

[MareNostrum user wins the 'SusChem Young Chemical Researchers'](#)

The study –classified by the journal as a 'Very Important Paper' (only 5% of the articles published in *Angew. Chem.* receive this distinction)– has been coordinated by the ICREA Research Professor Carme Rovira, leader of the Quantum Simulation of Biological Processes (SQPBIO) of the Co.S.Mo.LAB and member of the Institute of Theoretical Chemistry (IQTIC), University of Barcelona. The simulations have been carried out at the MareNostrum Barcelona Supercomputing Center (BSC-CNS).

In the study, Ardèvol and Rovira decipher the molecular mechanism of formation of glycosidic bonds by glycosyltransferases, the enzymes responsible for the structure of many carbohydrates. The results have important implications in the field of glycobiology, -area of biology that deals with the study of carbohydrates and their influence on the functions of cells - both for improving the synthesis of known carbohydrates in the laboratory, as well as for the search for new therapeutic agents.

In its decision the jury, chaired by Pilar Goya, vice president of the Royal Spanish Society of Chemistry (RSEQ) - has unanimously awarded the prize to Albert Ardèvol and described his scientific publication as "excellent".

Albert Ardèvol earned his Ph.D. in Chemistry on 20 January 2012 in the group Quantum Simulation of Biological Processes Laboratory of Computational simulation and modelling of the Barcelona Science Park, under the direction of Professor Carme Rovira, in the field of reaction mechanisms of carbohydrate-active enzymes. After receiving a grant from the European Molecular Biology Organization (EMBO), Ardèvol has recently joined the group of Professor M. Parrinello at ETH (Switzerland), to develop new methods for analyzing the dynamics of proteins.

The SusChem Young Chemical Researchers awards are promoted by the Spanish Technological Platform of Sustainable Chemistry (SusChem – ES) and aim to recognize, encourage and promote scientific research and dissemination among young chemists. They also support the development of the discipline of chemistry in Spain both as a pure science and with regard to its applications.

This year, in their fourth edition, the awards are presented in four categories –Innova Predoc, Postdoc and Future-, with a financial endowment of 1,500 Euros each. The Predoc Prize, awarded to Albert Ardèvol, grants recognition to the author of the best scientific publication (with page number 2011) in any area of chemistry and not holding a doctorate degree at December 31, 2011.

Barcelona Supercomputing Center - Centro Nacional de Supercomputación

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