Supporting Information

Fe_3O_4 Nanoparticle-Supported Cu(II)-β-Cyclodextrin Complex as a Magnetically Recoverable and Reusable Catalyst for the Synthesis of Symmetrical Biaryls and 1,2,3-Triazoles from Aryl Boronic Acids

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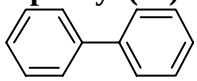
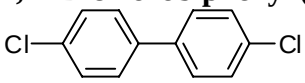
Biphenyl (2a)[2]



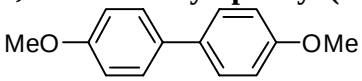
White solid; mp 68-71 °C (lit.[2] mp 67-69°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.60 (4H, d, *J*=7.1 Hz), 7.44 (4H, d, *J*=7.8 Hz), 7.36 (2H, d, *J*=7.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.2, 128.7, 127.2, 127.1; EI-MS: *m/z* 154 (M^+).

4,4´-Dichlorobiphenyl (2b)[2]



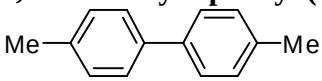
White solid; mp 146-148 °C (lit.[2] mp 149-154 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.45 (4H, d, *J*=8.6 Hz), 7.40 (4H, d, *J*=8.6 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ:138.5, 133.8, 129.1, 128.3; EI-MS: *m/z* 222 (M^+).

4,4´-Dimethoxybiphenyl (2c)[3]



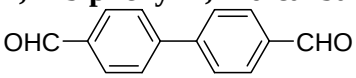
White solid; mp 173-175 °C (lit.[3] mp 173-174 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (4H, d, *J*=8.8 Hz), 6.96 (4H, d, *J*=8.8 Hz), 3.84 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ:158.8, 133.6, 127.8, 114.3, 55.4; EI-MS: *m/z* 214 (M^+).

4,4´-Dimethylbiphenyl (2d)[3]



White solid; mp 118-120 °C (lit.[3] mp 122-124 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.48 (4H, d, *J*=7.9 Hz), 7.24 (4H, d, *J*=7.9 Hz), 2.39 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.4, 136.8, 129.5, 126.9, 21.2; EI-MS: *m/z* 182 (M^+).

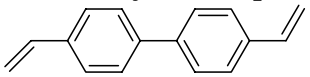
1,1´-biphenyl-4,4´-dicarbaldehyde (2e)[3]



2e

White solid; mp 146-148 °C; (Lit[3] mp 148–150 °C) ^{1}H NMR (400 MHz, $CDCl_3$) δ: 10.12 (2H, s), 8.03 (4H, d, *J*=8 Hz), 7.83 (4H, d, *J*=8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ:191.8, 145.6, 136.0, 130.4, 128.1

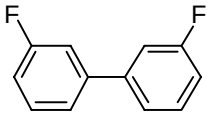
4,4´-Divinyl-1,1´-biphenyl (2f)[4]



2f

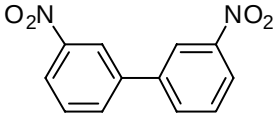
White solid; mp 140-142 (Lit[4] mp 151 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ:7.62 (4H, d, *J*=8.4 Hz), 7.53 (4H, d, *J*=8 Hz), 6.80 (2H, dd, *J*=17.6 Hz, 6.8 Hz), 5.84 (2H, d, *J*=17.6 Hz), 5.33 (2H, d, *J*=10.8 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ:140.1, 136.7, 136.4, 136.4, 127.1, 126.7, 114.0

3,3´-Difluorobiphenyl (2g)[3]



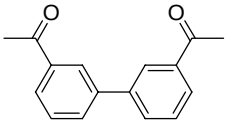
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44-7.34 (4H, m), 7.28-7.24 (2H, m), 7.09-7.04 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.2 (d, *J*=244.6 Hz), 142.3 (dd, *J*=7.7, 2.2 Hz), 130.5 (d, *J*=8.0 Hz), 122.8 (d, *J*=2.9 Hz), 114.8 (d, *J*=21.0 Hz), 114.1 (d, *J*=21.0 Hz); EI-MS: *m/z* 190 (M^+).

3,3´-Dinitrobiphenyl (2h)[3]



Yellow solid; mp 201-202 °C (lit. mp 201-202 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51 (2H, t, *J*=1.9 Hz), 8.31 (2H, dq, *J*=8.2, 1.9 Hz), 7.98 (2H, dq, *J*=8.2, 1.9 Hz), 7.72 (2H, t, *J*=8.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 148.9, 140.3, 133.1, 130.3, 123.3, 122.1; EI-MS: *m/z* 244 (M^+).

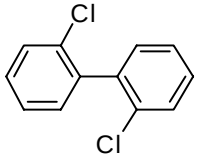
3,3´-Diacetylbiphenyl (2i)



2i

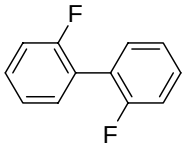
White solid; mp 106-108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.23 (2H, s), 8.00 (2H, d, *J*=7.6 Hz), 7.85 (2H, d, *J*=7.6 Hz), 7.61 (2H, t, *J*=8 Hz), 2.71 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 198.0, 140.8, 137.8, 131.8, 129.3, 127.8, 126.9, 26.8.

2,2´-Dichlorobiphenyl (2j)



White solid; mp 59-62 °C (lit.[2] mp 57-58 °C), ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.47 (2H, m), 7.37-7.33 (4H, m), 7.30-7.26 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.5, 133.6, 131.3, 129.6, 129.2, 126.7; EI-MS: *m/z* 222 (M^+).

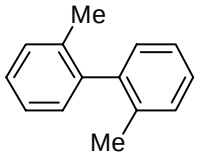
2,2´-Difluorobiphenyl (2k)



2k

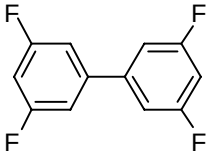
White solid; mp 118-120 °C (Lit[5] mp 117–118 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.45-7.39 (4H, m), 7.29-7.19 (4H, m); ^{13}C NMR (100 MHz, $CDCl_3$) ^{13}C NMR (100 MHz; $CDCl_3$) δ: 159.9 (dd, *J* = 248.6, 13.1 Hz), 131.7 (t, *J*=2.6 Hz), 129.9 (t, *J*=4.0 Hz), 124.2 (d, *J*=2.2 Hz), 115.9 (d, *J*=6.4 Hz), 115.6 (d, *J*=6.4 Hz).

2,2´-Dimethylbiphenyl (2l)[2]



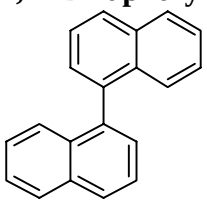
Colorless liquid; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.27–7.20 (6H, m), 7.10 (2H, d, *J*=7.0 Hz), 2.05 (6H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 141.7, 135.9, 129.9, 129.4, 127.2, 125.6, 19.9; EI-MS: *m/z* 182 (M^+).

3,3´-5,5´-Tetrafluorobiphenyl (2m)[5]



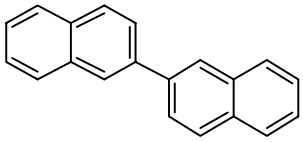
White solid; mp 82-84 °C (lit.[5] mp 85.5-87°); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.09-7.03 (4H, m), 6.87-6.81 (2H, tt, *J*=8.8, 2.3 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.2 (dd, *J* = 247.6, 13.1 Hz), 142.2 (t, *J*=11.9 Hz), 110.3 (d, *J*=26.2 Hz), 103.4 (t, *J*=25.4 Hz); EI-MS: *m/z* 226 (M^+)

1,1´-Binaphthyl (2o)[6]



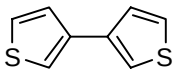
White solid; 142-144 °C (lit.[6] mp 141-143 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.97-7.94 (4H, m), 7.62-7.58 (2H, m), 7.51-7.46 (4H, m), 7.42-7.37 (2H, m), 7.27-7.24 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.5, 133.6, 132.9, 128.2, 128.0, 127.9, 126.6, 125.9, 125.7, 125.5; EI-MS: *m/z* 254 (M^+).

2,2´-Binaphthyl (2p)[7]



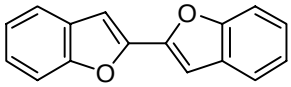
White solid; mp 184-186 °C (lit.[7] mp 188 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.17 (2H, s), 7.97–7.92 (4H, m), 7.90–7.87 (4H, m), 7.54–7.47 (4H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.5, 133.8, 132.8, 128.6, 128.4, 127.8, 126.5, 126.2, 126.1, 125.8; EI-MS *m/z* 254 (M^+).

3,3´-Bithiophene (2q)[8]



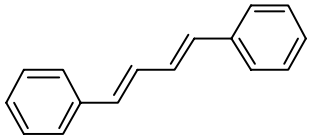
White solid; mp 130-131 °C (lit.[8] mp 130 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39 (2H, d, *J*=1.4 Hz,), 7.38-7.33 (4H, m). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.3, 126.5, 126.2, 119.9; EI-MS *m/z* 166 (M^+).

2,2´-Bibenzofuran (2r)[2]



White solid; mp 197-199 °C (lit.[2] mp 198–200 °C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.65-7.63 (2H, m), 7.56-7.54 (2H, m), 7.35 (2H, dt, *J*=7.3, 1.4 Hz), 7.28 (2H, dt, *J*=7.3, 0.9 Hz), 7.18 (2H, s). ^{13}C NMR (100 MHz, $CDCl_3$) δ:155.2, 147.8, 128.6, 125.2, 123.5, 121.5, 111.4, 103.8; EI-MS *m/z* 234 (M^+).

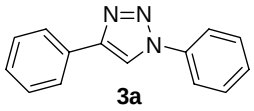
(1*E*,3*E*)-1,4-Diphenylbuta-1,3-diene (2s)[9]



White solid; mp 150-152 °C (lit.[9] mp 151–152°C); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47-7.45 (4H, m), 7.36-7.32 (4H, m), 7.28-7.24 (2H, m), 6.99-6.93 (2H, m), 6.72-6.66 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 137.4, 132.9, 129.3, 128.7, 127.6, 126.5; EI-MS *m/z* 206 (M^+).

Physical and spectroscopic data for the products 3

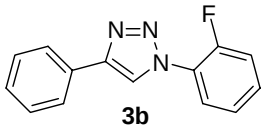
1,4-diphenyl-1H-1,2,3-triazole (3a):



3a

White solid; mp 170-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.27 (s, 1H), 7.95 (d, *J*=7.2 Hz, 2H), 7.83 (d, *J*=7.6 Hz, 2H), 7.58 (t, *J*=8 Hz, 2H), 7.48-7.51 (m, 3H), 7.40 (t, *J*=7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 132.6, 130.2, 129.8, 128.9, 128.8, 128.4, 128.0, 127.8, 125.8, 120.5; HRMS calcd for $C_{14}H_{12}N_3$ (MH^+): 222.1031 Found: 222.1031.

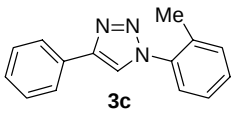
1-(*o*-Fluorophenyl)-4-phenyl-1,2,3-triazole (3b):



3b

White solid; mp 101-102 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (s, 1H), 8.04 (t, *J*=8 Hz, 1H), 7.95 (d, *J*=7.6 Hz, 2H), 7.44-7.51 (m, 3H), 7.34-7.43 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ: 153.2 (d, J_{CP}=249 Hz), 130.1 (d, J_{CP}=8 Hz), 130.1, 128.9, 128.5, 125.9, 125.3 (d, J_{CP}= 4 Hz), 125.3, 124.8, 117.1, 116.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -123.5; HRMS calcd for $C_{14}H_{11}N_3F(MH^+)$: 240.937 Found: 240.938.

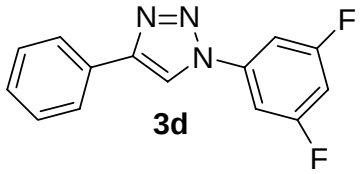
1-(*o*-Methylphenyl)-4-phenyl-1,2,3-triazole (3c): [10]



3c

Viscous oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.00 (1H, s), 7.95 (2H, d, *J*=7.2 Hz), 7.48 (2H, t, *J*=7.2 Hz), 7.46-7.39 (5H, M), 2.32 (1H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.5, 133.8, 131.6, 130.0, 129.0, 128.4, 126.9, 126.0, 125.8, 121.2, 29.7.

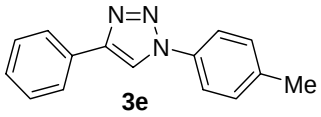
1-(3,5-Difluorophenyl)-4-phenyl-1,2,3-triazole (3d):



3d

White solid; mp 153-155 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.23 (s, 1H), 7.92 (d, *J*=7.6 Hz, 2H), 7.39-7.47 (m, 5H), 6.91-6.96 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 163.4 (dd, J_{CP}=250, 14 Hz), 138.6, 129.6, 129.0, 128.8, 125.9, 118.2, 104.0 (t, J_{CP}=25 Hz), 103.9(d, J_{CP}=20 Hz), 103.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ: -106.0; HRMS calcd for $C_{14}H_{10}N_3F_2$ (MH^+): 258.0843 Found: 258.0843.

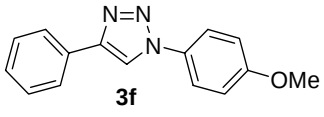
4-Phenyl-1-*p*-tolyl-1H-1, 2, 3-triazole (3e):



3e

White solid, mp 159-160 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.19 (s, 1H), 9.94 (d, *J*=7.2 Hz, 2H), 7.70 (d, J= 7.6 Hz, 2H), 7.49 (t, *J*=7.6 Hz, 2H), 7.36-7.41 (m, 3H), 2.47 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:138.9, 134.4, 130.4, 130.3, 128.9, 128.3, 125.8, 120.4, 117.6, 21.1; HRMS calcd for $C_{15}H_{14}N_3$ (MH^+): 236.1188 Found: 236.1198.

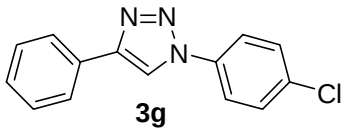
1-(*p*-Methoxyphenyl)-4-phenyl-1, 2, 3-triazole (3f):



3f

White solid, mp167-168 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.16 (s, 1H), 7.94 (d, *J*=7.6, 2H), 7.72 (d, *J*=8.8 Hz, 2H), 7.49 (t, *J*=7.2 Hz, 2H), 7.39 (t, *J*=7.2 Hz, 1H), 7.07 (d, *J*=8.6 Hz, 2H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.8, 130.4, 128.6, 128.3, 125.8, 122.4, 114.8, 55.6; HRMS calcd for $C_{15}H_{14}N_3O$ (MH^+): 252.1137 Found: 252.1143.

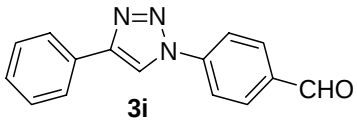
1-(*p*-Chlorophenyl)-4-phenyl-1,2,3-triazole (3g):



3g

White solid; mp 185-186 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ: 9.35 (s, 1H), 8.01 (d, *J*=8.8 Hz, 2H), 7.95 (d, *J*=7.2 Hz, 2H), 7.73 (d, *J*=8.8 Hz, 2H), 7.52 (t, *J*=7.6 Hz, 2H), 7.40 (t, *J*=7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ: 147.9, 135.9, 133.4, 130.5, 130.4, 129.3, 128.8, 125.8, 122.1, 120.1; HRMS calcd for $C_{14}H_{11}N_3Cl$ (MH^+): 256.0642 Found: 256.0642.

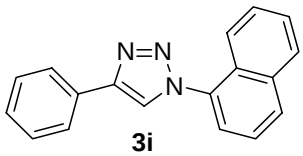
4-(4-phenyl-1H-1,2,3-triazol-1-yl)benzaldehyde (3h):



3i

Yellow solid; mp 220-221 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ: 10.10 (s, 1H), 9.49 (s, 1H), 8.24 (d, *J*=8.8 Hz, 2H), 8.18 (d, *J*=8.4 Hz, 2H), 7.97 (d, *J*= 7.6 Hz, 2H), 7.53 (t, *J*=8 Hz, 2H), 7.42 (t, *J*=7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ: 192.6, 148.1, 140.9, 136.1, 131.8, 130.4, 129.5, 128.9, 125.8, 120.6, 120.2; HRMS calcd for $C_{15}H_{12}N_3O$ (MH^+): 250.980 Found: 250.980.

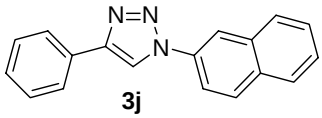
1-(α-Naphthyl)-4-phenyl-1,2,3-triazole (3i): [11]



3i

Viscous oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ:8.18 (1H, s), 8.06 (1H, d, *J*=8 Hz), 8.00 (3H, d, *J*=7.2 Hz), 7.73 (1H, d, *J*=8.4 Hz), 7.67-7.56 (4H, m), 7.51 (2H, t, *J*=7.2 Hz), 7.42 (1H, t, *J*=7.2 Hz); ^{13}C NMR (100 MHz, $CDCl_3$) δ:147.8, 134.2, 133.7, 130.5, 130.3, 129.0, 128.6, 128.5, 128.3, 128.0, 127.1, 125.9, 125.1, 123.6, 122.4, 122.3.

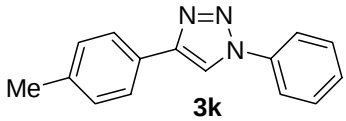
1-(β-Naphthyl)-4-phenyl-1,2,3-triazole (3j):



3j

White solid; mp 205-207 °C; ^{1}H NMR (400 MHz, DMSO-d6) δ: 9.48 (s, 1H), 8.55 (s, 1H), 8.21 (d, *J*=8.8 Hz, 2H), 8.05-8.16 (m, 2H), 8.06 (d, *J*=7.6 Hz, 2H), 7-61-7.68 (m, 2H), 7.53 (t, *J*=7.6 Hz, 2H), 7.41 (t, *J*=7.2 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d6) δ: 147.9, 134.5, 133.3, 132.8, 130.7, 130.4, 129.5, 128.7, 128.7, 128.4, 128.0, 127.4, 125.8, 120.2, 119.0, 118.0; HRMS calcd for $C_{18}H_{14}N_3$ (MH^+): 272.1188 Found: 272.1183.

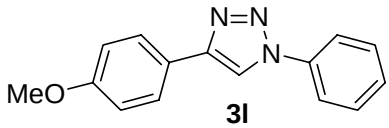
1-Phenyl-4-*p*-tolyl-1,2,3-triazole (3k):



3k

White solid; mp 171-172 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.19 (s, 1H), 7.83 (m, 4H), 7.57 (t, *J*=8 Hz, 2H), 7.48 (t, *J*=7.6, 1H), 7.30 (d, *J*=9.2 Hz, 2H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 138.3, 129.8, 129.6, 128.7, 127.4, 125.7, 120.5, 117.2, 21.3; HRMS calcd for $C_{15}H_{14}N_3$ (MH^+): 236.1188 Found: 236.1186.

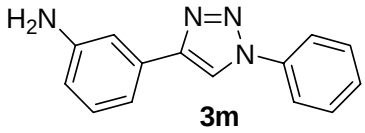
1-Phenyl-4-*p*-methoxyphenyl-1,2,3-triazole (3l): [12]



3l

White solid; mp 155–157 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.15 (1H, s), 7.87 (2H, d, *J* = 8.4 Hz), 7.81 (2H, d, *J*=7.6 Hz), 7.57 (2H, t, *J*=7.6 Hz), 7.48 (1H, t, *J*=7.6 Hz), 7.02 (2H, d, *J*=8.4 Hz), 3.89 (3H, s); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 159.8, 148.4, 137.2, 129.8, 128.7, 127.2, 123.0, 120.5, 116.8, 114.4, 55.4.

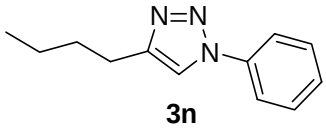
1-Phenyl-4-(*m*-aminophenyl)-1,2,3-triazole (3m):



3m

Yellow solid; mp 122-125 °C, ^{1}H NMR (400 MHz, acetone-d6) δ: 8.86 (s, 1H), 7.98 (d, *J*=8 Hz, 2H), 7.64 (t, *J*=7.6 Hz, 2H), 7.52 (t, *J*=7.6, 1H), 7.38 (d, *J*=1.6 Hz, 1H), 7.15-7.22 (m, 2H), 6.71 (dd, *J*=7.2, 1.2 Hz, 1H), 4.70-4.90 (br, 2H); ^{13}C NMR (100 MHz, acetone-d6) δ: 148.9, 148.55, 137.4, 131.4, 129.8, 129.4, 128.4, 120.0, 118.2, 114.2, 114.2, 111.3; HRMS calcd for $C_{14}H_{13}N_4$ (MH^+): 237.1140 Found: 237.1132.

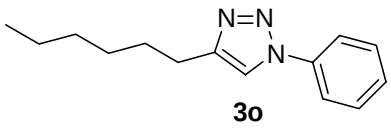
1-Phenyl-4-butyl-1,2,3-triazole (3n):



3n

White solid; mp 44-46 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (s, 1H), 7.67 (d, *J*= 8Hz, 2H), 7.43 (t, *J*=8 Hz, 2H), 7.33 (t, *J*=7.2 Hz, 1H), 2.74 (t, *J*=7.2 Hz, 2H), 1.65-1.68 (m, 2H), 1.34-1.37 (m, 2H), 0.90 (t, *J*=6.4, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 136.4, 130.1, 130.0, 129.4, 123.1, 128.8, 30.8, 24.2, 22.2, 13.7; HRMS calcd for $C_{12}H_{16}N_3$ (MH^+): 202.1344 Found: 202.1350.

1-Phenyl-4-hexyl-1,2,3-triazole (3o):



3o

White solid; mp 40-42 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.77 (s, 1H), 7.35 (d, *J*=7.6 Hz, 2H), 7.50 (t, *J*=7.2 Hz, 2H), 7.40 (t, *J*=7.2 Hz, 1H), 2.79 (t, *J*= 7.2 Hz, 2H), 1.70-1.78 (m, 2H), 1.32-1.40 (m, 6H), 0.89 (t, *J*= 6.8 Hz, 3H), ^{13}C NMR (100 MHz, $CDCl_3$) δ:137.3, 129.6, 128.3, 120.3, 118.8, 31.6, 29.3, 28.9, 25.6, 22.5, 14.7; HRMS calcd for $C_{14}H_{20}N_3$ (MH^+): 230.1657 Found: 230.1658.

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