

DrugScreener-G: an Integrated Environment for Grid-enabled Large-Scale Virtual Screening with Tools for Computer-Aided Drug Design and Modeling

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DrugScreener-G is an integrated environment for virtual screening with Grid computing. It implements basic ideas of Grid-enabled large-scale virtual screening into a concrete software suite, especially emphasizing user friendliness and accessibility to Grid computing. DrugScreener-G aims at providing users without knowledge of Grid computing with an intuitive and easy-to-use integrated environment for Grid-enabled large-scale virtual screening. We discuss architecture and design of DrugScreener-G in two aspects, extension and integration of different functions and virtual screening methods with plug-ins and application repository, and virtualization of Grid computing services under web service. DrugScreener-G is easily extensible with new virtual screening methods as it is developed in plug-in architecture. DrugScreener-G virtualizes different Grid computing services behind web service interface to hide technical details of grid computing from users and to provide interoperability among different types of Grid computing resources and middleware. It is also discussed how application-level interoperability in DrugScreener-G can be a simple and effective alternative to the recent approaches to Grid interoperability, such as SAGA and GIN, which are not yet agreed standards on Grid interoperability.