

Cut It, Pinch It, Twist It: A Theoretical look at Alizarin

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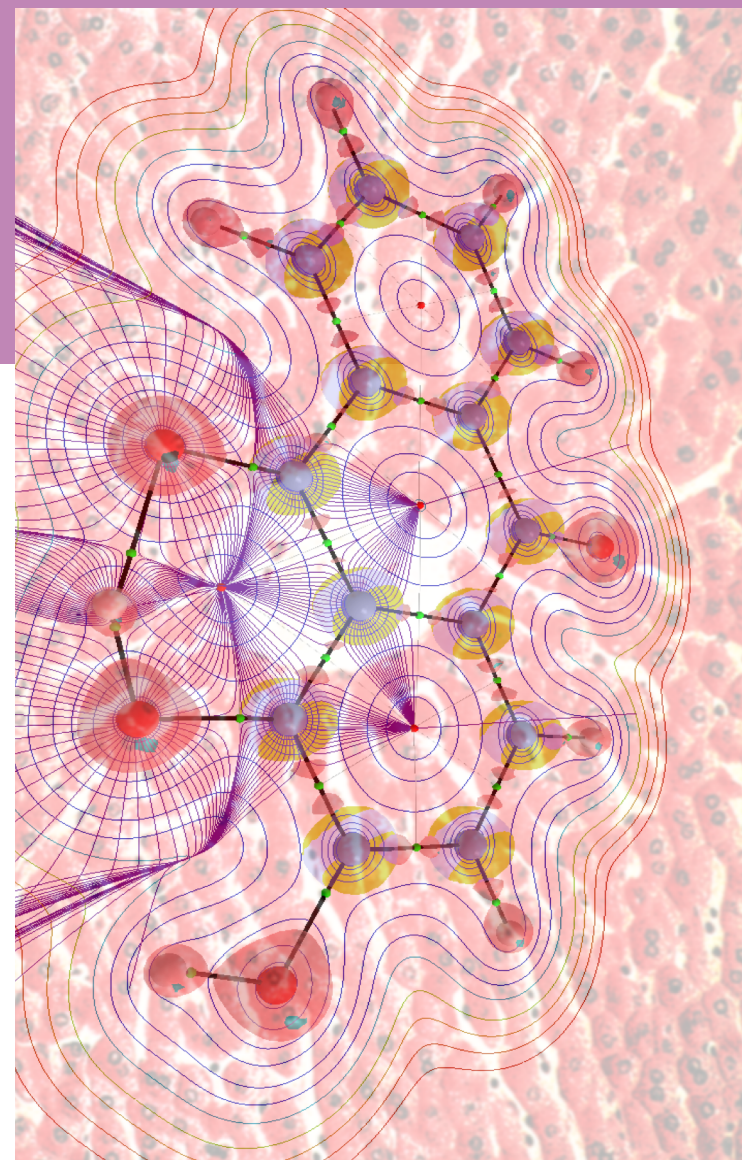
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A young Theoretical and Computational Chemist (born 1982) with a PhD in Sustainable Chemistry granted by the University of Porto and the Nova University of Lisbon, and pre-doctoral experience in tutoring, Food Chemistry, Organic Synthesis, and Environmental Chemistry. During his graduate research, he approached the limitations of the first study of Jacobsen catalyst using a combination of Density Functional Theory (DFT), Bader's Quantum Theory of Atoms In Molecules (QTAIM) and Multivariate

Analysis techniques. Current research interests include the refinement of Gillespie's VSEPR-derived model for the inner Valence Shell of transition metal atoms; the development of novel theoretical approaches to graphene-derived materials, vibrational analysis and the QTAIM description of inter-molecular interactions. Recently, he devoted his efforts to the time evolution of the topology of the electron density, trying to shed new lights on the vibrational spectra of historical pigments.



Alizarin lake pigment