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Global Discovery Chemistry

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Research at the interface between Computer-Aided Drug Discovery (CADD), Cheminformatics and Research Informatics is an exciting field and has become important in drug discovery. We help project teams to use the right data at the right time to take the best decisions to optimize small molecule compounds against multiple objectives. Over the course of a discovery project, a multitude of decisions are taken for each compound synthesized, thus describing how compound series are optimized. Typically, decisions are taken based on a complex underlying data structure known to the various scientists on the team and hence evolvement of a chemical series reflects this data implicitly. Understanding fully which decisions are taken when and under what circumstances is usually restricted to the team members. Transferring that knowledge between teams and over time can be a bottleneck in pharmaceutical research.

Our cross-departmental and scientific group structure of experts from different fields is set up to find novel methods to automatically extract, analyze, and understand that information from historical data. Leveraging on recent advances in the fields of machine learning and

behavioral analysis the derivation of those decision patterns taking into account biological (assay data) as well as chemical (reactions, building blocks) information has become a true possibility

Selected Publications

Chemical topic modeling: Exploring molecular datasets using a common text-mining approach [2].
Schneider N, Fechner N, Landrum GA, Stiefl N.
J Chem Inf Model. 2017 Aug; 57(8):1816-1831.

What's What: The (Nearly) Definitive Guide to Reaction Role Assignment. [3]
Schneider N, Stiefl N, Landrum GA.
J Chem Inf Model. 2016 Dec; 56(12):2336-2346.

Heterogeneous classifier fusion for ligand-based virtual screening: or, how decision making by committee can be a good thing. [4]
Riniker S, Fechner N, Landrum GA.
J Chem Inf Model. 2013 Nov; 53(11):2829-36.

Click here [5] for additional publications - Nikolaus Stiefl, PhD.

Click here [6] for additional publications - Nikolas Fechner, PhD.

Links
[1] https://www.novartis.com/our-science/postdoc-program/research-themes/chemistry/nikolaus-stiefl-phd
[2] https://www.ncbi.nlm.nih.gov/pubmed/28715190
[3] https://www.ncbi.nlm.nih.gov/pubmed/28024398
[4] https://www.ncbi.nlm.nih.gov/pubmed/24171408
[5] https://www.ncbi.nlm.nih.gov/pubmed/?term=stiefl%2C+nikolaus
[6] https://www.ncbi.nlm.nih.gov/pubmed/?term=fechner%2C+nikolas