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Bacterial type II dehydroquinase enzyme: From the reaction mechanism to the structure-based design of inhibitors

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The decreased effectiveness of antibacterial agents against infectious diseases caused by the development of drug resistance has become one of the most important public health issues of the early 21st century. Despite the recognized need for new antibiotics, only a few new classes of antibiotics have been brought to the market in the last three decades. Therefore, the discovery of novel drugs and therapies to treat antibiotic-resistant infections and, particularly of drugs with new mechanisms of action is needed. Today, there is a great and increasing interest in the detailed knowledge of the catalytic mechanism of selected enzymes for the rational design and development of new inhibitors that can be used as drugs. In recent years, computational methods have consolidated their value as important complementary tools that can assist in the elucidation of how these reactions are catalyzed and to derive QSAR models that help rationalize the determinants of binding affinity for inhibitors. Here we report results from computational, structural and biochemical studies that help understand in atomic detail the catalytic mechanism of two essential bacterial enzymes that are recognized to be attractive targets for the development of new antibacterial agents, the type II dehydroquinase enzyme (DHQ2). Comparative Binding Energy (COMBINE) analysis to quantify the importance of the hydrogen bonding interaction of the ligands with the water molecule involved in the enzymatic mechanism and the application of this knowledge in the structure-based designed of inhibitors will be also presented.

Biography

Concepción González-Bello has obtained her PhD at the University of Santiago de Compostela (USC, Spain) in 1994. She did two predoctoral stays in the University of Gent (Belgium) with Prof. Vandewalle and in the Scripps Research Institute (USA) with Prof. Nicolaou. After a postdoctoral stay in the University of Cambridge (UK) with Prof. Abell, she joined USC as an Assistant Professor, was promoted to Associate Professor in 2003 and obtained the Spanish habilitation to full Professor in 2011. She is author of more than 50 papers and several book chapters. She is a member of the ChemMedChem International Advisory Board.

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