

Application Name	Virtual Screening
Application Area	Computational Chemistry
Keywords	Virtual screening, molecular docking, computational chemistry, molecular design
Project/Dept. Affiliation	Georgia State University Chemistry Department
Value of grids to this application	This application needs millions of runs to dock a chemical database (about 1.5 million molecules). Only grids can provide enough computational resources to do such a timely calculation.
Originating institution	Georgia State University
Contact (s) Name, Email	Minyong Li, mli@gsu.edu Dr. Binghe Wang, wang@gsu.edu
Participating sites	Georgia State University, Kennesaw State University and others (available Linux cluster resources)
General description	<p>Virtual screening is a computational technique used in drug design research. To shorten the time-consuming drug design & discovery procedure, in the current project, millions of molecules will be docked into the receptor for the evaluation of receptor-based potency by molecular docking program DOCK 6.1. For more details, please refer to the following literatures:</p> <ol style="list-style-type: none"> 1. D.B. Kitchen, H. Decornez, J.R. Furr and J. Bajorath, <i>Docking and scoring in virtual screening for drug discovery: methods and applications</i>. Nat Rev Drug Discov, 2004. 3(11): p. 935-49. 2. B.K. Shoichet, <i>Virtual screening of chemical libraries</i>. Nature, 2004. 432(7019): p. 862-5.
Anticipated system requirements for SURAGrid nodes running this application	Any system having MPICH to run parallel applications and minimum 1GB of memory, Estimated Disk space required -: 10 GB
Anticipated non-system requirements for SURAGrid nodes running this application	DOCK 6.0, MPI (MPICH-1/2)
Grid focus (data sharing, computation, access to unique resources, collaboration)	Computation; Access to resources not present at Georgia State University
Network dependencies (bandwidth, latency, multicast, other)	Simple connection is sufficient.
Expected frequency of application run (one-time, occasional, monthly, weekly, daily...)	Daily/Weekly.
Estimated start date for application run	At the earliest.
Describe expected application invocation mechanism (by user submitting job, programmatically by	User submits MPI job via the SURAGrid portal.

SURAgid Application Description

some event or timing...)	
Is this application open to others to use with their own data or revisions?	Dock is available software for others who could use it for their own data and analysis if they wanted.
Additional comments	It is expected that this will be a long term capability and available via the SURAgid portal.