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5th International Conference on

Medicinal Chemistry &
Computer Aided Drug Designing and Drug Delivery

December 05-07, 2016   Phoenix, USA

Virtual flow: A flexible workflow system for virtual screening procedures on high-performance computers

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A vast arsenal of computational tools has been developed in the past which are useful for virtual screening, from the preparation of ligand databases to the postprocessing of the screening results. At the same time computer clusters such as high-performance computers or supercomputers became more and more available, which employ distributed resource management systems (batch systems) in order to handle and organize the jobs of the users. In order to be able to carry out large-scale virtual screening procedures in a fully automated fashion on computer clusters which are managed by a batch system we have developed VirtualFlow, a workflow system for virtual screening related tasks. Its features are: Scaling without limits with respect to the CPUs with essentially no overhead, monitoring and controlling of the workflow during the runtime and automatic compression /decompression/ archieving of the input and ouput files. The VirtualFlow framework has been implemented in two applications. The first one, VFLP (VirtualFlow for Ligand Preparation), is specialized on the preparation of ligand databases, taking SMILES as input and converting them into ready-to-dock molecules in any desired target format. The second implementation, VFVS (VirtualFlow for Virtual Screening), is specialized on the virtual screening procedure itself. VFLP and VFVS can be seamlessly joined to carry out virtual screenings on the largest scales.

Biography

Christoph Gorgulla has completed a BSc in Molecular Biology with Bioinformatics, as well as a BSc and MSc in Mathematics at the Free University of Berlin and the Berlin Mathematical School. Currently, he is a PhD candidate at the Int'l Max Planck Research School for Computational Biology and Scientific Computing of the Max Planck Institute for Molecular Genetics, the Berlin Mathematical School and the Free University of Berlin, and holds a Doctoral fellowship of the Einstein Center for Mathematics Berlin (ECMath).

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Med chem
ISSN: 2161-0444 Med chem, an open access journal

MedChem & CADD 2016
December 05-07, 2016

Volume 6, Issue 10(Suppl)

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