

Supplementary Informations

Table S1. pHis2 proton chemical shifts (ppm) in H₂O at 298 K.

	NH	α CH	β CH	Others
His1	-	4.07	3.22	C2 8.51; C4 7.28
Lys2	-	3.81	1.72	NHsc 8.14 ϵ 3.10 γ δ 1.35 1.20
β -Ala3	8.22	2.46	3.40	
Lys4	8.08	4.08	1.61	NHsc 8.14 NH ₂ t 7.52, 7.00 ϵ 3.10 γ δ 1.35 1.20
His5	-	4.07	3.22	C2 8.51; C4 7.28

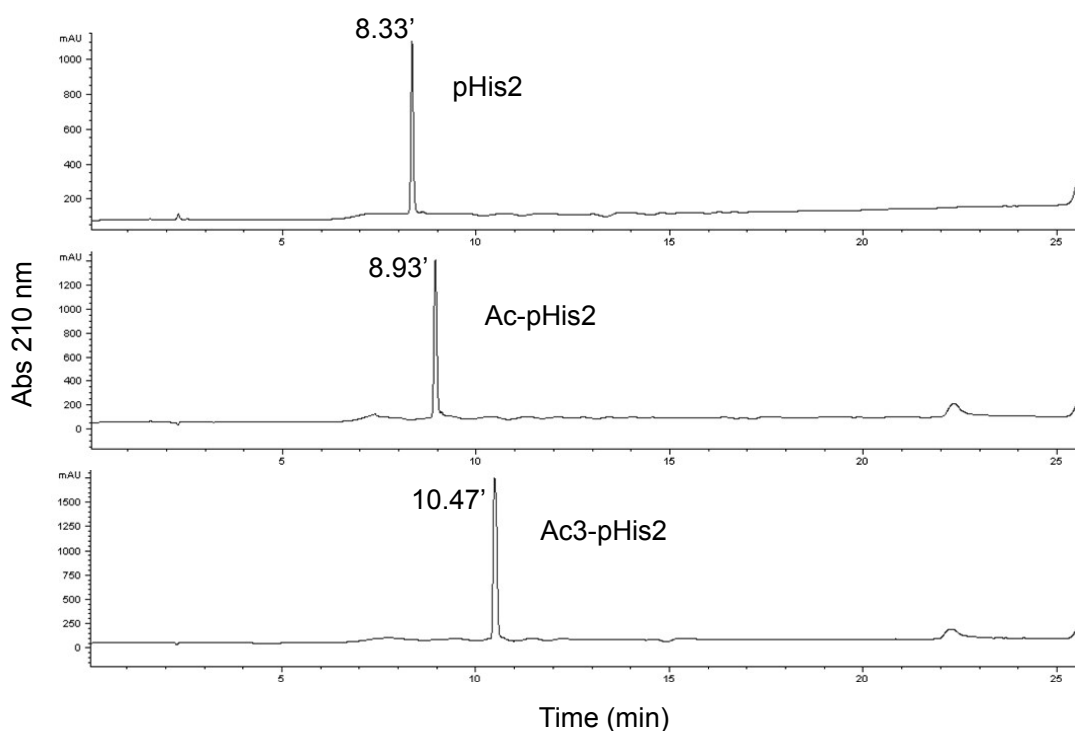


Figure S1: Analytical characterization by RP-HPLC of pHis2, Ac-pHis2 and Ac3-pHis2 peptides. Chromatograms were revealed reading the absorbance at 210 nm.

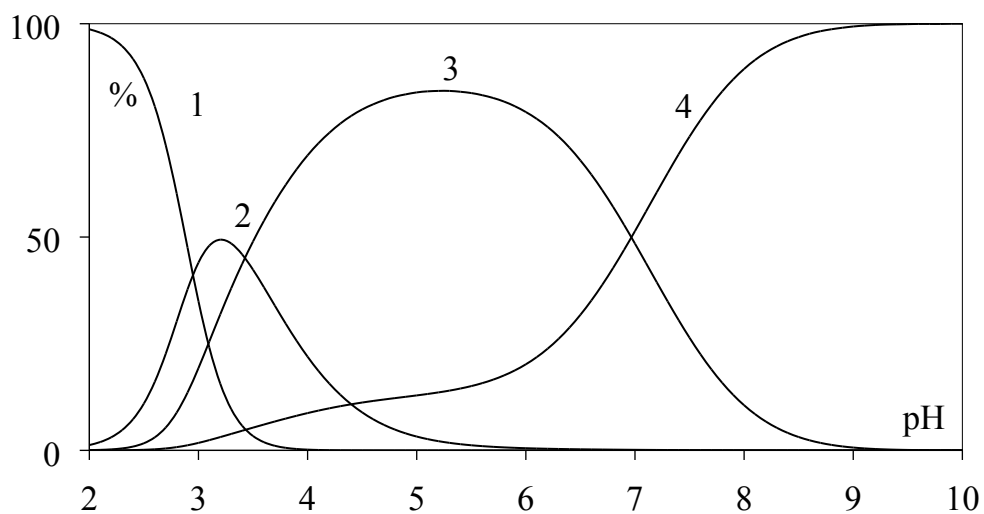


Fig.S2. Distribution diagram of Ga(III)-His system in 0.1 M NaClO₄ with $C_{Me} = 2.0 \cdot 10^{-3}$ M and $C_L = 4.0 \cdot 10^{-3}$ M (1: Ga³⁺; 2: Ga(OH)₂⁺; 3: Ga(OH)₂His⁺; 4: Ga(OH)₃).

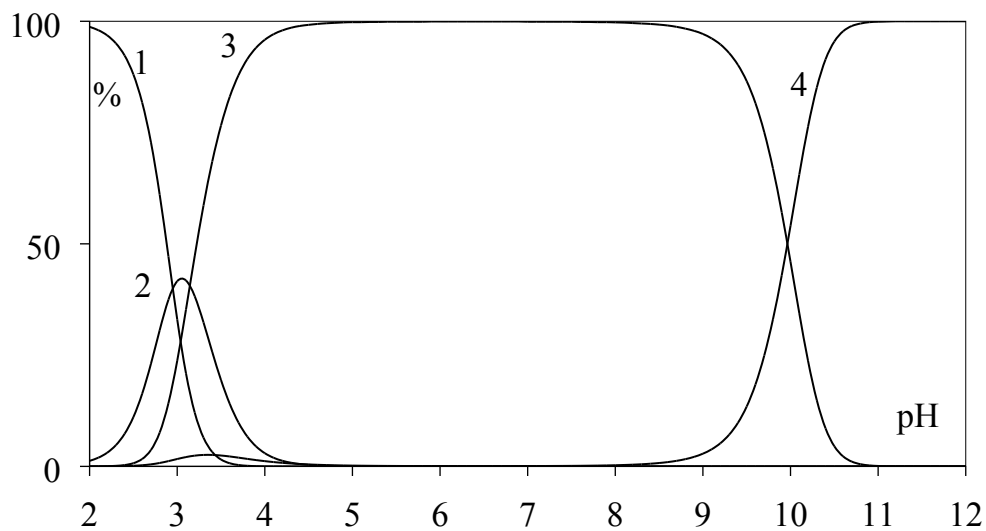


Fig.S3. Distribution diagram of Ga(III)-pHis2 system in 0.1 M NaClO₄ with $C_{Me} = 2.0 \cdot 10^{-3}$ M and $C_L = 4.0 \cdot 10^{-3}$ M (1: Ga³⁺; 2: Ga(OH)₂⁺; 3: Ga(OH)₂H₃L⁺; 4: Ga(OH)₃).

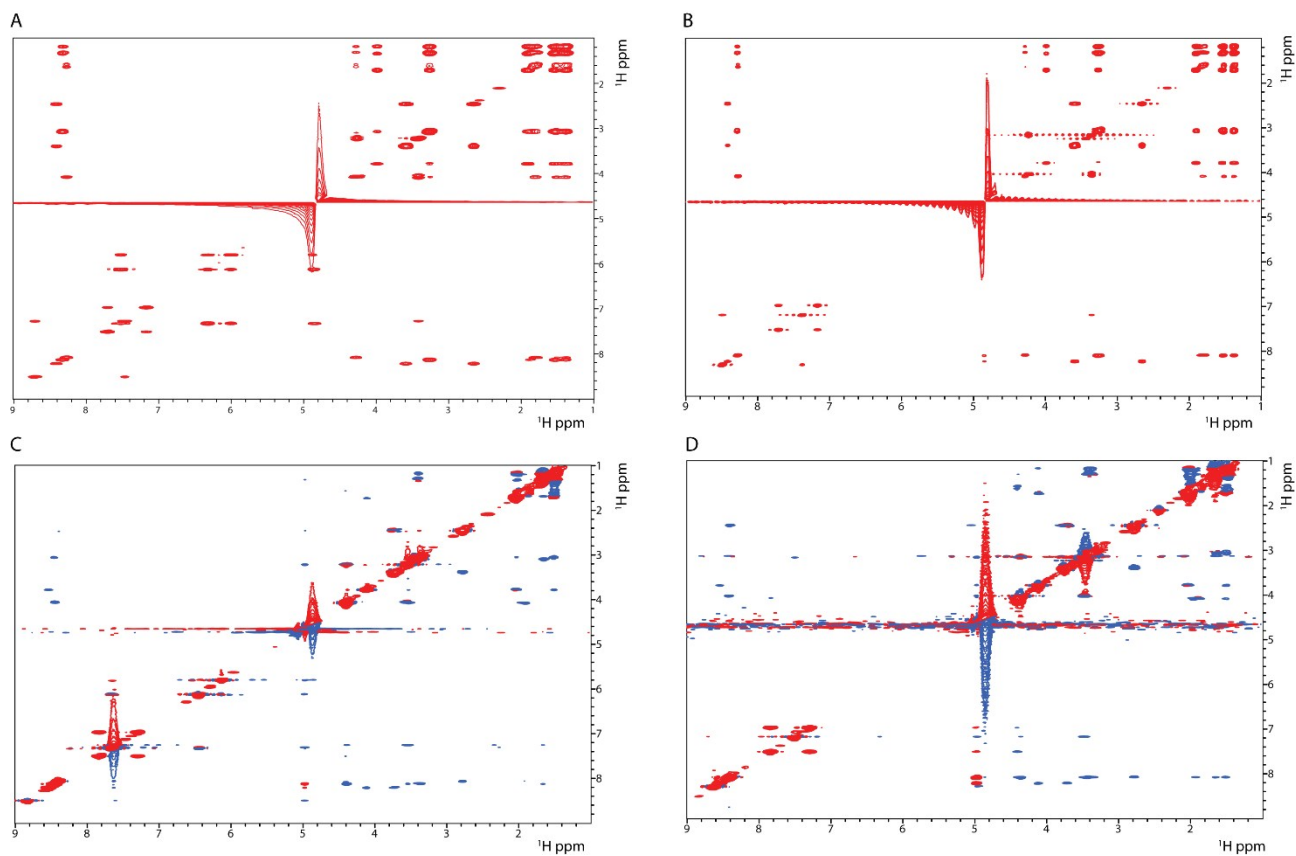


Fig.S4. ^1H - ^1H TOCSY and NOESY spectra of the *fac*- $[\text{Re}(\text{H}_2\text{O})_3(\text{CO})_3]^+$ -pHis2 (A and C, respectively) and of the Ga(III)-pHis2 complexes (B and D).

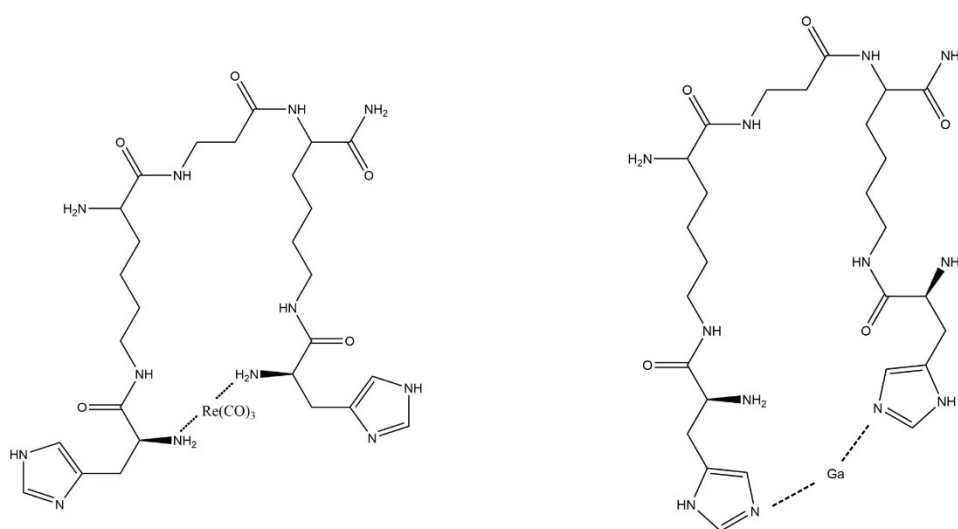


Fig.S5. Schematic representation of complex formed by pHis2 upon binding with *fac*- $[\text{Re}(\text{H}_2\text{O})_3(\text{CO})_3]^+$ (left) and with Ga(III) (right).