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New in silico descriptors for correlations with biological endpoints and drug design principles.

The Computer-Aided Drug Discovery (CADD) group has a strong focus on utilizing the vast Novartis knowledgebase to extract relationships between properties of molecules and their biological activity, and on developing approaches to make predictions based on those relationships using properties calculated from chemical structure (in silico descriptors). We work closely with experimentalists to design the compound sets for measurements of biological and physical properties in an effort to drive drug discovery and determine which molecular properties we can calculate that are predictive of the experimental properties. Two molecular properties that are not well described by the in silico descriptors commonly used in drug discovery are conformational flexibility and hydrogen-bonding strength. These properties play an important role in many biological activities, including various aspects of permeability (entry into mammalian cells, entry into gram-negative pathogens, blood-brain-barrier penetration, and passage across epithelial barriers). In order to better guide chemistry designs in drug discovery, we need better in silico descriptors to capture flexibility and hydrogen bonding strength. Our platform brings together computational, medicinal, and analytical chemistry, with the scientists that measure the relevant physicochemical and biological properties. This environment of experts, software, instruments, and data is particularly suited to develop new approaches for predicting these properties, including creating experimental datasets, and developing and evaluating new in silico descriptors. Applications of such descriptors include selection efforts (archive enhancement, library design, screening set design) as well as prospective chemistry designs during optimization.

Selected Publications

Profile-QSAR: A novel meta-QSAR method that combines activities across the kinase family to accurately

predict affinity, selectivity, and cellular activity.
Martin E, Mukherjee P, Sullivan D, Jansen J
J. Chem. Inf. Model. 2011 Aug 22;51(8):1942-56.

Target-biased scoring approaches and expert systems in structure-based virtual screening.
Jansen JM, Martin EJ
Curr Opin Chem Biol. 2004 Aug;8(4):359-64.

Click here for additional publications.

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List of links present in page

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