



IV ASBioSim – Advanced School on Biomolecular Simulation: Protein Engineering with Rosetta, from fundamental principles to tutorials

05 to 10/May, 2019, Recife/PE, Brazil

Optimizing the efficiency of enzymes in the shikimate pathway

Lousa D., Rocha I. and Soares C. M.

ITQB NOVA, Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da República, 2780-157 Oeiras, Portugal

Abstract: The Protein Modelling Lab of ITQB NOVA is currently participating in the European Project “SHIKIFACTORY100 - Modular cell factories for the production of 100 compounds from the shikimate pathway”, which aims to optimize the production of a universe of more than 100 high-added value compounds from the shikimate pathway, a hub in cell metabolism. This is a very ambitious project that will be implemented by a consortium covering research leading institutions in computational design and in vivo implementation of pathways and cell factories.

Our lab is responsible for developing an automated platform combining several structural bioinformatics tools that will be used in two tasks: gene selection and structure-based enzyme engineering. One of the aims of the project is to optimize the enzymes responsible for the limiting steps in the pathways, to enhance the production of the compounds of interest. This will be done using protein engineering methods, in order to optimize the catalytic efficiency of the target enzymes.