Grau en Biotecnologia

Comparative Modelling of Protein Structures

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0.1 Introduction

Summary The project involves the use of different bioinformatics tools to develop a model for an unknown protein structure. The different steps and tools used during the modelling process (template selection, sequence alignment, model building, loop refinement and model evaluation) will be connected through Python and R scripts in order to develop complete pipelines with general purpose. Each student will have a different project (protein target).

Software needed Python, R, Modeller

Covered topics evolution, multiple sequence analysis, homology modelling, protein 3D visualization.

References Some good references to start: [1]

0.2 Homology modelling essentials

Once a target sequence is chosen, the model building process consists on a series of steps that we will try to unravel through the course:

1. Looking for correct structural templates.
2. Obtain a signifficant multiple alignment between the target sequence and the templates.
3. Model building.
4. Structurally variable regions (SVR) building.

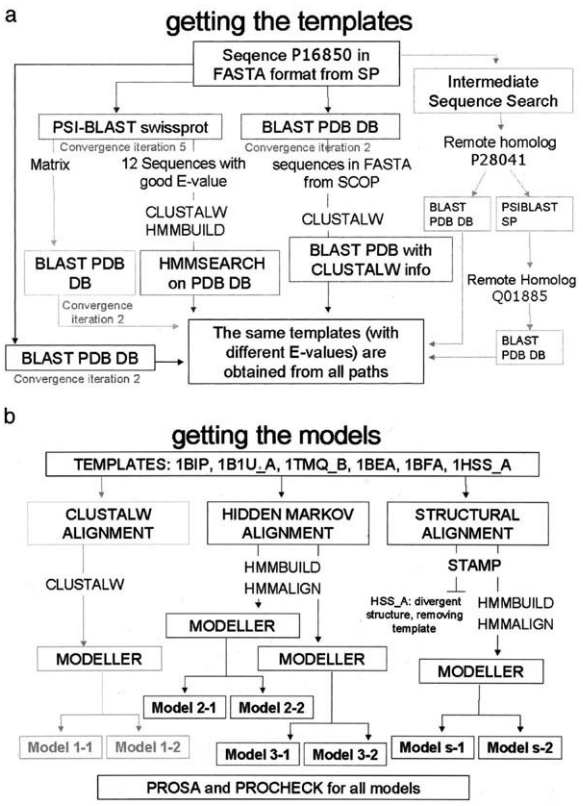

Figure 1: Sumary of a standard protocol for homology modelling[1]

5. Model refinement.
6. Model evaluation.

Appendix A

Enllaços d'interès

Referències generals d'interès:

LibreTexts Recull de continguts oberts en química `https://chem.libretexts.org/`

Institucions i fons d'informació primàries:

IUPAC International Union of Pure and Applied Chemistry (IUPAC): `https://iupac.org/`.

NIST National Institute of Standards and Technology US Dept. of Commerce `https://webbook.nist.gov/chemistry/`. Inclou bases de dades.

ChemSpider Recurs genèric de cerca de compostos i les seves propietats `http://www.chemspider.com/Default.aspx`.

Bases de dades:

PubChem `https://pubchem.ncbi.nlm.nih.gov/`. Cerca de compostos.

chemexper `https://www.chemexper.com/`. Cerca de compostos.

NMRShiftDB `http://nmrshiftdb.nmr.uni-koeln.de/`. Espectres de NMR de molècules d'interès.

NIST Chemical Kinetics Data `https://kinetics.nist.gov/kinetics/index.jsp`.

CCCBDB Computational Chemistry Comparison and Benchmark Database, NIST, `https://cccbdb.nist.gov/`. Inclou dades termodinàmiques verificades dels compostos més comuns.

IUPAC-NIST Solubility DB `https://srdata.nist.gov/solubility/`

Spectral Database for Organic Compounds SDBS `http://sdbs.db.aist.go.jp`.

CommonChemistry Cerca simple de molècules o del seu *CAS number* (`http://commonchemistry.org/`).

Symmetry @ Otterbein Interessant pàgina dedicada a la simetria química `http://symmetry.otterbein.edu/`.

MatWeb Informació sobre propietats de materials `http://www.matweb.com/index.aspx`.

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Bibliography

[1] Nuria B N B Centeno, Jordi Villà-Freixa, and Baldomero Oliva. "Teaching structural bioinformatics at the undergraduate level". In: *Biochemistry and Molecular Biology Education* 31.6 (2003), pp. 386–391. ISSN: 14708175. DOI: 10.1002/bmb.2003.494031060287.