

SORS: Receptor Sampling with Dpedmd for Virtual Screening

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Abstract

The genetic profile of patients directly affects their reaction against medication: sometimes in a positive manner (increasing the therapeutic effect), sometimes in a negative manner (increasing toxic side effects, or simply deactivating a drug response). Apparently trivial variations in the genome have a demonstrated impact in different aspects of drug therapy, among them a decrease of drug effect on receptors (Stingl et al. CPT 2010), which open a significant uncertainty on the impact of a given drug when applied to the population level. Experimental evaluation of the connection between genotype and pharmacological response is a priori possible, but its cost is prohibitive, forcing the use of in silico approaches (Alvarez, J. C.

J. C. Curr. Opin. Chem. Biol. 2004), which need to be improved and extended to tackle the formidable problem coming from world-wide genotyping initiatives. We aim to improve the screen of large collection of libraries developing an in silico platform that combines the classical structure-based and ligand-based approach. The platform increase the performance of predictions integrating determination of molecular receptor flexibility using computational modeling approaches, amongst which molecular dynamics (MD) and) and coarse grained dpED/MD simulations.

[The Presentation can be viewed here.](#)

Bio:

Dr. Ramon Goñi holds a PhD in Biotechnology from the University of Barcelona (UB, 2008). He graduated in Computer Science from the Universitat Politecnica de Catalunya (UPC, 2002).

He joined the Institute de Recerca Biomèdica de Barcelona (2004-2007) where he participated in several research projects like the study of anti-gene therapies, the development of gene-predictors or the study of the physical properties of genomic DNA.

In 2007 he joined the sales and marketing department of the bioinformatics company Integromics (2007-2009). He led the development genomics data analysis solutions for Pharma/Biotech industry.

From 2009 he joined the Barcelona Supercomputing Center as Senior Researcher and Project Manager of Technology Transfer projects. He taught bioinformatics in the University of Barcelona (UB, 2010) and in the Universitat de Vic (UVIC, 2005-2007).

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