Electronic Supplementary Material (ESI) for Medicinal Chemistry Communications

Supporting Information

Using Natural Potential of Chromone: Development of Small Molecules as Multi-ion Detectors

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Equation for calculation of binding constants

Binding constants of compound-anion complex were calculated using Benesi-Hildebrand Equation. $1/(A_f - A_{obs}) = 1/(A_f - A_{fc}) + 1/K(A_f - A_{fc})$ [Ligand]

Where A_f is absorbance of free host, A_{obs} is absorbance observed, A_{fc} is absorbance at saturation, K is the binding constant.

EXPERIMENTAL SECTION

Melting points were determined in capillaries and are uncorrected. ^1H and ^{13}C NMR spectra were recorded on JEOL 300 MHz and 75 MHz NMR spectrometer, respectively using $CDCl_3$ and/or DMSO-d_6 as solvent. Chemical shifts are given in ppm with TMS as internal reference. *J* values are given in Hertz. Signals are abbreviated as singlet, s; doublet, d; double-doublet, dd; triplet, t; multiplet, m. In ^{13}C NMR spectral data, +ve, -ve terms correspond to CH_3, CH, CH_2 signals in DEPT-135 NMR spectra. Chromatography was performed with silica 100-200 mesh and reactions were monitored by thin layer chromatography (TLC) with silica plates coated with silica gel HF-254. Elemental analysis was performed on Thermoelectron FLASH EA1112 CHN analyzer. Reactions under microwaves were performed using microwave oven (INALSA model 1MW17EG) with microwave power 700 W and operating frequency 2450 MHz. IR and UV spectral data were recorded on Varian 660-IR FT-IR Spectrometer and BioTek PowerWave XS instruments respectively.

Equation for calculation of correlation coefficient from linear regression analysis

$$r = \frac{\sum[(Xi-\bar{X})(Yi-\bar{Y})]}{\sqrt{\sum(Xi-\bar{X})^2 (Yi-\bar{Y})^2}}$$

Equation for calculation of correlation coefficient from partial regression analysis

$$r12.3 = \frac{r12-r13\times r23}{\sqrt{(1-r13^2)(1-r23^2)}}$$

Here, 1= compound 1, 2= Fe^{3+}, 3= Hg^{2+}
r12 = partial correlation between compound **3** and Fe^{3+}
r13 = partial correlation between compound **3** and Hg^{2+}
r12.3= partial correlation between compound **3** and Fe^{3+} eliminating the effect of Hg^{2+}
r13.2= partial correlation between compound **3** and Hg^{2+} eliminating the effect of Fe^{3+} (same formula as for r12.3)

1,3-Dimethyl-5-((4-oxo-4*H*-chromen-3-yl)methylene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (3): Creamish solid, 83% yield, mp 185 ^{o}C; ν_{max} (KBr): 1685, 1659, 1612 (C=O), ^{1}H NMR (300 MHz, $CDCl_3$): δ 3.45 (s, 3H, 2×CH_3), 7.46-7.71 (m, 2H, ArH), 7.73-7.77 (m, 1H, ArH), 8.28 (dd, J^3 = 7.8 Hz, J^4 = 1.5 Hz, 1H, ArH), 8.88 (s, 1H), 9.79 (s, 1H, 2-H). ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 28.4 (+ve, CH_3), 29.0 (+ve, CH_3), 117.9 (+ve, CH), 118.3 (+ve, CH), 118.3 (+ve, CH), 123.5 (+ve, CH), 126.3 (+ve, CH), 126.5 (+ve, CH), 134.5 (C), 148.7 (C), 151.0 (C), 155.6 (C), 161.2 (C), 161.7 (C), 163.50 (C), 175.2 (C). FAB mass *m/z* 312 (M^++1); (Found: C 61.56, H 4.13, N 9.27; $C_{16}H_{12}N_2O_5$ requires C 61.54, H 3.87, N 8.97).

5-((6-Isopropyl-4-oxo-4*H*-chromen-3-yl)methylene)-1,3-dimethylpyrimidine2,4,6(1*H*,3*H*, 5*H*)-trione (4): Creamish solid, 92% yield, mp 152 ^{o}C; ν_{max} (KBr): 1730, 1675, 1583 (C=O). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 1.27 (s, 3H; CH_3), 1.29 (s, 3H; CH_3), 3.01-3.05 (m, 1H; CH), 3.37 (s, 3H; CH_3), 3.40 (s, 3H; CH_3), 7.43 (d, *J* = 8.4 Hz, 1H; ArH), 7.57 (dd, ^{3}J = 8.5 Hz, ^{4}J = 2.4 Hz, 1H; ArH), 8.09 (d, *J* = 2.4 Hz, 1H; ArH), 8.88 (s, 1H; ArH), 9.77 ppm (s, 1H; 2-H); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 24.2 (+ve, CH_3), 28.8 (+ve, CH_3), 29.4 (+ve, CH_3), 34.2 (+ve, CH_3), 118.2 (+ve, CH), 118.5 (C), 118.6 (C), 123.8 (+ve, CH), 133.8 (+ve, CH), 147.9 (+ve, CH), 149.6 (C), 151.5 (C), 154.5 (C), 161.7 (C), 163.9 (+ve, CH), 175.8 (C). FAB mass *m/z* 355 (M^++1); (Found: C 64.40, H 5.12, N 7.91; $C_{19}H_{18}N_2O_5$ requires C 64.41, H 5.21, N 7.96).

5-((6-Bromo-4-oxo-4*H*-chromen-3-yl)methylene)-1,3-dimethylpyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (5): Creamish solid, 97% yield, mp 236 ^{o}C; ν_{max} (KBr): 1733, 1668, 1576 (C=O). ^{1}H NMR (300 MHz, $CDCl_3$) δ = 3.40 (s, 3H; CH_3), 3.47 (s, 3H; CH_3), 7.41 (d, *J* = 9 Hz, 1H; ArH), 7.79 (dd, ^{3}J = 8.8 Hz, ^{4}J = 2.7 Hz, 1H; ArH), 8.38 (d, *J* = 2.4 Hz, 1H; ArH), 8.78 (s, 1H; ArH), 9.71 (s, 1H; 2-H); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 24.7 (+ve, CH_3), 25.3 (+ve, CH_3), 114.3 (C), 115.1 (C), 116.5 (+ve, CH), 125.3 (+ve, CH), 133.7, (+ve, CH), 144.3 (+ve, CH), 150.6 (C), 157.4 (C), 159.3 (C); FAB mass *m/z* 392 (M^++1). (Found: C 49.13, H 2.83, N 7.16; $C_{16}H_{11}BrN_2O_5$ requires C 49.12, H 2.84, N 7.17).

1,3-Dimethyl-5-((6-nitro-4-oxo-4*H*-chromen-3-yl)methylene)pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione (6): Creamish solid, 95% yield, mp 200 ^{o}C; ν_{max} (KBr): 1734, 1672, 1623 (C=O). ^{1}H NMR (300 MHz, $CDCl_3$): δ = 2.00 (s, 3H; CH_3), 7.14-7.41 (m, 2H; ArH), 7.44-7.46 (m, 2H; ArH), 7.89-8.01 (m, 1H; ArH); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 28.5 (+ve, CH_3), 29.1

(+ve, CH_3), 118.7 (C), 120.2 (+ve, CH), 123.1 (+ve, CH), 123.8 (C), 128.7 (+ve, CH), 145.4 (C), 146.7 (+ve, CH), 150.8 (C), 158.4 (C), 161.0 (C), 161.3 (C), 162.4 (+ve, CH), 173.8 (C); FAB mass *m/z* 358 (M^++1). (Found: C 53.79, H 3.10, N 11.76; $C_{16}H_{11}N_3O_7$ requires C 53.80, H 3.09, N 11.77).

5-((6-Fluoro-8-nitro-4-oxo-4*H*-chromen-3-yl)methylene)-1,3-dimethylpyrimidine-2,4,6(1*H*, 3*H*,5*H*)-trione (7): Creamish solid, 97% yield, mp 190 ^oC; ν_{max} (KBr): 1681, 1593, 1537 (C=O). ^1H NMR (300 MHz, $CDCl_3$): δ = 3.38 (s, 3H; CH_3), 3.40 (s, 3H; CH_3), 8.12 (dd, ^3J = 7.2 Hz, ^4J = 3 Hz, 1H; ArH), 8.23 (dd, ^3J = 6.9 Hz, ^4J = 3.3 Hz, 1H; ArH), 8.66 (s, 1H; CH), 10.32 (s, 1H; =H); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 28.5 (+ve, CH_3), 29.1 (+ve, CH_3), 117.6 (+ve, CH), 117.9 (+ve, CH), 118.3 (C), 118.8 (+ve, CH), 119.2 (+ve, CH), 120.5 (C), 126.6 (C), 145.9 (+ve, CH), 150.8 (C), 160.9 (C), 161.2 (C), 161.8 (+ve, CH), 172.6 (C); FAB mass *m/z* 376 (M^++1). (Found: C 51.25, H 2.69, N 11.24; $C_{16}H_{10}FN_3O_7$ requires C 51.20, H 2.68, N 11.21).

5-(4-Oxo-4*H*-chromen-3-ylmethylene)-pyrimidine-2,4,6-trione (8) :

Creamish solid, 88% yield, mp >240 ^oC; ν_{max} (KBr): 3199, 3089 (NH), 1756, 1701 (C=O).

(4*Z*)-1-(3-Chlorophenyl)-3-methyl-4-((4-oxo-4*H*-chromen-3-yl)methylene)-1*H*-pyrazol-5(4*H*)-one (9): Orange solid, 87% yield, mp 227 ^oC; ν_{max} (KBr): 1680, 1610 (C=O). ^1H NMR (300 MHz, $CDCl_3$): δ = 2.39 (s, 3H; CH_3), 7.17-7.18 (m, 1H; ArH), 7.33 (t, *J* = 8.1 Hz, 1H; ArH), 7.50-7.58 (m, 2H; ArH), 7.74-7.79 (m, 1H; ArH), 7.88-7.91 (m, 1H; ArH), 8.01-8.04 (m, 2H; ArH), 8.29 (dd, ^3J = 8.1 Hz, ^4J = 1.5 Hz, 1H; ArH), 10.75 (s, 1H); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 13.2.5 (+ve, CH_3), 116.6 (+ve, CH), 118.2 (C), 118.7 (+ve, CH), 118.8 (+ve, CH), 123.6 (C), 124.9 (+ve, CH), 126.4 (+ve, CH), 126.5 (+ve, CH), 127.3 (C), 129.8 (+ve, CH), 134.5 (+ve, CH), 134.6 (+ve, CH), 136.6 (C), 139.2 (C), 151.5 (C), 156.0 (C), 162.5 (C), 164.1 (C), 175.3 (C); FAB mass *m/z* 365 (M^++1), 365:367 (3:1). (Found: C 66.13, H 3.73, N 7.70; $C_{20}H_{13}ClN_2O_3$ requires C 65.85, H 3.59, N 7.68).

(4*Z*)-1-(3-Chlorophenyl)-4-((6-isopropyl-4-oxo-4*H*-chromen-3-yl)methylene)-3-methyl-1*H*-pyrazol-5(4*H*)-one (10): Orange solid, 85% yield, mp 190 ^oC; ν_{max} (KBr): 1705 (C=O). ^1H NMR (300 MHz, $CDCl_3$): δ = 1.30 (s, 3H; CH_3), 1.31 (s, 3H; CH_3), 2.38 (s, 3H; CH_3), 3.00-3.10 (m, 1H; ArH), 7.11-7.15 (m, 1H; ArH), 7.31 (t, *J* = 8.1 Hz, 1H; ArH), 7.45 (d, *J* = 8.4 Hz, 1H; ArH), 7.61 (dd, ^3J = 8.8 Hz, ^4J = 2.4 Hz, 1H; ArH), 7.85-7.89 (m, 2H; ArH), 8.01-8.10 (m, 3H; ArH), 10.72 (s, 1H); ^{13}C NMR (normal/DEPT-135) ($CDCl_3$): δ 13.2 (+ve, CH_3), 23.8 (+ve, CH_3), 33.8 (+ve, CH_3), 116.6 (+ve, CH), 118.0 (+ve, CH), 118.5 (C), 118.8 (C), 123.3 (+ve,

CH), 124.8 (+ve, CH), 127.0 (C), 129.8 (+ve, CH), 133.5 (+ve, CH), 134.5 (C), 136.9 (+ve, CH), 139.2 (C), 147.5 (C), 151.6 (C), 154.4 (C), 162.5 (C), 164.1 (C), 175.4 (C). FAB mass *m/z* 407 (M^++1); (Found: C 67.90, H 4.71, N 6.89; $C_{23}H_{19}ClN_2O_3$ requires C 67.91, H 4.72, N 6.88).

(4*Z*)-4-((6-Bromo-4-oxo-4*H*-chromen-3-yl)methylene)-1-(3-chlorophenyl)-3-methyl-1*H*-pyrazol-5(4*H*)-one (11):

Orange solid, 91% yield, mp 210 ^oC; ν_{max} (KBr): 1673, 1624 (C=O); ^1H NMR (300 MHz, $CDCl_3$): δ = 2.32 (s, 3H; CH_3), 7.07-7.10 (m, 1H; ArH), 7.23 (t, *J* = 8.1 Hz, 1H; ArH), 7.40 (d, *J* = 8.7 Hz, 1H; ArH), 7.74-7.82 (m, 2H; ArH), 7.87 (s, 1H; ArH), 7.95 (t, *J* = 2.1 Hz, 1H; ArH), 8.33 (d, *J* = 2.4 Hz, 1H; ArH), 10.66 (s, 1H); FAB mass *m/z* 444 (M^++1). (Found: C 54.14, H 2.73, N 6.31; $C_{20}H_{12}BrClN_2O_3$ requires C 54.15, H 2.72, N 6.31).

(4*Z*)-1-(3-Chlorophenyl)-3-methyl-4-((6-nitro-4-oxo-4*H*-chromen-3-yl)methylene)-1*H*-pyrazol-5(4*H*)-one (12):

Orange solid, 87% yield, mp >240 ^oC; ν_{max} (KBr): 1684, 1662 (C=O). ^1H NMR (300 MHz, $CDCl_3$): δ = 2.34 (s, 3H; CH_3), 7.09-7.13 (m, 1H; ArH), 7.27 (t, *J* = 8.4 Hz, 1H; ArH), 7.68 (d, *J* = 9.3 Hz, 1H; ArH), 7.79-7.82 (m, 1H; ArH), 7.85 (d, *J* = 0.6 Hz, 1H; ArH), 7.95 (t, *J* = 2.1 Hz, 1H; ArH), 8.51 (dd, ^3J = 9 Hz, ^4J = 2.7 Hz, 1H; ArH), 9.08 (d, *J* = 2.4 Hz, 1H; ArH), 10.71 (s, 1H); FAB mass *m/z* 410 (M^++1); (Found: C 58.62, H 2.95, N 10.25; $C_{20}H_{12}ClN_3O_5$ requires C 58.63, H 2.95, N 10.24).

(4*Z*)-1-(3-Chlorophenyl)-4-((6-fluoro-8-nitro-4-oxo-4*H*-chromen-3-yl)methylene)-3-methyl 1*H*- pyrazol-5(4*H*)-one (13):

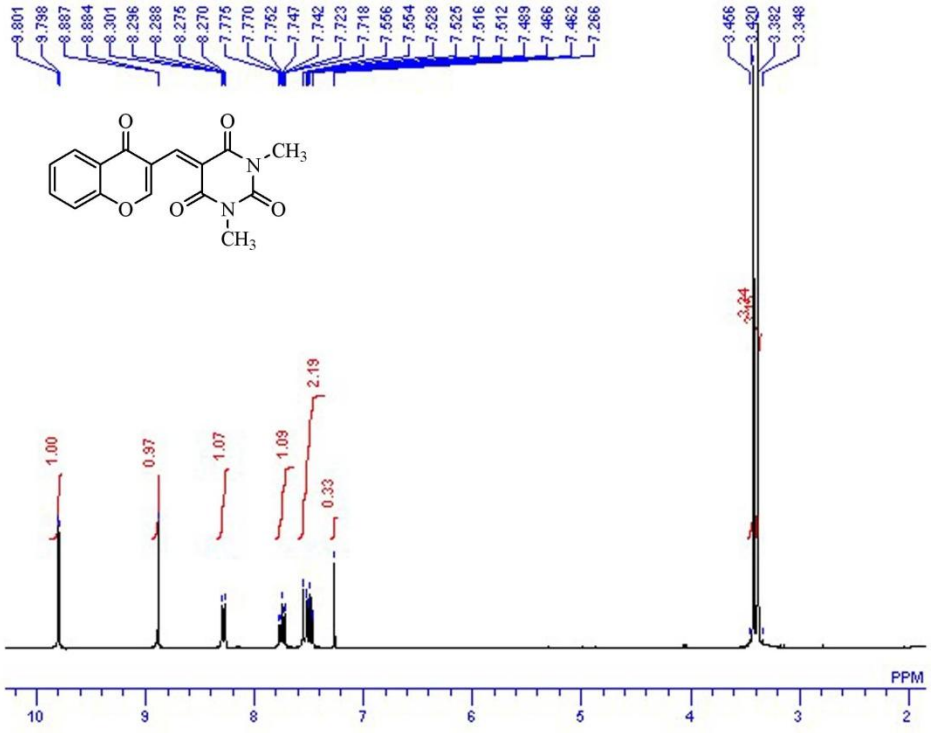
Orange solid, 89% yield, mp 230 ^oC; ν_{max} (KBr): 1730, 1653 (C=O). ^1H NMR (300 MHz, $CDCl_3$): δ = 2.33 (s, 3H; CH_3), 7.09-7.13 (m, 1H; ArH), 7.27 (t, *J* = 8.4 Hz, 1H; ArH), 7.78-7.83 (m, 2H; ArH), 7.94 (t, *J* = 2.1 Hz, 1H; ArH), 8.08 (dd, ^3J = 7 Hz, ^4J = 3 Hz, 1H; ArH), 8.18 (dd, ^3J = 7.2 Hz, ^4J = 3 Hz, 1H; ArH), 10.73 (s, 1H); FAB mass *m/z* 427 (M^++1); (Found: C 56.15, H 2.59, N 9.82; $C_{20}H_{12}ClFN_3O_5$ requires C 56.16, H 2.60, N 9.83).

3-(1,3-Dimethyl-2,4,6-trioxo-tetrahydro-pyrimidin-5-ylidenemethyl)-4-oxo-chroman-2-carbonitrile+3-(1,3-Dimethyl-2,4,6-trioxo-tetrahydro-pyrimidin-5-ylidenemethyl)-4-hydroxy-2H-chromene-2-carbonitrile (14):

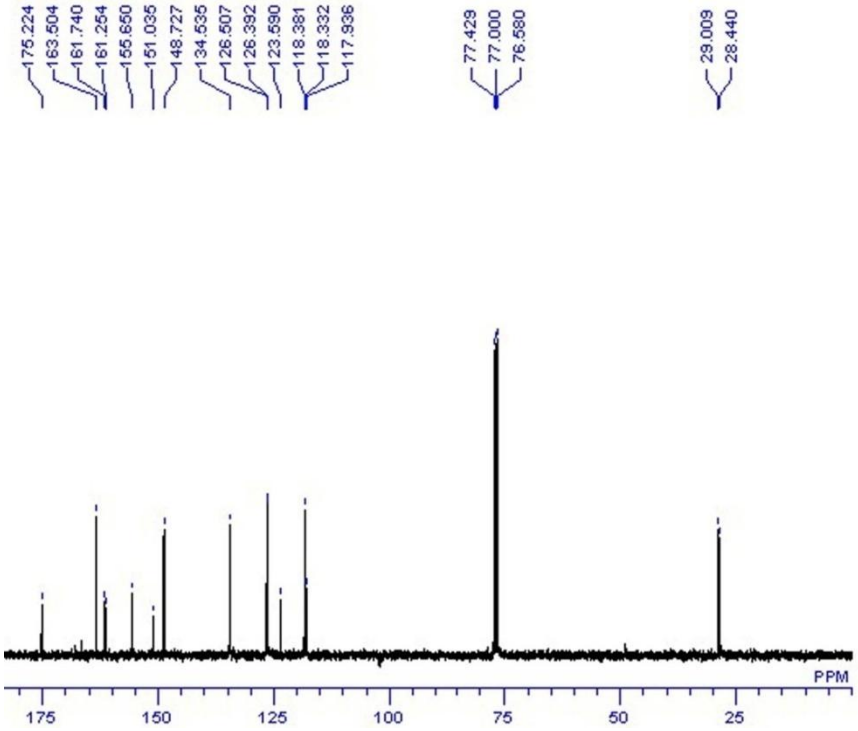
Yellow solid, 75% yield, mp >240 ^oC; ν_{max} (KBr): 2177 (C≡N), 1638, 1568 (C=O). ^1H NMR (300 MHz, MeOH-d_6+$CDCl_3$): δ = 3.18 (s, 3H; 2×CH_3), 5.58 (s, 1H; CH), 6.93 (d, *J* = 8.4 Hz, 1H; ArH), 7.04 (t, *J* = 7.2 Hz, 1H; ArH), 7.30-7.41 (m, 4H; ArH), 7.61 (t, *J* = 7.5 Hz, 1H; ArH),

7.84 (d, *J* = 7.8 Hz, 1H; ArH), 8.01 (d, *J* = 7.8 Hz, 1H; =H), 8.46 (s, 1H; ArH); ^{13}C NMR (normal/DEPT-135) (MeOH-d_4+$CDCl_3$): δ 23.6 (+ve, CH_3), 27.5 (+ve, CH_3), 27.9 (+ve, CH_3), 67.9 (+ve, CH), 81.9 (+ve, CH), 113.3 (C≡N), 117.9 (C), 118.4 (C), 119.0 (+ve, CH), 119.5 (+ve, CH), 120.5 (C), 122.9 (C), 123.4 (+ve, CH), 125.5 (+ve, CH), 127.5 (+ve, CH), 134.2 (C), 134.9 (C), 141.8 (+ve, CH), 153.6 (C), 156.5 (C), 156.5 (C), 156.7 (C), 157.8 (+ve, CH), 163.2 (C), 164.4 (C), 177.0 (C). FAB mass *m/z* 340 (M+1); (Found: C 60.18, H 3.86, N 12.38; $C_{17}H_{13}N_3O_5$ requires C 60.16, H 3.87, N 12.37).

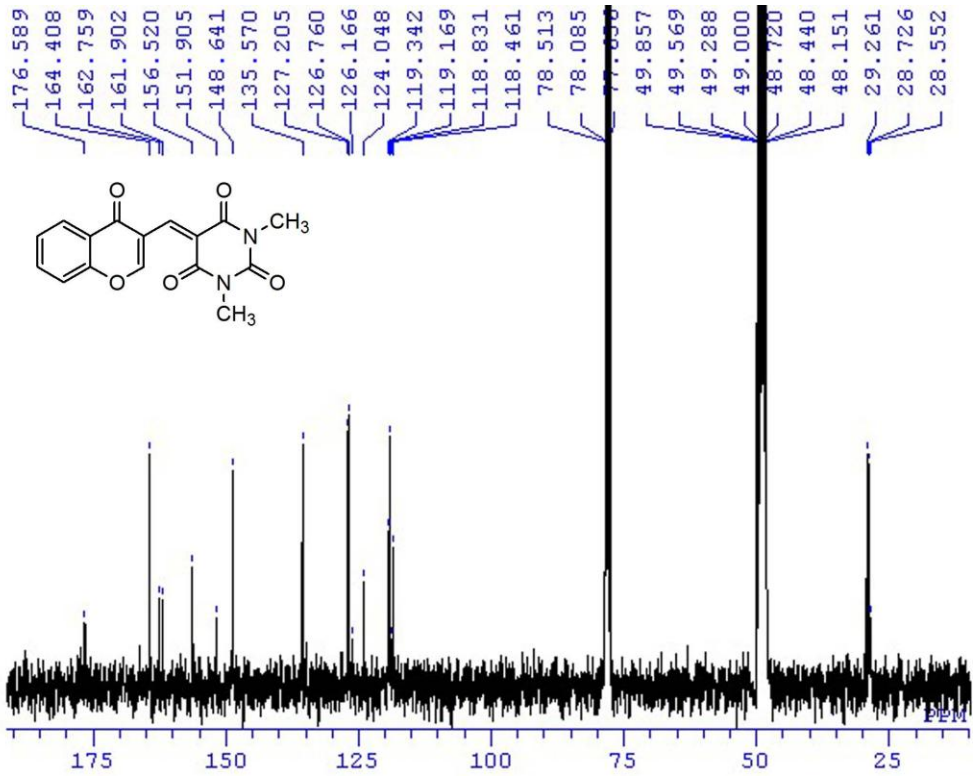
^{1}H NMR



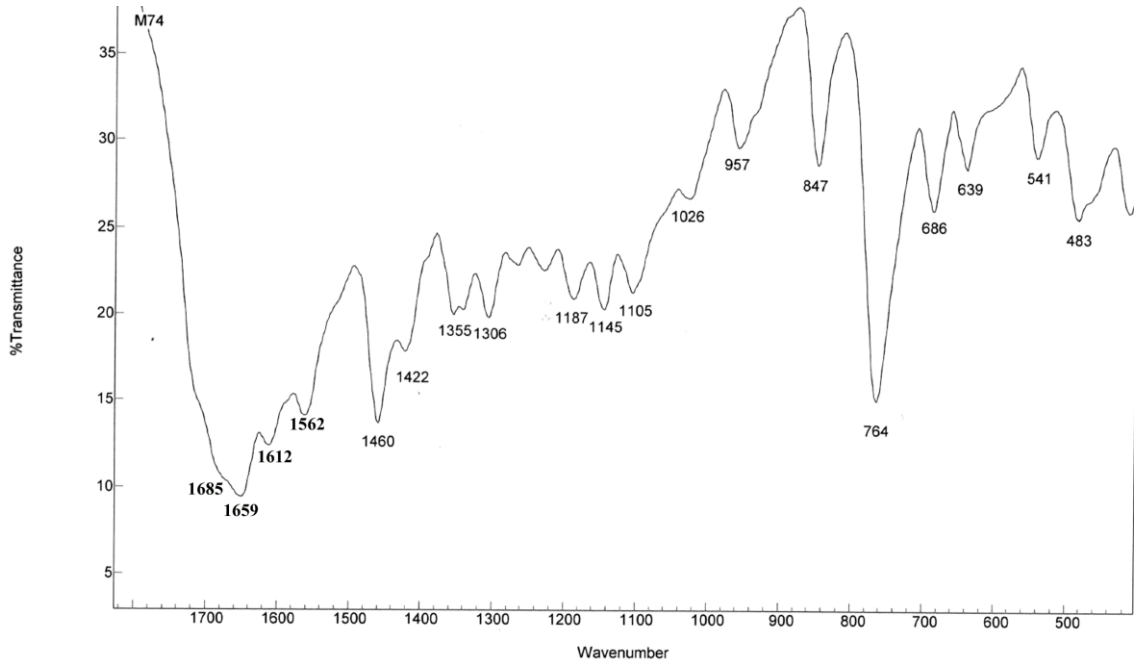
SI Figure 1. ^{1}H NMR spectrum of compound **3.**



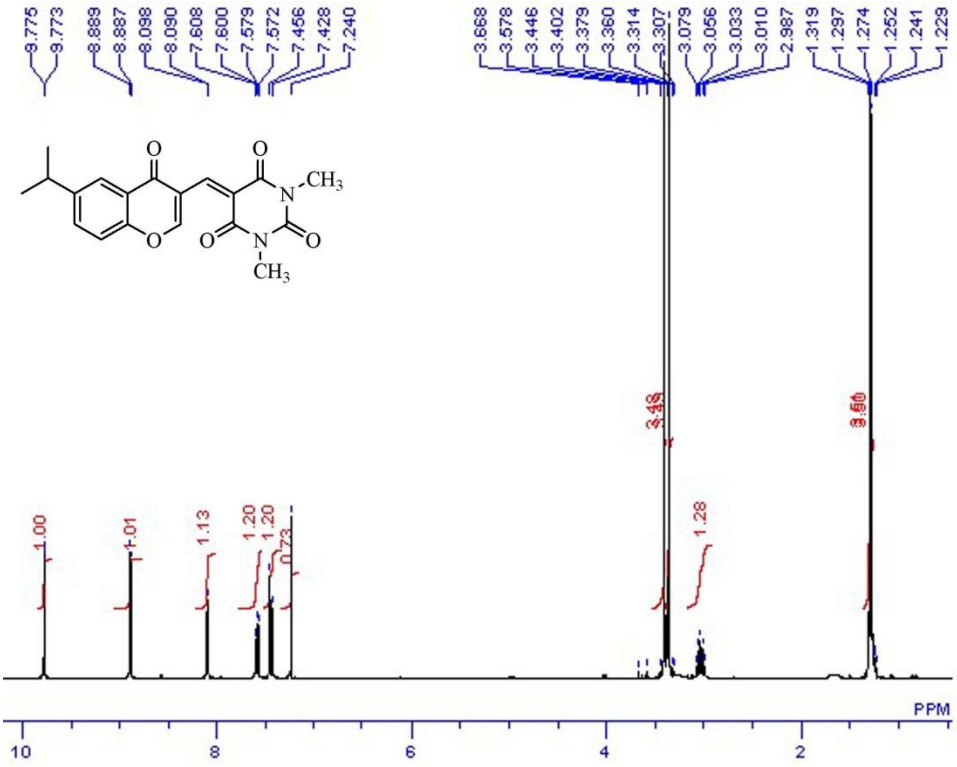
SI Figure 2. ^{13}C NMR spectrum of compound **3** ($CDCl_3$)**.**



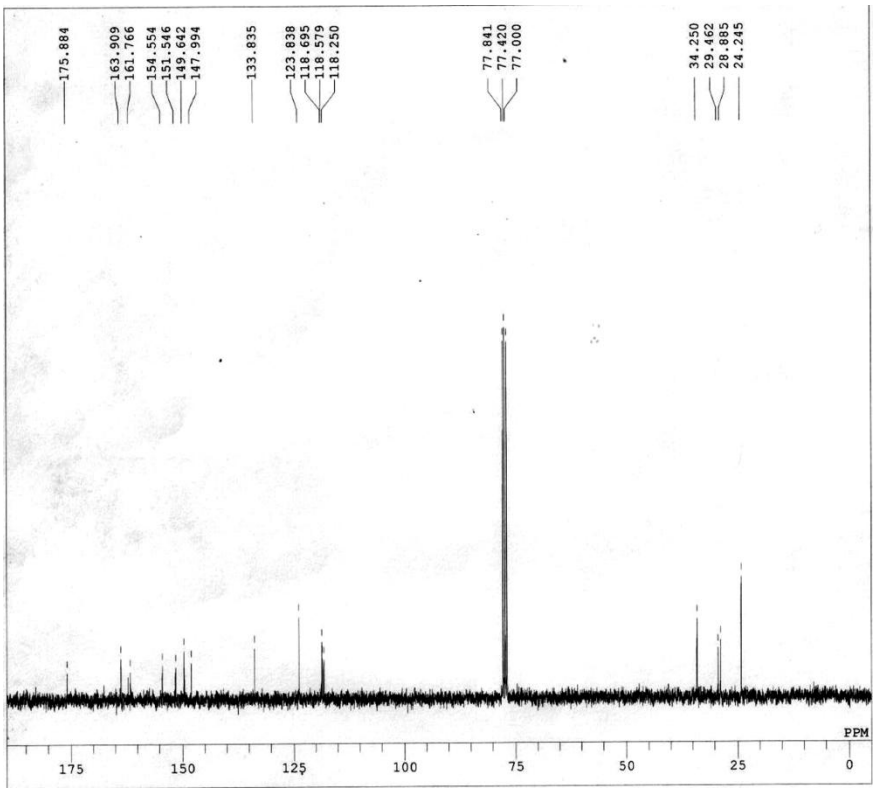
SI Figure 3. ^{13}C NMR spectrum of compound **3** in (MeOH-d_4+$CDCl_3$). Two tautomers were observed in MeOH.



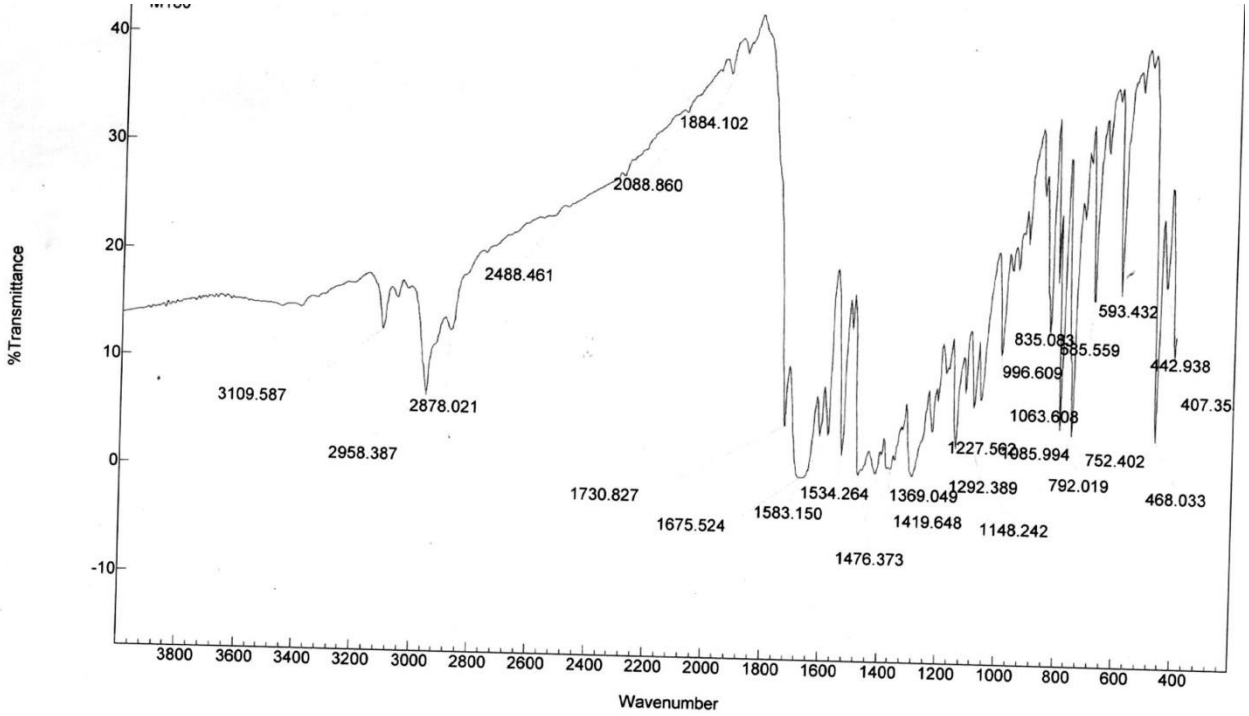
SI Figure 4. IR spectrum of compound **3.**



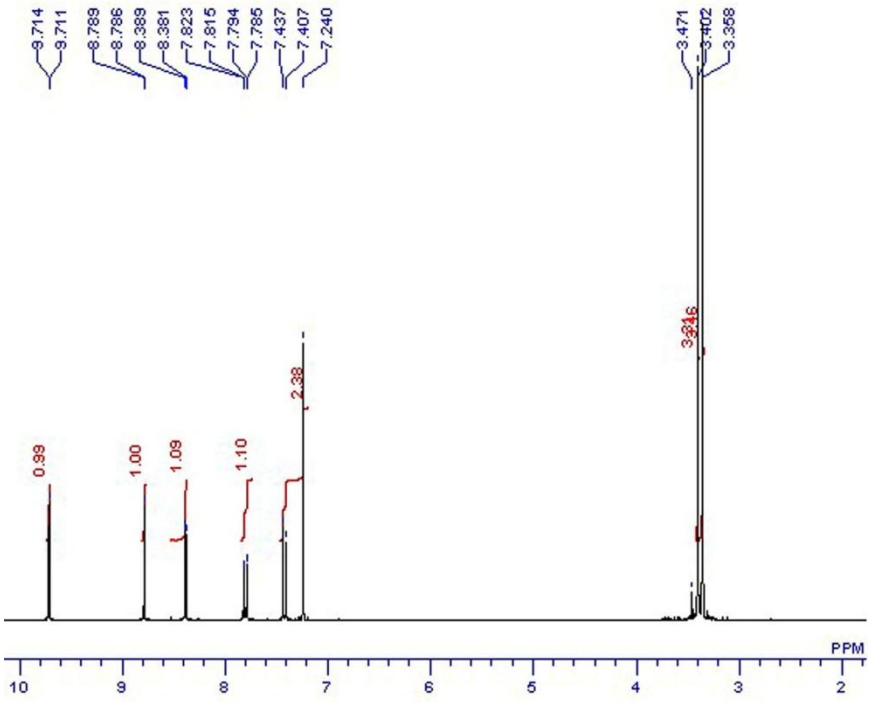
SI Figure 5. ^{1}H NMR spectrum of compound **4**.



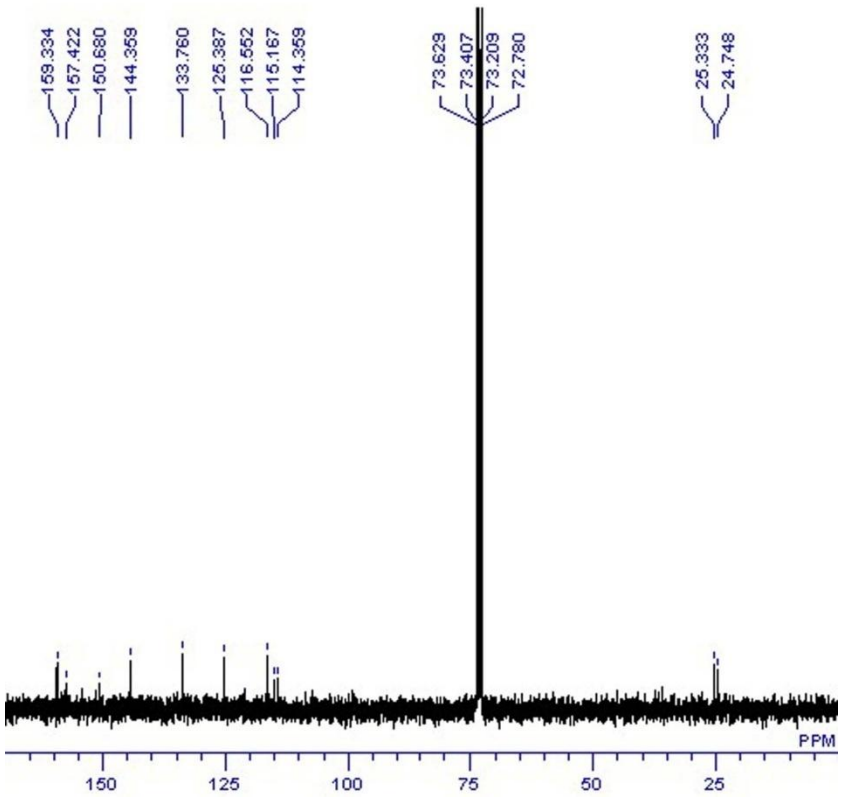
SI Figure 6. ^{13}C NMR spectrum of compound **4**.



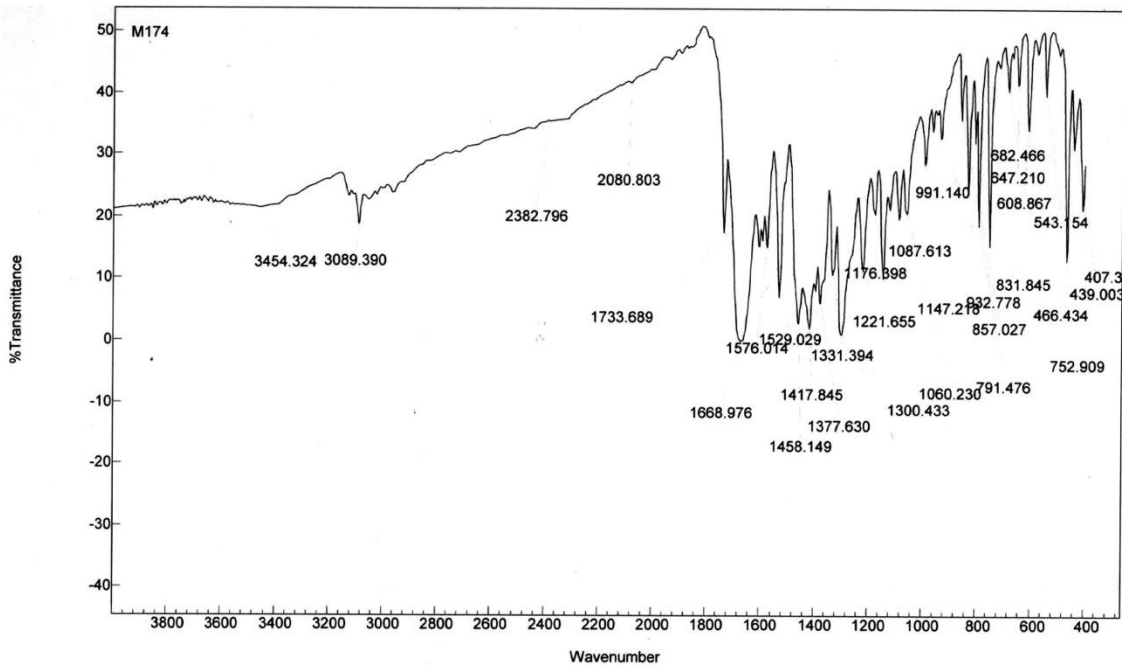
SI Figure 7. IR spectrum of compound **4**.



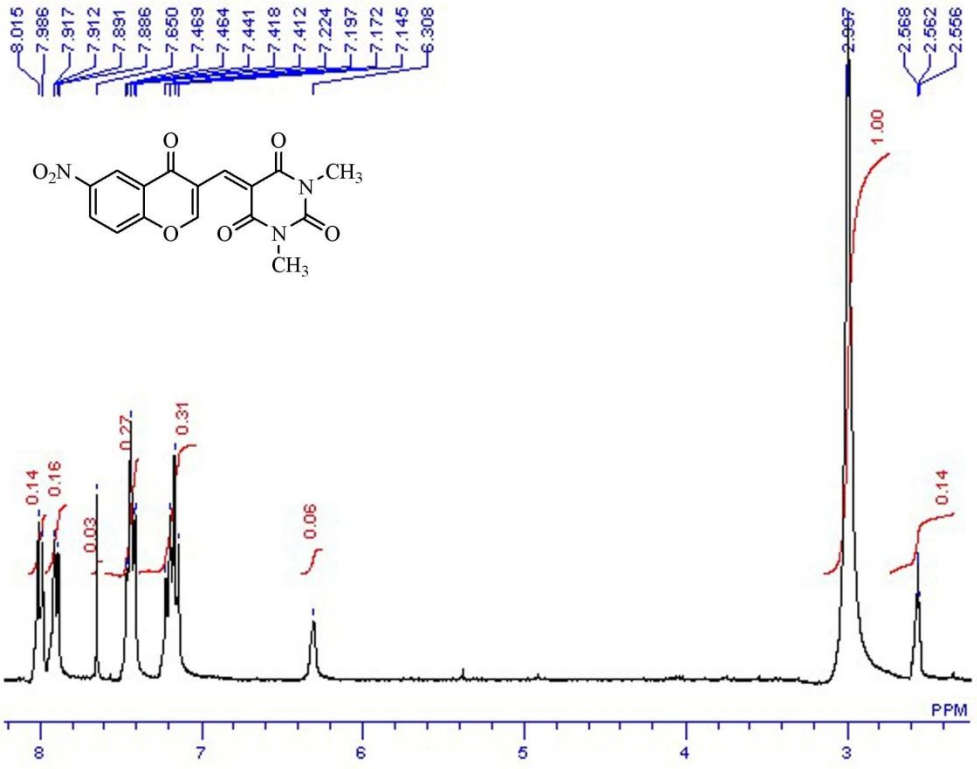
SI Figure 8. ^{1}H NMR spectrum of compound **5**.



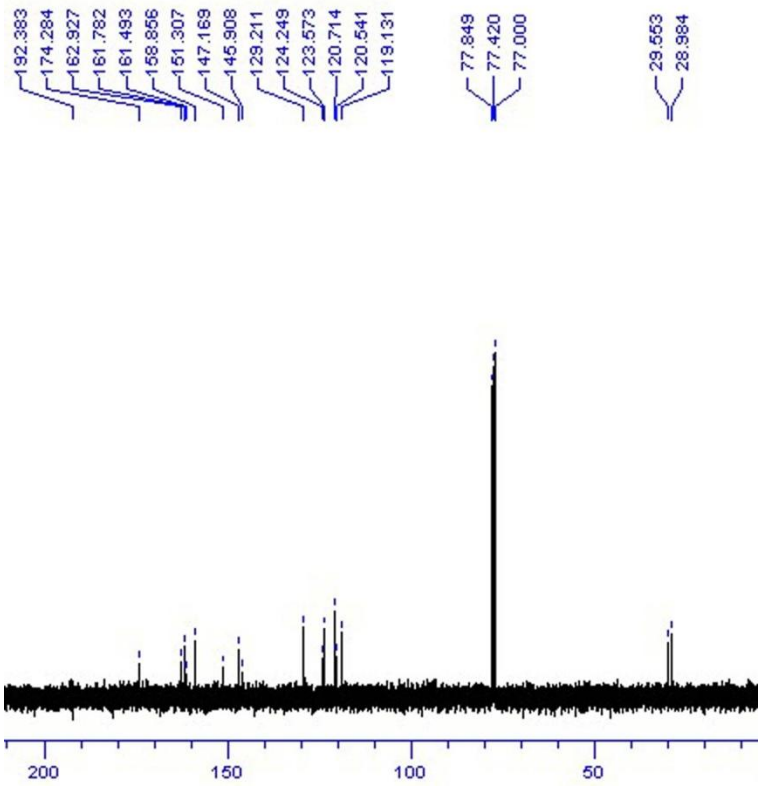
SI Figure 9. ^{13}C NMR spectrum of compound **5**.



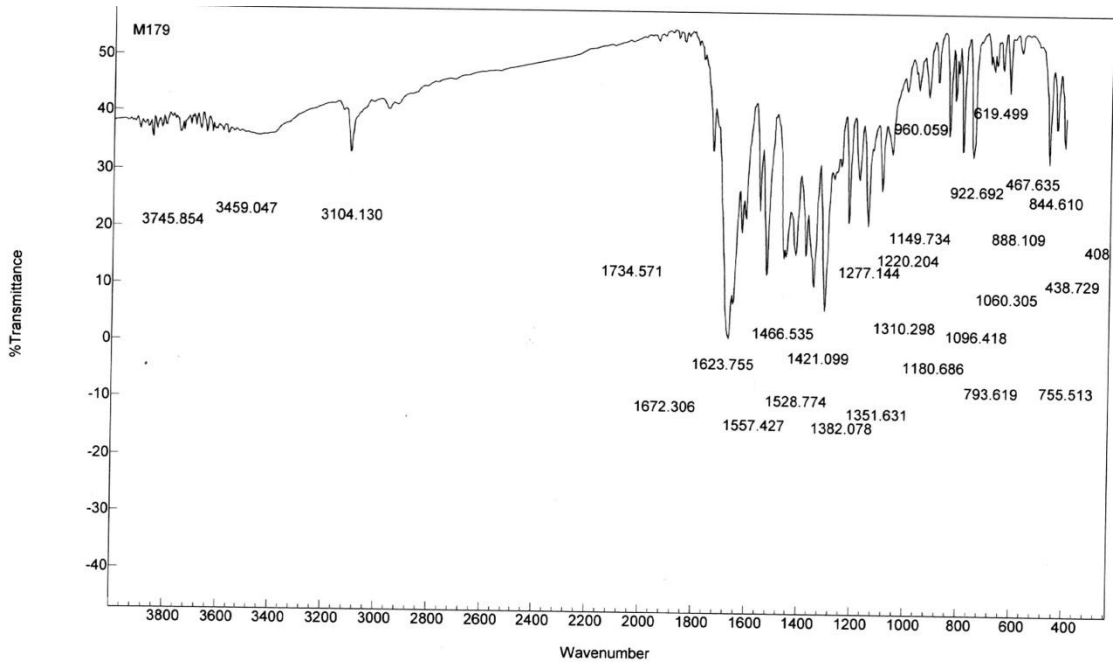
SI Figure 10. IR spectrum of compound **5**.



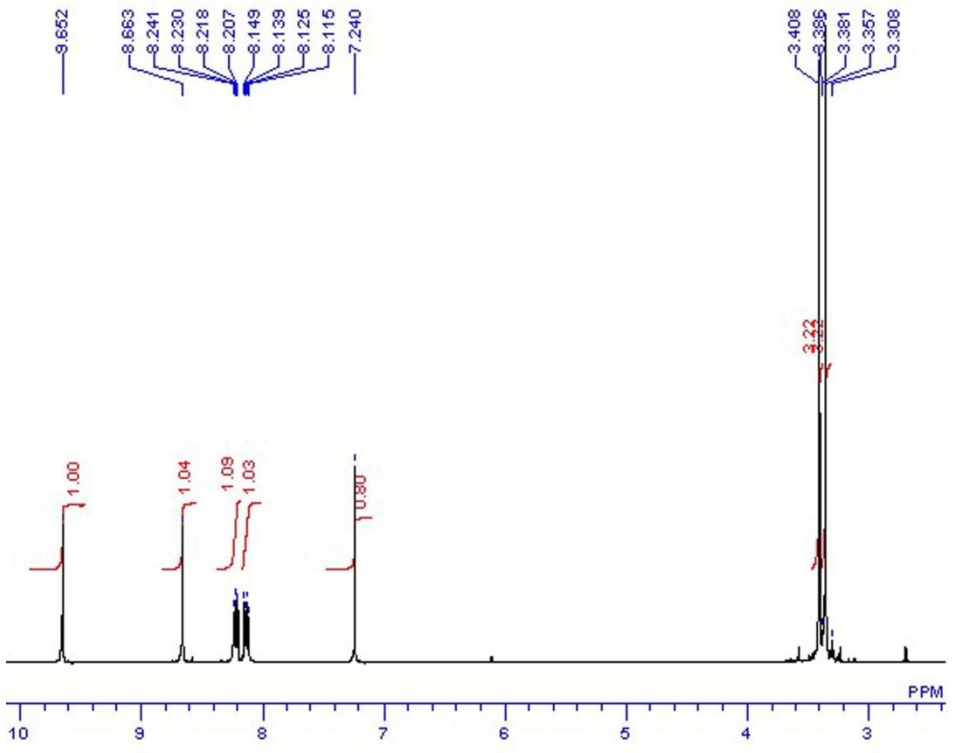
SI Figure 11. ^{1}H NMR spectrum of compound **6**.



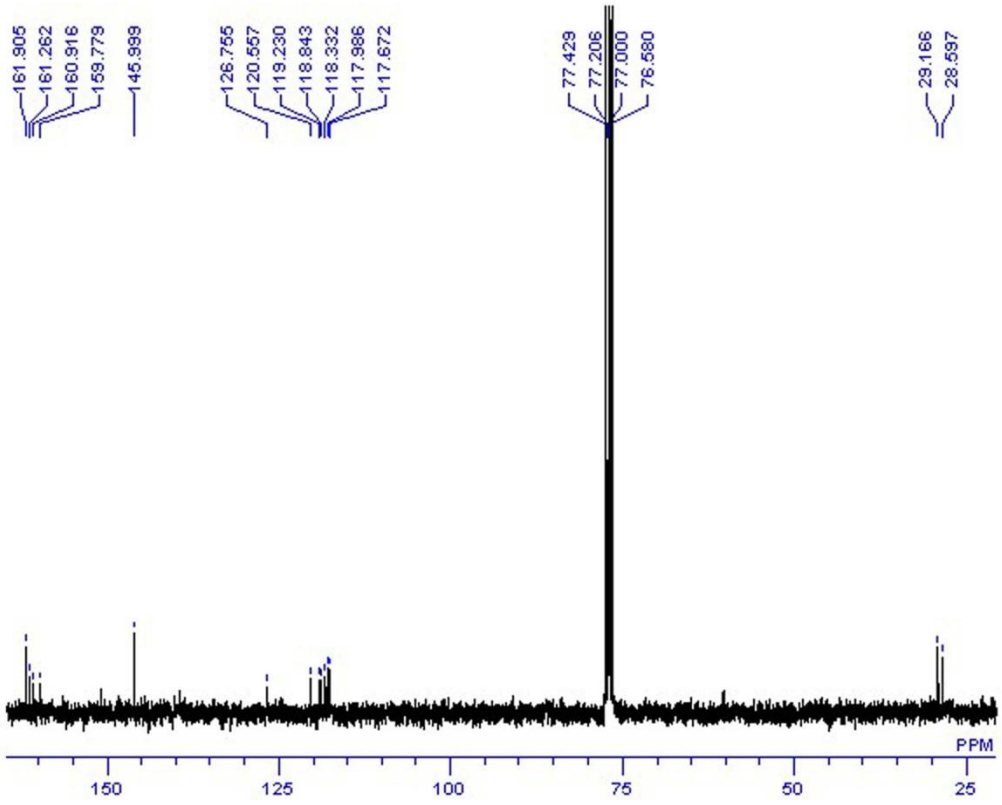
SI Figure 12. ^{13}C NMR spectrum of compound **6**.



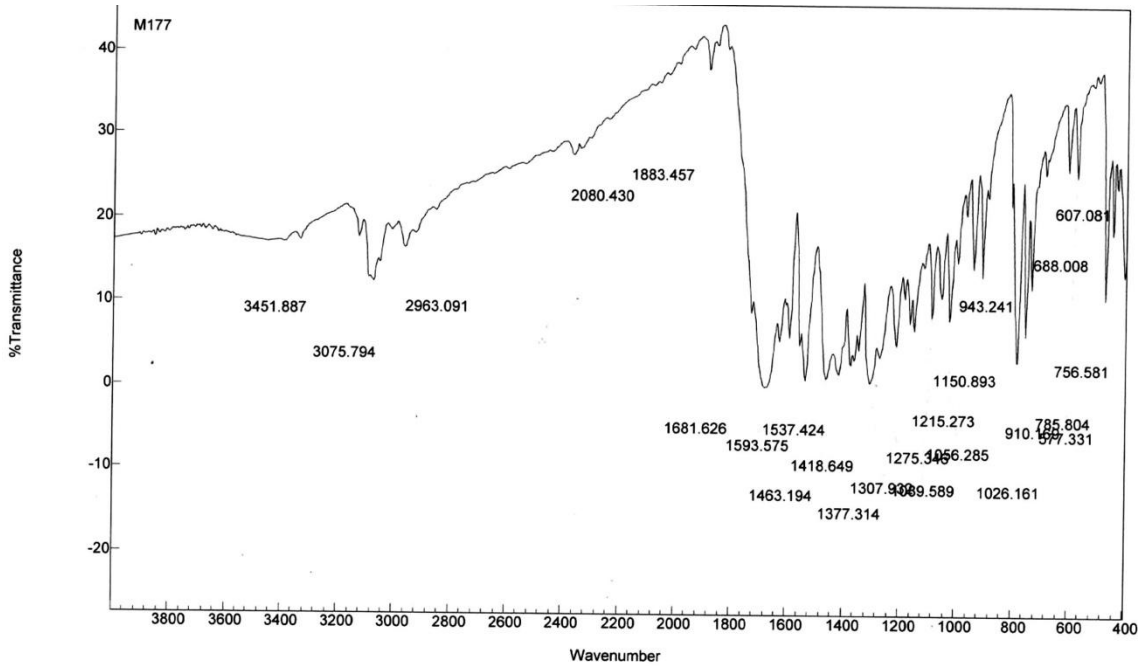
SI Figure 13. IR spectrum of compound **6**.



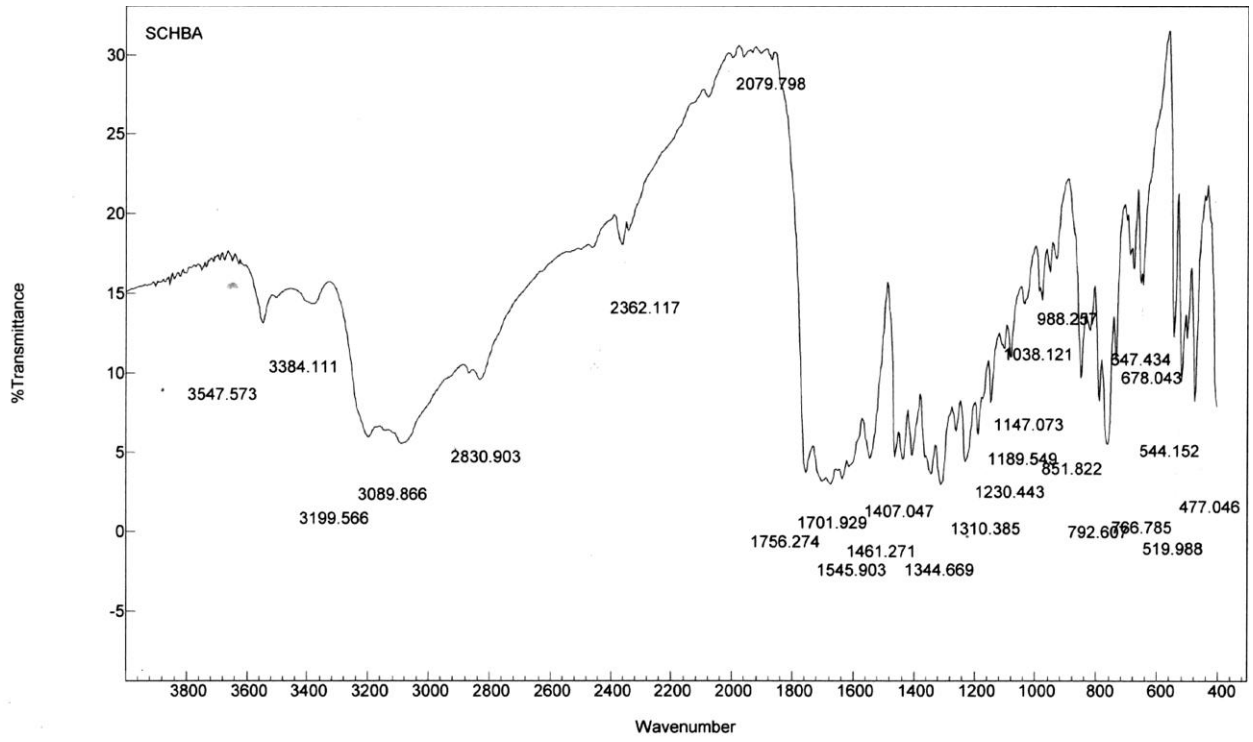
SI Figure 14. ^{1}H NMR spectrum of compound **7**.



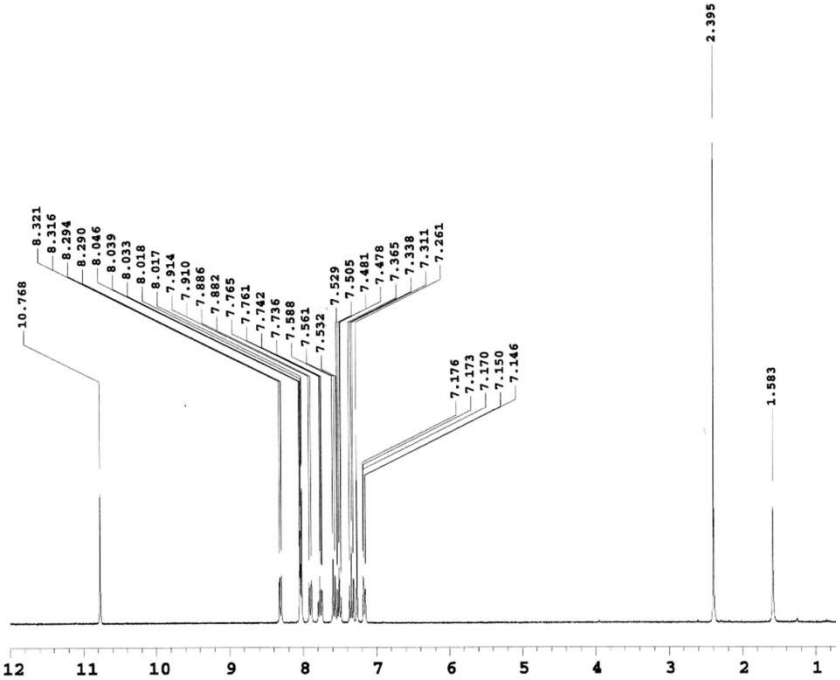
SI Figure 15. ^{13}C NMR spectrum of compound **7**.



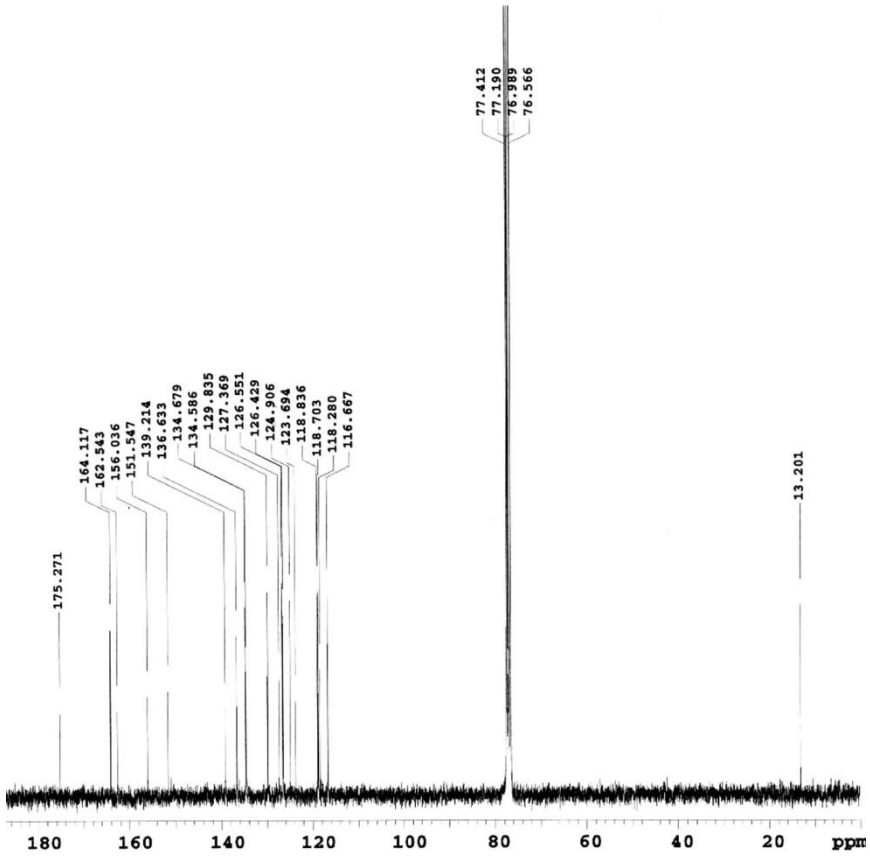
SI Figure 16. IR spectrum of compound **7**.



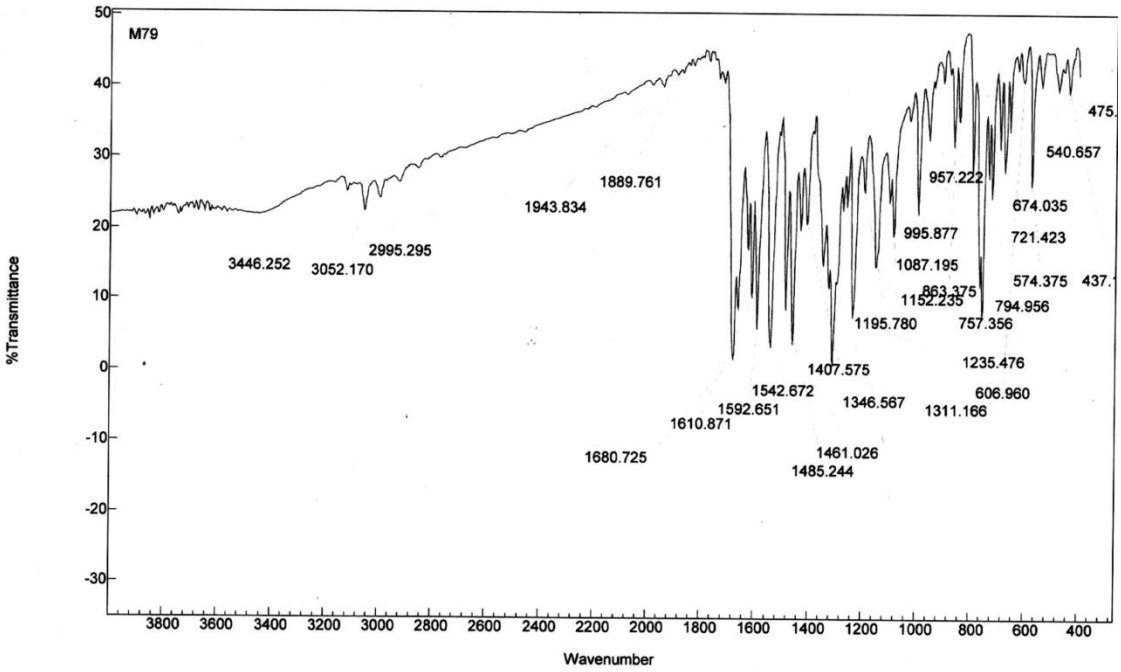
SI Figure 17. IR spectrum of compound **8**.



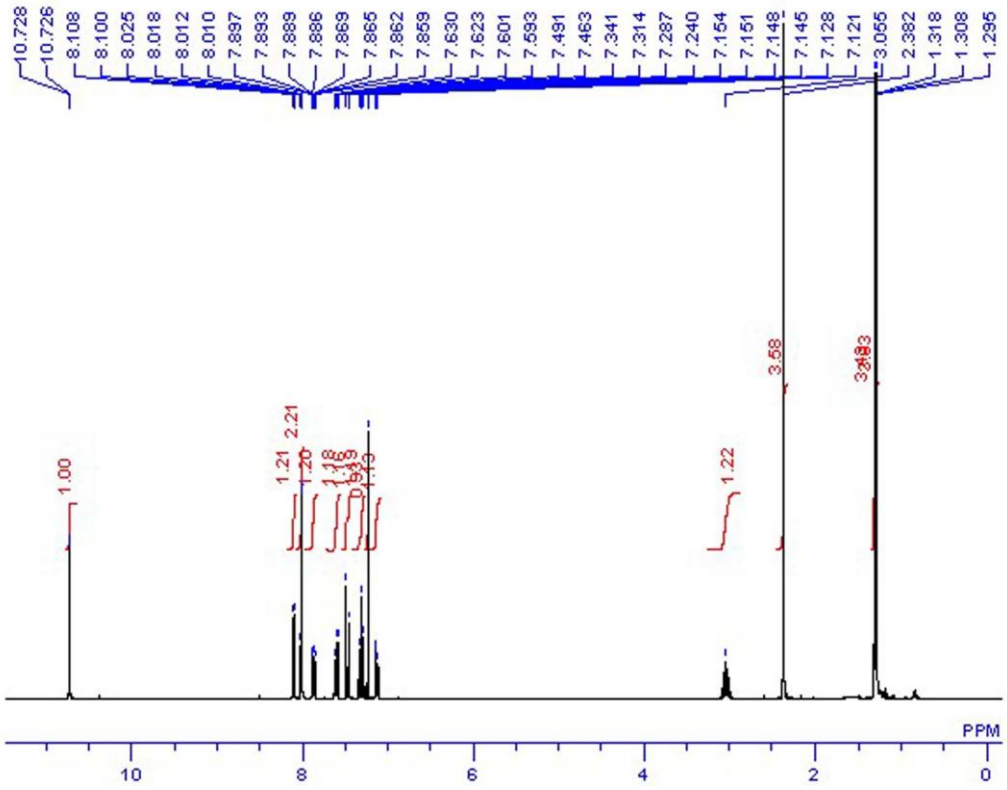
SI Figure 18. ^{1}H NMR spectrum of compound **9**.



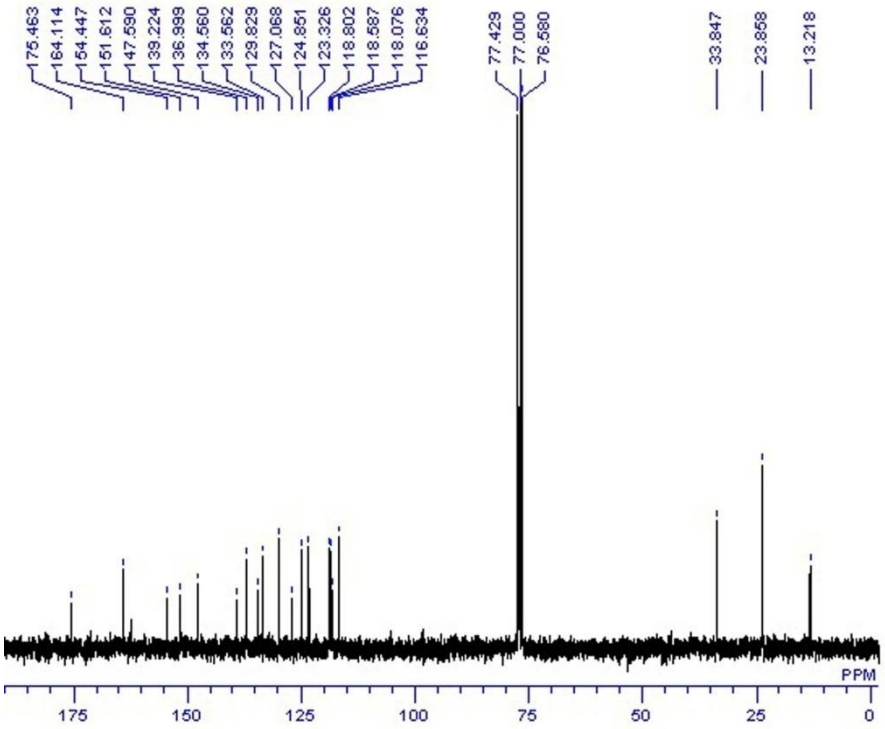
SI Figure 19. ^{13}C NMR spectrum of compound **9**.



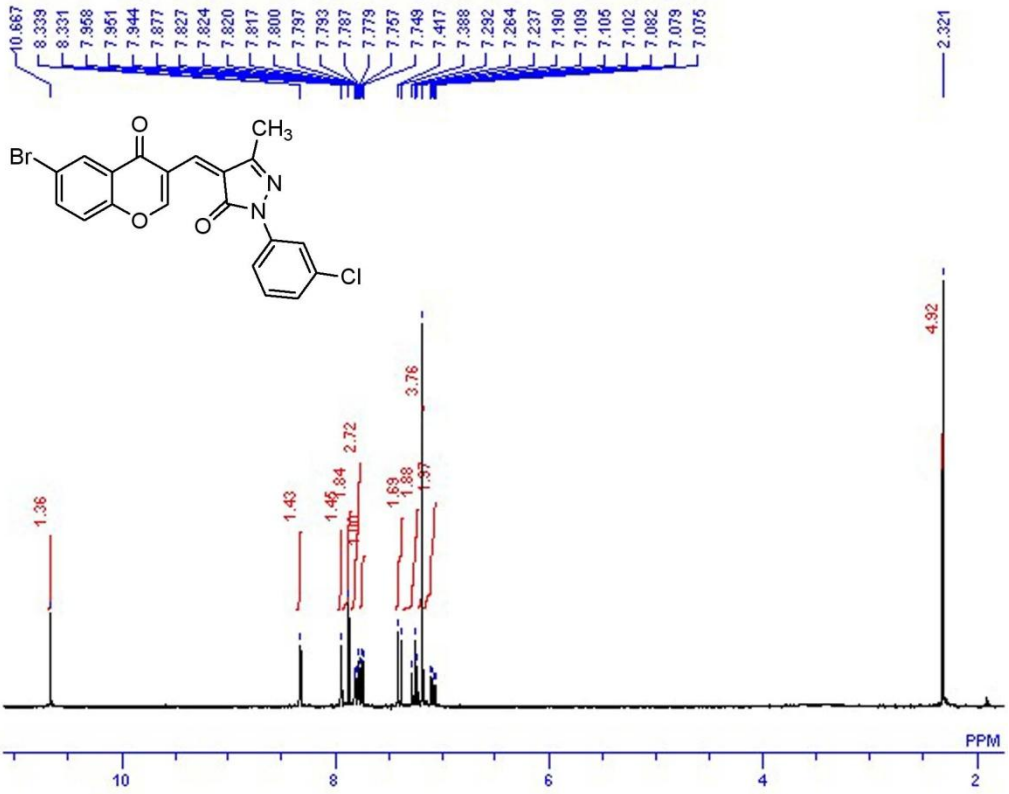
SI Figure 20. IR spectrum of compound **9**.



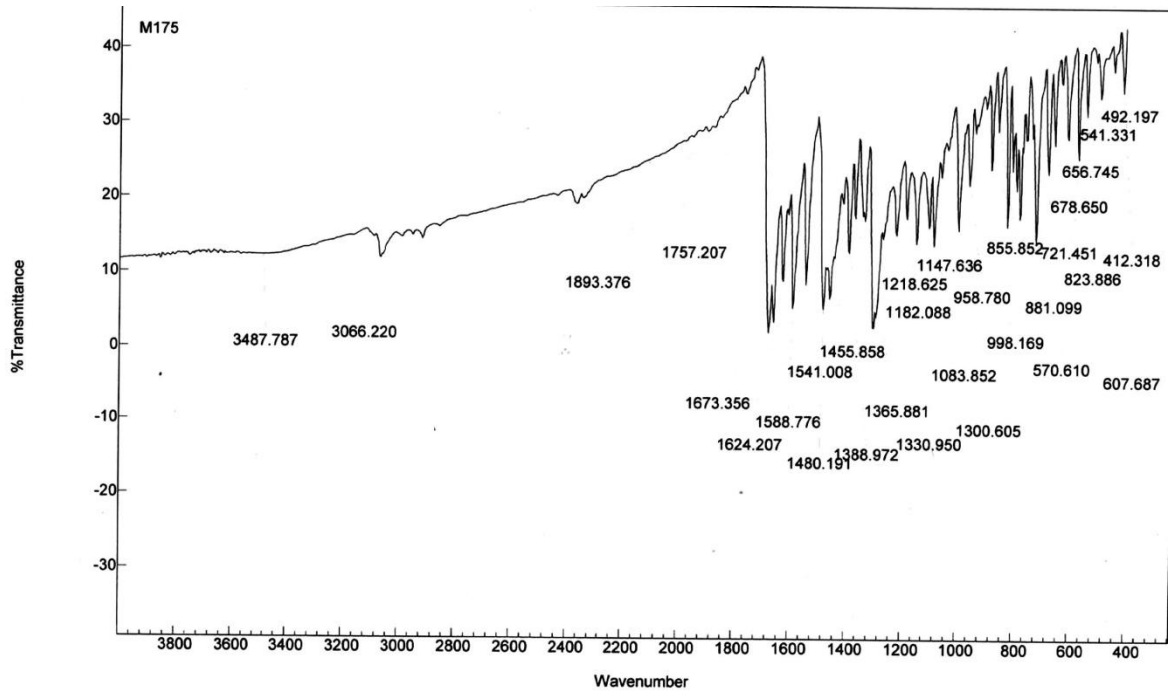
SI Figure 21. ^{1}H NMR spectrum of compound **10**.



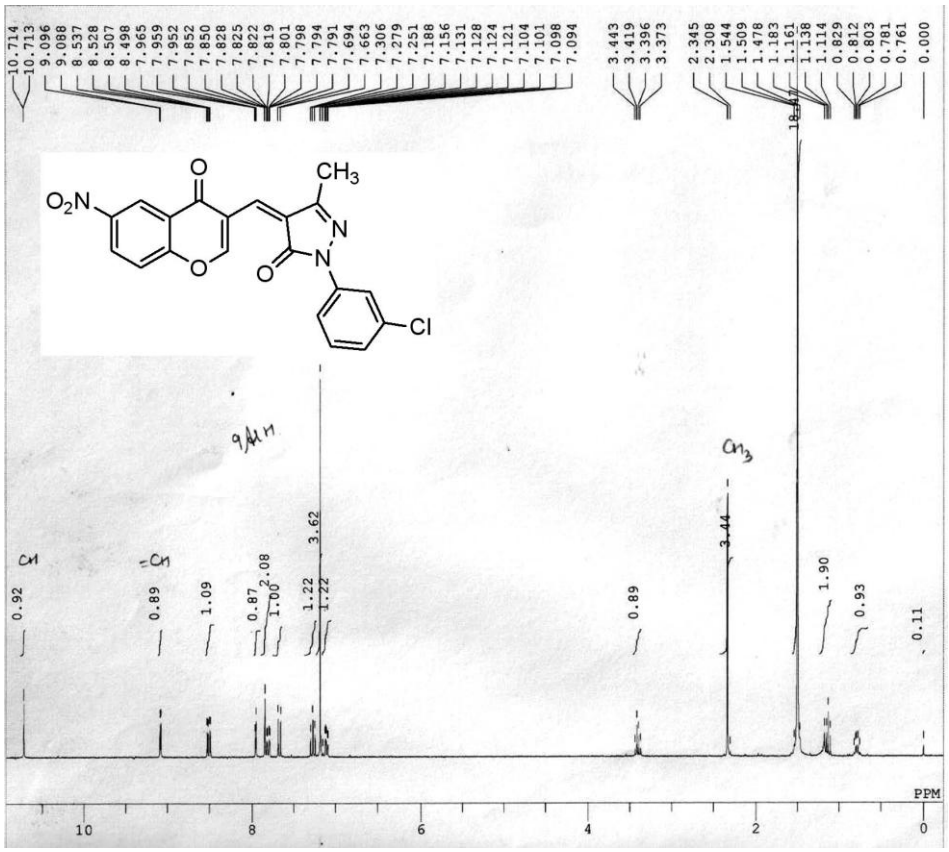
SI Figure 22. ^{13}C NMR spectrum of compound **10**.



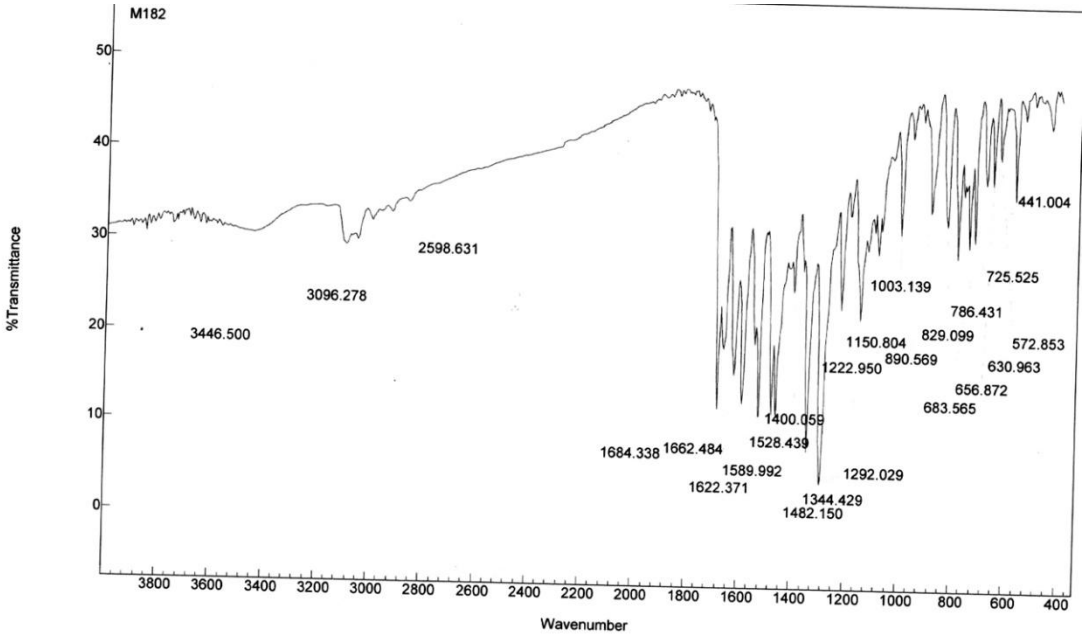
SI Figure 23. ^{1}H NMR spectrum of compound **11**.



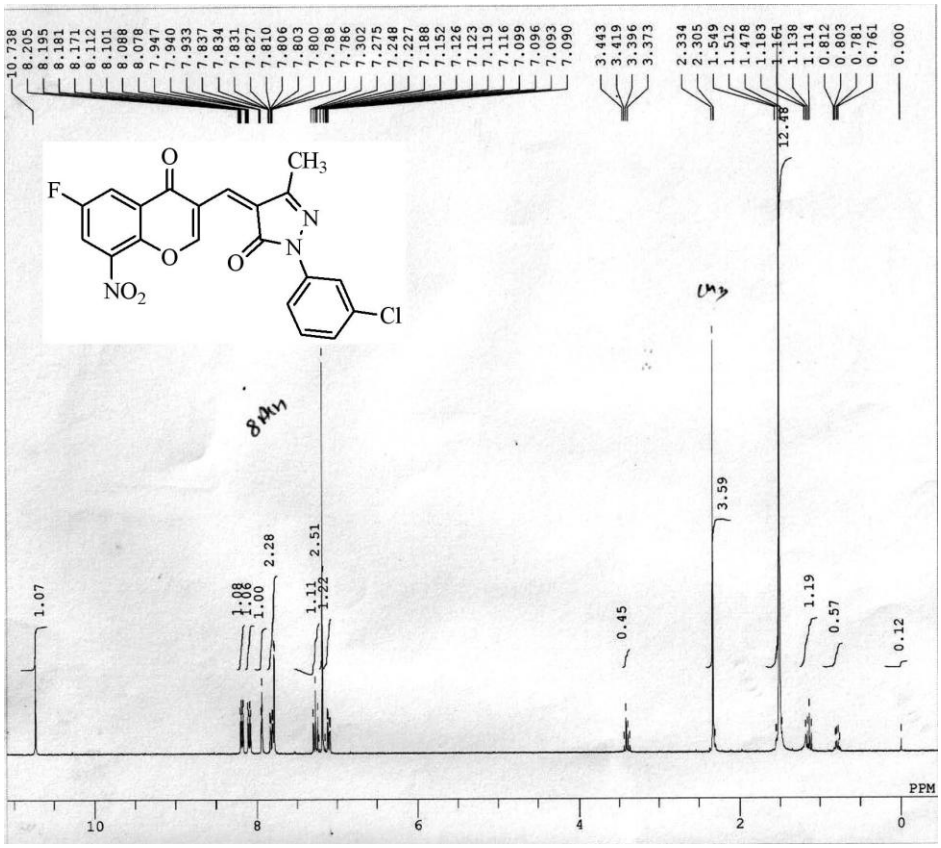
SI Figure 24. IR spectrum of compound **11**.



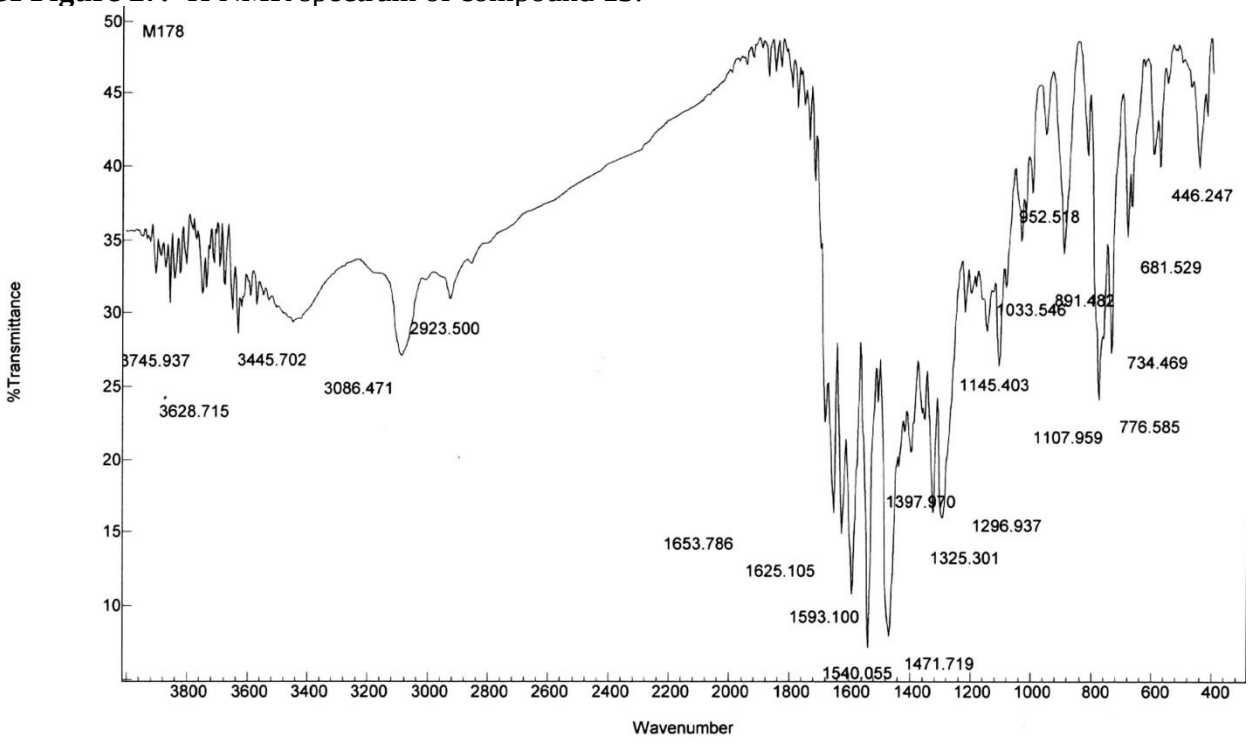
SI Figure 25. ^{1}H NMR spectrum of compound **12**.



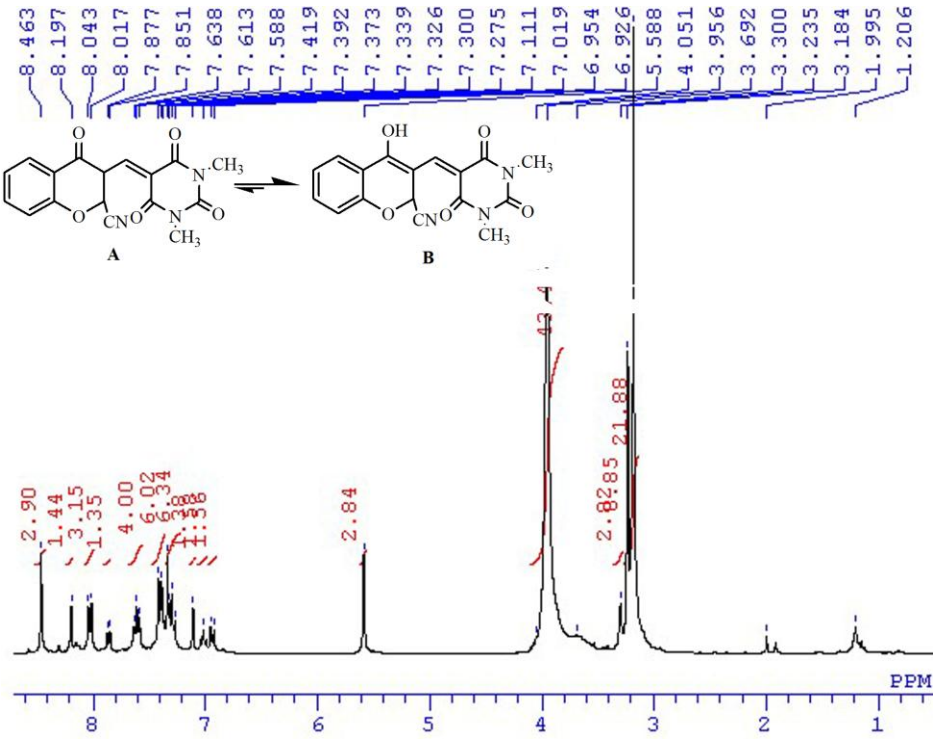
SI Figure 26. IR spectrum of compound **12**.



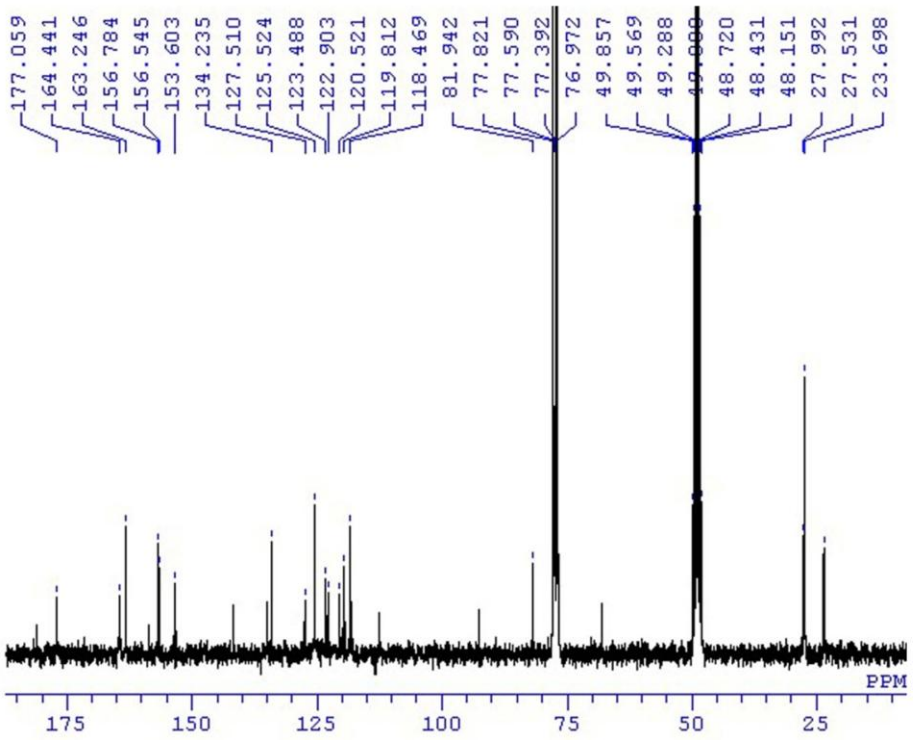
SI Figure 27. ^{1}H NMR spectrum of compound **13**.



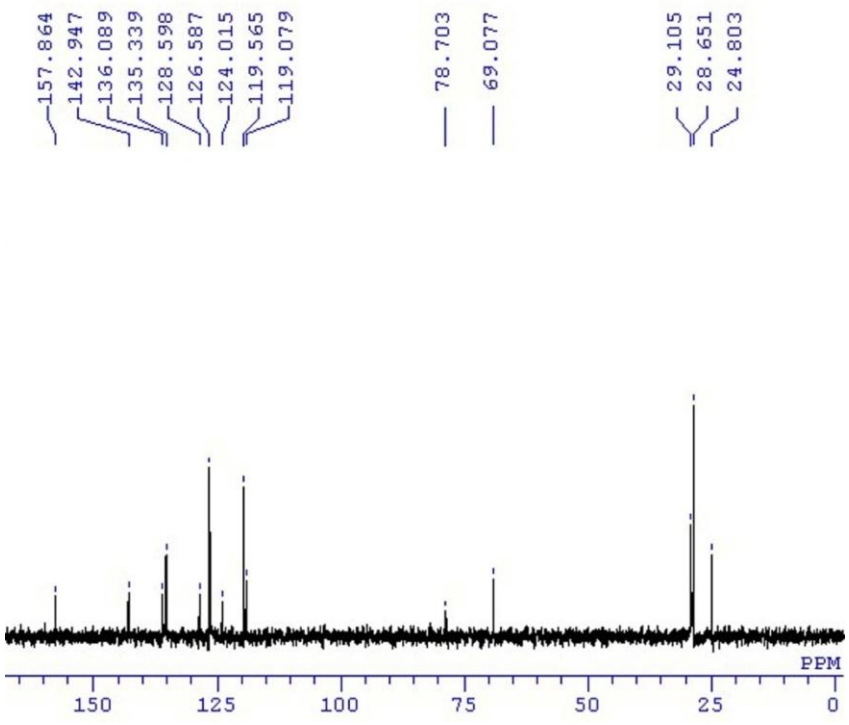
SI Figure 28. IR spectrum of compound **13**.



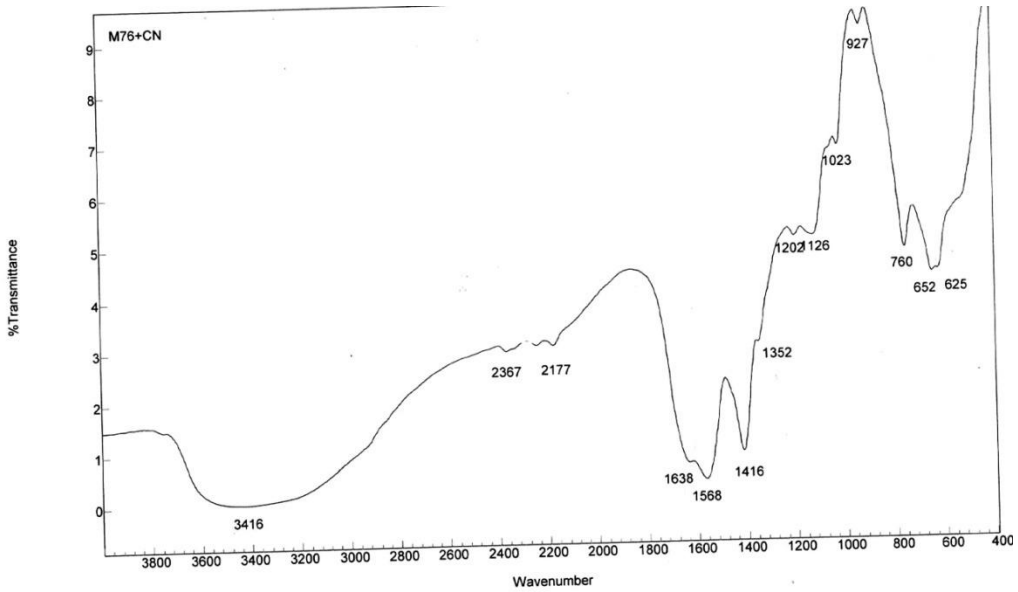
SI Figure 29. ^{1}H NMR spectrum of compound **14** (MeOH-d_4+$CDCl_3$). Two tautomers were observed in MeOH. Tautomer 'B' is major.



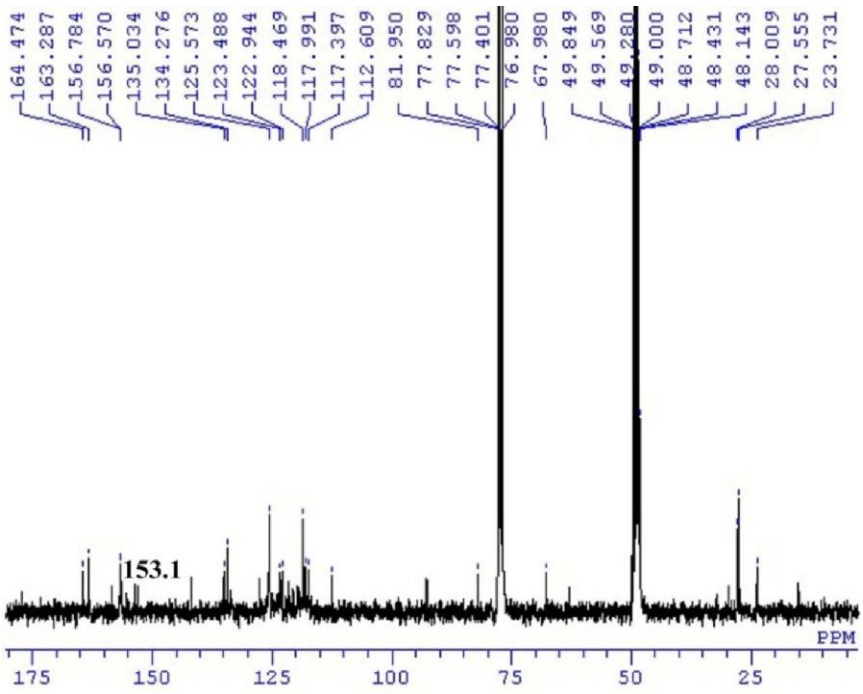
SI Figure 30. ^{13}C NMR spectrum of compound **14** (MeOH-d_4+$CDCl_3$).



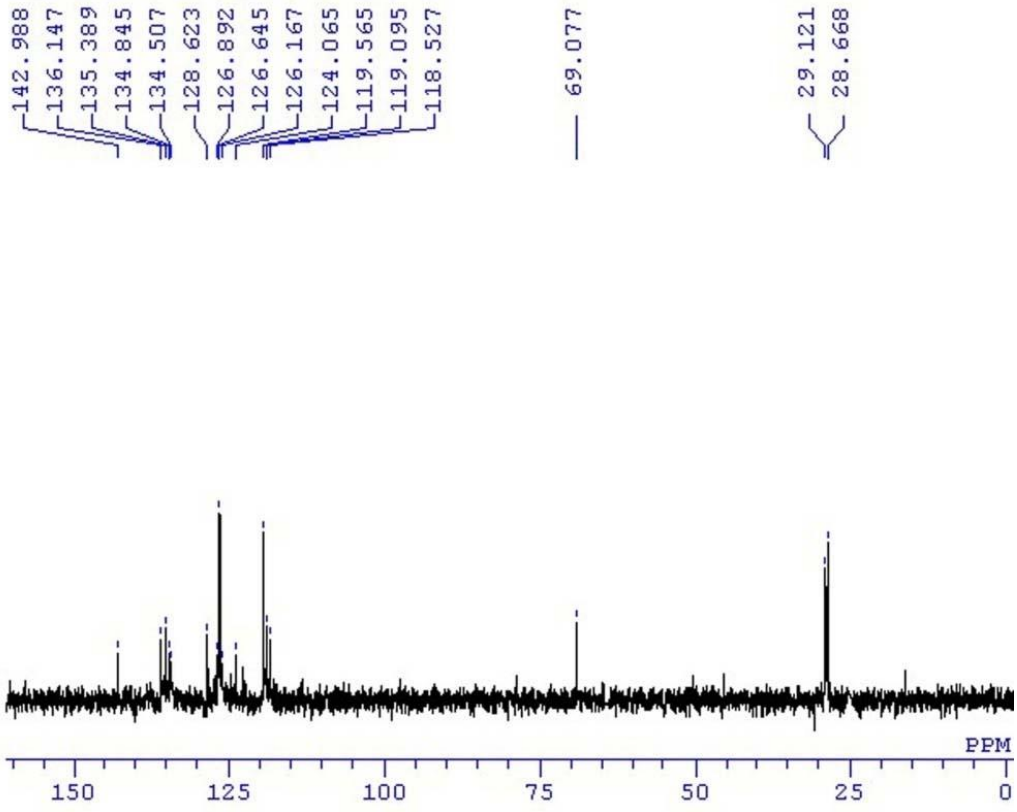
SI Figure 31. DEPT-135 NMR spectrum of compound **14**.



SI Figure 32. IR spectrum of compound **14**.

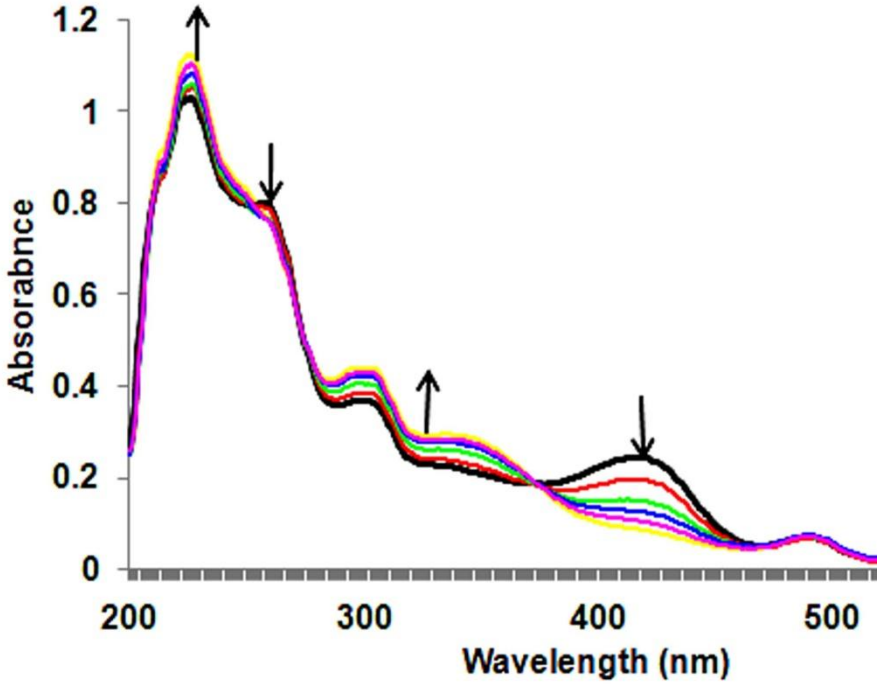


SI Figure 33. ^{13}C NMR spectrum of compound **3**+$Hg(ClO_4)_2$ in MeOH-d_4+$CDCl_3$.

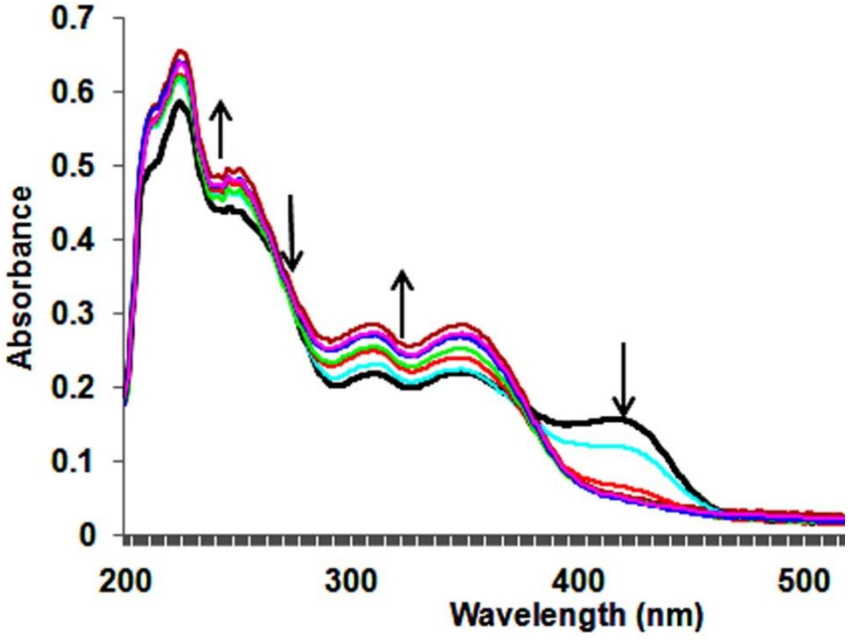


SI Figure 34. DEPT-135 NMR spectrum of compound **3**+$Hg(ClO_4)_2$ in MeOH-d_4+$CDCl_3$.

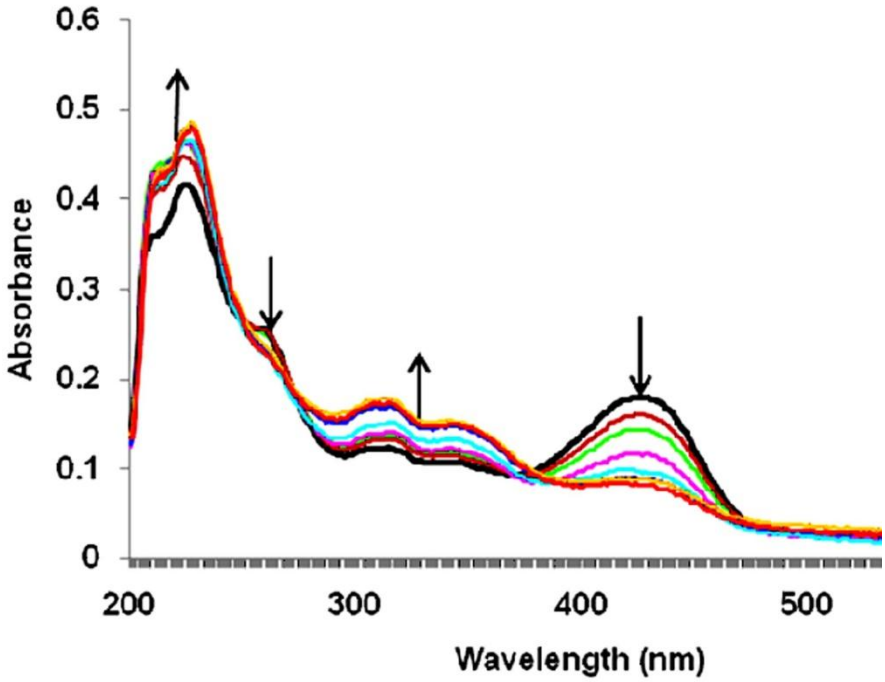
UV-vis titrations



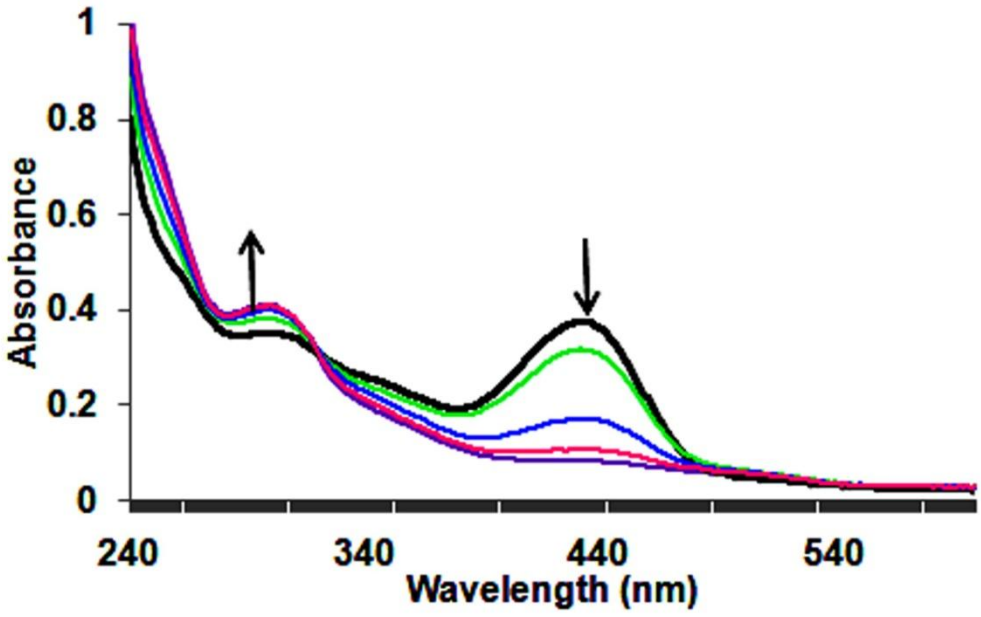
SI Figure 35. UV-vis spectra of compound **3** (5 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



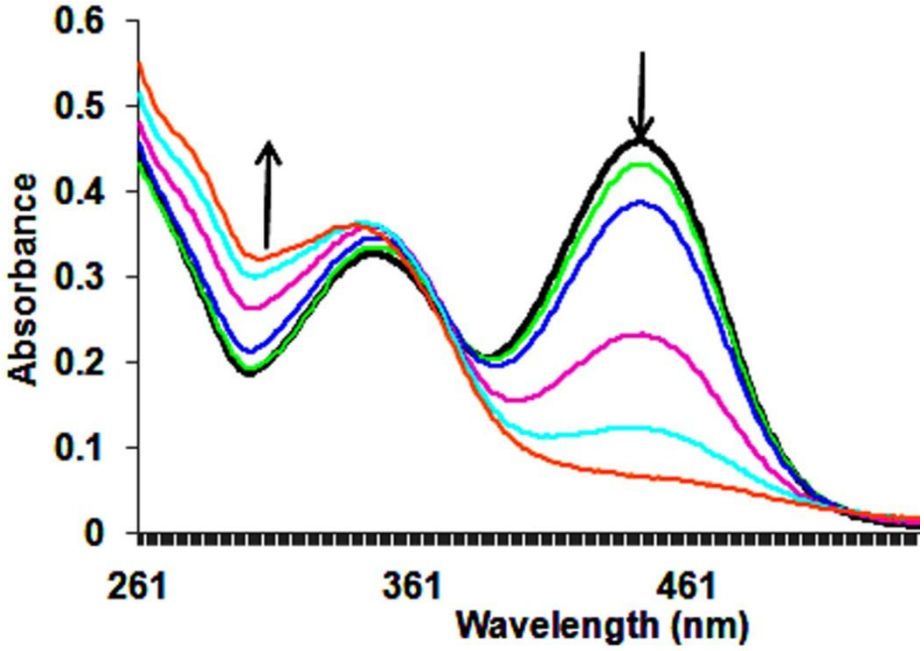
SI Figure 36. UV-vis spectra of compound **4** (5 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



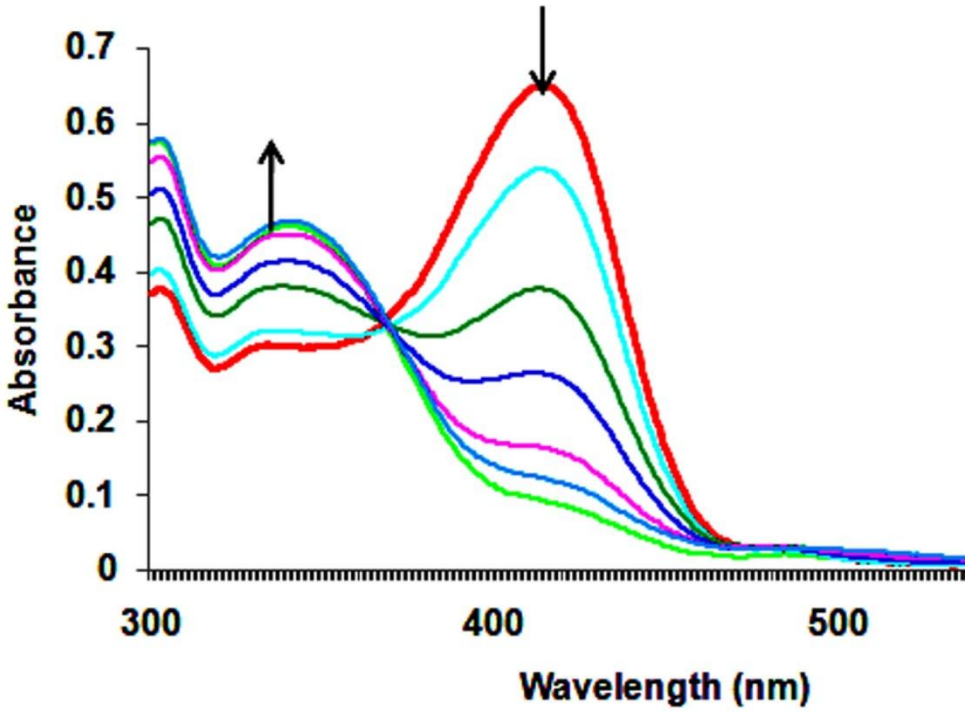
SI Figure 37. UV-vis spectra of compound **5** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



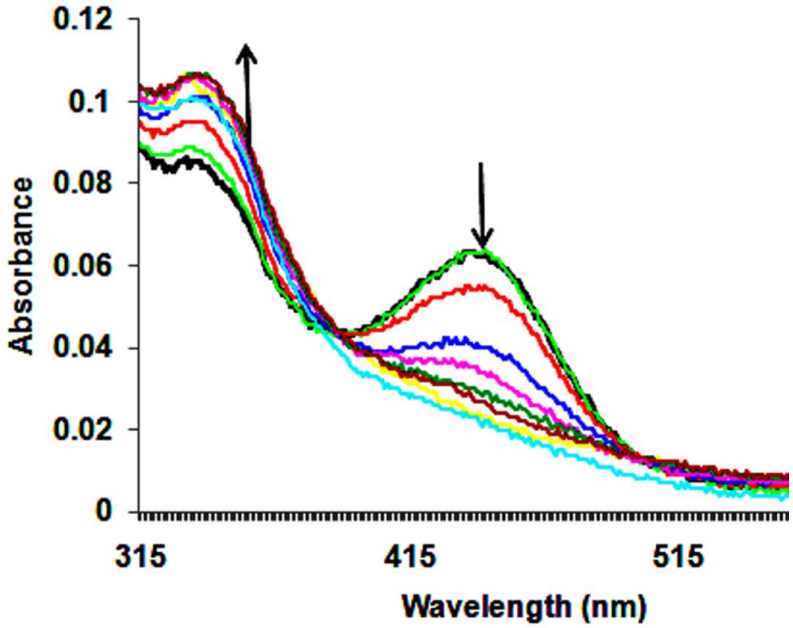
SI Figure 38. UV-vis spectra of compound **6** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



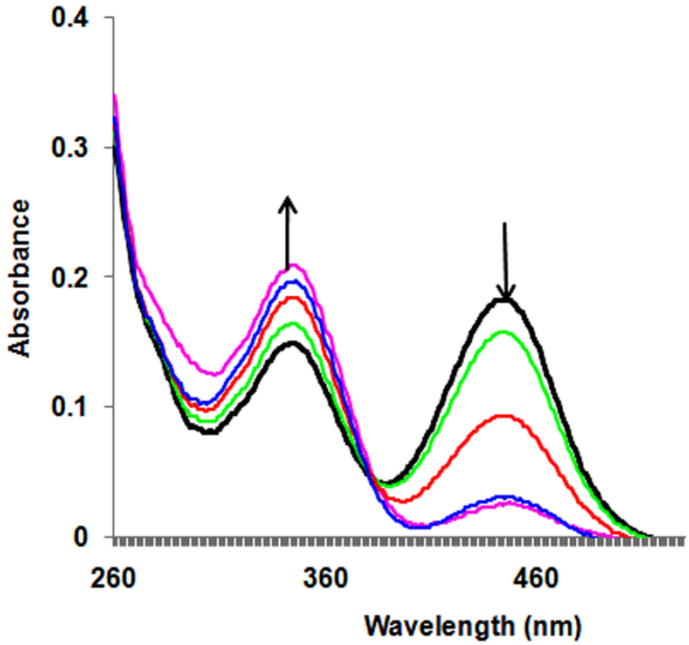
SI Figure 39. UV-vis spectra of compound **7** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



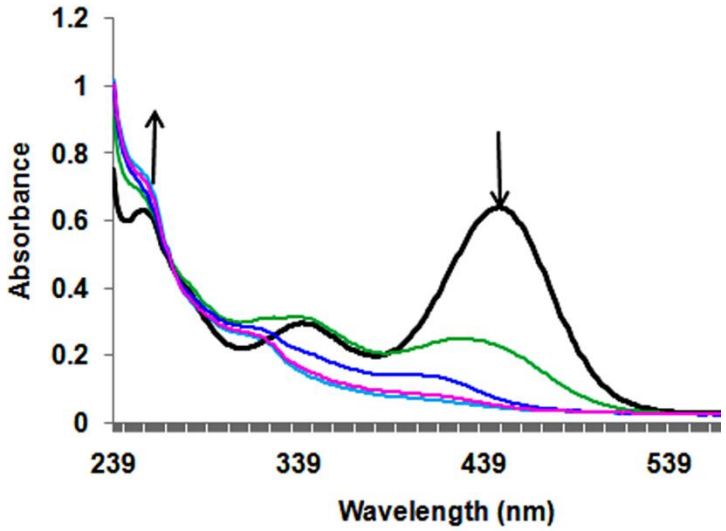
SI Figure 40. UV-vis spectra of compound **8** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



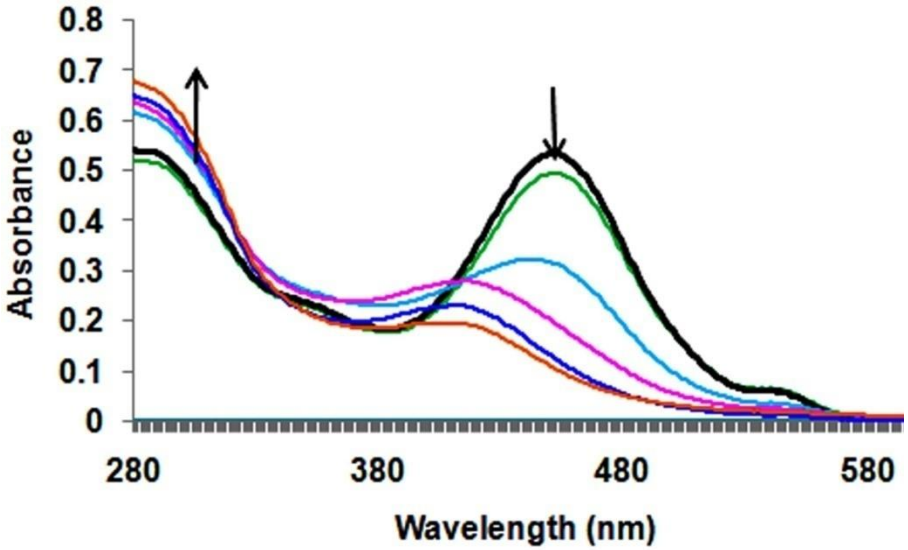
SI Figure 41. Changes in UV-vis spectra of compound **9** (5 µM) in water-ethanol (9:1 v/v, pH 7.2,) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



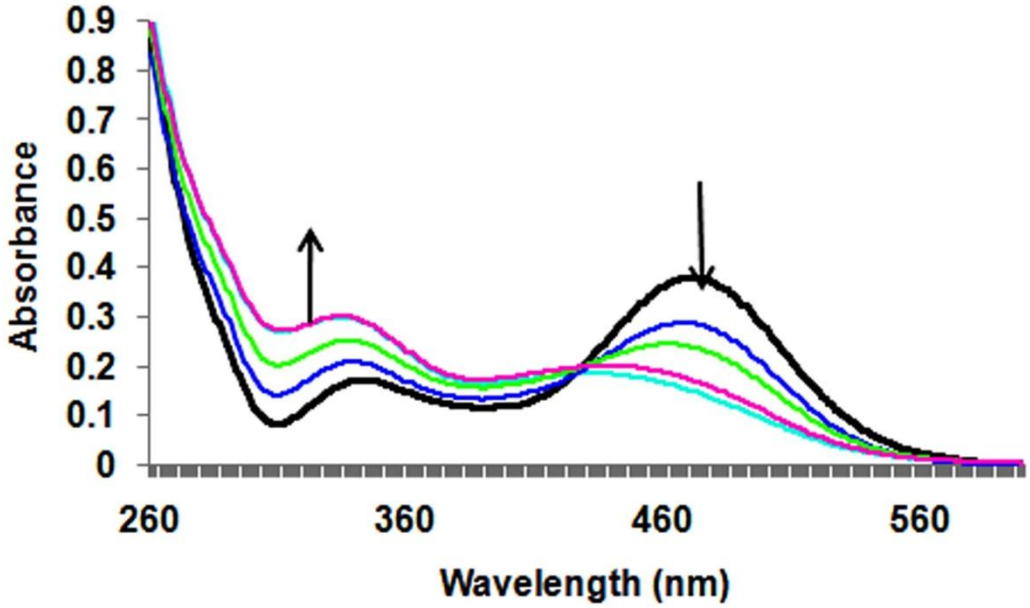
SI Figure 42. Changes in UV-vis spectra of compound **10** (5 µM) in water-ethanol (9:1 v/v, pH 7.2,) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



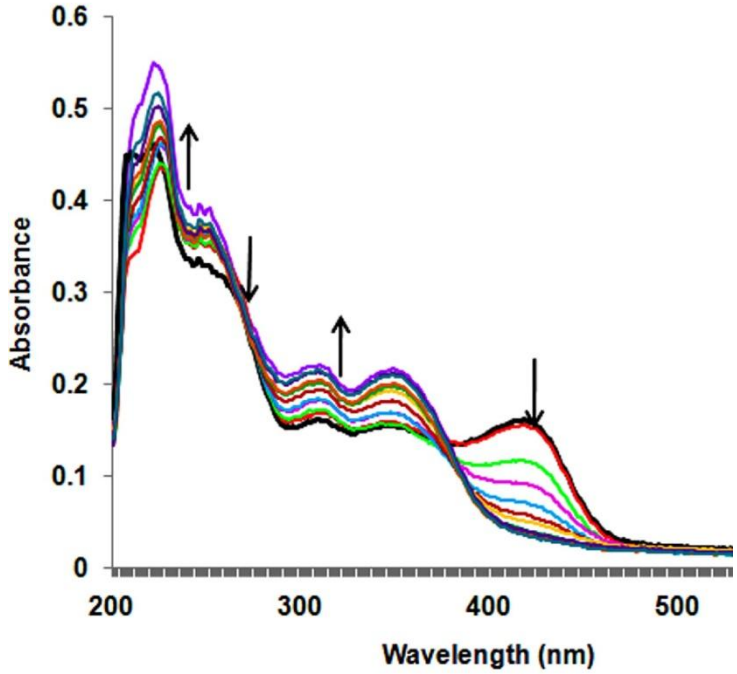
SI Figure 43. UV-vis spectra of compound **11** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



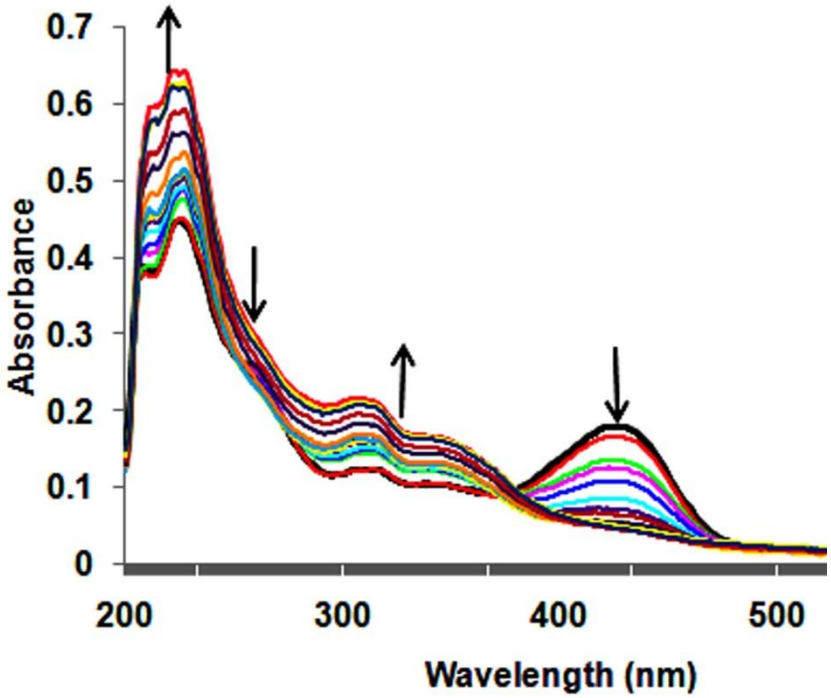
SI Figure 44. UV-vis spectra of compound **12** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



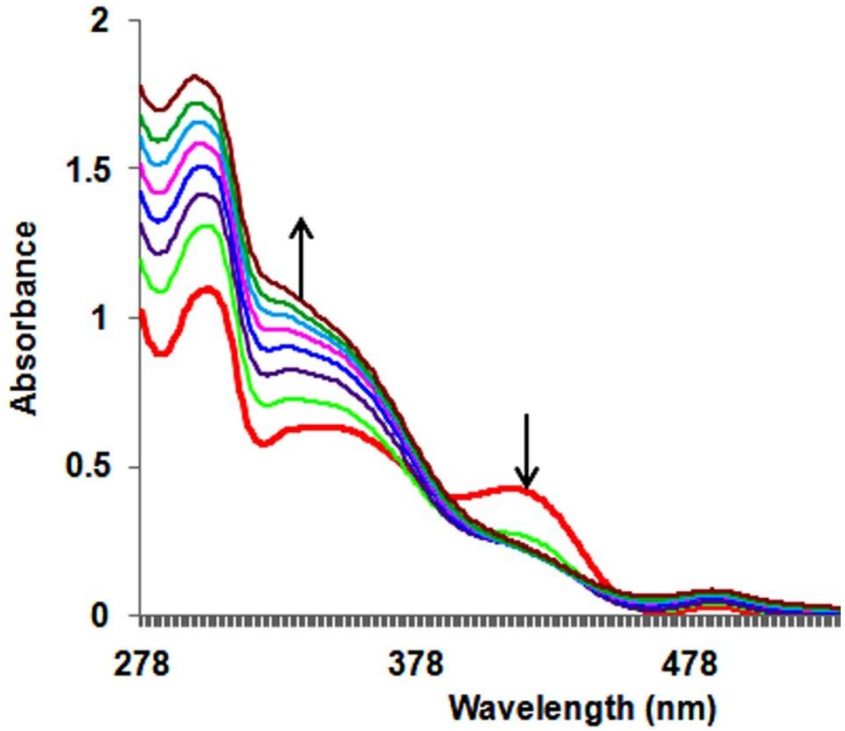
SI Figure 45. UV-vis spectra of compound **13** (10 µM) in aqueous solution (water-ethanol, pH 7.2, v/v 9:1) upon addition of increasing amount of $Hg(ClO_4)_2$ (0.1-1 equiv).



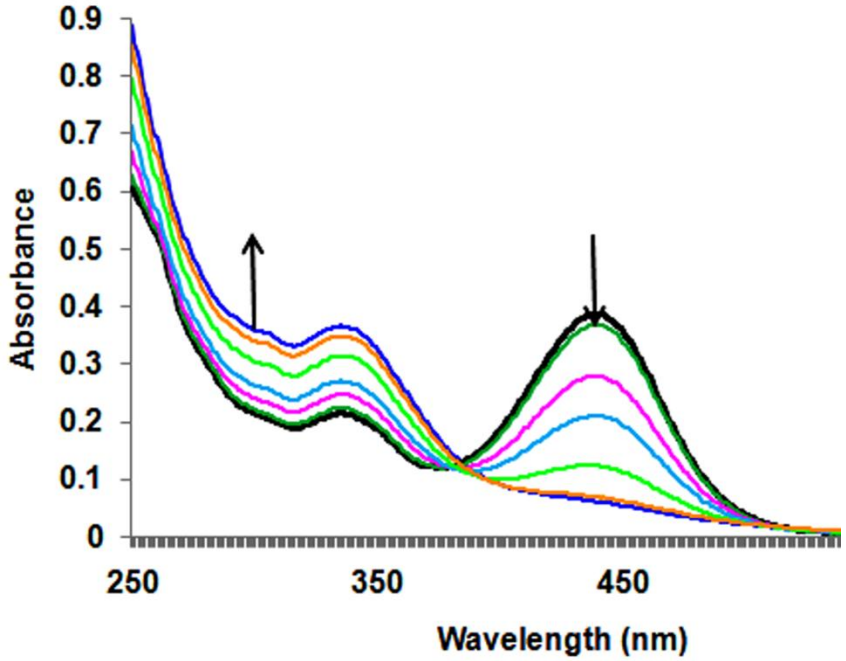
SI Figure 46. UV-vis spectra of compound **4** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amounts of $Fe(ClO_4)_3$ (0.1-1 equiv).



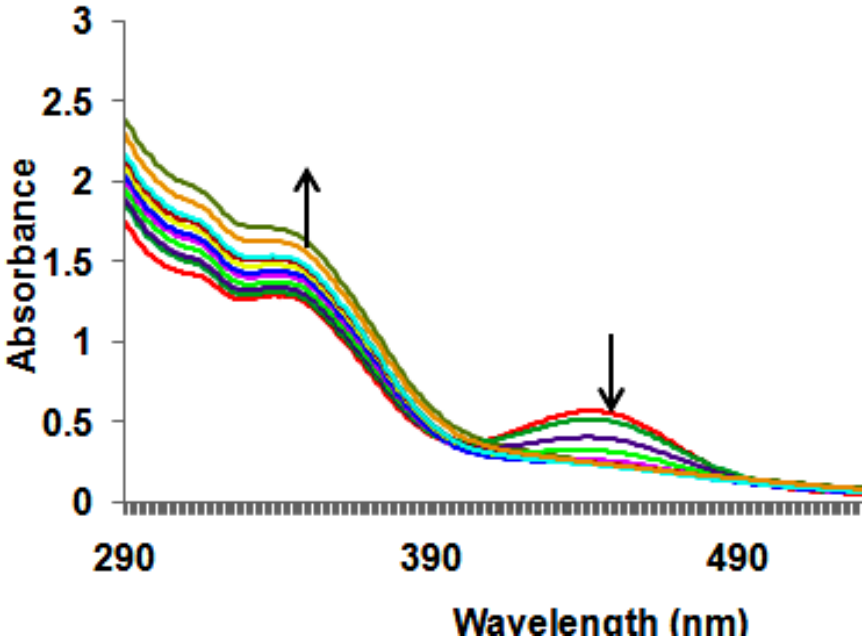
SI Figure 47. UV-vis spectra of compound **5** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Fe(ClO_4)_3$ (0.1-1 equiv).



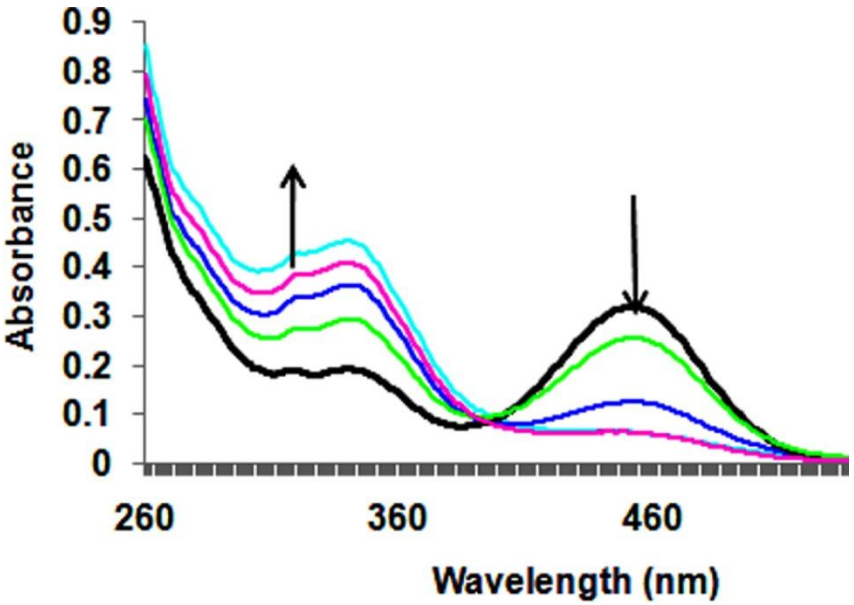
SI Figure 48. UV-vis spectra of compound **8** (10 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Fe(ClO_4)_3$ (0.1 - 1 equiv).



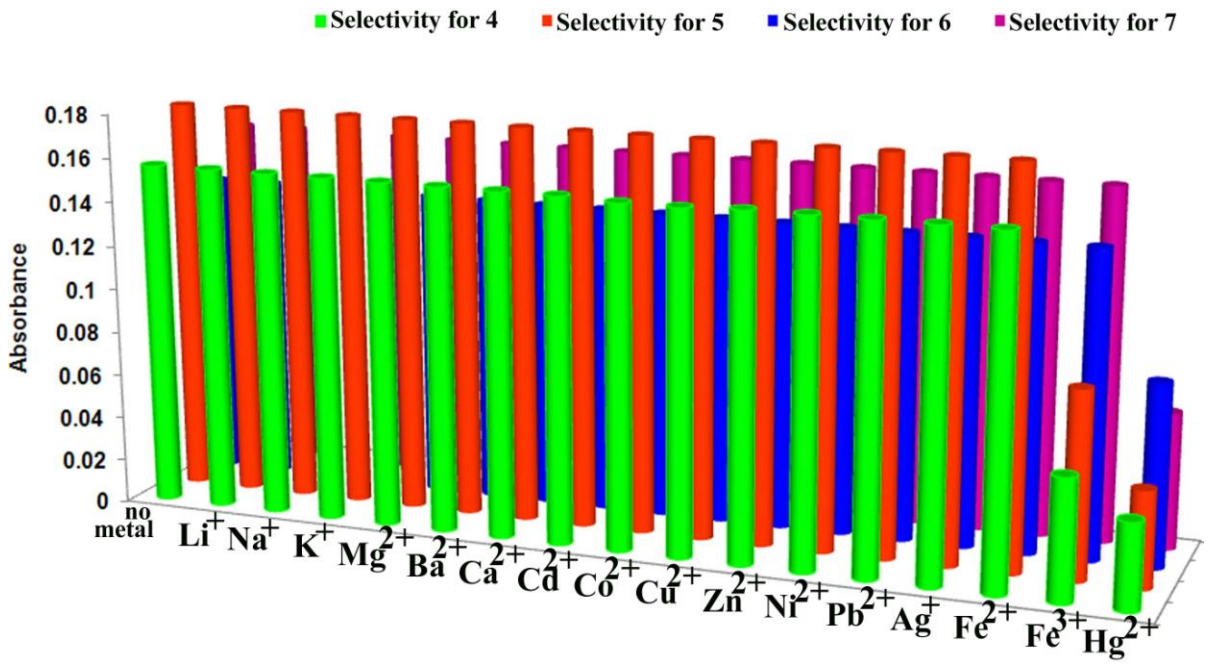
SI Figure 49. UV-vis spectra of compound **9** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Fe(ClO_4)_3$ (0.1-1 equiv).



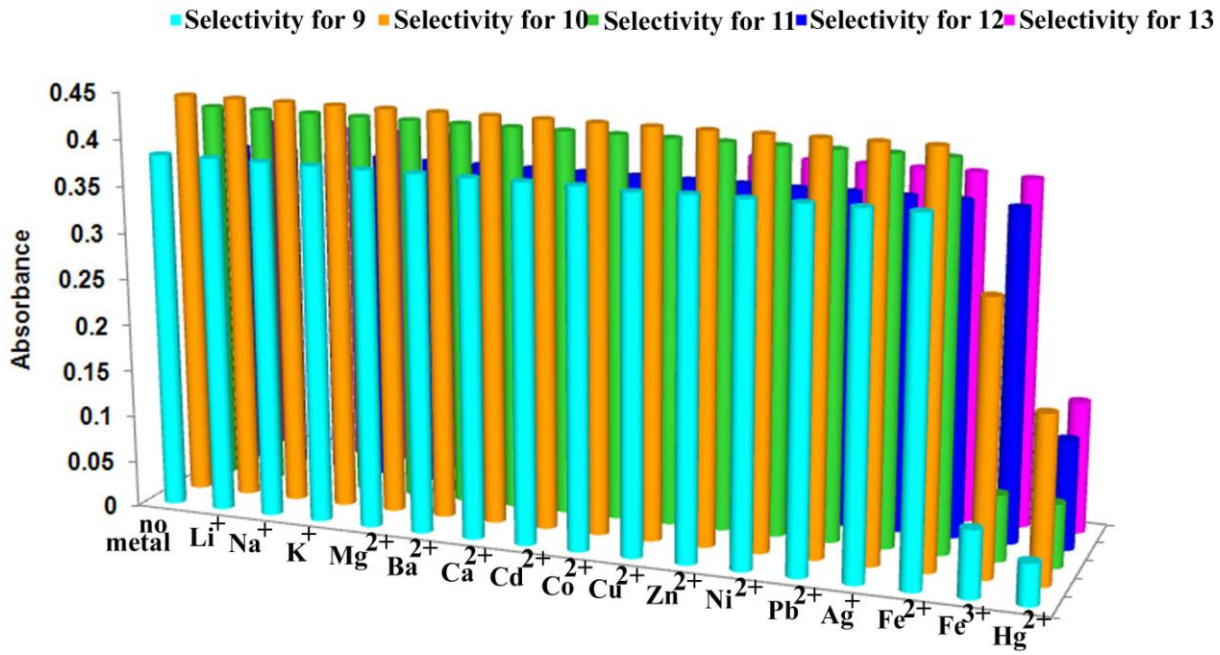
SI Figure 50. UV-vis spectra of compound **10** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Fe(ClO_4)_3$ (0.1-1 equiv).



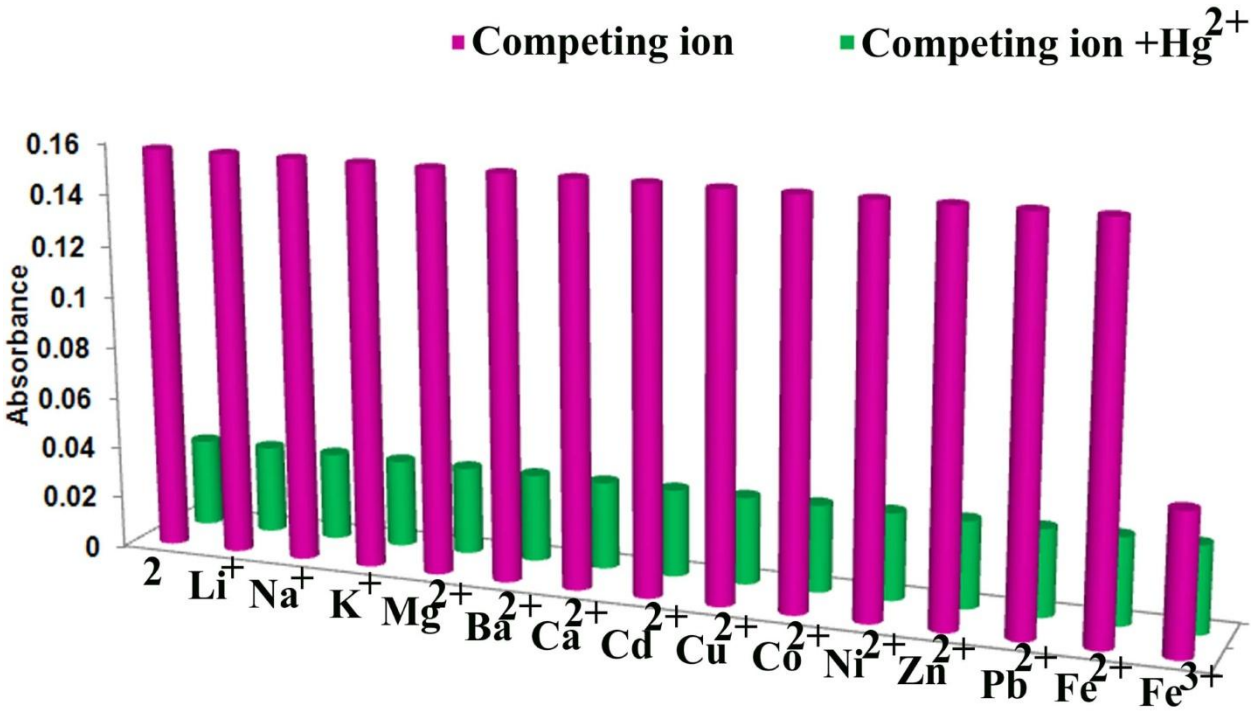
SI Figure 51. UV-vis spectra of compound **11** (10 μM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of $Fe(ClO_4)_3$ (0.1-1 equiv).



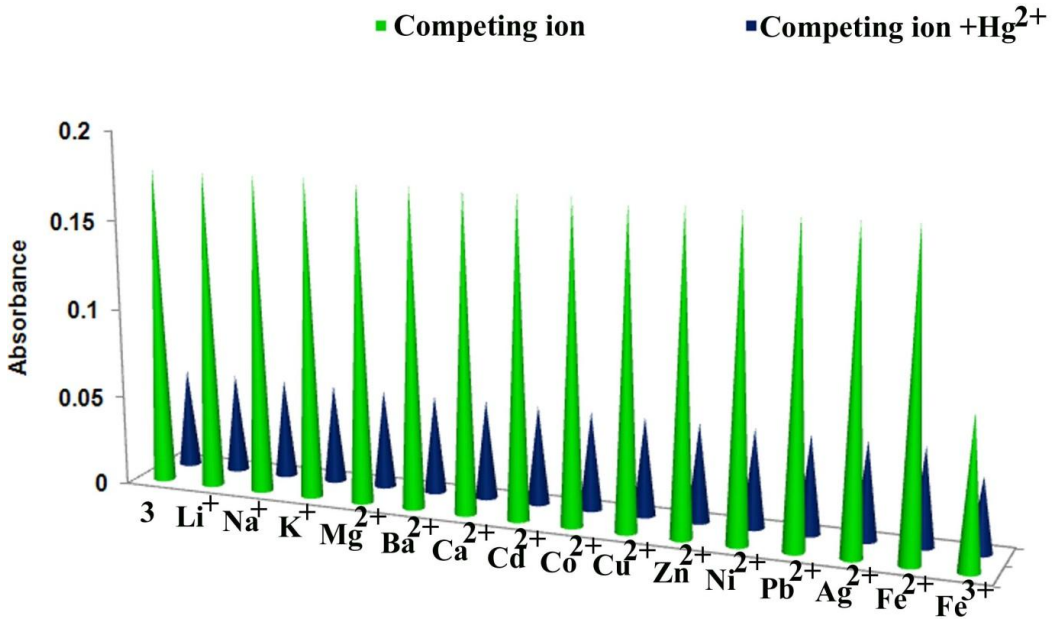
SI Figure 52. Selectivity of compounds **4**, **5**, **6** and **7** (5μM) towards Hg^{2+} among different cations.



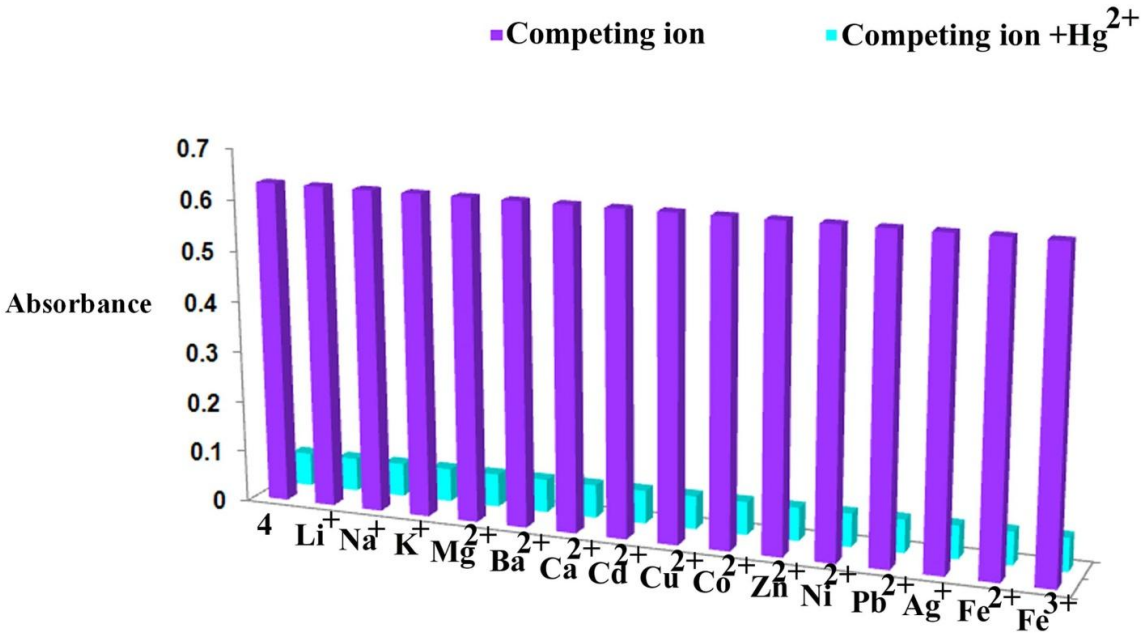
SI Figure 53. Selectivity of compounds **9**, **10**, **11**, **12** and **13** (10 µM) towards Hg^{2+} among different cations.



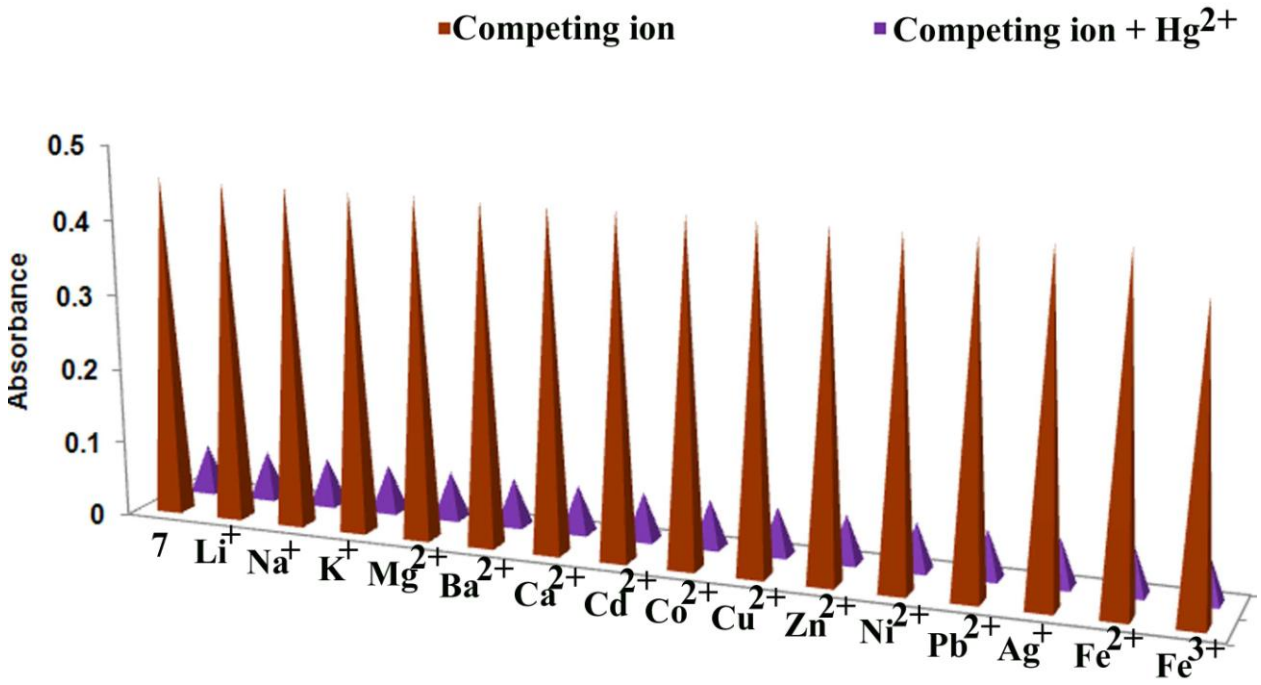
SI Figure 54. Response of compound **4** (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: **4** (5 µM) in presence of Hg^{2+} (1 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Fe^{2+} and Fe^{3+} (100 equiv).



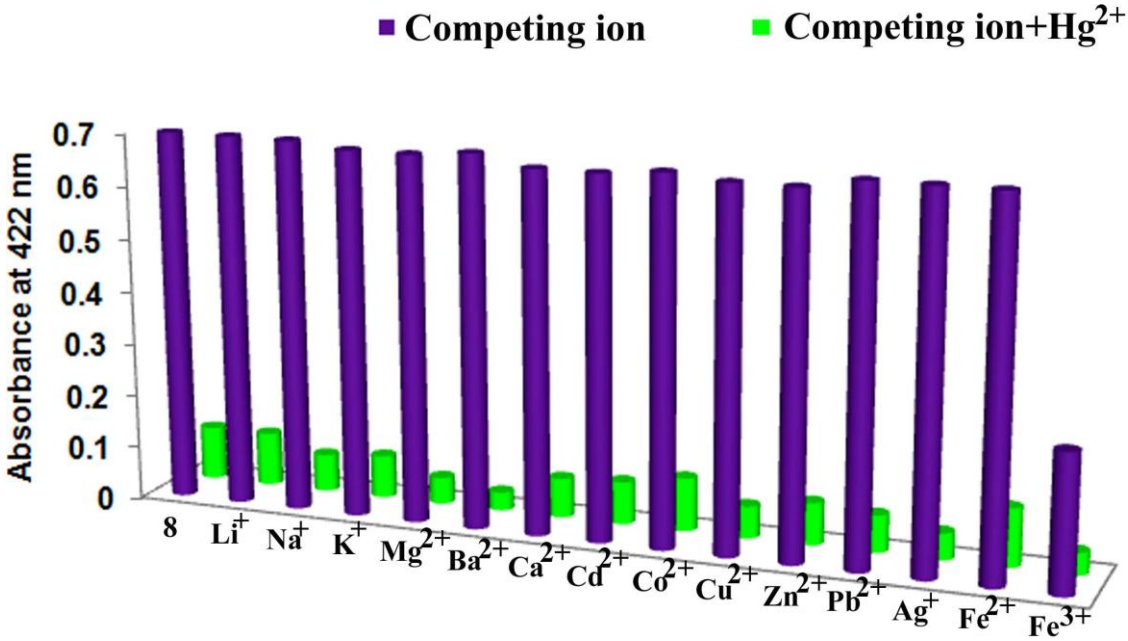
SI Figure 55. Response of compound **5** (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: **5** (5 µM) in presence of Hg^{2+} (1 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



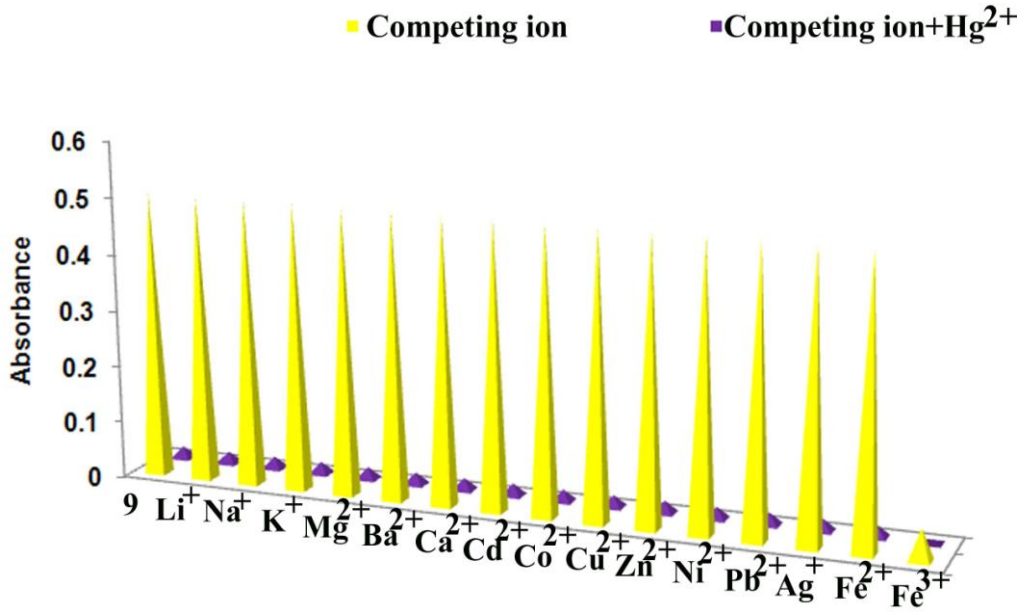
SI Figure 56. Response of compound **6** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 434 nm: **6** (2 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



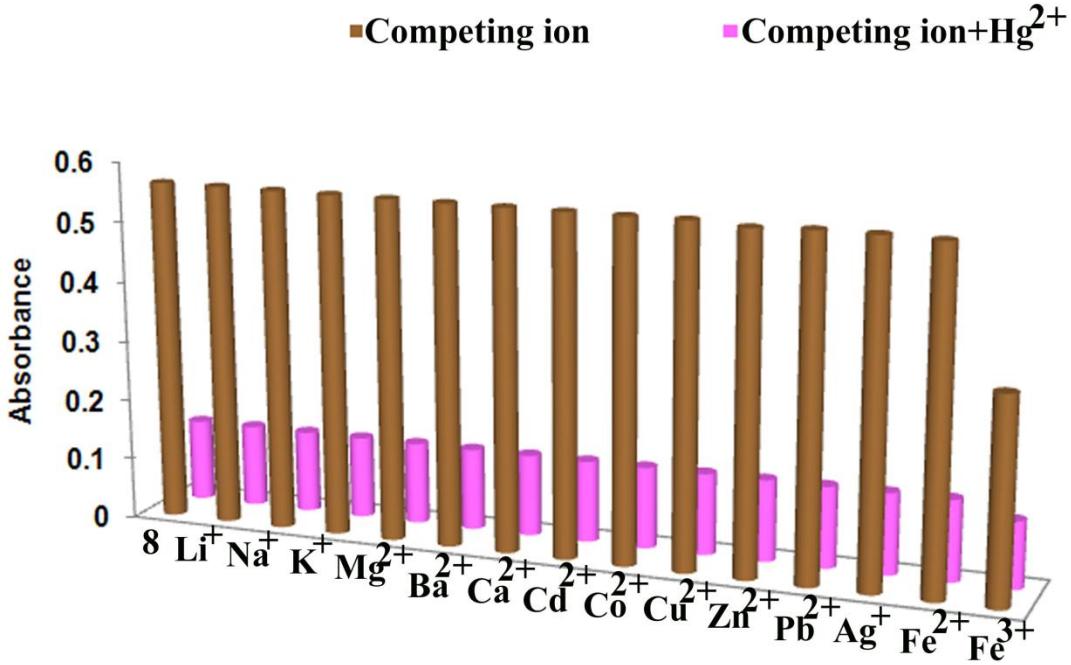
SI Figure 57. Response of compound **7** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 434 nm: **7** (10 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



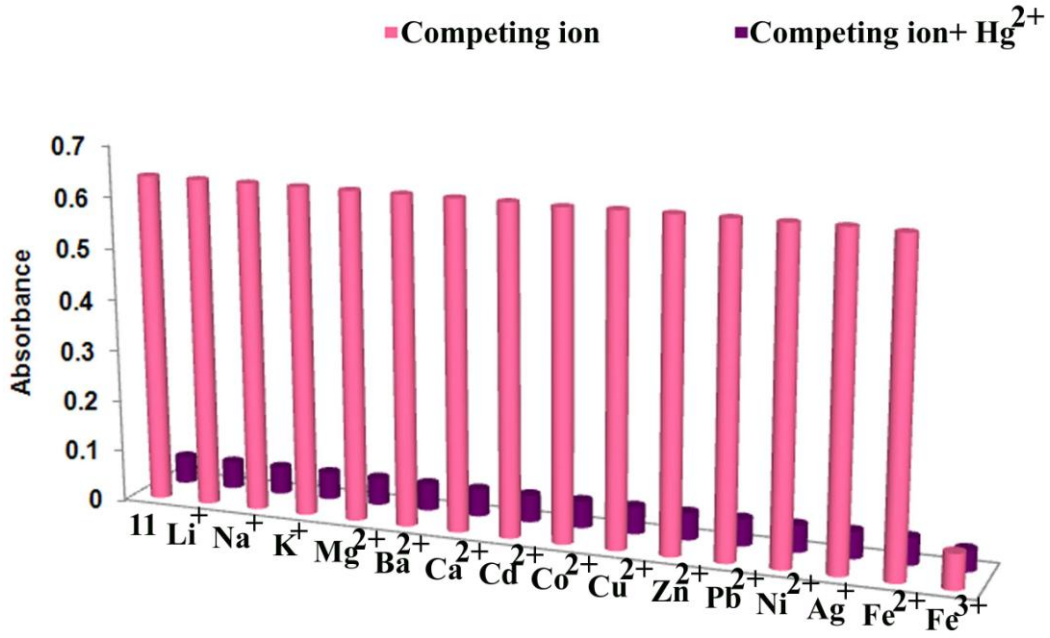
SI Figure 58. Response of compound **8** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: **8** (10 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



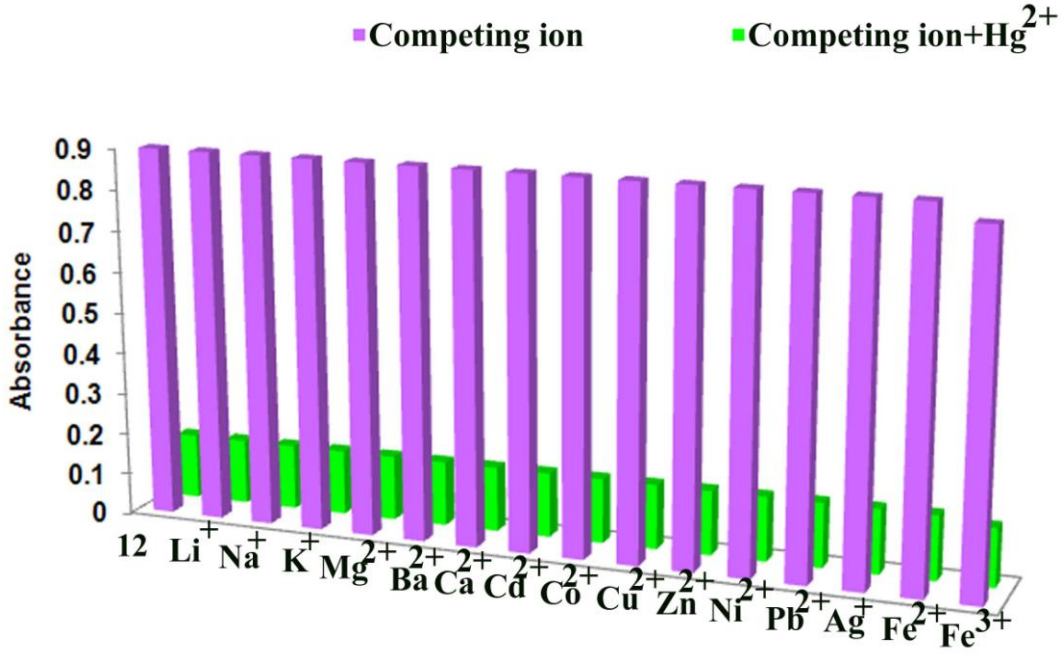
SI Figure 59. Response of compound **9** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: **9** (10 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



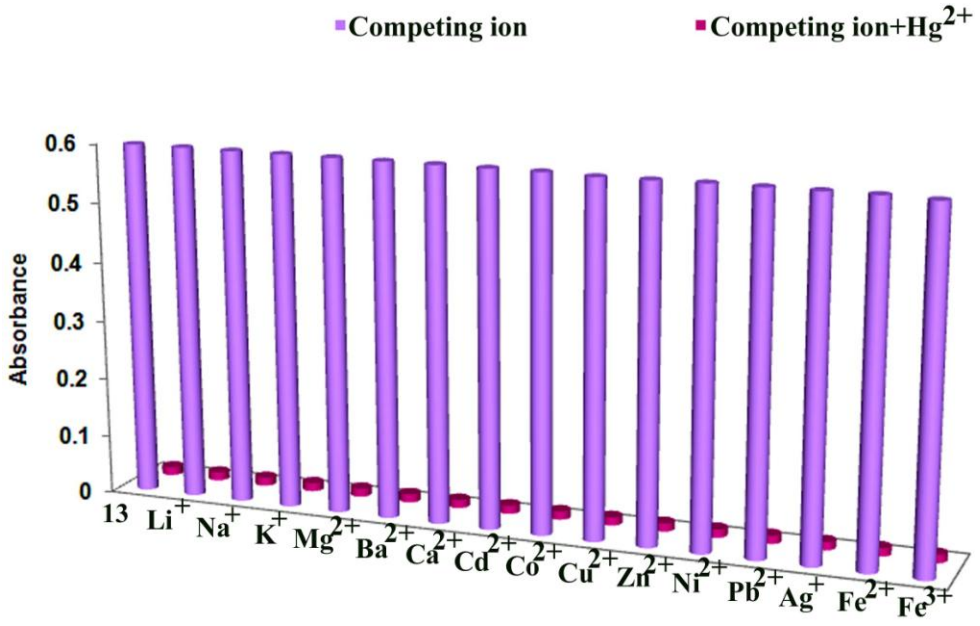
SI Figure 60. Response of compound **10** (5 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 442 nm: **10** (5 µM) in presence of Hg^{2+} (5 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



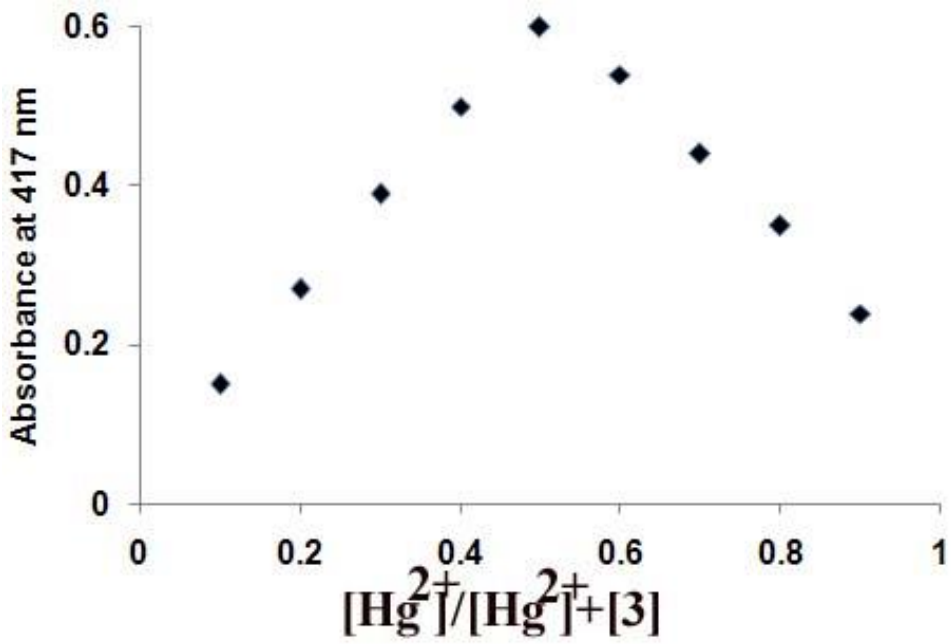
SI Figure 61. Response of compound **11** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 422 nm: **11** (10 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



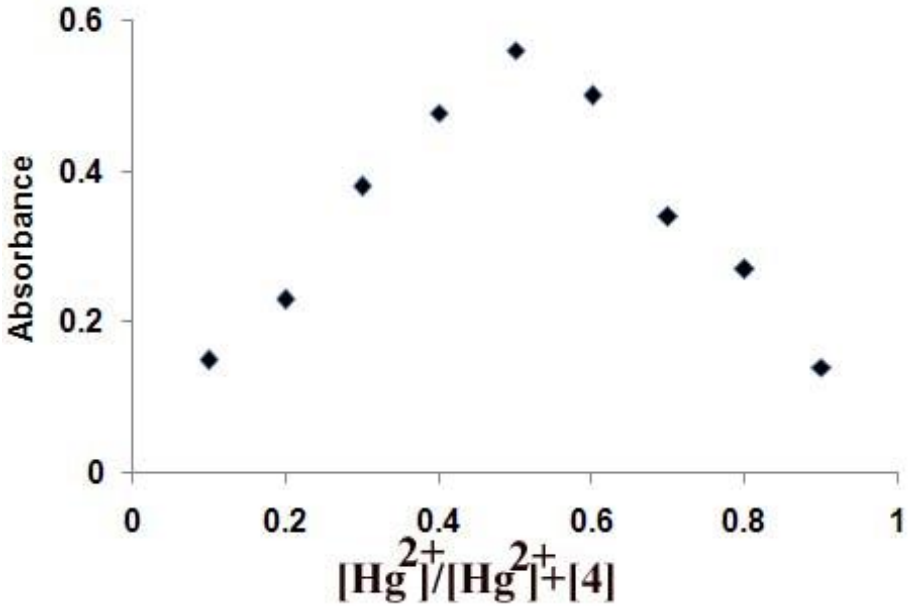
SI Figure 62. Response of compound **12** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 448 nm: **12** (10 µM) in presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



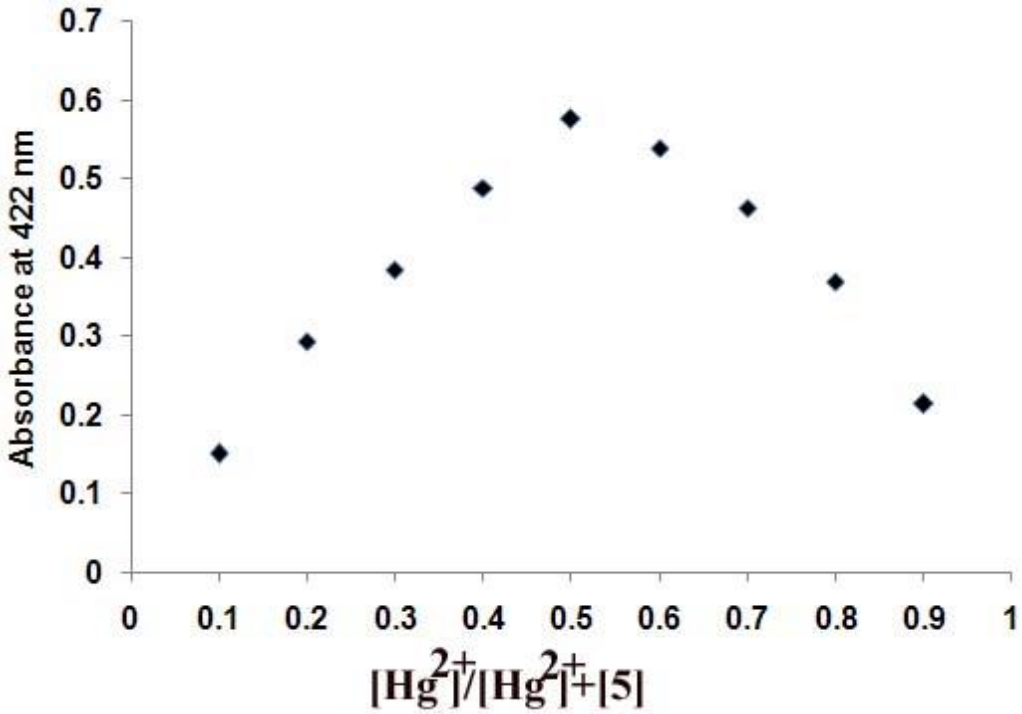
SI Figure 63. Response of compound **13** (10 µM) in water-ethanol (9:1 v/v) at pH 7.2 to various cations monitored at 467 nm **13** (10 µM) in the presence of Hg^{2+} (2 µM) and interfering ions Li^{+}, Na^{+}, K^{+} Mg^{2+}, Ba^{2+}, Ca^{2+}, Cd^{2+}, Co^{2+}, Cu^{2+}, Zn^{2+}, Pb^{2+}, Ag^{+}, Fe^{2+} and Fe^{3+} (100 equiv).



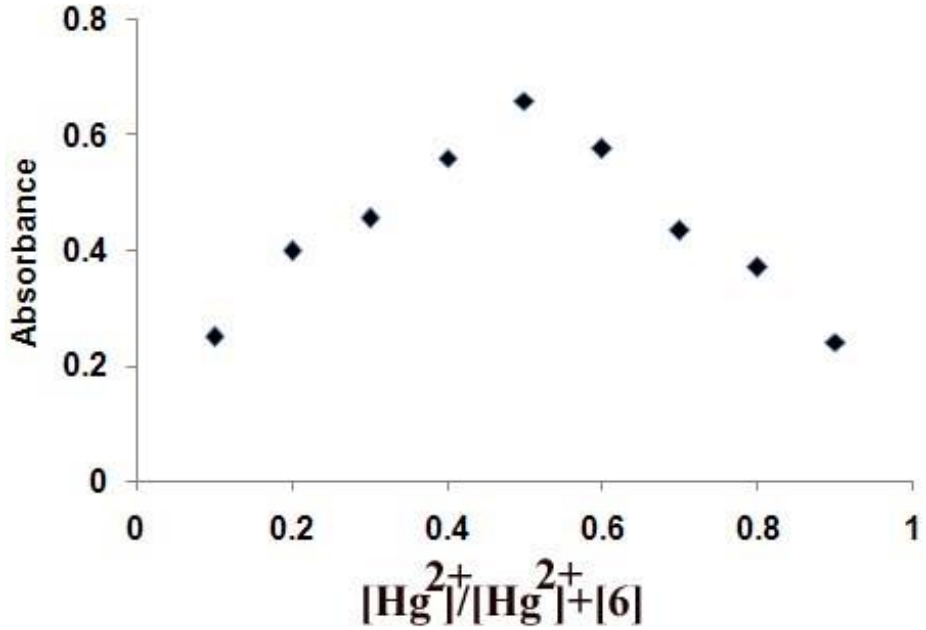
SI Figure 64. Job's plot for compound **3**, absorbance monitored at 417 nm.



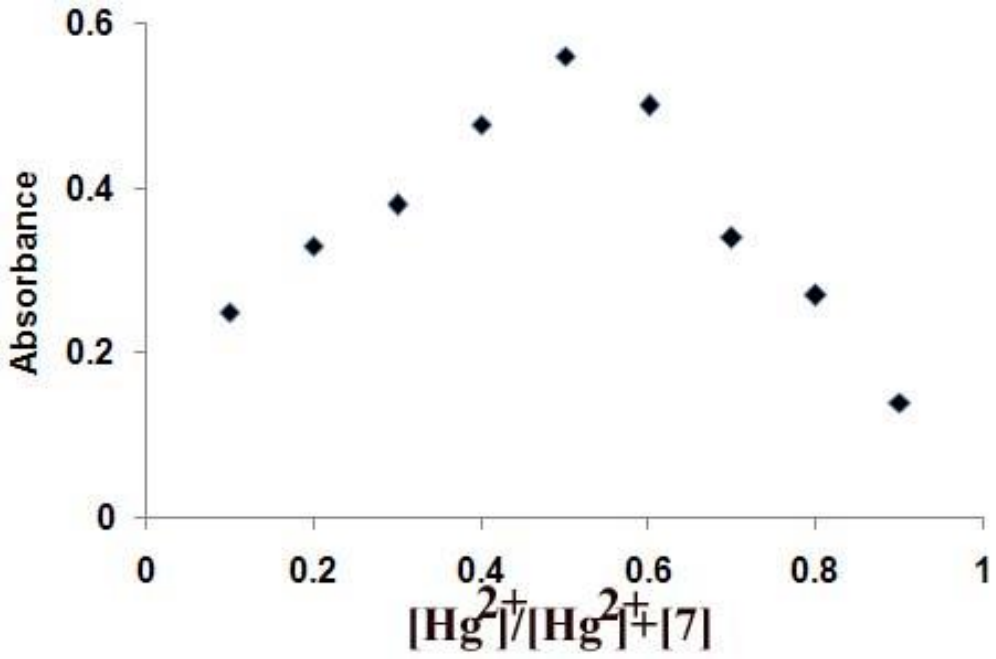
SI Figure 65. Job's plot for compound **4**, absorbance monitored at 422 nm.



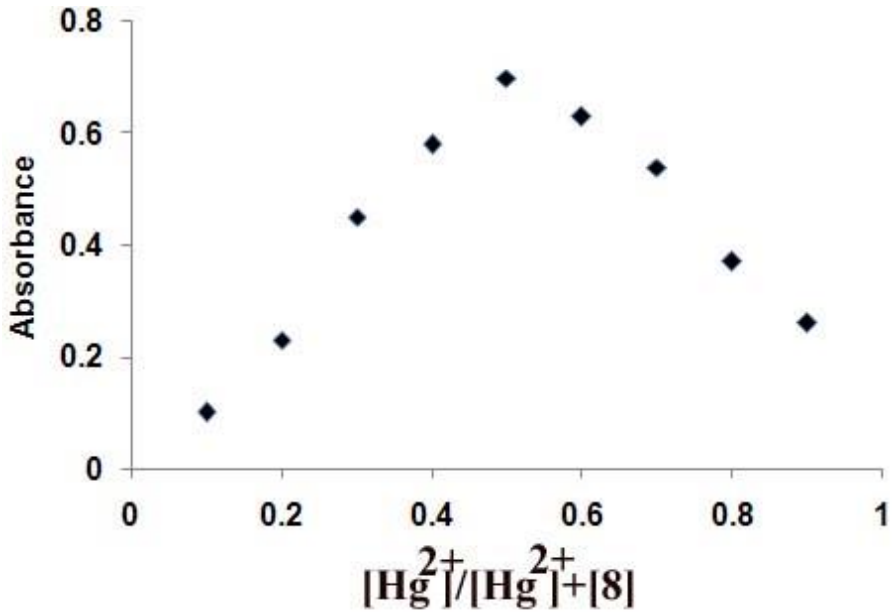
SI Figure 66. Job's plot for compound **5**, absorbance monitored at 422 nm.



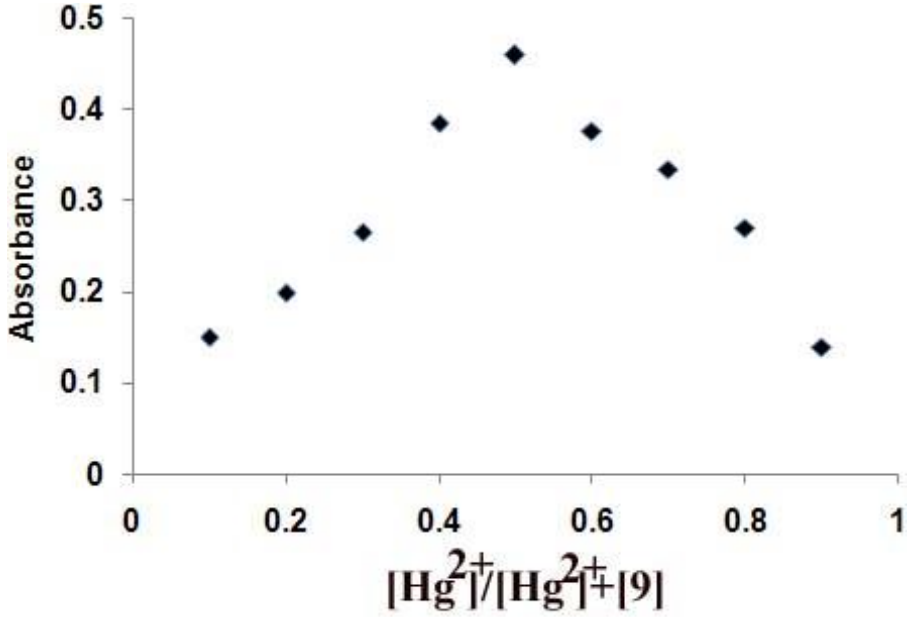
SI Figure 67. Job's plot for compound **6**, absorbance monitored at 434 nm.



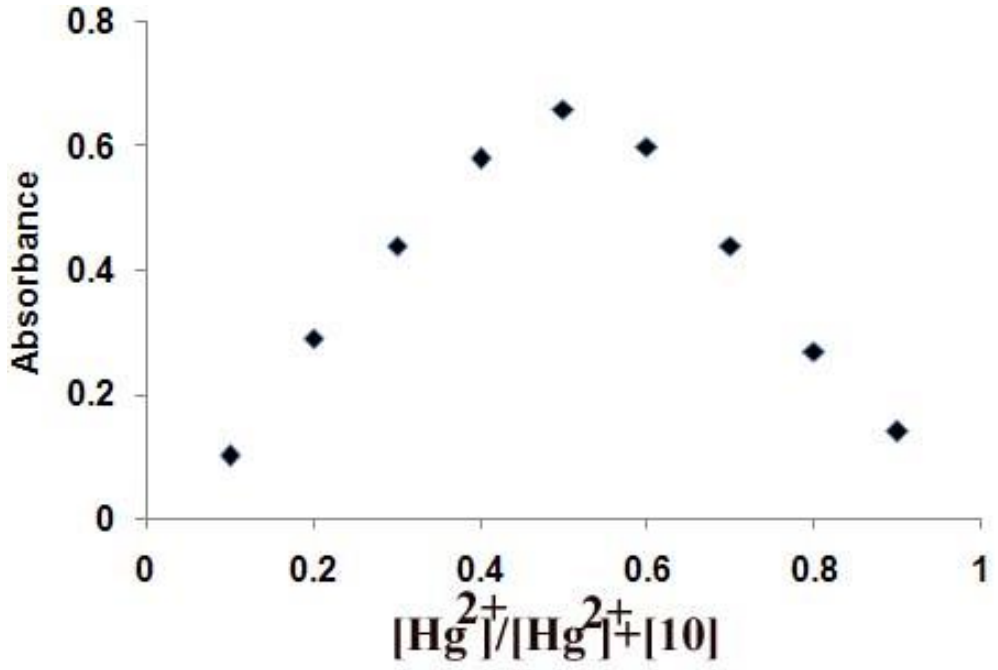
SI Figure 68. Job's plot for compound **7**, absorbance monitored at 422 nm.



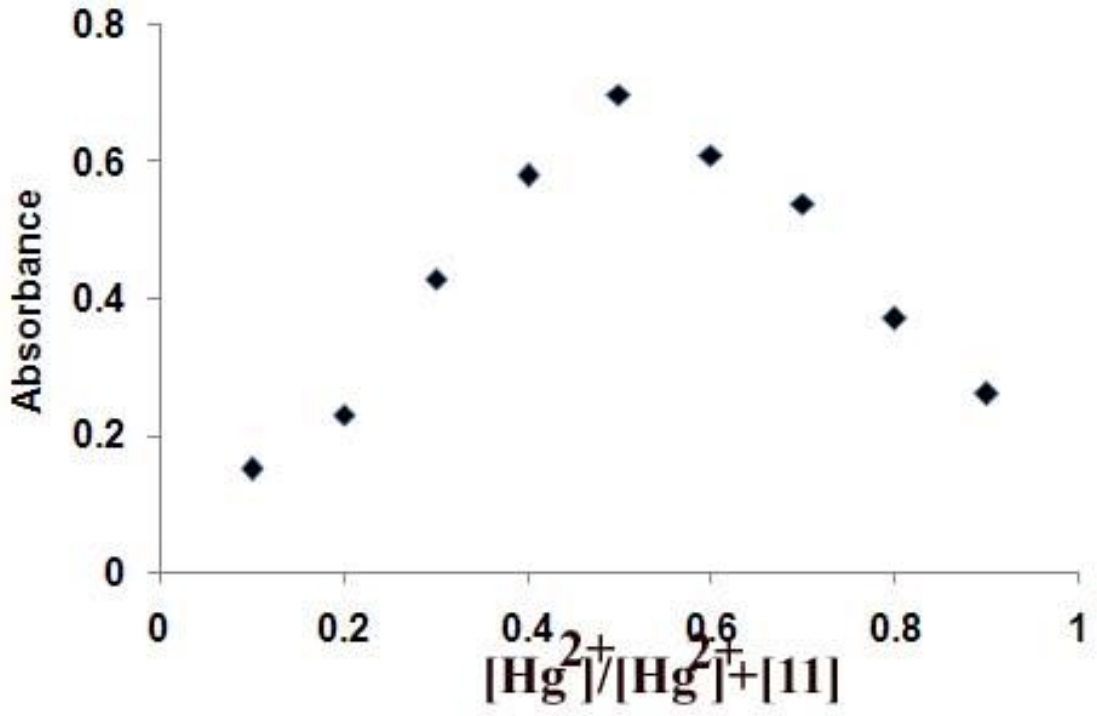
SI Figure 69. Job's plot for compound **8**, absorbance monitored at 422 nm.



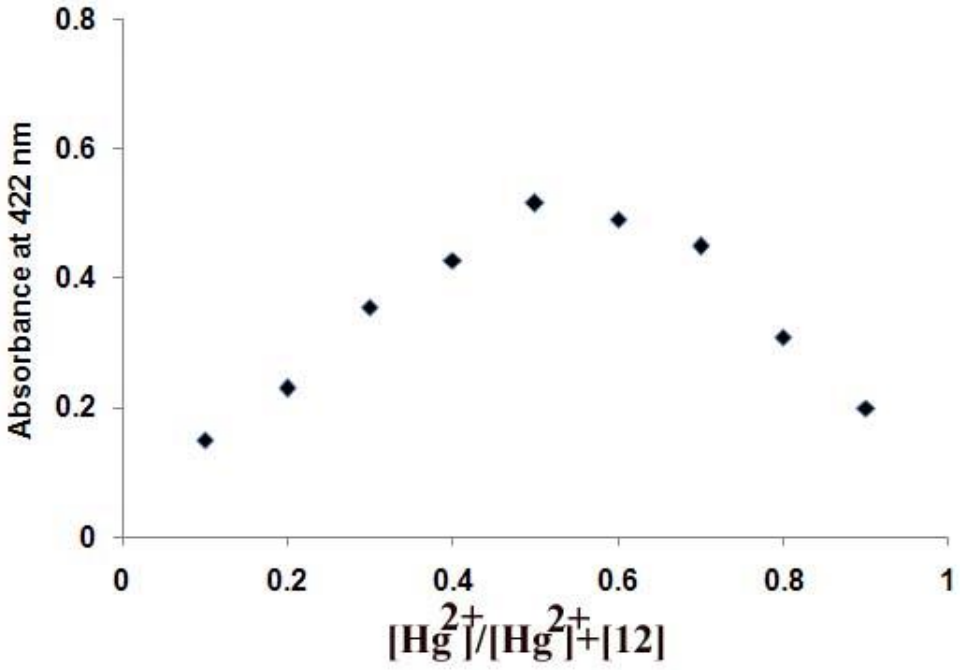
SI Figure 70. Job's plot for compound **9**, absorbance monitored at 422 nm.



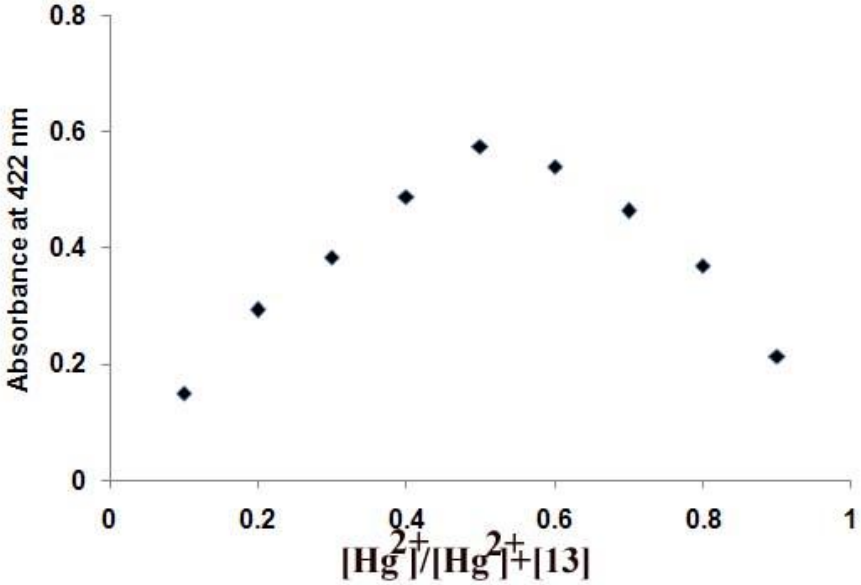
SI Figure 71. Job's plot for compound **10**, absobance monitored at 442 nm.



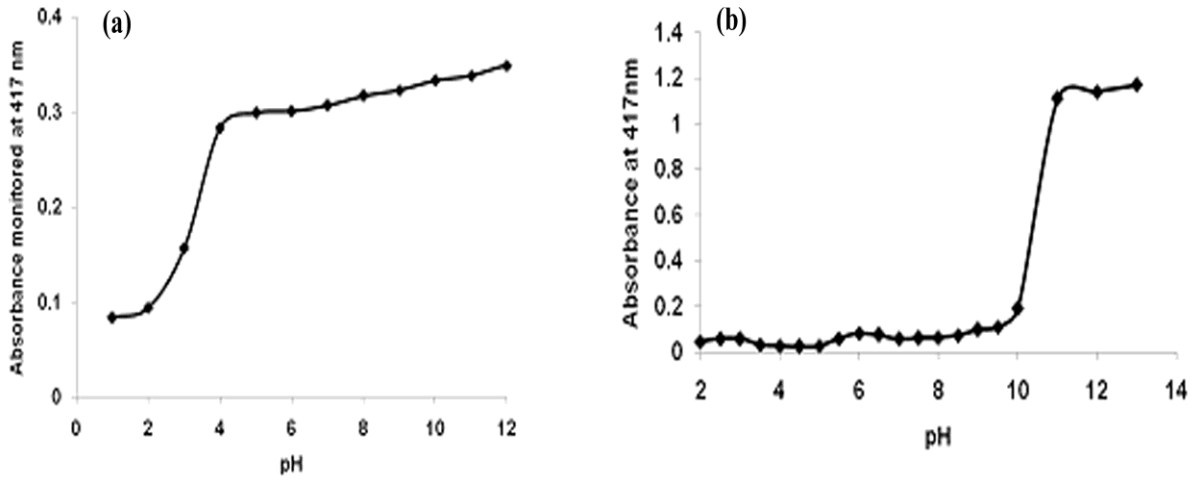
SI Figure 72. Job's plot for compound **11**, absorbance monitored at 439 nm.



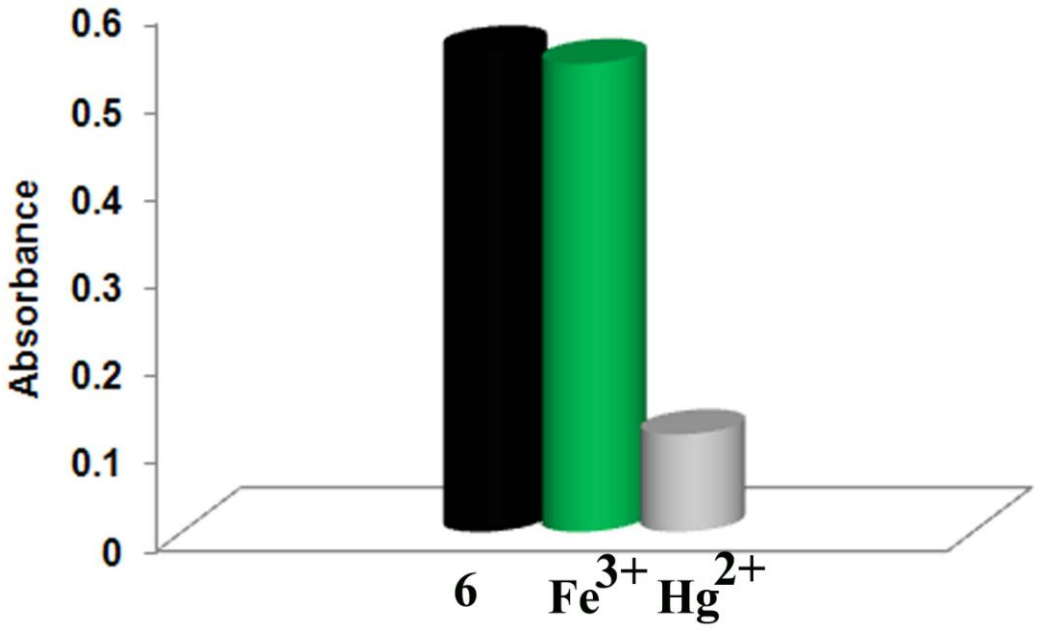
SI Figure 73. Job's plot for compound **12**, absorbance monitored at 448 nm.



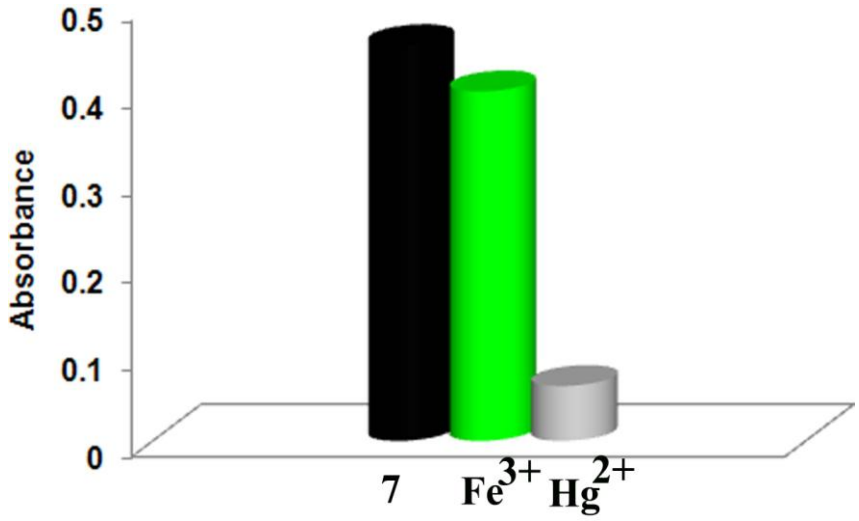
SI Figure 74. Job's plot for compound **13**, absorbance monitored at 467 nm.



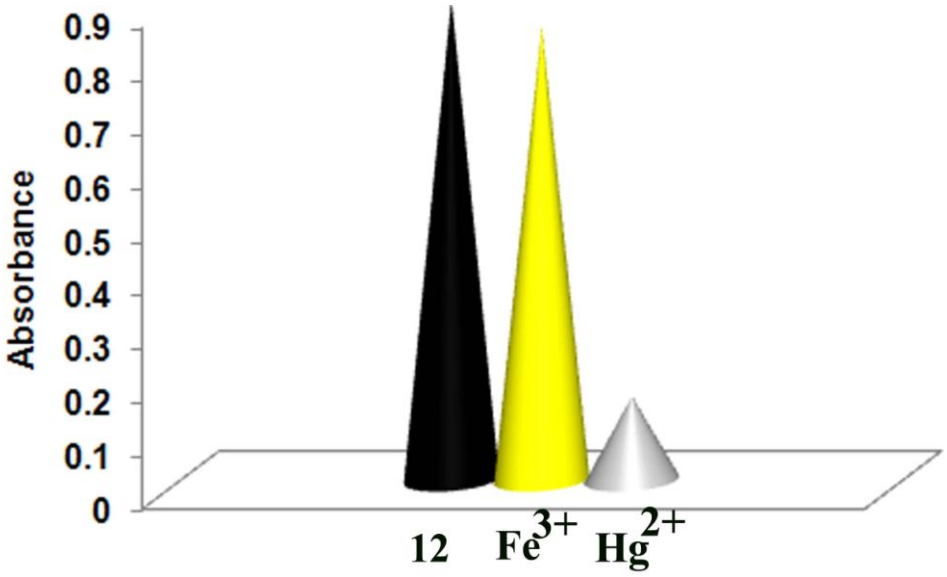
SI Figure 75. (a) Change in absorbance of compound **3** at 417 nm with pH, (b) Change in absorbance of compound **3** on addition of 1 equiv of Hg^{2+} (1 μM) at different pH.



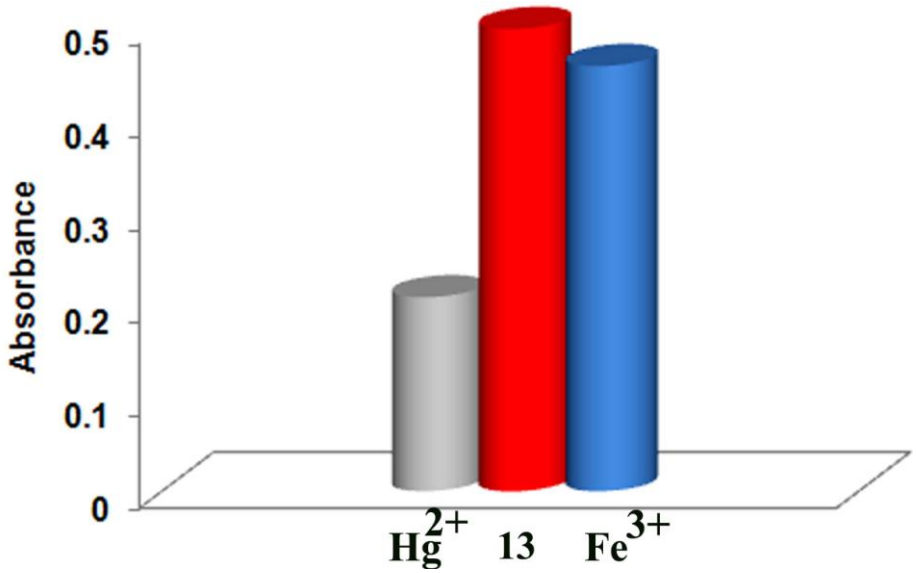
SI Figure 76. Bar graph showing the selectivity of compound **6** towards Hg^{2+} in presence of Fe^{3+} monitored at 434 nm.



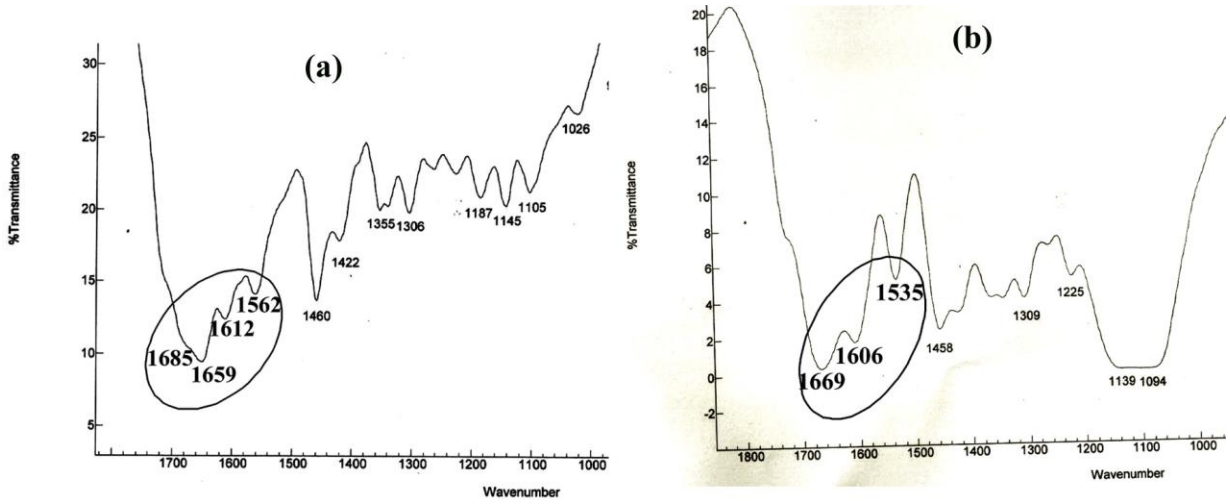
SI Figure 77. Bar graph showing the selectivity of compound **7** towards Hg^{2+} in presence of Fe^{3+} monitored at 439 nm.



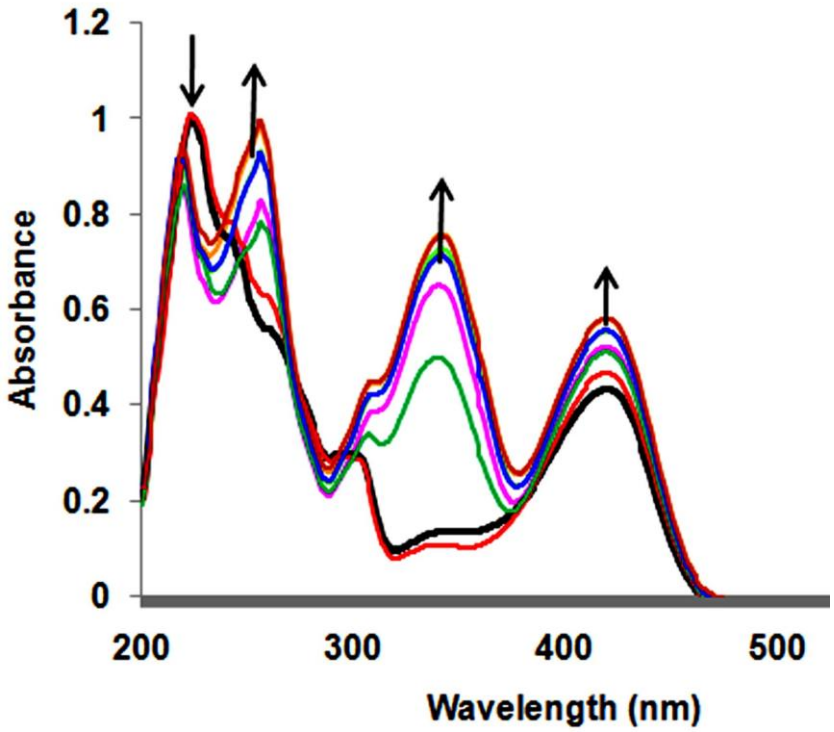
SI Figure 78. Bar graph showing selectivity of compound **12** towards Hg^{2+} in presence of Fe^{3+} monitored at 448 nm.



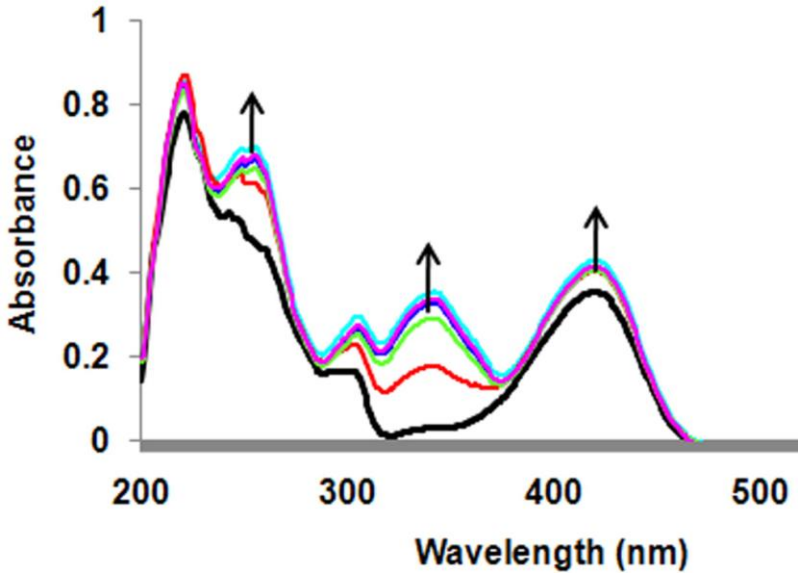
SI Figure 79. Bar graph showing the selectivity of compound **13** towards Hg^{2+} in presence of Fe^{3+} monitored at 467 nm.



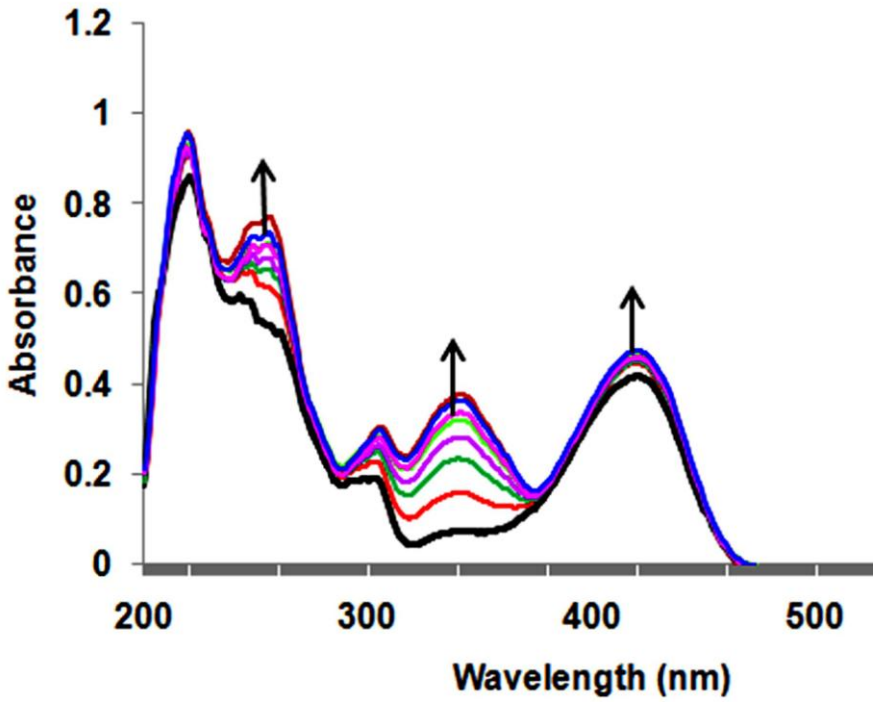
SI Figure 80. (a) A part of IR spectrum of compound **3**. (b) A part of IR spectrum of compound **3**.Hg^{2+}.



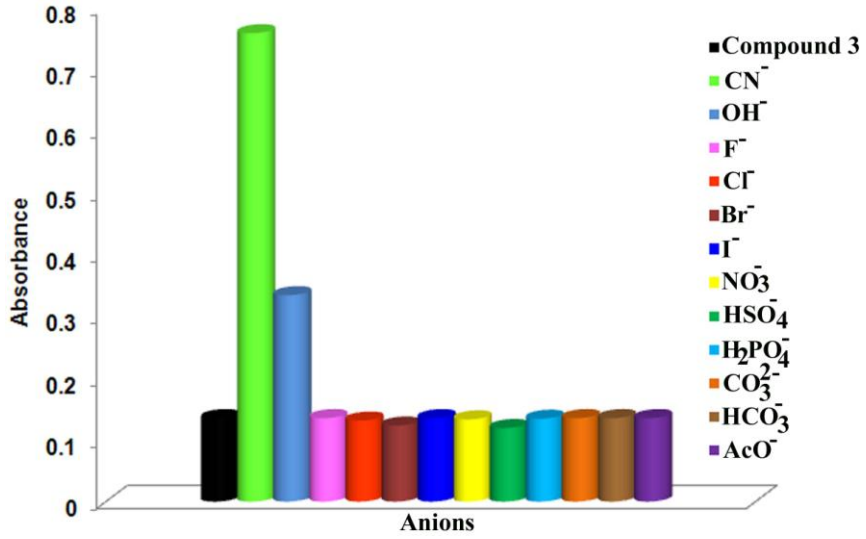
SI Figure 81. UV-vis spectra of compound **3** (5 µM) in water-ethanol (pH 7.2, v/v 9:1) upon addition of increasing amount of sodium cyanide (0.1-1 equiv).



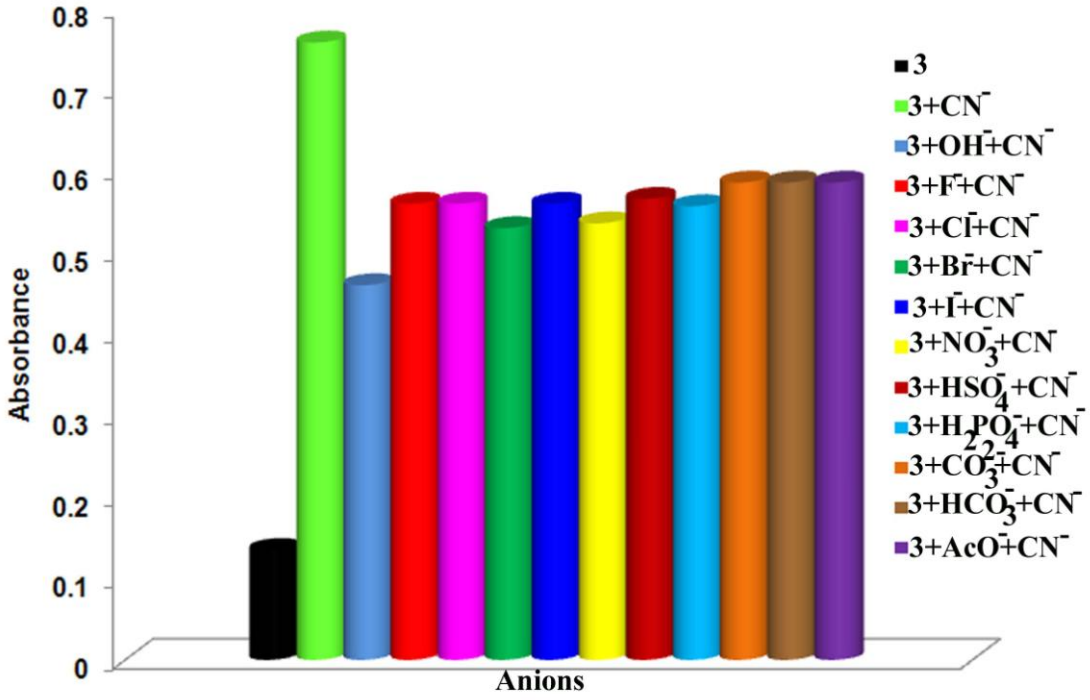
SI Figure 82. UV-vis spectra of compound **3** (5 µM) in acetonitrile (ACN) upon addition of increasing amount of TBACN (0.1-1 equiv).



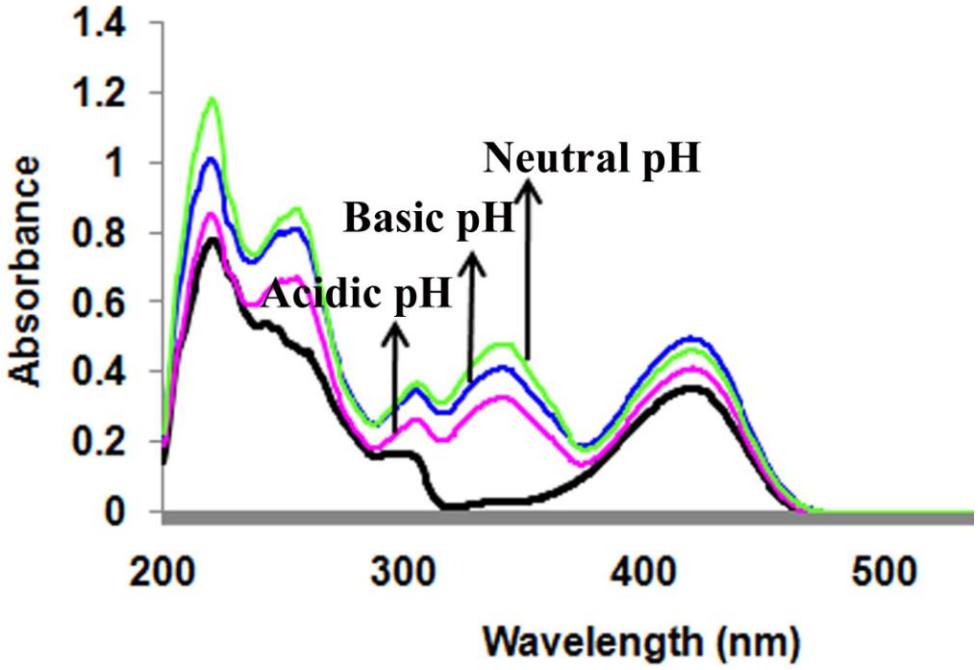
SI Figure 83. UV-vis spectra of compound **3** (5 μM) in chloroform ($CHCl_3$) upon addition of increasing amount of TBACN (0.1-1 equiv).



SI Figure 84. Bar graph shows absorbance of compound **3** at 341 nm in presence of 1 equiv of various anions.

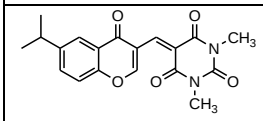
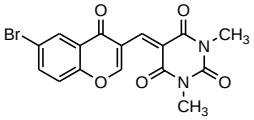
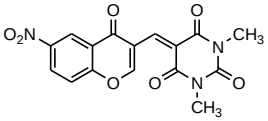
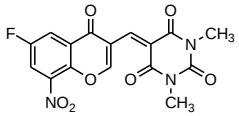
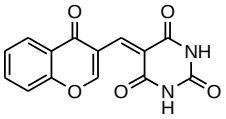
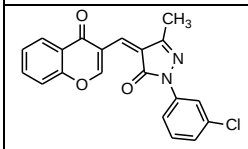
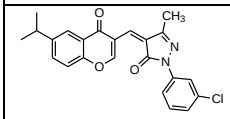
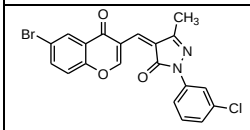
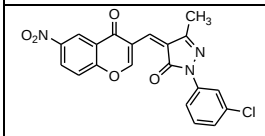
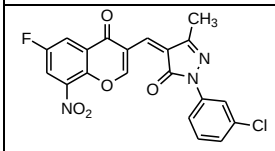


SI Figure 85. Competitive binding of compound **3** with CN^- in presence of other anions. Absorbance monitored at 341 nm.



SI Figure 86. Change in UV-vis spectrum of compound **3** (black trace) on addition of 1 equiv of CN^- (1 μM) at pH 6-8.

Table 1. Binding constants for compounds **4-13**.

Compound	Binding constant (M^{-1})	
	Hg^{2+}	Fe^{3+}
 **4**	7.1×10^{7}	2.8×10^{6}
 **5**	6.6×10^{8}	2×10^{8}
 **6**	3.8×10^{6}	-
 **7**	1.6×10^{7}	-
 **8**	1.5×10^{6}	2×10^{6}
 **9**	2.5×10^{6}	2.6×10^{6}
 **10**	3.9×10^{7}	1.6×10^{6}
 **11**	3.3×10^{7}	1.2×10^{6}
 **12**	4.7×10^{6}	-
 **13**	4.1×10^{6}	-