

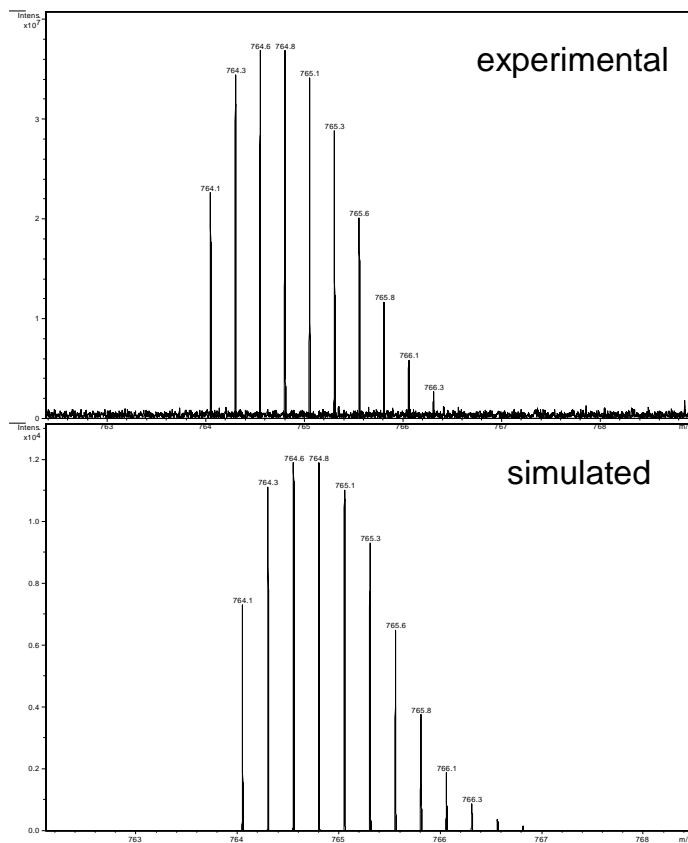
## Supplementary materials

### **The zinc-binding fragment of HypA from *Helicobacter pylori*: a tempting site also for nickel ions**

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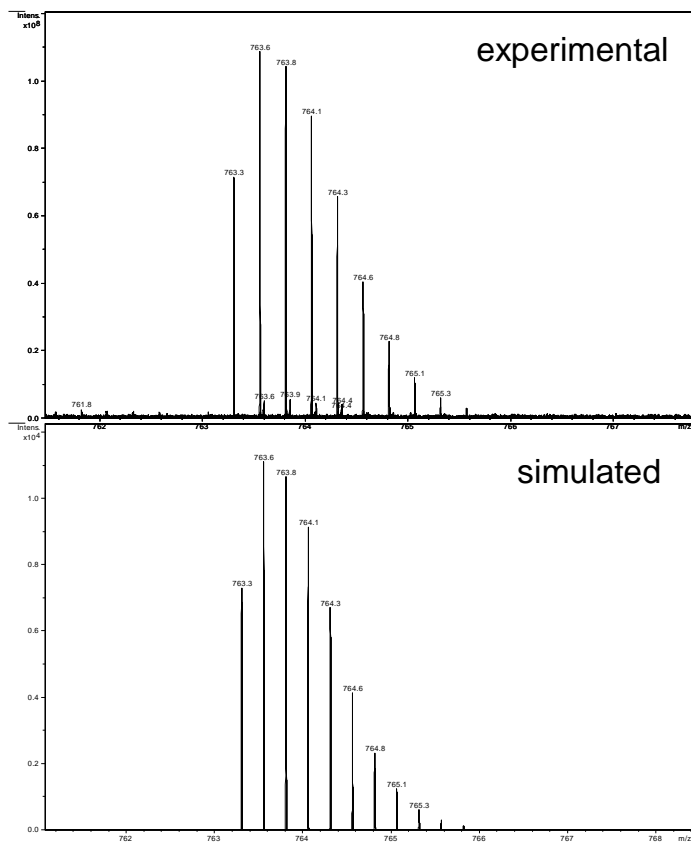
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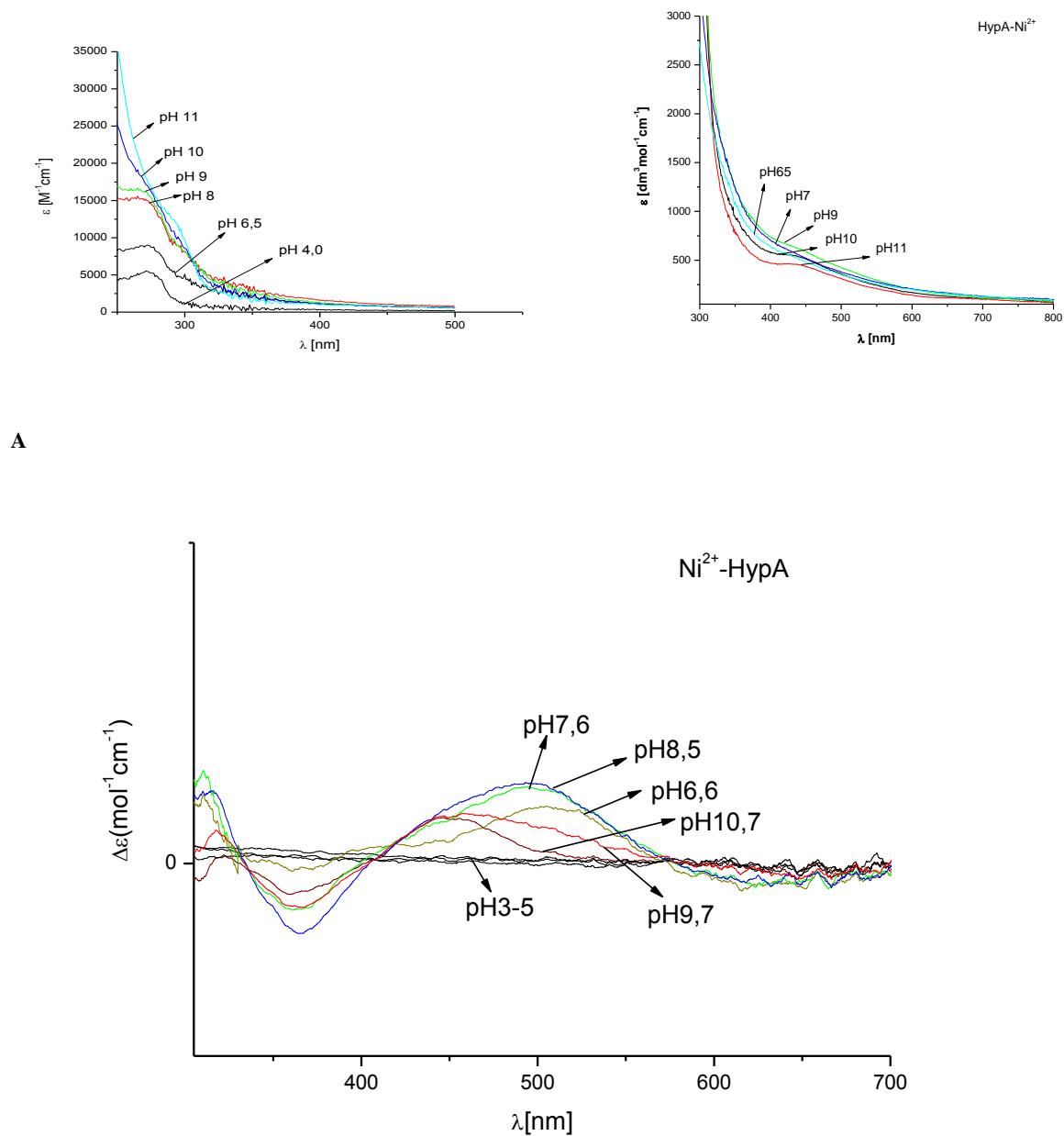
A

Ac-ELECKDCSHVFKPNALDYGVCEKCHS-NH<sub>2</sub> + 1eq. Ni<sup>2+</sup>



**B**

Fig. 1S. ESI-MS spectra of a system containing the HypA protein fragment Ac-ELECKDCSHVFKPNALDYGVCEKCHS-NH<sub>2</sub>, with (A) Zn<sup>2+</sup> and (B) Ni<sup>2+</sup> ions in a 1 : 1 stoichiometry. Signals that correspond to the complexes from Fig. 1 in the main text are shown in the upper part of each figure; below, simulated spectra are shown.. Initial pH was 7.4. M/z ratio of all the shown species = 4.



**B**  
Fig. 2S. UV-Vis (A) and CD spectra (B) for Ni<sup>2+</sup> complex of the HypA protein fragment (Ac-ELECKDCSHVFKPNALDYGVCEKCHS-NH<sub>2</sub>). Spectra were recorded at 298K, at the given pH values. The ligand concentration was 1 x 10<sup>-3</sup> M and metal to ligand molar ratios were 1:2 and 1:1.1.

ELECK**DCSH**VFKPNALDYGVCEKCHS

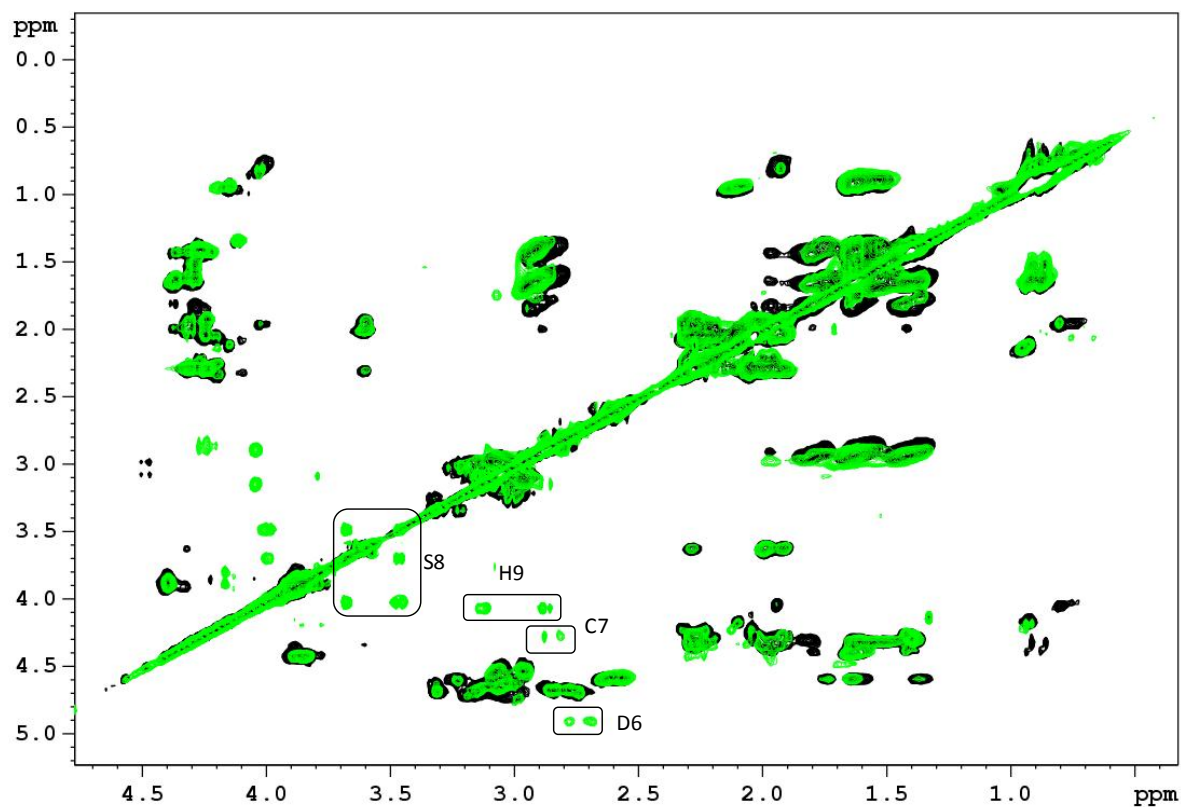


Fig. 3S. Aliphatic regions of  $^1\text{H}$ - $^1\text{H}$  TOCSY spectra of HypA  $1 \times 10^{-3}\text{M}$ , pH 10.5, T 298K in absence (black contours) and in presence (green contours) of 0.9  $\text{Ni}^{2+}$  eqs. The new appearing correlations are shown in the frames and the corresponding residues are shown in red in the peptide sequences.

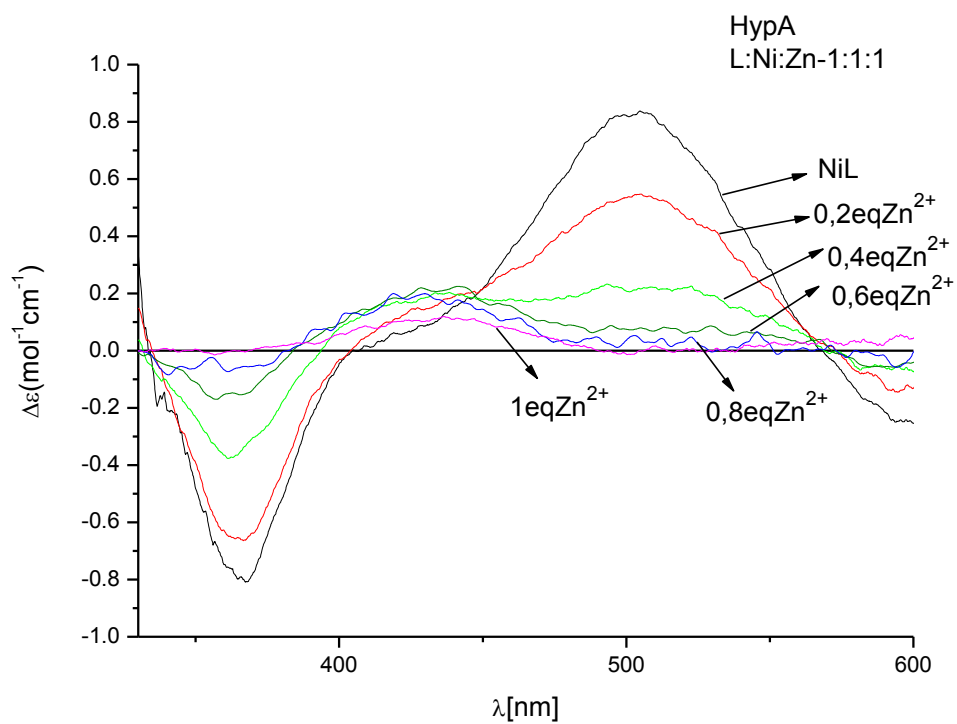


Fig. 4S. CD spectra of Ni<sup>2+</sup> complexes of the HypA protein fragment (Ac-ELECKDCSHVFKPNALDYGVCEKCHS-NH<sub>2</sub>) at pH 7.4, titrated with Zn<sup>2+</sup> ions at a step of 0.2 molar equivalents. Final Zn<sup>2+</sup> : Ni<sup>2+</sup> : L ratio = 1 : 1 : 1, pH= 7.4.