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#ICMolTalks

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Università della Calabria (Italia)

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Abstract

Exploiting computational approaches to study and characterize potential agents of pharmacological interest

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The use of multiscale computational methods, which combine quantum and molecular mechanics approaches such as DFT/TDDFT and MD, offers a detailed understanding of the molecular mechanisms involved in drug discovery. This significantly enhances the efficiency of experiments, greatly reducing both time and costs.

From cancer to bacterial infections, from inflammation to neurological diseases, in most cases the main goal is the synthesis of new molecules with minimal side effects in humans. Therefore, beyond exhibiting high bioavailability, a drug must possess high selectivity and very low toxicity.

In this context, transition metal ions involved in redox processes, together with light-dependent approaches, represent a progressive advancement over conventional medical strategies. Several coordination complexes , ligands and photo-responsive compounds have been proposed, showing promising biological and therapeutic activities by exploiting different mechanisms of action, even targeting distinct biological structures such as cellular membranes. Computational results will provide an insight into the chemical-physical and photophysical properties of the studied species and will be presented along with the support and validation of the experimental data.

Biography

lessandra was a student and later a thesis researcher at the Laboratory of “Progettazione Molecolare e Chimica dei Sistemi Complessi” (PROMOCS) of the Department of Chemistry and Chemical Technologies at the University of Calabria. In the same laboratory, Dr. Ritacca obtained her PhD in Translational Medicine (XXXIV Cycle) under the supervision of Prof. Emilia Sicilia. During her doctoral studies, her research activity focused on the characterization and investigation of the mechanism of action of copper complexes in their dual role as toxic and beneficial metals using various computational approaches. As a result of her work, seven articles were published. Of particular importance is a publication in the journal ACS Catalysis, concerning the detailed study of the CO oxidation mechanism to CO_2 by a particular enzyme containing a bimetallic MoCu center, and two articles, one published in JACS, on the mechanism of action of copper-containing anticancer compounds in collaboration with Prof. Peter Faller (University of Strasbourg), one of the leading experts in the field.

After obtaining her PhD, Dr. Ritacca continued with a postdoctoral research position at the Polytechnic University of Marche under the supervision of Prof. Luca Maragliano, also serving as a research affiliate at the Italian Institute of Technology (IIT), Center for Synaptic Neuroscience and Technology (NSYN), Genova, funded by the PRIN 2020 project titled “Structural modelling and molecular dynamics simulations of synthetic photosensitive molecules and their interactions with the cell membrane.” She then further consolidated her scientific profile as a postdoctoral researcher for the PRIN 2022 project titled “In silico-design, synthesis and characterization of innovative two-component Light-absorber (LA)-G-quadruplex (G4) binder conjugates: a new paradigm to afford a Dual Anti-Cancer Approach” in the group of Prof. Marta Erminia Alberto at the University of Calabria.

Her research activity focuses on topics of pharmacological interest, such as structural modelling and molecular dynamics of photosensitive molecules and their interactions with cell membranes; in silico design of innovative systems for anticancer strategies; theoretical studies of metal ions and bioactive complexes of medical relevance. She has also worked on materials research, in particular, on molecules that inhibit the corrosion of metallic surfaces.

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