Universität Hamburg
Bioinformatik Seminar

Donnerstag: 24.01.19 16:00 s.t.

Zentrum für Bioinformatik, Bundesstraße 43, Raum 16

Accelerated MD and QM to explore conformational preferences and molecular interactions

An application of accelerated molecular dynamics simulations to probe conformational preferences of small molecules and macrocycles is demonstrated along with an exploration of preferred pi-stacking geometries based on large-scale quantum-mechanical calculations.

Dr. Julian Fuchs
Boehringer-Ingelheim
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Everyone is welcome!