Supplementary Information

Synthesis, electrochemical, fluorescence and antimicrobial studies of 2-chloro-3-amino-1,4-naphthoquinone bearing mononuclear transition metal dithiocarbamate complexes [M{κ^2*S,S*-S_2C-piperazine-C_2H_4N(H)ClNQ}$_n$]

Sanjay K Verma and Vinay K Singh*

Department of Chemistry, Faculty of Science, The M. S. University of Baroda, Vadodara-390 002, India.

Email: vks.msu@gmail.com; vinay.singh-chem@msubaroda.ac.in

1. **IR spectra:** IR spectra of the 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**) and its complexes are summarized below as Fig. S1 to S5.

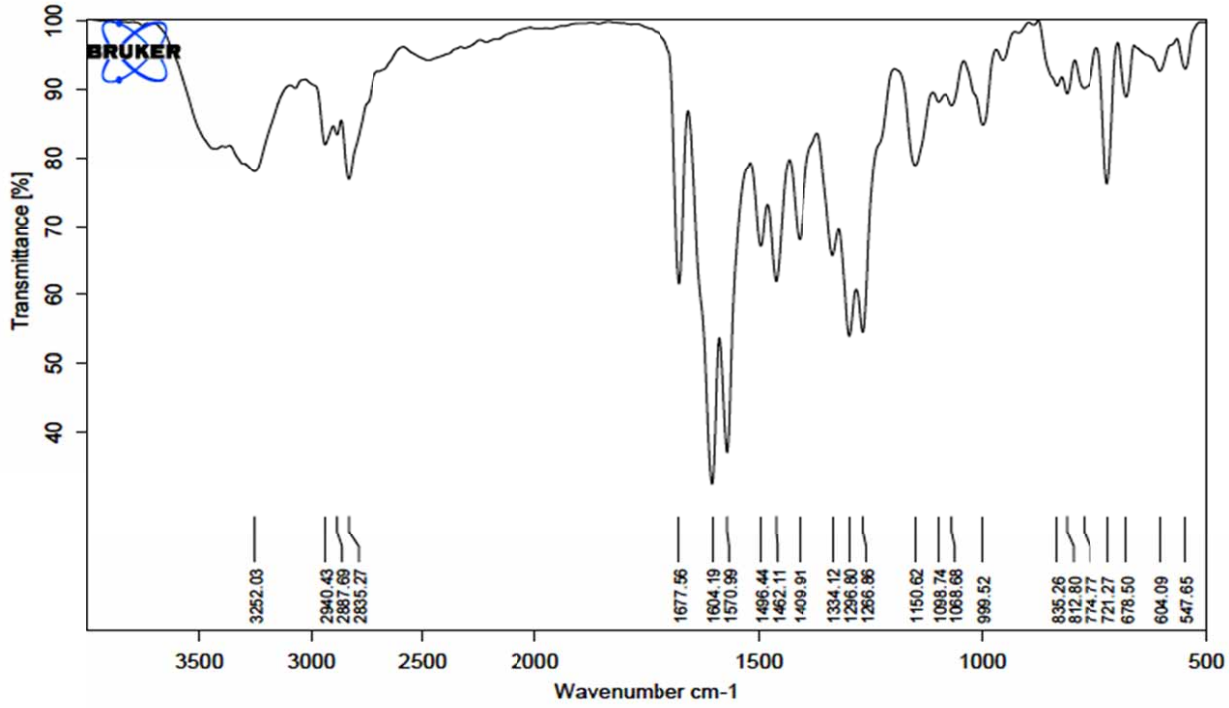

Fig. S1: IR Spectrum of the 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**)

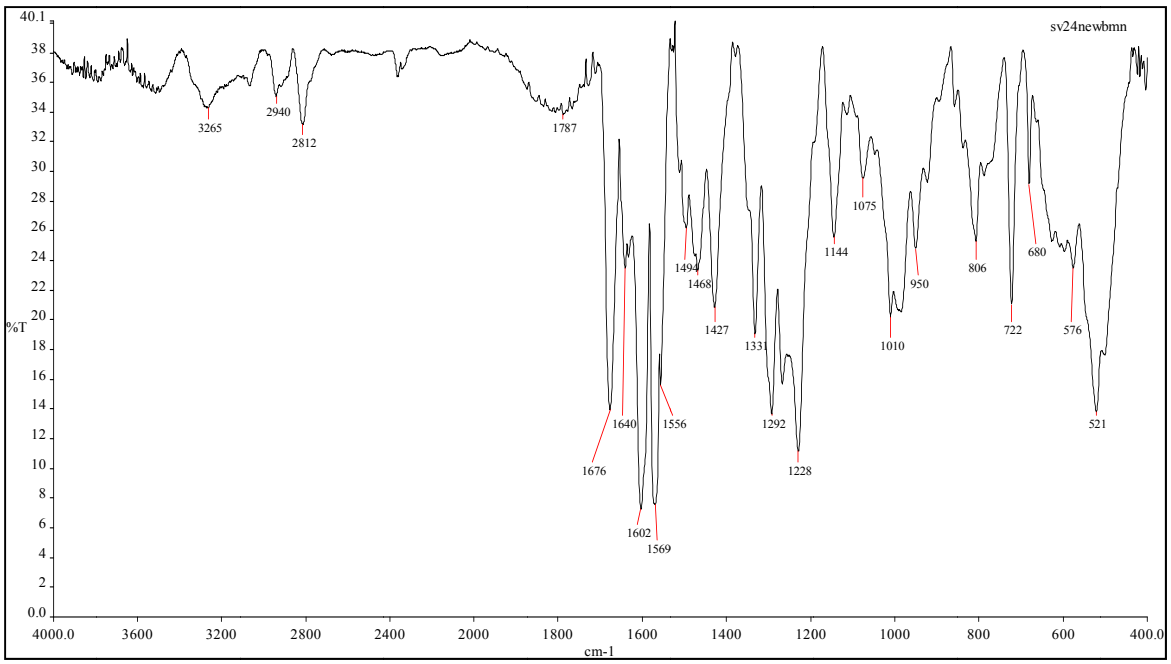

Fig. S2: IR Spectrum of compound 1

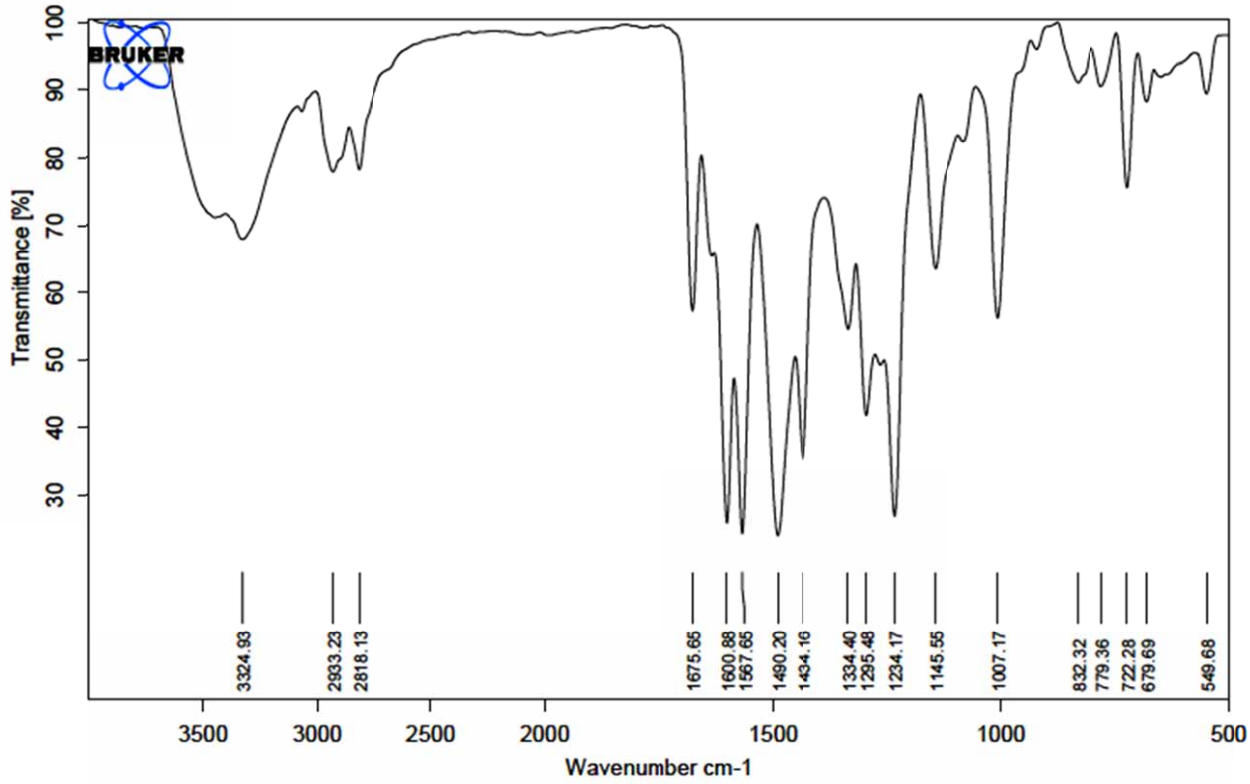

Fig. S3: IR Spectrum of compound 2

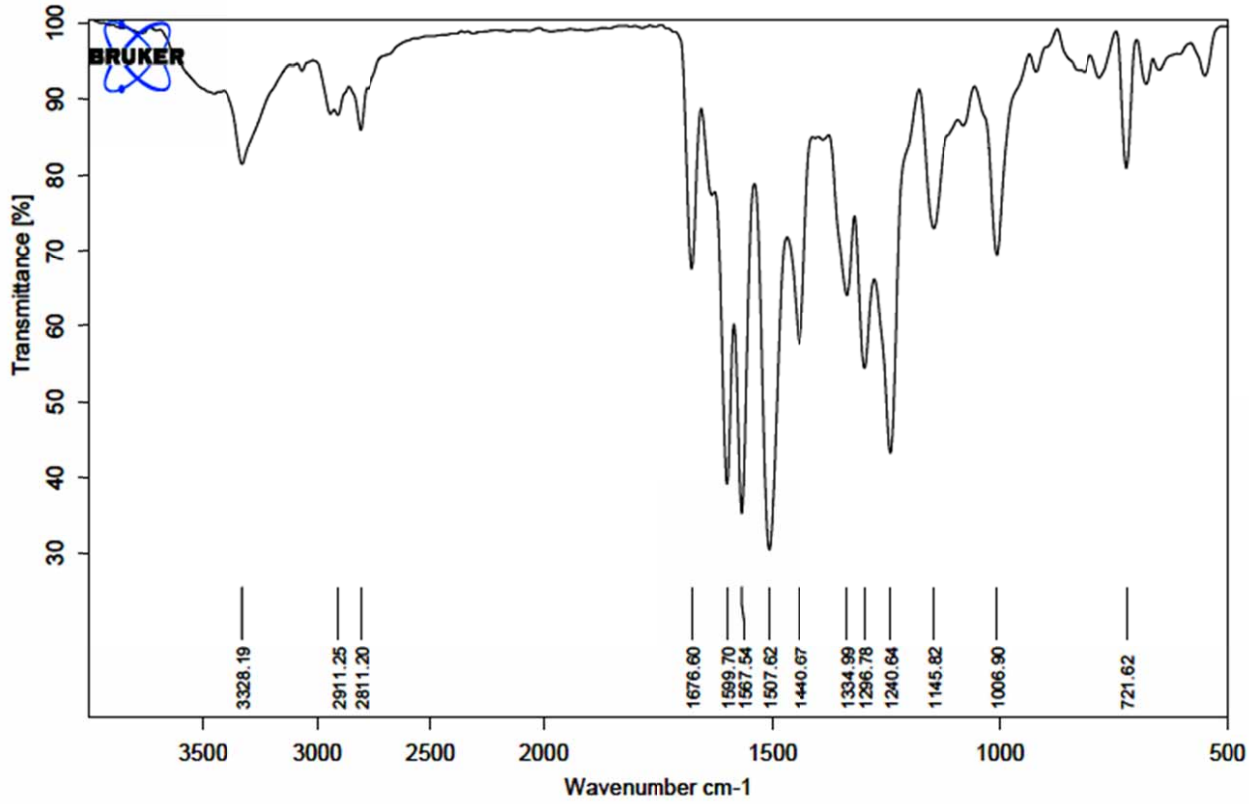

Fig. S4: IR Spectrum of compound 3

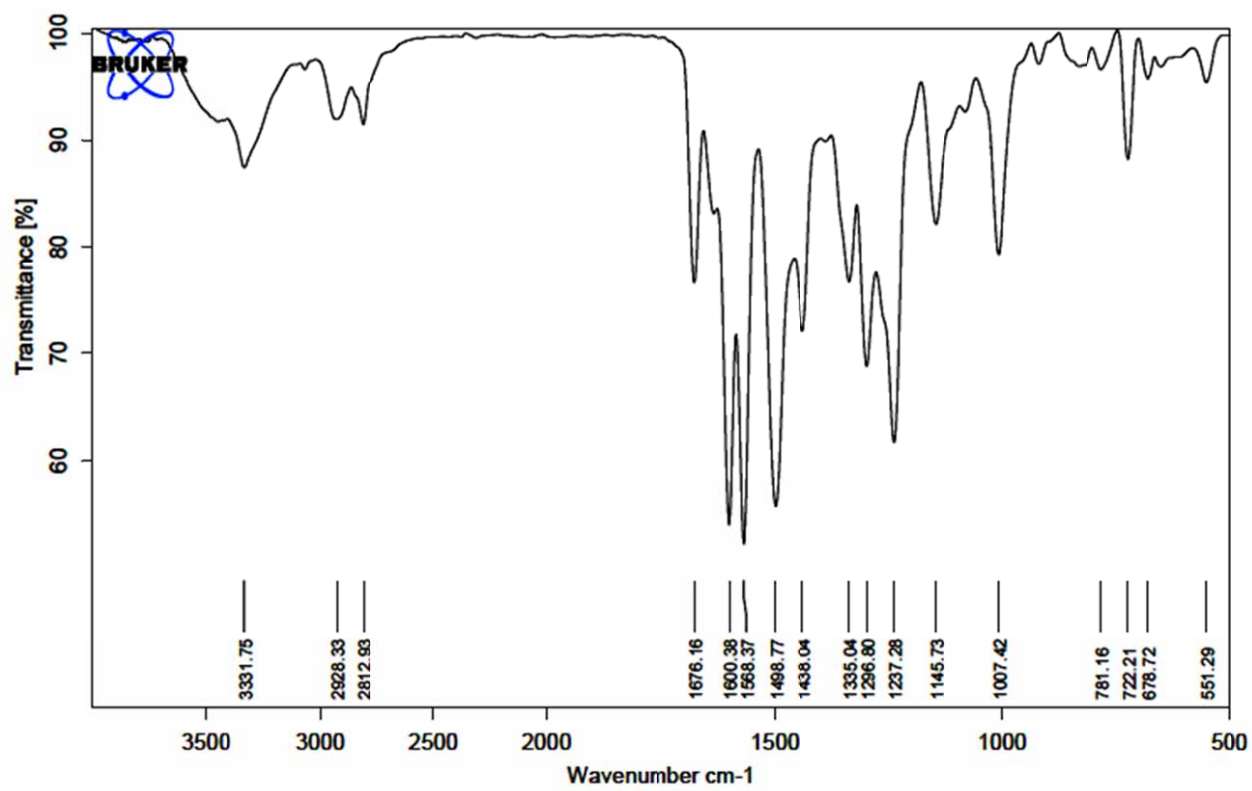

Fig. S5: IR Spectrum of compound 4

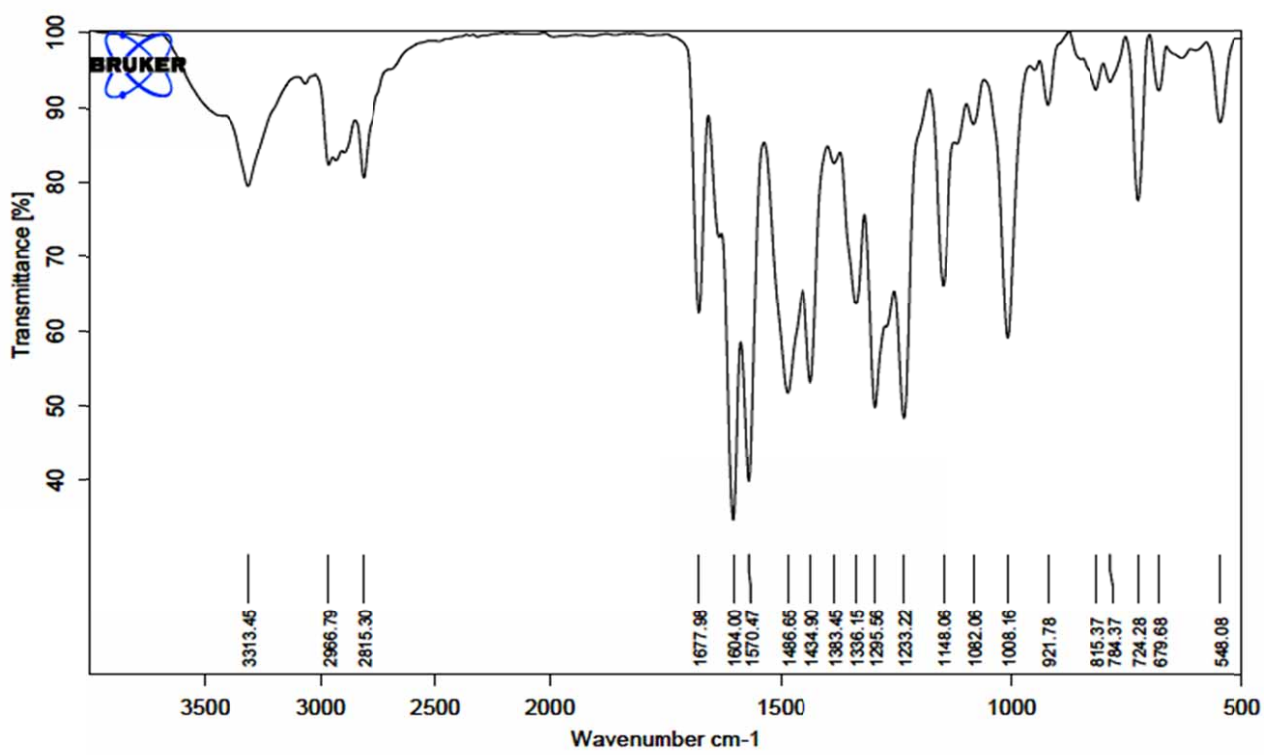

Fig. S6: IR Spectrum of compound 5

2. **NMR spectra:** The NMR spectra of the 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**), its triethyl ammonium dtc salt and complexes are summarized below as Fig. S7 to S12.

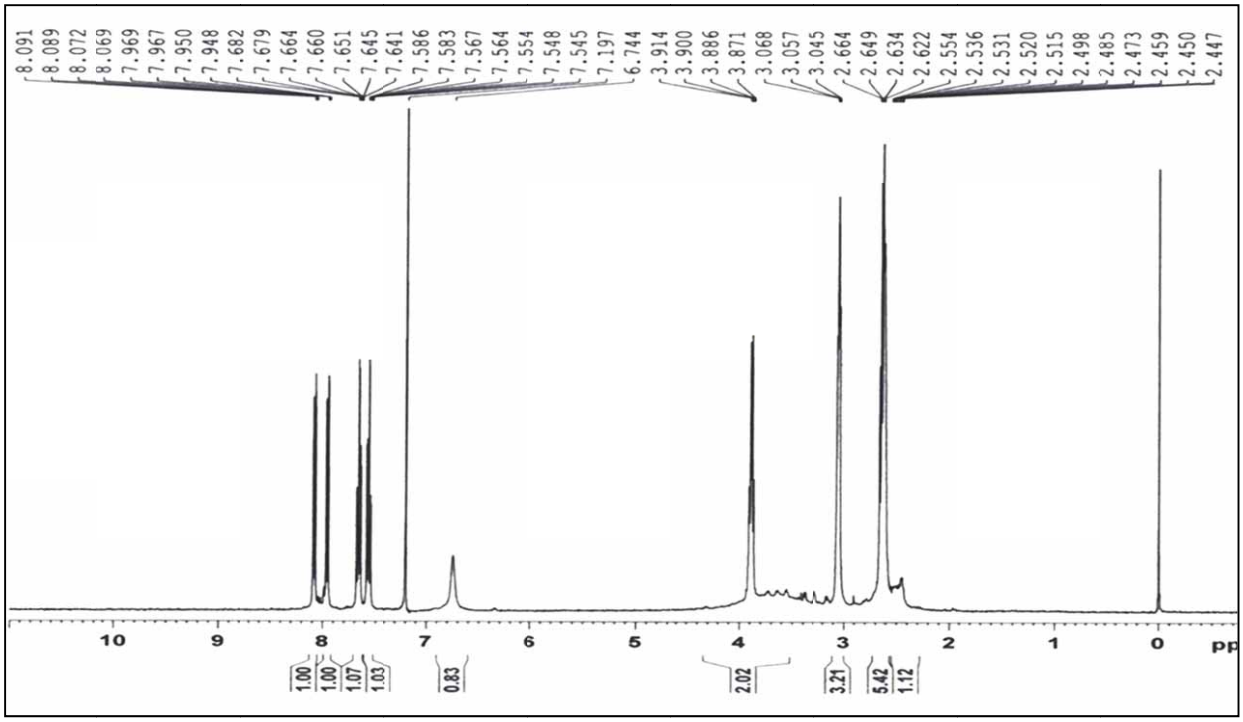

Fig. S7: ^{1}H NMR spectrum of the 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**).

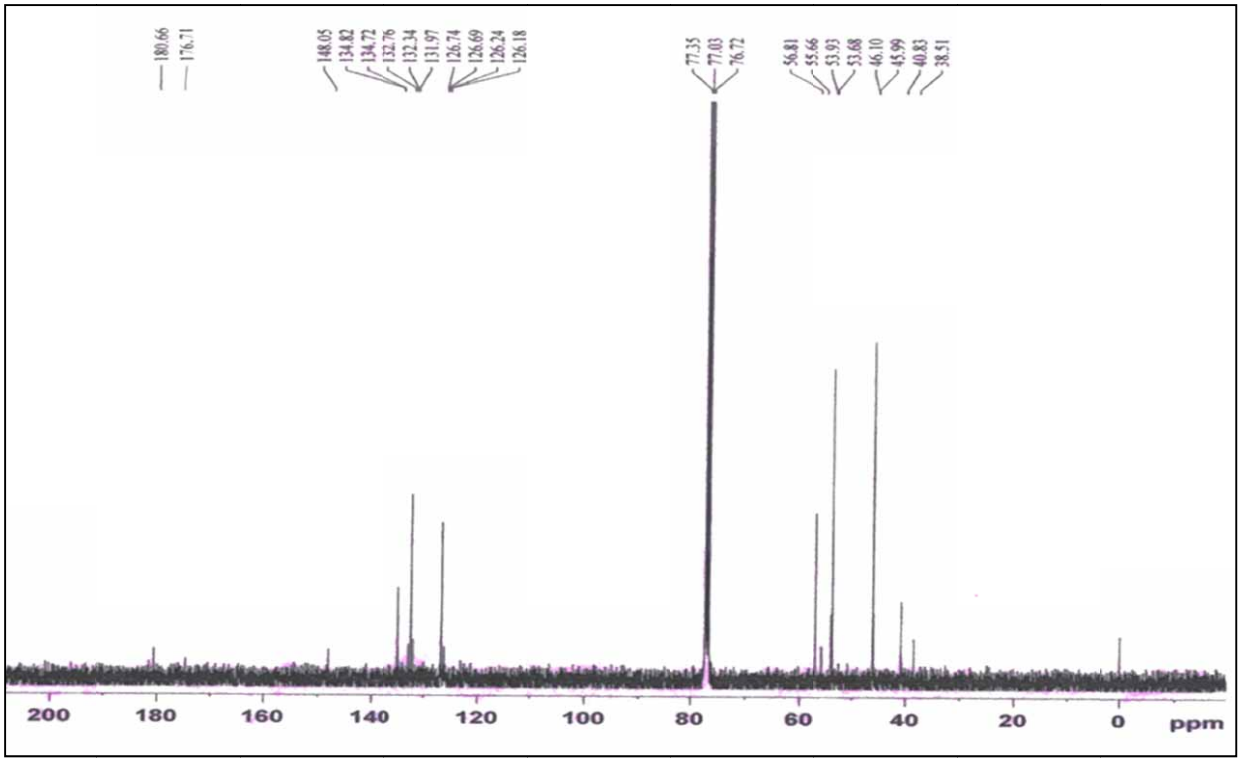

Fig. S8: ^{13}C NMR spectrum of 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**).

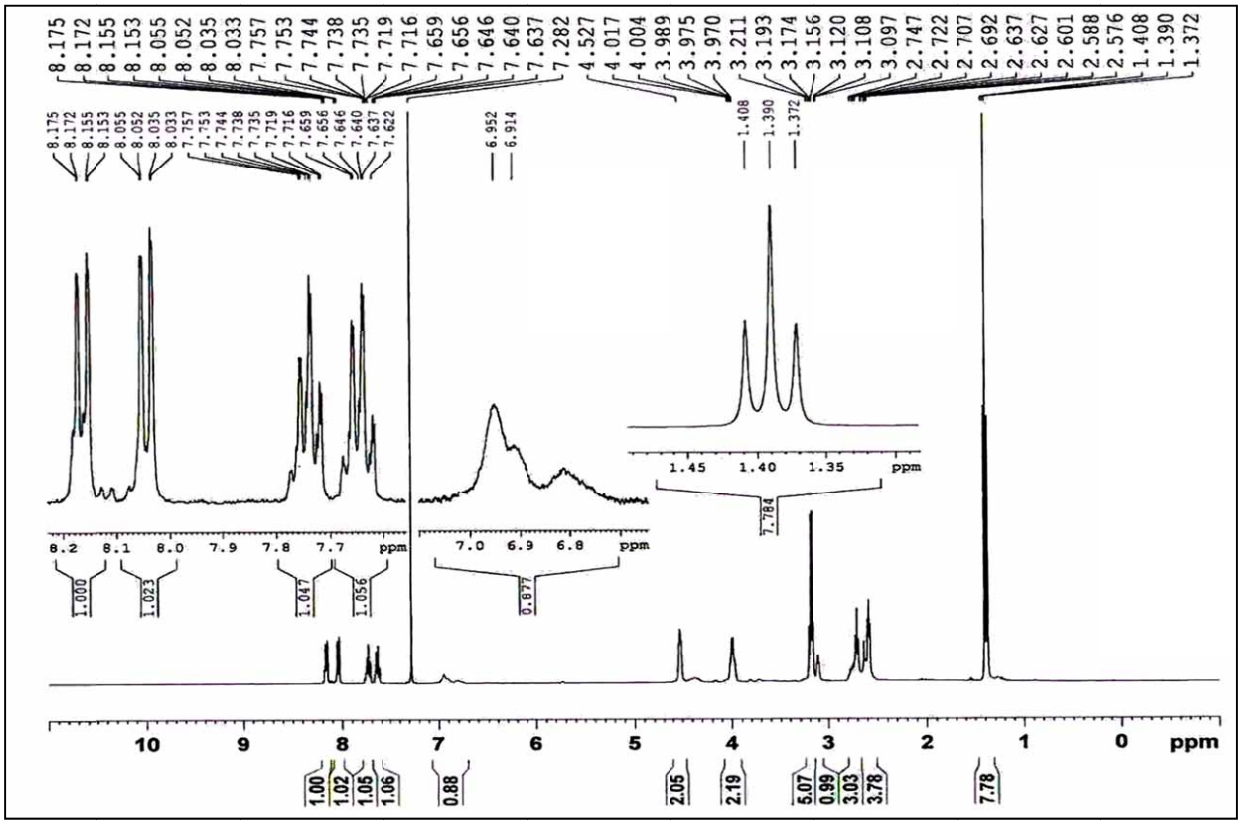

Fig. S9: ^{1}H NMR spectrum of triethyl ammonium dtc salt of the ligand precursor L.

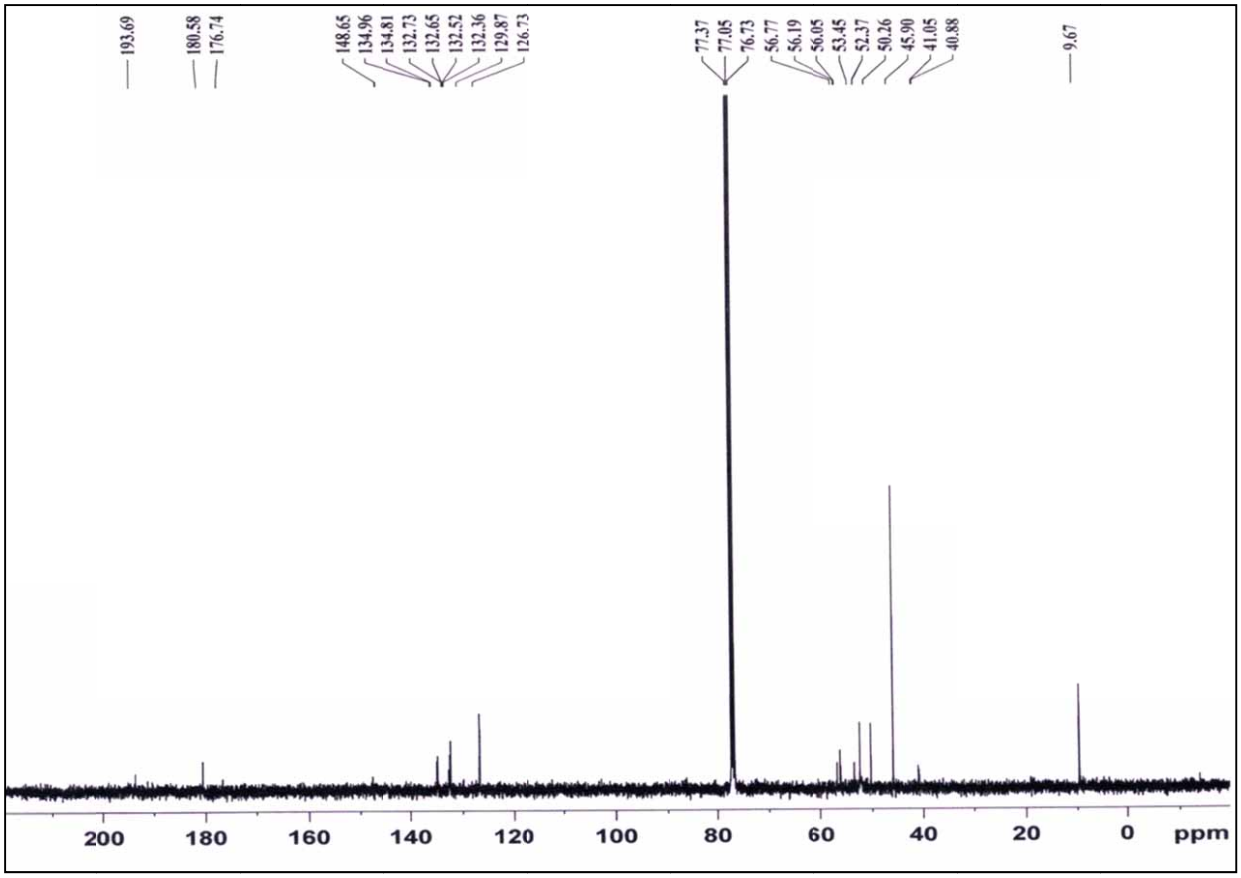

Fig. S10: ^{13}C NMR spectrum of triethyl ammonium dtc salt of the ligand precursor L.

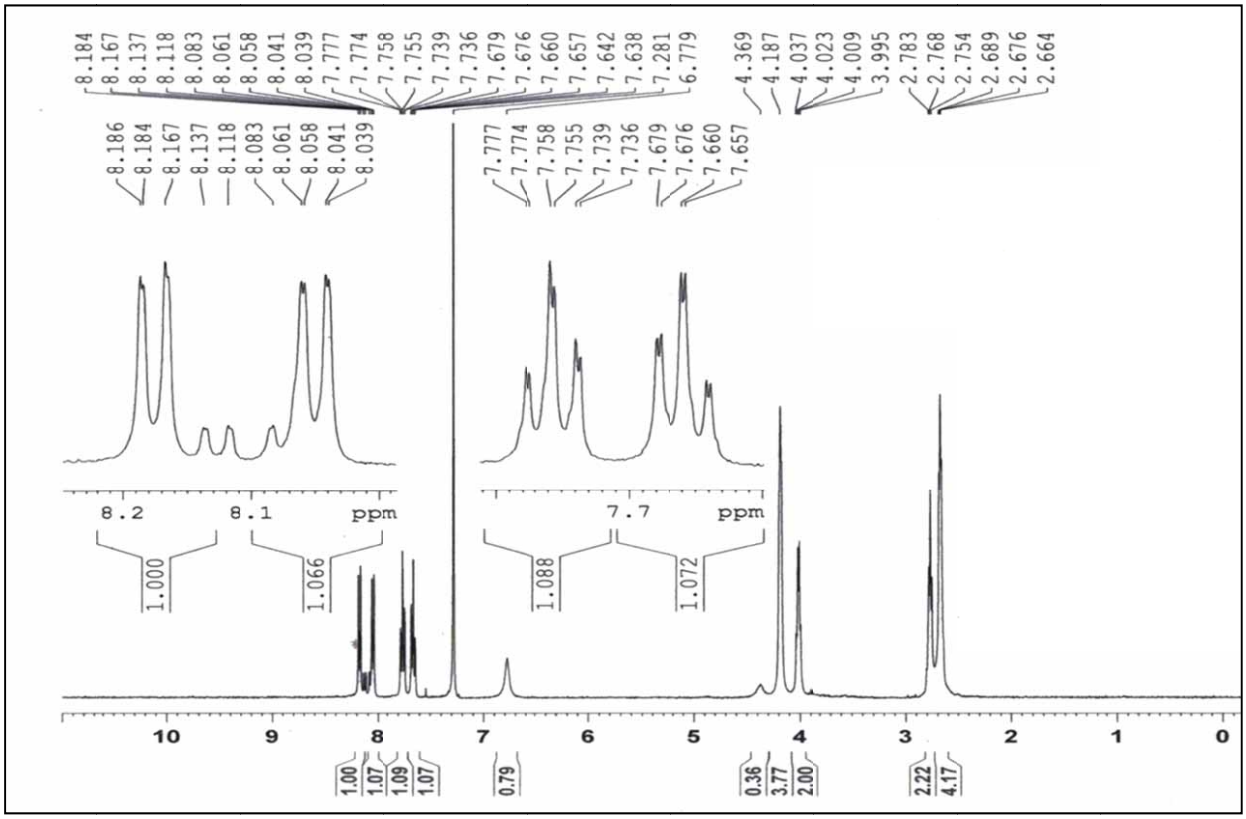

Fig. S11: ^{1}H NMR spectrum of compound 5.

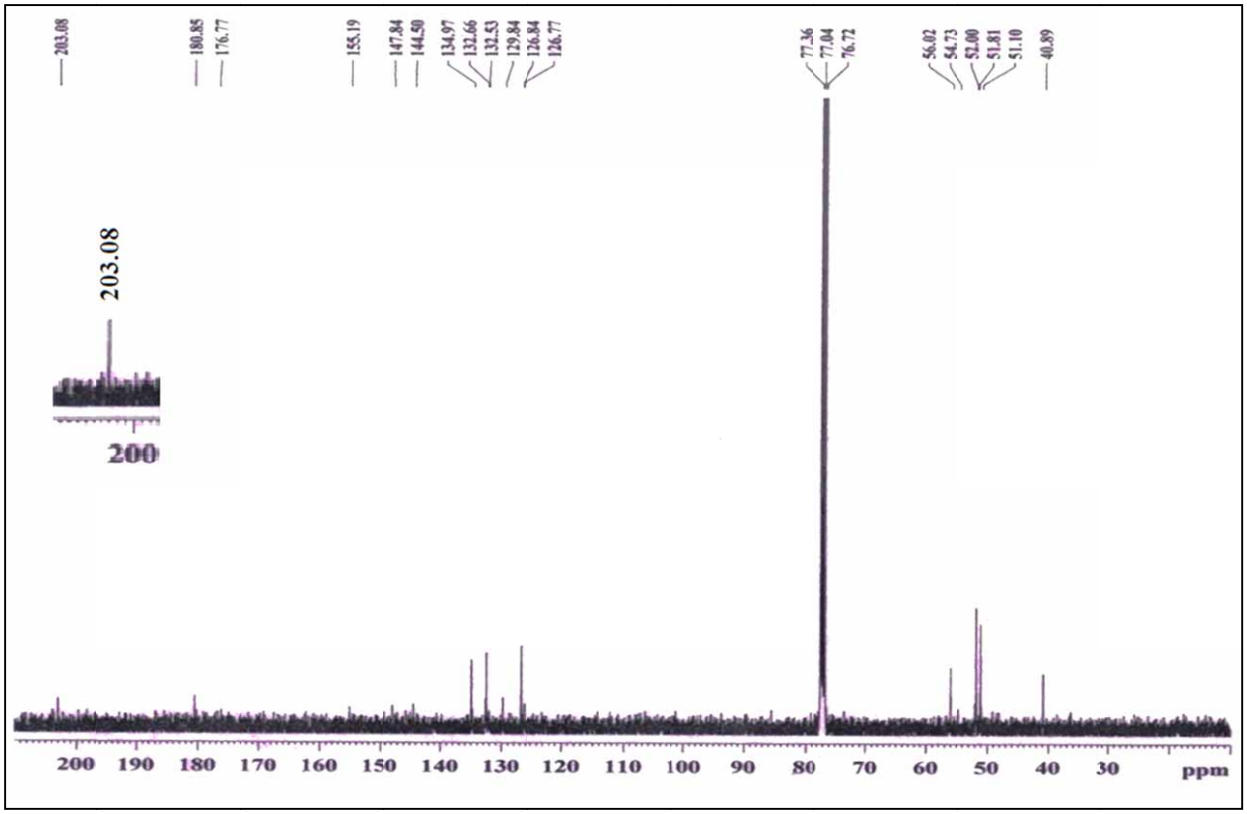

Fig. S12: ^{13}C NMR spectrum of compound 5.

3. **ESI MS spectra:** The ESI MS spectra of the dithiocarbamate metal complexes are summarized below as Fig. S13 to S18

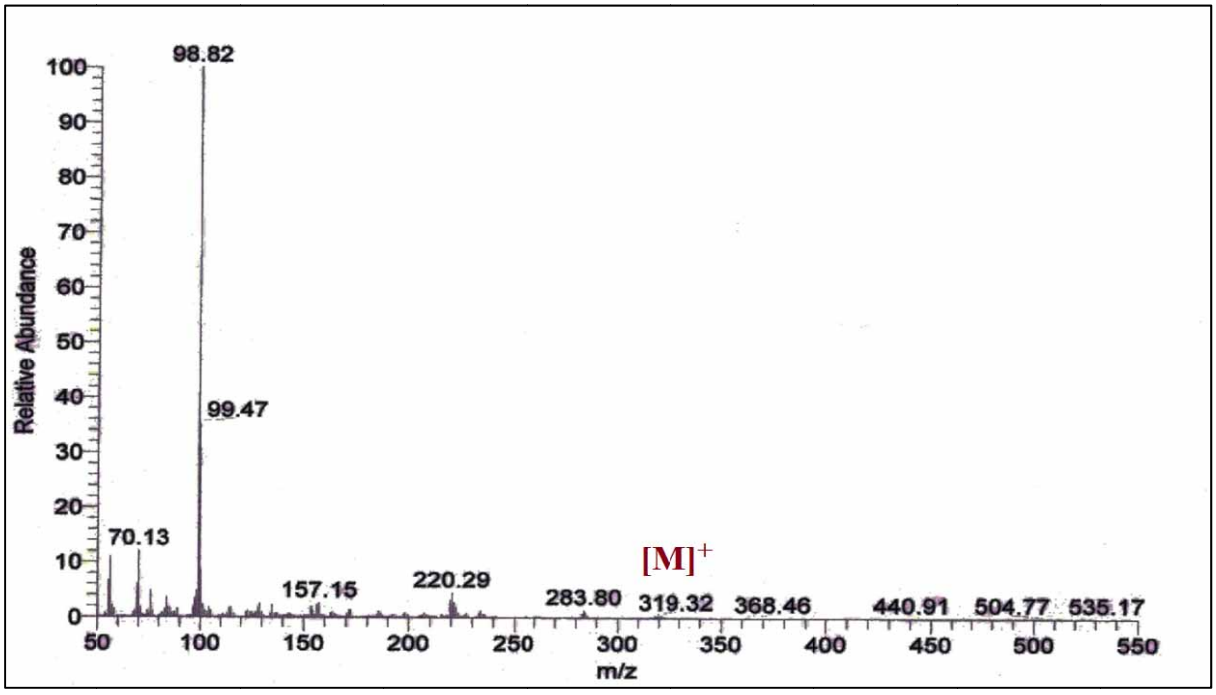

Fig. S13: GC MS spectrum of 2-chloro-3-{2-(piperazinyl)ethyl}-amino-1, 4-naphthoquinone (**L**).

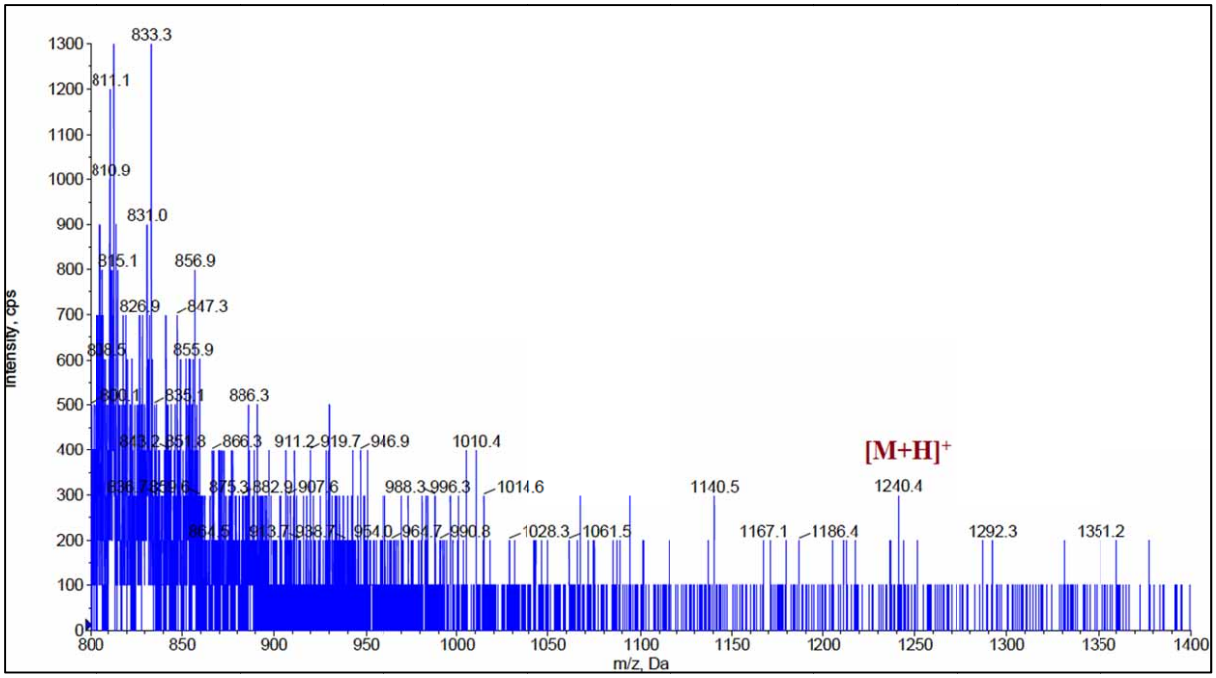

Fig. S14: LC MS spectra of compound **1**.

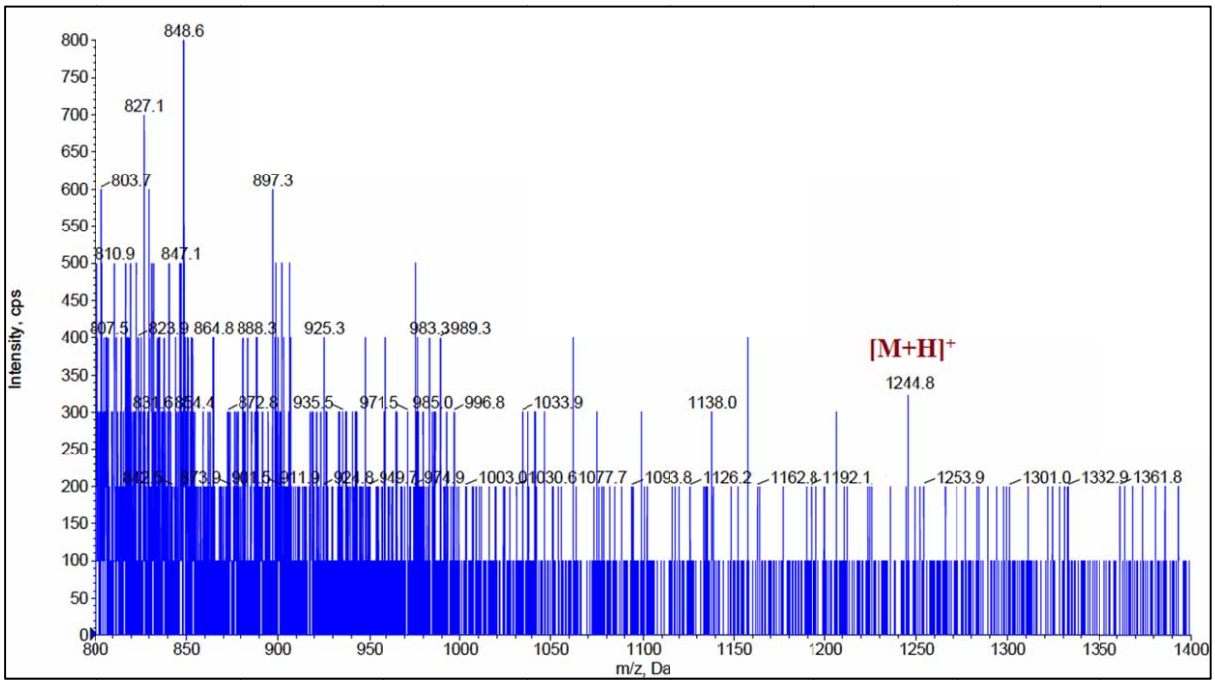

Fig. S15: LC MS spectra of compound **2**.

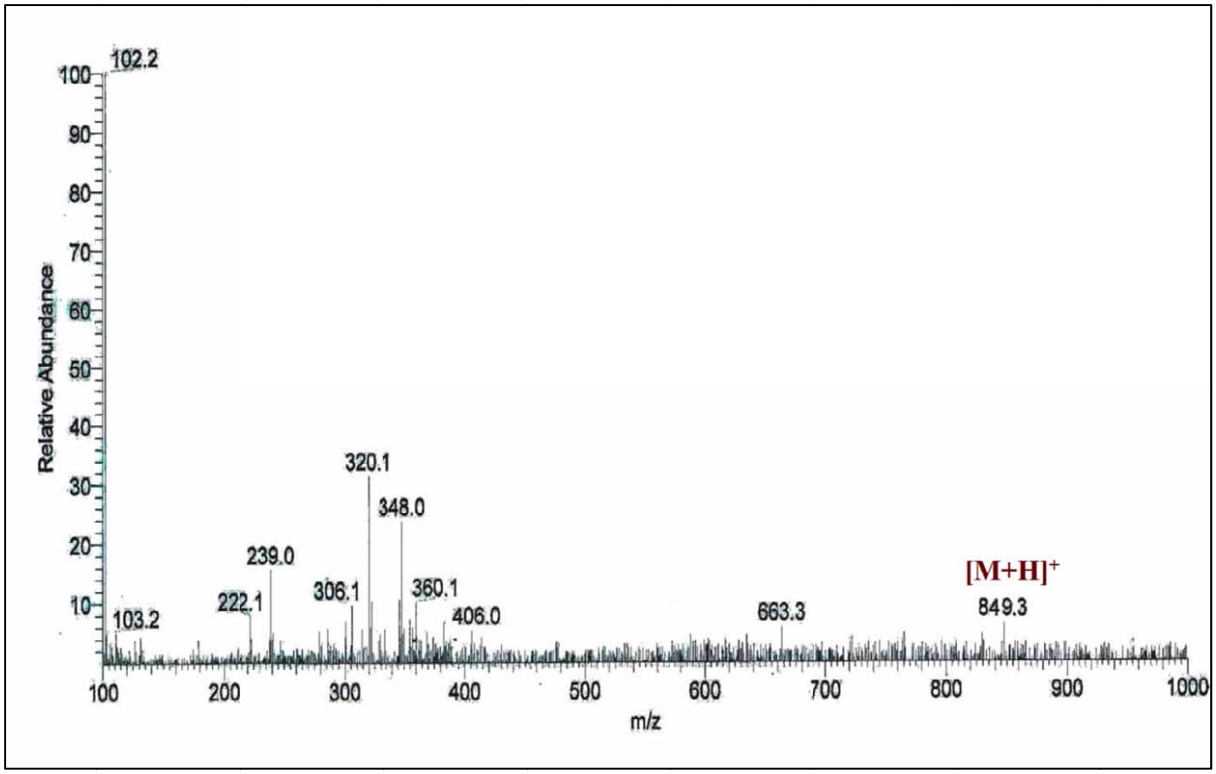

Fig. S16: ESI MS spectra of compound **3**.

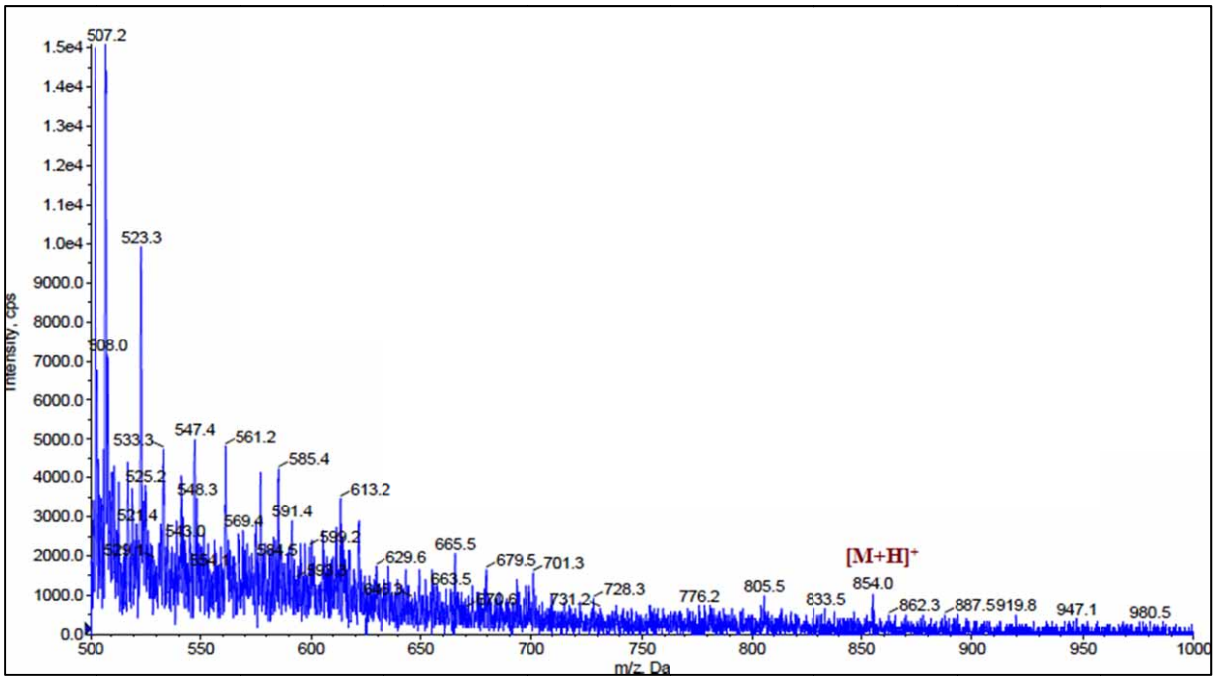

Fig. S17: LC MS spectra of compound **4**.

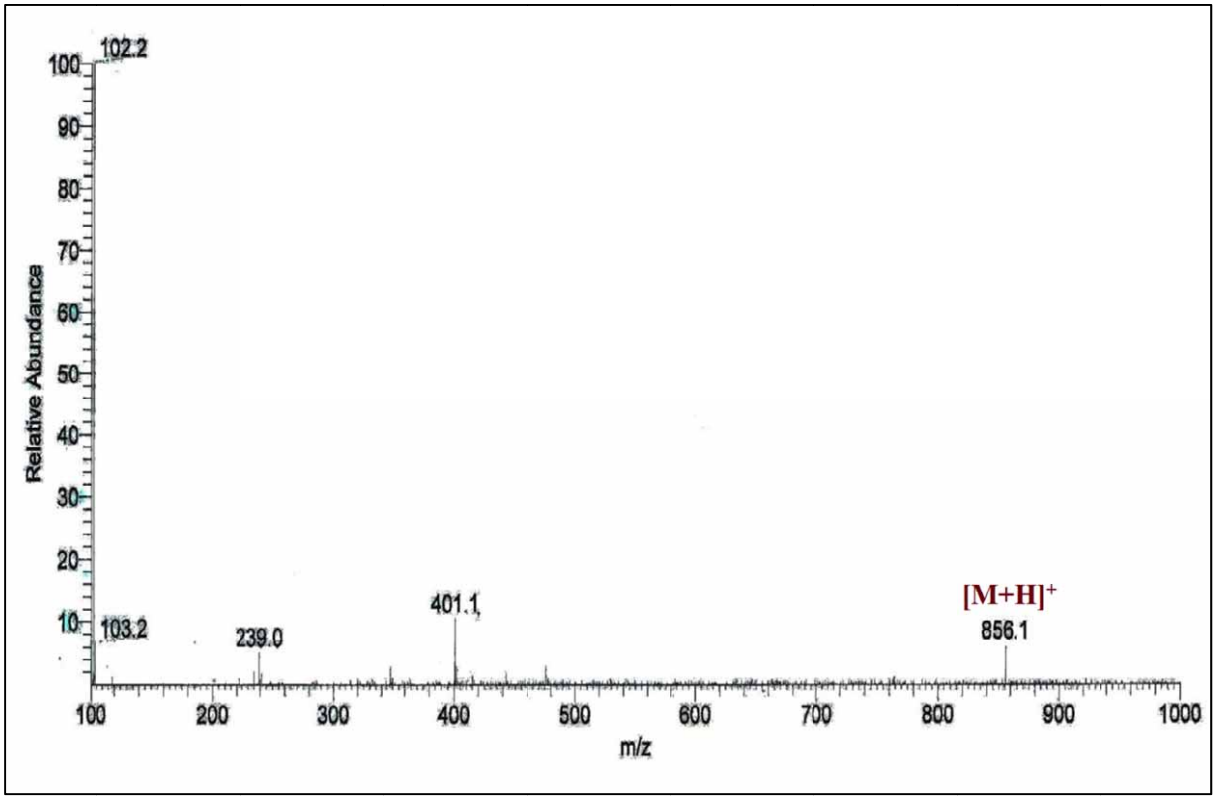

Fig. S18: ESI MS spectra of compound 5.

4. **TG/DTA:** TG/ DTA curve of the dithiocarbamate metal complexes are summarized below as Fig. S19 to S20

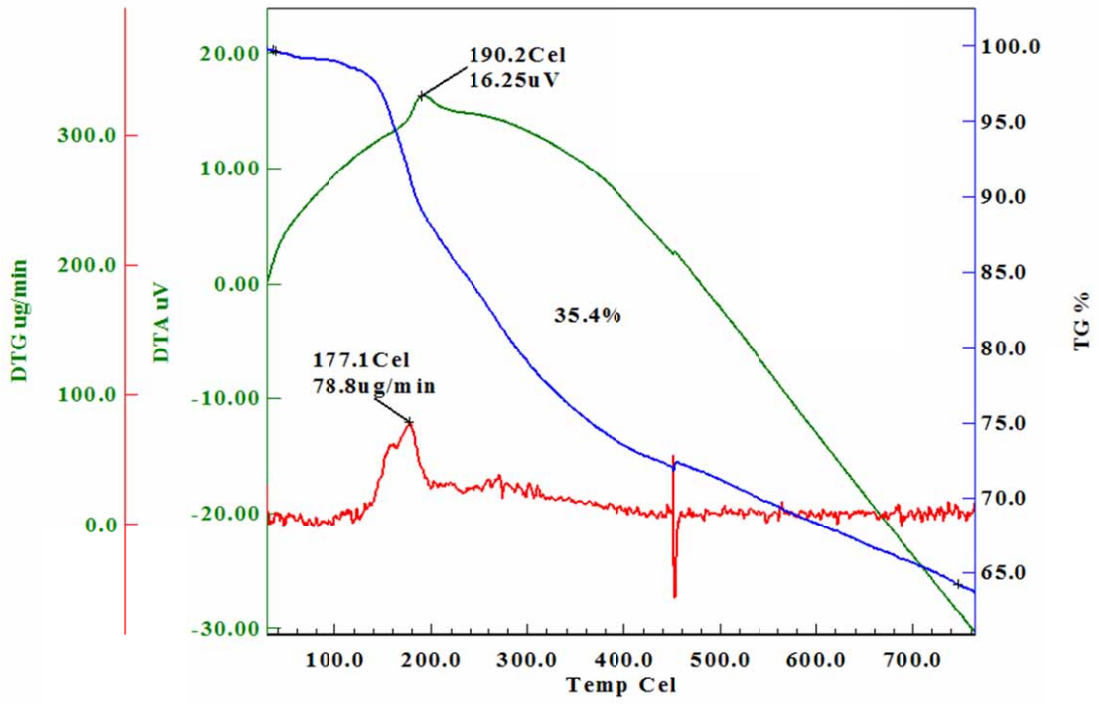

Fig. S19: TG/DTA curve of the dithiocarbamate metal complexes **1**

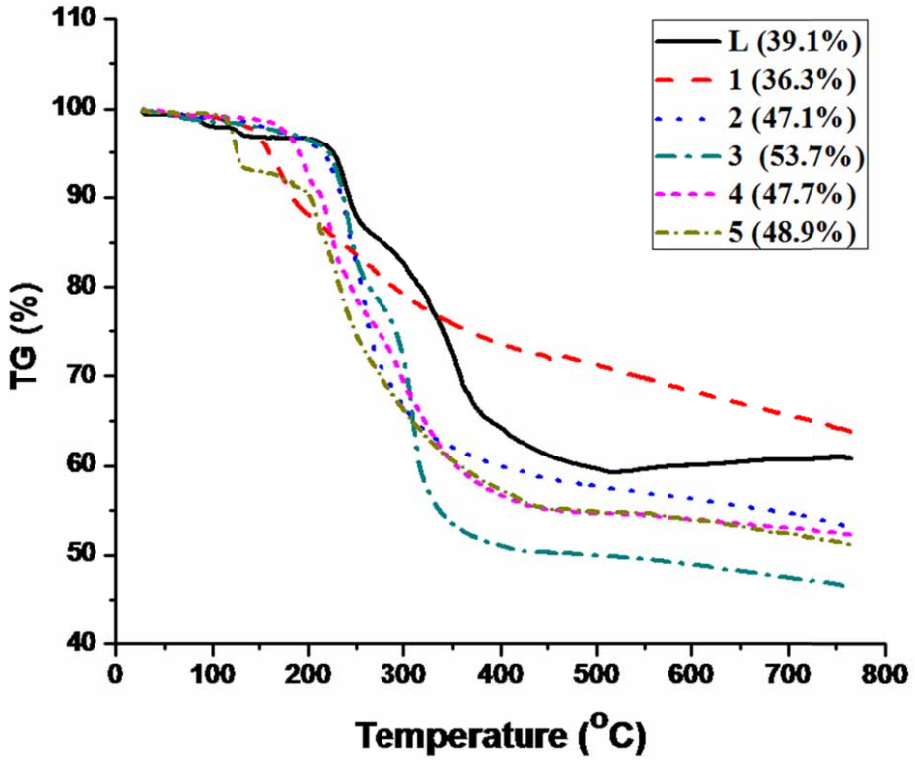

Fig. S20: TG curves of the dithiocarbamate metal complexes **1-5**

Table S1: Summary of the calculated values of ES-MS (other than [M+H] and $[M]^+$ ion peaks) matches well with the observed ones on MS spectra of **L** and **1-5**.

Entry	Loss of fragment	Corresponding weight	Remaining weight	Observed weight corresponding to base peak in MS
L	Piperazine moiety $[C_5H_{11}N_2]$	98.82	220.5	99
1	Loss of two molecules of naphthoquinone moiety $C_{20}H_8Cl_2N_2O_4$	410	830	833
2	Loss of two molecule of naphthoquinone moiety with chlorine and nitrogen $[C_{10}\ H_4O_2ClN]$	401.1	843	848.6
3	Two molecule of piperazinyl dithiocarbamate $[C_5N_2S_2]$	320.1	529.3	320
4	Remaining fragment after loss of two molecule of piperazinyl dithiocarbamate	523	321	523.3

	$[C_5H_8N_2S_2]$ $C_{29}H_{26}Cl_2N_4S_2Cu$			
5	**1**. Two molecule of naphthoquinone moiety with chlorine and nitrogen $[C_{10}H_4O_2ClN]$ **2**. Piperazine moiety $[C_5H_{12}N_2]$	401.1 102.2	455 754	410 100