PIC : Protein Interaction Calculator

HELP AND GUIDELINES

CONTENTS

1. OVERVIEW

Interactions amongst proteins, as well as interactions within a protein are essential for stability and function of the protein. There are several weak as well as strong interacting forces that typically govern interactions mediated by a protein. We aim to enumerate all such weak as well as strong non-covalent interactions that occur within a protein, as well as interactions that occur between proteins in a complex.
Protein Interaction Calculator (PIC) is a server which, given the coordinate set of three-dimensional structure of a protein or an assembly, computes various interactions such as disulphide bonds, interactions between hydrophobic residues, ionic interactions, hydrogen bonds, aromatic-aromatic interactions, aromatic-sulphur interactions and cation-pi interactions within a protein or between proteins. It also determines the accessible surface area as well as the residue-depth which is the distance of a residue from the surface of the protein. Interactions are calculated on the basis of standard, published criteria.

2. METHOD

For a given input all possible interacting residue pairs are enumerated along with the inter-atomic distances and angles. Interactions are identified using standard criteria available in the literature, Criteria Applied. However user has an option to input a different criterion to identify hydrophobic interactions, ionic interactions, aromatic-aromatic interactions, aromatic- sulphur interactions, cation-pi interactions.

3. INPUT

*** User may upload query structure in the three-dimensional coordinate set format of the protein data bank file.**
*** The input for intraprotein and solvent accessibility based calculations can be a monomeric or multimeric protein file.**
*** The input for protein-protein interactions should be a multimeric protein file.**
*** Use "Browse" button to upload the structure.**
*** User can mark on all or any of the check boxes as required.**
*** Click on the "Submit" button to initiate the calculations .**

4.OUTPUT

The format of the output will vary with the user defined options. The output-lists positions and chains of the interacting residues along with the inter-atomic distances and angles.

5.RASMOL VIEW

The coordinates of query protein colored by PIC programmes can be downloaded and conveniently displayed with structural viewers such as RASMOL.

How to view

1. Click on the link "Rasmol view"
2. Save the file.The file name will be "rasmol*.cgi"
3. Use rasmol -script rasmol.cgi command

Jmol is a Java based application and an applet for displaying 3D chemical information. you need to use a compatible operating system and browser. Windows, Mac, and Linux are all compatible with Jmol.

To view the structure in Jmol, click on the link given.Right click on the Jmol window for further options.

6.OPTIONS

The options available are

1. Intraprotein Interactions
2. Protein-Protein Interactions
3. Solvent accessibility (Ref 5) based Intraprotein and protein-protein Interactions.

For each of above options,

a. Hydrophobic Interactions
b. Disulphide bridges
c. Hydrogen Bonds (Ref 1)
d. Ionic Interactions
e. Aromatic-Aromatic Interactions (ref 2)
f. Aromatic-Sulphur Interactions (Ref 3)
g. Cation-Pi Interactions (Ref 4)

can be calculated.

4. Depth calculations (Ref 6)

For hydrophobic interactions, ionic interactions, aromatic-aromatic interactions, aromatic-sulphur interactions and cation-pi interactions the cut-off or range can be altered depending on the user's discretion.

7. REFERENCE

1. Overington J, et al .*Proc. Roy. Soc. Biol Sci.* 1990, pg.132-145
2. S.K.Burley, G.A.Petsko, *Science*, 1985, Vol 299, pg.23-28.
3. K.S.C Reid, P.F.Lindley and J.M. Thornton, *FEBS letter* 1985, Vol.190, pg.209-213.
4. R.Satyapriya and Saraswathi Vishveshwara, *Nucleic Acid Research* , 2004, Vol 32, pg.4109-4118.
5. Hubbard,S.J. & Thornton, J.M., 'NACCESS'. 1993.
6. Suvobrata Chakravarty and Raghavan Varadarajan, *Structure*, 1999, Vol 7, Pg.723–732.
7. Sayle RA, Milner-White EJ. *Trends Biochem Sci*, 1995,Vol 20, pg.374.
8. http://jmol.sourceforge.net/

PIC: Protein Interactions Calculator K. G. Tina, R. Bhadra and N. Srinivasan Molecular Biophysics Unit, Indian Institute of Science, Bangalore 560 012, India, Nucleic Acids Research, 2007, Vol. 35, Web Server issue W473–W476 [PDF]

http://nar.oxfordjournals.org/cgi/reprint/gkm423v1