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

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

ER-flow

See previous presentation by Kitti ☺

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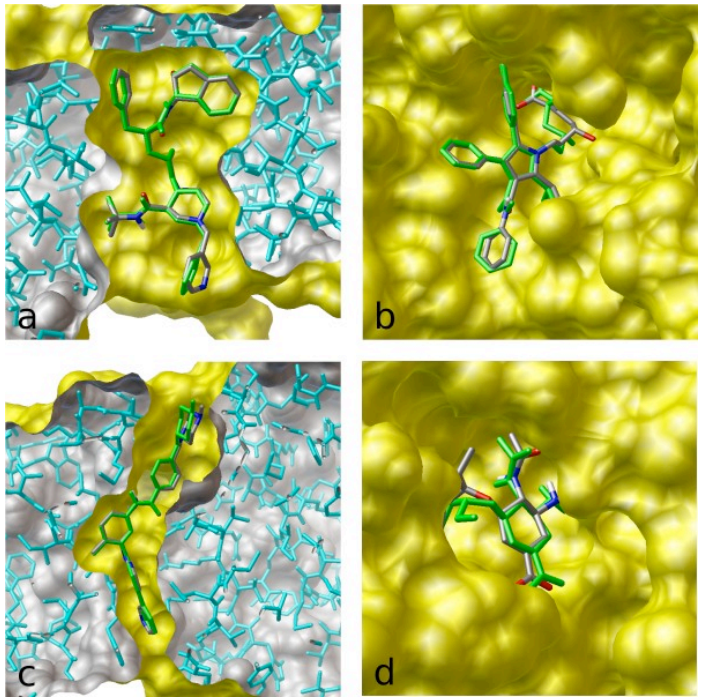
Application: Autodock Vina

- Purpose
  - Drug discovery
  - Molecular docking
  - Virtual screening



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

- Experiments demands large computing power

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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

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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

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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

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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.**

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SHIWA Repository

Mark Santcroos [active]

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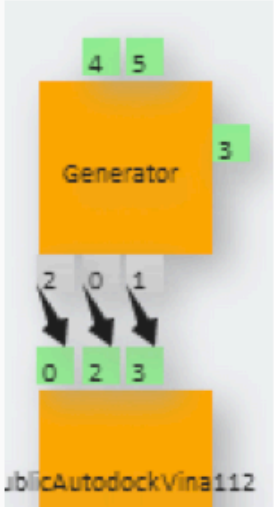
Workflow: PublicAutoDockVina112 | Engine: WS-PGRADE(3.4.5) | Implementation version: 1.00

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.

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Workflow details

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

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Implementation @ AMC

- Workflow was imported from the SHIWA Repository into the AMC portal

- Modified for the local usage scenario
  - PBS
  - gLite

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Porting issues

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

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The last mile

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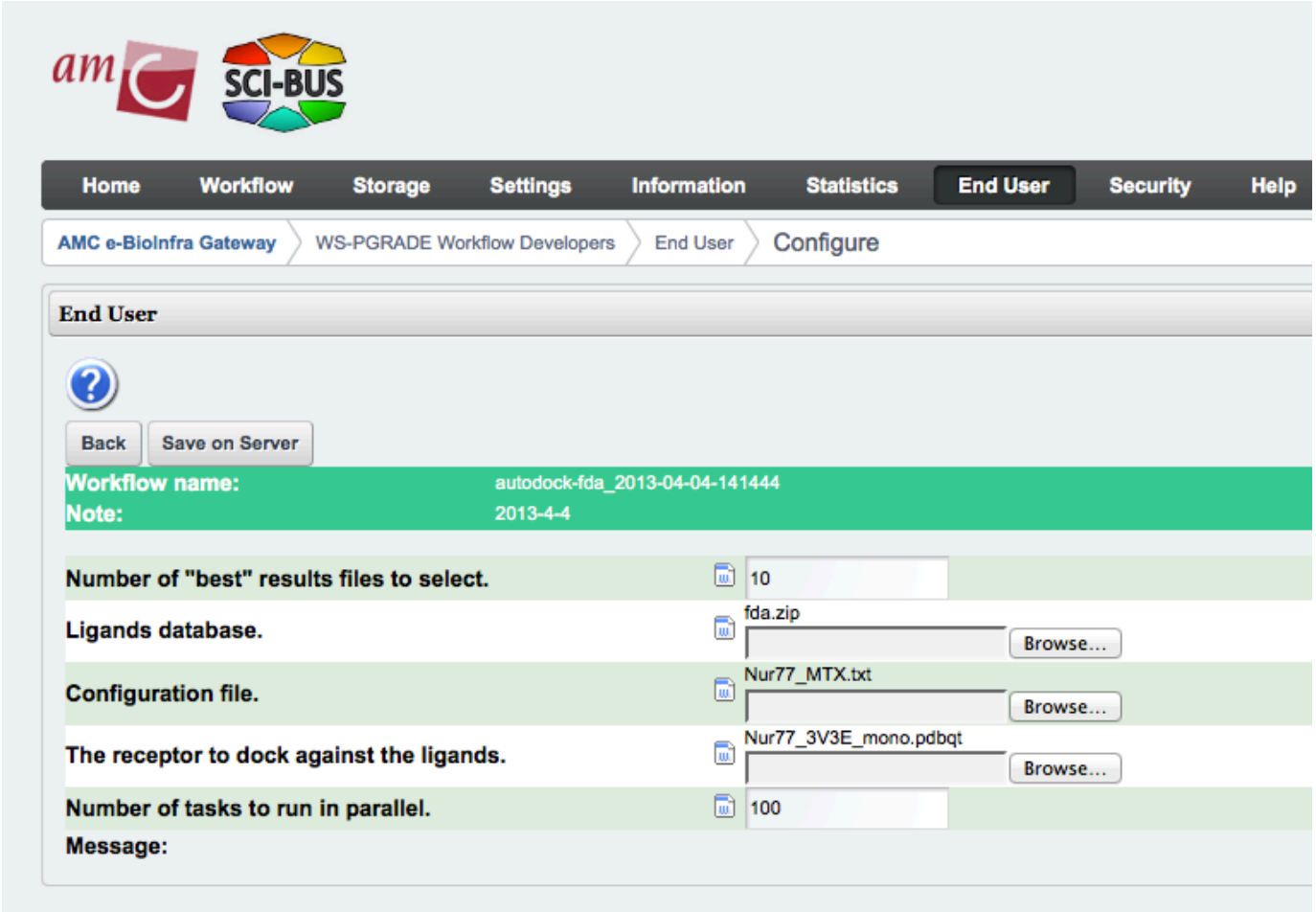
End-user view WS-PGRADE



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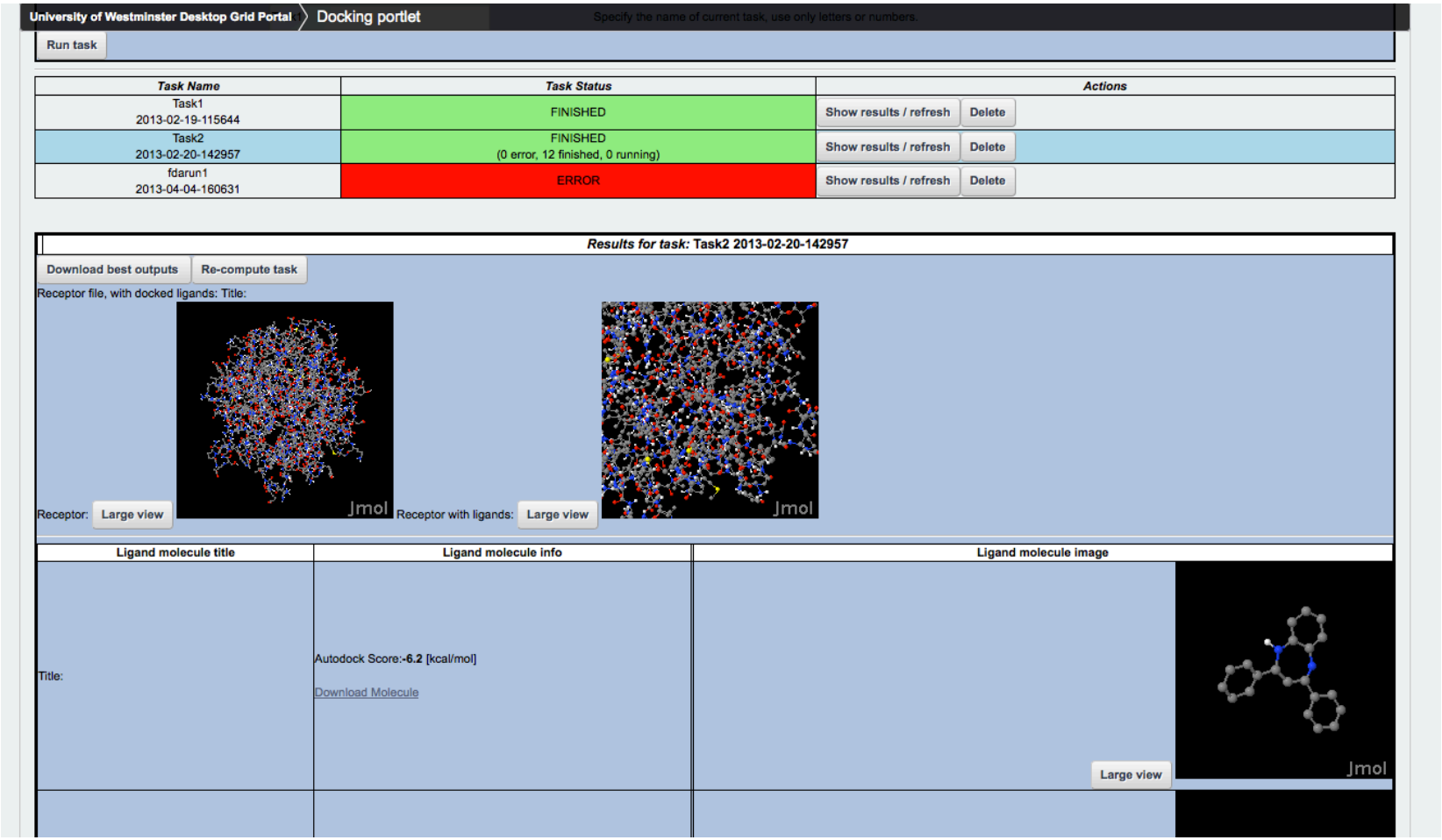
Customized Portlet (beta)



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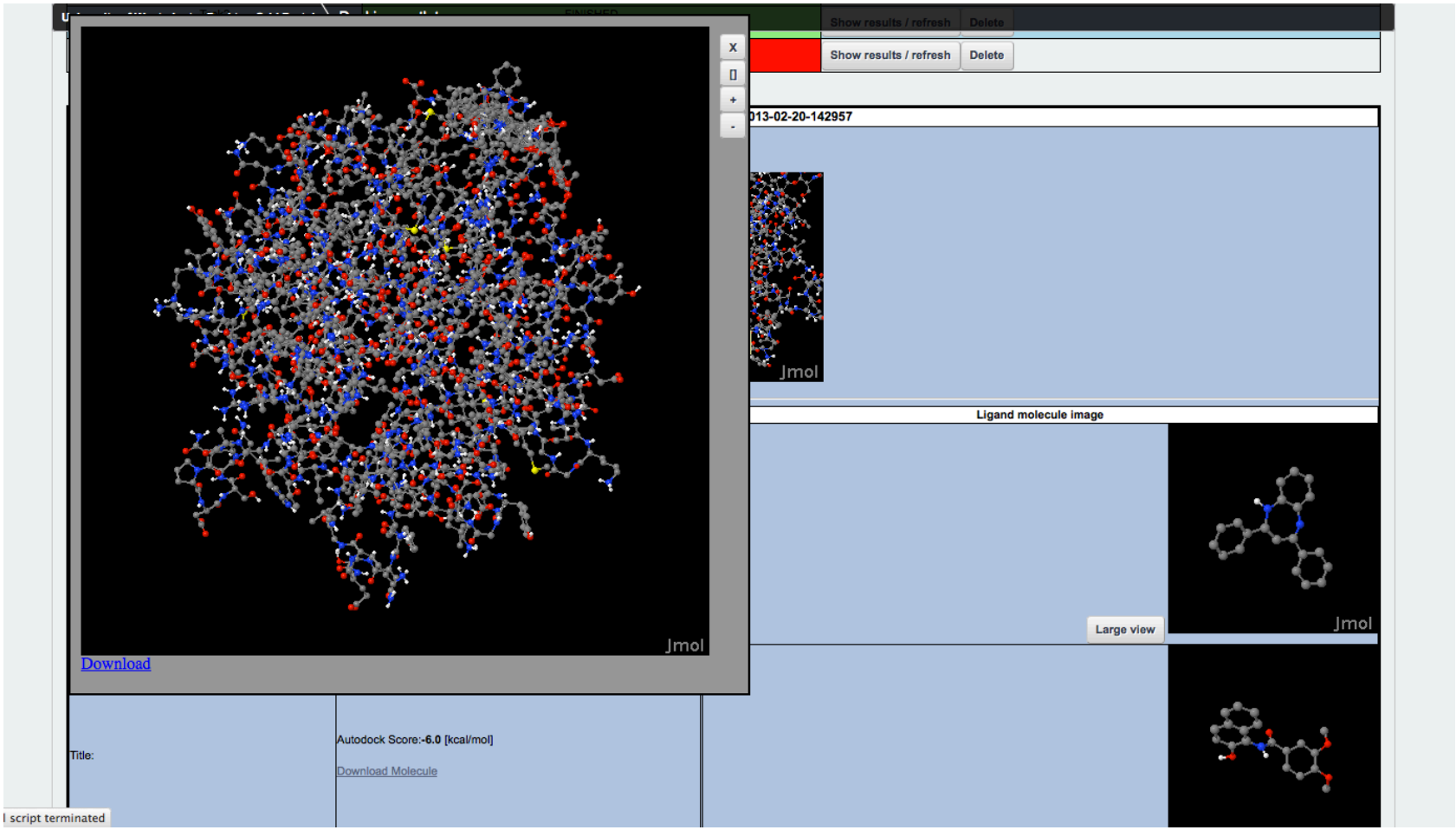
Interactive view



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Conclusions

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

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