PyRy3D: a tool for modeling of large macromolecular complexes

URL: http://genesilico.pl/pyry3d/

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How PyRy3D benefits biologists:

Our software PyRy3D is designed for experimental biologists who model structures of large macromolecular complexes. Ideal targets for structure prediction with PyRy3D are systems like the polymerases or editosome, where complex shape and most of its components' structures are known and there is also a lot of information about interactions between components from experiments like crosslinking or mass spectroscopy. Such hybrid approach may be the only possibility to retrieve structural details essential for planning further experiments (e.g. explaining mechanism of action of systems, for which experimental methods could not solve structures for many years).

Comparison to similar tools:

At the moment only IMP library is available (http://www.integrativemodeling.org/) for hybrid complex modeling, apart from our program. It is a powerful set of different methods devoted for modeling of large macromolecular systems.

However, our software PyRy3D has also various interesting features:

- the program is easy to use and there is no need of programming to run analysis. However, for more advanced users, PyRy3D is fully scriptable, thus users can write Python scripts and use PyRy3D for very specific tasks
- the program enables use of both electron density maps and ab initio models from SAXS as complex shape descriptors
- PyRy3D enables use of many different data taken from experiments and encodes them as distance restraints during modeling process
- a user can provide different components' representations as input data for the program. It is possible to work with crystal structures, NMR ensembles, homology/comparative models, crude models and even sequences with no structure. Furthermore to speed up analysis, for each of these a user can choose simplified representation type from several provided by the program.
- the program provides full control over the simulation (a complex model building) process. User can change simulation algorithm, scoring function weights, freeze components inside density map or define their move boundaries depending on available knowledge about a particular system

- PyRy3D enables modeling complexes built of structures with missing or disordered fragments. Our program can simulate these regions during complex building process and fit them into provided shape

- PyRy3D provides a graphical user interface with possibility to generate input files, setup simulation parameters and visualize complex building process in real time, among other functions.