Life Science Informatics in Bonn

- Research in our group mostly focuses on the development of computational methods for pharmaceutical research and chemical biology and on large-scale compound data mining.

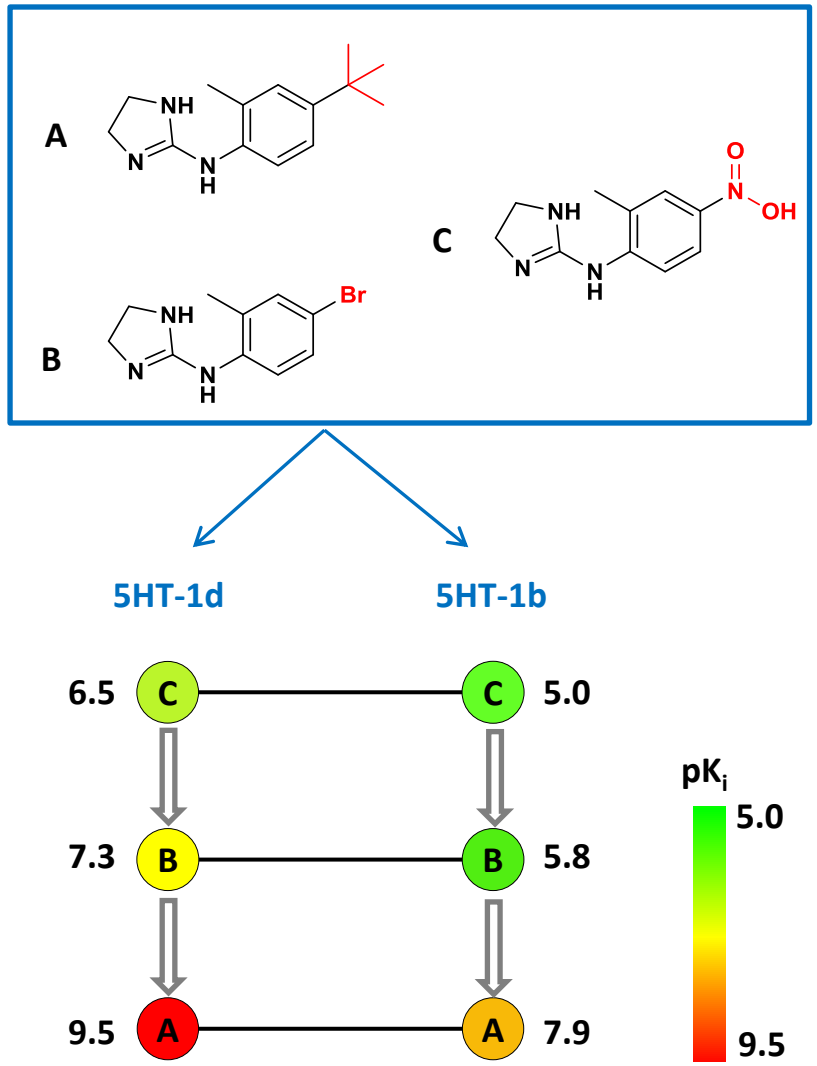
- Among others, these include topics like:

  - **Structure-activity relationship (SAR)**
  - **Activity cliffs**
  - **Machine learning & virtual screening**
  - **Data mining & compound activity analysis**
  - **Compound promiscuity**

http://www.limes-institut-bonn.de/forschung/arbeitsgruppen/unit-4/abteilung-bajorath/abt-bajorath-startseite/

Structure-Activity Relationship (SAR)

SAR visualization methods and graphical analysis tools have been developed that view local or global SAR characteristics of compound sets and extract SAR information from (heterogeneous) compound activity data.

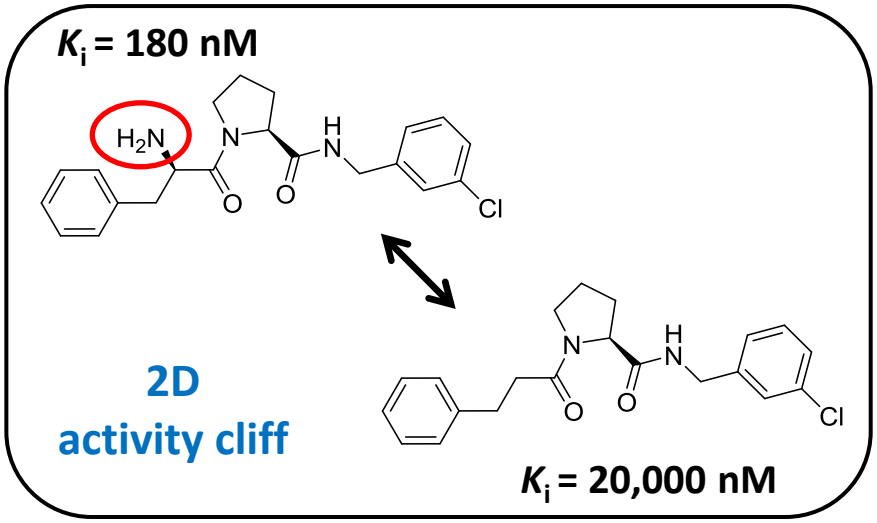


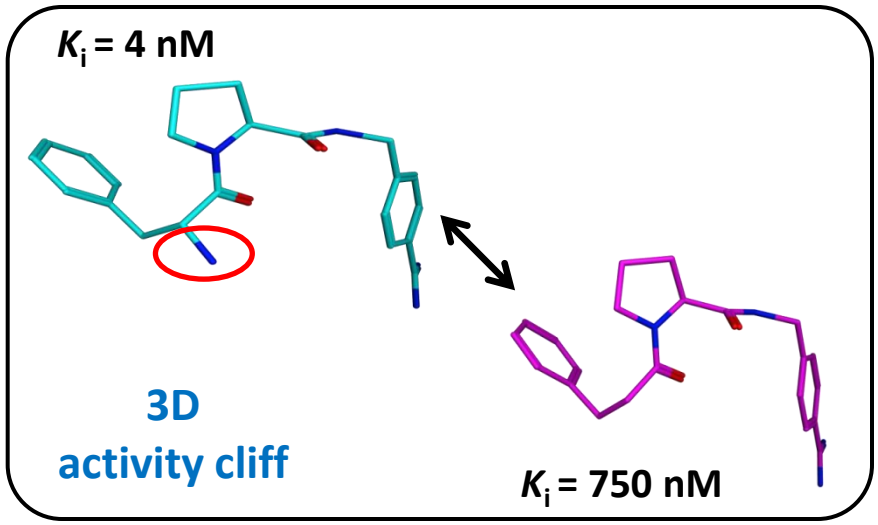
Series-based SAR transfer

Activity Cliffs

The study of activity cliffs is of prime interest because they reveal small chemical changes leading to large potency alterations.

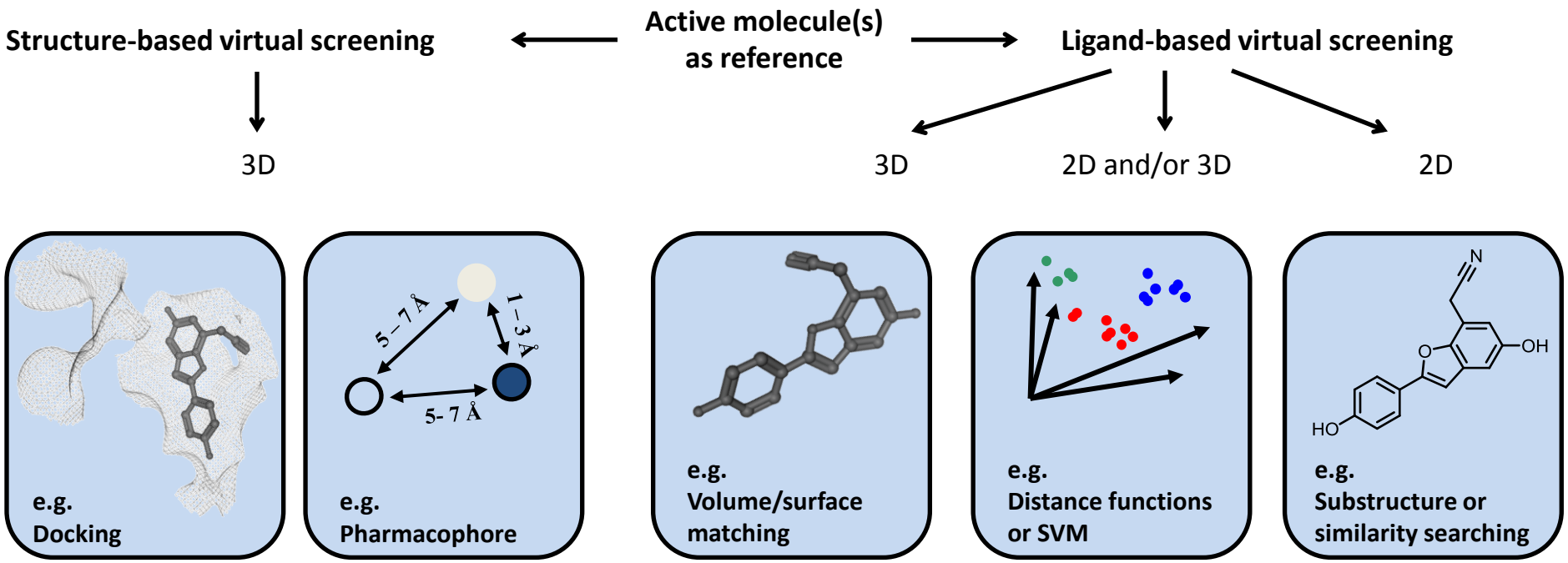
Research efforts in our group focus on the systematic identification and characterization of activity cliffs and their utilization in medicinal chemistry.





Machine Learning & Virtual Screening

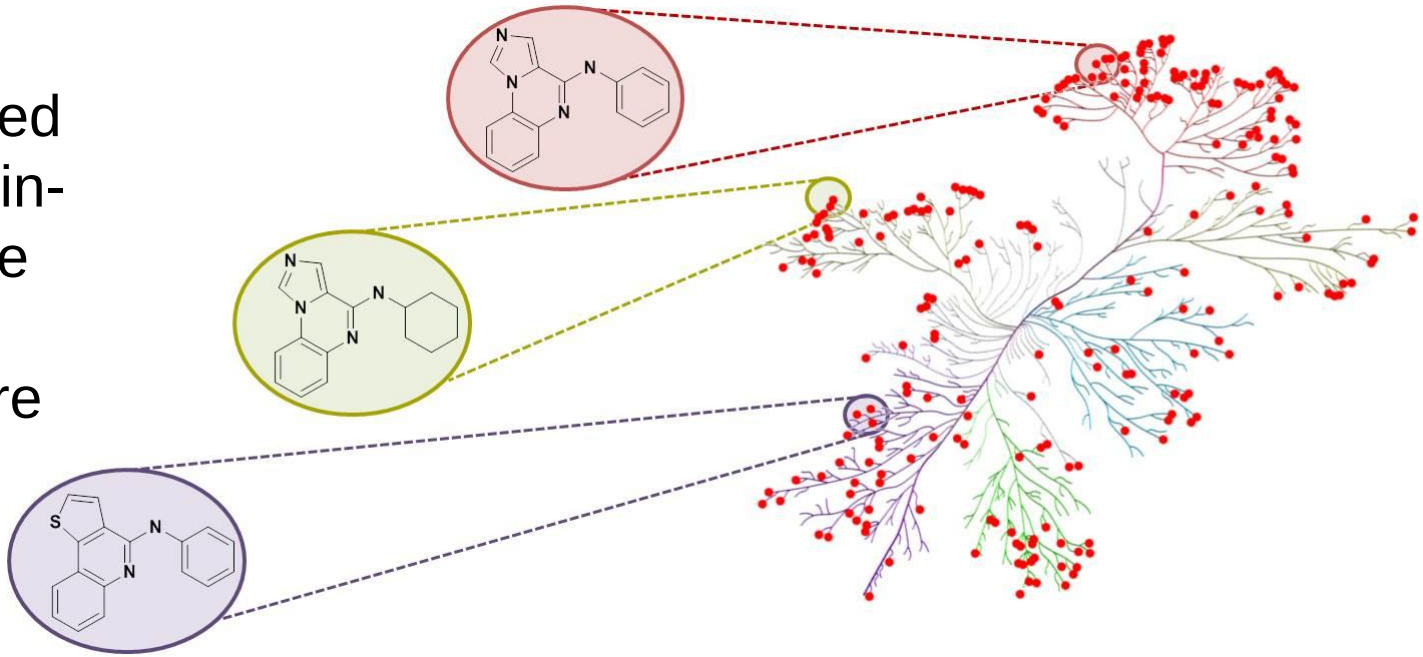
Structure- and ligand-based virtual screening refers to the process of computationally filtering large compound databases for ligands with desired properties.



Data Mining & Compound Activity Analysis

Only minor fractions of theoretically possible vast chemical space are currently accessible including small segments of biologically relevant chemical space populated with active compounds.

A variety of carefully curated data sets and in-house software tools for such applications are made publicly available.



Scaffold universe of kinase inhibitors

Compound Promiscuity

Compound promiscuity and polypharmacology are much discussed topics in pharmaceutical research.

Computationally, promiscuity degree (PD) can be estimated by mining of compound activity data and systematic promiscuity surveys (e.g. over time) can be monitored.