz, Ar-H), 7.22 (d, 2H, J = 7.8 Hz, Ar-H), 8.14 (d, 2H, J = 8.2 Hz, Ar-H), 8.39 (d, 2H, J = 8.2 Hz, Ar-H), 11.63 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 109.6, 110.2, 118.2, 121.5, 124.3, 125.8, 130.6, 141.2, 143.4, 155.3, 156.5; ESI–MS: 256 $[M+H]^+$; Anal. Calcd. For $C_{13}H_9N_3O_3$: C, 61.18; H, 3.55; N, 16.46%. Found: C, 61.20; H, 3.58; N, 16.45%.

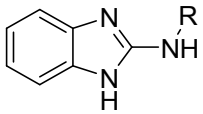
***N*-(3-chlorophenyl)benzo[*d*]oxazol-2-amine [3g']**

Prepared by reacting *in situ* generated **III** with 1-(3-chlorophenyl)urea (1 mmol, 0.17g); Off white solid, Yield: 87%,; mp 125–127 °C; IR (KBr, ν, cm^{-1}); 3447, 2993, 1594, 1521, 1443, 1136, 1050, 728. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.06 (t, 2H, J = 7.6 Hz, Ar-H), 7.14 (d, 2H, J = 7.6 Hz, Ar-H), 7.24 (s,1H, Ar-H), 7.32 (d, 1H, J = 8.0 Hz, Ar-H), 7.41 (m, 1H, Ar-H), 7.64 (d, 1H, J = 8 Hz, Ar-H), 10.76 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 110.3, 115.1, 119.5, 119.2, 121.7, 124.4, 127.9, 128.7, 128.4, 130.4, 142.8, 152.8, 162.2; ESI–MS: 246 $[M+H]^+$; Anal. Calcd. For $C_{13}H_9ClN_2O$: C, 63.81; H, 3.71; N, 11.45%. Found: C, 63.83; H, 3.69; N, 11.46%.

***N*-(3-nitrophenyl)benzo[*d*]oxazol-2-amine [3h']**

Prepared by reacting *in situ* generated **III** with 1-(3-nitrophenyl)urea (1 mmol, 0.18g); Golden yellow solid, Yield: 78%,; mp 125–127 °C; IR (KBr, ν, cm^{-1}); 3440, 3101, 1579, 1536, 1427, 1350, 1147, 1054. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 7.10 (t, 2H, J = 7.5 Hz, Ar-H), 7.17 (d, 2H, J = 7.5 Hz, Ar-H), 7.28 (s, 1H, Ar-H), 7.78 (d, 1H, J = 8.2 Hz, Ar-H), 7.86 (m, 1H, Ar-H), 8.05 (d, 1H, J = 8.2, Ar-H), 11.13 (s, 1H, NH); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 109.6, 110.2, 116.5, 117.2, 122.5, 124.3, 126.8, 129.1, 130.8, 142.2, 148.7, 155.3, 160.7; ESI–MS: 256 $[M+H]^+$; Anal. Calcd. For $C_{13}H_9N_3O_3$: C, 61.18; H, 3.55; N, 16.46%. Found: C, 61.21; H, 3.57; N, 16.44%.

Table S1 Derivatives of 2-amino substituted benzimidazoles (3a-h)



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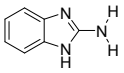
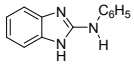
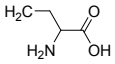
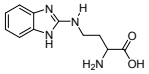
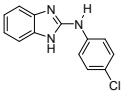
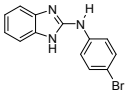
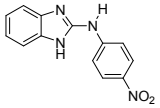
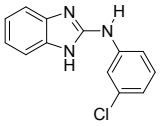
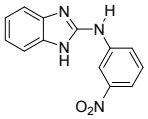
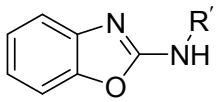
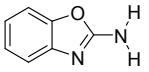
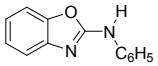
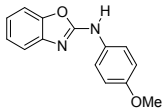
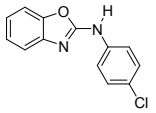
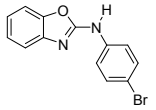
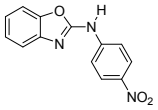
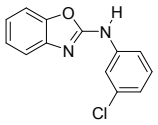
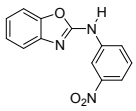
1	H		3a
2	C_6H_5		3b
3			3c
4	4-Cl C_6H_4		3d
5	4-Br C_6H_4		3e
6	4-NO_2 C_6H_4		3f
7	3-Cl C_6H_4		3g
8	3-NO_2 C_6H_4		3h

Compounds were characterized by IR, ^{1}H, ^{13}C NMR, ESI-MS and elemental analysis.

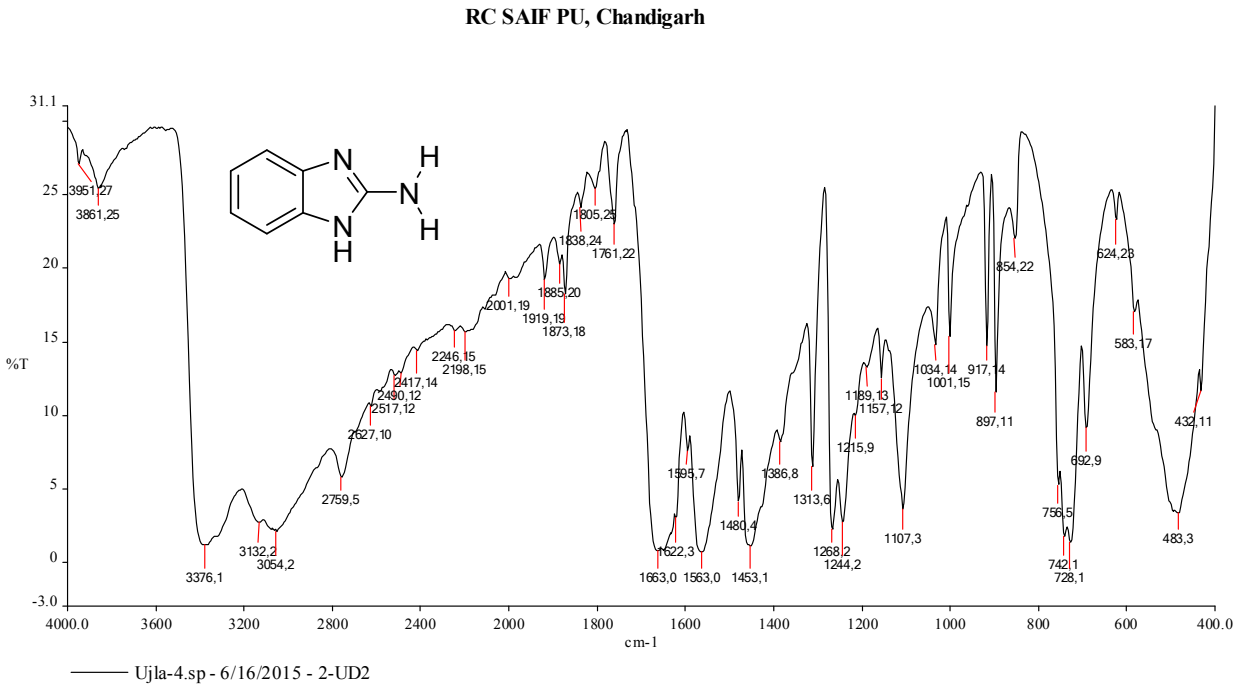
Table S2 Derivatives of 2-amino substituted benzoxazoles (3a'-h')



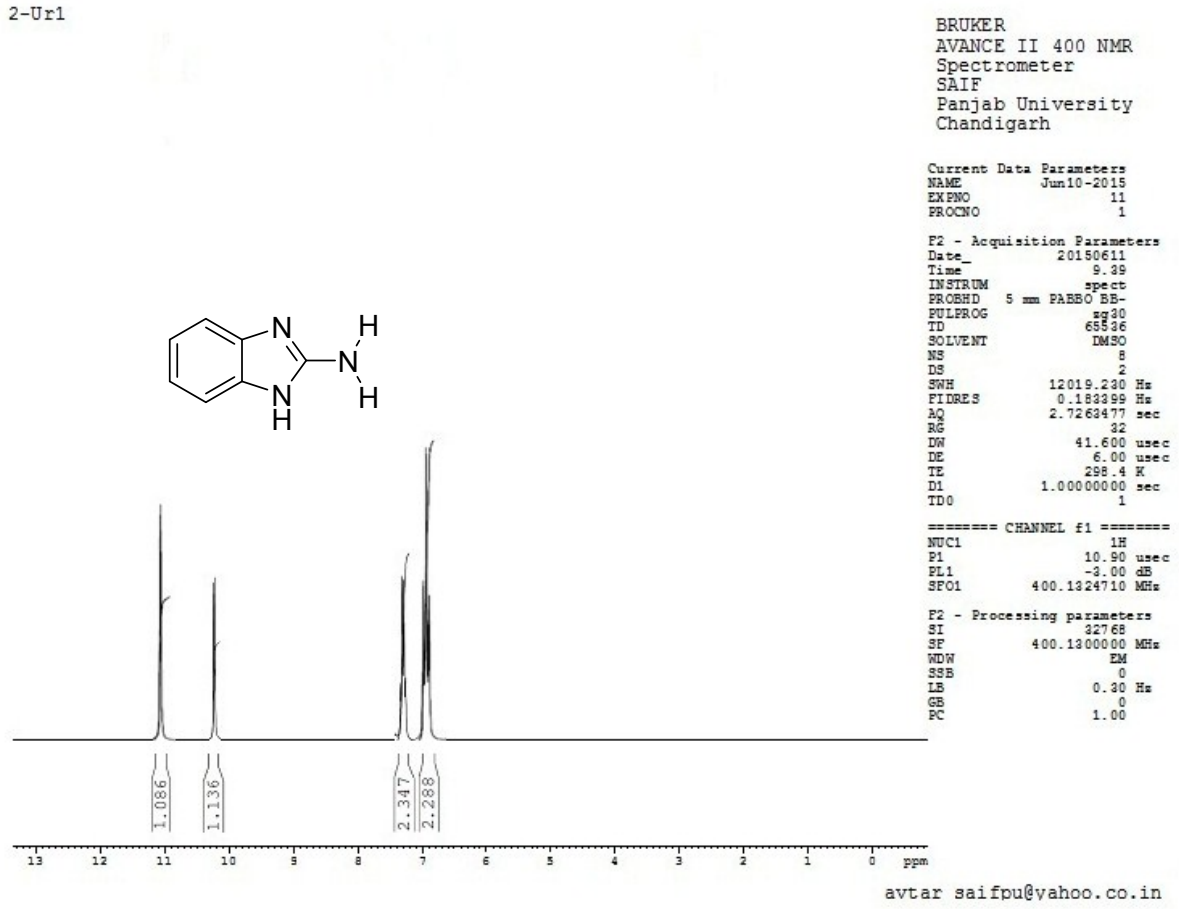
Entry	R'	Product	Product code
1	H		3a'
2	C_6H_5		3b'
3	4-OMe C_6H_4		3c'
4	4-Cl C_6H_4		3d'
5	4-Br C_6H_4		3e'
6	4-NO_2 C_6H_4		3f'
7	3-Cl C_6H_4		3g'
8	3-NO_2 C_6H_4		3h'

Compounds were characterized by IR, ^1H, ^{13}C NMR, ESI-MS and elemental analysis.

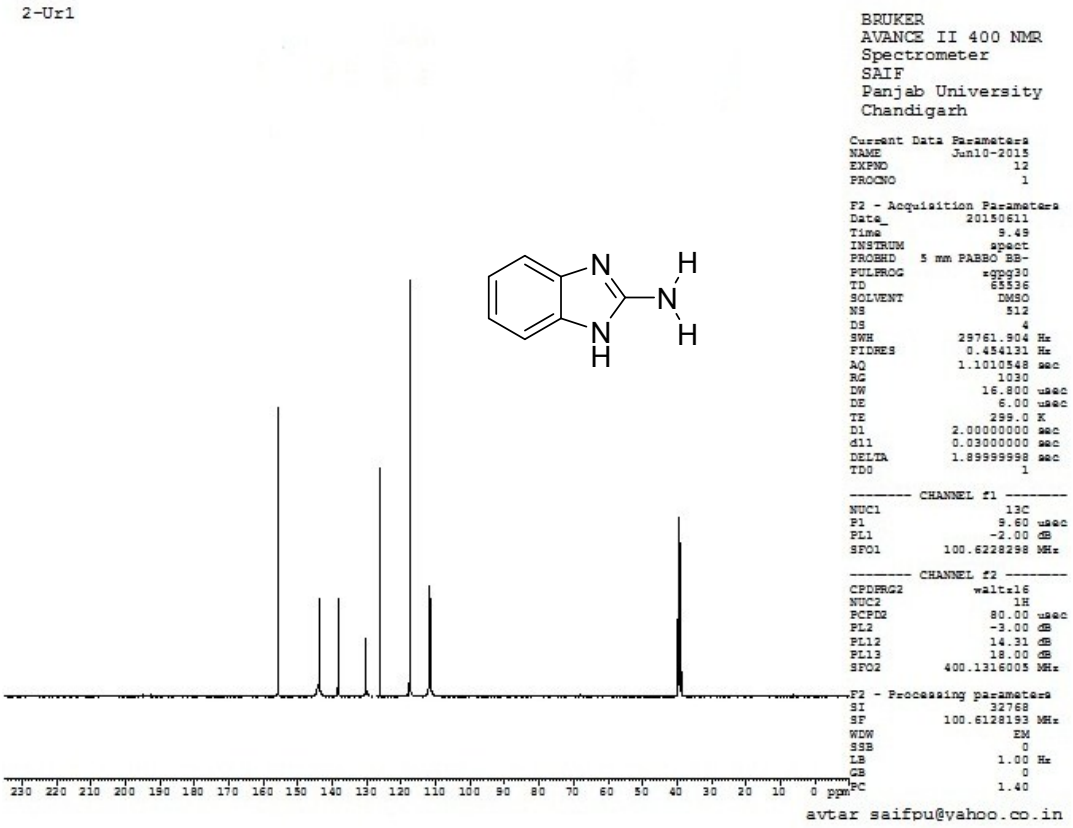
IR of 3a


RC SAIF PU, Chandigarh
%T
cm-1
3951,27
3861,25
3376,1
3132,2
3054,2
2759,5
2627,10
2517,12
2490,12
2417,14
2246,15
2198,15
2001,19
1919,19
1885,20
1873,18
1838,24
1805,25
1761,22
1663,0
1622,3
1595,7
1563,0
1480,4
1453,1
1386,8
1313,6
1268,2
1244,2
1215,9
1189,13
1157,12
1107,3
1034,14
1001,15
917,14
897,11
854,22
756,5
742,1
728,1
692,9
624,28
583,17
483,3
432,11
Ujla-4.sp - 6/16/2015 - 2-UD2

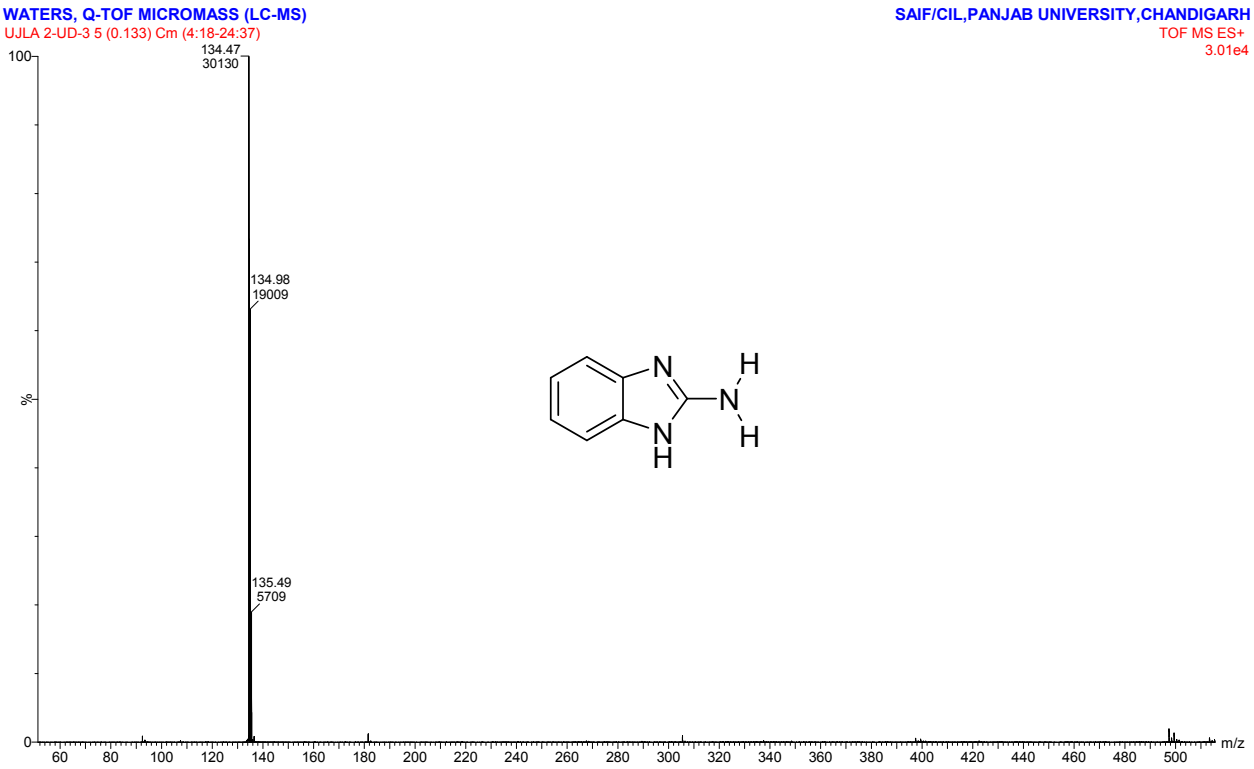
^{1}H NMR of 3a


2-Ur1
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Jun10-2015
EXPNO 11
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150611
Time 9.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 2
SWH 12019.230 Hz
FIDRES 0.183399 Hz
AQ 2.7263477 sec
RG 32
DW 41.600 usec
DE 6.00 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 10.90 usec
PL1 -3.00 dB
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
1.086
1.136
2.347
2.288
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
avtar saifpu@yahoo.co.in

^{13}C NMR of 3a


2-Ur1
BRUKER
AVANCE II 400 NMR
Spectrometer
SAIF
Panjab University
Chandigarh
Current Data Parameters
NAME Jun10-2015
EXPNO 12
PROCNO 1
F2 - Acquisition Parameters
Date_ 20150611
Time 9.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 1030
DW 16.800 usec
DE 6.00 usec
TE 299.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1
-------- CHANNEL f1 --------
NUC1 13C
P1 9.60 usec
PL1 -2.00 dB
SFO1 100.6228298 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -3.00 dB
PL12 14.31 dB
PL13 18.00 dB
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
avtar saifpu@yahoo.co.in

LC-MS of 3a


WATERS, Q-TOF MICROMASS (LC-MS)
UJLA 2-UD-3 5 (0.133) Cm (4:18-24:37)
SAIF/CIL,PANJAB UNIVERSITY,CHANDIGARH
TOF MS ES+
3.01e4
134.47
30130
134.98
19009
135.49
5709
100
%
0
60 80 100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460 480 500
m/z
N
H
N
N
H