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Contribution ID: **158** Type: **Workshop/BoF proposal**

Introduction to Schrödinger's drug discovery tools

Sunday, 3 December 2017 09:00 (8 hours)

Schrödinger is a leading provider of scientific software in the drug design industry. The workshop will give an overview of the drug discovery tools available from Schrödinger. Participants will be introduced to our new graphical interface, Maestro 11, and will work through hands-on examples for tasks like docking, pharmacophore based virtual screening and building homology models. The workshop will also touch on recent improvements on FEP+, our framework to run MD based free energy calculations. It will conclude with a general Q&A session were participants can discuss their own scientific projects.
A trial version of our software will be available to participants prior to the workshop. Please bring your own laptop!

HPC content

Modern computational drug discovery can help speed up the drug design process with the help of tools like GPGPU based molecular dynamics simulations or high throughput virtual screening with traditional CPUs. Since the chemical space that has to be covered can be very large, extensive use of computational resources can often help speed up projects and increase prediction accuracy.
The workshop will give an overview over the tools that are available from Schrödinger, and provide hand-on experience to the participants.

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Session Classification: Sunday Workshop: Introduction to Schrödinger's drug discovery tools

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