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SUPPLEMENTARY MATERIAL TO

Synthesis and antioxidant activity study of pyrazoline carrying an arylfuran/arylthiophene moiety

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

1-(4-Methylphenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one ***(2a)***. Mol. Form.: $C_{20}H_{15}NO_4$ (*FW*: 333.3); *m.p.*: 149–150 °C (Lit. 148–150 °C[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.56 (1H, *d*, *J* = 15.3 Hz, H-3), 6.83 (1H, *d*, *J* = 15.3 Hz, H-2), 7.0–8.2 (8H, *m*, Ar-H), 6.2 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4), 2.4 (3H, *s*, CH_3).

1-(4-Methoxyphenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one ***(2b)***. Mol. Form.: $C_{20}H_{15}NO_5$ (*FW*: 349.3); *m.p.*: 163–165 °C (Lit. 165–166[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.63 (1H, *d*, *J* = 15.3 Hz, H-3), 6.71 (1H, *d*, *J* = 15.3 Hz, H-2), 6.9–8.1 (8H, *m*, Ar-H), 6.3 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4) 3.8 (3H, *s*, OCH_3).

1-(4-Chlorophenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one ***(2c)***. Mol. Form.: $C_{19}H_{12}ClNO_4$; (*FW*: 353.7); *m.p.*: 155 °C (Lit. 156–157 °C[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.68 (1H, *d*, *J* = 15.4 Hz, H-3), 6.93 (1H, *d*, *J* = 15.4 Hz, H-2), 7.3–8.2 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4).

1-(2,4-Dichlorophenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one ***(2d)***. Mol. Form.: $C_{19}H_{11}Cl_2NO_4$ (*FW*: 388.2); *m.p.*: 157 °C (Lit. 157–158 °C[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.71 (1H, *d*, *J* = 15.5 Hz, H-3), 7.02 (1H, *d*, *J* = 15.5 Hz, H-2), 7.3–8.0 (7H, *m*, Ar-H), 6.2 (1H, *d*, *J* = 3.6Hz, furan H-3), 6.7 (1H, *d*, *J* = 3.6 Hz, furan H-4).

1-(4-Hydroxyphenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one ***(2e)***. Mol. Form.: $C_{19}H_{13}NO_5$ (*FW*: 335.3); *m.p.*: 152–153 °C (Lit. 152–154 °C[2]); ^{1}H-

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NMR (400 MHz, $CDCl_3$, δ / ppm): 6.64 (1H, *d*, *J* = 15.5 Hz, H-3), 7.12 (1H, *d*, *J* = 15.5 Hz, H-2), 7.3–8.0 (8H, *m*, Ar-H), 5.8 (1H, *s*, OH), 6.3 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4).

1-(4-Nitrophenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one (***2f***). Mol. Form.: $C_{19}H_{12}N_2O_6$ (*FW*: 364.3); *m.p.*: 205 °C (Lit. 205–206 °C[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.71 (1H, *d*, *J* = 15.3 Hz, H-3), 7.12 (1H, *d*, *J* = 15.3 Hz, H-2), 7.1–8.2 (8H, *m*, Ar-H), 6.6 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz furan H-4).

1-(4-Aminophenyl)-3-[5-(4-nitrophenyl)furan-2-yl]prop-2-en-1-one (***2g***). Mol. Form.: $C_{19}H_{12}N_2O_4$ (*FW*: 334.3); *m.p.*: 234–236 °C (Lit. 235–236 °C[1]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.89 (1H, *d*, *J* = 15.2 Hz, H-3), 7.10 (1H, *d*, *J* = 15.2 Hz, H-2), 7.3–8.0 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4), 9.1 (2H, *s*, NH_2).

1-(4-Methylphenyl)-3-[5-(2-nitrophenyl)furan-2-yl]prop-2-en-1-one (***2h***). Mol. Form.: $C_{20}H_{15}NO_4$ (*FW*: 333.3); *m.p.*: 133 °C (Lit. 134 °C[1]); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 6.71(1H, *d*, *J* = 15.2 Hz, H-3), 7.05 (1H, *d*, *J* = = 15.2 Hz, H-2), 7.3–7.6 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.2 Hz, furan H-3), 6.6 (1H, *d*, *J* = 3.2 Hz, furan H-4), 2.2 (3H, *s*, CH_3).

1-(4-Methylphenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (***2i***). Mol. Form.: $C_{20}H_{15}NO_3S$ (*FW*: 349.4); *m.p.*: 159 °C (Lit. 158–160 °C[2]); ^{1}H--NMR (400 MHz, $CDCl_3$, δ / ppm): 6.78 (1H, *d*, *J* = 15.3 Hz, H-3), 7.15 (1H, *d*, *J* = 15.3 Hz, H-2), 7.2–8.2 (8H, *m*, Ar-H), 7.0 (1H, *d*, *J* = 3.2 Hz, thiophene H-3), 6.8 (1H, *d*, *J* = 3.2 Hz, thiophene H-4), 2.13 (3H, *s*, CH_3).

1-(4-Methoxyphenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (***2j***). Mol. Form.: $C_{20}H_{15}NO_4S$ (*FW*: 365.4); *m.p.*: 152–153 °C (Lit. 151–153 °C[2]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.68 (1H, *d*, *J* = 15.3 Hz, H-3), 7.15 (1H, *d*, *J* = 15.3 Hz, H-2), 7.2–8.0 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* =3.6Hz, thiophene H-3), 6.6 (1H, *d*, *J* = 3.6 Hz, thiophene H-4), 3.89 (3H, *s*, CH_3).

1-(4-Chlorophenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (***2k***). Mol. Form.: $C_{19}H_{12}ClNO_3S$ (*FW*: 369.8); *m.p.*: 108–109 °C (Lit. 109–110 °C[2]); ^{1}H NMR (400 MHz, $CDCl_3$, δ / ppm): 6.73 (1H, *d*, *J* = 15.5 Hz, H-3), 7.02 (1H, *d*, *J* = 15.5 Hz, H-2), 7.3–8.0 (7H, *m*, Ar-H), 6.2 (1H, *d*, *J* = 3.6Hz, thiophene H-3), 6.6 (1H, *d*, *J* = 3.6 Hz, thiophene H-4).

1-(2,4-Dichlorophenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (***2l***). Mol. Form.: $C_{19}H_{11}Cl_2NO_3S$ (*FW*: 404.2); *m.p.*: 102 °C (Lit. 103 °C[2]); ^{1}H--NMR (400 MHz, $CDCl_3$, δ / ppm): 6.64 (1H, *d*, *J* = 15.3 Hz, H-3), 6.93 (1H, *d*, *J* = 15.3 Hz, H-2), 7.0–7.8 (7H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.7 (1H, *d*, *J* =3.6 Hz, thiophene H-4).

1-(4-Hydroxyphenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (***2m***). Mol. Form.: $C_{19}H_{13}NO_4S$ (*FW*: 351.3); *m.p.*: 134–135 °C (Lit. 135 °C[2]); ^{1}H--NMR (400 MHz, $CDCl_3$, δ / ppm): 6.58 (1H, *d*, *J* = 15.3 Hz, H-3), 6.98 (1H, *d*,

J = 15.3 Hz, H-2), 7.1–8.2 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, thiophene H-4).

*1-(4-Nitrophenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (**2n**)*: Mol. Form.: $C_{19}H_{12}N_2O_5S$ (*FW*: 380.3); *m.p.*: 175–176 °C (Lit. 176–177 °C[2]); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 6.81 (1H, *d*, *J* = 15.3 Hz, H-3), 7.14 (1H, *d*, *J* = 15.3 Hz, H-2), 7.1–7.9 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, thiophene H-4).

*1-(3-Nitrophenyl)-3-[5-(4-nitrophenyl)-2-thienyl]prop-2-en-1-one (**2o**)*. Mol. Form.: $C_{19}H_{12}N_2O_5S$ (*FW*: 380.3); *m.p.*: 119–120 °C (Lit. 118–220 °C[2]) ^{1}H--NMR (400 MHz, DMSO-d_6, δ / ppm): 6.83 (1H, *d*, *J* = 15.3 Hz, H-3), 7.2 (1H, *d*, *J* = 15.3 Hz, H-2), 7.1–7.9 (8H, *m*, Ar-H), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.7 (1H, *d*, *J* = 3.6 Hz, thiophene H-4).

*1-{3-(4-Methylphenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3a**)*. Yield: 78 %; *m.p.*: 143 °C; Anal. Calcd. for $C_{22}H_{19}N_3O_4$ (*FW*: 389.4): C, 67.86; H, 4.92; N, 10.79 %. Found: C, 67.83; H, 4.87; N, 10.74 %; IR (cm^{-1}): 1661 (C=O stretching of –N–$COCH_3$ group), 3238 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.3 (3H, *s*, $COCH_3$), 2.4 (3H, *s*, CH_3), 5.5 (1H, *dd*, *J* = 5.2 Hz, *J* = 12 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.2 Hz, *J* = 17.5 Hz, pyrazoline H-4), 3.7 (1H, *dd*, *J* = 12 Hz, *J* = 17.5 Hz, pyrazoline H-4 *trans*), 6.2 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4), 7.0––8.2 (8H, *m*, Ar-H); MS (*m*/*z*): 390.23 (M^++1).

*1-{3-(4-Methoxyphenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3b**)*. Yield: 81 %; *m.p.*: 152–153 °C; Anal. Calcd. for $C_{22}H_{19}N_3O_5$ (*FW*: 405.4): C, 65.18; H, 4.72; N, 10.36 %. Found: C, 65.11; H, 4.68; N, 10.29 %; IR (cm^{-1}): 1646 (C=O stretching of –N–$COCH_3$ group), 3103 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 3.8 (3H, *s*, OCH_3) 5.7 (1H, *dd*, *J* = 5.2 Hz, *J* = 12 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.6 (1H, *dd*, *J* = 12 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.7 (1H, *d*, *J* = 3.6 Hz furan H-4), 6.9–8.1 (8H, *m*, Ar-H). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 165.24 (C=O), 156.36 (C=N), 154.6, 151.9, 148.3, 145.7, 142.8, 134.2, 132.2, 130.2, 128.4, 127.3, 125.5, 122.4 (Ar-C), 75.2 (C-5 of pyrazoline), 68.3 (C-4 of pyrazoline), 21.21 (CO–**C**H_3), 12.5 (CH_3). MS (*m*/*z*): 406.53 (M^++1).

*1-{3-(4-Chlorophenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3c**)*. Yield: 73 %; *m.p.*: 136 °C; Anal. Calcd. for $C_{21}H_{16}ClN_3O_4$ (*FW*: 409.8): C, 61.54; H, 3.94; N, 10.25 %. Found: C, 61.50; H, 3.88; N, 10.21 %; IR (cm^{-1}): 1665 (C=O stretching of –N–$COCH_3$ group), 3246 (Ar–H): ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 5.7 (1H, *dd*, *J* =5.2 Hz, *J* = 12 Hz, pyrazoline H-5), 3.4 (1H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.6 (1H, *dd*, *J* = 12 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4) 7.4–8.2 (8H, *m*,

Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 165.52 (C=O), 156.77 (C=N), 154.3, 151.5, 148.7, 145.7, 142.8, 134.8, 132.6, 130.9, 128.1, 127.3, 125.9, 121.9 (Ar-C), 75.9 (C-5 of pyrazoline), 67.6 (C-4 of pyrazoline), 21.9 (CO–**C**H_3). MS (*m*/*z*): 410.14 (M^++1), 412.11 (M^++3).

*1-{3-(2,4-Dichlorophenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H-*pyrazol-1-yl}ethanone* (***3d***). Yield: 63 %; *m.p.*: 150–151 °C; Anal. Calcd. for $C_{21}H_{15}Cl_2N_3O_4$ (*FW*: 444.2): C, 56.77; H, 3.40; N, 9.46 %. Found: C, 56.73; H, 3.37; N, 9.40 %; IR (cm^{-1}): 1669 (C=O stretching of –N–$COCH_3$ group): ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.3 (3H, *s*, $COCH_3$), 5.6 (1H, *dd*, *J* = 5.2 Hz, *J* = 11.8 Hz, pyrazoline H-5), 3.4 (1H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.6 (1H, *dd*, *J* = 11.8 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.2 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.7 (1H, *d*, *J* = 3.6 Hz, furan H-4), 7.3–8.0 (7H, *m*, Ar-H); MS (*m*/*z*): 445.7 (M^++1).

*1-{3-(4-Hydroxyphenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H-*pyrazol-1-yl}ethanone* (***3e***). Yield: 69 %; *m.p.*: 225–226 °C; Anal. Calcd. for $C_{21}H_{17}N_3O_5$ (*FW*: 391.3): C, 64.45; H, 4.38; N, 10.74 %. Found: C, 64.40; H, 4.37; N, 10.71 %; IR (cm^{-1}): 1665 (C=O stretching of –N–$COCH_3$), 3198 (Ar-H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 5.5 (1H, *dd*, *J* = 5.2 Hz, *J* = 11.2 Hz, pyrazoline H-5), 3.2 (H, *dd*, *J* =5.2 Hz, *J* =17.4 Hz, pyrazoline H-4), 3.4 (1H, *dd*, *J* = 11.2 Hz, *J* = 17.4 Hz, pyrazoline H-4 *trans*), 5.8 (1H, *s*, OH), 6.3 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4) 7.3–8.0 (8H, *m*, Ar-H); MS (*m*/*z*): 392.09 (M^++1).

*1-{3-(4-Nitrophenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H-*pyrazol-1-yl}ethanone* (***3f***). Yield: 56 %; *m.p.*: 125–126 °C; Anal. Calcd. for $C_{21}H_{16}N_4O_6$ (*FW*: 420.3): C, 60.00; H, 3.84; N, 13.33 %. Found: C, 59.96; H, 3.85; N, 13.29 %; IR (cm^{-1}): 1666 (C=O stretching of –N–$COCH_3$ group), 3229 (Ar–H): ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 5.6 (1H, *dd*, *J* = 5.2 Hz, *J* = 11.8 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.5 (1H, *dd*, *J* = 11.8 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.6 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz furan H-4), 7.1–8.2 (8H, *m*, Ar-H); MS (*m*/*z*): 421.45 (M^++1).

*1-{3-(4-Aminophenyl)-5-[5-(4-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H-*pyrazol-1-yl}ethanone* (***3g***). Yield: 53 %; *m.p.*: 247–248 °C; Anal. Calcd. for $C_{21}H_{18}N_4O_4$ (*FW*: 390.3): C, 64.61; H, 4.65; N, 14.35 %. Found: C, 64.58; H, 4.59; N, 14.31%; IR (cm^{-1}): 1652 (C=O stretching of –N–$COCH_3$ group), 3248 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.3 (3H, *s*, $COCH_3$), 5.7 (1H, *dd*, *J* = 5.0 Hz, *J* = 12.0 Hz, pyrazoline H-5), 3.1 (1H, *dd*, *J* = 5.0 Hz, *J* = 17.8 Hz, pyrazoline H-4), 3.3 (1H, *dd*, *J* = 12.0 Hz, *J* = 17.8 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, furan H-4), 9.1 (2H, *s*, NH_2), 7.3–8.0 (8H, *m*, Ar-H); ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 166.3 (C=O), 157.0 (C=N), 155.3, 152.5, 148.9, 145.2, 144.8, 134.1, 132.5, 130.3,

128.9, 126.3, 125.1, 122.8 (Ar-C), 74.7 (C-5 of pyrazoline), 69.6 (C-4 of pyrazoline), 21.1 (CO–**C**H_3). MS (*m*/*z*): 391.23 (M^++1).

*1-{3-(4-Methylphenyl)-5-[5-(2-nitrophenyl)furan-2-yl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3h**)*. Yield: 85 %; *m.p.*: 149 °C; Anal. Calcd. for $C_{22}H_{19}N_3O_4$ (*FW*: 389.4): C, 67.86; H, 4.92; N, 10.79 %. Found: C, 67.80; H, 4.88; N, 10.75 %; IR (cm^{-1}): 1647 (C=O stretching of –N–$COCH_3$ group), ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 2.1 (3H, *s*, CH_3), 5.6 (1H, *dd*, *J* = 4.8 Hz, *J* = 11.4 Hz, pyrazoline H-5), 3.3 (H, *dd*, *J* = 4.8 Hz, *J* = = 17.6 Hz, pyrazoline H-4), 3.5 (1H, *dd*, *J* = 11.4 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.2 Hz, furan H-3), 6.6 (1H, *d*, *J* = 3.2 Hz, furan H-4), 7.3–7.6 (8H, *m*, Ar-H). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm):166.54 (C=O), 155.56 (C=N), 153.6, 151.9, 149.3, 145.2, 143.8, 134.5, 133.9, 131.4, 128.9, 127.7, 124.5, 123.4 (Ar-C), 77.2 (C-5 of pyrazoline), 68.9 (C-4 of pyrazoline), 21.3 (CO–**C**H_3), 13.6 (CH_3). MS (*m*/*z*): 390.18 (M^++1).

*1-{3-(4-Methylphenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3i**)*. Yield: 79 %; *m.p.*: 89–90 °C; Anal. Calcd. for $C_{22}H_{19}N_3O_3S$ (FW: 405.4): C, 65.17; H, 4.72; N, 10.36 %. Found: C, 65.18; H, 4.68; N, 10.31 %; IR (cm^{-1}): 1658 (C=O stretching of –N–$COCH_3$ group), ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 1.9 (3H, *s*, CH_3), 5.8 (1H, *dd*, *J* = 4.4 Hz, *J* = 11.6 Hz, pyrazoline H-5), 3.3 (1H, *dd*, *J* = 4.4 Hz, *J* = = 17.6 Hz, pyrazoline H-4), 3.7 (1H, *dd*, *J* = 11.6 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 7.0 (1H, *d*, *J* = 3.2 Hz, thiophene H-3), 7.0 (1H, *d*, *J* = 3.2 Hz, thiophene H-4), 7.2–8.2 (8H, *m*, Ar-H). ^{13}C-NMR (100 MHz, $CDCl_3$, δ / ppm): 165.24 (C=O), 156.36 (C=N), 154.6, 151.9, 148.3, 145.7, 142.8, 134.2, 132.2, 130.2, 128.4, 127.3, 125.5, 122.4 (Ar-C), 75.2 (C-5 of pyrazoline), 68.3 (C-4 of pyrazoline), 21.21 (CO–**C**H_3), 12.5 (CH_3); MS (*m*/*z*): 306.16 (M^++1).

*1-{3-(4-Methoxyphenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3j**)*: Yield: 81 %; *m.p.*: 89 °C; Anal. Calcd. for $C_{22}H_{19}N_3O_4S$ (*FW*: 421.4): C, 62.69; H, 4.54; N, 9.97 %. Found: C, 62.63; H, 4.51; N, 9.88 %; IR (cm^{-1}): 1656 (C=O stretching of –N–$COCH_3$ group); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 3.7 (3H, *s*, CH_3), 5.9 (1H, *dd*, *J* = 4.4 Hz, *J* = 11.6 Hz, pyrazoline H-5), 3.3 (H, *dd*, *J* = 4.4 Hz, *J* = = 17.6 Hz, pyrazoline H-4), 3.7 (1H, *dd*, *J* = 11.6 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* =3.6 Hz, thiophene H-3), 6.6 (1H, *d*, *J* = 3.6 Hz, thiophene H-4), 7.2–8.0 (8H, *m*, Ar-H); MS (*m*/*z*): 422.18 (M^++1).

*1-{3-(4-Chlorophenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3k**)*. Yield: 61 %; *m.p.*: 69–70 °C; Anal. Calcd. for $C_{21}H_{16}ClN_3O_3S$ (*FW*: 425.8): C, 59.22; H, 3.79; N, 9.87 %. Found: C, 59.17; H, 3.75; N, 9.84 %; IR (cm^{-1}): 1661 (C=O stretching of –N–$COCH_3$ group); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.2 (3H, *s*, $COCH_3$), 5.5 (1H, *dd*, *J* =5.2 Hz, *J* = 11.8 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline

H-4), 3.6 (1H, *dd*, *J* = 11.8 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.2 (1H, *d*, *J* = 3.6 Hz, furan H-3), 6.5 (1H, *d*, *J* = 3.6 Hz, furan H-4) 7.2–8.0 (7H, *m*, Ar-H); MS (*m*/*z*): 426.7 (M^++1).

*1-{3-(2,4-Dichlorophenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro--1*H*-pyrazol-1-yl}ethanone (**3l**)*. Yield: 63 %; *m.p.*: 94 °C; Anal. Calcd. for $C_{21}H_{15}Cl_2N_3O_3S$ (*FW*: 460.3): C, 54.79; H, 3.28; N, 9.13 %. Found: C, 54.75; H, 3.21; N, 9.09 %; IR (cm^{-1}): 1667 (C=O stretching of –N–$COCH_3$ group), 3255 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 5.7 (1H, *dd*, *J* = 5.0 Hz, *J* = 11.8 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.0 Hz, *J* = = 17.4 Hz, pyrazoline H-4), 3.5 (1H, *dd*, *J* = 11.8 Hz, *J* = 17.4 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.7 (1H, *d*, *J* =3.6 Hz, thiophene H-4), 7.0–7.8 (7H, *m*, Ar-H); MS (*m*/*z*): 461.63 (M^++1).

*1-{3-(4-Hydroxyphenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*--pyrazol-1-yl}ethanone (**3m**)*. Yield: 69 %; *m.p.*: 205–206 °C; Anal. Calcd. for $C_{21}H_{17}N_3O_4S$ (*FW*: 407.4): C, 61.90; H, 4.21; N, 10.31 %. Found: C, 61.86; H, 4.19; N, 10.28 %; IR (cm^{-1}): 1667 (C=O stretching of –N–$COCH_3$ group), 3242 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.2 (3H, *s*, $COCH_3$), 5.2 (1H, *dd*, *J* = 5.2 Hz, *J* = 11.8 Hz, pyrazoline H-5), 3.3 (H, *dd*, *J* = 5.2 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.5 (1H, *dd*, *J* = 11.8 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, thiophene H-4), 7.1– –8.2 (8H, *m*, Ar-H), 5.8 (1H, *s*, OH); MS (*m*/*z*): 408.14 (M^++1).

*1-{3-(4-Nitrophenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*-pyrazol--1-yl}ethanone* (***3n***). Yield: 61 %; *m.p.*: 137–138 °C; Anal. Calcd. for $C_{21}H_{16}N_4O_5S$ (*FW*: 436.4): C, 57.79; H, 3.70; N, 12.84 %. Found: C, 12.84; H, 3.67; N, 12.80 %; IR (cm^{-1}): 1663 (C=O stretching of –N–$COCH_3$ group), 3232 (Ar–H); ^{1}H-NMR (400 MHz, $CDCl_3$, δ / ppm): 2.3 (3H, *s*, $COCH_3$), 5.6 (1H, *dd*, *J* = 5.0 Hz, *J* = 12.0 Hz, pyrazoline H-5), 3.4 (H, *dd*, *J* = 5.0 Hz, *J* = 17.6 Hz, pyrazoline H-4), 3.5 (1H, *dd*, *J* = 12.0 Hz, *J* = 17.6 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.8 (1H, *d*, *J* = 3.6 Hz, thiophene H-4), 7.1– –7.9 (8H, *m*, Ar-H); MS (*m*/*z*): 437.26 (M^++1).

*1-{3-(3-nitrophenyl)-5-[5-(4-nitrophenyl)-2-thienyl]-4,5-dihydro-1*H*-pyrazol-1-yl}ethanone (**3o**)*. Yield: 52 %; *m.p.*: 117–118 °C; Anal. Calcd. for $C_{21}H_{16}N_4O_5S$ (*FW*: 436.4): C, 57.79; H, 3.70; N, 12.84 %. Found: C, 57.76; H, 3.65; N, 12.81 %; IR (cm^{-1}): 1669 (C=O stretching of –N–$COCH_3$ group), ^{1}H--NMR (400 MHz, DMSO-d_6, δ / ppm): 2.4 (3H, *s*, $COCH_3$), 5.7 (1H, *dd*, *J* = 5.2 Hz, *J* = 12.0 Hz, pyrazoline H-5), 3.3 (H, *dd*, *J* = 5.2 Hz, *J* = 17.4 Hz, pyrazoline H-4), 3.6 (1H, *dd*, *J* = 12.0 Hz, *J* = 17.4 Hz, pyrazoline H-4 *trans*), 6.4 (1H, *d*, *J* = 3.6 Hz, thiophene H-3), 6.7 (1H, *d*, *J* = 3.6 Hz, thiophene H-4), 7.1–7.9 (8H, *m*, Ar-H); MS (*m*/*z*): 437.59 (M^++1).

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