ICREA MEMOIR 2018

Osuna, Sílvia

Universitat de Girona (UdG)

Experimental Sciences & Mathematics

Sílvia Osuna received her PhD in 2010 from the University of Girona (UdG) at the Institut de Química Computacional (IQC). In 2010, she moved to the group of Prof. Houk at the University of California, Los Angeles (UCLA). Since then, Sílvia has worked in computational design of enzymes of medical and pharmaceutical interest. Sílvia has more than 65 research publications, and been awarded the Young Researcher award by the Royal Spanish Society of Chemistry (RSEQ 20116), the Research award by the Fundación Princesa de Girona (FPdGi 2016- Science category), and the 2017 Young Investigator Award of EuCheMS Organic Division. Her group is funded by the European Research Council project – Starting Grant (ERC-2015- STG-679001, NetMoDEzyme) and the Catalan government project for emergent research teams (2017-SGR-1701).

Research interests

Sílvia's research lies at the interface between computational chemistry and biology. Her research focuses on the study of biochemical processes mainly related to enzyme catalysis. Her lab is developing new computational tools for predicting which amino acid changes are required to the enzyme structure for allowing novel function, enhancing a promiscuous side reaction, or expanding its substrate scope. Her goal is to enable the routine computational design of proficient enzymes to boost their use in industry for the synthesis of pharmaceutically relevant targets. She also applies the developed methodologies to the study of the recognition and assembly process of biomolecules with carbon-based materials.

Selected publications

– Maria-Solano MA, Serrano-Hervas E, Romero-Rivera A, Iglesias-Fernandez J & **Osuna S** 2018, 'Role of conformational dynamics in the evolution of novel enzyme function', *Chemical Communications*, 54, 50, 6622 – 6634.

– Serrano-Hervas E, Casadevall G, Garcia-Borras M, Feixas F & **Osuna S** 2018, 'Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates', *Chemistry-a European Journal*, 24, 47, 12254 – 12258.

– Romero-Rivera A, Iglesias-Fernandez J & **Osuna S** 2018, 'Exploring the Conversion of a d-Sialic Acid Aldolase into a l-KDO Aldolase', *European Journal Of Organic Chemistry*, , 20-21, 2603 – 2608.

Selected research activities

Most relevant invited conference participations:

1. Osuna, S. Role of conformational dynamics in the evolution of novel enzyme function, **Invited lecture** at Rideal Conference, Oxford, UK March 2018.
2. Osuna, S. The role of conformational dynamics for novel enzyme function, **Invited lecture** at CECAM workshop**:**Proteins in realistic environments: Simulation meets experiments, Stuttgart, Germany, May 2018.
3. Osuna, S. Computational tools for enzyme design, **Invited lecture** at **Protein Engineering Canada 2018**, Vancouver, Canada, June 2018.
4. Osuna, S. The role of Conformational Dynamics on the evolution of novel enzymatic activities, **Invited lecture** at **254thACS meeting**, Boston, USA August 2018.
5. Osuna, S. The role of Conformational Dynamics on the evolution of novel enzymatic activities, **Invited lecture** at the European Young Chemist Network symposium at **7thEuChemS**, Liverpool, UK August 2018.
6. Osuna, S. The role of Conformational Dynamics on the evolution of novel enzymatic activities, **Invited lecture** at **The Future of Enzyme Modeling**, Stockholm, Sweden September 2018.
7. Osuna, S. Conformational heterogeneity in enzyme design, **Invited lecture** at the **Trenca meeting**, Benicassim, ESP November 2018.