Computational Molecular Design in Medicinal Chemistry

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The lead optimization phase of a small-molecule drug discovery program is a classical multi-parameter optimization. Up to 20 different properties need to be balanced to achieve an optimal profile of a candidate before entering clinical trials. The goal of computational molecular design is to make use of modern computational tools, ranging from molecular simulation to machine learning, to reduce the number of design cycles needed for the identification of a new drug candidate. The presentation will give an overview over optimization goals and how molecular properties can be predicted using a variety of different technologies.