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# BIOLOGY

PRINCIPLES & EXPLORATIONS



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on themes including but not limited to Modeling and simulations of metalloporphyrin enzymes and their catalytic molecular mechanisms Thermodynamics and kinetics of chemical processes in heme proteins Exploring the coupling of electron and proton transfer reactions and proton pumping function in biology by theory computation and experiments Protein cofactor interactions in natural and bioinspired heme protein structures Assessing the role of solvation and conformational dynamics by experimental and computational methods Cytochrome P450 enzymes and substrate drug metabolism Protein nanowires comprised of multi heme cytochromes and long range electron transfer Synthesis characterization and analysis of artificial heme proteins Biosensors with heme proteins Novel multiscale computational approaches incl hybrid QM MM QM MD QM SCE methods and AI ML based approaches Advanced experimental techniques incl high resolution crystallography Cryo EM NMR kinetic electrometric measurements time resolved optical spectroscopies Phylogenetic and structural analysis of heme proteins and specific subgroups The dysfunction of heme proteins including harmful mutations associated with severe health conditions

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