Supporting information:

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"Structural characterization of proteins with an attached ATCUN motif by paramagnetic relaxation enhancement NMR spectroscopy."

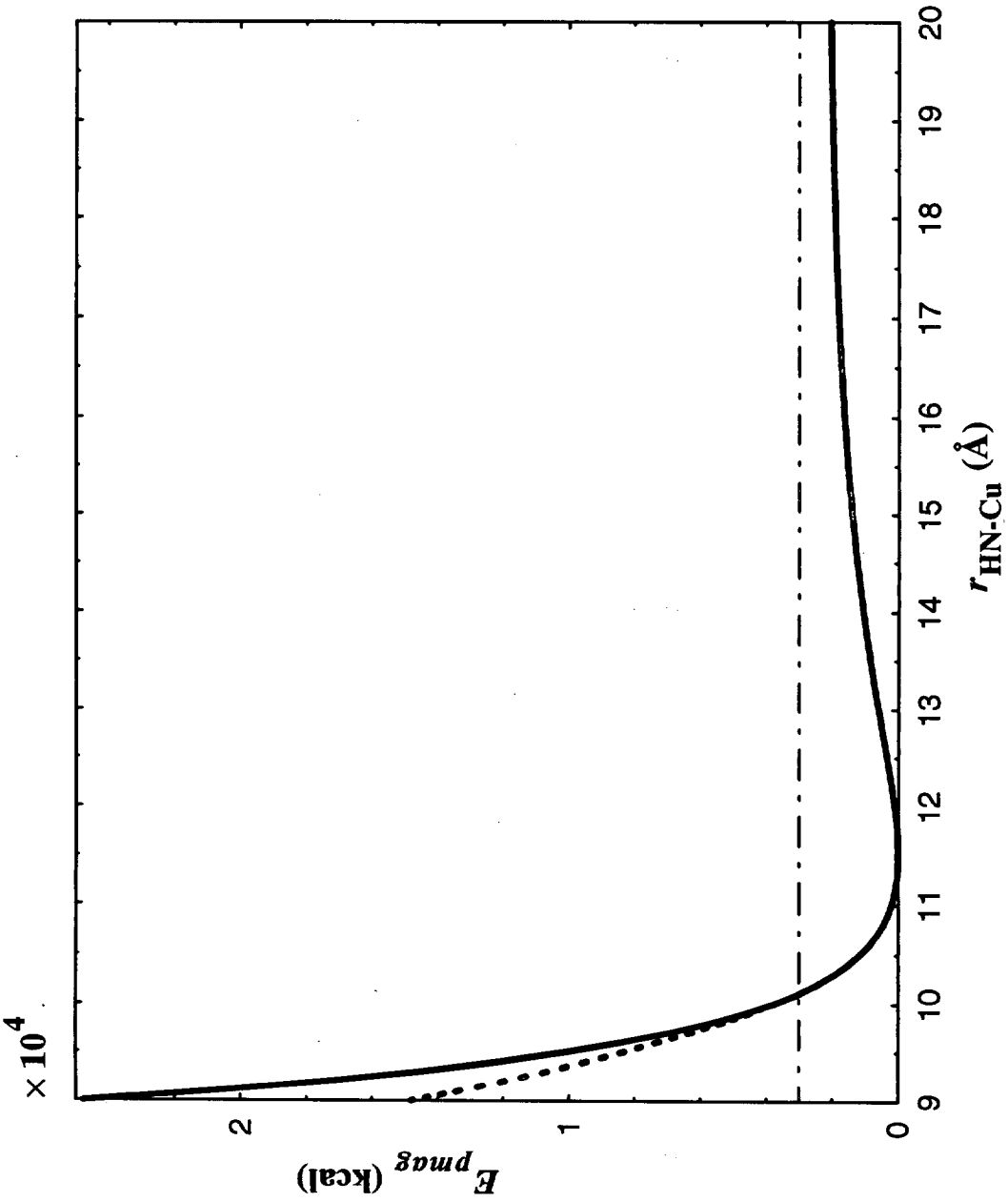
Figure S1. Pseudopotential E_{pmag} from the PMAG module as a function of the distance between Cu^{2+} and the amide proton, $r_{HN\text{-}Cu}$. The solid line denotes E_{pmag} calculated for a single HN proton according to

$$E_{pmag} = (\Gamma_2^{calc} - \Gamma_2^{obs})^2 [1 - \exp\{-(\Gamma_2^{calc} - \Gamma_2^{obs})^2 / 2\sigma_\Gamma^{obs2}\}]$$

using the following set of parameters: τ_c=2 ns, $\omega_H/2\pi$=600 MHz, σ_Γ^{obs}=1 s^{-1}, and Γ_2^{obs}=46.9 s^{-1} corresponding to $r_{HN\text{-}Cu}$=11.5 Å. The dashed line depicts the corrected pseudopotential function which includes the parabolic extension, $c_1(r_{HN\text{-}Cu} - c_2)^2$. This extension is employed when the energy exceeds a certain preset threshold level (in this case 3000 kcal, as indicated by the dot-dashed line) for distances that are on the short side of the minimum. The coefficients c_1, c_2 are automatically adjusted to ensure the continuity of the function and its first derivative. The E_{pmag} contributions for individual residues evaluated in this manner are subsequently summed, multiplied by the force constant k_{pmag} (see eq 2), and added to the overall target function within the CNS software.

Figure S2. Pseudopotential E_{pmag} (eq 2) as a function of the correlation time τ_c. The data are for the lowest energy structure from Figure 3. This type of curve is calculated on the fly by the PMAG module for each set of atomic coordinates generated by CNS in order to minimize E_{pmag} with respect to τ_c. The curve is sampled with a step size of 0.1 ns.

Figure S1



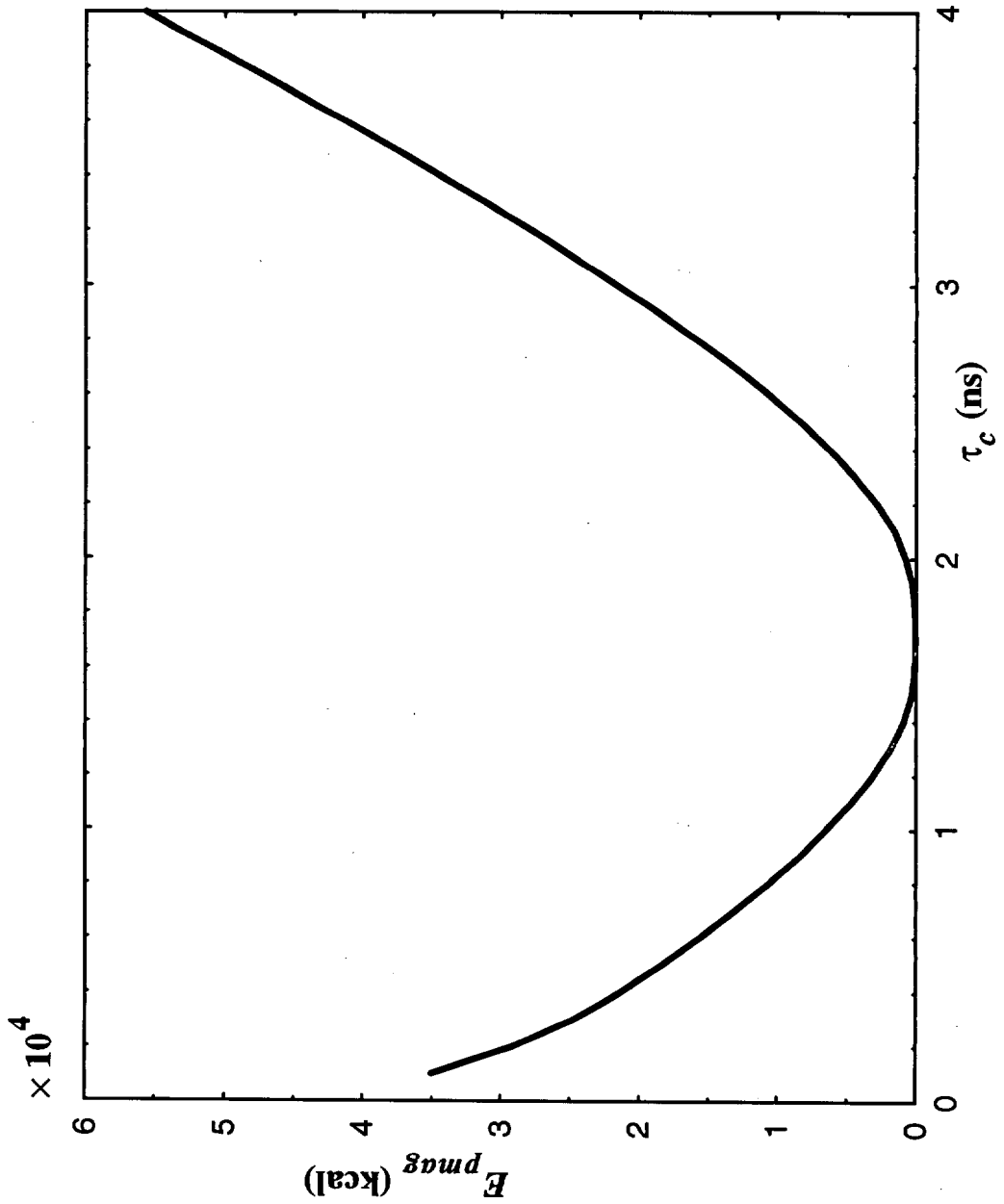


Figure S2