

Zn²⁺ and Cu²⁺ Interaction with the Recognition Interface of ACE2 for SARS-CoV-2 Spike Protein

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Supplementary Materials

Table S1. Hydrolysis constants for Cu(II) and Zn(II) ions for 0.1M ionic strength, T= 25°C.

Species	log β
Cu(OH) ⁺	-7.86
Cu(OH) ₂	-16.47
Cu(OH ₃) ⁻	-26.65
Cu(OH ₄) ²⁻	-39.29
Zn(OH) ⁺	-9.12
Zn(OH) ₂	-18.08
Zn(OH ₃) ⁻	-27.97
Zn(OH ₄) ²⁻	-39.50

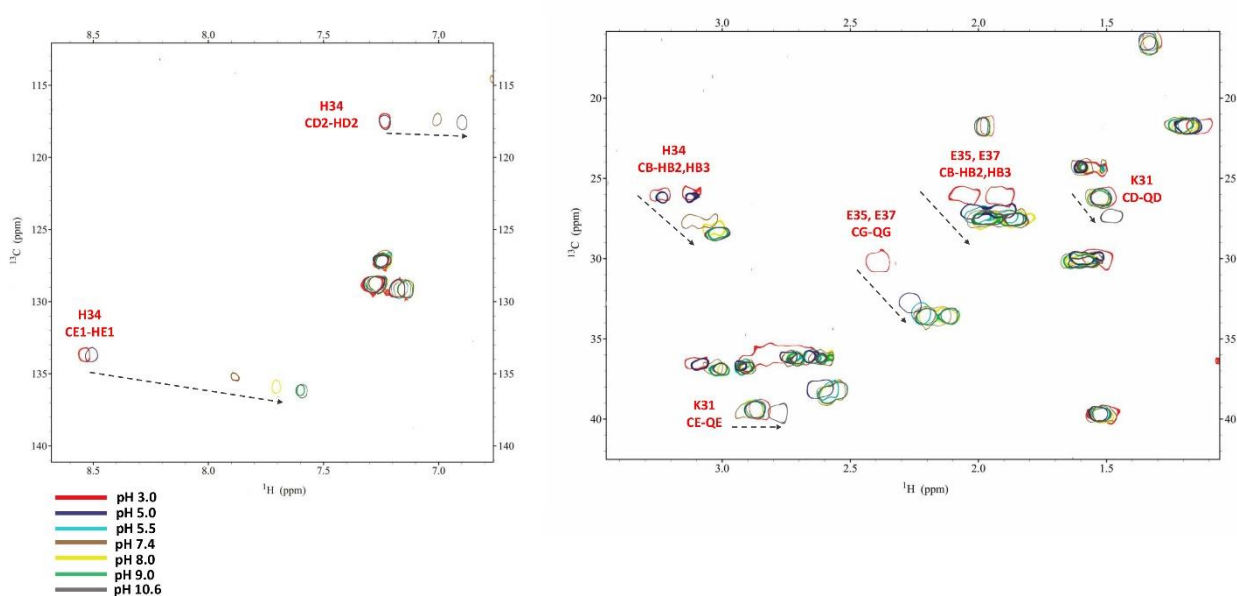


Figure S1. Superimposition of selected region of the ¹H-¹³C HSQC spectra for the free peptide P29-38 at various pH values.

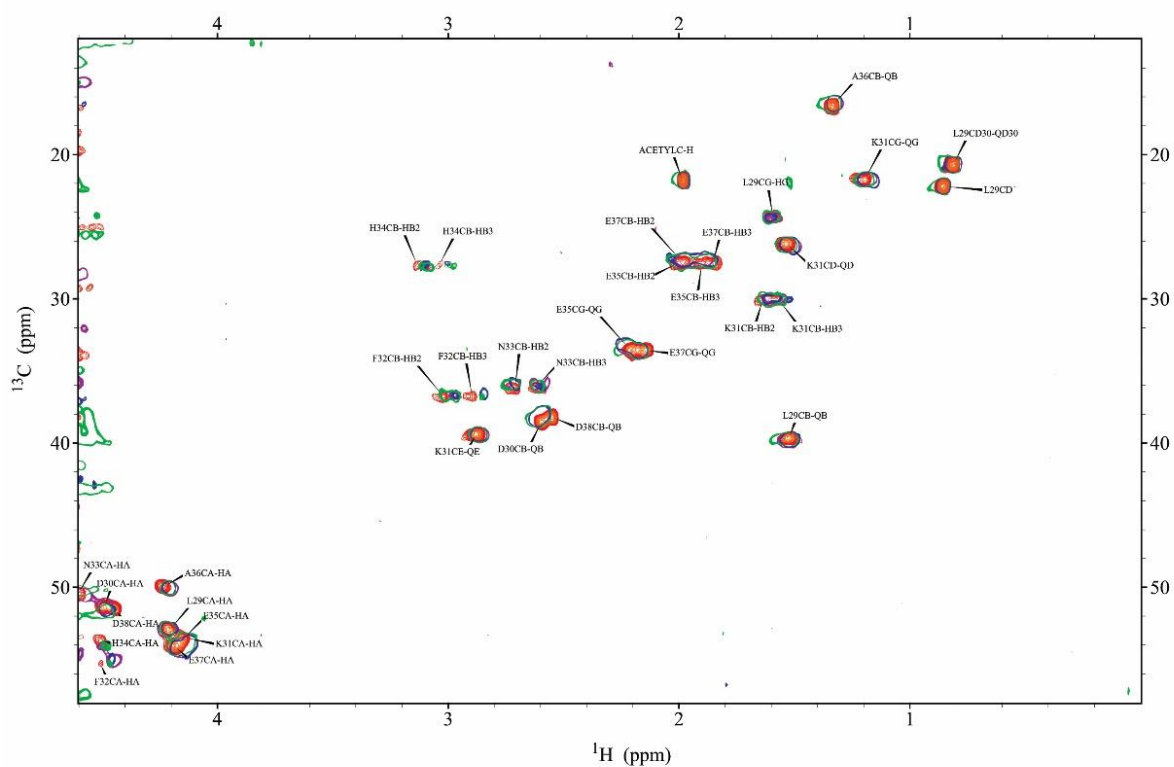


Figure S2. Superimposition of the aliphatic region of the ^1H - ^{13}C HSQC spectra for the free peptide P29-38 at pH 8 (orange) and the Zn(II)-P29-38 system at pH 8 (blue contours) and pH 9 (green contours).

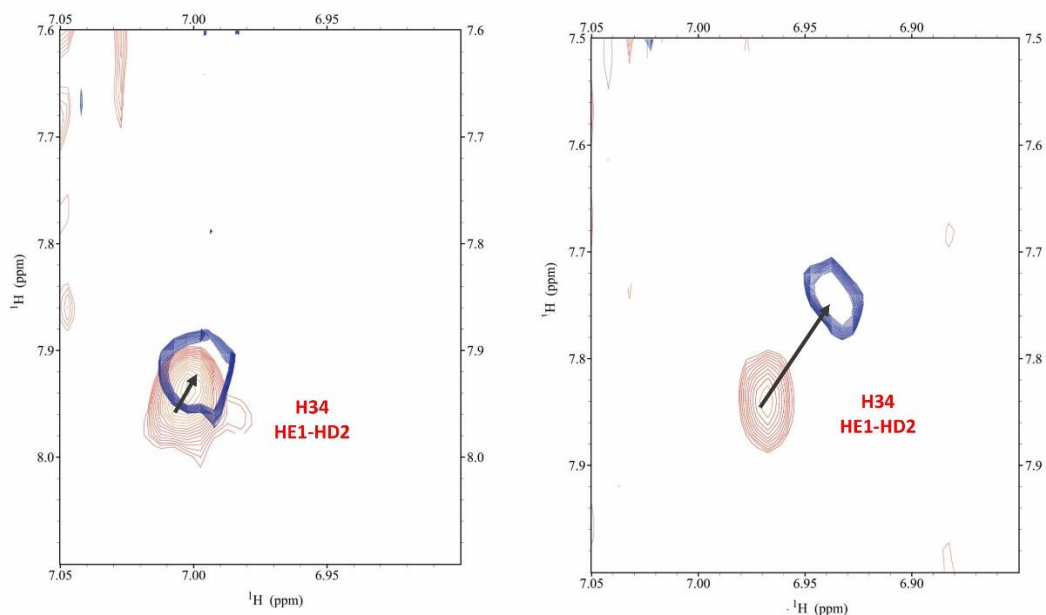


Figure S3. Superimposition of the selected region of the ^1H - ^1H TOCSY spectra for the free peptide P23-42 (orange) and the Zn(II)-P29-38 system (blue contours) at pH 7 (left) and pH 7.5 (right), related to the correlation signals of aromatic protons HE1 and HD2 of His34.

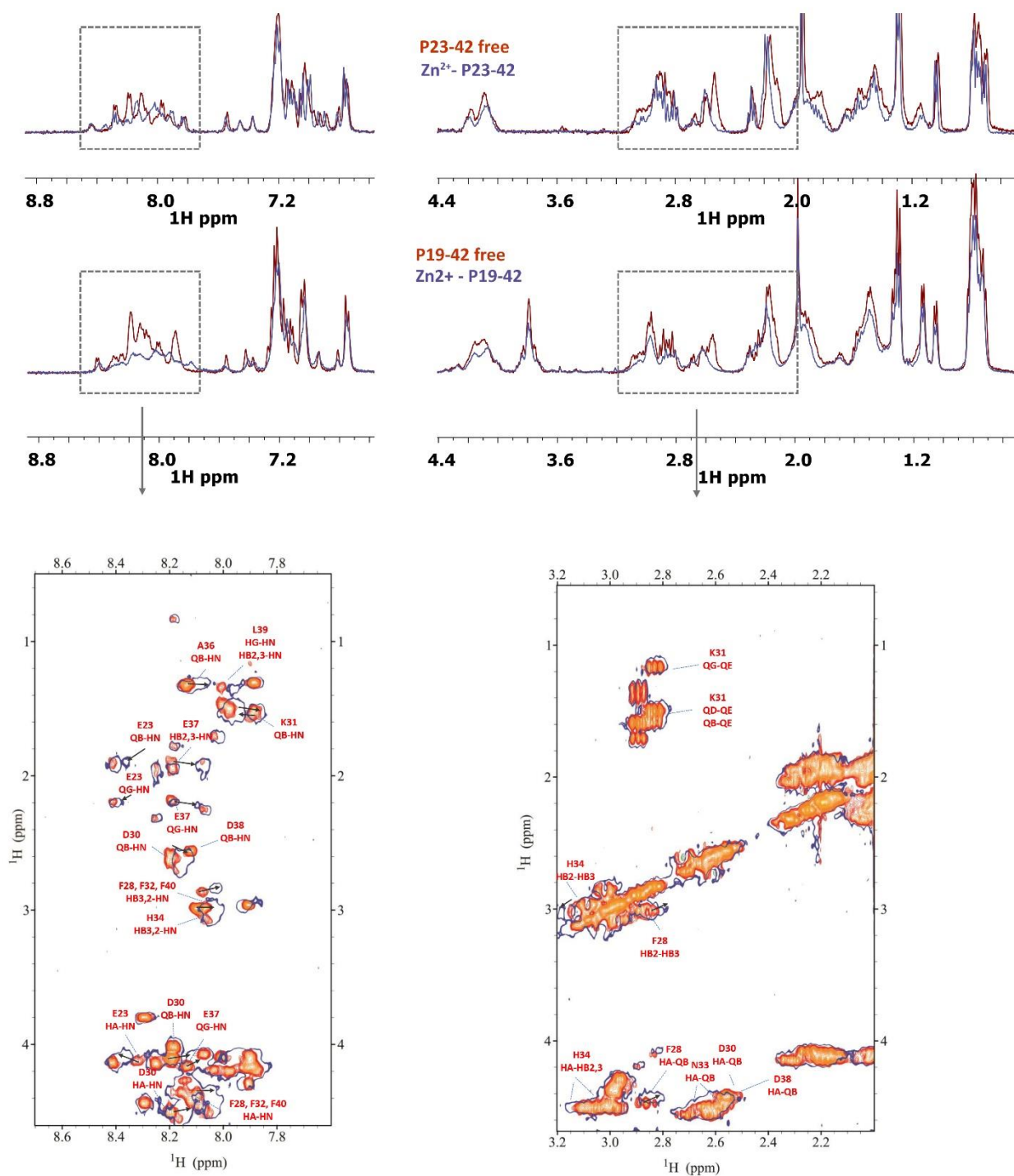


Figure S4. (up) Comparison of ^1H spectra for the free peptide P23-42 (orange) and Zn(II)-P23-42 system (blue) and P19-42 (orange) and Zn(II)-P19-42 system (blue) at pH 7.0; (down) selection of ^1H - ^1H TOCSY spectra for the free peptide P19-42 (orange) and Zn(II)-P19-42 system (blue) at pH 7.0.

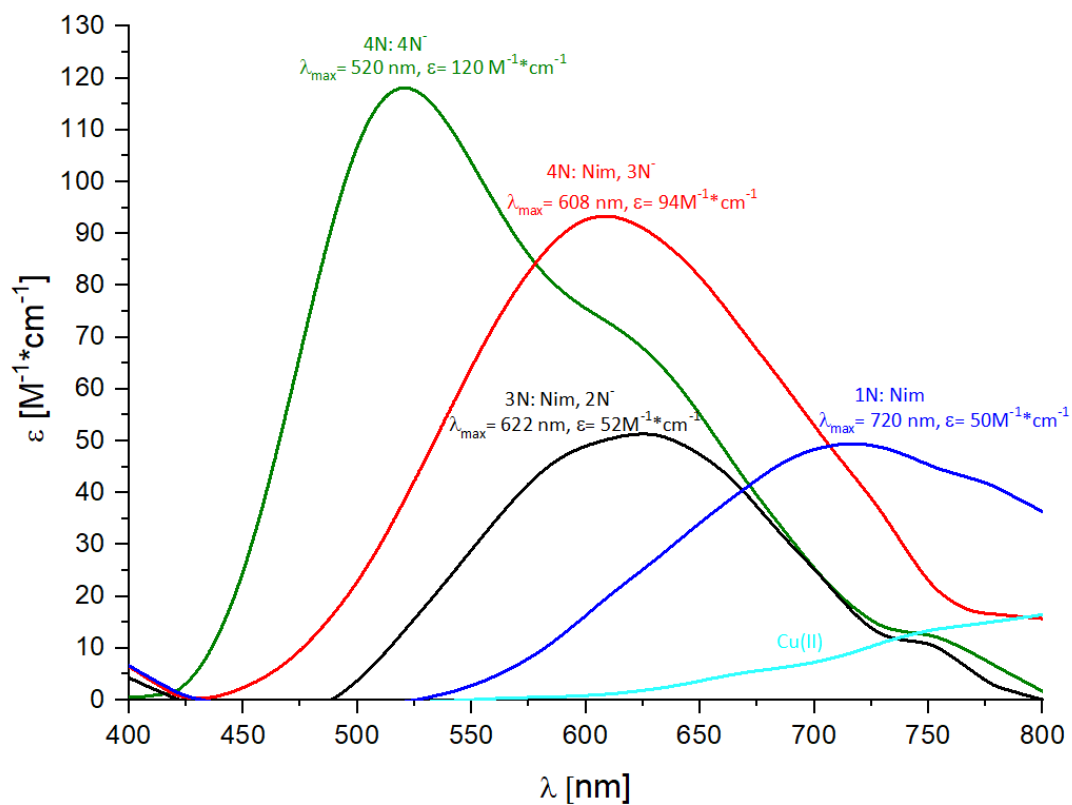


Figure S5. Calculated UV-Vis bands for various Cu(II) complex forms. Bands calculated and drawn by SPECFIT/32 software. cyano: free Cu(II), blue: $[\text{CuHL}]^-$, black: $[\text{CuLH}_2]^{3-}$, red: $[\text{CuLH}_2]^{4-}$, green: $[\text{CuLH}_3]^{5-}$.

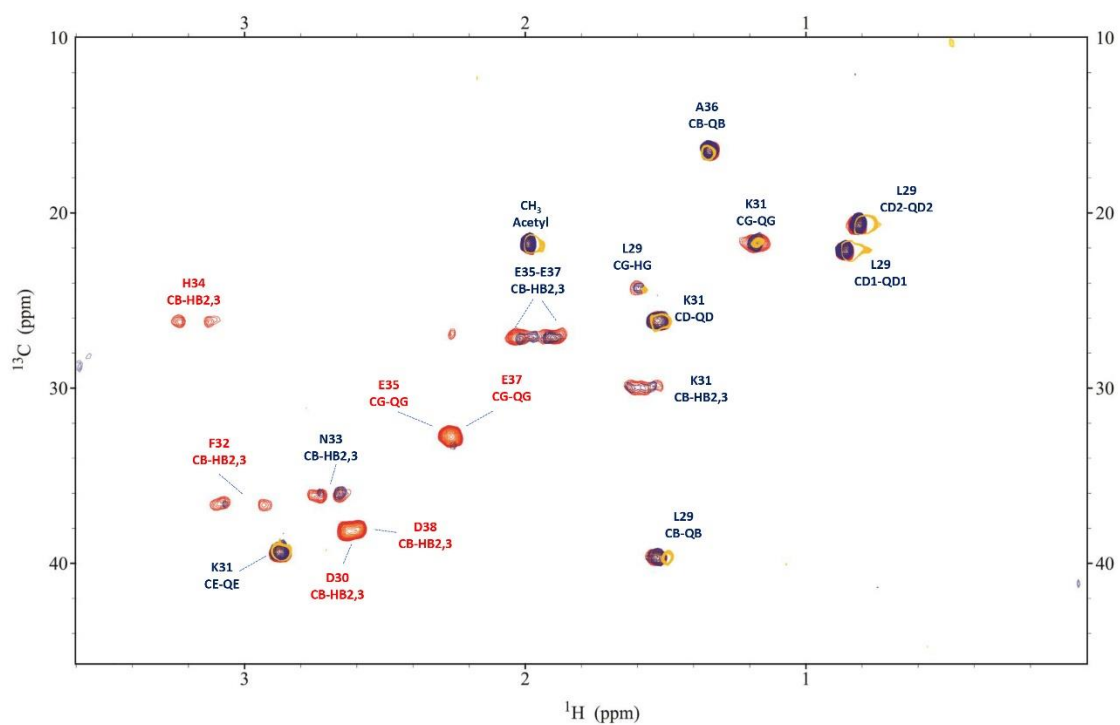


Figure S6. (up) Comparison of a selection aliphatic region of ^1H - ^{13}C HSQC spectra for the free peptide P29-38 (orange) and Cu(II)-P29-38 system in the molar ratio of 0.01:1 (blue) and 0.1:1 (yellow contours) at pH 5.5.

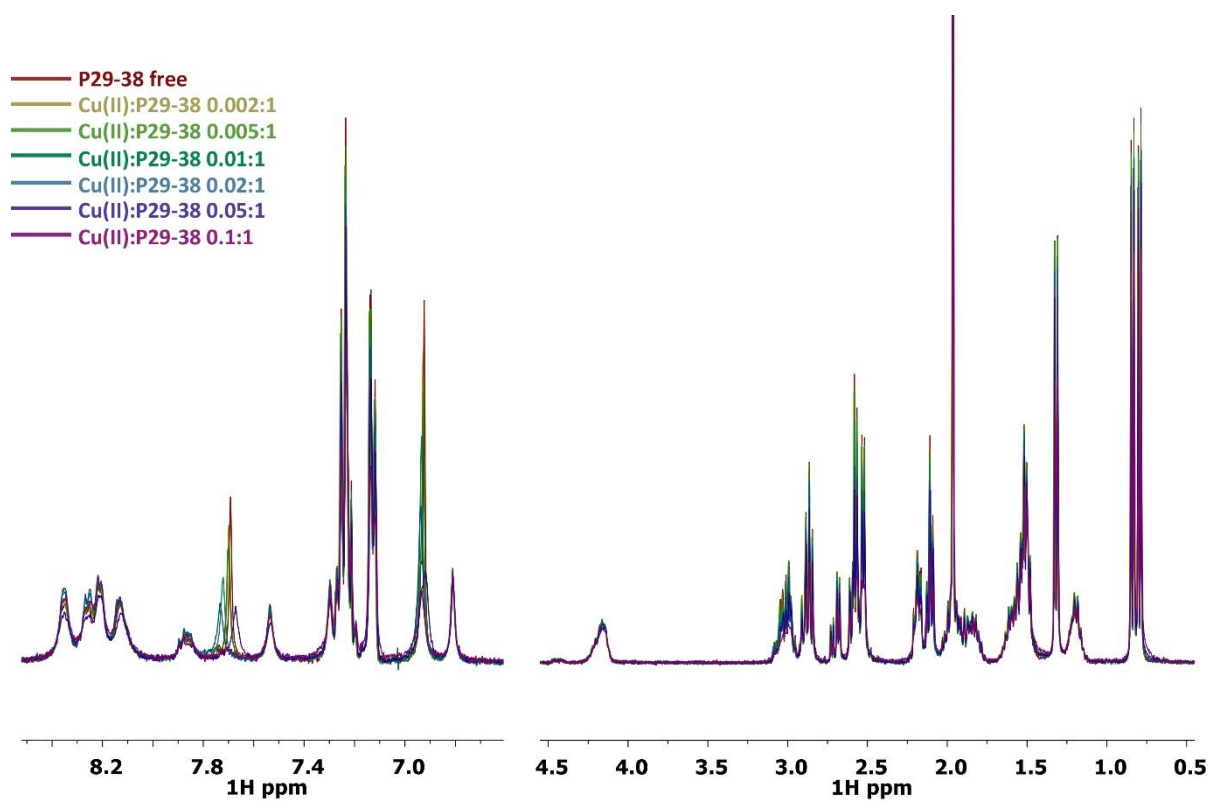


Figure S7. Comparison of ^1H spectra of P29-38 with increasing addition of Cu^{2+} at pH 7.4.

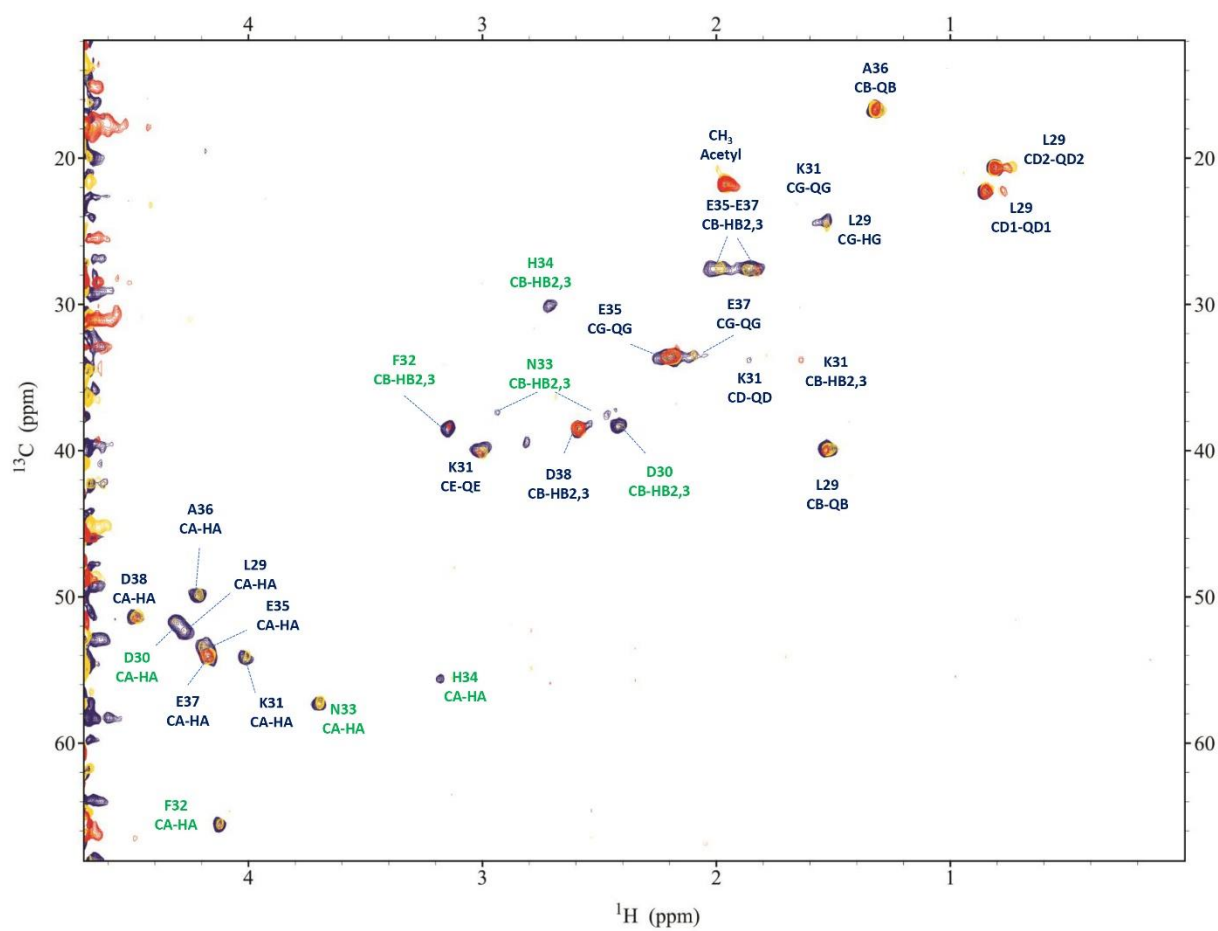


Figure S8. Comparison of aliphatic region of ^1H - ^{13}C HSQC spectra for the Ni(II)-P29-38 system (blue) with the subsequent addition of 0.4 (yellow) and 0.6 (red) equivalents of Cu(II) at pH 10.6.

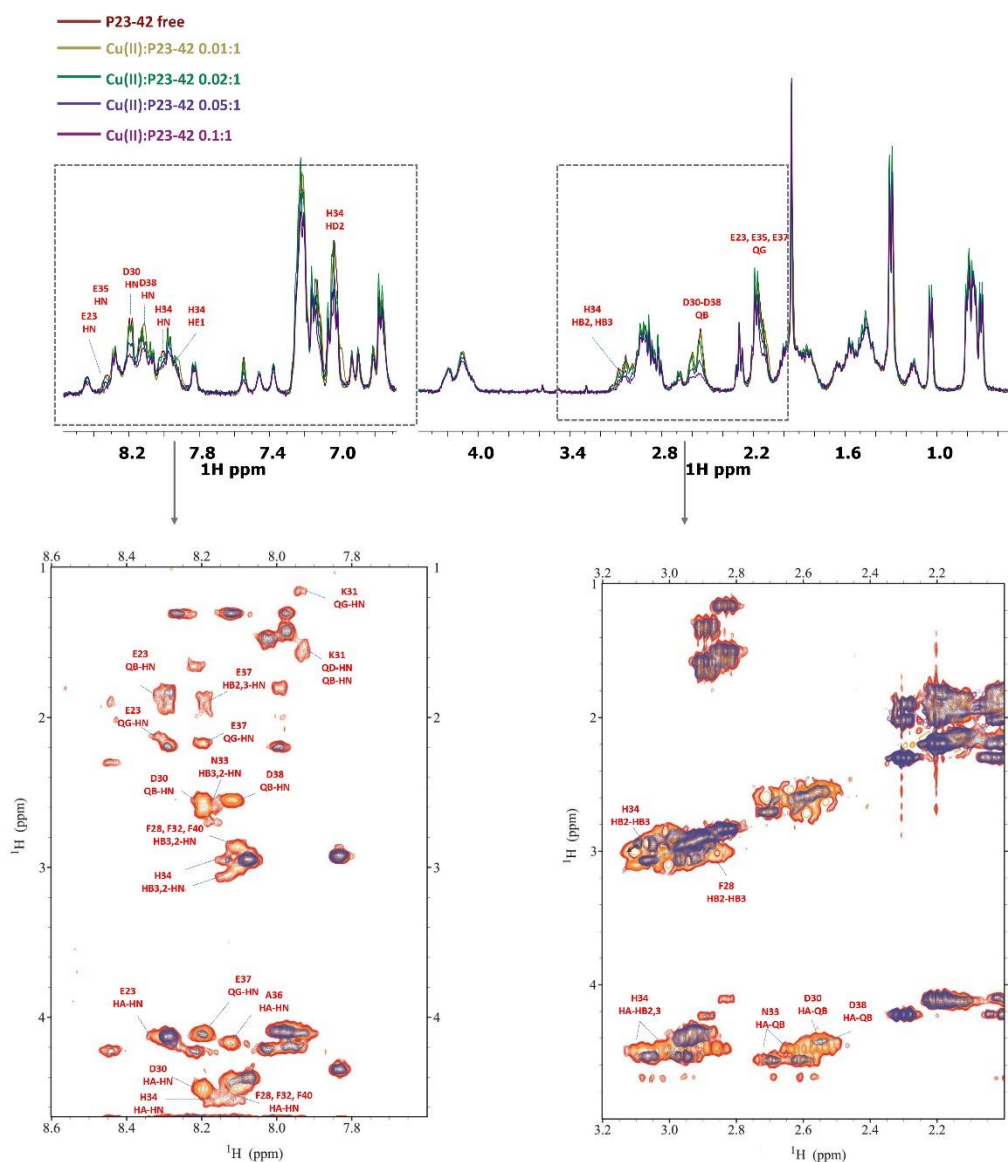


Figure S9. (up) Comparison of ^1H spectra of P23-42 with increasing addition of Cu^{2+} at pH 7.0; (down) selection of ^1H - ^1H TOCSY spectra for the free peptide P23-42 (orange) and Cu(II) -P23-42 system (blue), 0.1:1 molar ratio, at pH 7.0.

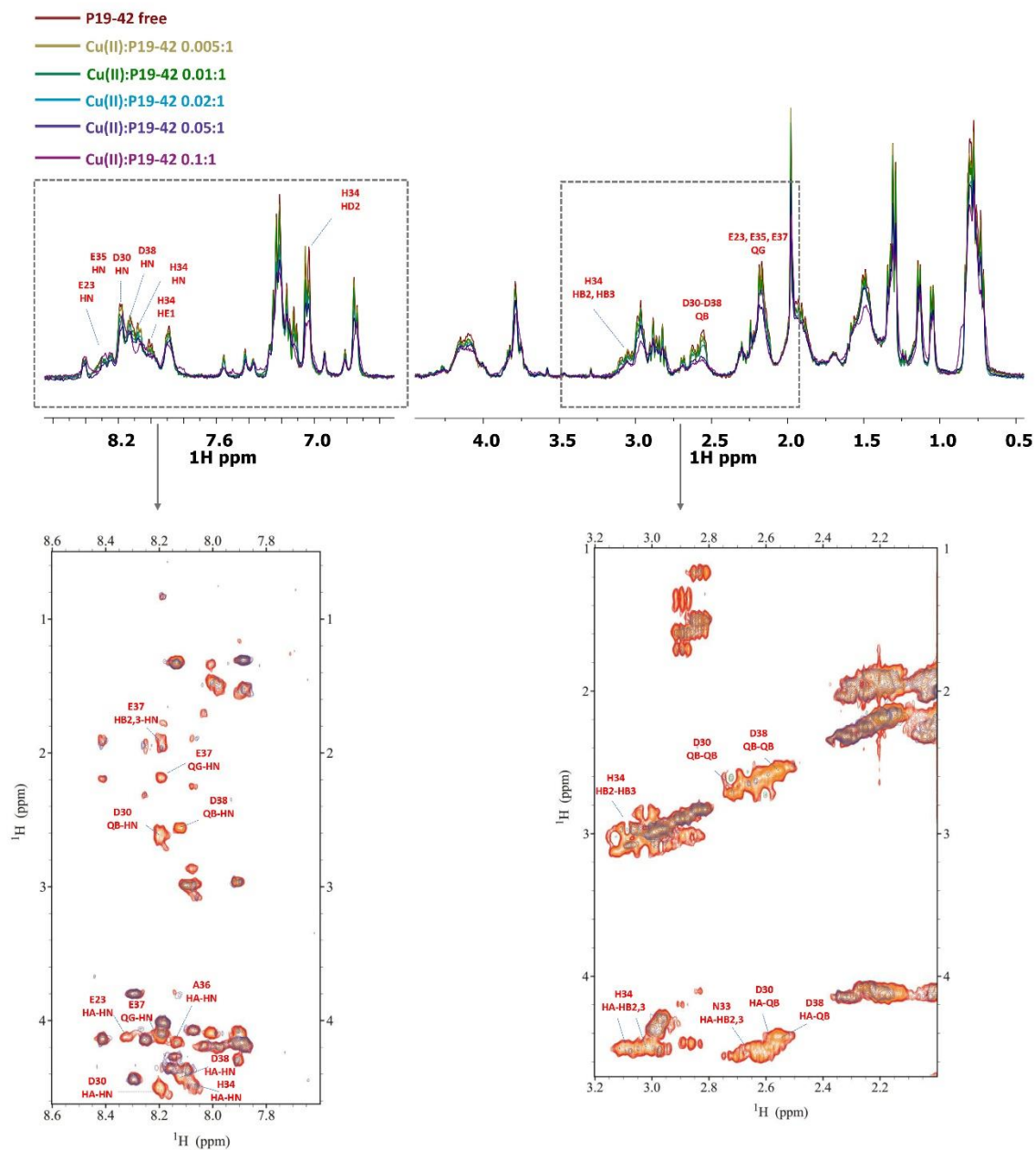


Figure S10. (up) Comparison of ^1H spectra of P19-42 with increasing addition of Cu^{2+} at pH 7.0; (down) selection of ^1H - ^1H TOCSY spectra for the free peptide P19-42 (orange) and $\text{Cu(II)}\text{-P23-42}$ system (blue), 0.1:1 molar ratio, at pH 7.0.

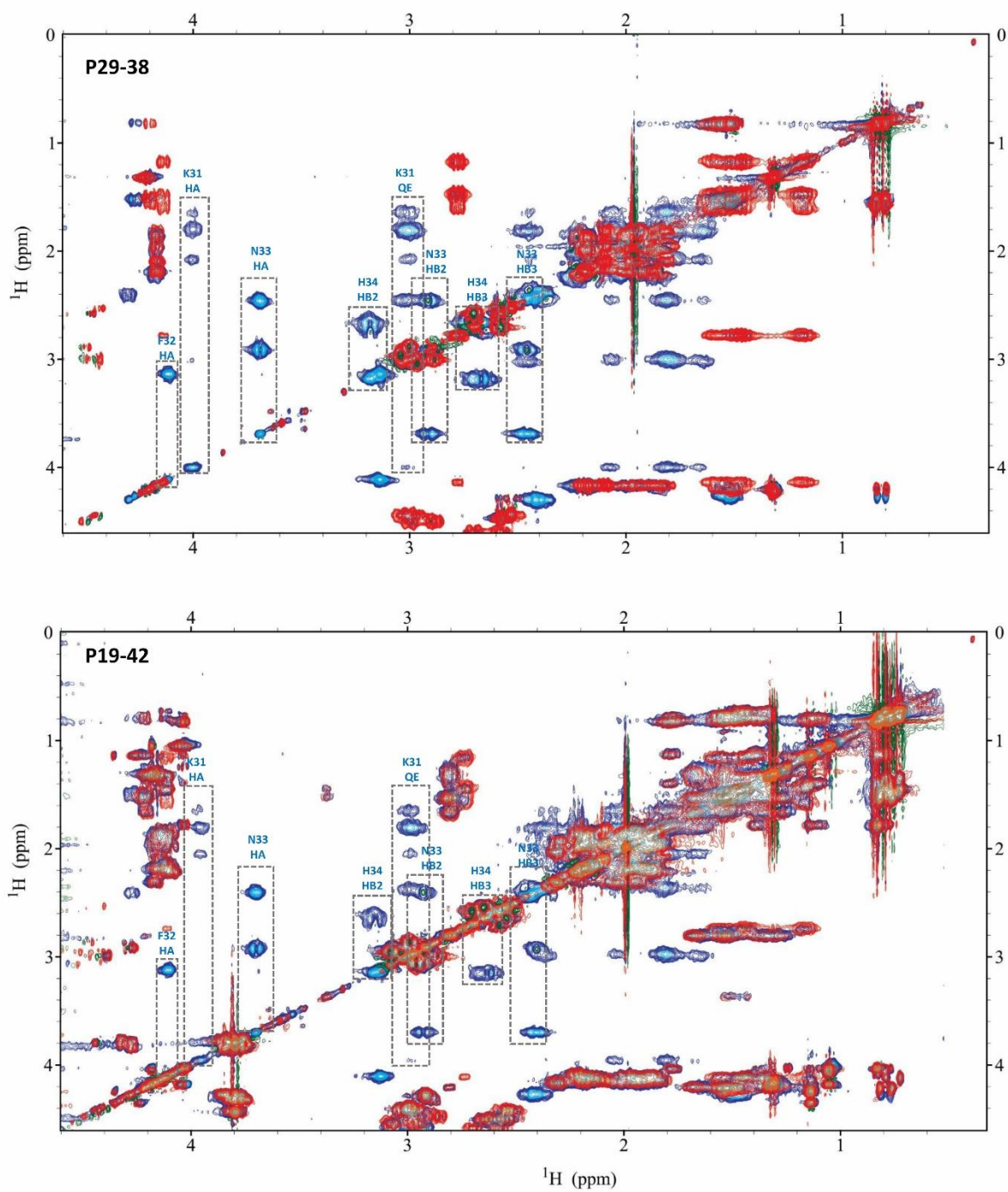


Figure S11. (up) Comparison of aliphatic ^1H - ^1H TOCSY spectra for the free peptide P29-38 (red) and Ni(II)-P29-38 system (blue) and (down) for P19-42 (red) and Ni(II)-P19-42 system (blue) at pH 10.6.

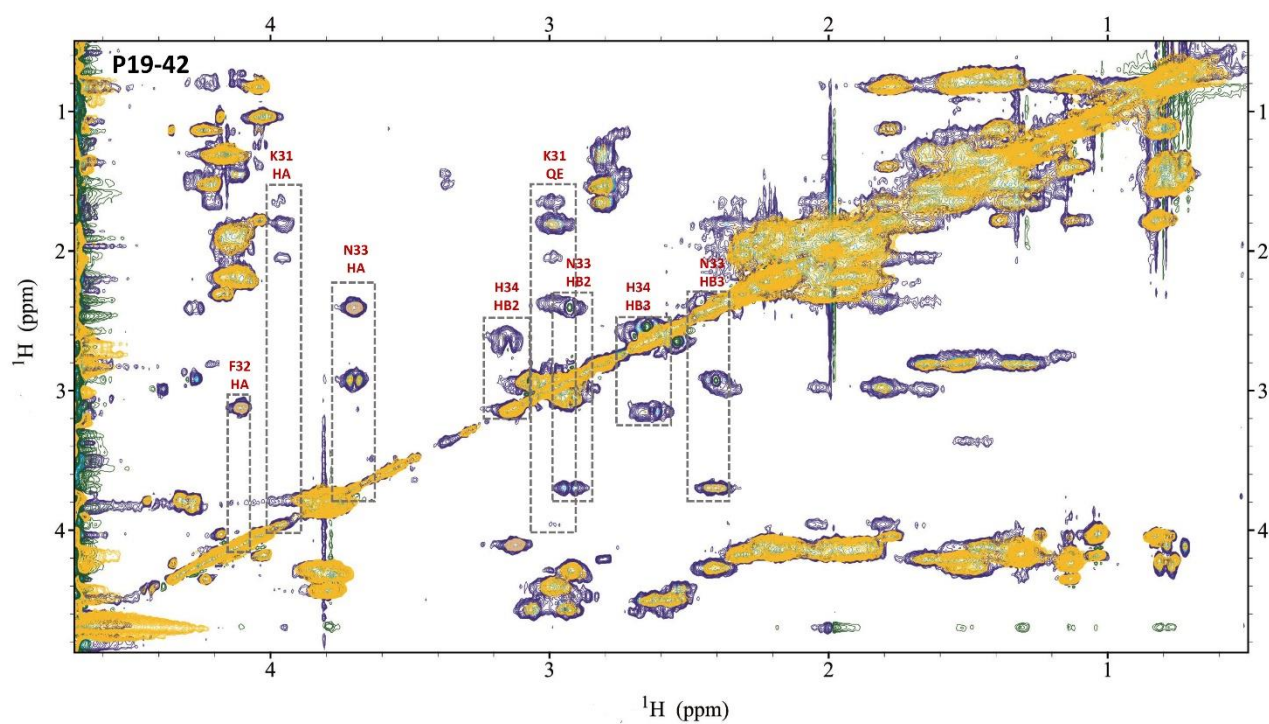


Figure S12. Comparison of aliphatic region of ^1H - ^1H TOCSY spectra for the Ni(II)-P19-42 system (blue) with the addition of 0.6 equivalents of Cu(II) (yellow), at pH 10.6.