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SUPPLEMENTARY MATERIAL TO

Efficient one-pot, four-component synthesis of *N,N*-dibenzyl--1-(5-aryl-1,3,4-oxadiazol-2-yl)cyclobutylamine derivatives from the reaction of (isocyanoimino)triphenylphosphorane, dibenzylamine, an aromatic carboxylic acid and cyclobutanone

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

N,N-*Dibenzyl-1-(5-phenyl-1,3,4-oxadiazol-2-yl)cyclobutylamine* ***(5a)***. Yellow crystal, Yield: 81 %; m.p. 99.8–102.6 °C; Anal. Calcd. for $C_{26}H_{25}N_3O$: C, 78.96; H, 6.37; N, 10.62 %. Found: C, 79.04; H, 6.42; N, 10.58 %; IR (KBr, cm^{-1}): 1554, 1447, 1363, 1257, 1076, 750, 698; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.71–1.92 (2H, *m*, cyclobutane), 2.17–2.38 (2H, *m*, cyclobutane), 2.40–2.61 (2H, *m*, cyclobutane), 3.65 (4H, *s*, $2CH_2$ of benzyl), 7.12–8.18 (15H, *m*, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.47 and 33.05 ($3CH_2$, cyclobutane), 53.85 ($2CH_2$ of benzyl), 62.66 (C_{ipso}, cyclobutane), 124.09, 126.88, 126.95, 128.01, 129.00, 129.12, 131.74 and 139.65 (aromatic carbons), 165.47 and 168.55 (2C=N); MS, *m*/*z* (%): 395 (M^+, 7), 304 (69), 276 (29), 250 (17), 196 (9), 173 (12), 130 (9), 91 (100), 65 (13), 41 (2).

N,N-*Dibenzyl-1-[5-(2-thienyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* ***(5b)***. Yellow crystal, yield: 85 %; m.p. 57.6–59.8 °C; Anal. Calcd. for $C_{24}H_{23}N_3OS$: C, 71.79; H, 5.77; N, 10.47 %. Found: C, 71.72; H, 5.79; N, 10.53 %; IR (KBr, cm^{-1}): 1553, 1450, 1363, 1254, 1075, 749, 696; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / / ppm): 1.70–2.04 (2H, *m*, cyclobutane), 2.15–2.40 (2H, *m*, cyclobutane), 2.42––2.62 (2H, *m*, cyclobutane), 3.65 (4H, *s*, $2CH_2$ of benzyl), 7.05–7.87 (13H, *m*, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.44 and 33.02 ($3CH_2$, cyclobutane), 53.88 ($2CH_2$ of benzyl), 62.67 (C_{ipso}, cyclobutane), 125.51 (C_{ipso}, thiophene), 126.86, 127.98, 128.16, 128.97, 129.68, 130.05 and 139.62 (aromatic carbons), 161.24 and 167.97 (2C=N); MS, *m*/*z* (%): 401 (M^+, 2), 310 (51), 282

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(29), 264 (6), 196 (10), 173 (18), 149 (7), 132 (12), 106 (38), 91(100), 65 (21), 41 (6).

N,N-*Dibenzyl-1-[5-(4-chlorophenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* ***(5c)***. Yellow crystal, yield: 80 %; m.p. 89.0–91.5 °C; Anal. Calcd. for $C_{26}H_{24}ClN_3O$: C, 72.63; H, 5.63; N, 9.77 %. Found: C, 72.70; H, 5.58; N, 9.70 %; IR (KBr, cm^{-1}): 1541, 1452, 1363, 1257, 1076, 748, 696; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.75–1.92 (2H, *m*, cyclobutane), 2.23–2.40 (2H, *m*, cyclobutane), 2.42–2.58 (2H, *m*, cyclobutane), 3.67 (4H, *s*, $2CH_2$ of benzyl), 6.98––7.38 (10H, *m*, aromatic CH), 7.54 (2H, *d*, $^3J_{HH}$ = 8.0 Hz, aromatic CH), 8.02 (2H, *d*, $^3J_{HH}$ = 8.0 Hz, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.39 and 32.98 ($3CH_2$, cyclobutane), 53.76 ($2CH_2$ of benzyl), 62.67 (C_{ipso}, cyclobutane), 122.62, 126.89, 128.00, 128.20, 128.94, 129.46, 137.91 and 139.51 (aromatic carbons), 164.20 and 168.88 (2C=N); MS, *m*/*z* (%): 429 (M^+, 2), 338 (59), 310 (39), 290 (7), 263(5), 196 (13), 173(22), 149 (10), 130 (12), 91 (100), 65 (17), 41 (4).

N,N-*Dibenzyl-1-[5-(3-chlorophenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* ***(5d)***. Yellow crystal, yield: 83 %; m.p. 131.1–133.2 °C; Anal. Calcd. for $C_{26}H_{24}ClN_3O$: C, 72.63; H, 5.63; N, 9.77 %. Found: C, 72.57; H, 5.67; N, 9.70 %; IR (KBr, cm^{-1}): 1551, 1438, 1364, 1259, 1080, 749, 696; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.72–1.96 (2H, *m*, cyclobutane), 2.22–2.43 (2H, *m*, cyclobutane), 2.45–2.61 (2H, *m*, cyclobutane), 3.68 (4H, *s*, $2CH_2$ of benzyl), 7.03––8.09 (14H, *m*, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.39 and 32.99 ($3CH_2$, cyclobutane), 53.76 ($2CH_2$ of benzyl), 62.68 (C_{ipso}, cyclobutane), 125.04, 125.75, 126.90, 128.00, 128.90, 128.94, 130.44, 131.68, 135.19 and 139.48 (aromatic carbons), 163.72 and 169.07 (2C=N).

N,N-*Dibenzyl-1-[5-(4-bromophenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* ***(5e)***. Yellow crystal, yield: 82 %; m.p. 121.3–123.1 °C; Anal. Calcd. for $C_{26}H_{24}BrN_3O$: C, 65.83; H, 5.10; N, 8.86 %. Found: C, 65.89; H, 5.13; N, 8.83 %; IR (KBr, cm^{-1}): 1563, 1452, 1361, 1257, 1080, 758, 703; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.81–1.98 (2H, *m*, cyclobutane), 2.28–2.48 (2H, *m*, cyclobutane), 2.52–2.68 (2H, *m*, cyclobutane), 3.73 (4H, *s*, $2CH_2$ of benzyl), 7.12––7.98 (10H, *m*, aromatic CH), 8.01 (2H, *d*, $^3J_{HH}$ = 8.5 Hz, aromatic CH), 8.19 (2H, *d*, $^3J_{HH}$ = 8.5 Hz, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.47 and 33.07 ($3CH_2$, cyclobutane), 53.96 ($2CH_2$ of benzyl), 62.78 (C_{ipso}, cyclobutane), 123.31, 126.87, 127.13, 128.00, 129.00, 129.08, 132.88 and 139.69 (aromatic carbons), 165.22 and 168.72 (2C=N).

N,N-*Dibenzyl-1-[5-(4-fluorophenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* ***(5f)***. Yellow crystal, yield: 80%; m.p. 91.3–93.5 °C; Anal. Calcd. for $C_{26}H_{24}FN_3O$: C, 75.52; H, 5.85; N, 10.16. Found: C, 75.50; H, 5.89; N, 10.12; IR (KBr, cm^{-1}): 1560, 1497, 1364, 1235, 1067, 745, 697; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.76–1.95 (2H, *m*, cyclobutane), 2.26–2.44 (2H, *m*, cyclobu-

tane), 2.46–2.61 (2H, *m*, cyclobutane), 3.68 (4H, *s*, $2CH_2$ of benzyl), 7.02–7.45 and 8.05–8.16 (14H, 2*m*, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.39 and 32.99 ($3CH_2$, cyclobutane), 53.82 ($2CH_2$ of benzyl), 62.68 (C_{ipso}, cyclobutane), 116.41 (2CH of aromatic carbons, *d*, $^2J_{CF}$ = 22.5 Hz), 120.52 (C, *d*, aromatic ,$^4J_{CF}$ =3.6 Hz), 126.88, 127.99, 128.94 and 139.56 (aromatic carbons), 129.19 (2CH of aromatic carbons, *d*, $^3J_{CF}$ = 8.1 Hz), 164.58 (C, *d*, aromatic, $^1J_{CF}$ = 231.1 Hz), 164.20 and 168.70 (2C=N).

N,N-*Dibenzyl-1-[5-(4-methylphenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* (***5g***). Yellow crystal, yield: 82 %; m.p. 55.5–57.9 °C; Anal. Calcd. for $C_{27}H_{27}N_3O$: C, 79.19; H, 6.65; N, 10.26 %. Found: C, 79.24; H, 6.62; N, 10.29 %; IR (KBr, cm^{-1}): 1560, 1454, 1364, 1258, 1078, 747, 696; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.75–1.91 (2H, *m*, cyclobutane), 2.22–2.62 (4H, *2m*, cyclobutane), 2.47 (3H, *s*, CH_3), 3.67 (4H, *s*, $2CH_2$ of benzyl), 7.12–7.45 (10H, *m*, aromatic CH), 7.33 (2H, *d*, $^3J_{HH}$ = 8.0 Hz, aromatic CH), 7.99 (2H, *d*, $^3J_{HH}$ = 8.0 Hz, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.44 and 33.03 ($3CH_2$, cyclobutane), 21.66 (CH_3), 53.95 ($2CH_2$ of benzyl), 62.71 (C_{ipso}, cyclobutane), 121.42, 126.83, 126.90, 127.97, 128.98, 129.78, 139.73 and 142.17 (aromatic carbons), 165.16 and 168.28 (2C=N).

N,N-*Dibenzyl-1-[5-(3-methylphenyl)-1,3,4-oxadiazol-2-yl]cyclobutylamine* (***5h***). Yellow crystal, yield: 81 %; m.p. 100.1–102.3 °C; Anal. Calcd. for $C_{27}H_{27}N_3O$: C, 79.19; H, 6.65; N, 10.26 %. Found: C, 79.25; H, 6.67; N, 10.22; IR (KBr, cm^{-1}): 1556, 1454, 1363, 1255, 1071, 750, 695; ^{1}H-NMR (250 MHz, $CDCl_3$, δ / ppm): 1.72–1.92 (2H, *m*, cyclobutane), 2.23–2.61 (4H, *2m*, cyclobutane), 2.49 (3H, *s*, CH_3), 3.67 (4H, *s*, $2CH_2$ of benzyl), 7.12–7.50 and 7.85––7.96 (14H, *2m*, aromatic CH); ^{13}C-NMR (62.5 MHz, $CDCl_3$, δ / ppm): 14.45 and 33.03 ($3CH_2$, cyclobutane), 21.40 (CH_3), 53.97 ($2CH_2$ of benzyl), 62.72 (C_{ipso}, cyclobutane), 124.03, 124.09, 126.85, 127.46, 127.97, 128.40, 128.98, 132.48, 138.97 and 139.70 (aromatic carbons), 165.17 and 168.47 (2C=N).