

## Electronic supplementary information

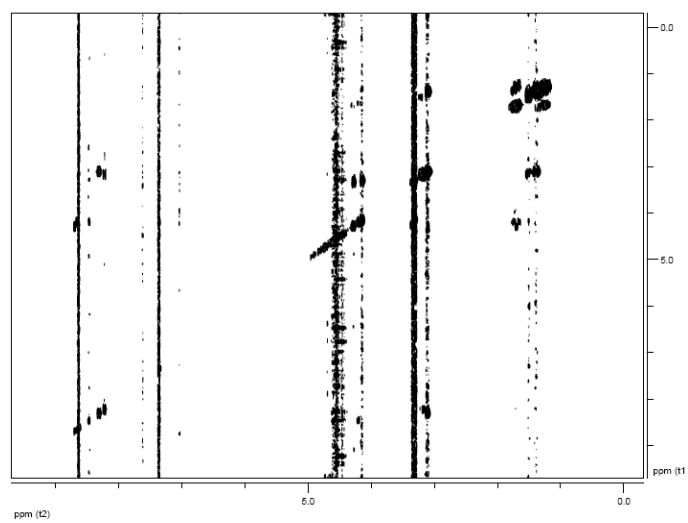
**Table S1.** The tentative assignment of the  $^1\text{H-NMR}$  signals: chemical shifts ( $\delta$ ) belonging to the Lys and His protons in the ligand at  $\text{pH}^* = 5.5$ .

Sort of H	$\delta(\text{ppm})$	
	Lys	His
$\alpha\text{-CH}$	4.18-4.20	4.13-4.69
$\beta\text{-CH}_2$	1.69-1.73	3.31-3.35
$\gamma\text{-CH}_2$	1.24-1.39	-
$\delta\text{-CH}_2$	1.38-1.51	-
$\varepsilon\text{-CH}_2$	3.12-3.18	-
$\text{C}^5\text{H}$	-	7.36
$\text{C}^2\text{H}$	-	8.65

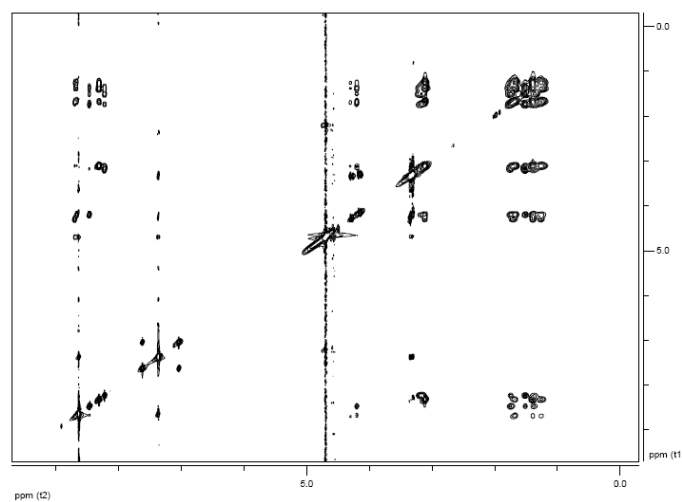
**Fig. S1** Two dimensional COSY spectra of the free ligand at  $\text{pH}^* = 5.5$  in  $\text{H}_2\text{O}$  (containing 10%  $\text{D}_2\text{O}$ ).

**Fig. S2** Two dimensional TOCSY spectra of the free ligand at  $\text{pH}^* = 5.5$  in  $\text{H}_2\text{O}$  (containing 10%  $\text{D}_2\text{O}$ ).

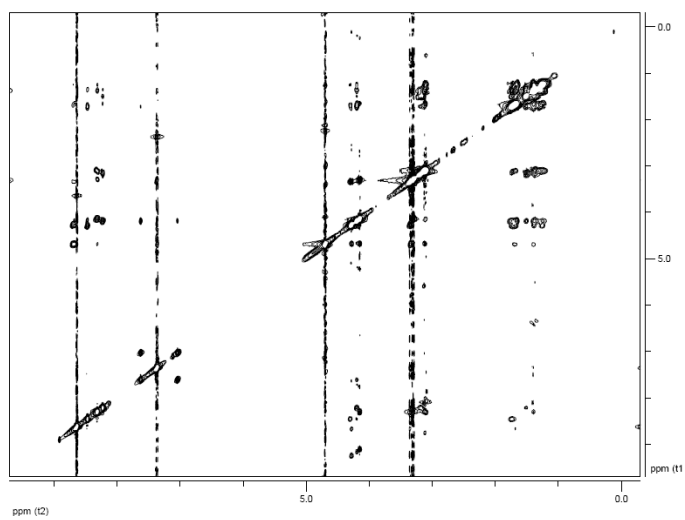
**Fig. S3** Two dimensional ROESY spectra of the free ligand at  $\text{pH}^* = 5.5$  in  $\text{H}_2\text{O}$  (containing 10%  $\text{D}_2\text{O}$ ).



**Fig. S1**



**Fig. S2**



**Fig. S3**