Enabling Drug Discovery with an Integrated Computational Approach. A Case Study in Schrödinger's Molecular Design Platform

T. Knehans[1]

[1]Schrödinger GmbH, Thierschstraße 27, 80538 München, Germany

In structure-based small molecule drug discovery a central challenge, once a protein target has been determined, is to design compounds that bind to the target with sufficient potency and specificity. Furthermore, molecules need to exhibit the right physico-chemical and ADMET property profile to become a drug candidate. Computational chemistry methods have always been an important component in this difficult endeavor and their contribution has increased dramatically over the last years.

The Schrödinger drug discovery platform integrates solutions for predictive modeling, machine learning, data analytics, and collaboration to enable more rapid discovery of such multi-parameter optimal novel chemical matter. Multiple examples of enterprise-wide deployment of these technologies have been demonstrated to increase the probability of success and shorten the length of time required for preclinical drug discovery.

In this presentation, we will examine a case study highlighting the different ways the Schrödinger Technology Platform may be utilized in a discovery project. We will follow the development of a previously described ACC inhibitor and show how predictive methods can help in targeted water displacement in binding sites to drive potency, enumerate compound analogues to optimize physico-chemical properties or address chemical stability issues.

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