Talk/Poster

Scipion-EM-ProDy: A Graphical Interface for the ProDy Python Package enabling Integration of Databases, Simulations and Cryo-Electron Microscopy Image Processing

James M. Krieger[1], David Herreros[1], Carlos Oscar Sanchez Sorzano[1] and Jose-Maria Carazo[1]

[1] *Biocomputing Unit, Centro Nacional de Biotecnología, Madrid, Spain*

jmkrieger@cnb.csic.es

The ProDy API is an application programming interface that enables protein dynamics analysis from ensembles of structures from experiments and computations through the use of an extensively developed Python package [1,2]. This software provides a broad range of classes, methods and functions that enable the creation of complex pipelines such as normal mode analysis of biomolecular assemblies taking account of their membrane environment [3], SignDy for signature dynamics analysis of protein families [4].

However, despite the existence of a handful of command-line applications and the normal mode wizard (NMWiz) plugin in VMD that provide the core functionalities, the primary method for using this software to date has required a sufficient knowledge of Python to integrate the various classes and functions into useful pipelines as mentioned above. On the other hand is Scipion, an integrative graphical software for combining other software packages into pipelines and workflows, especially for image processing for cryo-electron microscopy (CryoEM) [5].

Several major developments are under way to extract continuous information about protein dynamics from CryoEM data and we are now at the point where an integration between these purely image processing-based methods and structure- and biophysics-based methods is critical. I now present Scipion-EM-ProDy, a plugin for ProDy within Scipion which enables such integration and paves the way for improved methods for extraction of protein dynamics and energy landscapes from CryoEM and simulations.

References

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