Poster I-49

PROTEIN LIGAND CONTACTS ANALYSED IN AN INTEGRATED ENVIRONMENT WITH OTHER STRUCTURE AND SEQUENCE RELATED PARAMETERS

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Short Abstract: The Protein Ligand Contacts – the new STING module allows a user to compare the contacts established between the ligand and the protein together with the variety of other structure parameters within a simple yet intuitive set of interactive plots. The biologically important examples are presented in this work.

Long Abstract:
The structural Computational Biology and Bioinformatics is consistently trying to provide to the scientific community an ever increasingly interactive and complete environment for analysis of specific parameter relative to the sequence, structure or function of chosen structure. In addition, It is clear a tendency that the researchers need also to be able to compare obtained results from a specific parameter analysis, in context of other available descriptors of structure, sequence and stability for example. In this work we present the results of our effort to integrate the data on protein ligand contacts with the other structure descriptors which are available in the SITNG_DB (310 of them). This new STING module is based on a new algorithm which we have designed in order to calculate all potential contacts which can be established between the ligand and its hosting protein structure. For that we have followed the description of conditions available by Sobolev et al. (Sobolev V., Sorokine A., Prilusky J., Abola E.E. and Edelman M. (1999) Automated analysis of inter atomic contacts in proteins. Bioinformatics, 15, 327-332) with some significant adaptations which allowed us to make an robust approach with less problematic high throughput problems while applying it to the whole PDB. After the list of contacts is generated, the module is capable of displaying tables and graphical cartoons of established contacts. In addition, those inter molecular contacts are conveniently mapped into the complete map of structure descriptors so that the user can grasp the related parameters and analyze them within the same computational and graphical environment. In this work, we are presenting couple of structures and the importance of the integrated analysis of variety of parameters, given the spotlight dedication to the protein ligand contacts.