Lecture Title:

Schrödinger's Computational Molecular Design Platform

Speaker:
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Abstract: The Schrödinger molecular design platform integrates solutions for physics-based modeling, data analytics, and collaboration together with AI/machine learning methods, to enable more rapid discovery of multi-parameter optimal new molecules. Multiple examples of enterprise-wide deployment of these technologies have been demonstrated to increase the success for e.g. preclinical drug discovery. Here we will summarize the novel computational methods combined in the Schrödinger Technology Platform.

We have previously demonstrated a large-scale exploration of chemical space in the hit-to-lead process by coupling reaction-based enumeration, active learning and free energy calculations. We examine the utility of this combined workflow on an example from Schrodinger's internal drug discovery projects and demonstrate that a complete workflow can advance drug design projects faster than a traditional approach. The reported data suggest combining human expertise and machine learning enhanced simulations enables the rapid discovery of novel chemical matter within a predefined potency and property space.

About the speaker: Thomas Steinbrecher studied Chemistry at the University of Freiburg in Germany and earned a diploma with distinction in Physical Chemistry. He completed a Ph.D. thesis on “Computer Simulations of Protein-Ligand Interactions” in 2005.

He joined the developer team of the Amber MD package as a Postdoc at the Scripps Research Institute in San Diego and Rutgers University in New Jersey. The work focus was on efficient free energy calculation methods and QM/MM simulations of charge transfer.

After returning to Germany in 2008, Thomas established a junior research group at the Karlsruhe Institute of Technology, working on fast electron transfer phenomena in DNA and proteins.

He joined Schrodinger in 2013 where he was responsible for the large-scale application of free energy calculation methods in pharmaceutical drug design. Since 2017, he heads the Applications Science Department for Europe and supports customers in employing Schrödinger’s Drug Discovery Technology Platform for their research.