



EXPERIENCES FROM SHARING AN AUTODOCK VINA WORKFLOW FOR VIRTUAL SCREENING USING THE SHIWA WORKFLOW REPOSITORY



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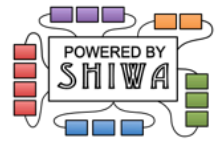
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ER-flow

See previous presentation by Kitti 😊

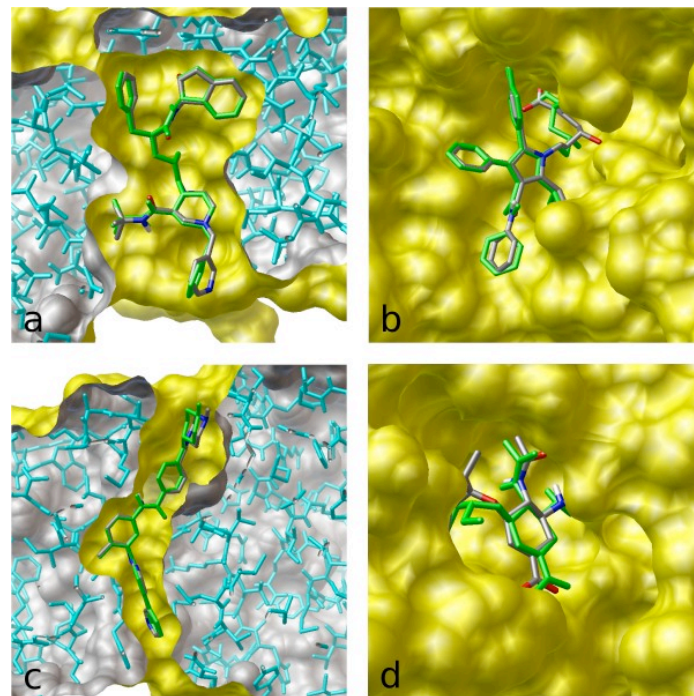
Application: Autodock Vina

- Purpose

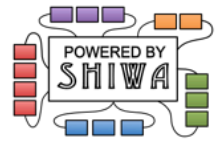
- Drug discovery
- Molecular docking
- Virtual screening

- Qualities

- Multi-core capabilities
- High performance
- Enhanced accuracy
- Ease of use



- Experiments demands large computing power



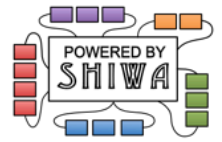
Vina @ Westminster

- Collaboration by researchers from School of Life Sciences and School of Electronics and Computer Science
- Composed workflow using the WS-PGRADE workflow system and science gateway framework
- Enabled the researchers to execute large scale virtual screening experiments from a high level science gateway interface



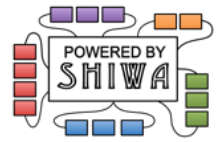
Vina @ AMC

- Scientists in the department of Medical Biochemistry also use Autodock Vina for virtual screening experiments
- Virtual screens of large databases are used as a starting point to identify small molecules that can interact with proteins and modulate activity
- Potential targets are further evaluated using conventional biochemical assays
- With the growth of databases, running their experiments on their local infrastructure became more and more challenging due to long computation times



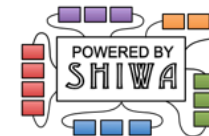
New collaboration

- Approached the e-BioScience team
- Experience with running Next Generation Sequencing and Medical Imaging applications on EGI through their e-BioInfra Gateway
- ER-flow and SCI-BUS partner



Westminster Workflow

- The workflow was originally supported to run on the BOINC-based local desktop grid
- Later ported to the public volunteer computing resources of EDGeS@home
- Published in the SHIWA Workflow Repository
 - Enabling other researchers to execute the workflow directly on the SHIWA Simulation Platform
 - **Allowing to download and customize the workflow according to their requirements.**



SHIWA Repository

Mark Santcroos [active]

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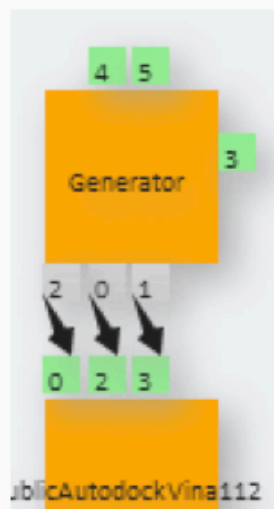
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Workflow: PublicAutoDockVina112 | Engine: WS-PGRADE(3.4.5) | Implementation version: 1.00

Graph



Implementation summary

Title: Public AutoDock Vina 1.1.2 - Virtual screening of a library of ligands

Workflow: [PublicAutoDockVina112](#)

Engine: WS-PGRADE(3.4.5)

Version: 1.00

Status: new

Language: WS-PGRADE

Licence: Apache License 2.0

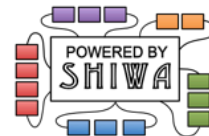
Definition: [workflow.xml](#)

Keywords: AutoDock, virtual screening, receptor, protein, ligand, molecule docking

Created: 06.11.12 0:00, **Modified:** 07.11.12 14:08

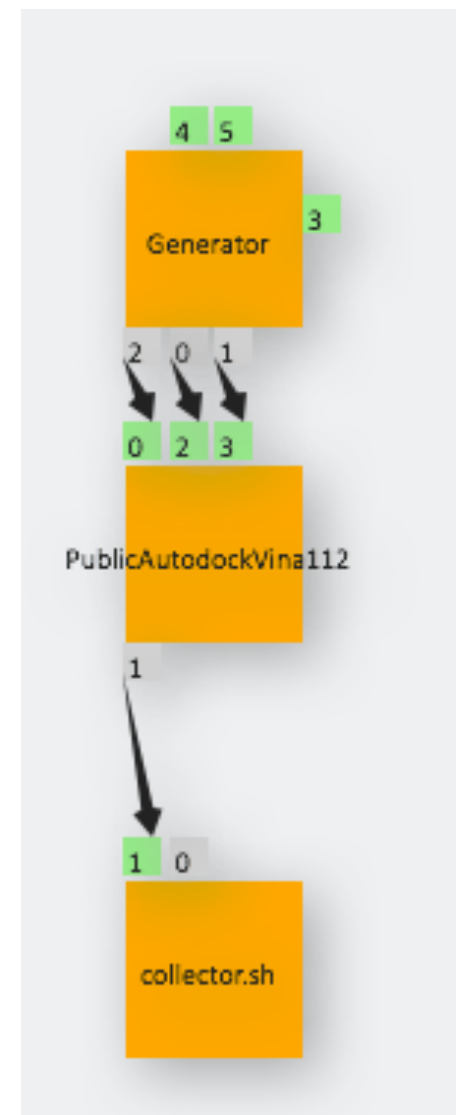
Description: This workflow performs virtual screening of molecules using version 1.1.2 of AutoDock Vina. It docks a library of small ligands on a selected receptor molecule. For further information, please download and contact the README file.

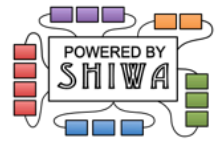




Workflow details

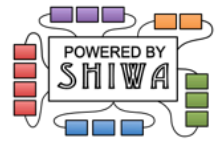
- Breaking up in work units to allow for parallelization
- Wrapper around binaries
- Merging the results and selecting the N best results





Implementation @ AMC

- Workflow was imported from the SHIWA Repository into the AMC portal
- Modified for the local usage scenario
 - PBS
 - gLite



Porting issues

- SHIWA Import vs “Download + Upload”
- Strong coupling to infrastructure (theory vs practice)
- “Missing” component reverse-engineering



The last mile





ER-Flow is supported by the FP7 INFRASTRUCTURES-2012-1 call under contract n°312579






End-user view WS-PGRADE



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[AMC e-BioInfra Gateway](#) > [WS-PGRADE Workflow Developers](#) > [End User](#) > [Configure](#)


End User





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Workflow name: autodock-fda_2013-04-04-141444


Note: 2013-4-4

Number of "best" results files to select. 

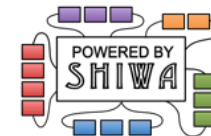
Ligands database.  fda.zip [Browse...](#)

Configuration file.  Nur77_MTX.txt [Browse...](#)

The receptor to dock against the ligands.  Nur77_3V3E_mono.pdbqt [Browse...](#)

Number of tasks to run in parallel. 

Message:



Customized Portlet (beta)

University of Westminster Desktop Grid Portal > Docking portlet

Specify the name of current task, use only letters or numbers.

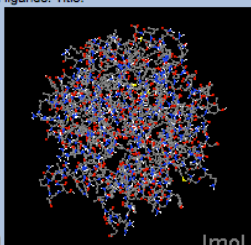
Run task

Task Name	Task Status	Actions	
Task1 2013-02-19-115644	FINISHED	Show results / refresh	Delete
Task2 2013-02-20-142957	FINISHED (0 error, 12 finished, 0 running)	Show results / refresh	Delete
fdarun1 2013-04-04-160631	ERROR	Show results / refresh	Delete

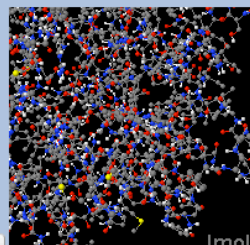
Results for task: Task2 2013-02-20-142957

Download best outputs Re-compute task

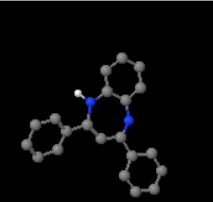
Receptor file, with docked ligands: Title:

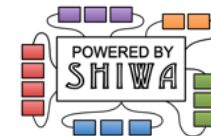


Receptor: Large view



Receptor with ligands: Large view

Ligand molecule title	Ligand molecule info	Ligand molecule image
Title:	Autodock Score:-6.2 [kcal/mol] Download Molecule	 <p>Large view</p>



Interactive view

013-02-20-142957

Jmol

Ligand molecule image

Large view

Jmol

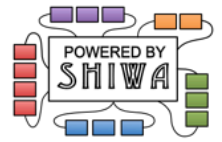
Download

Autodock Score: -6.0 [kcal/mol]

Download Molecule

script terminated





Conclusions

- Workflows for developing, describing, executing and sharing science works!
- Devil is in the details!
- Developers vs Users
- Generic vs Customized interface?

