## conferenceseries.com

6<sup>th</sup> International Conference on

## Structural Biology

August 22-23, 2016 New Orleans, USA

## Is molecular docking the holy grail of computational modeling?

Ihosvany Camps Federal University of Alfenas, Brazil

The molecular docking is the most used technique to theoretically study ligand-receptor interactions. The goal of the talk is to present the evolution and fundamental aspects behind the molecular docking together with other computational modeling methods capable of giving better information about the ligand-protein interactions than simple docking and ligands with better binding energy. In the first part of the talk, the types of docking (rigid-rigid, rigid-flexible and flexible-flexible) together with its different methods of implementation (mainly Monte Carlo, Genetic Algorism and Ant Colony Optimization) are analyzed side-by-side with other techniques like full complex optimization, quantum mechanics polarized ligand docking and fragment molecular orbital. The use and meaning of evaluation functions (score functions) is discussed together with the software where they are implemented and their possible relationship with experimental variables. The second part of the talk is dedicated to different methods used to generate new ligands with better interaction (binding) energy to specific targets. Such techniques include fragment based drug design and de novo design. These techniques generate libraries with thousands of molecules that should be filtered using criteria like the Tanimoto coefficient of similarity together with ADME (adsorption, distribution, metabolism, excretion) descriptors in order to obtain better drug candidates.

## Biography

Ihosvany Camps has completed his Bachelor degree in Physics from the Faculty of Physics, University of Havana (Cuba, 1995), Master degree in Physics from the Faculty of Physics, University of Havana (Cuba, 1996) and PhD in Physics from the Institute of Physics, Federal Fluminense University (Brazil, 2001). He has experience in Condensed Matter Physics and Computational Modeling. Currently, his research is on the study of electronic properties of nanostructures and the molecular modeling of organic and inorganic systems including the modeling of drugs (rational drug design, fragment-based drug design and de novo design), molecular docking and studies on polymorphism of pharmaceutical solids.

icamps@unifal-mg.edu.br

Notes: