

Grid-Enabled Virtual Screening Service Quick User Guide 1.0.1



**Academia Sinica Grid Computing
Centre**

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1. System Requirement

1.1. Windows

- Operating Systems
 - Windows 2000
 - Windows XP
 - Windows Vista
- Minimum Hardware
 - Pentium 4 2.4 GHz(Recommended: Intel Core 2 Duo or greater)
 - 1 GB RAM(Recommended: 2 GB or greater)
 - 100 MB hard drive space
- JRE 1.5 required

1.2. Mac

- Operating Systems
 - Mac OS X 10.3 and later
- Minimum Hardware
 - Macintosh computer with an Intel x86 or PowerPC G3, G4 or G5 processor
 - 512 MB RAM(Recommended: 1 GB RAM or greater)
 - 100 MB hard drive space
- JRE 1.5 required

1.3. Linux

- Operating Systems
 - Linux with X window environment
- Minimum Hardware
 - Pentium 4 2.4 GHz(Recommended: Intel Duo Core or greater)
 - 512 MB RAM(Recommended: 1 GB RAM or greater)
 - 100 MB hard drive space
- JRE 1.5 required

2. Before the Installation

2.1. Prepare your GRID Authority and environment

2.1.1. Certificate

2.1.1.1. Download the User Certificate Application Form

a. Download the User Certificate Application Form from

http://ca.grid.sinica.edu.tw/certificate/request/request_user_cert.html

b. Setup an interview with a local Registration Authority (RA)

You need to meet with a ASGCCA RA to verify your identity. Locate and contact your nearest RA: <http://ca.grid.sinica.edu.tw/contact.html>

Prepare the following documents for the your interview with the RA

c. Complete and submit your application form

2.1.1.2. Request for certificate online.

Before going through 2.1.1.2, make sure that you have finished 2.1.1.1 and a CA staff has confirmed with you.

Create a Certificate Signing Request(CSR) online on CA web page

(<http://ca.grid.sinica.edu.tw/certificate/request/nscert.php>). Please submit request on the computer that you want to store your public/private key.

2.1.2. Confirm the request.

ASGCCA will send a confirmation to your email address. Please click the url to confirm your application

2.1.3. Download and Import Your Certificate.

Once your certificate is issued, ASGC will publish it on the website and send out a email to inform you. You can simply download your certificate via the link provided in the e-mail and import it into your browser.

2.1.4. Export the Certificate

To use your certificate, you first need to export it from your browser. You can find the certificate export procedure here.

(http://ca.grid.sinica.edu.tw/certificate/request/certificate_management.html)

2.1.5. Convert certificate to pem format for the usage of GRID.

To use your certificate for Grid authentication, you need to convert your certificate(*.pfx or *.p12) to PEM format. You could find instructions here.

(<http://ca.grid.sinica.edu.tw/general/p12toserver.html>)

For Window users, you will need -

- Win32 OpenSSL -
 - You could find this from
 - <http://gnuwin32.sourceforge.net/packages/openssl.htm>

2.2. GAP Environment

2.2.1. Deploy your certificate for the usage of GRID

Create .globus directory in your Home directory.

The user HOME directory on the different Operation System, for example

1. Windows XP

'C:\Document and Settings\[UserName]'

2. Mac

'/Users/[UserName]'

3. Linux

'/home/[UserName]'

Put your userkey.pem and usercert.pem on \$HOME/.globus directory.

On Unix-like operation system

\$HOME/.globus/usercert.pem

\$HOME/.globus/userkey.pem

\$HOME/.globus/certificates

On Window-based operating system

%HOME%\globus\usercert.pem

%HOME%\globus\userkey.pem

%HOME%\globus\certificates

- NOTE! A directory with "." prefix on Windows needs to be created by command, there is no way to create such kind of directory via GUI.

2.2.2. Download ASGCCA certificate : PEM format

Download ASGCCA <http://ca.grid.sinica.edu.tw/publication/ASGCCA.pem>

Then rename ASGCCA.pem as 9cd75e87.0, and put it into .globus\certificates directory

2.3. You must import your certificate into your browser. Then you can apply the EUAsiaGRID VO and VQS account with this browser.

2.4. Join a VO(After 2.1 is finished)

After you get your user certificate, you need to join a VO for using the resource of GRID.

You have to apply for joining a VO with your browser which has your certificate.

- euasia - <https://vomrs.grid.sinica.edu.tw:8443/vomrs/euasia/vomrs>

2.5. Make sure you have Java Runtime Environment (JRE1.5+) installed.

2.6. Apply for a VQS account for using this Virtual Screening Service.

2.6.1. Apply via <https://vl01.grid.sinica.edu.tw:8443/vqsreg>

- Please make sure the browser you used contains your user certificate, the server will detect the user certificate and retrieve the DN(Distinguishing Name) from the user certificate for the registration.

The screenshot shows a web browser window titled "VQS Account Registration". The address bar shows the URL <https://t-04.grid.sinica.edu.tw:8443/vqsreg/webpages/vqsRegForm.jsp>. The page features a header with the "GAP" logo and the text "Grid Application Platform". Below the header, the title "VQS Account Registration" is centered. The registration form includes the following fields and controls:

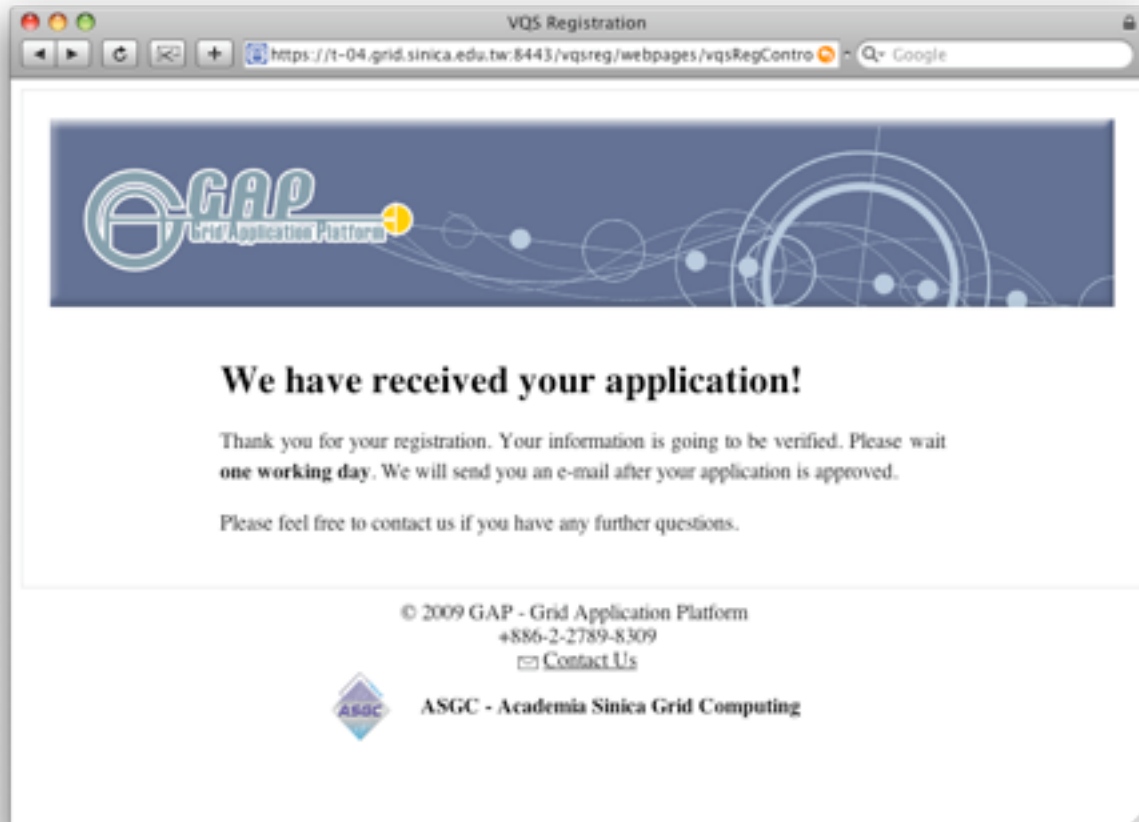
- *Title :
- *Full Name :
- *Your Account :
- *Your Password :
- *Confirm Password :
- *E-mail :
- *Country :
- *Address :
- *Phone :
- *Affiliation :
- *VO :

At the bottom of the form are "Submit" and "Reset" buttons. Below the form, a message states: "Your current certificate is "/C=TW/O=AS/OU=GRID/CN=Mason Hsiung 148117" certified by "/C=TW/O=AS/CN=Academia Sinica Grid Computing Certification Authority Mercury".

The footer contains the copyright notice "© 2009 GAP - Grid Application Platform", the phone number "4886-2-2789-8309", a "Contact Us" link, and the logo and name "ASGC - Academia Sinica Grid Computing".

- NOTE! Please select the corresponding VO(Virtual Organization) you belong to.

2.6.2. After you submit the application for the VQS account, you will receive a notification mail and need to wait one working day for approving your application.



2.6.3. Once your application is approved, you will receive an email telling you that your VQS account is approved and available. And follow the download link in the email to get the GUI client tool.



3. Installation

3.1. Download the installer package and follow the instructions of installer -

- Windows -
 - Double click the gvss-1.0.0.jar to startup the installer, and follow the instructions from the installer to complete the installation.
 - If you are not able to startup the installer by double clicking gvss-1.0.0.jar, please open the command line window and type 'java -jar gvss-1.0.0.jar'.
 - NOTE! Make sure you have JRE1.5+ installed on your window-based system.
- Linux -
 - Right click the gvss-1.0.0.jar and choose 'Open with Sun java ...' to startup the installer
 - Or open a terminal and type 'java -jar gvss-1.0.0.jar'
 - NOTE! Make sure you have JRE1.5+ installed on your Linux.
- Mac -
 - Double click gvss-1.0.0.dmg and drag the 'GVSS' application to 'Applications' folder or any place you want.

3.2. GAP environment

3.2.1. GAP_HOME environment variable

- You don't really have to modify this variable manually, the installer will set the GAP_HOME variable automatically.

3.2.2. Since this service is based on GAP and GAP uses globus toolkit, by default the GUI client will try to find your user certificate(usercert.pem and userkey.pem) under \$HOME/.globus/. Please make sure you have followed the previous instruction to put your user certificate into the right directory.

- Or you could change the location of the usercert.pem and userkey.pem later through the GUI.

4. After the Installation - How to start?

4.1. Windows -

4.1.1. Desktop Shortcut

- After the installation, there will be a shortcut icon created for quick launching this GUI client.

4.1.2. The startup batch script - vsautodock.bat

- There will be a startup batch script under the \$INSTALL_PATH/GVSS-1.0.0\opt\gap\bin, execute the script, eg

```
C:\> %INSTALL_PATH%\GVSS-1.0.0\opt\gap\bin\vsautodock
```

Or double click the batch script to launch this GUI client.

4.2. Linux -

4.2.1. Desktop Shortcut

- After the installation, there will be a shortcut icon created for quick launching this GUI client.

4.2.2. The startup bash script - vsautodock

- There will be a startup bash script under the \$INSTALL_PATH/GVSS-1.0.0/opt/gap/bin, execute the script. e.g. -
#> \$INSTALL_PATH/GVSS-1.0.0/opt/gap/bin/vsautodock

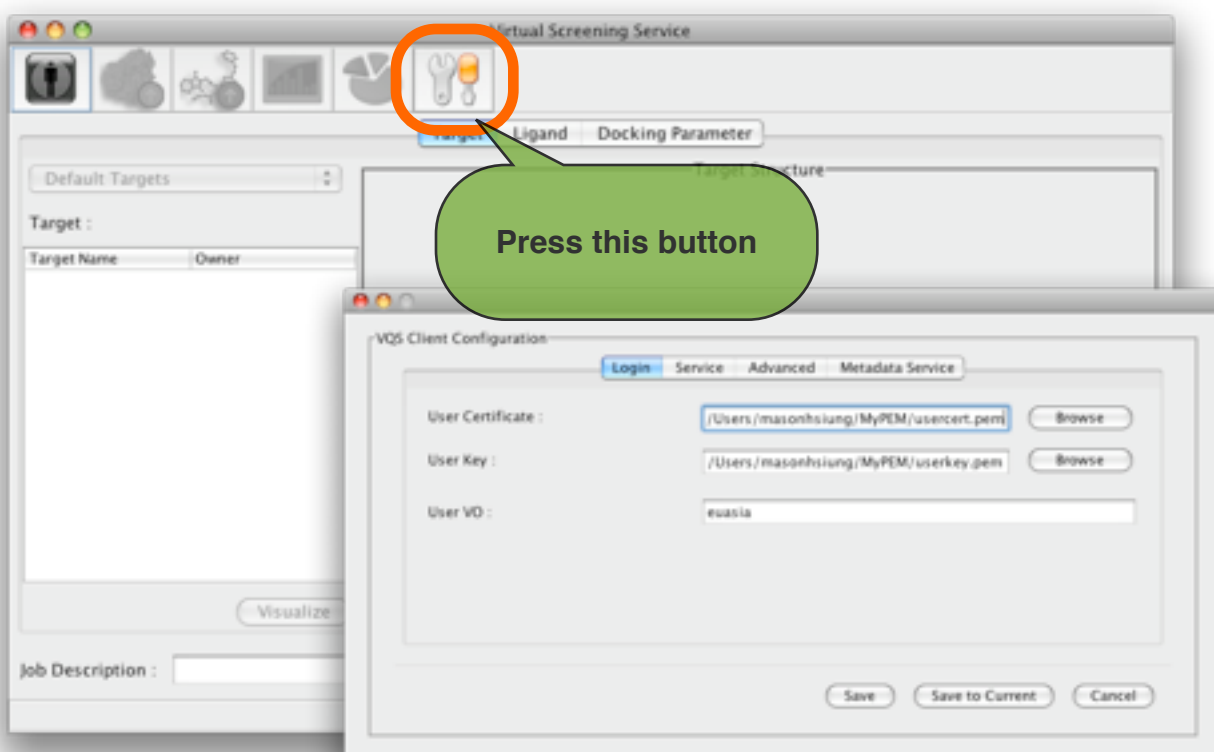
4.3. Mac -

4.3.1. Application Bundle

- Simply double click the GVSS application bundle.

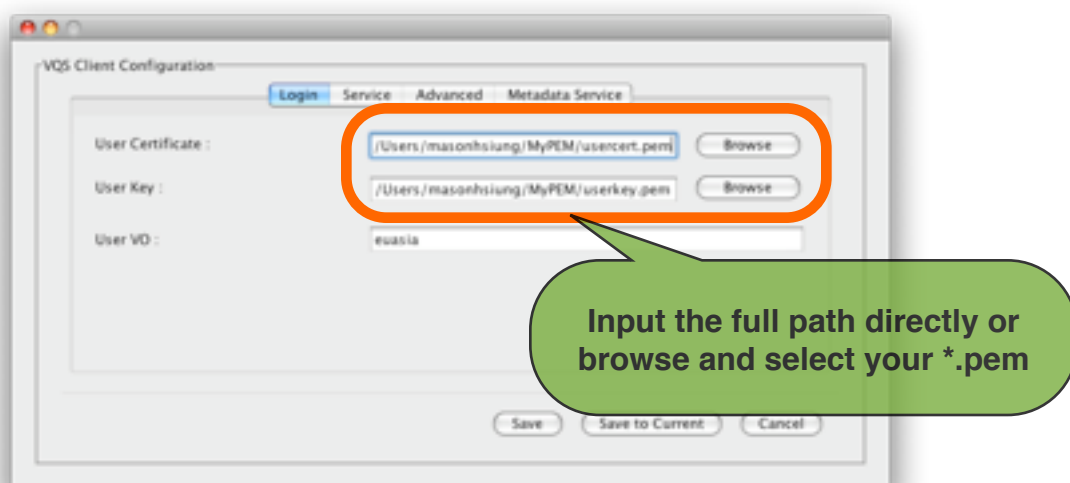
5. GUI Client Configuration

5.1. Show the configuration window.

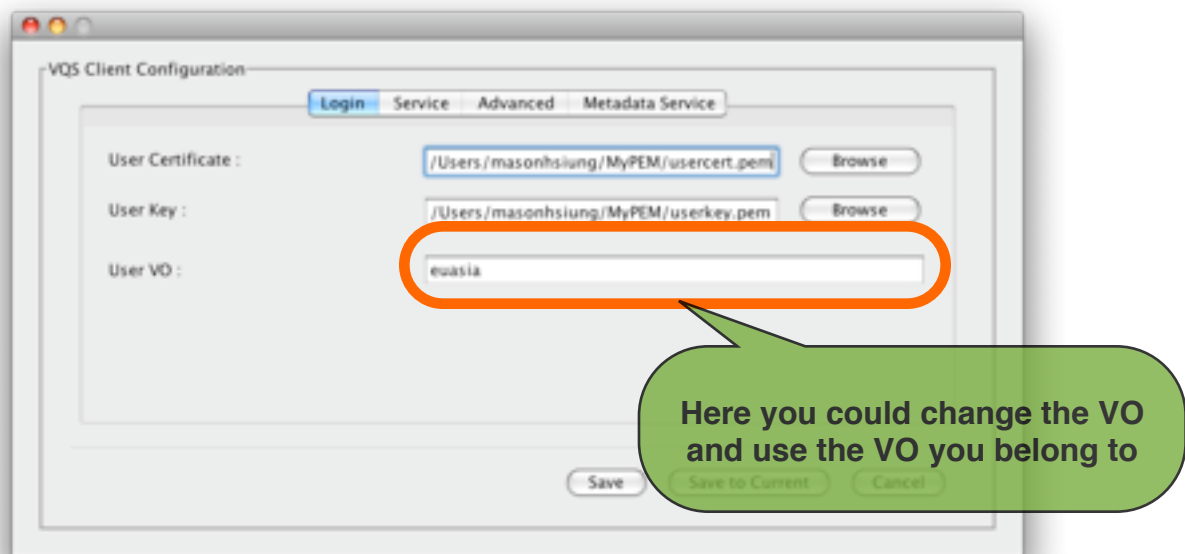


5.2. Change the location of your user certificate

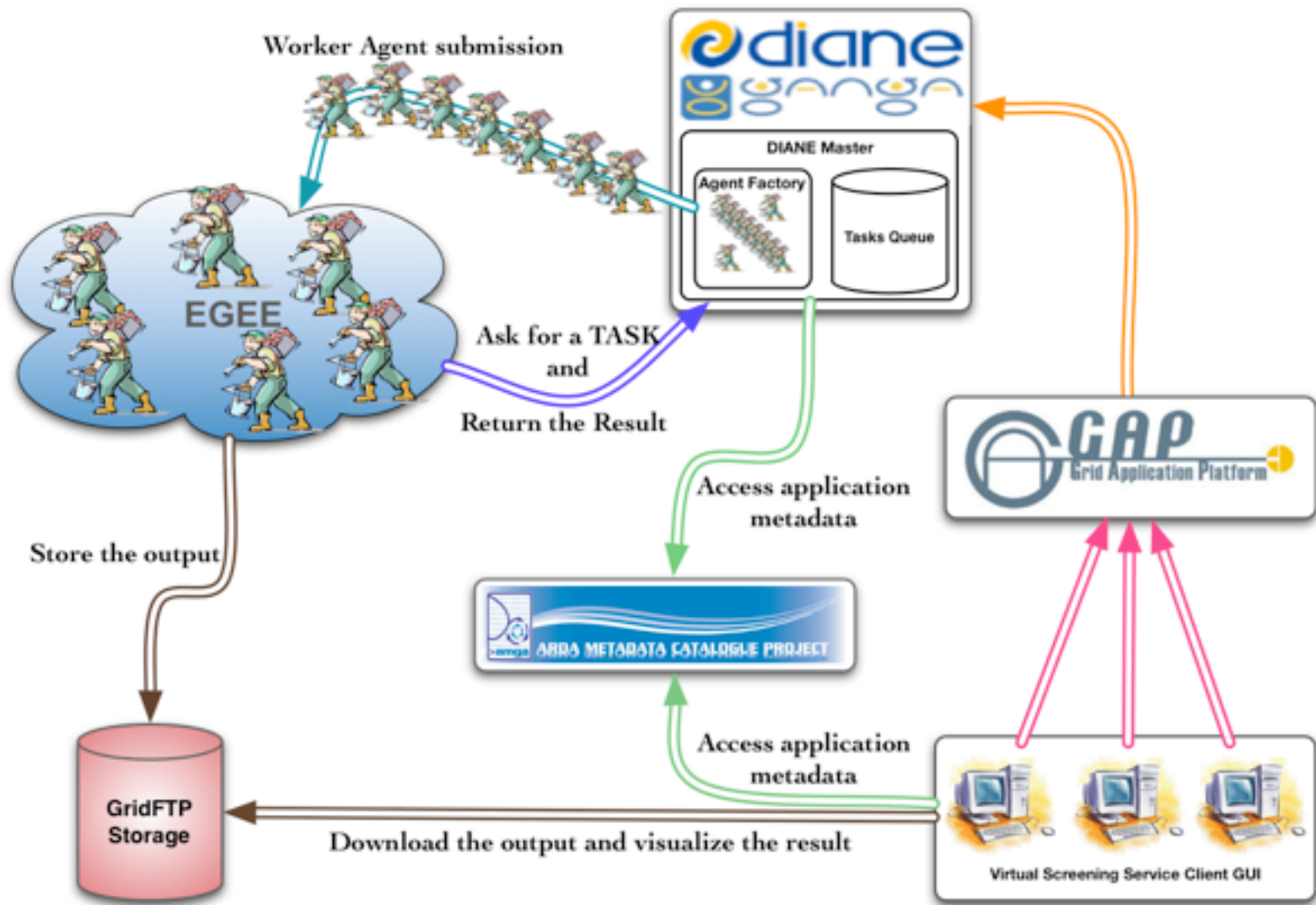
- Here you can change the location of your 'usercert.pem' and 'userkey.pem'



5.3. Change the default VO setting, the default one is 'euasia'.

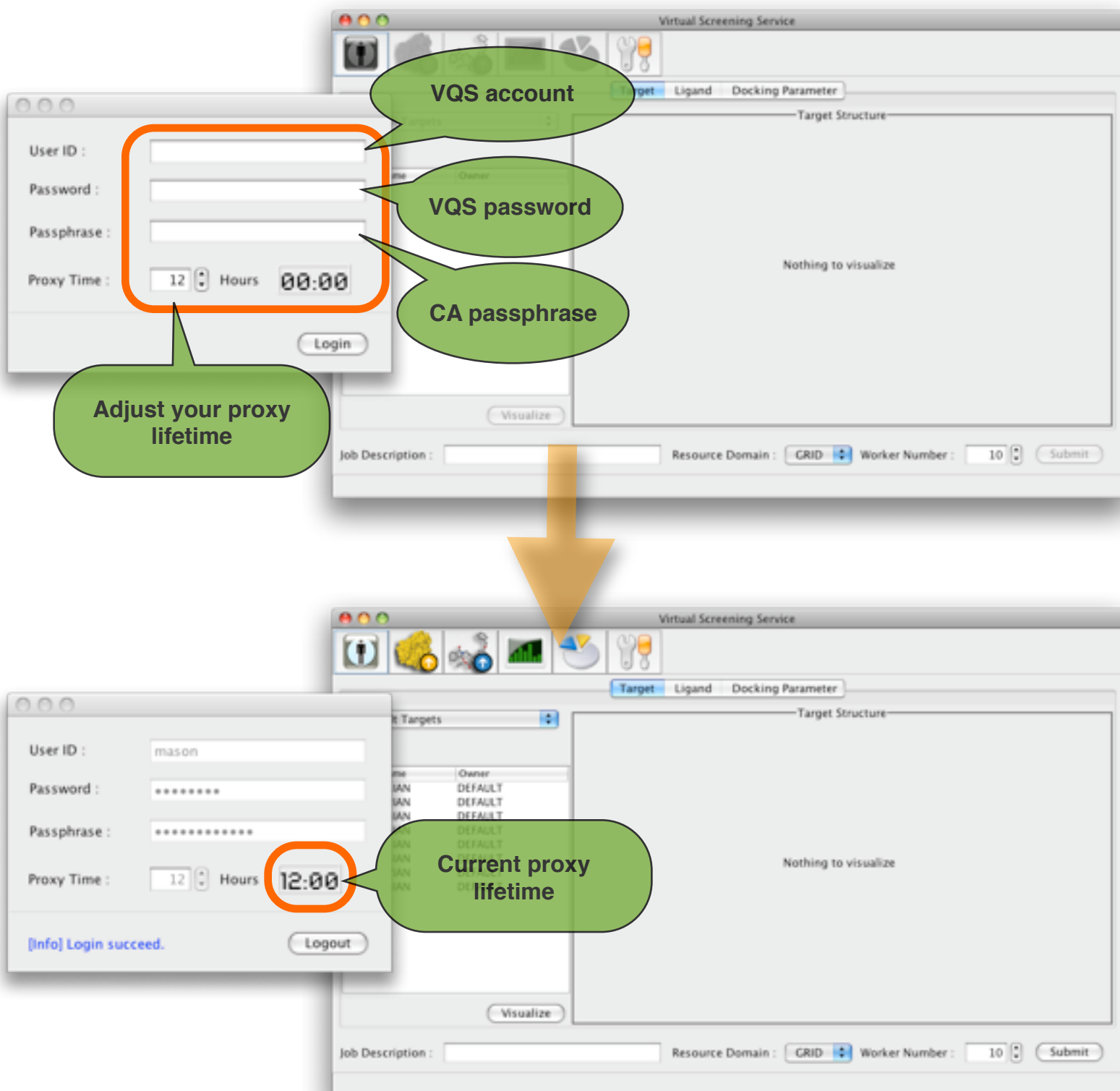


6. GRID Service Architecture



7. Virtual Screening Service GUI User Guide

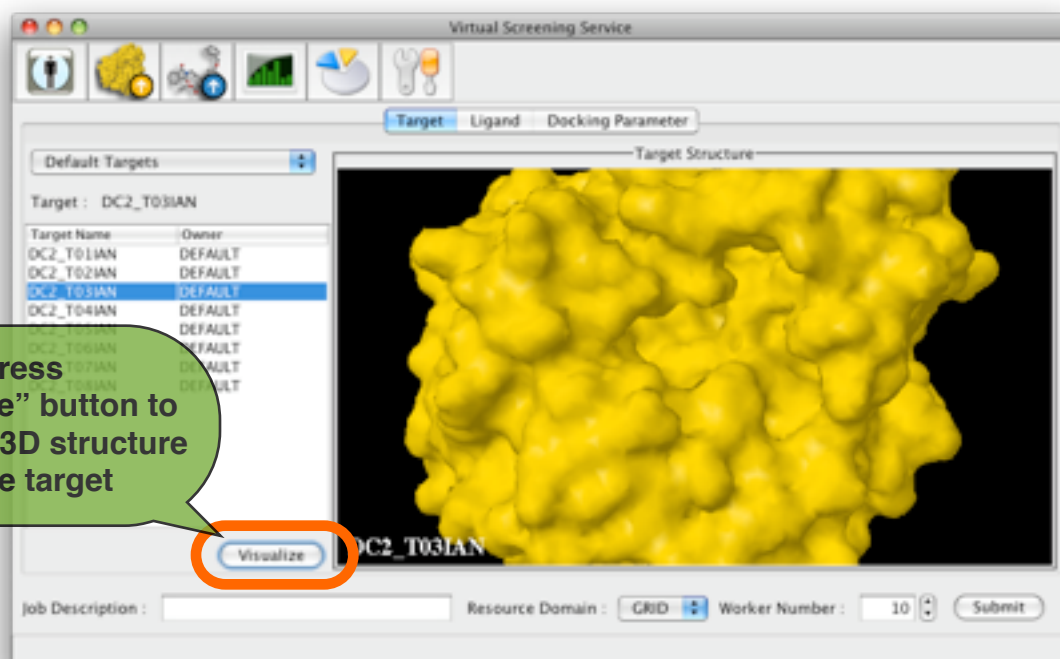
7.1. Login, input your VQS account and password, then input the passphrase of your certificate, finally decide your proxy life time



7.2. Initial Docking Simulation

7.2.1. Select Target

- Select the default target or your own target.
- And visualize the target if available and if you want.

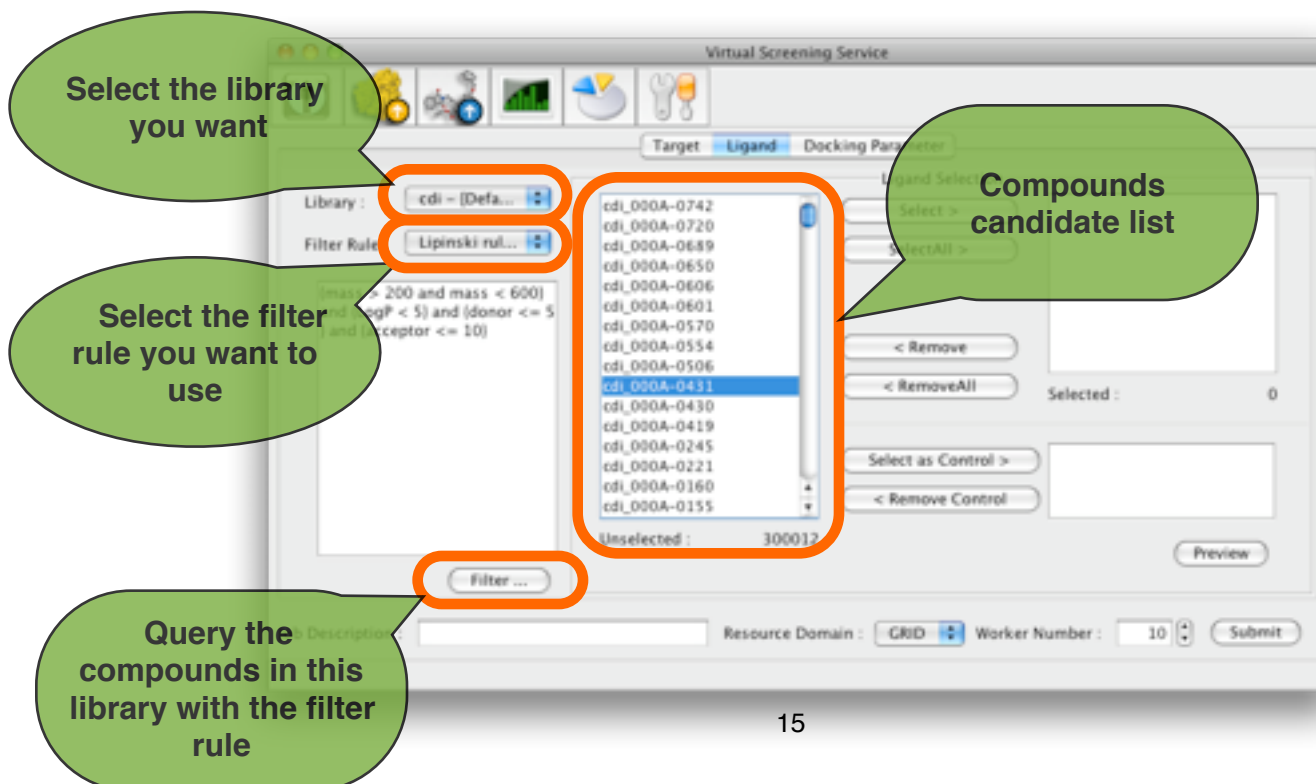


7.3. Select Ligands

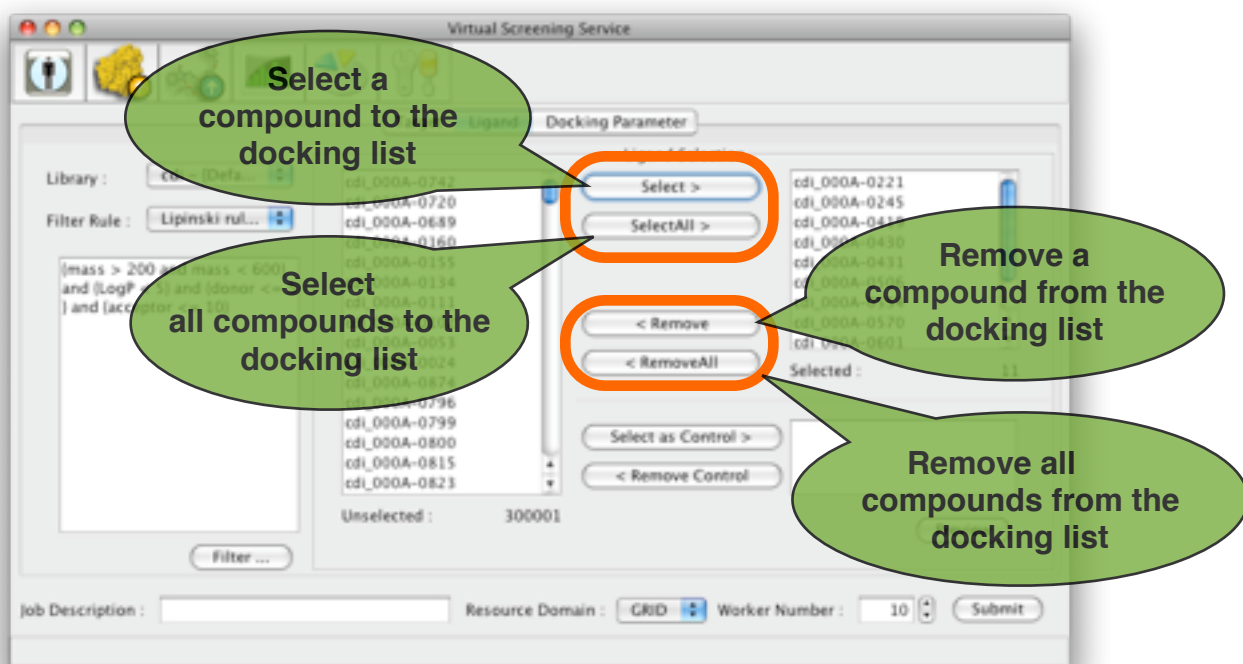
7.3.1. Select the library

7.3.2. Select the filter rule if needed

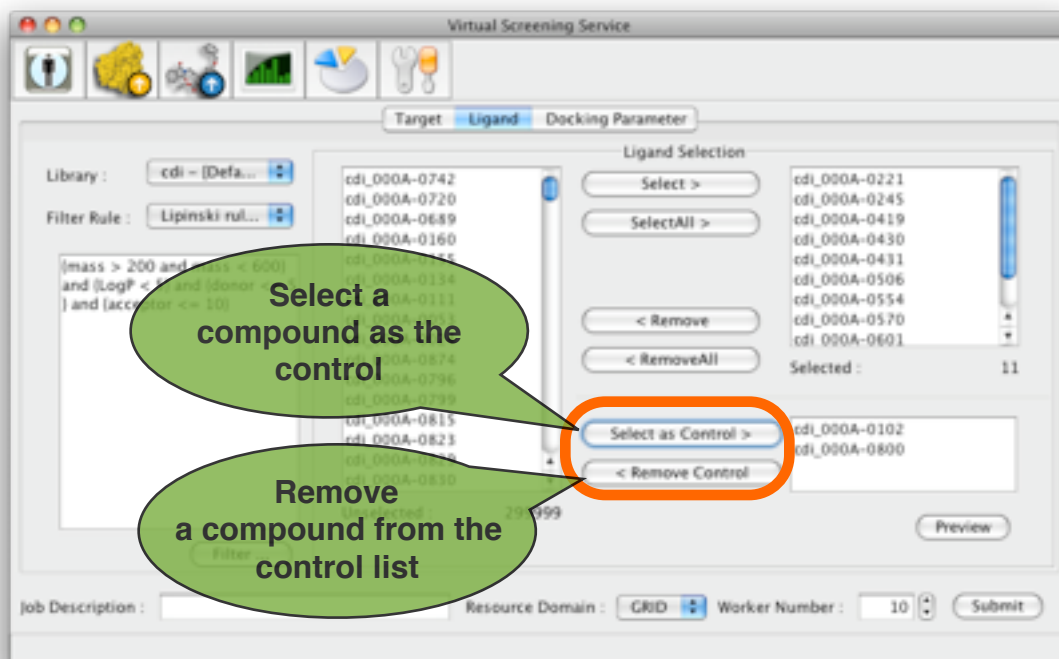
7.3.3. And push the 'Filter' button



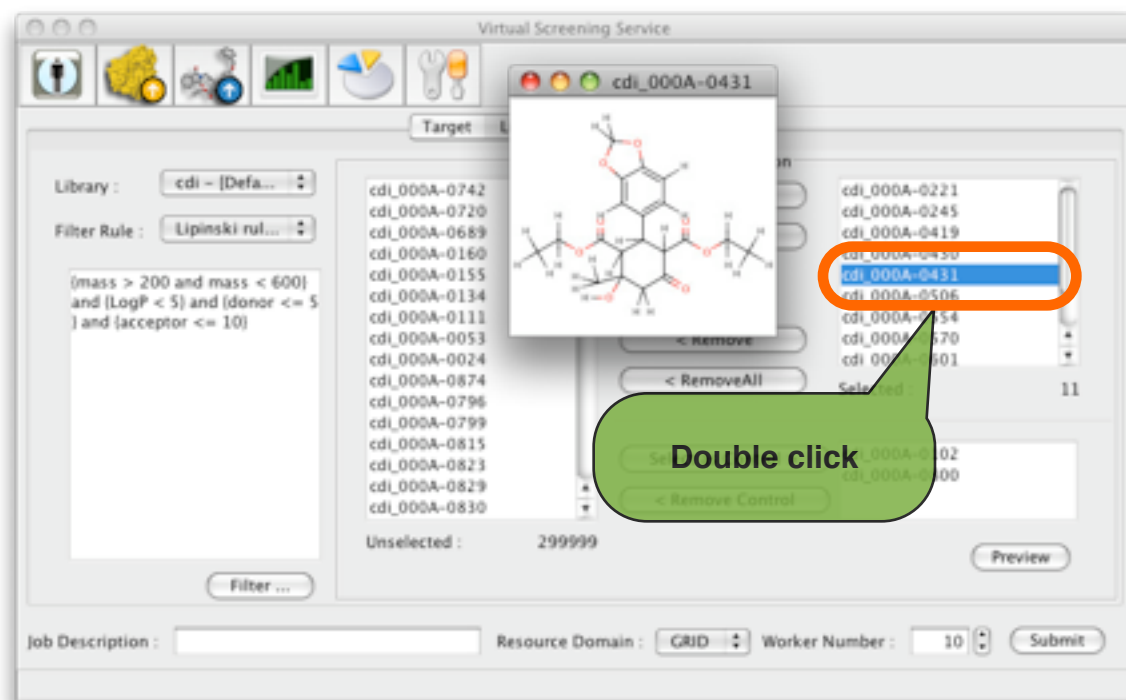
7.3.4. Select the ligands that you want to run the docking simulation.



7.3.5. Further more, you can select the ligand as the control if you want.

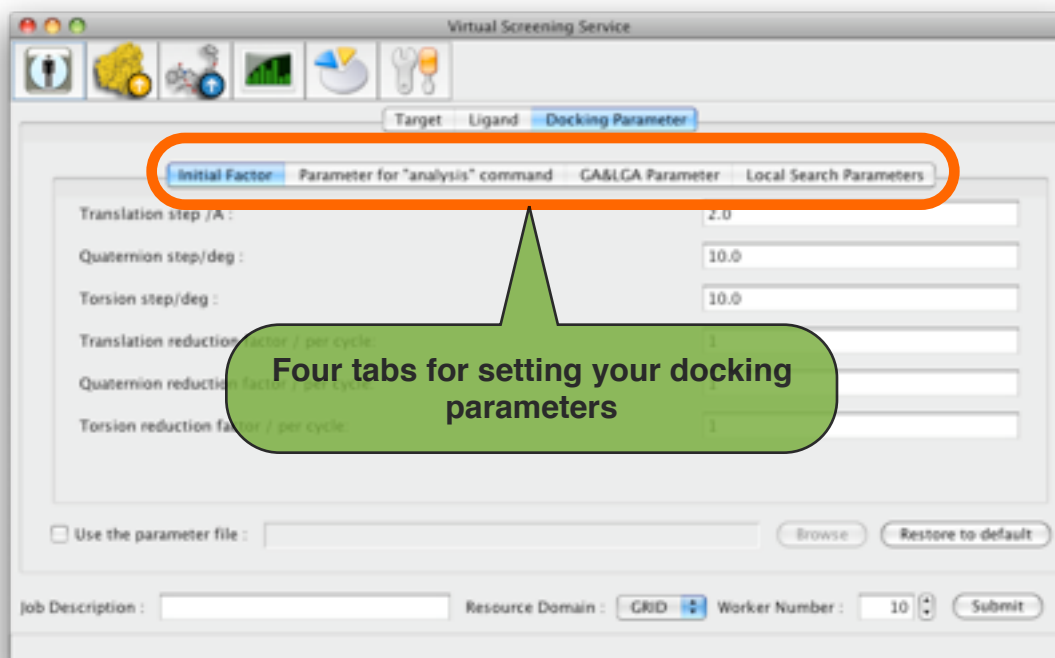


7.3.6. Double click the item of ligand, you can visualize the ligand 2D structure if available.

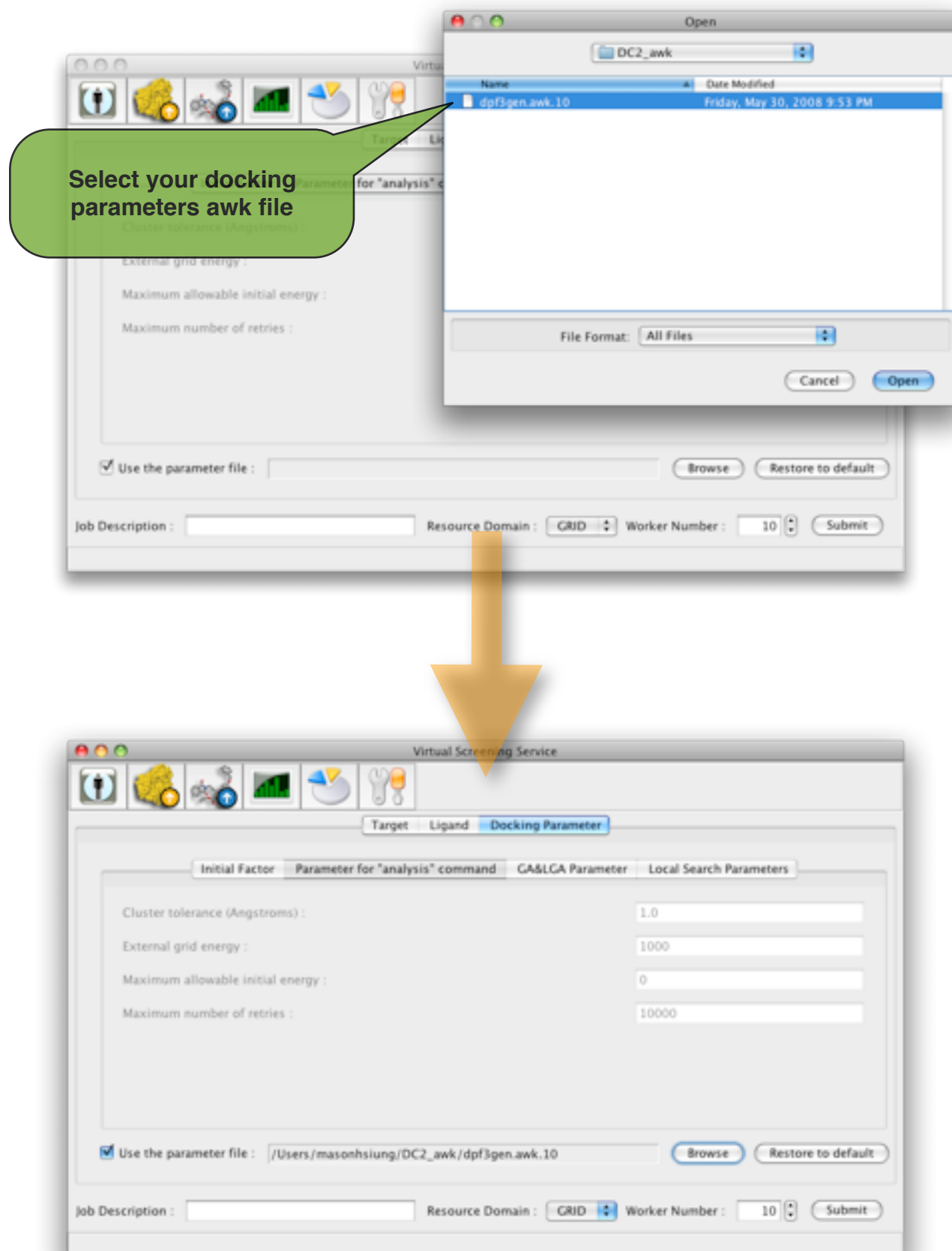


7.4. Modify your docking parameters

7.4.1. There are 4 tabs for setting your docking parameter. Just modify the parameters directly.



7.4.2. Or you can choose to use an existing docking parameter awk file.

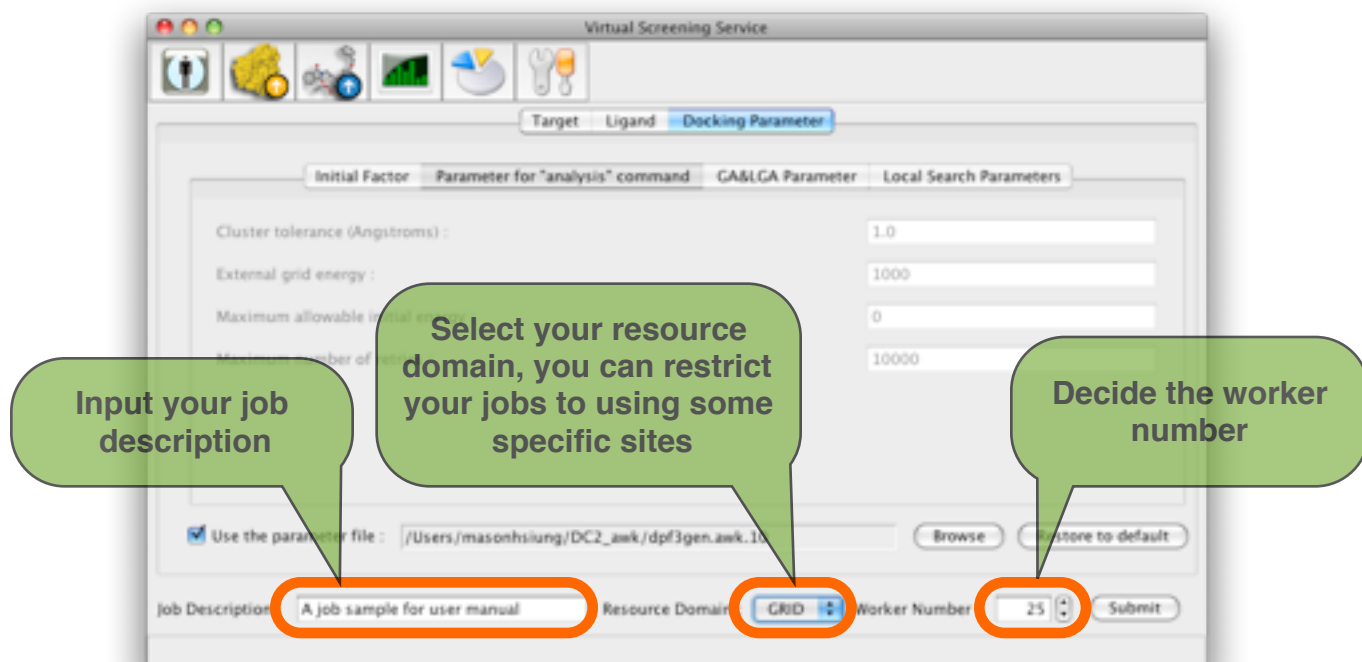


7.5. Configure your job

7.5.1. Input a simple job description.

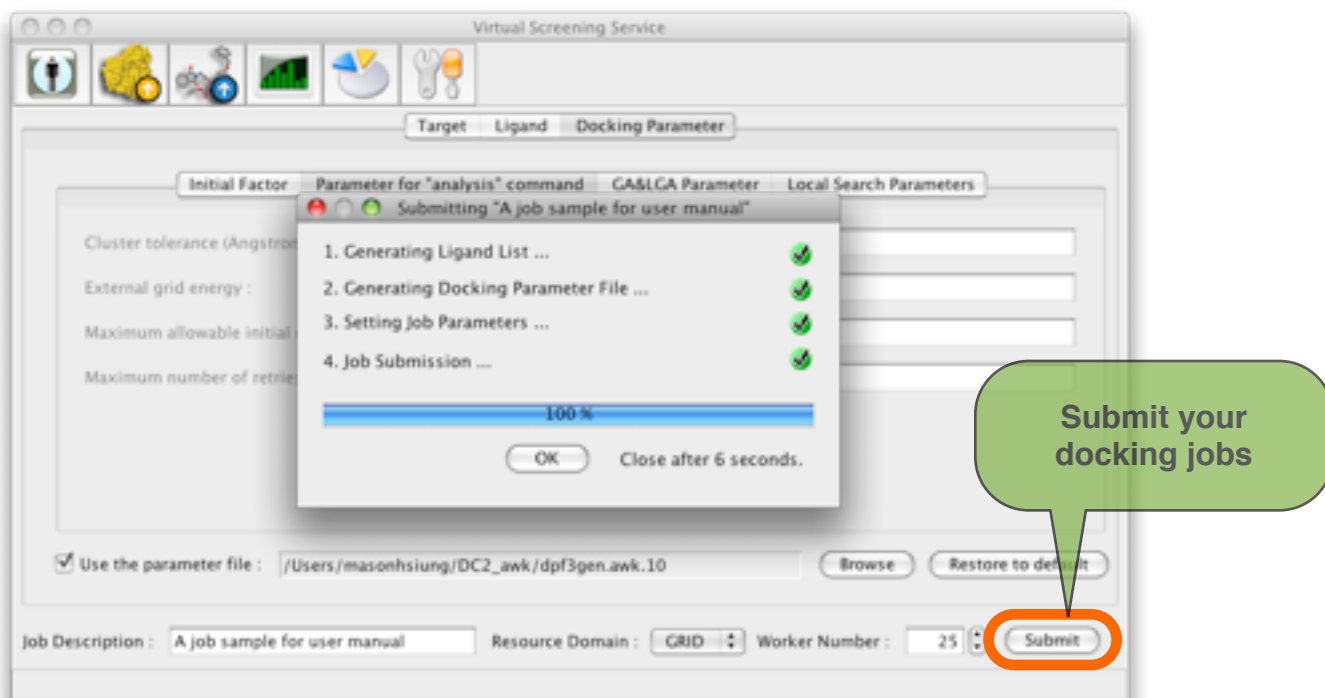
7.5.2. Select your resource domain

7.5.3. Decide how many workers(cpus) you want to use



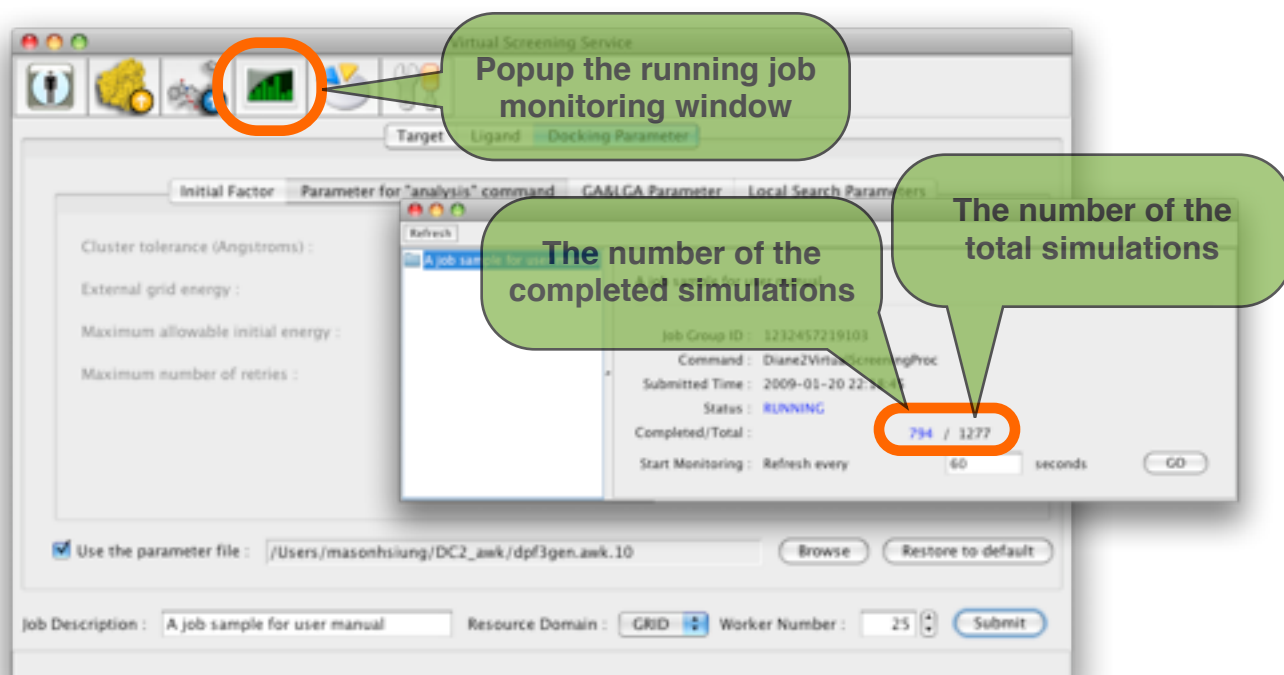
7.6. Job submission

7.6.1. Simply push the 'Submit' button

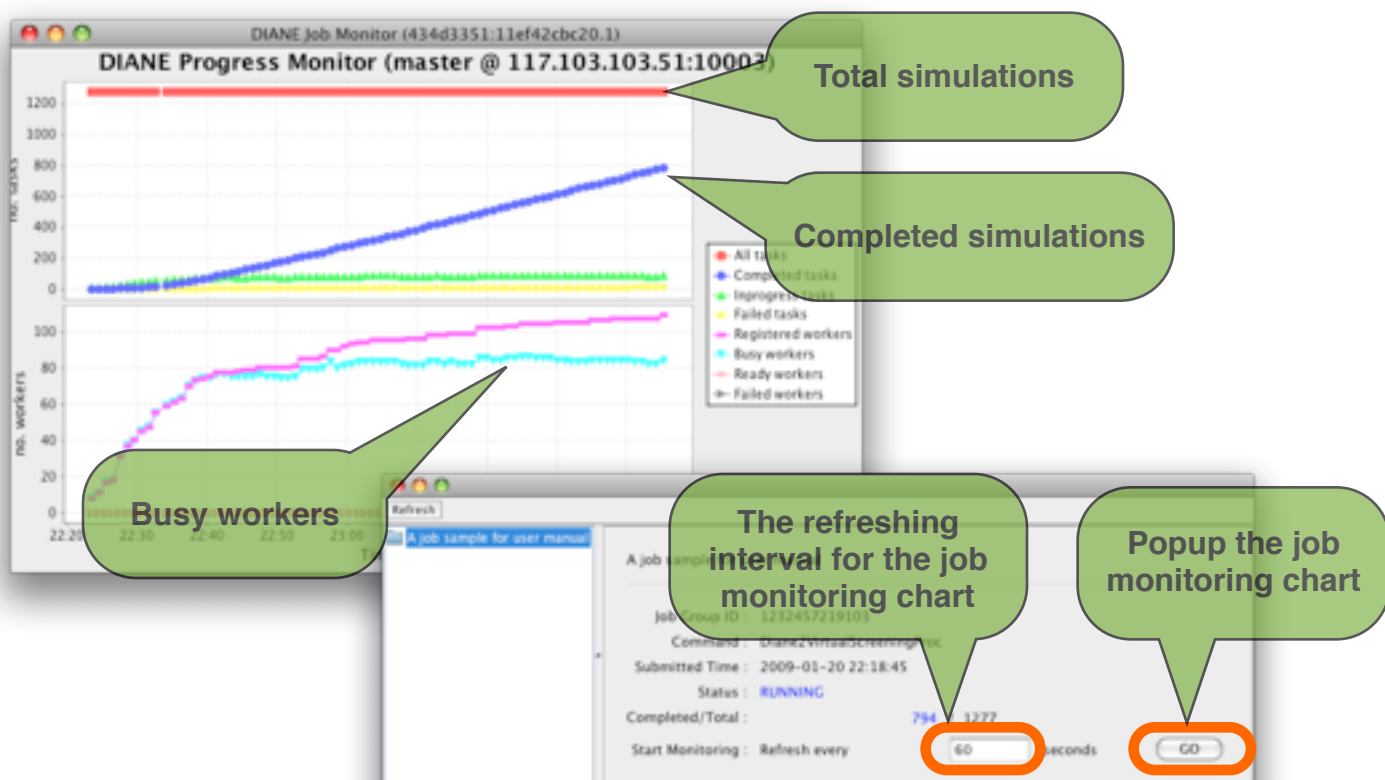


7.7. Job monitoring

7.7.1. Push the running job monitoring button

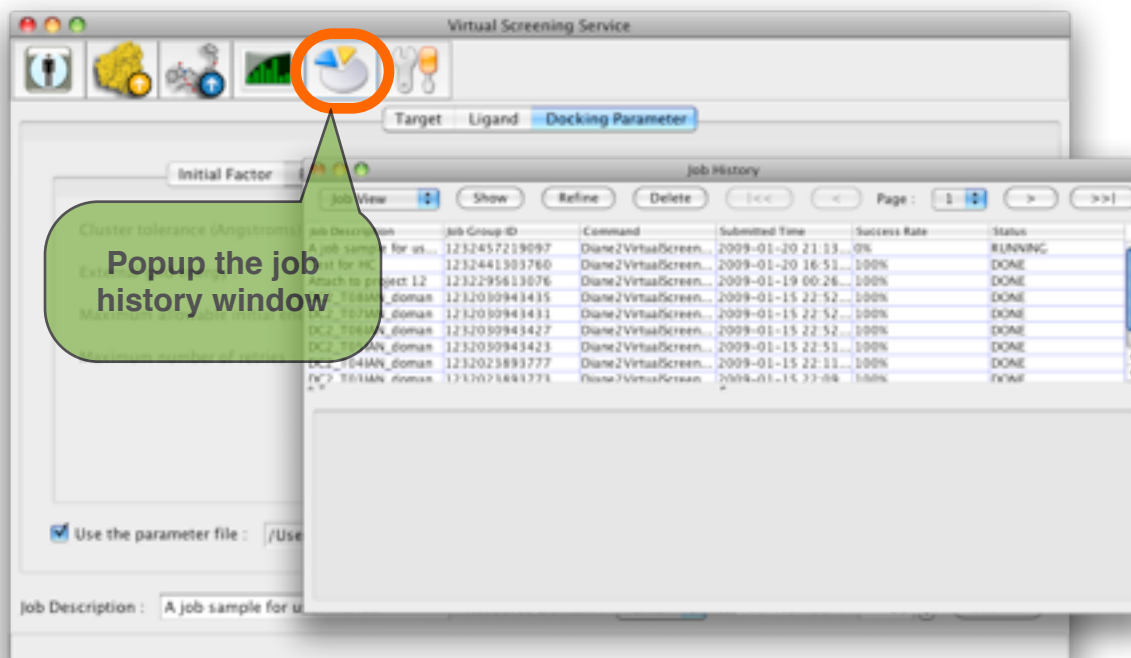


7.7.2. Monitor the job status via the dynamic job monitoring chart with a given refreshing interval.



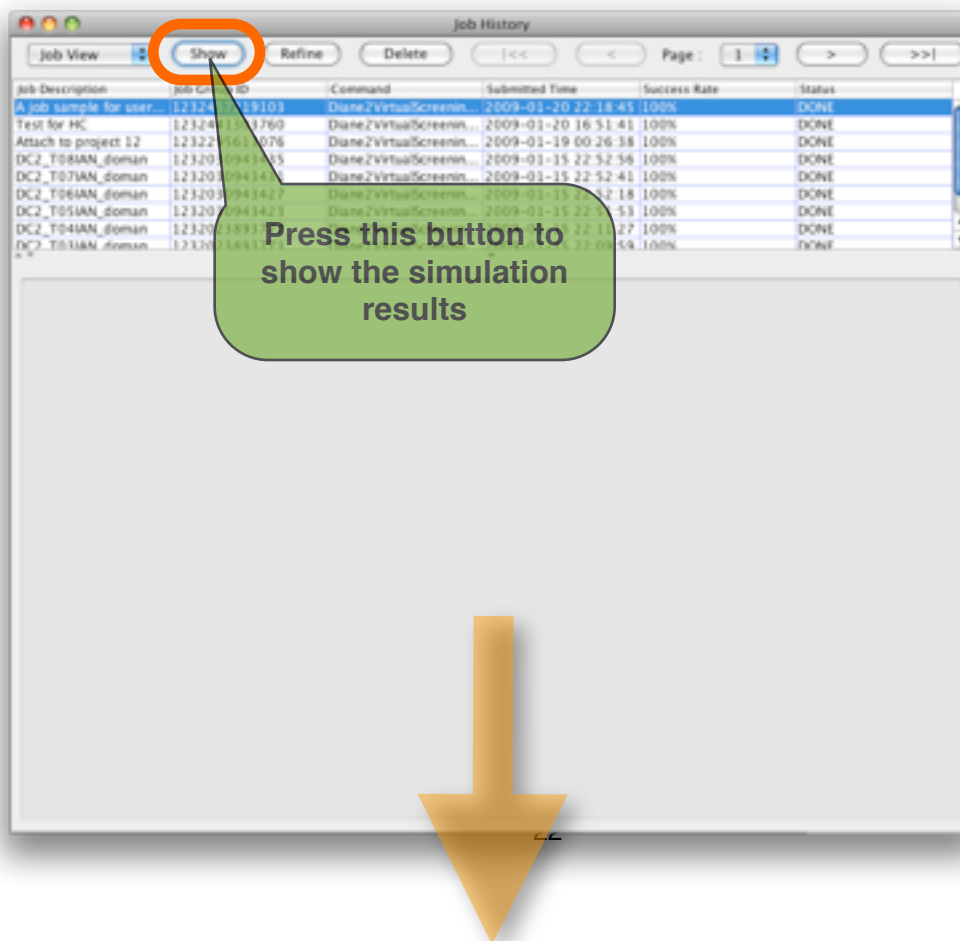
7.8. Check your docking simulation results

7.8.1. Push the job history button to popup the job history window.



7.8.2. Visualize your docking simulation results

a. Select the job you want to see, and push the 'Show' button.



The results of simulations in the project

Job Description	Job Group ID	Command	Submitted Time	Success Rate	Status
A job sample for user...	1232457219103	Diane2VirtualScreenin...	2009-01-20 22:18:45	100%	DONE
Test for HC	1232441303760	Diane2VirtualScreenin...	2009-01-20 16:51:41	100%	DONE
Attach to project 12	1232295613076	Diane2VirtualScreenin...	2009-01-19 00:26:38	100%	DONE
DC2_T01IAN_domain	1232030943435	Diane2VirtualScreenin...	2009-01-15 22:52:56	100%	DONE
DC2_T01IAN_domain	1232030943431	Diane2VirtualScreenin...	2009-01-15 22:52:41	100%	DONE
DC2_T01IAN_domain	1232030943427	Diane2VirtualScreenin...	2009-01-15 22:52:18	100%	DONE
DC2_T01IAN_domain	1232030943423	Diane2VirtualScreenin...	2009-01-15 22:51:53	100%	DONE
DC2_T01IAN_domain	1232021893777	Diane2VirtualScreenin...	2009-01-15 22:11:27	100%	DONE
DC2_T01IAN_domain	1232021893773	Diane2VirtualScreenin...	2009-01-15 22:09:59	100%	DONE

Below the table, there is a section for 'A job sample for user manual' with a list of energy targets and ligands. The 'Show Best Complex' button is highlighted.

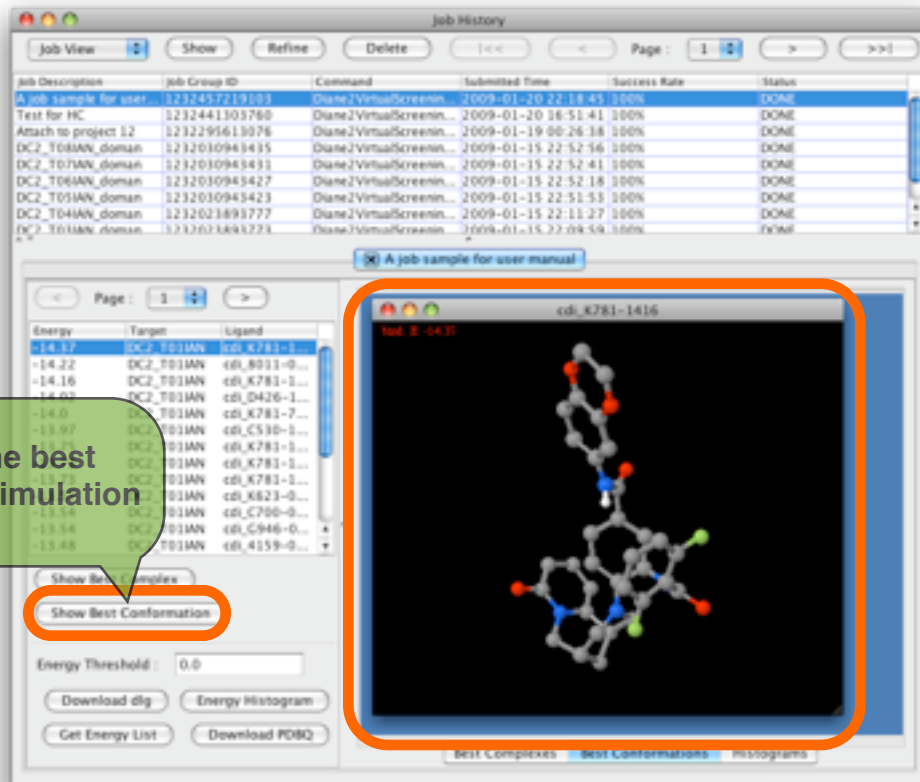
b. Show the best complex of a simulation.

Select a simulation

Press to show the best complex of a simulation

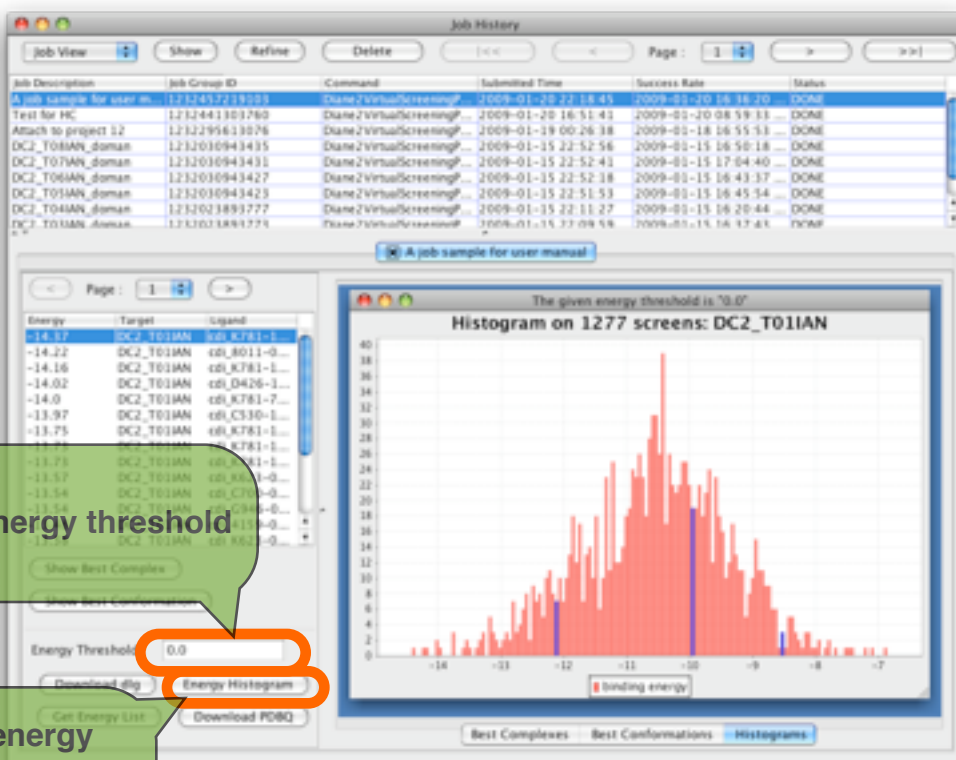
DC2_T01IAN vs cdi_K781-1416

c. Show the best ligand conformation of a simulation.



Press to show the best conformation of a simulation

d. Generate the energy histogram with controls from the best energies of all the simulations



Give an energy threshold

Generate the energy histogram with the given energy threshold

7.8.3. Download the simulation results

- Download the compound's PDBQ files with a given energy threshold

Job History

Job Description	Job Group ID	Command	Submitted Time	Success Rate	Status
A job sample for user m...	1232457219103	Dane2VirtualScreeningP...	2009-01-20 22:18:45	2009-01-20 16:16:20	DONE
Test for MC	1232441303760	Dane2VirtualScreeningP...	2009-01-20 16:51:41	2009-01-20 08:59:33	DONE
Attach to project 12	1232295613076	Dane2VirtualScreeningP...	2009-01-19 00:26:38	2009-01-18 16:55:53	DONE
DC2_T01IAN_domain	1232030943435	Dane2VirtualScreeningP...	2009-01-15 22:52:56	2009-01-15 16:30:18	DONE
DC2_T07IAN_domain	1232030943431	Dane2VirtualScreeningP...	2009-01-15 22:52:41	2009-01-15 17:04:40	DONE
DC2_T06IAN_domain	1232030943427	Dane2VirtualScreeningP...	2009-01-15 22:52:18	2009-01-15 16:43:37	DONE
DC2_T05IAN_domain	1232030943423	Dane2VirtualScreeningP...	2009-01-15 22:51:53	2009-01-15 16:45:54	DONE
DC2_T04IAN_domain	1232030943419	Dane2VirtualScreeningP...	2009-01-15 22:11:27	2009-01-15 16:20:44	DONE
DC2_T03IAN_domain	1232030943415	Dane2VirtualScreeningP...	2009-01-15 22:09:59	2009-01-15 16:17:41	DONE

Open

PDBQ Download

Name: Simulation_PDBQ Date Modified: Wednesday, January 21, 2009 11:00 AM

File Format: All Files

Cancel Choose

Energy Threshold: 0.0

Download dlg Energy Histogram

Download PDBQ

Download the PDBQ files with the given energy threshold

Job History

Job Description	Job Group ID	Command	Submitted Time	Success Rate	Status
A job sample for user m...	1232457219103	Dane2VirtualScreeningP...	2009-01-20 22:18:45	2009-01-20 16:16:20	DONE
Test for MC	1232441303760	Dane2VirtualScreeningP...	2009-01-20 16:51:41	2009-01-20 08:59:33	DONE
Attach to project 12	1232295613076	Dane2VirtualScreeningP...	2009-01-19 00:26:38	2009-01-18 16:55:53	DONE
DC2_T08IAN_domain	1232030943435	Dane2VirtualScreeningP...	2009-01-15 22:52:56	2009-01-15 16:30:18	DONE
DC2_T07IAN_domain	1232030943431	Dane2VirtualScreeningP...	2009-01-15 22:52:41	2009-01-15 17:04:40	DONE
DC2_T06IAN_domain	1232030943427	Dane2VirtualScreeningP...	2009-01-15 22:52:18	2009-01-15 16:43:37	DONE
DC2_T05IAN_domain	1232030943423	Dane2VirtualScreeningP...	2009-01-15 22:51:53	2009-01-15 16:45:54	DONE
DC2_T04IAN_domain	1232030943419	Dane2VirtualScreeningP...	2009-01-15 22:11:27	2009-01-15 16:20:44	DONE
DC2_T03IAN_domain	1232030943415	Dane2VirtualScreeningP...	2009-01-15 22:09:59	2009-01-15 16:17:41	DONE

Download PDBQ

Downloading: cdi_E715-0214 pdbq file ...

1 %

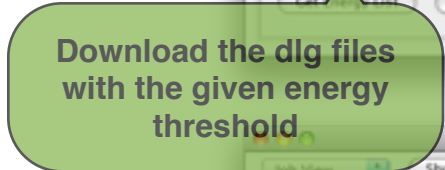
The given energy threshold is "0.0"

Histogram on 1277 screens: DC2_T01IAN

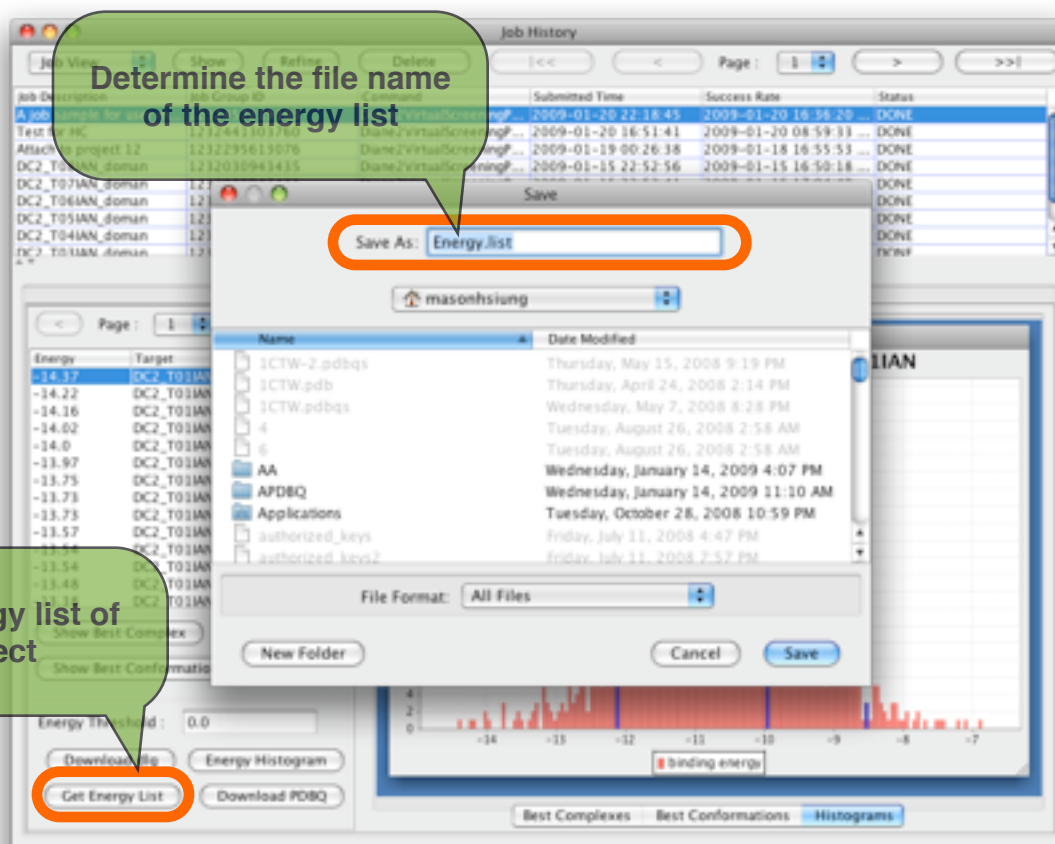
binding energy

Best Complexes Best Conformations Histograms

b. Download the dlg files(the output of 'autodock') with a given energy threshold

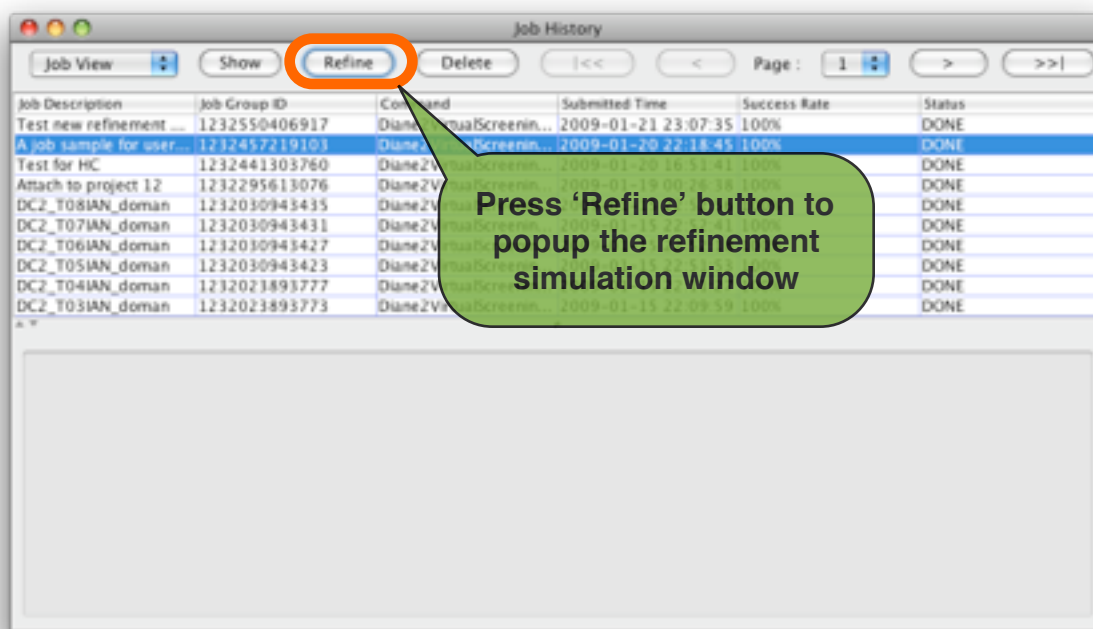


c. Generate the energy list of all the best energies of the simulations

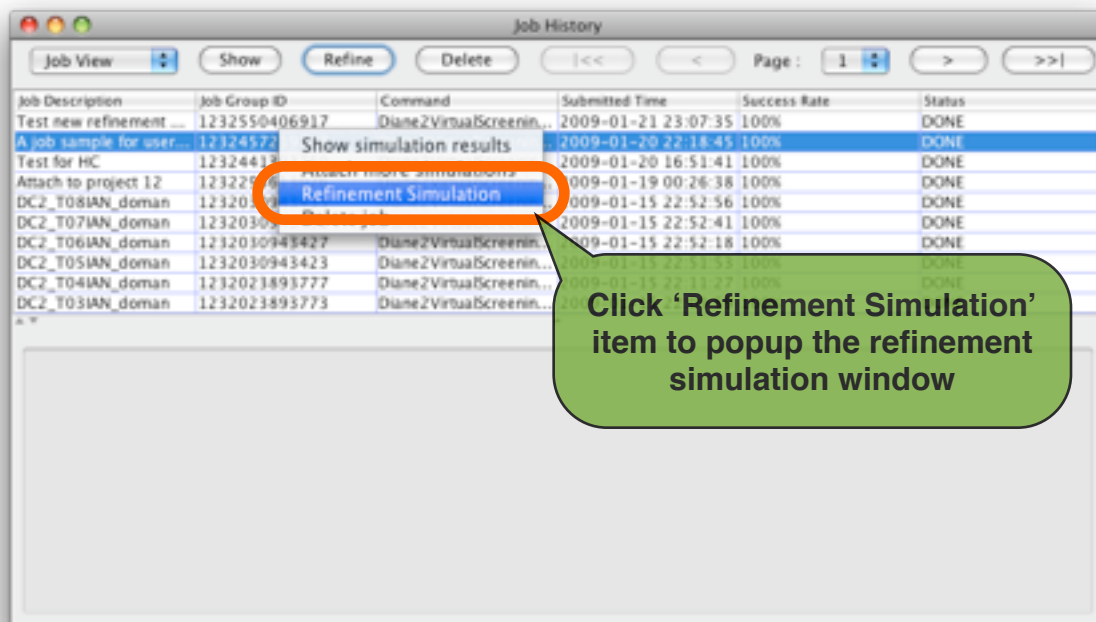


7.9. Advanced Refinement Docking Simulation

7.9.1. Select the item you want to refine and push 'Refine' button in the in job history window

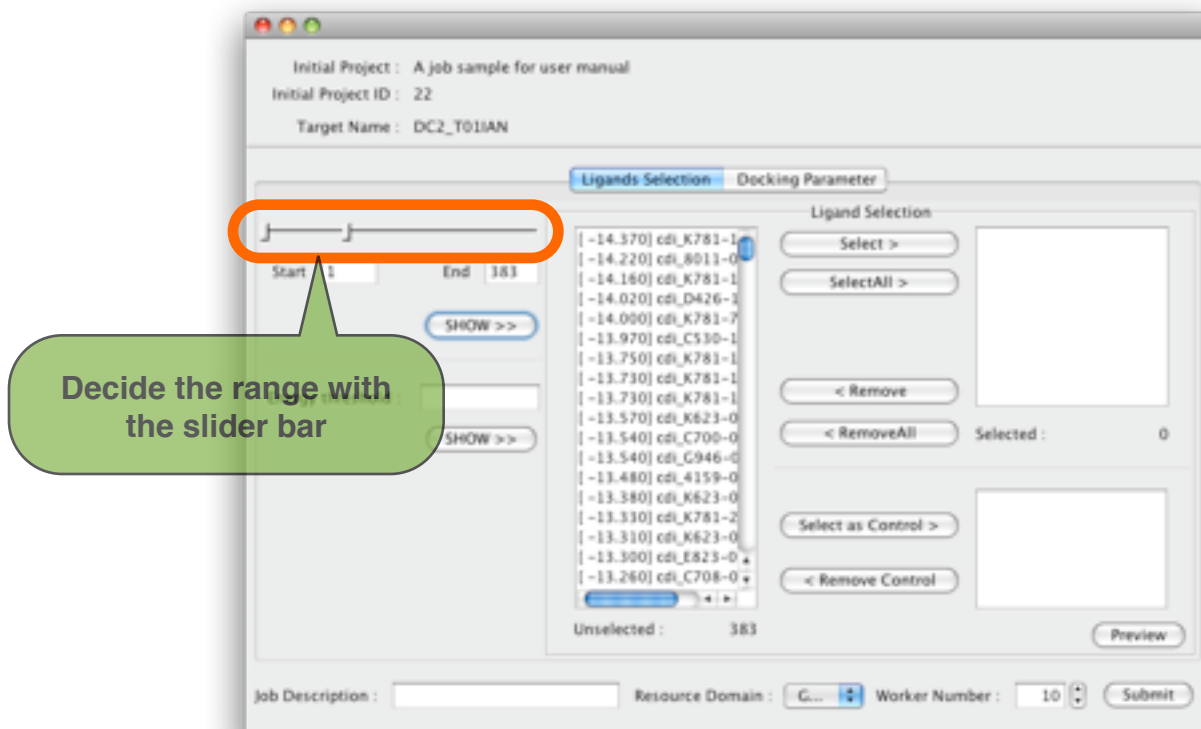


7.9.2. Or press the right button of mouse to popup the popup menu, and click 'Refinement Simulation' item in the job history window

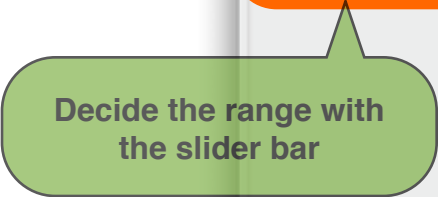


7.9.3. Ligands Selection, the ligands in the previous run have been sorted by each best energy. Remember that the target is determined by the previous run.

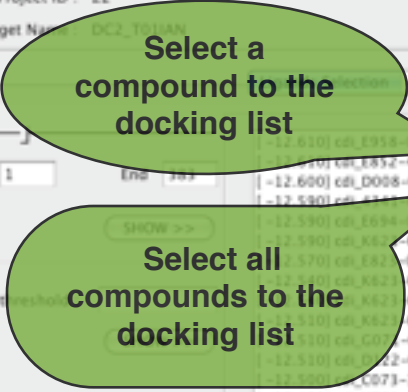
a. Filter the ligands by a range.



b. Filter the ligands with a given energy threshold



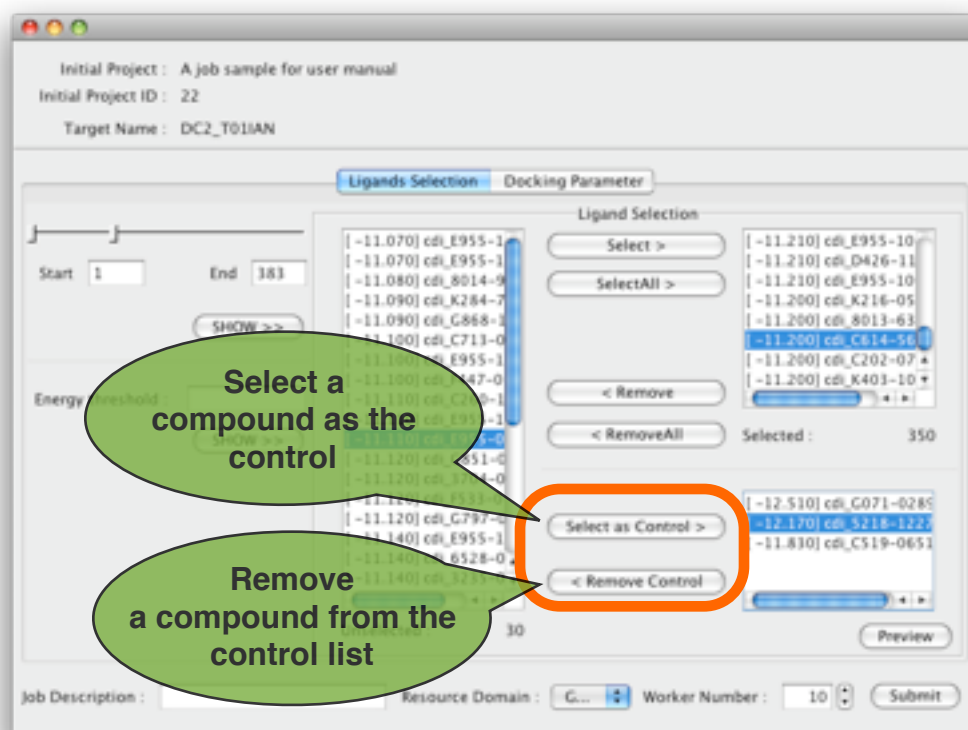
c. Select the ligands that you want to refine



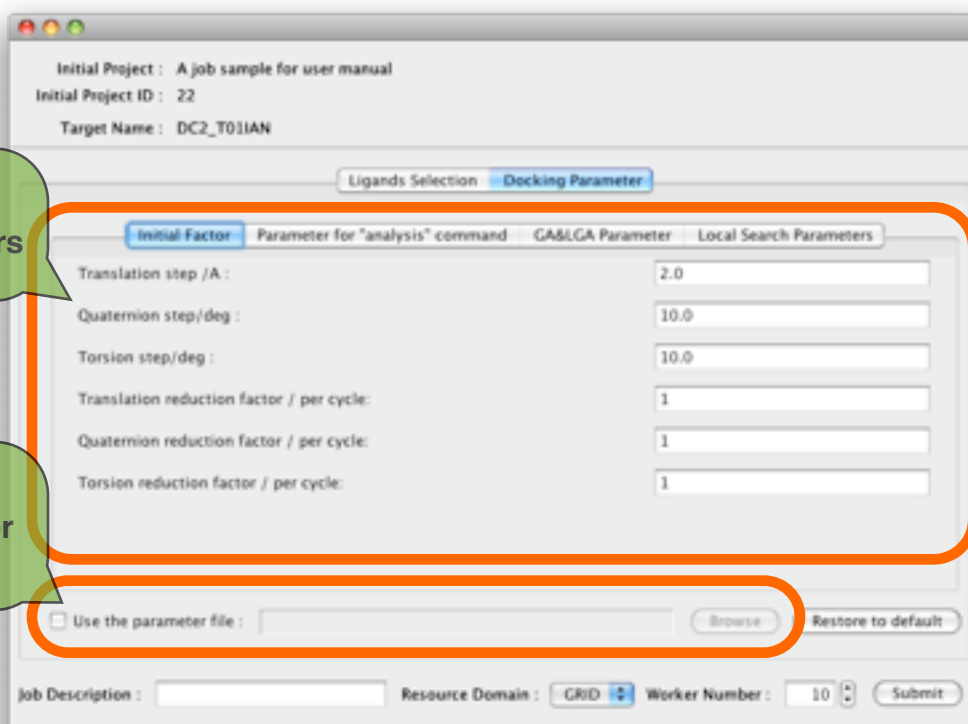
Remove a compound from the docking list

Remove all compounds from the docking list

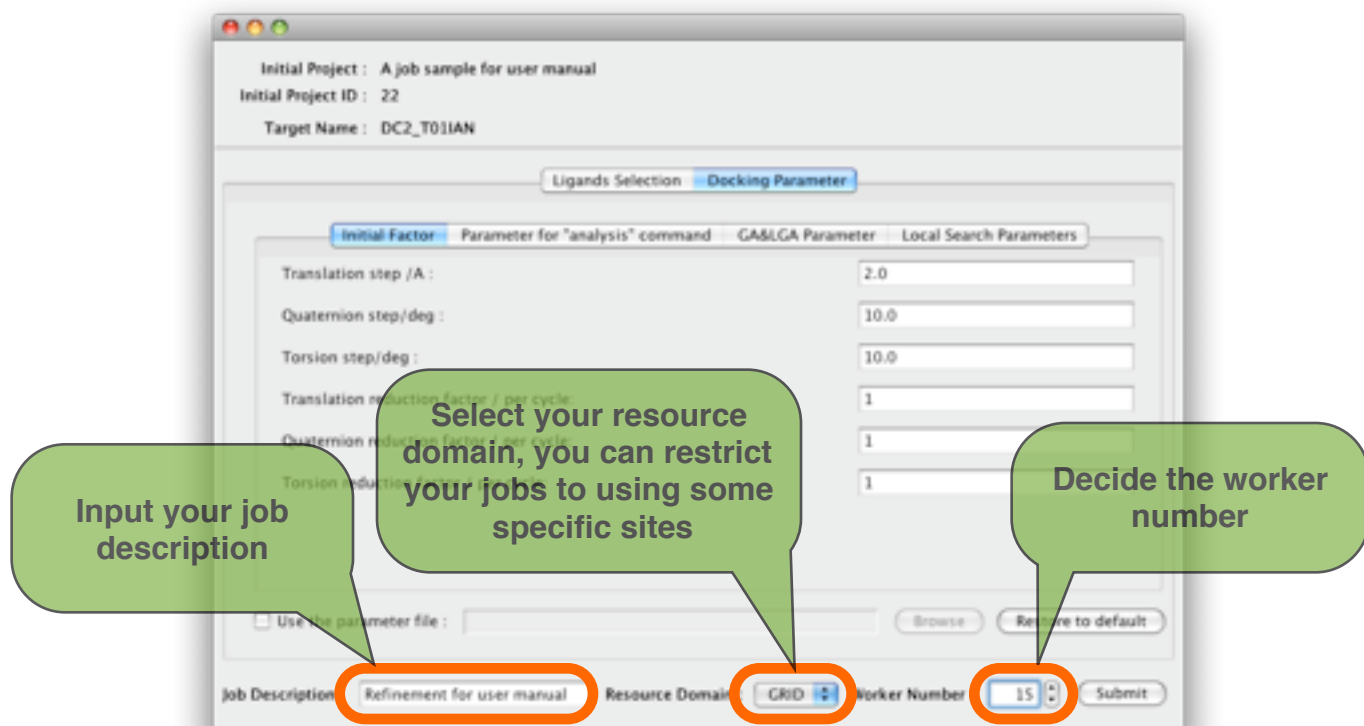
d. Just like the initial docking, you can select one or more ligands as the controls.



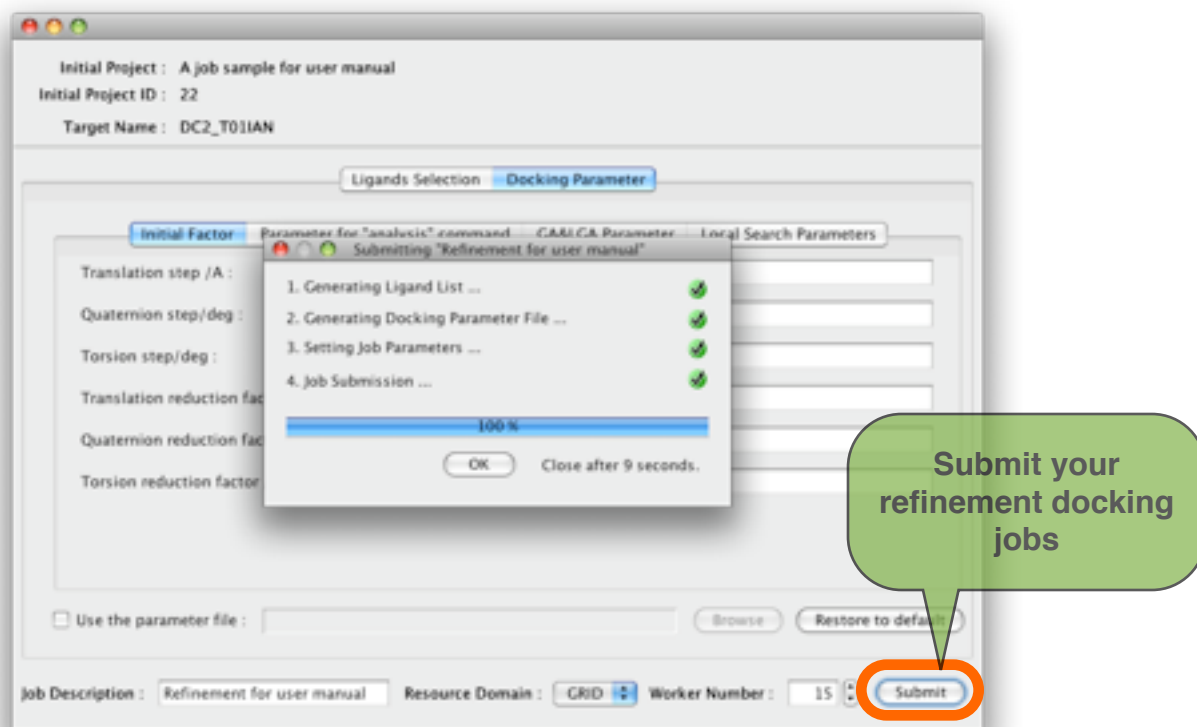
7.9.4. Modify the docking parameters for the refinement simulation, just like setting parameters in the initial docking, you can modify the parameters directly or just use your docking parameters awk file



- 7.9.5. Configure your job
- Input a simple job description.
 - Select your resource domain
 - Decide how many workers(cpus) you want to use

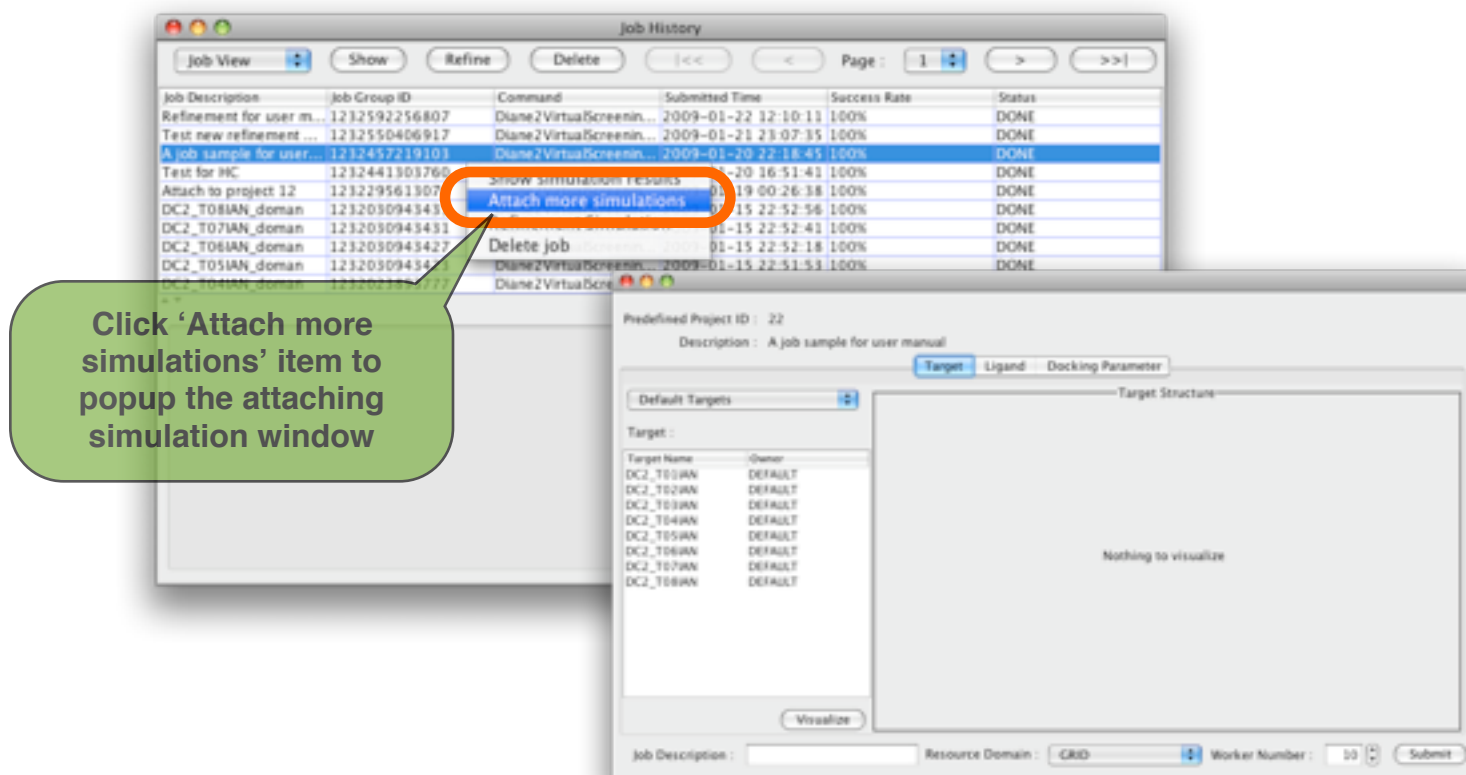


- 7.9.6. Push 'Submit' button to submit the refinement simulations job



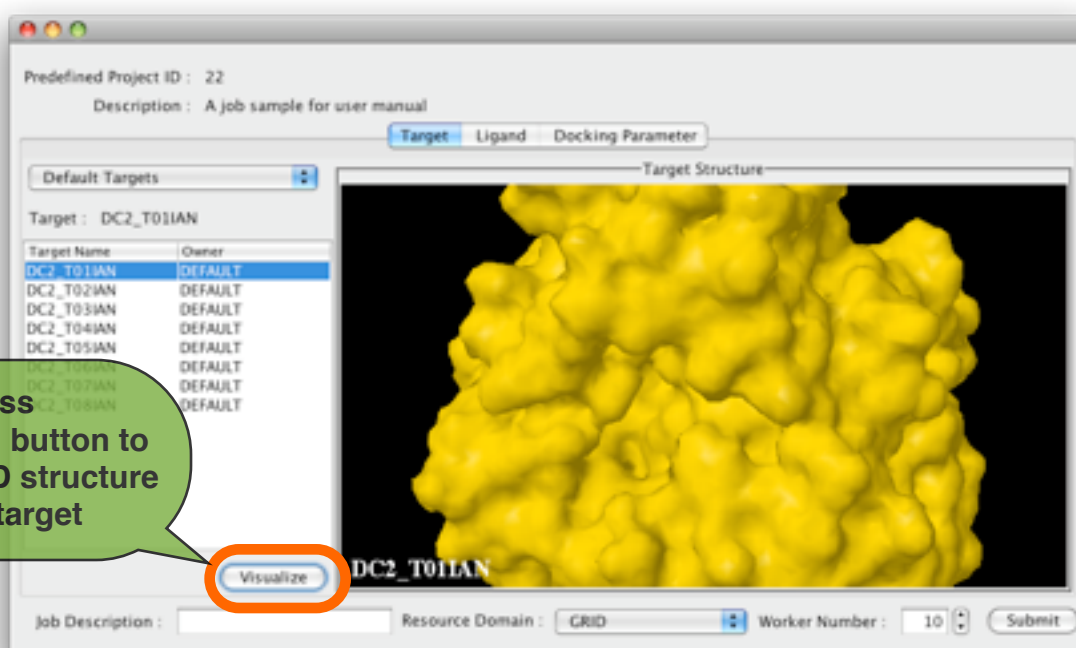
7.10. Attach more docking simulations to an existing project.

7.10.1. Select the item you want to attach and press the right button of mouse to popup the popup menu, and click 'Attach more simulations' item in the job history window

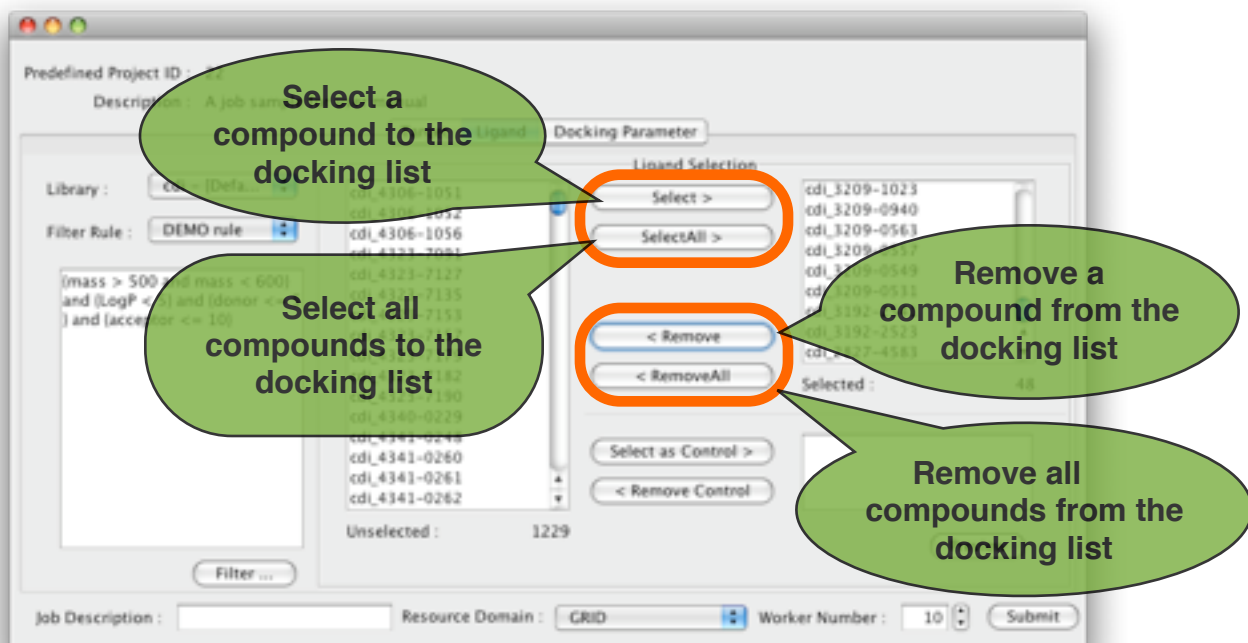


7.10.2. Select Target

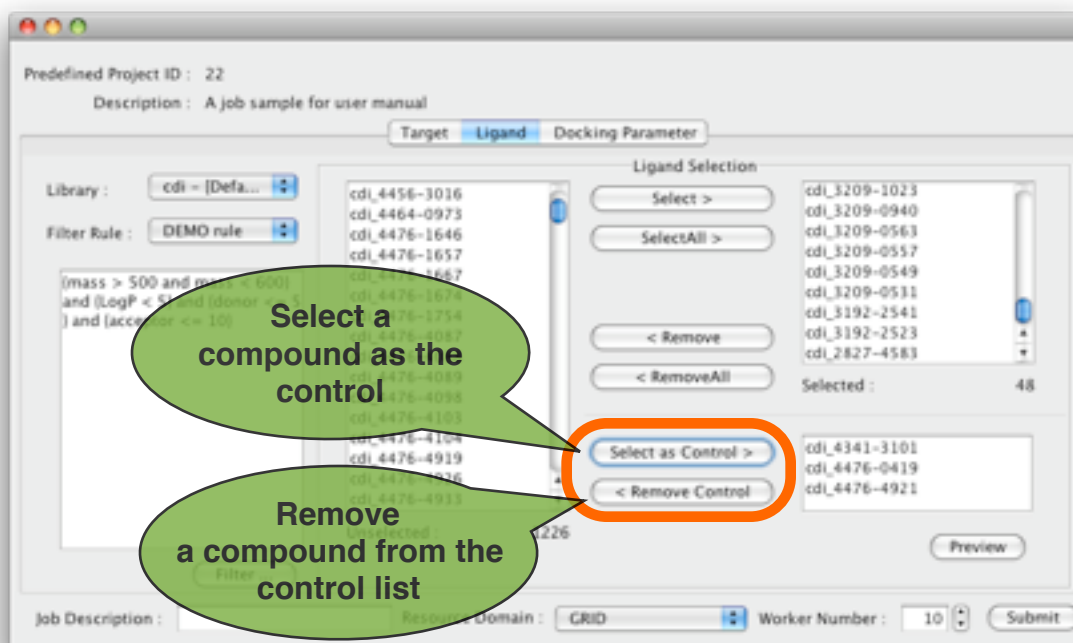
- Select the default target or your own target.
- Visualize the target if available and if you want.



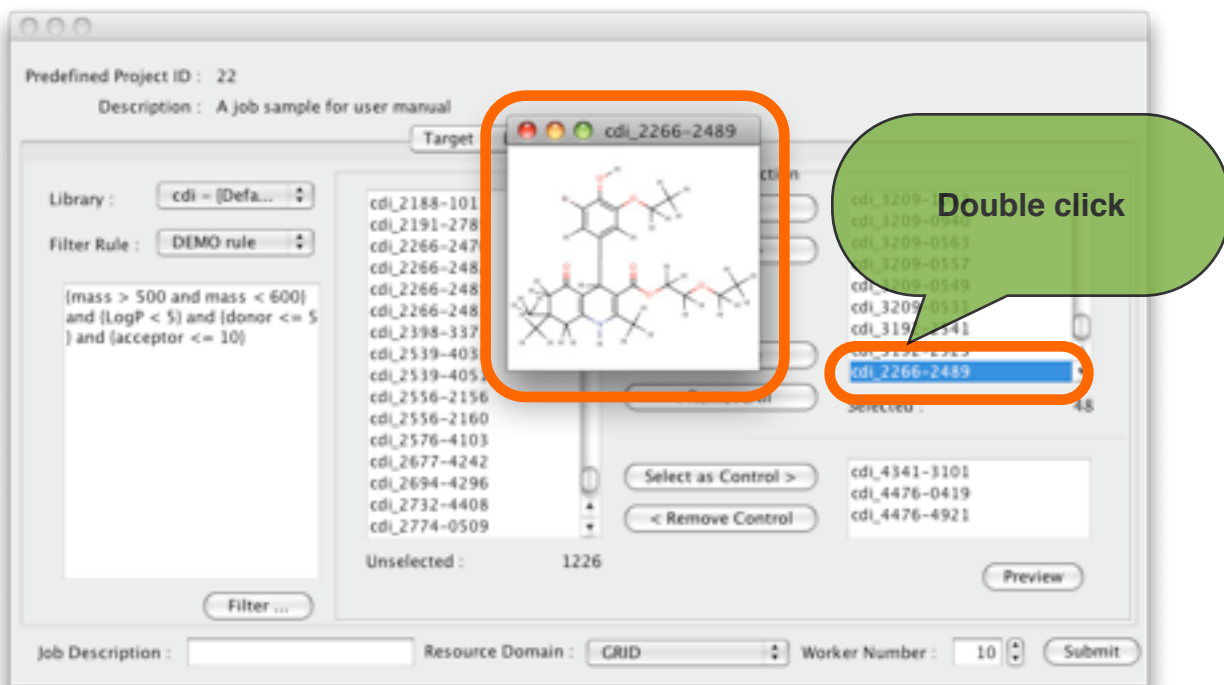
7.10.3. Select Ligands, just like the ligand selection in the initial docking.
 a. Select the ligands that you want to run the docking simulation.



b. You can select the ligand as the control if you want.

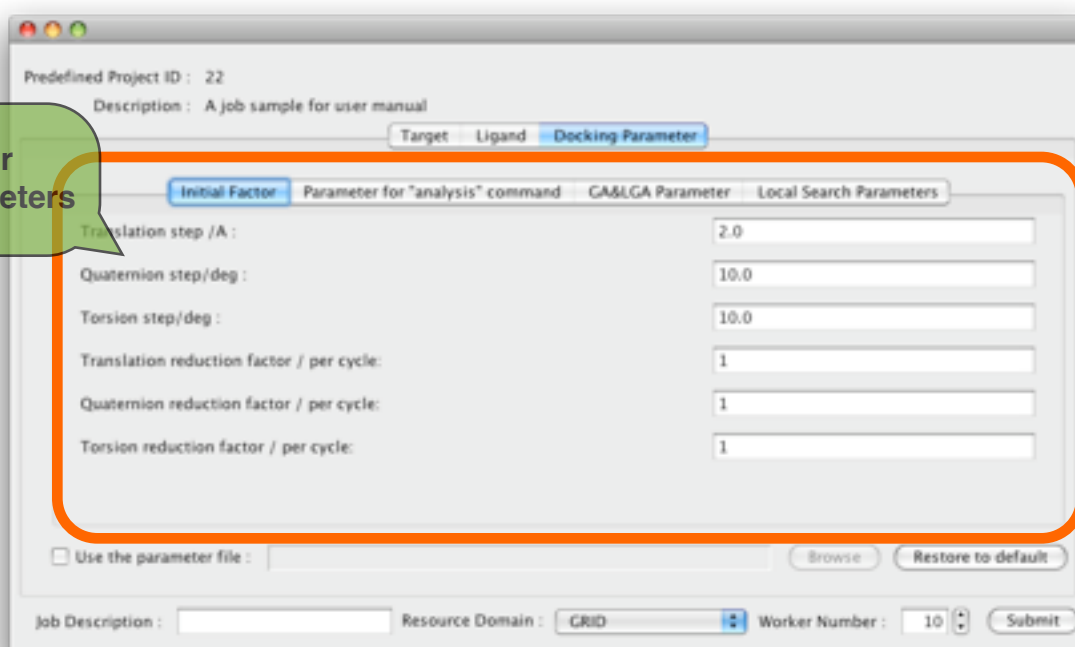


c. And of course, you can preview the 2D structure of ligand if available by double clicking the ligand in the list.

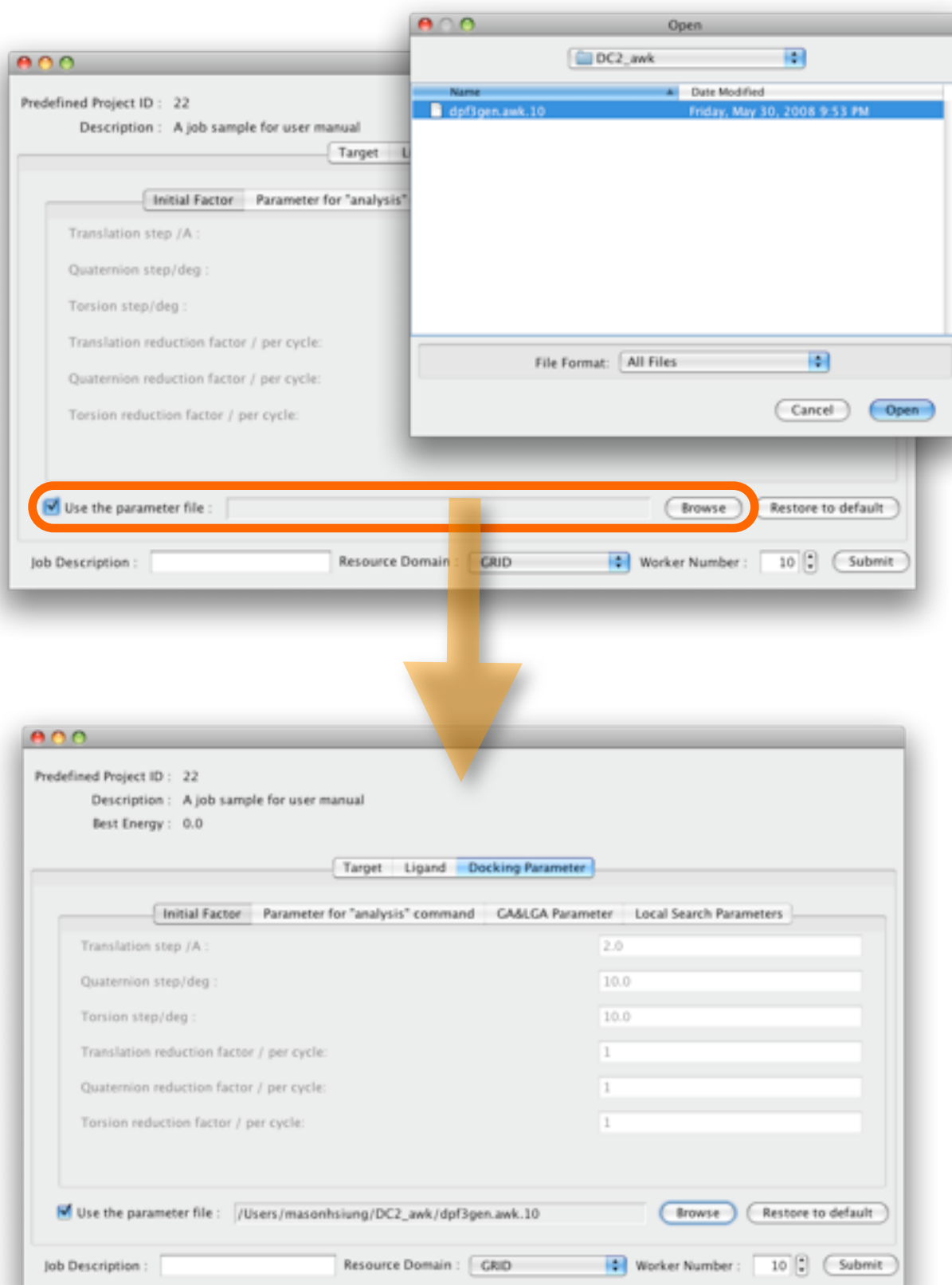


7.10.4. Modify your docking parameters

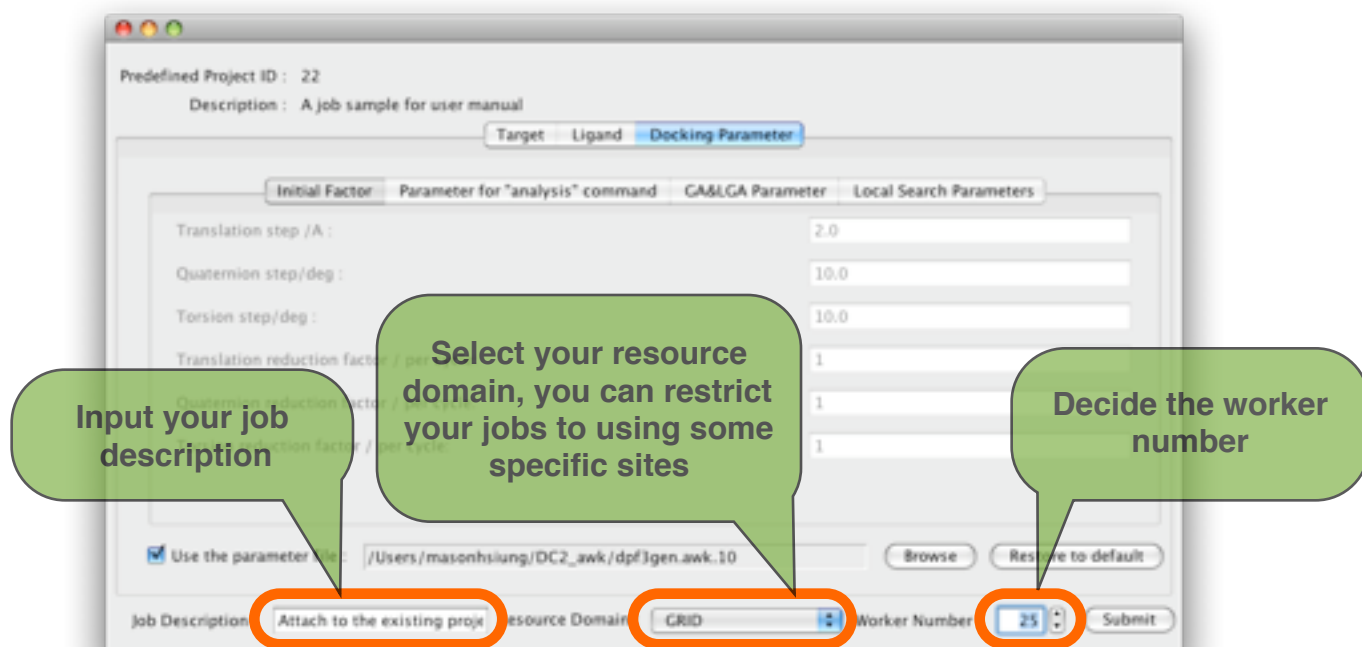
a. There are 4 tabs for setting your docking parameter. Just modify the parameters directly.



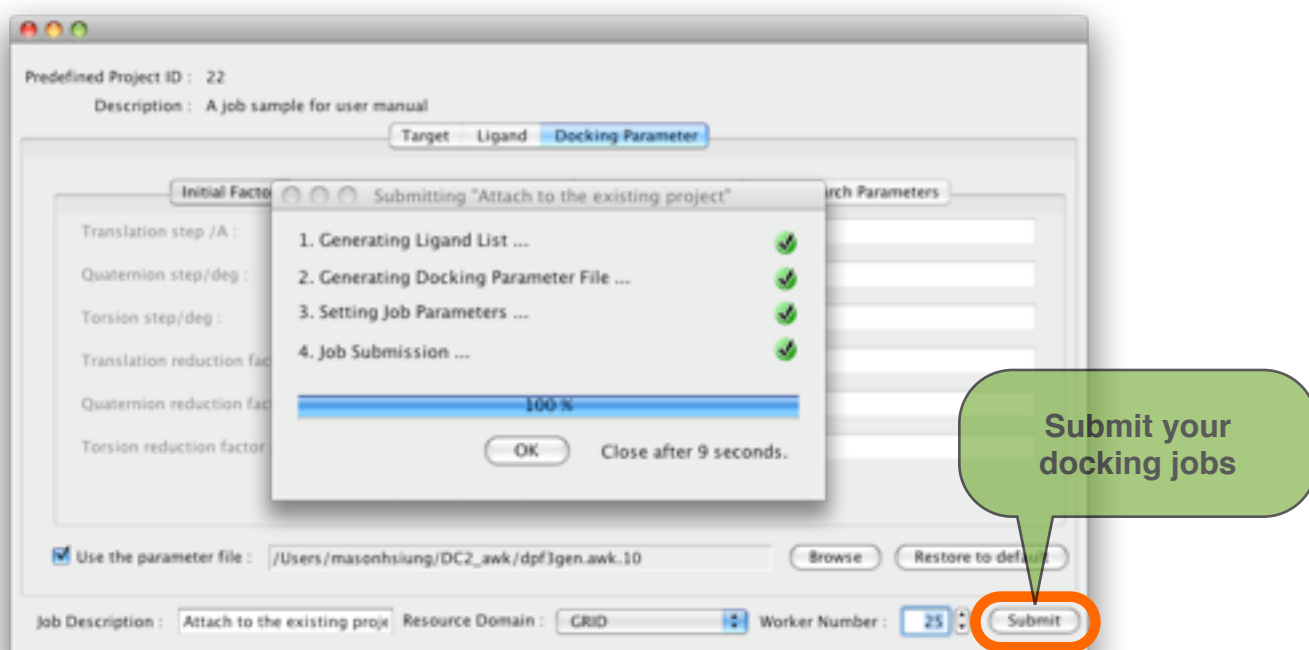
b. Or you can choose to use an existing docking parameter awk file.



- 7.10.5. Configure your job
- Input a simple job description.
 - Select your resource domain
 - Decide how many workers(cpus) you want to use



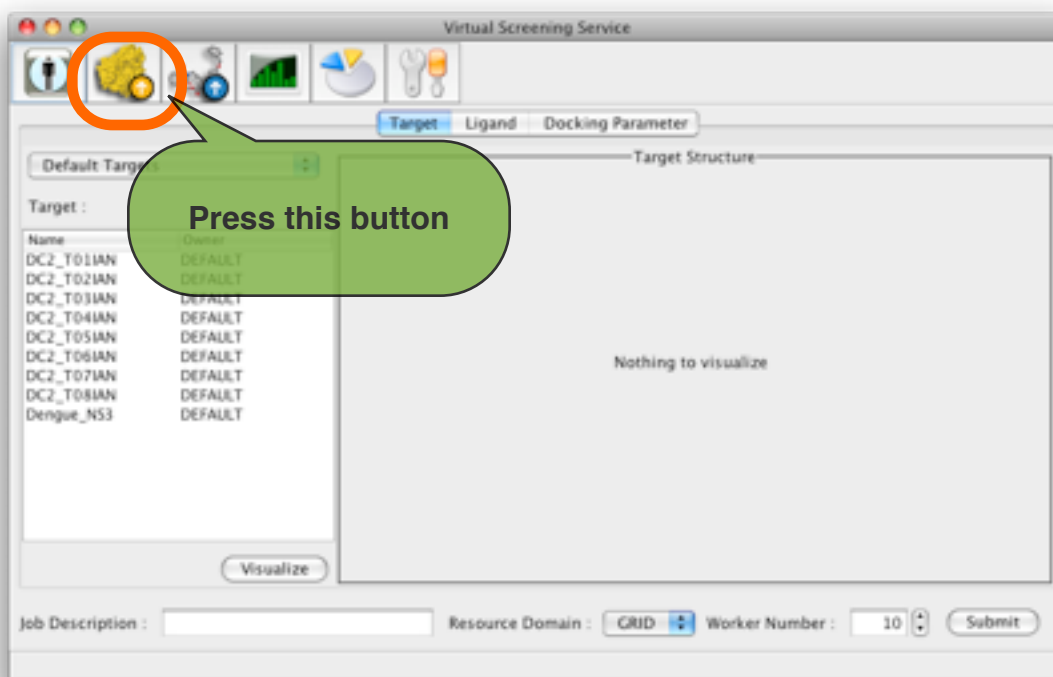
7.10.6. Attaching docking job submission



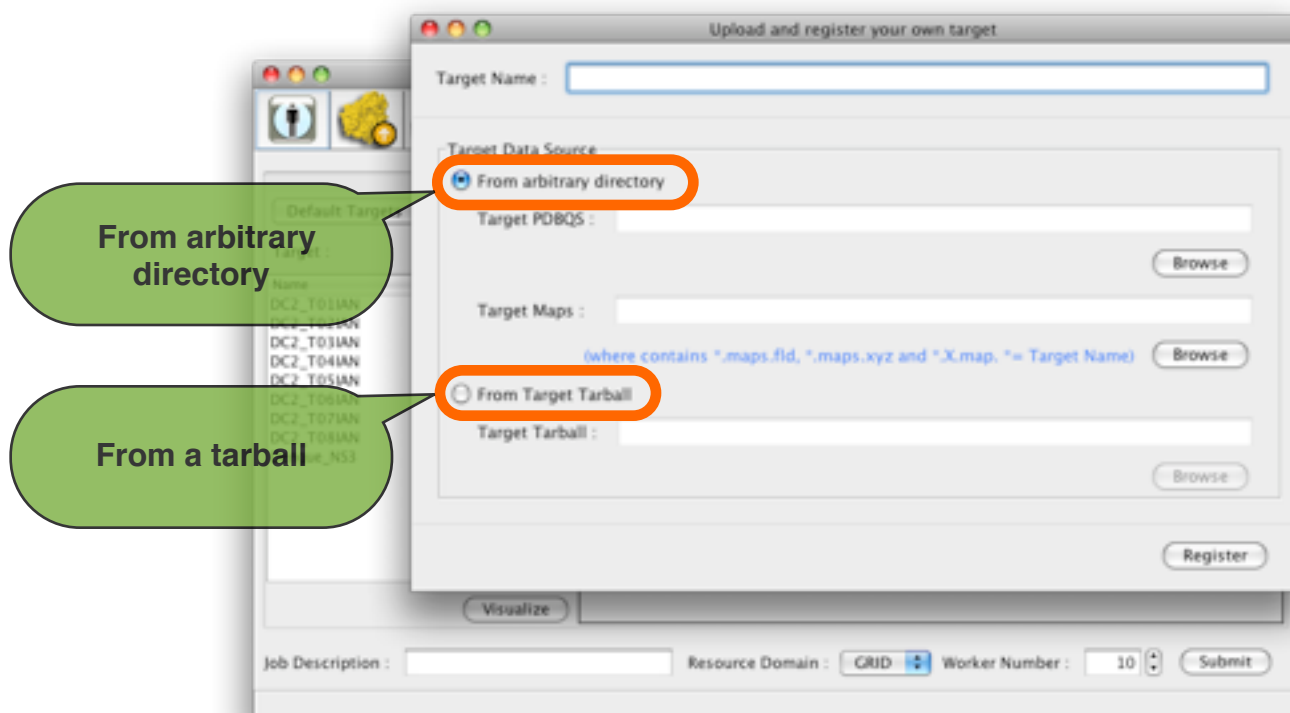
8. Upload your own target and ligands

8.1. Upload your own target

8.1.1. Press the target upload button



8.1.2. Choose how you want to upload your target



- a. From arbitrary directory (Please do this on Linux, unless you are sure your target map files are fine on case-insensitive OS.)
1. Select the target's pdbqs

Upload and register your own target

Target Name :

Target Data Source

☒ From arbitrary directory

Target PDBQS :

Target Maps :

(where contains *.maps.fld, *.maps.xyz and *.X.map, * = Target Name)

☐ From Target Tarball

Target Tarball :

2. Select the directory which contains the target's map, xyz and fld files. (NOTE : Make sure the map, xyz and fld files are under the directory, otherwise you will not be allowed to select the directory.)

Upload and register your own target

Target Name :

Target Data Source

☒ From arbitrary directory

Target PDBQS :

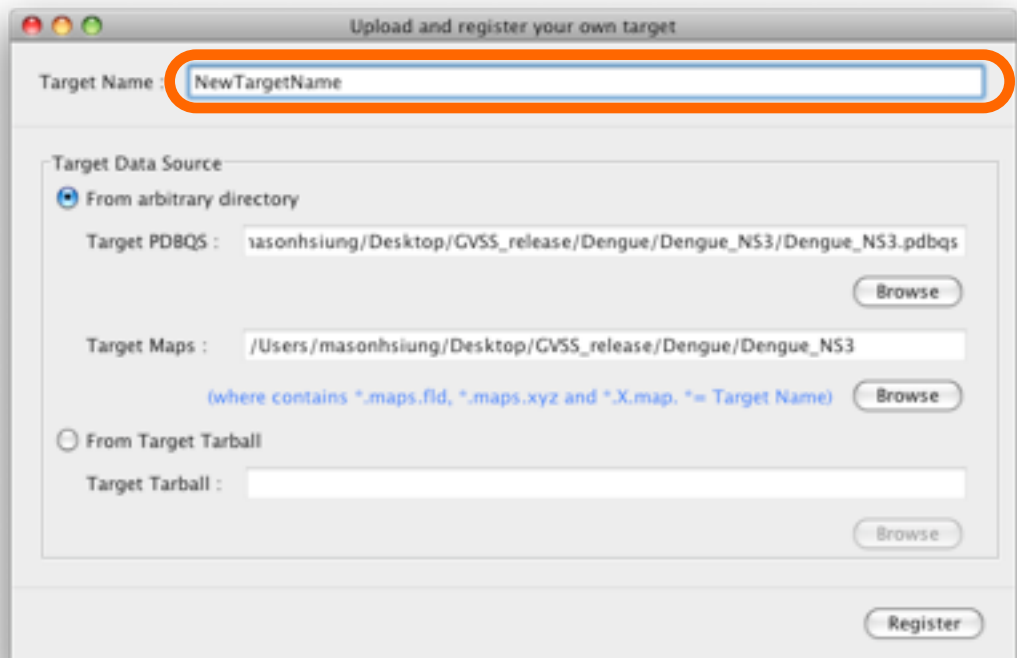
Target Maps :

(where contains *.maps.fld, *.maps.xyz and *.X.map, * = Target Name)

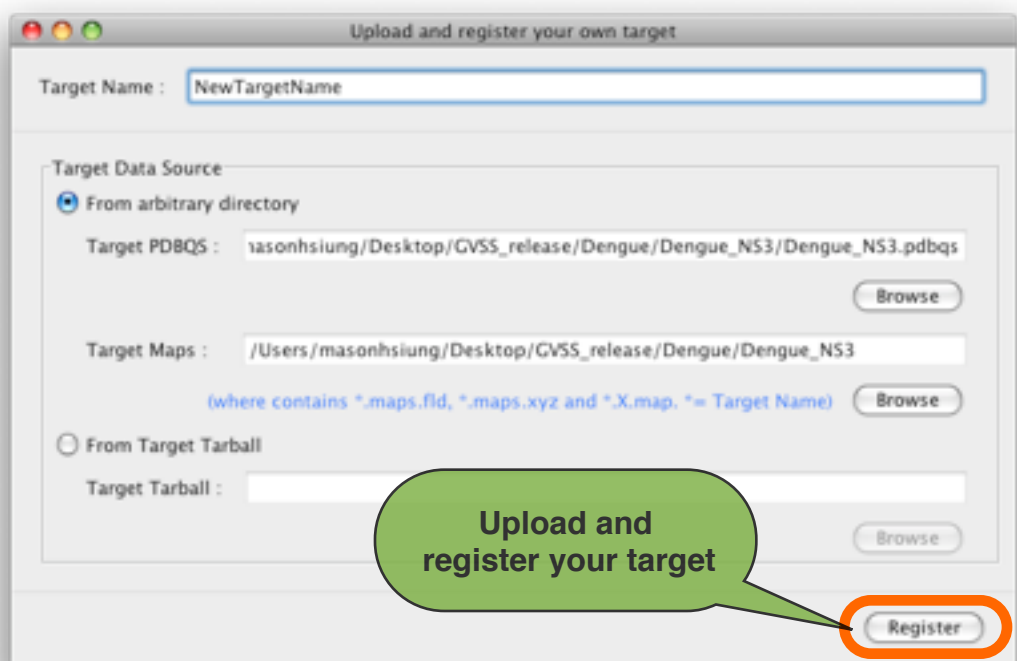
☐ From Target Tarball

Target Tarball :

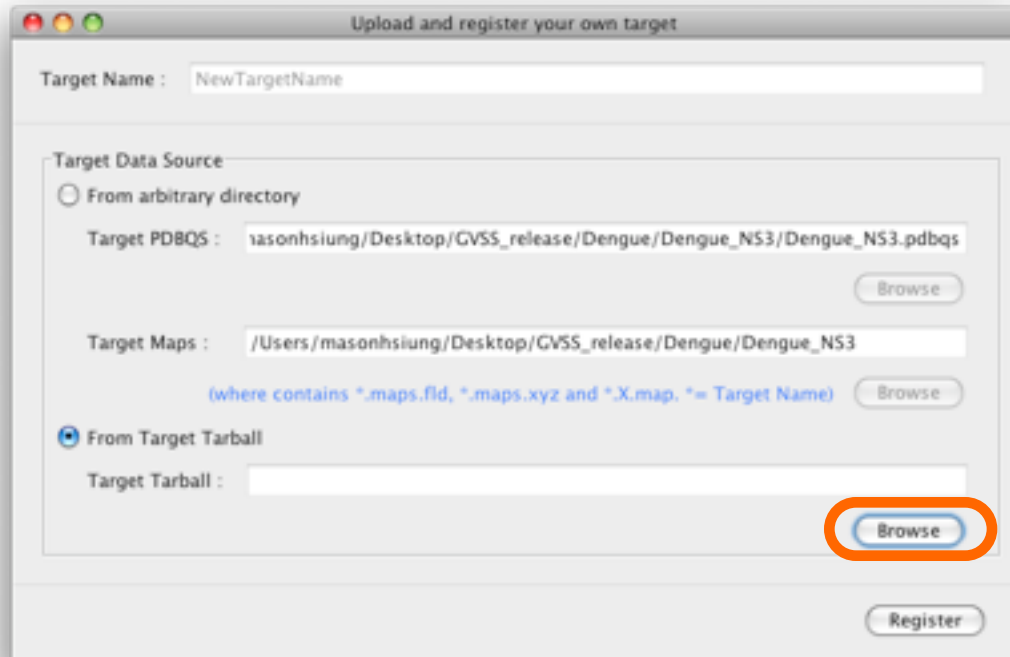
3. Name this target, this will automatically replace the old target name with the new name in all the files(pdbqs, *.map, xyz ...).



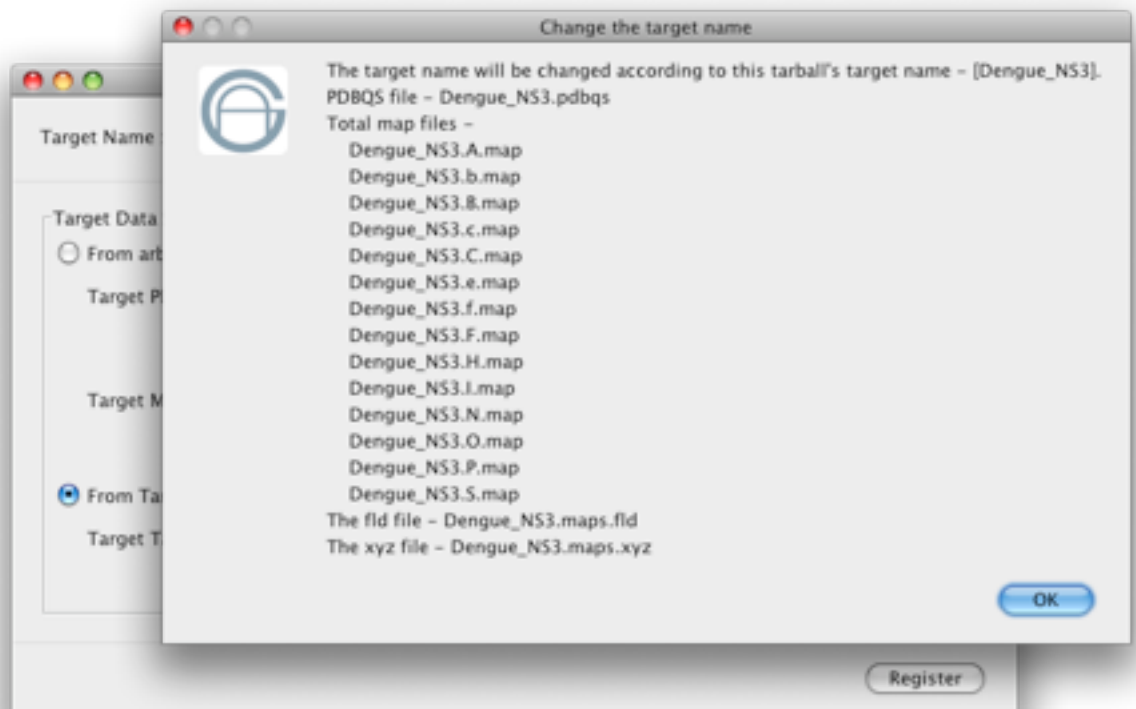
4. Finally, simply press the register button to upload and register your own target.



- b. From a well-packaged target tarball
1. Select the target tarball.



2. System will check the content of the tarball. If the tarball is invalid, you will not be allowed to select the tarball.



3. The target name will be determined automatically according to the target tarball. You are not able to change it.

Upload and register your own target

Target Name : Dengue_NS3

Target Data Source

☐ From arbitrary directory

Target PDBQS : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs Browse

Target Maps : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3
(where contains *.maps.fld, *.maps.xyz and *.X.map. *= Target Name) Browse

☒ From Target Tarball

Target Tarball : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3.tar.gz Browse

Register

4. Finally, simply press the register button to upload and register your own target.

Upload and register your own target

Target Name : Dengue_NS3

Target Data Source

☐ From arbitrary directory

Target PDBQS : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs Browse

Target Maps : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3
(where contains *.maps.fld, *.maps.xyz and *.X.map. *= Target Name) Browse

☒ From Target Tarball

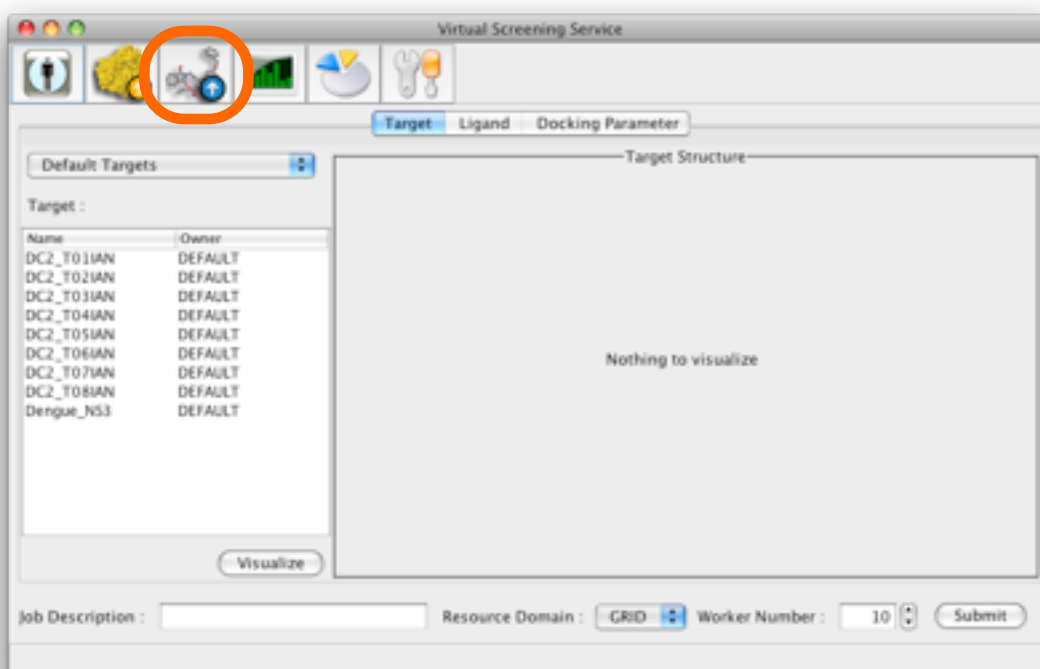
Target Tarball : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3.tar.gz Browse

Register

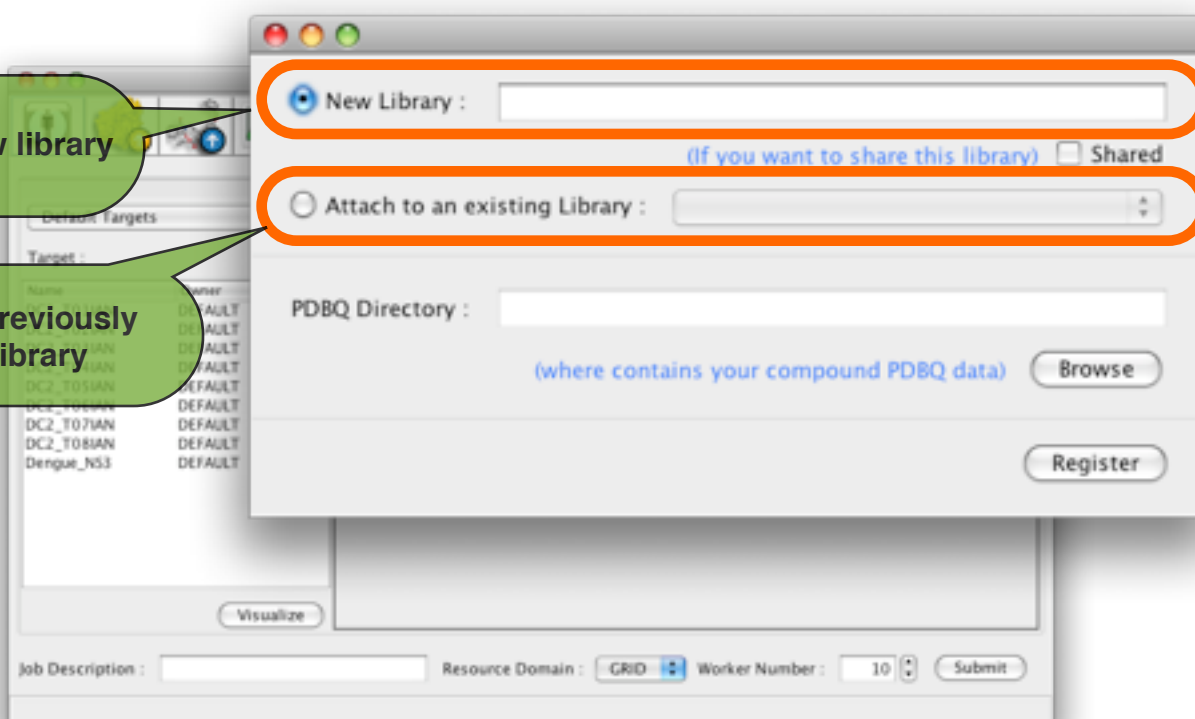
Upload and register your target

8.2. Upload your own ligands.

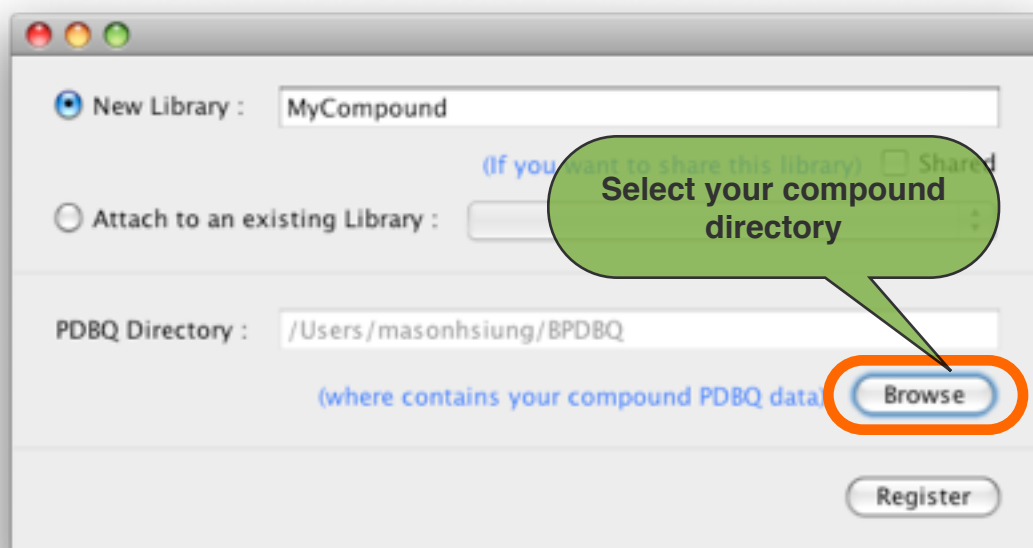
8.2.1. Press the ligand upload button.



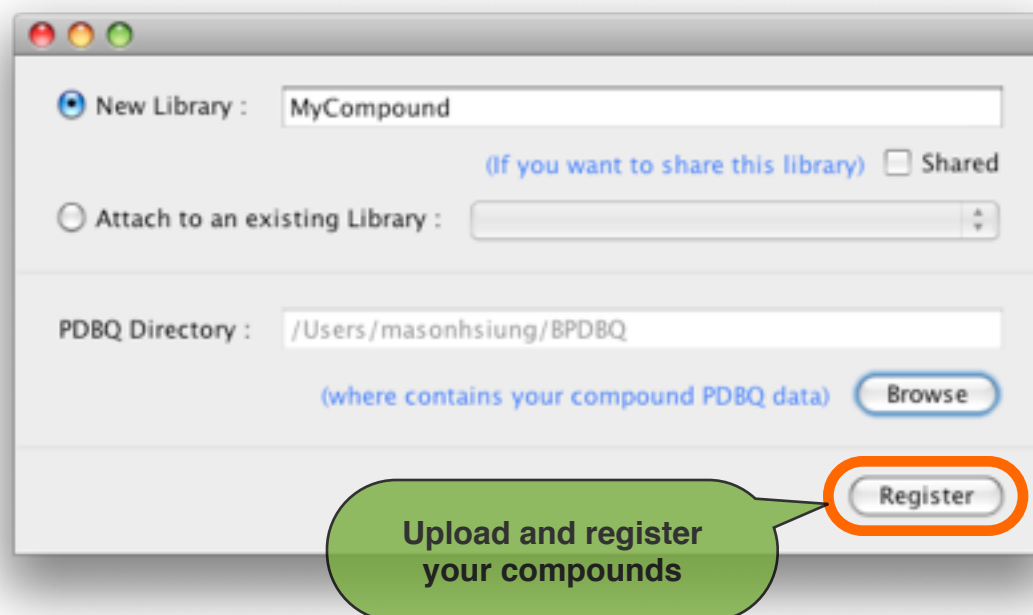
8.2.2. Decide either you want to create a compound library or attach to an existing compound library.



8.2.3. Select the directory which contains your compound PDBQ data.



8.2.4. Finally, simply press the register button to upload and register all the compounds under the directory.



9. References

- 9.1. GAP website - <http://gap.grid.sinica.edu.tw/>
- 9.2. EUAsiaGRID website - <http://www.euasiagrid.org/>
- 9.3. EUAsiaGRID voms website -
<https://vomrs.grid.sinica.edu.tw:8443/vomrs/euasia/vomrs>
- 9.4. MGLTools website - For preparing the target and ligands.
<http://mgltools.scripps.edu>