CHEMOINFORMATICS MEETS SYNTHETIC MEDICINAL CHEMISTRY

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At present, great amount of chemical information is accumulated in synthetic organic chemistry. They can be utilized for creation of computational tools assisting in synthesis planning, analysis and search of relevant information about chemical reactions. Practical utility and accuracy of such tools depends on two factors: data quality and effectiveness of underlying data mining approaches. The goal of presentation is to share experience and advancements achieved in our research group in development of computational tools relevant for synthetic medicinal chemistry.

The core of our technology is approach of Condensed Graph of Reaction (CGR) that fully encodes information about reaction transformation, can be used to depict reaction centers, and to represent reactions with the set of descriptors. We will show its application in reaction data curation, visualization, modeling reaction properties and conditions, visualization and analysis. Also, we show how combination of CGR can be used for discovery of novel chemical reactions. In the end, we'll show how computer-aided synthesis design can be combined with drug design to generate set of active compounds together with their synthesis strategy.

Reaction substructural and similarity searching

Analysis and visualisation of reaction data

Predictive models for optimal reaction conditions

Reaction data curation

- Incomplete reactions
- Atom-to-Atom Mapping

Reactions classification

Predictive models for kinetic and thermodynamic properties (rate constants, yield, reaction heats ...)