Multicriteria Decision Analysis and Optimization for Computational Chemistry and Drug Discovery

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In the tutorial we will provide an overview on methods from multicriteria decision analysis and optimization in the field of drug discovery.
Nowadays, data mining methods and machine learning are used to predict the properties of drugs. Multicriteria decision analysis can help to make use of these predictions in order to answer questions such as: What are the most promising compounds to select from a library for testing? How can we search the large chemical space for novel drug compounds? How can we assess the reliability of predictions with respect to various types of errors?
The first part of the tutorial will discuss common evaluation criteria in drug discovery, problem formulations, and contemporary optimisation and decision analysis methods. A focus will be on evolutionary multicriteria algorithms.
In the second part of the tutorial we will discuss the problem of experimental design in drug discovery in more detail, highlighting a new approach based on portfolio theory. In this scenario a set of molecules has to be selected for testing in vitro. Compound databases of vendors are typically large and only few molecules can be selected for testing. Such selection is partly based on the predicted quality of the selected molecules, but not only: In addition, the diversity of the selected set of molecules should be taken into account in order to mitigate the risk of failure of the selected set as a whole. The resulting mathematical programming models can also consider limited budget and other constraints, e.g. cardinality of the selected set.