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Contacts as the key elements for comparing two protein structures

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Short Abstract: TopSiMap (Topological Similarity Map) is and interactive tool which is part of the Star Sting Suite (http://sms.cbi.cnptia.embrapa.br/SMS).As contacts pattern is very conserved in each protein fold type, it makes possible to compare protein structures through their contact maps and also analyze what changes in contacts between two protein chains.

Long Abstract:

Many protein structures have been determined and reveal that proteins can adopt the same fold despite having dissimilar sequences. Chains with more than 30% of sequence in common, generally, adopt the same fold. What makes distant sequences fold in the same structure? We have verified that even for dissimilar sequences, there is a pattern of intrachain residue interactions for a fold family which composes its structural signature. As we showed in [1], contact maps of electrostatic and hydrophobic interactions and hydrogen bonds are a reliable representation of protein structure and can be used to compare them with high confidence.

We present a tool which makes possible to compare contact maps: Top-SiMap (Topological Similarity Map). It is part of the Star Sting Suite [2], available at the http://sms.cbi.cnptia.embrapa.br/SMS. Users can analyze any pair of PDB files or a personal protein model in PDB format. We show the maps containing: hydrophobic contacts; hydrogen bonds; charged attractive and repulsive interactions; dissulfide bonds and aromatic stacking. It is possible to select the types to be displayed as the connectivity of the contact (cross order), to zoom the map and click on the contacts seeing them in structure using JMol or Chime plug-ins. TopSiMap generates a report of the conserved and non-conserved interactions in the pair of chains as well as a table of their energies.

There is a wide range of applications to this tool. Users can compare proteins of the same family in different species, analyze structures obtained under different experimental conditions, with variety of ligands attached, etc. and verify what changes in the contacts signature. The users can also try to elucidate questions about folding and activity by contrasting wild and mutant proteins. From the tests we have done with single point mutations for structures present in the PDB, it is clear that a mutation can change contacts in residues very distant from the mutated one.

[1] F.A. Fernandes Jr and C.E.R. Lopes and R.C. Melo and R.L. Carceroni and M.M. Santoro

and C.H. Silveira and W. Meira Jr (2004). An Image-Matching Approach to Protein Similarity Analysis. XVII Brazilian Symposium on Computer Graphics and Image Processing, 17-24.

[2] G. Neshich and I. Mazoni and S.R.M. Oliveira and M.E.B. Yamagushi and P.R. Kuser-Falcão and L.C. Borro and D.U. Morita and K.R.R. Souza and G.V. Almeida and D.N. Rodrigues and J.G. Jardine and R.C. Togawa and A.L. Mancini and R.H. Higa and S.A.B. Cruz and F.D. Vieira and E.H. dos Santos and R.C. Melo and M.M. Santoro (2006). Star STING Server: A multiplatform environment for protein structure analysis. Submited.