

Supporting Information

Terphenyl-phenanthroline conjugate as a Zn^{2+} sensor: H_2PO_4^- induced tuning of emission wavelength

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General Experimental Procedures

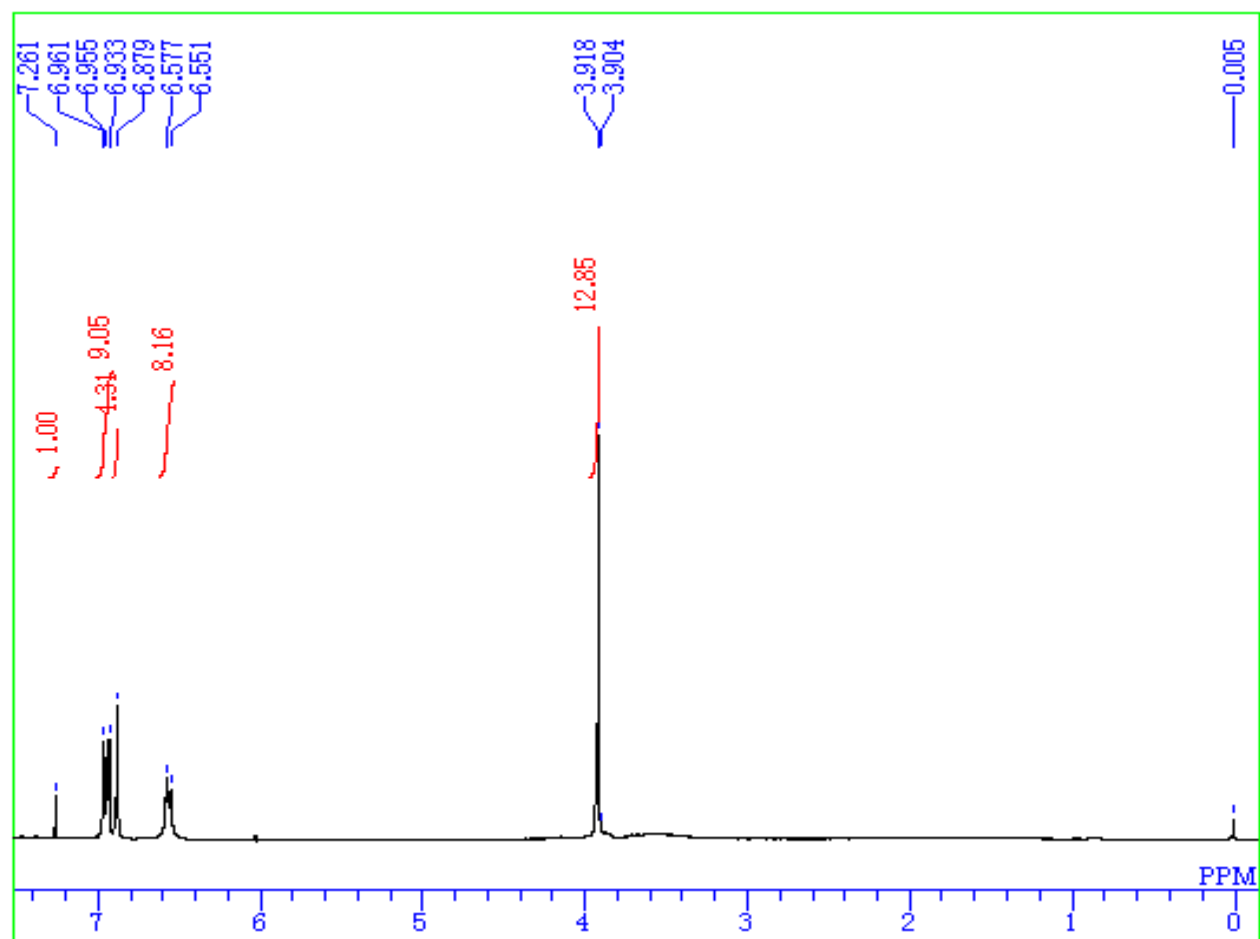
UV-Vis and fluorescence Titrations

UV-Vis and fluorescence titrations were performed with 1×10^{-5} M solution of receptor **5** and **7** in THF. Typically, aliquots of freshly prepared standard solutions (10^{-1} - 10^{-3} M in THF) of metal perchlorates (Pb^{2+} , Hg^{2+} , Ba^{2+} , Cd^{2+} , Ag^{+} , Zn^{2+} , Cu^{2+} , Ni^{2+} , Co^{2+} , K^{+} , Mg^{2+} , Na^{+} and Li^{+}) were added and the spectra of the samples were recorded. Similarly, aliquots of freshly prepared solutions of anions (F^{-} , Cl^{-} , Br^{-} , I^{-} , HSO_4^{-} , NO_3^{-} , $\text{H}_2\text{PO}_4^{-}$) were added to record the absorption and emission behaviour of **5** and **7**.

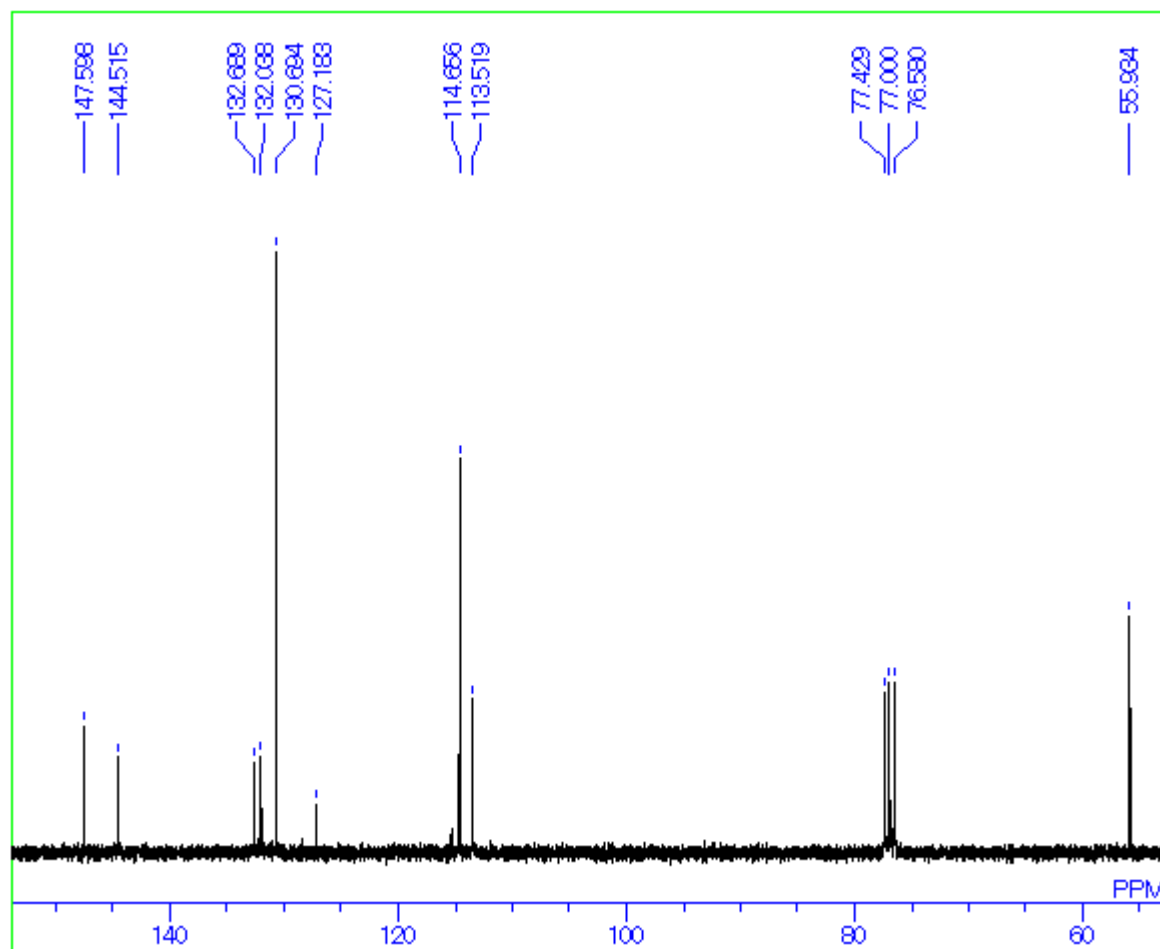
^1H NMR Experiments

The stock solution of compound **5** (10^{-2} M) was prepared in tetrachloroethane and perchlorate salts of Zn^{2+} (2×10^{-2} M) was prepared in CD_3CN for ^1H NMR titration experiments. The titration experiment was done in solvent mixture of tetrachloroethane and acetonitrile (7:3).

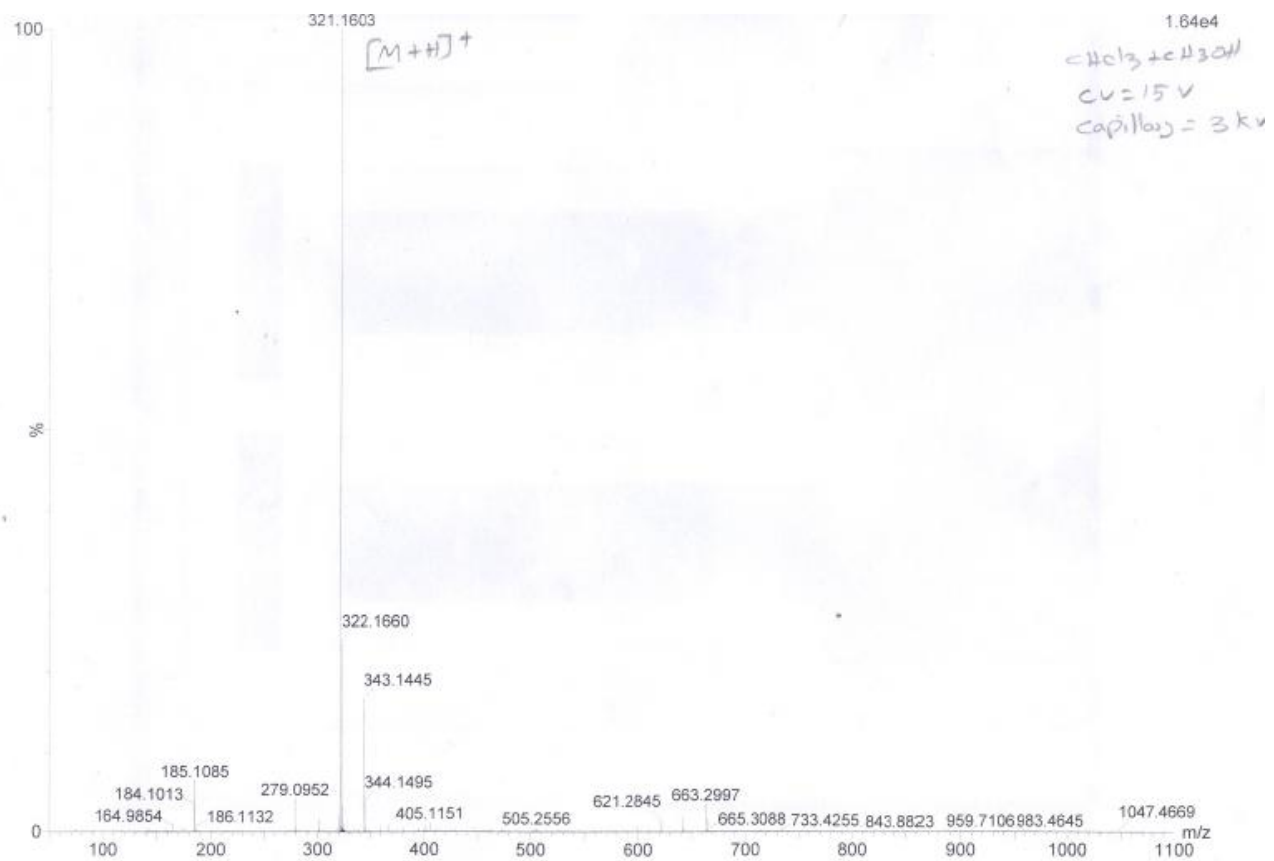
^1H NMR of compound 3



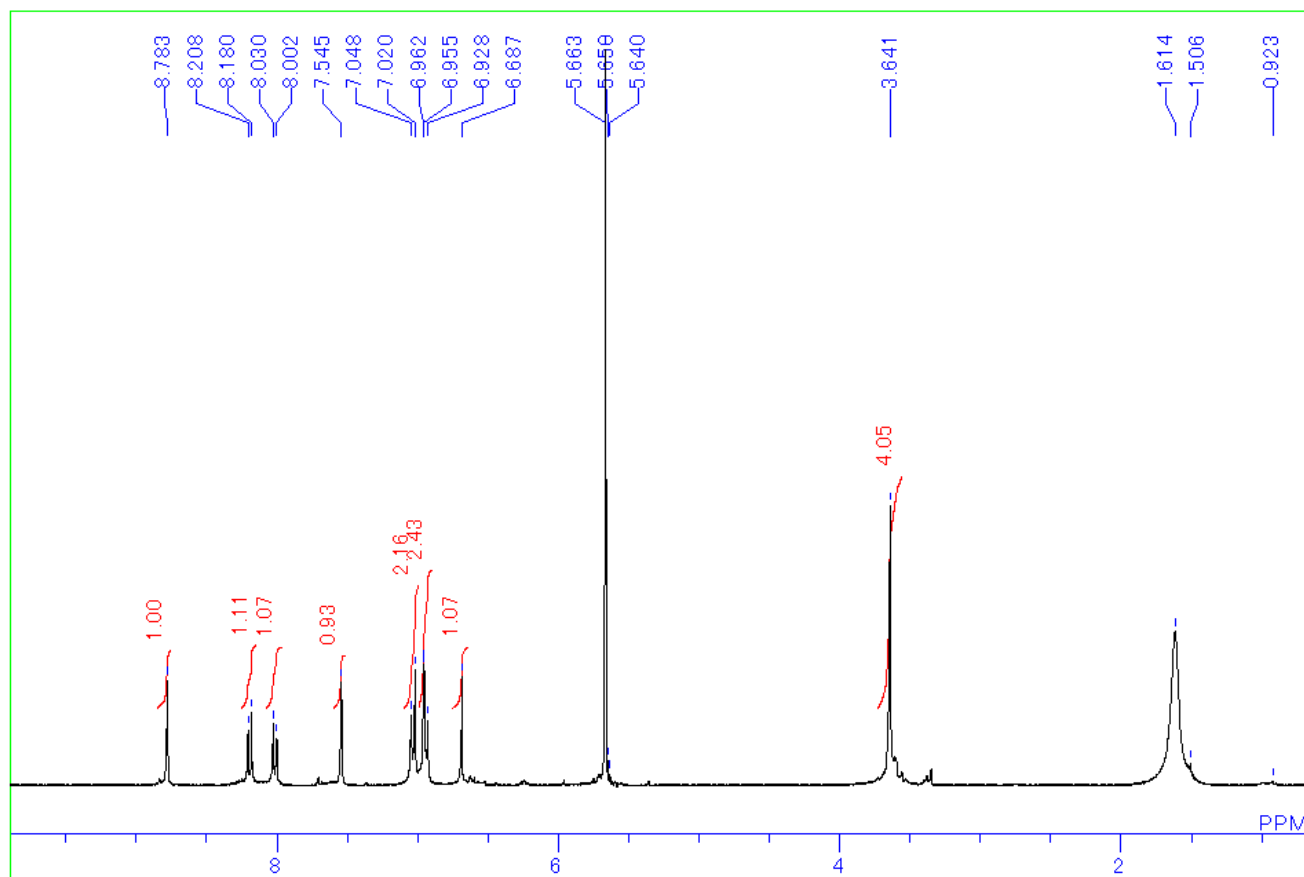
^{13}C NMR of compound 3



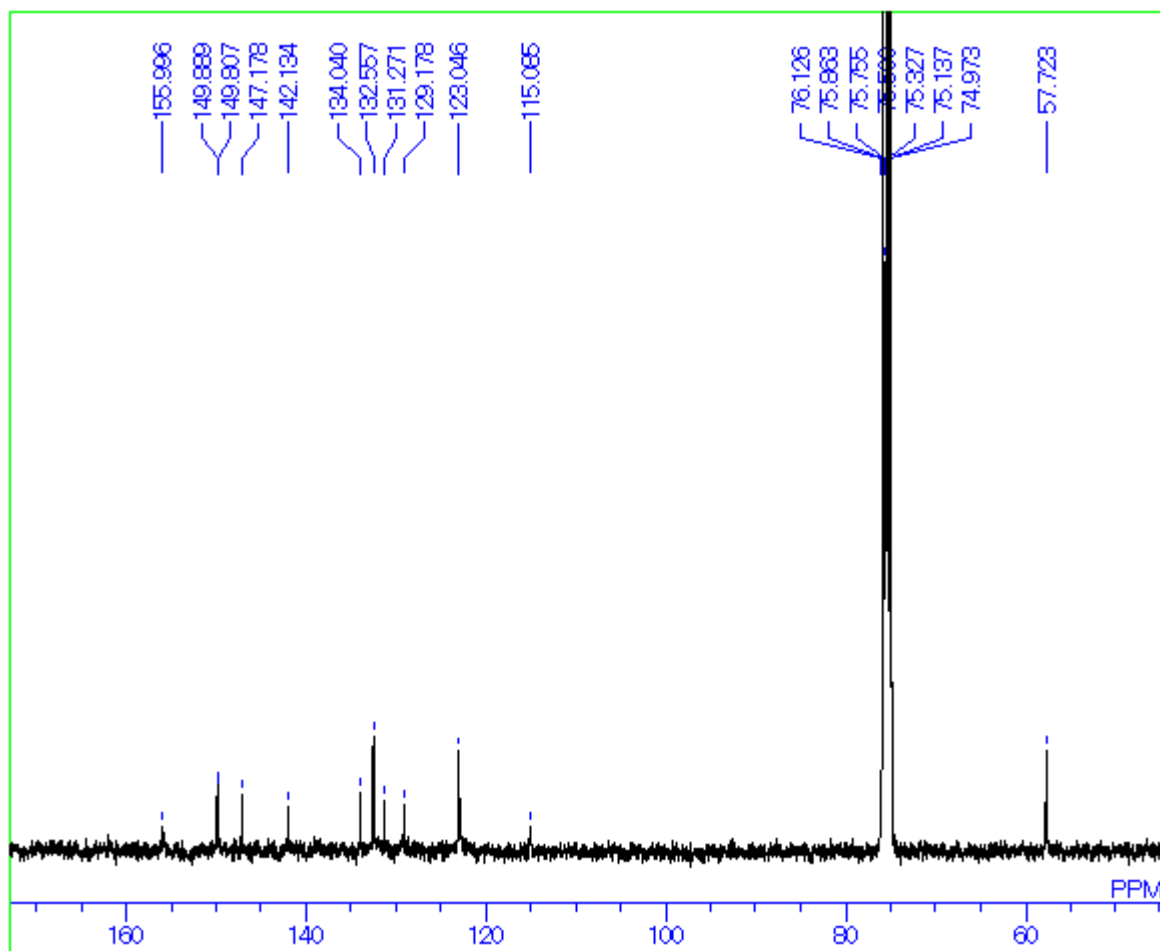
Mass Spectrum of compound 3



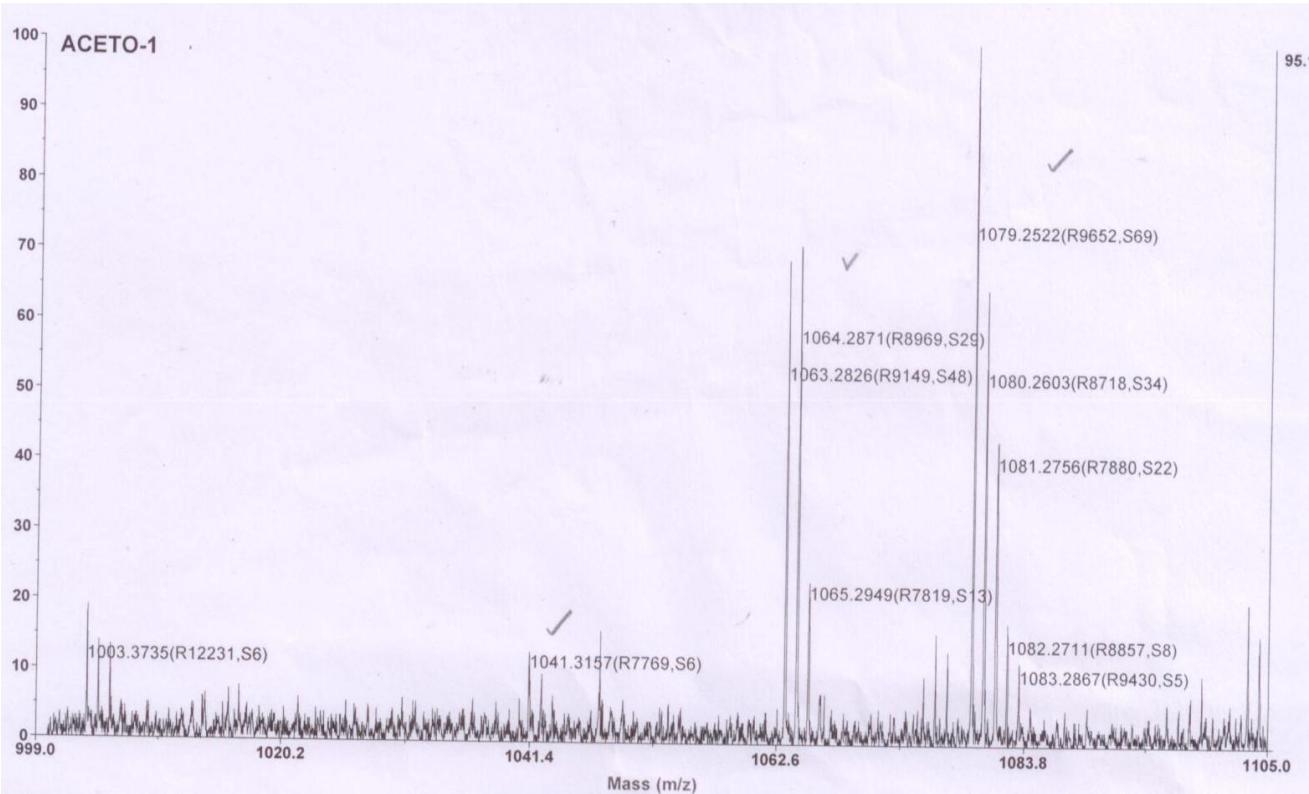
^1H NMR of compound 5



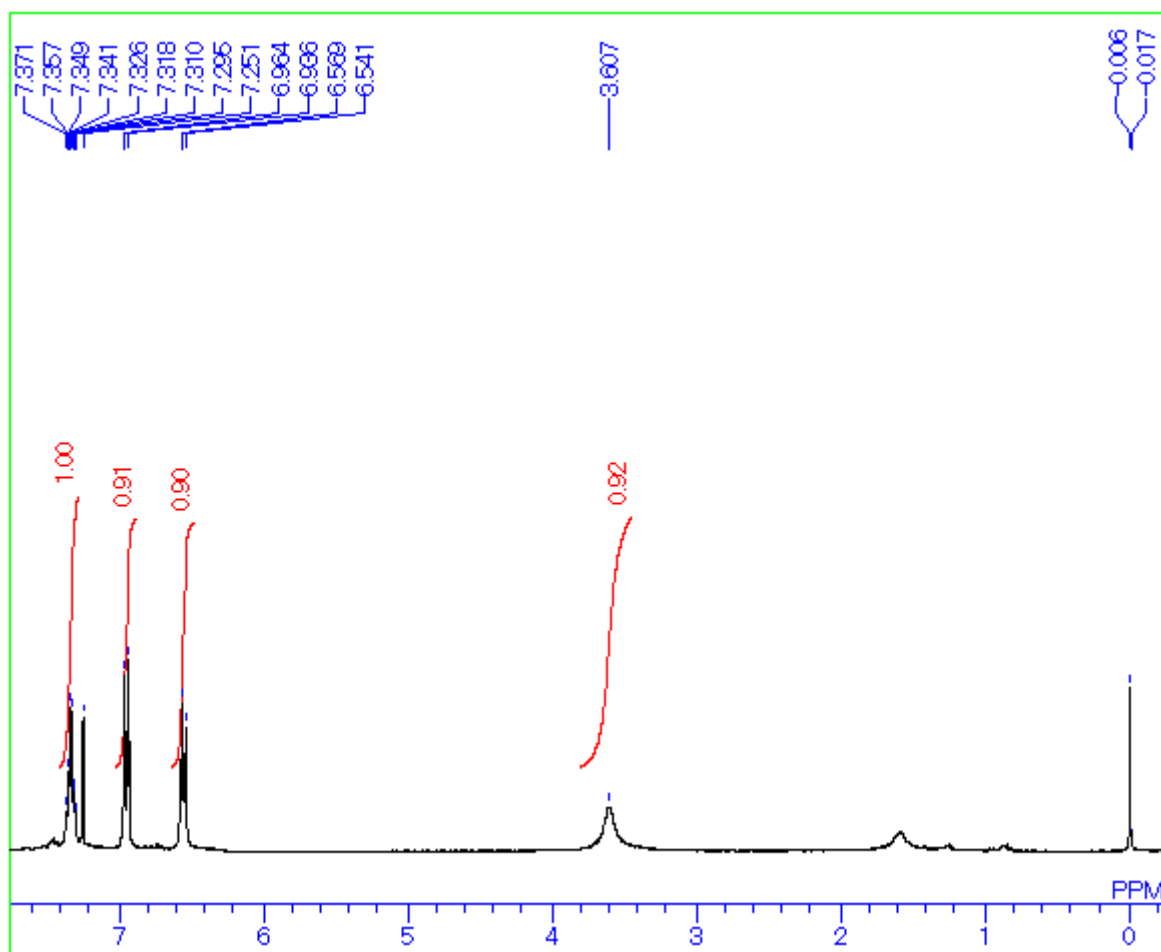
^{13}C NMR of compound 5



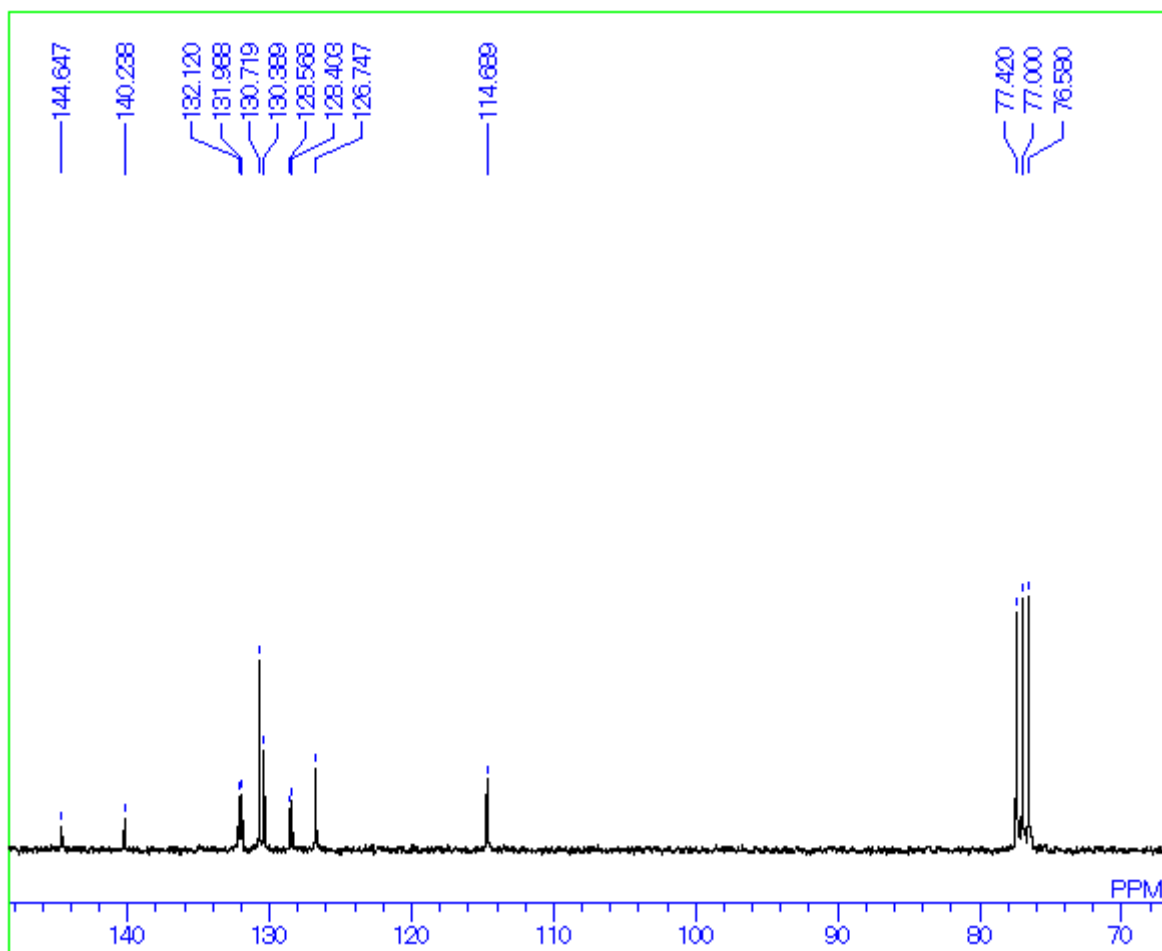
Mass spectrum of compound 5



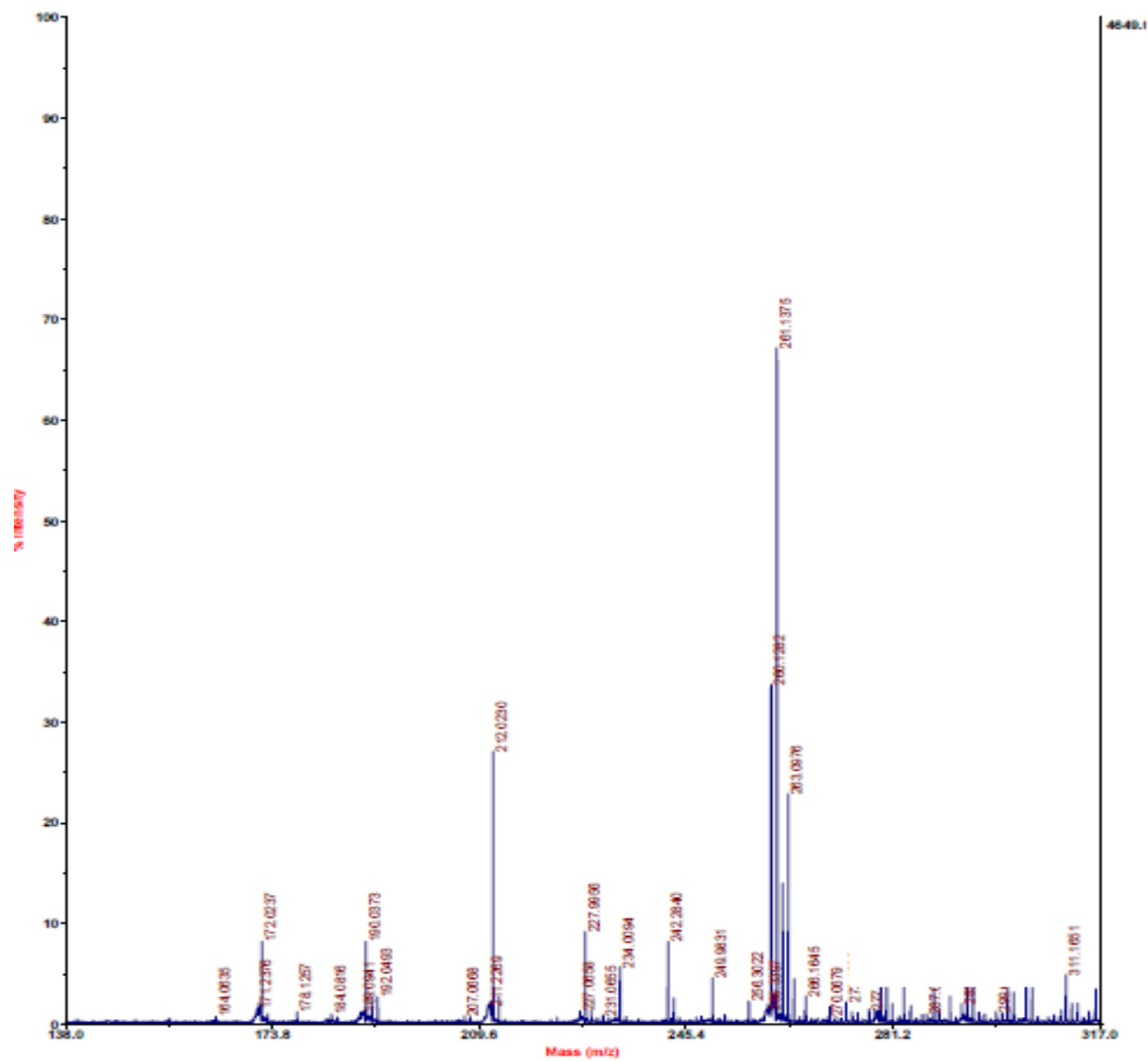
^1H NMR of compound 7



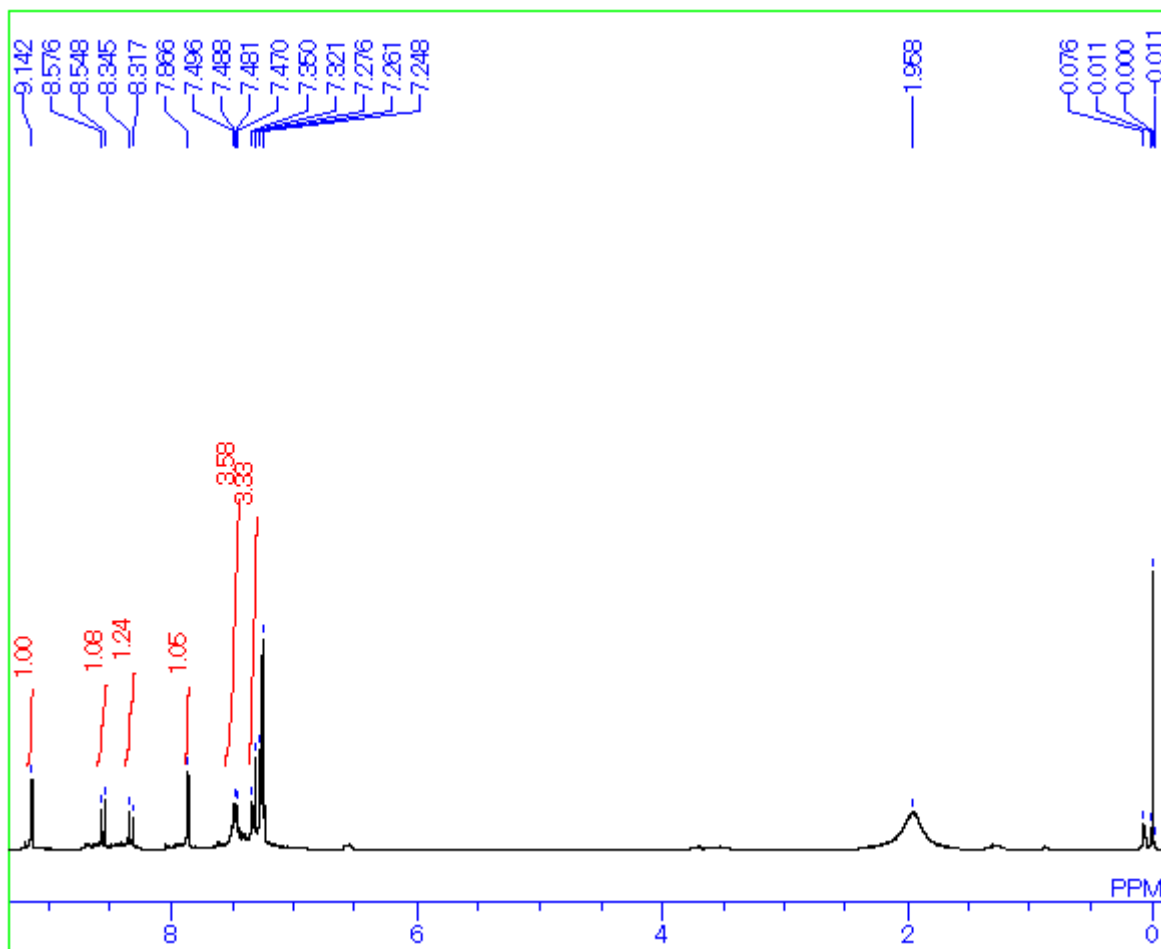
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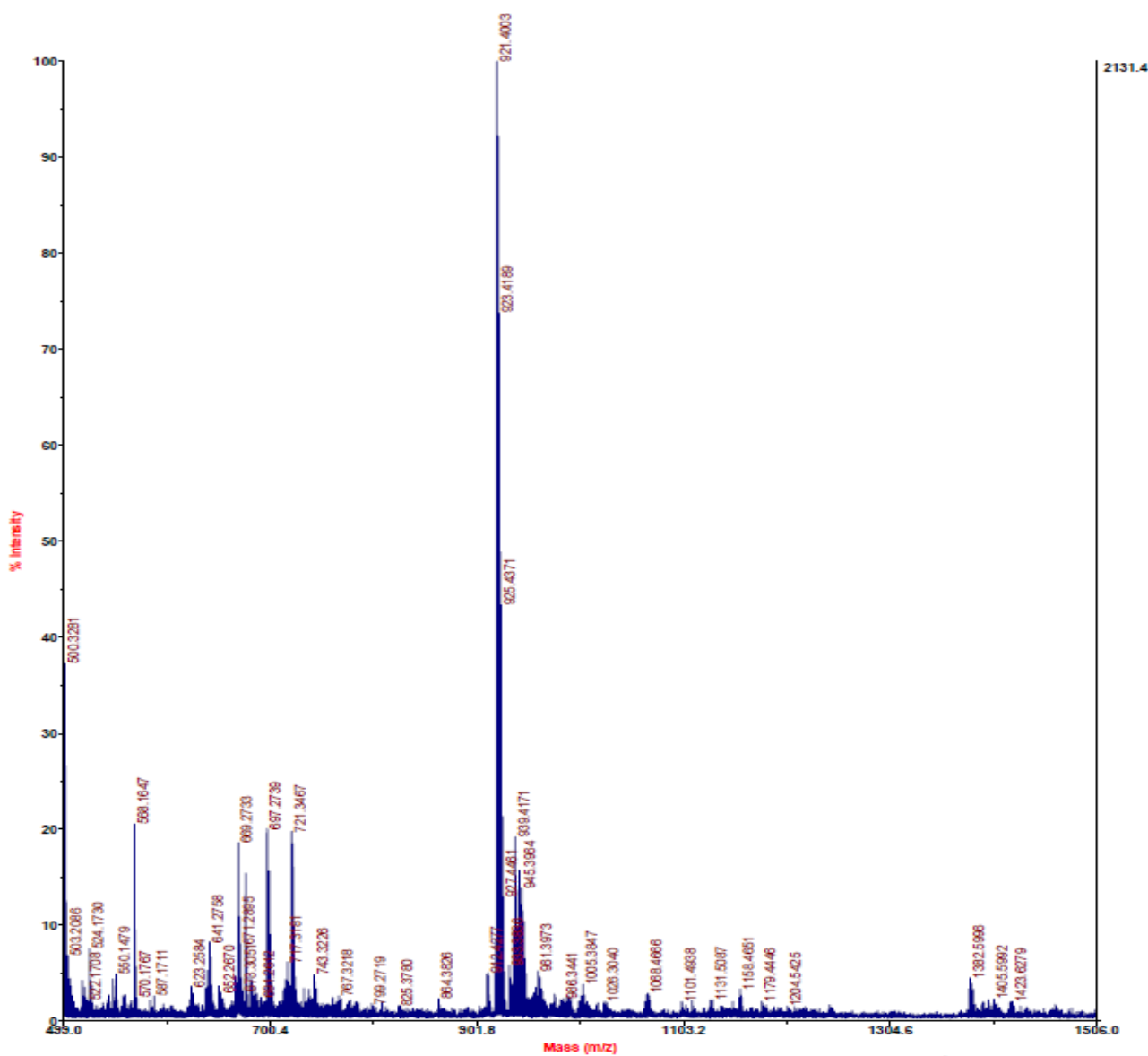
Mass spectrum of compound 7



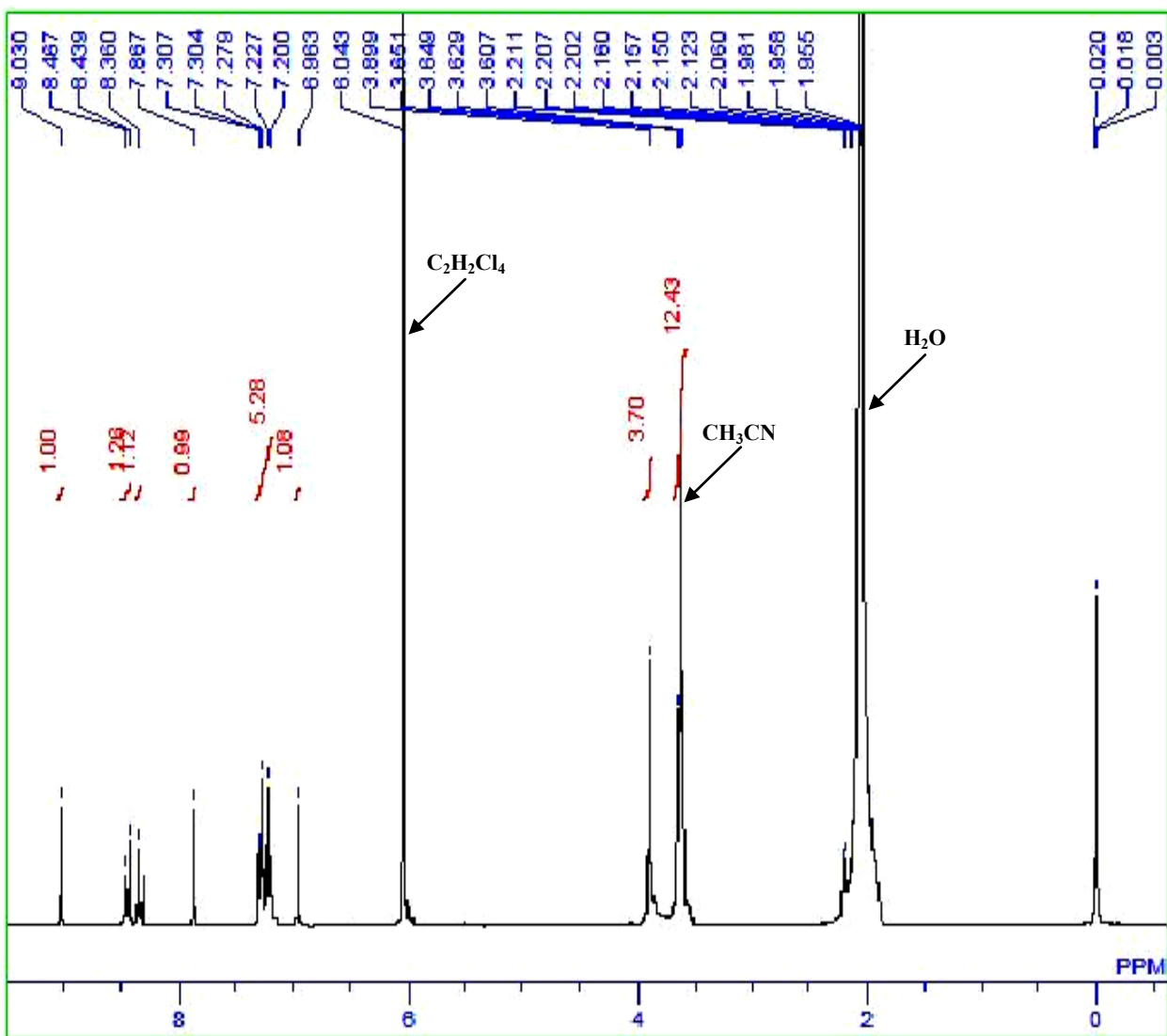
^1H NMR of compound 8



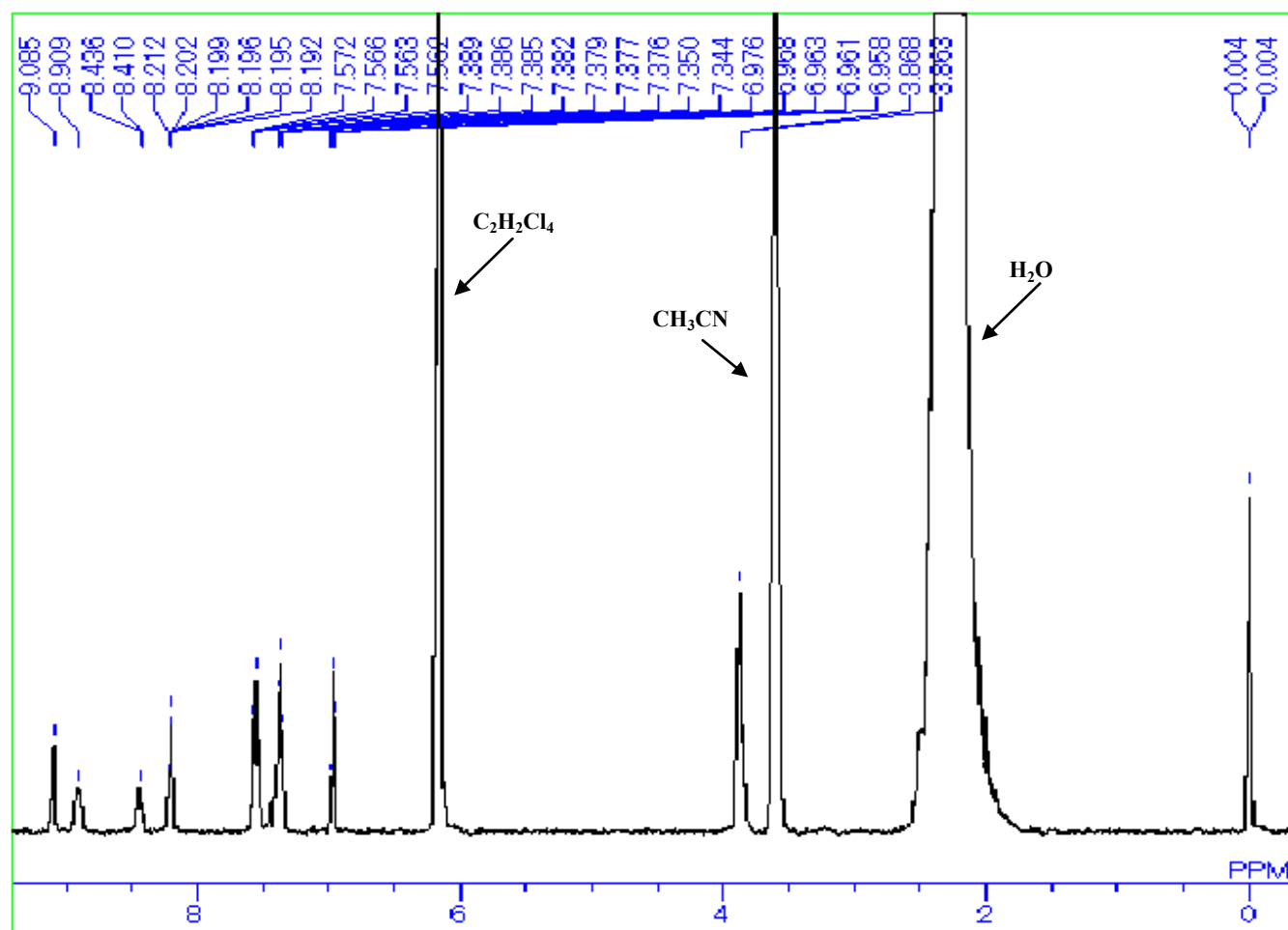
Mass spectrum of compound 8



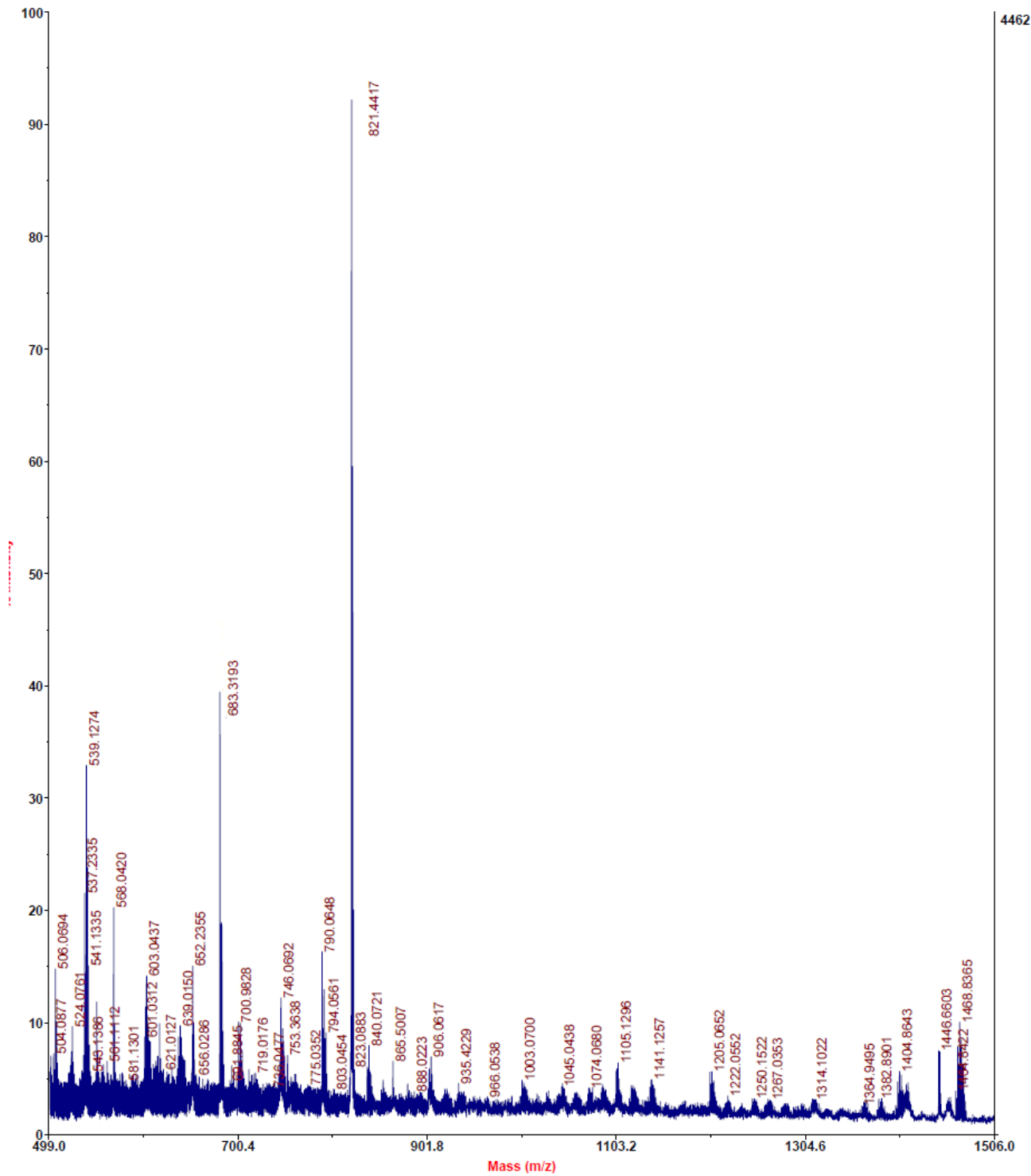
^1H NMR of compound 5 in Tetrachloroethane: CD_3CN (7:3)



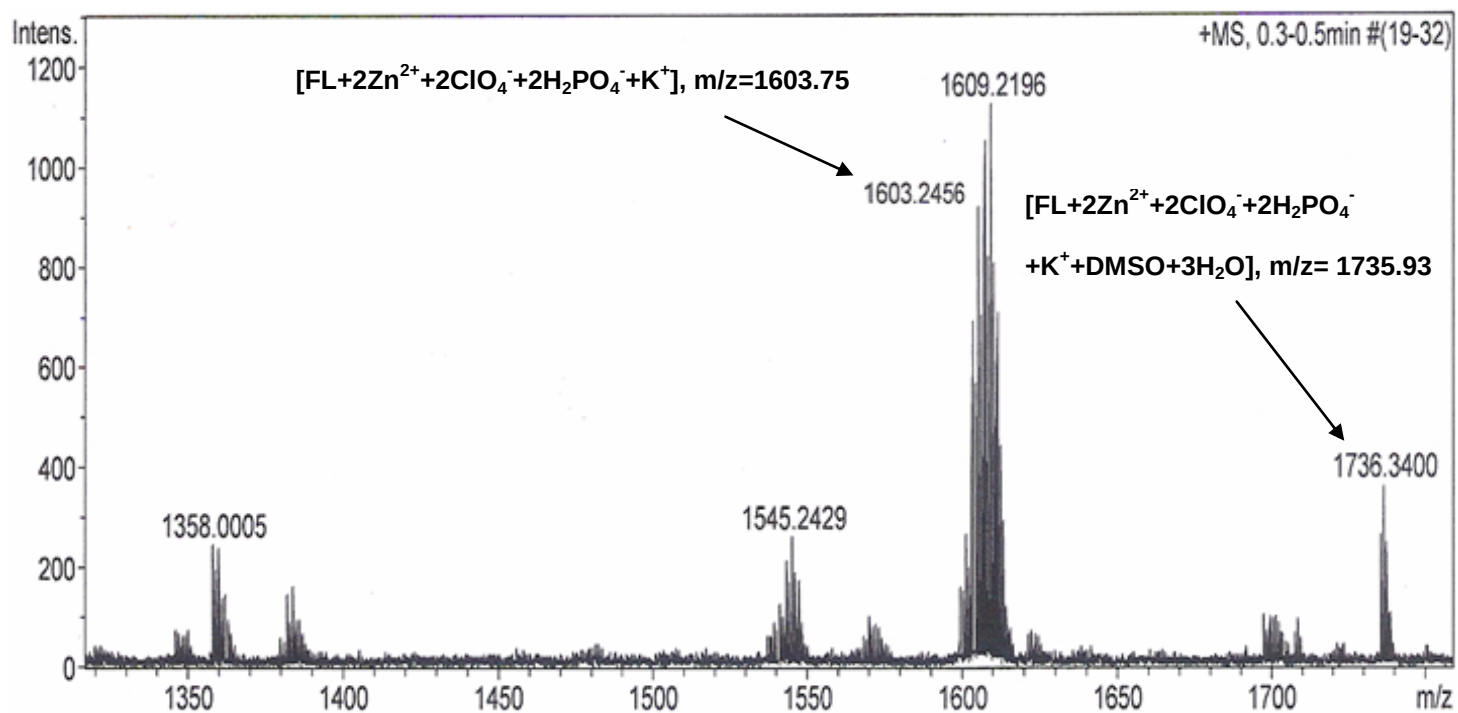
^1H NMR of compound 5 in Tetrachloroethane: CD_3CN (7:3) in presence of Zn^{2+} ions



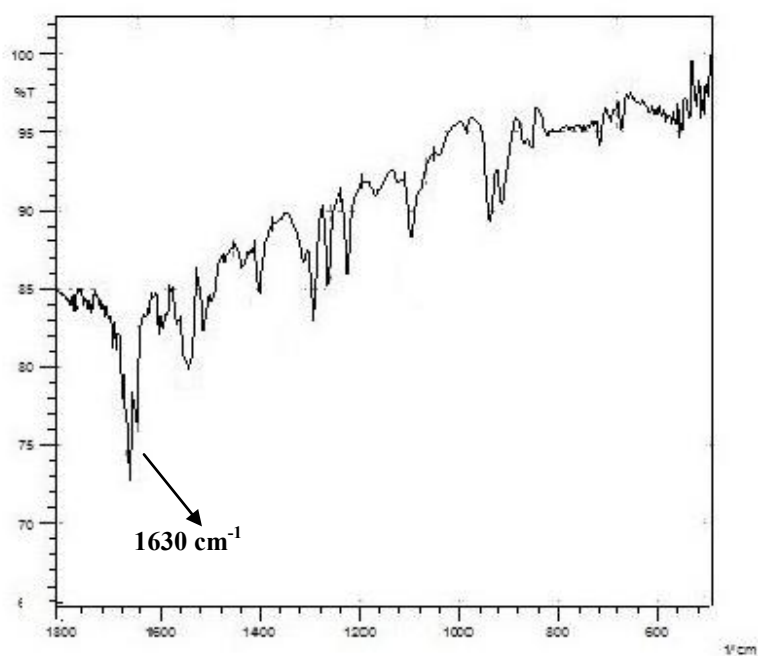
Mass spectrum of 5-Zn complex



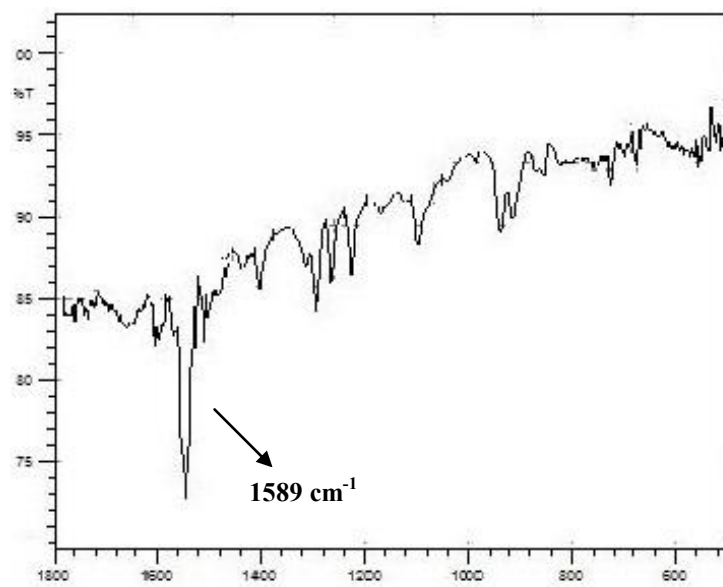
Mass spectrum of 5-Zn complex in the presence of H_2PO_4^-



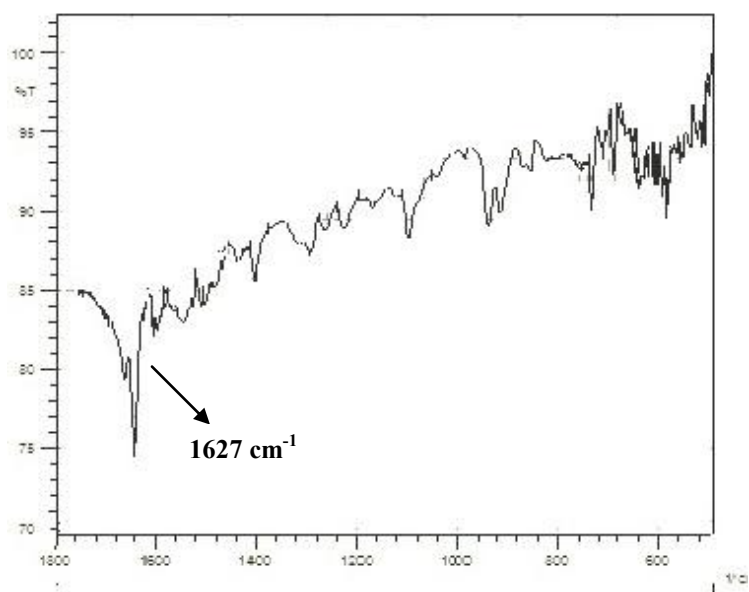
IR spectra of compound 5



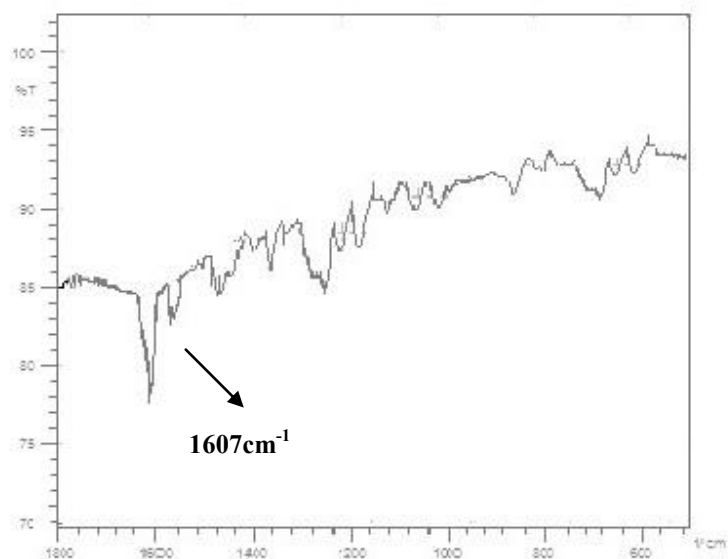
IR spectra of compound 5 + Zn



IR spectra of compound 5 + Zn²⁺ + OAc⁻



IR spectra of compound 5 + Zn + H_2PO_4^-



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Exp't Noise = 1.417E+00

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2	3.672E+05	8.242E+04	3.785E+00	Data Vector
3	7.088E+04	1.154E+04	1.417E+00	Data Vector
4	4.504E+03	7.038E+03	1.106E+00	Probably Noise
5	1.599E+03	5.439E+03	9.727E-01	Probably Noise

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2 1 0	False	1.05141E+01	+/- 3.55472E-01

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Convergence Found = 6.928E-05

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[STATISTICS]

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Goodness Of Fit, Chi^2 = 1.431E+02

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Goodness Of Fit, Chi^2 (raw data) = None

[COVARIANCE]

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[CORRELATION]

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[END FILE]

