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An integrated approach to virtual screening: From genomes to molecules

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In this talk we how the five axes of research in the Najmanovich Research Group (NRG) are integrated within a rational drug design approach to the detection of novel modulators of the function of biological macromolecules. Starting from the utilization of systems biology methods for the detection of essential targets, the utilization of ENCoM, a sequence-specific normal-modes-based method for the simulation of large-scale movements in proteins used to study dynamic aspects of protein function, predict the effect of mutations and generate conformational ensembles. The use of FlexAID, a genetic-algorithm-based docking method with ligand and side-chain flexibility. The detection of molecular similarities with IsoCleft and IsoMIF for the identification of potential cross-reactivity targets (or their exploitation in polypharmacology). We demonstrate these tools in the ligand-biased modelling of GPCRs and the virtual screening of peptidic inhibitors against Matriptase and screening against essential C. difficile targets. Such tools allow us to approach virtual screening in an integrated way from genomes to molecules.

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