Table S1. Spectroscopic parameters for Cu^{2+} complexes at 298K in aqueous solution. Metal/peptide ratio of 1:1.1. Standard deviation on the last significant figure is given in parentheses. Most abundant complex form at precise pH is bold.

		UV-Vis		CD		EPR		
Species	**pH**	λ [nm]	Ɛ [$M^{-1}cm^{-1}$]	Λ [nm]	ΔƐ [$M^{-1}cm^{-1}$]	$A_{\|\|}$ [G]	$g_{\|\|}$	Proposed donors
-	**2.07**	800	20.50	212.3 236	3.45 -27.68	-	-	-
[CuH_2L]	**3.00**	800	24.52	212.3 236	3.05 -26.90	121.3	2.41	-
[CuH_2L] [CuHL]	**3.99**	800 737	24.25 21.91	212.3 236	2.33 -23.74	120.1	2.42	-
[CuH_2L] **[CuHL]** [CuL]	**5.01**	716	39.98	236	-10.96	157.77	2.30	N_{im}, COO^-
[CuHL] **[CuL]** [$CuH_{-1}L$]	**6.08**	647	68.09	-	-	170.90	2.27	$2N_{im}$, COO^-
[CuHL] **[CuL]** [$CuH_{-1}L$]	**7.00**	635.5	83.58	257.1 525.7	34.33 0.83	178.10	2.26	$3N_{im}$ COO^-
[CuL] [$CuH_{-1}L$] [$CuH_{-2}L$]	**8.02**	619.5	93.08	257.1 525.7	40.68 2.33	185.01	2.23	$3N_{im}$ N^-
[$CuH_{-1}L$] **[$CuH_{-2}L$]**	**9.02**	597	97.68	262.8 316.8 525.7 609.9	42.46 7.075 3.20 4.97	189.42	2.22	$3N_{im}$, N^-

Bacterial M10 metallopeptidase as a medicinal target - coordination chemistry of possible metal-based inhibition

Paulina Potok,[1] Sławomir Potocki[1*]

slawomir.potocki@chem.uni.wroc.pl

[1] Faculty of Chemistry, University of Wroclaw, 14 Joliot-Curie St., 50-383 Wroclaw, Poland

[CuH$_{-2}$L] **[CuH$_{-3}$L]**	**10.07**	572.5	110.18	262.8 316.8 488.3 609.9	38.63 13.83 -4.05 7.41	189.56	2.22	3N$_{im}$, N$^-$
[CuH$_{-2}$L] **[CuH$_{-3}$L]**	**11.00**	538.5	127.13	262.8 316.8 488.3 609.9	32.43 17.65 -7.88 8.88	201.99	2.19	2N$_{im}$, 2N$^-$
[CuH$_{-3}$L]	**12.07**	526.5	136.33	262.8 316.8 488.3 609.9	28.61 17.53 -10.35 9.48			N$_{im}$, 3N$^-$

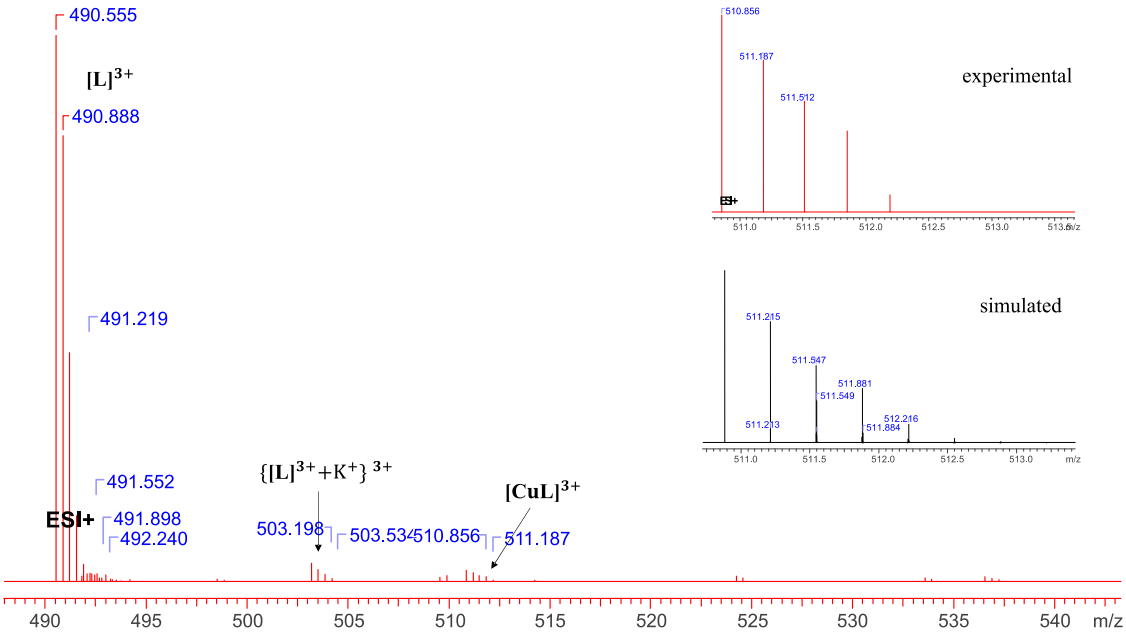

Figure S1. Mass spectrum for the Cu(II)-Ac-EHELGHAIGLDHT-NH$_2$ complex (metal to ligand molar ratio 1:1, [Cu(II)] = 2 mM). Experimental and simulated spectra for the [CuL]$^{3+}$ molecular ion with m/z 511.215 are presented in the right corner.

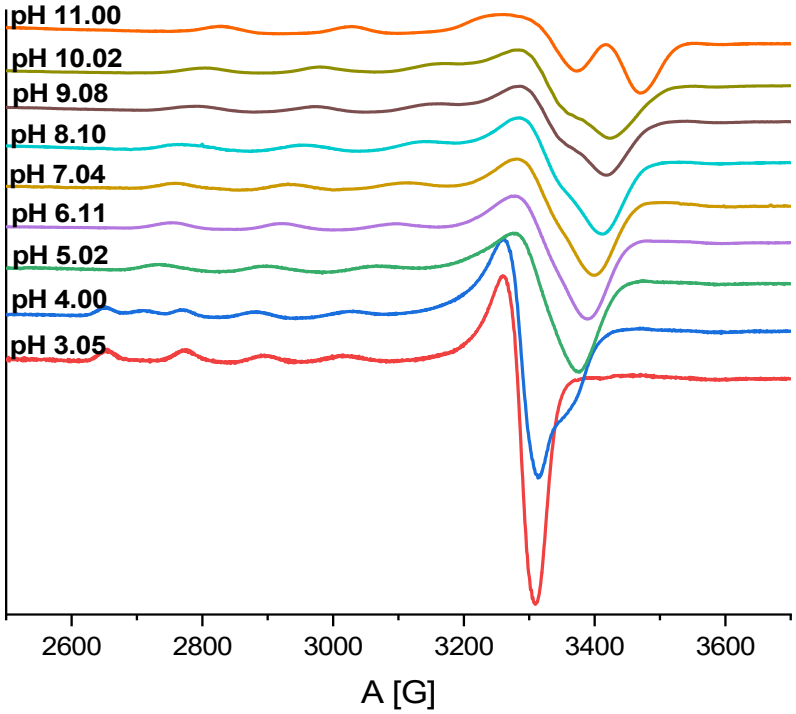

Figure S2. EPR spectra performed for the Cu(II)-Ac-EHELGHAIGLDHT-NH_2 complex, 5.00–11.00 pH range.

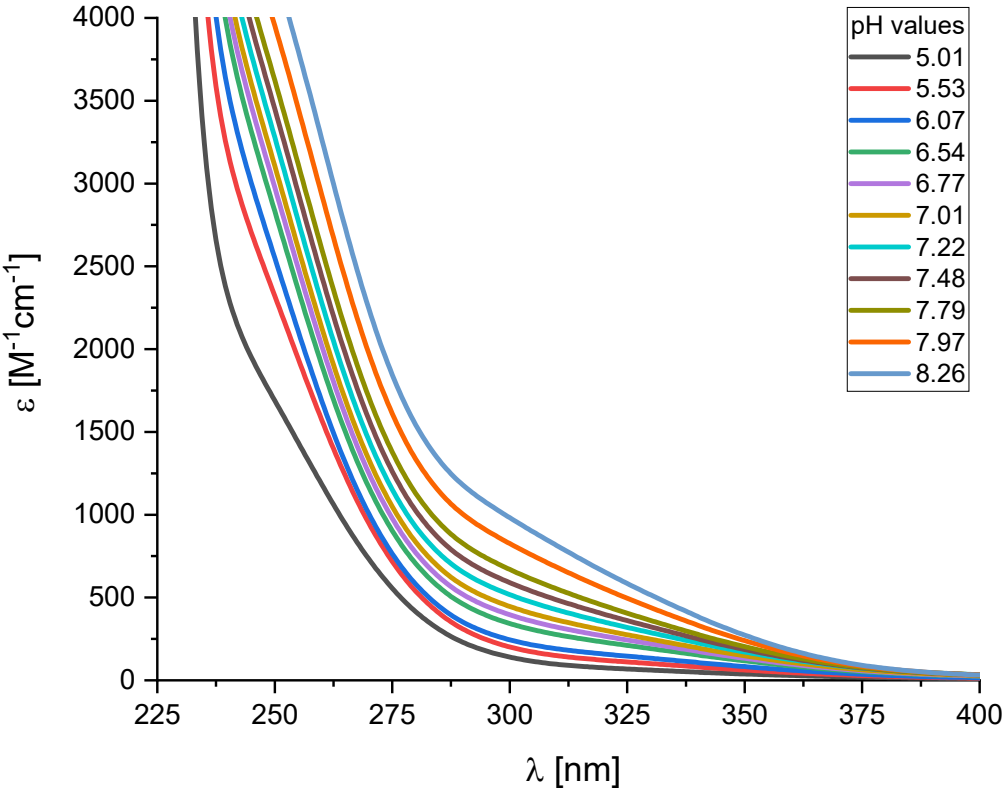

Figure S3. UV-Vis region for Cu(II) complexes of the Ac-EHELGHAIGLDHT-NH_2 peptide. Cu(II)/peptide ratio = 1:1.1

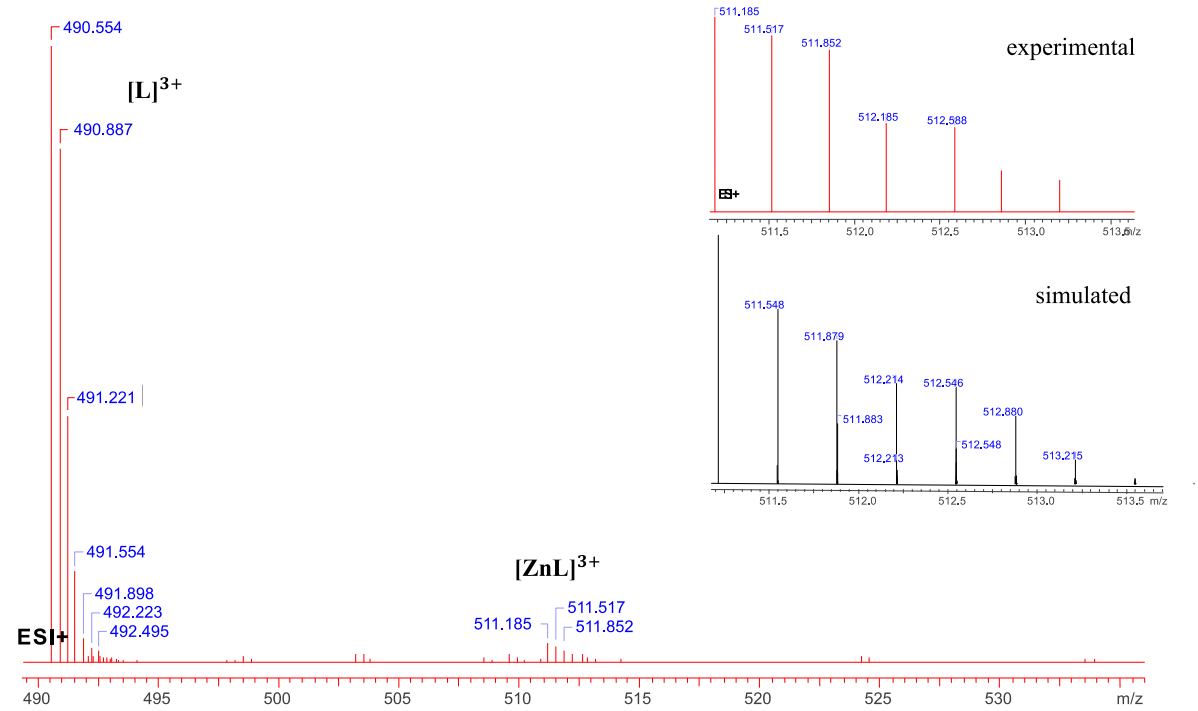

Figure S4. Mass spectrum for the Zn(II)-Ac-EHELGHAIGLDHT-NH_2 complex (metal to ligand molar ratio 1:1, [Zn(II)] = 2 mM). Experimental and simulated spectra for the $[ZnL]^{3+}$ molecular ion with m/z 511.539 are presented in the right corner.

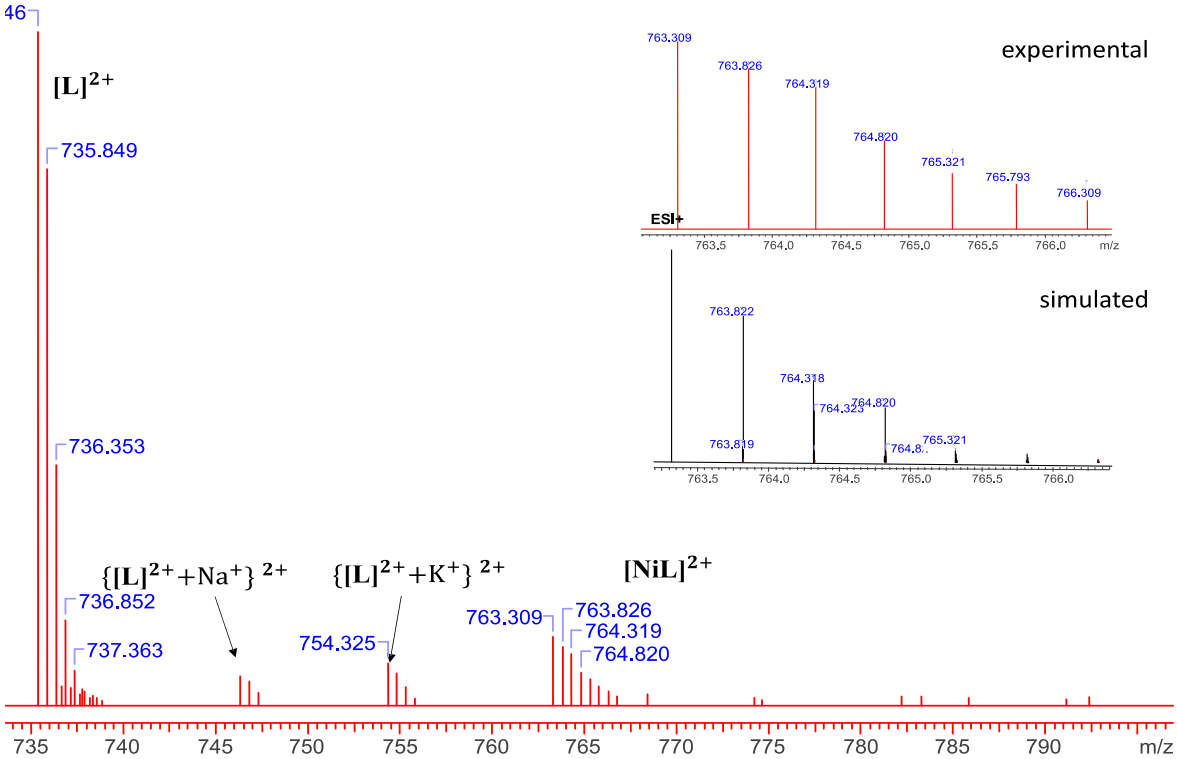

Figure S5. Mass spectrum for the Ni(II)-Ac-EHELGHAIGLDHT-NH_2 complex (metal to ligand molar ratio 1:1, [Ni(II)] = 2 mM). Experimental and simulated spectra for the $[NiL]^{2+}$ molecular ion with m/z 763.811 are presented in the right corner.

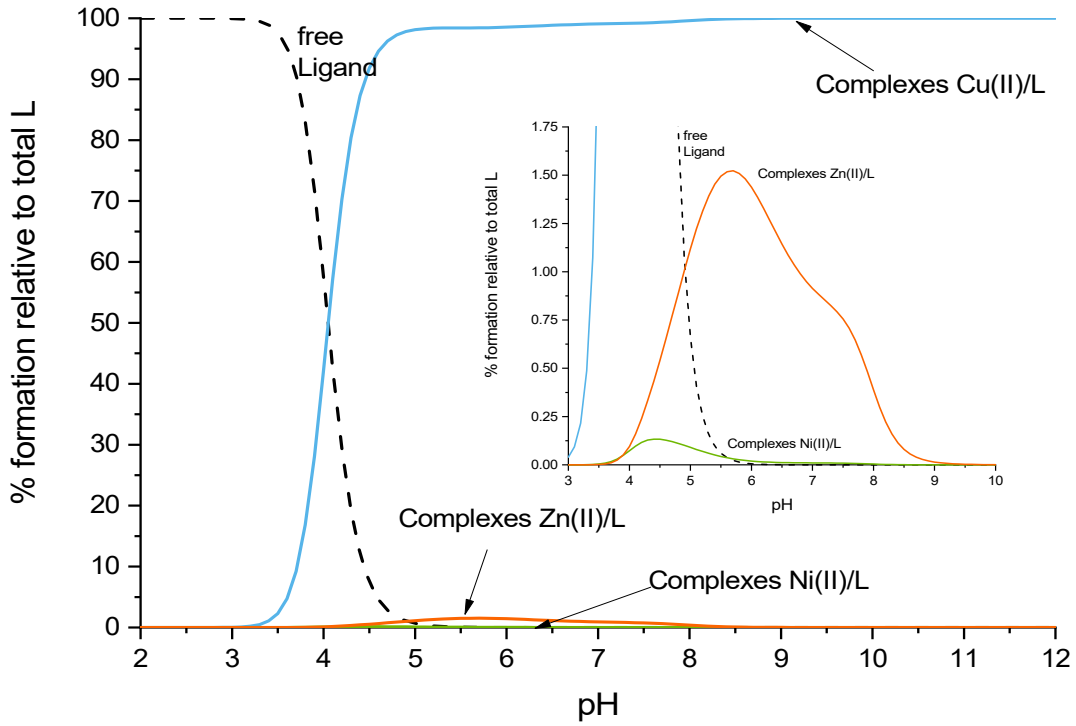

Figure S6. Competition plots showing the comparison of thermodynamic stability between complexes of Zn(II), Cu(II), and Ni(II) ions with ligand L – Ac-EHELGHAIGLDHT-NH2 peptide. The molar ratio for ligand and metal ions L : Zn(II) : Cu(II) : Ni(II) are 224:21:1.