ER-flow Application Description Template

Application Name: AutoDock Vina

Application domain: Medical Biochemistry

Brief description of application
AutoDock Vina is a toolbox to perform virtual screening experiments. It finds the preferred orientation of one molecule in respect to another considering a large set of binding affinities. Virtual screens of large databases are used as a starting point to identify small molecules that can interact with proteins and modulate activity in drug design. Potential targets are further evaluated using conventional biochemical assays.

Data:
input data format: PDBQT
output data format: csv, PDBQT
sample data: http://shiwa-repo.cpc.wmin.ac.uk/shiwa-repo/download?appid=4256&filename=Generator_input-ligands.zip
application http://vina.scripps.edu/
documentation http://vina.scripps.edu/tutorial.html
publication O. Trott, A. J. Olson, AutoDock Vina: improving the speed and accuracy of docking with a new scoring function, efficient optimization and multithreading, *Journal of Computational Chemistry 31 (2010) 455-461*

Execution environment
middleware: gLite / EGI / vlemed VO workflow system: WS-PGRADE

Execution characteristics
data size (per unit, typical number of units):
input: 1KB, thousands output: 1KB, thousands
processing time (per unit): 300s
memory usage: n.a. disk usage: minimal

Target users
Scientists of the Medical Biochemistry department and their collaborators at the AMC http://www.amc.nl/web/Research/Departments/Overview/Medical-Biochemistry/Medical-Biochemistry/Department.htm

number of users: 1 direct user who provides support for many other researchers
user type: end-user

Usage scenario for workflow in the ER-FLOW
An Autodock VINA workflow already existed in the SHIWA repo for a desktop grid infrastructure. The scenario in ER-Flow was to re-use this existing workflow to facilitate porting this application to the AMC execution environment (EGI gLite infrastructure). The workflow can be executed from the SHIWA Portal, as well as from a customized interface of the AMC SCI-BUS science gateway (under construction).

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