RACCOON 2 QUICKSTART

requirements:

- AutoDock|Raccoon2 installation, that is influded in the MGLTools 1.5.7rc1 installation:
  http://mgltools.scripps.edu/downloads/mgltools-1-5-7rc1
- example files available at:
  http://autodock.scripps.edu/resources/raccoon2/raccoon2
- user account on a Linux cluster/HPC with either PBS or SGE scheduler

A. PRELIMINARY SETUP

These steps should be done only when preparing a new server or when new libraries need to be uploaded on it. Once saved, connections will be available when re-opening the program. Libraries stored on the server will be available each time a connection is established.

SETUP TAB

1. CREATE A NEW SERVER CONNECTION

1.1 click on to open the Connection Manager
1.2 type a name in the *server name* field (i.e. “My Server”)
1.3 fill the *address* entry with the server IP or hostname (i.e. 192.1.68.1.1 or cluster.host.edu)
1.4 type the *username* of the account used to access the server
1.5 select one of the *authentication* methods and enter the appropriate values:
  1.5a) *password*: type the user password
  1.5b) *load key file*: select the public key to be used for the connection
  1.5c) *system key file*: use system public keys (Linux/Mac only)
1.6 save the connection by clicking on “ **Save**”
1.7 close the Connection manager

2. INSTALL A DOCKING SERVICE ON THE SERVER

2.1 connect to the server “My Server” by selecting it from the Connection menu
2.2 prepare the server ('*raccoonize*') by clicking on
2.3 open the Service manager by clicking on “ **Service manager**”
2.4 add a new service by clicking on
2.5 type a service *Name* (i.e. “Vina docking service”)
2.6 install Vina on the cluster by clicking on “ **Install AutoDock Vina on the server...**”
2.7 click on “**Yes**” and “**Yes**” to install AutoDock Vina by using the default download link
2.8 select the *multi-thread* value according to the number of CPU/cores on the nodes (if not sure, leave it at “1”)
2.9 save the service by clicking on “ **Save**”
2.10 close the Service manager
2.11 select the service “Vina docking service” from the **Available services** panel.

LIGANDS TAB

3. CREATE A NEW LIBRARY ON THE SERVER

3.1 create a new library by clicking on “ **New**” and open the Library Manager
3.2 click on “ **Add ligands->Scan directory**”, browse to **examples/ligands**, open it and press “**OK**” (Note: only PDBQT files are supported in this version)
3.3 close the Report window
3.4 click on “ Upload...” to open the “Upload library” interface
3.5 type the *Library name* (i.e. “Raccoon example library”) and press “Start”
3.6 wait for the download to complete, then press “Close”
3.7 Close the Library Manager

B. VIRTUAL SCREENING

These steps are performed each time a virtual screening is created, submitted and analyzed. It requires having at least a server connection already defined and a library uploaded on the server (see **A. PRELIMINARY SETUP**)

SETUP TAB

1. CONNECT TO A SERVER

1.1 connect to the server “My Server” by selecting it from the Connection menu

LIGANDS TAB

2. SELECT A LIBRARY FOR THE VIRTUAL SCREENING

2.1 Select the “Raccoon example library” in the **Remote libraries** panel then right-click on it to use it

RECEPTORS TAB

3. IMPORT RECEPTOR STRUCTURES

3.1 click on “ **Add->Scan directory**”, browse to **examples/targets**, open it and press “OK”
3.2 close the Report window

CONFIG TAB

4. DEFINE GRID BOX AND DOCKING SETTINGS

4.1 load a receptor structure in the **3D viewer** by clicking in items in the **Receptor list**
4.2 define the grid box to be used in dockings using one of the two methods

4.2a click on “ **Load...**”, browse to **examples/config/** and open the Vina config file “**active_site.conf**”
4.2b use the **Center** and **Size** thumbwheels to set the center to (0., 0., 0.) and the size to (20., 20., 20.). Numerical values can be entered by placing the mouse cursor a the thumbwheel, typing the number then pressing Enter.

4.3 [OPTIONAL] tweak the docking parameters (*exhaustiveness*, *num.modes* and *energy range*) by typing desired values in the entry fields.

JOB MANAGER TAB

5. JOB SUMBISSION

5.1 check that all **Cluster submission requirements** are satisfied (green).
5.2 start submission by clicking on “ **Submit...**” button
5.3 set the **Project** name to “<*new*>” and type a new name, i.e. “HIV”
5.4 set the **Experiment** name to “<*new*>” and type a new name, i.e. “Protease”
5.5 [OPTIONAL] define a tag to be used to identify the jobs (I.e.”FirstSubmission”)
5.6 Press “**OK**” and start the submission.
5.7 Depending on different factors (available computer power, library size, docking settings...) a calculation can take a variable amount of time. Although, once the calculation has been submitted, it is possible to close Raccoon, re-open it later and start from step **6** to update a job status at any time.

6. DOWNLOAD AND PROCESS RESULTS

6.1 expand the project to see the status of the experiment
6.2 update the status of the jobs by right-clicking on experiment name (“*Protease*”) or single jobs and select “**Update status**”. Server connection will be established automatically, if necessary.
6.3 When one or more jobs in the experiment are completed, download them individually by right-clicking on the job name (i.e. “*hiv_protease_frame1*”) or together by right-clicking on the experiment (“*Protease*”), then select “**Download results**”.

ANALYSIS TAB->DATA SOURCE

7. IMPORT RESULTS IN THE CURRENT SESSION

A. Import the results downloaded in step 6.

7.1a go to the "**Analysis->Data source**" tab

7.2a click on "**Add results->Select downloaded results**"

7.3a check the box to select at least one of projects, experiment or jobs to be imported and press "**OK**"

B. [OPTIONAL] Process and import results that were not generated using Raccoon

7.1b go to the "**Analysis->Data source**" tab

7.2b click on "**Add results->Process directory (Vina)...**"

7.3b Browse into the directory containing the results and press "**OK**"

7.4b Choose the receptor file used for the dockings to be used for processing the results

7.5b Select the name of the summary log file to be generated (default: "*DIRECTORYNAME_summary.log"*)

C. [OPTIONAL] Import results that were already processed (see step B)

7.1c go to the "**Analysis->Data source**" tab

7.2c click on "**Add results->Import from summary log file**"

7.3c Browse and load the desired summary file

8. FILTER RESULTS

8.1 Filter results by tuning energy and ligand efficiency sliders and press "**Apply filters**".

8.2 check the button to enable auto-filtering whenever values are modified.

8.3 reset energy and ligand efficiency filters to the defaults by clicking on

8.4 Add one or more interaction filters by clicking on in the **Target interactions** panel.

8.5 select the interaction type (i.e. "*HB any*") and the residue name (i.e. "*ASP25*"), then press **Enter**.

8.6 click on to set the interaction mode from "*wanted*" to "*unwanted*".

ANALYSIS TAB->VISUALIZATION

9. VISUALIZE AND SELECT RESULTS

9.1 go to the "**Analysis->Visualization**" tab

9.2 click on a ligand name in the **Results** panel to load the ligand-receptor complex in the **3D Viewer**

9.3 click on the checkbox under "**sel**" column to select a ligand

ANALYSIS TAB->EXPORT

10. EXPORT RESULTS

10.1 go to the "**Analysis->Export**" tab

10.2 select from the **Results** panel which results are going to be exported: "*Selected*" (only selected ligands), "*Filtered*" (all ligands that passed the filter) or "All" (all ligands imported in the session)

10.3 check the "**Ligands**" and "**Receptors**" to define which structure files are going to be exported

10.4 export structure files:

10.4a click on "**Save PDB...**" and specify a directory name where files will be converted to PDB and saved

10.4b click on "**Save PDBQT...**" and specify a directory where files will be saved as PDBQT

10.5 in **Summary log** panel, click on "**Save summary...**" to export the CSV (comma separated values) text summary file