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

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- 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 <u>http://ca.grid.sinica.edu.tw/certificate/request/request_user_cert.html</u>

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: <u>http://ca.grid.sinica.edu.tw/contact.html</u> 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 (<u>http://ca.grid.sinica.edu.tw/certificate/request/nscert.php</u>). 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
 - <u>http://gnuwin32.sourceforge.net/packages/openssl.htm</u>

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

VQS Account Registration VQS Account Registration Image: the state of the s
VQS Account Registration
· · ·
*Title :
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" © 2009 GAP - Grid Application Platform +886-2-2789-8309 © Contact Us 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

• The 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
 The 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.

5.1. Show the configuration window.

	Virtual Screenin	g Service
Default Targets Target : Target Name Owner	Press th	is button
	QS Client Configuration	Intervice Advanced Metadata Service
	User Key : User VD :	/Users/masonhsiung/MyPEM/userkey.pem Browse
Wsualize		
ob Description :		Save to Current Cancel

- 5.2. Change the location of your user certificate
 - Here you can change the location of your 'usercert.pem' and 'userkey.pem'

/QS Client Configuration	ogin Service Advanced Metadata Service
User Certificate :	/Users/masonhsiung/MyPEM/usercert.pem Browse
User Key :	/Users/masonhsiung/MyPEM/userkey.pem Browse
User VO :	eusta
	Input the full path directly or browse and select your *.pen

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

User Certificate :	/Users/masonhsiung/MyPEM/usercert.pemi Browse
User Key :	/Users/masonhsiung/MyPEM/userkey.pem Browse
User VO :	euasia
	and use the VO you belong t
	Save Save to Current Cancel

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
 - a. Select the default target or your own target.
 - b. 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.

000	Virtual Screening Service	
Select compound docking	a to the used Decking Parameter	
Filter Rule : Lipinski ruL. Control Co	Select > Select > Select All > SelectAll	CdL090A-0221 cdL090A-0245 cdL000A-0245 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL000 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cdL00 cd
Filter	000A-0799 000A-0799 000A-0800 000A-0815 000A-0823 elected : 300001	Remove all compounds from the docking list
Job Description :	Resource Domain : GRID 🔹 V	Worker Number : 10 Submit

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

000	Virtual Screening Service	
🔃 💰 💑 🛲	🅙 💘	
	Target Ligand Docking Parameter	
Library : cdi - [Defa Filter Rule : Lipinski rul (mass > 200 and cos < 600) and (LogP < rul donor Se) and (accutor <= 10)	Ligand Selection cd_000A-0742 cd_000A-0720 cd_000A-020 cd_000A-0289 cd_000A-0689 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0431 cd_000A-0431 cd_000A-0431 cd_000A-0431 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0430 cd_000A-0554 cd_000A-0601 cd_000A-0601	ļ
R	Off_050A-0815 Select as Control > cdi_000A-0102 cdi_050A-0823 Remove Control emove 199 199	Preview
Job Description :	Resource Domain : CRID 🔮 Worker Number : 10 🕃	Submit

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

000	Virtual Screening	Service	
Library : cdi - [Defa 0] Filter Rule : Lipinski rul 0 (mass > 200 and mass < 600) and il on R < St and idence <= S	Virtual Screening	Service $cdi_000A-0431$ $f_{+}^{+}f_{+}^{+}f_{+}^{+}$ $r_{+}^{+}f_{+}^{+}f_{+}^{+}$ $cdi_000A-0221$ $cdi_000A-0225$ $cdi_000A-0419$ $cdi_000A-0430$ $cdi_000A-0430$ $cdi_000A-0430$	
and (LogP < 5) and (donor <= 5) and (acceptor <= 10)	cdi_000A-0111 cdi_000A-0053 cdi_000A-0024 cdi_000A-0874 cdi_000A-0796 cdi_000A-0799 cdi_000A-0815 cdi_000A-0823 cdi_000A-0829 edi_000A-0830	< Remove	11
Filter	Unselected : 299999		Preview
Job Description :	Resource Dom	ain : GRID 🗘 Worker Number : 10	Submit

7.4. Modify your docking parameters7.4.1. There are 4 tabs for setting your docking parameter. Just modify the parameters directly.

800	Virtual Screening Service	
1 🍪 🔧 🗈	I 🕙 👯	
	Target Ligand Docking Par	rameter
Initial Factor	Parameter for "analysis" command GA&LG	A Parameter Local Search Parameters
Translation step /A :	٨	2.0
Quaternion step/deg :		10.0
Torsion step/deg :		10.0
Translation reduction facto	r / per cycle:	1
Quaternion reduction facto	Four tabs for setting you	ur docking
Torsion reduction factor /	parameters	
Use the parameter file :		Browse Restore to default
Job Description :	Resource Domain :	GRD 😧 Worker Number : 10 🗘 (Submit)

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

	Virtu		
1 🔁 🛃 💑 🔼 🕙	dpf3gen awk.	Date N Date N Friday	odnied , May 30, 2008 9:53 PM
	-		
Select your docking	nalysis" ¢		
parameters awk file			
Maximum allowable initial energy :			
Maximum number of retries :		en e Callena	
		File Format: All Files	
			Cancel Ope
	-		
S Use the parameter file :		Browse	Restore to default
lob Description :	Resource Domain :	GBID D Worker Number :	10 Submit
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non 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	Virtual Screen ing Service		
	Virtual Screen Ag Service	rameter	
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Initial Factor Parameter for "ar Cluster tolerance (Angstroms) : External grid energy : Maximum allowable initial energy : Maximum number of retries :	Virtual Screen ng Service	A Parameter Local Search Pa 1.0 1000 0 10000	rameters
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Image: Second system Image: Second system Image: Second	Virtual Screen Ag Service	A Parameter A Parameter 1.0 1000 0 10000	rameters

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

Initial Factor	Parameter for "analysis" comm	and GA&LGA Parameter sample for user manual"	r Local Search Pa	irameters	
Cluster tolerance (Angstroe	1. Generating Ligand List		3]
External grid energy :	2. Generating Docking Para	meter File	3		1
Maximum allowable initial	3. Setting Job Parameters		3		1
Maximum number of retriev	4. Job Submission		3		
	0	Close after 6 sec	conds.		Submit your locking jobs
Use the parameter file : 70	sers/masonhsiung/DC2_awk/d	pf3gen.awk.10	Browse	Restore to def	

7.7.Job monitoring

7.7.1. Push the running job monitoring buttion



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.

	Target	t Ligand De	cking Parameter			
			ink	No. 100		_
Initial Factor		(0mm) (1	Job			000
	Configura 1.		une (beere)	0000	C reger (1 10)	00
Cluster tolerance (Angstrom	5. Job Description	Job Group ID	Command	Submitted Time	Success Rate	Status
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Use the parameter file : /U	se					
A job sample for						_

7.8.2. Visualize your docking simulation results a. Select the job you want to see, and push the 'Show' button.



Interview Show Refine Delete <	4		_		History	fol		
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Stor Standyold for Units (221433/2110) Dater Virsus/Streets	-		late	Success	Submitted Time	Command	Job Group ID	ob Description
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Much to project 12 1232295613076 Date2VthatGreenen, 2099-01-19 00 26 35 100% DOW The result SQ_T058/M_doman 1232039643431 Date2VthatGreenen, 2099-01-15 22 52 46 100% SIMULATIONS IN t CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 52 41 100% SIMULATIONS IN t CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 51 43 100% DOW DATE CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DATE CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DATE CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DATE CQ_T054/M_doman 1232039643433 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DATE CQ_T054/M_doman 1232023893777 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DOW DATE CQ_T054/M_doman 1232023893777 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW DOW DATE CQ_T054/M_doman 1230021893777 Date2VthatGreenen, 2099-01-15 22 51 53 100% DOW		L		\$1:41 100%	2009-01-20 16	Diane2VirtualScreenin.	1232441303760	Test for HC
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conformation of a simulation 13.14 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 13.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54 15.54	Press to show th	e best	101IAN 66.K781-1				
Conformation of a simulation of a simulation of the second		-13.73 DC2	101HN cdi_K781-1				
-13.54 DC2 D1MN c0(_CPH6-04 -13.54 DC2 D1MN c0(_CPH6-04 -13.48 DC PD1MN c0(_4159-04 Show Brst Conformation Energy Threshold : 0.0 Download dlg Energy Histogram Get Energy List Dewnload PD80	conformation of a s	Imulation	101MN cdi_K623-0	h		31	
-15.34 DC2 (510N) (d) (540-0) * -15.45 DT011N) (d) (540-0) * Show Bry Complex Show Bry Complex * Show Bry Complex Forenyy Histogram Cet Energy List Download PD8Q		-13.54 DC2	011MN cdi_C700-0	- L.			
Show Best Conformation Energy Threshold : 0.0 Download dig Energy Histogram Get Energy List Download PDBQ		-13.34 DC2	101MN 68_C946-0				
Show Bot Conformation Energy Threshold : 0.0 Download dlg Energy Histogram Get Energy List Download PD8Q Best Complexes Best Conformations Postograms		1.2.48	1111MA 00(4123-4	Para 19			
Show Best Conformation Energy Threshold : Download elig Energy Histogram Get Energy List Download PD8Q		C Show Berry Com	olex				
Show Best Conformation Energy Threshold : Download dbg Energy Histogram Get Energy List Download PDBQ						P 10.0	
Energy Threshold : 0.0 Download dlg Energy Histogram Get Energy List Download PDBQ Best Complexes Best Conformations Plotograms		Show Best Conf	ormation				
Energy Threshold : 0.0 Download dlg Energy Histogram Get Energy List Download PD8Q Best Complexes Best Conternations Pistograms							
Cet Energy List Complexes Best Complexes Best Conformations Bistograms					\sim	<i>1</i>	
Oownload dig Energy Histogram Get Energy List Download PDBQ Best Complexes Best Complexes		Energy Threshold	0.0				
Get Energy List Download PDBQ Best Complexes Best Conformations Pristograms		Download dig) (Energy Histogr	um)			
Best Complexes Best Conternations Pristograms							
His Complexes desicontentations missioners		Centermation	C. Described and				
		Cet Energy Lis	t Download PC	80			

c. Show the best ligand conformation of a simulation.

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



7.8.3. Download the simulation results

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





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

00		Job History	
Job View 🔹	Show Refin	e) Delete I<< Page: 1	
lob Description	Job Group ID	Convend Submitted Time Success Rate	Status
lest new refinement	1232550406917	Diane mualScreenin 2009-01-21 23:07:35 100%	DONE
job sample for user	1232457219103	Diane2 Configure Discreterin 2009-01-20 22:18:45 100%	DONE
est for HC	1232441303760	Diane24 muabcreenin 2009-01-20 16:51:41 100%	DONE
ttach to project 12	1232295613076	Diane2V/nualScreenin 2009-01-19 00:26:38 100%	DONE
C2_T08IAN_doman	1232030943435	our Press 'Refine' button to	DONE
C2_T07IAN_doman	1232030943431	Diane 21 mualScreenin 2009-01-15 22:52:41 100%	DONE
C2_T06IAN_doman	1232030943427	puezy popup the retinement	DONE
C2_T05IAN_doman	1232030943423	Dane2v multicreener 2000 politics 22:51:53 pont	DONE
C2_T04IAN_doman	1232023893777	Dune 2V subset Simulation window	DONE
C2_T03IAN_doman	1232023893773	Diane2VirtualScreenin 2009-01-15 22:09:59 100%	DONE
_	_	21	

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

00		Job I	History	
Job View	Show Refi	ne Delete (: 1 : >>>
Job Description	Job Group ID	Command	Submitted Time Succe	ss Rate Status
Test new refinement	1232550406917	Diane2VirtualScreenin.	. 2009-01-21 23:07:35 100%	DONE
A job sample for user	12124572 Show	simulation results	2009-01-20 22:18:45 100%	DONE
Test for HC	12324412		2009-01-20 16:51:41 100%	DONE
Attach to project 12	123225 6	more simulations	009-01-19 00:26:38 100%	DONE
DC2_T08IAN_doman	123203 (g) Refine	ment simulation	009-01-15 22:52:56 100%	DONE
DC2_T07IAN_doman	12320303		2009-01-15 22:52:41 100%	DONE
DC2_T06IAN_doman	1232030943427	Diane2VirtualScreenin.	. 09-01-15 22:52:18 100%	DONE
DC2_T05IAN_doman	1232030943423	Diane2VirtualScreenin.	2009-01-15 22:51:53 100%	DONE
DC2_T04IAN_doman	1232023893777	Diane2VirtualScreenin	2009-01-15 22:11:27 100%	DONE
DC2_T03IAN_doman	1232023893773	Diane2VirtualScreenin.	Click 'Befine	ment Simulation'
			simulat	ion 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.

Initia Initial P Targ	l Project : A job sample for o roject ID : 22 et Name : DC2_T01IAN	iser manual		
		Ligands Selection Doc	king Parameter	
			Ligand Selection	
Start	5HOW>>	[-14.370] cdi_K781-1 [-14.220] cdi_8011-0 [-14.160] cdi_K781-1 [-14.020] cdi_K781-1 [-14.020] cdi_K781-7 [-11.970] cdi_K781-7	Select >	
Decide the range the slider bar	with	-13.750 cft (X781-1 -13.730) cft (X781-1 -13.730) cft (X781-1 -13.730) cft (X781-1 -13.570) cft (X781-1 -13.570) cft (X781-1 -13.570) cft (X781-0 -11.540) cft (X700-0 -11.540) cft (X700-0	<pre>< Remove </pre> Selected	: 0
		-11.480 cd, 4159-0 -13.380 cd, K623-0 -13.380 cd, K623-0 -13.310 cd, K623-0 -13.300 cd, E823-0 -13.260 cd, C708-0 +	Select as Control >	
		Unselected : 383		Preview
Job Descri	ption :	Resource Domain	: G 😫 Worker Number :	10 🕄 Submit

b. Filter the ligands with a given energy threshold

	Target Name : DC2	T01IAN			
			igands Selection De	cking Parameter	
				Ligand Selection	
	Start 1	nd 383	-14.370] cdi_K781-141 -14.220] cdi_8011-010 -14.160] cdi_K781-155 -14.020] cdi_D426-110	Select >	
		HOW >>	-14.000] cdi_K781-769		
	Energy threshold : -14	.0		< Remove	
		HOW >>		< RemoveAli Selected :	0
				Select as Control >	
Decide the	range with				
the slid	er bar			(< Remove Control	
		U	nselected : 5		Preview

c. Select the ligands that you want to refine

Target Na	Select a compound to the Decking Pa	rameter
Start 1	docking list	Select > [-12.840] cdl_C397-00 1-12.890] cdl_C073-26 SelectAll > [-12.890] cdl_E713-02
Energy Tresholo	Select all compounds to the docking list	< Remove All Selected
	(-12.490) cft (X781-0 (-12.480) cft (4186-0 (-12.480) cft (4186-0 (-12.480) cft (4186-0 (-12.480) cft (55-3) (-12.460) cft (55-3) (-12.460) cft (5692-1) (-12.460) cft (5692-1) (-12.46	Remove Control > 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

	00	
	Initial Project : A job sample for user manual nitial Project ID : 22 Target Name : DC2_T01IAN	
Modify your	Ligands Selection	Docking Parameter
docking parameters	Translation step /A :	2.0
	Quaternion step/deg :	10.0
	Torsion step/deg :	10.0
	Translation reduction factor / per cycle:	1
	Quaternion reduction factor / per cycle:	1
Or choose a docking parameter awk file	Torsion reduction factor / per cycle:	1
	Use the parameter file :	Restore to default
jot	Description : Resource Dom	sain : CRID 🗘 Worker Number : 10 🗘 Submit
	30	1

7.9.5. Configure your job

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

6	800			
	Initial Project : A job sample for user manual Initial Project ID : 22			
	Target Name : DC2_T01IAN			
	Ugands Selection De	cking Parameter		
	Initial Factor Parameter for "analysis" command	GA&LGA Parameter	r Local Search Parameters	
	Translation step /A :	2	2.0	
	Quaternion step/deg :	1	10.0	
	Torsion step/deg :	1	10.0	
	Select your resourc	e	1	
	domain, you can rest	rict	Deside the workey	
Input you	r job	me	number	
descript	ion specific sites			
	Use Ste partmeter file :		Browse Recore to default	
	Job Description Refinement for user manual Resource Domain	CRID : No	orker Number	

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

	Ligands Selection Do	cking Parameter				
Initial Factor	A Submitting Refinement	CARLCA Parameter for user manual*	Local	Search Paramet	ers	
Oustamion step/dep:	1. Generating Ligand List		2	-	_	
Quaternion scept bog :	2. Generating Docking Parameter I 3. Setting Job Parameters	ile	2	_	_	
Torsion step/deg :	4. Job Submission		õ l	_		
Translation reduction fac	100 %		_			-
Quaternion reduction fac	(())	Close after 0 secon		(- Cu	hmit vour
Torsion reduction factor		close after 9 secon	us.		rofino	onnt your popt dooki
					rennei	ioho
						Jobs

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
 - a. Select the default target or your own target.
 - b. 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.

		Target Li	pand Dockin	g rarameter		
				Ligand Selection		
Library : edi	i - (Defa	cdi_4456-3016	<u> </u>	Select >	cdi_3209-1023	ñ
in the second	MO cula	cdl_4464-0973			cdl_5209-0940	- 11
riber Kulé : Ebe	NO THE	cd_4476-1646 cdi 4476-1657	e	SelectAll >	cdi 3209-0557	- 11
(mars > 500 mm	1 m 2 com	cdi 4476 1667			cdi_3209-0549	
and (LogP < S	nd (donor <= 5	cdL4476-1674			cdi_3209-0531	
) and (acce cor		t a			cdi_3192-2541	U
	compound	d as the		< Remove	cdi 2827-4583	-
	compound	cdi 4476-4089		< RemoveAll	Enlasted :	
	cont	rol 476-4098	$\langle \rangle$		selected :	48
		401_4478-4104		Select as Control >	cdi_4341-3101	_
		cdi_4476-4919		Server as control >	cdi_4476-0419	
		cdi 4476-4933		< Remove Control	cdi_4476-4921	
	Rem	ove				
		Unselected :	1226			-

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

ocomposition region antipic re	Target	• O O cdi_2266-2489		
Library : cdi = [Defa ¢] Filter Rule : DEMO rule ¢ (mass > 500 and mass < 600) and {LogP < 5} and (donor <= 5)) and (acceptor <= 10)	cdi_2188-101 cdi_2191-278 cdi_2266-247 cdi_2266-248 cdi_2266-248 cdi_2266-248 cdi_2339-337 cdi_2539-403 cdi_2539-403 cdi_2556-2166 cdi_2556-2166 cdi_2556-2160 cdi_2576-4103 cdi_2677-4242 cdi_2694-4296 cdi_2694-4296 cdi_2573-4408	Select as Control 2	cdi 3209- Doub cdi 3209- 0500 cdi 3209-0549 cdi 3209-0549 cdi 3209 cdi 3200 cdi 3200	le click
	cd_2774-0509 Unselected :	Remove Control 1226	cdl_4476-4921	eview -

7.10.4. Modify your docking parameters

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

Modify your	Description : A job sample for user manual Target Ligand Docking Parameter for "analysis" command GA&LG	A Parameter
parameter	Translation step /A :	2.0
	Quaternion step/deg :	10.0
	Torsion step/deg :	10.0
	Translation reduction factor / per cycle:	1
	Quaternion reduction factor / per cycle:	1
	Torsion reduction factor / per cycle:	1
	Use the parameter file :	Browse Restore to default

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

00	DC2_awk
redefined Project ID : 22 Description : A job sample for user manual	Name Dute Modified Dute Modified Priday, May 30, 2008 9-53 PM
Target	L
Initial Factor Parameter for "analysis	c
Translation step /A :	1
Quaternion step/deg :	
Torsion step/deg :	
Translation reduction factor / per cycle:	
Quaternion reduction factor / per cycle:	File Format: All Files
Torsion reduction factor / per cycle:	Cancel
SUse the parameter file :	Browse Restore to default
Job Description : Resource	Domain : CRID 🗣 Worker Number : 10 🕻 Submit
Resource Resource Predefined Project ID : 22 Description : A job sample for user manual But foremer: 0.0	Domain : CRUD 😵 Worker Number : 10 🕄 Submit
Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0	Domain : CRID Vorker Number : 10 Submit
Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target	Domain : CRID Vorker Number : 10 Submit
Resource Res	Domain : CRUD Vorker Number : 10 Submit
Job Description : Resource Resource Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target i Initial Factor Parameter for "analysis Translation step /A : Quaternion step/deg : Parameter for "analysis	Domain : CRID Vorker Number : 10 Submit
Job Description : Resource Resource Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target Initial Factor Parameter for "analysis Translation step /A : Quaternion step/deg : Torsion step/deg :	Domain : CRID Worker Number : 10 Submit
Job Description : Resource Resource Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target : Initial Factor: Parameter for "analysis Translation step /A : Quaternion step/deg : Torsion step/deg : Translation reduction factor / per cycle:	Ligand Docking Parameter s* command GA&LGA Parameter Local Search Parameters 2.0 10.0 1
Job Description : Resource Resource Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : Best Energy : 0.0 Target Initial Factor Parameter for "analysis Translation step /A : Quaternion step/deg : Translation reduction factor / per cycle: Quaternion reduction factor / per cycle:	Comain : CRUD Vorker Number : 10 Submit
Job Description : Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target : Initial Factor Parameter for "analysis Translation step /A : Quaternion step/deg : Torsion step/deg : Translation reduction factor / per cycle: Quaternion reduction factor / per cycle: Torsion reduction factor / per cycle:	Comain : CRID Worker Number : 10 Submit
Job Description : Resource Predefined Project ID : 22 Description : A job sample for user manual Best Energy : 0.0 Target : Initial Factor: Parameter for "analysi Translation step /A : Quaternion step/deg : Torsion step/deg : Translation reduction factor / per cycle: Quaternion reduction factor / per cycle: Torsion reduction factor / per cycle: Wise the parameter file : Use the parameter file :	Ligand Docking Parameter s ^c command GA&LGA Parameter Local Search Parameters 2.0 10.0 1 1 1 1 2.0 10.0 1 2.0 10.0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

7.10.5. Configure your job

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



7.10.6. Attaching docking job submission

Initial Facto	○ ○ ○ Submitting "Attach to the existing project"	rch Parameters	
Translation step /A :	1. Generating Ligand List	3	
Quaternion step/deg :	2. Generating Docking Parameter File	3	
Torsion step/deg :	3. Setting Job Parameters	3	
Translation reduction fac	4. Job Submission	3	
Quaternion reduction fac	100 %	_	Cubmit
Torsion reduction factor	OK Close after 9 sec	conds.	docking jobs

8. Upload your own target and ligands

- 8.1. Upload your own target
 - 8.1.1. Press the target upload button

	1	Virtual Screening Service
Default Target Target : Name DC2_T01IAN DC2_T03IAN DC2_T03IAN DC2_T03IAN DC2_T05IAN	Press this Overal Default Default Default	Target Ligand Docking Parameter Target Structure
DC2_T05IAN DC2_T05IAN DC2_T07IAN DC2_T07IAN DC2_T08IAN Dengue_NS3	DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT	Nothing to visualize
Job Description :		Resource Domain : GRUD 🔹 Worker Number : 10 🗘 Submit

8.1.2. Choose how you want to upload your target

	000	Upload and register your own target
	Target Name :	
	Target Data Source From arbitrary dis	rectory
From arbitrary	Target PDBQS :	Browse
DC2_T01IAN DC2_T01IAN DC2_T01IAN DC2_T01IAN	Target Maps :	ere contains ".maps.fld, ".maps.xyz and ".X.map. "= Target Name) Browse
Erom a tarball	From Target Tarb Target Tarball :	
Troin a tarbai		Browse
		Register
	(Visualize)	
Job Description :		Resource Domain : GRID 🗣 Worker Number : 10 🗘 Submit
		37

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
irectory
1asonhsiung/Desktop/GVS5_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs
Browse Select target's pdbqs here contains *.maps. (1 * maps.xyz and * X maps. * Target ame) Browse
ball
Browse
Register

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.)

Target Data Source	
• From arbitrary d	rectory
Target PDBQS :	hasonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs
	Browse
Target Maps :	/Users/masonhsiung/Desktop/GV55_release/Dengue/Dengue_NS3
(w)	tere contains *.maps.fid, *.maps.xyz and *.X.map. *= Target Name Browse
From Target Tarl	lila
Target Tarball :	Select the directory
	Browse

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

Target Data Source		
From arbitrary d	irectory	
Target PDBQS :	asonhsiung/Desktop/GVS5_release/Dengue/Dengue_NS3/Dengu	e_NS3.pdbqs
		Browse
Target Maps :	/Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS	3
(w	here contains *.maps.fld, *.maps.xyz and *.X.map, *= Target Name)	Browse
From Target Tar	ball	
Target Tarball :		
		Brown

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

00	Upload and register your own target
Target Name :	NewTargetName
Target Data So	urce
From arbitr	ary directory
Target PD8	QS : hasonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs
	Browse
Target Map	s : /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3
	(where contains *.maps.fld, *.maps.xyz and *.X.map. *= Target Name) Browse
🖯 From Targe	t Tarball
Target Tarb	all :
	Upload and register your target
	Register

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

Upload and register your own target
NewTargetName
urce
rary directory
IQS : hasonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs
Browse
s: /Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3
(where contains *.maps.fld, *.maps.xyz and *.X.map. *= Target Name) Browse
et Tarball
ball :
Browse
Register

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.

Target Data Source	
O From arbitrary di	rectory
Target PDBQS :	hasonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3/Dengue_NS3.pdbqs
	Browse
Target Maps :	/Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3
(wł	ere contains *.maps.fld, *.maps.xyz and *.X.map. *= Target Name) Browse
From Target Tart	sall
Target Tarball :	/Users/masonhsiung/Desktop/GVSS_release/Dengue/Dengue_NS3.tar.gz
	Browse

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



8.2. Upload your own ligands.

8.2.1. Press the ligand upload button.

		Target Ligand Docking Parameter
Default Target	s 💀	Target Structure
Name DC2_T014AN DC2_T024AN DC2_T024AN DC2_T044AN DC2_T054AN DC2_T054AN DC2_T054AN DC2_T074AN DC2_T074AN DC2_T084AN Dengue_NS3	Owner DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT DEFAULT	Nothing to visualize
b Description :		Resource Domain : GRID Vorker Number : 10 Submit

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

	000	
	• New Library :	
Name this new library	(If you want to share this library)	Shared
Delast Targets	Attach to an existing Library :	•
Select the previously created library	PDBQ Directory : AT AT AT AT AT (where contains your compound PDBQ data)	rowse
DC2_T07IAN DEFA DC2_T08IAN DEFA Dengue_NS3 DEFA	ar ar ar	gister
	Visualize	
Job Description :	Resource Domain : GRID 😫 Worker Number : 10 🕃 Submit	

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

New Library :	MyCompound
Attach to an ex	isting Library :
PDBQ Directory :	/Users/masonhsiung/BPDBQ
	(where contains your compound PDBQ data)
	Register

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

• New Library :	MyCompound
Attach to an ex	disting Library :
PDBQ Directory :	/Users/masonhsiung/BPDBQ
	(where contains your compound PDBQ data) Browse
	Register

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 <u>https://vomrs.grid.sinica.edu.tw:8443/vomrs/euasia/vomrs</u>
- 9.4. MGLTools website For preparing the target and ligands. http://mgltools.scripps.edu