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EPR discrimination of N-ligands coordinating copper in peptide complexes in solution

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A complete strategy for discriminating nitrogen ligands coordinating copper in metal-peptide solutions for fast tumbling copper spectra has been developed. The use of EPR spectra computer simulation in combination with isotopic substitution, second derivative display, and multifrequency and Fourier Transform analysis was attempted with the aim of providing confirmation of the biological validity to the models directly at room temperature. This approach permitted the determination with good precision of a set of spin Hamiltonian input parameters for the Cu-GlyHis and Cu-HisGly complexes. Different arrangements in the first coordination sphere of copper were determined and a definitive discrimination of nitrogen ligands in solution was achieved.