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Computational approaches for understanding the origin of antioxidant properties in Hemocyanin enzymes

Hemocyanins (Hc), proteins commonly known for its extracellular roles in oxygen (O2) sensing, transport, and storage in many invertebrates,[1] have an intriguing and poorly understood intracellular presence. Emerging evidence suggests a significant correlation between oxidative stress and increased intracellular Hcs levels, implicating an active role of Hcs in the antioxidant response.[2] In this study, we employ ab initio calculations (DFT and QM/MM) to unravel the binding features of reactive oxygen species (ROS) at the Hcs active site, using hemocyanin from the arthropod Limulus polyphemus as a model system, to elucidate its potential function in mitigating oxidative stress and contributing to cellular defense mechanisms. Our findings reveal novel states of the Hcs active site, unprecedented insights into its function as a ROS-scavenging enzyme, and a detailed elucidation of its mode-of-action, which highlights the pivotal role of Hcs in oxidative stress management and its potential contribution to the immune response. These insights broaden our understanding about the functional versatility of Hcs and serve as a foundation for the rational design and development of novel artificial enzymatic systems with ROS scavenging properties.

Primary author(s) : Dr. TERÁN, Aarón (Department of Physics "Ettore Pancini", University of Naples Federico II, Complesso Universitario Monte Sant'Angelo Via Cintia 21, Naples 80126, Italy.)

Co-author(s) : Dr. FASULO, Francesca (Department of Physics "Ettore Pancini", University of Naples Federico II, Complesso Universitario Monte Sant'Angelo Via Cintia 21, Naples 80126, Italy.); Mr. TATSIS, Polychronis (Metazoa Phylogenomics and Genome Evolution Lab, Institute of Evolutionary Biology (CSIC-Universitat Pompeu Fabra), Passeig Marítim de la Barceloneta 37-49, 08003, Barcelona, Spain.); Ms. MARTÍNEZ-REDONDO, Gemma I. (Metazoa Phylogenomics and Genome Evolution Lab, Institute of Evolutionary Biology (CSIC-Universitat Pompeu Fabra), Passeig Marítim de la Barceloneta 37-49, 08003, Barcelona, Spain.); Dr. FERNÁNDEZ, Rosa (Metazoa Phylogenomics and Genome Evolution Lab, Institute of Evolutionary Biology (CSIC-Universitat Pompeu Fabra), Passeig Marítim de la Barceloneta 37-49, 08003, Barcelona, Spain.); Dr. ORTEGA-HERNÁNDEZ, Javier (Museum of Comparative Zoology and Department of Organismic and Evolutionary Biology, Harvard University, Cambridge, MA 02138, USA.); Prof. PAVONE, Michele (Department of Chemical Sciences, University of Naples Federico II, Complesso Universitario Monte Sant'Angelo, Via Cintia 21, Naples 80126, Italy.); Prof. MUÑOZ-GARCÍA, Ana Belén (Department of Physics "Ettore Pancini", University of Naples Federico II, Complesso Universitario Monte Sant'Angelo Via Cintia 21, Naples 80126, Italy.)

Presenter(s) : Dr. TERÁN, Aarón (Department of Physics "Ettore Pancini", University of Naples Federico II, Complesso Universitario Monte Sant'Angelo Via Cintia 21, Naples 80126, Italy.)