CiQUS

Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares

Conferencia:

New Computational Developments for the Design of Chemobiological Architectures

Jean-Didier Maréchal

Universidad Autónoma de Barcelona

12/06/18

Aula de Seminarios do CIQUS

12:15 h

Más información:
www.usc.es/ciqus

XUNTA DE GALICIA
CONSELLERÍA DE CULTURA, EDUCACIÓN E ORDENACIÓN UNIVERSITARIA

USC UNIVERSIDADE DE SANTIAGO DE COMPOSTELA

CAMPUS VIDA
CAMPUS DE EXCELENCIA INTERNACIONAL

New Computational Developments for the Design of Chemobiological Architectures

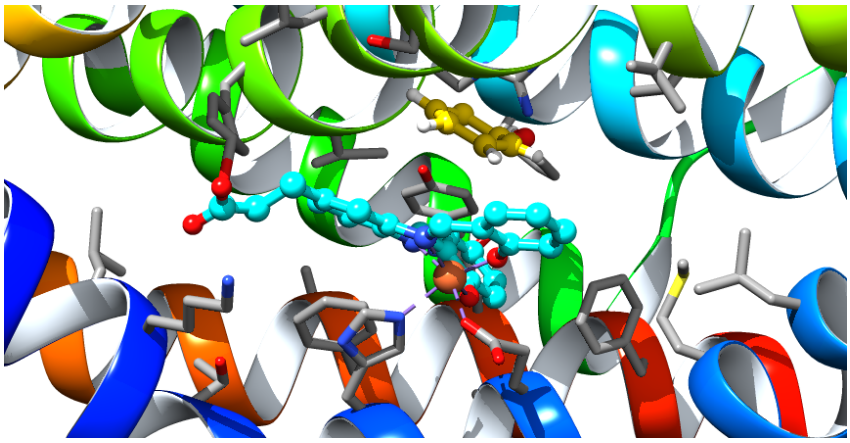
Jean-Didier Maréchal

Departament de Química, Universitat Autònoma de Barcelona, Edifici C.n., 08193 Bellaterra, Spain
Jeandidier.marechal@uab.cat

In the recent years, our group developed, tested and applied a series of computational strategies for the study and design of novel chemobiological architectures with a clear focus toward bioinorganic systems. From standard protein-ligand dockings to multi-scale approaches and including the development of our multi-objective molecular constructor GaudiMM[1], our work allowed to better understand the molecular mechanism of some of these species and how to design new ones.

Our most important contribution has focused on artificial metalloenzymes, a novel kind of biocatalysts obtained by the incorporation of homogenous catalysts into biological frameworks[2-3]. But with time and experience we added novel activities like the prediction of the binding of metallodrugs to protein, the formation to siderophores or the development of biosensors.

Here, we present the underpinning concepts of our strategies and summarize the most important results. Focus will be given on our updates on protein-ligand docking approaches and how this had a positive impact on our prediction of metal-protein interactions.



Literature:

1. J. Rodríguez-Guerra, G. Sciortino, M. Municoy, J. Guasp and J.-D. Maréchal *J. Comput. Chem.* 2017 **38**, 2126
2. V. Muñoz Robles, E. Ortega-Carrasco, L. Alonso-Cotchico, J. Rodríguez-Guerra, A. Lledós, A. and J.-D. Maréchal, *ACS Catal.* 2015, **5**, 2469
3. L. Villarino, Splan K., Reddem E., Gutiérrez de Souza C., Alonso-Cotchico L., Lledós A., Maréchal J-D., Thunnissen A-M. and Roelfes G. 2018 *Angew. Chem. Int. Ed.* DOI: anie.201802946