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The introduction of high-throughput experimental technology over the last decades has led to a massive increase in volume of compound-activity pharmacological data. High throughput experiments are however costly and their impact on R&D productivity has often not met the initial expectations. In recent years, advances in the field of machine learning technologies and artificial intelligence suggest that these new approaches might transform how we discover new drugs driven by the data pharmaceutical industry has collected.

Machine-learning models trained on large volume of structure-activity data are consistently improving. Such models allow us become more efficient in the selection and prioritization of small molecules for chemical synthesis and biological testing, and will therefore contribute to the reduction of drug discovery costs. It has been shown recently that multi-task models trained to predict many biological activity outcomes at the same time bring a performance advantage compare to single task models.

With this new finding, Novartis has joined the MELLODDY consortium within EU's IMI initiative

aiming at the federation of the preclinical pharmacology data of ten pharmaceutical companies for machine learning in a privacy preserving way. This project will change how pharma currently trains their machine learning model by leveraging not only data resulting from conventional dose response assays, but also adding other experimental results linked to small molecules such as high-throughput screening data and high-content cellular imaging data. This cross - departmental and cross-company project offers the opportunity to work within a large team of scientists with cutting-edge expertise on structure-activity modelling.

Selected Publications

Identification of SPPL2a Inhibitors by Multiparametric Analysis of a High-Content Ultra-High-Throughput Screen. [2]
Zhang X, Götte M, Ibig-Rehm Y, Schuffenhauer A, Kamke M, Beisner D, Guerini D, Siebert D, Bonamy GMC, Gabriel D, Bodendorf U.
SLAS Discov. 2017 Jul; 22(9): 1106–1119.

Latent hit series hidden in high-throughput screening data. [3]
Varin T, Didiot MC, Parker CN, Schuffenhauer A.
J Med Chem. 2012 Feb 9;55(3):1161-70.

The scaffold tree--visualization of the scaffold universe by hierarchical scaffold classification. [4]
Schuffenhauer A, Ertl P, Roggo S, Wetzel S, Koch MA, Waldmann H.
J Chem Inf Model. 2007 Jan-Feb;47(1):47-58.

Click here [5] for additional publications.

Links
[1] https://www.novartis.com/our-science/postdoc-program/research-themes/computational-sciences/ansgar-schuffenhauer-phd
[2] https://www.ncbi.nlm.nih.gov/pubmed/28731783
[3] https://www.ncbi.nlm.nih.gov/pubmed/22185196
[4] https://www.ncbi.nlm.nih.gov/pubmed/17238248
[5] https://www.ncbi.nlm.nih.gov/pubmed/?term=ansgar%20schuffenhauer%5Bau%5D