Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

A Molecular Dynamics and Quantum Mechanical Investigation of Intermolecular Interaction and Electron-transfer Mechanism between Copper-containing Nitrite Reductase and Redox Partner Pseudoazurin

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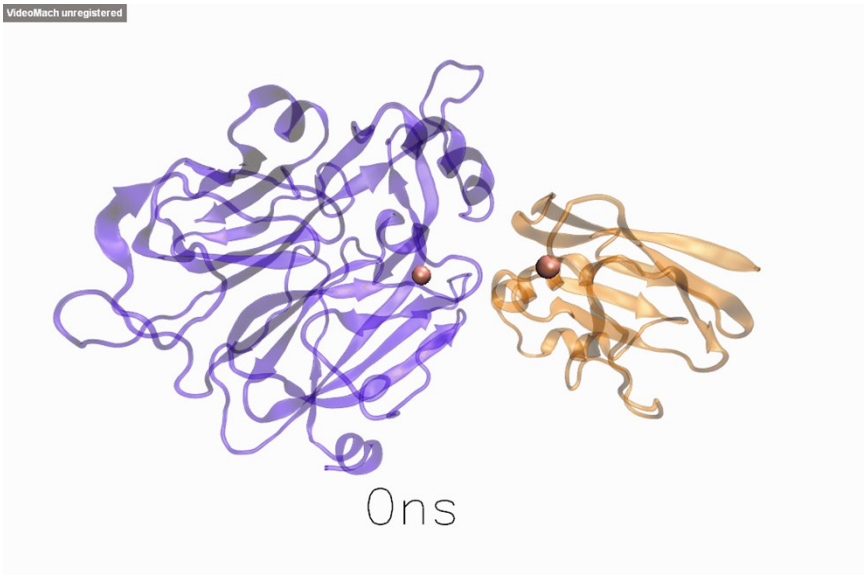

Fig. S1 100ns dynamic trajectory GIF of the chain C (CuNiR, purple) and D (PAz, yellow) in the CuNiR-PAz complex.

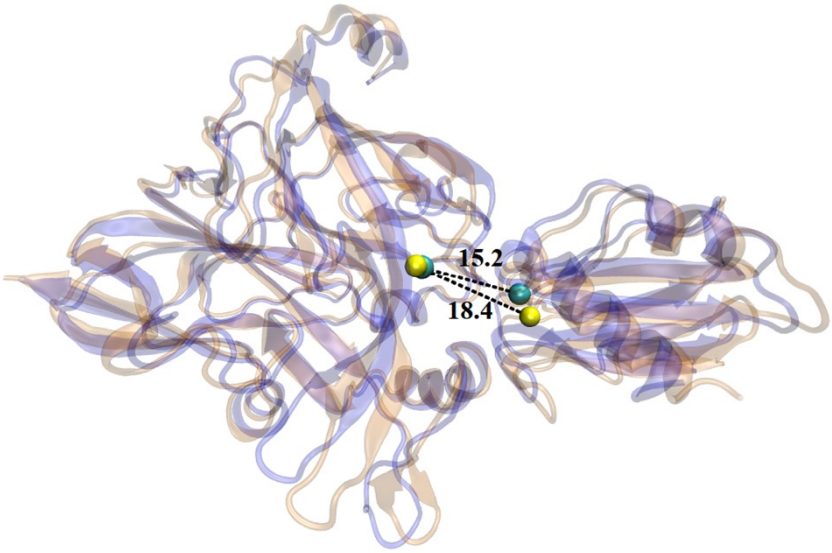

Fig. S2 Superposition of the last frame of 100ns production simulation and the crystal structure (purple, PDB code: 2P80) shows that the overall backbone similarity is high, and the distance between two T1Cu centers does not deviate too much (15.2Å vs 18.4Å).

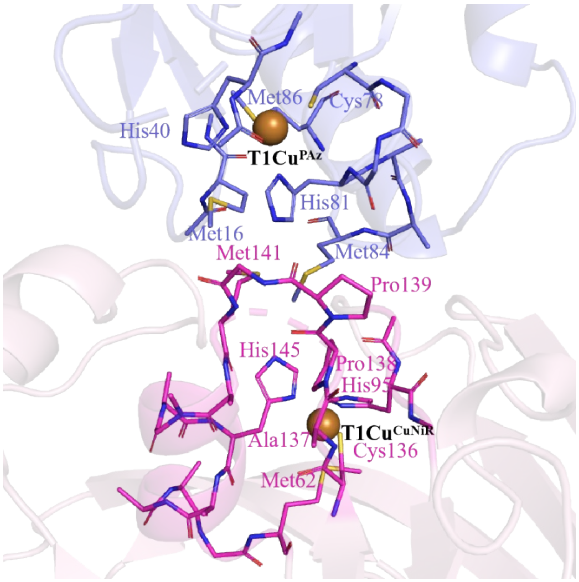

Fig. S3 The quantum calculation model (shown in the stick) including CuNiR residues His95, His145, Cys136, Met150, Pro138, Pro139, and Ala137, and PAz residues His81, His40, Met86, Met16, Cys78, and Met84. Every boundary residue was truncated at the first C-atom and substituted with H atoms.

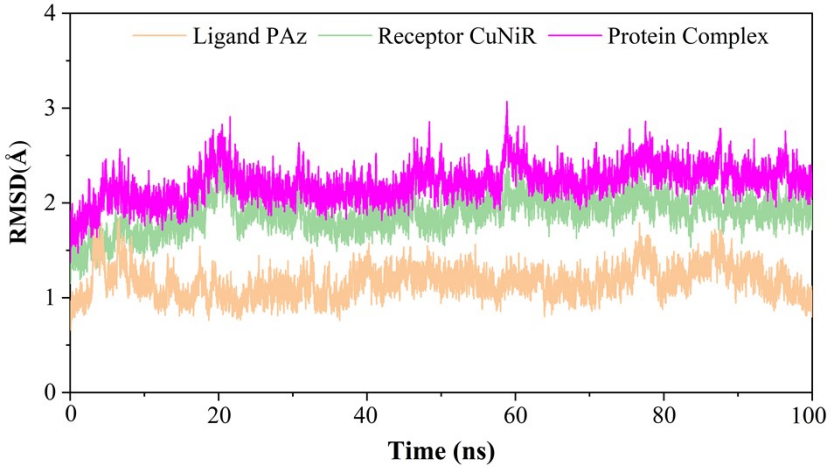

Fig. S4 Root mean square deviation (RMSD) of the Cα atoms of the protein-protein complex and protein(s) only. RMSD plots showing: (a) the CuNIR-PAz complex (magenta), (b) proteins: the receptor protein CuNiR (light green), (c) the ligand protein PAz (light orange) from classical molecular dynamics simulation.

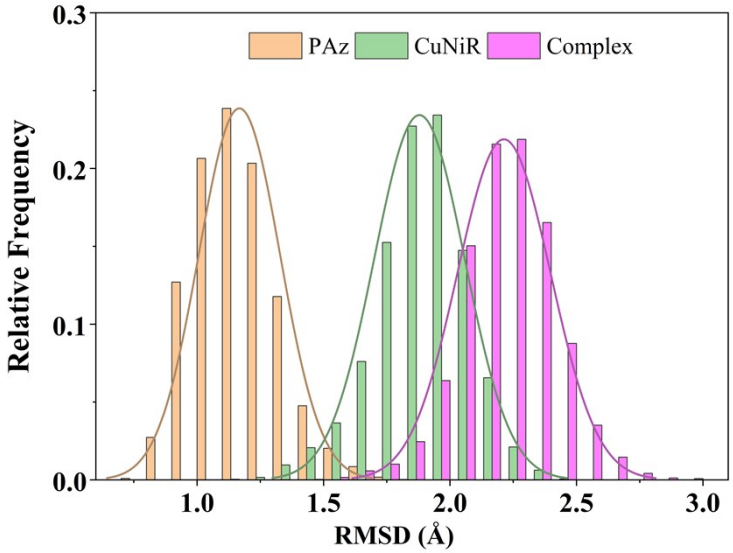

Fig. S5 Root mean square histograms of PAz, CuNiR and the complex.

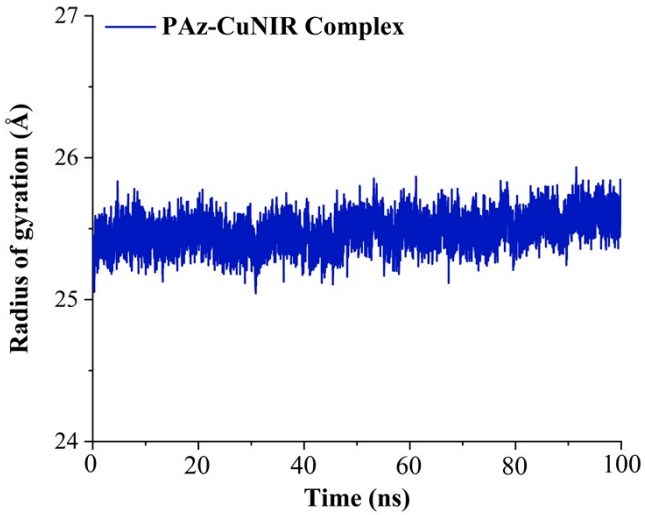

Fig. S6 Radius of the gyration of the CuNiR-PAz complex.

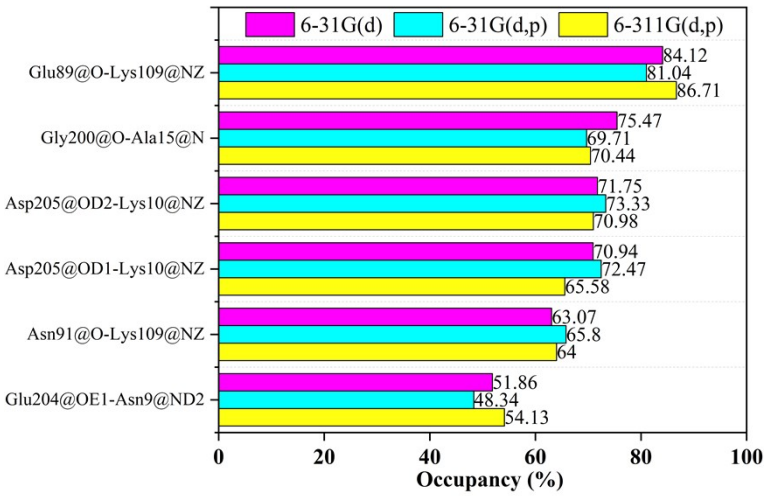

Fig.S7 Hydrogen bond analysis between CuNiR and PAz from three MD trajectories. The basis sets at three different levels (6-31G*, 6-31G**, and 6-311G**, respectively) were used to deal with the missing force field

parameters for the nonstandard residues.

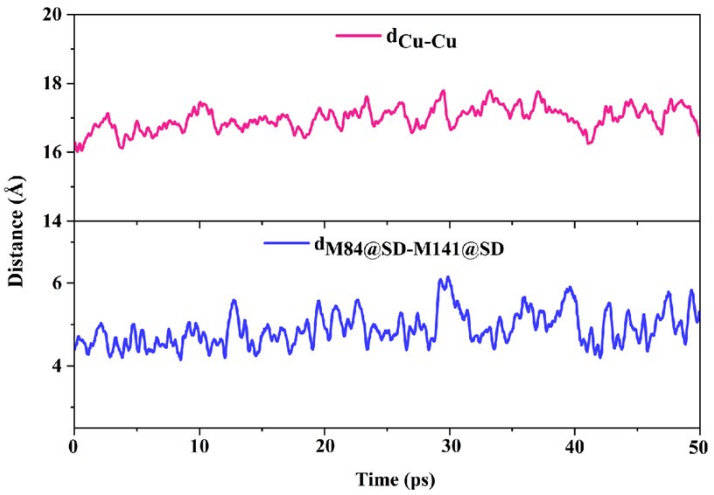

Fig. S8 The distances between PAz T1Cu and CuNiR T1Cu (upper) and between the SD@Met84 atom and the SD@Met141 atom obtained by 50ps QM/MM simulation (lower).