Project Report

Proteomes Interactomes and Biological Networks

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Report Outlines

- Title
- Abstract: Summary of the work
- Introduction: Description of the Hemoglobin function
- Methods: Detailed information about the methodologies used for the analysis
- Results: Quantitative results of the analysis
- Discussion: Short summary of the results
- References: List of articles and web pages
- Supplementary Materials: Information not included in the main report

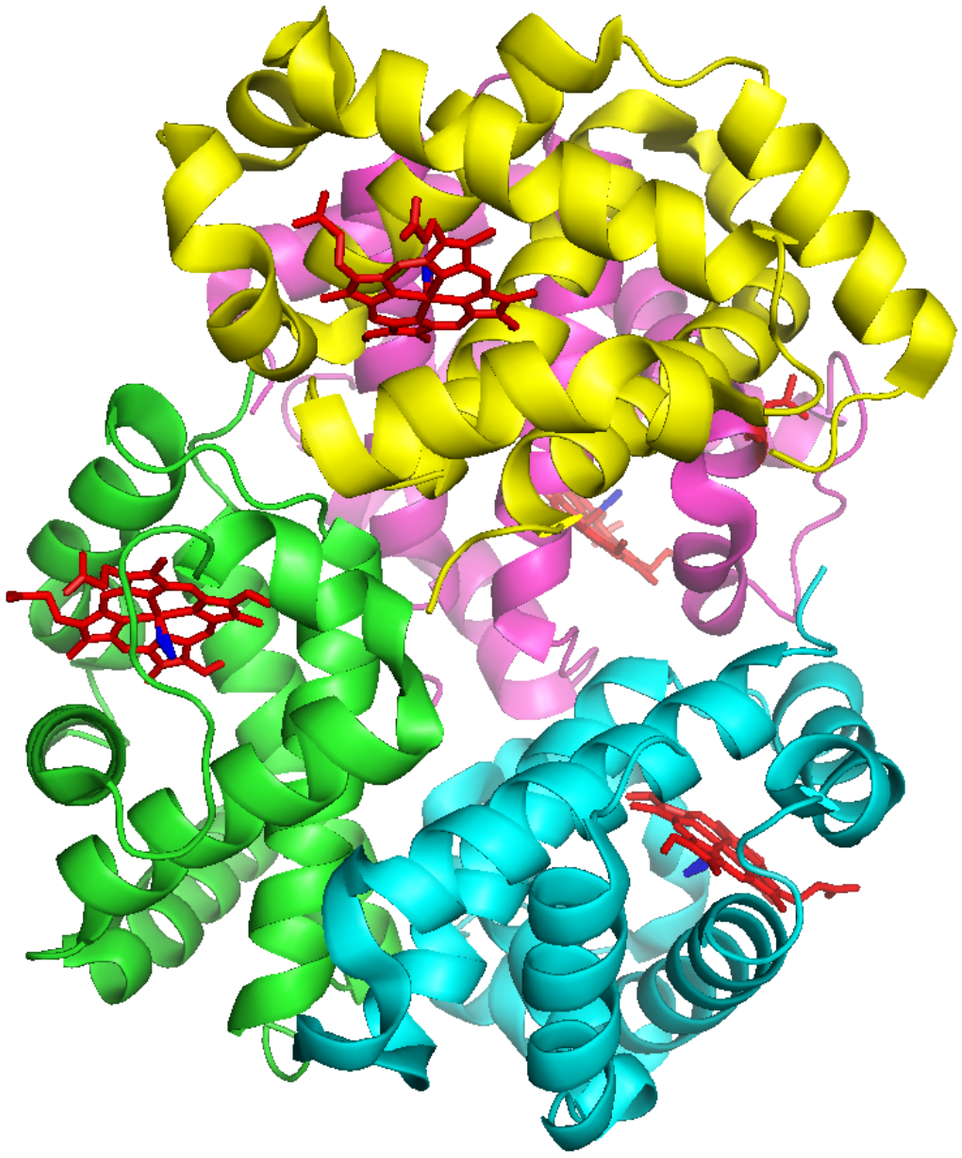
Introduction

Description of the hemoglobin function and the protein complex

- Oxygen transport

- Tetramer composed by 2 types of monomers (α and β subunits)

- Each monomer interact with a Heme group



Methods

Detailed description of the data and methodologies used for the development of the project.

- Details about the protein structure used for the analysis of the Hemoglobin complex (1GZX).

- Programs used for the analysis of complex.

- Procedure used for the analysis of the hemoglobin complex: Calculation of the physical interactions (heme-monomers and between monomers) and the surface of interaction between monomers.

Results (I)

Quantitative results of the analysis divided in two main parts:

- Analysis of the physical interactions heme and oxygen groups and monomers and between monomers. What are the atoms and residues below 3.5 Å?

The mean donor-acceptor distances in protein secondary structure elements are close to 3.0 Å. Since many pdb files lack hydrogen atoms, the presence of an energetically significant hydrogen bond can be inferred when a probable donor and acceptor are within 3.5 Å of each other (https://proteopedia.org/wiki/index.php/Hydrogen_bonds).

The distance between the residues participating in the salt bridge is less than 4 Å (https://proteopedia.org/wiki/index.php/Salt_bridges).

Table (I)

Heme - monomer interactions:

Chain	Residue	Hetero	Atoms (≤3.5Å)
A	HIS58	OXY1143	NE2-O2, …..
	HIS87	HEM1142	NE2-FE, …..

Interactions between monomers:

Chain1	Residue1	Chain2	Residue2	Atoms (≤3.5Å)
A	ARG141	C	ASP526	NH2-OD2, ….

Highlights the salt bridges that stabilizes the interactions and show some figures

Results (II)

Quantitative results of the analysis divided in two main parts:

- Analysis of the surface of interaction between monomers and the lost of accessibility of the single residues

Calculate the surface of interaction for each pair of chains to calculate which chains has stronger interaction.

Determine the possible interaction hot-spots considering the hydrophobic residues with large value of relative solvent accessibility lost.

Table (II)

Surface of interaction between monomers:

Chain1	Chain2	SA (Å^2)
A	B	994

Lost relative solvent accessibility for each residue

Chain	Residue	RSA(M)	RSA(C)	RSA(M)-RSA(M)
A	LEU34	0.74	0.44	0.31

Show the residues with more than 10% of difference and highlight the hydrophobic residues with high difference

Facultative Problem

Using the protein-protein interaction network from IntAct database:

- Extract the sub network of interactions between human proteins from Uniprot database. (Use “uniprotkb” as a key for the identifiers).

- Reduce the network considering only the nodes with maximum path length of 2 from the α and β subunits of the hemoglobin. The grep command in the shell can reduce the time for selecting the nodes.

- Calculate the degree, betweenness and clustering coefficient for the α and β subunits of the hemoglobin.

- Identify the proteins with direct interactions (path length = 1) and calculate degree, betweenness and clustering coefficient for the interacting proteins.

Project Submission

- The report of the project should be a PDF file named *lastname_pibn.pdf*

- A directory containing the supplementary materials should be send as a unique zipped file named *lastname_supmat.zip*.

- All the report should be send by email to emidio.capriotti@unibo.it by December 23, 2019.

- The subject of the mail should be “lastname - PIBN project”.