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# *Integrated high throughput virtual screening tools*

In this talk, we present a range of tools developed in the Najmanovich Research Group (NRG) for an integrated high throughput virtual screening approach. Among these: 1. ENCoM, a sequence-specific normal-modes-based method for the simulation of large-scale movements in proteins used to generate conformational ensembles, and 2. FlexAID, a genetic-algorithm-based docking method with ligand and side-chain flexibility. We demonstrate these tools in the ligand-biased modelling of GPCRs and the virtual screening of peptidic inhibitors against Matriptase. We will present additional tools developed or implemented in our group integrating systems biology approaches for the determination of essential targets and the analysis of binding-site similarities for the detection of potential cross-reactivity targets. Such tools allow us to approach virtual screening in an integrated way from genomes to molecules.

**Rafael Najmanovich** graduated in 1994 with a degree in molecular sciences from the University of Sao Paolo in Brazil. He then obtained a Masters degree in statistical physics with Professor Vera Bohomoletz Henriquez at the same University. In 2003, he obtained his PhD in physics and biology from the Weizmann Institute of Science in Israel with professors Meir Edelman (biology) and Eytan Domany (physics), on side chain flexibility upon ligand binding. He then pursued postdoctoral studies with Janet Thorton at the European Bioinformatics Institute (EMBL-EMI) in Cambridge. He was hired in 2009 as an assistant professor in the biochemistry department at the Université de Sherbrooke. His research group is focused on molecular recognition, particularly between small molecules and biological macromolecules, combining computational structural biology, systems biology, chemoinformatics and experimental molecular biophysics techniques.