Séminaire HélioBio du 6 mars 2017

Lessons from (co)evolution in the structural modeling and design of protein interactions

Jessica Andreani et Raphaël Guerois

Laboratoire de Biologie Structurale et Radiobiologie (LBSR), IBITECS, CEA Saclay

Protein-protein interactions are central to most biological processes. Understanding how binding partners coevolved can provide essential clues to improve the structural prediction of protein interfaces. Our team focuses on the analysis and prediction of protein interactions through the combined use of structural data and evolutionary information. In a study of over 1,000 couples of homologous interfaces, we uncovered significant plasticity in the way interface structure coevolved [1, 2]. We also identified rather invariant features which provided tracks for the development of InterEvDock, a server for protein-protein docking designed to integrate evolutionary information in the docking process [3, 4]. We successfully used this pipeline in the CAPRI international prediction challenge [5] and in a variety of biological applications. Understanding how interfaces coevolve also opens interesting perspectives in the design of novel binders to modulate protein-protein interaction networks.

1. Faure, G., J. Andreani, and R. Guerois, *InterEvol database: exploring the structure and evolution of protein complex interfaces.* Nucleic Acids Res, 2012. **40** (Database issue): D847-56.
2. Andreani, J., G. Faure, and R. Guerois, *Versatility and invariance in the evolution of homologous heteromeric interfaces*. PLoS Comput Biol, 2012. **8**(8): p. e1002677.
3. Yu, J., et al., *InterEvDock: a docking server to predict the structure of protein-protein interactions using evolutionary information.* Nucleic Acids Res, 2016. **44**(W1):W542-9.
4. Andreani, J., G. Faure, and R. Guerois, *InterEvScore: a novel coarse-grained interface scoring function using a multi-body statistical potential coupled to evolution.* Bioinformatics, 2013. **29**(14): p. 1742-9.
5. Yu, J., et al., *Lessons from (co-)evolution in the docking of proteins and peptides for CAPRI Rounds 28-35.* Proteins, 2016.