

“Synthesis of benzylidene amino arylpyridinones and their AIE Studies: Dual metal sensing of Fe³⁺ and Hg²⁺”

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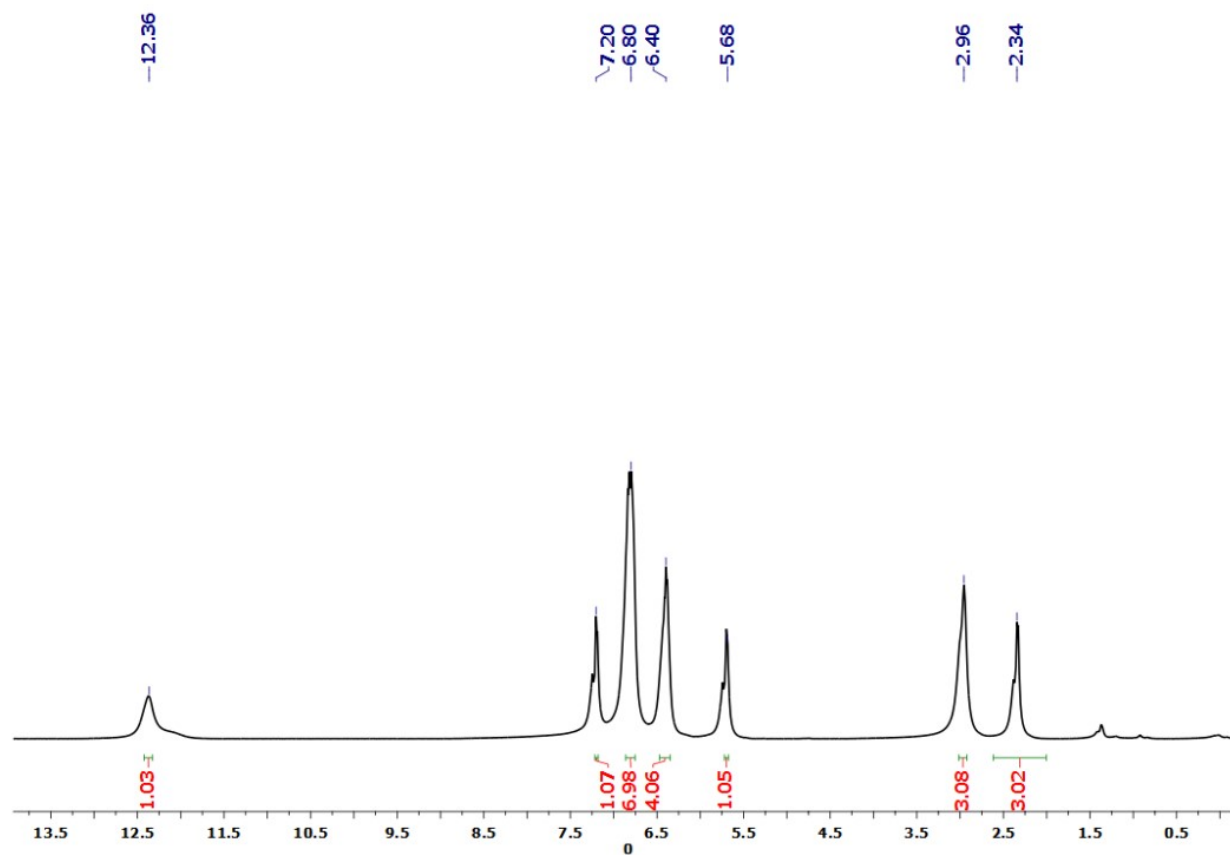


Figure S.1: ¹H NMR Spectrum of 4a

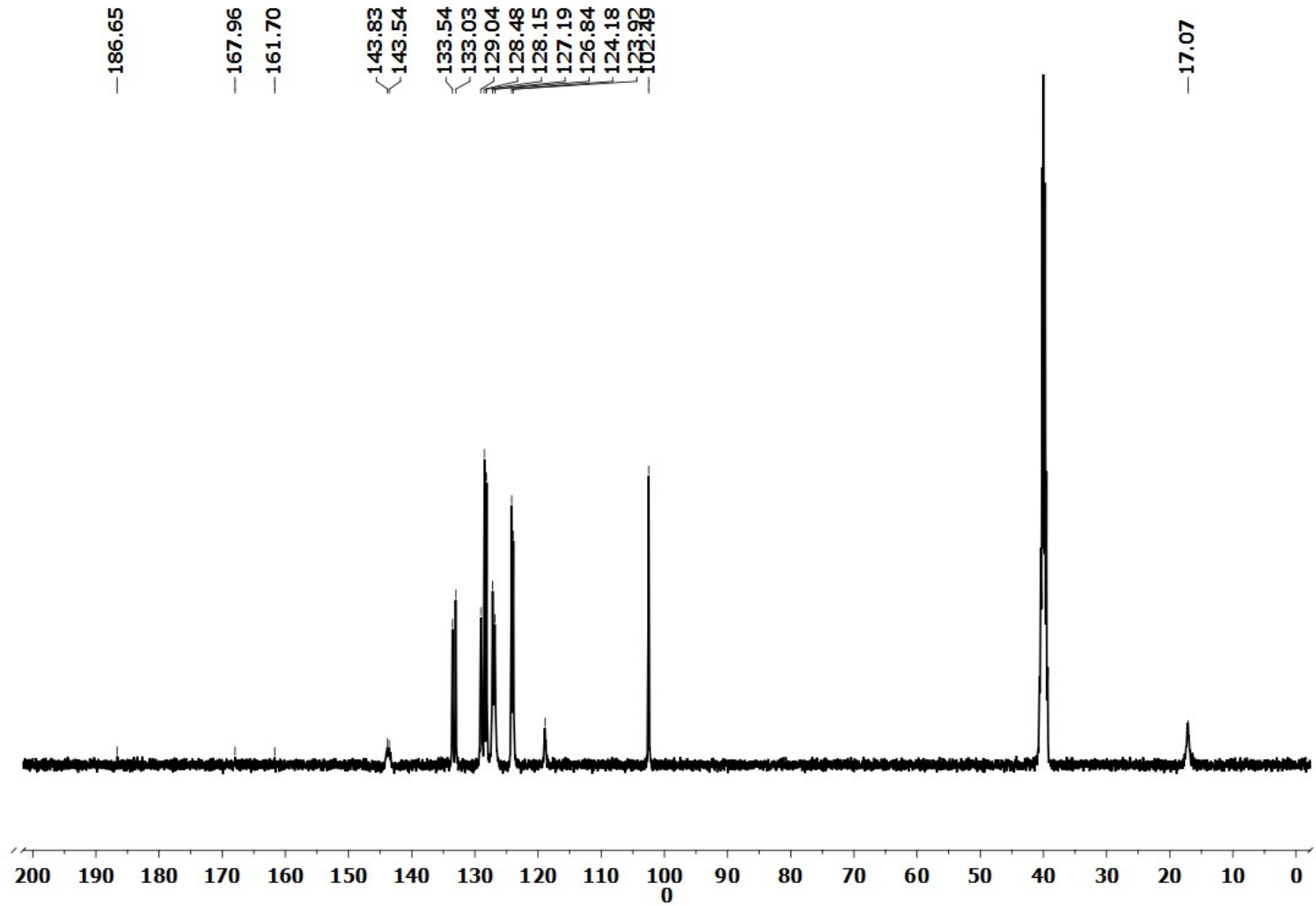


Figure S.2: ^{13}C NMR Spectrum of 4a

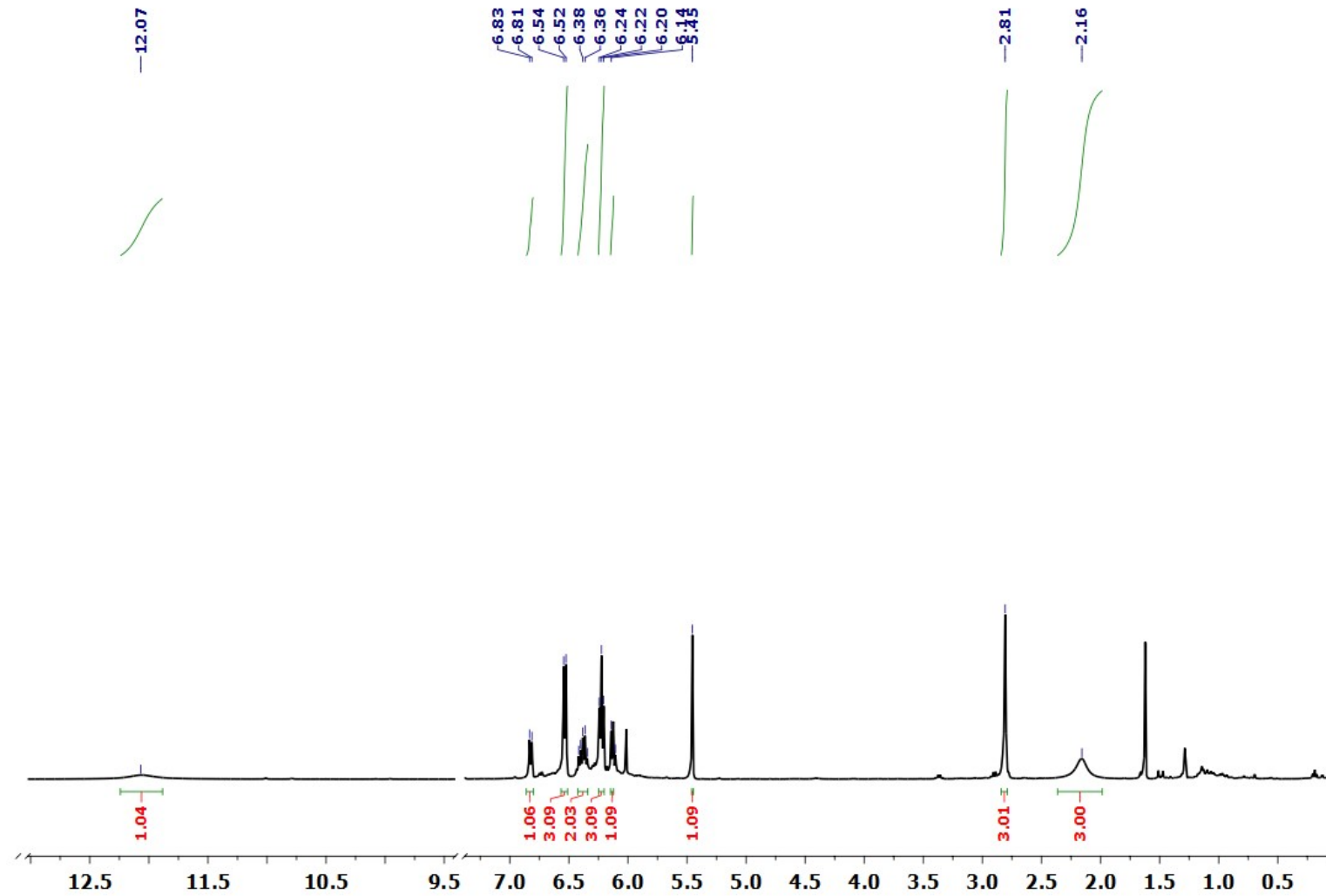


Figure S.3: ¹H NMR Spectrum of 4b

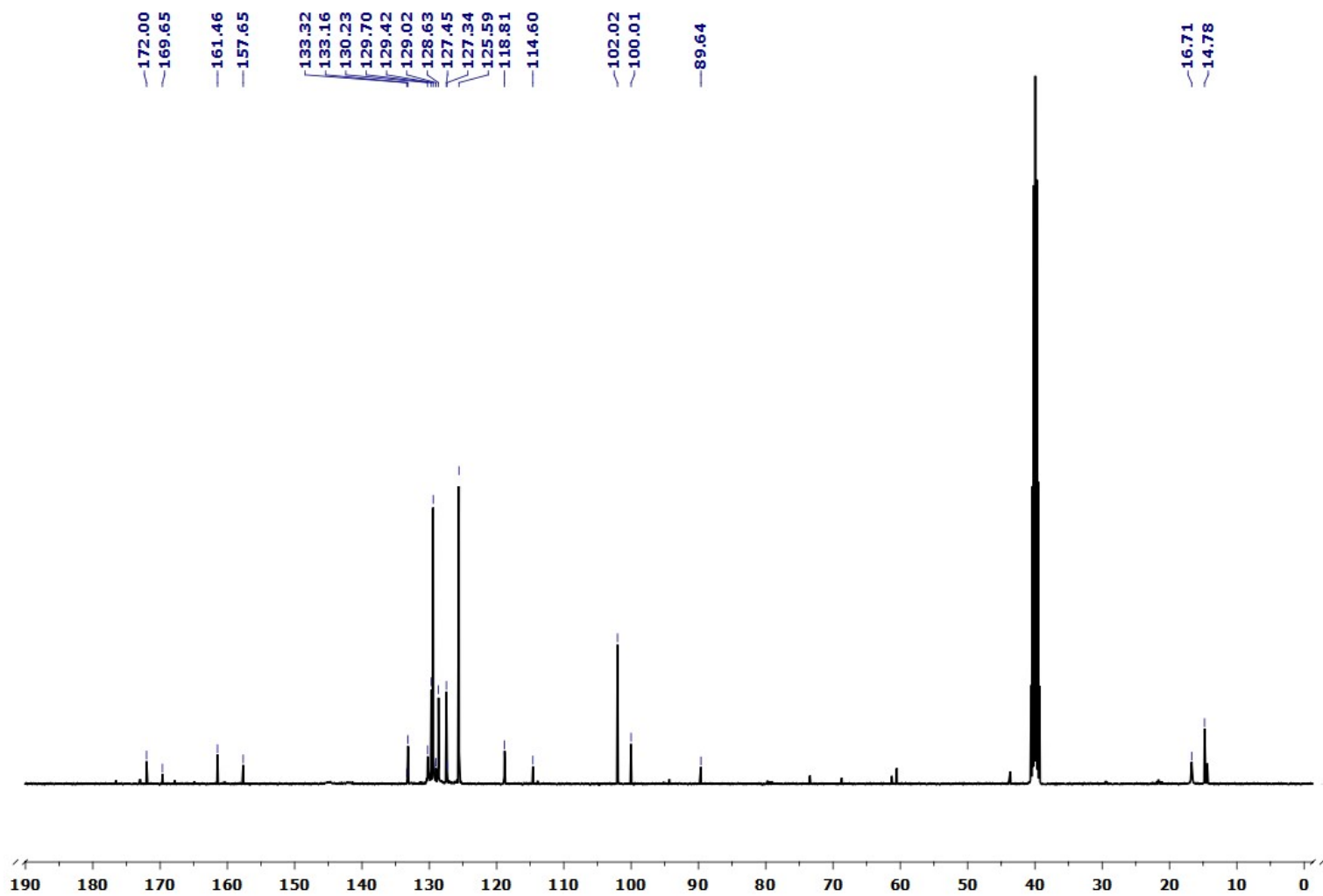


Figure S.4: ^{13}C NMR Spectrum of 4b

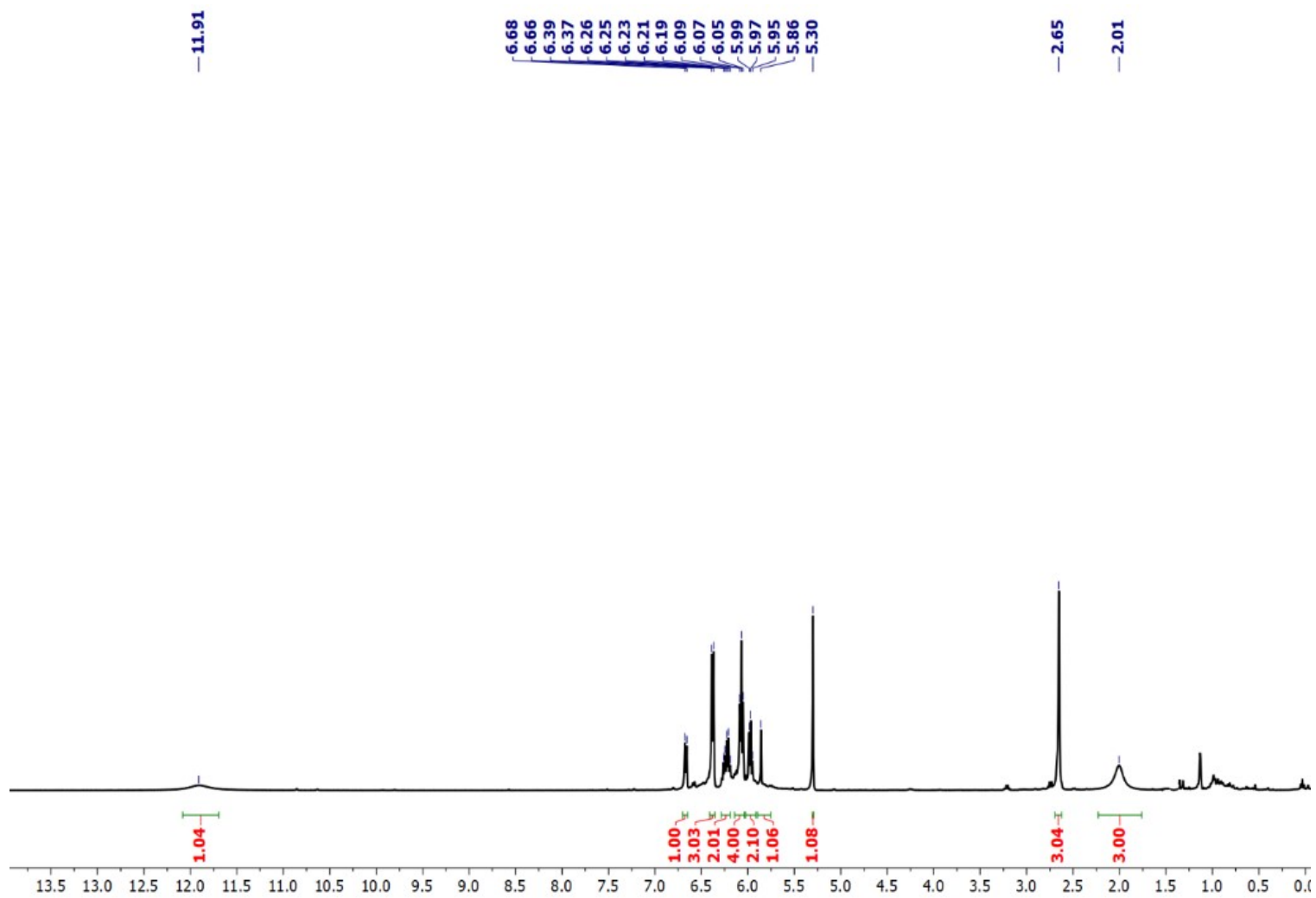


Figure S.5: ¹H NMR Spectrum of 4c

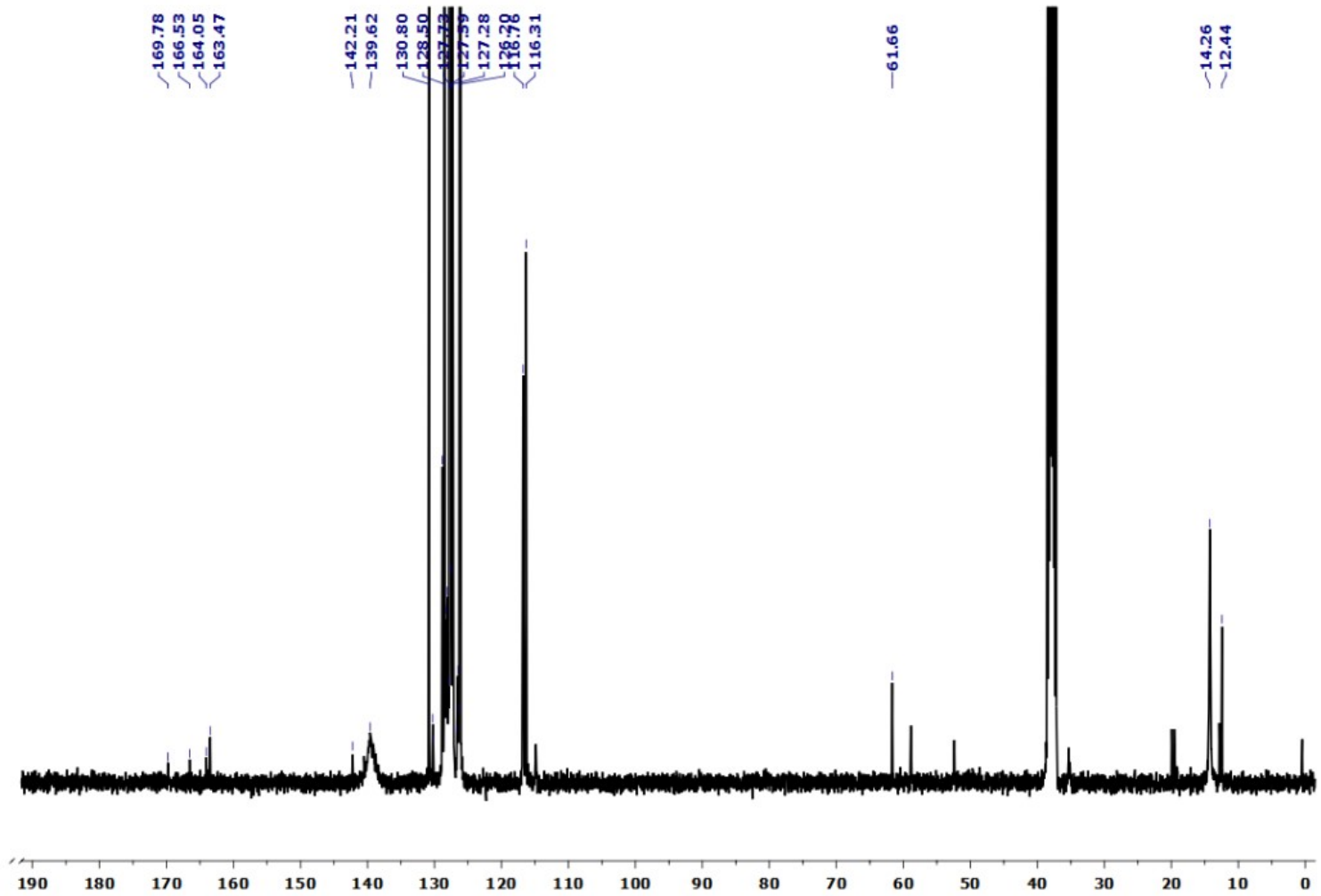


Figure S.6: ^{13}C NMR Spectrum of 4c

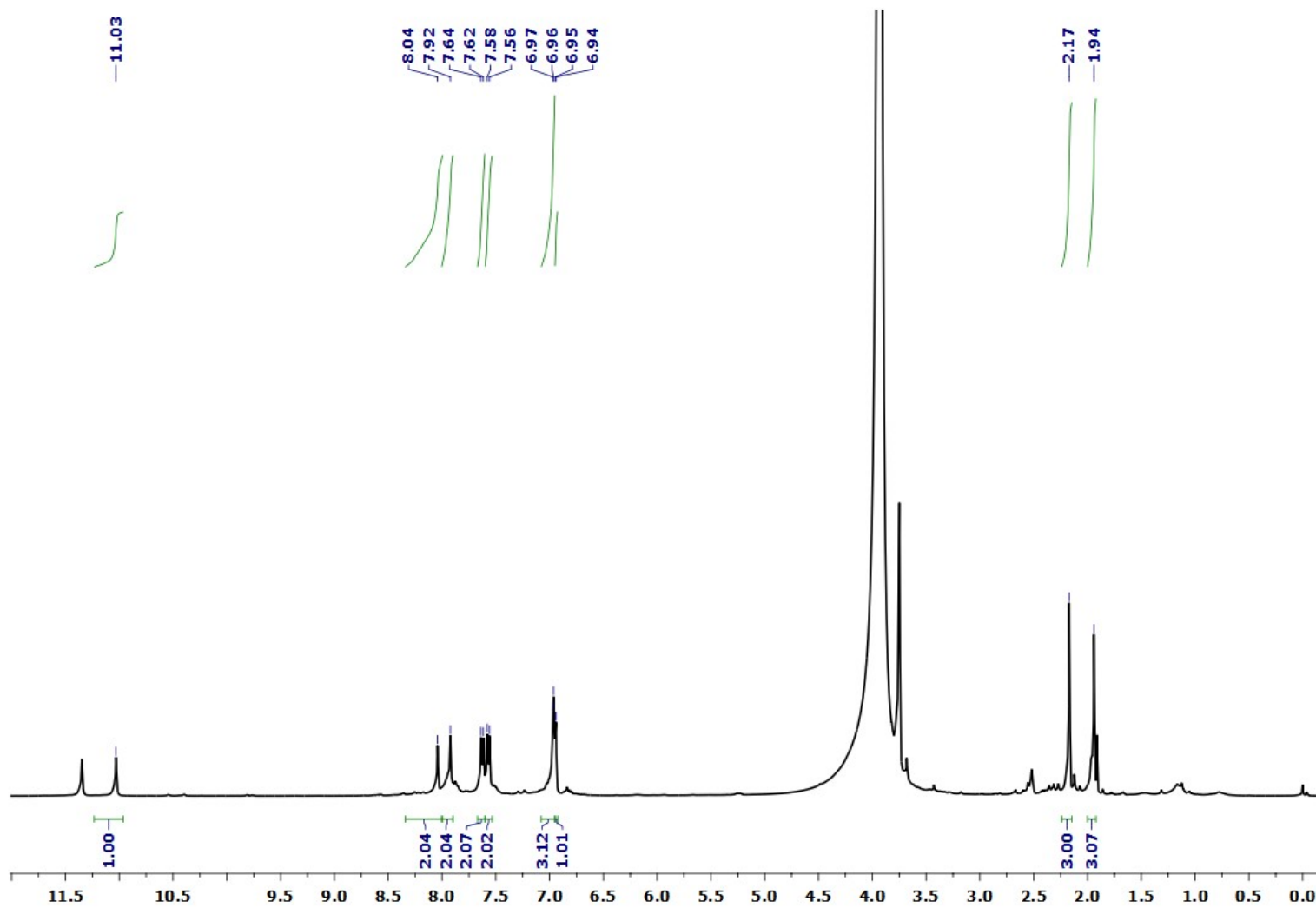


Figure S.7: ^1H NMR Spectrum of 4d

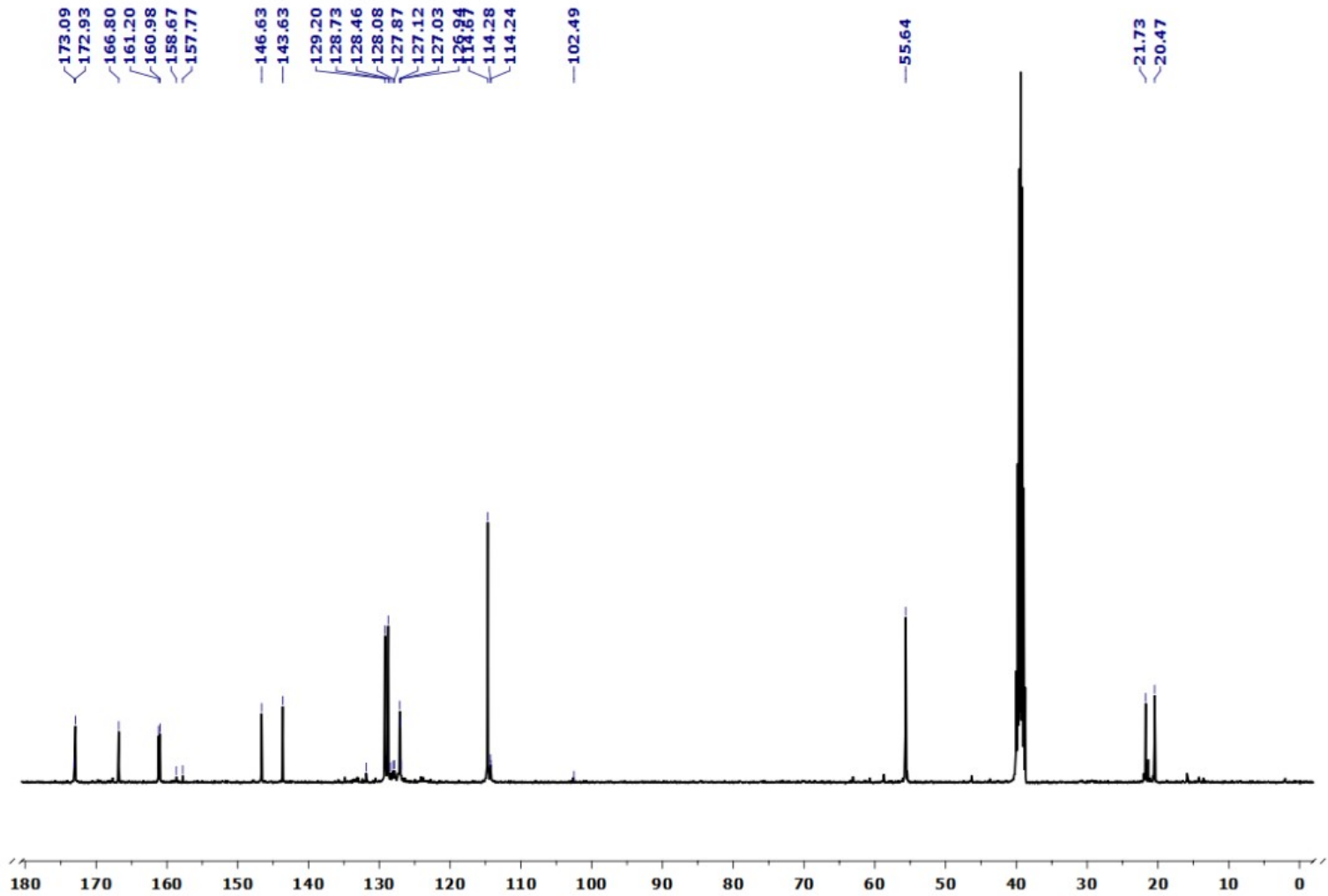


Figure S.8: ^{13}C NMR Spectrum of 4d

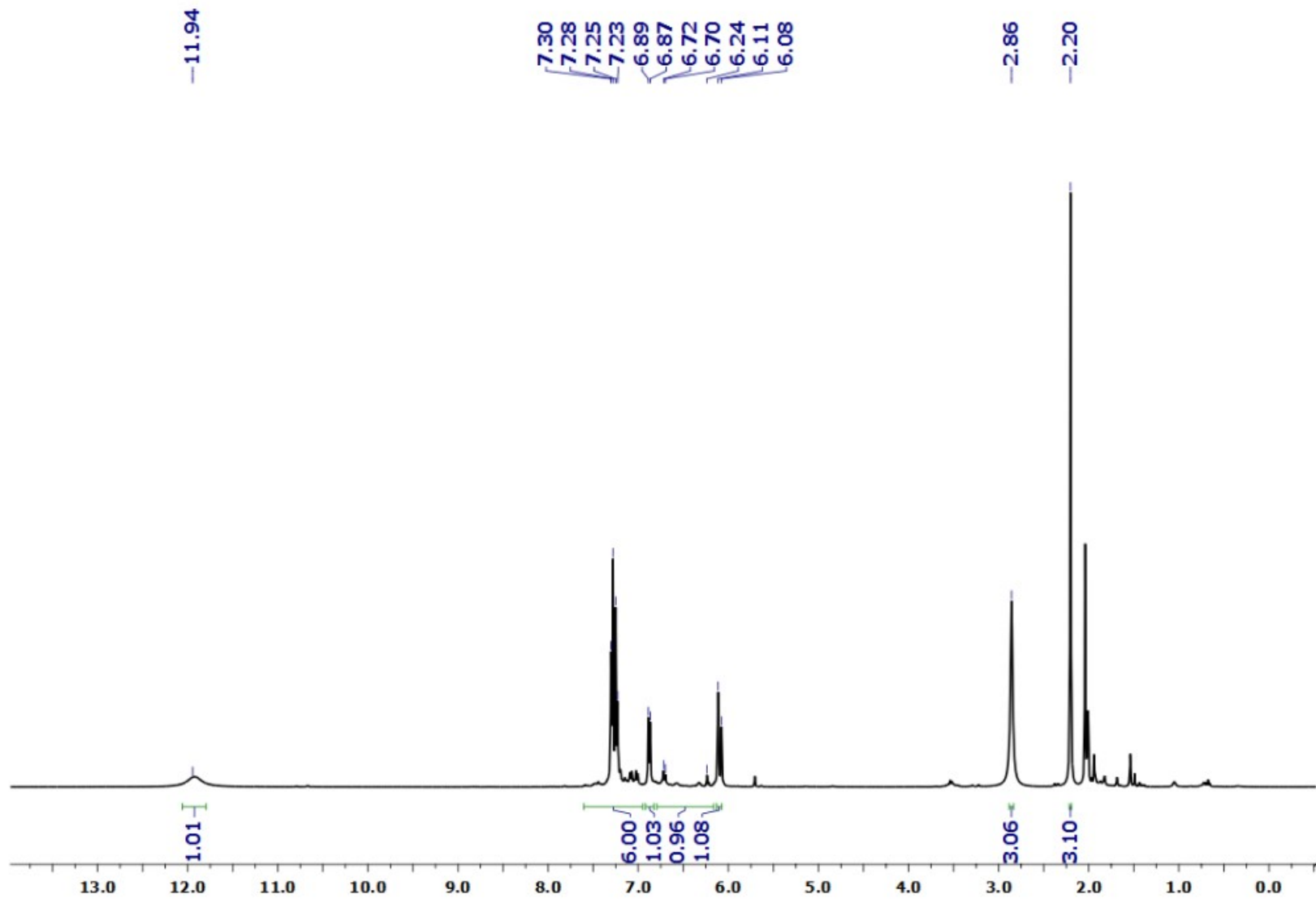


Figure S.9: ^1H NMR Spectrum of **4e**

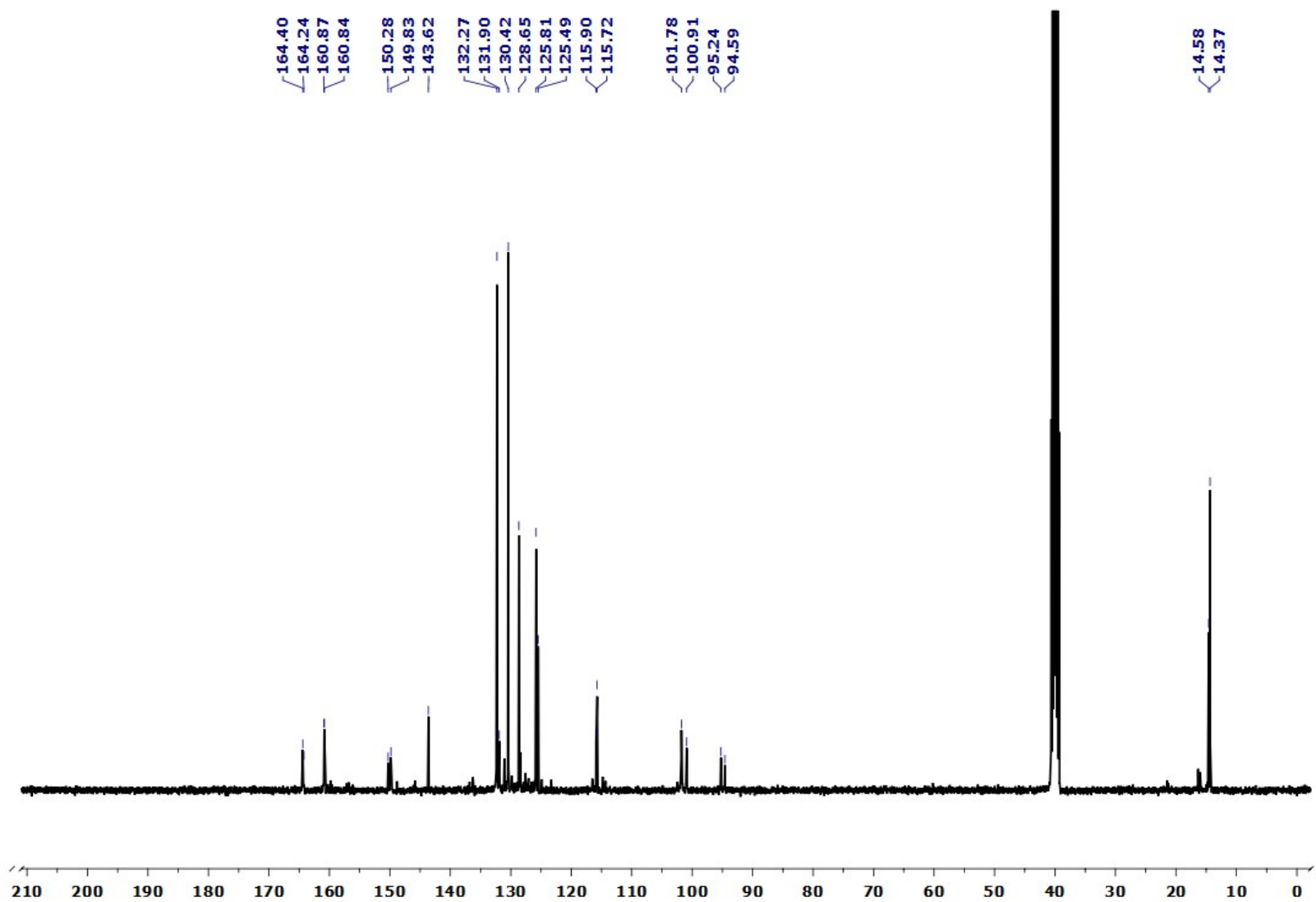


Figure S.10: ^{13}C NMR Spectrum of 4e

TB

IISER BERHAMPUR
CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

23-Aug-2024 16:50:49

TB-SM-GP-03 New 16 (0.310) AM2 (Ar,22000.0,556.28,0.00,LS 10)

1: TOF MS ES+
3.64e6

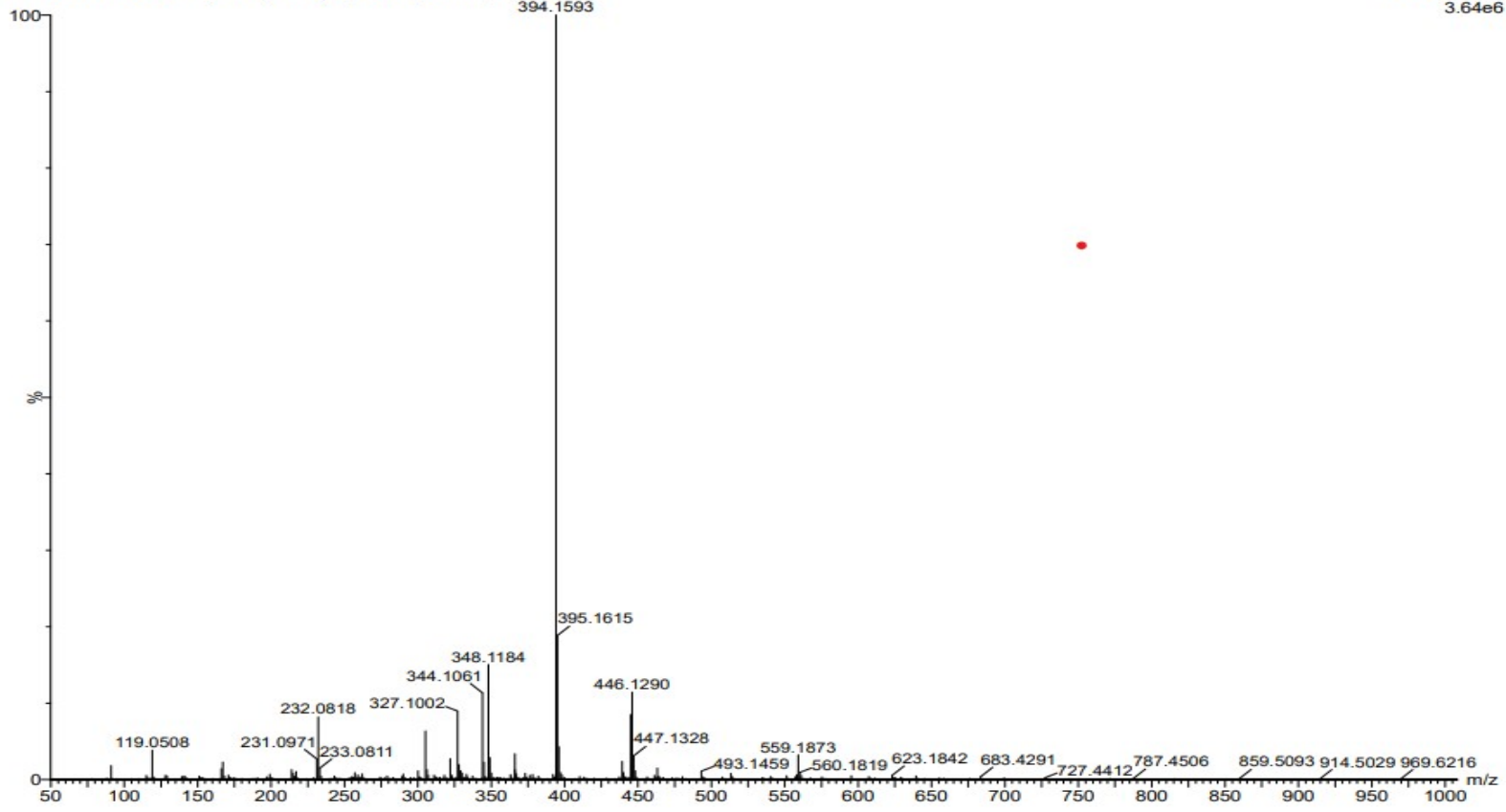


Figure S.11: HRMS-Spectrum of 4a

BBC-46
23022023_31 56 (0.537) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (56-408:420)

IISc Organic Chemistry

23-Feb-2023
1: TOF MS ES+
2.24e4

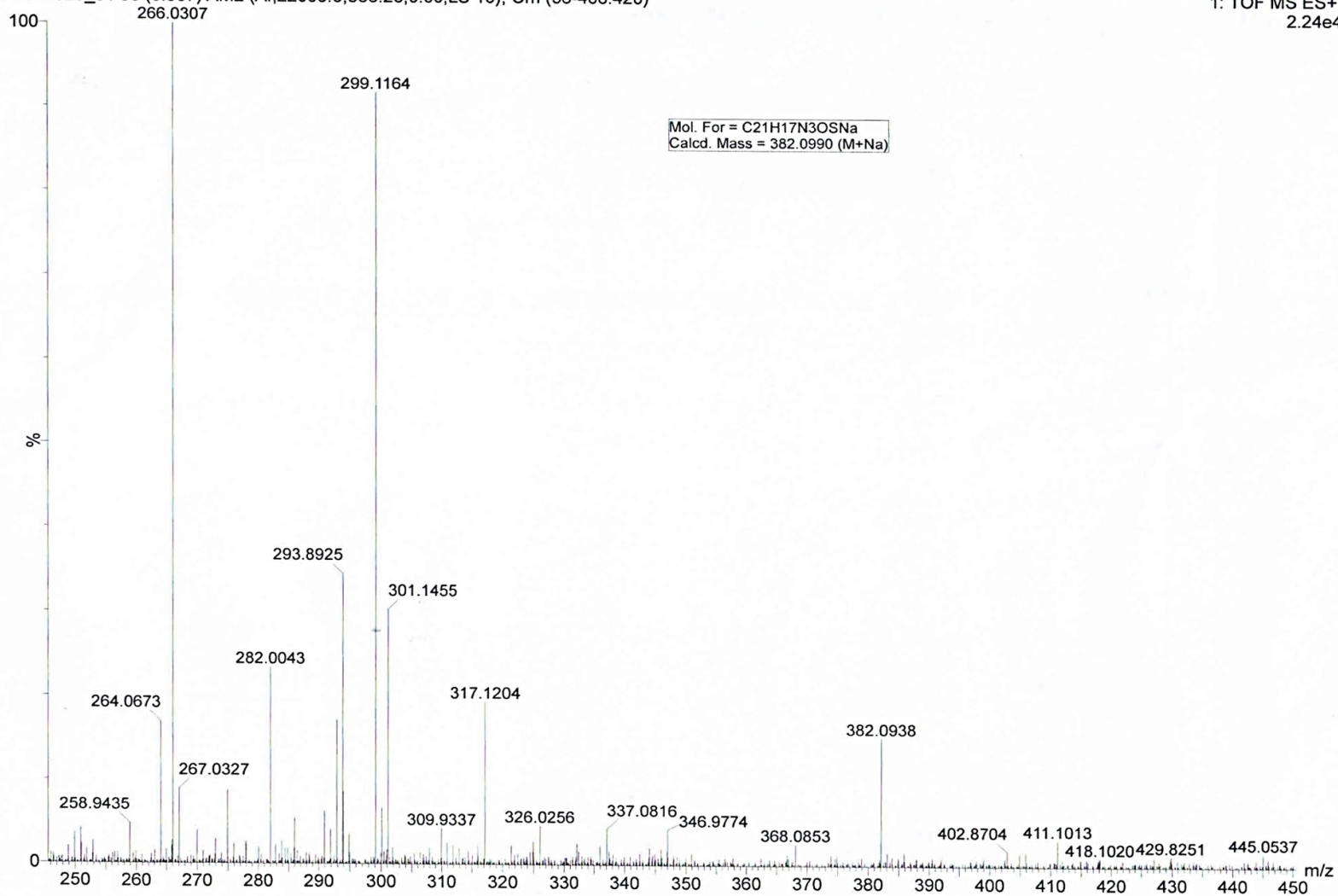


Figure S.12: HRMS-Spectrum of 4b

TB

IISER BERHAMPUR
CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

23-Aug-2024 16:09:37

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1: TOF MS ES+
3.00e6

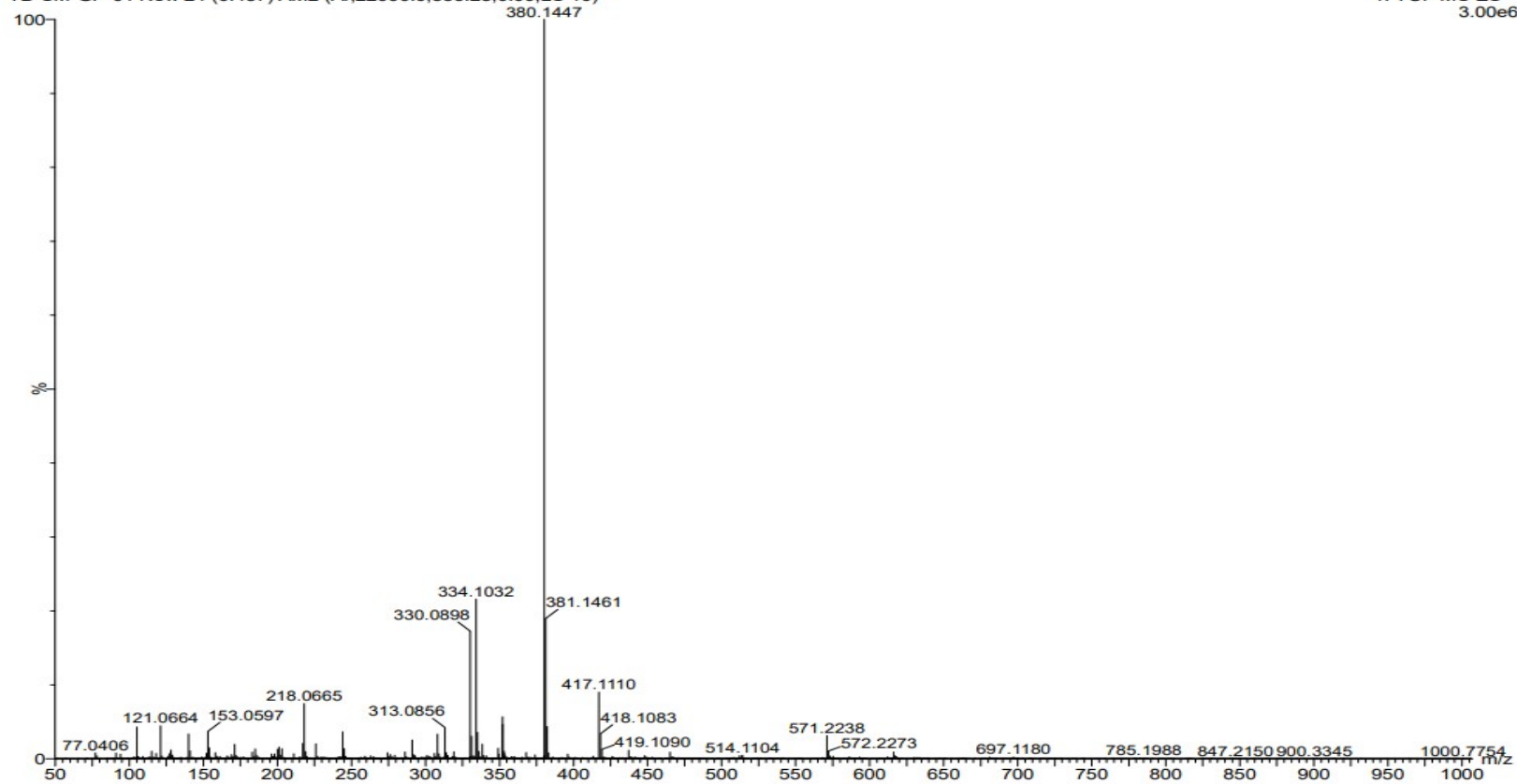


Figure S.13: HRMS-Spectrum of 4c

TB

IISER BERHAMPUR
CAIF HRMS FACILITY
XEVO-G2XSQTOF#YFA1829

23-Aug-2024 15:22:19

TB-SM-GP-05 73 (0.700) AM2 (Ar,22000.0,556.28,0.00,LS 10); Cm (37:80)

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8.61e7

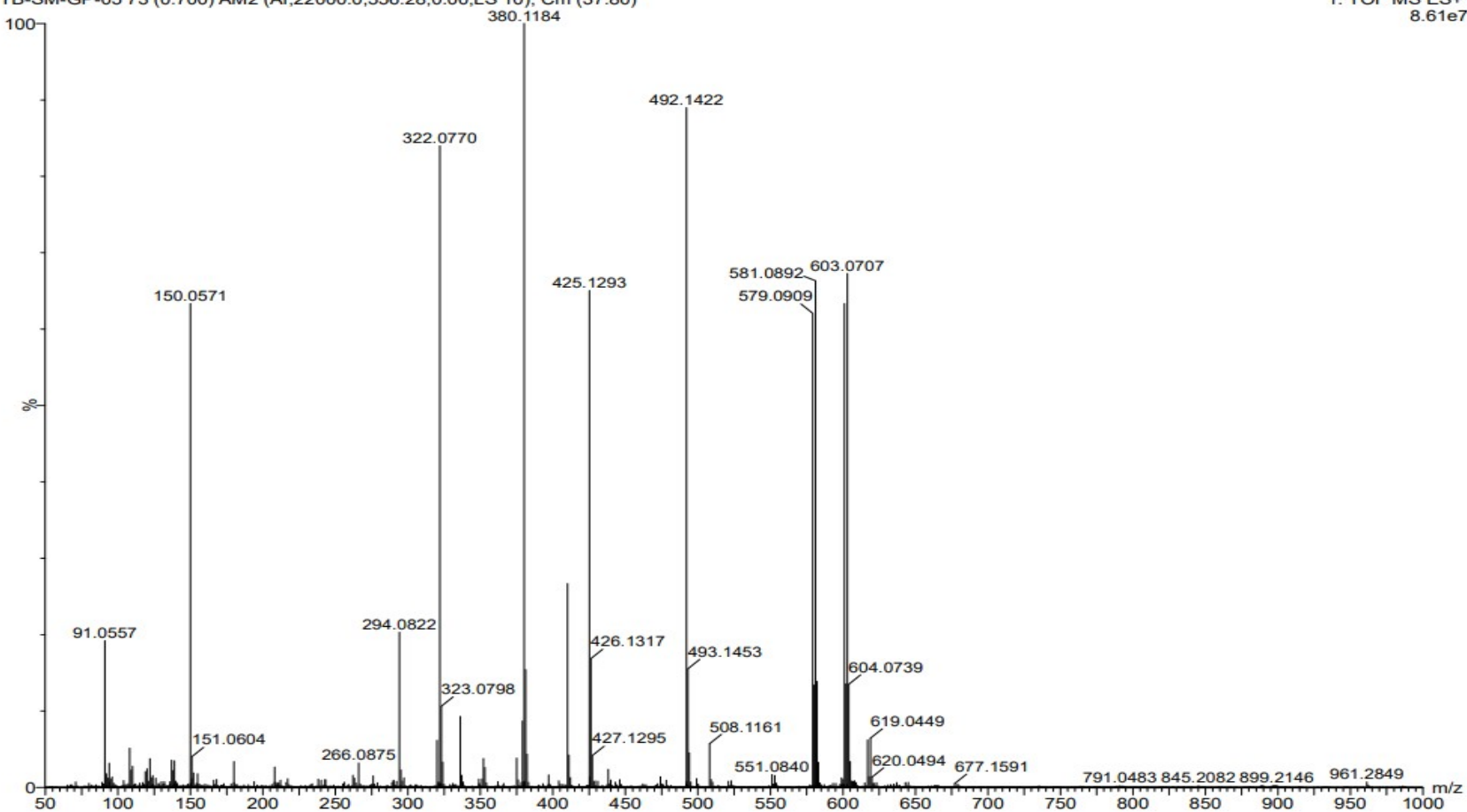


Figure S.14: HRMS-Spectrum of 4d

TB

23-Aug-2024 16:17:09

IISER BERHAMPUR
CAIF HRMS FACILITY
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1: TOF MS ES+
6.75e6

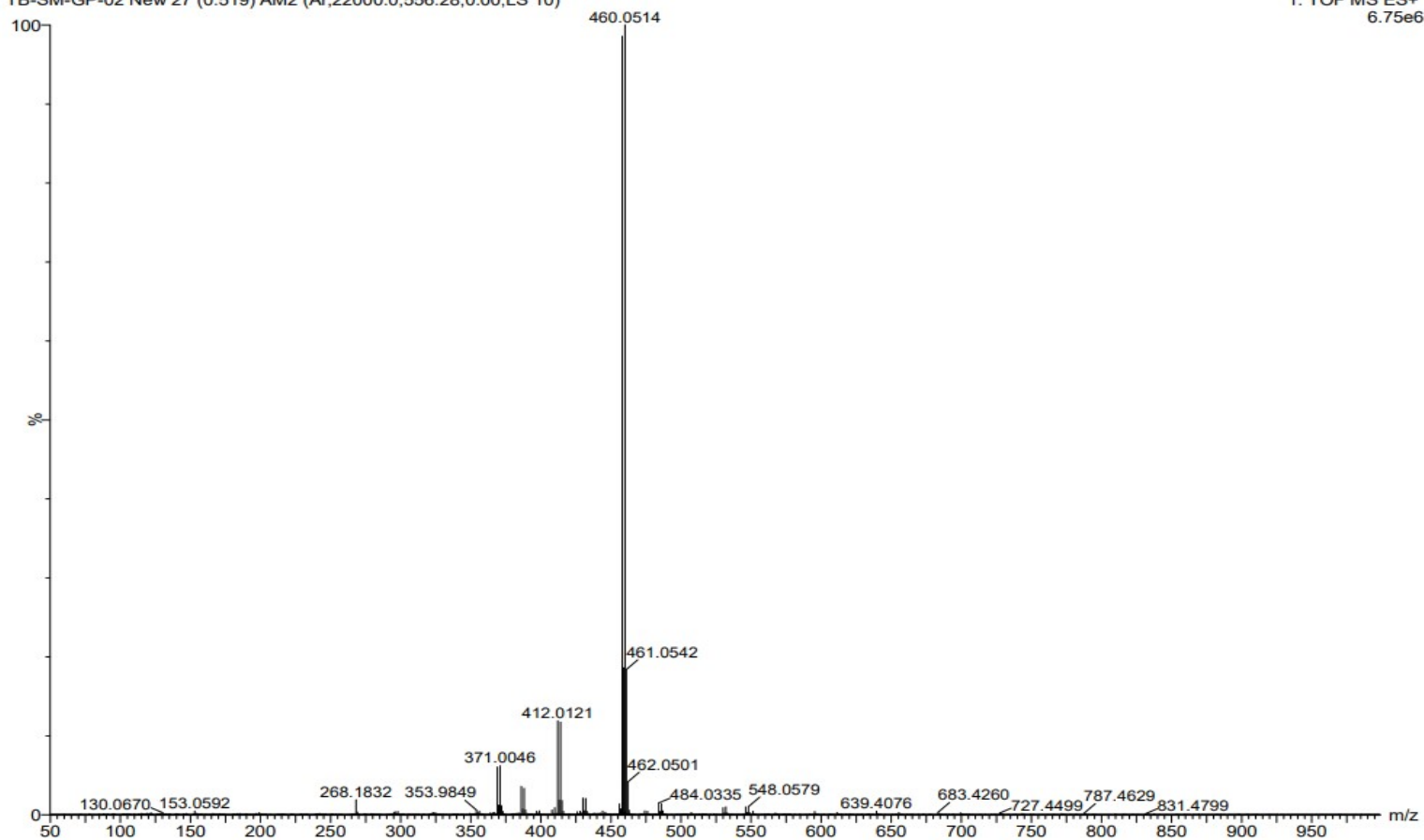


Figure S.15: HRMS-Spectrum of **4e**

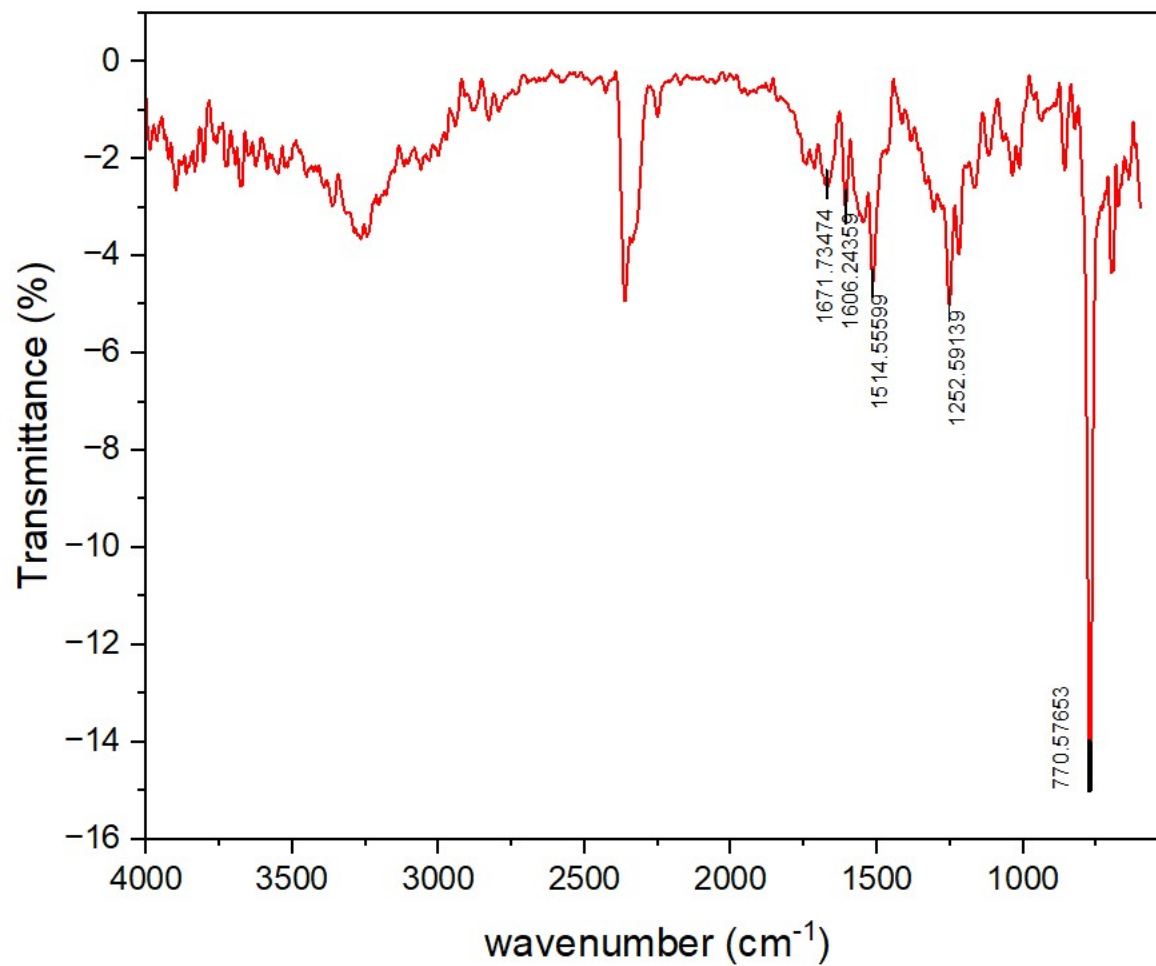


Figure S.16: FTIR-Spectrum of 4a

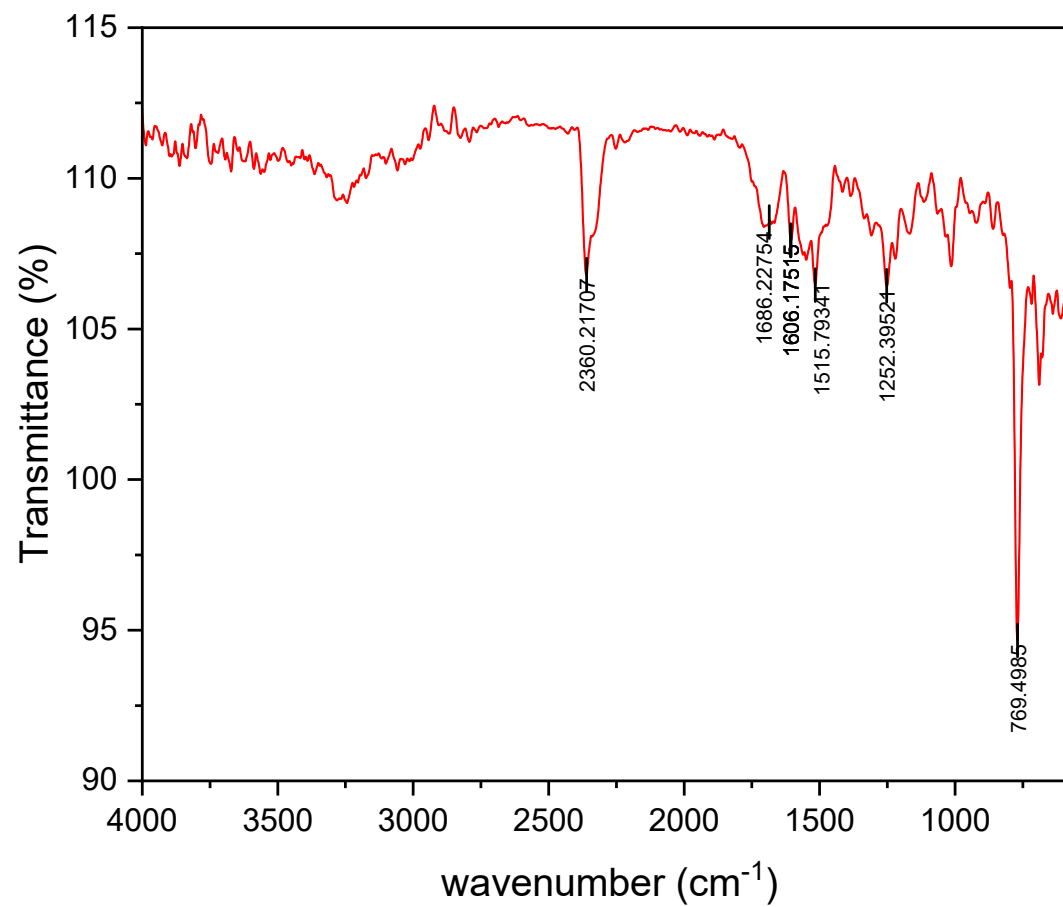


Figure S.17: FTIR-Spectrum of 4b

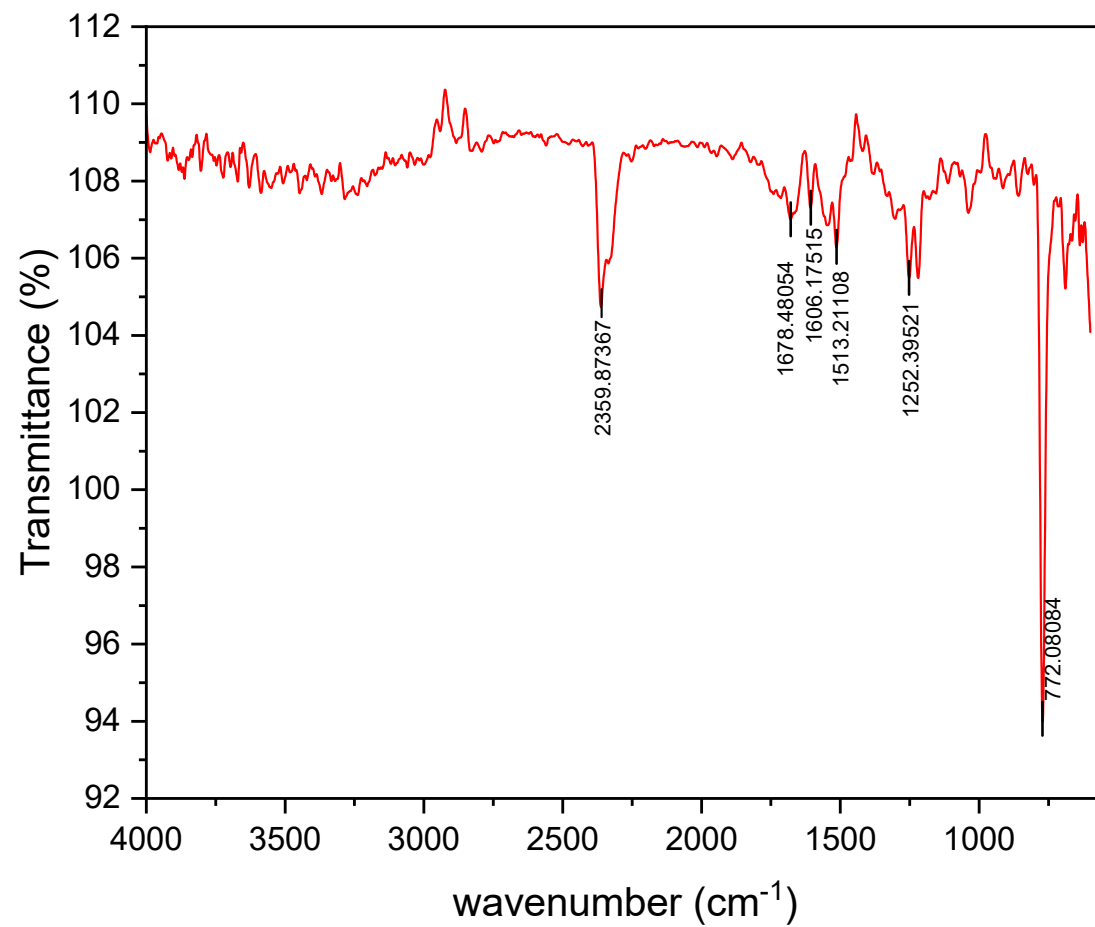


Figure S.18: FTIR-Spectrum of 4c

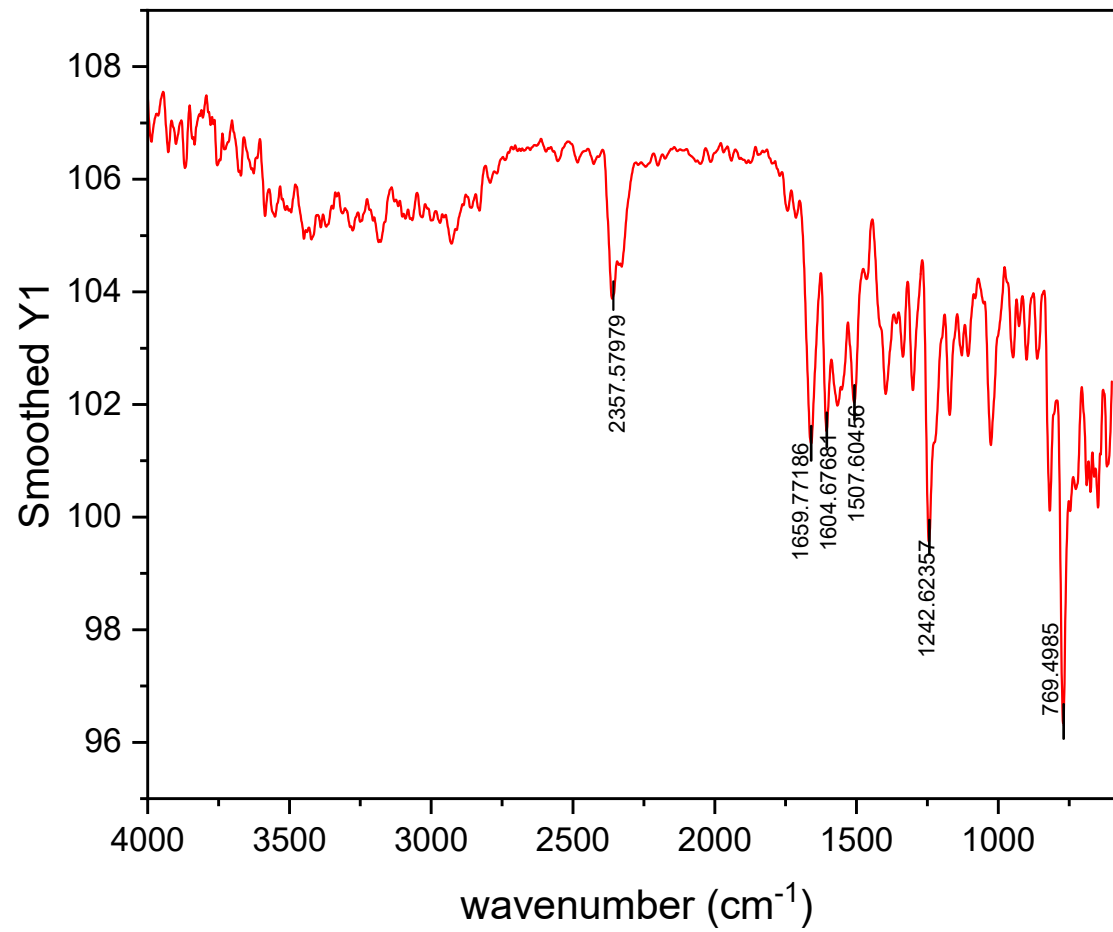


Figure S.19: FTIR-Spectrum of 4d

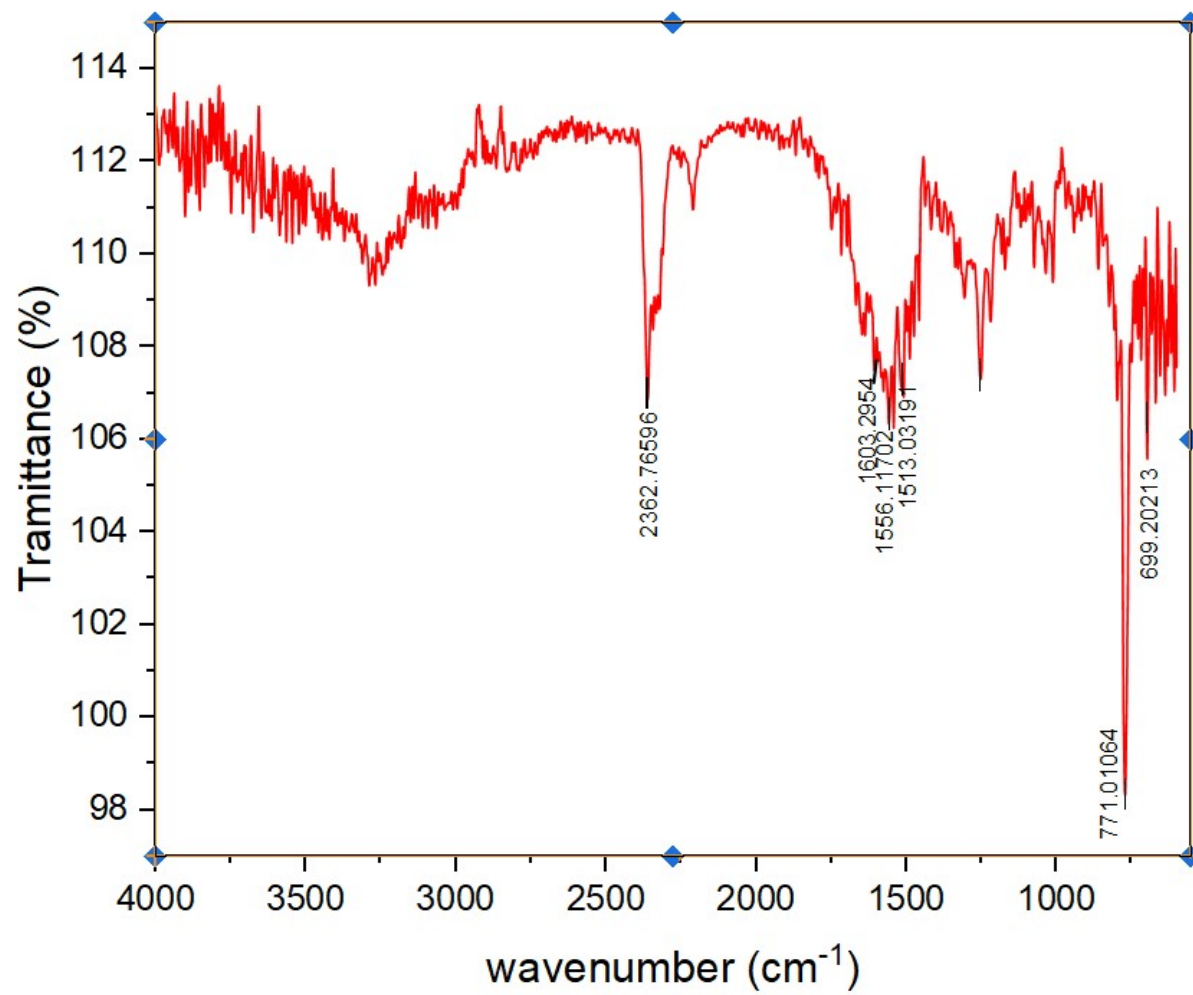


Figure S.20: FTIR-Spectrum of 4e

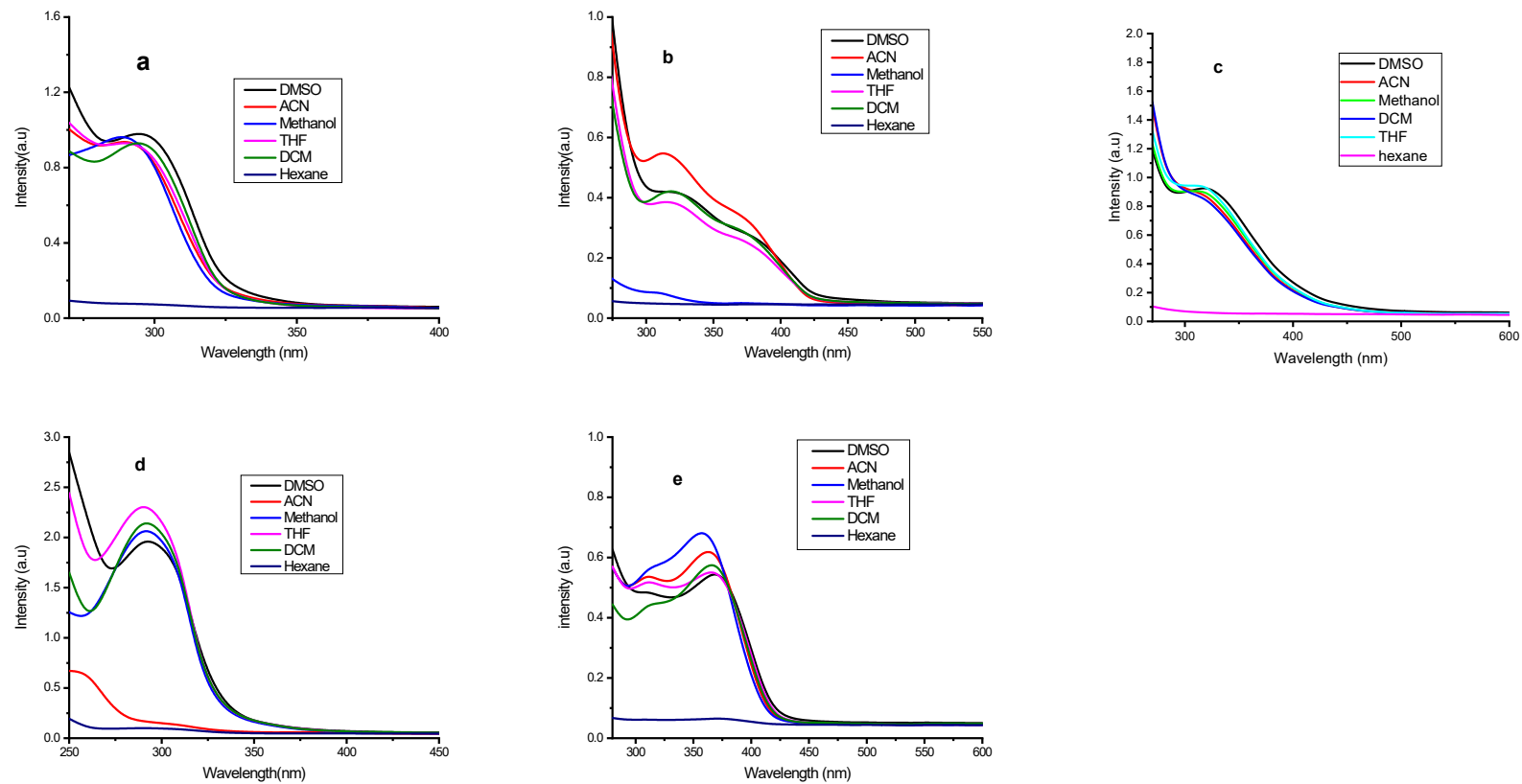


Figure S.21. Uv-Vis spectra of 4e (5×10^{-5} M) in Various solvents

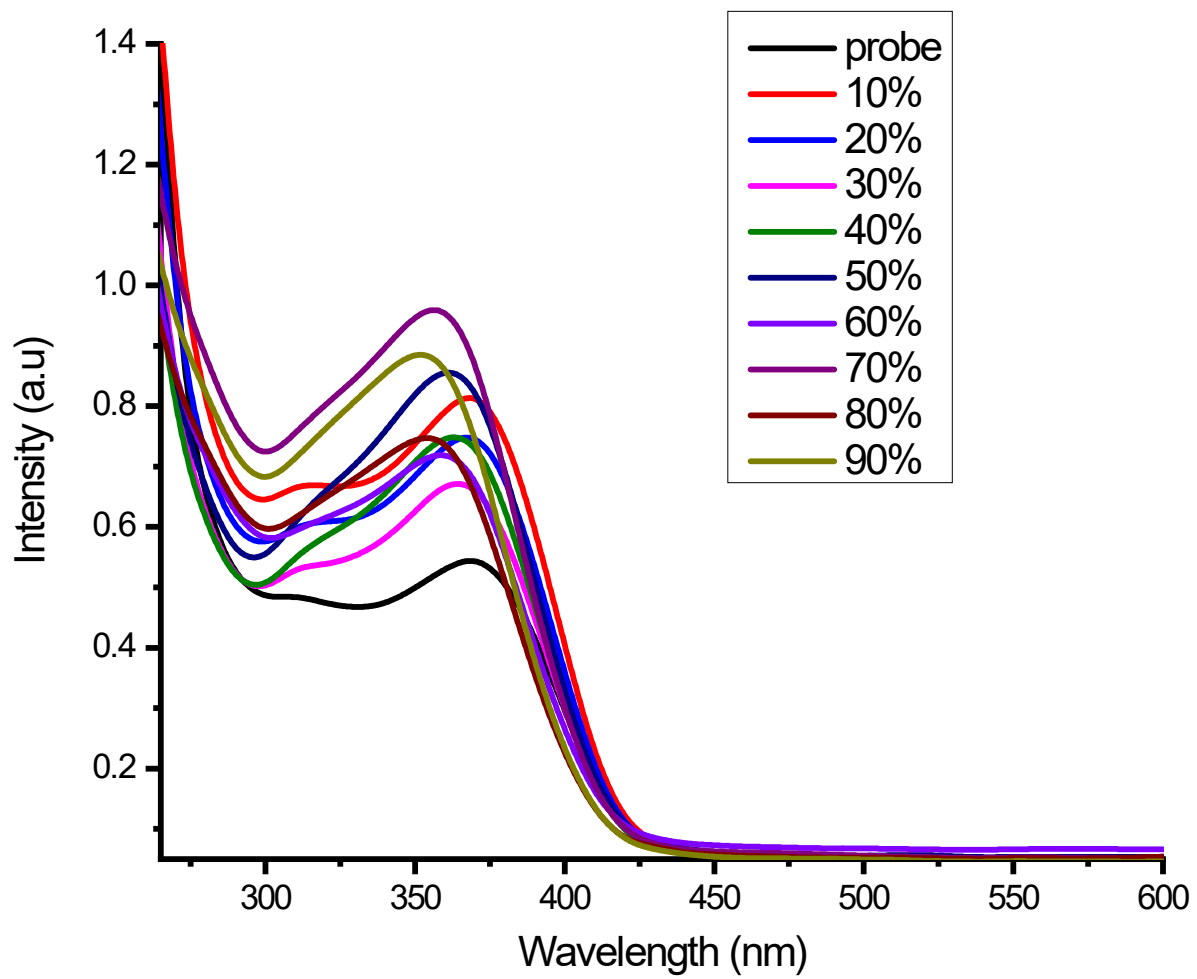


Figure S.22. UV- Vis spectra of 4e (5×10^{-5} M) in DMSO: water solvent mixtures

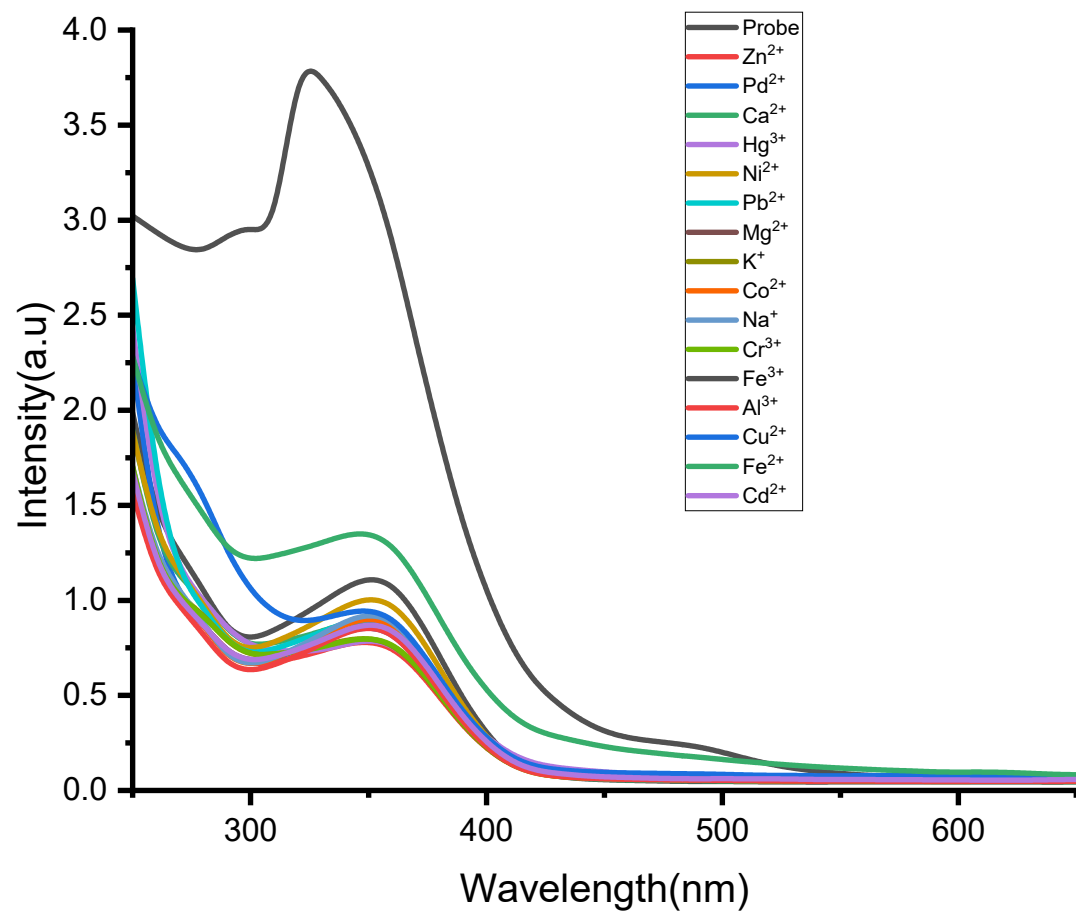


Figure S.23. UV- Vis spectra of 4e (5×10^{-5} M) in different metal cations (300 μ l)

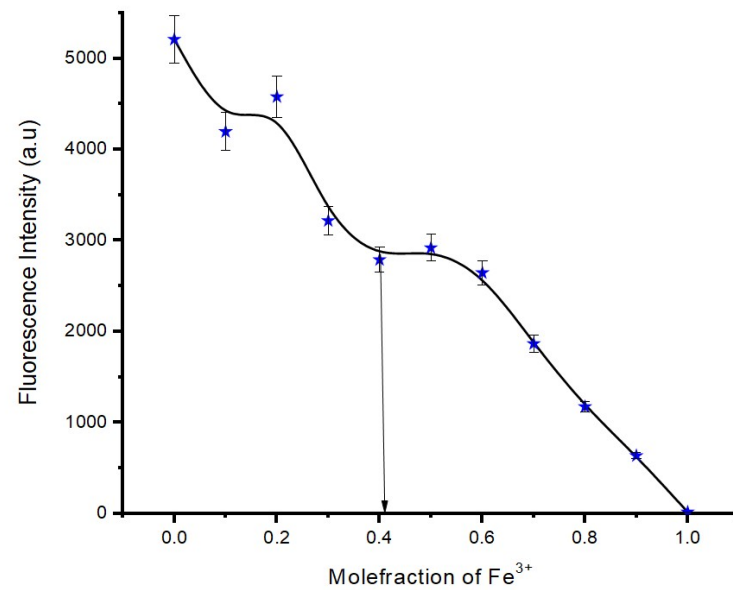
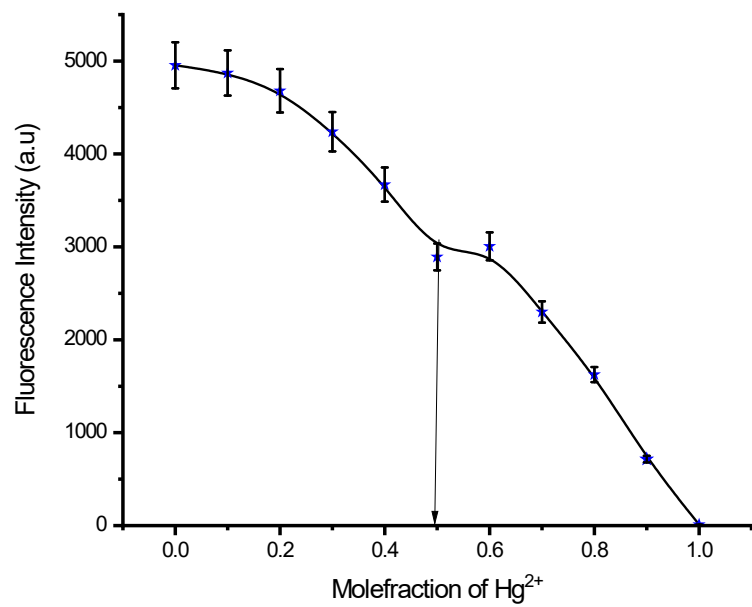
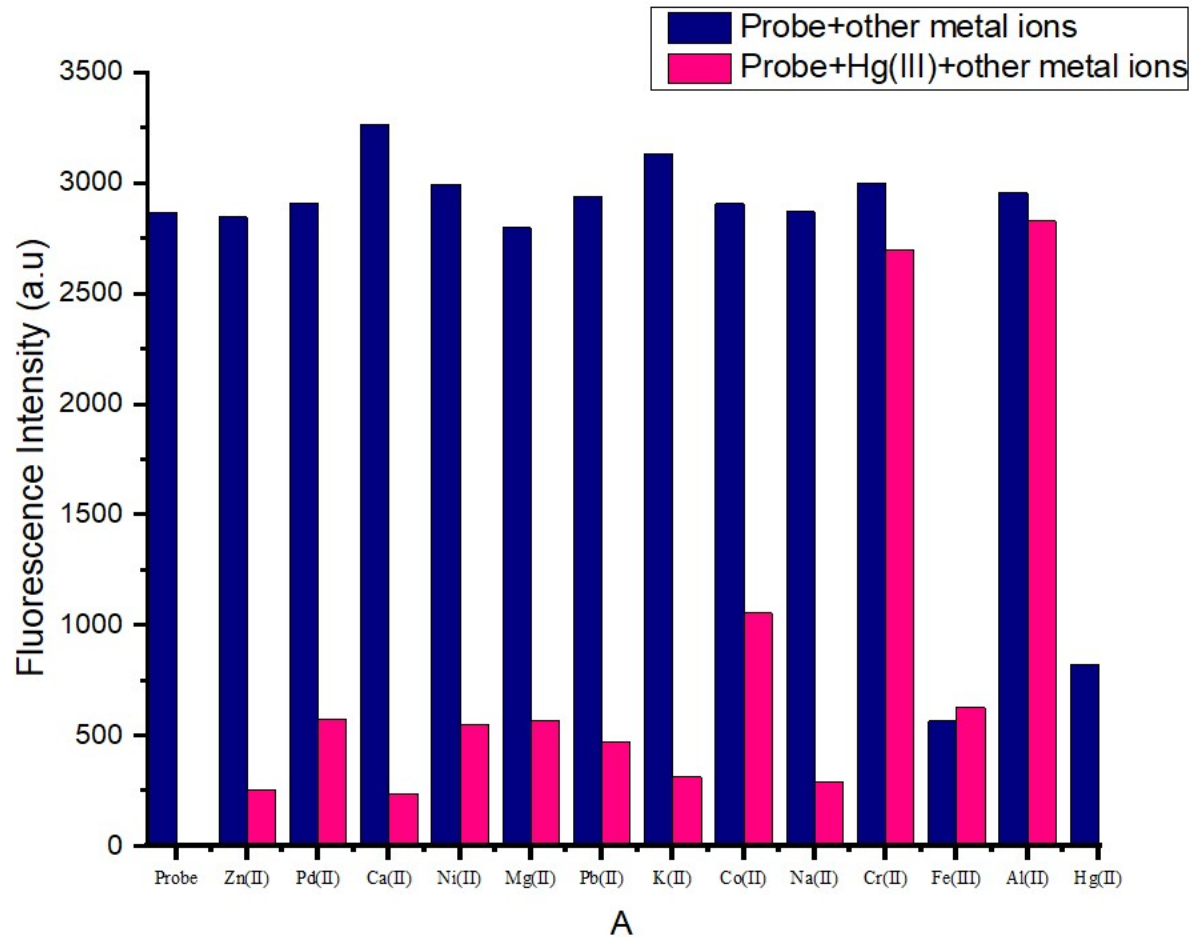
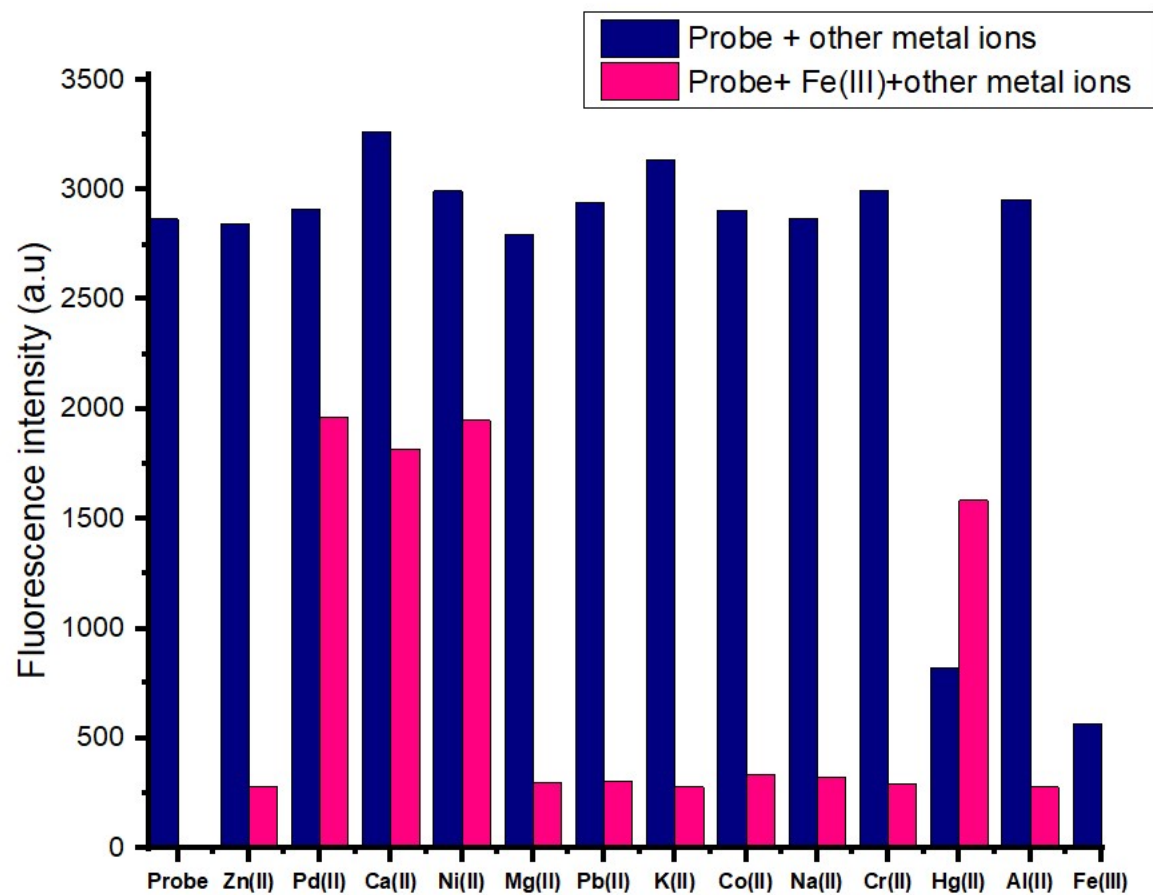


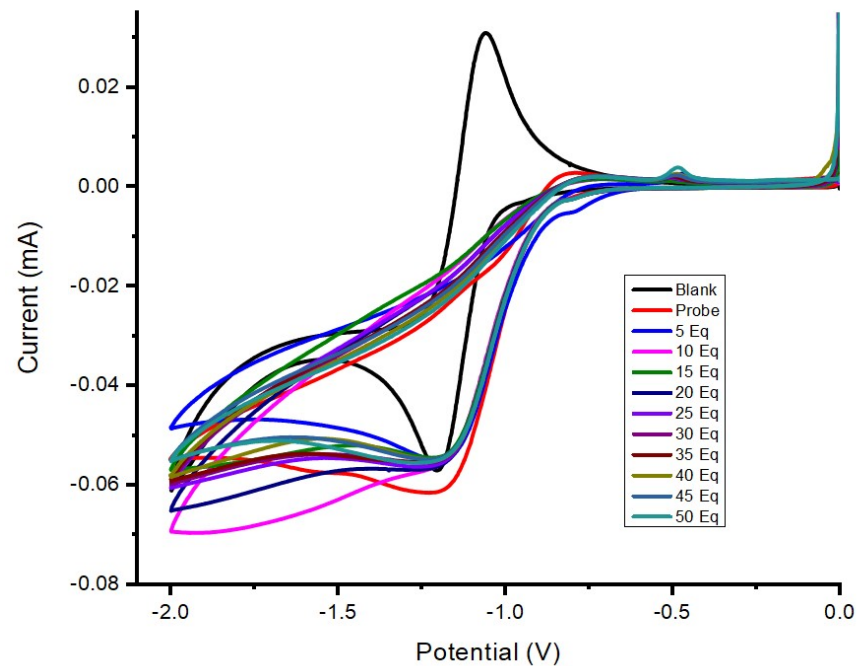
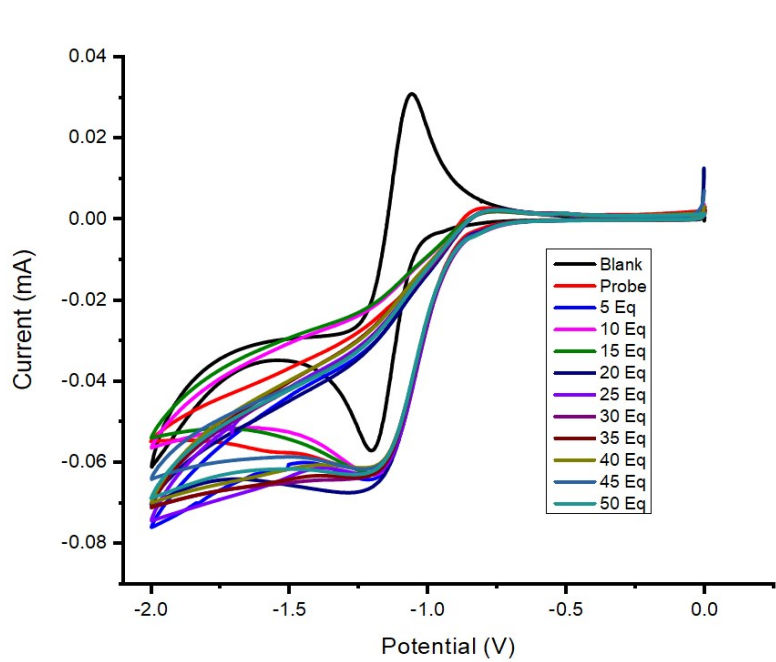
Figure S.24: Job's plot between the Fluorescence intensity of 4e and the mole fraction of Fe³⁺ and Hg²⁺



Figures S.25. Interference study of A-4e (5×10^{-5} M) in DMSO solvent presence of various metal ions. Blue bars represent the Fluorescence intensity of A-4e + metal cation systems; Pink bars represent the Fluorescence intensity of Hg²⁺ + metal cation systems.



Figures S.26. Interference study of A-4e (5×10^{-5} M) in DMSO solvent presence of various metal ions. Blue bars represent the Fluorescence intensity of A-4e + metal cation systems; Pink bars represent the Fluorescence intensity of Fe^{3+} + metal cation systems.



Figures S.27: (a) Cyclic voltammetry titration of A-4e with Fe^{3+} ions (0-50 μl) (b) Cyclic voltammetry titration of A-4e with Hg^{2+} ions (0-50 μl).

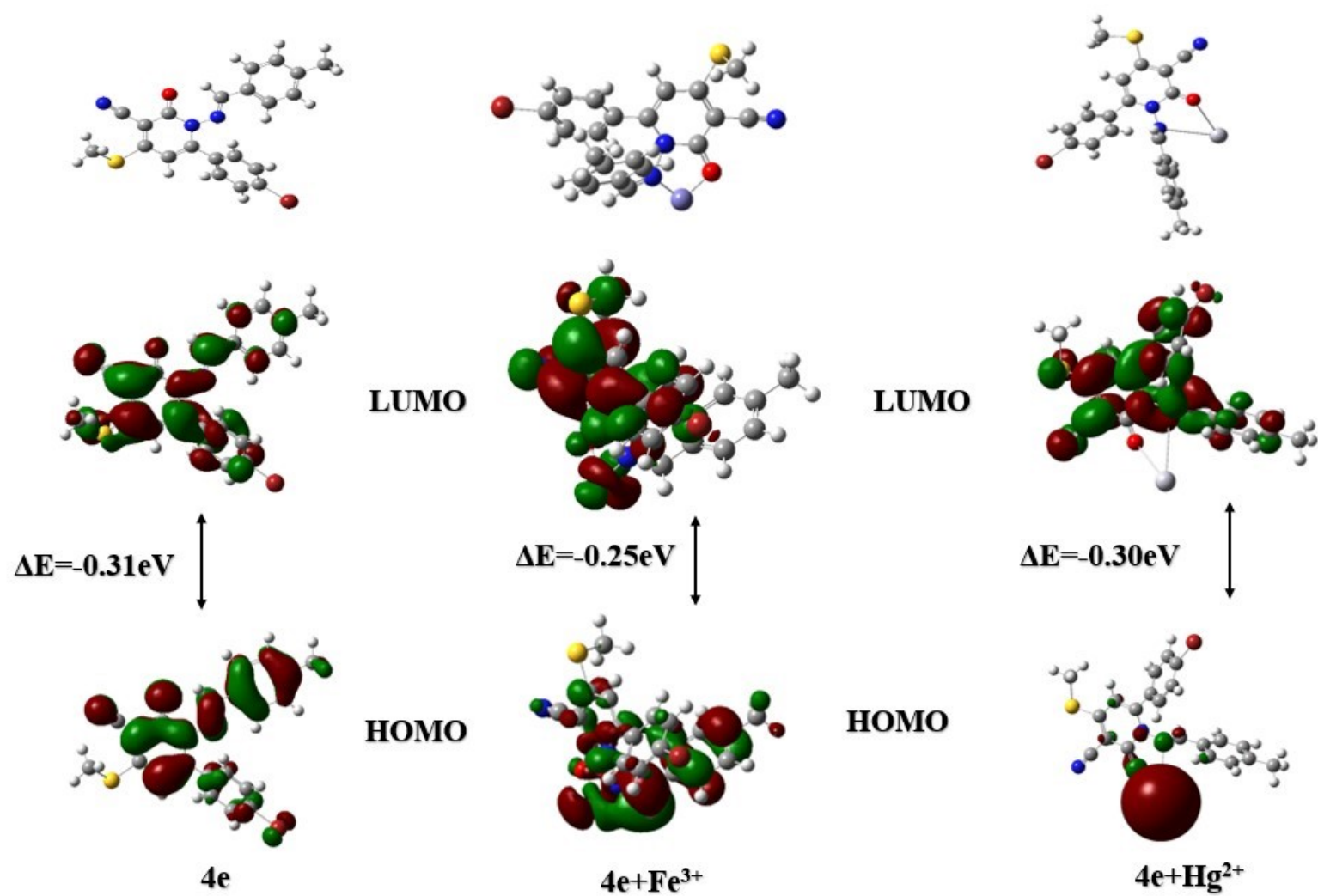


Figure S.28: Calculated HOMOs and LUMOs of 4e and 4e+Fe³⁺ and 4e+Hg²⁺

	λ_{ex}	λ_{em}	τ_1 (rel%)	τ_2 (rel%)	τ_3 (rel%)	$T_{\text{average(ns)}}$	χ^2
4e (Probe)	350nm	450nm	0.255636	4.77261	-	0.96	1.357502
A-4e	350nm	470nm	0.304501	1.68946	-	1.54	1.009198
A-4e+Fe ³⁺	350nm	470nm	0.21956	1.63526	-	1.47	1.044633
A-4e+Hg ²⁺	350nm	470nm	0.215328	1.01693	4.76184	0.89	1.137985

TCSPC – (Time correlated single photon counting) spectrometer for probe

4e, A-4e, A-4e+Fe³⁺ and A-4e+Hg²⁺

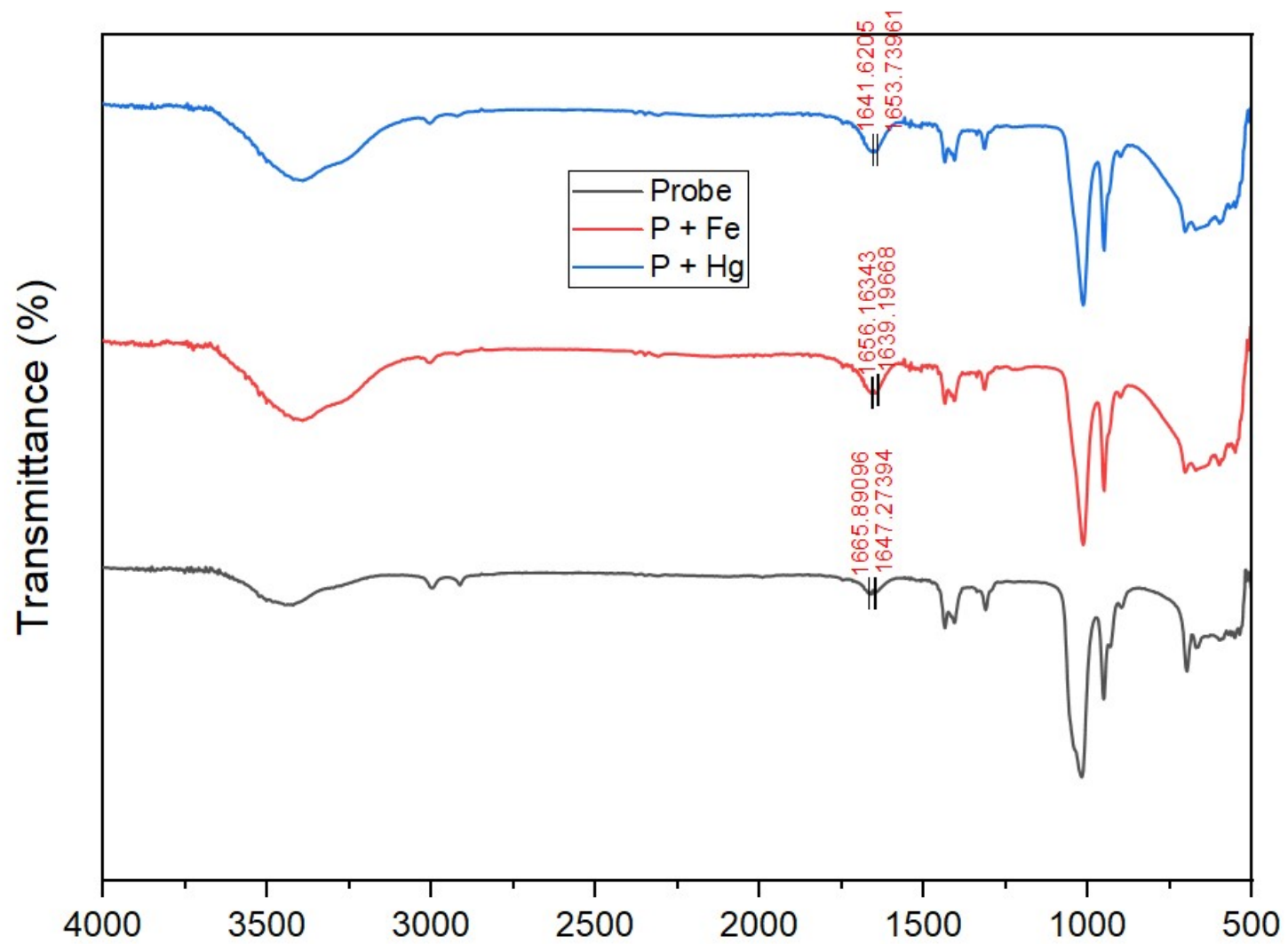


Figure S.29: FTIR spectra of 4e in the presence of Fe^{3+} and Hg^{2+}