

Comparative Analysis of Protein -Protein Interface Methods

Alexandre de Brevern, Jérémy Esque

▶ To cite this version:

Alexandre de Brevern, Jérémy Esque. Comparative Analysis of Protein -Protein Interface Methods. Groupe Graphisme Modélisation Moléculaire (GGMM), May 2017, Reims, France. inserm-01586501

HAL Id: inserm-01586501 https://inserm.hal.science/inserm-01586501

Submitted on 12 Sep 2017

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Comparative Analysis of Protein - Protein Interface Methods

A.G. de Brevern¹ and J. Esque²



¹ Laboratoire DSIMB, INSERM, U 1134, Univ Paris Diderot, Univ. Sorbonne Paris Cité, INTS, Laboratoire d'Excellence GR-Ex, F-75739 Paris, France. ² Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés, INSA, CNRS, INRA, Université de Toulouse 135 Avenue de Rangueil, F-31077 Toulouse, France

E-mail: alexandre.de-brevern@inserm.fr; esque@insa-toulouse.fr





In the cells, proteins are never alone. All proteins interact with other molecules to become functional. Protein interactions (PPIs) are essential for a broad range of cellular processes including signal transduction, cell-to-cell communication, transcription, replication, and membrane transport. So, studying PPIs is crucial to better understand the relationship between different protein partners and their functions. These interactions result in physical contacts of high specificity as a result of biochemical events steered by electrostatic forces including hydrophobic effect. Residues close in space determine protein contacts and computational approaches finding these residues are interesting for PPI studies.



Threshold Method

C station S

ViP (Voronoï Interface Protein) ^[1-3]

ASA (Accessible Surface Area)



RESULTS & DISCUSSION

Global View

DataSet

- 4742 non-redundant complex proteins from InterEvol



Frequencies (%) of Residues defined at the interface







Stratification from VIP Network Chain A Chain B





Conclusion

ViP is an extension of VLDP software [1-3] and is an open source program available on request. Depending on scientific community interest, a webserver could be developped. Instrinsically, ViP identifies the nearest neighbouring residue (contacts) and an interface that does not suffer from the limitations of standard methods, For example, an arbitrary distance parameter must be defined in the threshold method, and results of the ASA method depend on the choice of probe sphere radius. One limitation of ViP could be the assignments, which can be verified by slightly varying the values and checking for any network changes (contacts). Moreover, further addition of solvent, for example from a dynamics trajectory, is important in protein complexes. This comparative analysis showed that ViP is particularly promising as both common and supplementary types of residues not found by other metric methods (threshold and ASA) or MMPBSA energy calculations could be identified. To conclude, ViP is a powerful, mathematically robust and efficient, geometric tool for analysing interface and environments in protein complexes.

[1] Esque J, Oquey C and AG de Brevern. A novel evaluation of residue and protein volumes by means of Laguerre tessellation. J. Chem. Inf. Mod. (2010) 50:947-60 [2] Esque J, Oquey C and AG de Brevern. Comparative analysis of threshold and tessellation methods for determining protein contacts. J. Chem. Inf. Mod. (2011) 51:493-507 [3] Esque J, Léonard S, AG de Brevern and Oguey C. VLDP web server : a powerful geometric tool for analysing protein structures in their environment. NAR (2013) 41:W373-8 [4] Faure G, Andreani J and Guerois R. InterEvol database : Exploring the structure and evolution of protein complex interfaces. NAR (2012) 40:D847-56