Supporting Information

Development of fluorophoric [2]pseudorotaxanes and [2]rotaxane: Selective sensing of Zn(II)

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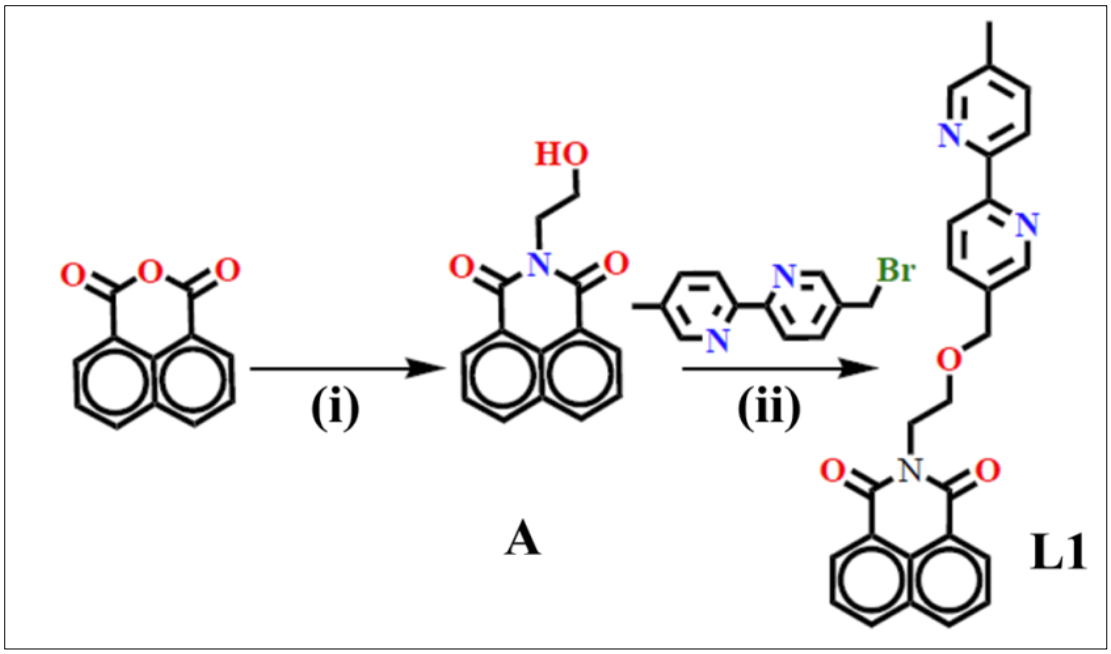
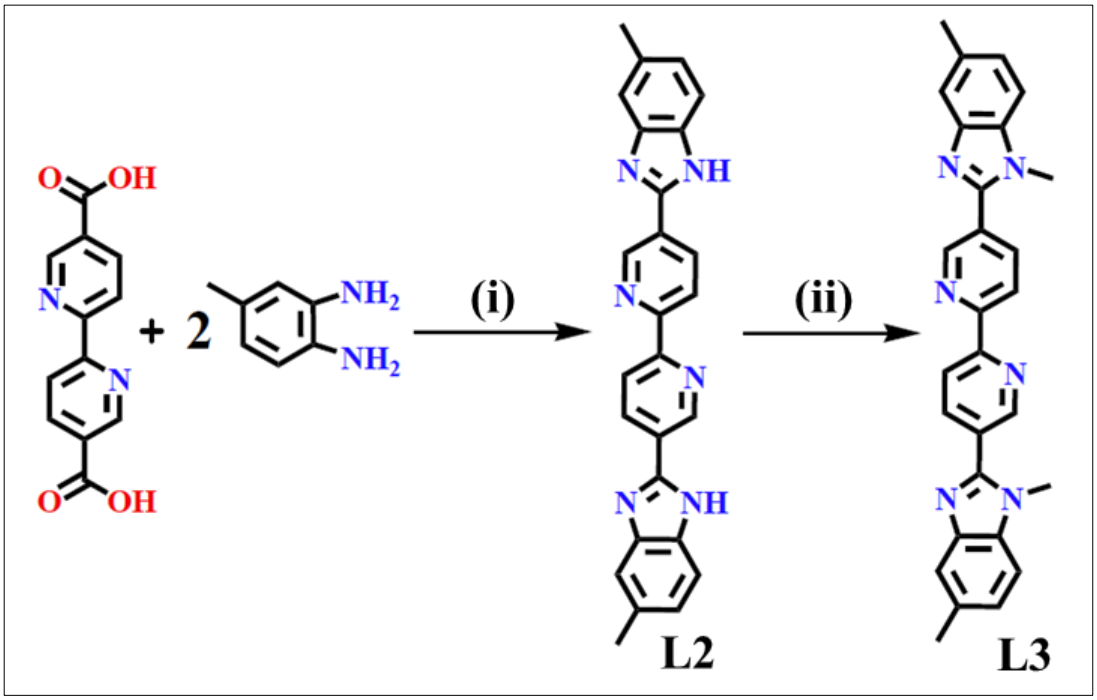
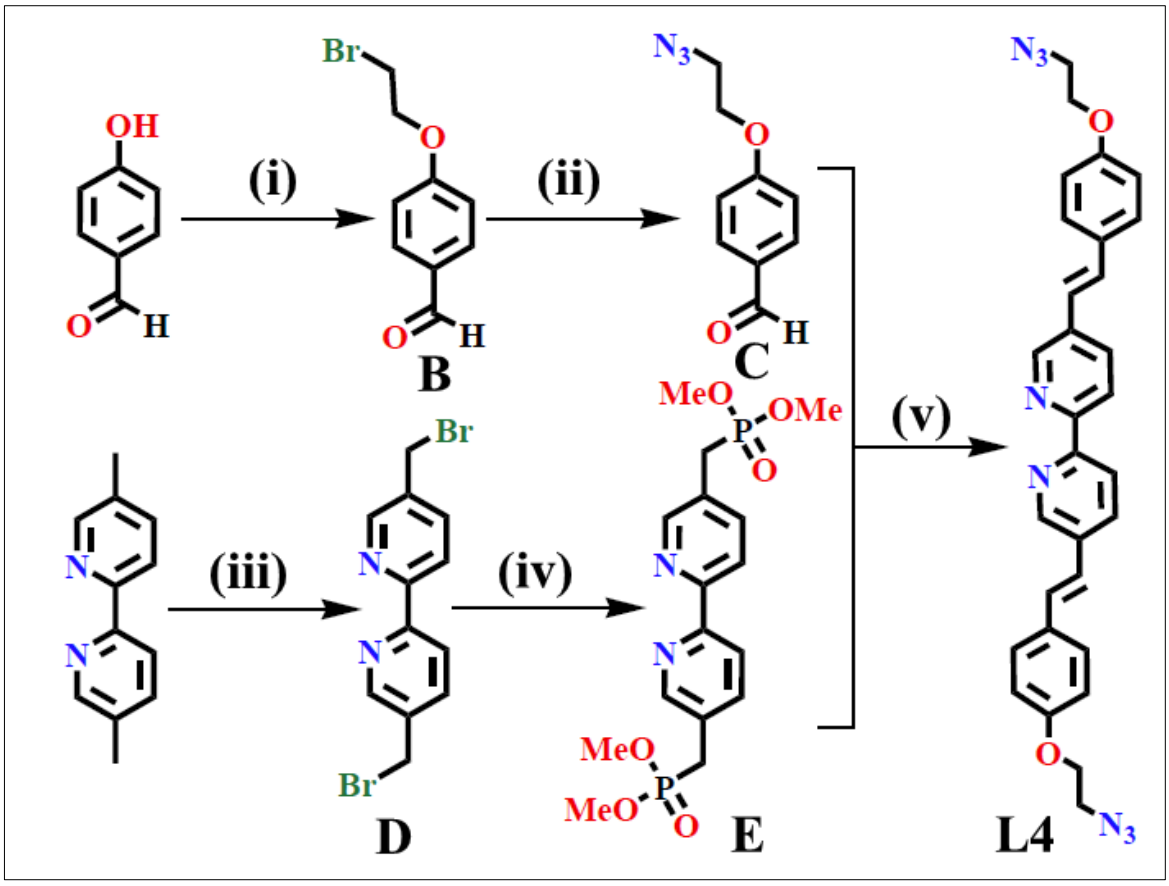


Scheme 1S. Synthetic path of **L1**: (i) 2-amino ethanol, CH_3CH_2OH, reflux, 14h; (ii) NaH, THF, stirring at 0 °C followed by stirring at RT for 12 h.



Scheme 2S. Synthetic path of **L2** and **L3**: (i) PPA, reflux, 18h; (ii) Methyl iodide, NaH, THF, stirring at 0^0C followed by stirring at RT for 12 h.



Scheme 3S. Synthetic path of **L4**: (i) 1,2-dibromo ethane, CH_3CN, K_2CO_3, reflux; (ii) NaN_3, DMF, reflux, 8h; (iii) NBS, AIBN, CCl_4, reflux; (iv) trimethyl phosphite, reflux; (v) potassium tertbutoxide, DMF, 0^0C, stirring, 10 h.

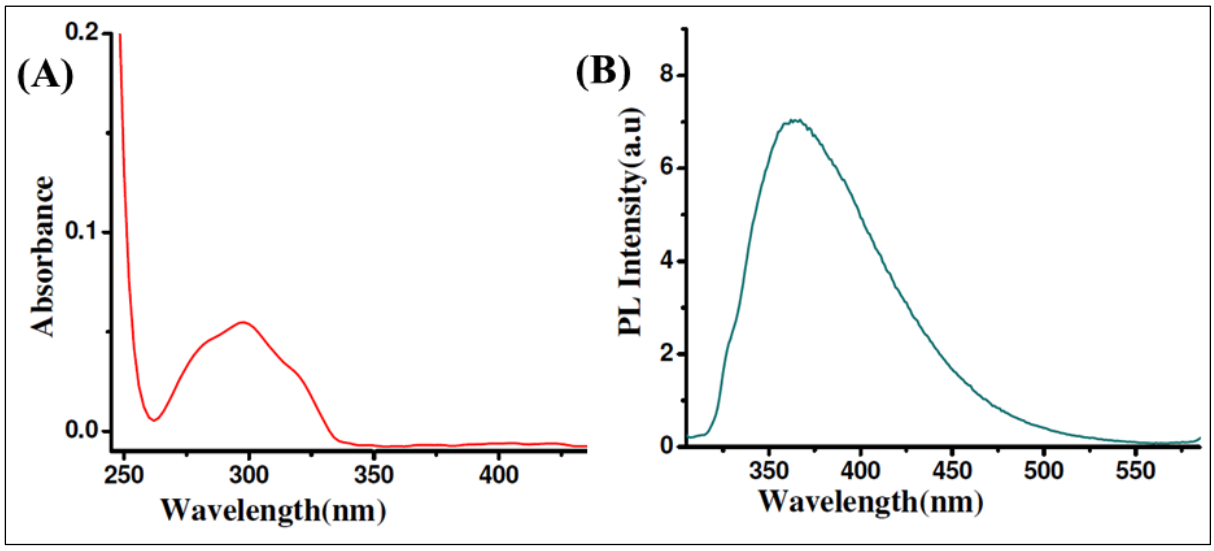


Figure 1S. (A) UV/Vis and (B) emission spectra of **NaphMC** at 298K.

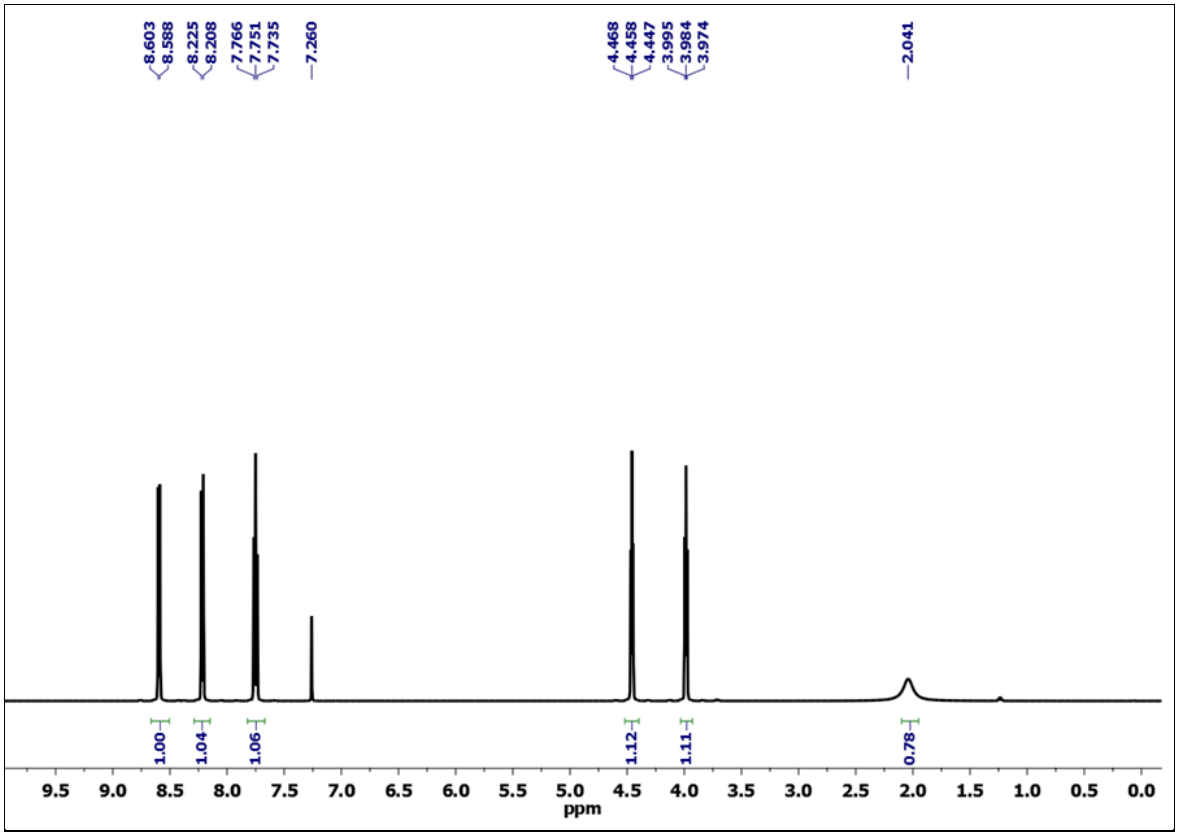


Figure 2S. ^{1}H-NMR spectrum of **A** in $CDCl_3$ in 500 MHz at 298K.

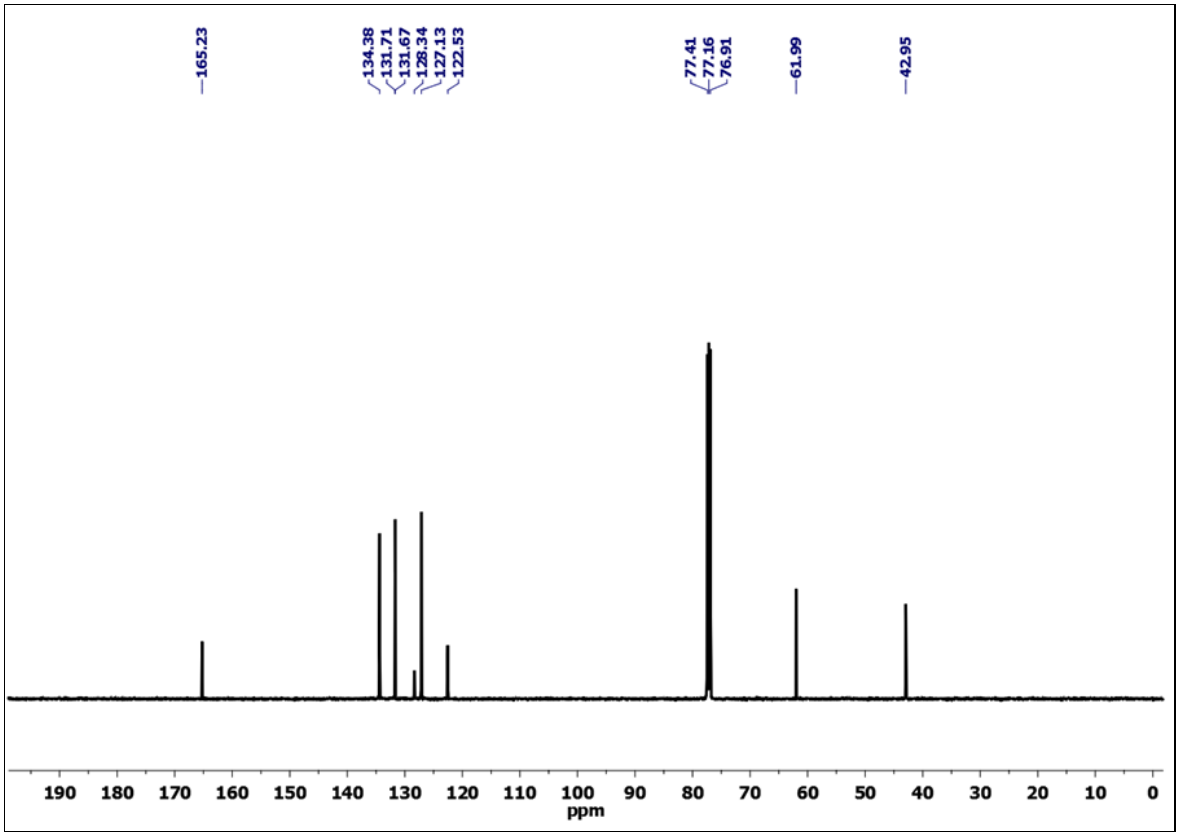


Figure 3S. ^{13}C-NMR spectrum of **A** in $CDCl_3$ in 125 MHz at 298K.

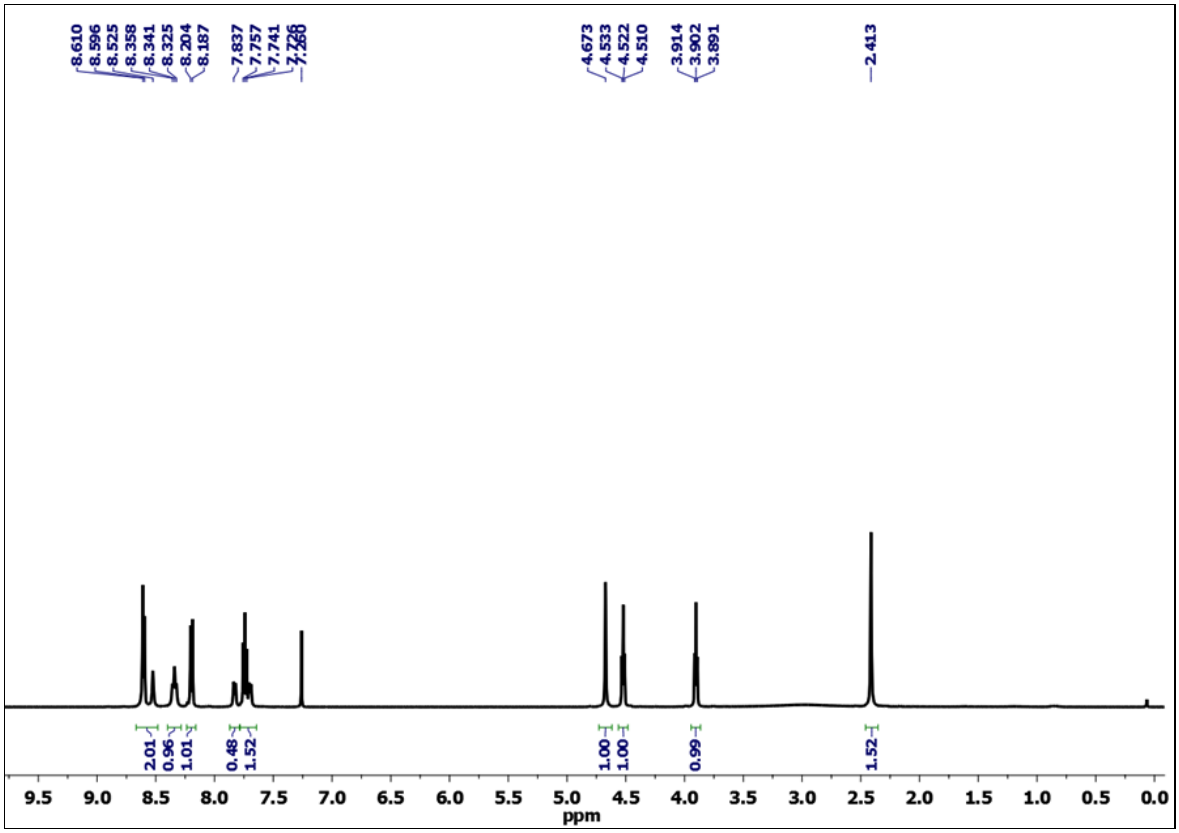


Figure 4S. ^{1}H-NMR spectrum of **L1** in $CDCl_3$ in 500 MHz at 298K.

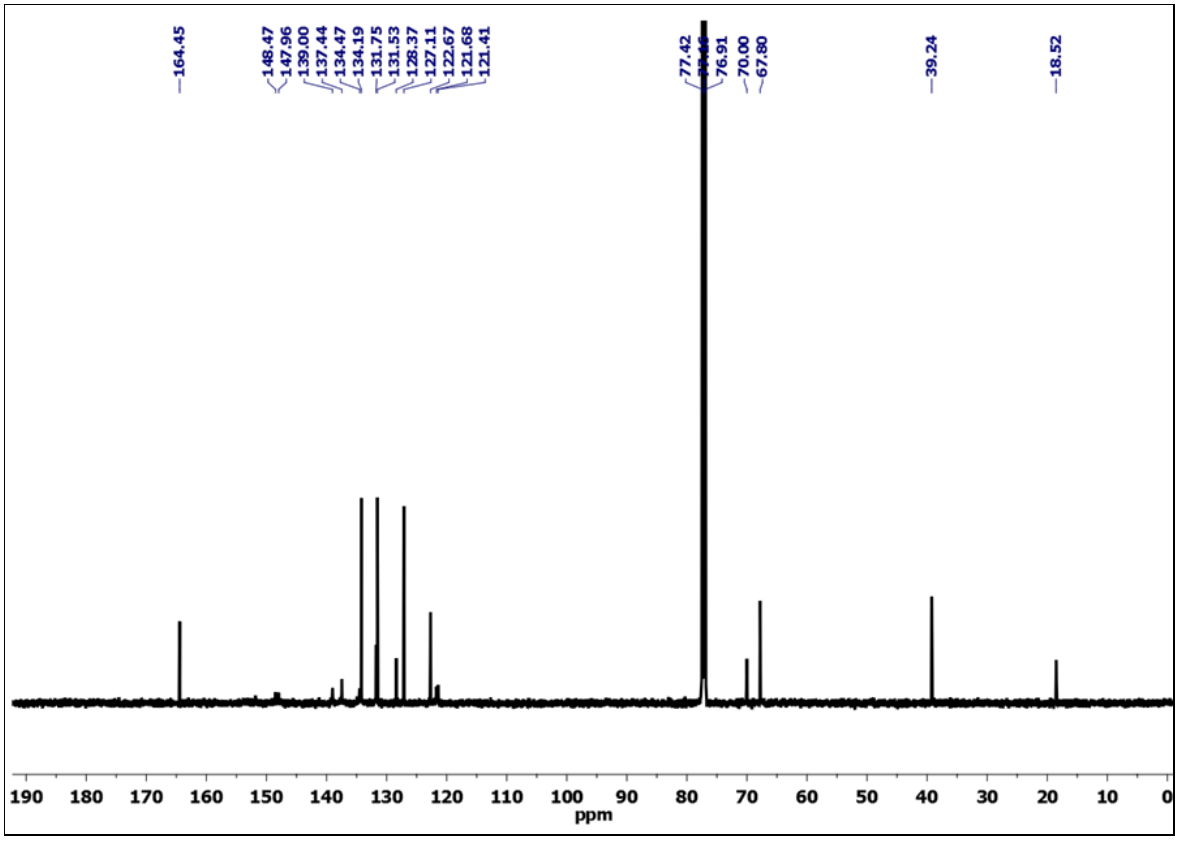


Figure 5S. ^{13}C-NMR spectrum of **L1** in $CDCl_3$ in 125 MHz at 298K.

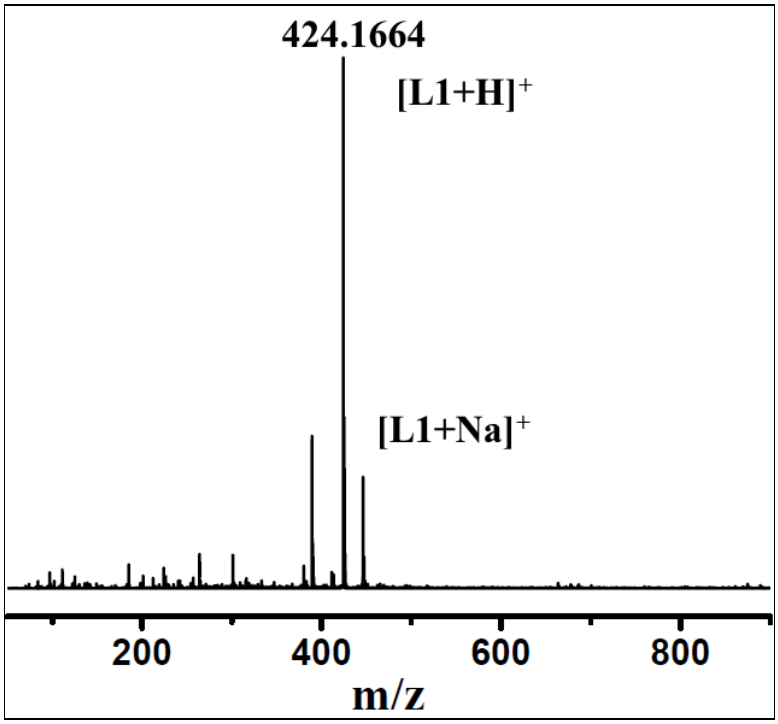


Figure 6S. ESI-MS (+ve) spectrum of **L1** at 298K.

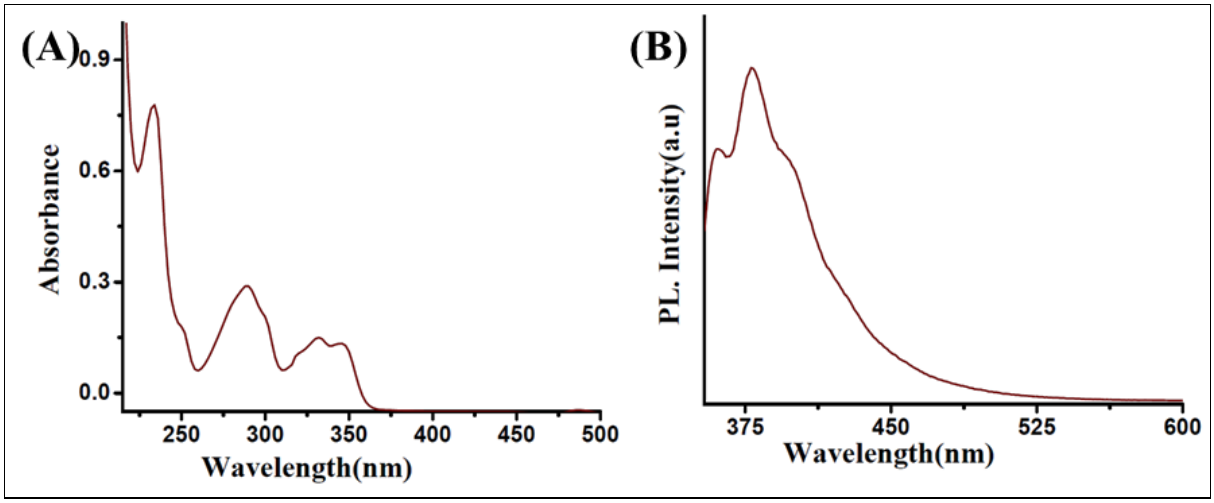


Figure 7S. (A) UV/Vis and (B) Emission spectra of **L1** at 298K.

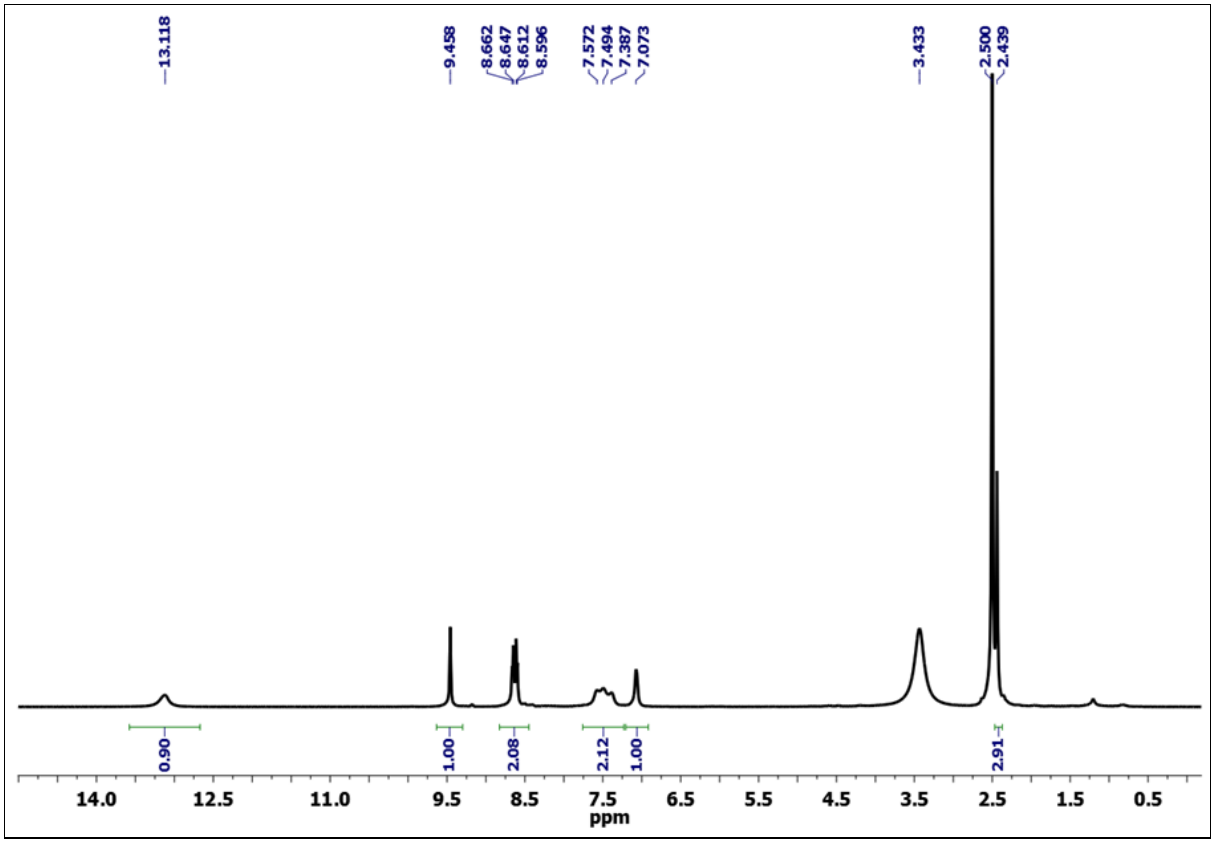


Figure 8S. ^{1}H-NMR spectrum of **L2** in DMSO-d_6 in 500 MHz at 298K.

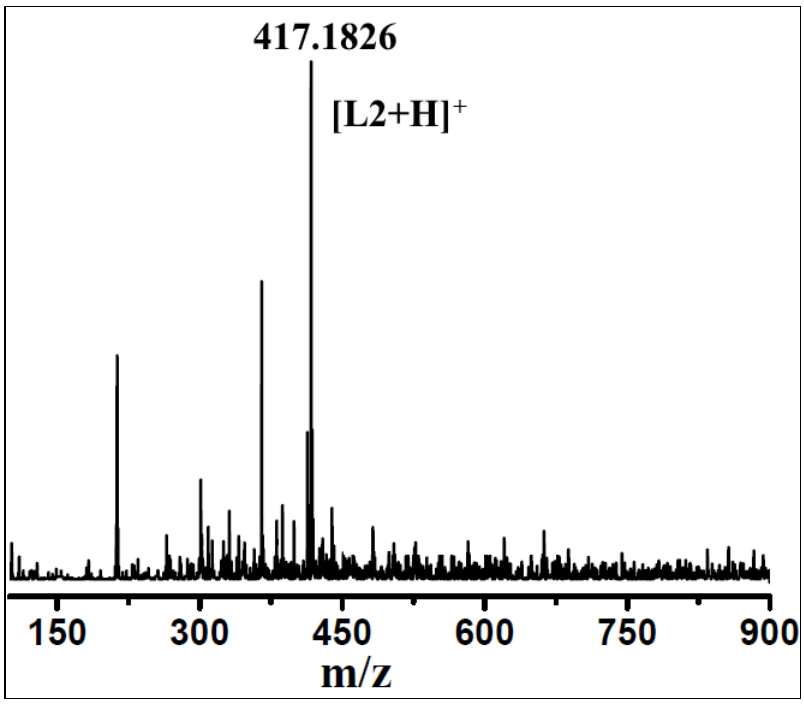


Figure 9S. ESI-MS (+ve) spectrum of **L2** at 298K.

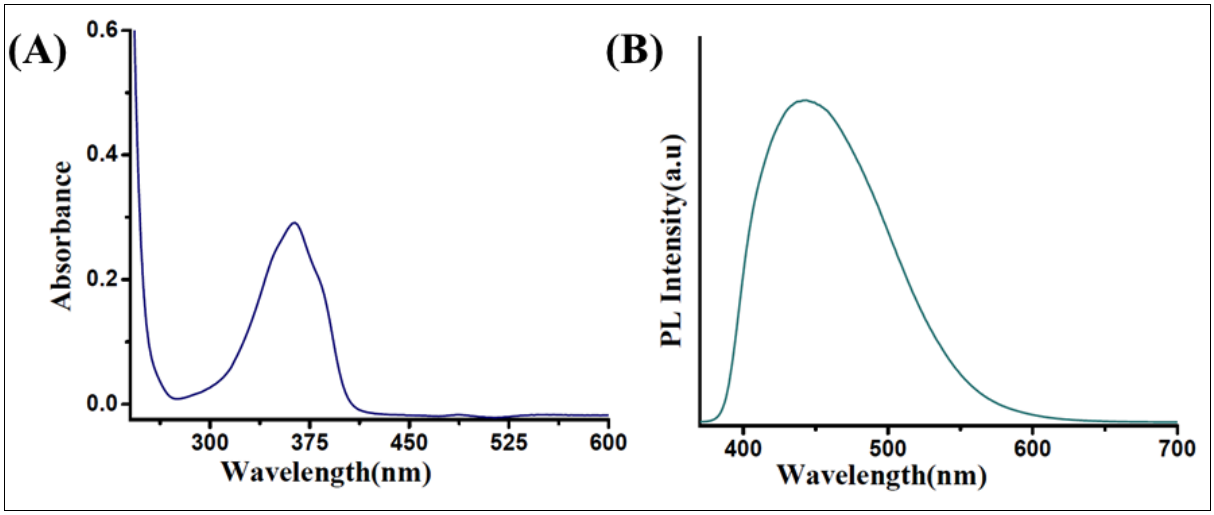


Figure 10S. (A) UV/Vis and (B) Emission spectra of **L2** (λ_{exc} = 363 nm) at 298K.

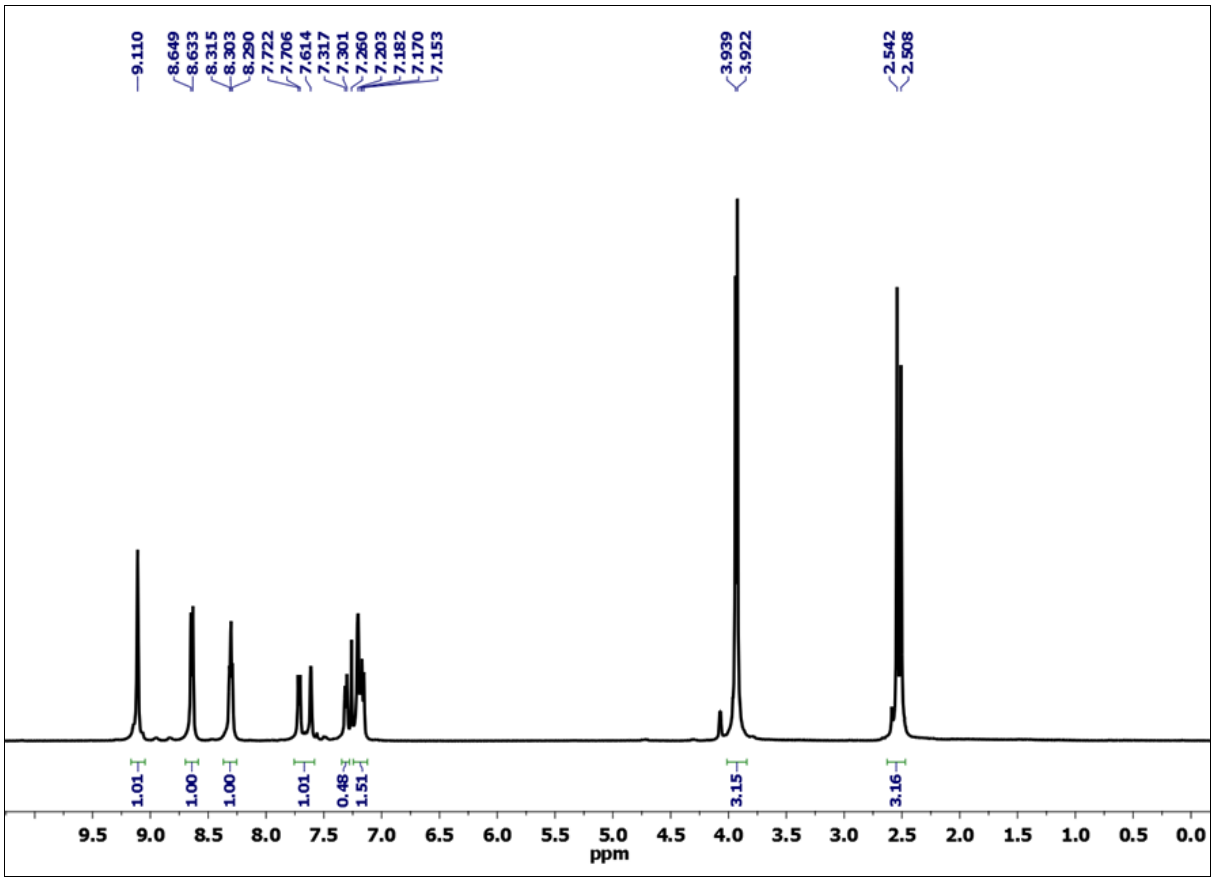


Figure 11S. ^{1}H-NMR spectrum of **L3** in $CDCl_3$ in 500 MHz at 298K.

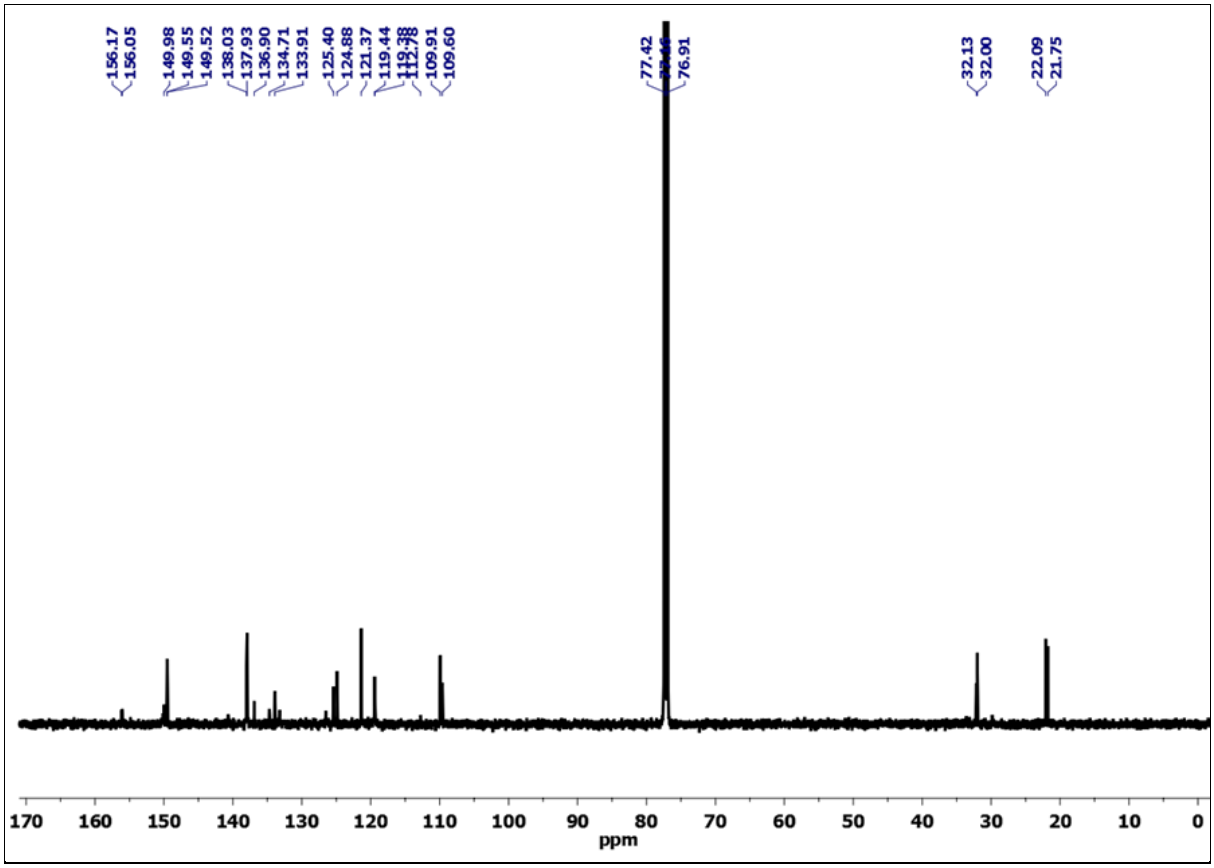


Figure 12S. ^{13}C-NMR spectrum of **L3** in $CDCl_3$ in 500 MHz at 298K.

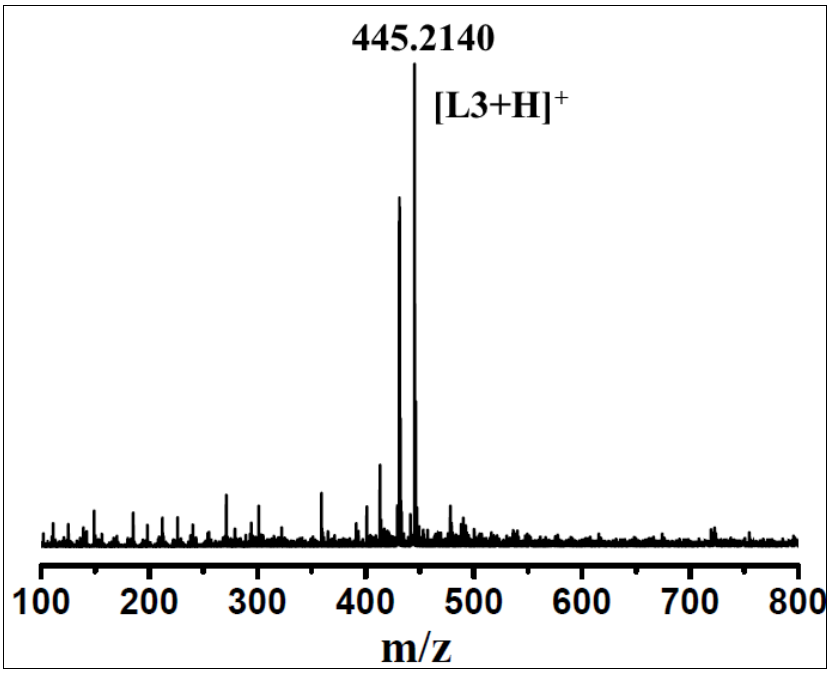


Figure 13S. ESI-MS (+ve) spectrum of **L3** at 298K.

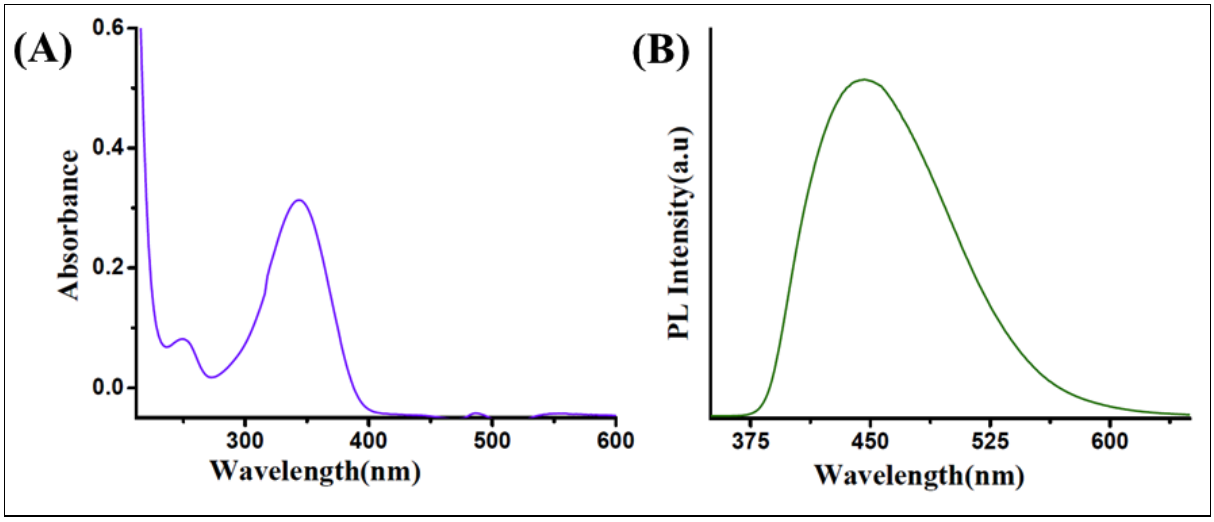


Figure 14S. (A) UV/Vis and (B) Emission spectra of **L3** (λ_{exc} = 345 nm) at 298K.

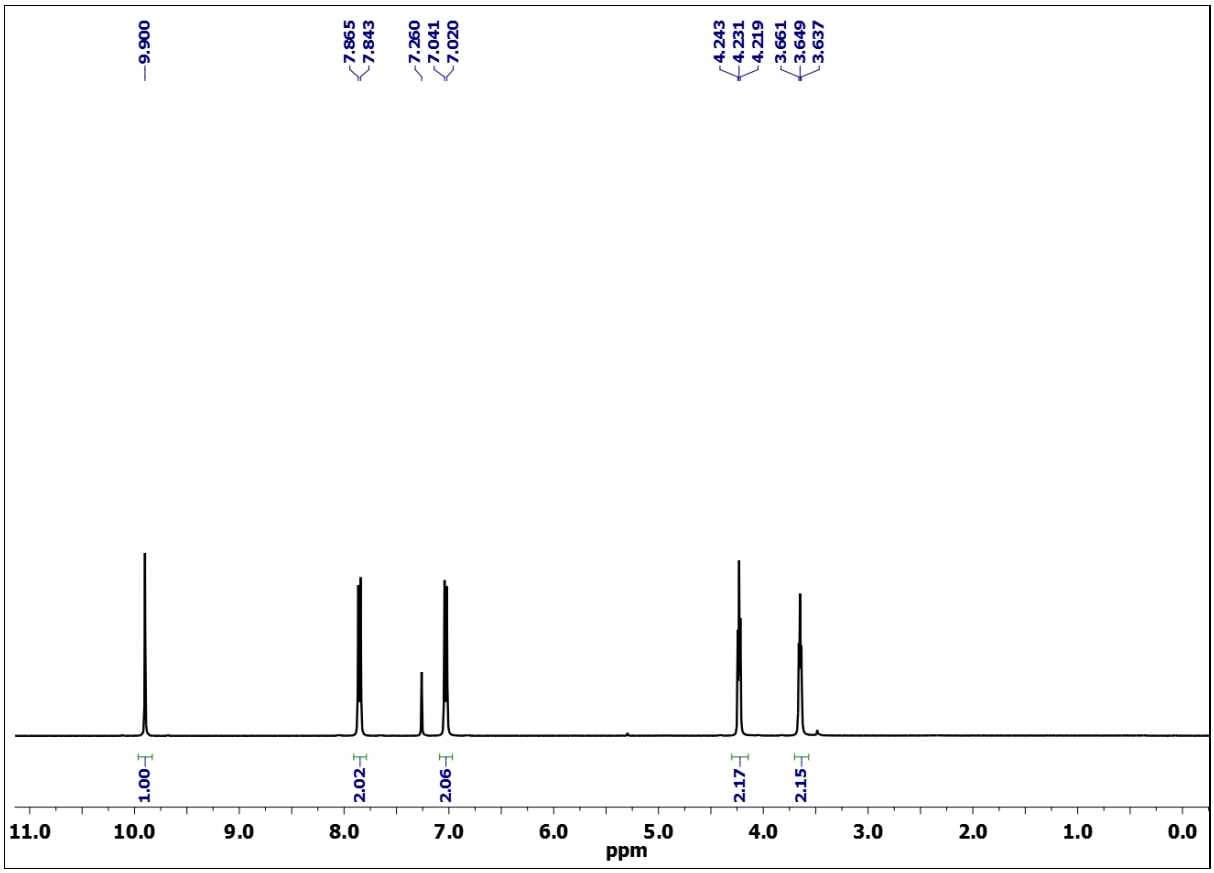


Figure 15S. ^{1}H-NMR spectrum of compound **C** in $CDCl_3$ in 400 MHz at 298K.

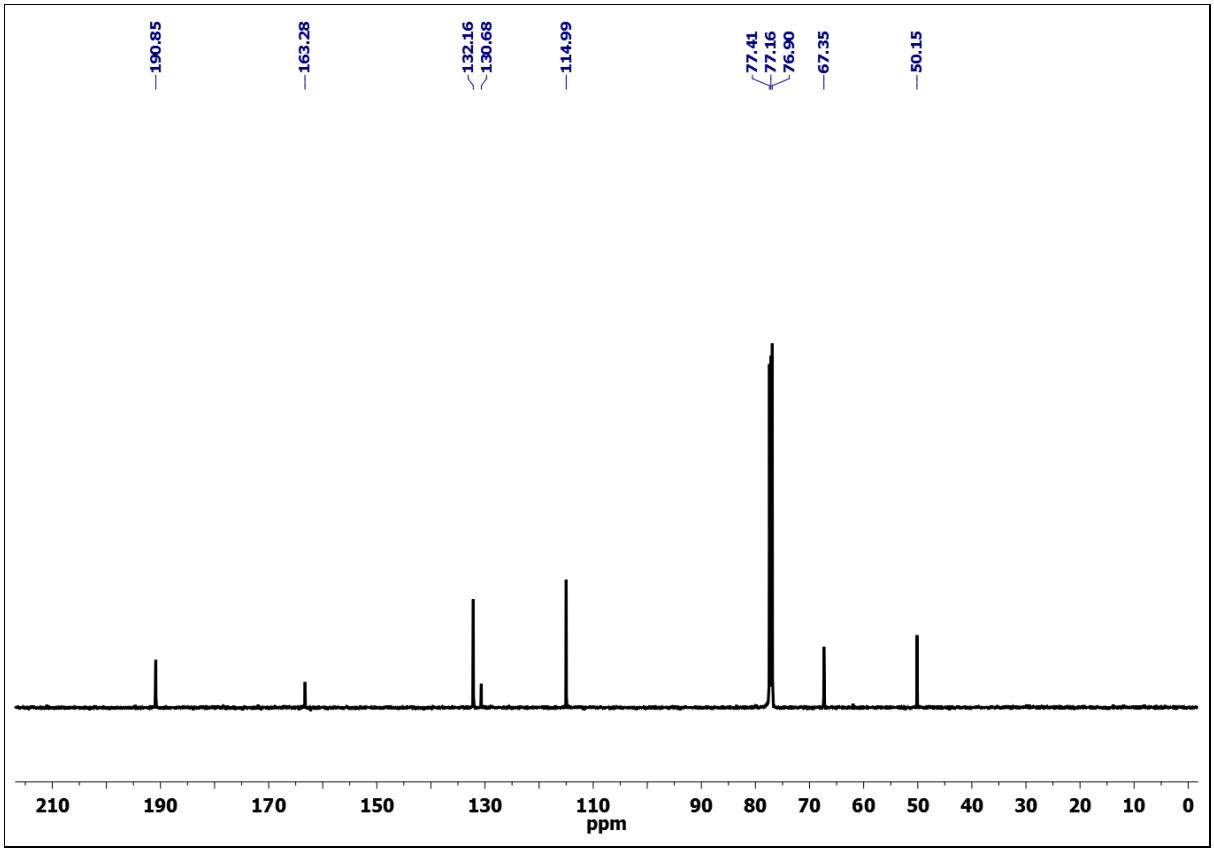


Figure 16S. [13] C-NMR spectrum of compound **C** in $CDCl_3$ in 125 MHz at 298K.

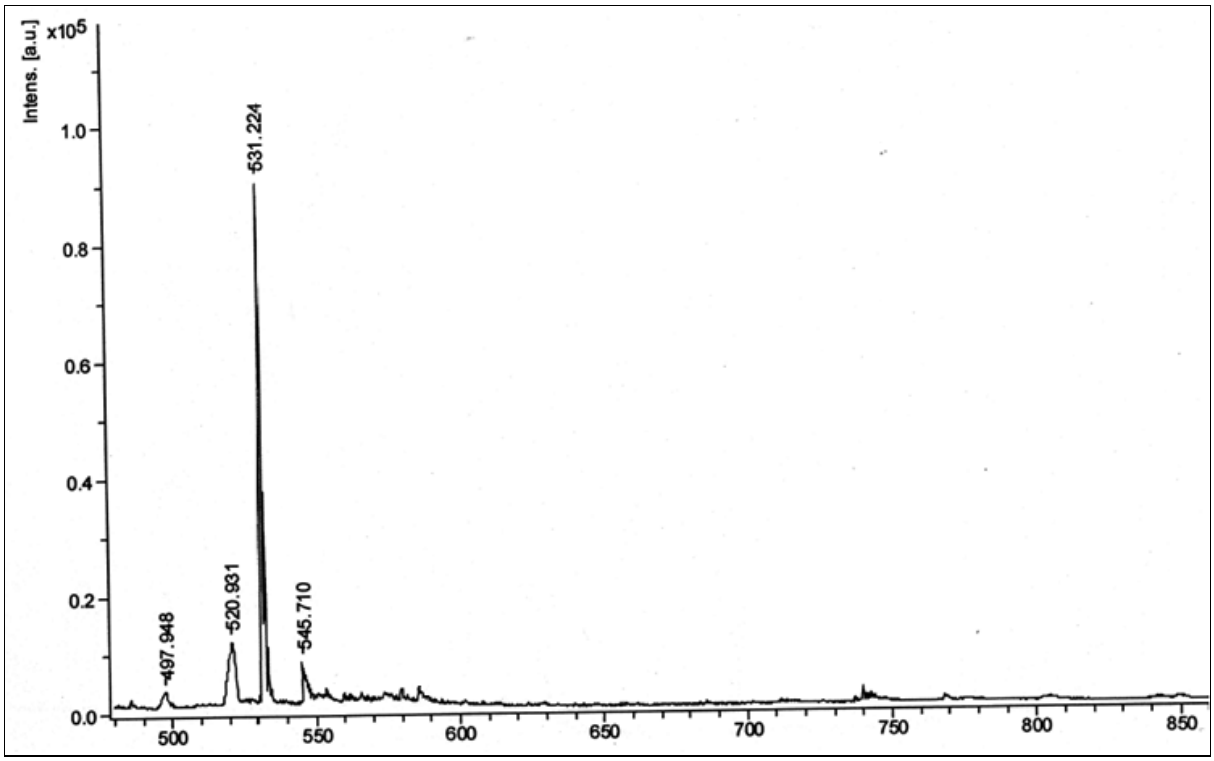


Figure 17S. MALDI-mass (+ve) spectrum of compound **L4** at 298K.

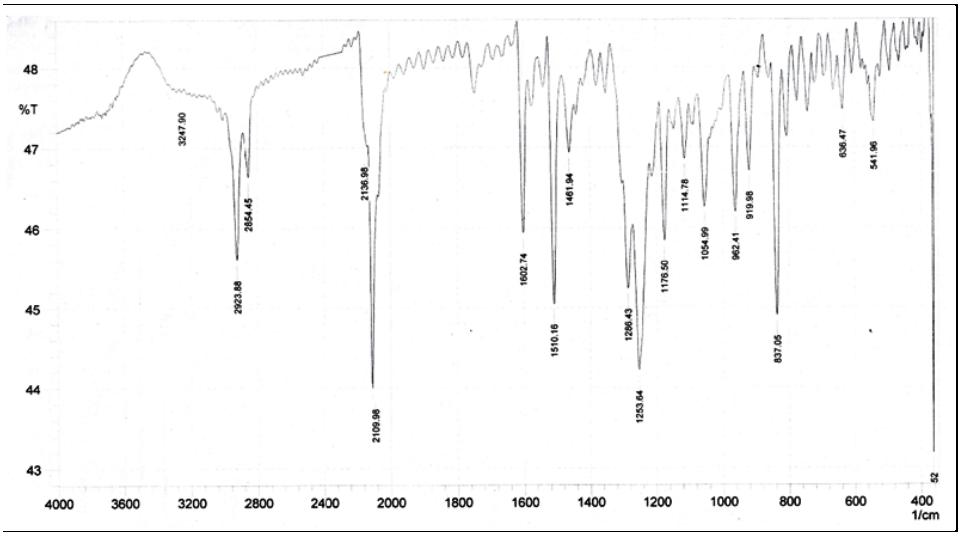


Figure 18S. IR spectrum of compound **L4**.

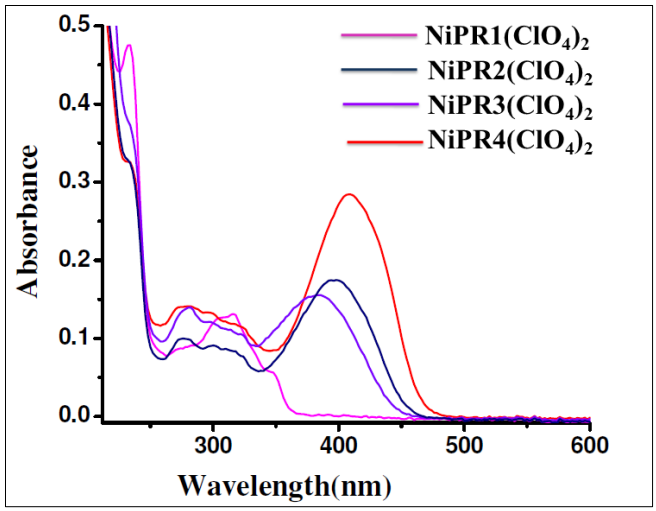


Figure 19S. Characteristic UV/Vis spectra of ternary complexes **{NiPR1(ClO$_4$)$_2$-NiPR4(ClO$_4$)$_2$}** in CH_3CN at 298K.

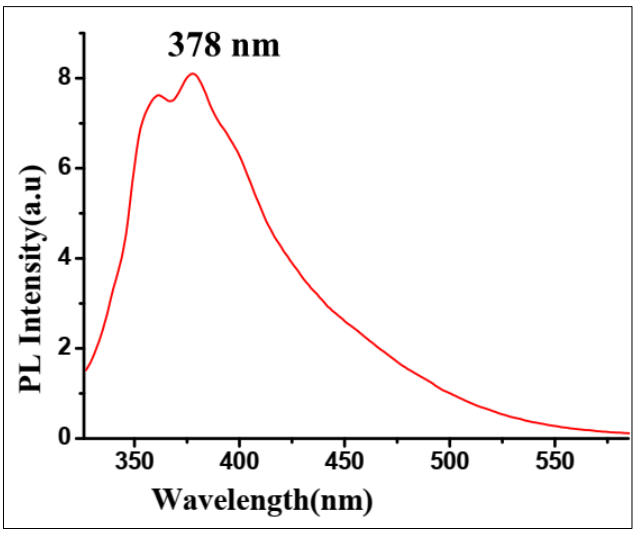


Figure 20S. Emission spectrum of **NiPR1(ClO$_4$)$_2$** in CH_3CN at 298K (λexc = 317 nm).

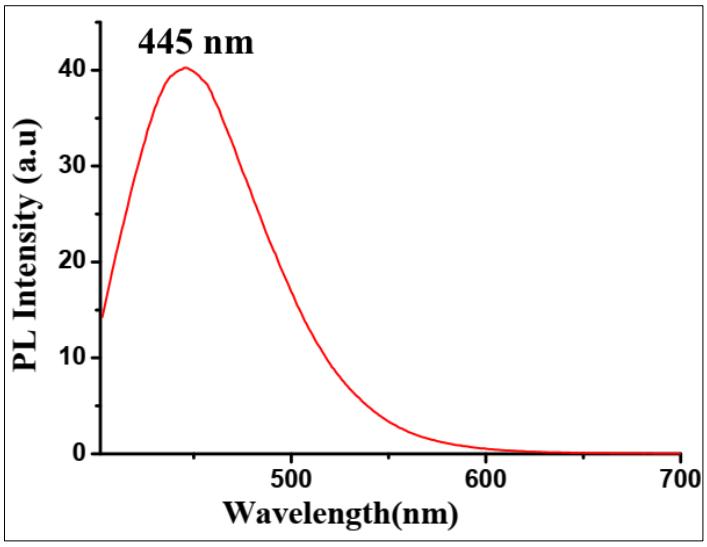


Figure 21S. Emission spectrum of **NiPR2(ClO$_4$)$_2$** in CH_3CN at 298K (λexc = 396 nm).

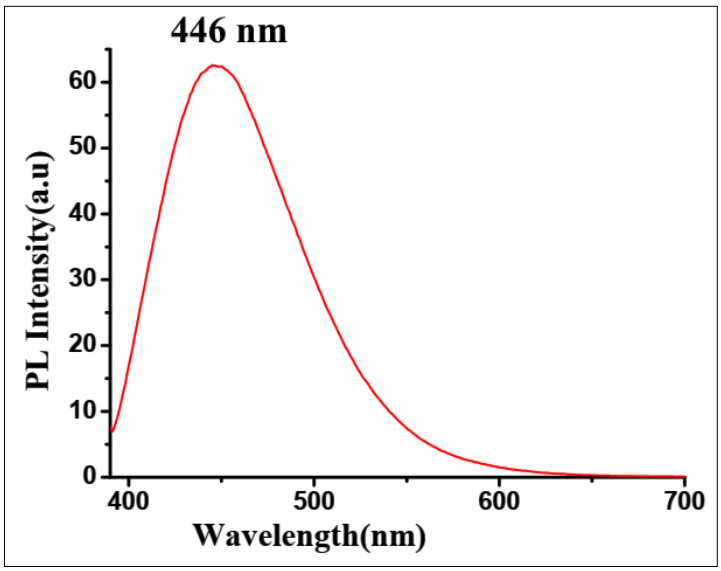


Figure 22S. Emission spectrum of **NiPR3(ClO$_4$)$_2$** in CH_3CN at 298K (λexc = 385 nm).

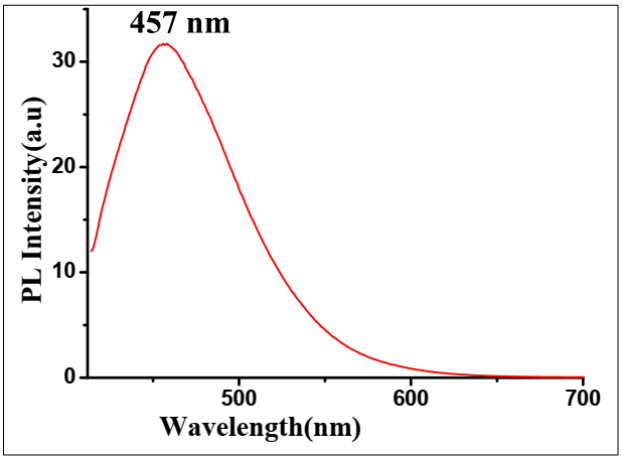


Figure 23S. Emission spectrum of **NiPR4(ClO$_4$)$_2$** in CH_3CN at 298K (λexc = 408 nm).

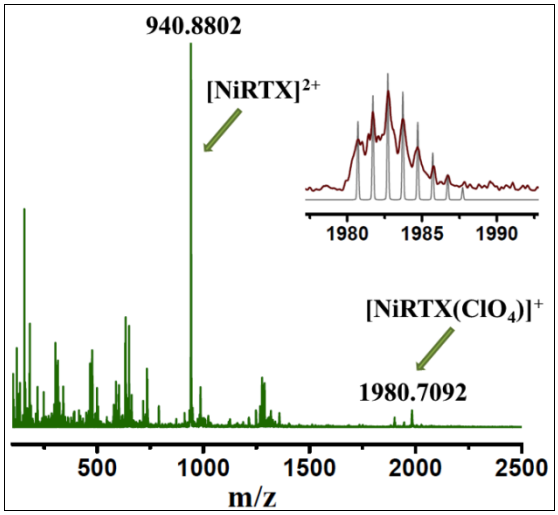


Figure 24S. ESI-MS (+ve) spectrum of Ni(II) templated rotaxane [**NiRTX(ClO$_4$)$_2$**] at 298K.

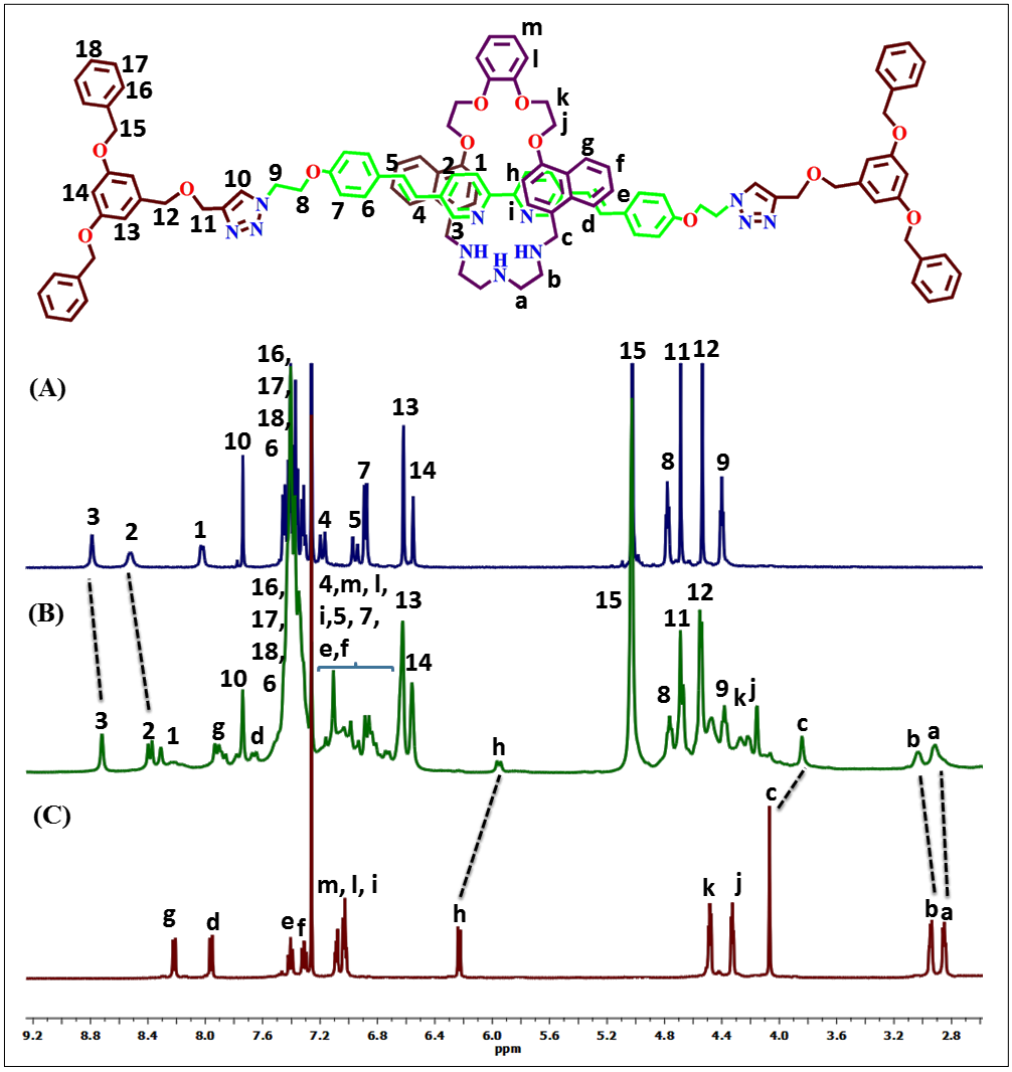


Figure 25S. Stacked ^{1}H NMR spectra of (A) **ConAx**, (B) **RTX**, and (C) **NaphMC** in $CDCl_3$ at 298 K. The labels of protons are shown correspond to **NaphMC** and **ConAx** in **RTX** in the above mentioned structure.

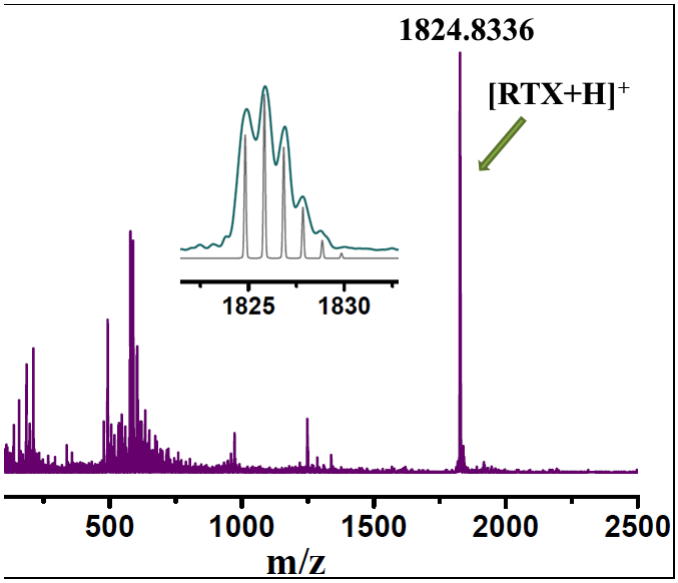


Figure 26S. ESI-MS (+ve) spectrum of metal free rotaxane [**RTX**] at 298K.

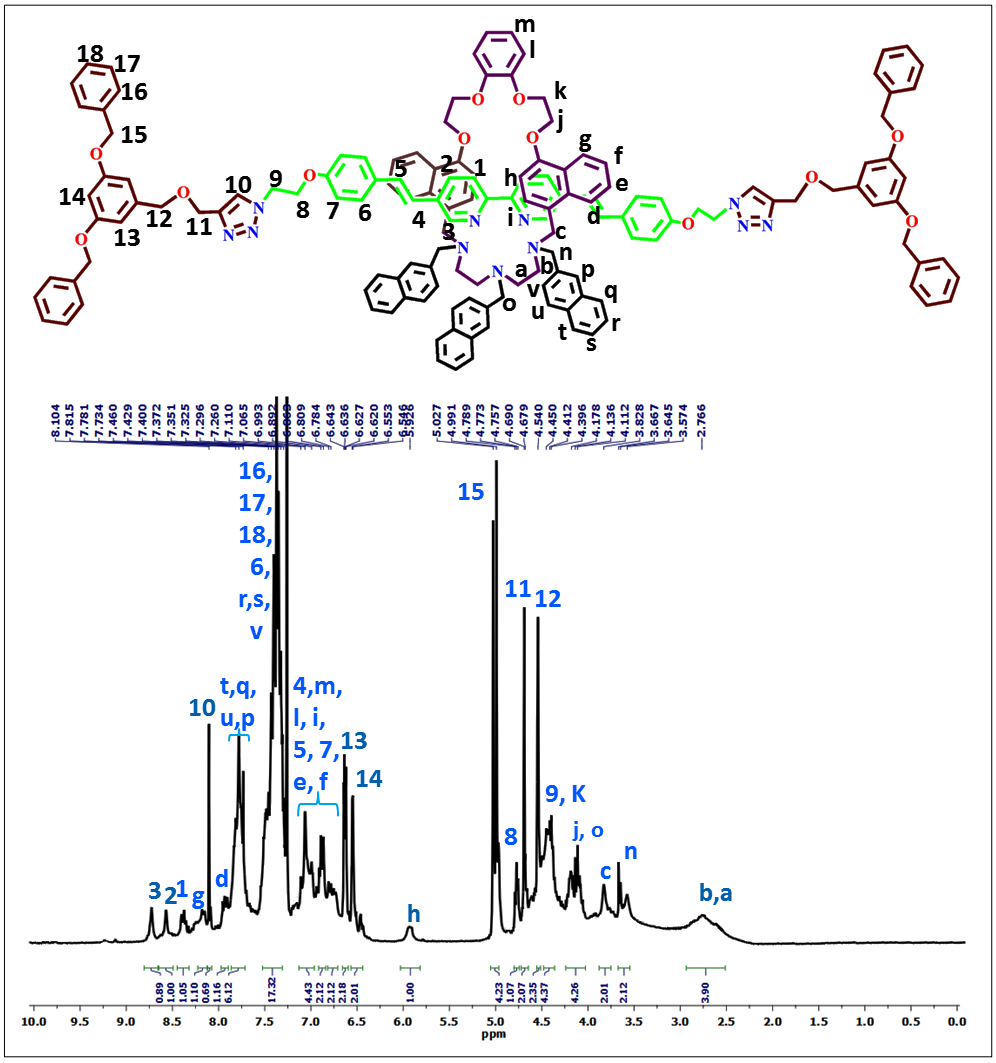


Figure 27S. ^{1}H-NMR spectrum of **NAPRTX** in $CDCl_3$ in 300 MHz at RT.

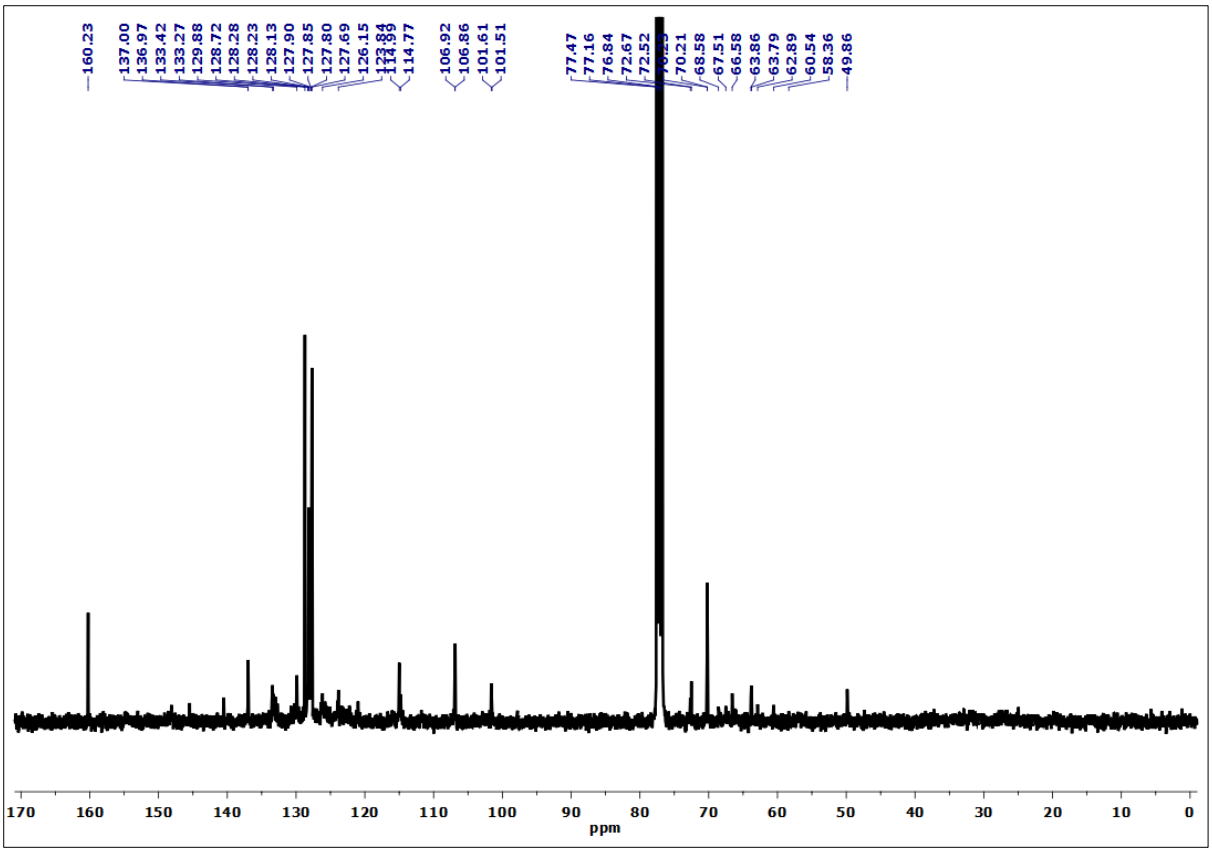


Figure 28S. ^{13}C-NMR spectrum of **NAPRTX** in $CDCl_3$ in 300 MHz at RT.

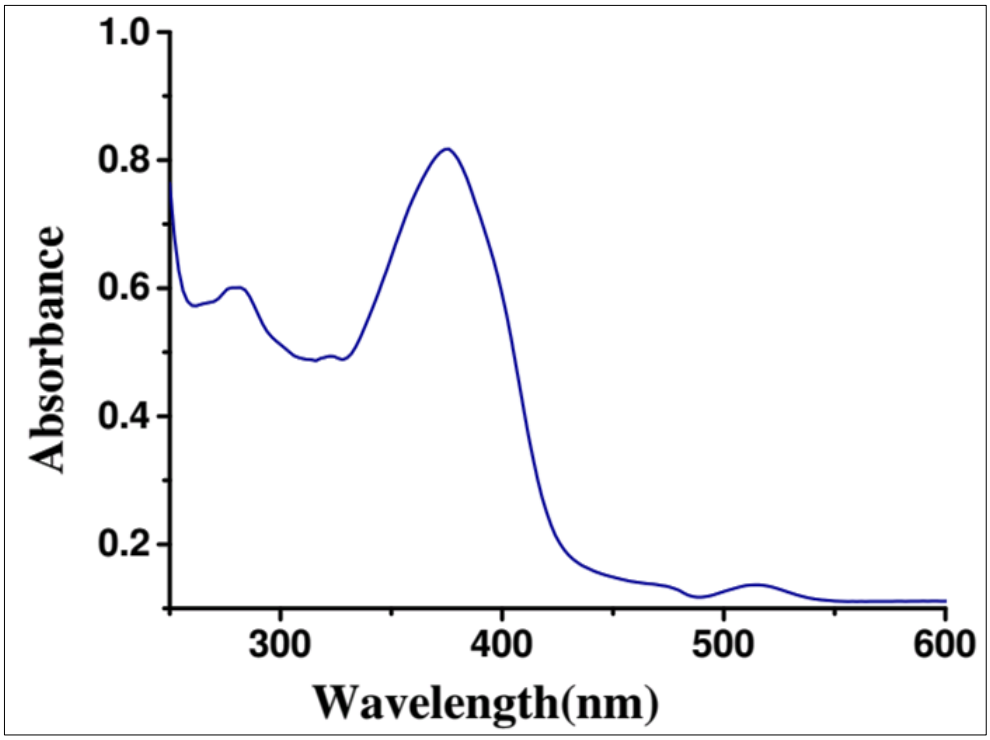


Figure 29S. UV/Vis spectrum of **NAPRTX** at 298K.

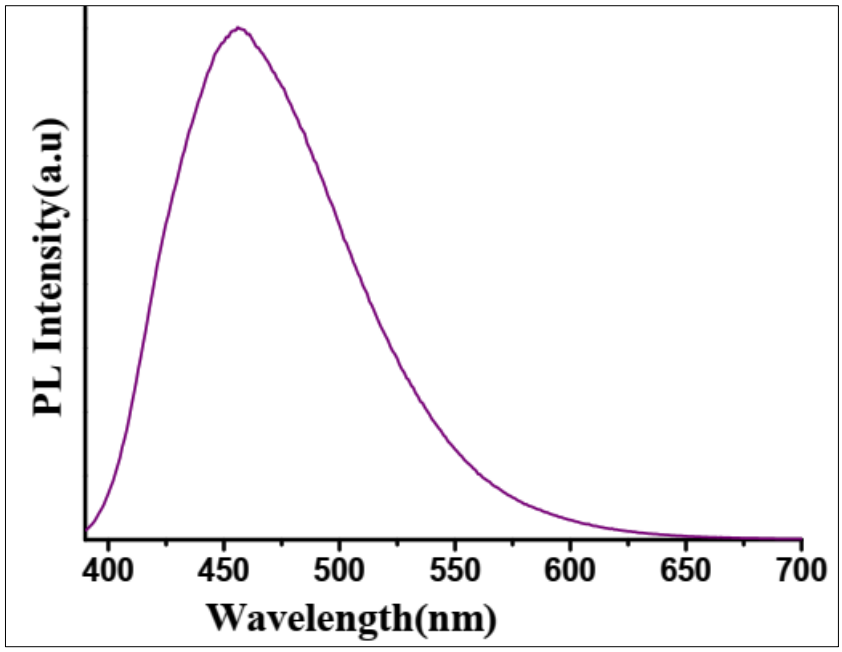


Figure 30S. Emission spectrum of **NAPRTX** exc at 375 nm at 298K.

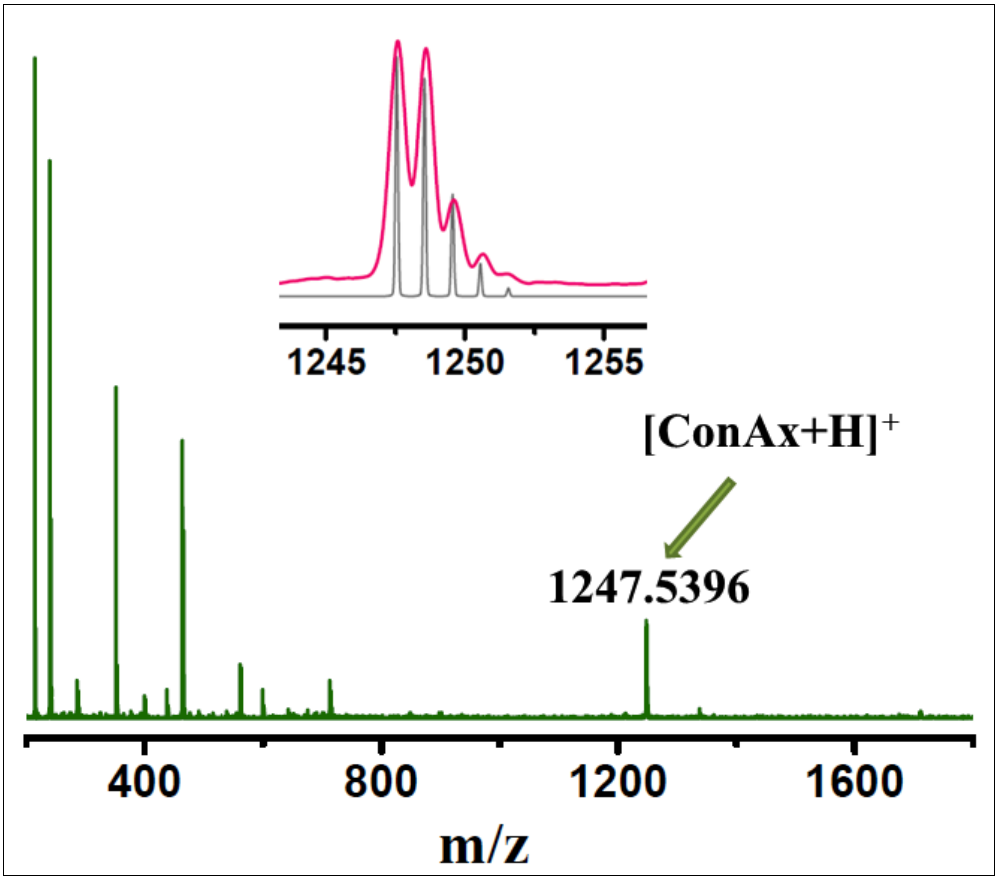


Figure 31S. ESI-MS (+ve) spectrum of **ConAx** at 298K.

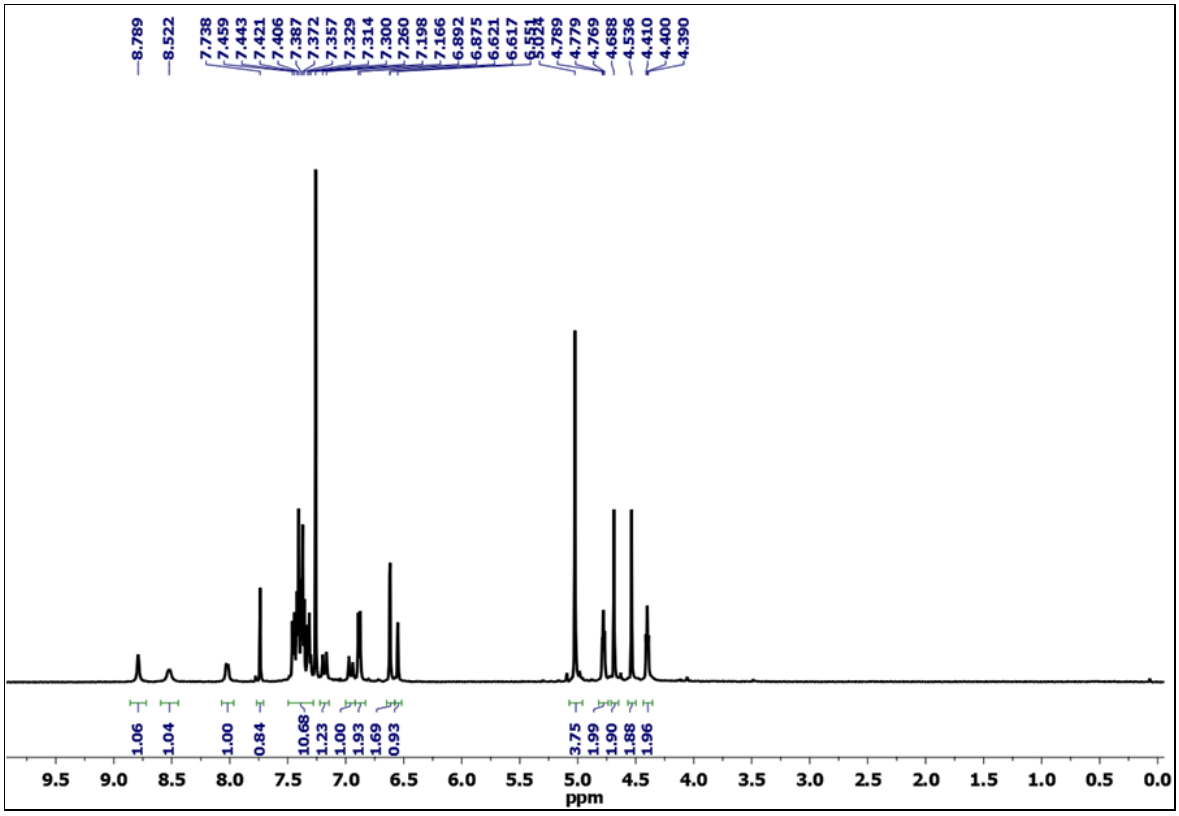


Figure 32S. ^{1}H-NMR spectrum of **ConAx** in $CDCl_3$ in 500 MHz at 298K.

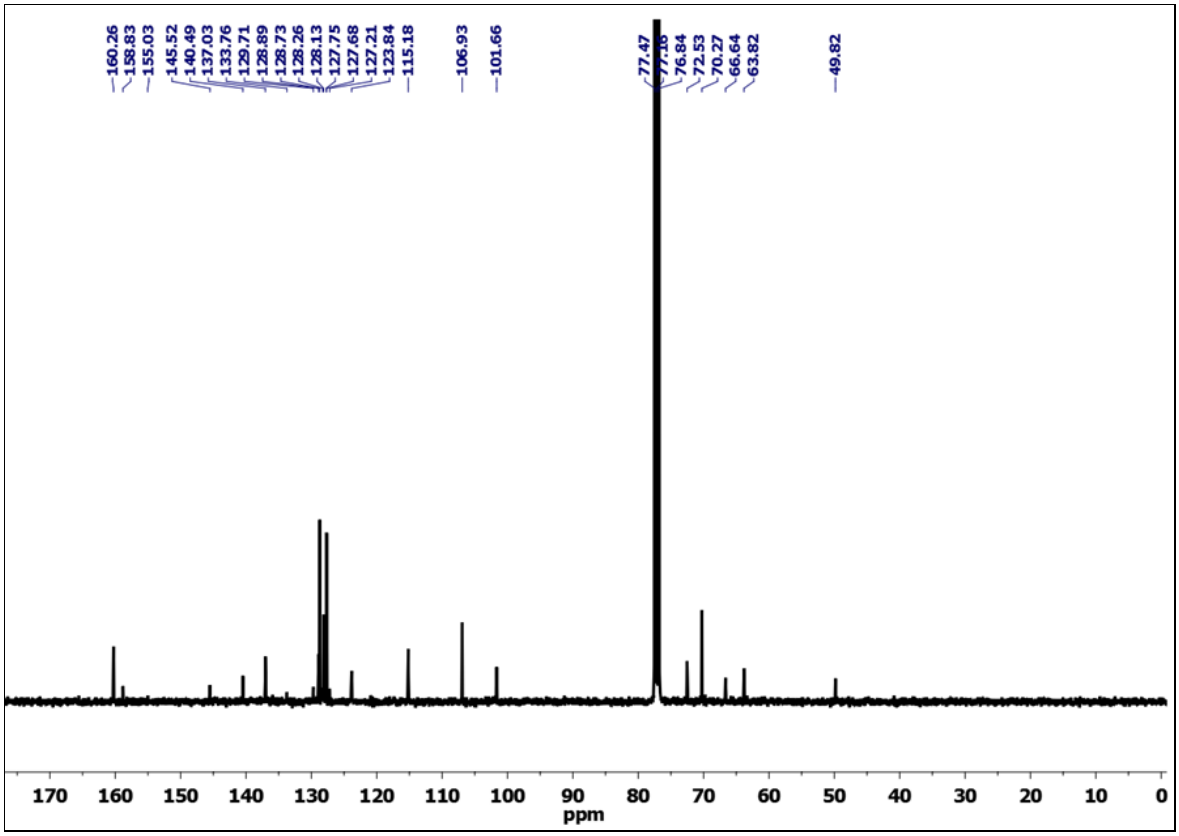


Figure 33S. ^{13}C-NMR spectrum of **ConAx** in $CDCl_3$ in 100 MHz at 298K.

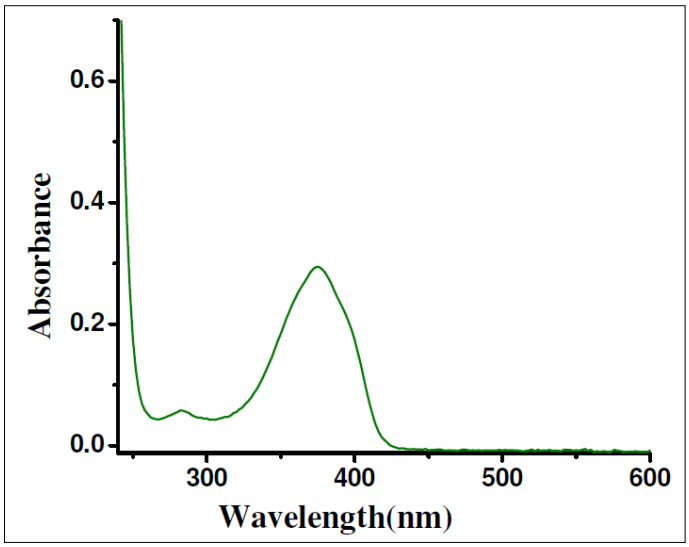


Figure 34S. UV/Vis spectrum of **ConAx** in DMF-CH_3CN (2:8) at 298K.

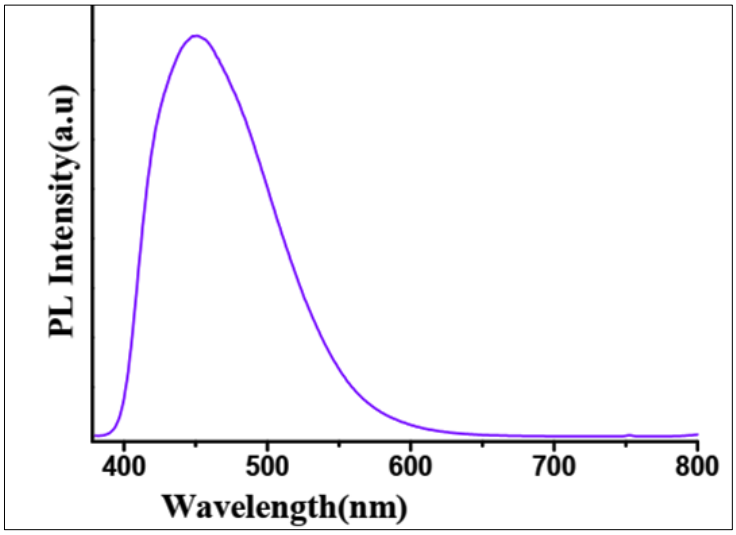


Figure 35S. Emission spectrum of **ConAx** ($5x10^{-6}$ M) in DMF-CH_3CN (2:8) exc at 375 nm at 298K.

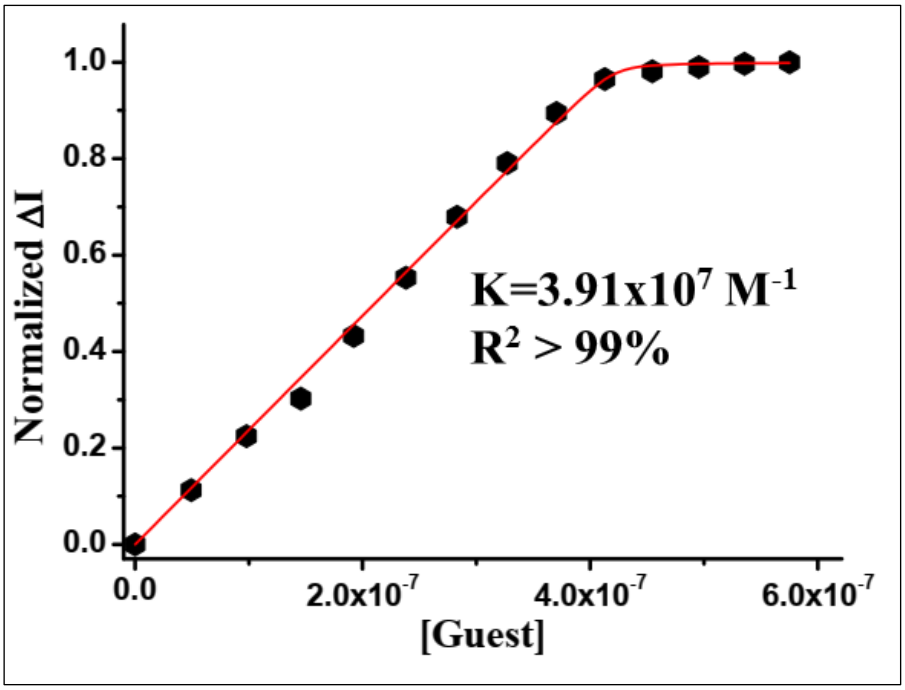


Figure 36S. Non-linear 1 : 1 curve fitting plot from PL titration data between **NAPRTX** and Zn^{2+} ion at 298 K, λ_{exc}= 375 nm.

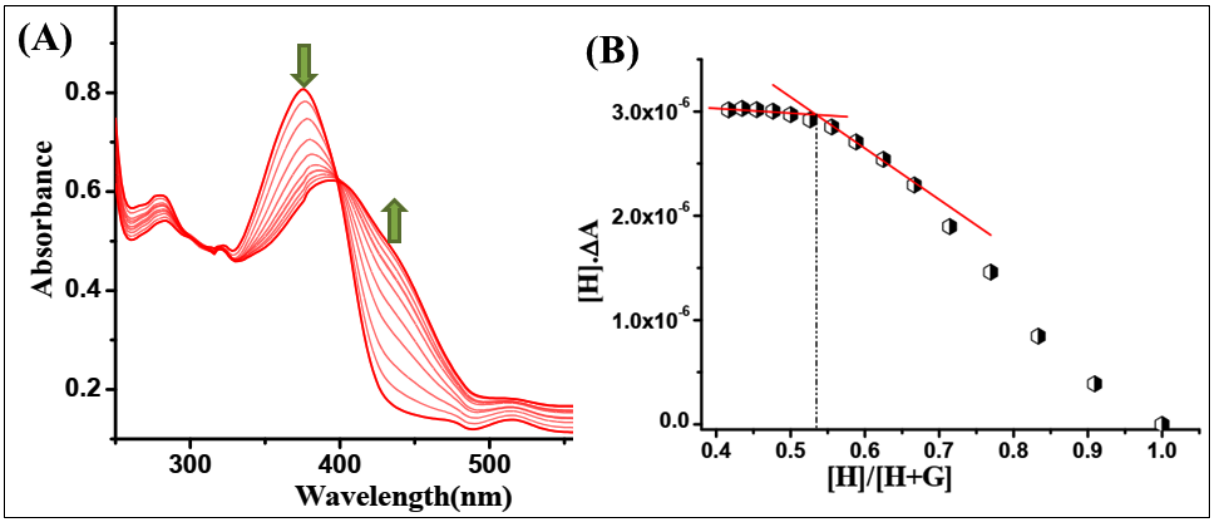


Figure 37S. (A) UV titration of **NAPRTX** with **$Zn(ClO_4)_2$** in solvent mixture {3% water in mixture of solvent} at 298 K. (B) Molar ratio plot.

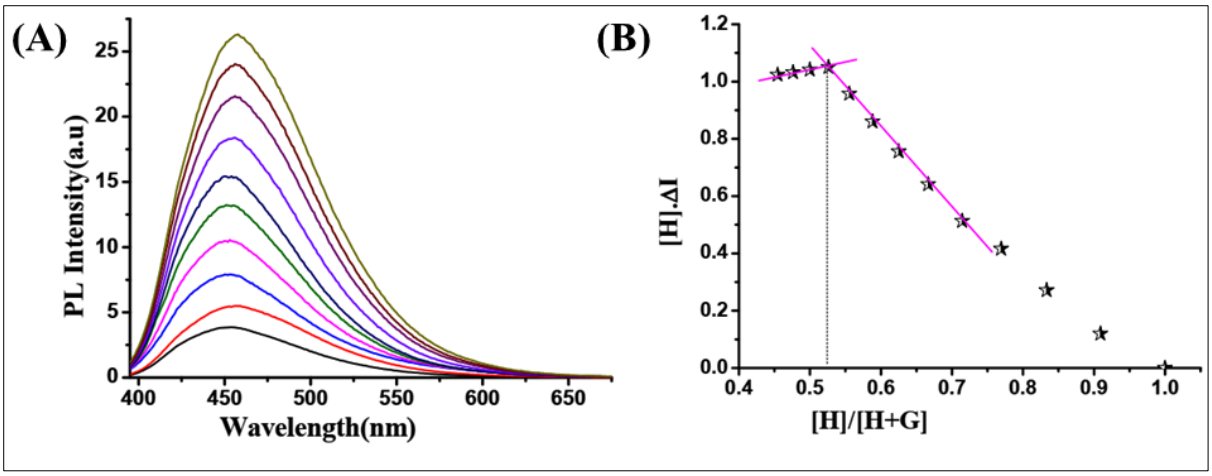


Figure 38S. (A) PL titration of **NAPRTX** with **$Zn(ClO_4)_2$** in solvent mixture {3% water in mixture of solvent} at 298 K. (B) Molar ratio plot.