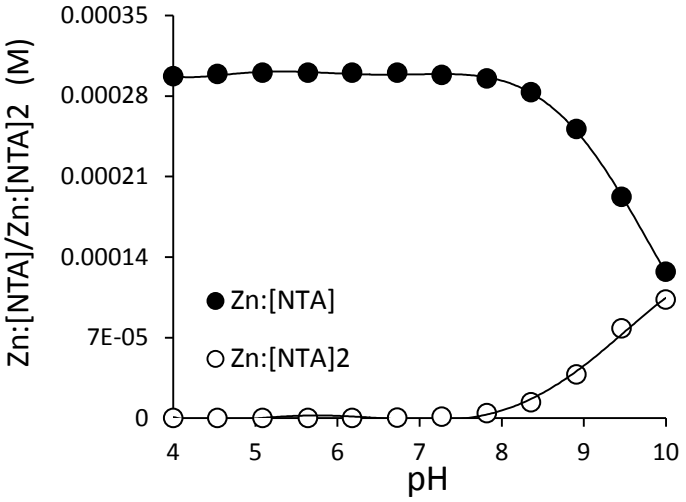
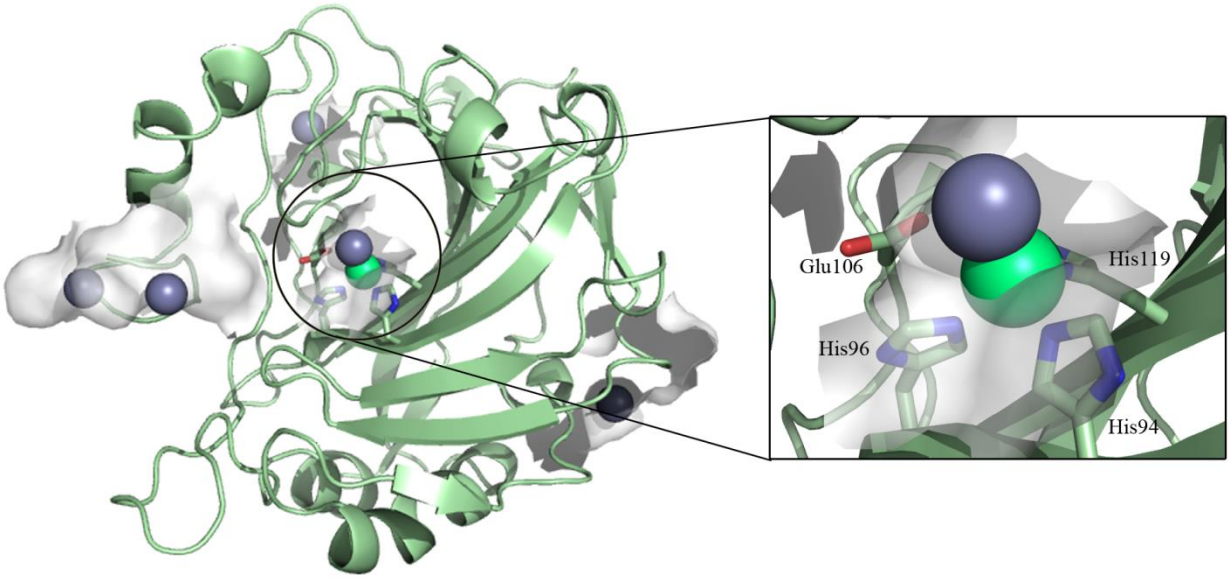
Electronic Supplementary Material (ESI) for Metallomics.



Supplementary Figure S1. *Zn:[NTA] species distribution at different pH values.* 1 mM NTA was the input into MINEQL+ 4.6 software in order to model and determine the distribution of both the Zn:[NTA] and Zn:$[NTA]_2$ species at different pH values. The Zn:[NTA] species predominates at acidic pH and decreases as the pH increases, while the Zn:$[NTA]_2$ species follows the opposite pattern.

Figure S1



Supplementary Figure S2. *Predicted binding of Zn^{2+} on carbonic anhydrase II.* Result of docking simulation performed on a carbonic anhydrase II (CA) X-ray crystal structure (PDB id: 1CAM); details of the catalytic site are shown in the square frame. Protein structure is in pale green, Zn^{2+} ions as grey spheres, and relevant amino acids as sticks. The zinc atom localized originally in the crystal structure of CA is shown in green.

Carbonic Anhydrase II (PDB id: 1CAM, res.: 1.70 Å)	Pose 1	Pose 2	Pose 3	Pose 4	Pose 5
Estimate binding Energy (kcal/mol)	-26.0211	-25.5656	-23.7628	-23.499	-22.5137
Amino acids within 4 Å	His94 His96 Glu106 His119 Ala199	Tyr51 Asp52 Ala54 Asp180	His3 His10	Asp32 Asp34	His3 His4

Supplementary Table 1. Results of docking simulations on Carbonic Anhydrase II.