

Result files

Once the computation has ended, the server prepares a tgz compressed tar archive containing several result files organized by folders as:

- project[XXX]_[xxx].pdb: The top one hundred conformation sorted by PyDock scoring function.

- project[XXX].ene: Example output of the pyDock scoring function.

Conf	Ele	Desolv	VDW	Total	RANK
 7031	-25.253	-22.058	74.407	-39.870	1
9002	-23.131	-19.566	51.752	-37.522	2
5706	-16.856	-22.852	53.149	-34.393	3
3693	-27.846	-10.676	47.051	-33.816	4

- project[XXX].eneRST: Example output of the pyDock scoring function and constraints applied.

Conf	Ele	Desolv	VDW	relRST	Total#	RANK
2509	-10.757	-40.523	47.310	12.245	-58.794	1
9217	-11.841	-42.381	68.484	10.204	-57.578	2
8610	-14.009	-33.178	91.284	19.388	-57.447	3
3550	-7.846	-18.799	66.162	33.673	-53.702	4

Conf: Column containing the conformation number of the docking pose as in the rot file (last column).

Ele: Electrostatic energy component.

Desolv: Desolvation energy component.

relRST: Percentage of the restrictions imposed that the

conformation complies with.

VDW: Van der Waals energy component (term weighted to

0.1 by default).

Total: Total binding energy (representing the sum of the

3 previous energies).

Total: Total binding energy without Desolv and

subtracting the relRST value.

RANK: Conformation rank according to its computed

binding energy.

- project[xxx].ftdock: FTDock application output.

- project[xxx].rot: rotation angles for each of the poses generated by FTDock.

- project[xxx] rec.pdb: Receptor PDB file parsed pyDockWEB.
- project[xxx] lig.pdb: Ligand PDB file parsed pyDockWEB.
- project[xxx]_setup.log: A log file of the pyDock setup process (PDB files parsing).
- project[xxx].ene: a table with a list of generated conformations scored and ranked by the energy scoring selected.
- project[xxx]_- .pdb: One of the top 100 conformations in PDB file format. They correspond with the first 100 rows in project[xxx] [scoring].ene file.

If any distance restraint has been chosen:

- project[xxx].rst: contains a table with the top 10000 conformations scored using the restraints applied.
- project[xxx].eneRST: a table with a list of generated conformations scored and ranked by the energy scoring selected and one extra column with the restraint scoring.

Note: ["xxx"] is the conformation number given by FTDOCK. ["XXX"] is the job number generated by pyDockWEB server.

- makePDB.py: With the help of this script you can generate the 10,000

conformations generated by FTDOCK.

Usage: ./makePDB.py dock name starting rank ending rank eneTab.

(Rank according to its computed binding energy).

Example: ./makePDB.py project902 1 10000 project902.ene

(If the eneTab is not provided the ene file in the

folder is used)

To cite pyDock, please reference:

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