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SUPPLEMENTARY MATERIAL TO

Microwave-assisted synthesis of 1*H*-tetrazole-based flavonoid derivatives and their antimicrobial activity

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CHARACTERIZATION DATA

*(*E*)-3-(4-(1*H*-tetrazol-5-yl)phenyl)-1-(2-hydroxyphenyl)prop-2-en-1-one* (**4a**). Anal. Calcd. for $C_{16}H_{12}N_4O_2$: C, 65.78; H, 4.15; N, 19.18 %. Found: C, 65.75; H, 4.14; N, 19.17 %; IR (KBr, cm^{-1}): 3595*w* (OH), 3498*w* (NH), 1641*s* (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 12.41 (1H, *s*, OH), 8.27 (1H, *d*, J = 7.03 Hz, Ar-H), 8.18–8.14 (5H, *m*, Ar-H & H_β), 7.89 (1H, *d*, J = 15.56 Hz, H_α), 7.59 (*t*, 1H, J = 7.03 Hz, Ar-H), 7.05–7.01 (2H, *m*, Ar-H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 193.4, 161.7, 143.1, 137.0, 136.4, 130.9, 130.0, 127.3, 125.9, 123.6, 120.8, 119.2, 117.7; MS-ESI (*m*/*z*): 293 $(M+H)^+$ (100 %).

*(*E*)-1-(5-Fluoro-2-hydroxyphenyl)-3-(4-(1*H*-tetrazol-5-yl)phenyl)-prop-2-en--1-one (**4b**)*. Anal. Calcd. for $C_{16}H_{11}FN_4O_2$: C, 61.95; H, 3.58; N, 18.07 %. Found: C, 61.93; H, 3.57; N, 18.06 %; IR (KBr, cm^{-1}): 3539*w* (OH), 3473*w* (NH), 1641*s* (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 12.26 (1H, *s*, OH), 8.18–8.10 (6H, *m*, Ar-H & H_β), 7.88 (1H, *d*, J = 15.41 Hz, H_α), 7.41 (1H, *d*, J = 8.44 Hz, Ar-H), 6.92 (1H, *d*, J = 8.44 Hz, Ar-H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 192.4, 157.7, 154.7 (*d*, ^1J = 234 Hz), 143.7, 136.6, 129.9, 127.3, 126.5, 123.5, 121.2, 119.1, 115.8 (*d*, ^2J = 23.9 Hz); MS-ESI (*m*/*z*): 311 $(M+H)^+$ (100 %).

*(*E*)-1-(5-Chloro-2-hydroxyphenyl)3-(4-(1*H*-tetrazol-5-yl)phenyl)-prop-2-en--1-one (**4c**)*. Anal. calcd. for $C_{16}H_{11}ClN_4O_2$: C, 58.85; H, 3.41; N, 17.12 %. Found: C, 58.82; H, 3.39; N, 17.15 %; IR (KBr, cm^{-1}): 3537*w* (OH), 3475*w* (NH), 1643*s* (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 12.33 (1H, *s*, OH), 8.32–8.04 (6H, *m*, Ar-H & H_β), 7.82 (1H, *d*, J = 15.00 Hz, H_α), 7.65 (1H, *d*, J = 7.78 Hz, Ar-H), 6.96 (1H, *d*, J = 7.78 Hz, Ar-H); ^{13}C-NMR (100 MHz,

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DMSO-d_6, δ / ppm): 188.4, 142.8, 138.0, 137.7, 134.4, 133.9, 131.9, 131.2, 130.9, 129.4, 127.7, 126.7, 124.0, 122.7; MS-ESI: (*m*/*z*) 327 $(M+H)^+$ (100 %).

*(*E*)-1-(2-Hydroxy-5-methylphenyl)3-(4-(1*H*-tetrazol-5-yl)phenyl)-prop-2-en--1-one* ***(4d)***. Anal. Calcd. for $C_{17}H_{14}N_4O_2$: C, 66.68; H, 4.63; N, 18.31 %. Found: C, 66.66; H, 4.61; N, 18.29 %; IR (KBr, cm^{-1}): 3473*w* (OH), 3361*w* (NH), 1643*s* (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 12.26 (1H, *s*, OH), 8.18–8.10 (6H, *m*, Ar-H & H_β), 7.88 (1H, *d*, *J* = 15.41 Hz, H_α), 7.41 (1H, *d*, *J* = 8.44 Hz, Ar-H), 6.92 (1H, *d*, *J* = 8.44 Hz, Ar-H), 2.34 (3H, *s*, CH_3); ^{13}C--NMR (100 MHz, DMSO-d_6, δ / ppm): 193.3, 159.8, 143.1, 137.4, 136.9, 131.4, 130.4, 129.9, 128.0, 127.3, 126.0, 123.5, 120.3, 117.5, 19.9; MS-ESI (*m*/*z*) 307 $(M+H)^+$ (100 %).

*(*E*)-1-(5-Bromo-2-hydroxyphenyl)3-(4-(1*H*-tetrazol-5-yl)phenyl)-prop-2-en--1-one* ***(4e)***. Anal. Calcd. for $C_{16}H_{11}BrN_4O_2$: C, 51.79; H, 3.00; N, 15.11 %. Found: C, 51.77; H, 2.99; N, 15.09 %; IR (KBr, cm^{-1}): 3543*w* (OH), 3361*w* (NH), 1639*s* (C=O); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 12.21 (1H, *s*, OH), 8.26–8.08 (6H, *m*, Ar-H & H_β), 7.87 (1H, *d*, *J* = 15.41 Hz, H_α), 7.59 (1H, *d*, *J* = 8.80 Hz, Ar-H), 7.05 (1H, *d*, *J* = 8.80 Hz, Ar-H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 189.9, 156.5, 139.7, 134.0, 133.6, 127.0, 126.6, 124.7, 124.0, 122.7, 120.1, 117.0, 114.1; MS-ESI (*m*/*z*): 371 $(M+H)^+$ (100 %).

*(*Z*)-2-(4-(1*H*-Tetrazol-5-yl)benzylidene)benzofuran-3(2*H*)-one* ***(5a)***. Anal. Calcd. for $C_{16}H_{10}N_4O_2$: C, 66.23; H, 3.49; N, 19.32 %. Found: C, 66.20; H, 3.47; N, 19.30 %; IR (KBr, cm^{-1}): 3353*w* (NH), 1681*s* (C=O), 1135*s* (C–O–C); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 8.05 (2H, *d*, *J* = 7.78 Hz, Ar-H), 7.64 (2H, *d*, *J* = 7.78 Hz, Ar-H), 7.31 (1H, *d*, *J* = 7.53 Hz, Ar-H), 7.24 (1H, *d*, *J* = 7.53 Hz, Ar-H), 6.93–6.88 (2H, *m*, benzylidene & Ar-H); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 177.7, 157.9, 141.3, 132.7, 128.4, 127.6, 125.9, 121.3, 119.2, 117.8, 114.5, 106.8, 104.4; MS-ESI (*m*/*z*): 291 $[M+H]^+$ (100 %).

*(*Z*)-5-Fluoro-2-(4-(1*H*-tetrazol-5-yl)benzylidene)-benzofuran-3(2*H*)-one* ***(5b)***. Anal. Calcd. for $C_{16}H_9FN_4O_2$: C, 62.36; H, 2.96; N, 18.19 %. Found: C, 62.34; H, 2.94; N, 18.17 %; IR (KBr, cm^{-1}): 3400*w* (NH), 1682*s* (C=O), 1049*s* (C–O–C); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 7.99 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.74 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.49–7.32 (3H, *m*, Ar-H), 6.85 (1H, *s*, benzylidene); ^{13}C-NMR (100 MHz, DMSO-d_6, ppm): 175.1, 156.6 (*d*, ^1J = 228.3 Hz),138.8, 130.2, 125.9, 125.0, 123.4, 118.8, 118.7, 116.6, 115.3, 112.0, 104.3, 101.0; MS-ESI (*m*/*z*): 309 $[M+H]^+$ (100 %).

*(*Z*)-5-Chloro-2-(4-(1*H*-tetrazol-5-yl)benzylidene)-benzofuran-3(2*H*)-one* ***(5c)***. Anal. Calcd. for $C_{16}H_9ClN_4O_2$: C, 59.23; H, 2.82; Cl, 10.95; N, 17.27 %. Found: C, 59.18; H, 2.79; Cl, 10.92; N, 17.25. IR (KBr, cm^{-1}): 3318*w* (NH), 1670*s* (C=O), 1057*s* (C–O–C); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 8.20 (2H, *d*, *J* = 8.28 Hz, Ar-H), 8.14 (2H, *d*, *J* = 8.28 Hz, Ar-H), 7.50–7.32 (3H, *m*, Ar-H), 6.85 (1H, *s*, benzylidene); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 175.6,

165.4, 155.8, 151.0, 138.7, 134.4, 133.4, 131.9, 127.4, 125.2, 123.8, 120.3, 112.8, 110.4; Mass spectrum: ESI (*m/z*): 325 $[M+H]^+$ (100 %).

*(Z)-5-Methyl-2-(4-(1*H*-tetrazol-5-yl)benzylidene)benzofuran-3(2*H*)-one(**5d**)*. Anal. Calcd. for $C_{17}H_{12}N_4O_2$: C, 67.12; H, 3.99; N, 18.44 %. Found: C, 67.10; H, 3.97; N, 18.41 %; IR (KBr, cm^{-1}): 3347*w* (NH), 1679*s* (C=O), 1134*s* (C–O–C); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 8.06 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.81 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.53–7.45 (3H, *m*, Ar-H), 6.90 (1H, *s*, benzylidene), 2.33 (3H, *s*, CH_3); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 183.6, 163.9, 147.3, 138.7, 134.4, 133.6, 131.9, 127.3, 125.2, 123.8, 120.5, 112.8, 110.4, 20.1; MS-ESI (*m/z*): 305 $[M+H]^+$ (100 %).

*(Z)-5-Bromo-2-(4-(1*H*-tetrazol-5-yl)benzylidene)benzofuran-3(2*H*)-one (**5e**)*. Anal. Calcd. for $C_{16}H_9BrN_4O_2$: C, 52.07; H, 2.48; N, 15.20 %. Found: C, 52.05; H, 2.46; N, 15.18 %; IR (KBr, cm^{-1}): 3423*w* (NH), 1683*s* (C=O), 1133*s* (C–O–C); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 7.99 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.59 (2H, *d*, *J* = 8.53 Hz, Ar-H), 7.48–7.35 (3H, *m*, Ar-H), 6.85 (1H, *s*, benzylidene); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 184.0, 164.3, 147.7, 139.0, 134.8, 133.9, 132.3, 127.6, 125.5, 124.2, 120.9, 113.2, 110.8; MS-ESI (*m/z*): 369 $[M+H]^+$ (100 %).