CAPI : Computational Analysis of Protein Interactions

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 noncovalent interactions that occur within a protein, as well as interactions that occur between proteins in a complex.

Computational Analysis of Protein Interactions (CAPI) 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. 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-caromatic 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 tool can be a monomeric or multimeric protein file.
- Use "Browse" button to upload the structure.
- User can go for any calculation by clicking the appropriate tab
- 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.

6.OPTIONS

The options available are

1. Protein-Protein Interactions
    a. Hydrophobic Interactions

b. Disulphide bridges
c. Hydrogen Bonds
d. Ionic Interactions
e. Aromatic-Aromatic Interactions
f. Aromatic-Sulphur Interactions
g. Cation-Pi Interactions

can be calculated.

7. REFERENCE

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DEVELOPED AND MAINTAIED

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