

## Supplementary Information

### Hydrolytically active tetranuclear $[\text{Ni}^{\text{II}}_2]_2$ complexes: synthesis, structure, spectroscopy and phosphoester hydrolysis

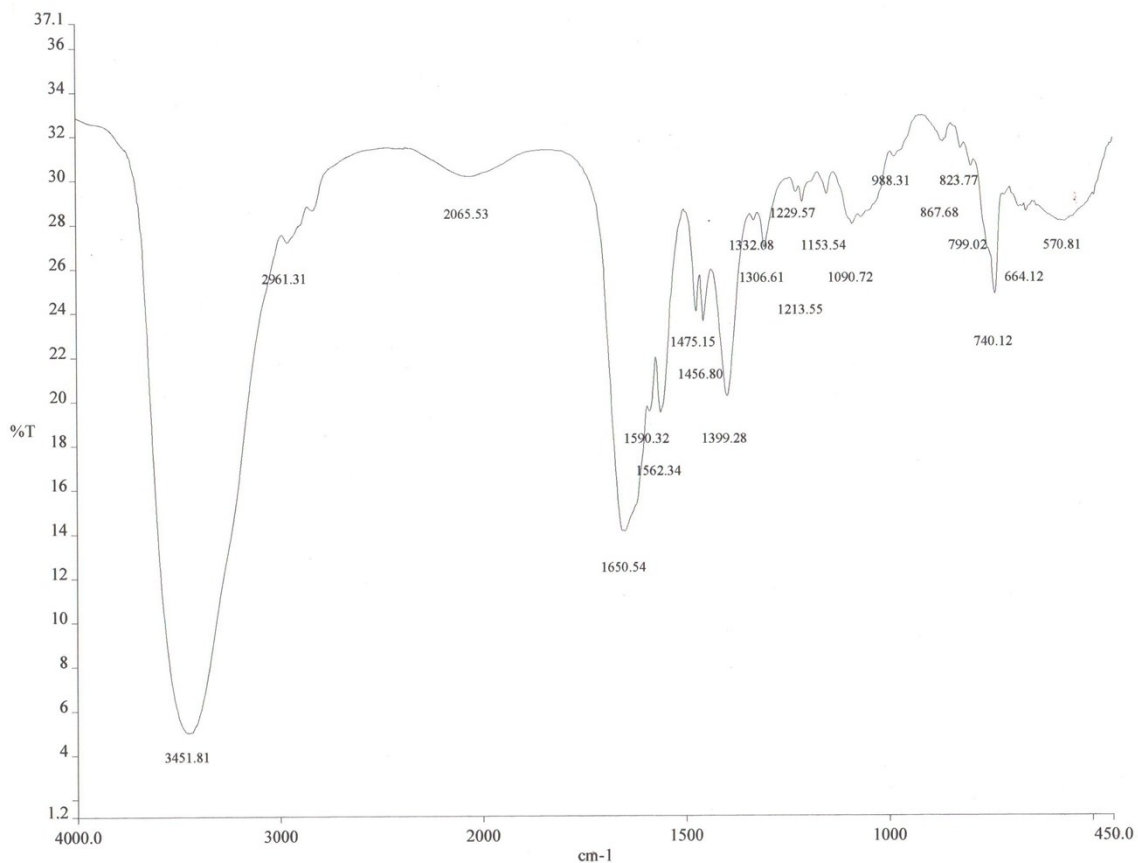
Gopal C. Giri,<sup>a</sup> Ayan Patra,<sup>a</sup> Gonela Vijaykumar,<sup>b</sup> Luca Carrella,<sup>c</sup> and Manindranath Bera<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, University of Kalyani, Kalyani, West Bengal-741235, INDIA. E-mail: mbera2009@klyuniv.ac.in; <http://www.klyuniv.ac.in>; Fax: +91 33 25828282; Tel: +91 33 25828282 x306

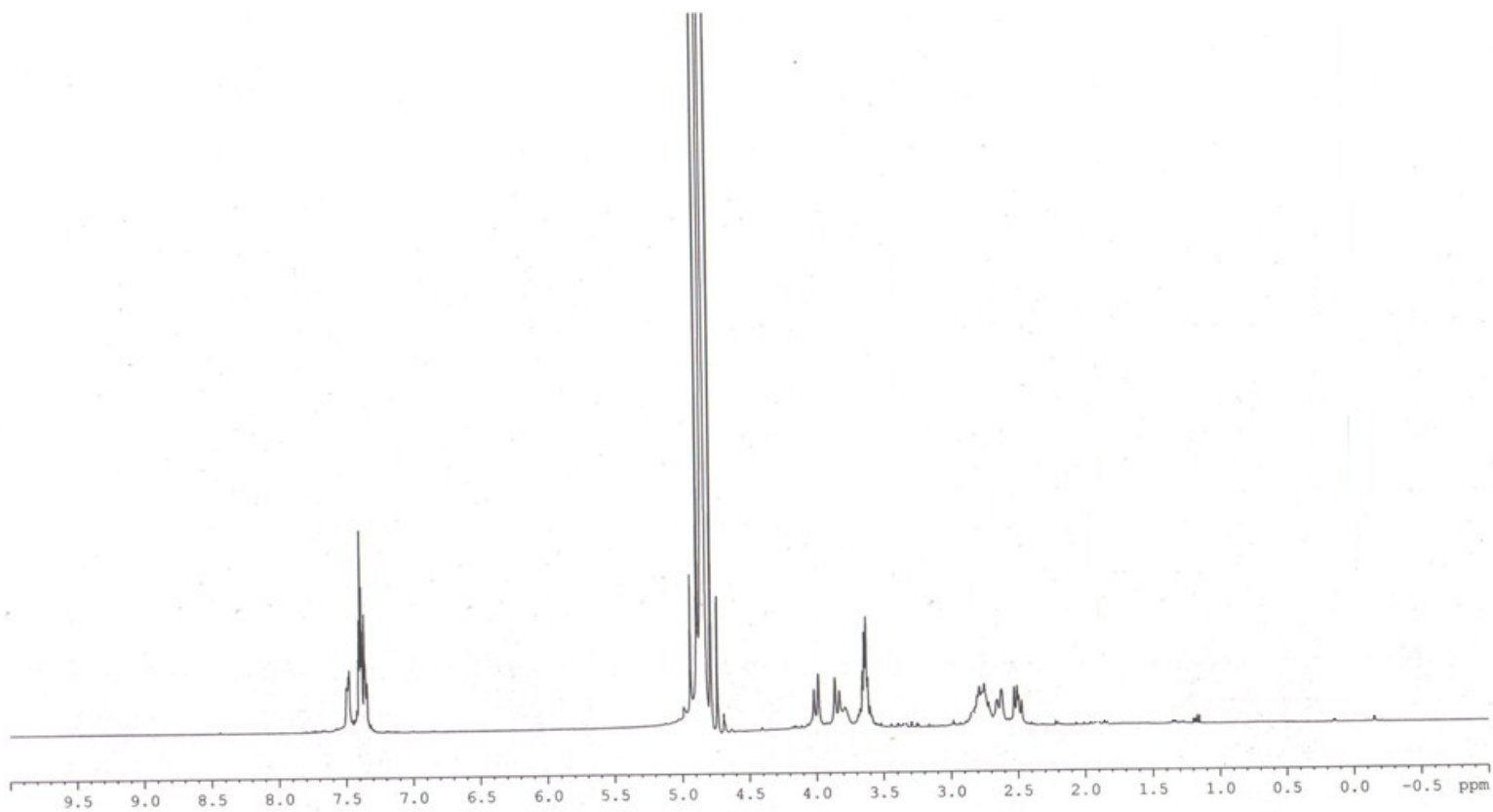
<sup>b</sup>Department of Chemical Sciences, Indian Institute of Science Education & Research Kolkata, Mohanpur, West Bengal-741246, INDIA.

<sup>c</sup>Institut für Anorganische Chemie und Analytische Chemie, Johannes-Gutenberg Universität Mainz, Duesbergweg 10-14, D-55128 Mainz, Germany.

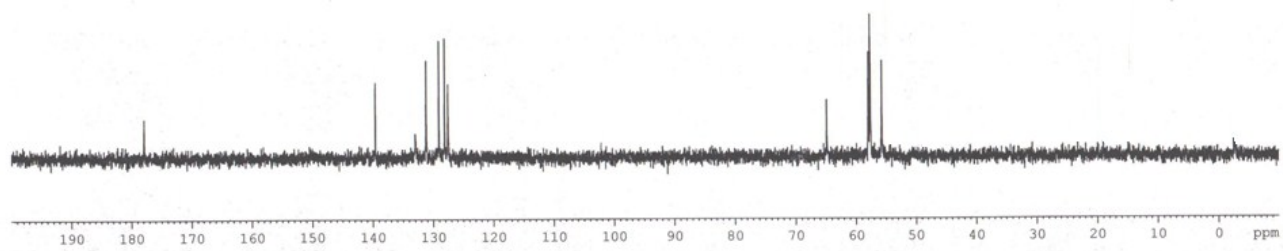
### Figures with Captions



**Fig. S1** FTIR spectrum of the ligand H<sub>5</sub>chdp in the region of 4000-450 cm<sup>-1</sup>.



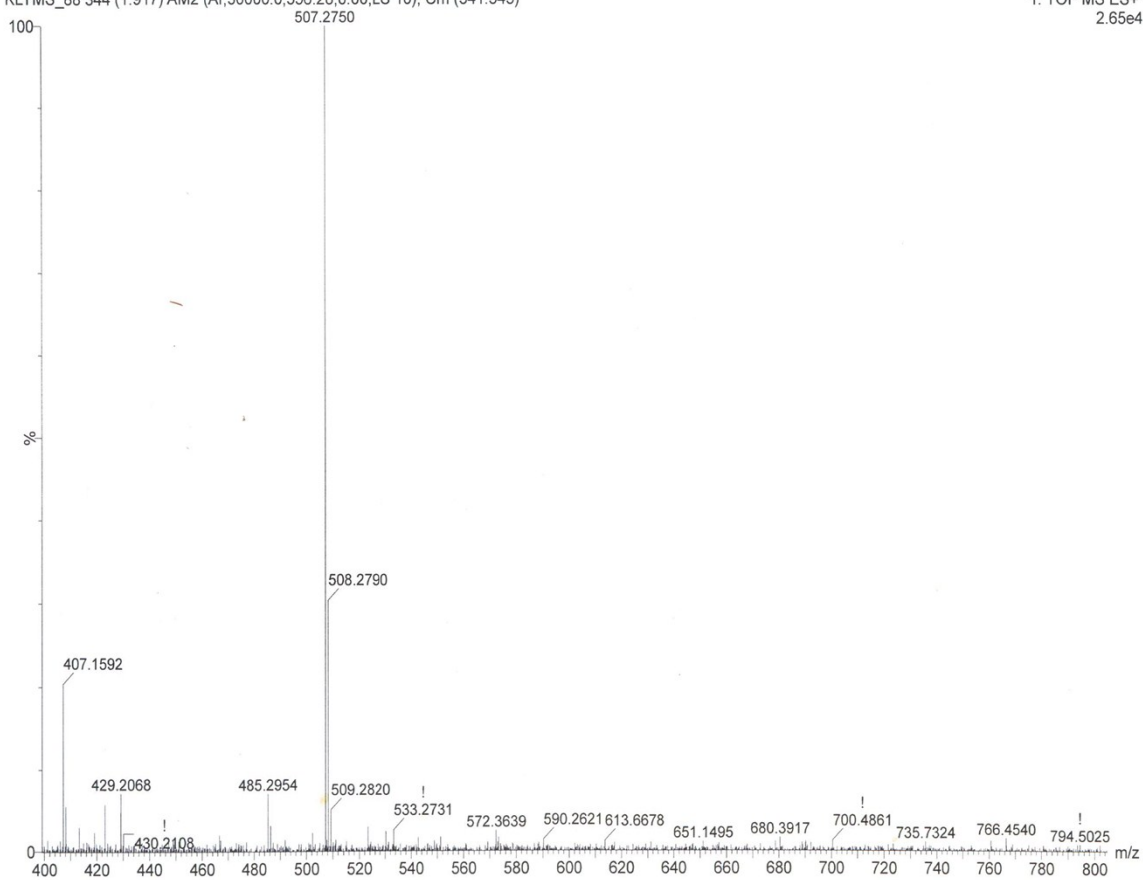
**Fig. S2**  $^1\text{H}$  NMR spectrum of the ligand  $\text{H}_5\text{chdp}$  in  $\text{D}_2\text{O}$ .



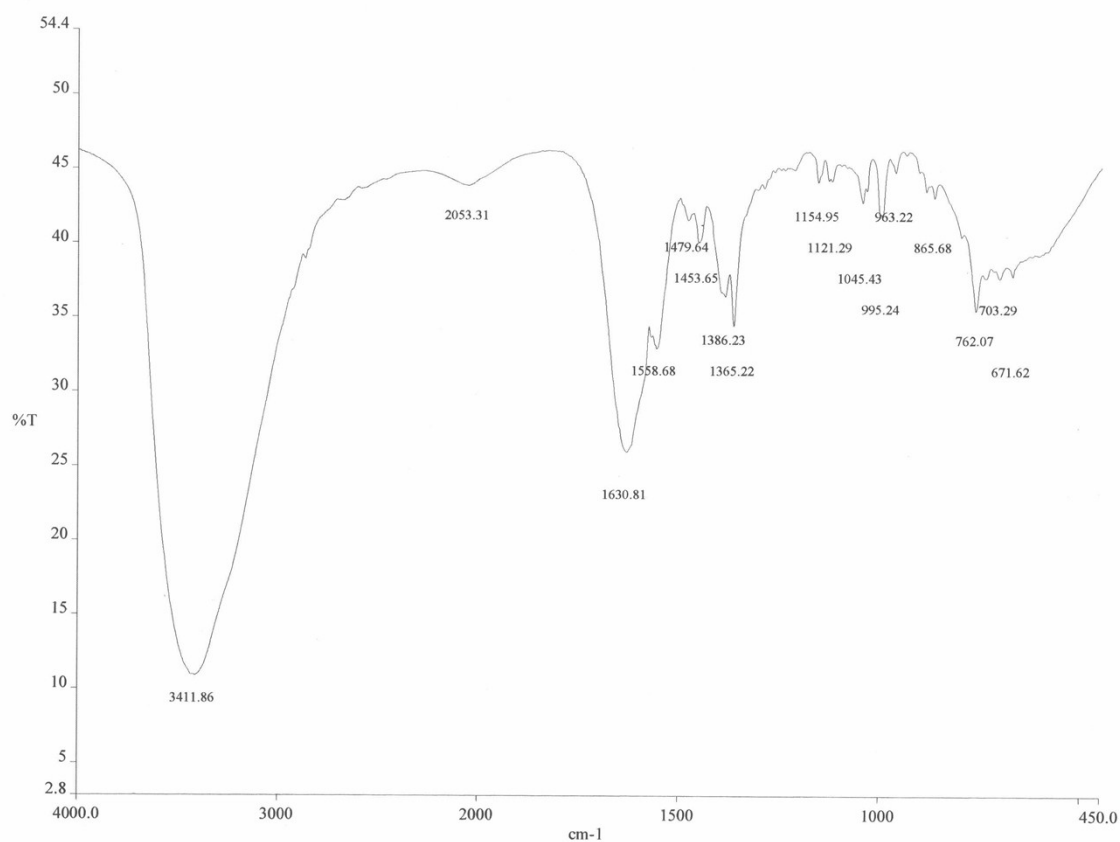
**Fig. S3**  $^{13}\text{C}$  NMR spectrum of the ligand  $\text{H}_5\text{chdp}$  in  $\text{D}_2\text{O}$ .

GG\_I\_OH  
13-Aug-2015  
KLYMS\_88 344 (1.917) AM2 (Ar,30000.0,556.28,0.00,LS 10); Cm (341:345)

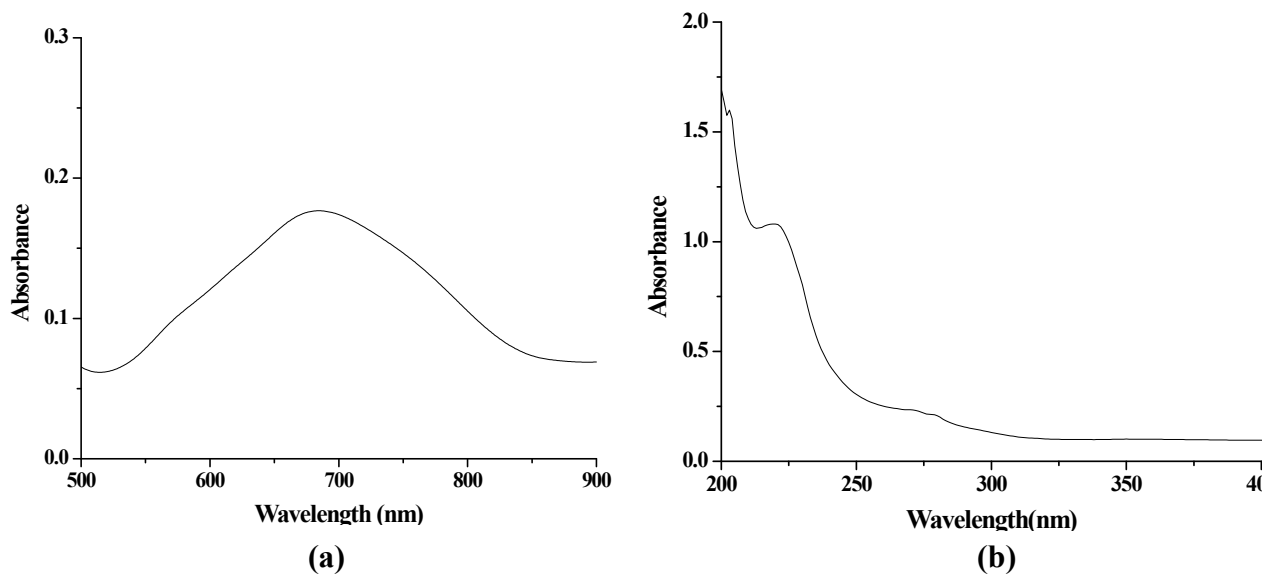
1: TOF MS ES+  
2.65e4



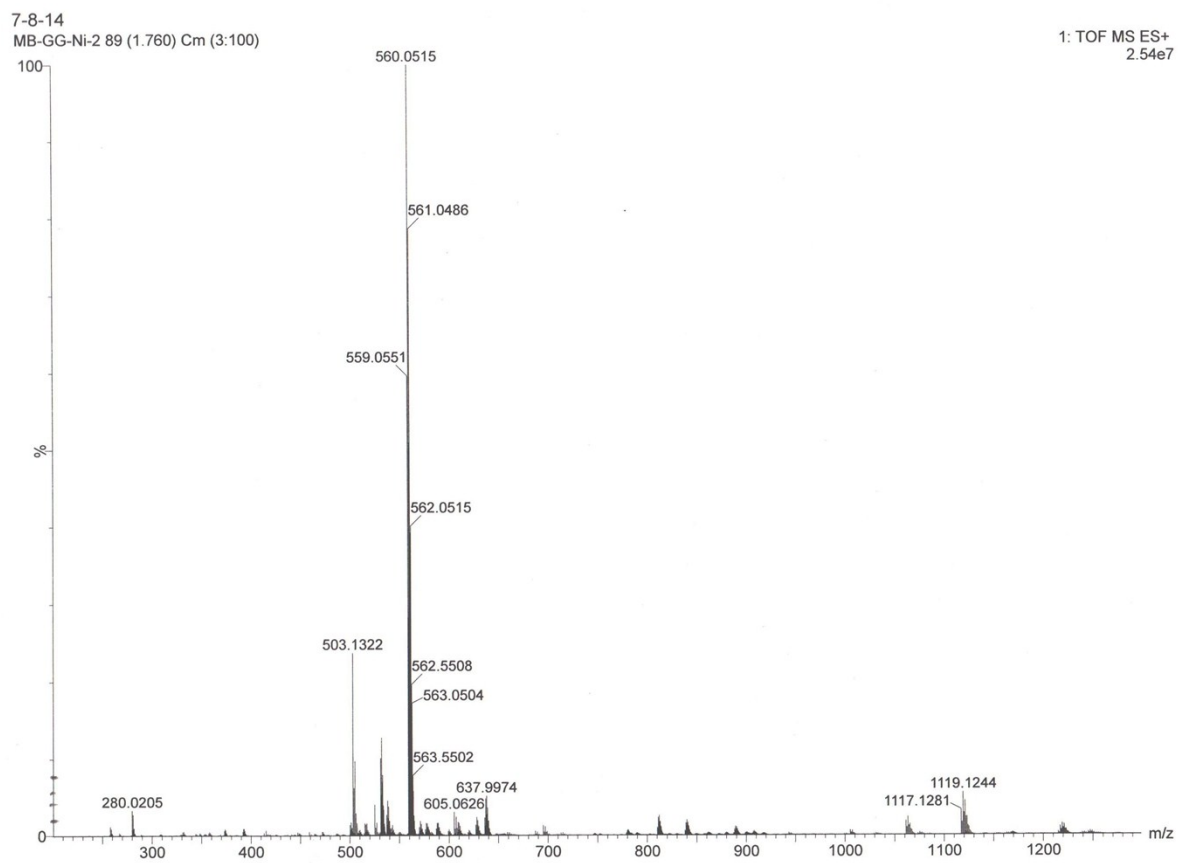
**Fig. S4** ESI mass spectrum (positive ion mode) of the ligand H<sub>5</sub>chdp in methanol.



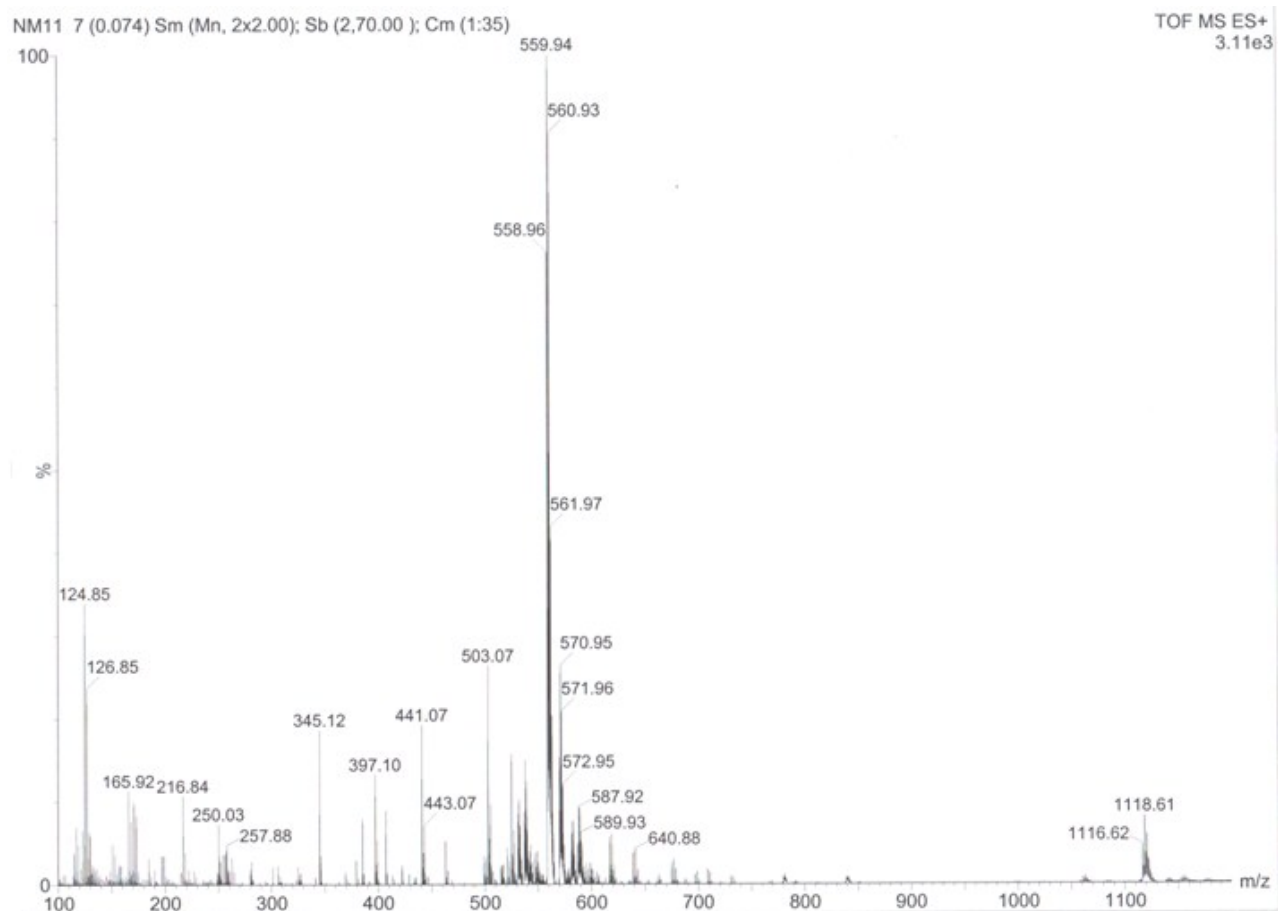
**Fig. S5** FTIR spectrum of complex **1** in the region of 4000-450 cm<sup>-1</sup>.



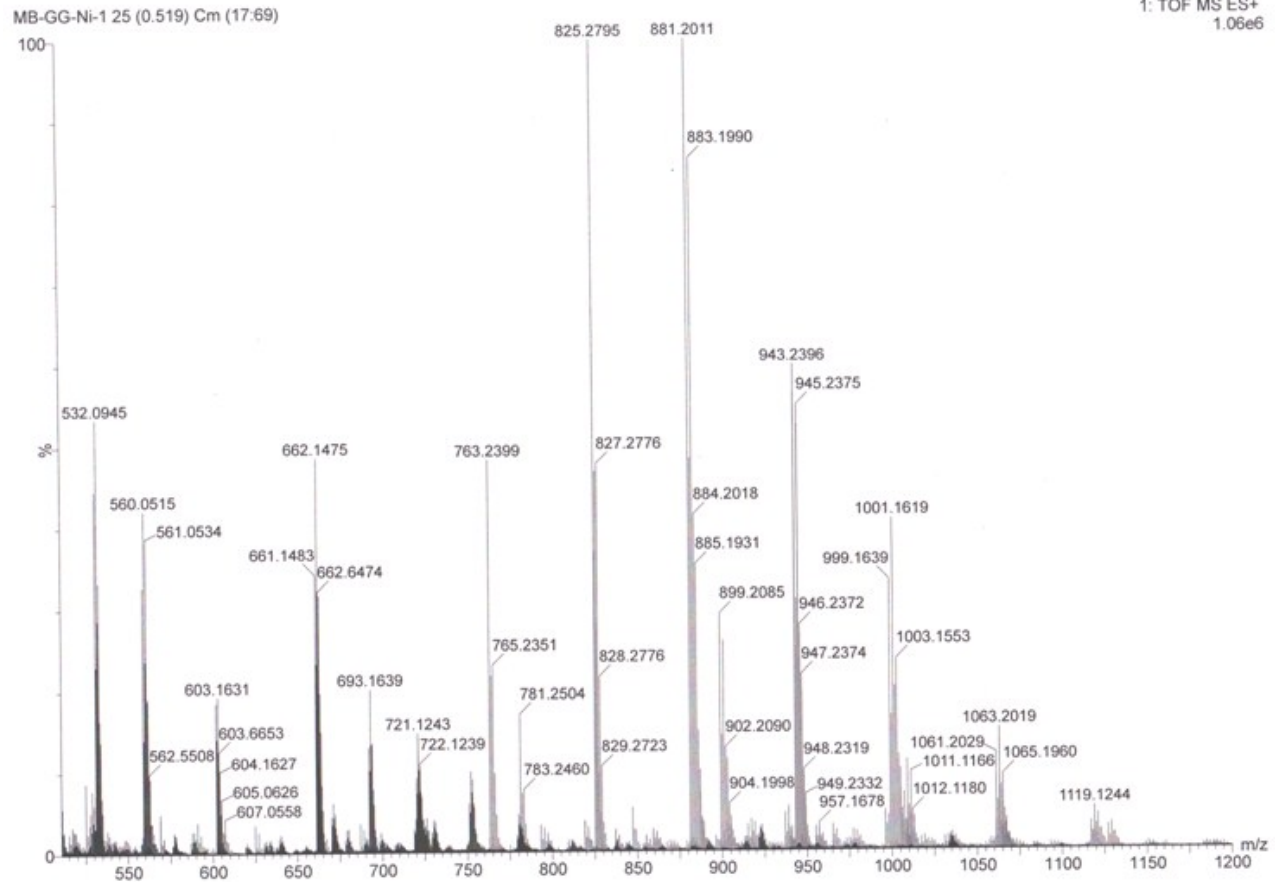
**Fig. S6** UV-Vis spectra of complex **1** at (a) 10<sup>-3</sup>(M) and (b) 10<sup>-4</sup> (M) in methanol-water (1:1; v/v) solution at pH~7.5.



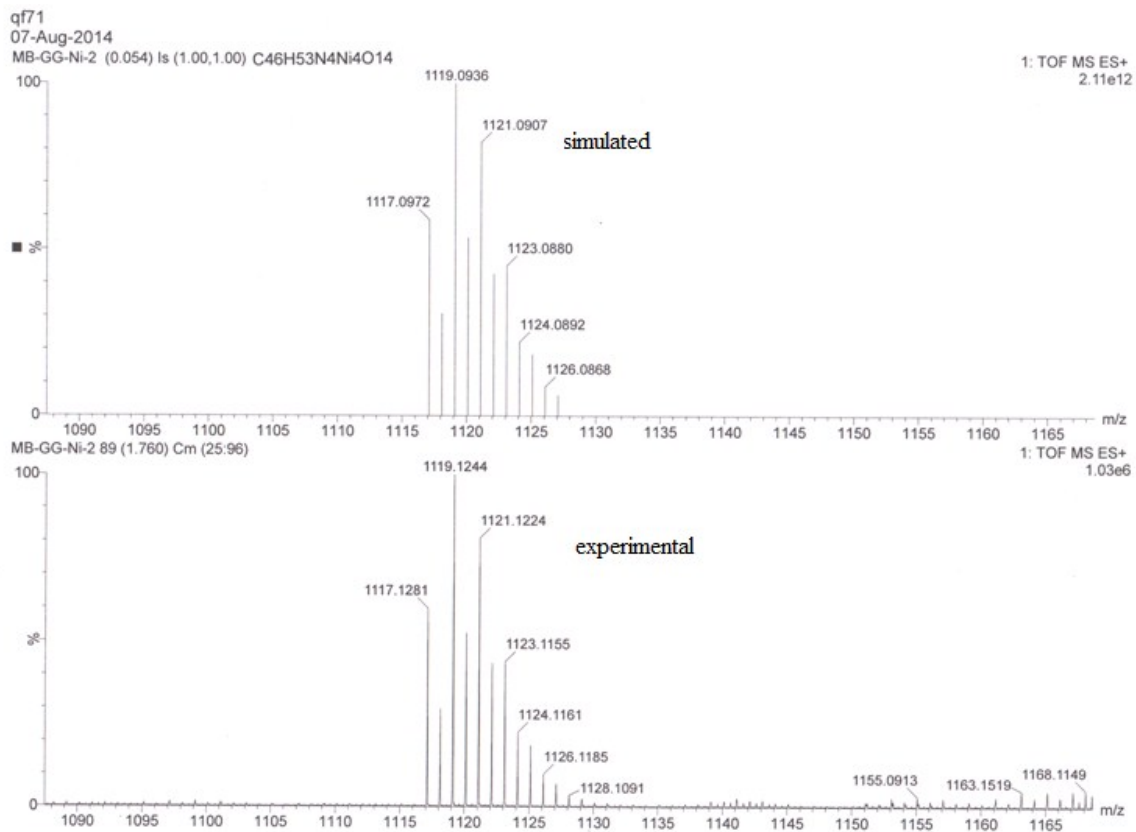
**Fig. S7** ESI mass spectrum (positive ion mode) of complex **1** in methanol-water solution at pH~7.5.



**Fig. S8** ESI mass spectrum (positive ion mode) of complex **2** in methanol-water solution at pH~7.5.

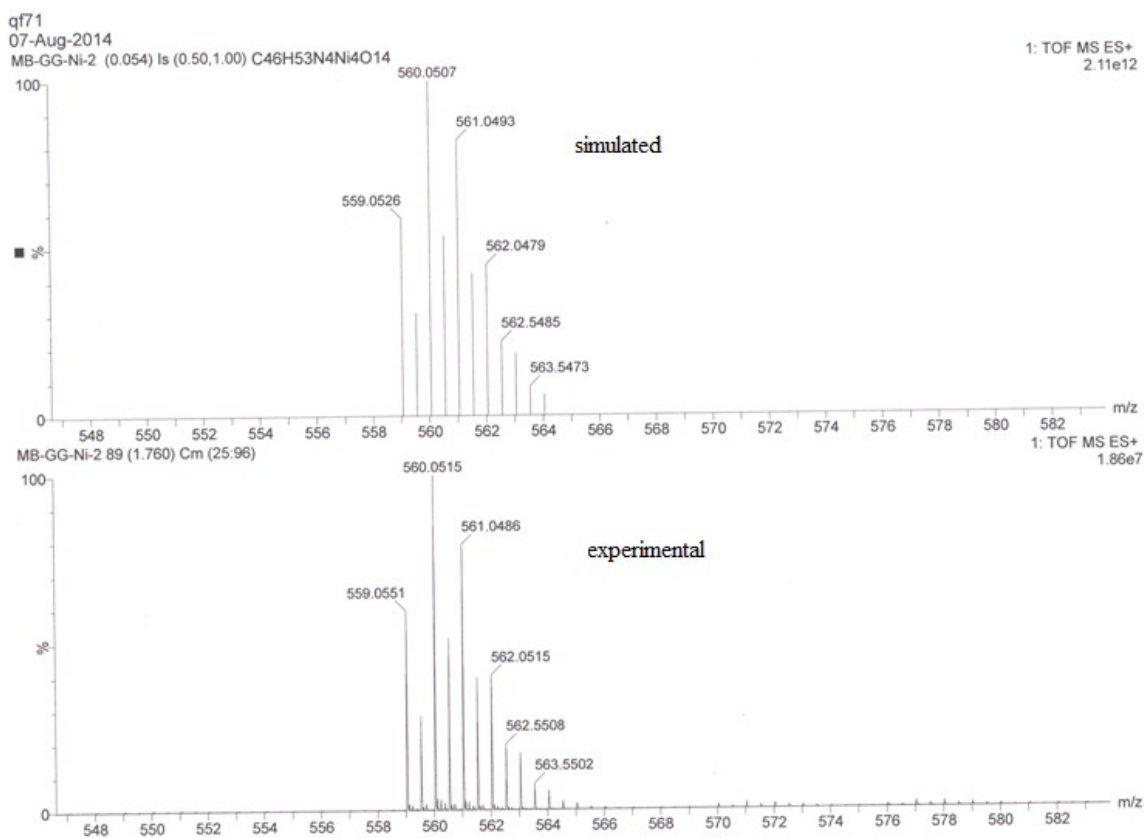


**Fig. S9** ESI mass spectrum (positive ion mode) of complex **3** in methanol-water solution at pH~7.5.

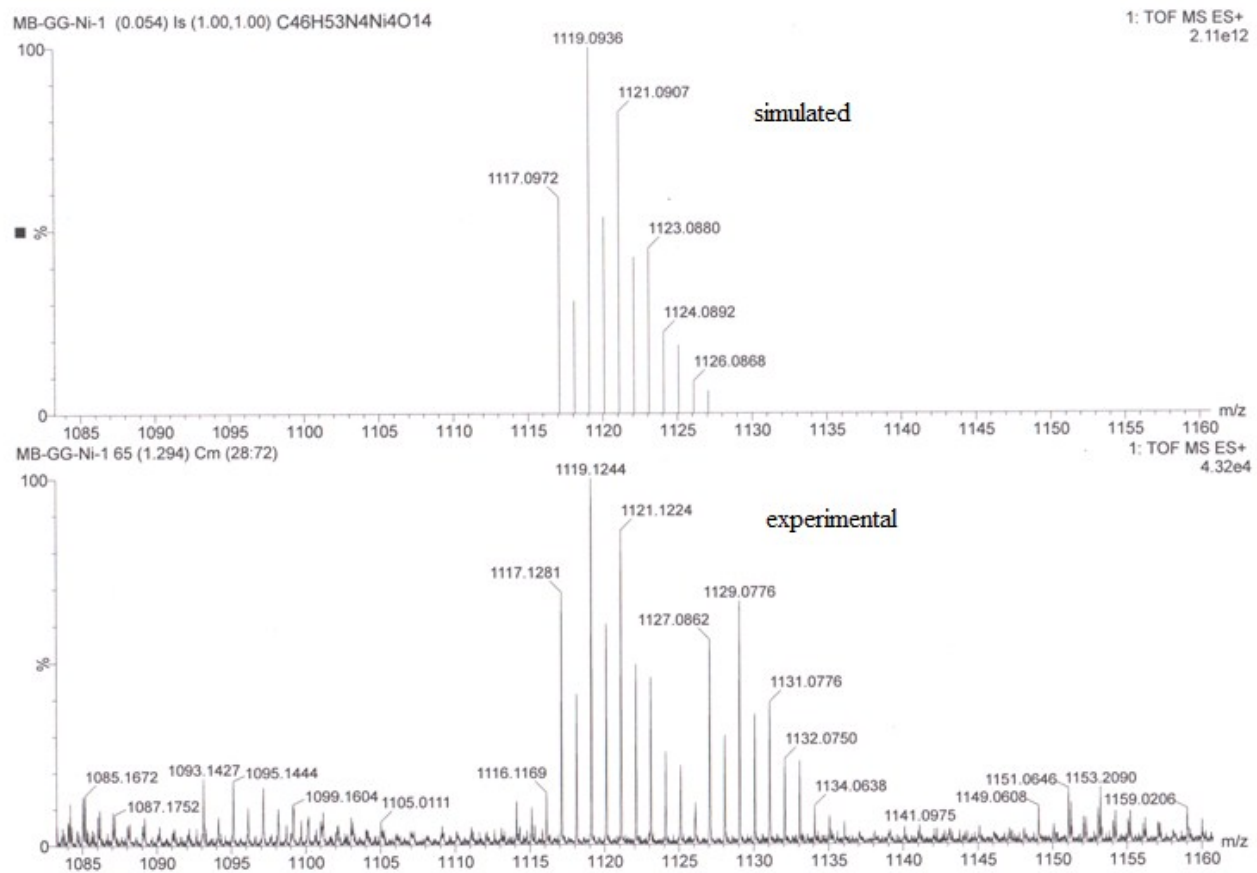


**Fig. S10(a)** The experimental and simulated mass spectra of the peak at  $m/z = 1119$  for complex **1** in methanol-water solution at pH~7.5.

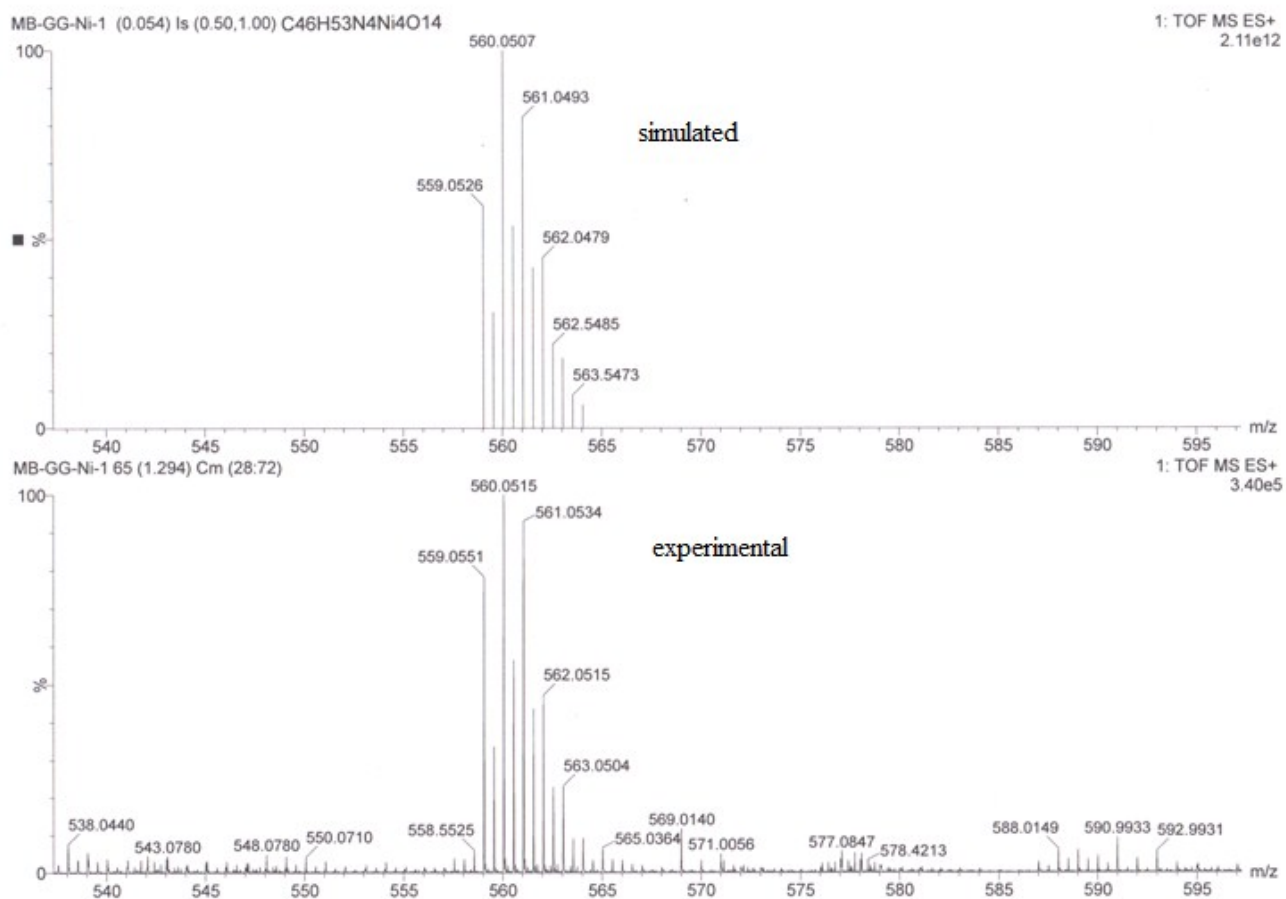




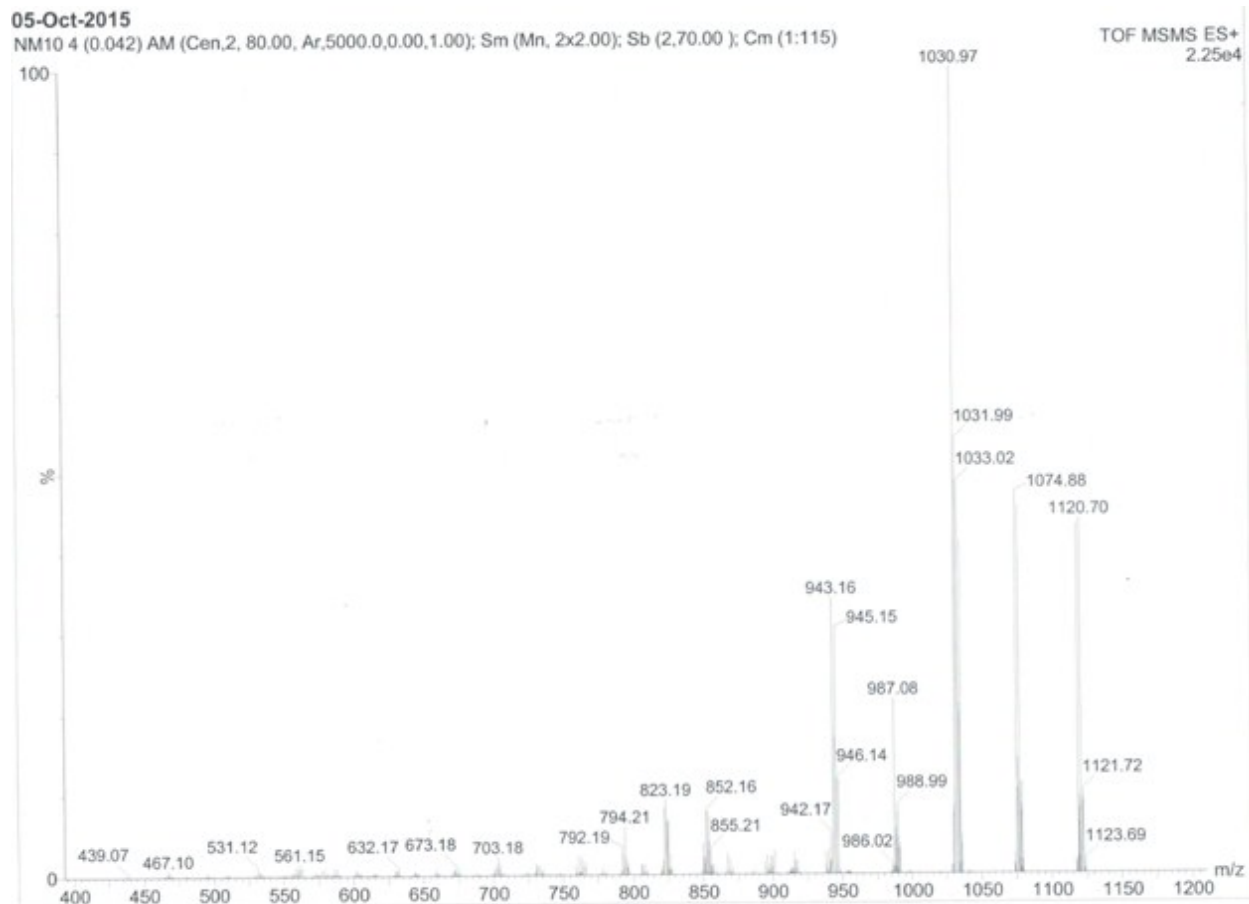
**Fig. S10(b)** The representative experimental and simulated mass spectra of the peak at  $m/z = 560$  for complex **1** in methanol-water solution at pH~7.5.



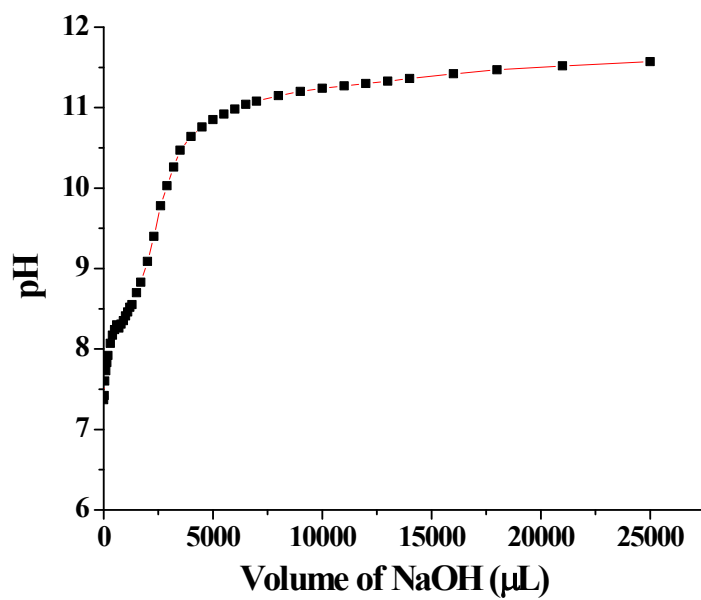
**Fig. S11(a)** The representative experimental and simulated mass spectra of the peak at  $m/z = 1119$  for complex **3** in methanol-water solution at pH~7.5.



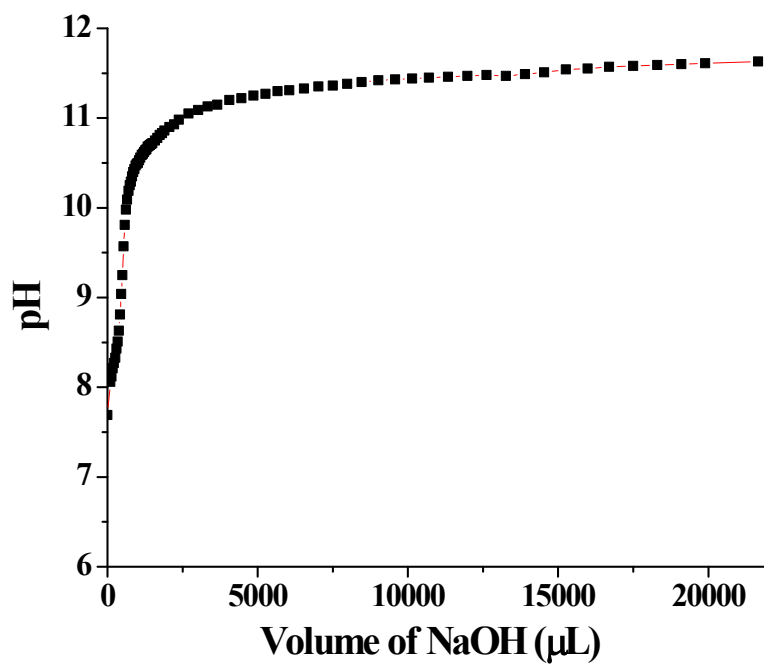
**Fig. S11(b)** The representative experimental and simulated mass spectra of the peak at  $m/z = 560$  for complex **3** in methanol-water solution at pH~7.5.



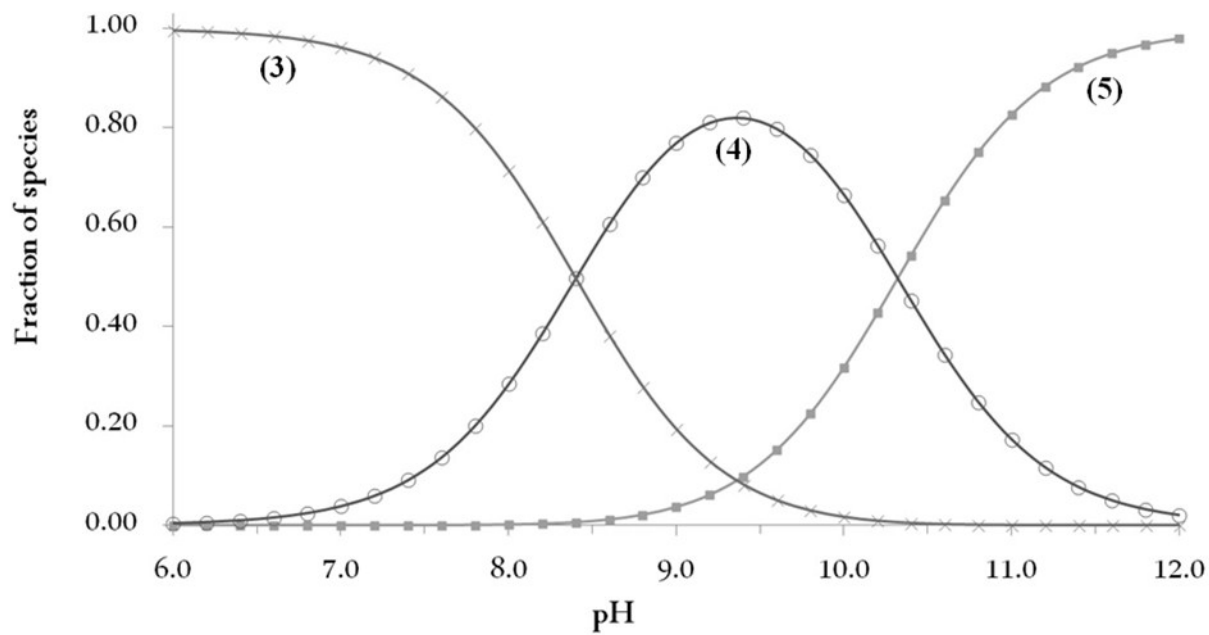
**Fig. S12** MS/MS spectrum (positive ion mode) of the peak at  $m/z = 1119$  for complex **1** in methanol-water solution at pH~7.5.



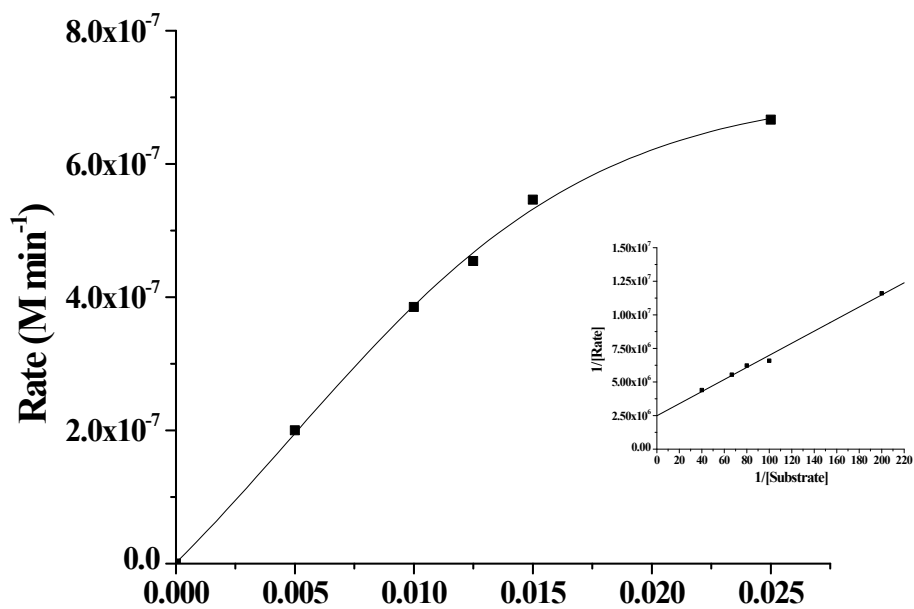
**Fig. S13** Potentiometric titration curve obtained by titrating complex **2** with 0.01 M NaOH. The experimental points (black squares) are in good agreement with the theoretical curve (red line).



**Fig. S14** Potentiometric titration curve obtained by titrating complex **3** with 0.01 M NaOH. The experimental points (black squares) are in good agreement with the theoretical curve (red line).

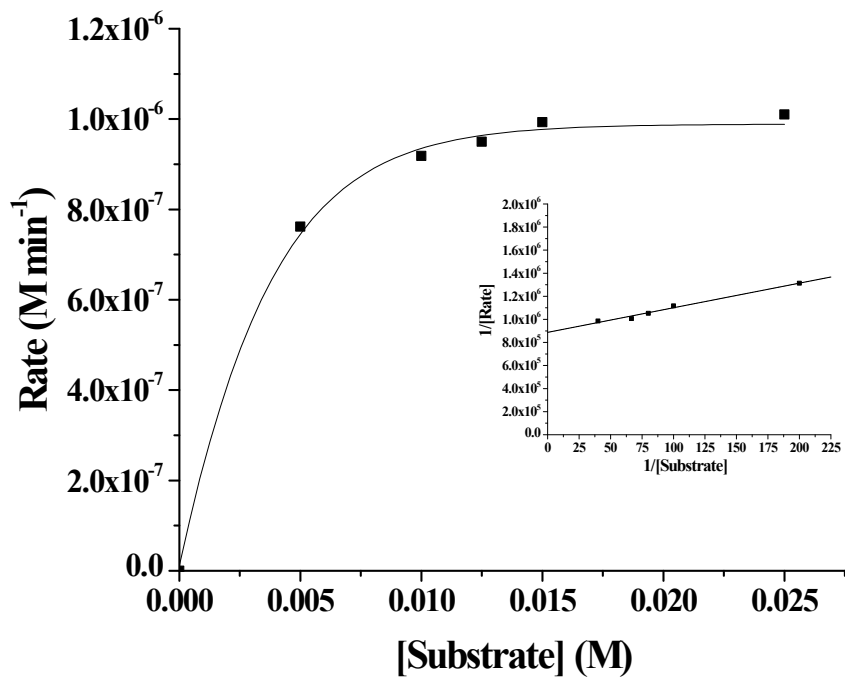


**Fig. S15** Species distribution curves of complex **3** as a function of pH.

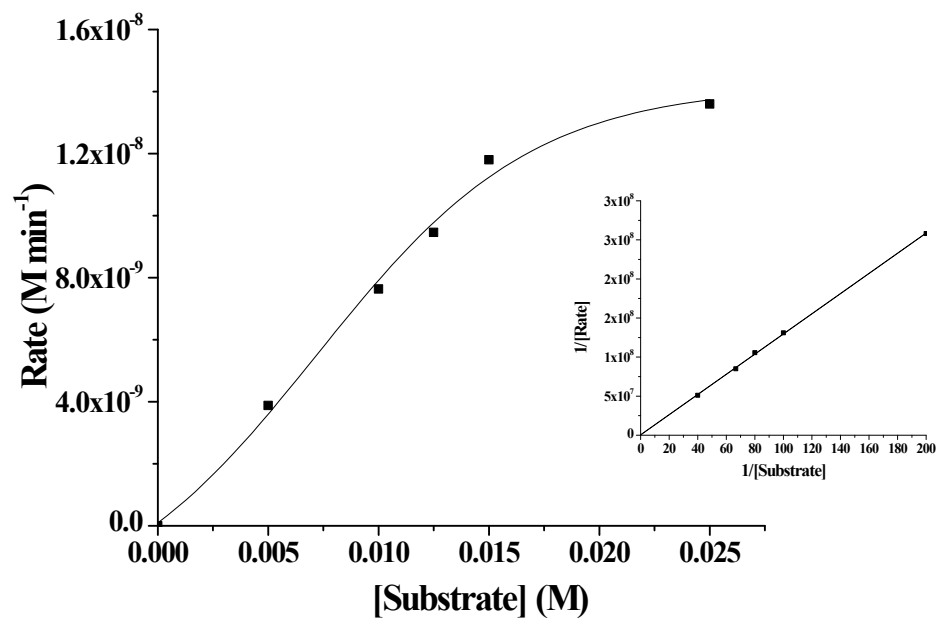


**Fig. S16** Dependence of the rate on the concentration of substrate (BNPP) for complex **1**. Inset shows Lineweaver-Burk plot. [Complex] =  $25 \times 10^{-5}$  M; [Buffer] =  $20 \times 10^{-3}$  M; pH~11.8;  $I = 0.1$  M (NaClO<sub>4</sub>) in MeOH-H<sub>2</sub>O (1:1; v/v) at 30°C.





**Fig. S17** Dependence of the rate on the concentration of substrate (BNPP) for complex **2**. Inset shows Lineweaver-Burk plot. [Complex] =  $25 \times 10^{-5}$  M; [Buffer] =  $20 \times 10^{-3}$  M; pH~11.8;  $I = 0.1$  M (NaClO<sub>4</sub>) in MeOH-H<sub>2</sub>O (1:1; v/v) at 30°C.



**Fig. S18** Dependence of the rate on the concentration of substrate (BNPP) for complex **3**. Inset shows Lineweaver-Burk plot. [Complex] =  $25 \times 10^{-5}$  M; [Buffer] =  $20 \times 10^{-3}$  M; pH~11.8;  $I = 0.1$  M (NaClO<sub>4</sub>) in MeOH-H<sub>2</sub>O (1:1; v/v) at 30°C.