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SUPPLEMENTARY MATERIAL TO

Microwave-assisted multi-component synthesis of 3'-indol-3-yl substituted pyrano[2,3-*c*]pyrazoles and their antimicrobial activity

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ANALYTICAL AND SPECTRAL DATA OF THE SYNTHESIZED COMPOUNDS

*6-Amino-3-methyl-4-(2-phenyl-1*H*-indol-3-yl)-1,4-dihydropyrano[2,3-*c*]pyrazole-5-carbonitrile (**5a**)*. Anal. Calcd. for $C_{22}H_{17}N_5O$ (FW: 367.14): C, 71.92; H, 4.66; N 19.06 %. Found: C, 71.86; H, 4.48; N, 19.15 %; IR (KBr, cm^{-1}): 3410 and 3385, 3270 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2210 (–C≡N str.), 1220 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.53 (3H, *s*, CH_3), 4.99 (1H, *s*, H4), 6.82 (2H, *s*, NH_2), 6.84–8.31 (9H, *m*, Ar–H), 11.21 (1H, *s*, NH of indole ring), 11.94 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 9.85 (CH_3), 27.41 (C4), 57.38 (C5), 97.59 (pyran C5), 111.71, 112.38, 114.55, 119.21, 120.92, 121.08, 126.11, 126.35, 127.25, 130.33, 135.21, 136.05, 136.93, 156.56 (Ar–C and C≡N), 158.32 (C7a), 162.38 (C6); MS (*m*/*z*): 368 (M^++1).

*6-Amino-3-methyl-4-(2-(4-methylphenyl)-1*H*-indol-3-yl)-1,4-dihydropyrano-[2,3-*c*]pyrazole-5-carbonitrile (**5b**)*. Anal. Calcd. for $C_{23}H_{19}N_5O$ (FW: 381.16): C, 72.42; H, 5.02; N, 18.36 %. Found: C, 72.33; H, 5.11; N, 18.24 %; IR (KBr, cm^{-1}): 3395 and 3360, 3285 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2190 (–C≡N str.), 1235 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.52 (3H, *s*, CH_3), 2.47 (3H, *s*, CH_3), 4.91 (1H, *s*, H4), 6.85 (2H, *s*, NH_2), 6.95–8.13 (8H, *m*, Ar–H), 11.15 (1H, *s*, NH of indole ring), 11.94 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 9.96 (CH_3), 21.42 (CH_3), 27.15 (C4), 58.25 (C5), 97.46 (C3a), 112.05, 112.67, 115.28, 120.11, 120.87, 121.45, 127.05, 127.88, 128.31, 131.18, 135.33, 136.81,

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137.25, 157.36 (Ar–C and C≡N), 158.92 (C7a), 161.81 (C6); MS (*m*/*z*): 382.1 (M^++1).

*6-Amino-4-(2-(4-methoxyphenyl)-1*H*-indol-3-yl)-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (**5c**)*. Anal. Calcd. for $C_{23}H_{19}N_5O_2$ (FW: 397.15): C, 69.51; H, 4.82; N, 17.62 %. Found: C, 69.85; H, 4.75; N, 17.59 %; IR (KBr, cm^{-1}): 3415 and 3320, 3250 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2195 (–C≡N str.), 1250 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.54 (3H, *s*, CH_3), 3.08 (3H, *s*, OCH_3), 4.95 (1H, *s*, H4), 6.82 (2H, *s*, NH_2), 7.03–7.60 (8H, *m*, Ar–H), 11.11 (1H, *s*, NH of indole ring), 11.92 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 9.87 (CH_3), 27.52 (C4), 55.69 (OCH_3), 57.31 (C5), 97.88 (C3a), 111.76, 112.49, 114.71, 119.09, 121.48, 121.72, 125.37, 125.95, 127.00, 130.54, 135.88, 135.97, 136.74, 155.27 (Ar–C and C≡N), 159.51 (C7a), 161.32 (C6); MS (*m*/*z*): 398 (M^++1).

*6-Amino-4-(2-(4-chlorophenyl)-1*H*-indol-3-yl)-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (**5d**)*. Anal. Calcd. for $C_{22}H_{16}ClN_5O$ (FW: 401.10): C, 65.76; H, 4.61; N, 17.43 %. Found: C, 65.69; H, 4.72; N, 17.57 %; IR (KBr, cm^{-1}): 3410 and 3355, 3280 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2200 (–C≡N str.), 1210 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.57 (3H, *s*, CH_3), 5.00 (1H, *s*, H4), 6.88 (2H, *s*, NH_2), 7.05–8.11 (8H, *m*, Ar–H), 11.25 (1H, *s*, NH of indole ring), 11.96 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 10.03 (CH_3), 27.45 (C4), 58.38 (C5), 97.23 (C3a), 112.13, 113.21, 114.77, 119.25, 120.99, 121.37, 125.12, 125.77, 126.89, 131.22, 136.05, 136.28, 138.45, 157.31 (Ar–C and C≡N), 158.66 (C7a), 161.27 (C6); MS (*m*/*z*): 402.0 (M^++1).

*6-Amino-4-(2-(4-bromophenyl)-1*H*-indol-3-yl)-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (**5e**)*. Anal. Calcd. for $C_{22}H_{16}BrN_5O$ (FW: 445.05): C, 59.21; H, 3.61; N, 15.69 %. Found: C, 59.44; H, 3.82; N, 15.38 %; IR (KBr, cm^{-1}): 3405 and 3360, 3285 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2190 (–C≡N str.), 1255 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.61 (3H, *s*, CH_3), 4.96 (1H, *s*, H4), 6.81 (2H, *s*, NH_2), 6.95–7.89 (8H, *m*, Ar–H), 11.20 (1H, *s*, NH of indole ring), 11.97 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 10.15 (CH_3), 27.50 (C4), 57.17 (C5), 97.68 (C3a), 111.88, 112.95, 114.03, 120.11, 121.12, 121.89, 125.23, 126.17, 126.93, 130.73, 135.27, 137.34, 138.36, 148.86 (Ar–C and C≡N), 156.27 (C7a), 162.09 (C6); MS (*m*/*z*): 445.9 (M^++1).

*6-Amino-4-(2-(4-fluorophenyl)-1*H*-indol-3-yl)-3-methyl-1,4-dihydropyrano[2,3-c]pyrazole-5-carbonitrile (**5f**)*. Anal. Calcd. for $C_{22}H_{16}FN_5O$ (FW: 385.13): C, 68.56; H, 4.18; N, 18.17 %. Found: C, 68.81; H, 4.03; N 17.98 %; IR (KBr, cm^{-1}): 3400 and 3370, 3285 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2190 (–C≡N str.), 1255 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz,

DMSO-d_6, δ / ppm): 1.54 (3H, *s*, CH_3), 5.01 (1H, *s*, H4), 6.79 (2H, *s*, NH_2), 6.93–8.03 (8H, *m*, Ar–H), 11.11 (1H, *s*, NH of indole ring), 11.92 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 9.91 (CH_3), 27.36 (C4), 57.49 (C5), 97.48 (C3a), 112.08, 113.25, 114.92, 116.08, 120.06, 120.86, 125.03, 126.28, 126.73, 131.25, 134.93, 136.23, 137.48, 156.49 (Ar–C and C≡N), 159.29 (C7a), 161.45 (C6); MS (*m*/*z*): 386.0 (M^++1).

*6-Amino-3-methyl-4-(2-(4-(methylsulphonyl)phenyl)-1*H*-indol-3-yl)-1,4-dihydropyrano[2,3-*c*]pyrazole-5-carbonitrile (**5g**)*. Anal. Calcd. for $C_{23}H_{19}N_5O_3S$ (FW: 445.12): C, 62.01; H, 4.30; N, 15.72 %. Found: C, 61.92; H, 4.19; N, 15.69 %; IR (KBr, cm^{-1}): 3385 and 3345, 3270 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2195 (–C≡N str.), 1250 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.58 (3H, *s*, CH_3), 3.35 (3H, *s*, SO_2CH_3), 5.07 (1H, *s*, H4), 6.86 (2H, *s*, NH_2), 6.91–8.09 (8H, *m*, Ar–H), 11.43 (1H, *s*, NH of indole ring), 11.97 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 10.00 (CH_3), 27.48 (C4), 44.00 (SO_2CH_3), 57.06 (C5), 97.57 (C3a), 112.19, 114.88, 119.50, 119.66, 121.55, 112.64, 126.79, 127.86, 129.77, 134.03, 136.02, 137.30, 138.00, 140.18 (Ar–C and C≡N), 155.25 (C7a), 161.29 (C6); MS (*m*/*z*): 446.1 (M^++1).

*6-Amino-3-methyl-4-(2-(4-nitrophenyl)-1*H*-indol-3-yl)-1,4-dihydropyrano-[2,3-*c*]pyrazole-5-carbonitrile (**5h**)*. Anal. Calcd. for $C_{22}H_{16}N_6O_3$ (FW: 412.13): C, 64.07; H, 3.91; N, 20.38 %. Found: C, 64.15; H, 4.22; N, 20.06 %; IR (KBr, cm^{-1}): 3395 and 3350, 3240 (asym. and sym. str. of $–NH_2$ and –NH– str.), 2185 (–C≡N str.), 1245 (asym. str. of cyclic C–O–C ether); ^{1}H-NMR (400 MHz, DMSO-d_6, δ / ppm): 1.55 (3H, *s*, CH_3), 4.99 (1H, *s*, H4), 6.98 (2H, *s*, NH_2), 7.11–8.15 (8H, *m*, Ar–H), 11.24 (1H, *s*, NH of indole ring), 12.01 (1H, *s*, NH of pyrazole ring); ^{13}C-NMR (100 MHz, DMSO-d_6, δ / ppm): 9.78 (CH_3), 27.39 (C4), 57.00 (C5), 97.65 (C3a), 112.23, 114.72, 120.13, 120.54, 121.31, 123.25, 125.68, 125.99, 130.72, 135.21, 135.98, 137.53, 139.05, 149.35 (Ar–C and C≡N), 157.43 (C7a), 161.63 (C6); MS (*m*/*z*): 413.0 (M^++1).

REPRESENTATIVE SPECTRA OF COMPOUNDS **5e** AND **5f**

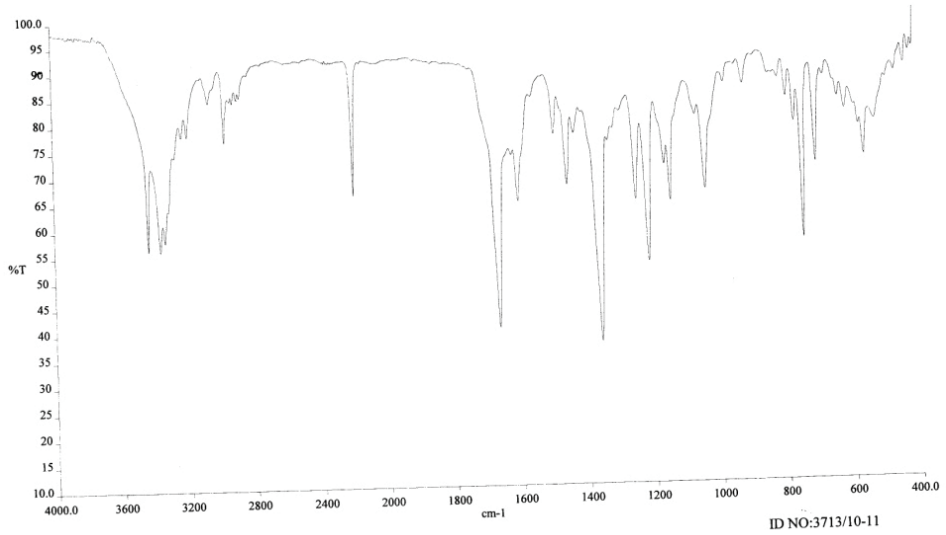

Fig. S1. IR Spectrum of compound **5e**.

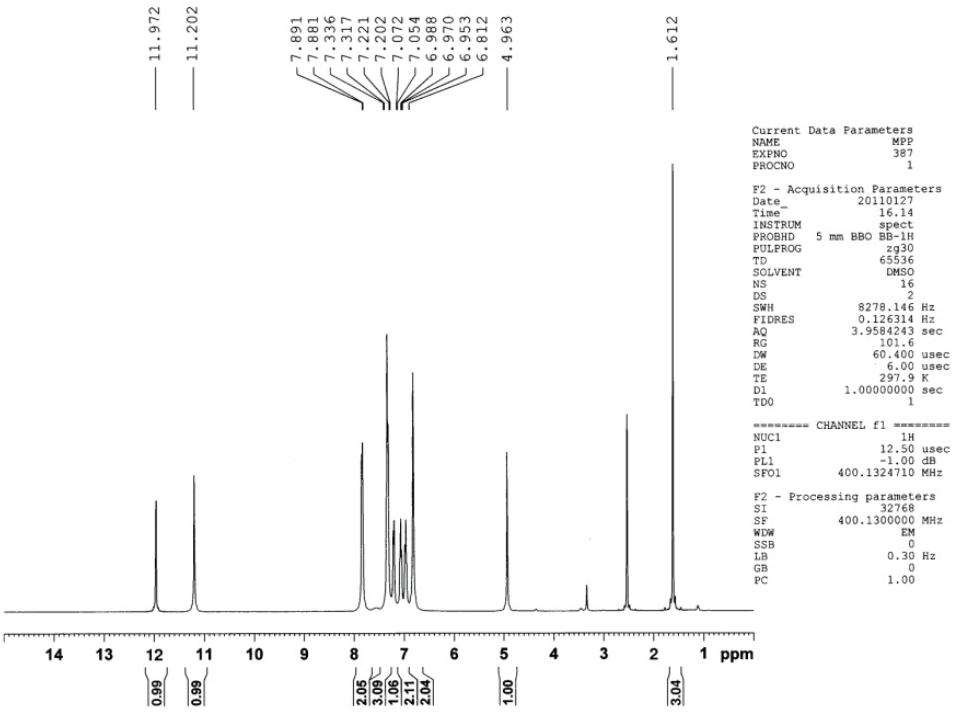

Fig. S2. ^{1}H-NMR Spectrum of compound **5e**.

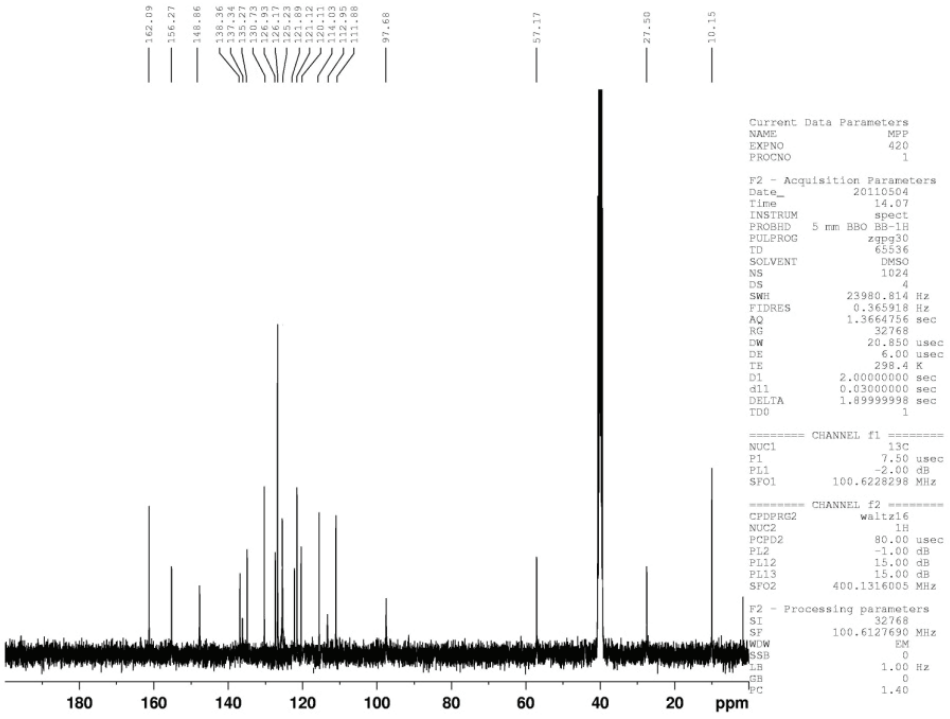

Fig. S3. ^{13}C-NMR Spectrum of compound **5e**.

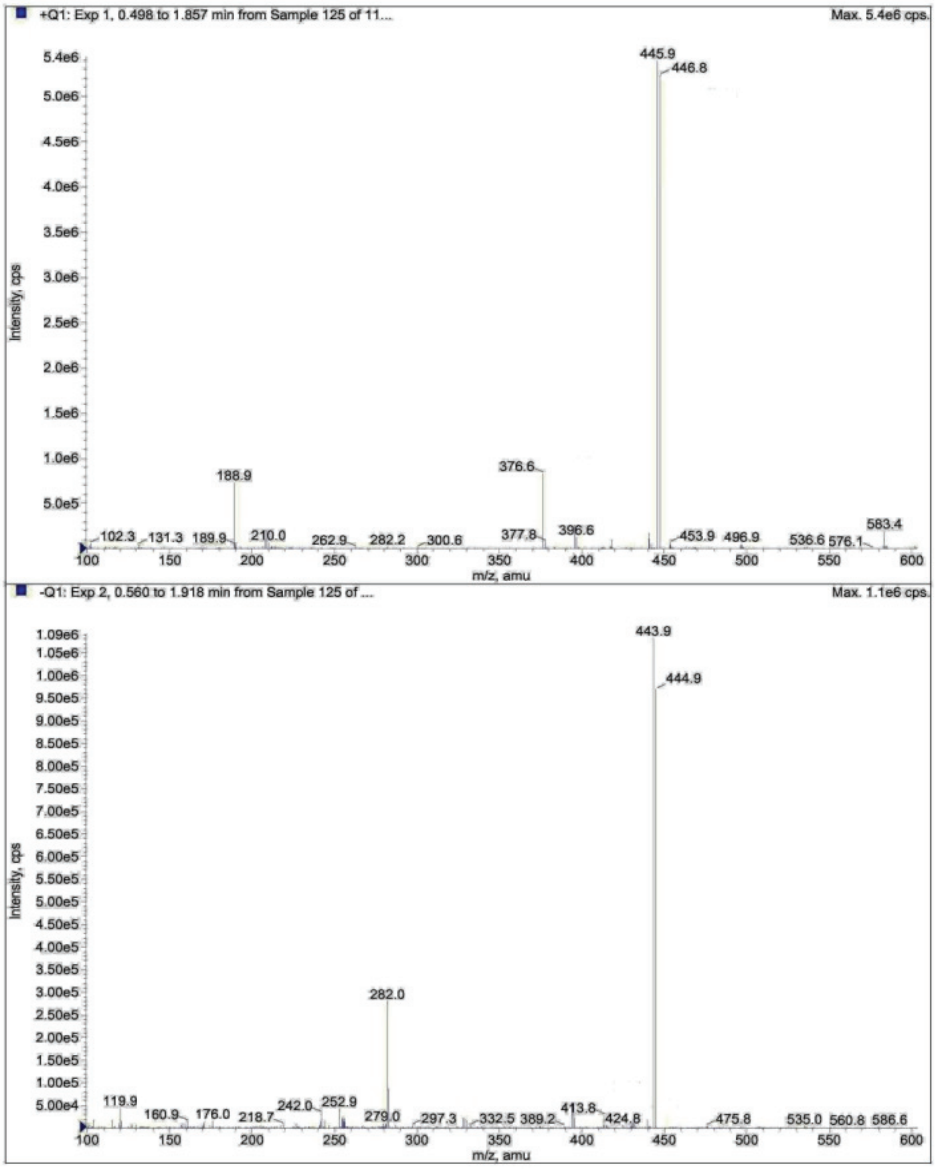

Fig. S4. Mass spectrum of compound **5e**.

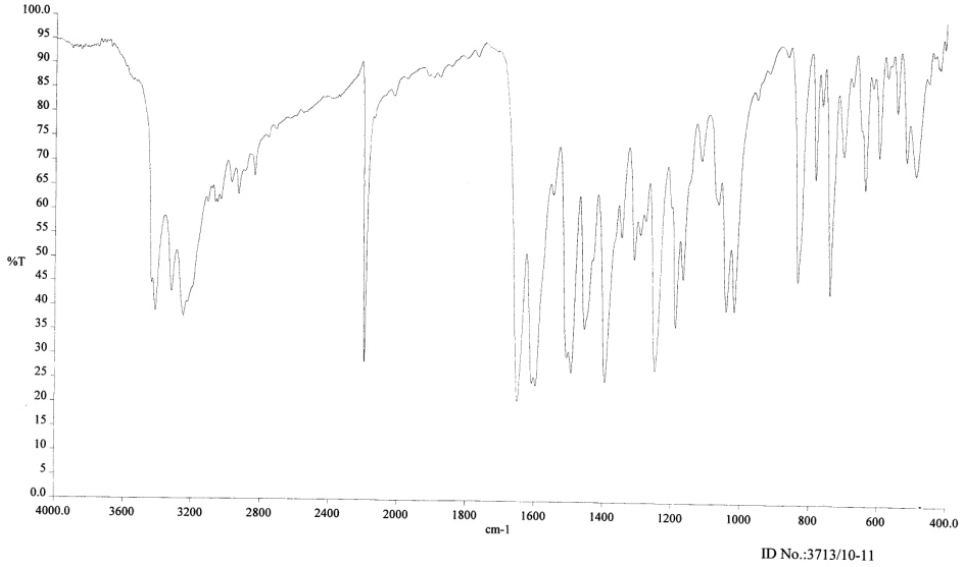

Fig. S5. IR Spectrum of compound **5f**.

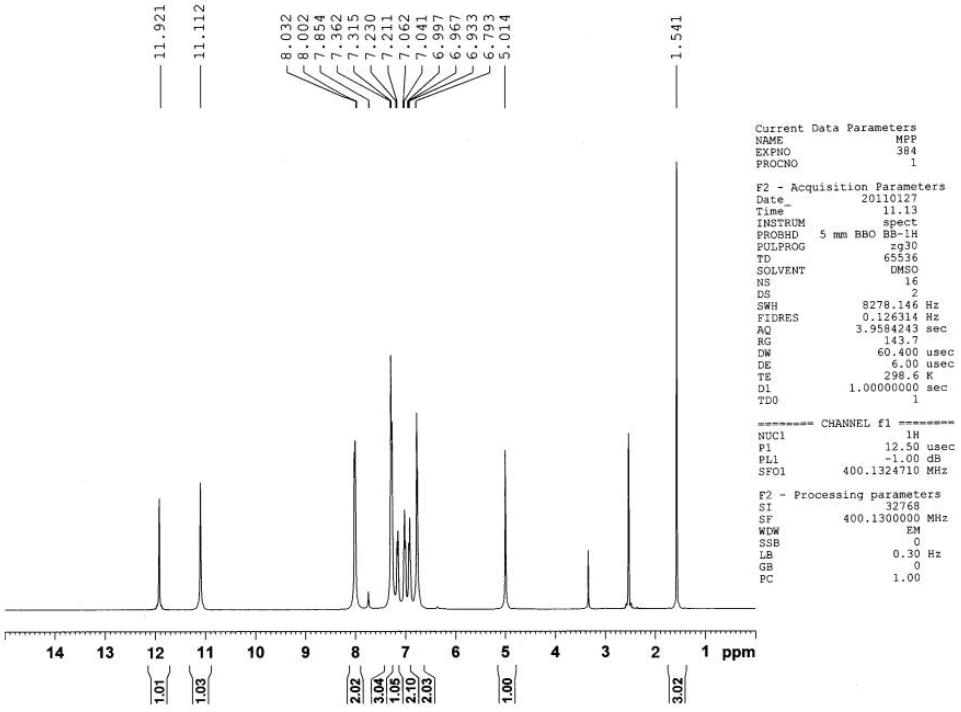

Fig. S6. ^{1}H-NMR Spectrum of compound **5f**.

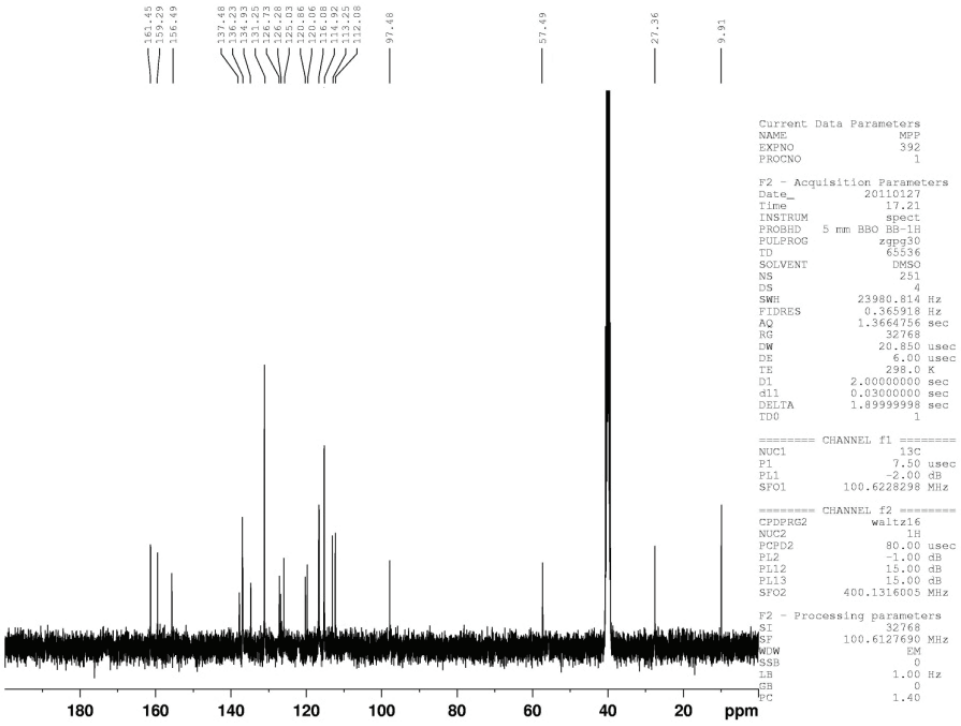

Fig. S7. ^{13}C-NMR Spectrum of compound **5f**.

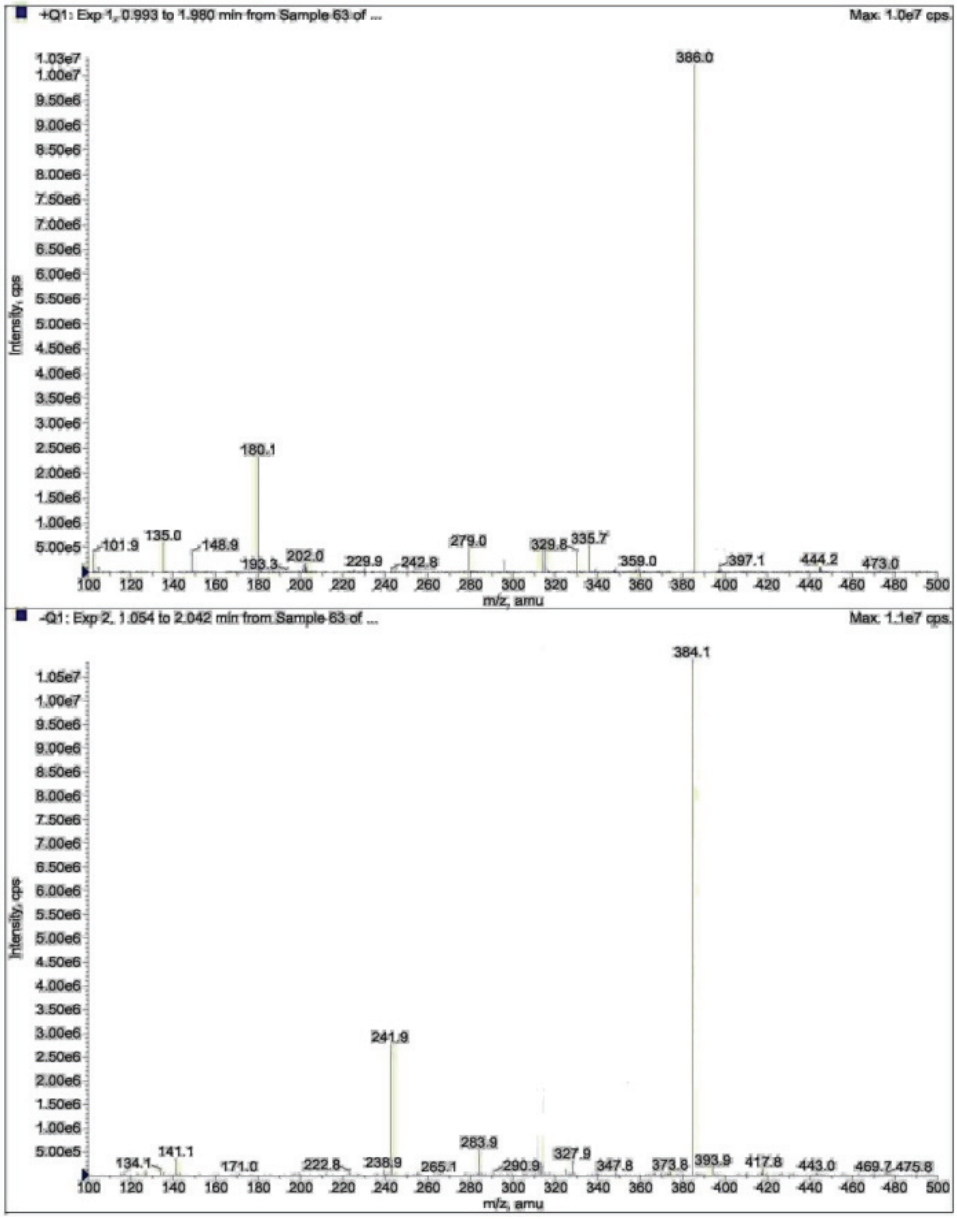

Fig. S8. Mass spectrum of compound **5f**.