Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Coordination behaviour of new open chain and macrocyclic peptidomimetic compounds with copper(II).

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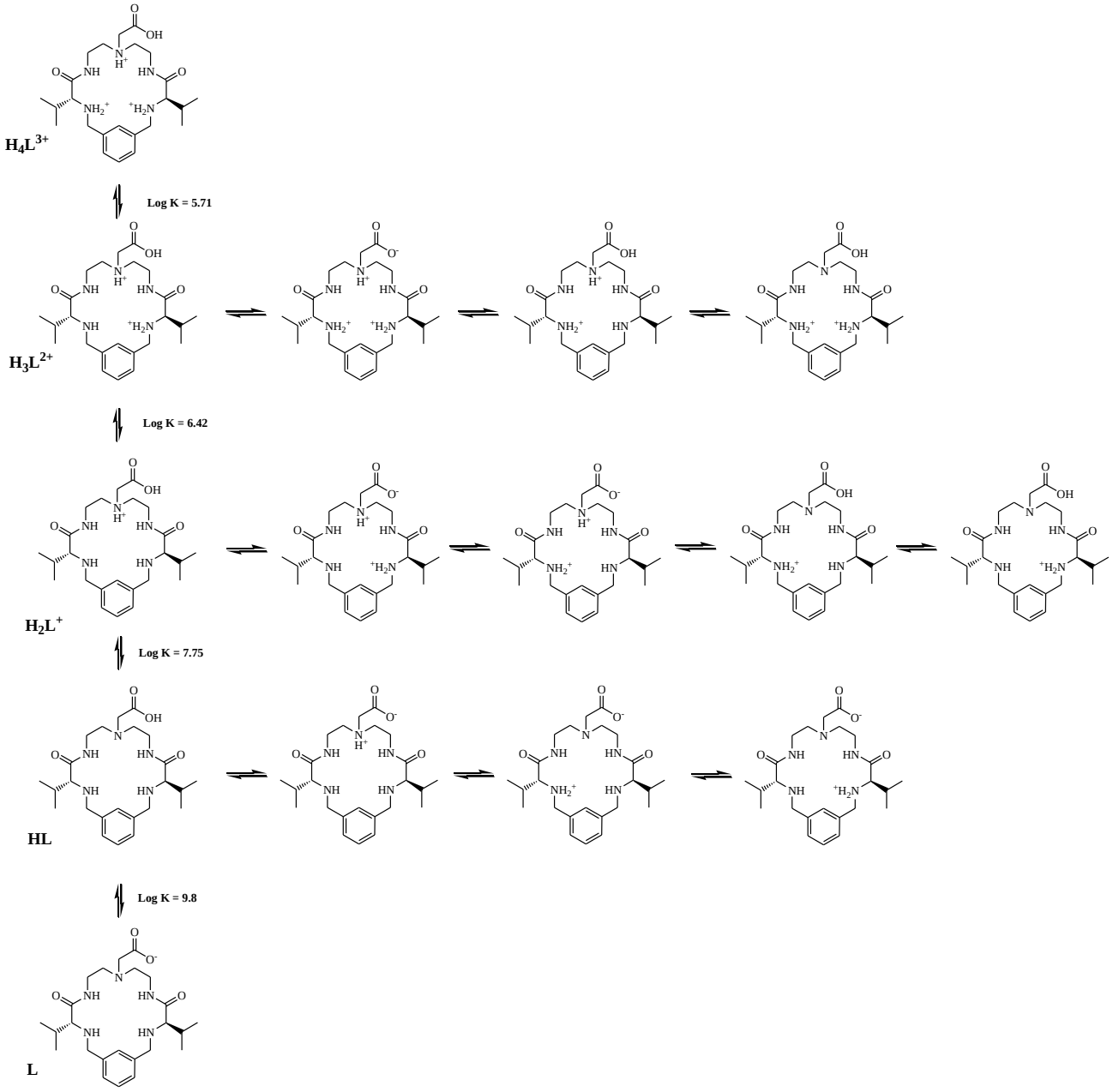
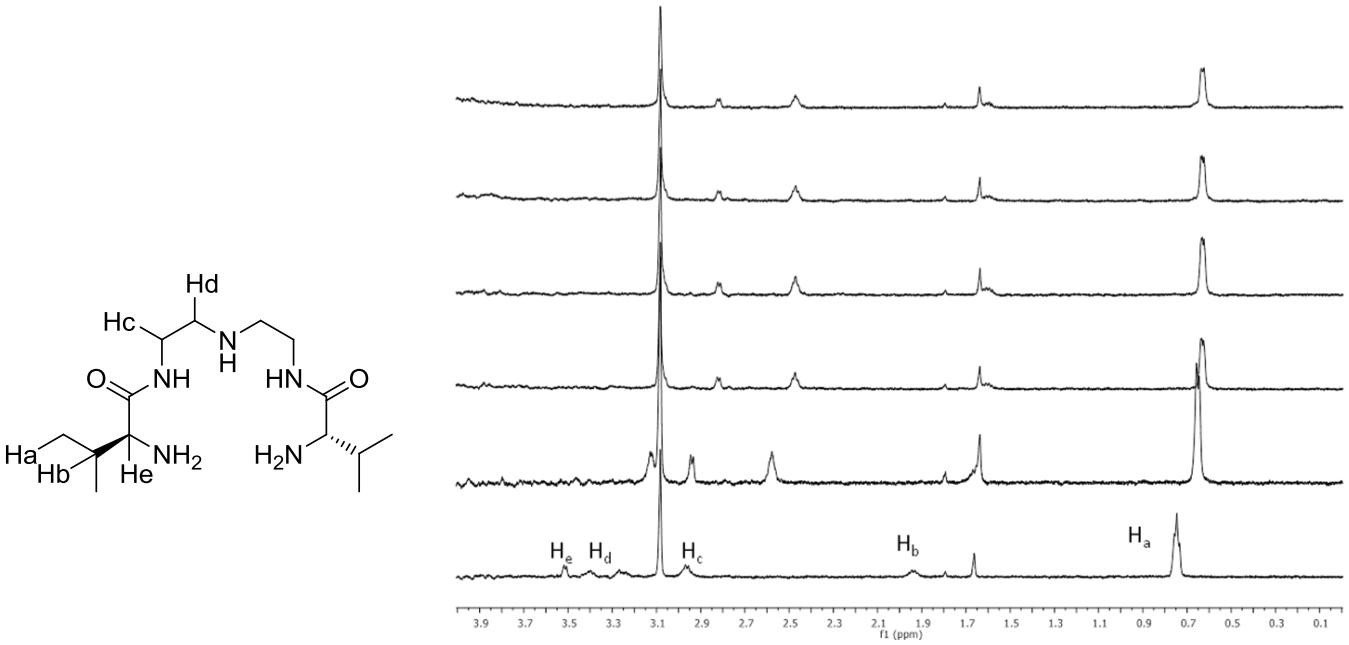
S1 Potential protonation equilibria for pseudopeptide 2.

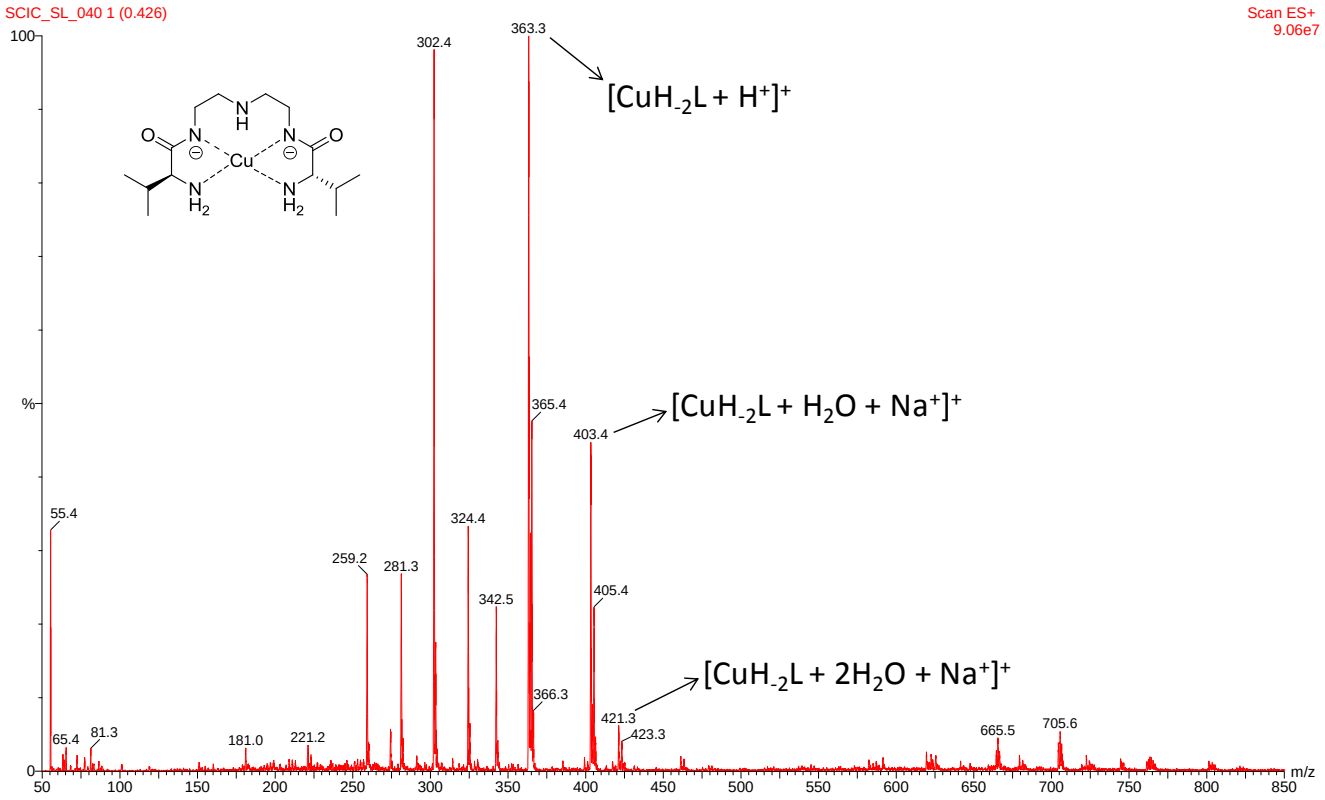


S2 Proton induced shifts for Compound 1 upon changing pH

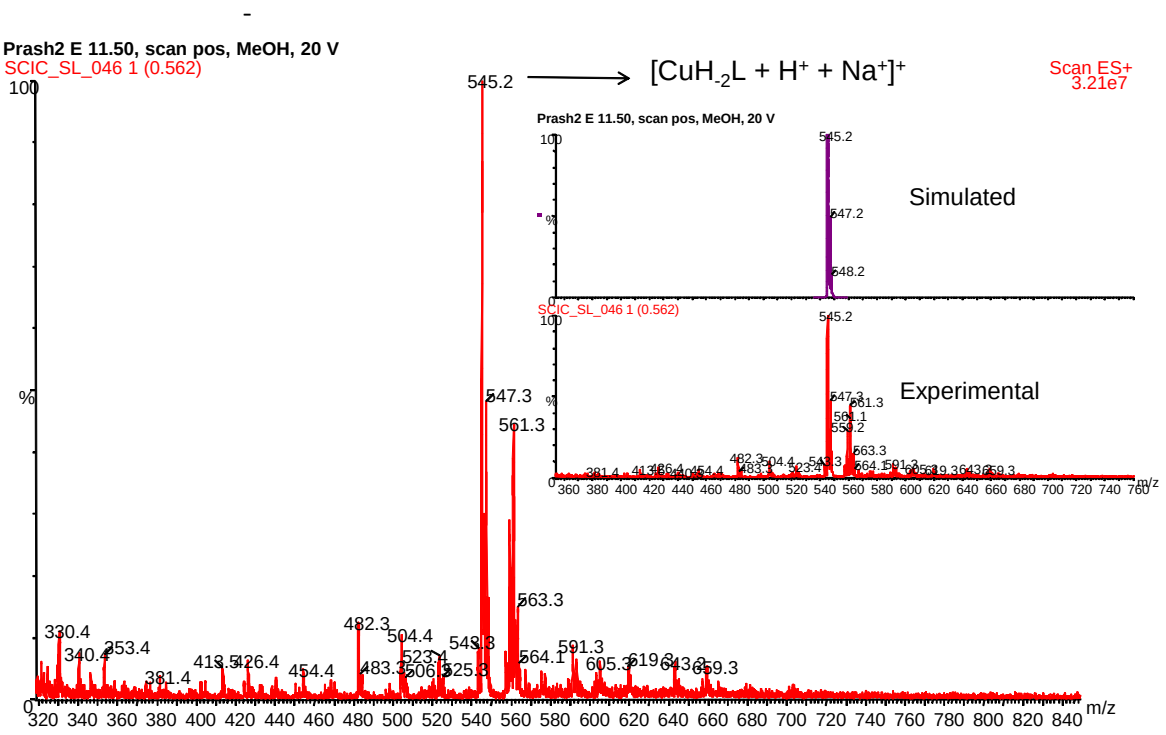


^{1}H NMR of compound **1** (1 mM) at different pH values in H_2O/D_2O 9:1 (from top to bottom, pH values are: 11.3; 10.3; 9.1; 8.6; 6.9 and 5.3).

S3. ESI-MS spectra for Cu (II) complexes.



ESI-MS for **1+Cu** at pH 9.0.

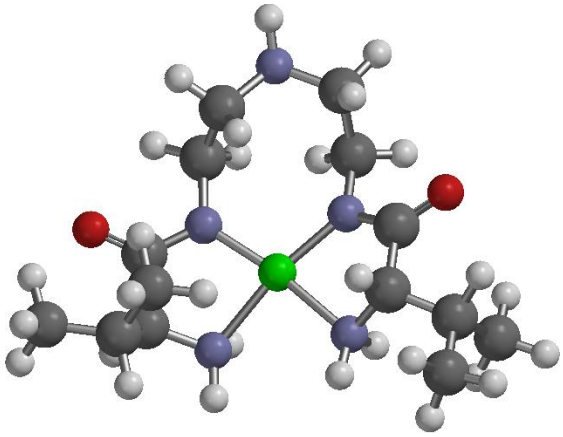


ESI-MS for **2+Cu** at pH 11.5. The species $[CuH_{-2}L+H^{+}+Na^{+}]^{+}$ is monocationic taking into consideration that **L** for **2** has been defined as a monoanionic species.

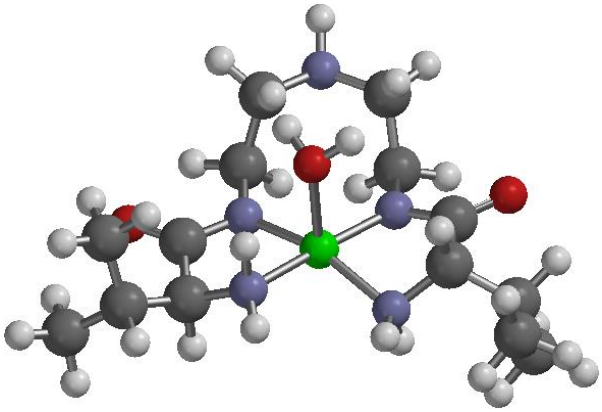
S4. Theoretical studies for Cu(II) Complexes

The calculations were carried out with the program Spartan'14 (version 1.1.0), using the Monte Carlo conformational search performed at the Merck molecular force field (MMFF). The most stable conformers obtained in the conformational search were then optimized by means of density functional theory using the non local hybrid Becke's three-parameter exchange functional (denoted as B3LYP) with LanL2DZ pseudopotential and the associated basis set for Cu and the 6-31G(d) basis set for the rest of atoms using the Gaussian 09 program. The stationary points have been characterized as true minima by the calculation of the normal vibration modes, being all the values positive.

Calculated **1+Cu** complex geometries for [$CuH_{-2}L$] species



square planar

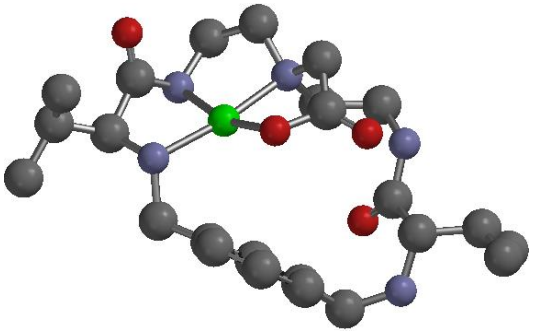


pyramidal

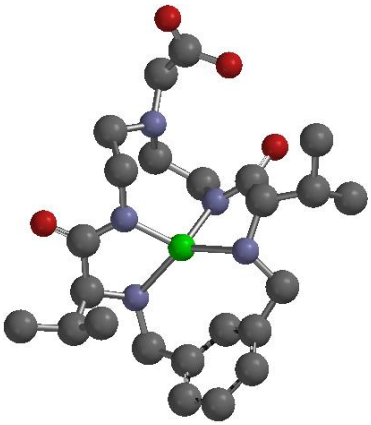
	Square planar	Pyramidal
d (N1-Cu)	1.851 Å	1.877 Å
d (N2-Cu)	1.865 Å	1.879 Å
d (N3-Cu)	2.067 Å	2.067 Å
d (N4-Cu)	2.090 Å	2.089 Å
d (O1-Cu)	-	2.179 Å
d (O2-Cu)	-	-
a (N1-Cu-N2)	105.8°	106.9 °
a (N2-Cu-N4)	83.3°	83.7 °
a (N1-Cu-N3)	85.3 °	84.2 °
a (N3-Cu-N4)	85.9 °	87.2 °
planar distortion	6.1º	15.2º
Relative energy*	1.9	0.0

*Energy difference in kcal/mol

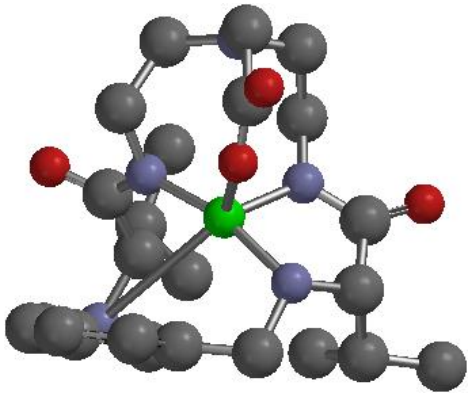
Calculated **2+Cu** complex geometries for $[CuH_{-2}L]$ species



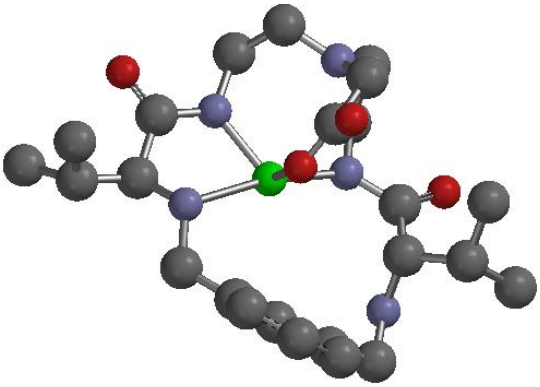
A



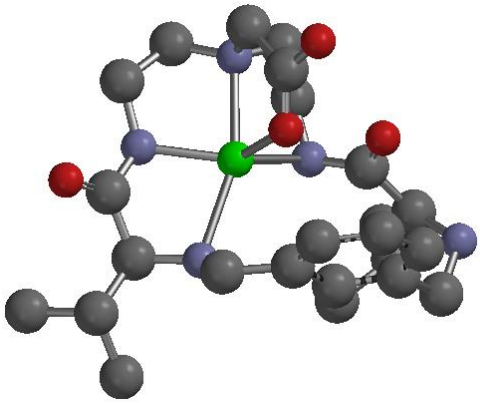
B



C



D



E

	A	B	C	D	E
d (N1-Cu)	2.171 Å	1.839 Å	1.865 Å	2.035 Å	2.091 Å
d (N2-Cu)	-	1.838 Å	1.845 Å	2.047 Å	2.127 Å
d (N3-Cu)	2.025 Å	2.327 Å	2.076 Å	2.431 Å	2.339 Å
d (N4-Cu)	-	2.213 Å	4.103 Å	-	-
d (N5-Cu)	2.024 Å	-	2.113 Å	-	2.237 Å
d (O-Cu)	2.068 Å	-	-	1.904 Å	2.027 Å
Relative energy*	7.6	0.9	3.7	2.5	0.0

*Energy difference in kcal/mol