Sample Scenario (20, translated)

Determine the 3D structure of a biologically important protein

Summary

1 Determine the 3D structure of a biologically important protein

2 Procedure

- Find a few proteins relevant to your curriculum.
- Preferably select 3D structures from this MM PDB poster http://mm.rcsb.org/

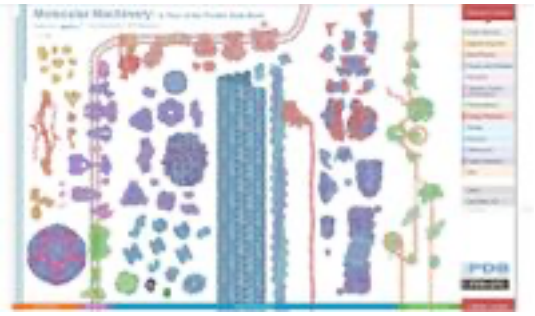


Figure 1: PDB Protein Poster (thumb): click http://mm.rcsb.org/ to enlarge

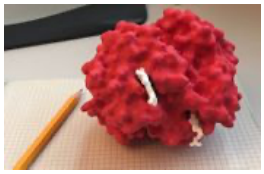
- For proteins related to health and drugs: select from the 3D structures proposed by PDB (from this poster) http://pdb101.rcsb.org/browse/you-and-your-health

Figure 2: Poster of some health-related proteins at PDB.org (thumb: click http://mm.rcsb.org/thumb to enlarge)

3 Many proteins with their structure and STL file - ready for printing

List offered during teacher training in Geneva with Dr Marie-Claude Blatter.

Table 1: Selection of proteins, and data offered (Selection, see full table at the WikiMedia platform.

Selected Protein name	UniProtKB Entry	PDB Entry	Picture of protein A-model	Ready-to-print STL files
Human Hemoglobin	HBB_HUMAN HBA_HUMAN	1a00 4hhb* 2hhb	 Hemoglobin (2x2 subunits red, 4x heme white)	Hemoglobin.stl Heme group.stl
Human Insulin	INS_HUMAN	2hiu* 1ben	 Insulin	InsulineReady2print.stl
Nucleosome Human	H4_HUMAN	5b40	 Nucleosome (histone + 1 DNA loop only)	5B40_histone-protein-only.stl DNA-filament-2-circles.stl
Immunoglobulin IgG (mouse)	GCAA_MOUSE IGH1M_MOUSE	1igt* 1igy	 ImmunoglobulinG	IgG1-ready-2-print.stl.zip With pockets for magnets to simulate affinity in antigen-binding pockets
tRNA	Not a protein!	4tna	 ARNt Phe	4TNA-ready2print.stl
CFTR Causes Cystic Fibrosis when defect)	CFTR_HUMAN P13569	5uak	 CFTR normal-form	CFTR-ready-to-print.stl

NB: not all 3D structures in the database contain all the chains that make up a macromolecule in vivo (example hemoglobin: many 3D structures in PDB contain 2 chains instead of 4...)
NB: not all 3D structures 'span' the full length of the peptide chain

Repository of numerous-protein-structures-in-stl format

These structures were chosen in collaboration between Dr Marie-Claude Blatter of the Swiss Institute for Bioinformatics and Dr. François Lombard. They were printed by (Julien Dacosta, Stephane Morand, Vincent Widmer), coordinated by Prof. Daniel K. Schneider, all from TECFA, Geneva university. The Sevice Ecole et Medias of Departement de l'Instruction Publique, Geneva, (SEM) 3D Printing Service also printed some.
GFP was printed by Romain Deweale, COX1 et the AINS were offered by Pr. Vincent Zoete, SIB Swiss Institute of Bioinformatics, University of Lausanne

4 Examples of questions for biology learning activities to be selected and adapted by teacher.

• It is sometimes said that the sequence of amino acids (a.a.) determines the function of the protein. To which extent is this correct and in which ways is it incomplete?
• How is the secondary and tertiary structure established with what you have learned so far? (In which cell structures? How?)
• Can we currently predict from its sequence the 3D shape that a protein will take?
• How does the observed shape determine the activity of the protein?
• Compare the sequence on UniProtKB, then the 3D shape for various proteins:
    o Insulin (http://www.rcsb.org/structure/1ben ; alternative (with protein sequence: https://www.rcsb.org/3d-view/1ben/))
    o Immunoglobulin IgG (http://www.rcsb.org/structure/1igy ; alternative (with protein sequence: https://www.rcsb.org/3d-view/1igy/))
• Which parts of the structure of the hormone, o the antibody can to be related to their function?
• Does form alone determine function?
• Try to determine (partly) how the shape of an Ig antibody determines its function?
• For these two proteins, which areas of the protein sequence could – in your opinion – change a little following a mutation without seriously jeopardizing its functioning and ultimately reducing the fertility of the animal with this genome?
• In what other areas could a change affect the functioning of the protein?
    o Same for histone HIST1H4A
    o Same for INS insulin
    o Ditto for the MC1R melanotropin receptor
• Conclude on the link between form and function, the limits of the "key-lock" model

5 External links

- 3D-printing service at Sevice Ecole et Medias of Departement de l'Instruction Publique, Geneva, (SEMLab): specially for local schools.

6 Related Scenarios

- Could follow Scenario 17, or prepare for scenario 21

6.1 References

Scenario established with scientific advice from Dr. Marie-Claude Blatter of SIB Swiss Institute of Bioinformatics