Synthesis of thiocarbonyl analogues of colourimetric coumarin-based chemosensors: altering the selectivity from Fe to Hg(II) and Cu(II) ions Supplementary Information

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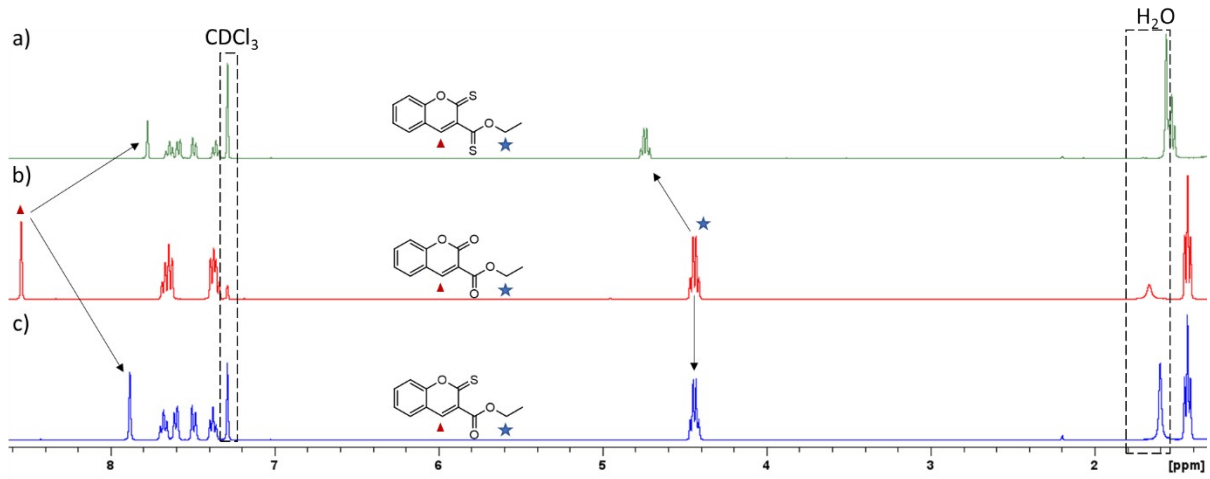

***Figure S 1**: [1]H NMR spectra of a) **S1c**, b) **S1a**, and c) **S1b**, showing the shifts in the proton peaks.*

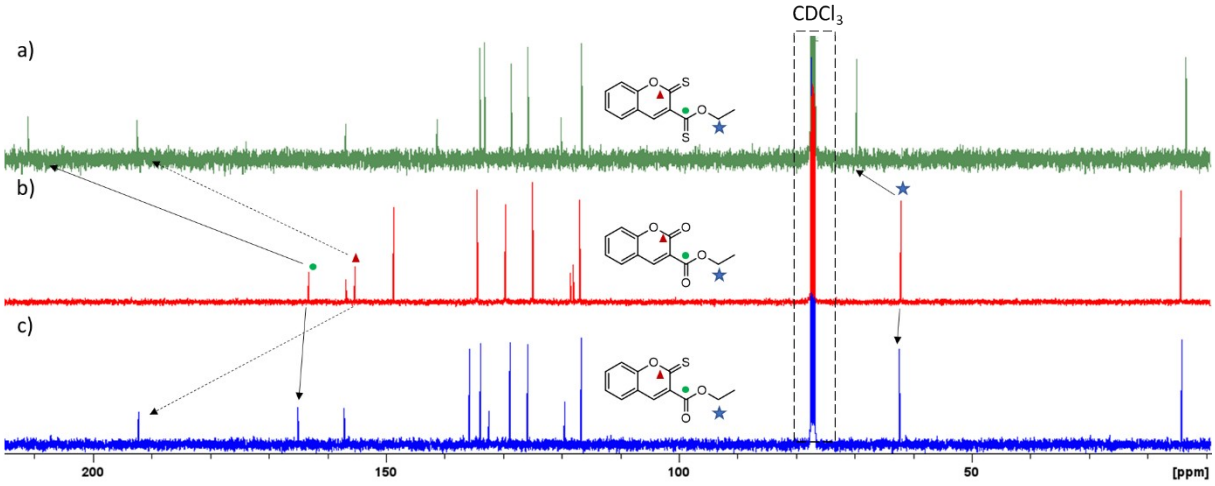

***Figure S 2**: [13]C NMR spectra of a) **S1c**, b) **S1a**, and c) **S1b**, showing the shifts in the carbon peaks.*

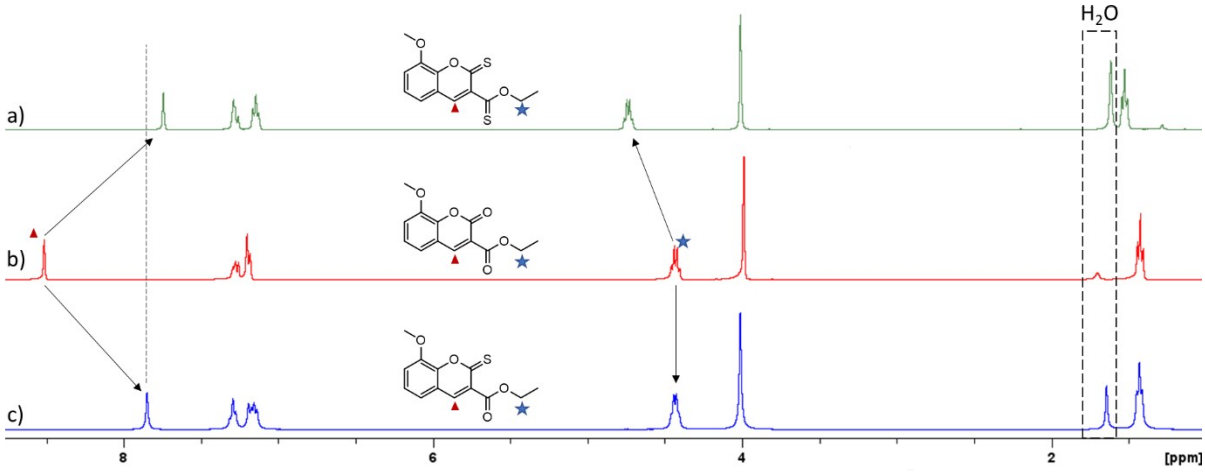

***Figure S 3**: [1]H NMR spectra of a) **S2c**, b) **S2a**, and c) **S2b**, showing the shifts in the proton peaks.*

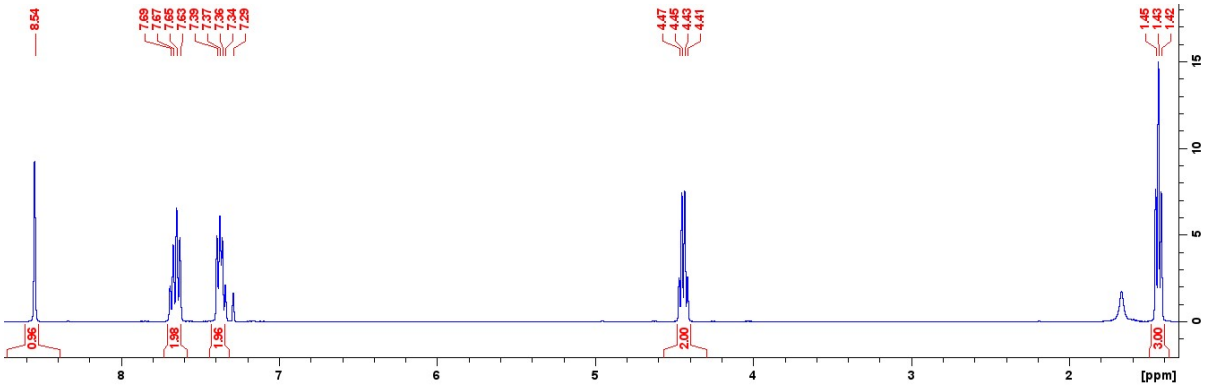

***Figure S 4**: [1]H NMR of **S1a**.*

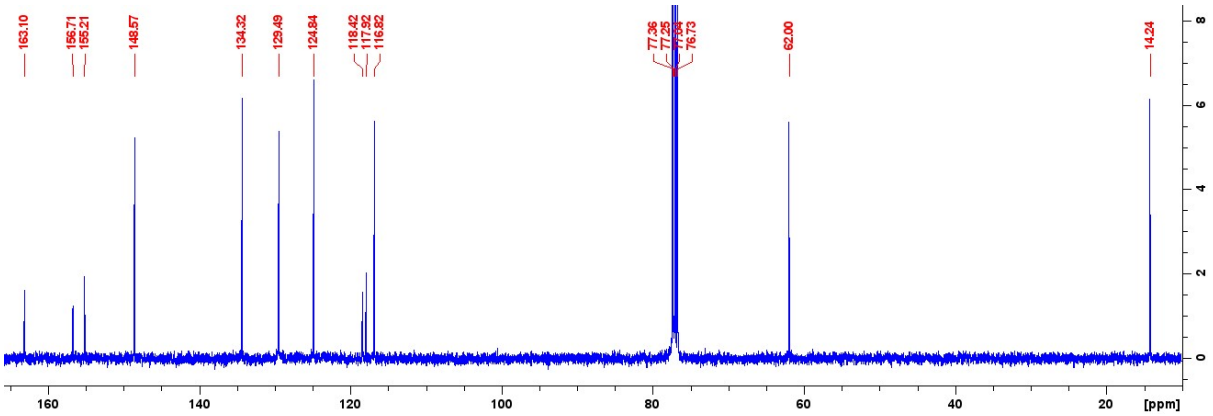

***Figure S 5**: [13]C NMR of **S1a**.*

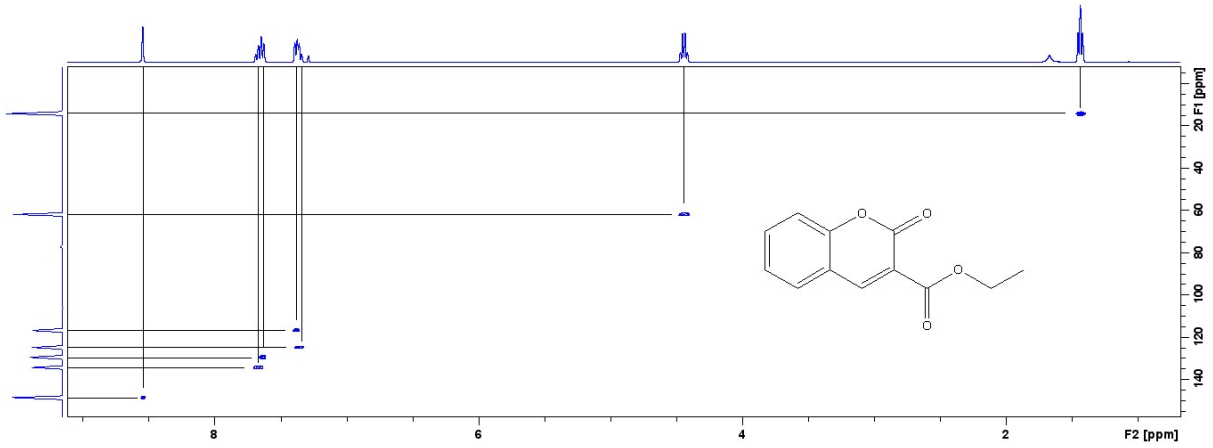

***Figure S 6:** HSQC of **S1a**.*

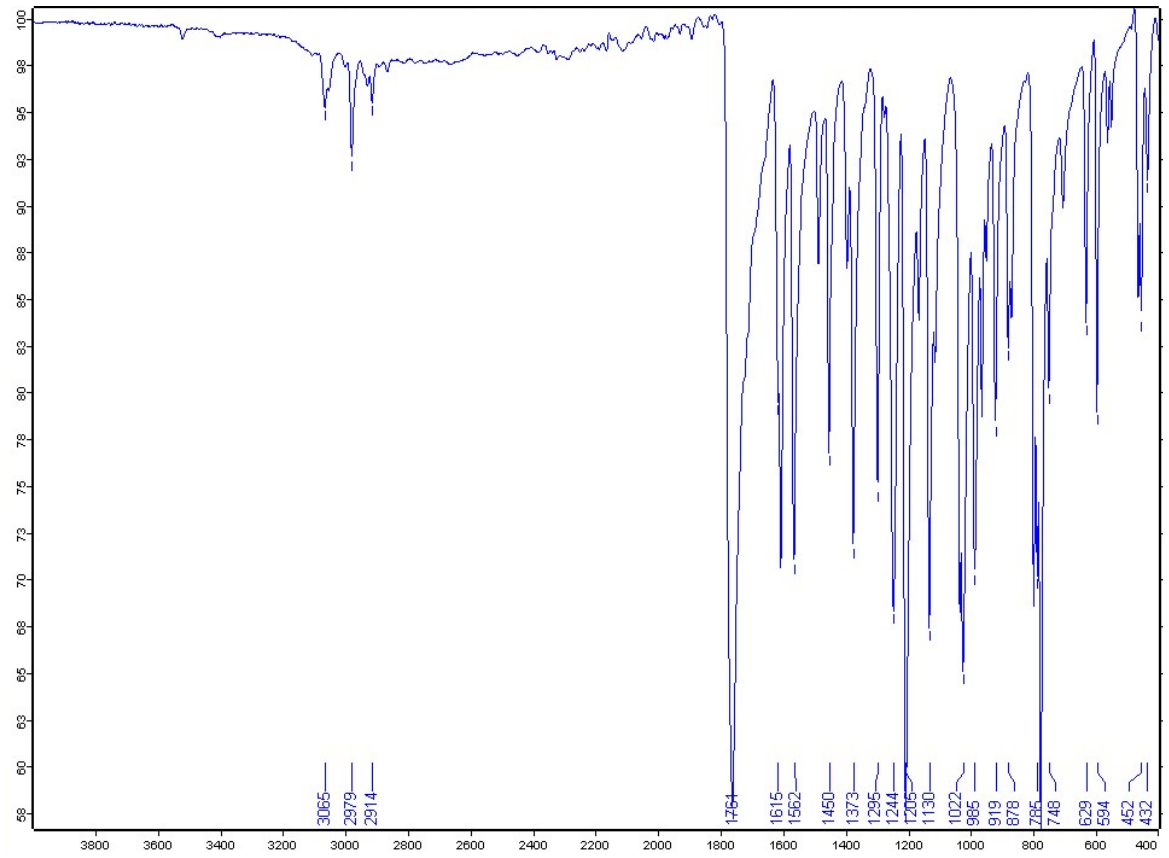

***Figure S 7**: FT-IR spectrum of **S1a**.*

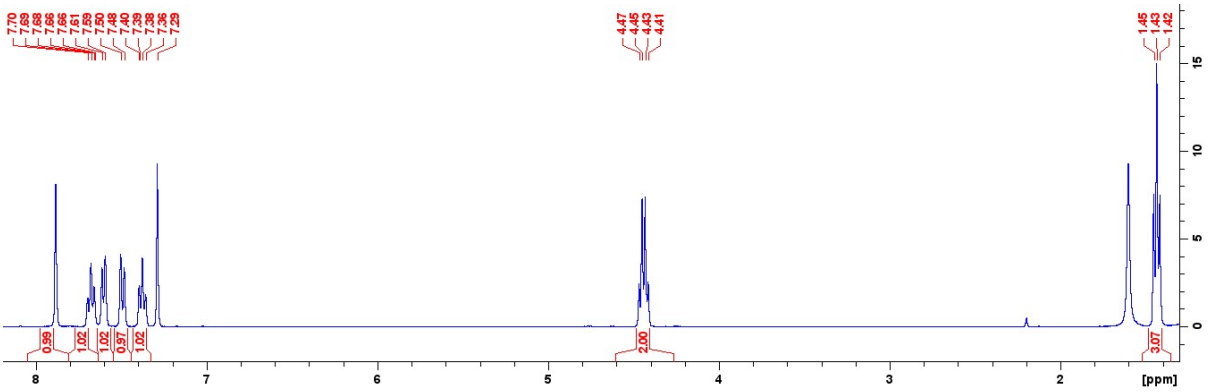

***Figure S 8**: ^{1}H NMR of **S1b**.*

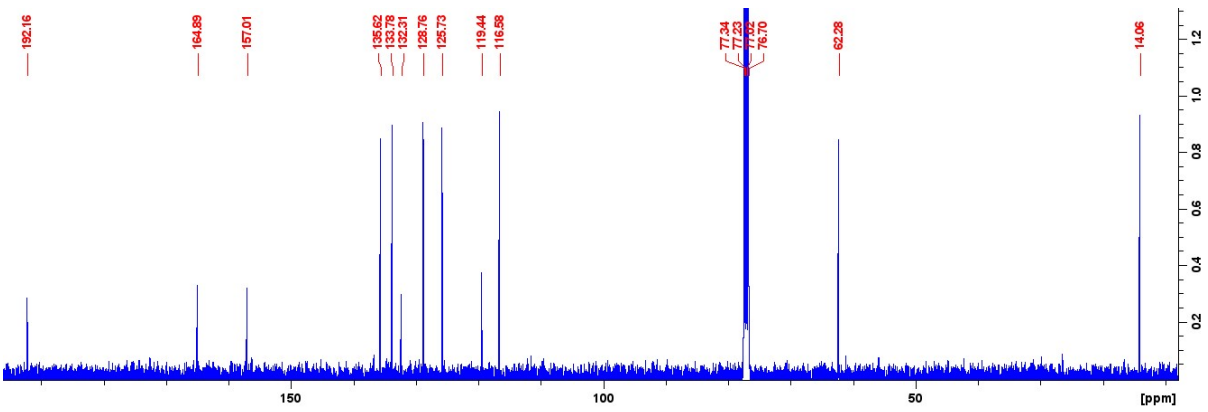

***Figure S 9**: ^{13}C NMR of **S1b**.*

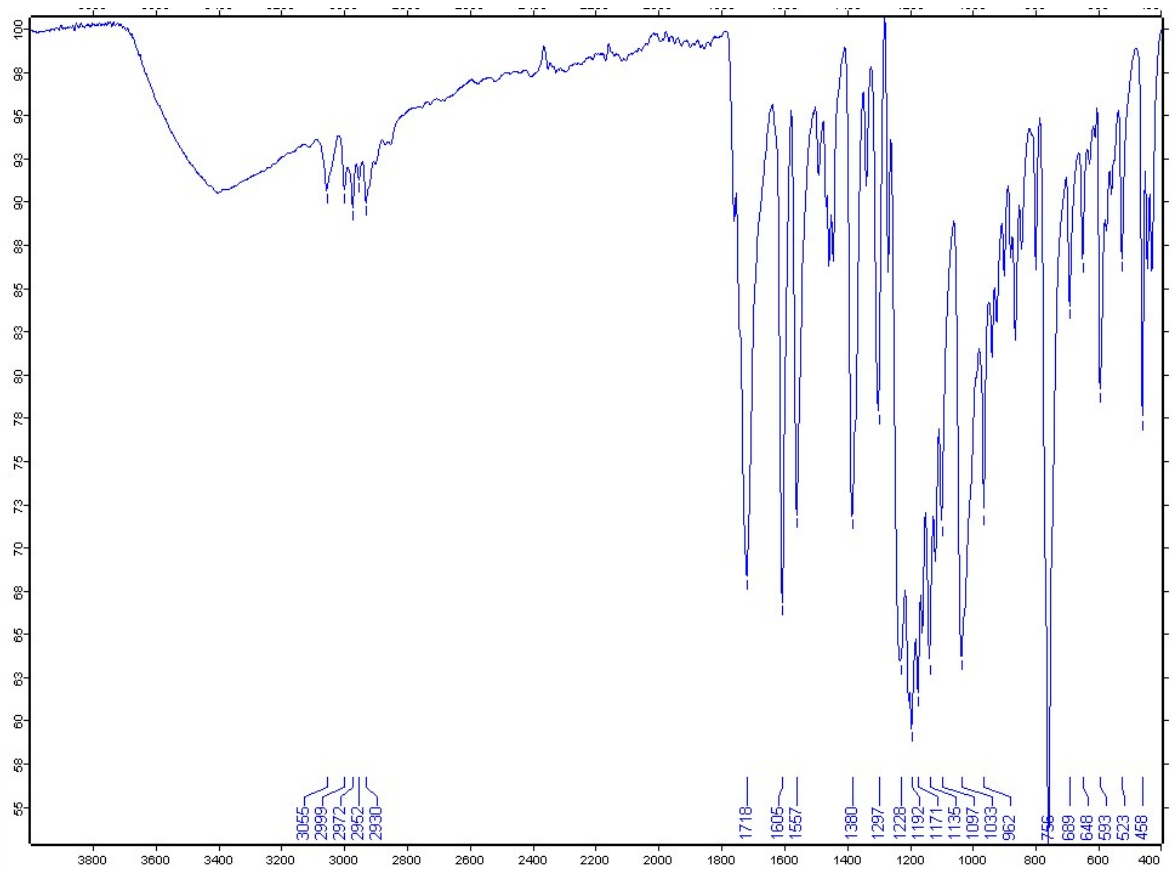

***Figure S 10**: FT-IR spectrum of **S1b**.*

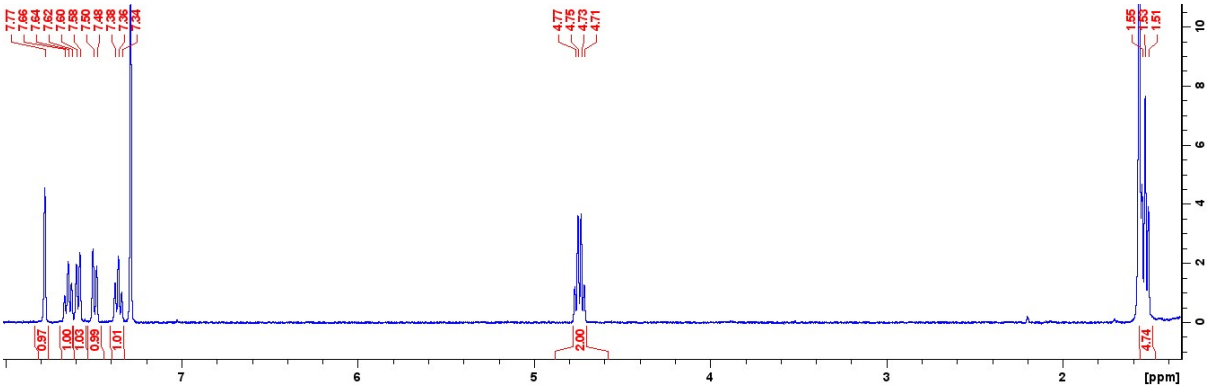

***Figure S 11:** ^{1}H NMR of **S1c**.*

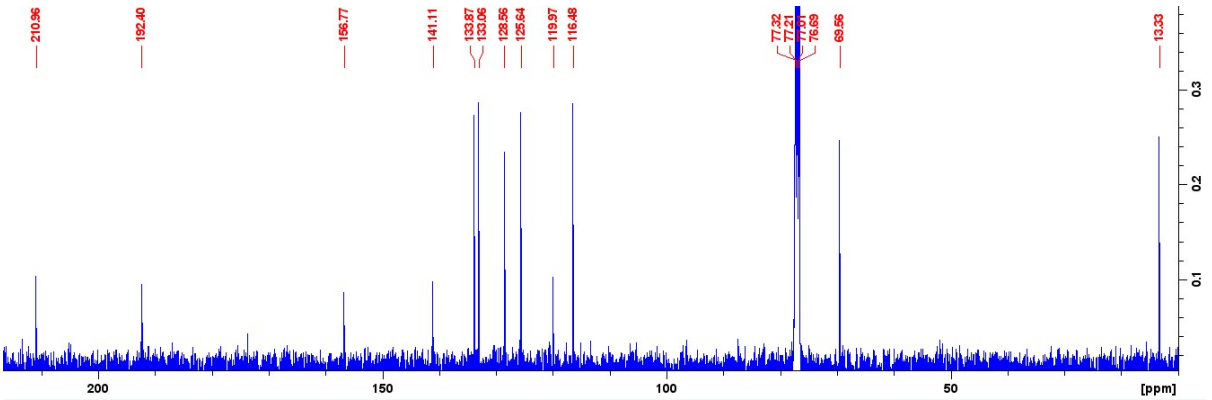

***Figure S 12**: ^{13}C NMR of **S1c**.*

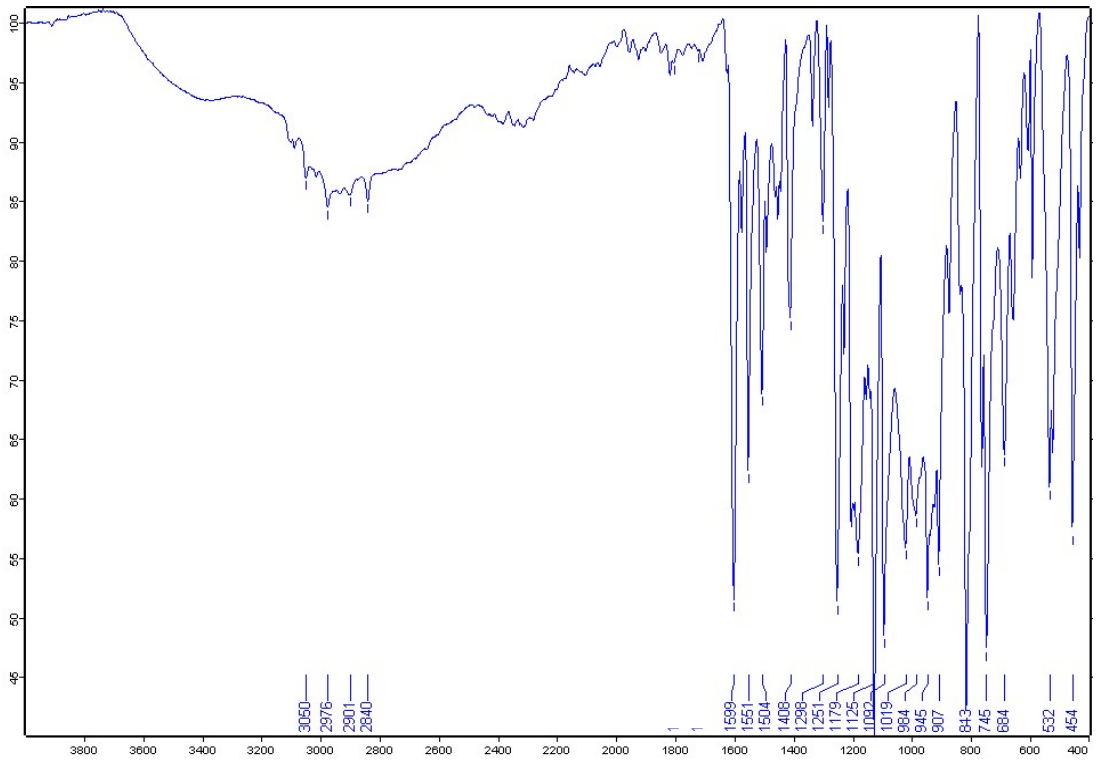

***Figure S 13**: FT-IR spectrum of **S1c**.*

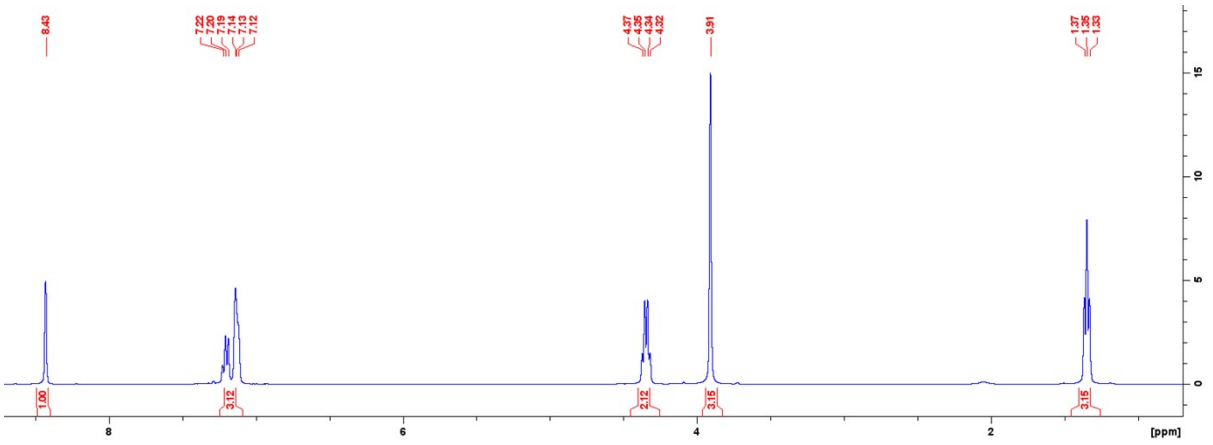

***Figure S 14:** ^{1}H NMR of **S2a**.*

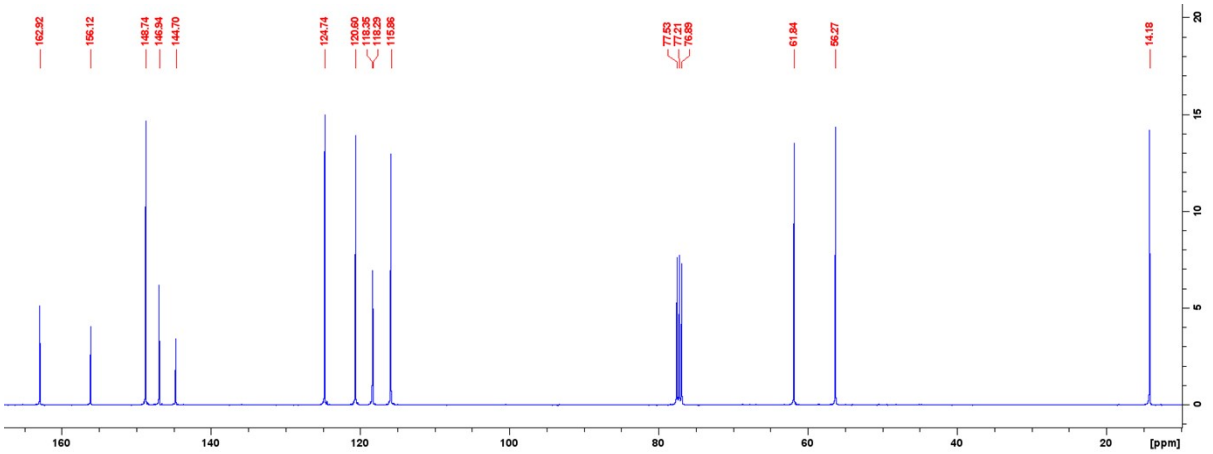

***Figure S 15**: ^{13}C NMR of **S2a**.*

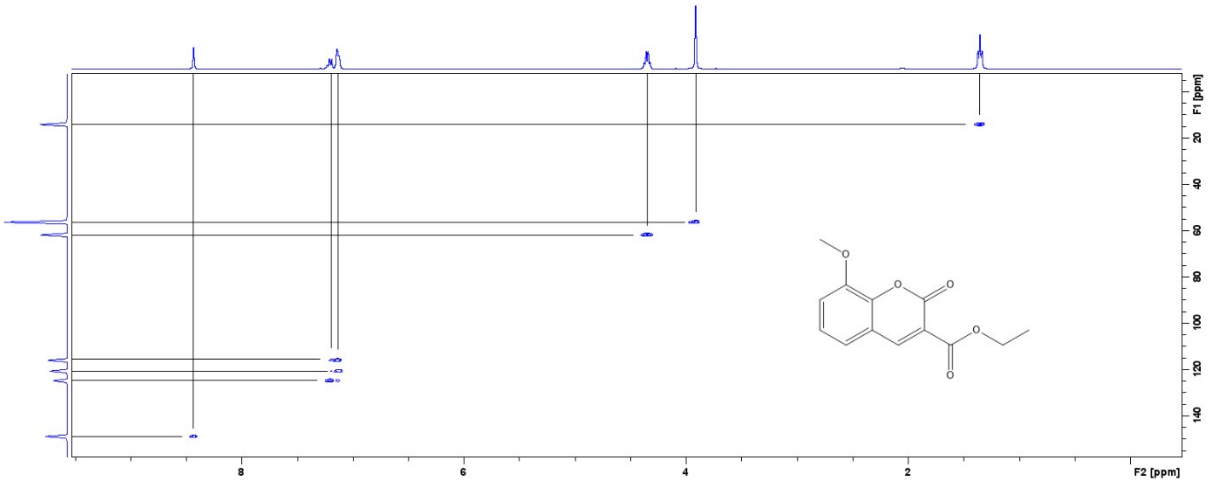

***Figure S 16**: HSQC of **S2a**.*

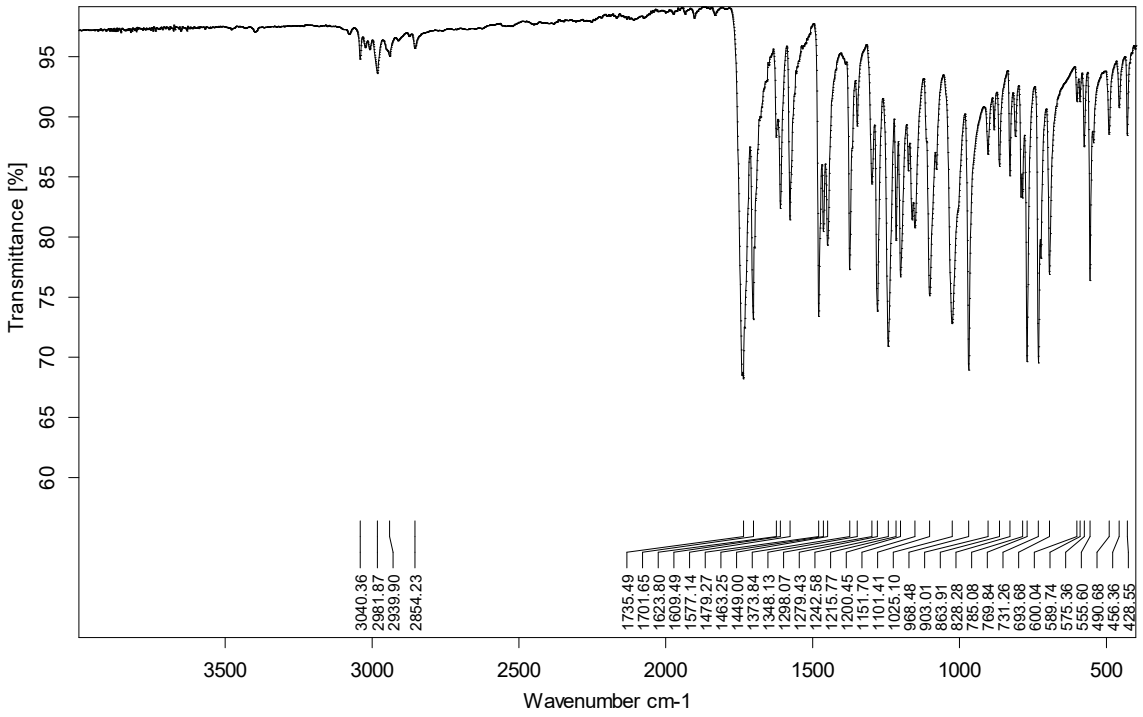

***Figure S 17**: FT-IR spectrum of **S2a**.*

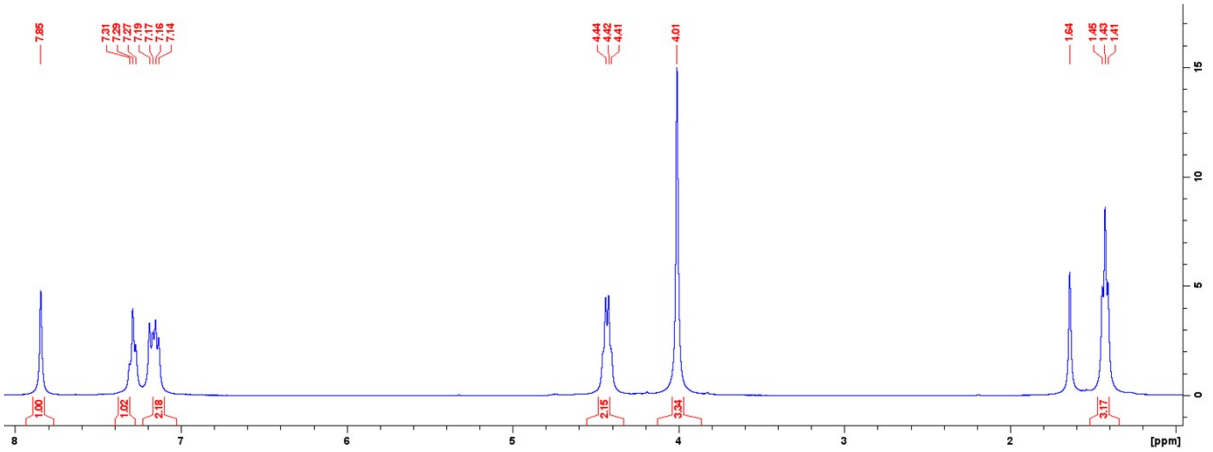

***Figure S 18**: ^{1}H NMR of **S2b**.*

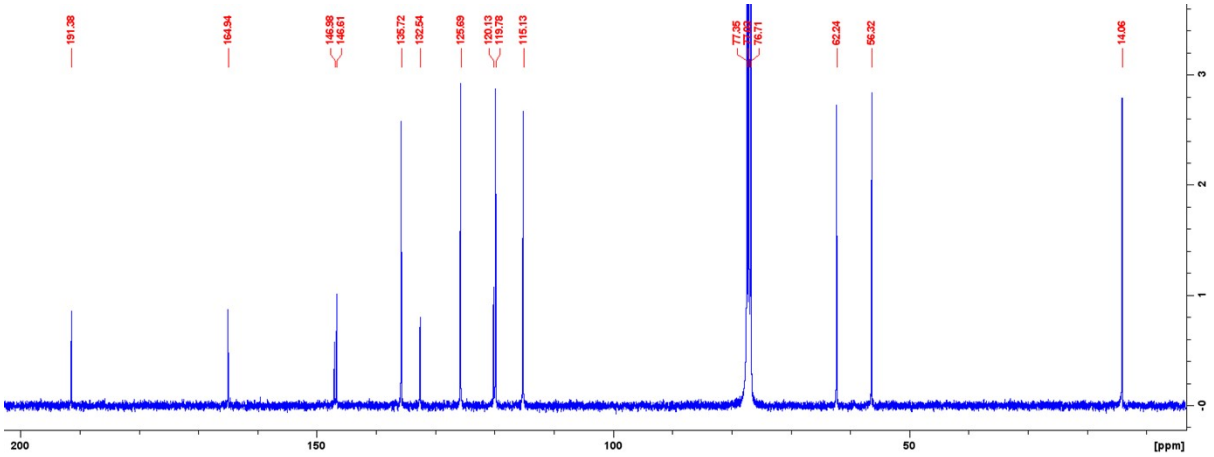

***Figure S 19**: ^{13}C NMR of **S2b**.*

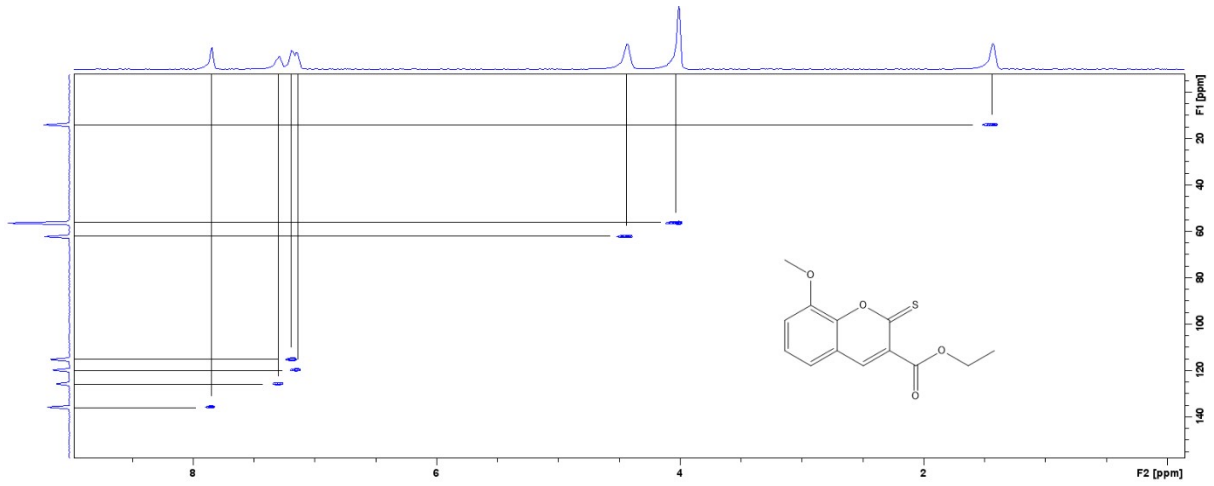

***Figure S 20**: HSQC of **S2b**.*

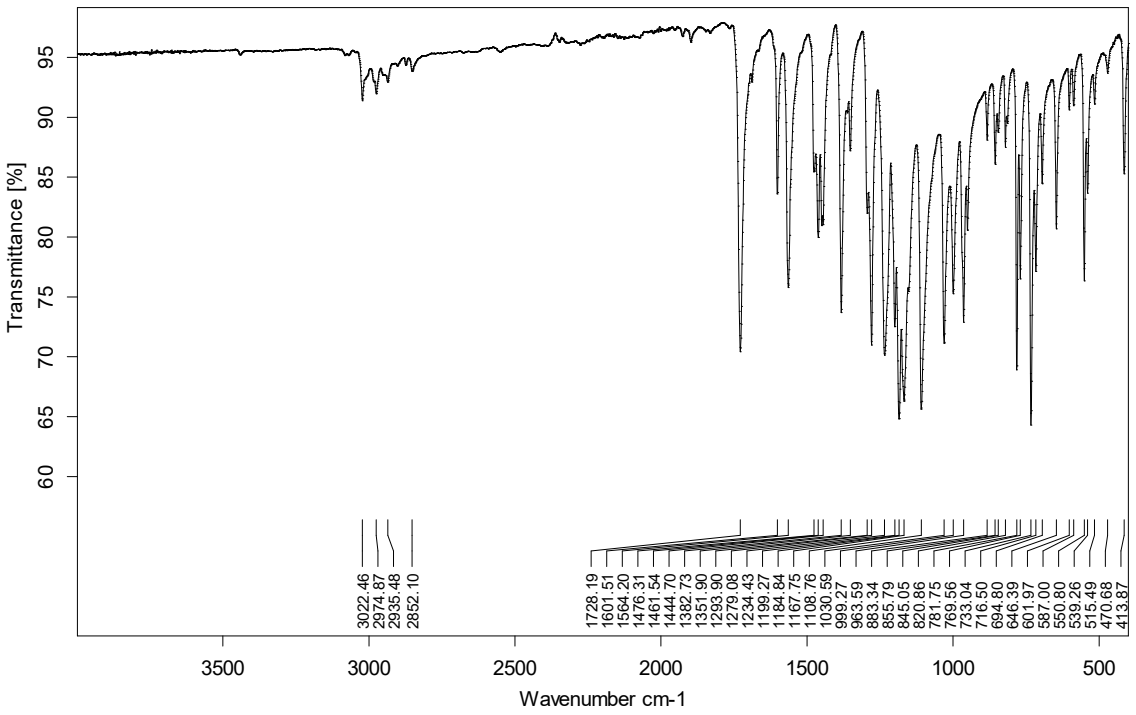

***Figure S 21**: FT-IR spectrum of **S2b**.*

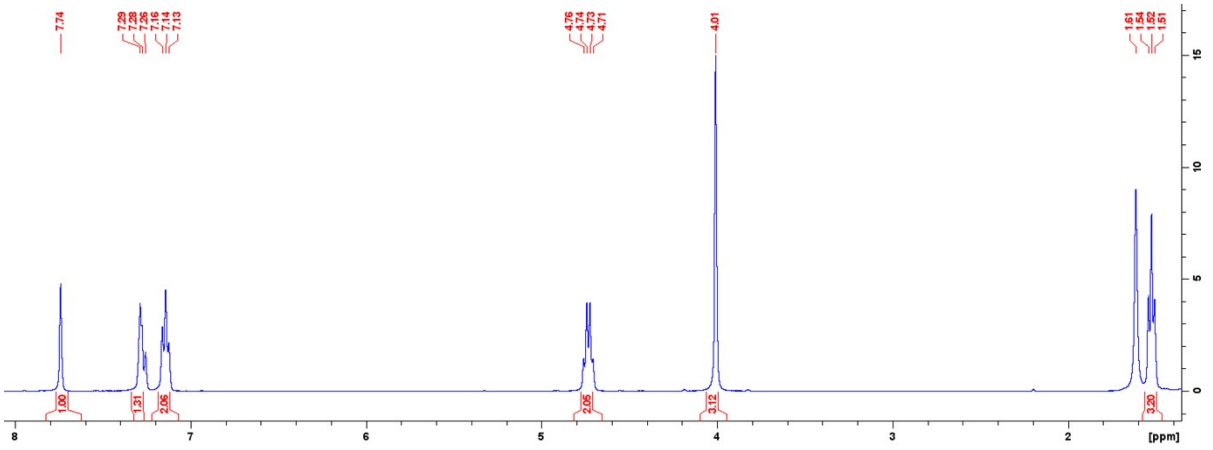

***Figure S 22**: [1]H NMR of **S2c**.*

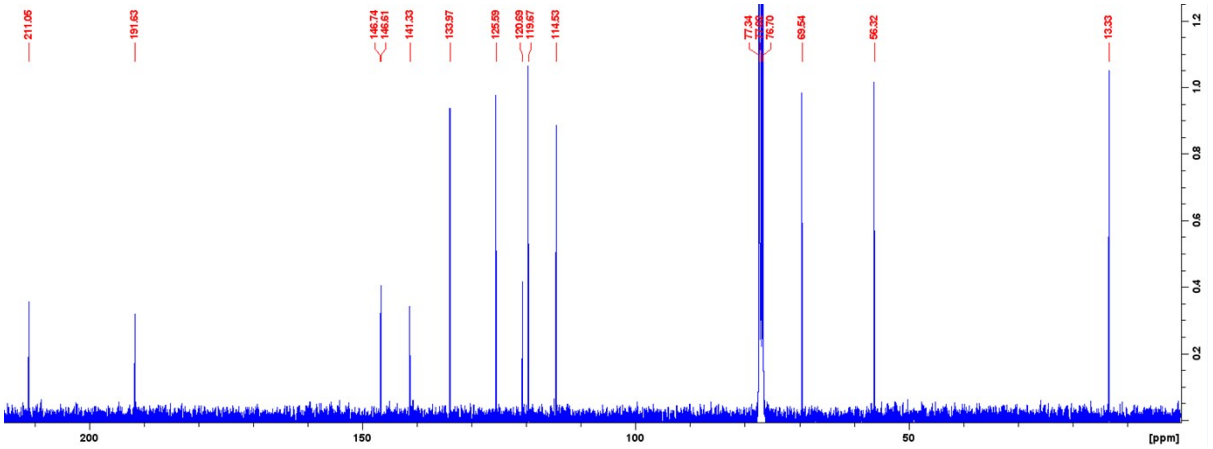

***Figure S 23**: [13]C NMR of **S2c**.*

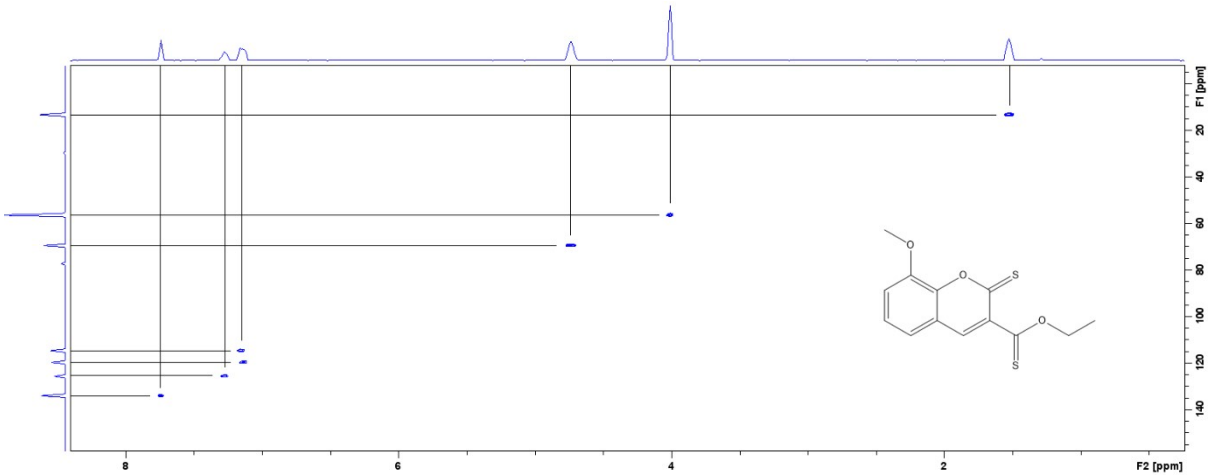

***Figure S 24**: HSQC of **S2c**.*

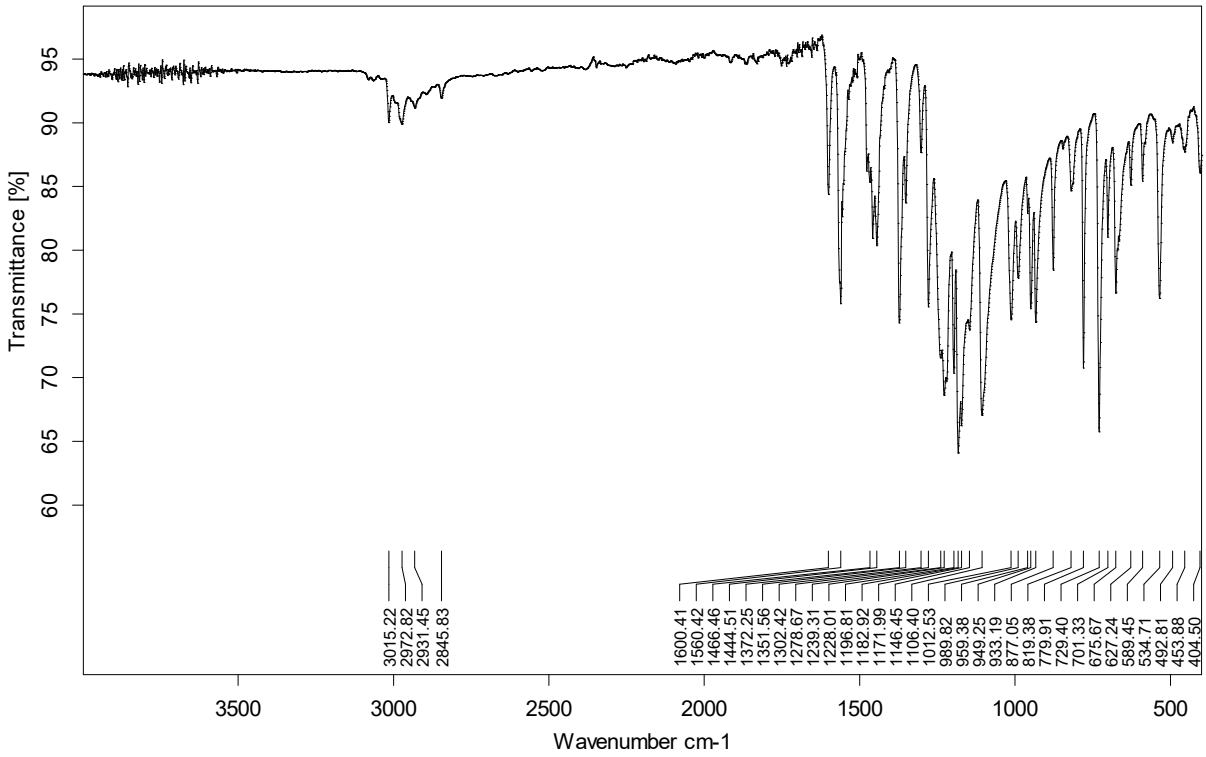

***Figure S 25**: FT-IR spectrum of **S2c**.*

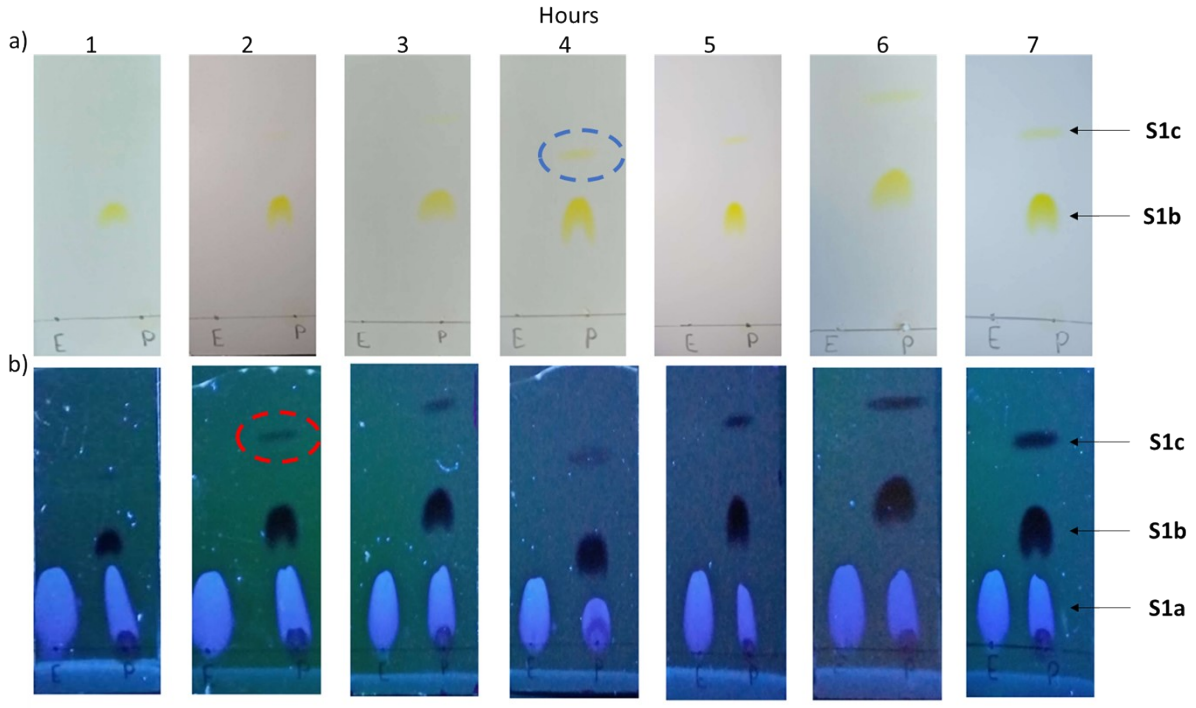

***Figure S 26**: TLC plates during the reaction forming **S1b** and **S1c** under a) ambient light and b) UV light.*

***Table S 1**: Selected ^{13}C NMR peaks (in ppm) of all synthesised compounds.*

	Lactone Carbonyl (▲) (ppm)	*Ester Carbonyl (●) (ppm)*	*Ethyl Carbon (★) (ppm)*
S1a	155.21	163.10	62.00
S2a	156.12	162.92	61.84
S1b	192.16	164.89	62.28
S2b	191.83	164.94	62.24
S1c	192.40	210.96	69.54
S2c	191.63	211.05	69.54

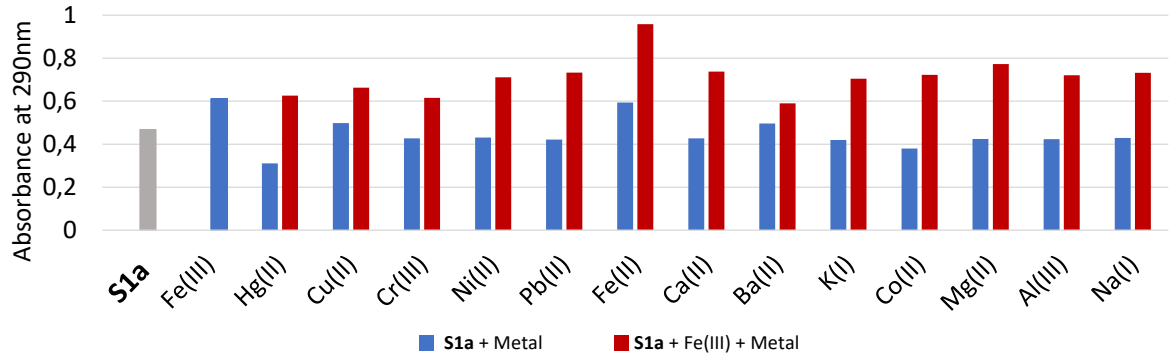

***Figure S 27**: Selectivity studies of **S1a** towards Fe^{3+}.*

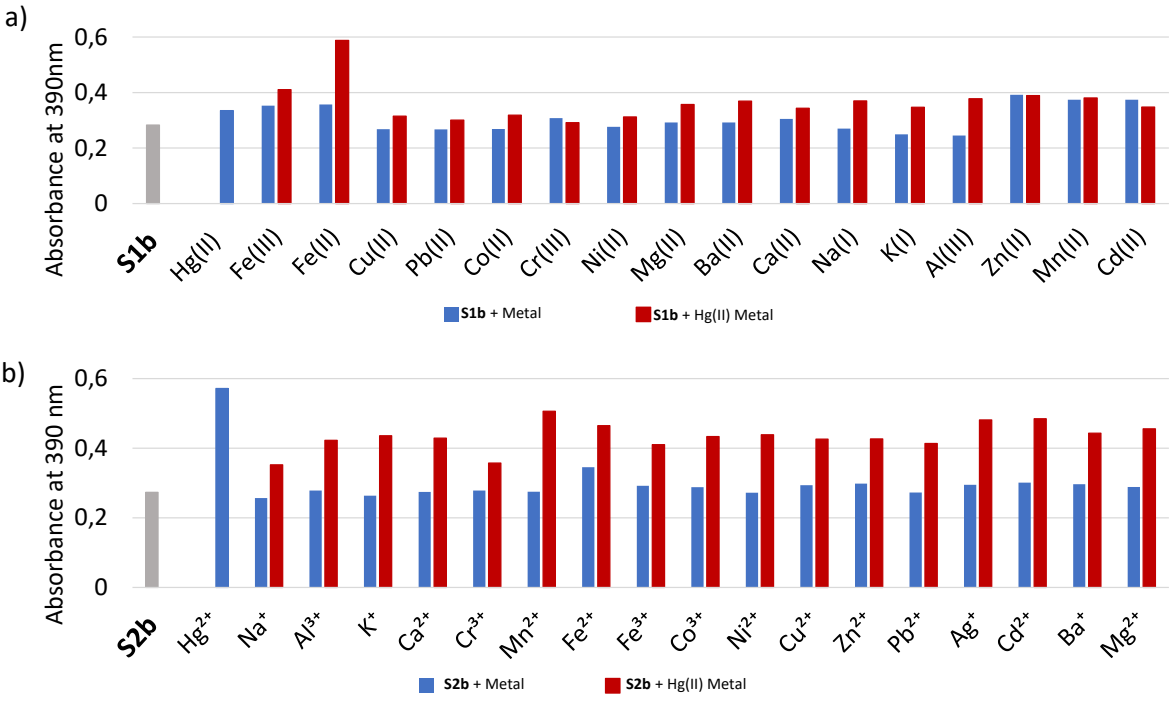

***Figure S 28**: Selectivity studies of a) **S1b** and b) **S2b** towards Hg^{2+}.*

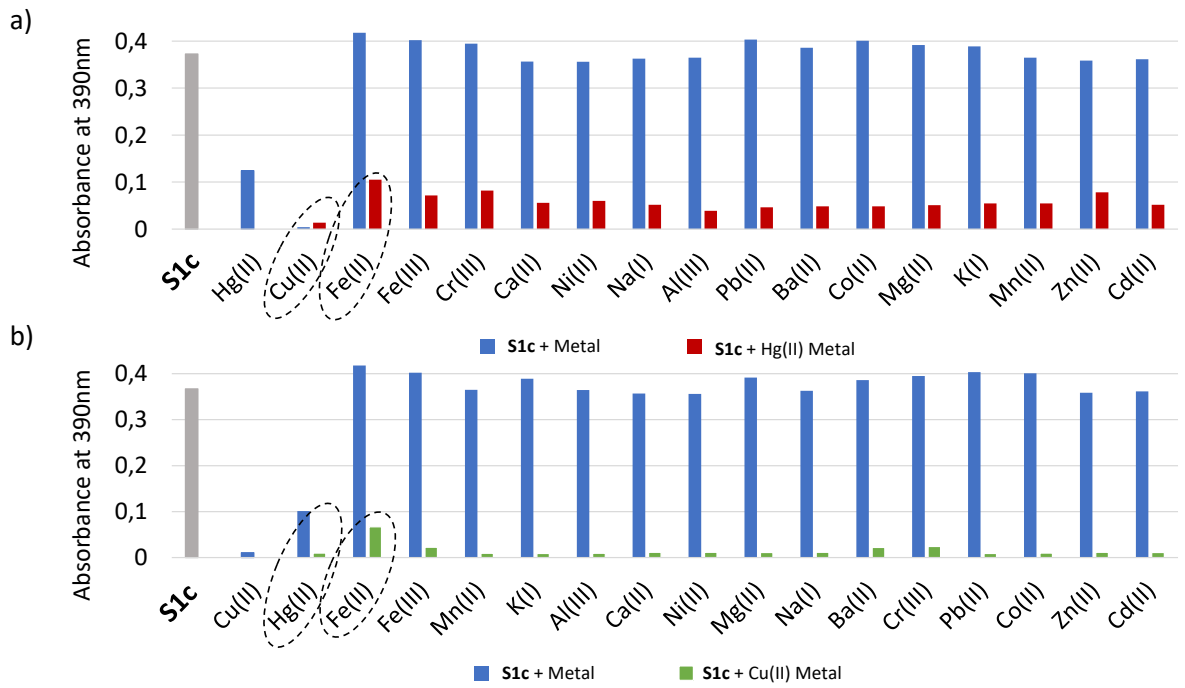

***Figure S 29**: Selectivity studies of **S1c** towards a) Hg^{2+} and b) Cu^{2+}.*

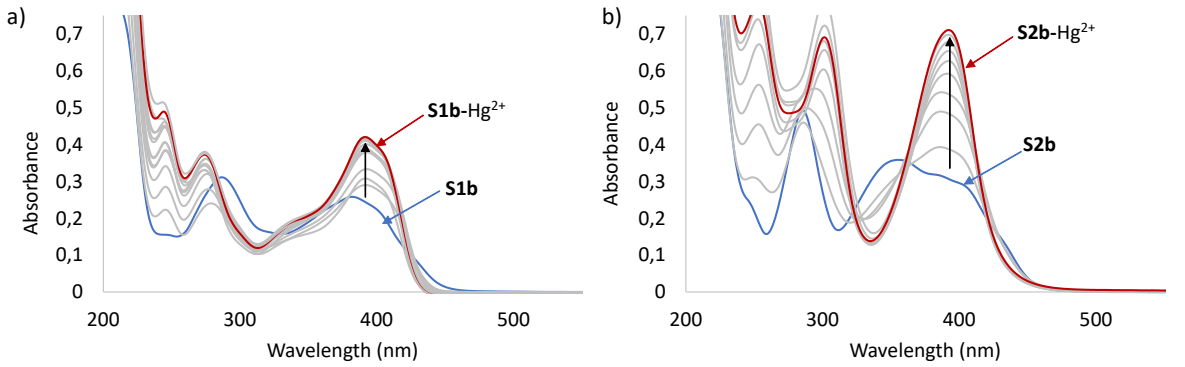

***Figure S 30**: Titration studies of a) **S1b** and b) **S2b** with increasing amounts of Hg^{2+}.*

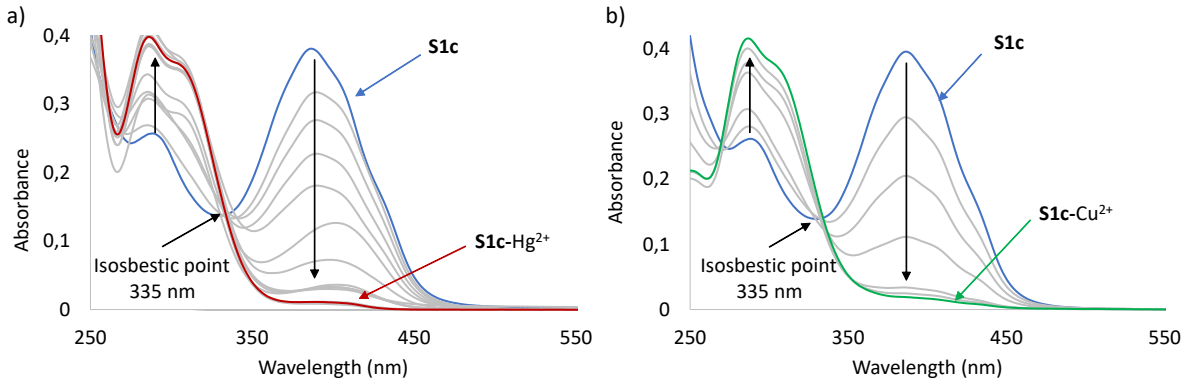

***Figure S 31**: Titration studies of **S1c** with increasing amounts of a) Hg^{2+} and b) Cu^{2+}.*

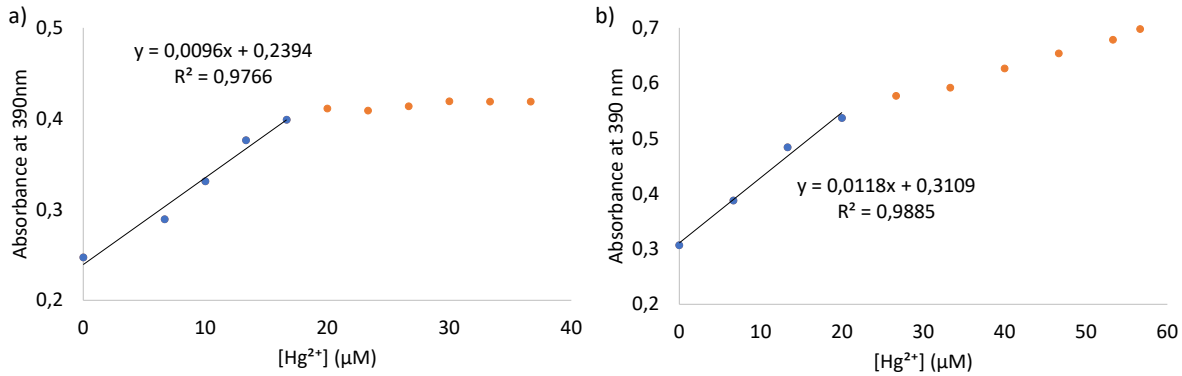

***Figure S 32**: Calibration curve for a) **S1b** and b) **S2b** in the presence of Hg^{2+}.*

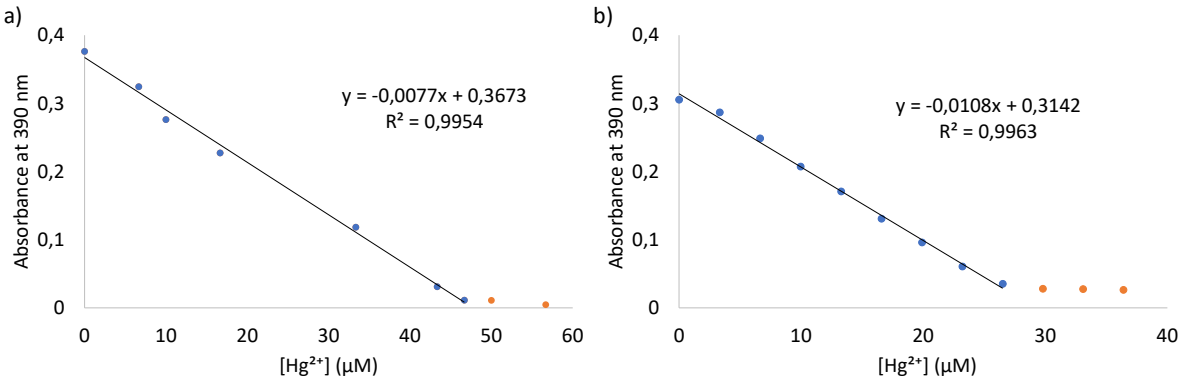

***Figure S 33**: Calibration curve for a) **S1c** and b) **S2c** with increasing amounts of Hg^{2+}.*

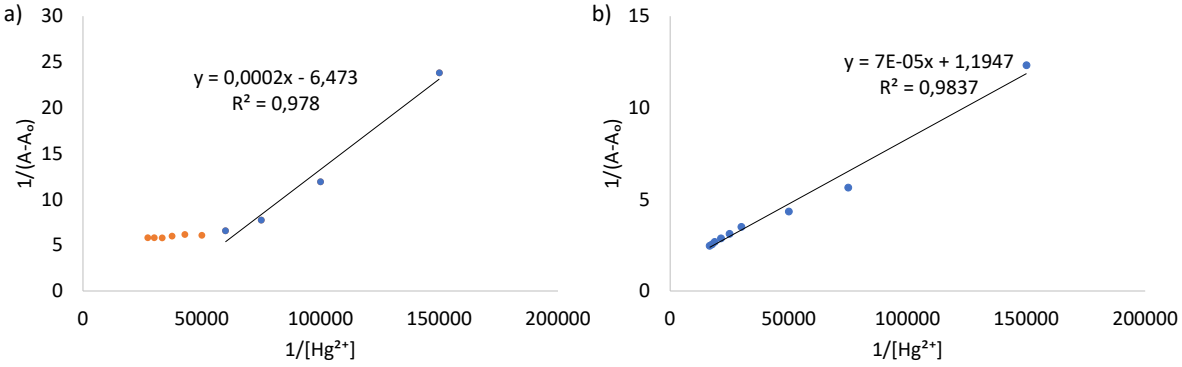

***Figure S 34**: The Benesi Hildebrand plot for a) **S1b** and b) **S2b** in the presence of Hg^{2+}.*

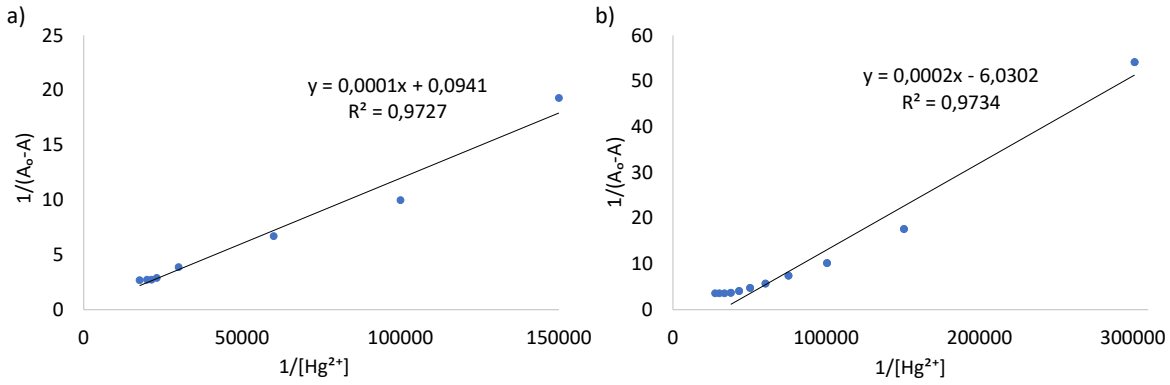

***Figure S 35**: The Benesi Hildebrand plot for a) **S1c** and b) **S2c** in the presence of Hg^{2+}.*

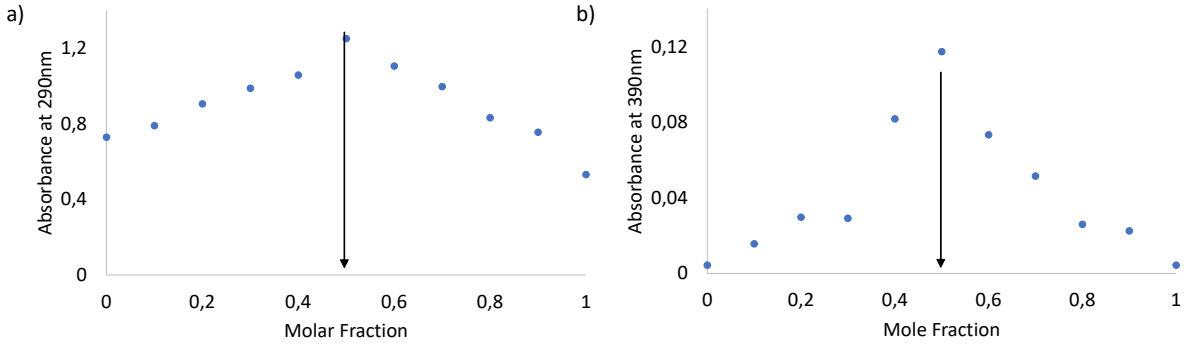

***Figure S 36**: Jobs plots of a) **S1a** and b) **S1c** with various mole fractions of Hg^{2+}.*

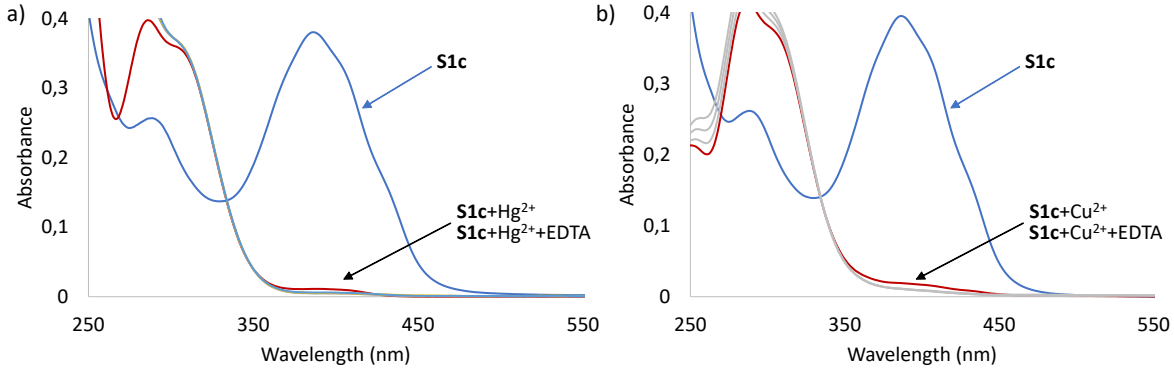

***Figure S 37**: Reversibility studies of **S1c** with a) Hg^{2+} and b) Cu^{2+} in the presence of EDTA.*