Supplementary materials

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

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Ac-ELECKDCSHVFKNALDYGVCEKCHS-NH₂ + 1eq. Zn²⁺
Fig. 1S. ESI-MS spectra of a system containing the HypA protein fragment Ac-ELECKDCSHVFKNALDYGVCEKCHS-NH$_2$, with (A) Zn$^{2+}$ and (B) Ni$^{2+}$ 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 $= 4.$
Fig. 2S. UV-Vis (A) and CD spectra (B) for Ni^{2+} complex of the HypA protein fragment (Ac-ELECKDCSHVFKNALDYGVCKCHS-NH2). Spectra were recorded at 298K, at the given pH values. The ligand concentration was $1 \times 10^{-3}$ M and metal to ligand molar ratios were 1:2 and 1:1.1.
Fig. 3S. Aliphatic regions of $^1$H-$^1$H TOCSY spectra of HypA 1x10$^{-3}$M, pH 10.5, T 298K in absence (black contours) and in presence (green contours) of 0.9 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$^{2+}$ complexes of the HypA protein fragment (Ac-ELECKDCSHVFKPNALDYGVCEKCHS-NH$_2$) at pH 7.4, titrated with Zn$^{2+}$ ions at a step of 0.2 molar equivalents. Final Zn$^{2+}$ : Ni$^{2+}$ : L ratio = 1 : 1 : 1, pH= 7.4.