



SUPPLEMENTARY MATERIAL TO
**Microwave-assisted synthesis and antimicrobial evaluation of
6-[3-aryl-1-phenyl-4',5'-dihydro[4,5'-bi-1*H*-pyrazol]-3'-yl]-
-2*H*-chromen-5-ols**

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¹H-, ¹³C-NMR AND MASS SPECTRA OF COMPOUNDS **6a–j**

6-[1,3-diphenyl-4',5'-dihydro[4,5'-bi-1*H*-pyrazol]-3'-yl]-2*H*-chromen-5-ol (6a):
Anal. Calcd. for C₂₇H₂₂N₄O₂: C, 74.46; H, 5.10; N, 12.89; Found: C, 74.41; H, 5.12; N, 12.85; IR (KBr, cm⁻¹): 3435 (OH), 3254 (NH), 1590 (C=N); ¹H NMR (400 MHz, CDCl₃, δ / ppm): 3.11 (1H, *dd*, *J* = 8.68 Hz, *J* = 16.80 Hz, H_A), 3.50 (1H, *dd*, *J* = 9.82 Hz, *J* = 16.80 Hz, H_B), 4.81 (2H, *s*, OCH₂), 5.04–5.10 (1H, *m*, H_X), 5.73–5.77 (1H, *m*, OCH₂–CH=CH), 6.35 (1H, *d*, *J* = 8.30 Hz, Ar-H), 6.88 (1H, *d*, *J* = 9.63 Hz, OCH₂–CH=CH), 6.95 (1H, *d*, *J* = 8.49 Hz, Ar-H), 7.29 (1H, *d*, *J* = 7.17 Hz, Ar-H), 7.38–7.50 (6H, *m*, Ar-H), 7.70 (4H, *t*, *J* = 7.28 Hz, Ar-H), 7.99 (1H, *s*, pyrazole-H), 11.36 (1H, *br.-s*, OH); ¹³C NMR (100 MHz, CDCl₃, δ / ppm): 40.6, 53.6, 65.1, 106.6, 109.8, 110.0, 118.5, 118.7, 119.1, 122.0, 125.2, 126.1, 127.3, 127.6, 127.8, 128.3, 128.9, 132.4, 139.3, 150.7, 153.5, 154.7, 155.5; LC–MS (*m/z*) 435 ([M+H]⁺, 100%).

**6-[3-(4-bromophenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1*H*-pyrazol]-3'-yl]-2*H*-
-chromen-5-ol (6b):** Anal. Calcd. for C₂₇H₂₁BrN₄O₂: C, 63.17; H, 4.12; N, 10.9; Found: C, 63.19; H, 4.16; N, 11.02; IR (KBr, cm⁻¹): 3439 (OH), 3260 (NH), 1593 (C=N); ¹H NMR (400 MHz, CDCl₃, δ / ppm): 3.08 (1H, *dd*, *J* = 8.68 Hz, *J* = 16.05 Hz, H_A), 3.48 (1H, *dd*, *J* = 10.00 Hz, *J* = 16.05 Hz, H_B), 4.82 (2H, *s*, OCH₂), 5.04 (1H, *dd*, *J* = 8.68 Hz, *J* = 10.00 Hz, H_X), 5.72–5.78 (1H, *m*, OCH₂–CH=CH), 6.35 (1H, *d*, *J* = 8.49 Hz, Ar-H), 6.87 (1H, *d*, *J* = 10.00 Hz, OCH₂–CH=CH), 6.93 (1H, *d*, *J* = 8.49 Hz, Ar-H), 7.31 (1H, *d*, *J* = 7.36 Hz, Ar-H), 7.44 (2H, *t*, *J* = 8.49 Hz, Ar-H), 7.59 (4H, *s*, Ar-H), 7.71 (3H, *d*, *J* = 7.74 Hz,

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Ar-H), 7.99 (1H, *s*, pyrazole-H), 11.39 (1H, *s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 40.5, 53.5, 65.1, 106.7, 107.5, 109.7, 110.1, 118.6, 118.7, 119.2, 122.0, 125.5, 126.3, 127.3, 129.0, 129.1, 131.3, 131.4, 139.2, 149.4, 153.5, 154.7, 155.6. LC-MS (m/z) 513 ($[\text{M}+\text{H}]^+$, 515 $[\text{M}+\text{H}+2]^+$, 100%).

6-[3-(4-chlorophenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (6c): Anal. Calcd. for $\text{C}_{27}\text{H}_{21}\text{ClN}_4\text{O}_2$: C, 69.15; H, 4.51; N, 11.95; Found: C, 69.19; H, 4.54; N, 11.91; IR (KBr, cm^{-1}): 3438 (OH), 3257 (NH), 1591 (C=N); ^1H NMR (400 MHz, CDCl_3 , δ / ppm): 3.07 (1H, *dd*, $J = 8.87$ Hz, $J = 16.05$ Hz, H_A), 3.48 (1H, *dd*, $J = 10.19$ Hz, $J = 16.05$ Hz, H_B), 4.80–4.82 (2H, *m*, OCH_2), 5.03 (1H, *dd*, $J = 8.87$ Hz, $J = 10.19$ Hz, H_X), 5.71–5.77 (1H, *m*, $\text{OCH}_2\text{-CH=CH}$), 5.89 (1H, *broad-s*, NH), 6.34 (1H, *d*, $J = 8.68$ Hz, Ar-H), 6.87 (1H, *d*, $J = 10.00$ Hz, $\text{OCH}_2\text{-CH=CH}$), 6.92 (1H, *d*, $J = 8.49$ Hz, Ar-H), 7.30 (1H, *d*, $J = 7.36$ Hz, Ar-H), 7.41–7.46 (4H, *m*, Ar-H), 7.64–7.71 (4H, *m*, Ar-H), 7.99 (1H, *s*, pyrazole-H), 11.33 (1H, *s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 40.5, 53.5, 65.1, 106.6, 109.7, 110.0, 118.5, 118.6, 119.2, 122.0, 125.5, 126.3, 127.3, 128.5, 128.8, 129.0, 131.0, 133.8, 139.2, 149.4, 153.5, 154.7, 155.6. LC-MS (m/z) 469 ($[\text{M}+\text{H}]^+$, 100%).

6-[1-phenyl-3-p-tolyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (6d): Anal. Calcd. for $\text{C}_{28}\text{H}_{24}\text{N}_4\text{O}_2$: C, 74.98; H, 5.39; N, 12.49; Found: C, 74.95; H, 5.43; N, 12.46; IR (KBr, cm^{-1}): 3440 (OH), 3258 (NH), 1594 (C=N); ^1H NMR (400 MHz, CDCl_3 , δ / ppm): 2.40 (3H, *s*, Ar- CH_3), 3.08 (1H, *dd*, $J = 8.49$ Hz, $J = 16.25$ Hz, H_A), 3.46 (1H, *dd*, $J = 10.19$ Hz, $J = 16.25$ Hz, H_B), 4.80–4.84 (2H, *m*, 2H, OCH_2), 5.04 (1H, *dd*, $J = 8.49$ Hz, $J = 10.19$ Hz, H_X), 5.72–5.77 (1H, *m*, $\text{OCH}_2\text{-CH=CH}$), 5.88 (1H, *br.-s*, NH), 6.34 (1H, *d*, $J = 8.68$ Hz, Ar-H), 6.87 (1H, *d*, $J = 10.00$ Hz, $\text{OCH}_2\text{-CH=CH}$), 6.94 (1H, *d*, $J = 8.30$ Hz, Ar-H), 7.27 (3H, *d*, $J = 7.74$ Hz, Ar-H), 7.42 (2H, *t*, $J = 7.74$ Hz, Ar-H), 7.57 (2H, *d*, $J = 7.93$ Hz, Ar-H), 7.71 (2H, *d*, $J = 7.93$ Hz, Ar-H), 7.97 (1H, *s*, pyrazole-H), 11.40 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 20.8, 40.5, 53.5, 65.0, 106.6, 109.8, 110.0, 118.4, 118.6, 119.2, 121.9, 125.1, 126.0, 127.3, 127.4, 128.9, 129.0, 129.4, 137.6, 139.3, 150.6, 153.5, 154.7, 155.4. LC-MS (m/z) 449 ($[\text{M}+\text{H}]^+$, 100%).

6-[3-(4-hydroxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (6e): Anal. Calcd. for $\text{C}_{27}\text{H}_{22}\text{N}_4\text{O}_3$: C, 71.99; H, 4.92; N, 12.44; Found: C, 71.94; H, 4.95; N, 12.41; IR (KBr, cm^{-1}): 3443 (OH), 3256 (NH), 1591 (C=N); ^1H NMR (400 MHz, CDCl_3 , δ / ppm): 3.09 (1H, *dd*, $J = 8.12$ Hz, $J = 15.86$ Hz, H_A), 3.47 (1H, *dd*, $J = 10.57$ Hz, $J = 15.86$ Hz, H_B), 4.81 (2H, *s*, OCH_2), 5.01 (1H, *dd*, $J = 8.12$ Hz, $J = 10.57$ Hz, H_X), 5.73–5.77 (1H, *m*, $\text{OCH}_2\text{-CH=CH}$), 6.35 (1H, *d*, $J = 8.30$ Hz, Ar-H), 6.85–6.95 (5H, *m*, Ar-H), 7.28 (1H, *d*, $J = 7.53$ Hz, Ar-H), 7.40–7.54 (6H, *m*, Ar-H), 7.95 (1H, *s*, pyrazole-H), 8.04 (1H, *s*, OH), 11.38 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 40.5, 53.5, 65.1, 106.7, 109.7, 110.0, 118.5, 118.5, 118.6, 119.2, 121.9,

125.5, 126.3, 127.3, 128.5, 128.8, 129.0, 133.8, 139.18, 149.4, 153.5, 154.8, 156.6. LC-MS (m/z) 451 ($[M+H]^+$, 100%).

6-[3-(4-methoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6f**): Anal. Calcd. for $C_{28}H_{24}N_4O_3$; C, 72.40; H, 5.21; N, 12.06; Found: C, 72.43; H, 5.18; N, 12.10; IR (KBr, cm^{-1}): 3445 (OH), 3261 (NH), 1595 (C=N); 1H NMR (400 MHz, $CDCl_3$, δ / ppm): 3.11 (1H, *dd*, $J = 8.68$ Hz, $J = 16.05$ Hz, H_A), 3.48 (1H, *dd*, $J = 10.00$ Hz, $J = 16.05$ Hz, H_B), 3.86 (3H, *s*, Ar-OCH₃), 4.81–4.83 (2H, *m*, OCH₂), 5.02–5.08 (1H, *m*, H_X), 5.73–5.78 (1H, *m*, OCH₂-CH=CH), 5.87 (1H, *br.-s*, NH), 6.35 (1H, *d*, $J = 8.68$ Hz, Ar-H), 6.87 (1H, *d*, $J = 10.19$ Hz, OCH₂-CH=CH), 6.95 (1H, *d*, $J = 8.49$ Hz, Ar-H), 7.00 (2H, *d*, $J = 8.68$ Hz, Ar-H), 7.28 (1H, *d*, $J = 7.55$ Hz, Ar-H), 7.43 (2H, *t*, $J = 8.49$ Hz, Ar-H), 7.62 (2H, *d*, $J = 8.68$ Hz, Ar-H), 7.71 (2H, *d*, $J = 7.93$ Hz, Ar-H), 7.97 (1H, *s*, pyrazole-H), 11.38 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, $CDCl_3$, δ / ppm): 40.5, 53.6, 54.9, 65.1, 106.6, 109.8, 110.0, 113.7, 118.4, 118.6, 119.2, 121.7, 124.9, 125.1, 126.0, 127.3, 128.8, 128.9, 139.3, 150.5, 153.5, 154.7, 155.5, 159.2. LC-MS (m/z) 465 ($[M+H]^+$, 100%).

6-[3-(4-ethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6g**): Anal. Calcd. for $C_{29}H_{26}N_4O_3$; C, 72.79; H, 5.48 ; N, 11.71; Found: C, 72.76; H, 5.51; N, 11.75; IR (KBr, cm^{-1}): 3442 (OH), 3261 (NH), 1596 (C=N); 1H NMR (400 MHz, DMSO- d_6 , δ / ppm): 1.35 (3H, *t*, $J = 6.18$ Hz, CH₃), 3.08 (1H, *dd*, $J = 10.76$ Hz, $J = 16.61$ Hz, H_A), 3.58 (1H, *dd*, $J = 10.57$ Hz, $J = 16.61$ Hz, H_B), 4.08 (2H, *q*, $J = 7.68$ Hz, Ar-OCH₂), 4.75–4.78 (2H, *m*, OCH₂), 4.86–4.95 (1H, *dd*, $J = 10.76$ Hz, $J = 10.57$ Hz, H_X), 5.84 (1H, *m*, OCH₂-CH=CH), 6.33 (1H, *d*, $J = 8.49$ Hz, Ar-H), 6.73 (1H, *d*, $J = 10.00$ Hz, OCH₂-CH=CH), 7.01 (2H, *d*, $J = 8.68$ Hz, Ar-H), 7.06 (1H, *d*, $J = 8.49$ Hz, Ar-H), 7.30 (1H, *d*, $J = 7.55$ Hz, Ar-H), 7.48 (2H, *t*, $J = 8.49$ Hz, Ar-H), 7.65 (3H, *dd*, $J = 3.77$ Hz, $J = 8.68$ Hz, Ar-H), 7.87 (2H, *d*, $J = 7.74$ Hz, Ar-H), 8.57 (1H, *s*, pyrazole-H), 11.72 (1H, *s*, OH); ^{13}C NMR (100 MHz, DMSO- d_6 , δ / ppm): 14.5, 40.3, 53.1, 62.9, 64.8, 106.7, 109.5, 110.4, 113.7, 114.2, 118.1, 118.9, 120.5, 120.7, 122.3, 126.2, 127.5, 127.9, 129.4, 129.6, 134.1, 139.3, 150.2, 152.8, 153.6, 154.7, 158.5. LC-MS (m/z) 479 ($[M+H]^+$, 100%).

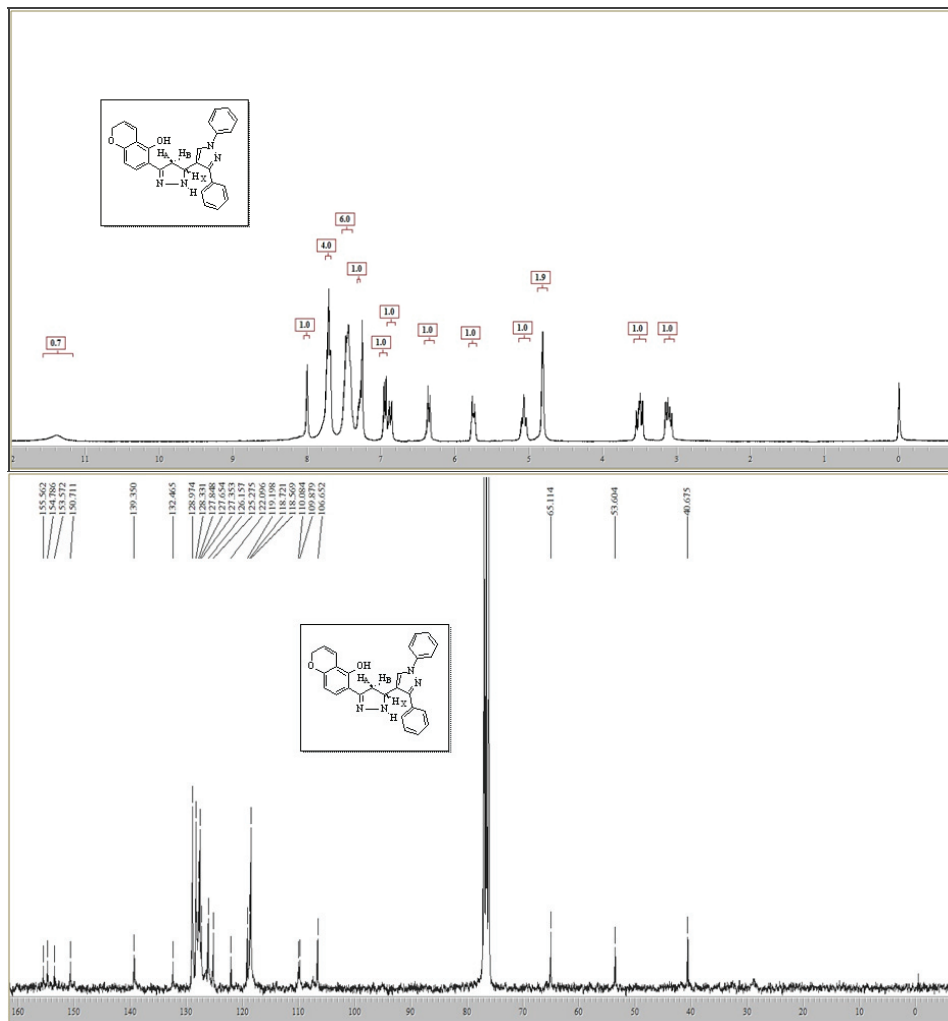
6-[3-(3-ethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6h**): Anal. Calcd. for $C_{29}H_{26}N_4O_3$; C, 72.79; H, 5.48 ; N, 11.71; Found: C, 72.76; H, 5.44; N, 11.75; IR (KBr, cm^{-1}): 3464 (OH), 3268 (NH), 1599 (C=N); 1H NMR (400 MHz, $CDCl_3$, δ / ppm): 1.43 (3H, *t*, $J = 5.45$ Hz, CH₃), 3.09 (1H, *dd*, $J = 8.87$ Hz, $J = 16.24$ Hz, H_A), 3.48 (1H, *dd*, $J = 10.19$ Hz, $J = 16.24$ Hz, H_B), 4.09 (2H, *q*, $J = 7.15$ Hz, Ar-OCH₂), 4.80–4.82 (2H, *m*, OCH₂), 5.08 (1H, *dd*, $J = 8.87$ Hz, $J = 10.19$ Hz, H_X), 5.74 (1H, *m*, OCH₂-CH=CH), 5.90 (1H, *br.-s*, NH), 6.34 (1H, *d*, $J = 8.49$ Hz, Ar-H), 6.87 (1H, *d*, $J = 10.00$ Hz, OCH₂-CH=CH), 6.93 (2H, *d*, $J = 8.49$ Hz, Ar-H), 7.29 (2H, *d*, $J = 7.55$ Hz, Ar-H), 7.34–7.46 (4H, *m*, Ar-H), 7.71 (2H, *d*, $J = 7.74$ Hz, Ar-H), 7.98 (1H, *s*,

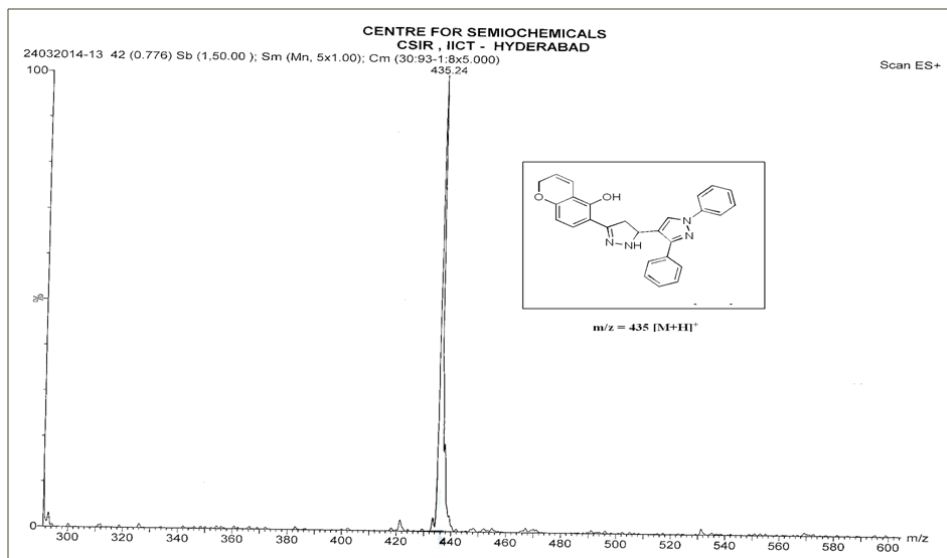
pyrazole-H), 11.38 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 14.8, 40.9, 54.1, 63.5, 65.5, 107.0, 110.3, 110.5, 114.7, 118.9, 119.1, 119.6, 122.2, 125.2, 125.5, 126.4, 127.8, 129.3, 129.4, 139.8, 151.0, 154.0, 155.2, 156.0, 159.1. LC-MS (m/z) 479 ($[\text{M}+\text{H}]^+$, 100%).

6-[3-(3,4-dimethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6i**): Anal. Calcd. for $\text{C}_{29}\text{H}_{26}\text{N}_4\text{O}_4$: C, 70.43; H, 5.30; N, 11.33; Found: C, 70.39; H, 5.33; N, 11.38; IR (KBr, cm^{-1}): 3444 (OH), 3261 (NH), 1596 (C=N); ^1H NMR (400 MHz, CDCl_3 , δ / ppm): 3.11 (1H, *dd*, $J = 8.87$ Hz, $J = 16.05$ Hz, H_A), 3.47 (1H, *dd*, $J = 10.19$ Hz, $J = 16.05$ Hz, H_B), 3.93 (3H, *s*, Ar-OCH₃), 3.93 (3H, *s*, Ar-OCH₃), 4.81 (2H, *s*, OCH₂), 5.07 (1H, *dd*, $J = 8.87$ Hz, $J = 10.19$ Hz, H_X), 5.72–5.78 (1H, *m*, OCH₂-CH=CH), 6.34 (1H, *d*, $J = 8.49$ Hz, Ar-H), 6.86–6.99 (3H, *m*, Ar-H), 7.19 (1H, *d*, $J = 8.49$ Hz, Ar-H), 7.35 (1H, *s*, Ar-H), 7.42–7.49 (3H, *m*, Ar-H), 7.71 (2H, *d*, $J = 7.74$ Hz, Ar-H), 7.82 (1H, *d*, $J = 7.93$ Hz, Ar-H), 7.97 (1H, *s*, pyrazole-H), 11.38 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 40.3, 53.7, 55.5, 55.6, 65.1, 109.8, 110.8, 111.1, 118.5, 118.7, 118.9, 119.1, 120.0, 121.6, 125.4, 126.1, 126.5, 126.7, 127.3, 128.9, 129.0, 139.3, 148.8, 148.8, 153.6, 154.0, 154.8, 155.6. LC-MS (m/z) 495 ($[\text{M}+\text{H}]^+$, 100%).

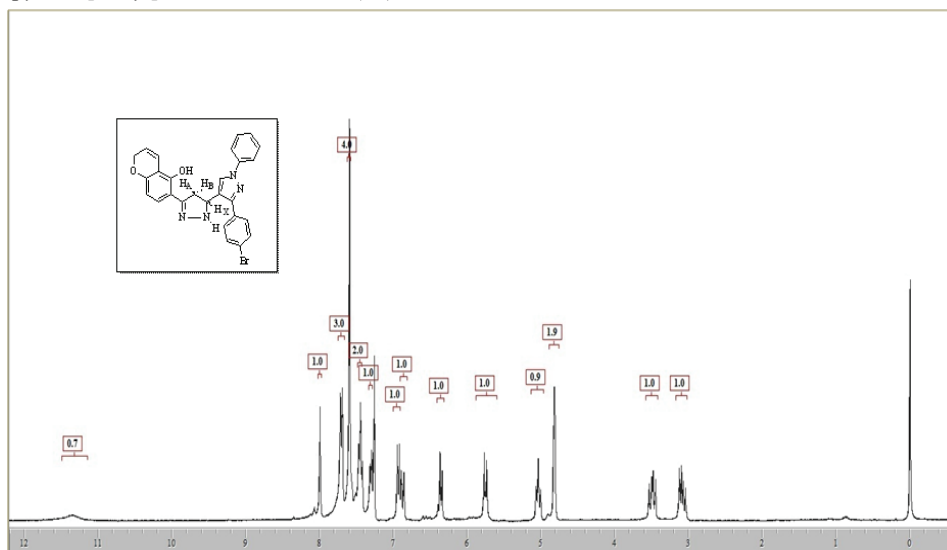
6-[3-(naphthalen-2-yl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6j**): Anal. Calcd. for $\text{C}_{31}\text{H}_{24}\text{N}_4\text{O}_2$: C, 76.84; H, 4.99; N, 11.56; Found: C, 76.81; H, 5.02; N, 11.52; IR (KBr, cm^{-1}): 3441 (OH), 3257 (NH), 1590 (C=N); ^1H NMR (400 MHz, CDCl_3 , δ / ppm): 3.14 (1H, *dd*, $J = 8.80$ Hz, $J = 16.26$ Hz, H_A), 3.53 (1H, *dd*, $J = 10.14$ Hz, $J = 16.26$ Hz, H_B), 4.81–4.82 (2H, *m*, OCH₂), 5.19 (1H, *dd*, $J = 8.80$ Hz, $J = 10.14$ Hz, H_X), 5.72–5.78 (1H, *m*, OCH₂-CH=CH), 6.33 (1H, *d*, $J = 8.43$ Hz, Ar-H), 6.87 (1H, *d*, $J = 9.90$ Hz, OCH₂-CH=CH), 6.93 (1H, *d*, $J = 8.43$ Hz, Ar-H), 7.31 (1H, *d*, $J = 7.33$ Hz, Ar-H), 7.46 (2H, *t*, $J = 7.33$ Hz, Ar-H), 7.51–7.53 (2H, *m*, Ar-H), 7.76 (2H, *d*, $J = 8.12$ Hz, Ar-H), 7.87–7.92 (4H, *m*, Ar-H), 7.95 (1H, *d*, $J = 8.55$ Hz, Ar-H), 8.03 (1H, *s*, Ar-H), 8.14 (1H, *s*, pyrazole-H), 11.39 (1H, *br.-s*, OH); ^{13}C NMR (100 MHz, CDCl_3 , δ / ppm): 41.0, 54.0, 65.5, 107.0, 110.2, 110.4, 119.0, 119.1, 125.8, 126.3, 126.4, 126.6, 127.0, 127.7, 127.7, 128.2, 128.4, 129.4, 130.3, 132.9, 133.3, 139.7, 150.9, 153.9, 155.2, 155.9. LC-MS (m/z) 485 ($[\text{M}+\text{H}]^+$, 100%).

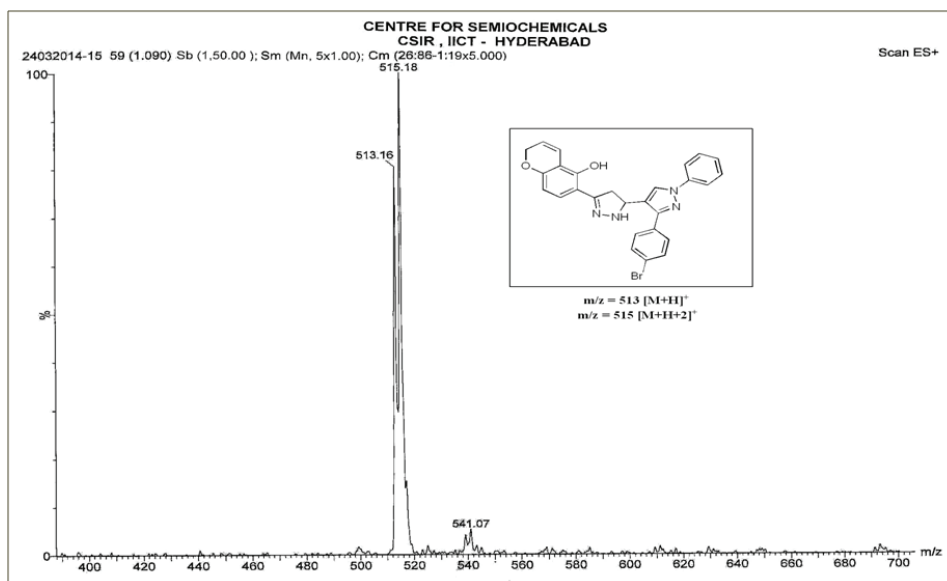
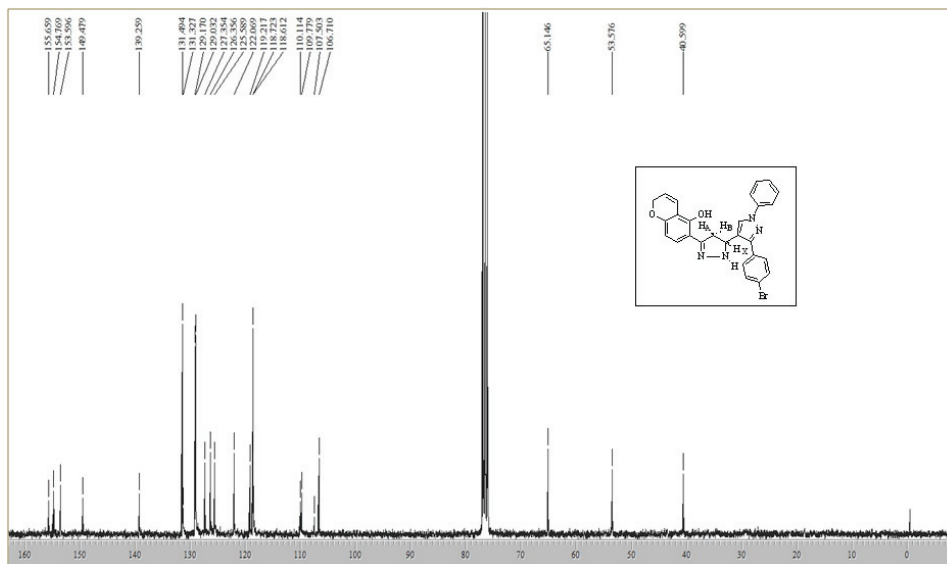
^1H -, ^{13}C -NMR and mass spectra of 6-[1,3-diphenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6a**)



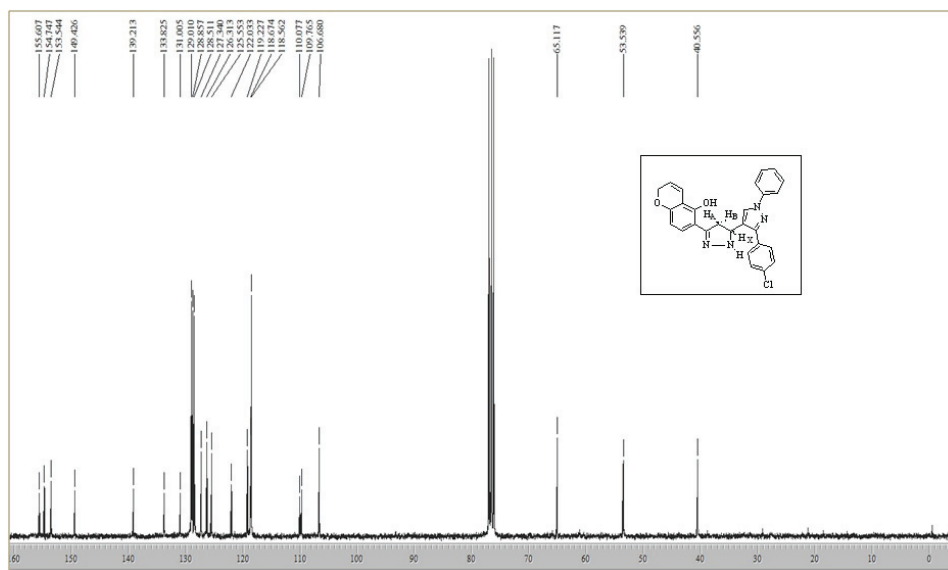
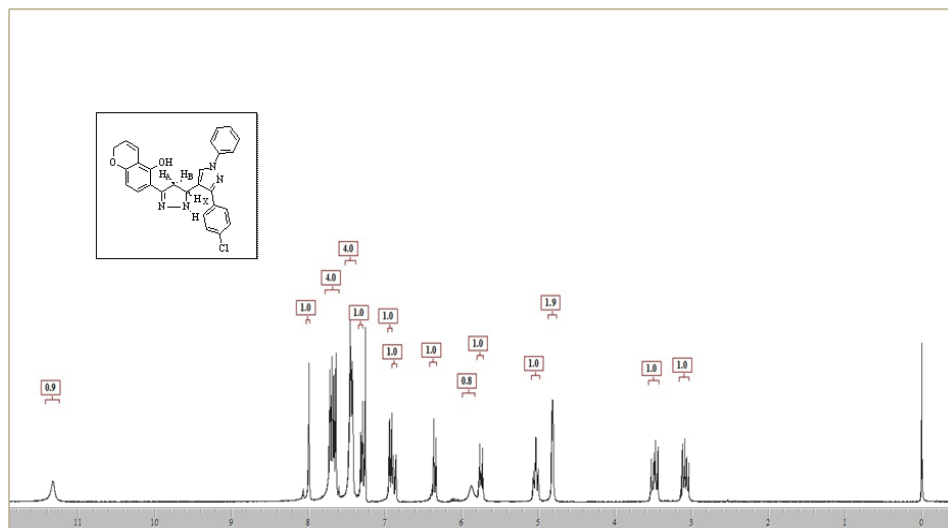


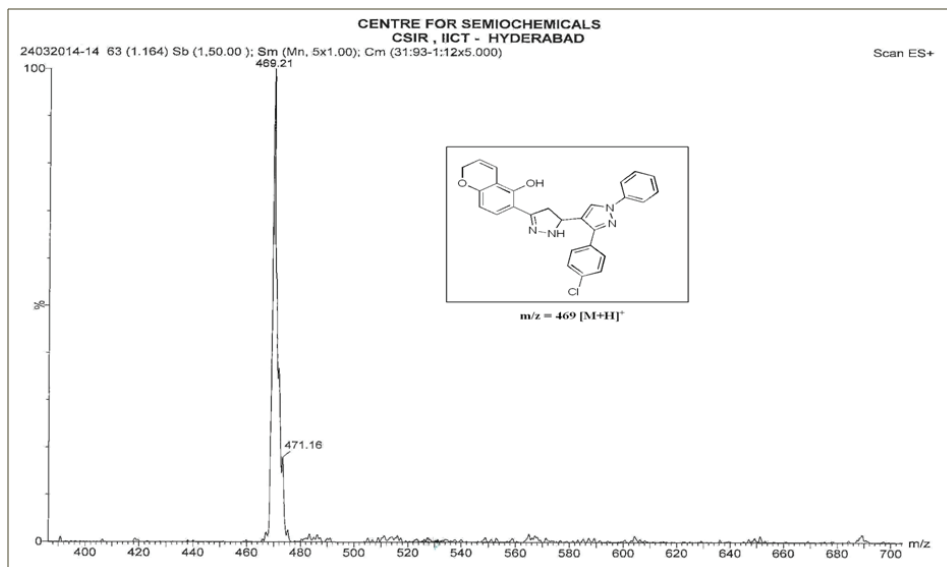
¹H-, *¹³C*-NMR and mass spectra of 6-[3-(4-bromophenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6b**)



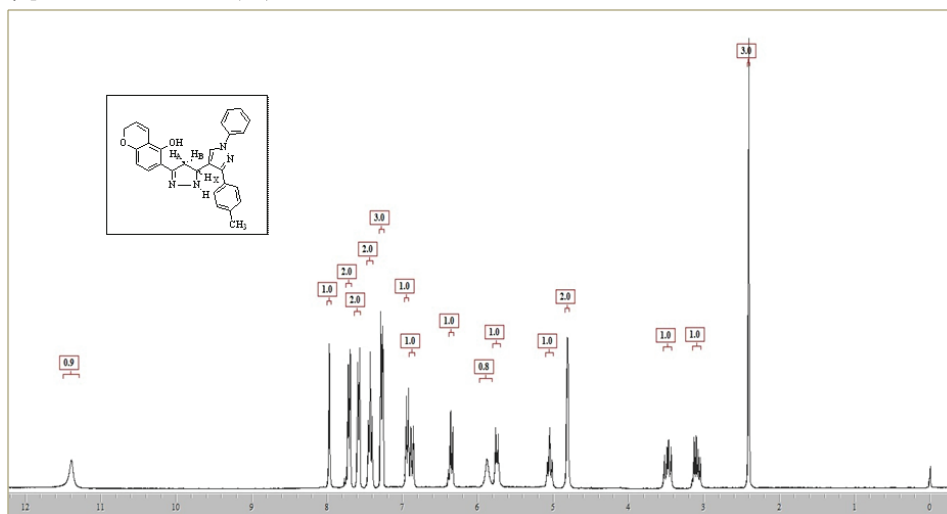


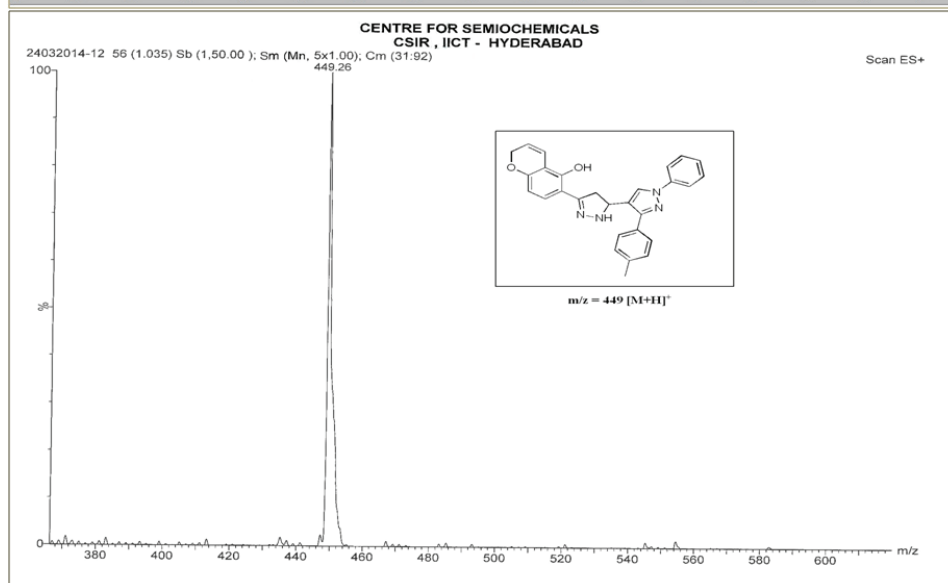
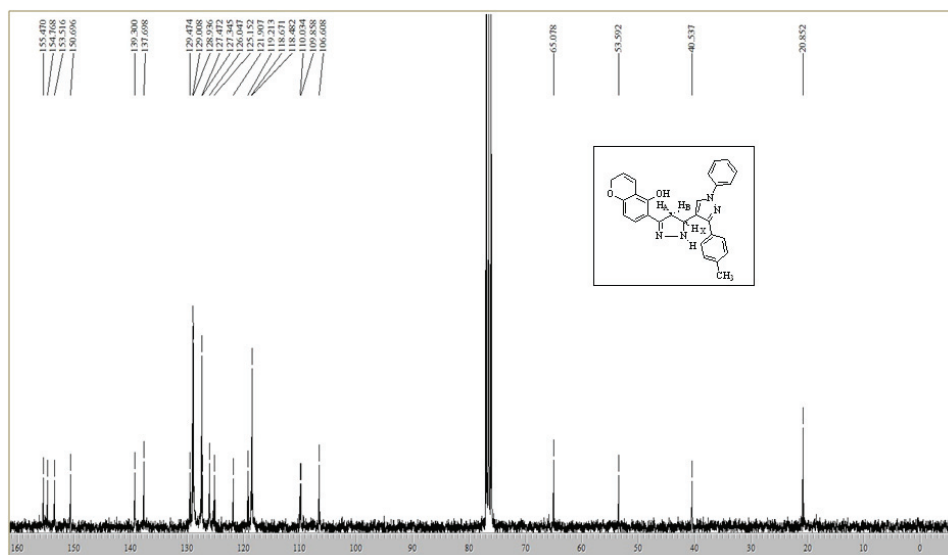
^1H -, ^{13}C -NMR and mass spectra of 6-[3-(4-chlorophenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6c**)



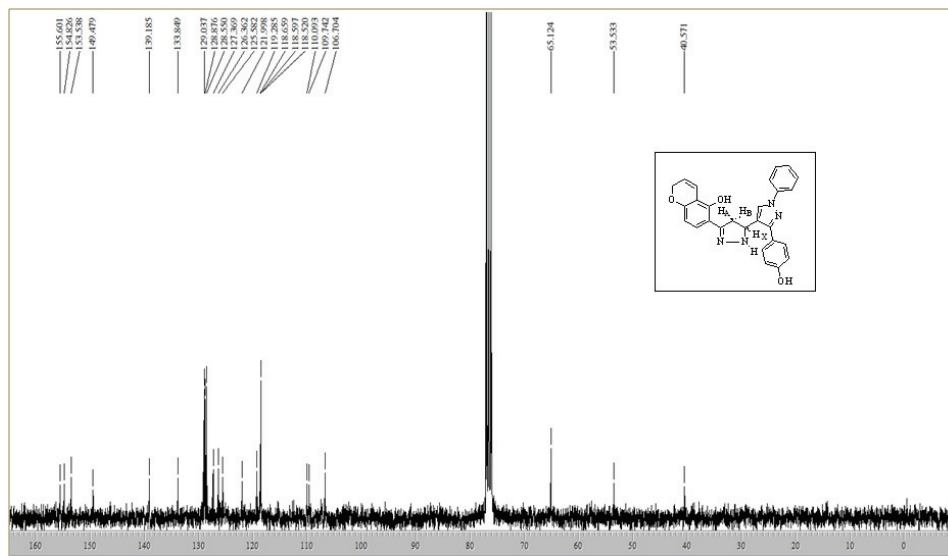
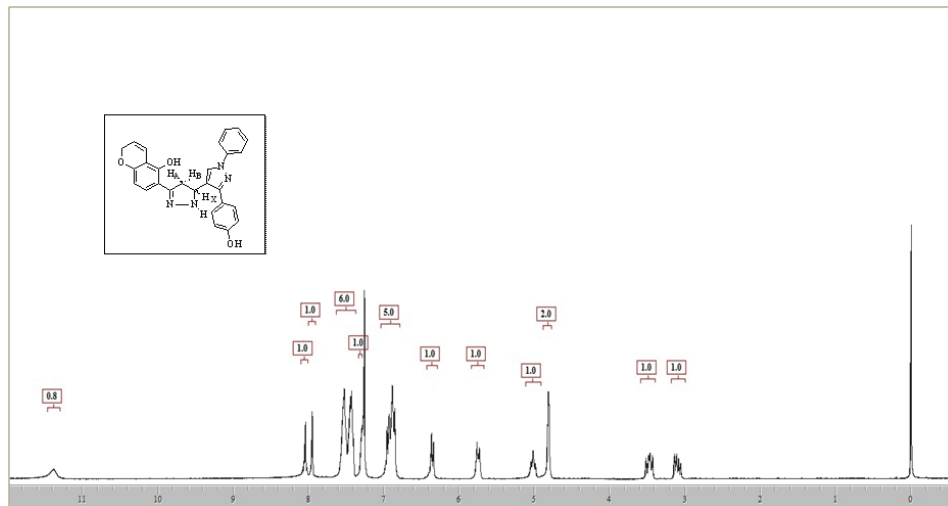


^1H -, ^{13}C -NMR and mass spectra of 6-[1-phenyl-3-p-tolyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6d**)

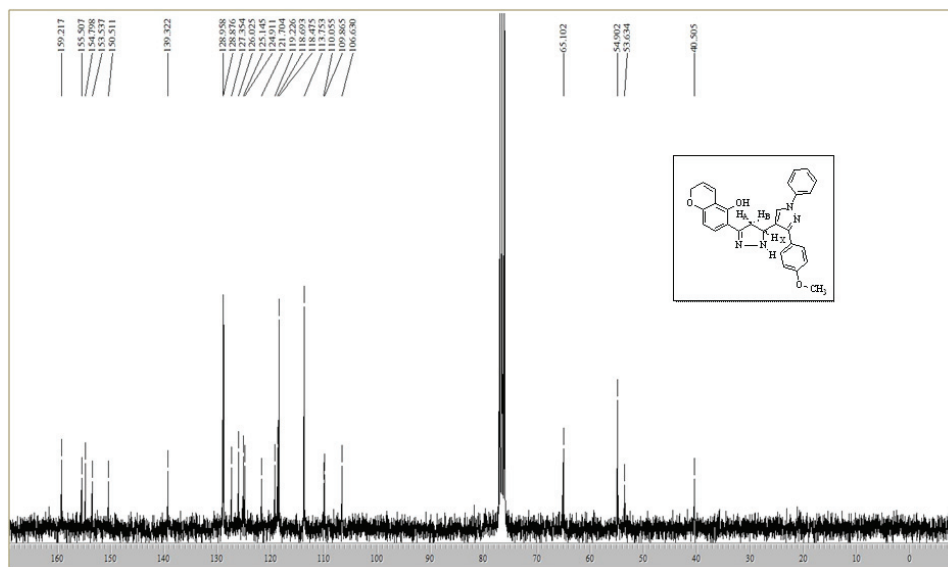
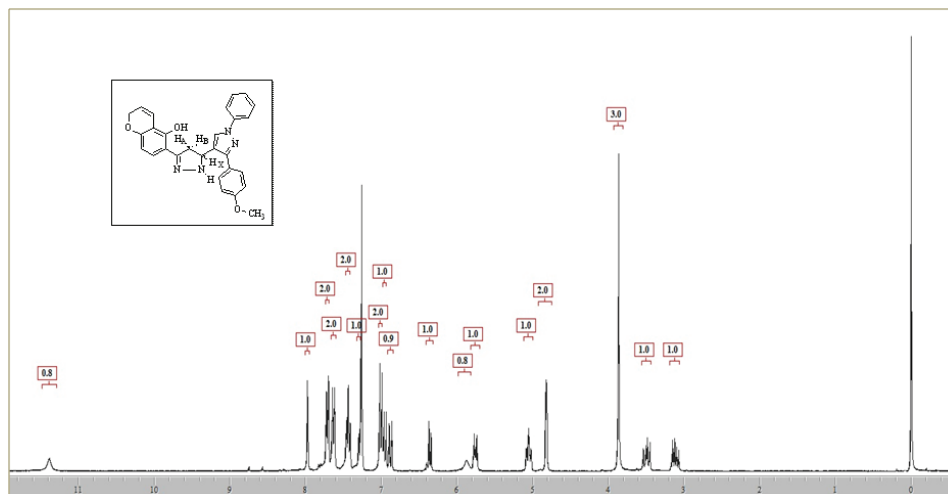




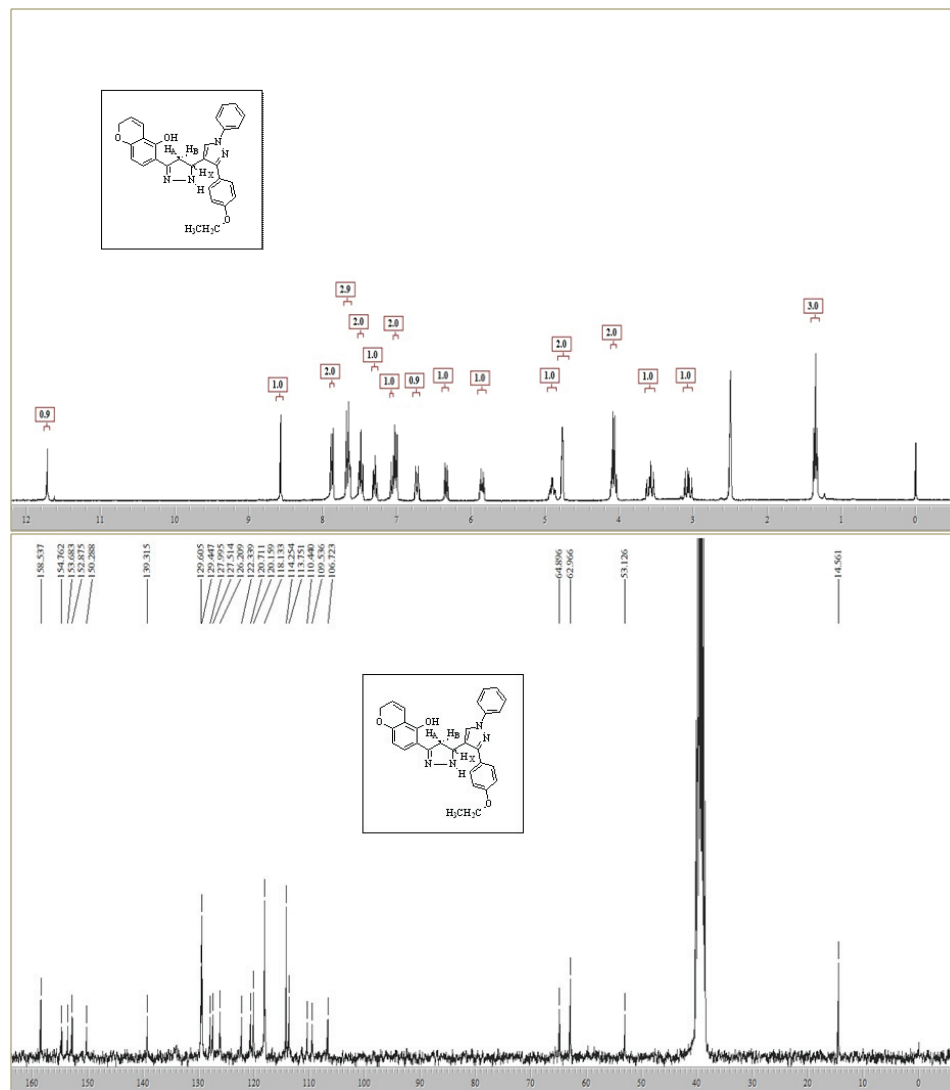
^1H - and ^{13}C -NMR spectra of 6-[3-(4-hydroxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6e**)

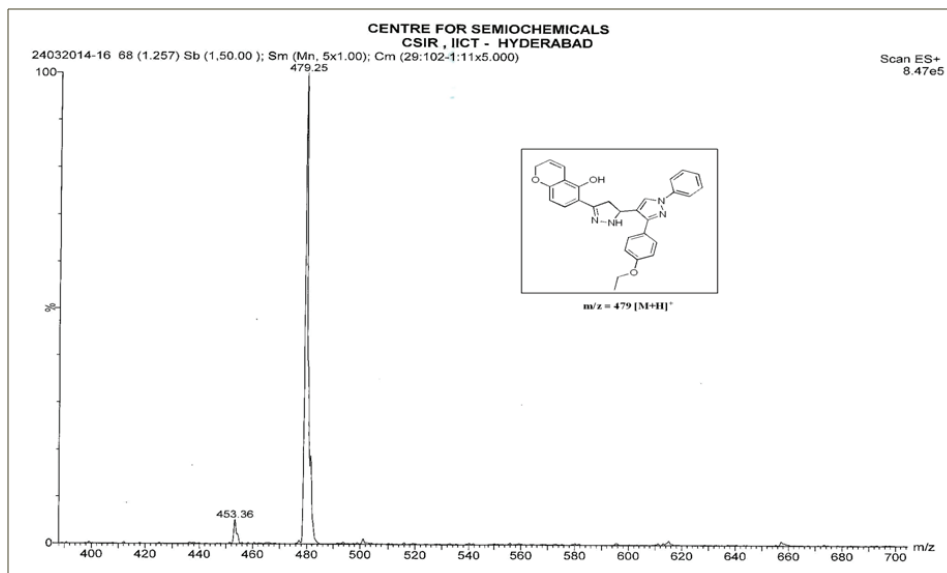


^1H -, ^{13}C -NMR spectra of 6-[3-(4-methoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6f**)

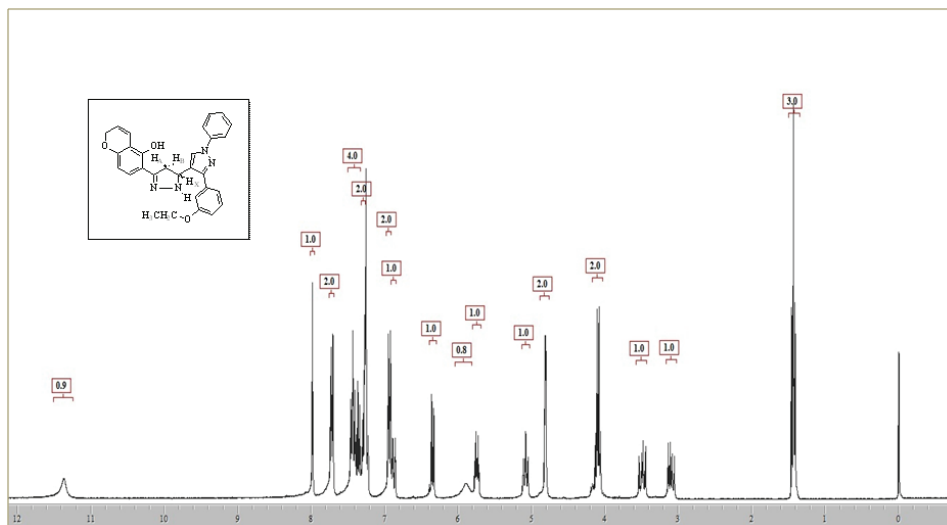


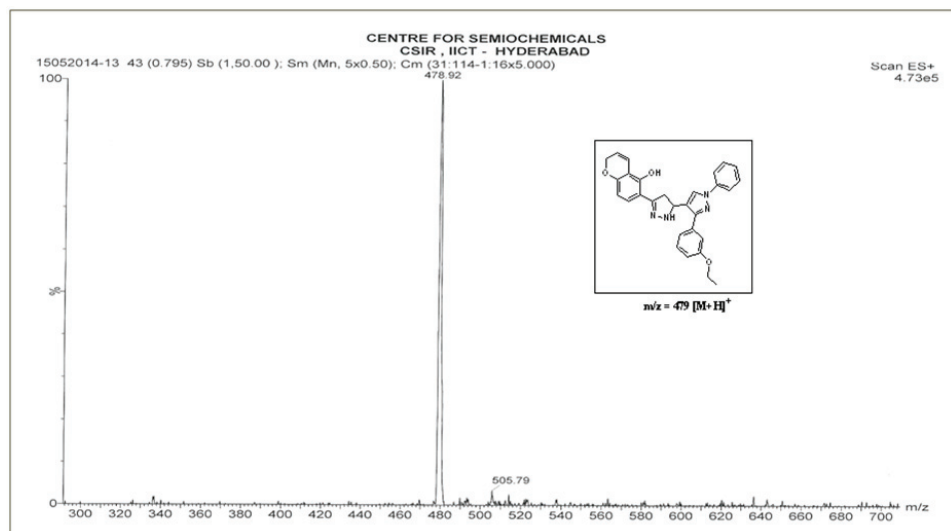
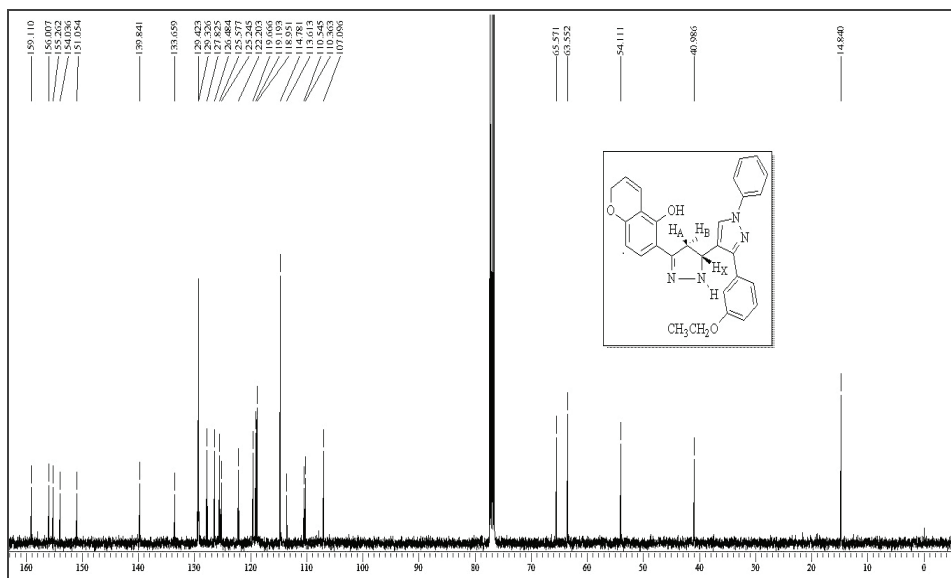
^1H -, ^{13}C -NMR and mass spectra of 6-[3-(4-ethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6g**)





¹H-, ¹³C-NMR and mass spectra of 6-[3-(3-ethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6h**)





^1H -, ^{13}C -NMR and mass spectra of 6-[3-(3,4-dimethoxyphenyl)-1-phenyl-4',5'-dihydro[4,5'-bi-1H-pyrazol]-3'-yl]-2H-chromen-5-ol (**6i**)

