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

Abstract

Brief summary of the work ~200 words describing the aims and the results of the work.

- Motivation: Study of the Hemoglobin and its function

- Methodology: Analysis of the protein structure

- Results: Generic description of the results with minimal details.

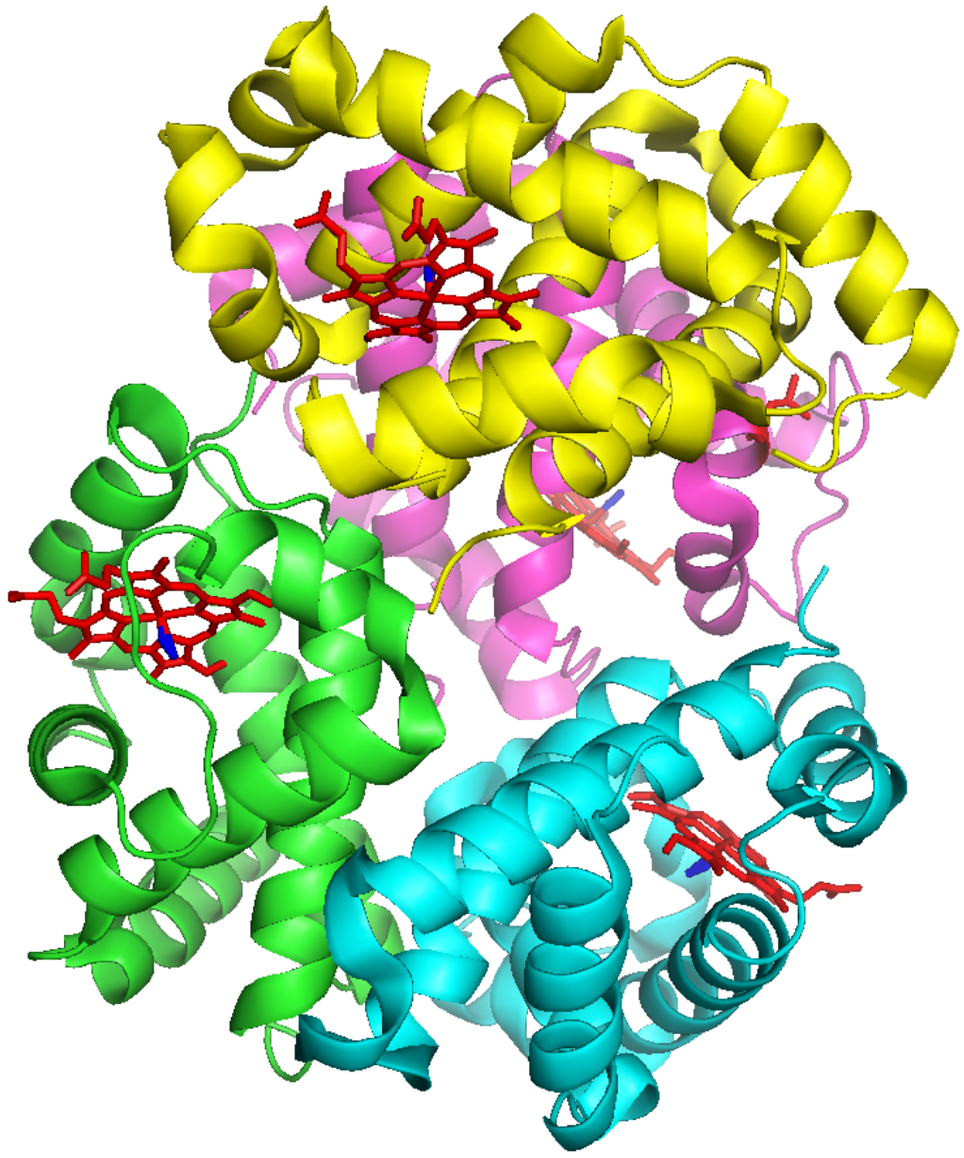
Introduction

Description of the function and the structure of the Hemoglobin

- 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.

- Data: The protein structure used for the analysis of the Hemoglobin complex (1GZX), the database used for the analysis of the protein-protein interaction network

- 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

Results (III)

Analysis of the protein-protein interaction network from IntAct

- Characterization of the protein-protein interaction network from IntAct considering only direct interactions.

  How many nodes and unique edges are present?

  What is the node with highest degree? etc.

- Focus on the α and β subunits of the Hemoglobin.

  What is their degree, and what are the proteins directly interacting with them?
  What is fraction proteins higher degree than the subunit with highest degree?

  Calculate clustering coefficient and betweenness (not normalized)? What is the change of the betweenness of α and β subunits when one of them is removed?

Discussion

Summary of the results highlighting the following points:

- What are the key residues for the function of the proteins and their interactions?

- What are the main electrostatic interactions stabilizing the structure of the hemoglobin?

- What are the important residues at the interface between the different subunits?

References

Include in the final part of the manuscript a list of articles, books and websites used as a reference for writing your report. Some examples are:

- Reference the manuscript describing the function of the hemoglobin

- Article describing the experimental determination of the structure of the Hemoglobin

- Citation of the program used for calculating the solvent accessibility

- What is the scale used for the normalization of the solvent accessibility?

Suggestion: use Zotero to collect the bibliography. It can be combined with Word or Latex.

Supplementary Materials

All the material important for the reproducibility of the results that is too long to be included in main manuscripts.

- Full table with all the list of interacting atoms.

- Full list of residues at the interface between the α and β subunits of the Hemoglobin

- Python code used fo the analysis of the data

Important: the supplementary material should be referenced in the main manuscript

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 31, 2020.

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