

## **SUPPLEMENTARY MATERIAL**

### **Microwave assisted synthesis, characterization and investigation of antibacterial activity of 3-(5-(substituted-phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one derivatives**

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*Microwave assisted synthesis of 3-cinnamoyl-2H-chromen-2-one (2)*

Catalytic amount of piperidine (5 drops) was added to 3-acetyl coumarin (3.00 g, 16.00 mmol) followed by benzaldehyde (1.62 mL, 16.00 mmol). The mixture was swirled and was transferred into microwave oven where it was irradiated for 1 min. The completion of reaction was monitored using TLC (eluting solvent: Dichloromethane). The product was recrystallized from ethanol to afford compound **2**. The detail of the spectral data of reactive intermediates **2a-j** were as presented in supplementary material.

*3-Cinnamoyl-2H-chromen-2-one (2a)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), benzaldehyde (0.50 mL, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 3 min., 140 °C. Purification: recrystallization (ethanol).  $\lambda_{\max}$  (Log  $\epsilon$ ): 224 (3.99), 348 (3.47), 375 (3.01s). IR (KBr): 1740, 1673, 1606, 1363  $\text{cm}^{-1}$ .  $^1\text{H-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{H}}$ : 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.33-7.84 (m, 9H, Benzofused coumarin-4H and Ar-5H), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H).  $^{13}\text{C-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{C}}$ : 183.7 (C=O), 159.4 (C=O), 153.0, 147.2, 142.2, 135.2, 134.2, 128.6, 128.6, 128.5, 128.5, 128.3, 127.9, 127.9, 125.4, 125.4, 118.1, 116.1 ppm. MS:  $m/z$  276 ( $\text{M}^+$ , 75%), 199 (60%), 173 (100%).

*3-(3-(4-dimethylaminophenyl)acryloyl)-2H-chromen-2-one (2b)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), 4-(*N,N*-dimethylamino)benzaldehyde (1.27 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 2½ min., 140 °C. Purification: recrystallization (ethanol).  $\lambda_{\max}$  (Log  $\epsilon$ ): 208 (4.00), 327 (3.90s), 344 (3.97), 448 (3.84). IR (KBr): 1746, 1685, 1594, 1375  $\text{cm}^{-1}$ .  $^1\text{H-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{H}}$ : 3.06 (s, 6H, 2 ×  $\text{CH}_3$ ), 6.71 (d, 2H, Ar-H), 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.72 (d, 2H, Ar-H), 7.42-7.84 (m, 4H, Ar-H), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H).  $^{13}\text{C-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{C}}$ : 183.7 (C=O), 159.4 (C=O), 153.0, 150.3, 147.2, 142.2, 134.2, 129.7, 129.7, 128.3, 127.9, 125.4, 125.4, 124.7, 118.1, 116.1, 111.7, 111.7, 41.3 (2 ×  $\text{CH}_3$ ) ppm. MS:  $m/z$  319 ( $\text{M}^+$ , 70 %), 199 (100%).

*3-(3-(4-hydroxy-3-methoxyphenyl)acryloyl)-2H-chromen-2-one (2c)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), vanillin (0.81 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 1 min., 140 °C. Purification: recrystallization (ethanol).  $\lambda_{\max}$  (Log  $\epsilon$ ): 208 (4.03), 244 (3.91), 352 (3.42). IR (KBr): 1740, 1685, 1600, 1338  $\text{cm}^{-1}$ .  $^1\text{H-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{H}}$ : 3.83 (s, 3H,  $\text{OCH}_3$ ), 5.35 (s, 1H, OH,  $\text{D}_2\text{O}$  exchangeable), 6.79 (d, 1H, Ar-H), 6.99 (d, 1H, Ar-H), 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.16 (s, 1H, Ar-H), 7.42-7.84 (m, 4H, Benzofused coumarin-H), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H).  $^{13}\text{C-NMR}$  ( $\text{CD}_3\text{OD}$ , 400 Hz)  $\delta_{\text{C}}$ : 183.7 (C=O), 159.4 (C=O), 153.0, 149.1 ( $\underline{\text{C}}-\text{OCH}_3$ ), 147.9 (C-OH), 147.2, 142.2, 134.2, 128.3, 127.9, 127.6, 125.4, 125.4, 122.9, 118.1, 116.8, 116.1, 111.9, 56.1( $\text{OCH}_3$ ) ppm. MS:  $m/z$  323 ( $\text{M}^+$ , 68%), 275 (60%), 199 (50%).

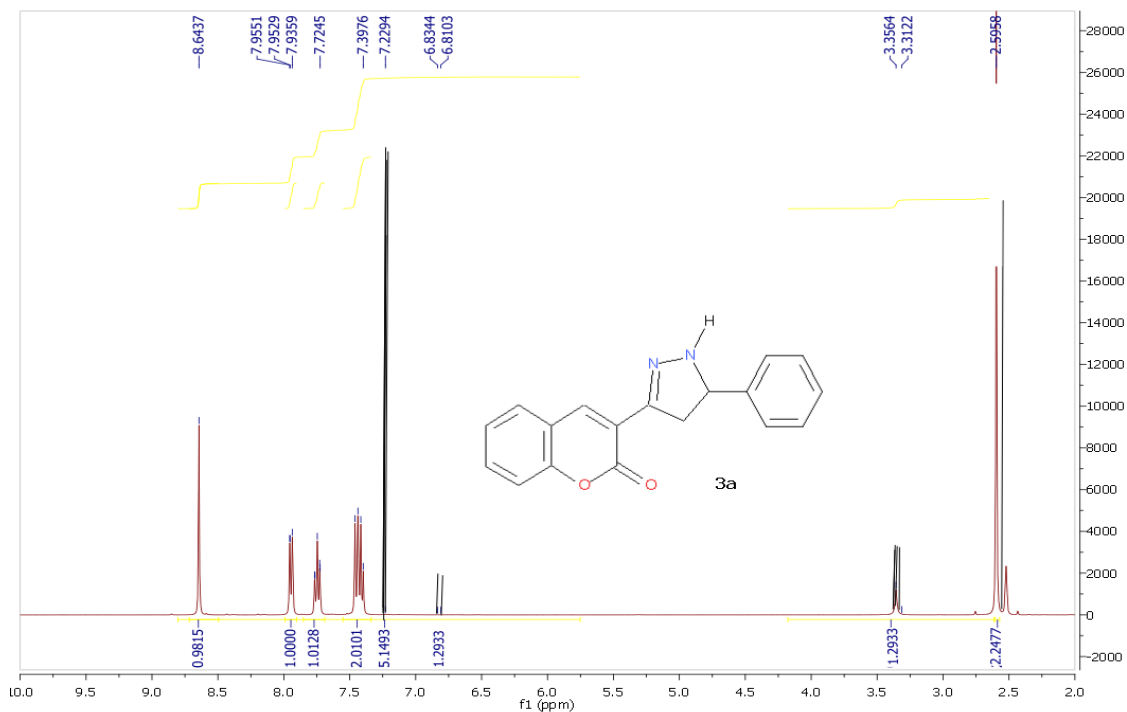
*3-(3-(4-chlorophenyl)acryloyl)-2H-chromen-2-one (2e)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), *p*-chlorobenzaldehyde (0.74 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 1½ min., 140 °C. Purification: recrystallization (methanol).  $^1\text{H-}$

NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{H}}$ : 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 7.44 (d, 2H, Ar-H), 7.68 (d, 2H, Ar-H), 7.42-7.84 (m, 4H, Benzofused coumarin-H), 8.57 (s, 1H, Coumarin-H). <sup>13</sup>C-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{C}}$ : 183.7, 159.4, 153.0, 147.2, 142.2, 134.2, 133.5, 133.3, 129.0, 129.0, 128.7, 128.7, 128.3, 127.9, 125.4, 125.4, 118.1, 116.1 ppm. MS:  $m/z$  310.5 (M<sup>+</sup>, 80%), 275 (40%).

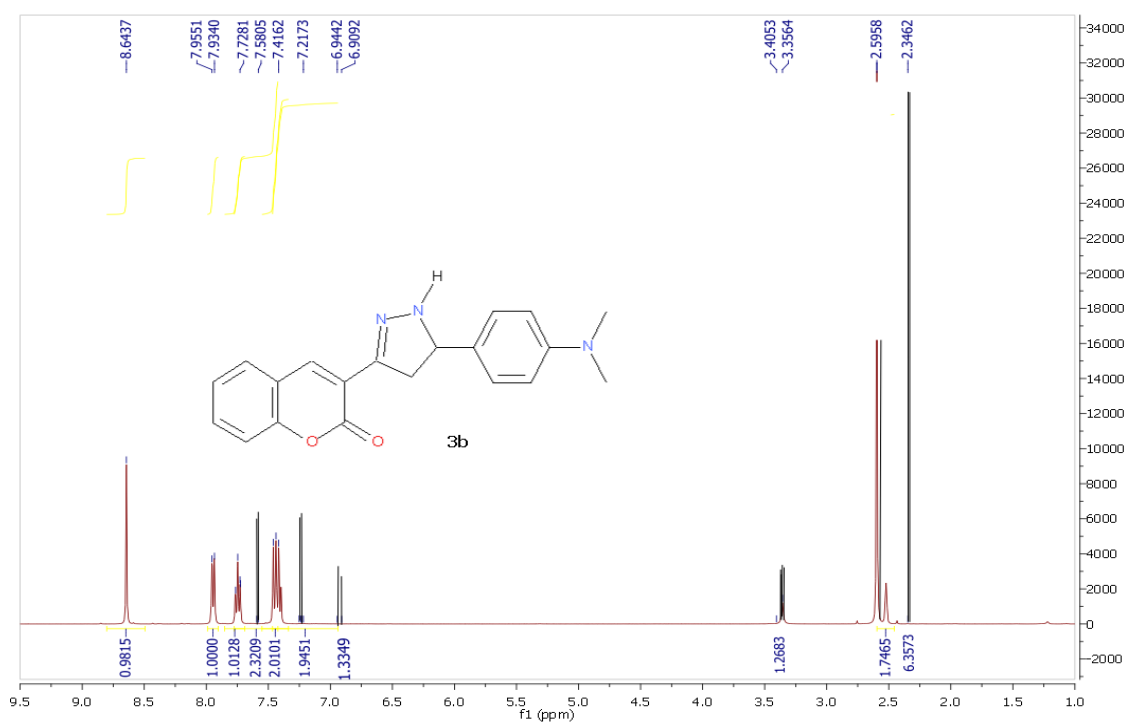
*3-(3-(3-hydroxyphenyl)acryloyl)-2H-chromen-2-one (2f)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), *m*-hydroxybenzaldehyde (0.65 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 2 min., 140 °C. Purification: recrystallization (methanol).  $\lambda_{\text{max}}$  (Log  $\epsilon$ ): 208 (3.82), 280 (3.32), 348 (3.46), 361 (3.46), 369 (3.45). IR (KBr): 3302, 1703, 1648, 1600, 1375 cm<sup>-1</sup>. <sup>1</sup>H-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{H}}$ : 5.35 (s, 1H, OH, D<sub>2</sub>O exchangeable), 6.70 (s, 1H, Ar-H), 6.83 (d, 1H, Ar-H), 7.03 (d, 1H,  $J = 8.8$  Hz, CO-CH=C), 7.16 (d, 1H, Ar-H), 7.42-7.84 (m, 4H, Benzofused coumarin-H), 7.53 (t, 1H, Ar-H), 7.96 (d, 1H,  $J = 8.8$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H). <sup>13</sup>C-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{C}}$ : 183.7 (C=O), 159.4 (C=O), 158.4, 153.0, 147.2, 142.2, 135.4, 134.2, 130.0, 128.3, 127.9, 125.4, 125.4, 121.1, 118.1, 117.6, 116.1, 115.1 ppm. MS:  $m/z$  292 (M<sup>+</sup>, 30%), 275 (50%), 199 (25%), 145 (100%).

*3-(3-(4-hydroxyphenyl)acryloyl)-2H-chromen-2-one (2g)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), *p*-hydroxybenzaldehyde (0.65 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 3 min., 140 °C. Purification: recrystallization (ethanol).  $\lambda_{\text{max}}$  (Log  $\epsilon$ ): 211 (3.52), 336 (3.41), 368 (3.56). IR (KBr): 3241, 1734, 1685, 1612, 1375 cm<sup>-1</sup>. <sup>1</sup>H-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{H}}$ : 5.35 (s, 1H, OH, D<sub>2</sub>O exchangeable), 6.65 (d, 2H, Ar-H), 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.42-7.84 (m, 4H, Benzofused coumarin-H), 7.56 (d, 2H, Ar-H), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H). <sup>13</sup>C-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{C}}$ : 183.7, 159.4, 157.7 (C-OH), 153.0, 147.2, 142.2, 134.2, 130.6, 130.6, 128.3, 127.9, 127.8, 125.4, 125.4, 118.1, 116.1, 115.8 ppm. MS:  $m/z$  292 (M<sup>+</sup>, 40%), 275 (75%), 199 (50%), 145 (100%).

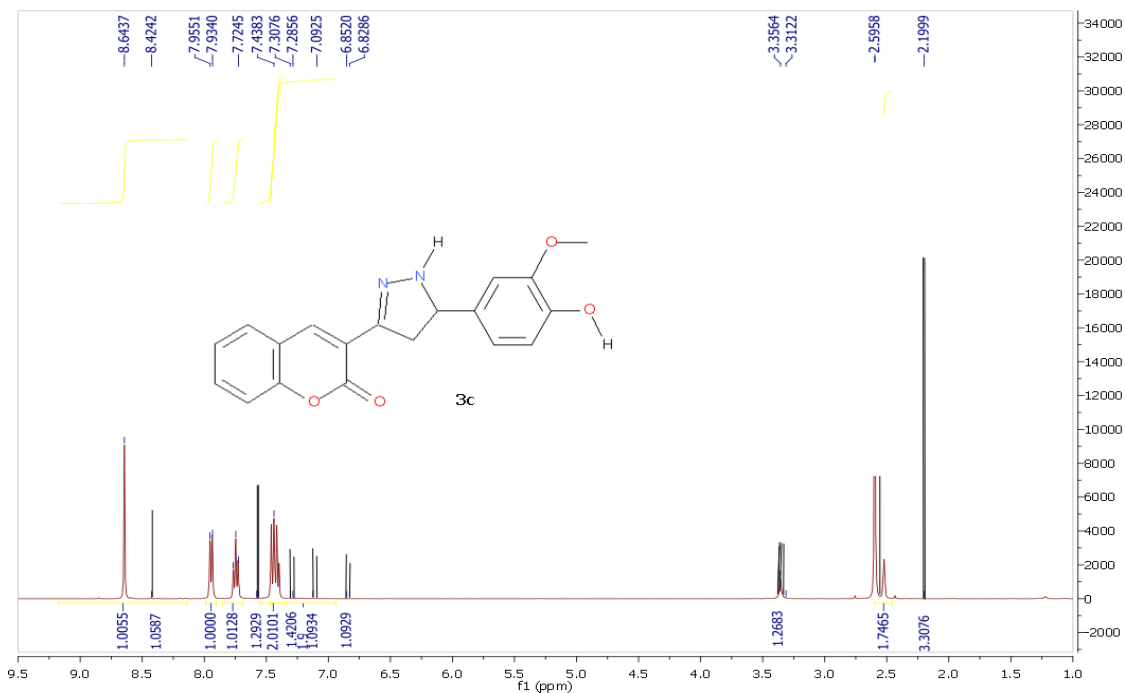
*3-(3-(4-(diethylamino)phenyl)acryloyl)-2H-chromen-2-one (2j)*. Reagents: Compound **1** (1.00 g, 5.30 mmol), 4-(*N,N*-dimethylamino)benzaldehyde (1.01 g, 5.30 mmol), piperidine (0.20 mL). Conditions: MWI for 3 min., 140 °C. Purification: recrystallization (ethanol). <sup>1</sup>H-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{H}}$ : 2.33-2.32 (t,  $J = 2.44$  Hz, 4H, 2 × CH<sub>3</sub>-CH<sub>2</sub>), 3.14-3.13 (q,  $J = 2.44$  Hz, 4H, 2 × CH<sub>2</sub>-CH<sub>3</sub>), 6.71 (d, 2H, Ar-H), 7.03 (d, 1H,  $J = 8.5$  Hz, CO-CH=C), 7.72 (d, 2H, Ar-H), 7.42-7.84 (m, 4H, Ar-H), 7.82 (d, 1H,  $J = 8.5$  Hz, CO-C=CH), 8.57 (s, 1H, Coumarin-H). <sup>13</sup>C-NMR (CD<sub>3</sub>OD, 400 Hz)  $\delta_{\text{C}}$ : 183.7 (C=O), 159.4 (C=O), 153.0, 150.3, 147.2, 142.2, 134.2, 129.7, 129.7, 128.3, 127.9, 125.4, 125.4, 124.7, 118.1, 116.1, 111.7, 111.7, 50.8 (2 × CH<sub>2</sub>), 19.5 (2 × CH<sub>3</sub>) ppm.  $\lambda_{\text{max}}$  (Log  $\epsilon$ ): 208 (4.00), 327 (3.90s), 344 (3.97), 448 (3.84). IR (KBr): 2925 (CH aliphatic), 1746 (C=O of ester), 1690 (C=O of conjugated ketone), 1594, 1375 (C-O), 1226 (C-N), 725 (Ar-H) cm<sup>-1</sup>.



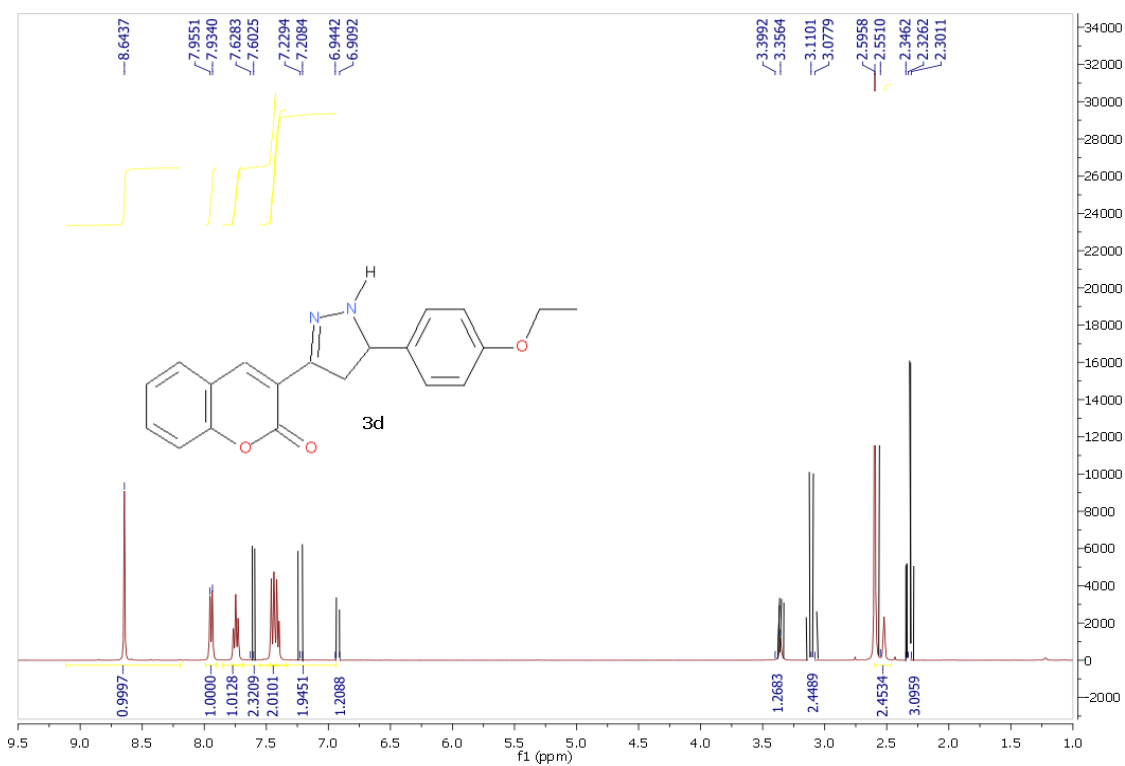
**Fig. S1:**  $^1\text{H}$  NMR spectrum of 3-(5-phenyl-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3a**.



**Fig. S2:**  $^1\text{H}$  NMR spectrum of 3-(5-(4-(dimethylamino)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3b**



**Fig. S3:**  $^1\text{H}$  NMR spectrum of 3-(5-(4-hydroxy-3-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3c**



**Fig. S4:**  $^1\text{H}$  NMR spectrum of 3-(5-(4-ethoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3d**

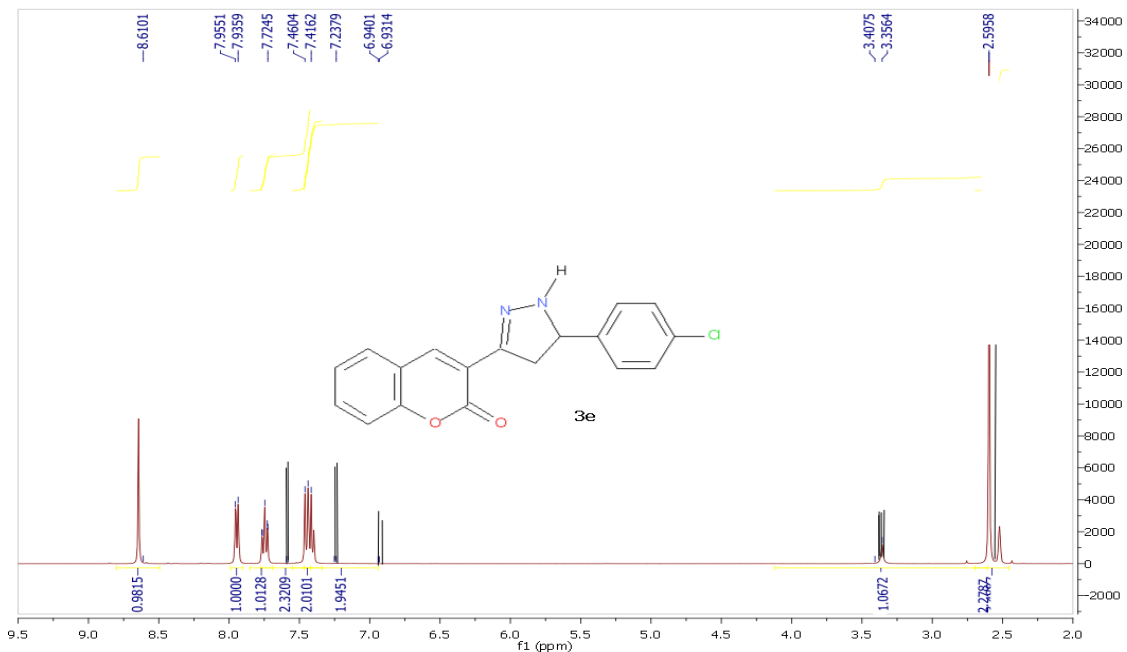


Fig. S5:  $^1\text{H}$  NMR spectrum of 3-(5-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3e**

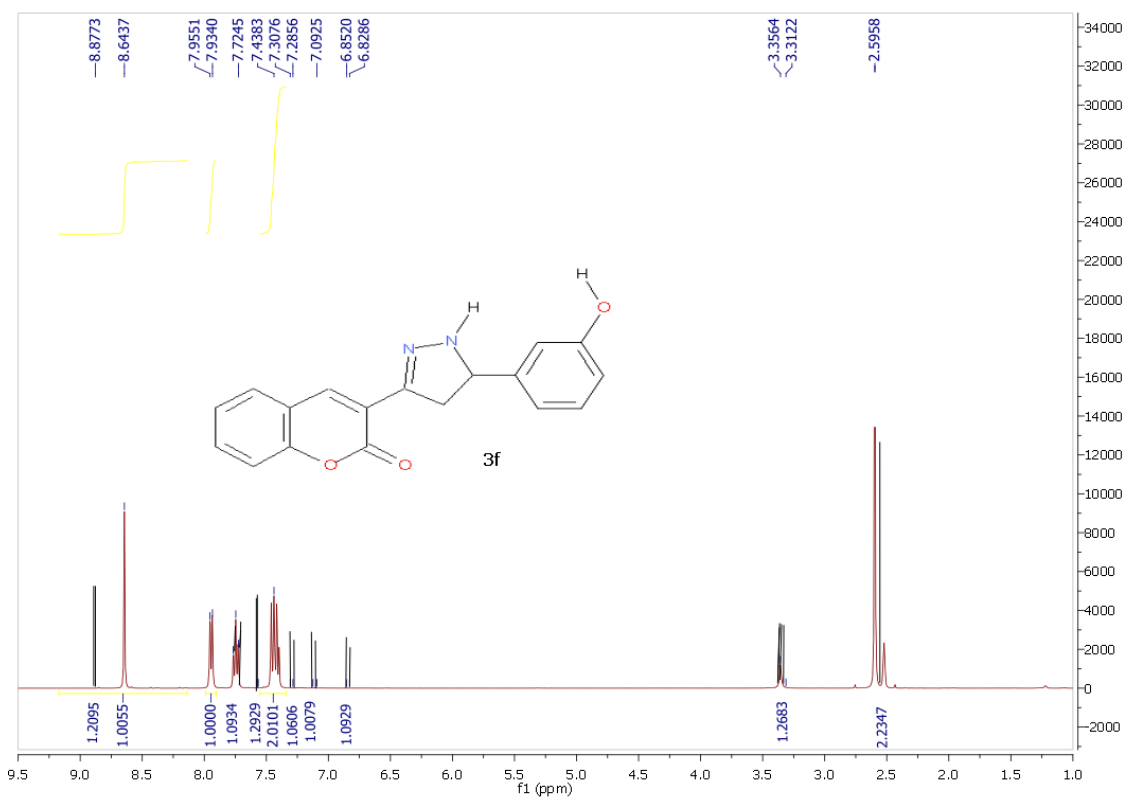
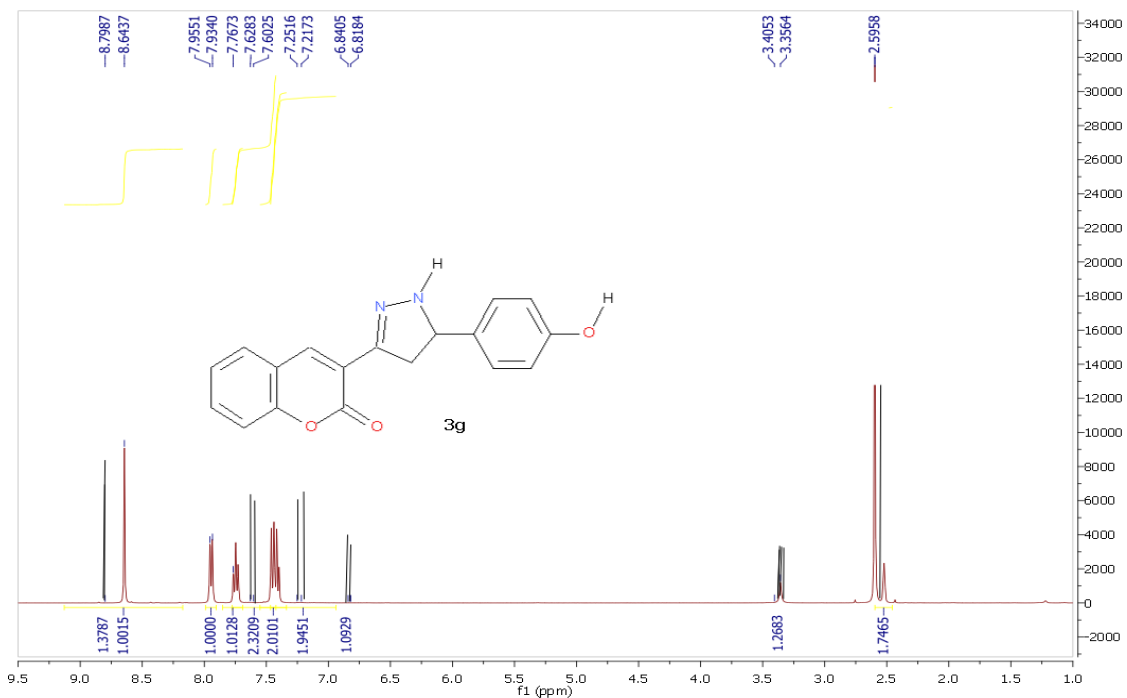
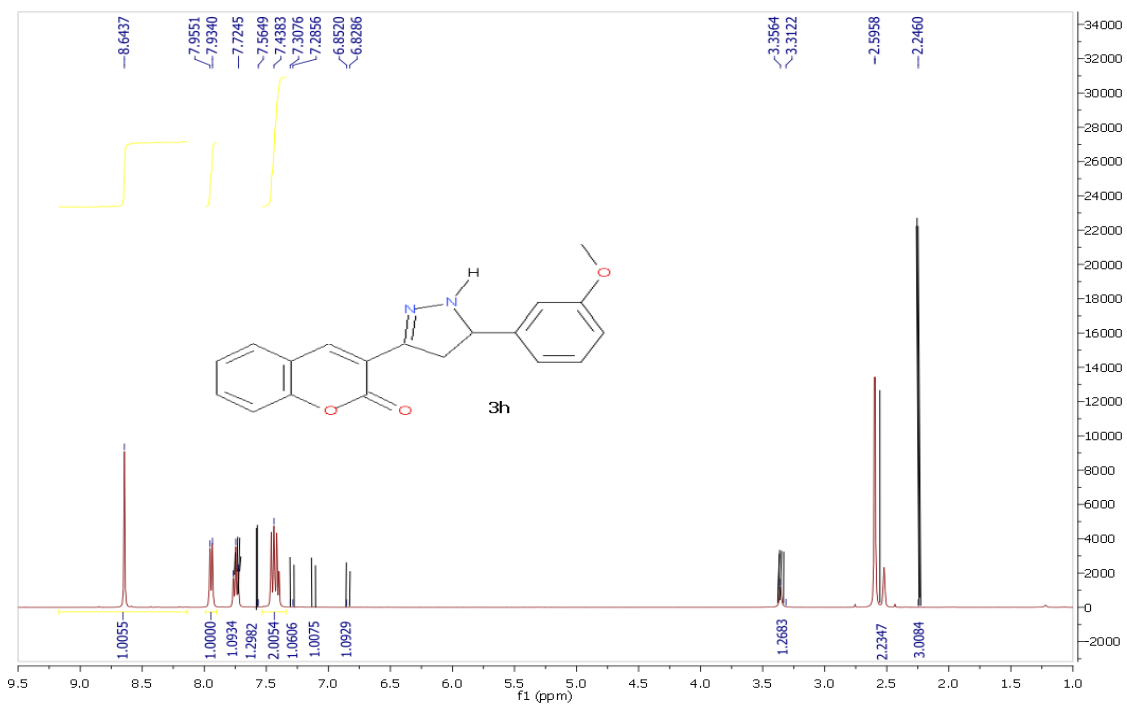


Fig. S6:  $^1\text{H}$  NMR spectrum of 3-(5-(3-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3f**

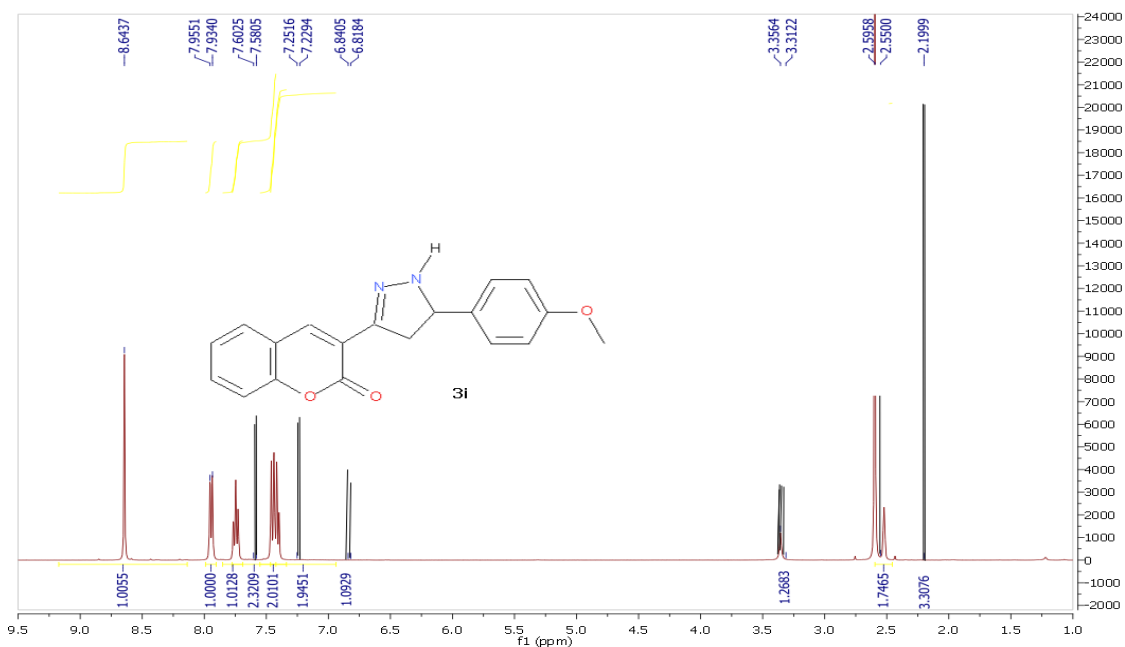


**Fig.S7:** <sup>1</sup>H NMR spectrum of 3-(5-(4-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3g**

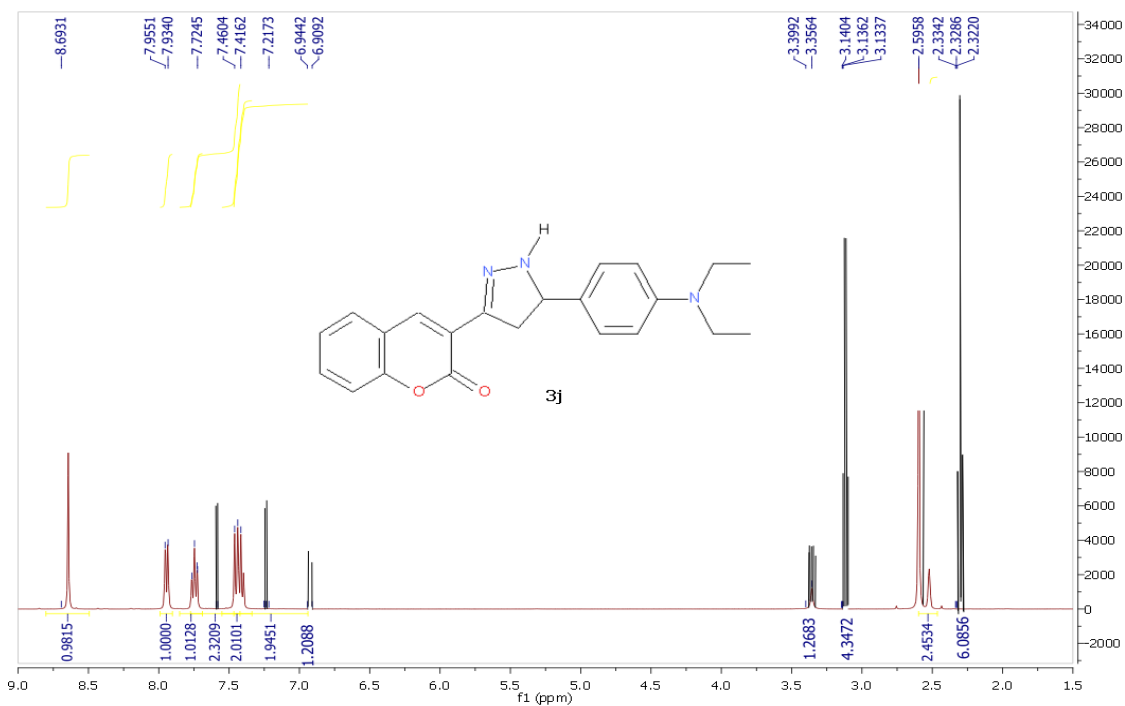


**Fig. S8:** <sup>1</sup>H NMR spectrum of 3-(5-(3-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3h**

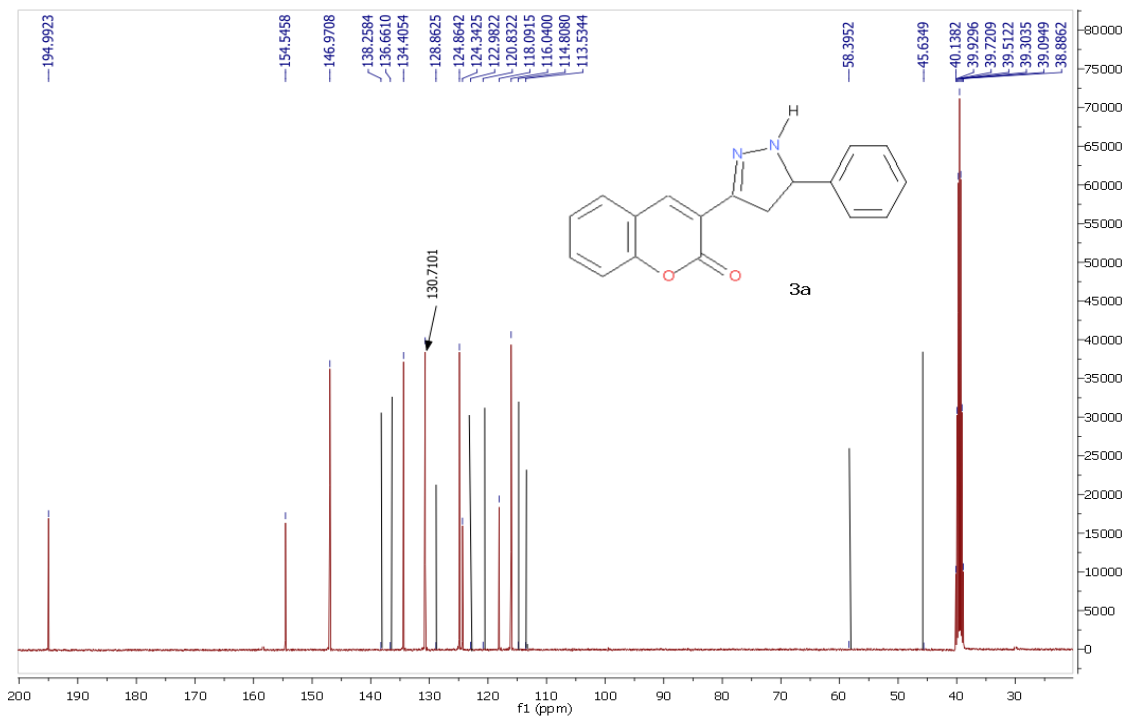




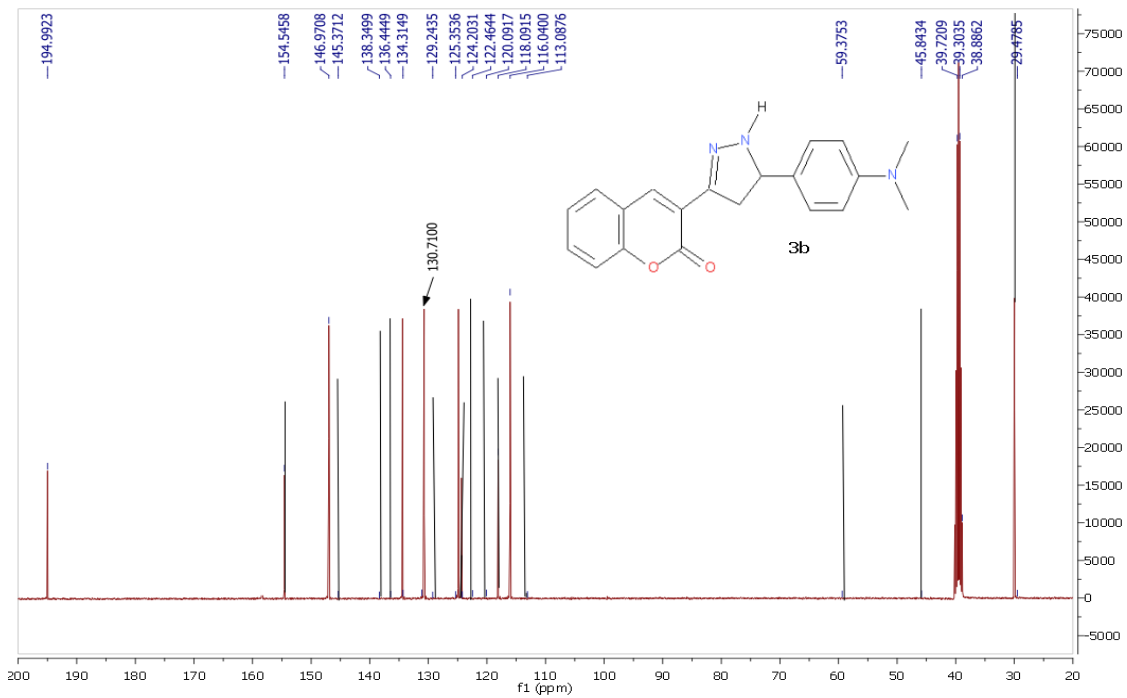
**Fig. S9:**  $^1\text{H}$  NMR spectrum of 3-(5-(4-methoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3i**



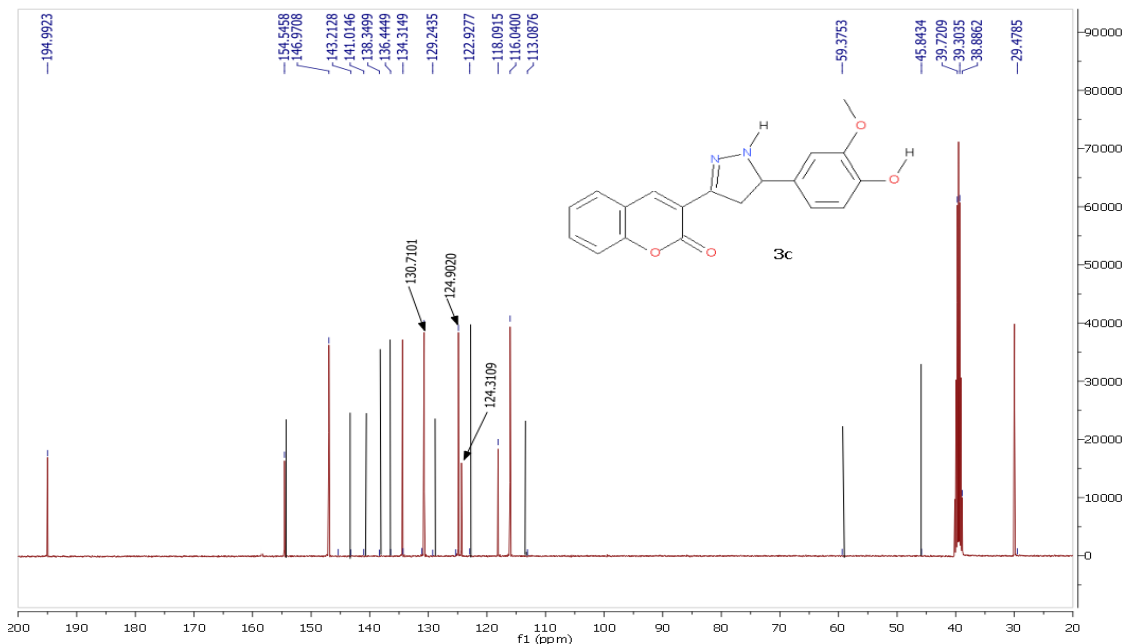
**Fig. S10:**  $^1\text{H}$  NMR spectrum of 3-(5-(4-(diethylamino)phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3j**



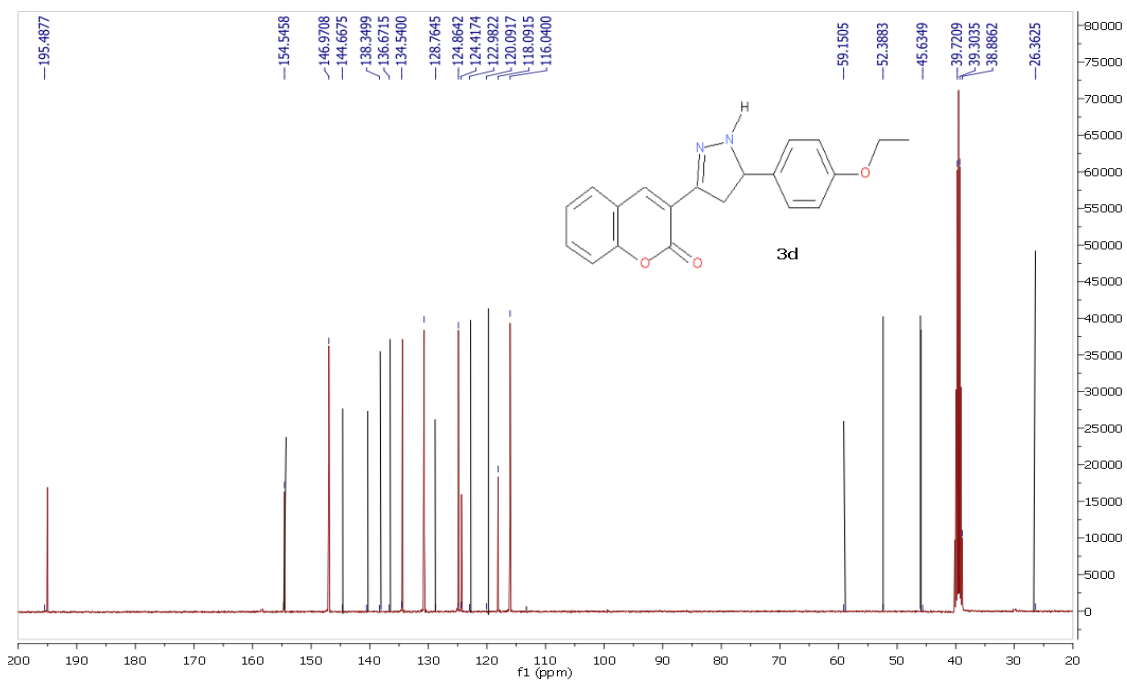
**Fig. S11:**  $^{13}\text{C}$  NMR spectrum of 3-(5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3a**.



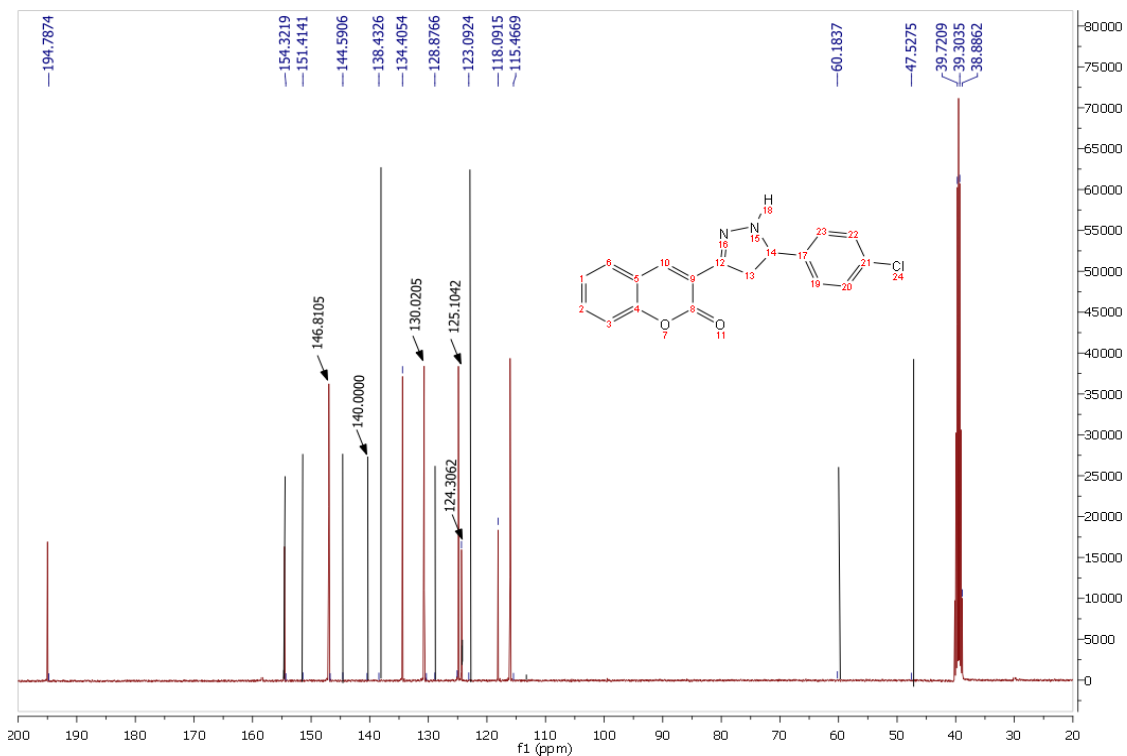
**Fig. S12:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-(dimethylamino)phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3b**



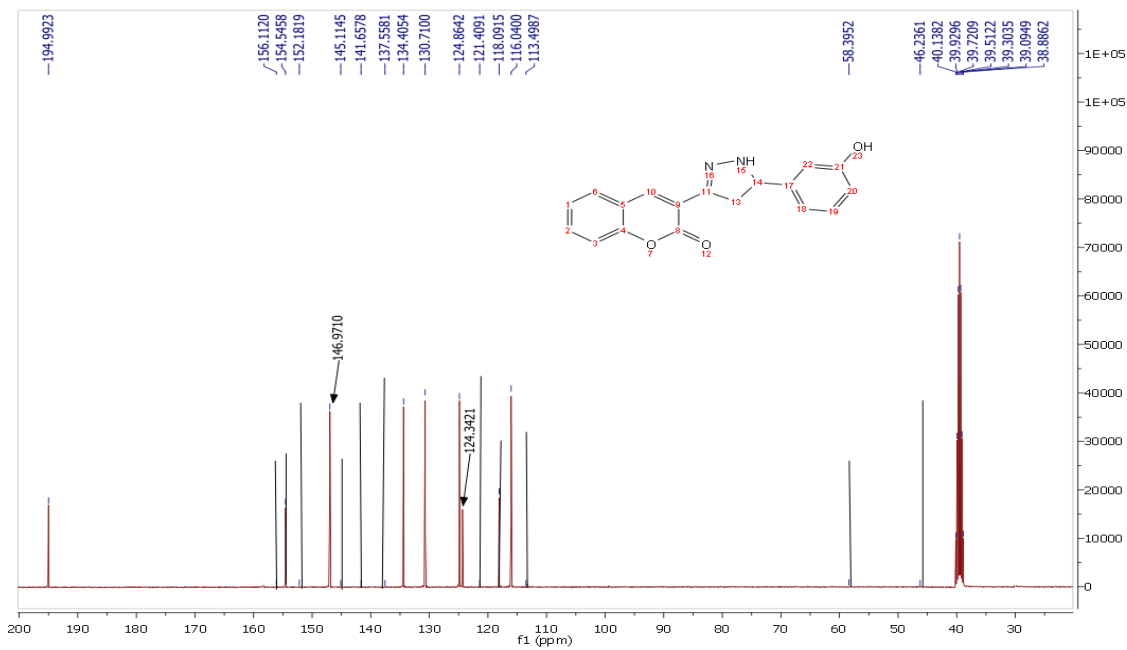
**Fig. S13:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-hydroxy-3-methoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3c**



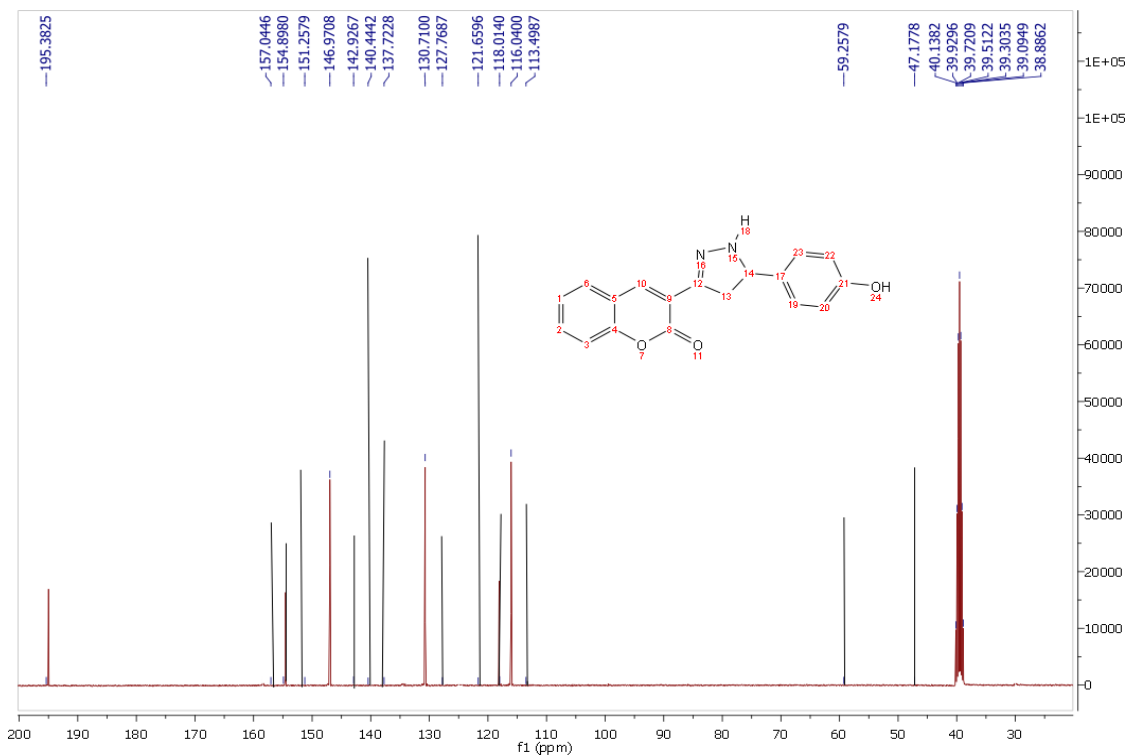
**Fig. S14:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-ethoxyphenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3d**



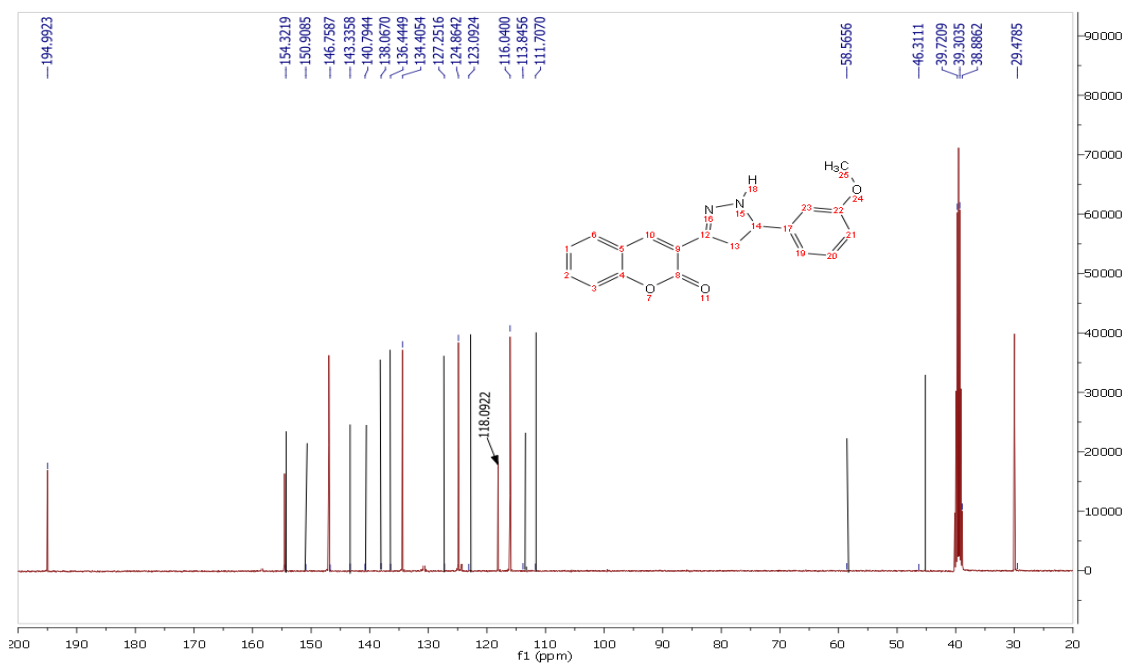
**Fig. S15:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3e**



**Fig. S16:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(3-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3f**



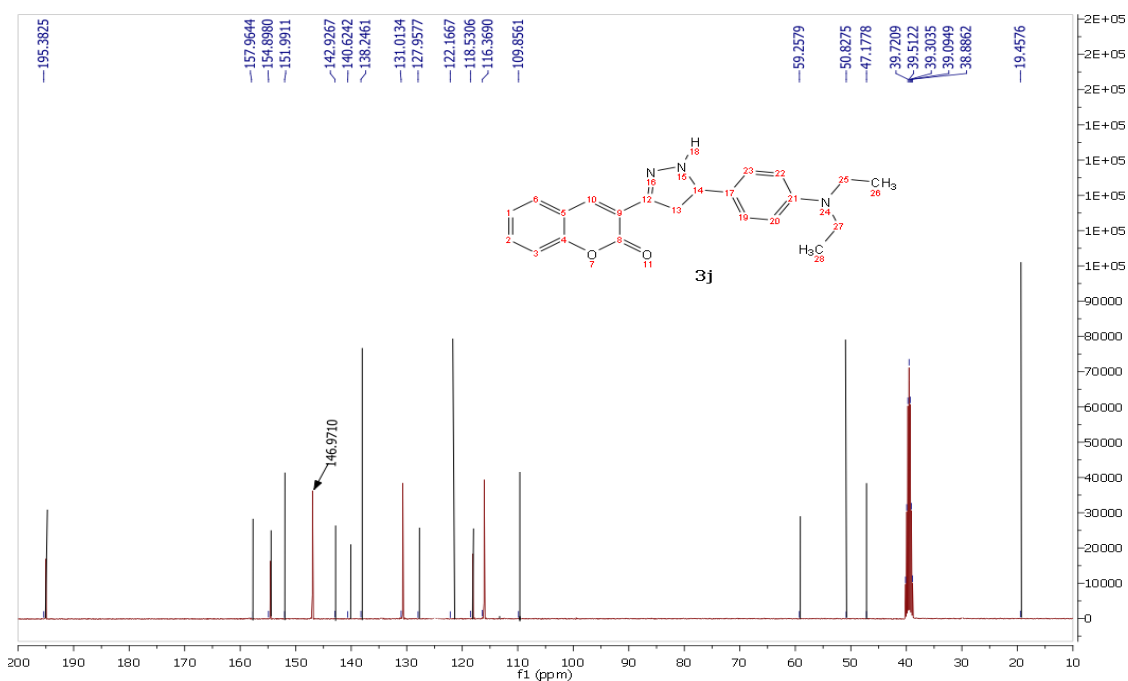
**Fig.S17:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3g**



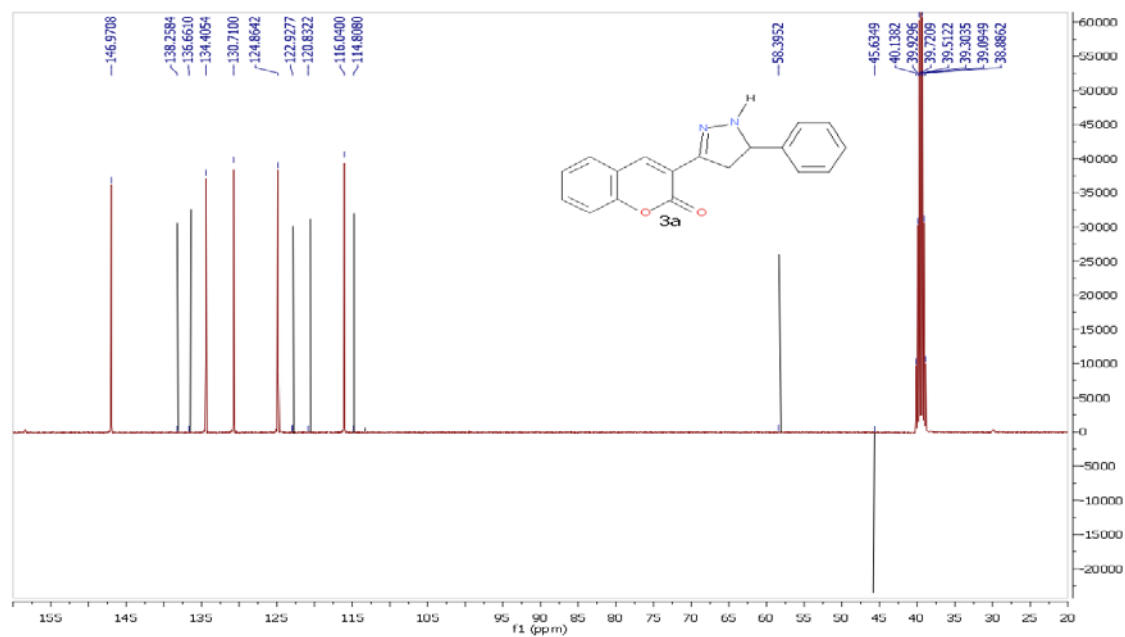
**Fig. S18:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(3-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3h**



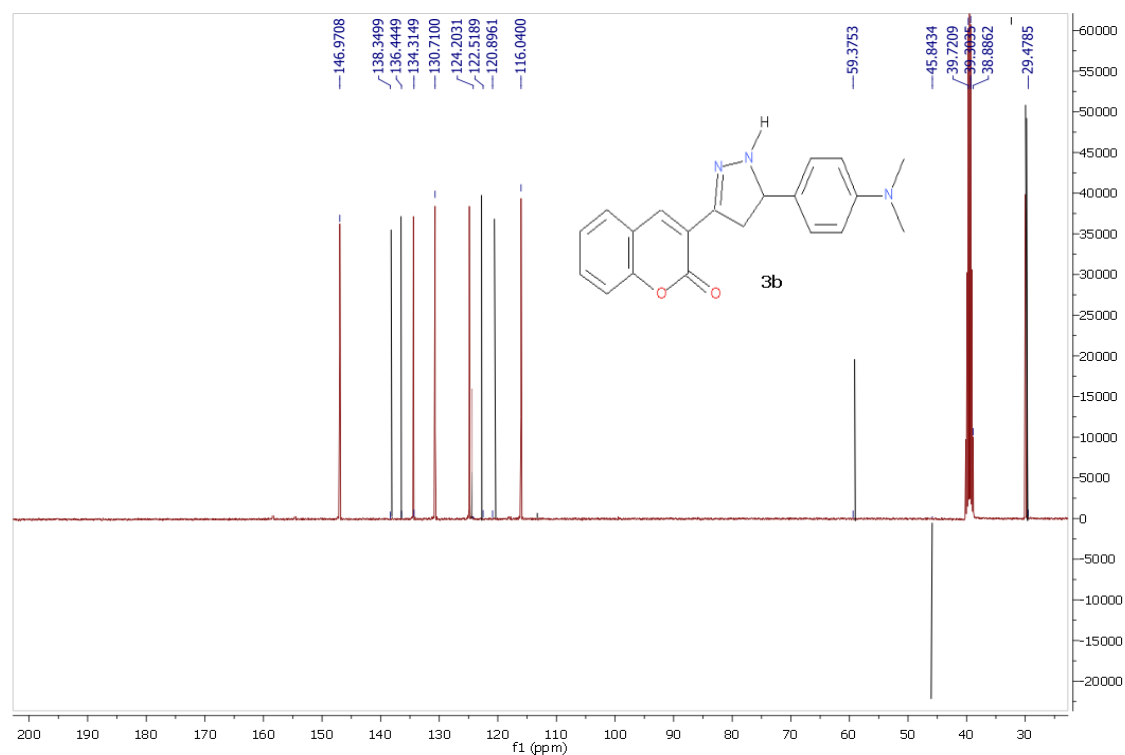
**Fig. S19:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3i**



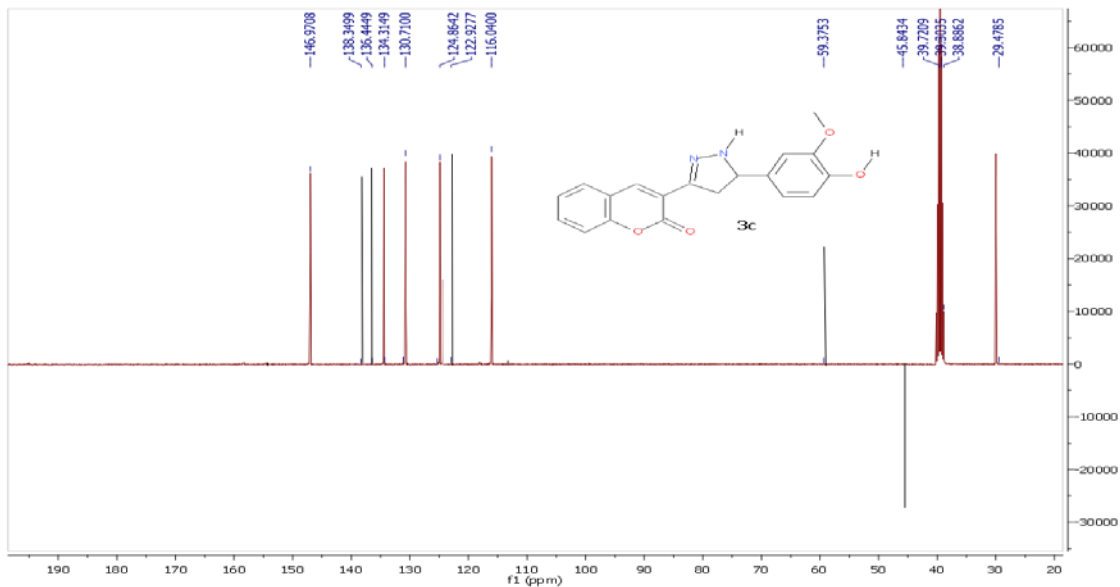
**Fig. S20:**  $^{13}\text{C}$  NMR spectrum of 3-(5-(4-(diethylamino)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3j**



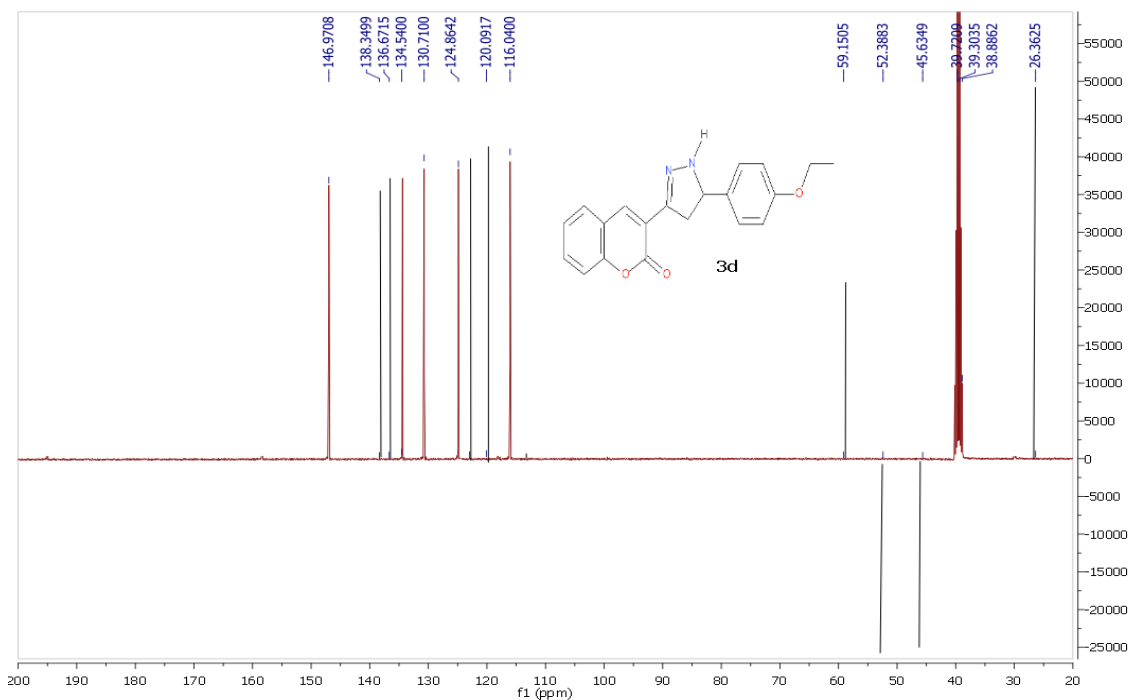
**Fig. S21:** DEPT 135 NMR spectrum of 3-(5-phenyl-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3a**.



**Fig. S22:** DEPT 135 NMR spectrum of 3-(5-(4-(dimethylamino)phenyl)-4,5-dihydro-1*H*-pyrazol-3-yl)-2*H*-chromen-2-one, **3b**

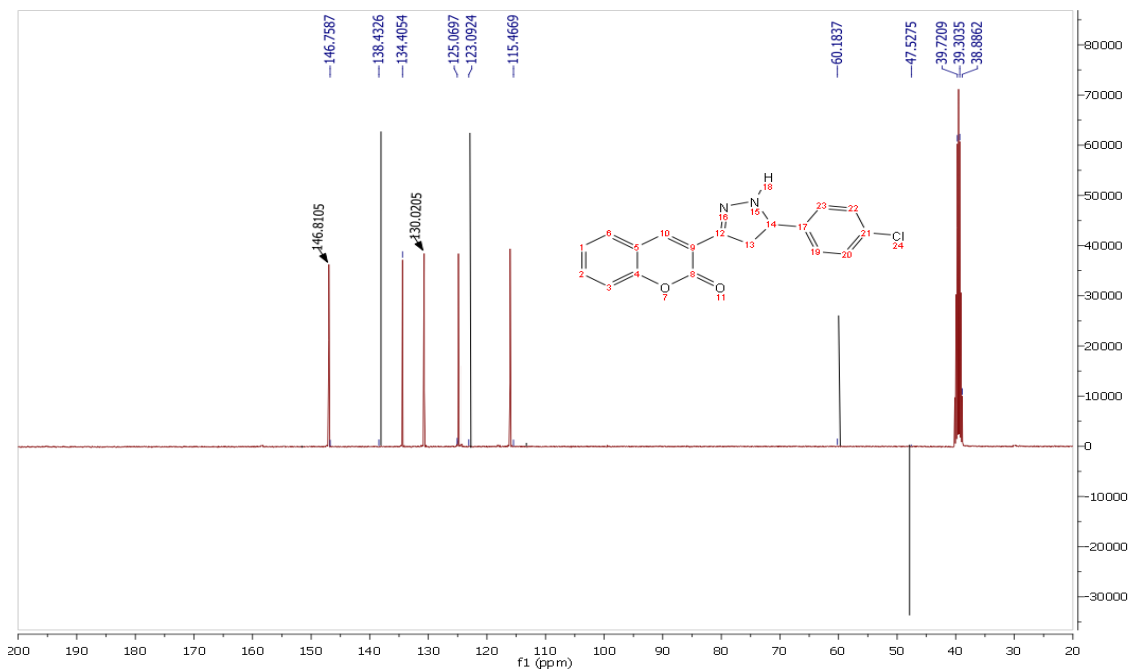


**Fig. S23:** DEPT 135 NMR spectrum of 3-(5-(4-hydroxy-3-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3c**

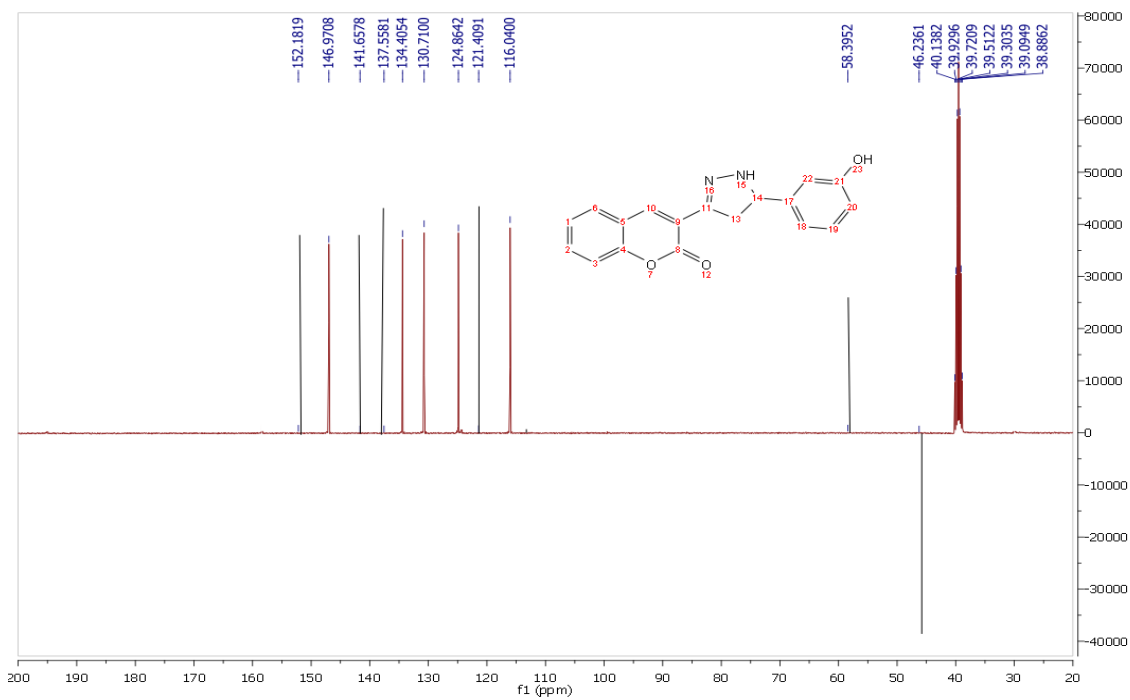


**Fig. S24:** DEPT 135 NMR spectrum of 3-(5-(4-ethoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3d**

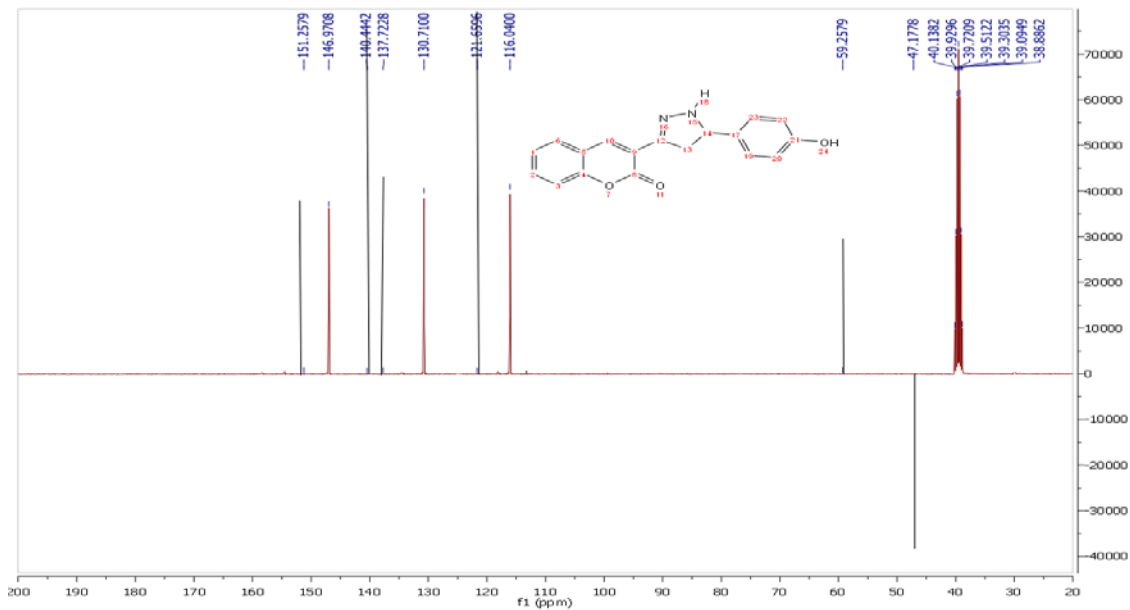




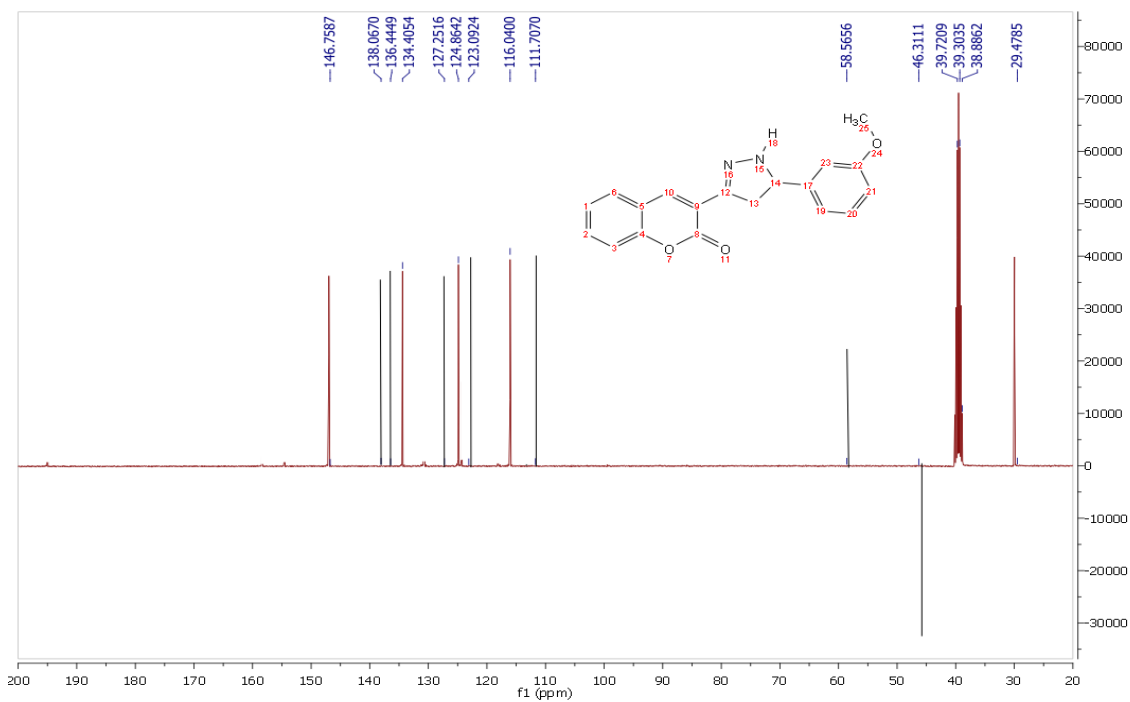
**Fig. S25:** DEPT 135 NMR spectrum of 3-(5-(4-chlorophenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3e**



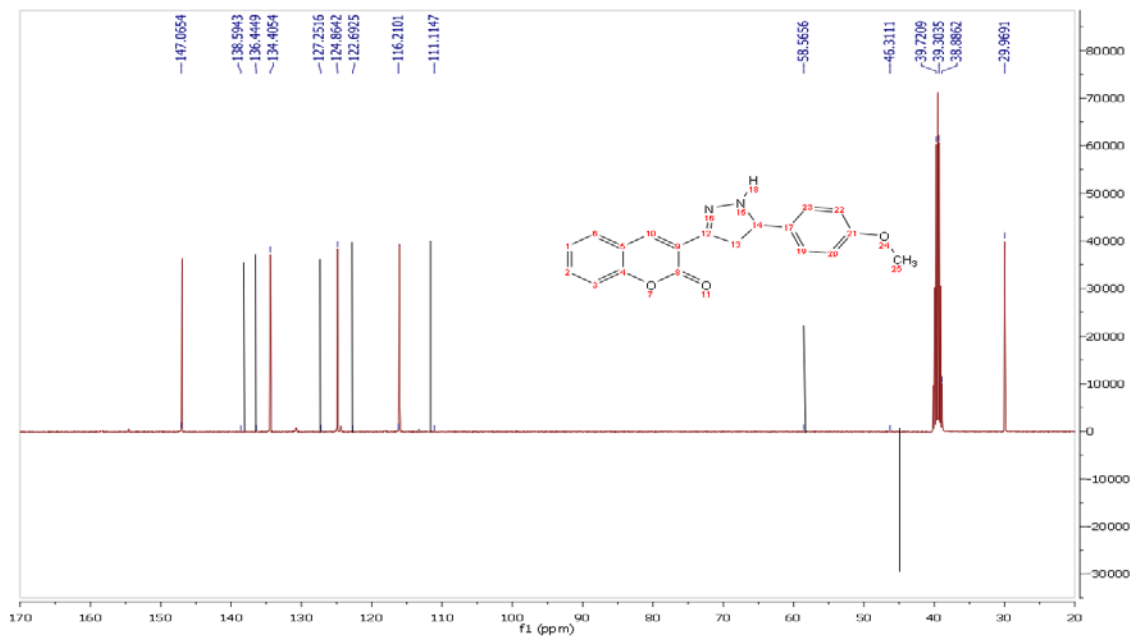
**Fig. S26:** DEPT 135 NMR spectrum of 3-(5-(3-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3f**



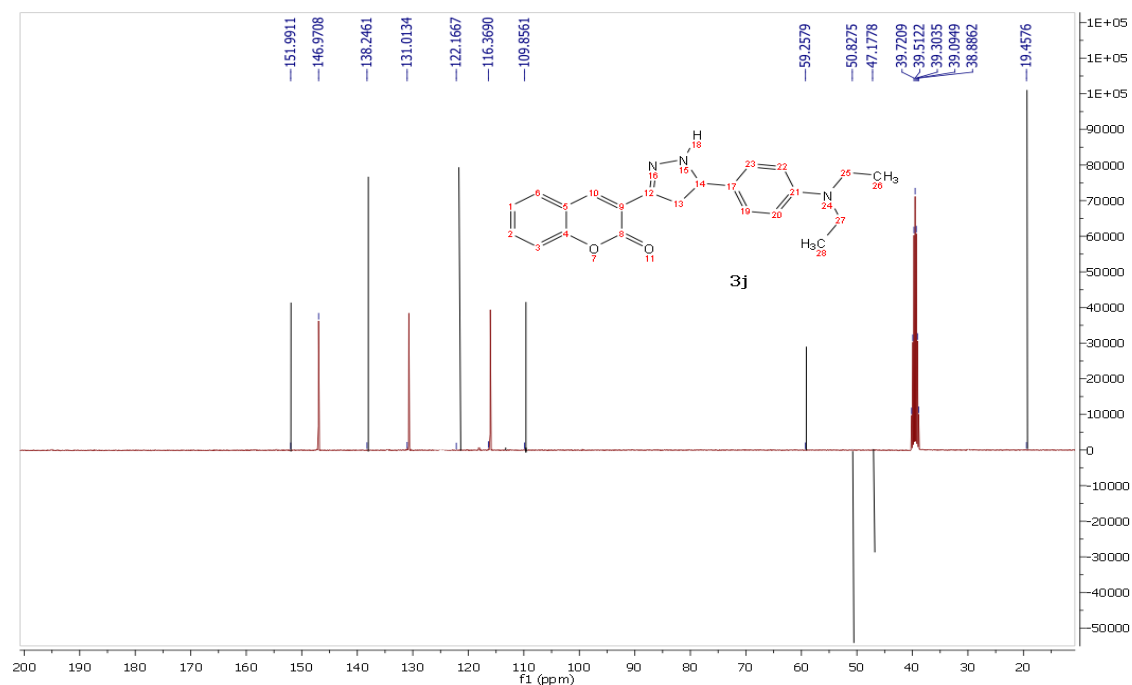
**Fig.S27:** DEPT 135 NMR spectrum of 3-(5-(4-hydroxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3g**



**Fig. S28:** DEPT 135 NMR spectrum of 3-(5-(3-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3h**



**Fig. S29:** DEPT 135 NMR spectrum of 3-(5-(4-methoxyphenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3i**



**Fig. S30:** DEPT 135 NMR spectrum of 3-(5-(4-(diethylamino)phenyl)-4,5-dihydro-1H-pyrazol-3-yl)-2H-chromen-2-one, **3j**