



# 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**

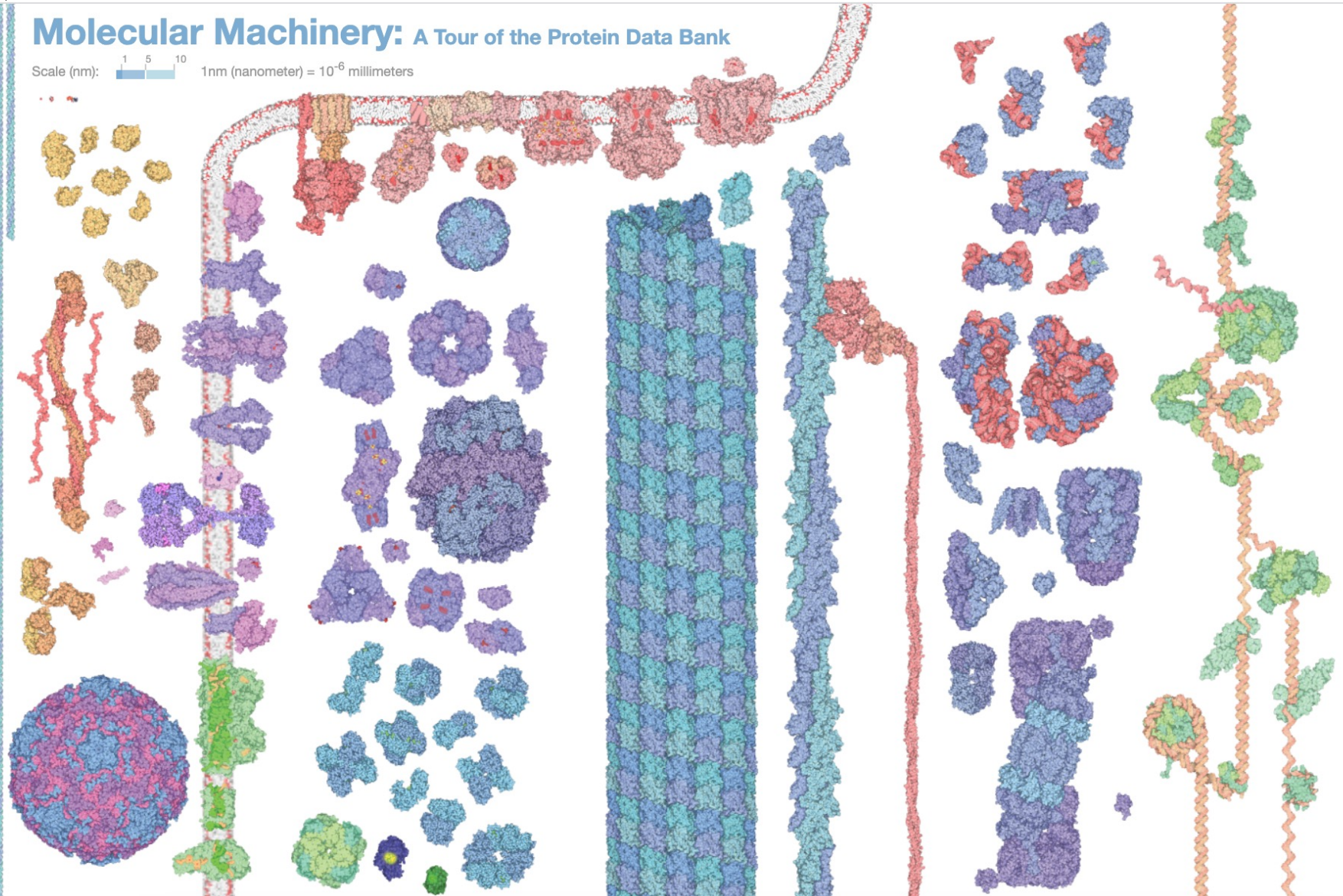


# Understanding Life Sciences relies on understanding Structural Biology

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

## Molecular Machinery: A Tour of the Protein Data Bank

Scale (nm): 1 5 10  
1nm (nanometer) =  $10^{-6}$  millimeters



Extracellular

Membrane

Intracellular/Cytosol

Intracellular/Nucleus

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





# RCSB PDB - Structural data for researchers

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

The screenshot shows the RCSB PDB website interface. At the top, there is a navigation bar with links for Deposit, Search, Visualize, Analyze, Download, Learn, More, Documentation, and Careers. A search bar is prominently displayed with the text "Enter search terms or PDB ID(s)". Below the search bar, there are logos for PDB-101, PDB, EMDataResource, Nucleic Acid Database, and Worldwide Protein Data Bank Foundation. A banner for "Developers: Join the RCSB PDB Team" is also visible. The main content area features a "Welcome" message, a sidebar with navigation options (Deposit, Search, Visualize, Analyze, Download), and a section titled "A Structural View of Biology" which describes the resource's purpose and its role in curating and annotating PDB data. To the right, there is a section for the "October Molecule of the Month" featuring a 3D molecular model.

## How much data is available?

Enough to have confidence in protein structure prediction!



Proc Natl Acad Sci U S A. 2005 Jan 25; 102(4): 1029-1034.  
Published online 2005 Jan 14. doi: 10.1073/pnas.0407152101  
Biophysics

PMCID: PMC545829  
PMID: 15653774

### 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<sup>1</sup> and Yang Zhang<sup>1,2,\*</sup>

From the <sup>1</sup>Department of Computational Medicine and Bioinformatics, <sup>2</sup>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

Search Molecule of the Month articles and more

Go

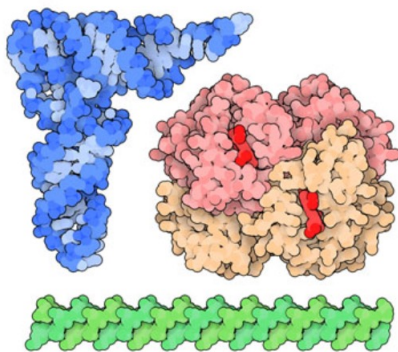
Celebrating  50 YEARS OF  
Protein Data Bank



Educational portal 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

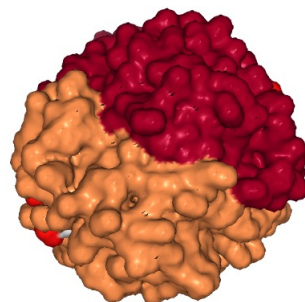
- Cartoon
- Spheres
- Surface

Color

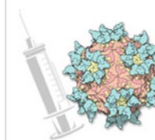
- Rainbow
- Chain
- Structure

Spin

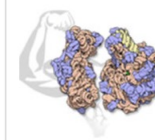
- On
- Off



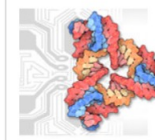
Browse resources by category >



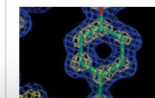
▾ Health and Disease



▾ Molecules of Life

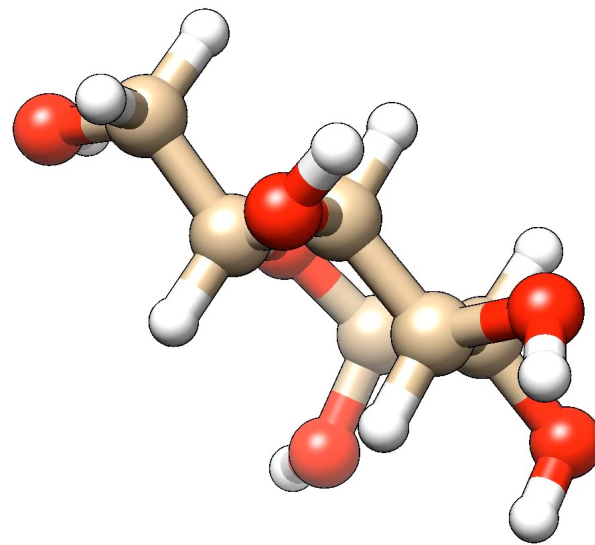
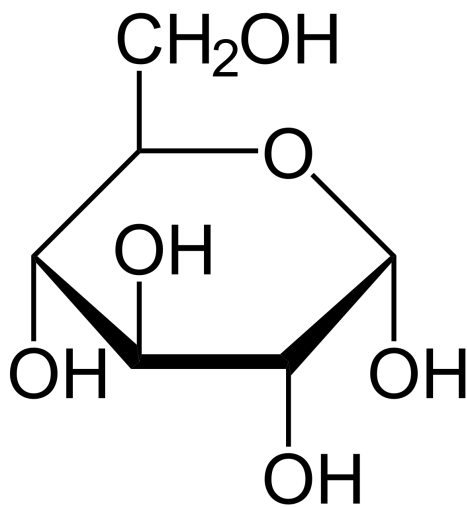


▾ Biotech and Nanotech



▾ Structures and Structure  
Determination





$\alpha$ -D-glucopyranose

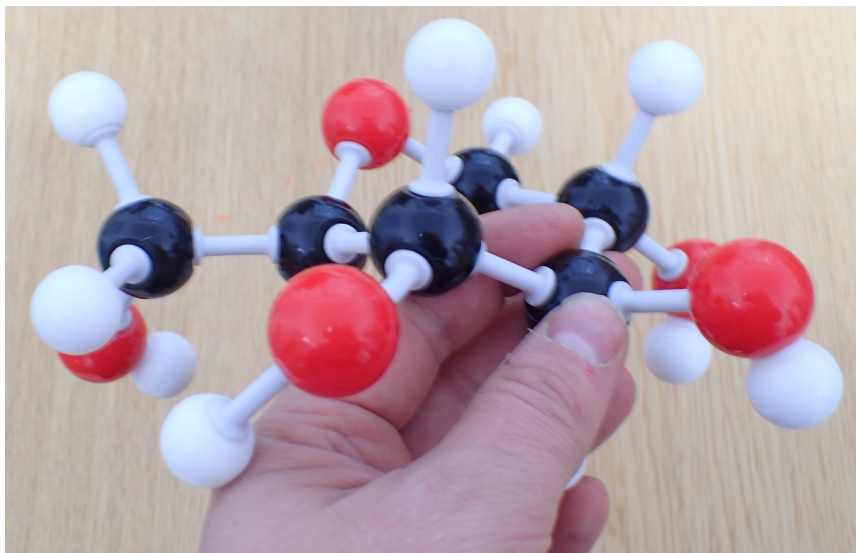


# Molecular models to aid teaching - Molymod

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

## **molymod**<sup>®</sup>

The *original* dual-scale system of molecular models

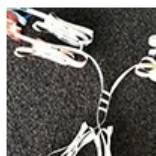


[http://www.molymod.com/MMS-004\\_Inorganic\\_\\_Organic\\_Teacher\\_Set.jpg](http://www.molymod.com/MMS-004_Inorganic__Organic_Teacher_Set.jpg)



# Molecular models to aid teaching – Paper models

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Antibody  
(Paper Model)



DNA  
(Paper Model)



Dengue Virus  
(Paper Model)



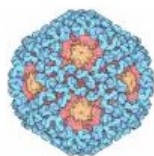
Green and Red  
Fluorescent Proteins  
(Paper Model)



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)



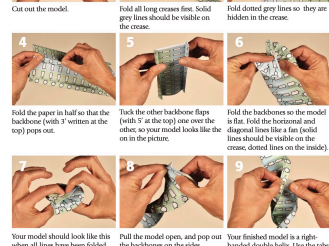
tRNA  
(Paper Model)



Zika Virus with and  
without antibodies  
(Paper Model)

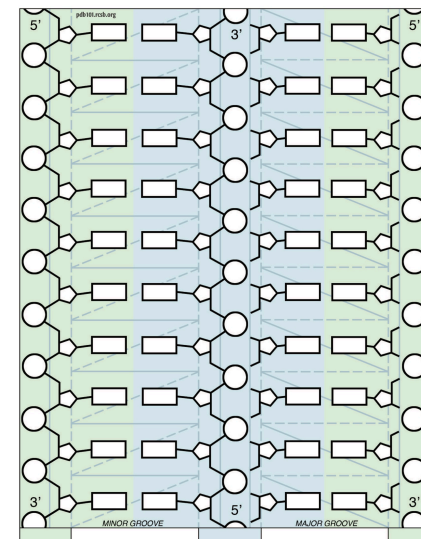
## Build a Paper Model of DNA

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).



**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-C. 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](http://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)



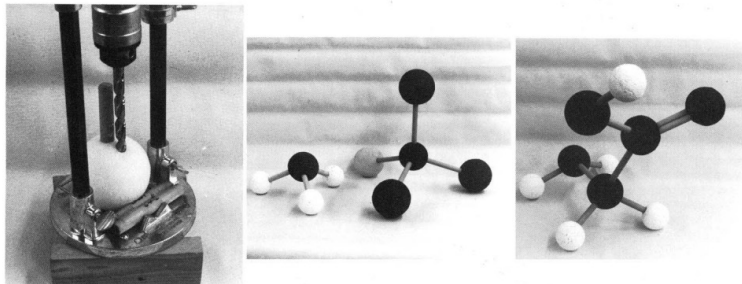
PDB 101 is the educational portal of RCSB Protein Data Bank (rcsb.org)





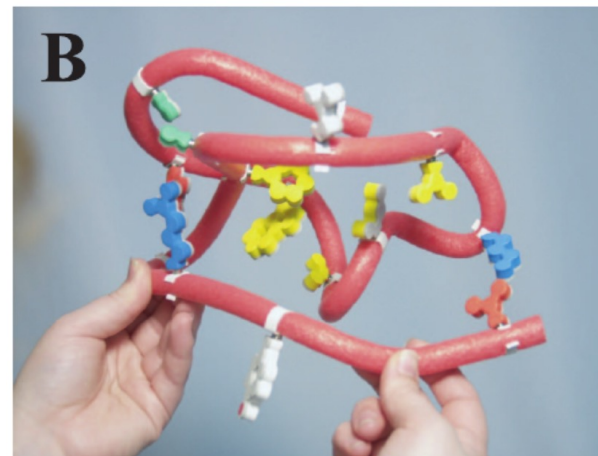
# Molecular models to aid teaching – DIY

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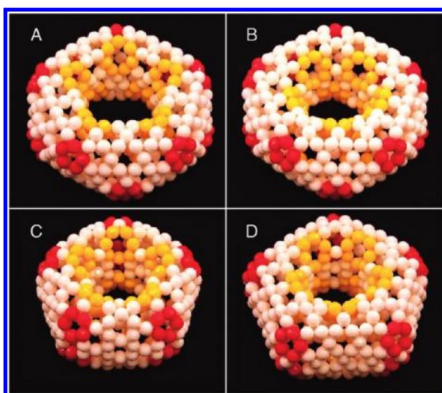
## Styrofoam balls and copper wires

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



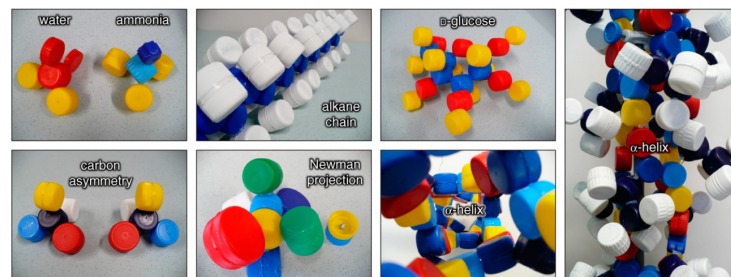
## Flexible foam, wires and foam cut-outs

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



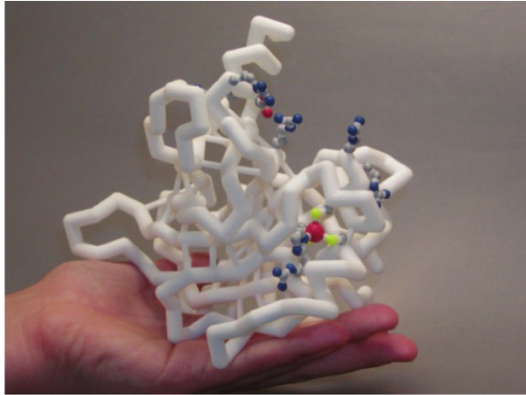
## Screw-on bottle caps

Siodlak, D. Building Molecular Models Using Screw-On Bottle Caps. *J. Chem. Educ.* 2013, 90, 1247–1249.



# Molecular models to aid teaching – 3D printed models

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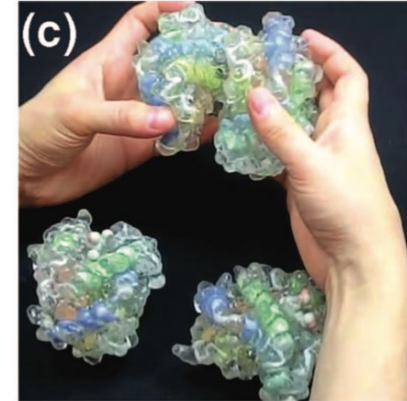
**p53 tumor suppressor protein**

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



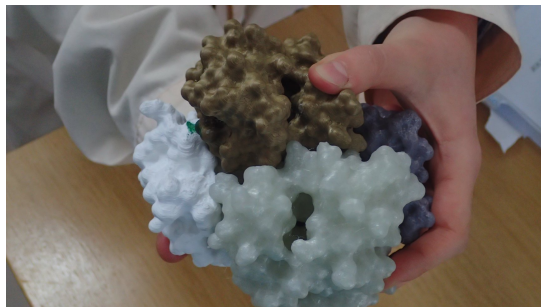
**Leucine zipper**

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

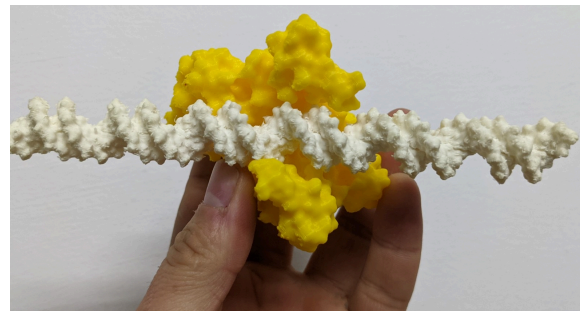


**Human haemoglobin**

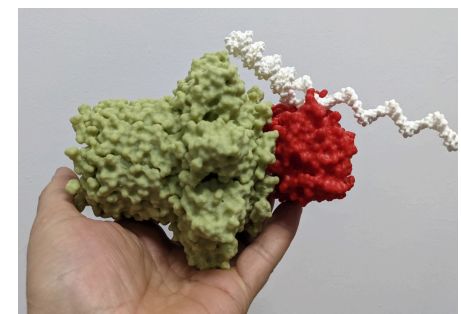
Kawakami M. A soft and transparent handleable protein model. *Rev Sci Instrum.* 2012; 83(8): 084303.



**Human deoxyhaemoglobin**



**EcoRI endonuclease and DNA**



**Nanopore sequencing complex**



# Molecular models to aid teaching – 3D printed models

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## 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

molecular visualization software  
Chimera, PyMol

Over the internet, print when required

 **PDBe**  
Protein Data Bank in Europe

 **PDB**  
PROTEIN DATA BANK

 **PDBj**  
Protein Data Bank Japan  
27.10.2021





# 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:

## Molecular Models

3D Printing for the Life Sciences

[Home](#) [Examples of our work](#) [FAQs](#) [Contact Us](#)

### SARS-CoV-2 Spike Protein



Molecular Models in collaboration with [Lee 3D](#), have been working with life-science researchers and scientists across the UK and beyond to bring molecular structures to life using colour 3D printing. We printed the SARS-Cov-2 spike trimer for Prof. Jason McLellan (University of Texas at Austin).

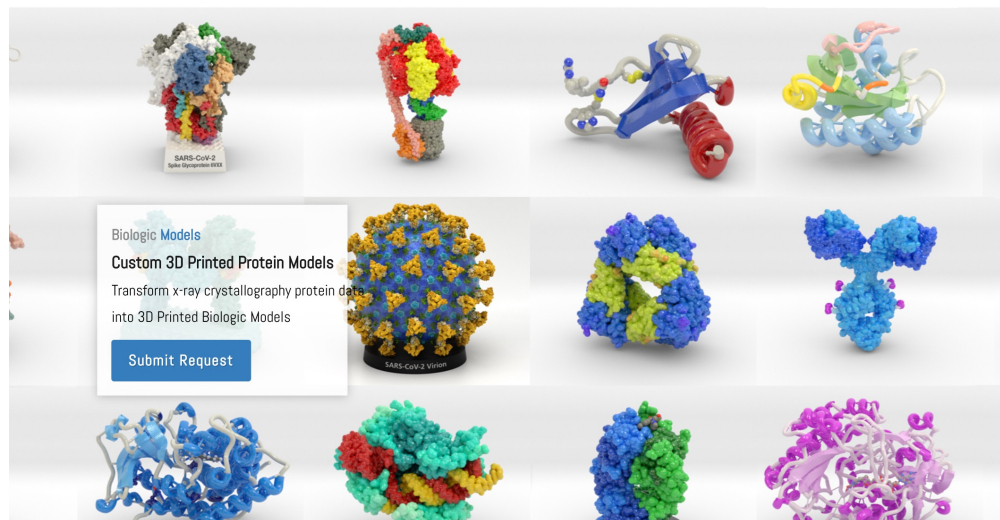
Copies of the model have been gifted to the vaccine development teams at Oxford University and

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

## BIOLOGIC MODELS

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0 items



<https://biologicmodels.com/>



# 3D printed models – how to get them

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The almost easy, but clearly much cheaper way:

**A1. Find an already available model at:**

<https://3dprint.nih.gov/>

<https://modelemolculare.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://modelemolculare.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](http://printari-3d.ro) [3dp.ro](http://3dp.ro) [fablab.ro](http://fablab.ro)

**NIH 3D PRINT EXCHANGE**



DISCOVER



SHARE



CREATE



LEARN



ENGAGE

3D printing technology is advancing at a rapid pace, but it is difficult to find or create 3D-printable models that are scientifically accurate or medically applicable. The NIH 3D Print Exchange provides models in formats that are readily compatible with 3D printers, and offers a unique set of tools to create and share 3D-printable





# Take-away message

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

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

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<https://modelemolculare.ro/>

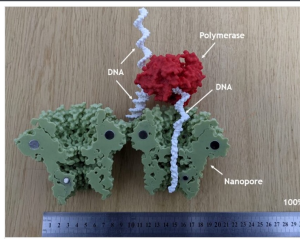
EXPLOREAZĂ UNIVERSUL MOLECULAR CU AJUTORUL MODELELOR IMPRIMATE 3D!



Despre noi Cum obținem modelele ▼ Modele noi Modele gratuite

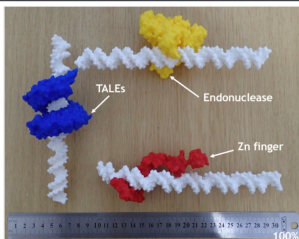
Modele noi

Modele noi



**Nanopor proteic secvețiind un fragment de ADN**

9 October 2021

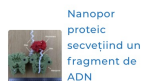


**Domenii proteice ce interacționează cu ADN-ul**

27 September 2021

Căutare

Modele recente:



9 OCTOBER 2021 / 0 COMMENTS



27 SEPTEMBER 2021 / 0 COMMENTS

Contact:

Marius Mihașan, Grupul de cercetare BioActive, Facultatea de Biologie, Universitatea Alexandru Ioan Cuza din Iași

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**Email:**  
marius.mihasan@modelemolculare.ro

**Website:**  
www.modelemolculare.ro

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Modele recente



Nanopor proteic secvețiind un fragment de ADN  
9 OCTOBER 2021 / 0 COMMENTS

Noutăți

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**Identification and Characterization of Biological Active Molecules**

@BioActive.bio.uaic.ro · Science Website

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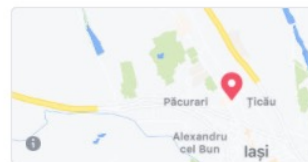
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About

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The group is based at the Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania. It consists of several academia members and researchers, technicians as well as students and Ph.D's which share common research interests.

The group is based at the Faculty of Biology, Alexandru Ioan Cuza University of Iasi, Romania. It consists of several academia members and researcher... See More

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<http://www.bio.uaic.ro/cercetare/grupuri/bioactive/content/people/people.html>

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**Identification and Characterization of Biological Active Molecules**

March 9 at 2:09 PM · 🌐

Ever wondered how an antibody looks like? Now you can print your own molecular model of an antibody using a 3D printer. Instructions and printable files available at <https://3dprint.nih.gov/discover/3DPX-015554> Details in the molecule are available at <https://pdb101.rcsb.org/motm/21>

V-ați întrebat cu arată în realitate un anticorp? Acum poate vizualizat și manipulat sub forma unui model tipărit la imprimanta 3D! Modelele tridimensionale gata de tipărit pentru doi anticor... See More



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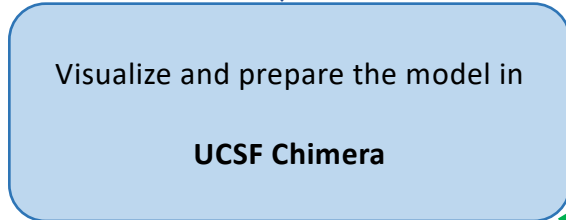
# 3D printed models – how to get them

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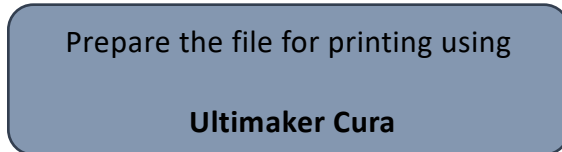
## The hard way:



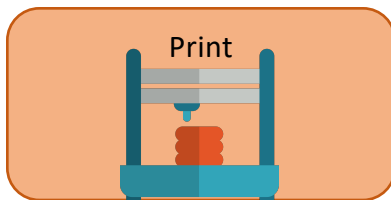
PDB or CIF file



STL file



GCODE file

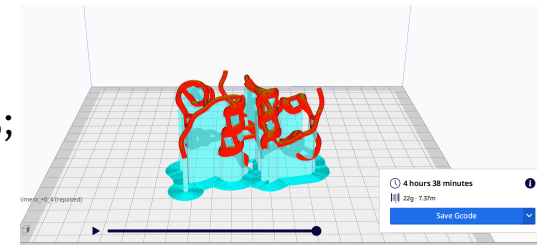


1. Chose or combine **visualization styles**;
2. Add **H bonds** or **create struts** to make the model more **sturdy** (mandatory for cartoon and balls and sticks models, not required for surface);
3. **Increase the thickness** of each printed element and/or **improve the smoothness** for molecular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



Support material  
removal

## C. Clean up and finalize the physical 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<sup>1</sup>, James Tyrwhitt-Drake<sup>2</sup>, Ian Roy<sup>3</sup>, Raed Shalaby<sup>4</sup>, Jakob Suckale<sup>4</sup>, Daniel Pomeranz Krummel<sup>5</sup>

<sup>1</sup>Department of Physics, Brandeis University

<sup>2</sup>Bioinformatics and Computational Biosciences Branch (BCBB), NIH/NIAD/OD/OSMO/OCICB

<sup>3</sup>Library/LTS/MakerLab, Brandeis University

<sup>4</sup>Interfaculty Institute of Biochemistry (IFIB), University of Tübingen

<sup>5</sup>Winship Cancer Institute, Emory University School of Medicine

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

URL: <https://www.jove.com/video/55427>

DOI: [doi:10.3791/55427](https://doi.org/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](https://doi.org/10.3791/55427) (2017).

JOURNAL OF  
**CHEMICAL EDUCATION**

Communication

[pubs.acs.org/jchemeduc](https://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,<sup>†</sup> Hamel N. Taylor,<sup>‡</sup> Vincent F. Scalfani,<sup>§</sup> and Nabyl Merbouh<sup>\*†‡</sup>

<sup>†</sup>Science Technical Center and <sup>‡</sup>Department of Chemistry, Simon Fraser University 8888 University Drive Burnaby, British Columbia V5A 1S6, Canada

<sup>§</sup>University Libraries, Rodgers Library for Science and Engineering, The University of Alabama, Tuscaloosa, Alabama 35487, United States

Supporting Information

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Article

[pubs.acs.org/jchemeduc](https://pubs.acs.org/jchemeduc)

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

Oliver A. H. Jones<sup>\*†‡</sup> and Michelle J. S. Spencer<sup>\*‡‡</sup>

<sup>†</sup>Australian Centre for Research on Separation Science (ACROSS), School of Science, RMIT University, GPO Box 2476, Melbourne, Victoria 3001, Australia

<sup>‡</sup>School of Science, RMIT University, GPO Box 2476, Melbourne, Victoria 3001, Australia

**Biochemistry and Molecular Biology Education**

**Biochemistry and Molecular Biology Education**



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>



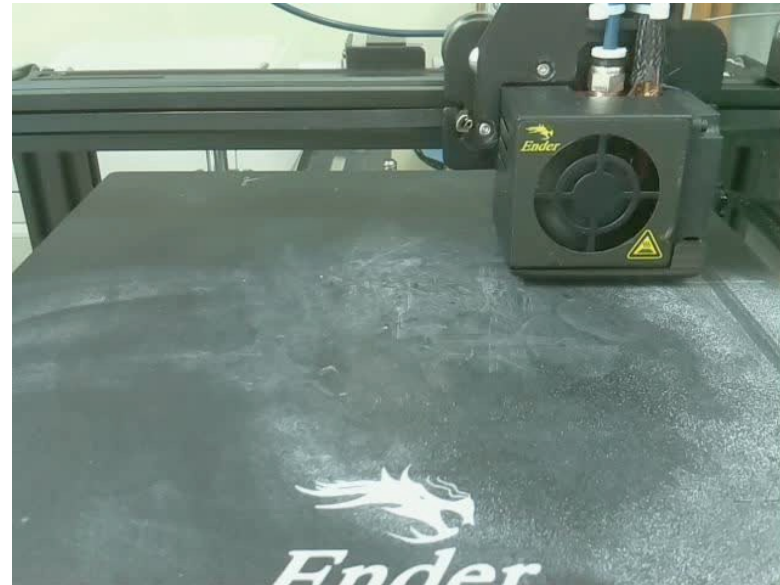
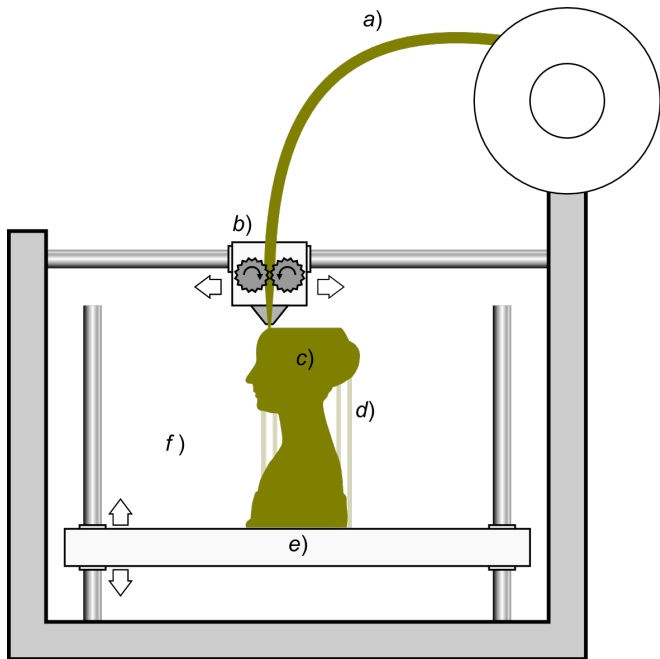


# What is 3D printing and how does it work

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)



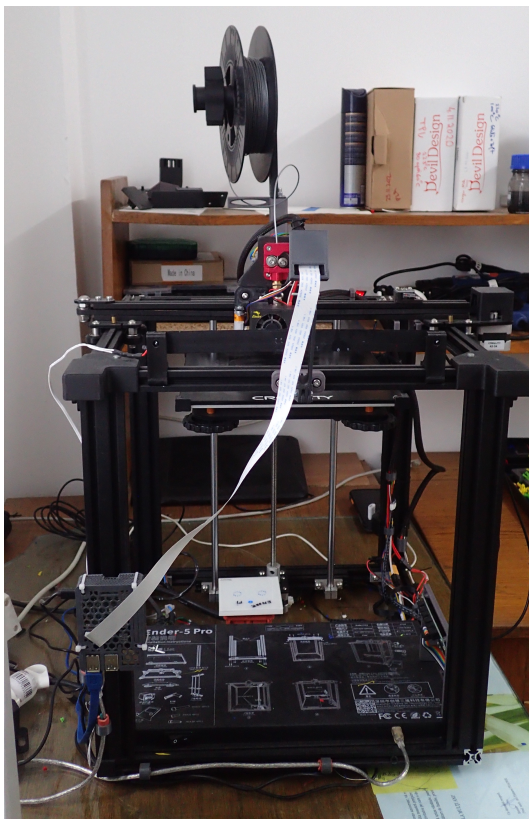


# 3D printing using FFF is accessible

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

Under 500\$ printer

20\$ - 40\$ Kg of plastic



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**3D Printing Materials**  
 ABS  
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**3D Printer Filament Diameter**  
 1.75 mm  
 2.85 mm  
 3.00 mm

**3D Printer Filament Weight**  
 Up to 499 g  
 500 to 999 g  
 1 to 1.9 kg  
 2 kg & above

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