



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].ene`: Example output of the pyDock scoring function.

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- project[XXX].eneRST: Example output of the pyDock scoring function and
constraints applied.
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Conf: Column containing the conformation number of the docking pose as in the rot file (last column).

Desolv: Desolvation energy component.

VDW: Van der Waals energy component (term weighted to 0.1 by default).

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:

Jimenez-Garcia B., Pons C. and Fernandez-Recio J. pyDockWEB: a web server for rigid-body protein-protein docking using electrostatics and desolvation scoring. *Bioinformatics* (2013) 29(13):1698-1699.