Supporting information

Design and Synthesis of coumarin based pyrazole-pyrazoline hybrid derivatives and their photophysical, antimicrobial, sensing and computational studies

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Characterization of coumarin based pyrazole-pyrazoline hybrid derivatives (4a-4r):

Compound 4a: White solid, 87% yield, IR (KBr): 3598, 3203, 3108, 1732, 1670, 1610, 1561,1470,1381, 1227,1116, 960 cm^{-1}. ^1H NMR ($CDCl_3$) δ (ppm): 1.33 (3H, t, $COCH_2C\mathbf{H_3}$), 3.49 (1H, d, pyrazoline ring), 4.08 (1H, d, pyrazoline ring), 4.30 (2H, q, $COC\mathbf{H_2}CH_3$), 5.02 (1H, d, pyrazoline ring), 7.19 (N-H), 7.39 (1H, d, coumarin ring), 7.41 (1H, t, coumarin ring), 7.47 (1H, t, phenyl ring),7.58 (2H, t, phenyl ring), 7.63 (1H, t, coumarin ring),7.89 (2H, d, phenyl ring), 7.95 (1H, d, coumarin ring), 8.65 (1H, s, pyrazole proton), 13.37 (1H, s, OH).^{13}C NMR ($CDCl_3$) δ (ppm): 13.92; 38.05; 43.65; 51.69; 60.88; 92.19; 116.60; 119.47; 120.76; 123.92; 124.93; 127.22; 127.80; 128.66; 129.67; 133.69; 138.43; 139.72; 142.45; 153.22; 153.79; 160.54; 162.41; 176.48.

Compound 4b: White solid, 91% yield, IR (KBr): 3674, 3619, 2976, 1708, 1693, 1545, 1334,1237, 1112, 995cm^{-1}. ^1H NMR ($CDCl_3$) δ (ppm):1.48 (3H, t, $\mathbf{CH_3}$-CH_2-COO-), 2.48 (3H, s, $C\mathbf{H_3}CO$-), 3.72 (1H, d, pyrazoline ring), 4.02 (1H, d, pyrazoline ring), 4.50 (2H, q, CH_3-$\mathbf{CH_2}$-COO-), 6.12 (1H, d, pyrazoline ring), 7.39 (3H, dd, one is coumarin ring and two in pyrazole ring), 7.42 (2H, t, one is coumarin ring and second is pyrazole ring), 7.59 (1H, s, pyrazole proton), 7.69 (3H, d, one is coumarin ring and two in phenyl ring), 8.02 (1H,d, coumarin ring), 13.5 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm):14.39; 22.16; 29.70; 45.47; 51.26; 61.35; 76.71; 96.06; 114.98; 116.84; 120.30; 124.44; 124.55; 126.36; 126.88; 127.80; 129.40; 134.20; 139.39; 140.82; 153.38, 157.76; 160.38; 162.16; 167.51; 167.72.

Compound 4c: White solid, 87% yield, IR (KBr):3674, 3618, 2973, 1714, 1653, 1551, 1425, 1244, 1114, 1005, 959cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 2.36 (3H, s, COC**H$_3$**), 3.59 (1H, d, pyrazoline ring), 3.91 (3H, s, COOC**H$_3$**), 4.15 (1H, d, pyrazoline ring), 5.92 (1H, d, pyrazoline ring), 7.26-7.30 (3H, 2t,1d, 1proton phenyl ring and 2H in coumarin ring), 7.39 (2H, t, phenyl ring), 7.59 (1H, s, pyrazole ring), 7.63 (3H, t, d, one proton in coumarin ring and two in phenyl ring), 7.96 (1H, d, coumarin ring), 13.38 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 22.16; 29.70; 45.33; 51.13; 52.27; 76.71; 96.07;115.00; 116.85; 120.29; 124.45; 124.54; 126.56; 127.03; 127.88; 129.44; 134.19; 139.34; 140.51;153.39; 157.71; 160.38; 162.59; 167.55; 167.72.

Compound 4d: White solid, 87% yield, IR (KBr): 3674, 3619, 3207, 1708,1699, 1552, 1476, 1234, 1114, 1060, 951cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.90 (3H, s, COOC**H$_3$**), 3.79 (1H, d, pyrazoline ring proton), 4.05 (1H, d, pyrazoline ring proton), 5.12 (1H, d, pyrazoline ring proton),7.10 (1H, s, NH), 7.35 (1H, s, coumarin proton), 7.39 (1H, t, coumarin proton), 7.40 (1H, t, pyrazole ring attached phenyl proton), 7.49 (2H, t, pyrazole ring attached phenyl proton), 7.62(1H, t, coumarin proton), 7.76 (2H, d, pyrazole ring attached phenyl proton), 7.85 (1H, d, coumarin proton), 8.63 (1H, s, pyrazole ring proton), 13.02 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 23.69; 30.29; 40.80; 51.25; 52.38; 92.36; 116.99; 119.55; 124.01; 125.68; 128.05; 128.34; 130.03; 133.83; 133.95; 139.49; 141.34; 153.95; 159.21; 162.57; 162.87; 165.32; 166.87; 169.35.

Compound 4e: White solid, 89% yield, IR (KBr): 3673, 3618, 2977, 2360, 1701, 1635, 1525, 1333, 1241,1116, 1012, 963 cm^{-1}.^{1}H NMR ($CDCl_3$) δ (ppm): 1.21 (3H, t, $COOCH_2$-C**H$_3$**), 2.01 (3H, s, COC**H$_3$**), 3.02 (1H, d, pyrazoline ring proton), 4.02 (1H, d, pyrazoline ring proton), 4.41 (2H, q, COOC**H$_2$**), 5.57 (1H, d, pyrazoline ring proton), 7.41 (1H, d, coumarin proton), 7.60 (1H, t, coumarin proton), 7.85 (2H, d, pyrazole ring attached phenyl proton), 8.01 (2H, d, pyrazole ring attached phenyl proton), 8.18 (1H, t, coumarin proton), 8.61(1H, d, coumarin proton), 8.88 (1H, s, pyrazole ring proton), 12.49 (1H, s, OH).^{13}C NMR ($CDCl_3$) δ (ppm): 18.66; 20.10; 22.54; 38.48; 39.63; 41.50; 42.64; 56.00; 77.54; 89.74; 91.32; 106.83; 120.62; 121.34; 134.84; 135.41; 151.21; 167.29; 168.44; 170.30; 174.47; 180.36.

Compound 4f: White solid, 87% yield, IR (KBr):3672, 3618, 3194, 2986, 2360, 1689, 1524, 1239, 1119, 1047, 959cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.37 (3H, t, COOCH2-C**H$_3$**), 3.52 (1H, d, pyrazoline ring proton), 3.59 (1H, d, pyrazoline ring proton), 4.20 (1H, d, pyrazoline ring proton),

4.47 (2H, q, COOC**H$_2$**), 5.90 (1H,s, NH), 7.39 (1H, d, coumarin proton), 7.42 (1H, t, coumarin proton), 7.60 (1H, t, coumarin proton), 7.69 (2H, d, pyrazole ring attached phenyl proton), 7.80 (2H, d, pyrazole ring attached phenyl proton), 7.90 (1H, s, pyrazole ring proton), 8.0 (1H, d, coumarin proton), 13.39 (1H, s, OH).

Compound 4g: Pale yellow solid, 94% yield, IR (KBr): 3674, 3618, 3253, 2977, 2361, 1694, 1605, 1513, 1416, 1327, 1236, 1164, 1111, 976 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 3.72 (1H, d, pyrazoline ring proton), 4.15 (3H, s, COC**H$_3$**), 4.39 (1H, d, pyrazoline ring proton), 5.93 (1H, d, pyrazoline ring proton), 7.01 (2H, d, pyrazoline ring attached phenyl proton), 7.35 (1H, d, coumarin proton), 7.39 (1H, t, pyrazole ring attached phenyl proton), 7.40 (1H, s, pyrazole ring proton), 7.46 (3H, t, 1H in coumarin ring and 2H proton is pyrazole attached phenyl ring),7.59 (2H, d, pyrazoline ring attached phenyl proton), 7.62 (2H, d, pyrazole ring attached phenyl proton), 7.70 (1H, t, coumarin proton), 8.05 (1H, d, coumarin proton), 13.59 (1H, s, OH).^{13}C NMR ($CDCl_3$) δ (ppm): 41.21; 46.23; 52.27; 75.67; 100.23; 113.30; 116.31; 116.89; 120.04; 122.34; 123.49; 124.64; 126.22; 126.94; 128.09; 128.80; 129.67; 133.40; 135.98; 137.13; 139.43; 143.02; 154.65; 160.68; 162.26; 181.65; 190.84.

Compound 4h: White solid, 90% yield, IR (KBr): 3673, 3618, 2978, 2359, 1918, 1695, 1524, 1237, 1173, 1113, 1010, 835 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.30 (3H, t, $COCH_2C$**H$_3$**),1.46(3H, t, $COOCH_2C$**H$_3$**), 2.30 (2H, q, COC**H$_2$**CH_3), 3.64 (1H, d, pyrazoline ring), 4.10 (1H, d, pyrazoline ring), 4.50 (2H, q, COOC**H$_2$**CH_3), 5.93 (1H, d, pyrazoline ring), 7.28-7.32 (3H, m, aromatic proton), 7.39 (2H, t, phenyl ring), 7.59 (2H, t, phenyl ring), 7.61 (1H, t, coumarin ring), 7.72 (1H, s, pyrazole proton), 7.94 (1H, d, coumarin ring), 13.45 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 9.20; 14.51; 22.69; 29.64; 31.69; 32.71; 44.98; 51.31; 61.54; 76.26; 116.54; 120.42; 124.10; 124.92; 126.76; 127.58; 128.39; 129.42; 131.26; 132.28; 134.12; 153.34; 157.63; 162.33.

Compound 4i: White solid, 88% yield, IR (KBr): 3674, 3618, 2973, 2361, 1714, 1654, 1548, 1339, 1245, 1182, 1113, 1011, 886 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.16 (3H, t, $COCH_2C$**H$_3$**), 2.78 (2H, q, COC**H$_2$**CH_3), 3.65 (1H, d, pyrazoline ring), 4.00 (3H, s, COOC**H$_3$**), 4.12 (1H, d, pyrazoline ring), 6.02 (1H, d, pyrazoline ring), 7.37 (2H, t, aromatic proton(1H is phenyl ring & 1H in coumarin ring)), 7.39 (1H, d, coumarin ring), 7.48 (2H, t, phenyl ring), 7.65 (1H, t, coumarin ring),7.71 (2H, d, phenyl ring), 7.75 (1H, s, pyrazole proton), 8.12 (1H, d, coumarin ring), 13.45

(1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 8.68; 27.74; 29.71; 45.04; 50.90; 51.14; 52.29; 76.72; 96.12; 115.04; 116.84; 120.27; 124.42; 124.54; 126.62; 127.18; 127.87; 129.44; 134.15; 139.32; 140.48; 153.35; 157.41; 160.45; 162.58; 167.68; 170.95.

Compound 4j: Yellow solid, 88% yield, IR (KBr): 3675, 3616, 3105, 2982, 2361, 1709, 1653, 1552, 1466, 1337, 1235, 1108, 1009, 958cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.19 (3H, t, $NCOCH_2C\mathbf{H_3}$ proton), 1.49 (3H, t, $COOCH_2C\mathbf{H_3}$ proton), 2.62 (2H, q, $NCOC\mathbf{H_2}CH_3$ proton), 3.52 (1H, d, pyrazoline ring proton), 4.02 (1H, d, pyrazoline ring proton), 4.50(2H, q, $COOC\mathbf{H_2}CH_3$ proton), 6.00 (1H, d, pyrazoline ring proton), 7.40 (1H, d, coumarin ring proton), 7.45 (1H, t, coumarin ring proton), 7.59 (1H, t, coumarin ring proton), 7.62(2H, d, pyrazole attached phenyl ring proton), 7.70 (2H, d, pyrazole attached phenyl ring proton), 7.85 (1H, s, pyrazole ring proton), 8.02 (1H, d, coumarin ring proton), 13.49 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 13.64; 29.29; 30.29; 61.60; 80.27; 96.92; 97.64; 116.17; 117.17; 119.61; 120.19; 121.19; 130.10; 134.12; 134.84; 137.56; 159.53; 160.54; 174.04; 175.04; 187.25; 188.54.

Compound 4k: Yellow puffy solid, 90% yield, IR (KBr): 3674, 3618, 2980, 2361, 1918, 1699, 1516, 1409, 1328, 1232, 1107, 1016, 885 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.51 (3H, t, $COOCH_2C\mathbf{H_3}$), 3.76 (1H, d, pyrazoline ring), 4.37 (1H, d, pyrazoline ring), 4.57 (2H, q, $COOC\mathbf{H_2}CH_3$), 5.58 (1H, d, pyrazoline ring), 6.99 (2H, d, 4-CN phenyl ring), 7.30-7.47 (5H, m, aromatic proton), 7.54 (2H, d, phenyl ring), 7.60 (3H, t, 1 is coumarin ring and 2 in phenyl ring), 7.62 (1H, s, pyrazole proton), 8.06 (1H, d, coumarin ring), 13.57 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 14.43; 29.70; 46.09; 54.33; 61.64; 76.71; 96.46; 102.19; 112.89; 115.16; 116.77; 119.59; 120.14; 120.24; 124.55; 126.49; 126.71; 128.09; 129.51; 133.75; 133.79; 139.11; 140.78; 145.51; 153.17; 153.65; 160.52; 162.32; 166.61.

Compound 4l: Yellow solid, 96% yield, IR (KBr):3673, 3618, 2979, 2359, 1696, 1518, 1410, 1230, 1056, 1001, 836 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.42 (3H, t, $COOCH_2C\mathbf{H_3}$), 3.62 (1H, d, pyrazoline ring proton), 4.25 (1H, d, pyrazoline ring proton), 4.49 (2H, q, $COOC\mathbf{H_2}CH_3$), 6.05 (1H, d, pyrazoline ring proton), 6.86 (2H, d, pyrazoline ring attached phenyl ring proton), 7.02 (2H, d, pyrazoline ring attached phenyl ring proton), 7.29 (1H, d, coumarin ring proton), 7.38 (1H, t, coumarin ring proton), 7.49 (2H, d, pyrazole attached phenyl ring proton), 7.58 (2H, d, pyrazole attached phenyl ring proton), 7.62 (1H, t, coumarin ring proton), 7.70 (1H, s, pyrazole ring proton),

7.79 (1H, d, coumarin ring proton), 13.48 (1H, s, OH).^{13}C NMR ($CDCl_3$) δ (ppm): 13.86; 14.56; 39.34; 40.17; 40.38; 40.59; 61.18; 61.72; 96.25; 100.37; 110.24; 113.39; 116.92; 118.77; 119.87; 120.22; 120.45; 124.38; 124.49; 124.59; 127.64; 131.00; 133.40; 133.93; 134.51; 134.60; 141.97; 142.17; 148.80; 153.96; 160.39; 161.79.

Compound 4m: Yellow solid, 89% yield, IR (KBr):3674, 3618, 2982, 2362, 1701, 1640,1515, 1405, 1328, 1233, 1108, 971cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.50 (3H, t, $COOCH_2C\mathbf{H_3}$), 2.29 (3H, s, tolyl proton), 3.60 (1H, d pyrazoline proton), 4.30 (1H, d, pyrazoline proton), 4.56 (2H, q, $COOC\mathbf{H_2}CH_3$), 5.57 (1H, d, pyrazoline proton), 6.91 (2H, d, tolyl ring), 7.11 (2H, d, tolyl ring), 7.30-7.38 (3H, m, 2H in coumarin and 1H in phenyl ring), 7.42 (2H, t, phenyl ring), 7.60 (1H, t, coumarin ring), 7.69 (2H, d, phenyl ring), 7.75 (1H, s, pyrazole ring proton), 8.07 (1H, d, coumarin ring), 14.10 (1H, s, OH peak). ^{13}C NMR ($CDCl_3$) δ (ppm): 14.43; 20.52; 29.71; 45.61; 55.92; 61.46; 76.71; 77.34; 96.76; 113.61; 115.65, 116.65; 120.07; 124.05; 124.30; 126.96; 127.79; 128.06; 129.40; 129.89; 130.14; 133.08; 139.29; 140.87; 141.66; 150.89; 152.97; 160.86; 162.36;166.09.

Compound 4n: Yellow solid, 96% yield, IR (KBr): 3674, 3618, 2982, 2361, 1919, 1700, 1519, 1412, 1237, 1110, 1049, 982 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 2.34 (3H, s, tolyl proton), 3.59 (1H, d, pyrazoline ring), 4.09 (3H, s, $COOC\mathbf{H_3}$), 4.47 (1H, d, pyrazoline ring), 5.58 (1H, d, pyrazoline ring), 6.92 (2H, d, tolyl ring proton), 7.10 (2H, d, tolyl ring proton), 7.30-7.7.39 (3H, t, d, one in coumarin ring (d), two proton present in phenyl ring (t)), 7.43 (2H, t, one in coumarin ring and second one is pyrazole attached phenyl ring), 7.62 (1H, t, coumarin ring), 7.69 (2H,d, pyrazole attached phenyl ring), 7.75 (1H, s, pyrazole ring), 8.03 (1H, d, coumarin ring),14.10 (1H, s, OH peak). ^{13}C NMR ($CDCl_3$) δ (ppm): 20.52; 29.70; 45.55; 52.35; 55.80; 76.71; 96.76; 113.64; 115.65; 116.65; 120.07; 124.05; 124.29; 126.99; 127.86; 128.28; 129.43; 129.89; 130.17; 133.08; 139.25; 140.54; 141.65; 150.90; 152.98; 160.85; 162.78; 166.09.

Compound 4o: Pale yellow solid, 95% yield, IR (KBr): 3615, 3355, 2918, 2362, 1921,1700, 1607, 1516, 1461, 1382, 1226, 1107, it959 cm^{-1}. ^{1}H NMR ($CDCl_3$) δ (ppm): 1.39 (3H, t, $COOCH_2C\mathbf{H_3}$), 2.22 (3H, s, Ph-$C\mathbf{H_3}$), 3.51(1H, d, pyrazoline proton), 4.21 (1H, d, pyrazoline proton), 4.47 (2H, q, $COOC\mathbf{H_2}CH_3$), 5.16 (1H, d, pyrazoline proton), 6.82 (2H, d, pyrazoline ring attached phenyl ring proton), 7.02 (2H, d, pyrazoline ring attached phenyl ring proton), 7.29 (1H, d, coumarin ring

proton), 7.32 (1H, t, coumarin ring proton), 7.52 (1H, t, coumarin ring proton), 7.62 (2H, d, pyrazole attached phenyl ring proton), 7.70 (2H, d, pyrazole attached phenyl ring proton), 7.79 (1H, s, pyrazole ring proton), 7.90 (1H, d, coumarin ring proton), 13.92 (1H, s, OH).

Compound 4p: Yellow solid, 93% yield, IR (KBr):3672, 3617, 2979, 2361, 1697, 1546, 1502, 13931321,1219, 1097, 987 cm^{-1}. ^1H NMR ($CDCl_3$) δ (ppm): 1.52 (3H, t, C**H₃**-CH_2-COO-), 3.65 (1H, d, pyrazoline ring), 4.27 (1H, d, pyrazoline ring), 4.57 (2H, q, CH_3-C**H₂**-COO-), 5.82(1H, d, pyrazoline ring),6.89 (1H, t, phenyl ring), 6.95 (2H, d, phenyl ring), 7.31 (3H, d, one is coumarin ring and two in pyrazole ring), 7.38 (2H, t, pyrazole ring), 7.42 (2H, t, one is coumarin ring and second is pyrazole ring), 7.63 (2H, d, pyrazole ring attached phenyl ring proton), 7.67 (1H, t, coumarin ring), 7.77 (1H, s, pyrazole ring), 8.12 (1H, d, coumarin proton), 14.2 (1H, s, OH peak). ^{13}C NMR ($CDCl_3$) δ (ppm): 14.44; 45.69; 55.54; 61.49; 76.72; 77.04; 77.36; 96.74; 113.40, 115.56; 116.66; 120.08; 120.56; 124.07; 124.33;126.93; 127.82; 127.97; 129.41; 129.67; 133.18; 139.27; 140.82; 143.64; 151.18; 152.99; 160.81; 162.35; 166.10.

Compound 4q: Yellow solid, 95% yield, IR (KBr): 3673, 3618, 2981, 2359, 1918, 1699, 1521, 1405, 1329, 1222, 1149, 1099, 1058, 997 cm^{-1}. ^1H NMR ($CDCl_3$) δ (ppm): 3.65 (1H, d, pyrazoline ring), 4.07 (3H, s, COOC**H₃**), 4.39 (1H, d, pyrazoline ring), 5.85 (1H, d, pyrazoline ring), 6.92 (1H, t, pyrazoline ring attached phenyl proton), 7.02 (2H, d, pyrazoline ring attached phenyl proton), 7.23 (2H, t, pyrazoline ring attached phenyl ring proton), 7.40 (1H, d, coumarin ring proton), 7.42 (2H, t, 1H in coumarin ring and 1H proton is pyrazole attached phenyl ring), 7.60 (2H, d, pyrazole ring attached phenyl proton), 7.68 (3H, t, 1H in coumarin ring and 2H is pyrazole attached phenyl ring), 7.80 (1H, s, pyrazole ring proton), 8.12 (1H, d, coumarin proton), 14.02 (1H, s, OH). ^{13}C NMR ($CDCl_3$) δ (ppm): 45.66; 52.44; 55.42; 96.75; 113.47; 115.66; 116.67; 120.01; 120.65; 124.03; 124.39; 126.94; 127.94; 128.12; 129.31; 129.71; 133.26; 138.82; 139.22; 140.58; 143.12; 143.59; 151.21; 153.07; 160.72; 162.19; 162.77; 166.17.

Compound 4r: Yellow solid, 96% yield, IR (KBr): 3675, 3618, 2987, 2361, 1699,1517,1395,1323, 1223, 1103, 1049, 998 cm^{-1}. ^1H NMR ($CDCl_3$) δ (ppm): 1.5 (3H, t, $COOCH_2C$**H₃**), 3.67 (1H, d, pyrazoline ring), 4.34 (1H, d, pyrazoline ring), 4.57 (2H, q, COOC**H₂**CH_3), 5.81 (1H, d, pyrazoline ring), 6.90 (1H, t, pyrazoline ring attached phenyl ring), 7.02 (2H, d, pyrazoline ring attached phenyl ring), 7.25 (2H, t, pyrazoline attached phenyl ring

proton), 7.36 (1H, d, coumarin ring proton), 7.39 (1H, t, coumarin ring), 7.62 (1H, t, coumarin ring), 7.74 (2H, d, pyrazole ring attached [redacted]ng), 7.81 (2H, d, pyrazole ring attached phenyl ring), 7.87 (1H, s, pyrazole ring proton), [redacted] d, coumarin ring), 13.95 (1H, s, OH peak). ^{13}C NMR ($CDCl_3$) δ (ppm): 14.02; 14.13; 29.71; 61.65; 76.71; 95.64; 110.42; 111.68; 115.81; 116.01; 116.58; 119.94; 123.88; 123.99; 124.12; 128.03; 129.14; 132.62; 133.07; 133.62; 133.87; 139.10; 141.69; 143.79; 148.28; 152.70; 160.59; 164.17.

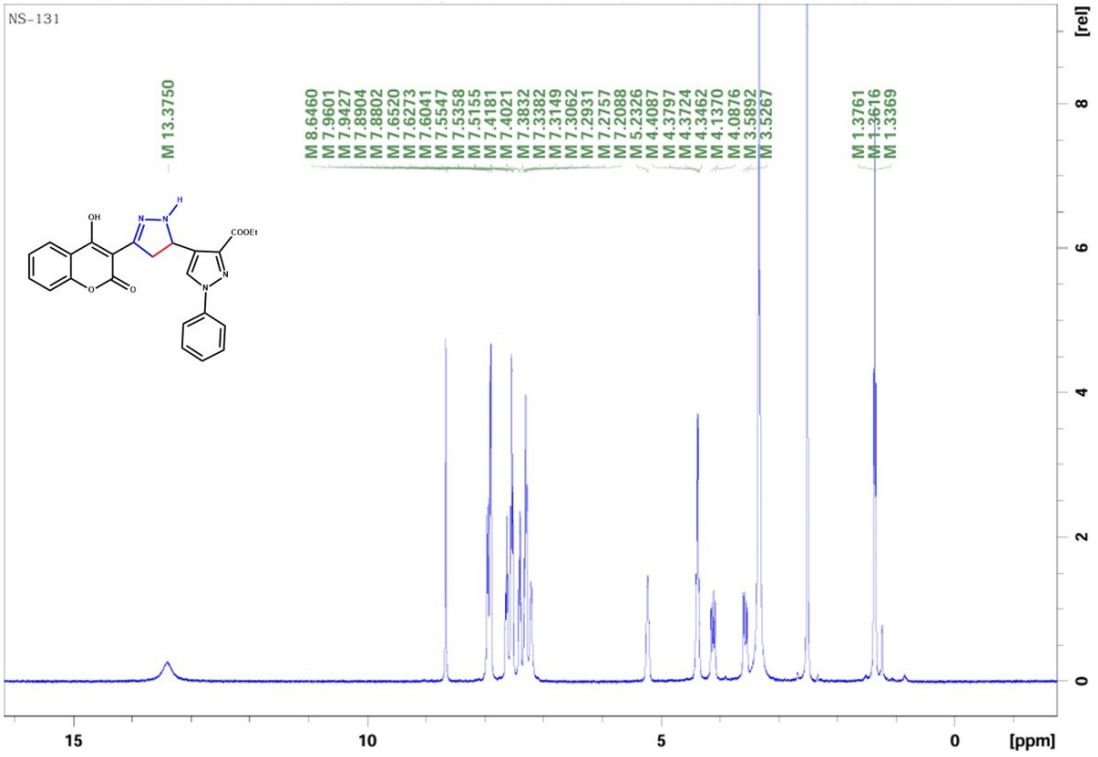


Figure S1. ^{1}H proton NMR spectra of compound **4a**.

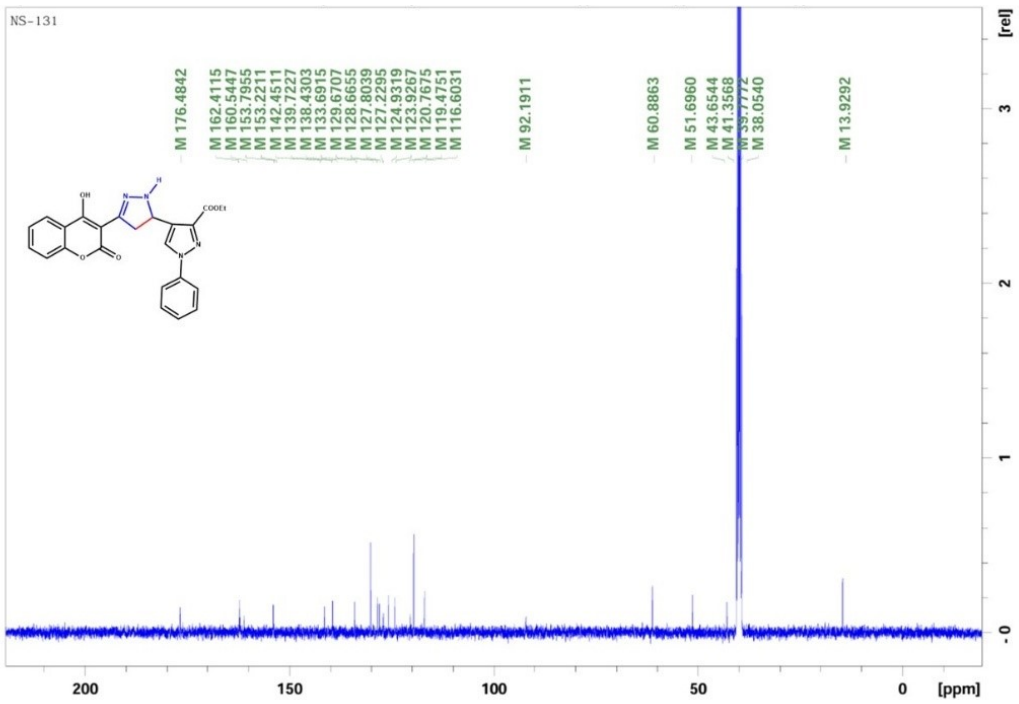


Figure S2. ^{13}C NMR spectra of compound **4a**.

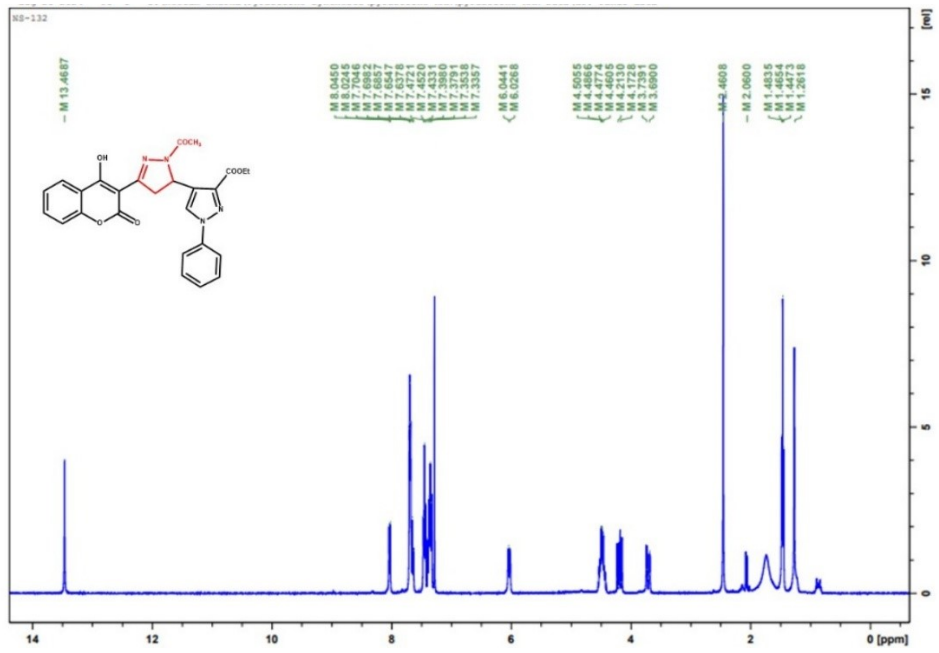


Figure S3. ^{1}H proton NMR spectra of compound **4b**.

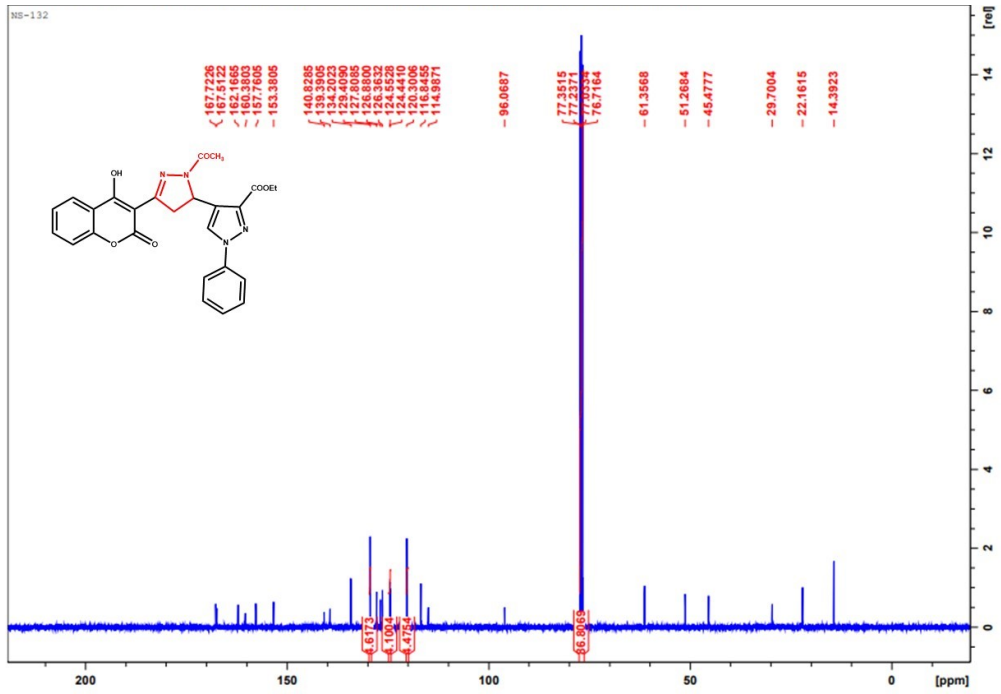


Figure S4. ^{13}C NMR spectra of compound **4b**.

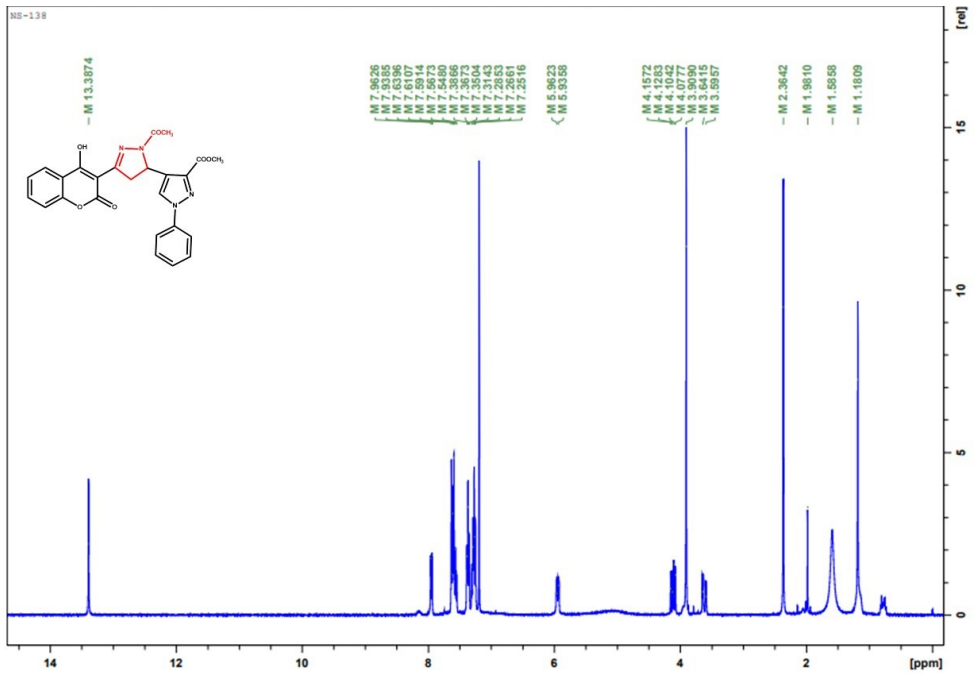


Figure S5. ^{1}H proton NMR spectra of compound **4c**.

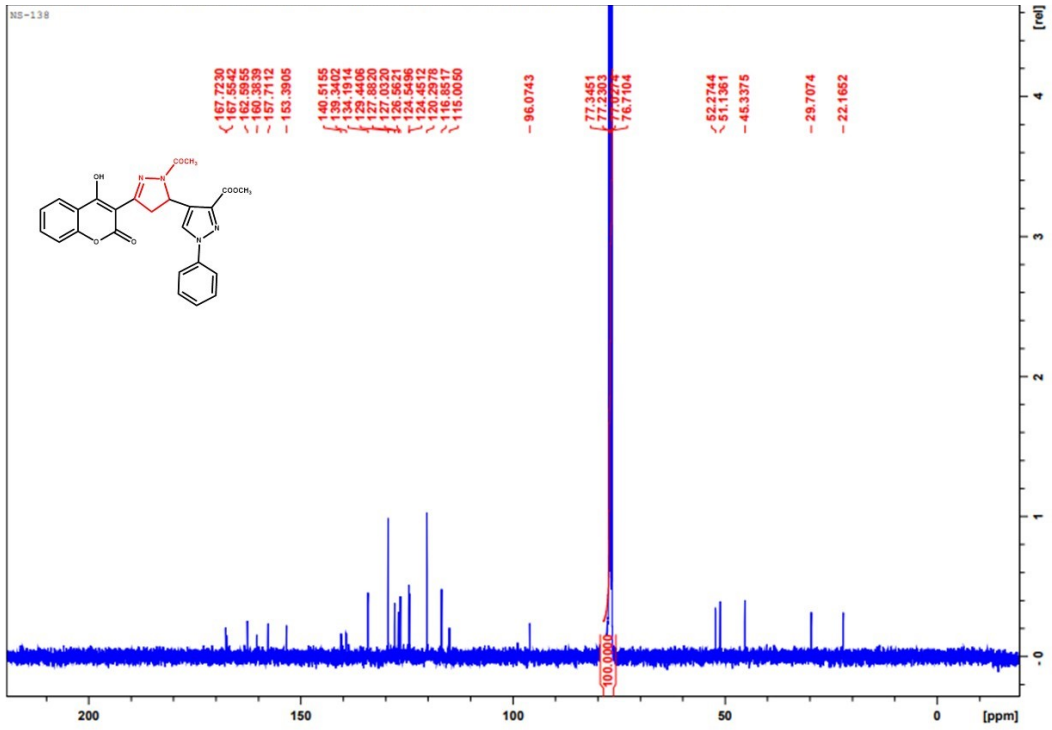


Figure S6. ^{13}C NMR spectra of compound **4c**.

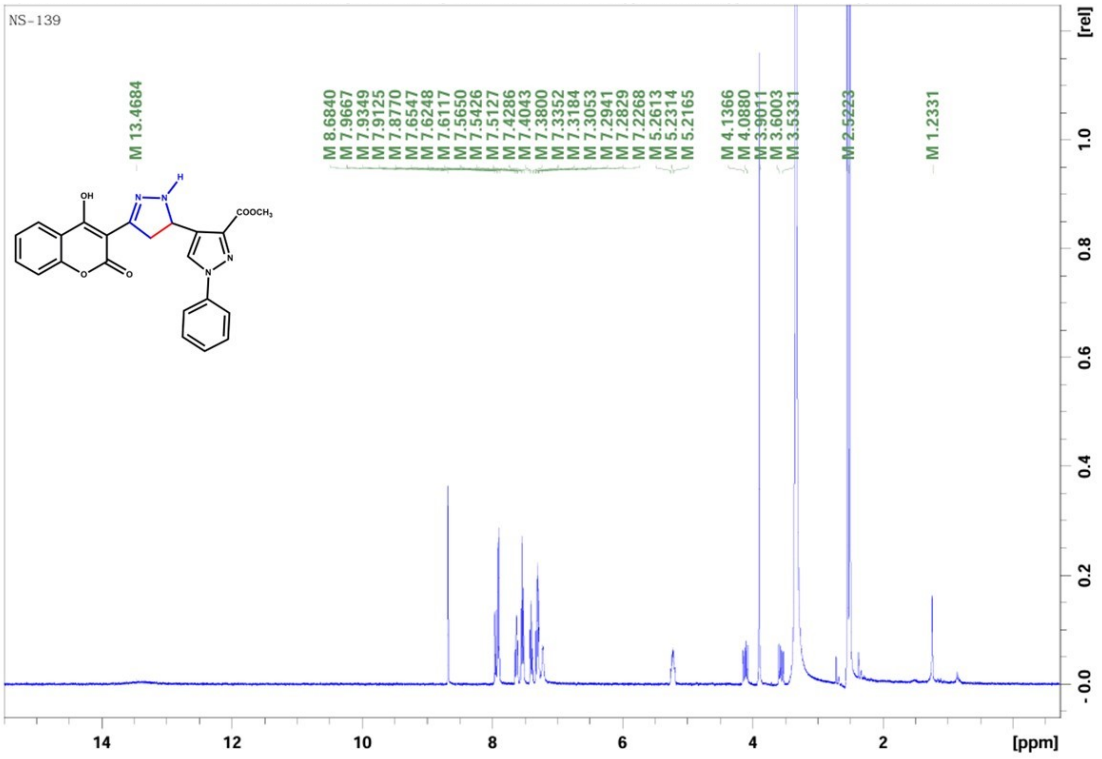


Figure S7. ^{1}H proton NMR spectra of compound **4d**.

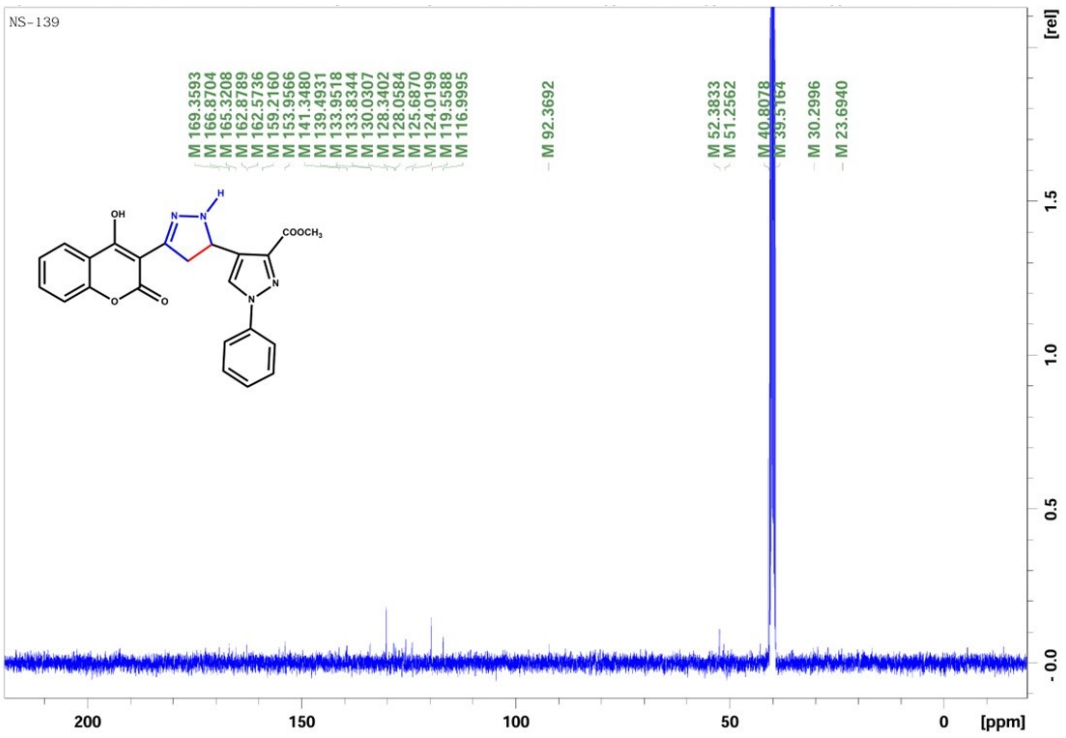


Figure S8. ^{13}C NMR spectra of compound **4d**.

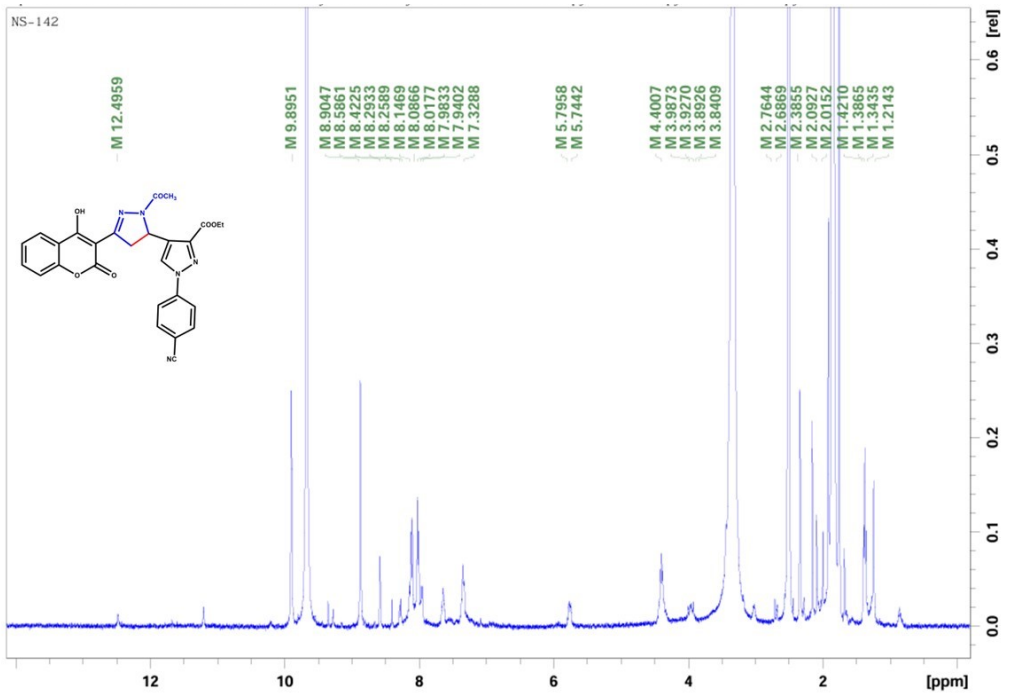


Figure S9. ^{1}H proton NMR spectra of compound **4e**.

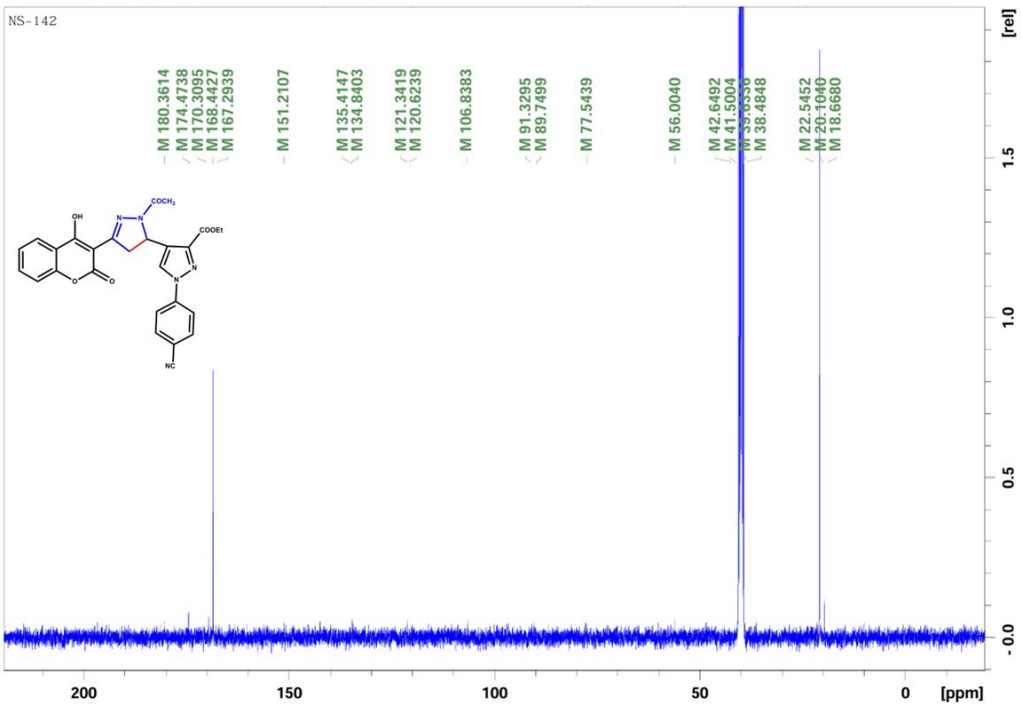


Figure S10. ^{13}C NMR spectra of compound **4e**.

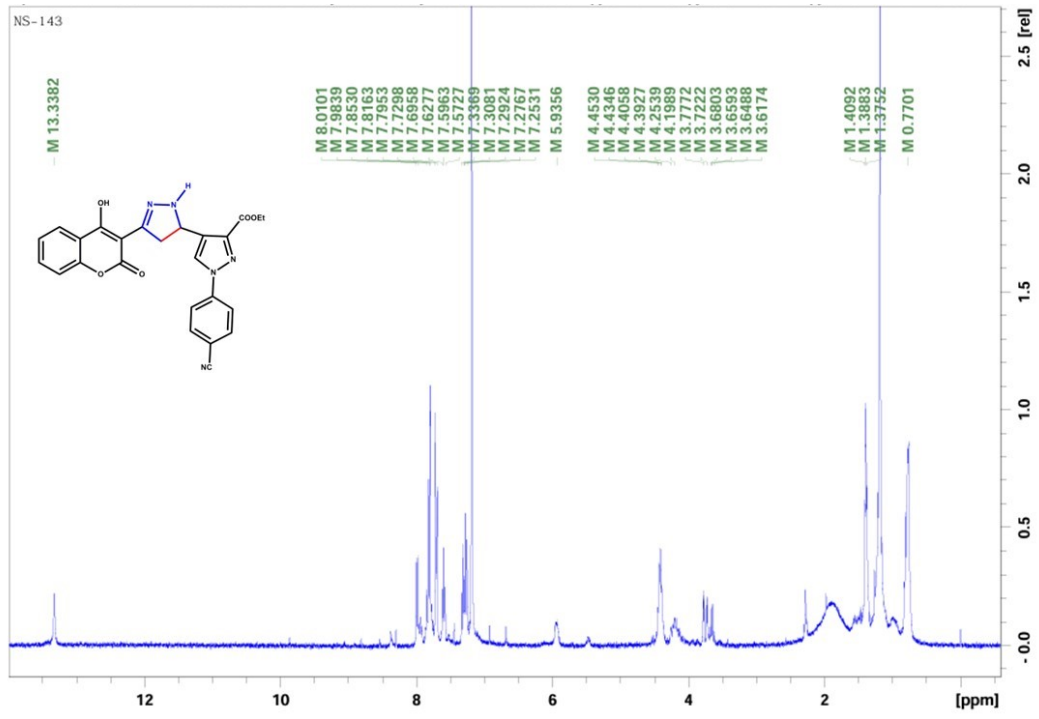


Figure S11. ^{1}H proton NMR spectra of compound **4f**.

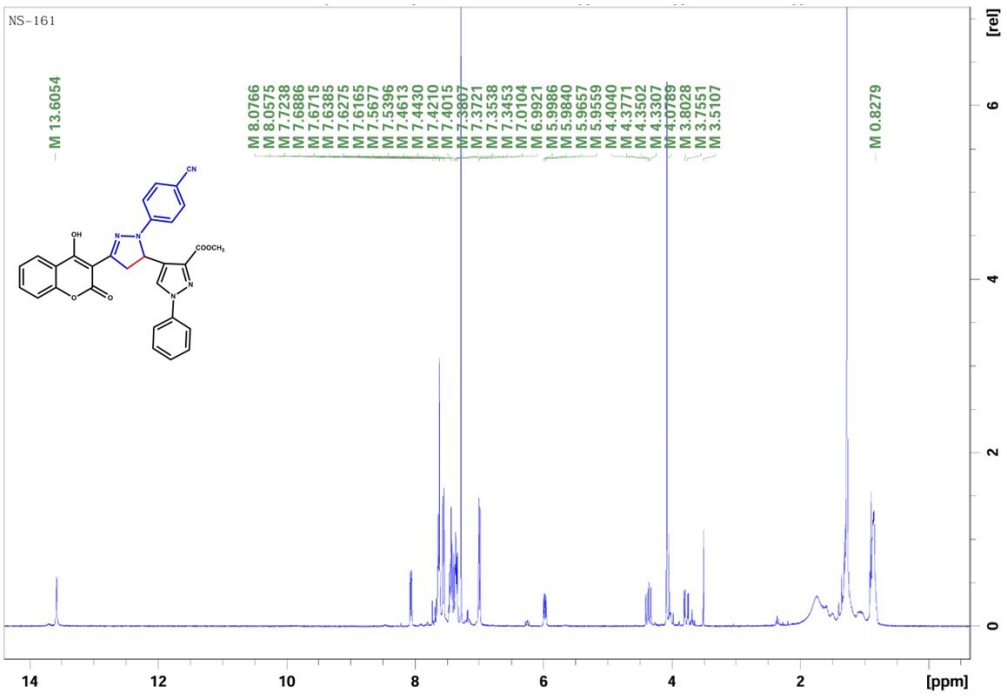


Figure S12. [1]H proton NMR spectra of compound **4g**.

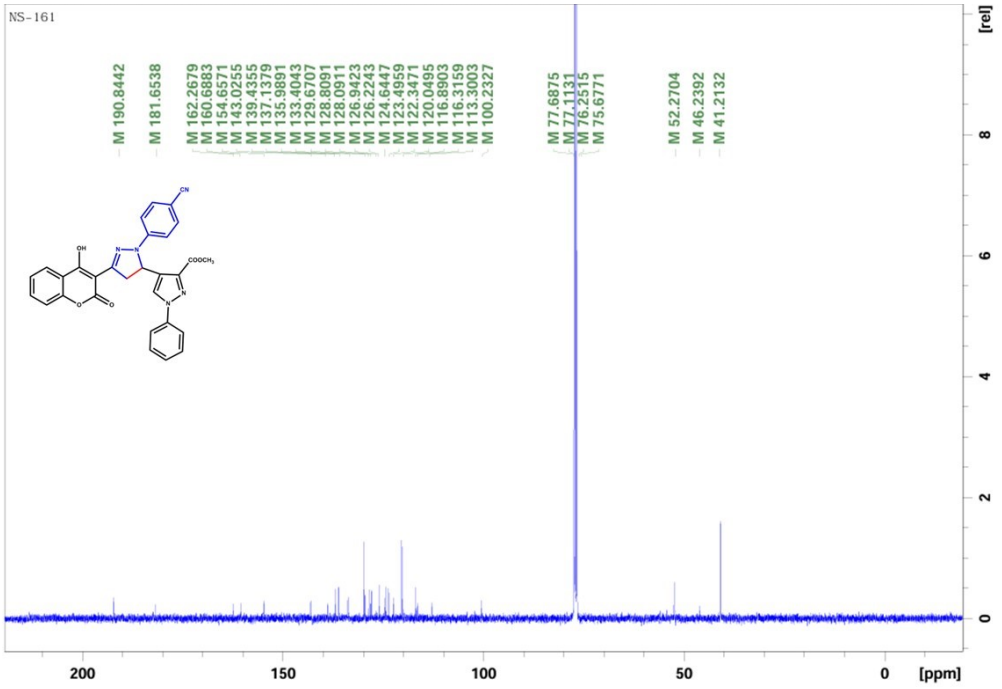


Figure S13. [13]C NMR spectra of compound **4g**.

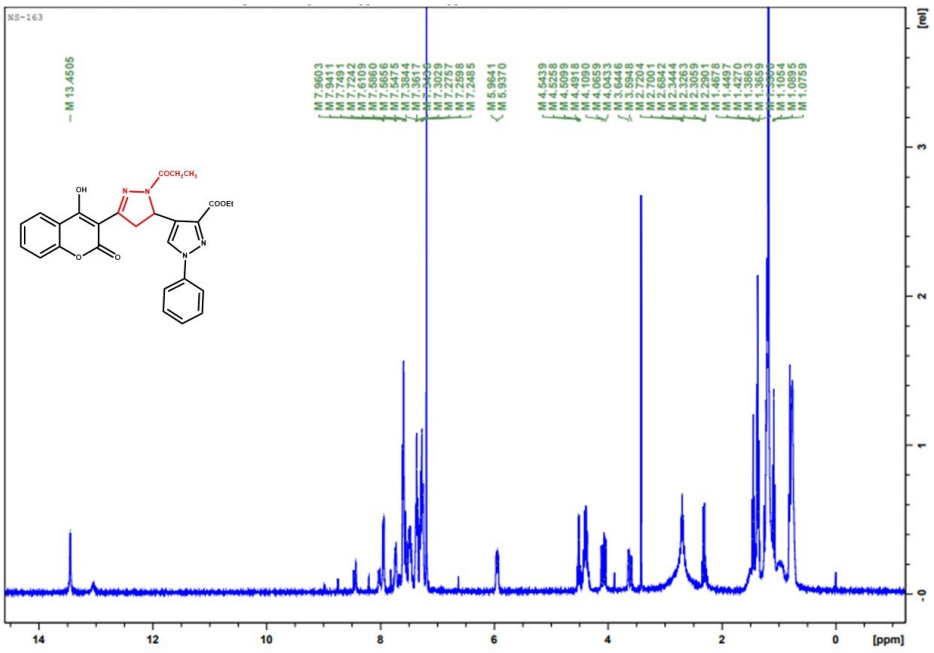


Figure S14. ^{1}H proton NMR spectra of compound 4h.

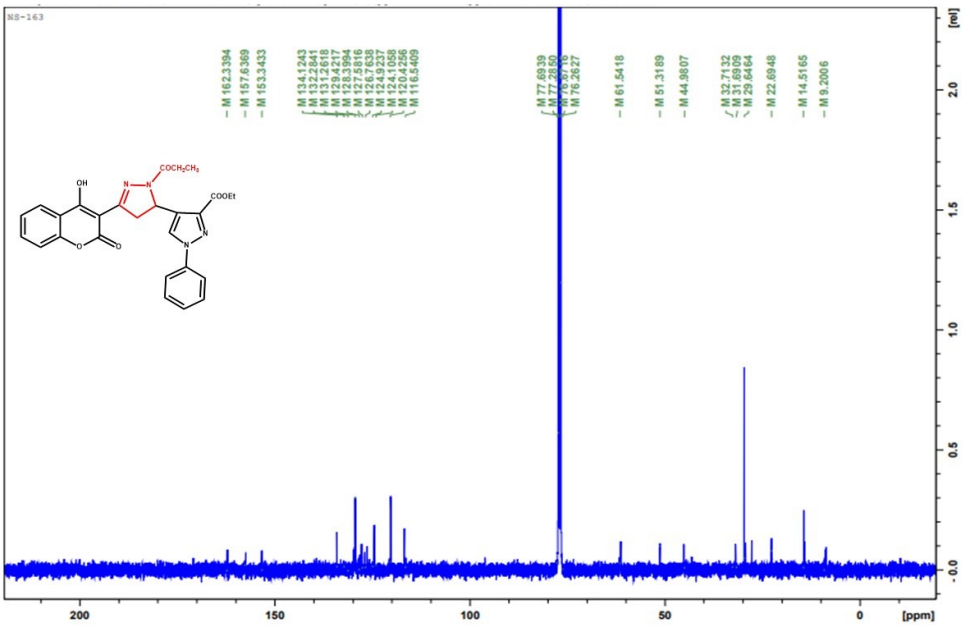


Figure S15. ^{13}C NMR spectra of compound **4h**.

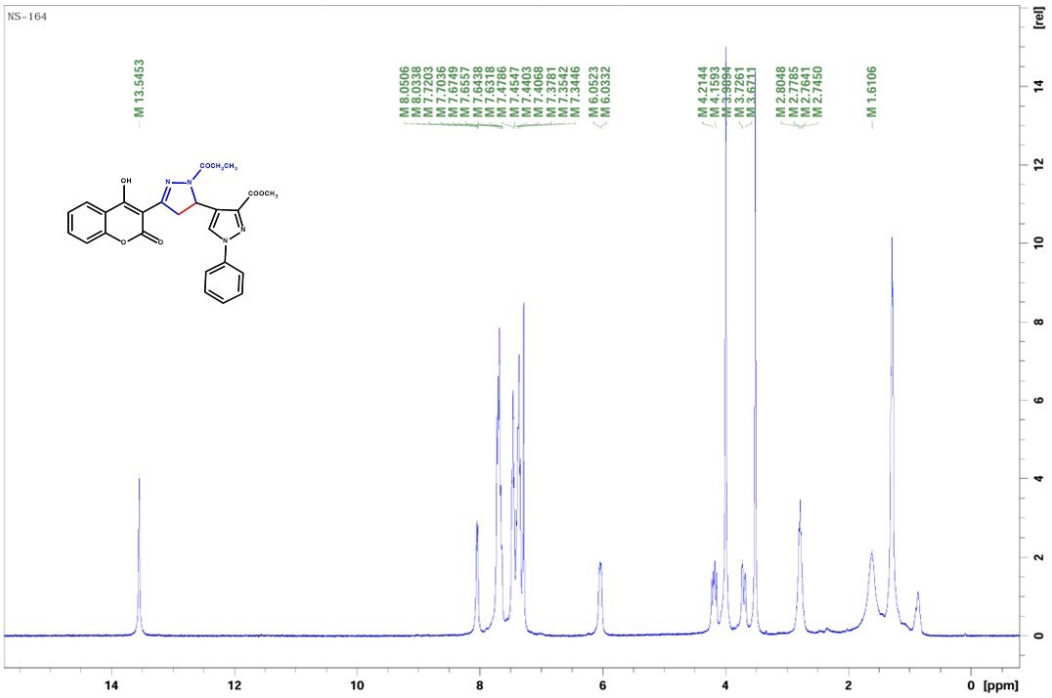


Figure S16. ^{1}H proton NMR spectra of compound **4i**.

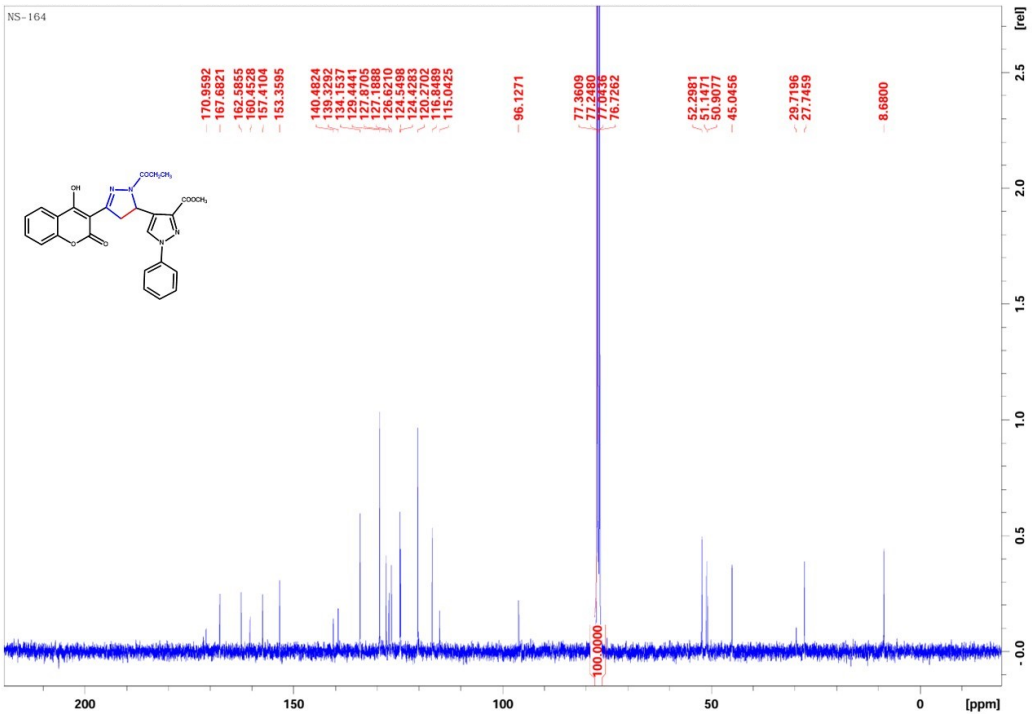


Figure S17. ^{13}C NMR spectra of compound **4i**.

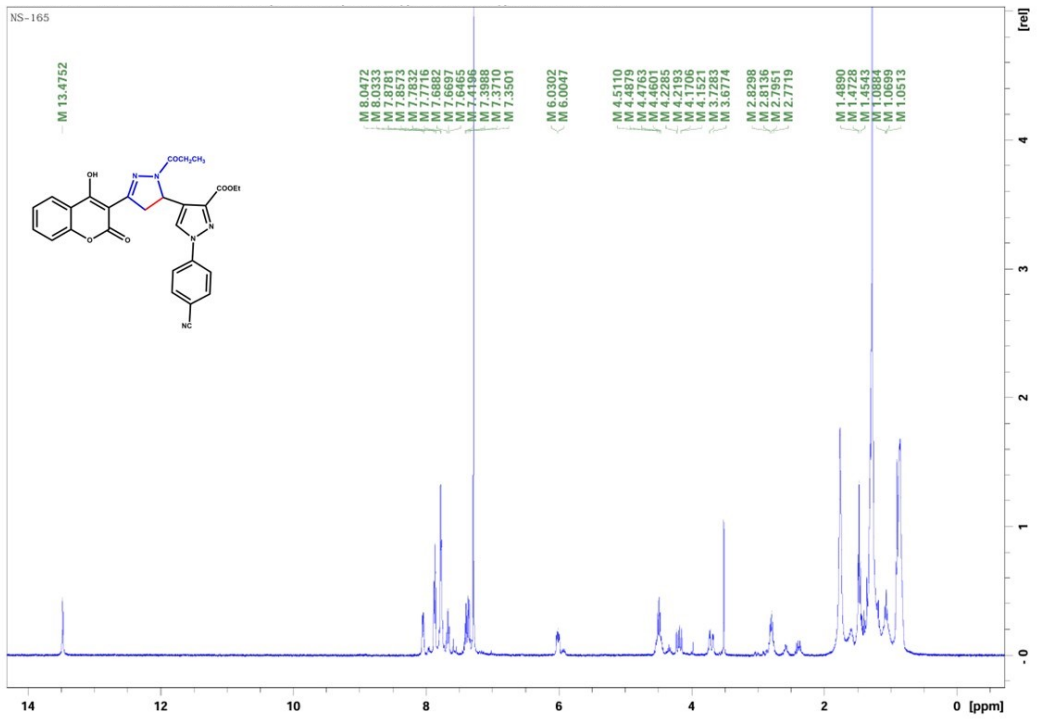


Figure S18. ^{1}H proton NMR spectra of compound **4j**.

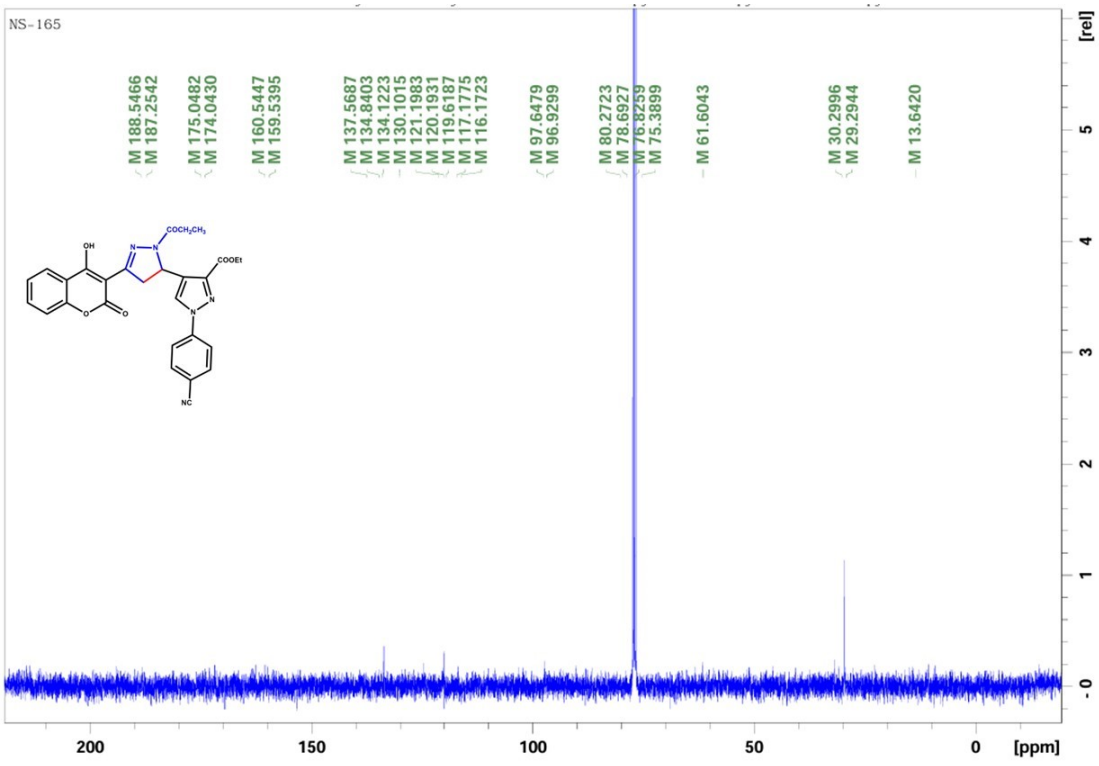


Figure S19. ^{13}C NMR spectra of compound **4j**.

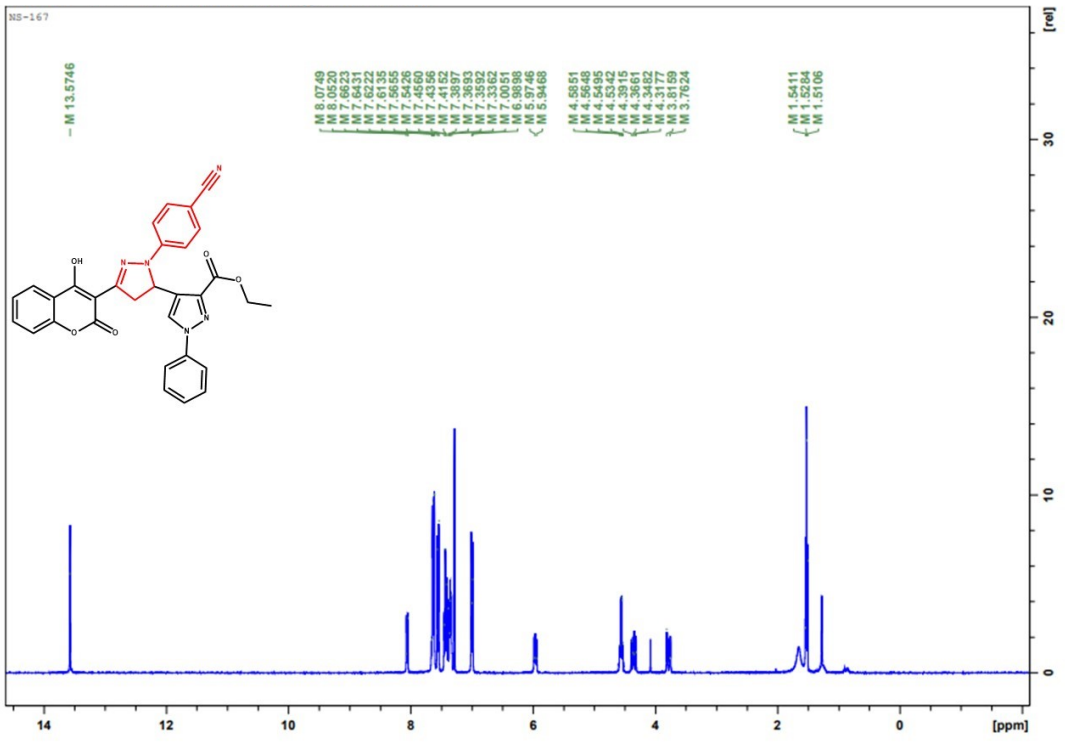


Figure S20. [1]H proton NMR spectra of compound **4k**.

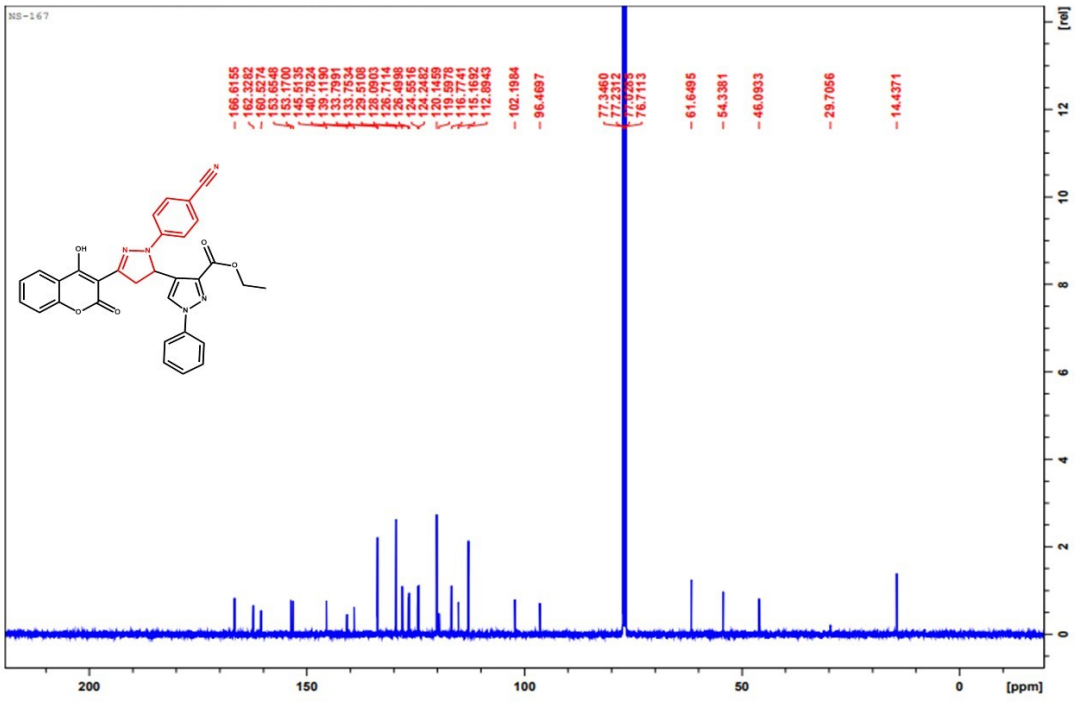


Figure S21. [13]C NMR spectra of compound **4k**.

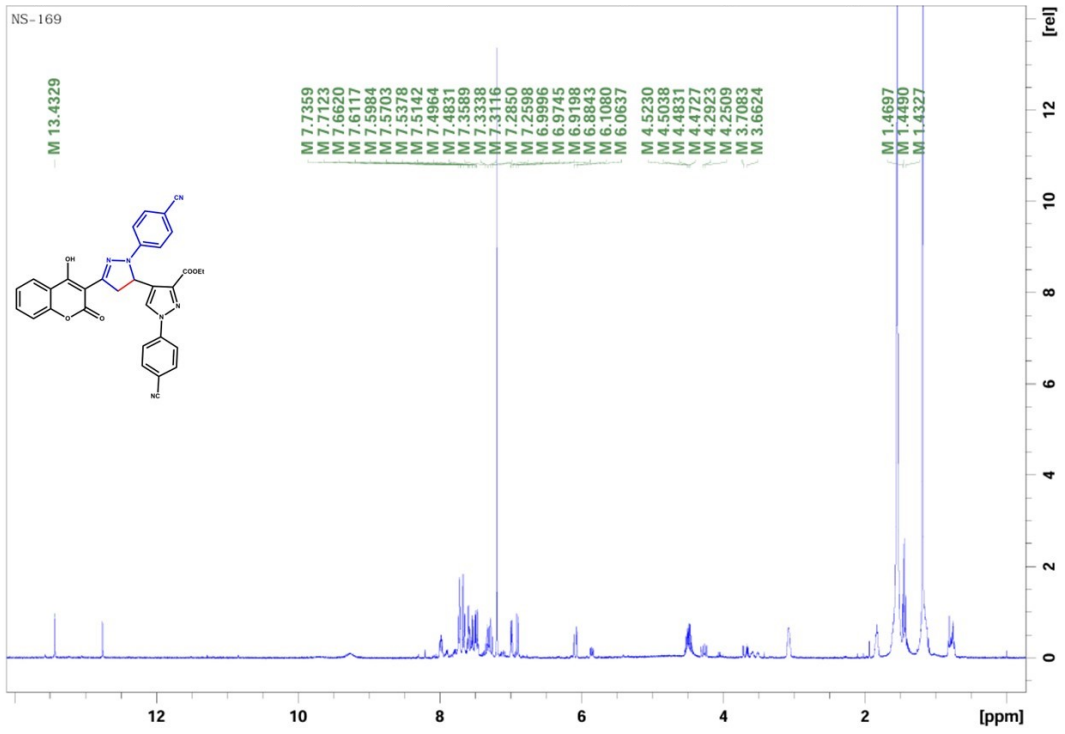


Figure S22. ^{1}H proton NMR spectra of compound **4l**.

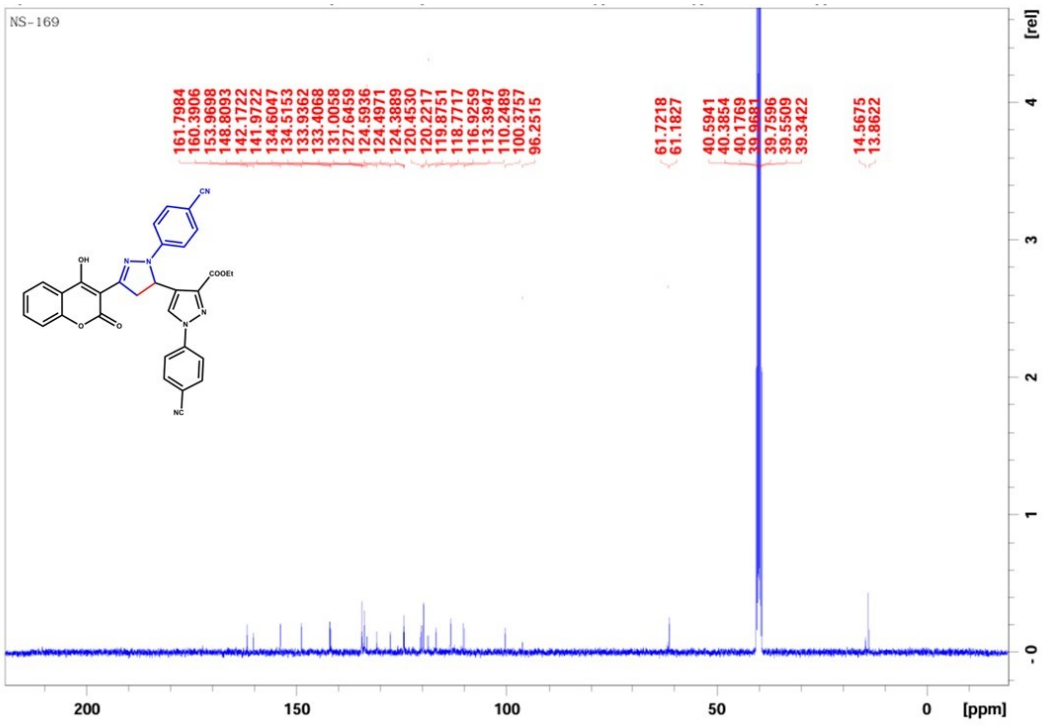


Figure S23. ^{13}C NMR spectra of compound **4l**.

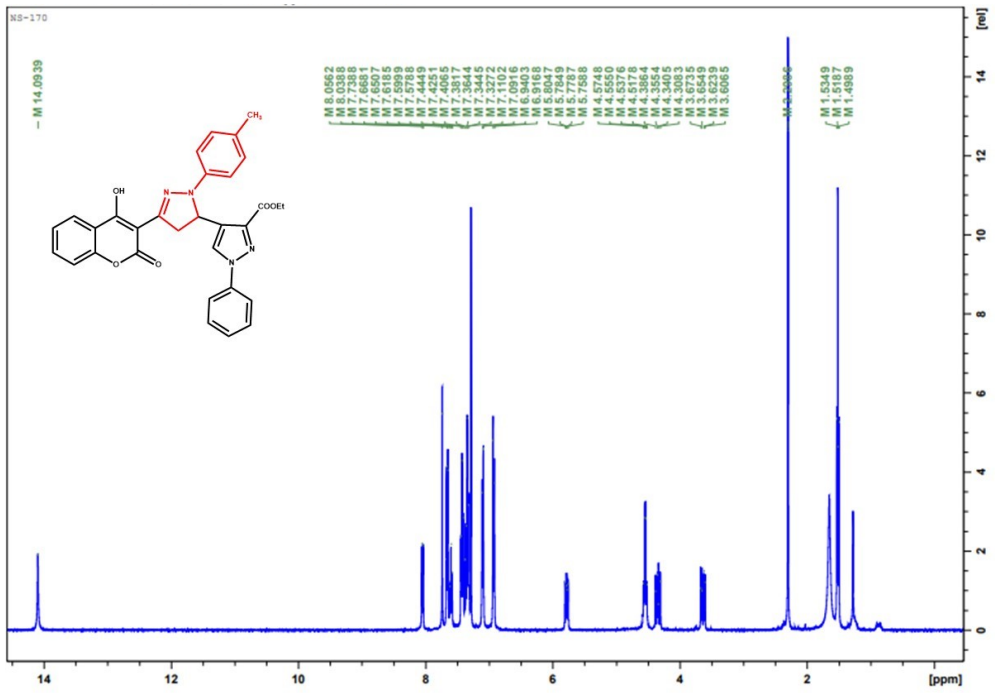


Figure S24. ^{1}H proton NMR spectra of compound **4m**.

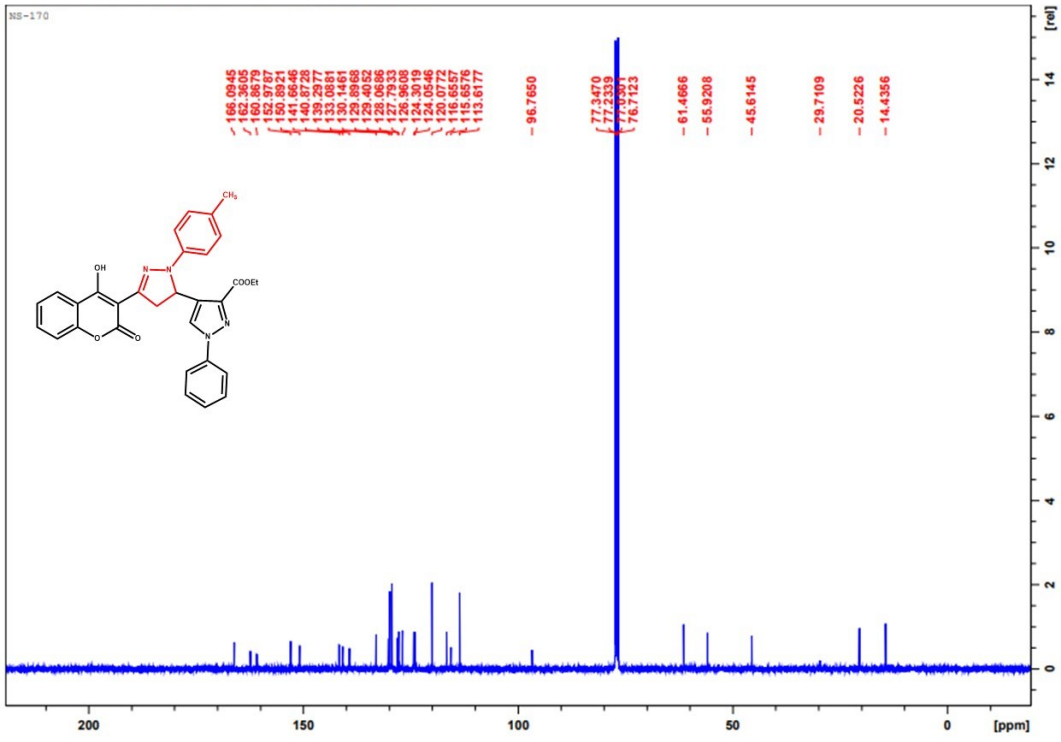


Figure S25. ^{13}C NMR spectra of compound **4m**.

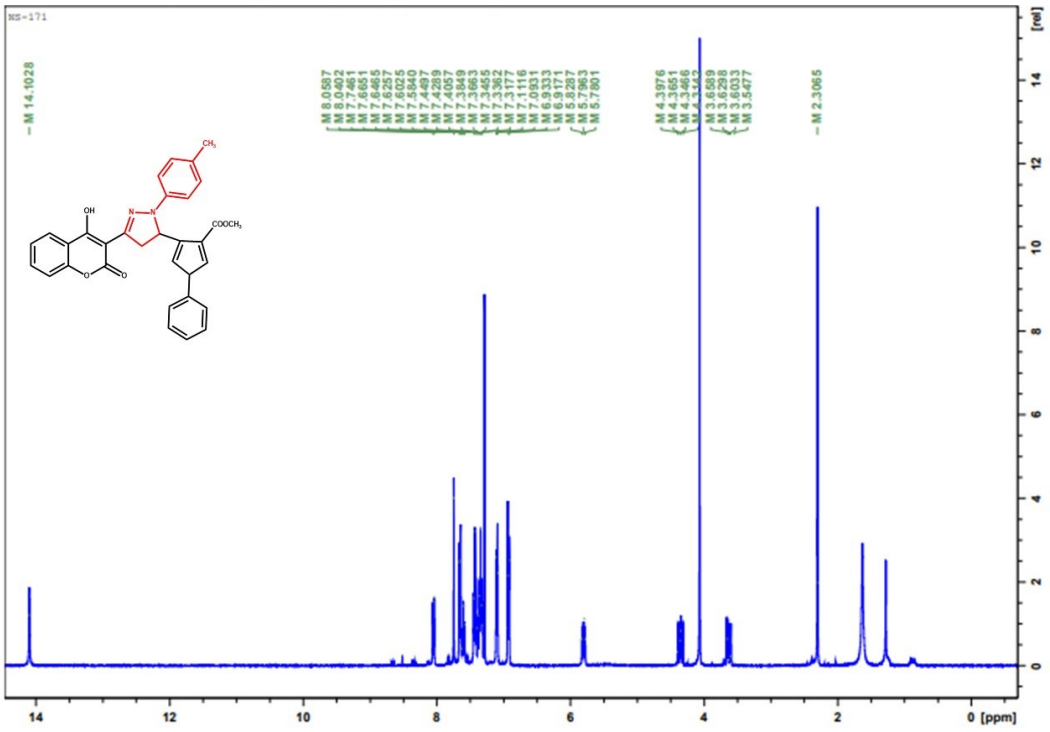


Figure S26. [1]H proton NMR spectra of compound **4n**.

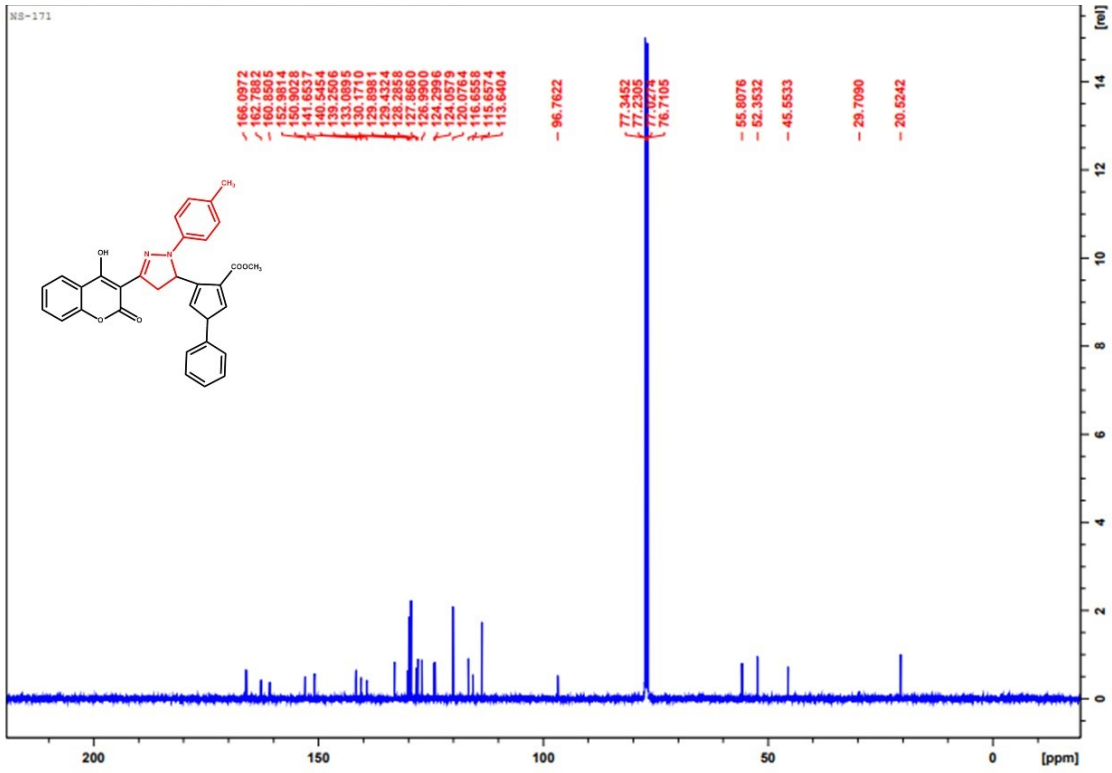


Figure S27. [13]C NMR spectra of compound **4n**.

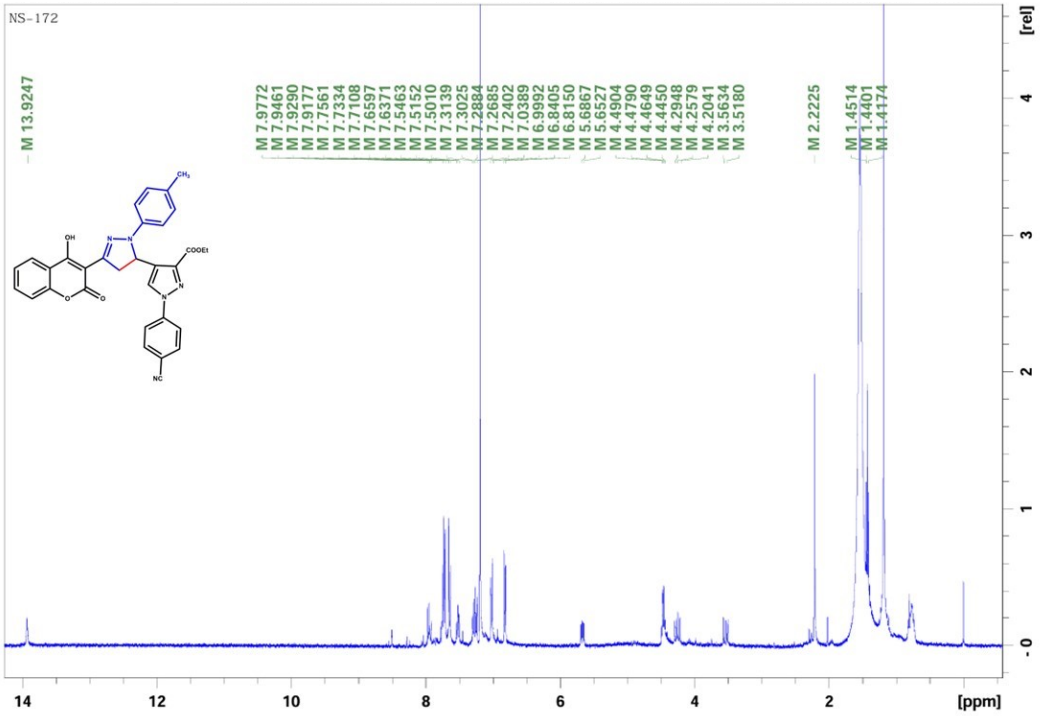


Figure S28. [1]H proton NMR spectra of compound **4o**.

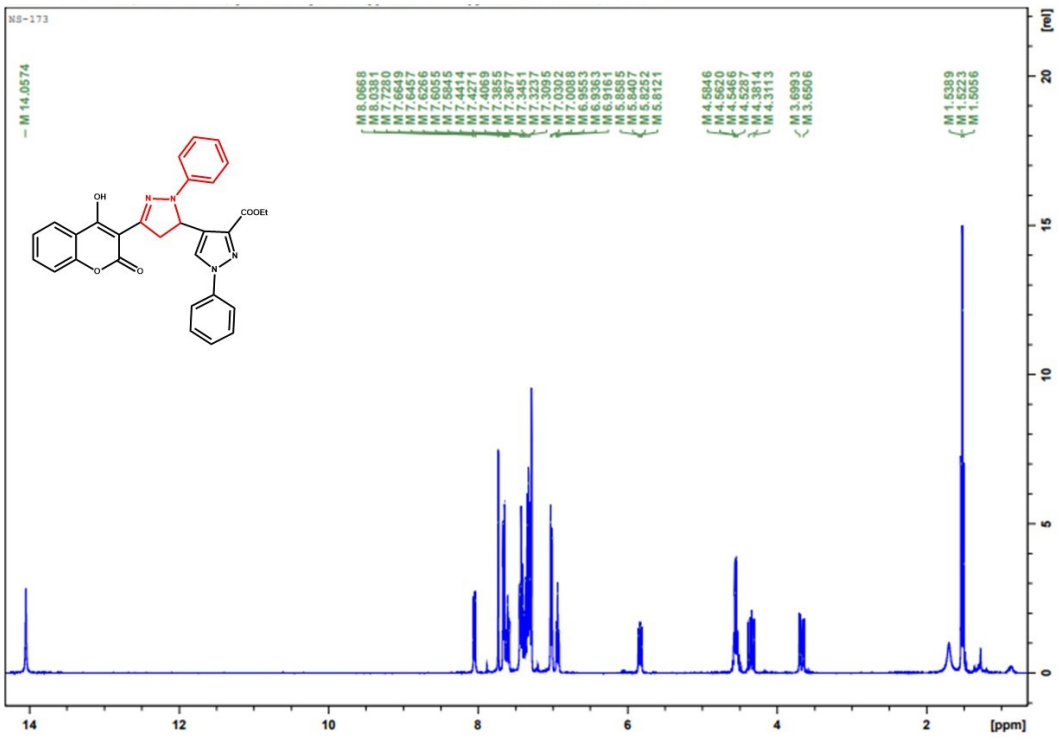


Figure S29. [1]H proton NMR spectra of compound **4p**.

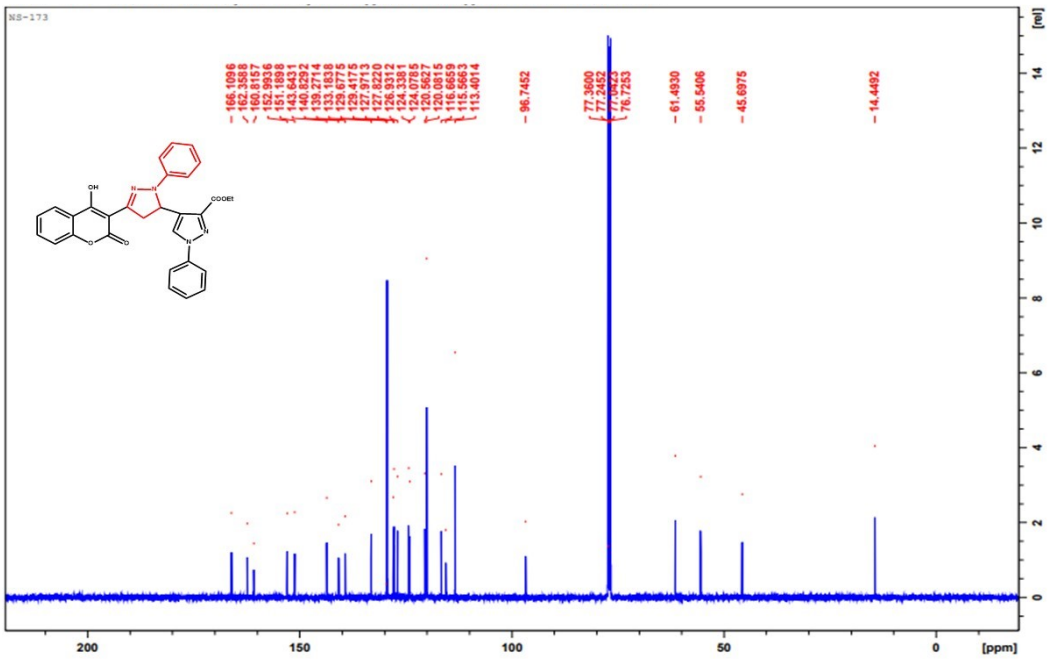


Figure S30. ^{13}C NMR spectra of compound **4p**.

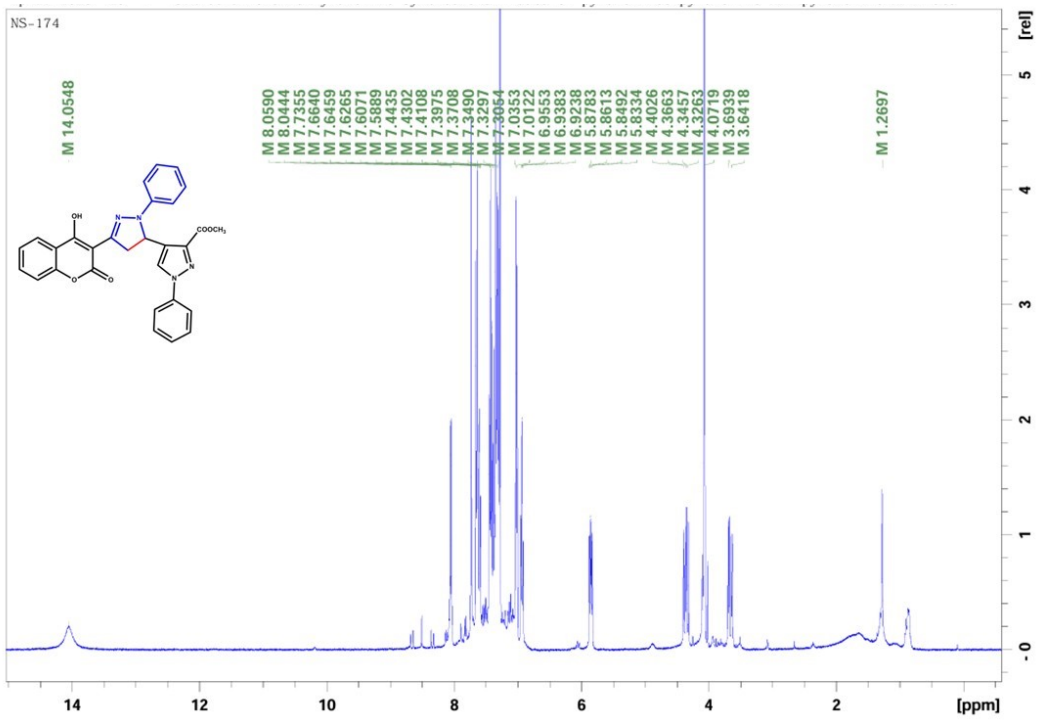


Figure S31. ^{1}H proton NMR spectra of compound **4q**.

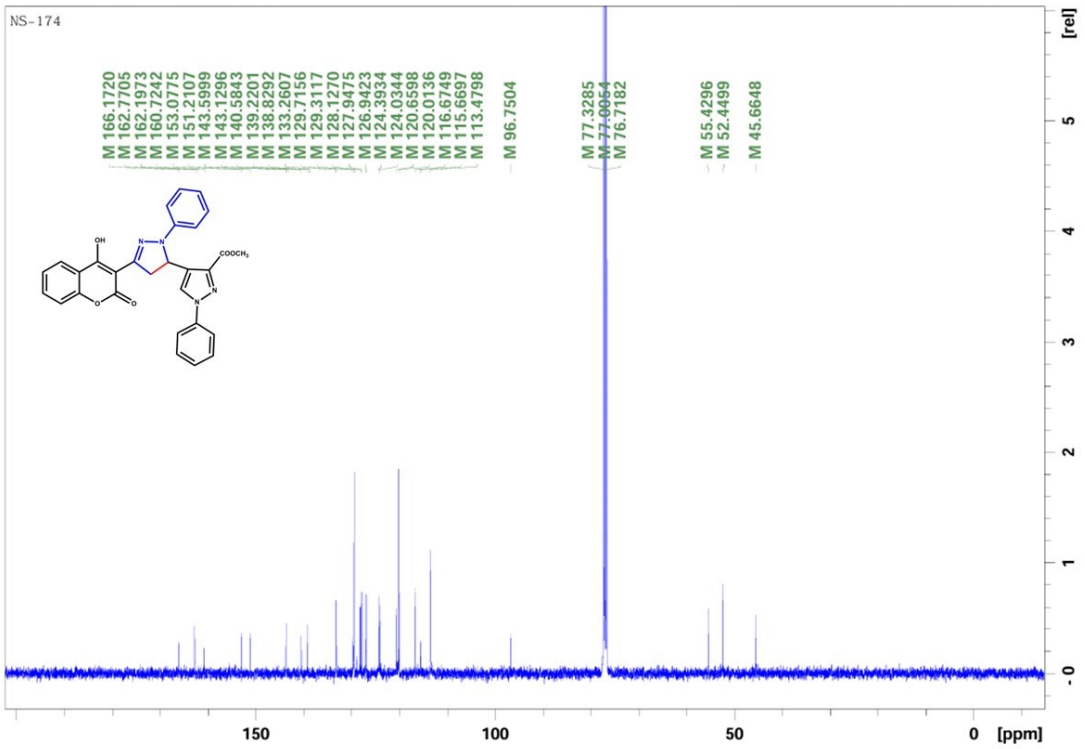


Figure S32. ^{13}C NMR spectra of compound **4q**.

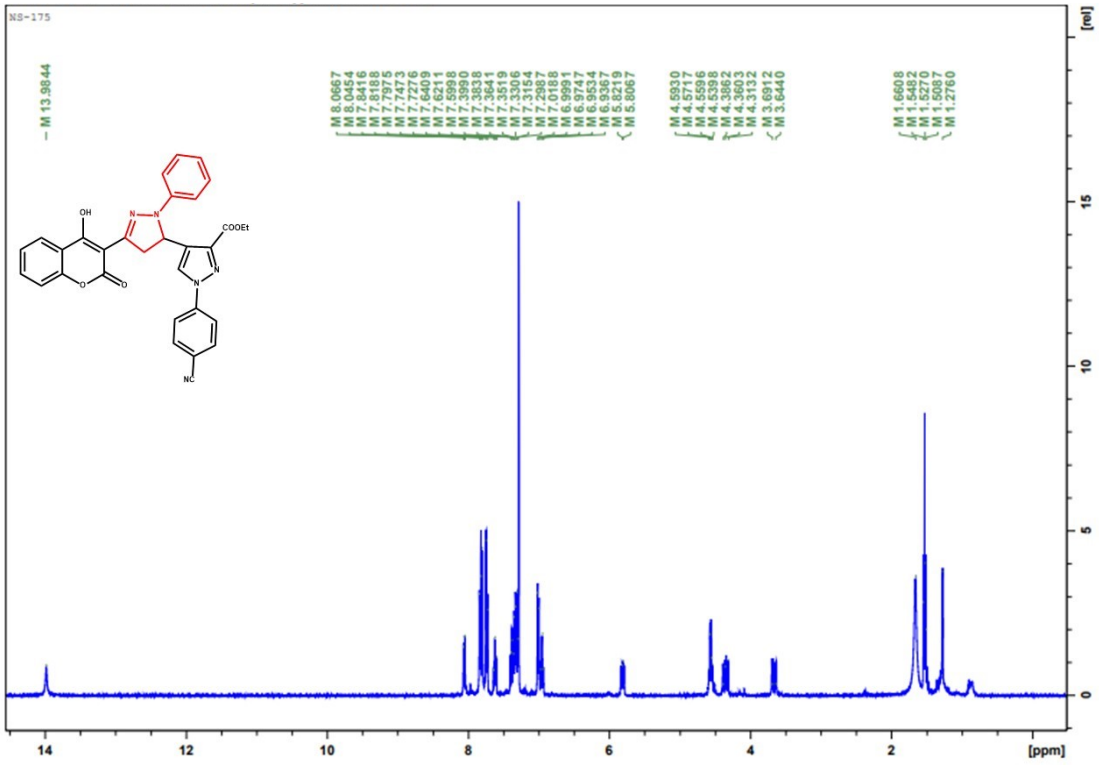


Figure S33. ^{1}H proton NMR spectra of compound **4r**.

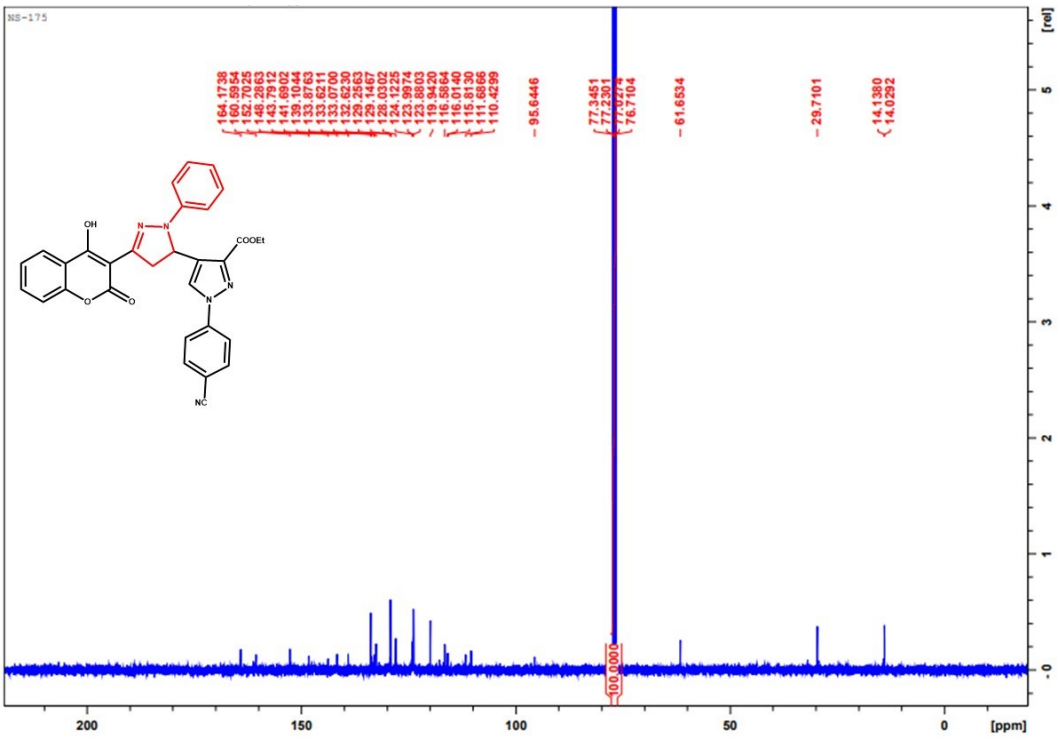


Figure S34. ^{13}C NMR spectra of compound **4r**.

Green chemistry metrics analysis

The following formulae were used for calculating Effective Mass Yield (EMY), Atom Economy (AE), Atom Efficiency (AEf), Reaction Mass Efficiency (RME), Optimum Efficiency (OE), Carbon Efficiency (CE), Mass Intensity (MI), Process Mass Intensity (PMI), Mass Productivity (MP), E-factor, and Solvent Intensity (SI). Calculated data for compounds 4a – 4r are presented in Table 4 and 5.

$$EMY\ (\%) = \frac{Mass\ of\ product}{Mass\ of\ non-benign\ reagents} \times\ 100$$

$$AE\ (\%) = \frac{Molecular\ weight\ of\ product}{Total\ molecualr\ weight\ of\ reactants} \times\ 100$$

$$AEf\ (\%) =\ AE \times Yield\%$$

$$CE(\%) = \frac{Amount\ of\ carbon\ in\ the\ product}{Total\ carbon\ present\ in\ reactants} \times 100$$

$$RME(\%) = \frac{Mass\ of\ isolated\ product}{Total\ mass\ of\ reactants} \times 100$$

$$OE(\%) = \frac{RME}{AE} \times 100$$

$$PMI = \frac{Total\ mass\ of\ input\ material\ in\ the\ whole\ process\ (including\ solvent(s)\ used\ during\ workup)}{Mass\ of\ product}$$

$$MI = \frac{Total\ mass\ used\ in\ the\ whole\ process\ step\ (excluding\ water)}{Mass\ of\ product}$$

$$MP(\%) = \frac{1}{MI} \times 100$$

$$SI = \frac{Total\ mass\ of\ solvents\ excluding\ water\ in\ the\ whole\ process}{Mass\ of\ product}$$

$$E - factor = \frac{Totalmass\ of\ wastes}{Mass\ of\ product} = \frac{Mass\ of\ raw\ materials - Mass\ of\ product}{Mass\ of\ product}$$

Materials used for calculations of metrics:

Chalcones (**1**, mmol), hydrazine hydrate (**2**, mmol), 3ml of ethanol/acetic acid/propionic acid for performing a reaction, and another 1ml of ethanol used for washing purpose only when ethanol used as a solvent in the reaction.

Respective amounts-

Reagents- ethyl pyruvate chalcones 1eq (MW 430.41); methyl pyruvate chalcones 1eq (MW 416.38); cyno ethyl pyruvate chalcones 1eq (MW 455.42); hydrazine hydrate 2eq (MW 50.06); Phenylhydrazine hydrochloride 2eq (MW 144.61); 4-CN phenylhydrazine hydrochloride 2eq (MW 169.61); 4-CH_3 phenylhydrazine hydrochloride 2eq (MW 158.63).

Solvents: Reaction media- ethanol (3.0 ml), acetic acid (3.0 ml), propionic acid (3.0 ml).

Solvent for washing purpose: ethanol (1.0 ml)

products- 4a 0.0896g (MW 444.14); **4b** 0.102g (MW 486.48); **4c** 0.0976g (MW 472.45); **4d** 0.0898g (MW 430.41); **4e** 0.099g (MW 511.49); **4f** 0.089g (MW 469.45); **4g** 0.120g (MW 531.52); **4h** 0.104g (MW 500.50); **4i** 0.102g (MW 486.48); **4j** 0.101g (MW 525.51); **4k** 0.114g

(MW 545.54); **4l** 0.119g (MW 570.55); **4m** 0.110g (MW 534.56); **4n** 0.119g (MW 520.54); **4o** 0.115g (MW 559.57); **4p** 0.112g (MW 520.54); **4q** 0.115g (MW 506.51); **4r** 0.114g (MW 545.54);

Representative calculations of green metrics for 4a-

$$EMY\ (\%) = \frac{Mass\ of\ product}{Mass\ of\ non-benign\ reagents} \times\ 100 \quad = \quad \frac{0.0896g}{(0.1+0.023)g} \times\ 100 \quad = 72.84\%$$

$$AE\ (\%) = \frac{Molecular\ weight\ of\ product}{Total\ molecualr\ weight\ of\ reactants} \times\ 100 \ = \ \frac{444.14}{(430.41+2*50.06)} \times\ 100 = 83.71\%$$

$$AEf\ (\%) = \ AE \times Yield\% \qquad\qquad = 83.71 * 86.99\% \ = \ 72.81\%$$

$$CE(\%) = \frac{Amount\ of\ carbon\ in\ the\ product}{Total\ carbon\ present\ in\ reactants} \times 100 \quad = \quad \frac{24*0.00020}{24*0.00023} \times 100 \ = 86.95\%$$

$$RME(\%) = \frac{Mass\ of\ isolated\ product}{Total\ mass\ of\ reactants} \times 100 \qquad = \frac{0.0896g}{(0.1+0.023)g} \times 100 \ = \ 72.84\%$$

$$OE(\%) = \frac{RME}{AE} \times 100 \quad = \frac{72.84}{83.71} \times 100 \quad = 87.01\%$$

$$PMI = \frac{Total\ mass\ of\ input\ material\ in\ the\ whole\ process\ (including\ solvent(s)\ used\ during\ workup)}{Mass\ of\ product} = \frac{(0.1+0.023+3.15)g}{0.0896g} = 36.52g/g$$

$$MI = \frac{Total\ mass\ used\ in\ the\ whole\ process\ step\ (excluding\ water)}{Mass\ of\ product} = \frac{(0.1+0.023+2.36)g}{0.0896g} = 27.71g/g$$

$$MP(\%) = \frac{1}{MI} \times 100 \quad \frac{1}{27.71} \times 100 \ = \ 3.60\%$$

$$SI = \frac{Total\ mass\ of\ solvents\ excluding\ water\ in\ the\ whole\ process}{Mass\ of\ product} = \frac{3.156g}{0.0896g} = 35.22g/g$$

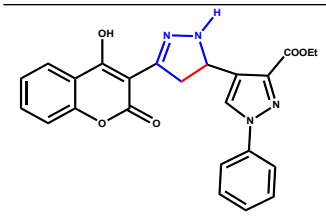
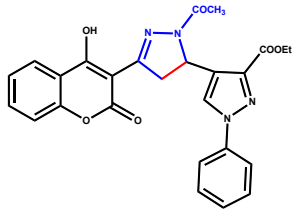
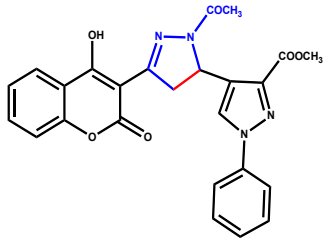
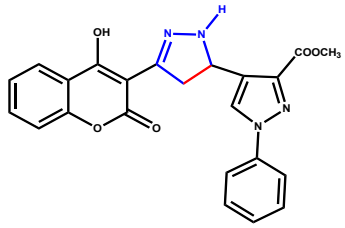
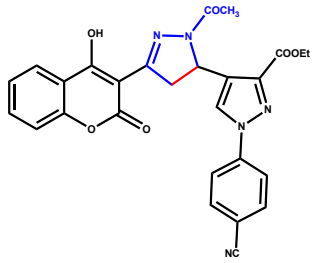
$$E-factor = \frac{Total\ mass\ of\ wastes}{Mass\ of\ product} = \frac{Mass\ of\ raw\ materials - Mass\ of\ product}{Mass\ of\ product} = \frac{(0.1+0.023)g - 0.0896g}{0.0896g} = 0.37$$

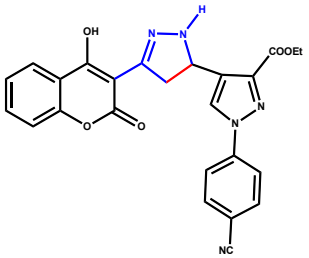
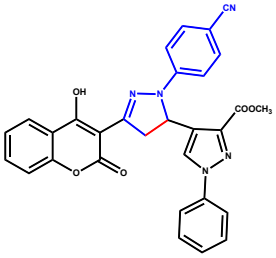
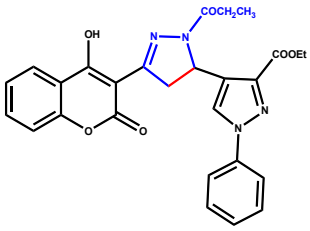
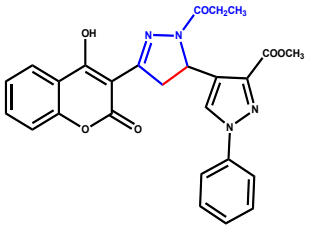
[note:

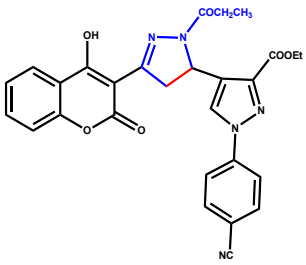
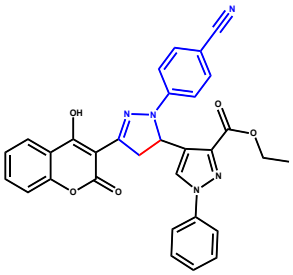
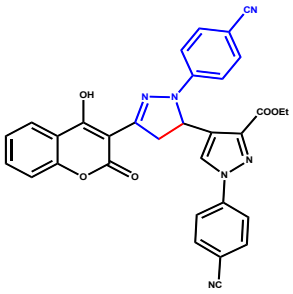
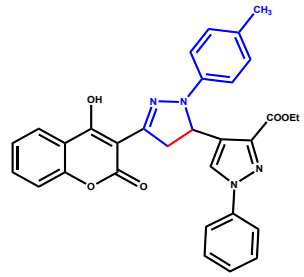
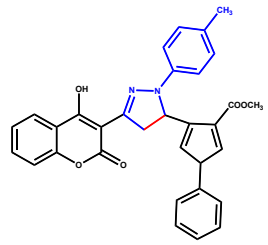
Photophysical properties-

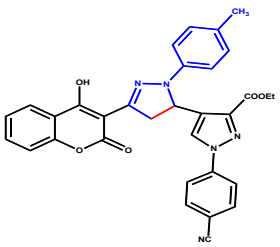
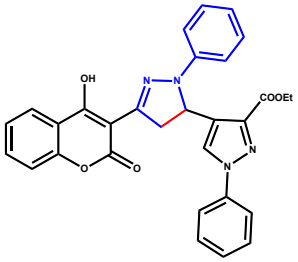
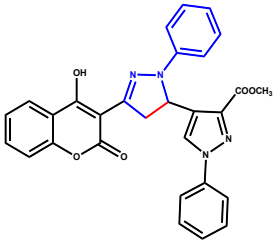
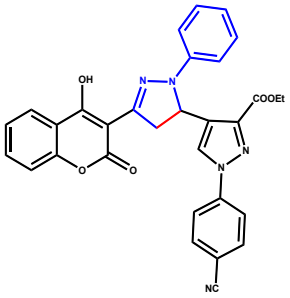
Table S1: The photophysical properties of the coumarin based pyrazole-pyrazoline hybrid heterocyclic molecules.

structure	solvent	λ_{abs}/nm	λ_{em}/nm	ΔνSS/cm^{-1}	($Eg_{em)\ (eV)}$

 4a	ACN	345	436	6050	2.84
	DMSO	347	429	5508	2.89
	MeOH	336	431	6560	2.87
	DMF	346	426	5427	2.91
	THF	347	427	5399	2.90
	DCM	342	438	6408	2.83
	EtOAc	341	425	5796	2.91
 4b	ACN	351	441	5815	2.81
	DMSO	343	436	6219	2.84
	MeOH	339	439	6719	2.82
	DMF	343	436	6219	2.84
	THF	351	438	5659	2.83
	DCM	350	433	5477	2.86
	EtOAc	348	434	5694	2.85
 4c	ACN	350	442	5947	2.80
	DMSO	341	452	7202	2.74
	MeOH	341	432	6177	2.87
	DMF	344	442	6445	2.80
	THF	352	429	5099	2.89
	DCM	356	431	4888	2.87
	EtOAc	346	430	5646	2.88
 4d	ACN	339	427	6079	2.90
	DMSO	344	429	5759	2.89
	MeOH	341	428	5961	2.89
	DMF	349	420	4844	2.95
	THF	344	435	6081	2.85
	DCM	345	430	5730	2.88
	EtOAc	343	427	5735	2.90
	ACN	353	446	5907	2.78
	DMSO	348	428	5371	2.89
	MeOH	341	434	6284	2.85
	DMF	343	429	5844	2.89
	THF	351	427	5071	2.90
	DCM	349	431	5452	2.87

4e 	EtOAc	346	433	5807	2.86
	ACN	341	483	8622	2.56
	DMSO	341	402	4450	3.08
	MeOH	344	427	5650	2.90
	DMF	354	429	4938	2.89
	THF	344	432	5921	2.87
4f	DCM	338	424	6001	2.92
	EtOAc	342	421	5487	2.94
	ACN	370	479	6151	2.58
	DMSO	356	427	4670	2.90
	MeOH	354	425	4719	2.91
	DMF	357	429	4701	2.89
	THF	371	484	6293	2.56
4g	DCM	378	418	2532	2.96
	EtOAc	381	428	2882	2.89
	ACN	344	447	6698	2.77
	DMSO	344	447	6698	2.77
	MeOH	344	433	5975	2.86
	DMF	343	447	6783	2.77
	THF	345	442	6361	2.80
4h	DCM	352	430	5154	2.88
	EtOAc	348	438	5904	2.83
	ACN	349	442	6029	2.80
	DMSO	347	444	6296	2.79
	MeOH	347	434	5777	2.85
	DMF	343	447	6783	2.77
	THF	349	444	6131	2.79
4i	DCM	359	429	4545	2.89
	EtOAc	344	430	5814	2.88
	ACN	354	436	5313	2.84
	DMSO	291	438	11533	2.83
	MeOH	347	431	5617	2.87

 4j	DMF	343	438	6323	2.83
	THF	353	427	4909	2.90
	DCM	356	430	4834	2.88
	EtOAc	346	429	5591	2.89
 4k	ACN	408	517	5167	2.39
	DMSO	382	506	6416	2.45
	MeOH	373	494	6567	2.51
	DMF	379	506	6623	2.45
	THF	409	505	4648	2.45
	DCM	409	503	4569	2.46
	EtOAc	408	503	4629	2.46
 4l	ACN	345	488	8494	2.54
	DMSO	353	432	5180	2.87
	MeOH	344	426	5595	2.91
	DMF	348	496	8574	2.5
	THF	359	496	7694	2.5
	DCM	378	496	6294	2.5
	EtOAc	353	495	8126	2.50
 4m	ACN	406	551	6482	2.25
	DMSO	371	435	3966	2.85
	MeOH	390	545	7293	2.27
	DMF	370	547	8746	2.26
	THF	415	539	5544	2.30
	DCM	417	549	5766	2.25
	EtOAc	409	547	6168	2.26
	ACN	390	423	2001	2.93
	DMSO	363	430	4293	2.88
	MeOH	360	427	4358	2.90
	DMF	362	431	4423	2.87
	THF	370	428	3663	2.89
	DCM	383	430	2854	2.88

4n 	EtOAc	371	424	3370	2.92
	ACN	288	345	5737	3.59
	DMSO	291	422	10668	2.93
	MeOH	287	348	6108	3.56
	DMF	289	346	5701	3.58
	THF	291	341	5039	3.63
	DCM	282	342	6221	3.62
4o	EtOAc	275	346	7462	3.58
	ACN	401	542	6487	2.28
	DMSO	366	427	3903	2.90
	MeOH	370	527	8052	2.35
	DMF	358	427	4513	2.90
	THF	412	524	5188	2.36
4p	DCM	397	521	5995	2.38
	EtOAc	404	522	5595	2.37
	ACN	384	550	7860	2.25
	DMSO	363	434	4507	2.85
	MeOH	366	540	8804	2.29
	DMF	359	431	4654	2.87
	THF	385	525	6927	2.36
4q	DCM	387	524	6756	2.36
	EtOAc	390	524	6558	2.36
	ACN	369	535	8409	2.31
	DMSO	360	431	4576	2.87
	MeOH	357	429	4701	2.89
	DMF	361	434	4659	2.85
	THF	370	522	7870	2.37
	DCM	368	429	3863	2.89
4r	EtOAc	365	426	3923	2.91

Absorption (λ_{abs}) and fluorescence emission (λ_{em}) maximum; Stokes shift ($\Delta\nu SS$); Energy band gap of PL (Eg_{em}).

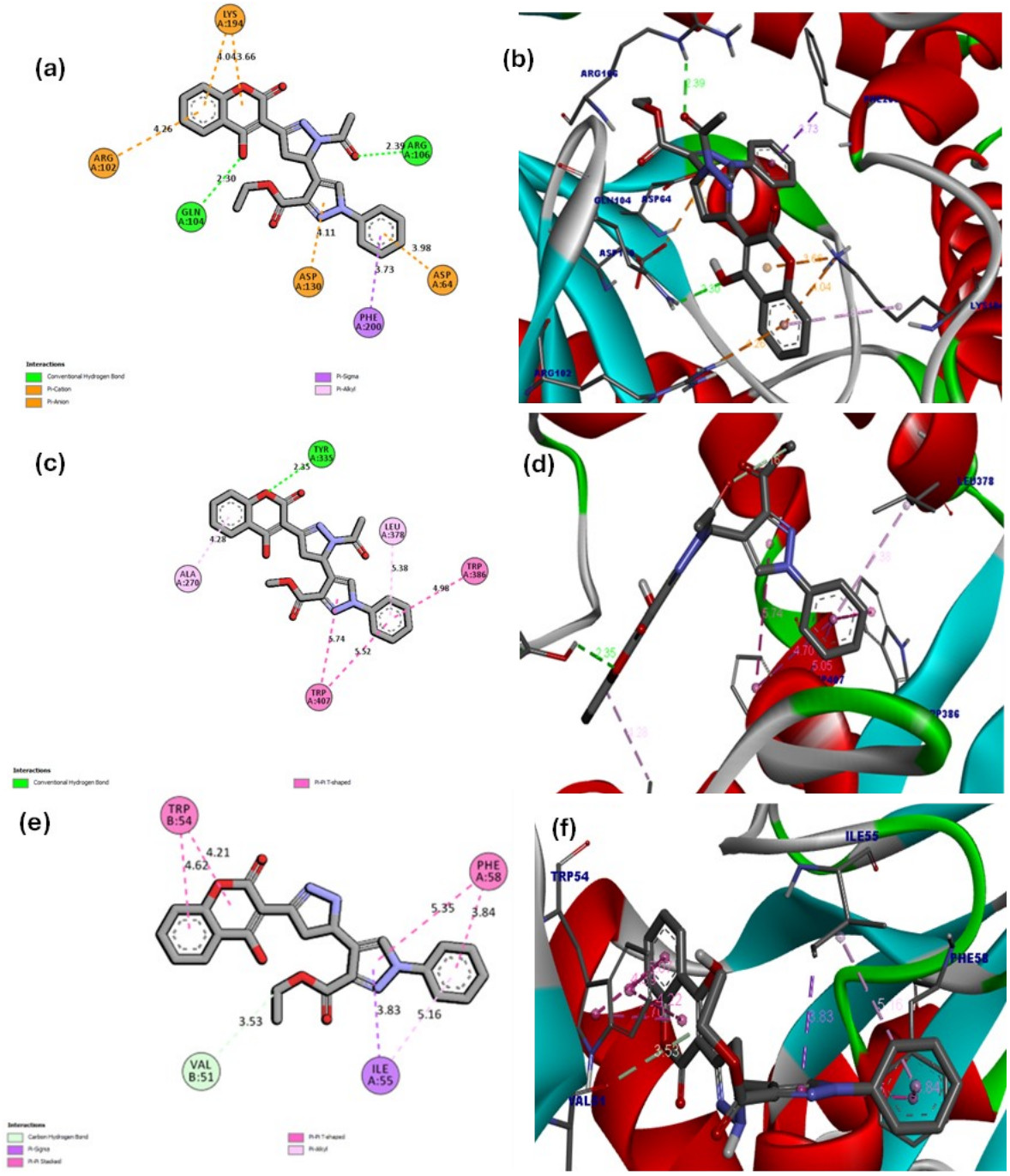


Figure S 35. The selected docked poses of coumarin based pyrazole-pyrazoline hybrid heterocyclic molecules (a) 2D Docked poses of **4b** with 6P8U; (b) 3D Docked poses of **4b** with

6P8U; (c) 2D Docked poses of 8BBX with **4c**; (d) 3D Docked poses of 8BBX with **4c**; (e) 2D Docked poses of 5TZ1 with **4a**; (f) 3D Docked poses of 5TZ1 with **4a**

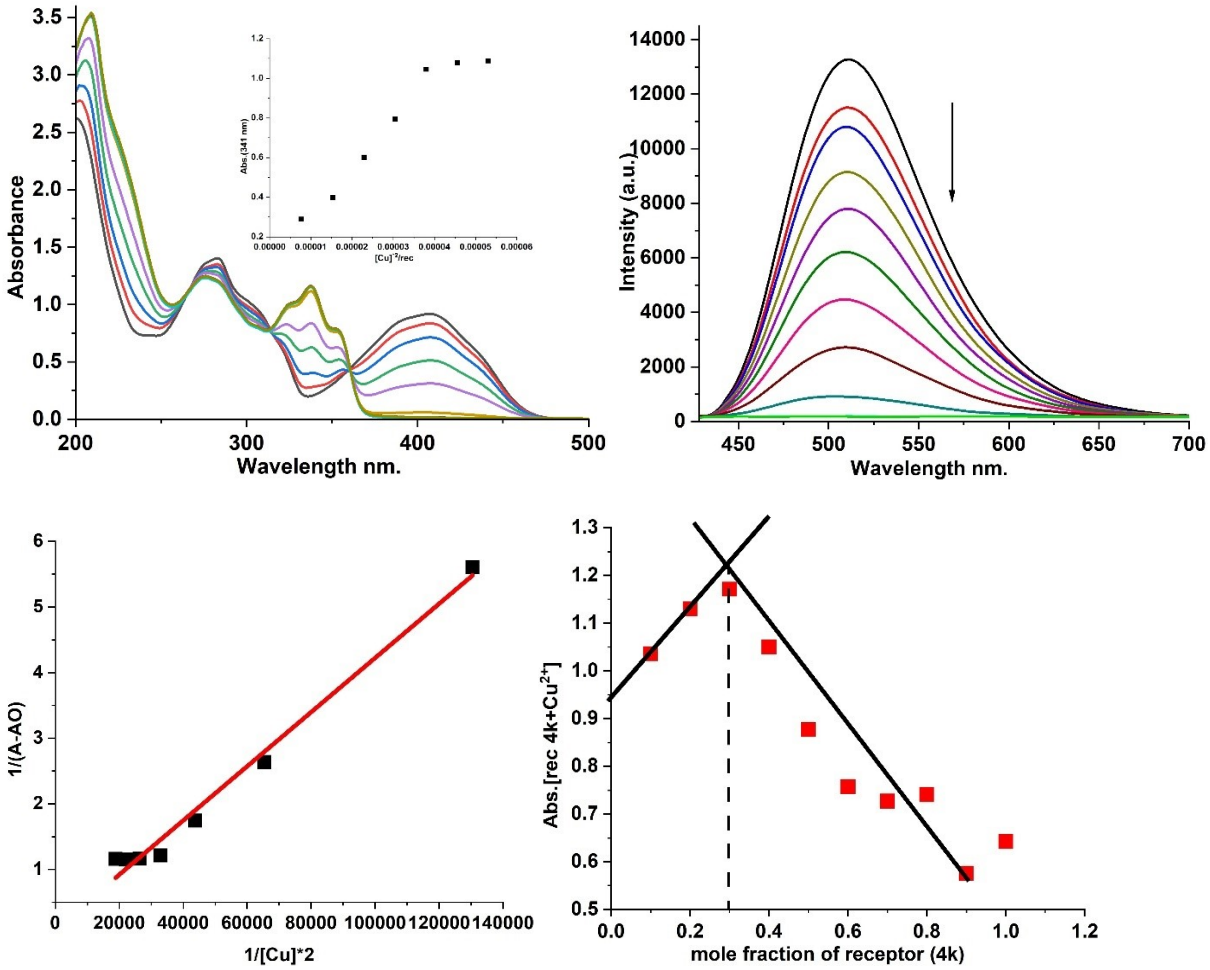


Figure S 36: The UV titration spectra of receptor **4k,** The emission spectra of **4k**, Benesi-Hildebrand plot of compound 4k, **and** Job's continuation variation graph of compound **4k** with (a) with Cu^{2+}.

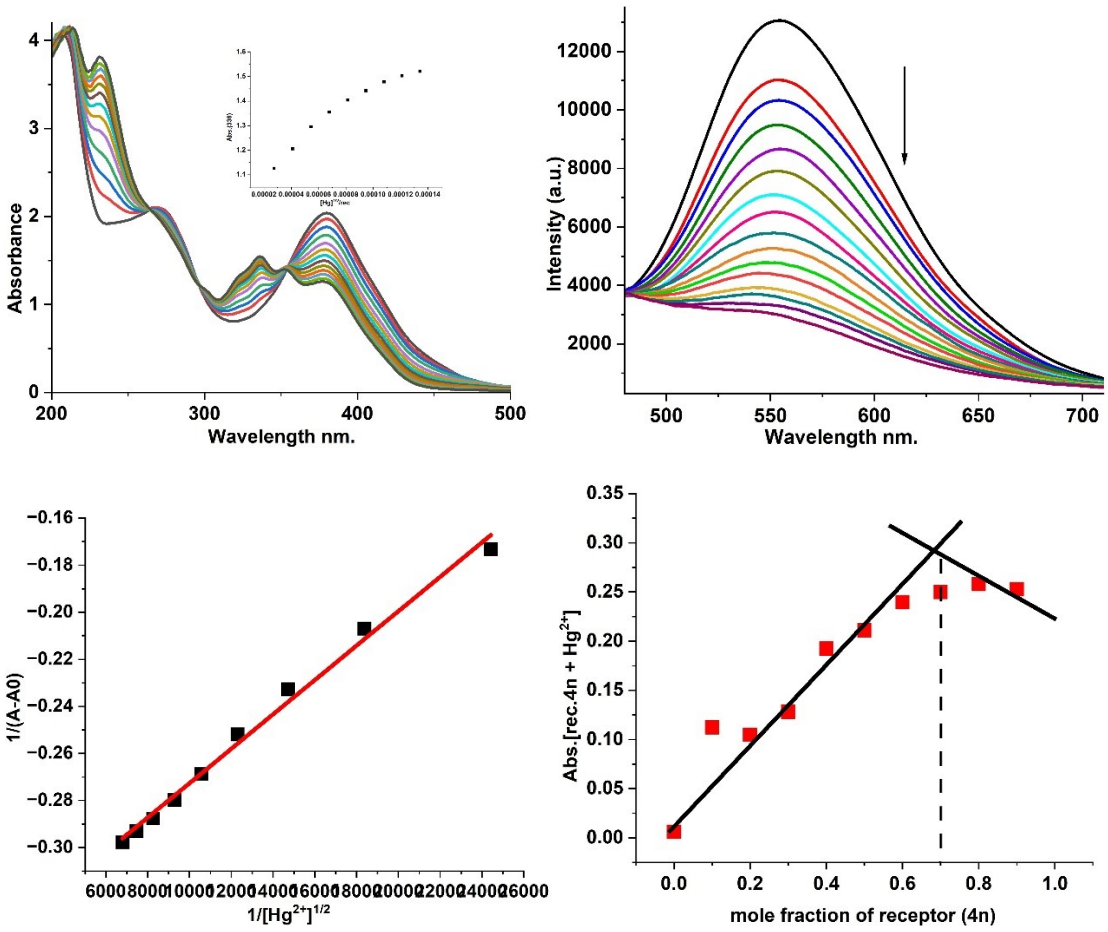
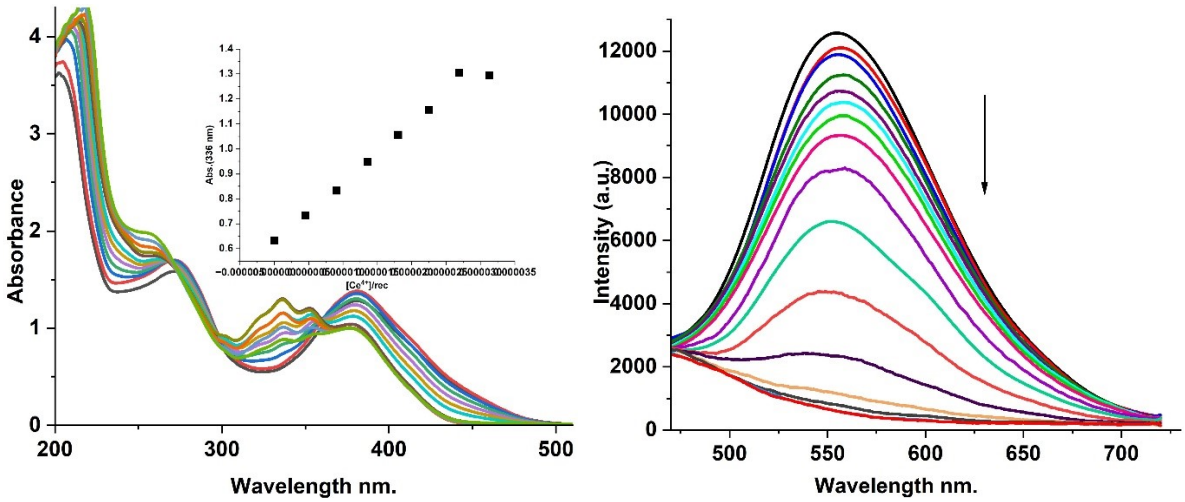


Figure S 37: The UV titration spectra of receptor **4n,** The emission spectra of **4n**, Benesi-Hildebrand plot of compound 4n, **and** Job's continuation variation graph of compound **4n** with (a) with Hg^{2+}.



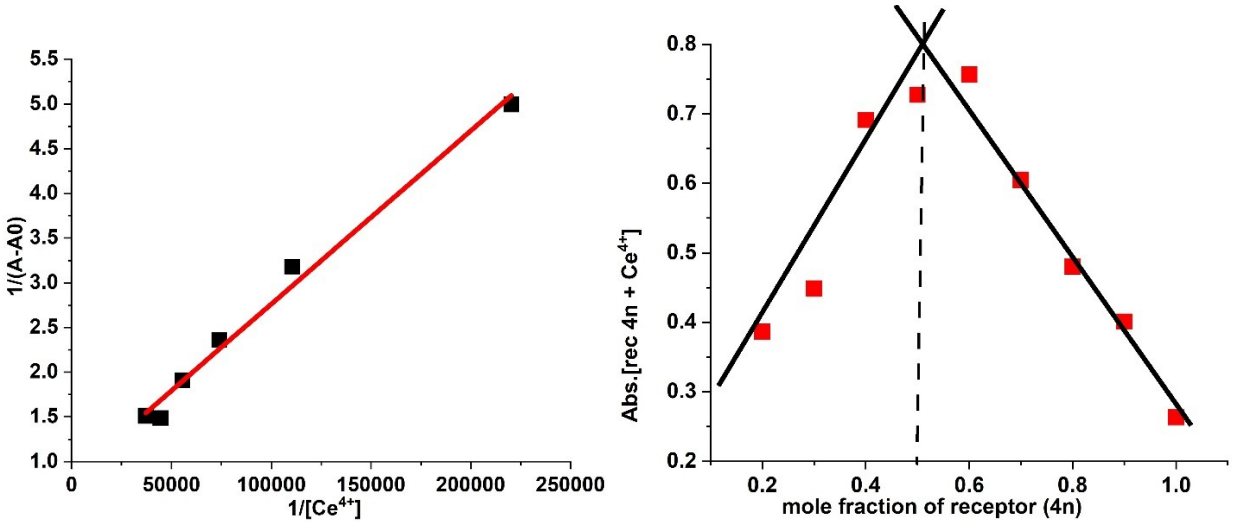


Figure S 38: The UV titration spectra of receptor **4n,** The emission spectra of **4n**, Benesi-Hildebrand plot of compound 4n, **and** Job's continuation variation graph of compound **4n** with (a) with Ce^{4+}.

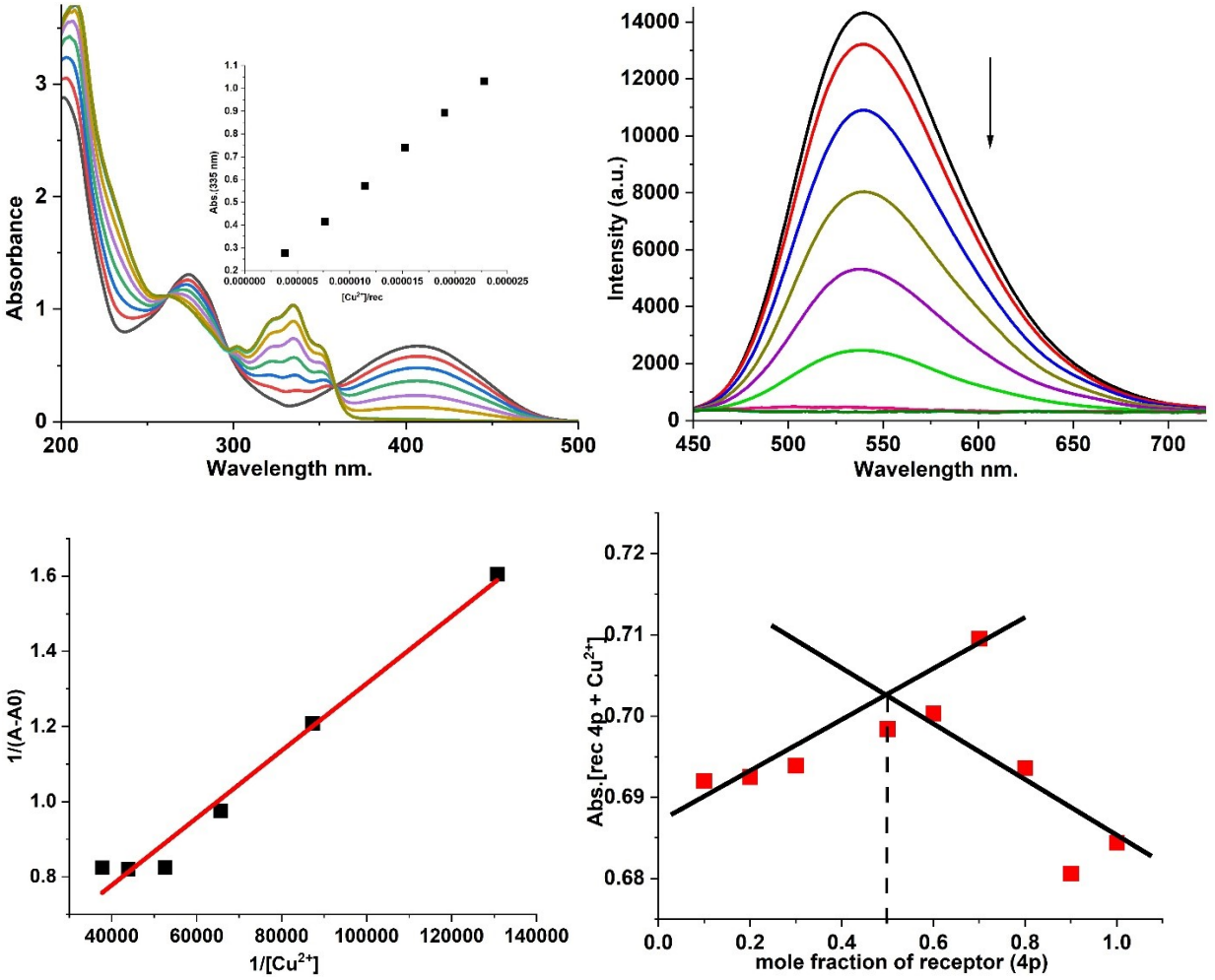


Figure S 39: The UV titration spectra of receptor **4p,** The emission spectra of **4p**, Benesi-Hildebrand plot of compound 4p, **and** Job's continuation variation graph of compound **4p** with (a) with Cu^{2+}.

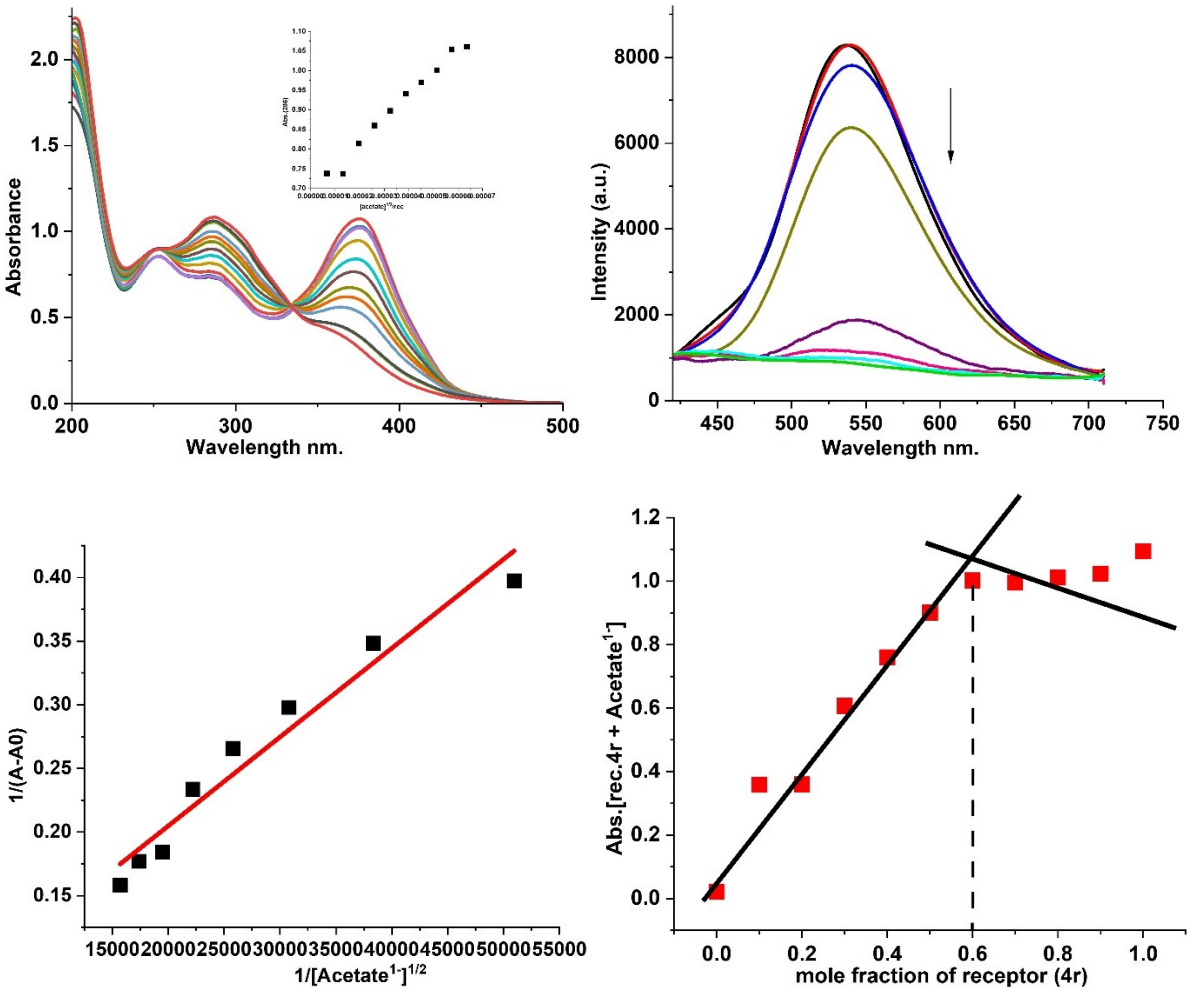


Figure S 40: The UV titration spectra of receptor **4r,** The emission spectra of **4r**, Benesi-Hildebrand plot of compound 4r, and Job's continuation variation graph of compound **4r** with (a) with $Acetate^{1-}$.