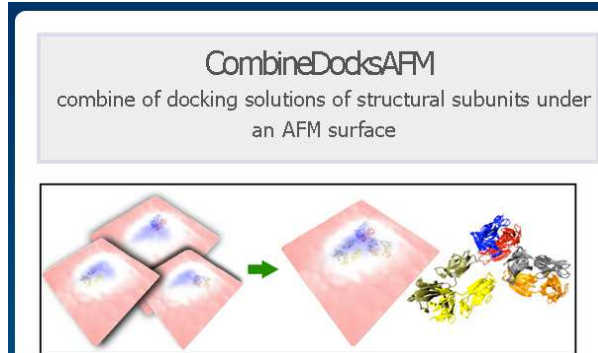# CombineDocksAFM
v1.0
http://biodev.cea.fr/combinedocksafm

In this tool the 3D structure of a multi-component protein can be assembled. The principle is based on the hypothesis that large proteins are essentially constituted by structural parts already known and common to other large proteins. Therefore, by considering experimental information at the shape level, such as the data provided by AFM, computational reconstruction can be performed. Given a list of structural components and their respective docking into an experimental envelope, CombineDocksAFM allows the computation that combines docking possibilities while imposing bump checks and distances constraints.

To use CombineDocksAFM, it is necessary to perform first the docking of each structural component to be considered in the reconstruction with the tool: **http://biodev.cea.fr/dockafm**

After obtaining the docking solutions (a *.e6d file) from DockAFM, please upload the PDB file of each component (on the left) and their respective *.e6d files (on the right).

Several types of constraints can be imposed during reconstruction:
1) To avoid overlapping in structural components, a bump range in Å can be entered as well as the total number of allowed bumps.

2) To reduce computational time, a set of distance constraints can be provided. In the table (above) distances are set from structural components (a is the first PDB file, b the second, …) In the test sample provided, the assembly concerns 3 consecutive components; i.e. component 1 is linked to component 2, and component 2 is linked to component 3. A constraint is defined by three values: min, max, and ideal. A constraint is defined between one XYZ coordinates of each component. Multiple constraints are allowed. **However**, if you change the number of distance constraints

in the pull-down menu on the top of the page, names of input files will be lost and their names should be re-entered.

A z threshold, that should take in consideration the attractive layer used in docking $z_{threshold}$ = T-L is necessary for computing the ranking score. Finally, the last set of parameters deal with the selection of docked components. To reduce computation time, a partial number of docking solutions is considered after filtering (coarse filter) the complete docking list (*.e6d file). A docking orientation is kept if it represents a set of close neighbors defined by distance and orientation parameters. Then, a second combination run is made by selecting docking solution (from the *.e6d file) around the top solution obtained at coarse level: distance and orientation parameters can be adjusted for this second finer filter.

File-in your email address to receive a link on the output results.
Then, click on "Run analysis" to submit the job.

Any comments or suggestions please use the link to the coordinator email.