

Electronic Supplementary Information

Coordination properties of Cu(II) ions towards a phosphorylated fragment from the R1 domain of the tau protein and the effect of Ser phosphorylation on Cu(II) binding affinity

Dimitra Kyriakou, Eleni Bletsas, Vassilios Moussis, Yiannis Deligiannakis
and Gerasimos Malandrinos

Footnote: Electronic supplementary information (ESI) available: 1 and 2D NMR (Figures S1-S10), EPR (Figures S12, S13) and CD (Figure S14) spectra, and NMR data for both peptides (Tables S1 and S2)

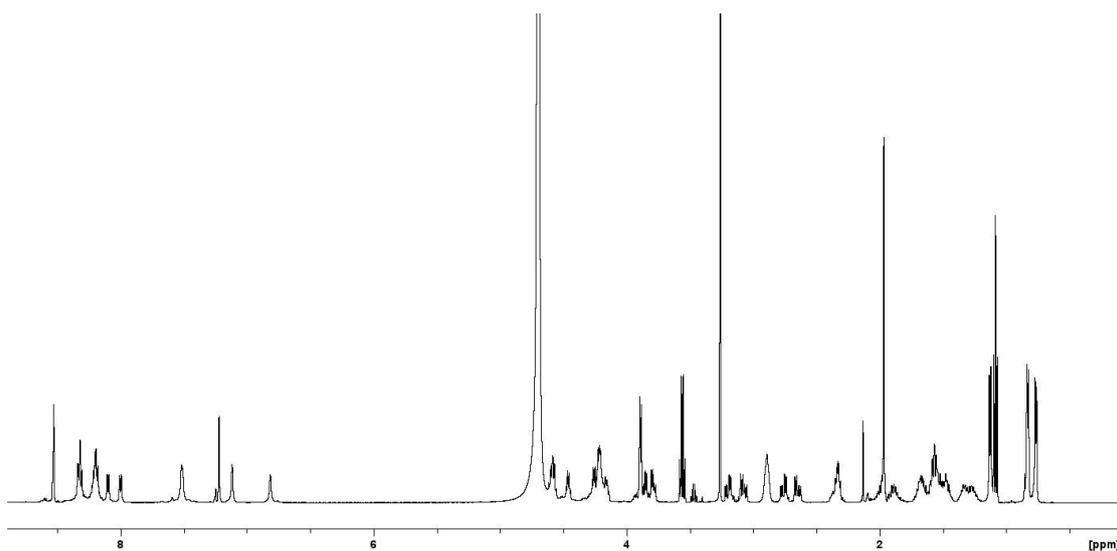


Figure S1. 1D ¹H NMR spectrum of the peptide Ac-GSTENLKH-NH₂ (C=2 mM and T=298K)

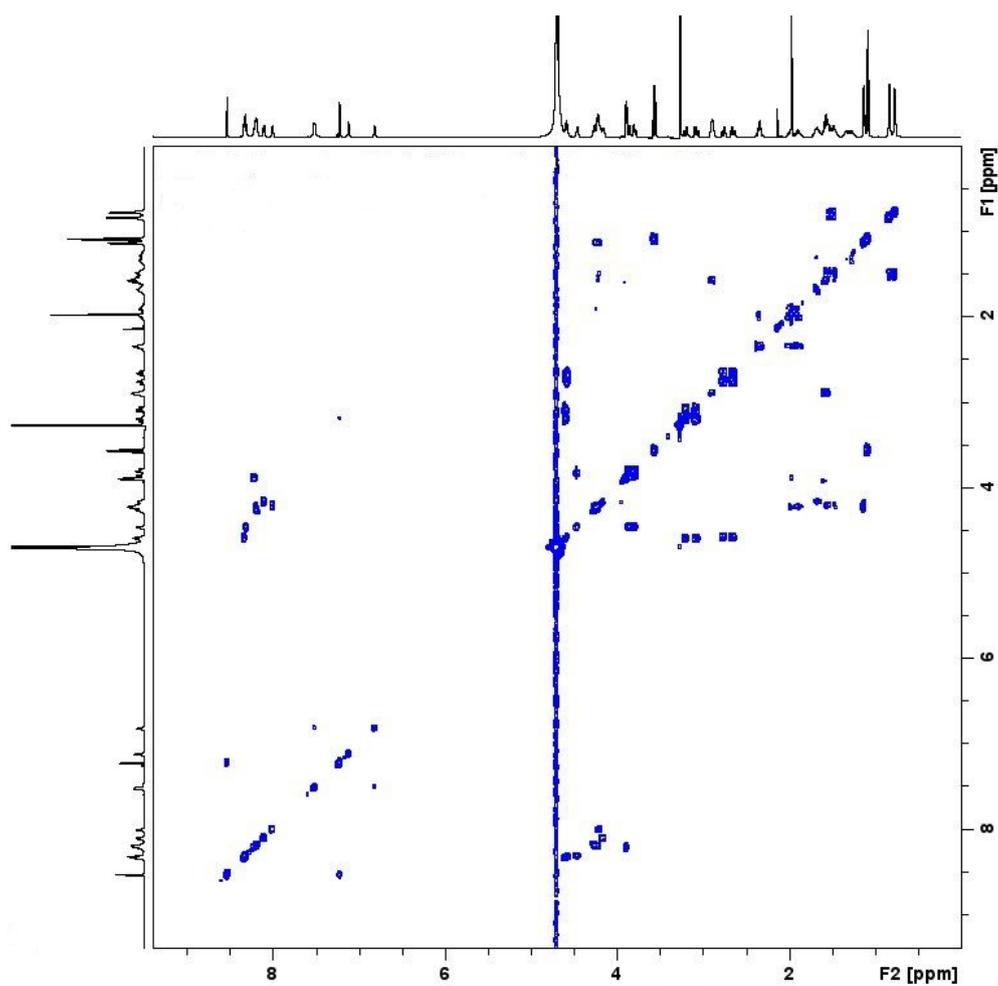


Figure S2. ¹H ¹H COSY NMR spectrum of the peptide Ac-GSTENLKH-NH₂ (C=2 mM and T=298K)

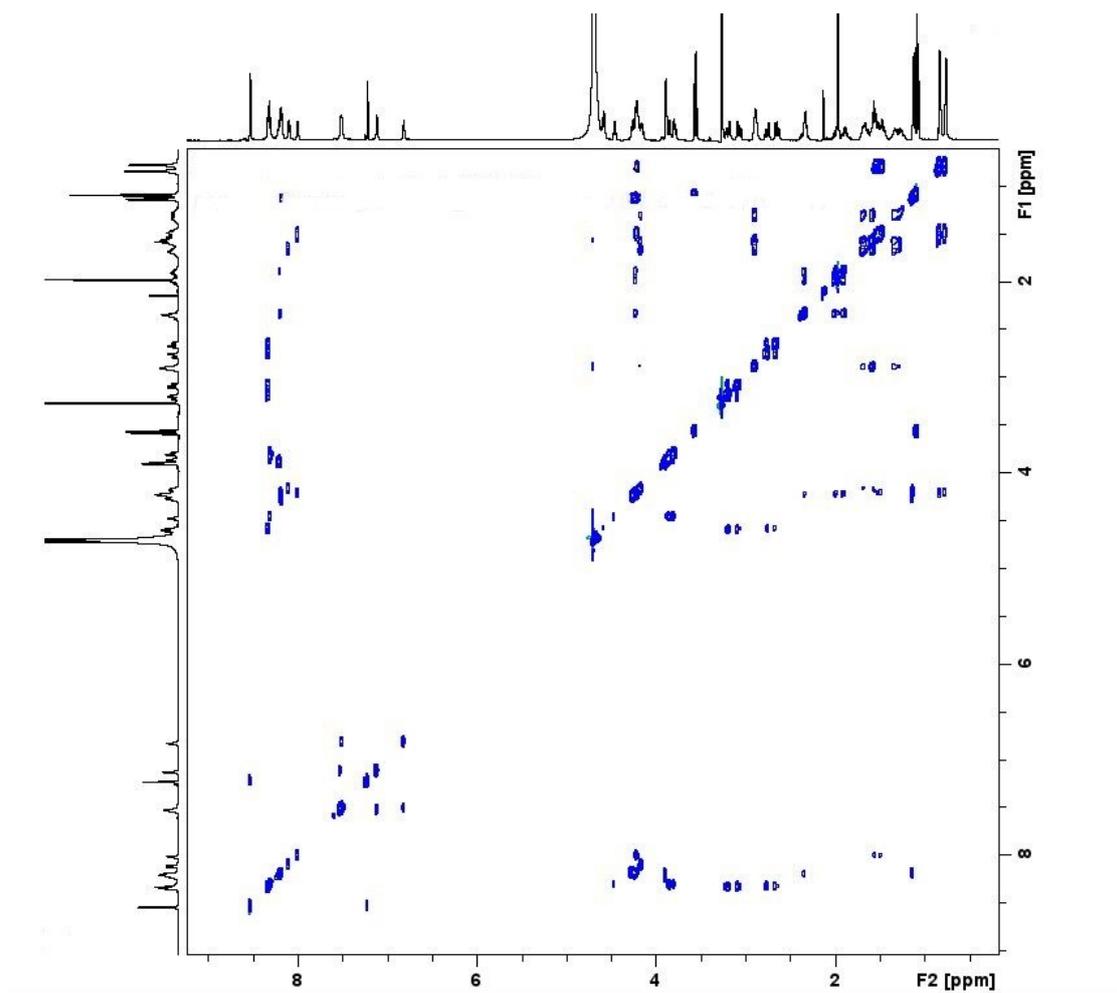


Figure S3. ^1H ^1H TOCSY NMR spectrum of the peptide Ac-GSTENLKH-NH₂ (C=2 mM and T=298K)

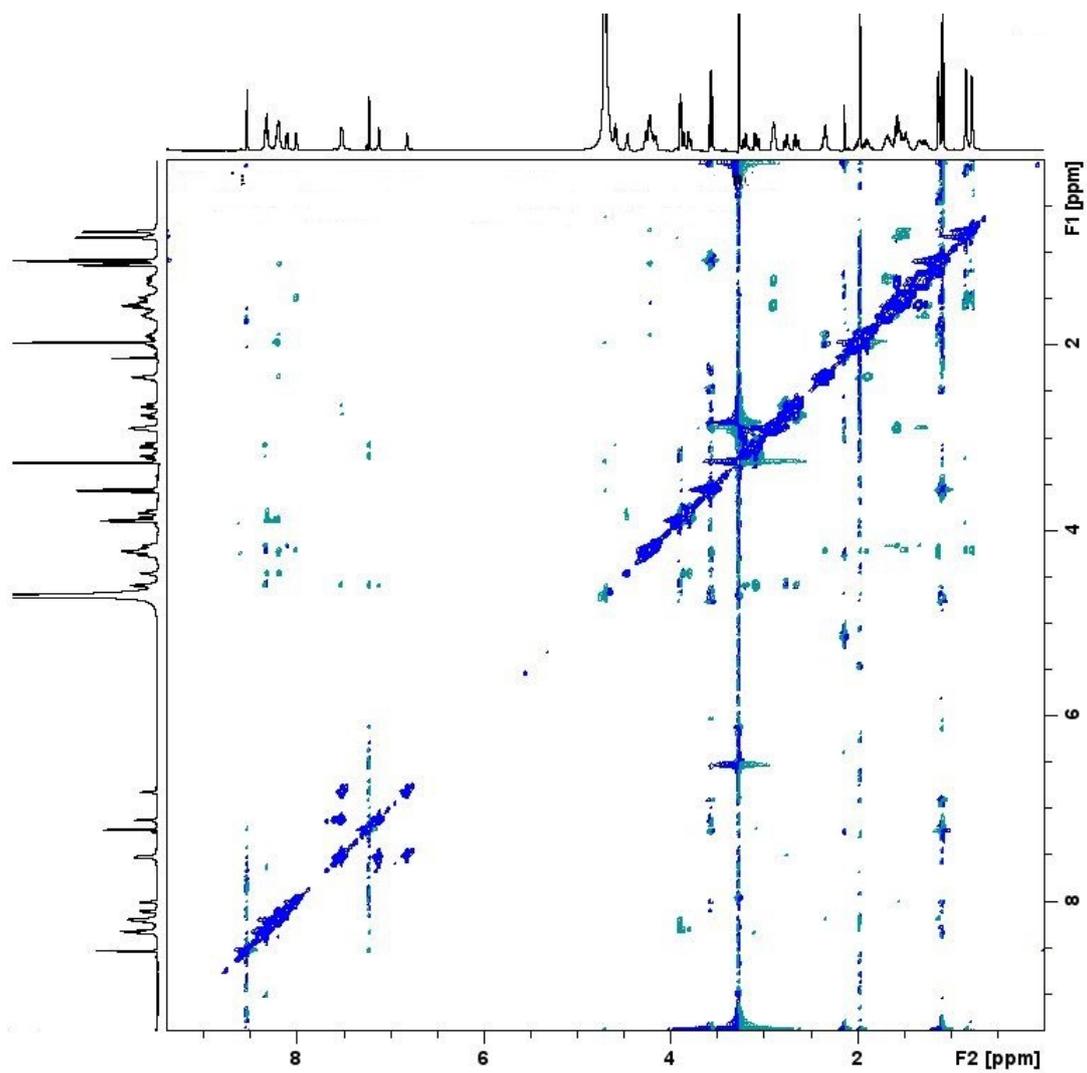


Figure S4. ^1H ^1H NOESY NMR spectrum of the peptide Ac-GSTENLKH-NH₂ (C=2 mM and T=298K)

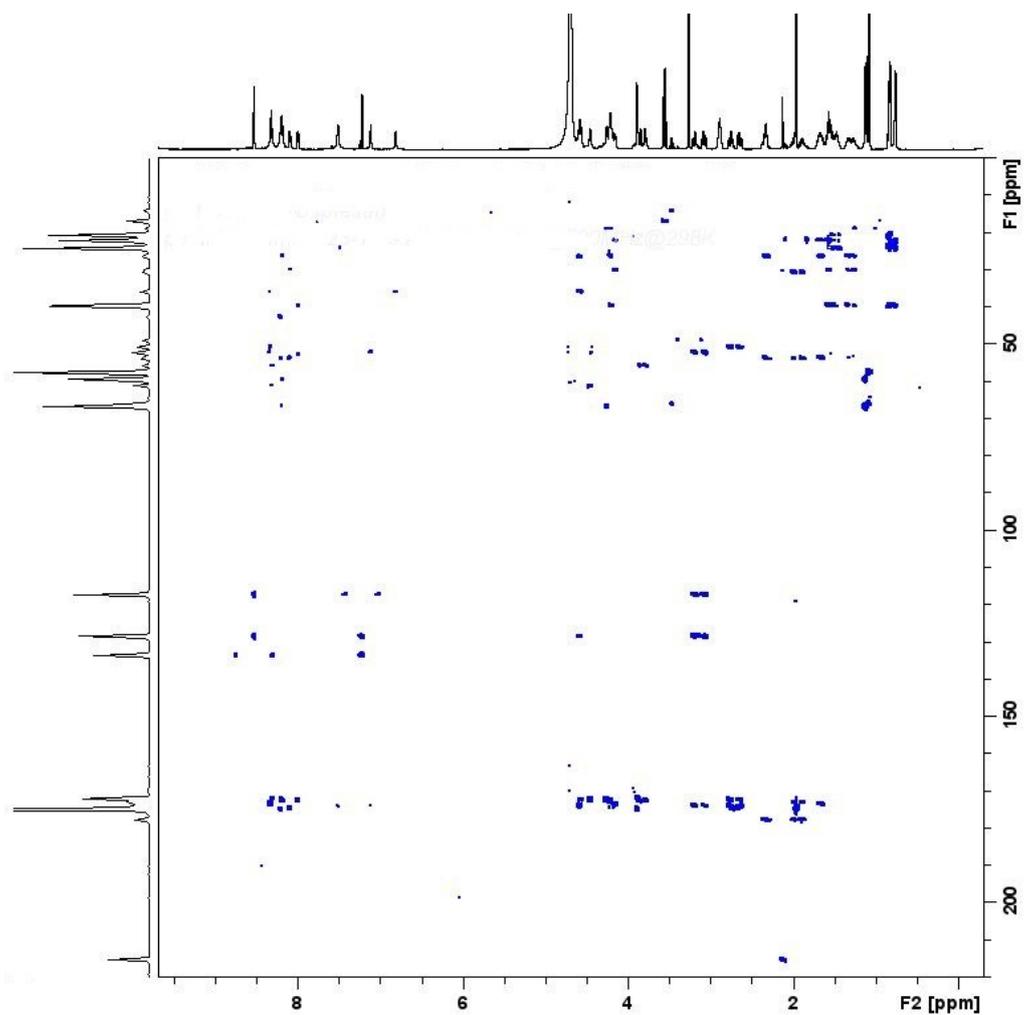


Figure S5. ^1H ^{13}C HBMBC NMR spectrum of the peptide Ac-GSTENLKH-NH₂ (C=2 mM and T=298K)

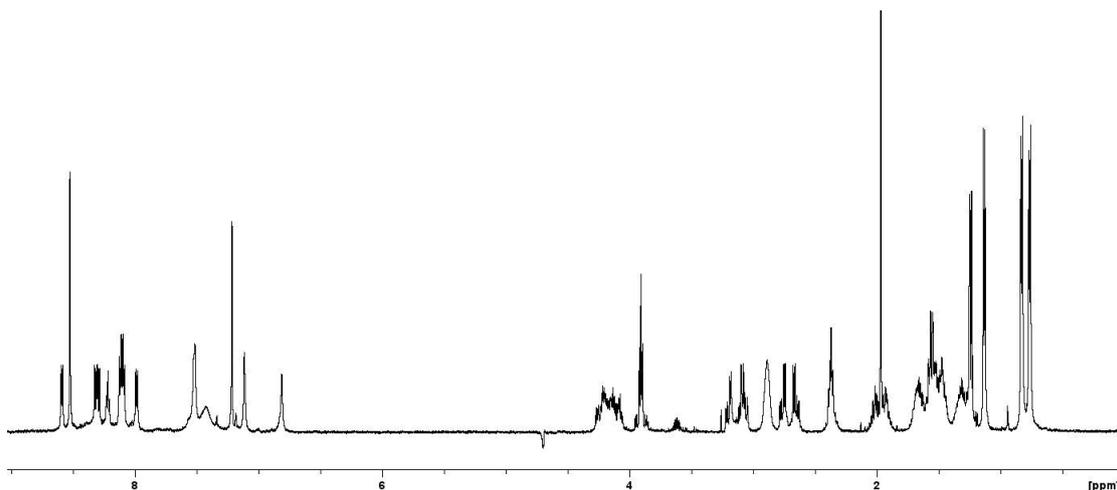


Figure S6. 1D ^1H NMR spectrum of the peptide Ac-GS(P)TENLKH-NH₂ (C=2 mM and T=298K)

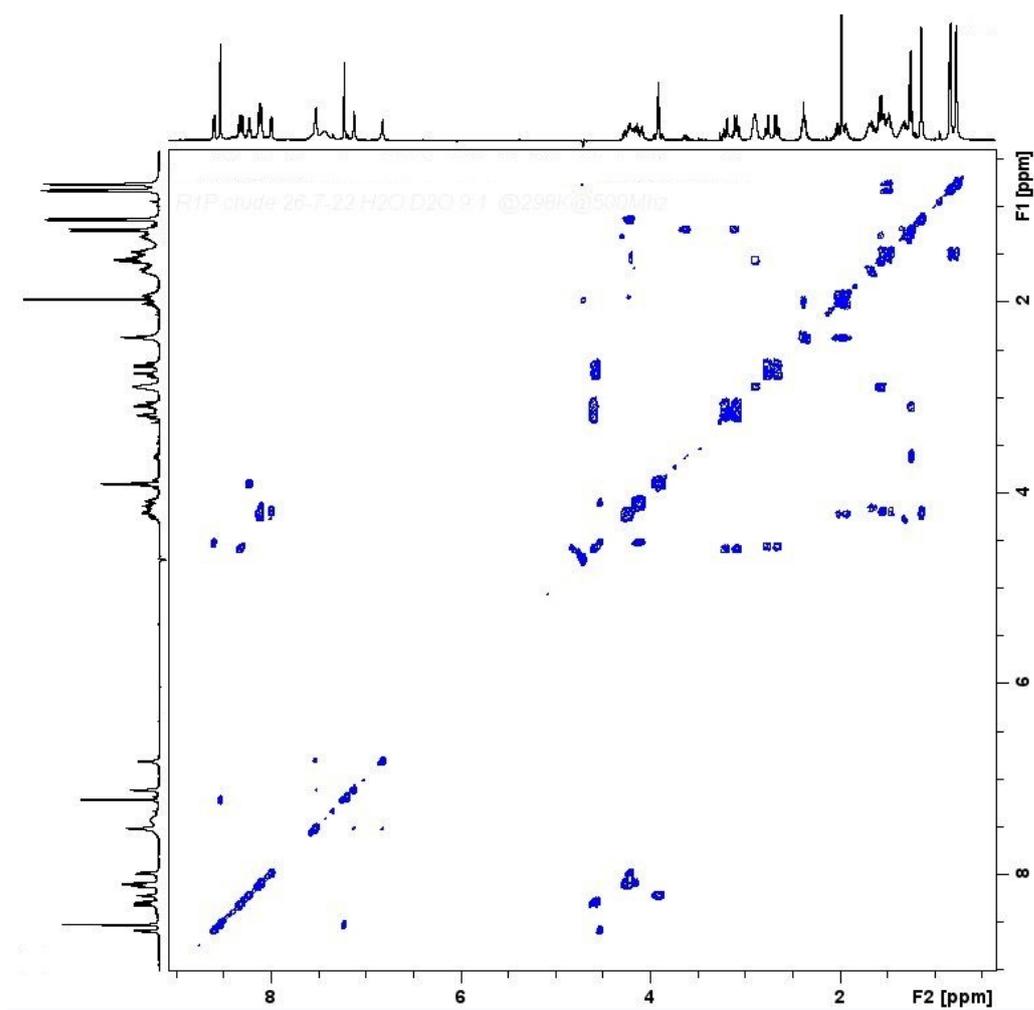


Figure S7. ^1H ^1H COSY NMR spectrum of the peptide Ac-GS(P)TENLKH-NH₂ (C=2 mM and T=298K)

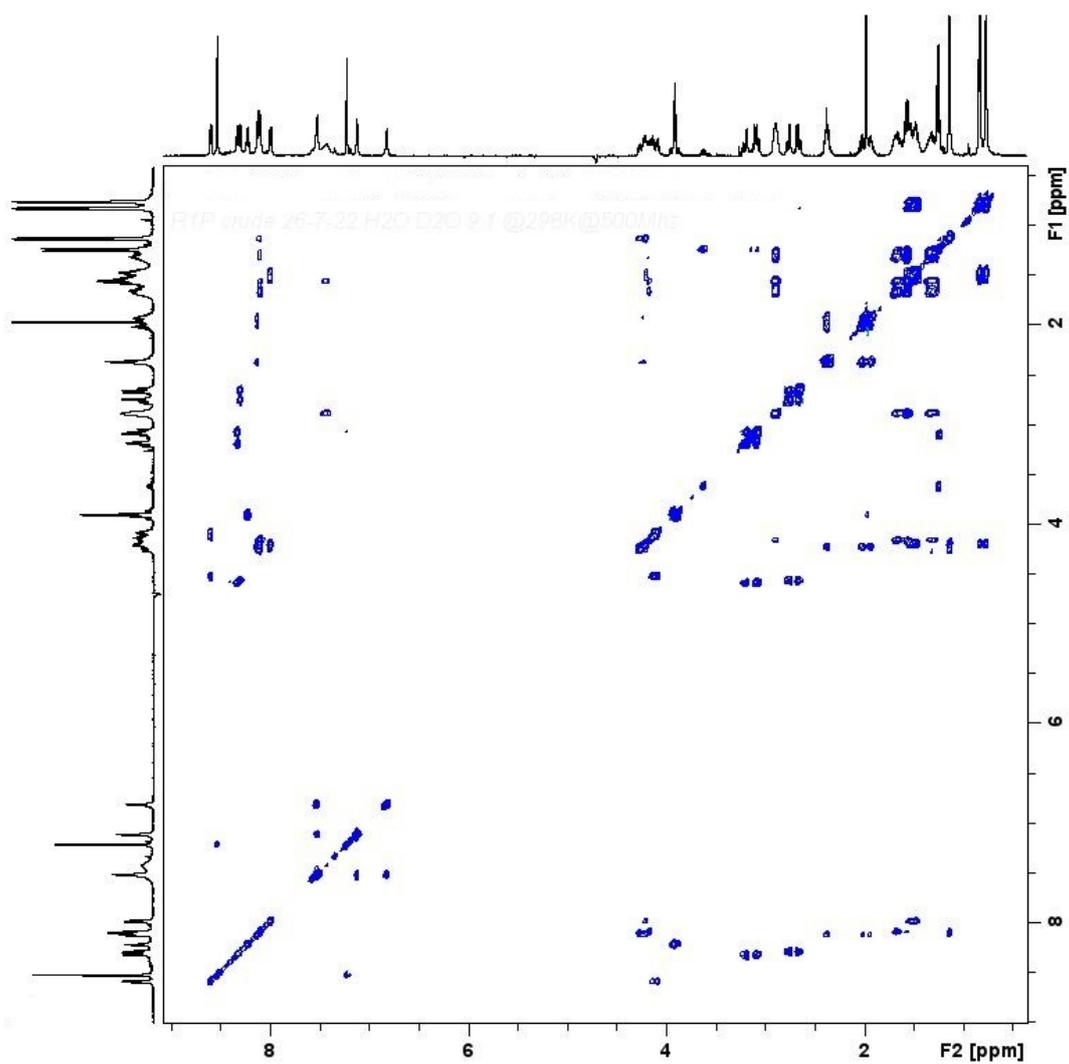


Figure S8. ^1H ^1H TOCSY NMR spectrum of the peptide Ac-GS(P)TENLKH-NH₂ (C=2 mM and T=298K)

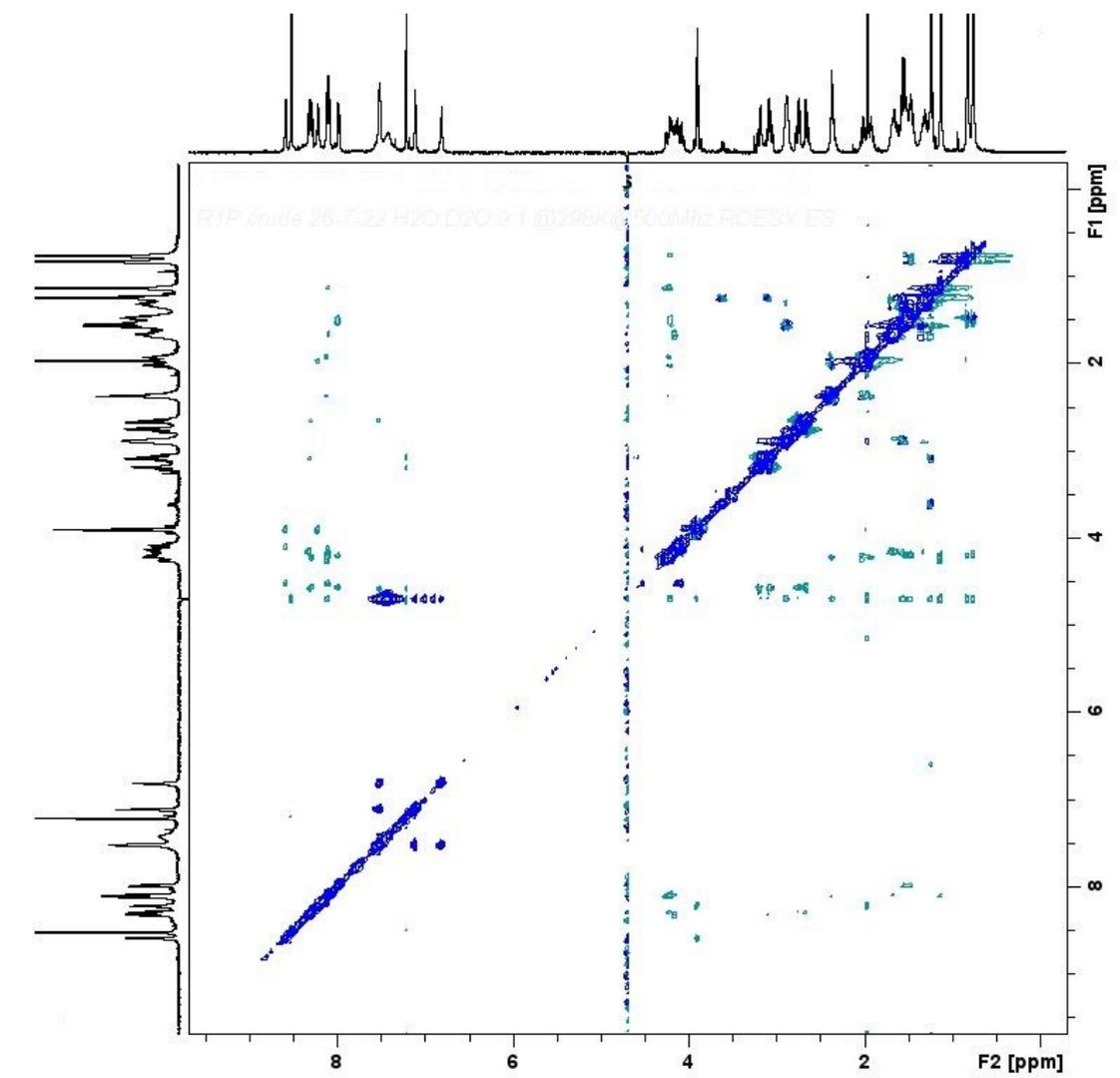


Figure S9. ^1H ^1H ROESY NMR spectrum of the peptide Ac-GS(P)TENLKH-NH₂ (C=2 mM and T=298K)

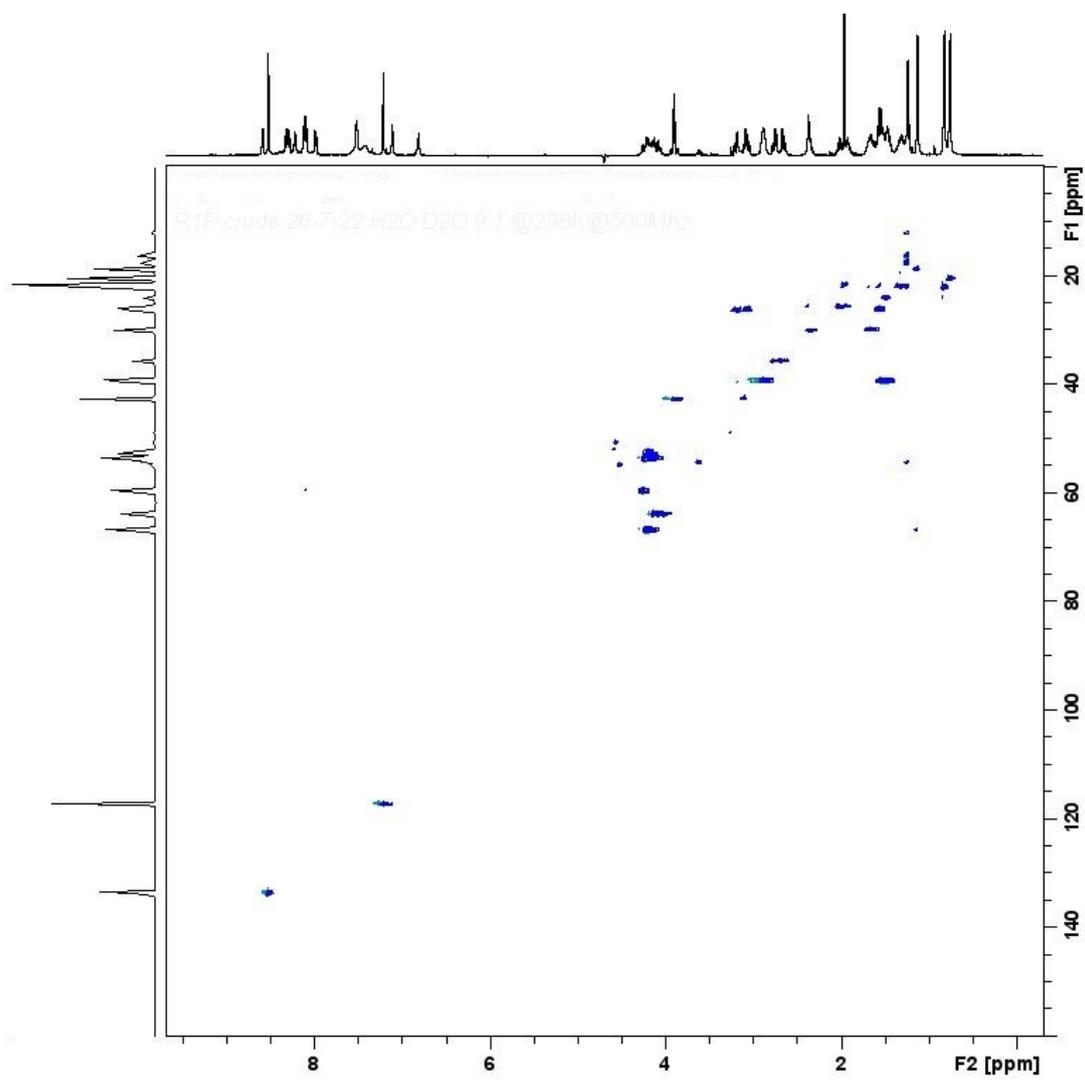


Figure S10. ^1H ^{13}C HSQC NMR spectrum of the peptide Ac-GS(P)TENLKH-NH₂ (C=2 mM and T=298K)

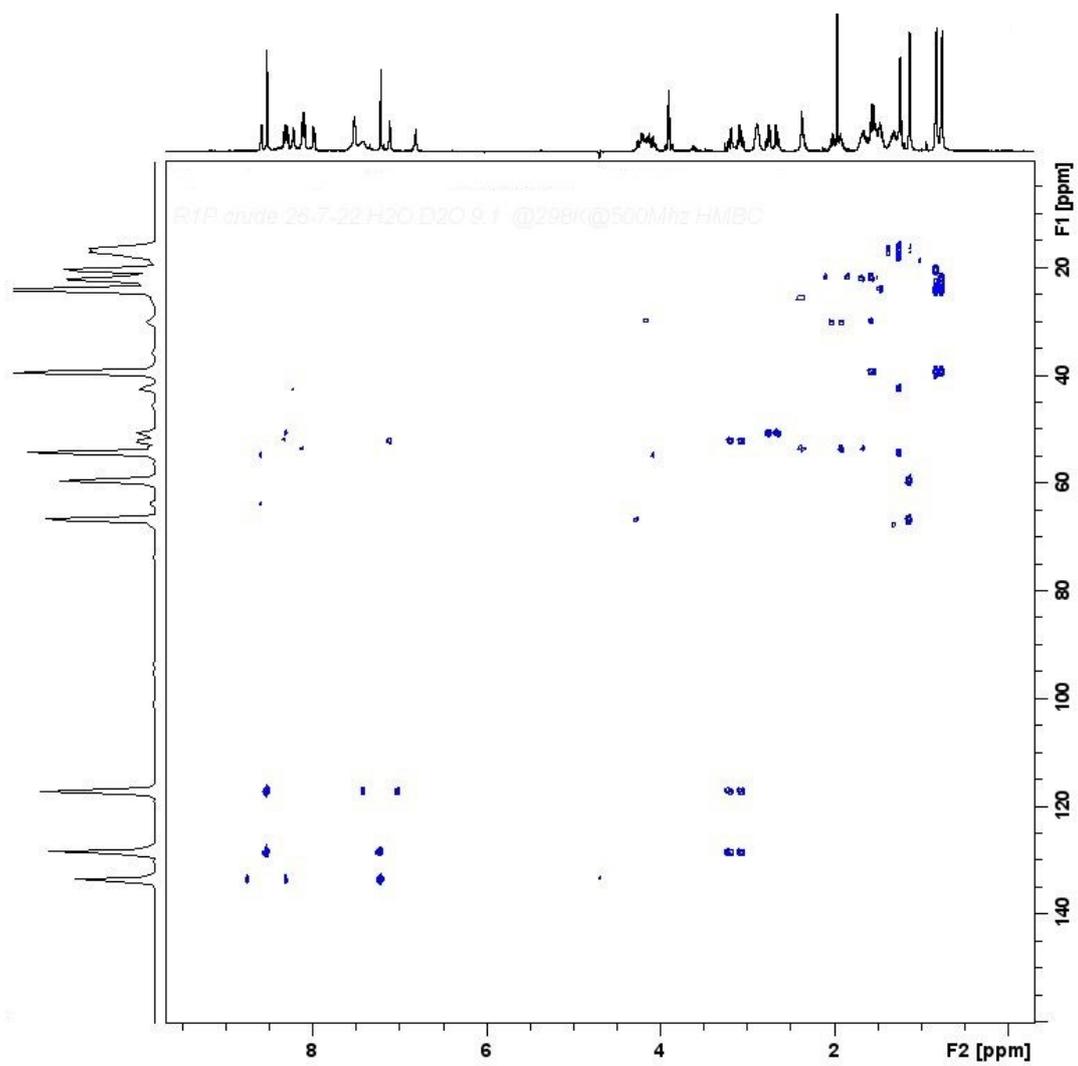


Fig S11. ^1H ^{13}C HMBC NMR spectrum of the Ac-GS(P)TENLKH-NH₂ peptide (2 mM and T=298K)

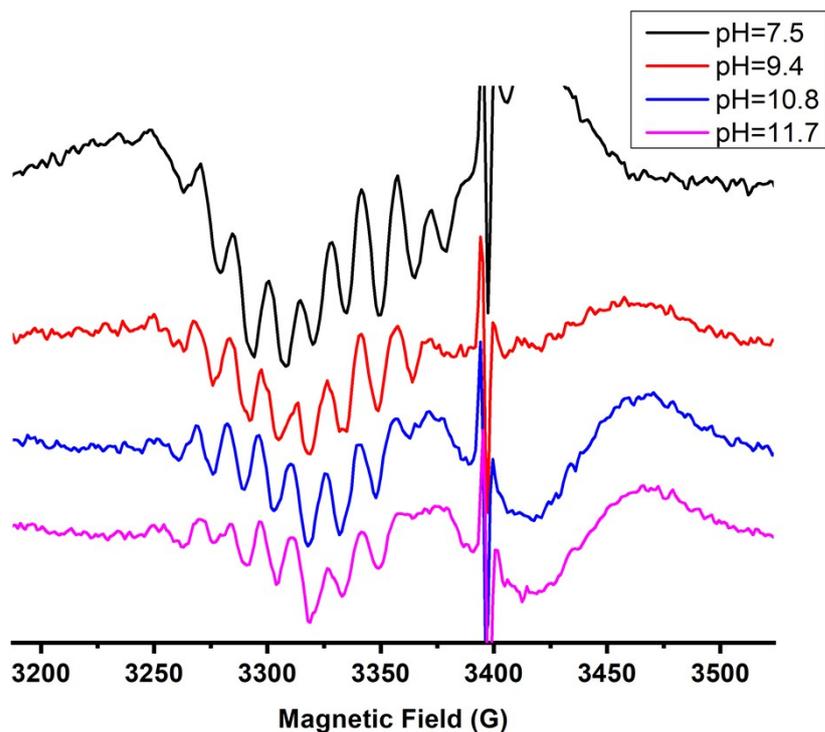


Fig S12 The second derivative of the perpendicular region of EPR spectra for the system Cu(II): R1P recorded at the indicated pH values

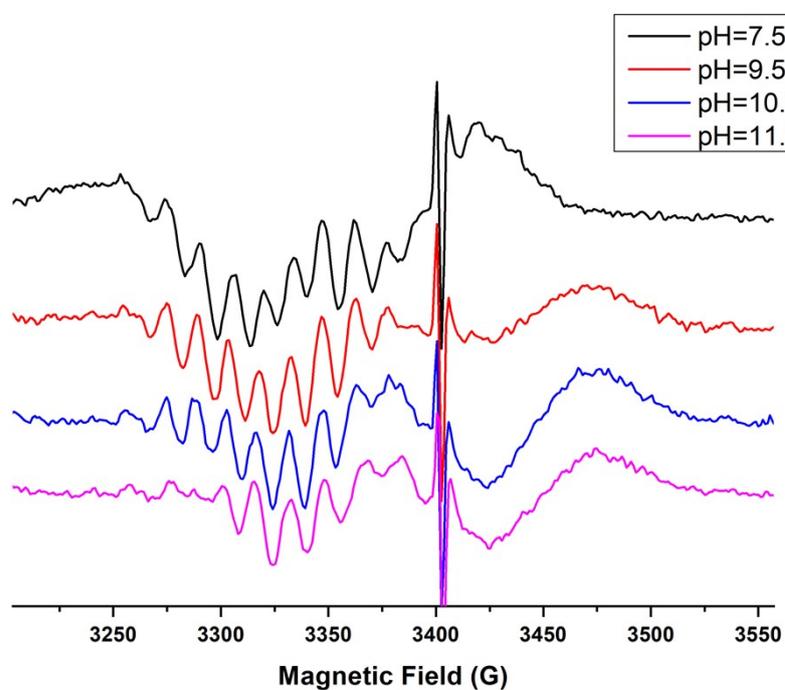


Fig S13 The second derivative of the perpendicular region of EPR spectra for the system Cu(II): R1 recorded at the indicated pH values

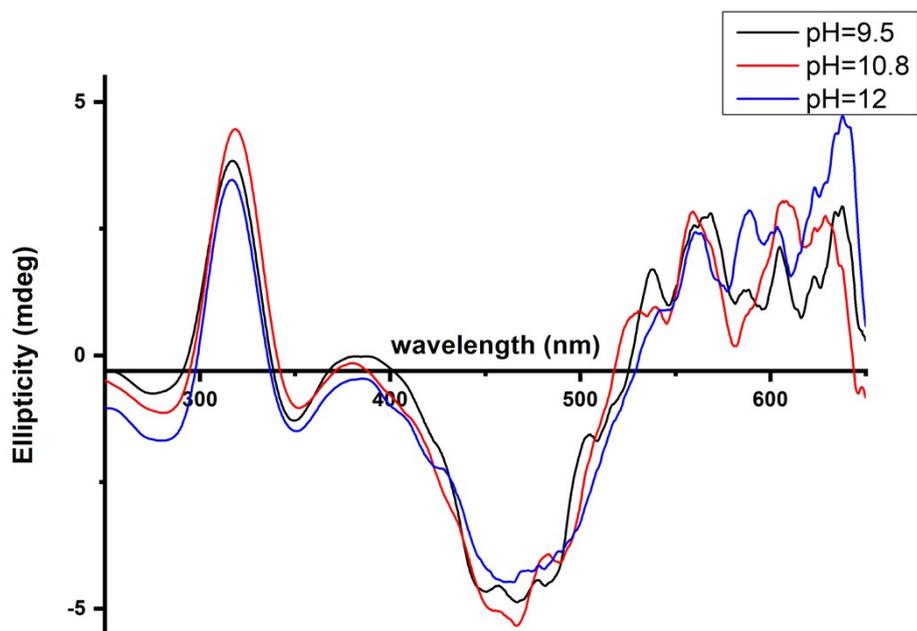


Fig S14 Circular dichroism spectra of solutions of Cu(II) and R1 (Cu(II):R1 1:1.2), recorded at the indicated pH values.