USING MOLECULAR MODELS FOR A BETTER EDUCATION IN LIFE SCIENCES

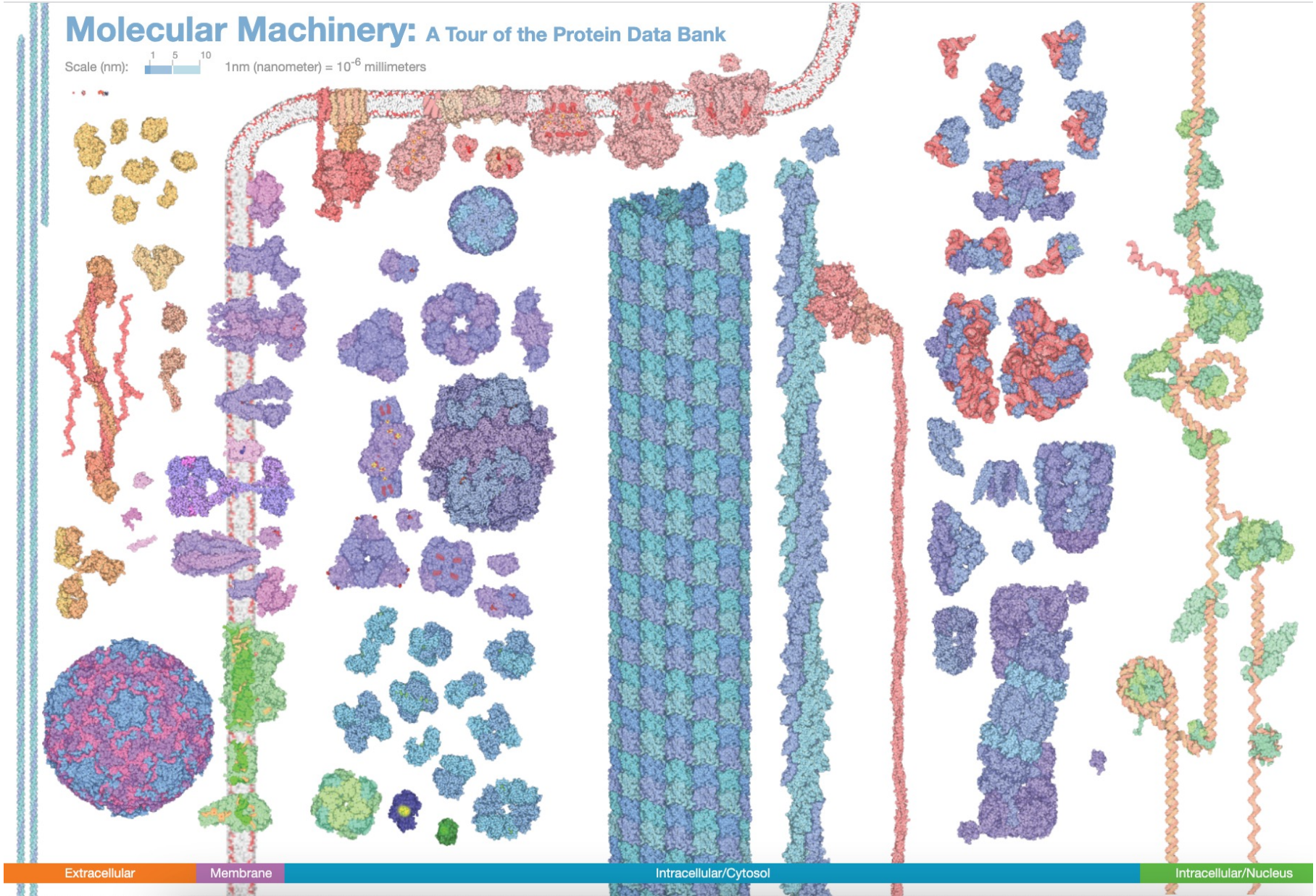
Round table event associated with:

Faculty of Biology Scientific Session

New trends in Biology:
from molecules to complex systems

Understanding Life Sciences relies on understanding Structural Biology

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania



https://cdn.rcsb.org/pdb101/molecular-machinery/

RCSB PDB - Structural data for researchers

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

How much data is available?

Enough to have confidence in protein structure prediction!

PNAS
Proceedings of the National Academy of Sciences of the United States of America
Proc Natl Acad Sci U S A. 2005 Jan 25; 102(4): 1029–1034.
Published online 2005 Jan 14. doi: 10.1073/pnas.0407152101
PMCID: PMC545829
PMID: 15653774
Biophysics

The protein structure prediction problem could be solved using the current PDB library

Yang Zhang and Jeffrey Skolnick*

JBC REVIEWS

Toward the solution of the protein structure prediction problem

Received for publication, April 20, 2021, and in revised form, June 7, 2021 Published, Papers in Press, June 11, 2021,
https://doi.org/10.1016/j.jbc.2021.100870

Robin Pearce and Yang Zhang
From the Department of Computational Medicine and Bioinformatics, Department of Biological Chemistry, University of Michigan, Ann Arbor, Michigan, USA

Edited by Wolfgang Peti

Article | Open Access | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

John Jumper, Richard Evans, [...] Demis Hassabis

Nature 596, 583–589 (2021) | Cite this article
415k Accesses | 69 Citations | 2798 Altmetric | Metrics

PDB-101 – PDB for pupils, students and teachers

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

PDB-101 | Molecule of the Month | Browse | Learn | Global Health | Teach | SciArt | Events | More

RCSB PDB-101 — Molecular explorations through biology and medicine

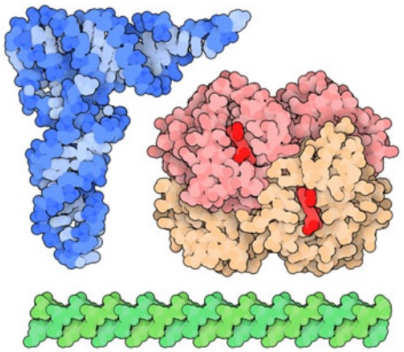
Educational portal of RCSB PDB PROTEIN DATA BANK

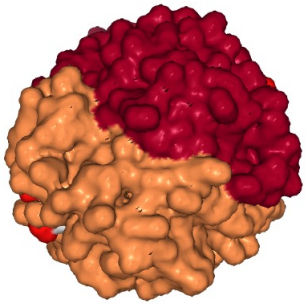
Search Molecule of the Month articles and more — Go

Celebrating 50 YEARS OF Protein Data Bank

Molecule of the Month

October 2021





Fifty Years of Open Access to PDB Structures

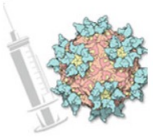
The Protein Data Bank is celebrating its golden anniversary!

More

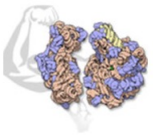
3D View: 2DHB

Style	Color	Spin
○ Cartoon	○ Rainbow	◉ On
○ Spheres	◉ Chain	○ Off
◉ Surface	○ Structure	

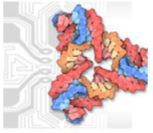
Browse resources by category



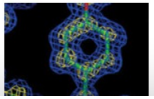
Health and Disease



Molecules of Life



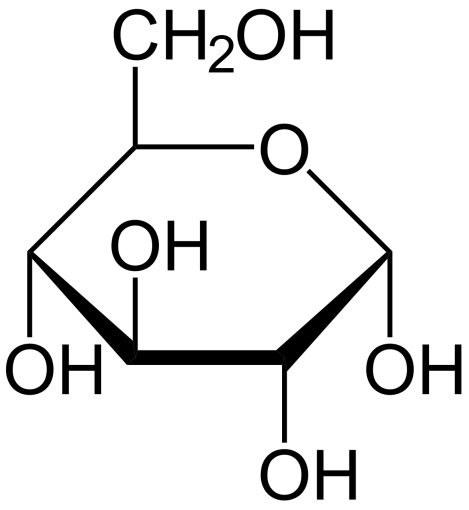
Biotech and Nanotech

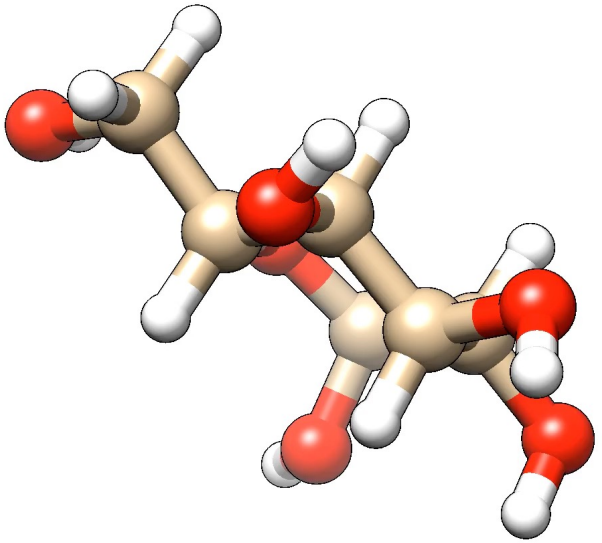


Structures and Structure Determination

Teaching Structural Biology relies on structural formulae

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania





α-D-glucopyranose

Molecular models to aid teaching - Molymod

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

molymod®

The *original* dual-scale system of molecular models

http://www.molymod.com/MMS-004_Inorganic__Organic_Teacher_Set.jpg

Molecular models to aid teaching – Paper models

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

Antibody
(Paper Model)

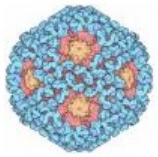
DNA
(Paper Model)

Dengue Virus
(Paper Model)

Green and Red Fluorescent Proteins
(Paper Model)

G Protein-Coupled Receptor (GPCR)
(Paper Model)

HIV Capsid
(Paper Model)



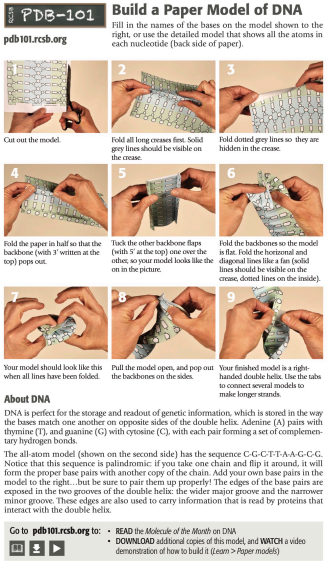
Human Papillomavirus (HPV)
(Paper Model)

Insulin
(Paper Model)

Quasisymmetry in Icosahedral Viruses
(Activity Page)

tRNA
(Paper Model)

Zika Virus with and without antibodies
(Paper Model)



PDB-101

Build a Paper Model of DNA

pdb101.rcsb.org

Fill in the names of the bases on the model shown to the right, or use the detailed model that shows all the atoms in each nucleotide (back side of paper).

1 Cut out the model.

2 Fold all long creases first. Solid grey lines should be visible on the crease.

3 Fold dotted grey lines so they are hidden in the crease.

4 Fold the paper in half so that the backbone (with 3' written at the top) pops out.

5 Tuck the other backbone flaps (with 5' at the top) one over the other, so your model looks like the on in the picture.

6 Fold the backbones so the model is flat. Fold the horizontal and diagonal lines like a fan (solid lines should be visible on the crease, dotted lines on the inside).

7 Your model should look like this when all lines have been folded.

8 Pull the model open, and pop out the backbones on the sides.

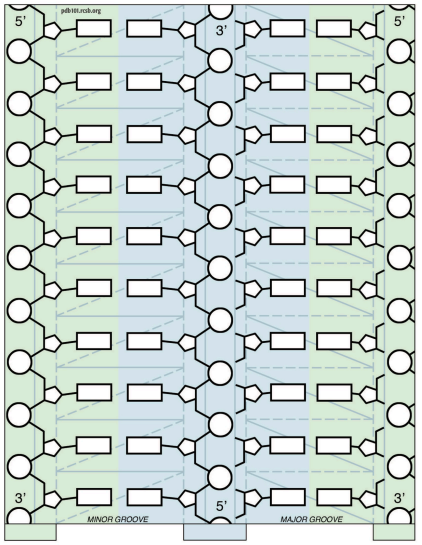
9 Your finished model is a right-handed double helix. Use the tabs to connect several models to make longer strands.

About DNA

DNA is perfect for the storage and readout of genetic information, which is stored in the way the bases match one another on opposite sides of the double helix. Adenine (A) pairs with thymine (T), and guanine (G) with cytosine (C), with each pair forming a set of complementary hydrogen bonds.

The all-atom model (shown on the second side) has the sequence C-G-C-T-T-A-A-G-C-G. Notice that this sequence is palindromic: if you take one chain and flip it around, it will form the proper base pairs with another copy of the chain. Add your own base pairs in the model to the right…but be sure to pair them up properly! The edges of the base pairs are exposed in the two grooves of the double helix: the wider major groove and the narrower minor groove. These edges are also used to carry information that is read by proteins that interact with the double helix.

Go to **pdb101.rcsb.org** to:
- READ the *Molecule of the Month* on DNA
- **DOWNLOAD** additional copies of this model, and **WATCH** a video demonstration of how to build it (*Learn > Paper models*)

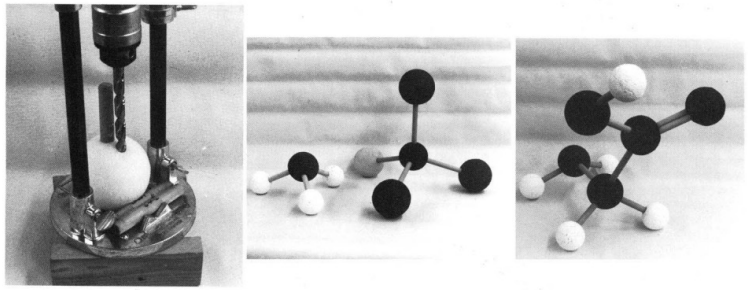


PDB-101 is the educational portal of RCSB Protein Data Bank (rcsb.org)

https://pdb101.rcsb.org/learn/paper-models

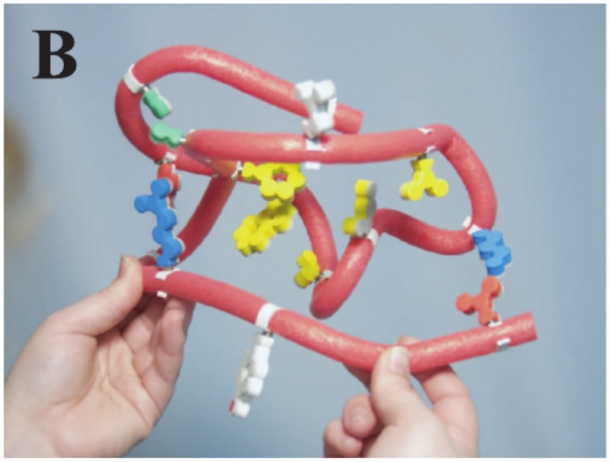
Molecular models to aid teaching – DIY

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania



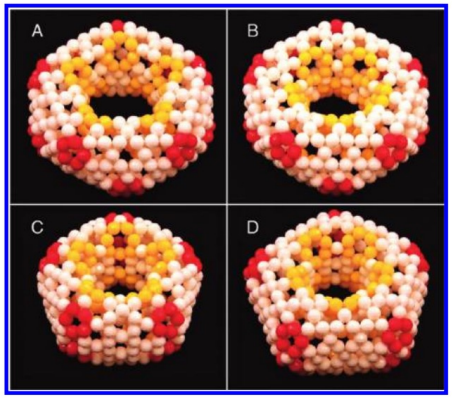
Styrofoam balls and copper wires

Birk, J. P.; Foster, J. Molecular models for the do-it-yourselfer. J. Chem. Educ. 1989, 66, 1015−1018.



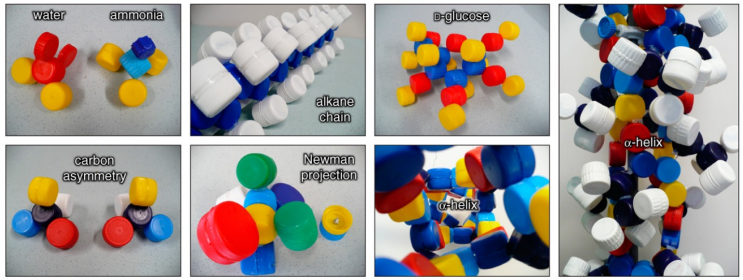
Flexible foam, wires and foam cut-outs

Herman T., et. al. Tactile teaching: Exploring protein structure/function using physical models. Biochem. Mol. Biol. Educ. **34**: 247–254.



Glass Beads

Chuang, C. et al. Molecular Modeling of Fullerenes with Beads. J. Chem. Educ. 2012, 89, 414−416

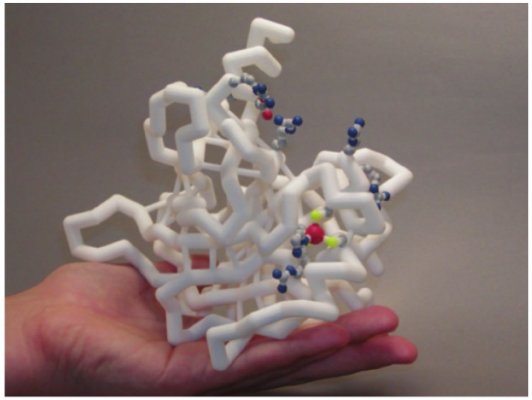


Screw-on bottle caps

Siodłak, D. Building Molecular Models Using Screw-On Bottle Caps. J. Chem. Educ. 2013, 90, 1247−1249.

Molecular models to aid teaching – 3D printed models

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

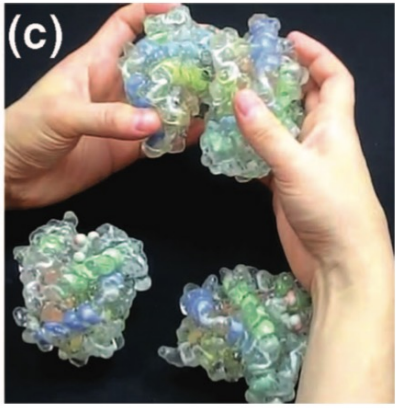


p53 tumor suppressor protein

Herman T., et. al. Tactile teaching: Exploring protein structure/function using physical models. Biochem. Mol. Biol. Educ. 34: 247–254.

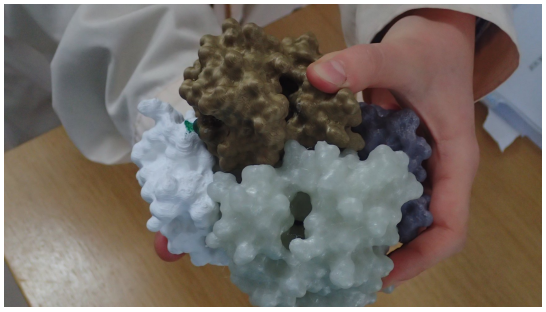
Leucine zipper

Meyer S.C. 2015. 3D Printing of Protein Models in an Undergraduate Laboratory: Leucine Zippers. J. Chem. Educ. 92: 2120–2125.

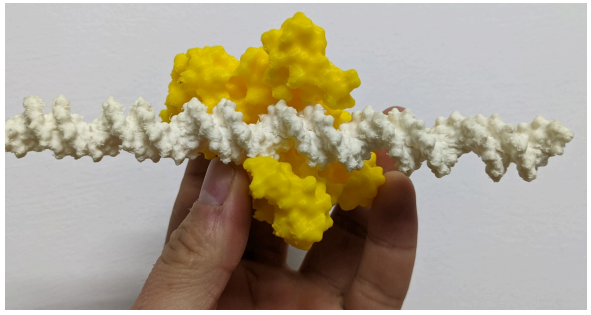


Human haemoglobin

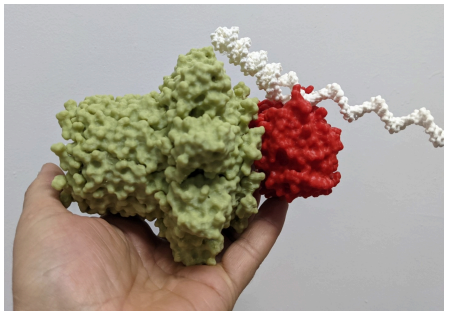
Kawakami M. A soft and transparent handleable protein model. Rev Sci Instrum. 2012; 83(8): 084303.



Human deoxyhaemoglobin



EcoRI endonuclease and DNA



Nanopore sequencing complex

Molecular models to aid teaching – 3D printed models

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

Advantages of 3D printed molecular models:

Based on real scientific data;

Depicted using standardized representations;

Easy to edit and adapt to the outcomes of a specific lesson;

Cheap to fabricate and reproduce;

Easy to distribute

183584 structures freely available

PDBe Protein Data Bank in Europe

RCSB PDB PROTEIN DATA BANK

PDBj Protein Data Bank Japan

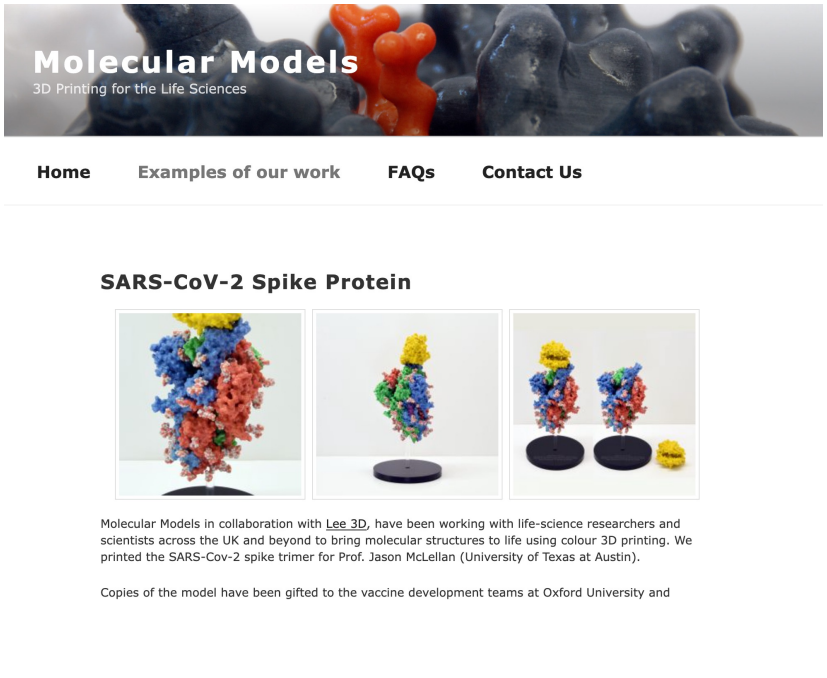
molecular visualization software
Chimera, PyMol

Over the internet, print when required

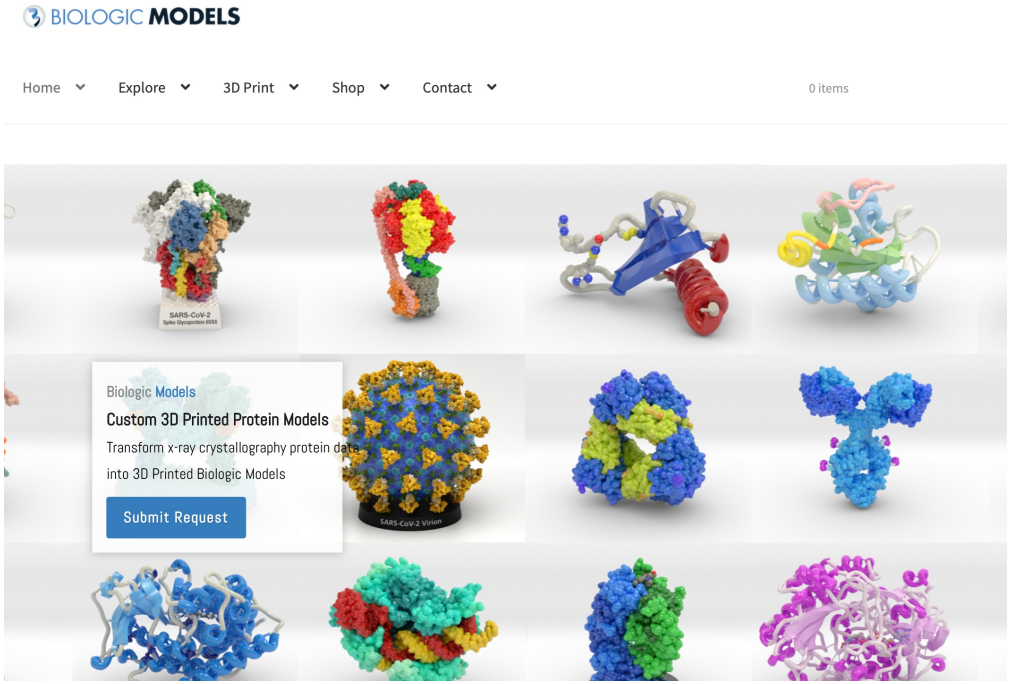
3D printed models – how to get them

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

The easy, but certainly not cheap the way:



http://www.molecmodels.co.uk/



https://biologicmodels.com/

3D printed models – how to get them

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

The almost easy, but clearly much cheaper way:

A1. Find an already available model at:
https://3dprint.nih.gov/
https://modelemoleculare.ro/

OR

A2. Automatically create your own model at:
https://3dprint.nih.gov/create

OR

A3. Ask somebody else to do it such as:
https://modelemoleculare.ro/product-category/modele-la-cerere/

B. Fabricate your model using your own 3D printer or access an on demand 3D printing service
printari-3d.ro 3dp.ro fablab.ro

Take-away message

Usage of physical models of (macro)molecules improves learning outcomes, but is better to be tailored to teachers needs

3D printing offers a cheap way of fabricating and distributing molecular models

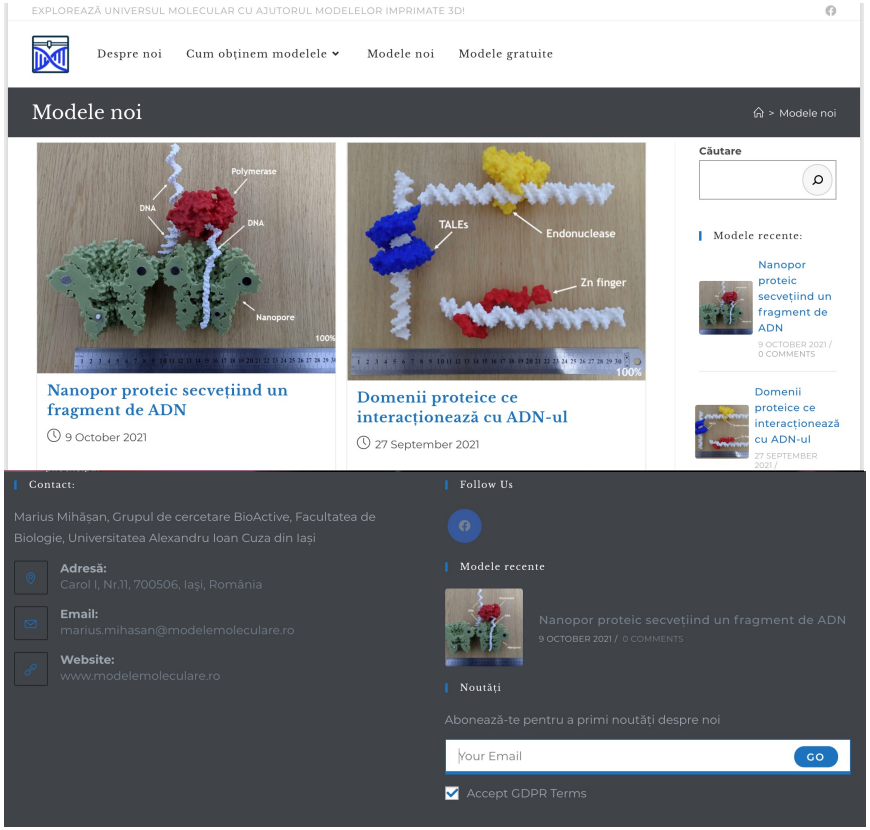
Models and workflows for printing macromolecular models from PDB are available

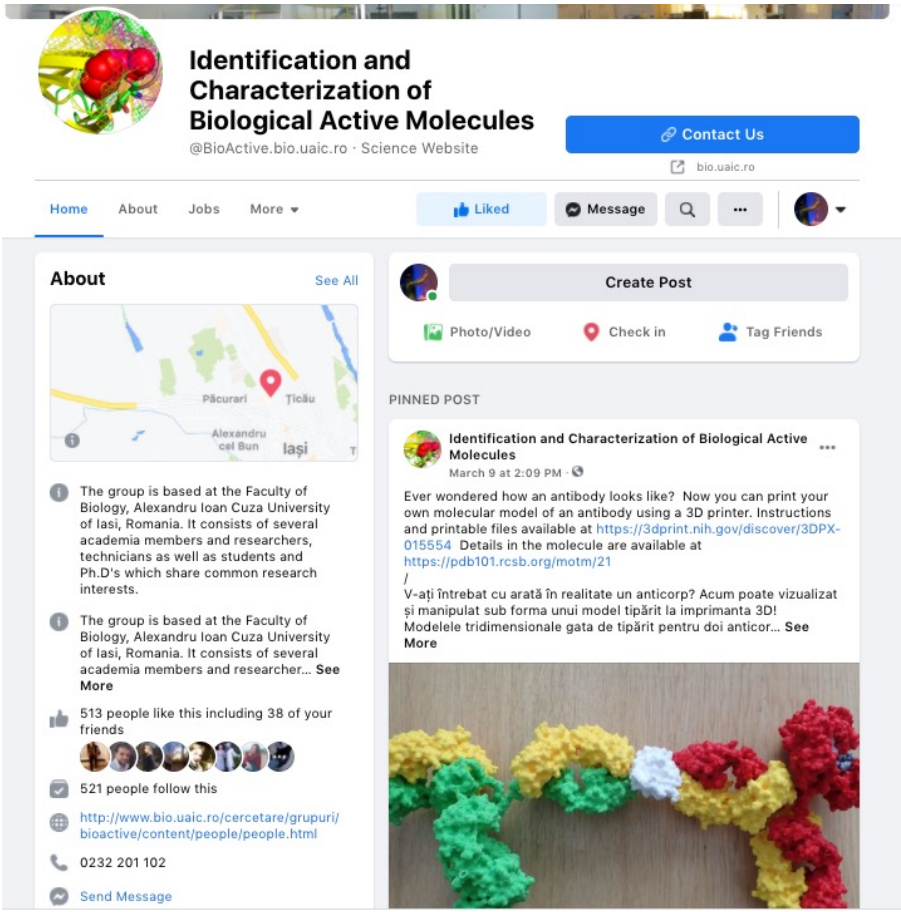
Proof of concept demonstrated. Please spread the word!

Updates and new printed models

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

https://modelemoleculare.ro/





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3D printed models – how to get them

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

The hard way:

Download structure from

PDBe Protein Data Bank in Europe | RCSB PDB PROTEIN DATA BANK | PDBj Protein Data Bank Japan

PDB or **CIF** file

Visualize and prepare the model in

UCSF Chimera

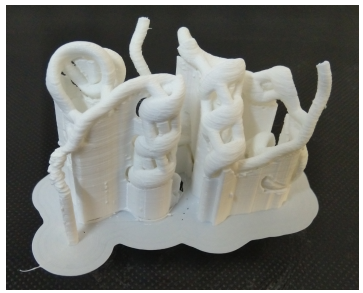
STL file

Prepare the file for printing using

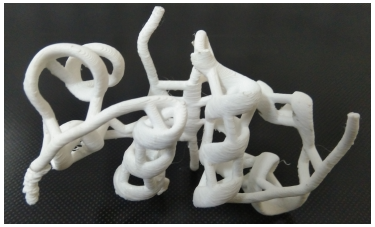
Ultimaker Cura

GCODE file

Print

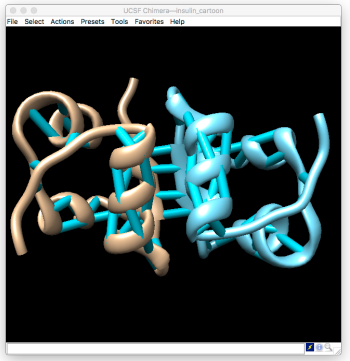


Support material removal



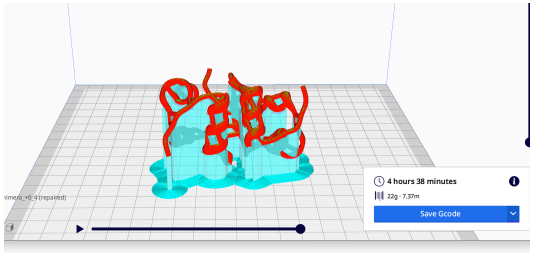
C. Clean up and finalize the physical model

1. **Chose or combine visualization styles;**
2. **Add H bonds or create struts to make the model more sturdy** (mandatory for cartoon and balls and sticks models, not required for surface);
3. **Increase the thickness** of each printed element and/or **improve the smoothness** for molecular surfaces.



A. Generate the computer model

1. Set the printing **scale**;
2. **Orient** the model on printing bed;
3. Set printing **resolution**;
4. Set shell **wall thickness** and **infill** %;
5. Automatically **add support**;
6. **Slice** the model;
7. **Send** the resulting gcode to printer (via SD-Card, USB or WiFi)



B. Print the model

3D printed models – how to get them

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

jove Journal of Visualized Experiments www.jove.com

Video Article

3D Printing of Biomolecular Models for Research and Pedagogy

Eduardo Da Veiga Beltrame[1], James Tyrwhitt-Drake[2], Ian Roy[3], Raed Shalaby[4], Jakob Suckale[4], Daniel Pomeranz Krummel[5]

[1]Department of Physics, Brandeis University
[2]Bioinformatics and Computational Biosciences Branch (BCBB), NIH/NIAID/OD/OSMO/OCICB
[3]Library/LTS/MakerLab, Brandeis University
[4]Interfaculty Institute of Biochemistry (IFIB), University of Tübingen
[5]Winship Cancer Institute, Emory University School of Medicine

Correspondence to: Jakob Suckale at jakob.suckale@uni-tuebingen.de, Daniel Pomeranz Krummel at dapk@brandeis.edu

URL: https://www.jove.com/video/55427
DOI: doi:10.3791/55427

Keywords: Engineering, Issue 121, 3D printing, molecular biology, education, structure, biomolecules, models, extrusion printers

Date Published: 3/13/2017

Citation: Da Veiga Beltrame, E., Tyrwhitt-Drake, J., Roy, I., Shalaby, R., Suckale, J., Pomeranz Krummel, D. 3D Printing of Biomolecular Models for Research and Pedagogy. *J. Vis. Exp.* (121), e55427, doi:10.3791/55427 (2017).

JOURNAL OF CHEMICAL EDUCATION Communication

pubs.acs.org/jchemeduc

Rapid Access to Multicolor Three-Dimensional Printed Chemistry and Biochemistry Models Using Visualization and Three-Dimensional Printing Software Programs

Ken Van Wieren,[†] Hamel N. Tailor,[‡] Vincent F. Scalfani,[§] and Nabyl Merbouh*[,‡]

[†]Science Technical Center and [‡]Department of Chemistry, Simon Fraser University 8888 University Drive Burnaby, British Columbia V5A 1S6, Canada
[§]University Libraries, Rodgers Library for Science and Engineering, The University of Alabama, Tuscaloosa, Alabama 35487, United States

Supporting Information

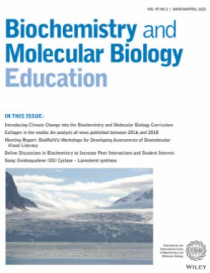
JOURNAL OF CHEMICAL EDUCATION Article

pubs.acs.org/jchemeduc

A Simplified Method for the 3D Printing of Molecular Models for Chemical Education

Oliver A. H. Jones*[,†] and Michelle J. S. Spencer*[,‡]

[†]Australian Centre for Research on Separation Science (ACROSS), School of Science, RMIT University, GPO Box 2476, Melbourne, Victoria 3001, Australia
[‡]School of Science, RMIT University, GPO Box 2476, Melbourne, Victoria 3001, Australia



Biochemistry and Molecular Biology Education

A beginner's guideline for low-cost 3D printing of macromolecules usable for teaching and demonstration

Marius Mihasan

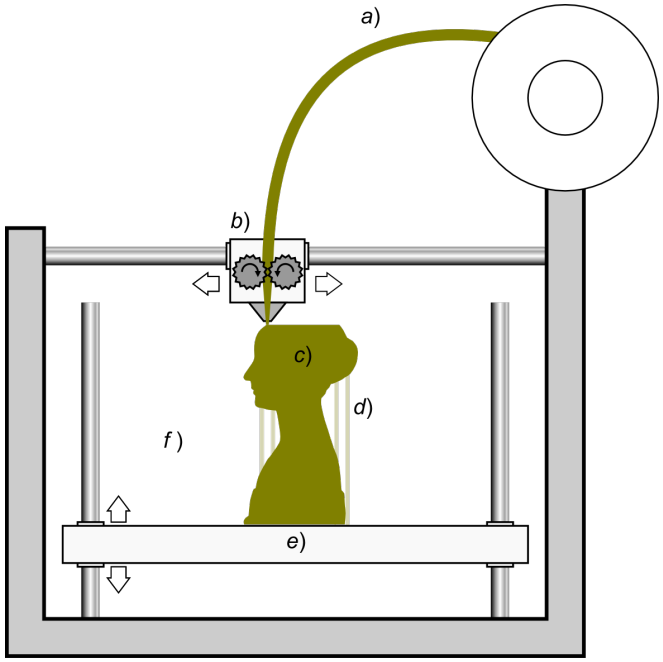
First published: 23 March 2021 | https://doi.org/10.1002/bmb.21493

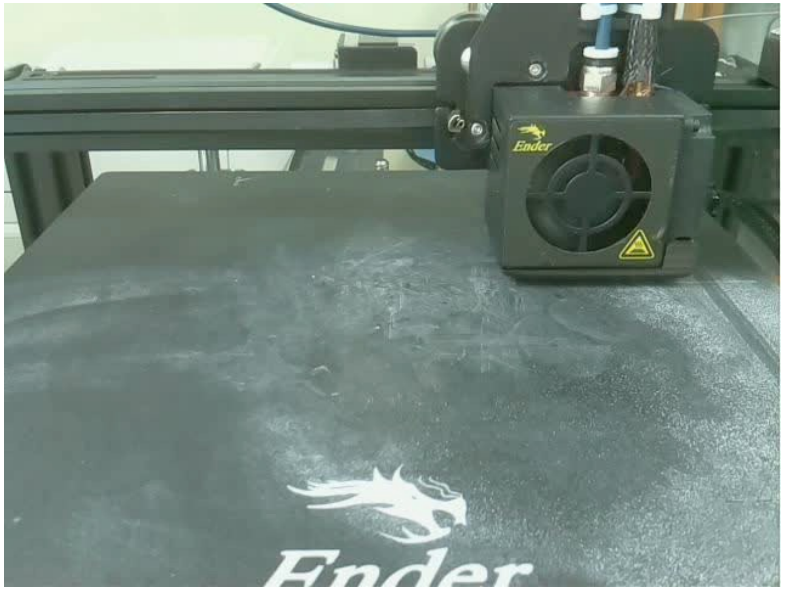
What is 3D printing and how does it work

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

3D printing - construction of a three-dimensional object from a digital 3D model. Also termed **additive manufacturing**.

Material extrusion / Fused filament fabrication (FFF) / fused deposition modeling (FDM)

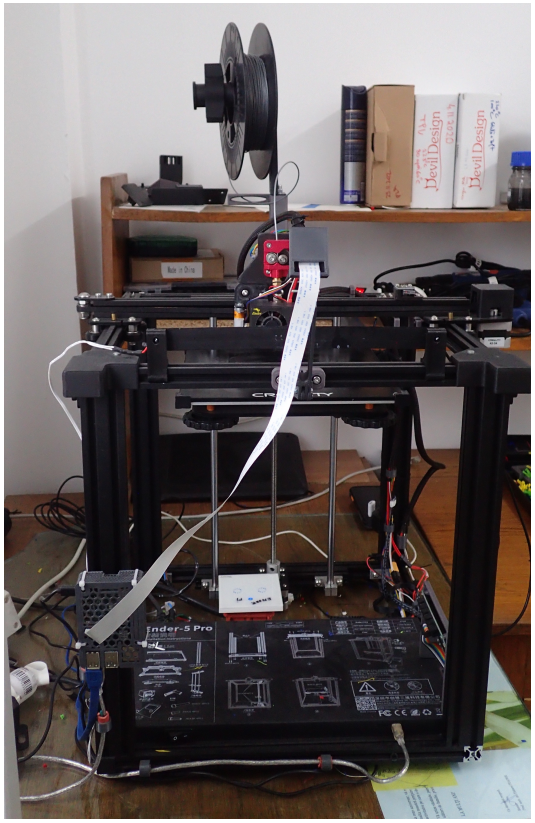




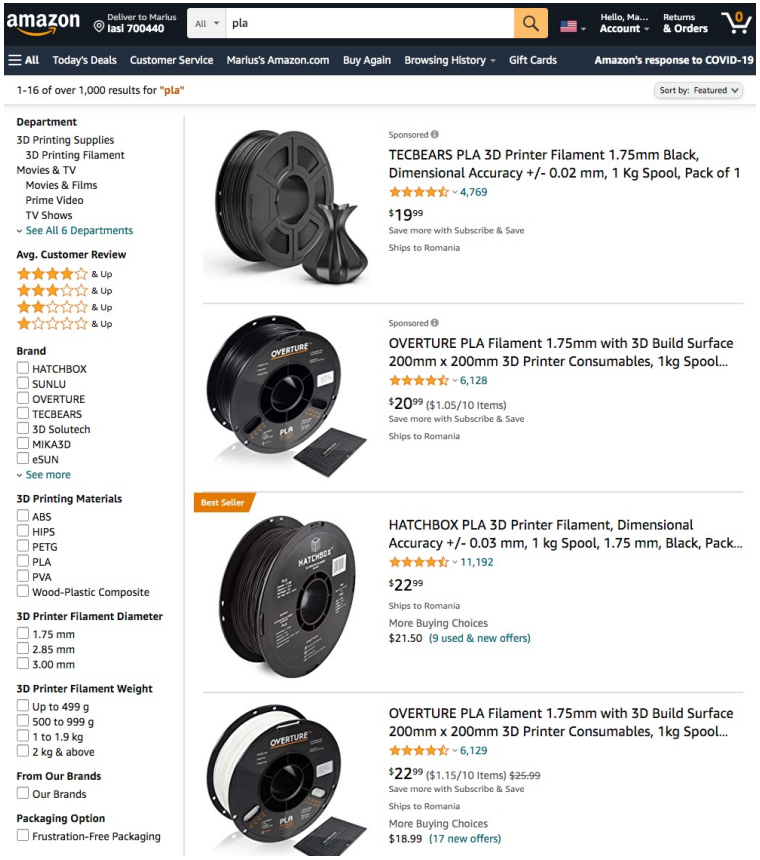
3D printing using FFF is accessible

Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania

Under 500$ printer



20$ - 40$ Kg of plastic



3D printing can pe used in high schools/universities from low income countries to fabricate macromolecular models adapted to teachers needs