3DP-Jmol: Bridging Structural Bioinformatics and Physical Models for Teaching and Outreach

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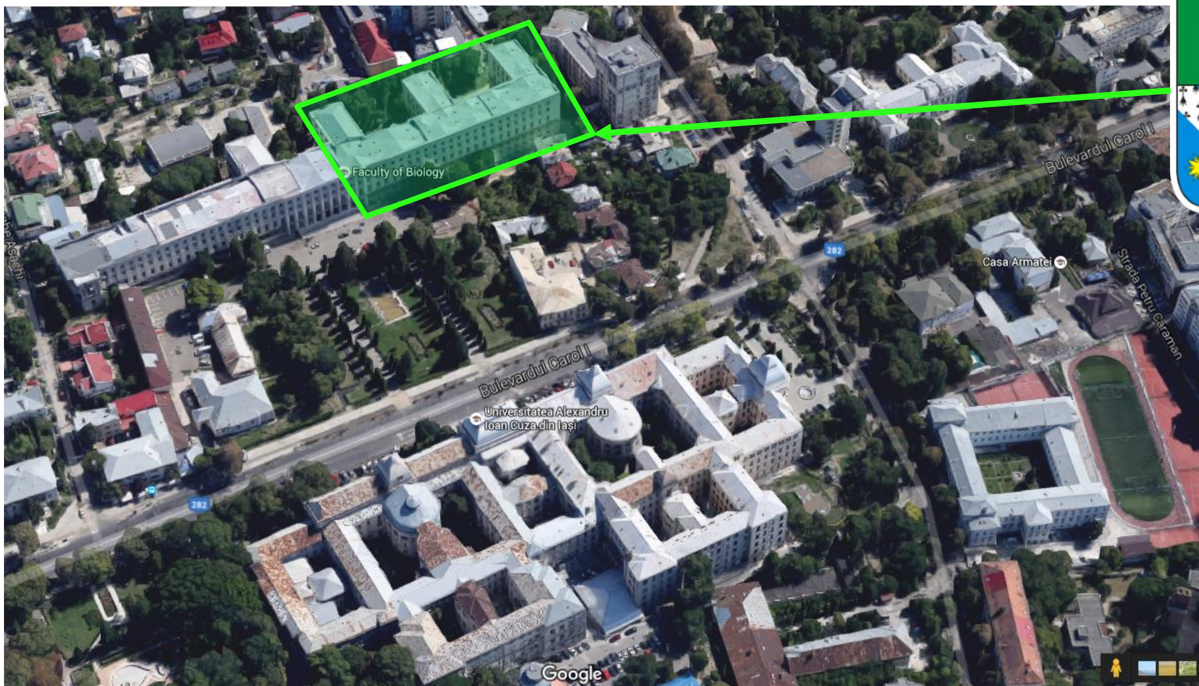
https://github.com/mariusmihasan/3DP-Jmol

Department of Biology



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www.bio.uaic.ro

Founded in **1948**

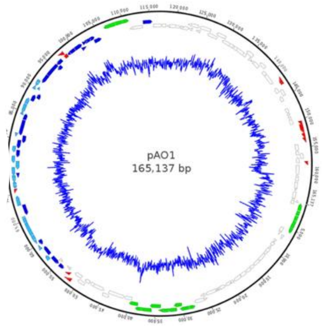
BioActive research group

- Isolation
- Identification
- Characterization
- Biological effects (neurological effects, citotoxycity, oxidative stress, antimicrobial activity

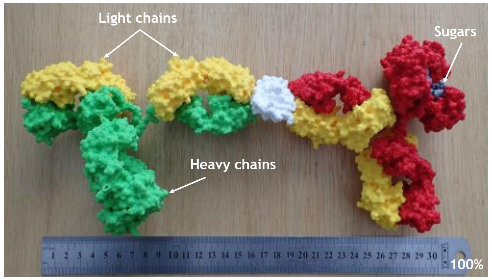
of biological active molecules with potential applications in biotechnology.

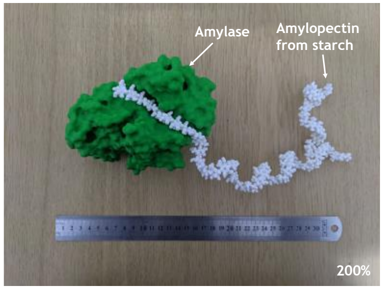
Main research subjects:

- molecular biology of pAO1 megaplasmid related to nicotine catabolism, stress induced by nicotine degradation and biotechnological applications.

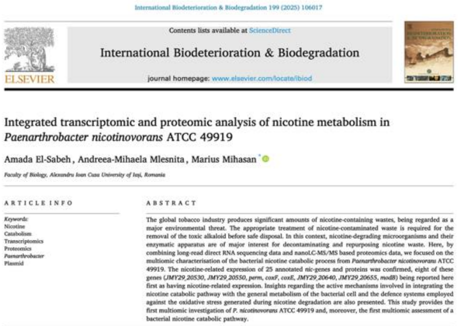


- using 3D printing for creating teaching materials to support molecular bioscience education.





Latest paper:



International Biodeterioration & Biodegradation 199 (2025) 106017

Contents lists available at ScienceDirect

International Biodeterioration & Biodegradation

journal homepage: www.elsevier.com/locate/ibiod

Integrated transcriptomic and proteomic analysis of nicotine metabolism in *Paenarthrobacter nicotinovorans* ATCC 49919

Amada El-Sabeh, Andreea-Mihaela Mlesnita, Marius Mihasan

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Nicotine
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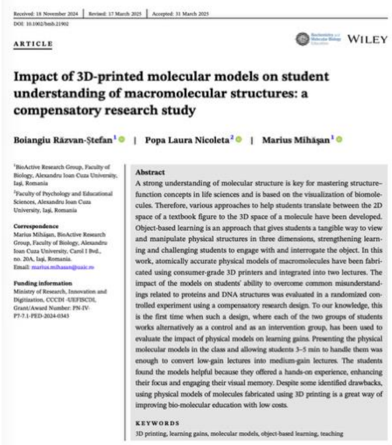
ICMB2025

Wed 05.11, 18:10
Tiberius Iustin Munteanu
Thu 6.11, 9:55 – 10:15
Andreea Mihaela Mlesnita

Latest paper:



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ARTICLE

WILEY

Impact of 3D-printed molecular models on student understanding of macromolecular structures: a compensatory research study

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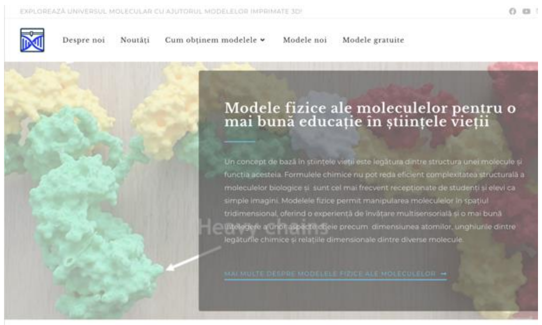
Correspondence

Abstract

Developed educational resources:



https://modelemoleculare.ro/

The plan for today

Theoretical part - This presentation

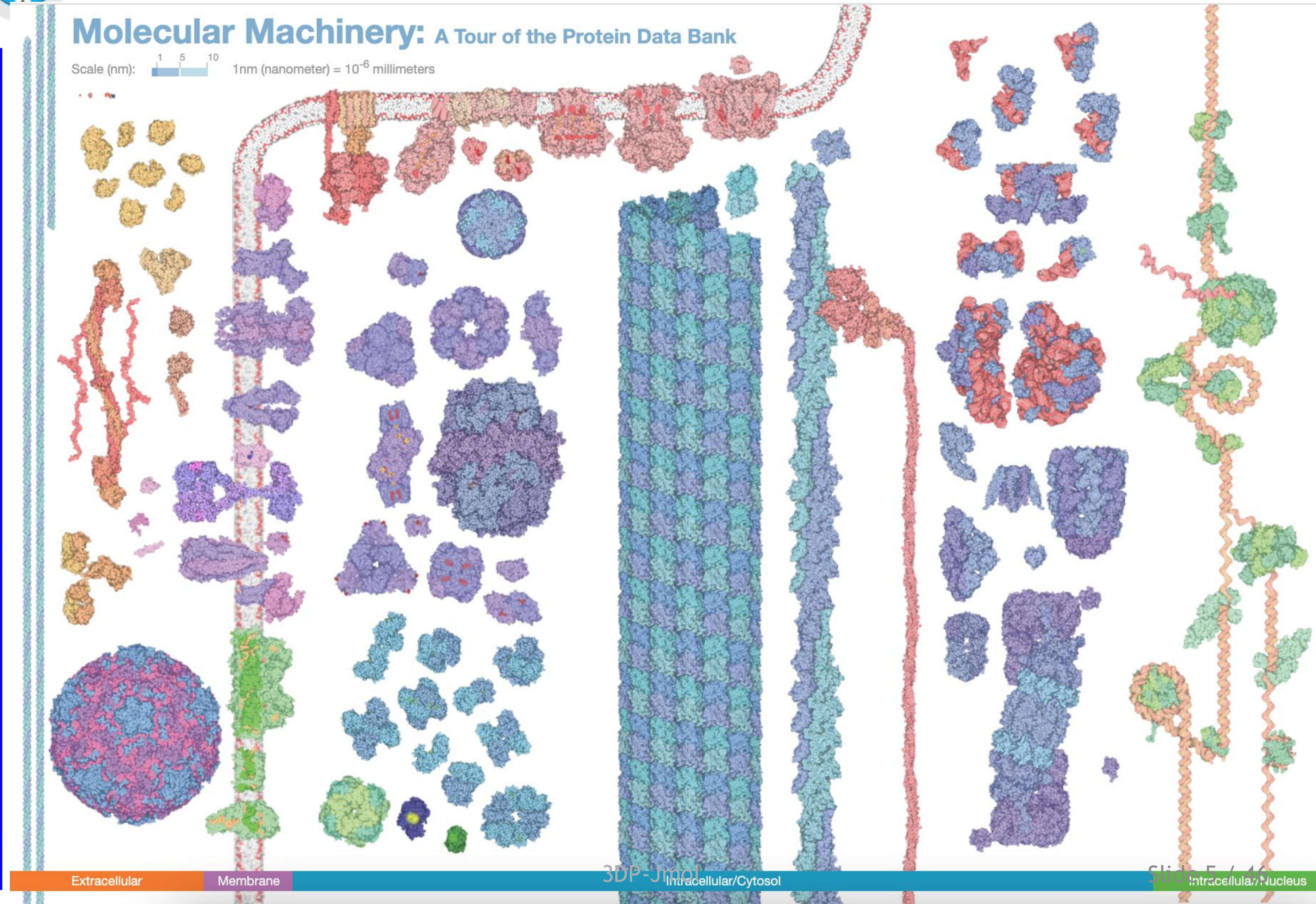
- Why are 3D printed molecular models needed?
- Are these models efficient?
- How and from where can I get 3D printed models ?

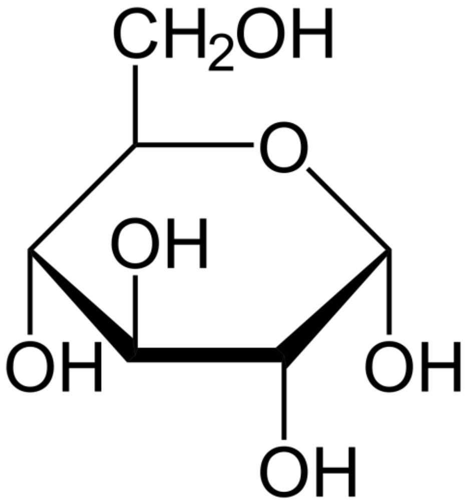
Hands-on part - the workshop

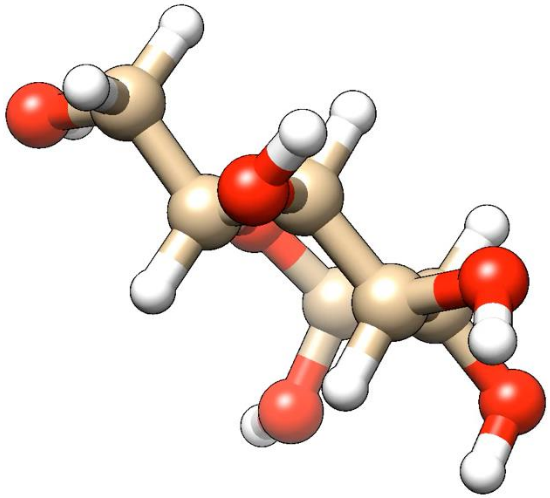
- .PDB to .STL files - software and steps
- Practical considerations when 3D printing molecular models

Understanding Life Sciences relies on understanding Structural Biology

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

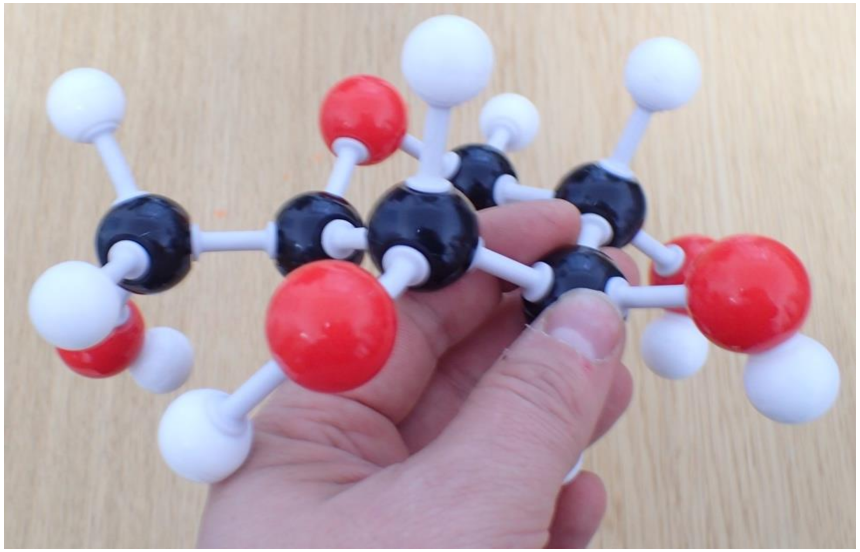






α-D-glucopyranose

Molecular models to aid teaching - Molymod

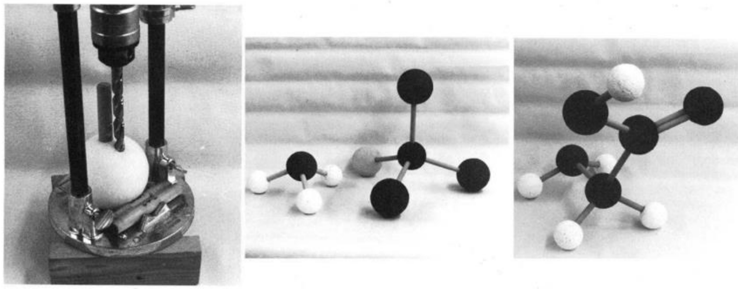


http://www.molymod.com/MMS-004_Inorganic__Organic_Teacher_Set.jpg

molymod®

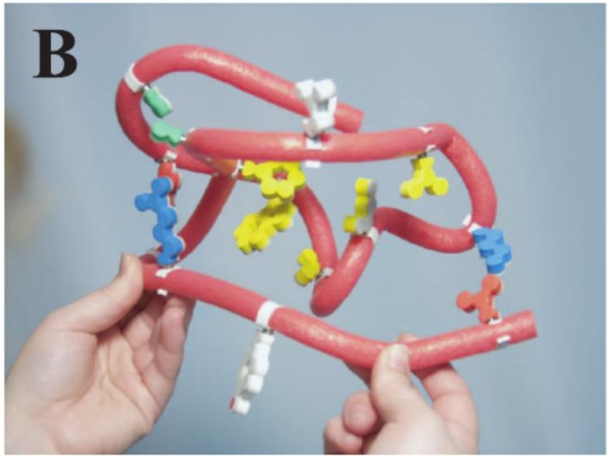
The *original* dual-scale system of molecular models

Molecular models to aid teaching - DIY



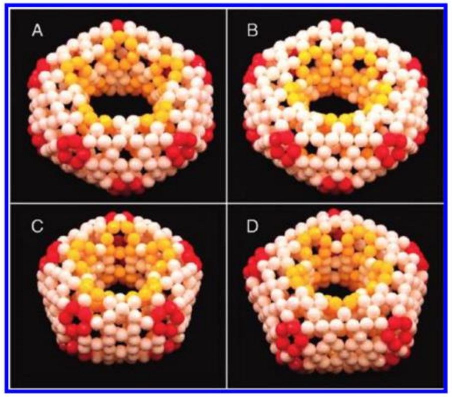
Styrofoam balls and copper wires

10.1021/ed066p1015



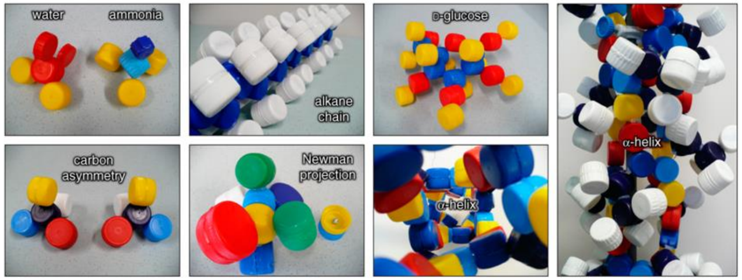
Flexible foam, wires and foam cut-outs

10.1002/bmb.2006.494034042649



Glass Beads

10.1021/ED200142G



Screw-on bottle caps

10.1021/ed400126p

Molecular models to aid teaching – Paper models

Antibody
(Paper Model)

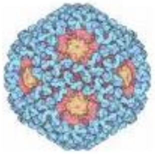
DNA
(Paper Model)

Dengue Virus
(Paper Model)

Green and Red Fluorescent Proteins
(Paper Model)

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

HIV Capsid
(Paper Model)



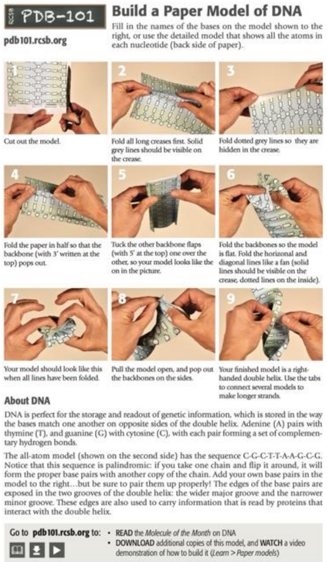
Human Papillomavirus (HPV)
(Paper Model)

Insulin
(Paper Model)

Quasisymmetry in Icosahedral Viruses
(Activity Page)

tRNA
(Paper Model)

Zika Virus with and without antibodies
(Paper Model)



PDB-101

pdb101.rcsb.org

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).

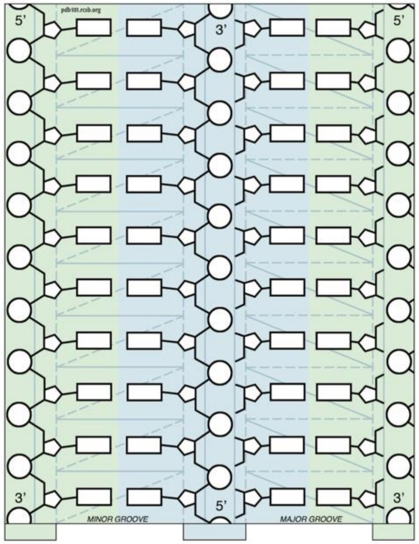
1. Cut out the model.
2. Fold all long creases first. Solid grey lines should be visible on the crease.
3. Fold dotted grey lines so they are hidden in the crease.
4. Fold the paper in half so that the backbone (with 3' written at the top) pops out.
5. Tuck the other backbone flaps (with 5' at the top) 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 horizonal 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.

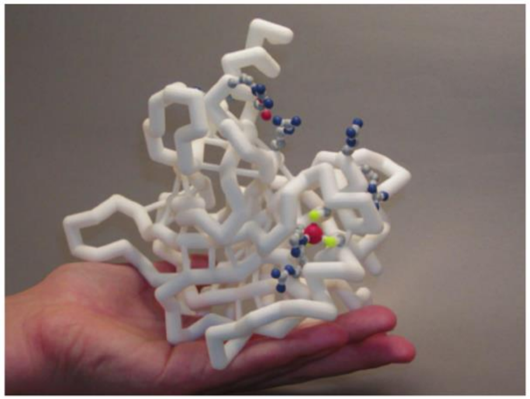
Go to **pdb101.rcsb.org** to:
- **READ** the *Molecule of the Month* on DNA
- **DOWNLOAD** additional copies of this model, and **WATCH** a video demonstration of how to build it (*Learn > Paper models*)



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 – 3D printed models



p53 tumor suppressor protein

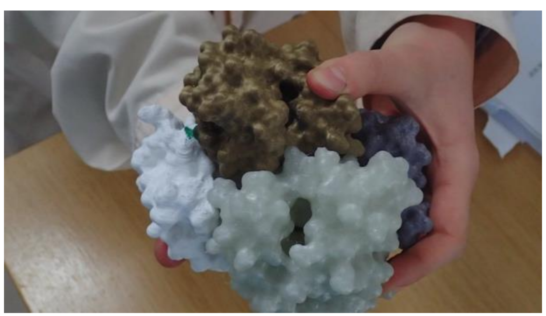
10.1002/bmb.2006.494034042649

Leucine zipper

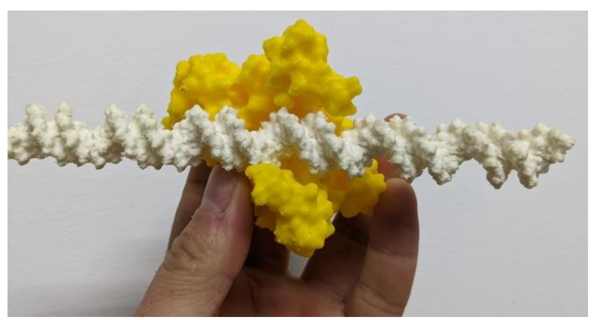
0.1021/acs.jchemed.5b00207

Human haemoglobin

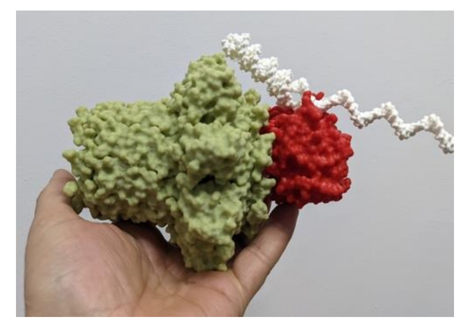
10.1063/1.4739961



Human deoxyhaemoglobin

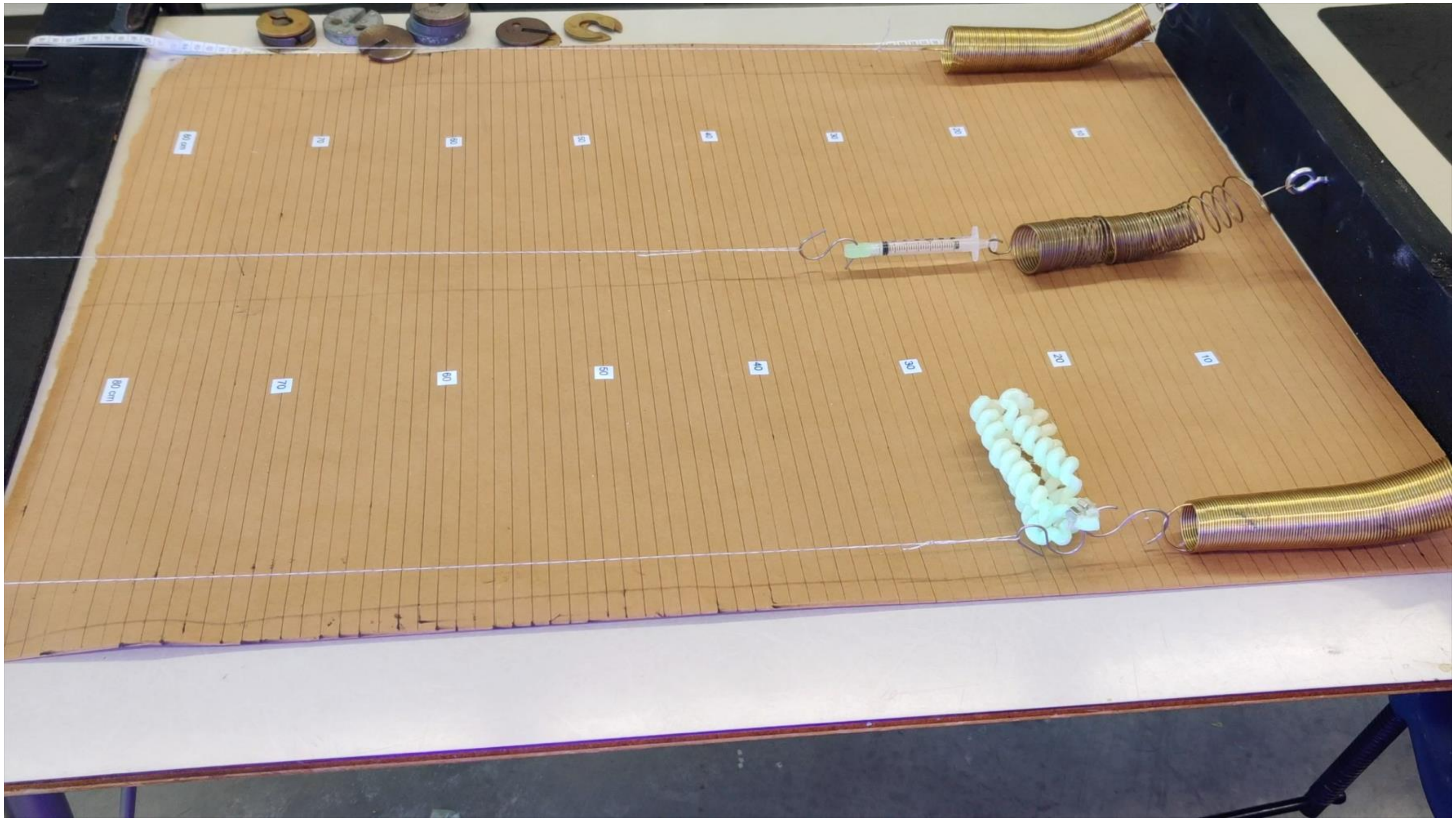


EcoRI endonuclease and DNA



Nanopore sequencing complex

Molecular models to aid teaching – 3D printed models



10.1021/acs.jchemed.2c00231

Custom macromolecular models, adapted to the teacher's/demonstrator's requirements are needed !!!

Custom macromolecular models for teaching are need it

The custom macromolecular models should be:

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

✓

224 572 structures
1 068 577 CSM
freely available

PDBe Protein Data Bank in Europe

RCSB PDB PROTEIN DATA BANK

PDBj Protein Data Bank Japan

✓

molecular visualization software
Chimera, Jmol, PyMol

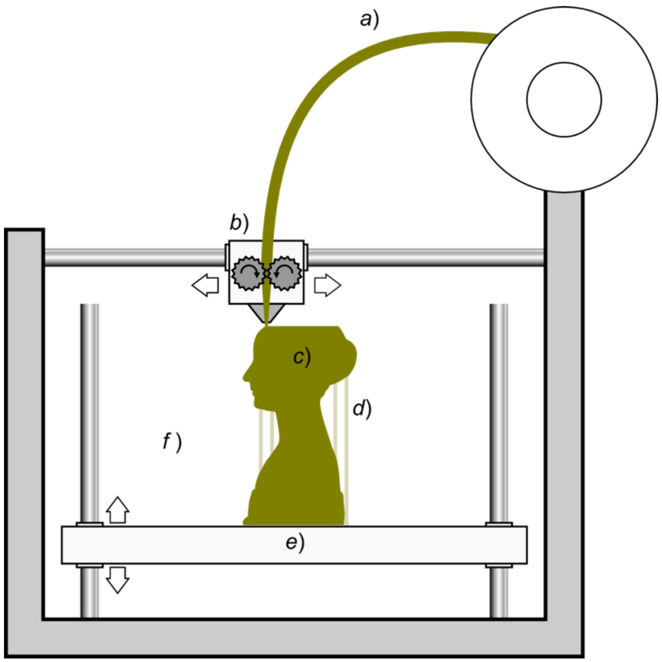
✓

3D printing can do that

What is 3D printing?

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

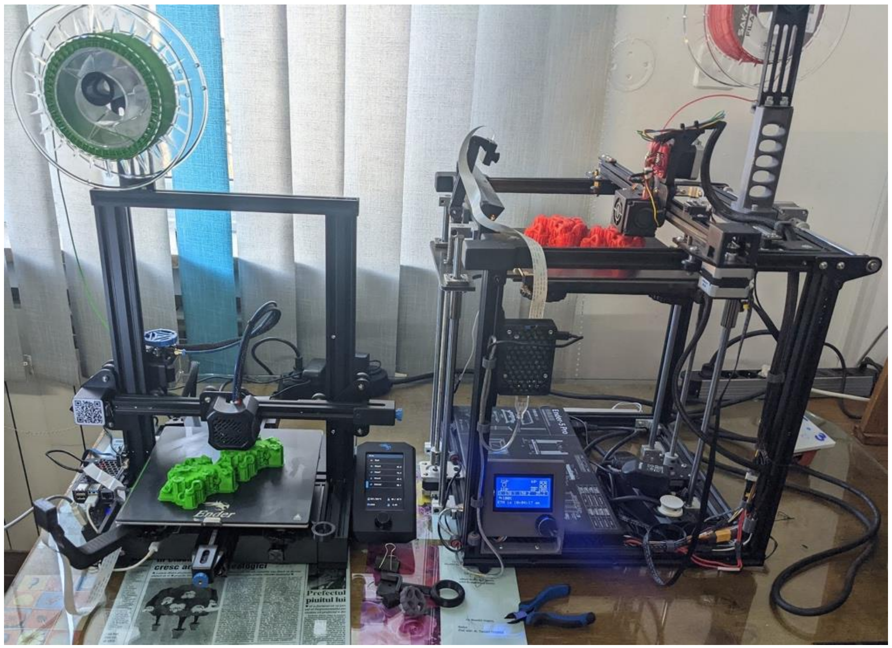
Material extrusion / Fused filament fabrication (FFF) / fused deposition modeling (FDM)



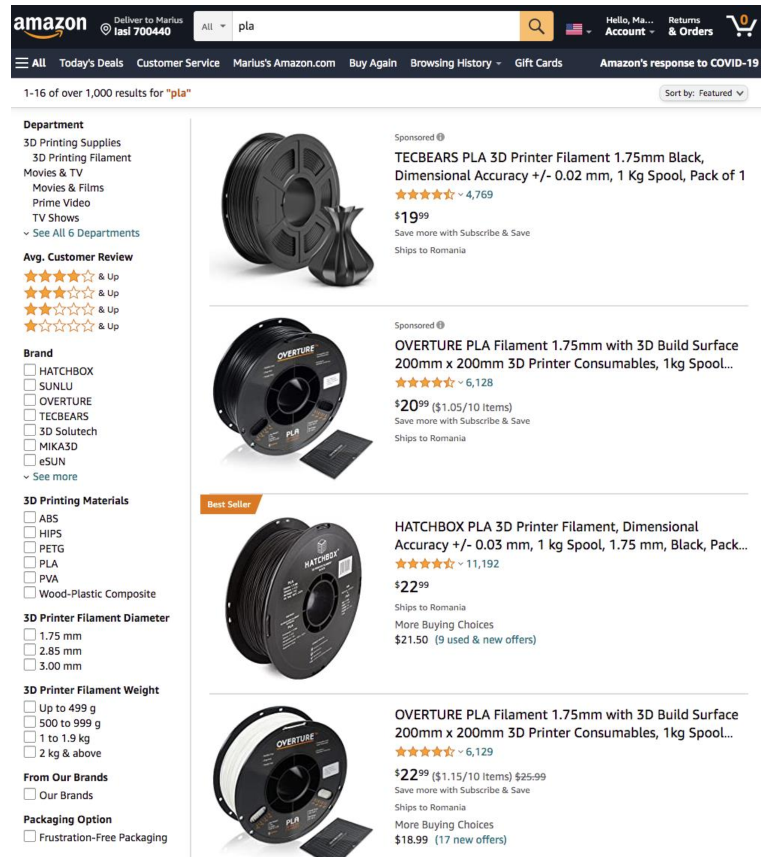
Scopigno R et al. (2017). "Digital Fabrication Techniques for Cultural Heritage: A Survey". Computer Graphics Forum 36 (1): 6-21

3D printing using FFF is accessible

Under 500$ printers



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

Do these models make a difference in teaching?

A compensatory research study


Laura Nicoleta P.


Razvan Stefan B.

	Week 1	Week 2			Week 3			Week 4 - Week 7
		Pre-test 1	Lecture 1 - Proteins Structure	Post-test 1	Pre-test 2	Lecture 2 - DNA structure	Post-test 2	
Group A	Announcement Recruitment Consent	2 days before lecture, 30 minutes, 13 questions	No intervention	2 days after lecture, 30 minutes, 13 questions	2 days before lecture, 30 minutes, 10 questions	Intervention	2 days after lecture, 30 minutes, 10 questions	Intervention and Feedback form
Group B			Intervention			No intervention		

The project was approved by the ethics committee at the Department of Phycology and Education Sciences, Alexandru Ioan Cuza University of Iași (no 186/29.01.2024). Students were informed prior to the start of instruction of the purpose and objectives of the investigation. Student participation was anonymous and voluntarily, and each student was presented with the opportunity to exclude him/herself from the study at any time. Information regarding data security, the type of information obtained, data storage procedures, and the measures taken to protect participants' anonymity was provided. Furthermore, students were assured that participation would have no bearing on any score assignment and that the results could be used for publication.

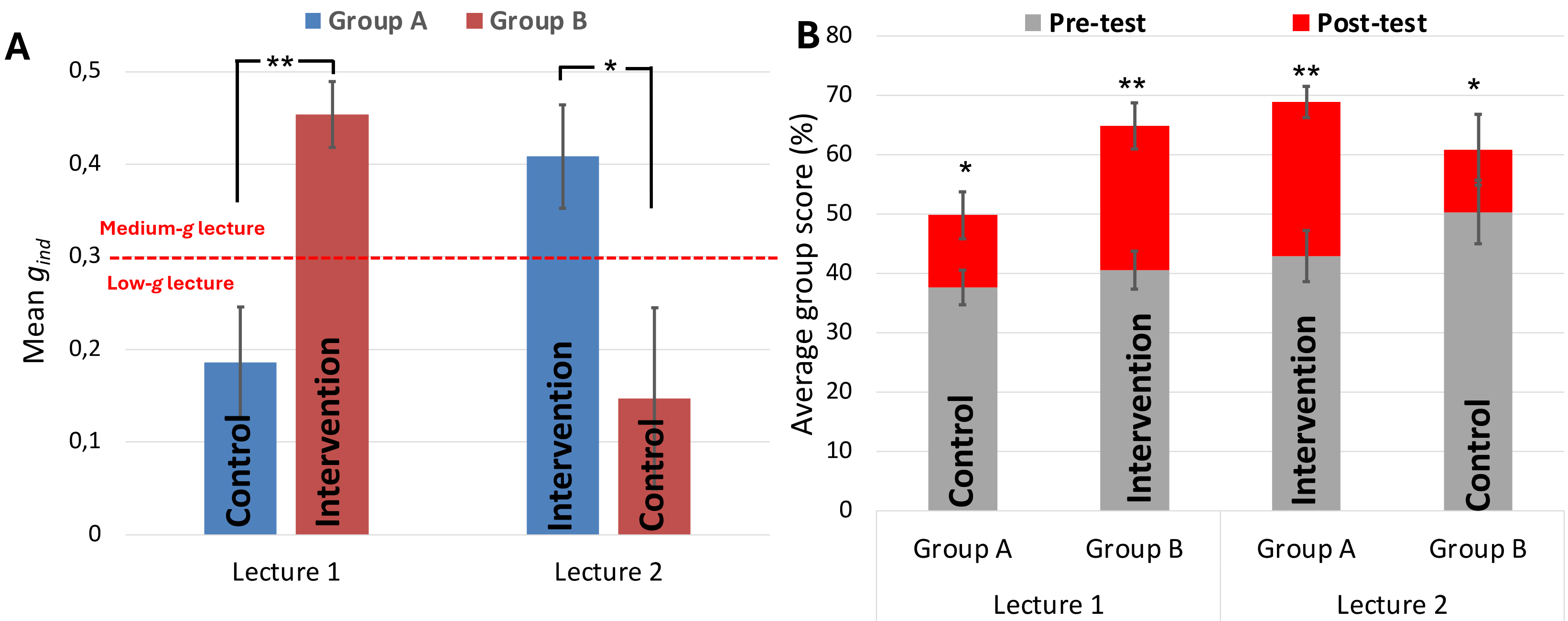
Do these models make a difference in teaching?

Evaluation of impact is key

Models	NIH 3D DOI:	Assessment questions	Learning objective	Biomolecular visualization learning goals
Amino acids, peptides and proteins				
4 amino acids (L-Glycine, L-Tryptophan, L-Proline, L-Arginine) in different representations	10.60705/3dpx/21049.1	Q2, Q4	Recognize a variety of molecular representations (i.e. stick and space fill).	AR2.02 students will describe the atoms that are represented in different renderings. (novice)
Two insuline chains (PDBID 4ins, chains C and D) in 4 representations: sticks, balls and sticks, cartoon and surface	10.60705/3dpx/21051.1	Q1, Q2, Q3, Q4, Q7	Recognize a variety of molecular representations (i.e. stick and space fill). Identify features of the peptide backbone, including the amino and carboxyl ends, peptide bonds, and alpha carbon. N to C direction	MR1.01 given a rendered structure of a biological polymer students will be able to identify the ends of a biological polymer. (novice, amateur, expert) MR1.02 given a rendered structure, students will be able to divide the polymer into its monomer units. (novice)
Quaternary structure of human deoxihaemoglobin with removable hem	10.60705/3dpx/14895.2	Q10, Q11	Describe why and how protein subunits interact to make the “quaternary structure”	TC2.06 Students can identify the levels of protein structure (e.g., parse a tertiary/quaternary structure into a series of secondary structures/motifs) and the ways in which they are connected from a three-dimensional structure. (Novice, Amateur, Expert)
Nucleotides and nucleic acids				
Deoxyribonucleotides and ribonucleotides in in different representations.	10.60705/3dpx/21050.1	Q2,	Recognize a variety of molecular representations (i.e. stick and space fill).	AR2.02 students will describe the atoms that are represented in different renderings. (novice)
B-DNA dodecamer printed in flexible	10.60705/3dpx/14893.2	Q5	Understand the flexibility of DNA due to the higher number of rotable bonds.	AG3.01 Students can identify a dihedral/torsion angle in a three-dimensional representation of a macromolecule. (Novice) AG3.02 Students can identify the planes between which a dihedral/torsion angle exists within a three-dimensional representation of a macromolecule. (Novice)

https://biomolviz.org/. Biochem Mol Biol Educ. 2017 Jan 2;45(1):69-75. doi: 10.1002/bmb.20991.

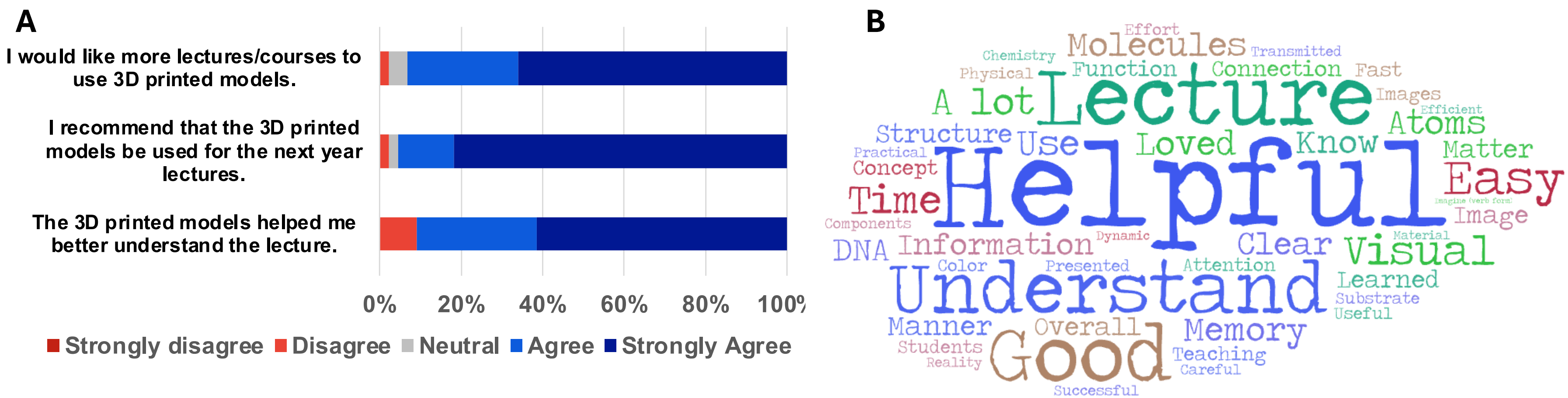
Individual learning gain



10.1002/bmb.21902

Results

Free-form assessment



Boiangiu RS, Popa LN, Mihasan M. *Journal of Science Education and Technology*, submitted manuscript

"The 3D models were **very useful** as the **information and images were transformed into something physical that I could touch**. And this helped me better understand the content presented. **It is easier to understand a notion or a concept if one can hold it in its hand and turn it around to evaluated it from all the angles**".

10.1002/bmb.21902

Asking students to paint the models to recognize different structures

Guiding students to create and print their own models for presentations

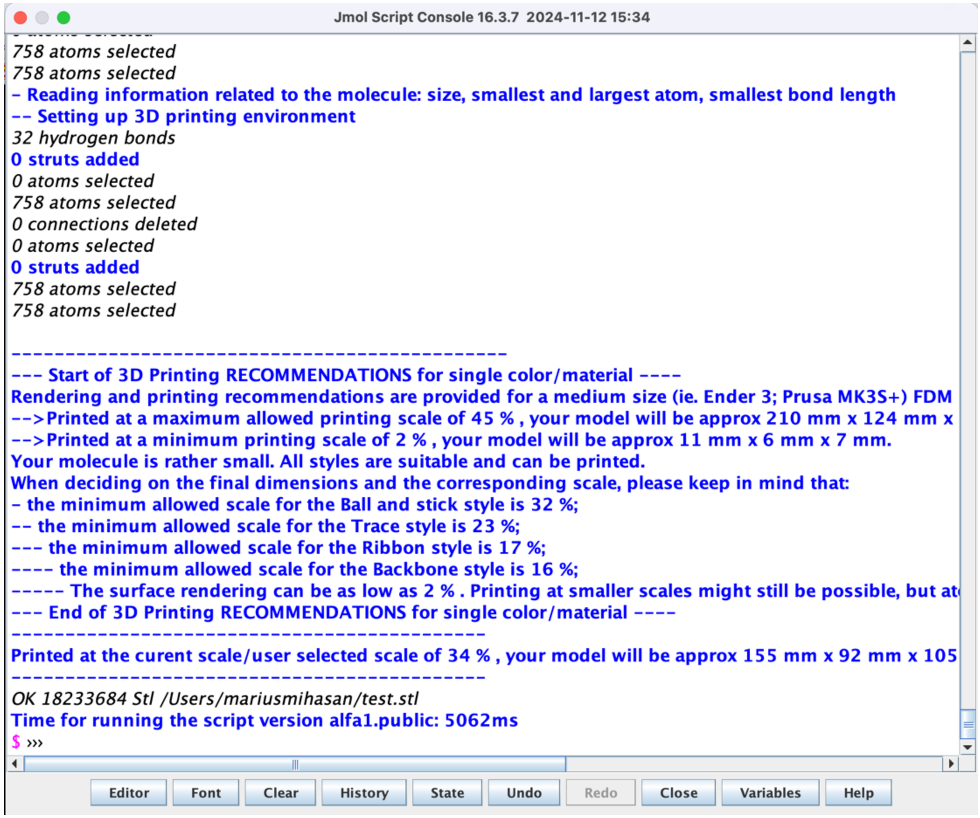
Hard learned truth:

Most teachers/students are very enthusiastic about the models,

but verry few can/want to use structural data and design models.

Introducing 3DP-Jmol – a script for automatic generation of 3D printable molecular models

```
///This is where user input is required
load =4BNA //Please type here the 4-character code of the macromolecule of interest from PDB - https://www.rcsb.org/. Alternatively, PubChem molecules can be loaded using this command load :nicotine and codes from https://www.ebi.ac.uk/pdbe/ using this command load *8jiv
var opt = "ballandstick" // works for ballandstick; backbone; trace; ribbon; sesurface and sasurface.
var LigStruts = true // If ligands are to be connected with the macromolecule. Recommended to be true for backbone; trace; ribbon; for surface (sesurface and sasurface) needs to be false.
var NucProtStruts = 1 // If nucleic acids are to be connected with the macromolecule. 0 or 1.
var PrintScaleFactorUser = 0; //This is where the size of the printed model is indicated by the user as print scale. Should be 0 when first running the script to generate a model printable at the maximum size. Based on the feedback from the console, smaller scales could be selected by the user based on his preference. The scale in the console is %, but here should be divided by 100. For example, for a scale of 30%, here should be 0.3
var colorPrinter = 'no' # 'yes' or 'no' // Please leave it to 'no' for now. Experimental feature, not yet fully tested.
///This is where the required user input ends and the process starts. No edits below this line should be required.
//=====================================================
```



3DP-Jmol

Development of 3DP-Jmol is supported by EDUMOL3D, Project PN-IV-P7-7.1-PED-2024-0343 financed by the Ministry of Research, Innovation and Digitization, UEFISCDI, Romania.

Introducing 3DP-Jmol – a script for automatic generation of 3D printable molecular models

Angel Herráez
University of Alcalá,
Madrid, Spain

Make file for 3D printer

User options:

- **include H atoms**
- **PDB ID:** 4ins
- **Style:** Ball & Stick Backbone (protein/nucleic) Trace (protein/nucleic) Ribbon (protein/nucleic) Cartoon (protein) Blocks (nucleic) Spacefill Solvent-accesible surface Molecular surface
- **Ligands connected to macromolecule.** (Recommended for backbone, trace or ribbon. Disabled for surfaces)
- **Create support links** (struts) between protein and nucleic chains.
- **Size of printed model:** 0.2
  This should be 0 when first running the script to generate a model printable at the maximum size. Based on the feedback from the console, smaller scales could be selected by users based on their preference. Scale in the console is %, but here it should be divided by 100. For example, enter 0.3 here for a scale of 30%.
- **Prepare for color printing.**
  Very experimental. A decision is needed here if required to implement. If checked, output will be OBJ and color, if not, output will be STL and monochrome. OBJ files are nor properly scaled yet, but can be done.

Updated: 2025-02-26 , 10:21:10.000Z

--- Start of 3D Printing RECOMMENDATIONS ----
Rendering and printing recommendations are provided for a medium size (ie. Ender 3; Prusa MK3S+) FDM 3D printer. Using SLA printers is possible, but not yet tested.
-->Printed at a maximum allowed printing scale of 40% , your model will be approx 210 mm x 202 mm x 108 mm.
-->Printed at a minimum printing scale of 3% , your model will be approx 16 mm x 15 mm x 8 mm.
Your molecule is medium-sized. All styles except Ball and Stick can be printed.
When deciding on the final dimensions and the corresponding scale, please keep in mind that:
- the minimum allowed scale for the Ball and stick style is 48%;
-- the minimum allowed scale for the Trace style is 23%;
--- the minimum allowed scale for the Ribbon style is 17%;
---- the minimum allowed scale for the Backbone style is 16%;
----- The surface rendering can be as low as 3%. Printing at smaller scales might still be possible, but atomic details (H atoms) will be lost.
--- End of 3D Printing RECOMMENDATIONS ----

Printed at the current scale/user selected scale of 20% , your model will be approx 105 mm x 101 mm x 54 mm.

Help:

STL file viewers: online :: ModuleWorks STLView :: Cravesoft STL Viewer

WRL file viewers: online :: FreeWRL

TasksBoard | Desktop ap

https://biomodel.uah.es/JSmol2/Marius_Mihasan/PDB2STL.htm

3DP-Jmol

Development of 3DP-Jmol is supported by EDUMOL3D, Project PN-IV-P7-7.1-PED-2024-0343 financed by the Ministry of Research, Innovation and Digitization, UEFISCDI, Romania.

3DP-Jmol – integration with Proteopedia

journal | discussion | edit this page | history | watch

Journal of Biological Inorganic Chemistry

A publication of the Society of Biological Inorganic Chemistry

Structure of Anticancer Ruthenium Half-Sandwich Complex Bound to Glycogen Synthase Kinase 3ß

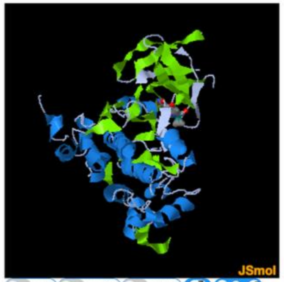
G. Atilla-Gocumen, L. Di Costanzo, E. Meggers [1]

Molecular Tour

A crystal structure of an **organometallic half-sandwich ruthenium complex** bound to the protein kinase glycogen synthase kinase 3ß (GSK-3ß) has been determined (PDB entry 3m1s) and reveals that the inhibitor binds to the **ATP binding site** via an induced fit mechanism utlizing several **hydrogen bonds** and **hydrophobic interactions.** Importantly, the metal is not involved in any direct interaction with the protein kinase but fulfills a purely structural role. The unique, bulky molecular structure of the half-sandwich complex with the CO-ligand oriented perpendicular to the pyridocarbazole heterocycle allows the complex to stretch the whole distance **sandwiched between the faces of the N- and C-terminal lobes** and to interact tightly with **the flexible glycine-rich loop.** Although this complex is a conventional ATP-competitive binder, the unique shape of the complex allows novel interactions with the glycine-rich loop which are crucial for binding potency and selectivity. It can be hypothesized that coordination spheres which present other ligands towards the glycine-rich loop might display completely different protein kinase selectivities.

PDB reference: Structure of Ruthenium Half-Sandwich Complex Bound to Glycogen Synthase Kinase 3, 3m1s.

References



spin quality labels

PDB ID 3rec

Drag the structure with the mouse to rotate

Export Animated Image Print3D

1.

Proteopedia Page Contributors and Editors (what is this?)

David Canner, Alexander Berchansky, Jaime Prilusky

This page complements a publication in scientific journals and is one of the Proteopedia's **Interactive 3D Complement** pages. For aditional details please see **I3DC.**

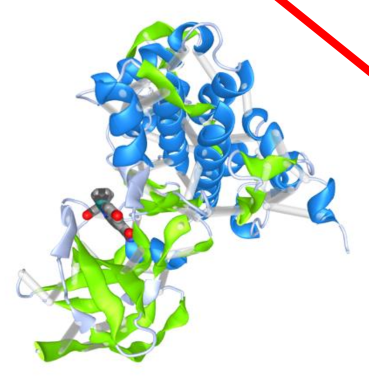
Please choose the parameters to tailor the aspect of the resulting printed model on page *Journal:JBIC:2*

Scheme	Proteopedia Scene	
Hydrogen atoms	OFF	Recommended to be off unless you have particular reasons to have the hydrogen atoms shown in the model. H atoms might be required when the model is represented as ball and sticks, or when ligands are present. If not H atoms are not mandatory, keep in mind that keeping this option on will increase the minimum scale at which the model can be printed.
Nuclear struts	ON	If nucleic acids are to be connected with the macromolecule.
Ligand struts	ON	If ligands are to be connected with the macromolecule.
Printer	Multimaterial/Multicolor	
Printer scale	32 %	You may set from 2% to 32%. With the current scale, your model will be approximately (x,y,z) **192 x 210 x 194 mm.**

Make printer files

2.

Note: Before processing, we removed from the structure solvent (UREA, SO4, PO4, HOH, DOD, WAT), NA,K,CL,BR,GOL,DIO,DOX,NO,NO3,EDO,DMS,FMT,ACT,IPA, and they **will not appear** on the printed model.



Drag the model with the mouse to rotate

Page: Journal:JBIC:2

Scheme: scene

Scale: 32%

Ligand struts: true

Nucleic acids struts: true

Download Files | Download SCRIPT

3.

With these OBJ and MTL files, your printer will generate a **Scene** model of **Journal:JBIC:2**

The size of your model will be approximately (x,y,z) **192 x 210 x 194 mm.**

Generate files for the Same structure with different parameters.

Programming and implementation by Jaime Prilusky. STL/OBJ/MTL files generated with Jmol and 3DP-Jmol. Model preview powered with Online 3D viewer

PROTEOPEDIA — LIFE IN 3D —

3DP-Jmol

Development of 3DP-Jmol is supported by EDUMOL3D, Project PN-IV-P7-7.1-PED-2024-0343 financed by the Ministry of Research, Innovation and Digitization, UEFISCDI, Romania.

Summary

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

3D printing offers a cheap way of fabricating and distributing molecular models applicable in low-income countries

The 3D printed models were received by students as being helpful as it provided a hands-on advantage. Allowing students 3-5 minutes to handle models converted a low-g lecture into a medium-g lecture.

Workflows for printing macromolecular models from PDB are available and are based on free software

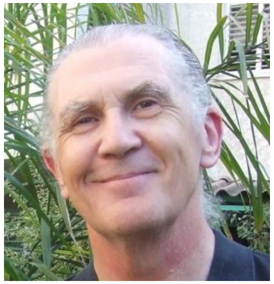
Biochemistry students
Class 2022 - 2025 and 2023-2026

Popa Laura Nicoleta
Faculty of Psychology and Educational Sciences

Boiangiu Răzvan-Ștefan
Faculty of Biology

Angel Herráez
University of Alcalá,
Madrid, Spain

Jaime Prilusky
Weizmann Institute of Science
Rehovot, Israel



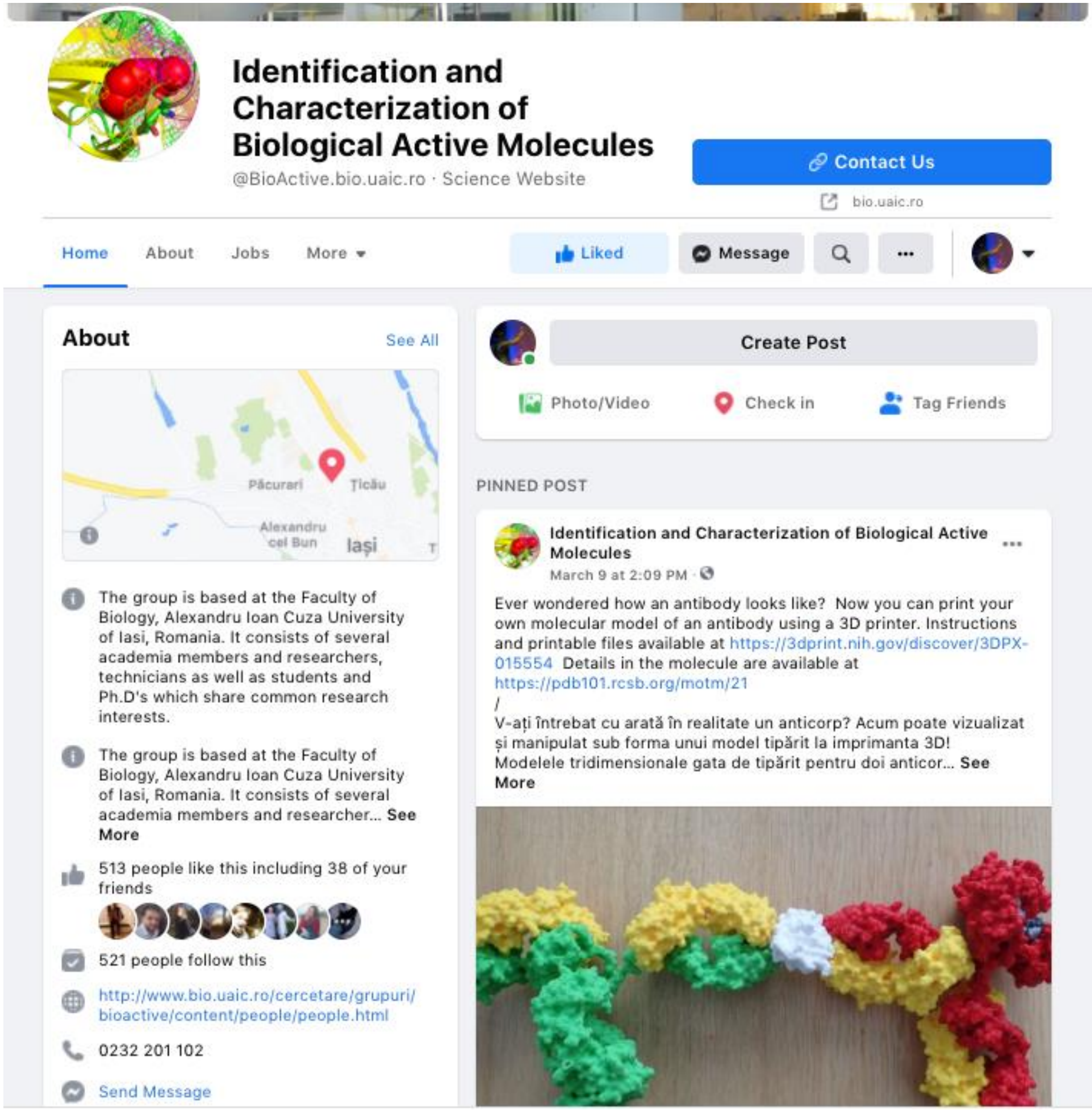
Amada

Anda

Tiberius

Development of 3DP-Jmol is supported by EDUMOL3D, Project PN-IV-P7-7.1-PED-2024-0343
financed by the Ministry of Research, Innovation and Digitization, UEFISCDI, Romania

Updates and new printed models



Find us on Facebook @BioActive.bio.uaic.ro

A Practical Introduction to 3DP-Jmol and 3D Printing

ALEXANDRU IOAN CUZA UNIVERSITY of IAȘI

www.uaic.ro

Marius Mihășan, PhD.

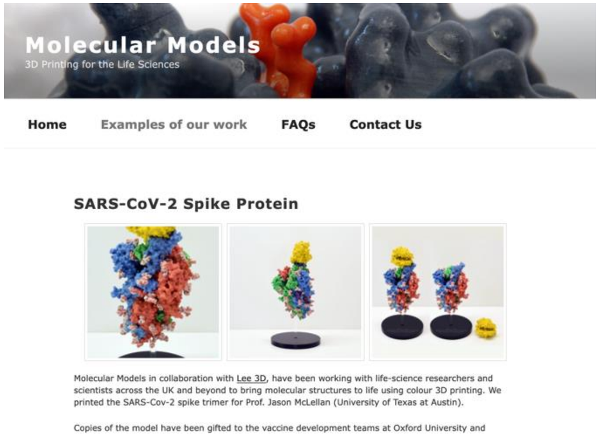
Faculty of Biology
Alexandru Ioan Cuza University of Iași, Romania
E-mail: marius.mihasan@uaic.ro
https://github.com/mariusmihasan/3DP-Jmol

How difficult it is to create your own 3D printable molecular model?

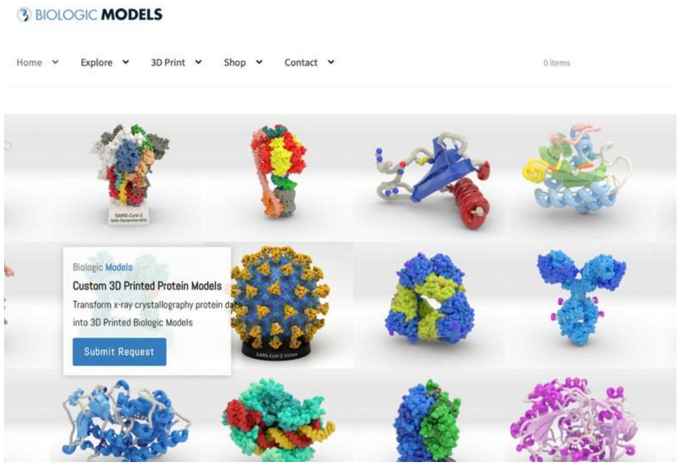
Let’s walk through the process together, and judge yourself

3D printed models - how to get them

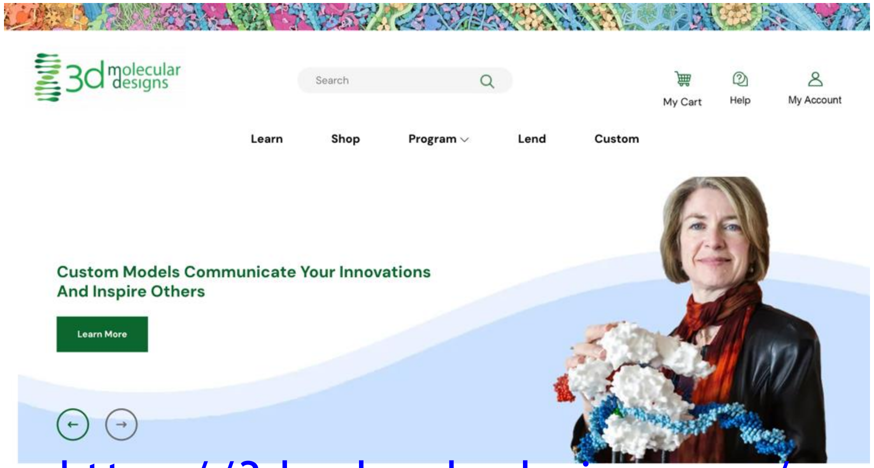
The easy, but not necessarily the cheap way:



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



https://biologicmodels.com/



https://3dmoleculardesigns.com/

3D printed models - how to get them

The almost easy, but a bit cheaper way:

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

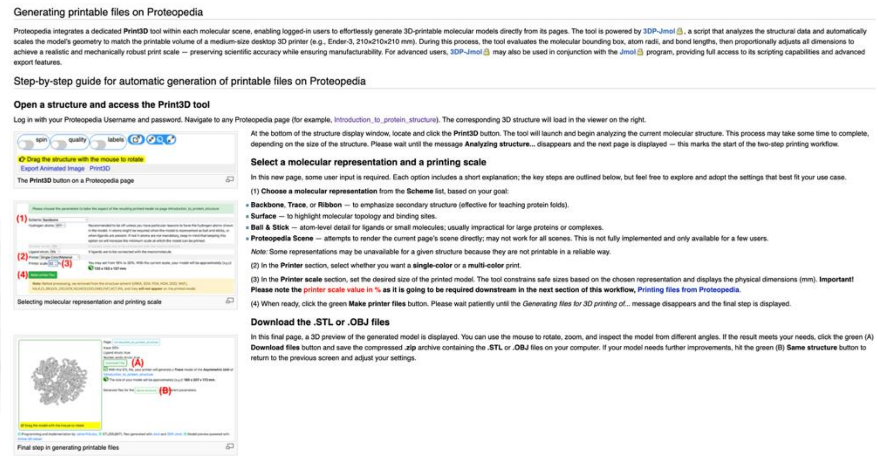
OR

A2. Automatically create your own model with
Proteopedia Print3D tool
or

OR

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

AND



Generating printable files on Proteopedia

Proteopedia integrates a dedicated **Print3D** tool within each molecular scene, enabling logged-in users to effortlessly generate 3D-printable molecular models directly from its pages. The tool is powered by 3DP-Jmol, a script that analyzes the structural data and automatically scales the model's geometry to match the printable volume of a medium-size desktop 3D printer (e.g., Ender-3, 210×210×210 mm). During this process, the tool evaluates the molecular bounding box, atom radii, and bond lengths, then proportionally adjusts all dimensions to achieve a realistic and mechanically robust print scale — preserving scientific accuracy while ensuring manufacturability. For advanced users, 3DP-Jmol may also be used in conjunction with the Jmol program, providing full access to its scripting capabilities and advanced export features.

Step-by-step guide for automatic generation of printable files on Proteopedia

Open a structure and access the Print3D tool

Log in with your Proteopedia Username and password. Navigate to any Proteopedia page (for example, Introduction_to_protein_structure). The corresponding 3D structure will load in the viewer on the right.

The **Print3D** button on a Proteopedia page

At the bottom of the structure display window, locate and click the **Print3D** button. The tool will launch and begin analyzing the current molecular structure. This process may take some time to complete, depending on the size of the structure. Please wait until the message **Analyzing structure...** disappears and the next page is displayed — this marks the start of the two-step printing workflow.

Select a molecular representation and a printing scale

In this new page, some user input is required. Each option includes a short explanation; the key steps are outlined below, but feel free to explore and adopt the settings that best fit your use case.

(1) **Choose a molecular representation** from the **Scheme** list, based on your goal:

- **Backbone**, **Trace**, or **Ribbon** — to emphasize secondary structure (effective for teaching protein folds).
- **Surface** — to highlight molecular topology and binding sites.
- **Ball & Stick** — atom-level detail for ligands or small molecules; usually impractical for large proteins or complexes.
- **Proteopedia Scene** — attempts to render the current page's scene directly; may not work for all scenes. This is not fully implemented and only available for a few users.

Note: Some representations may be unavailable for a given structure because they are not printable in a reliable way.

(2) In the **Printer** section, select whether you want a **single-color** or a **multi-color** print.

(3) In the **Printer scale** section, set the desired size of the printed model. The tool constrains safe sizes based on the chosen representation and displays the physical dimensions (mm). **Important! Please note the printer scale value in % as it is going to be required downstream in the next section of this workflow,** Printing files from Proteopedia.

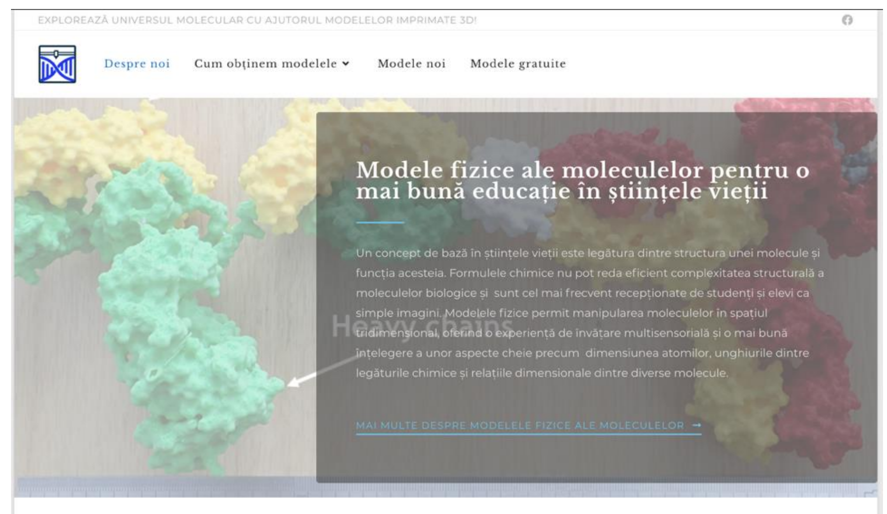
(4) When ready, click the green **Make printer files** button. Please wait patiently until the *Generating files for 3D printing of...* message disappears and the final step is displayed.

Selecting molecular representation and printing scale

Download the .STL or .OBJ files

In this final page, a 3D preview of the generated model is displayed. You can use the mouse to rotate, zoom, and inspect the model from different angles. If the result meets your needs, click the green (A) **Download files** button and save the compressed **.zip** archive containing the **.STL** or **.OBJ** files on your computer. If your model needs further improvements, hit the green (B) **Same structure** button to return to the previous screen and adjust your settings.

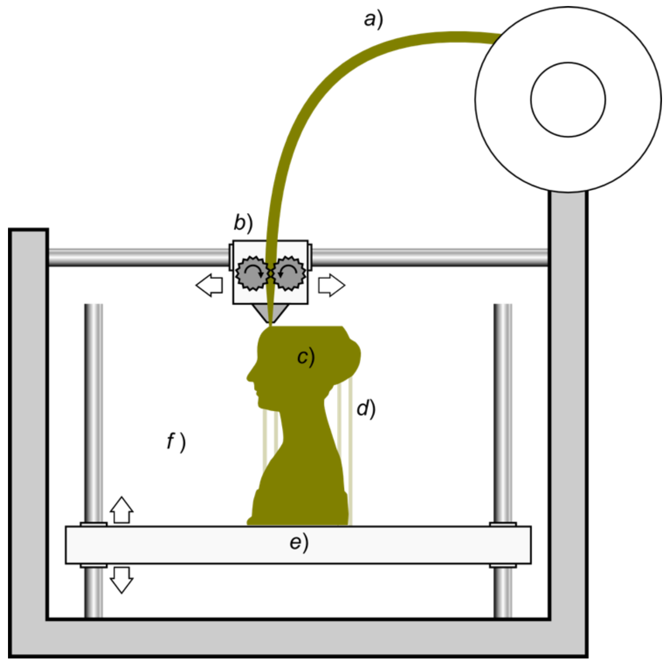
Final step in generating printable files



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

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)



Scopigno R et al. (2017). "Digital Fabrication Techniques for Cultural Heritage: A Survey". Computer Graphics Forum 36 (1): 6-21

Steps involving fabricating a macromolecular model

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 ChimeraX / Jmol

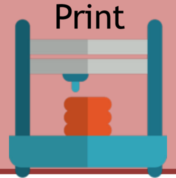
STL file

Prepare the file for printing using

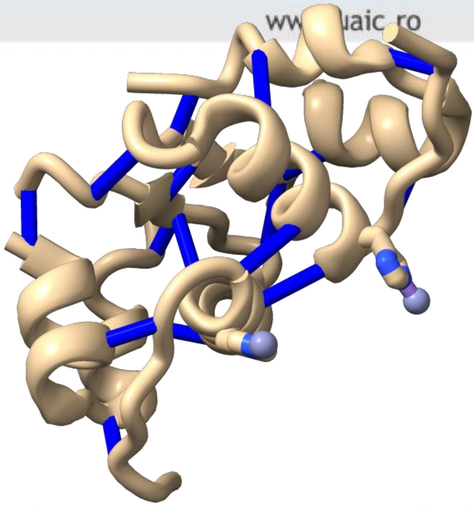
Cura/PrusaSlicer/BambooStudio

GCODE file

Print

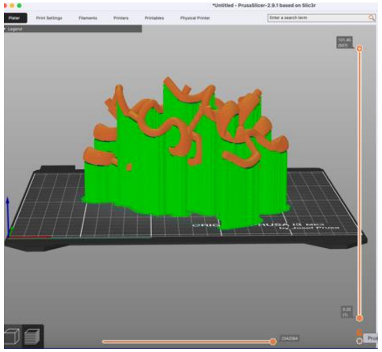


1. **Chose or combine visualization styles;**
2. **Add H bonds or create struts to make the model more sturdy** (mandatory for cartoon and balls and sticks models, not required for surface);
3. **Increase the thickness** of each printed element and/or **improve the smoothness** for molecular surfaces.



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

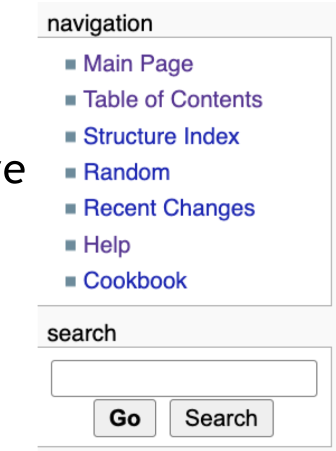
Support material removal

C. Clean up and finalize the physical model

10.37917/55427 ; 10.1002/bmb.21493

A. How to generate of the computer model (or .STL/.OBJ file)

A1. Using Proteopedia and Print3D tool;



- Navigate to https://proteopedia.org/wiki/index.php/Main_Page

Alternatively, search in Google for "Proteopedia" to navigate to the link above

- Log-in with your username and password

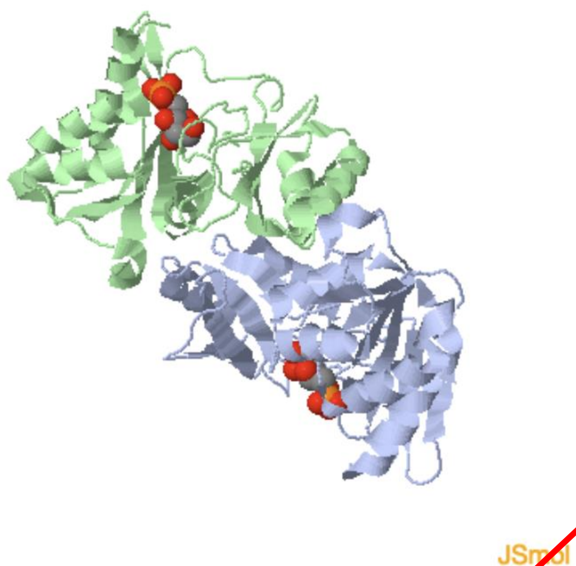
- On the left side, locate the Navigation panel and hit Table of Contents

- Expand the folders and chose your molecule of interest. ***Alternatively***, if you know already a PDB ID of interest, type it in the Search box.

- The new page that opens has on the right-side a section displaying a structure. Most, if not all pages in Proteopedia, have such a **Structure Section**. The content of the **Structure Section** can be modified by clicking in any on any of the green links. The **Structure Section is** initially opened in view only mode – recognizable by the Display Interactive Model button.

A. How to generate of the computer model (or .STL/.OBJ file)

- Click on the **Display Interactive Model** button to activate an extra set of controls, including the **Print3D** tool. Clicking the **Print3D** will start **the two-step interactive** conversion process;



spin quality labels

Ribose-5-phosphate isomerase A dimer complex with ribulose-5-phosphate, 3enw

Show: ○ *Asymmetric Unit*

◉ *Biological Assembly, QSbio confidence: Medium*

Drag the structure with the mouse to rotate

Export Animated Image Print3D

Please choose the parameters to tailor the aspect of the resulting printed model on page *Ribose-5-phosphate_isomerase*

Scheme	Trace	
Hydrogen atoms	OFF	Recommended to be off unless you have particular reasons to have the hydrogen atoms shown in the model. H atoms might be required when the model is represented as ball and sticks, or when ligands are present. If not H atoms are not mandatory, keep in mind that keeping this option on will increase the minimum scale at which the model can be printed.
Nuclear struts	ON	If nucleic acids are to be connected with the macromolecule.
Ligand struts	ON	If ligands are to be connected with the macromolecule.
Printer	Single Color/Material	
Printer scale	25 %	You may set from 23% to 25%. With the current scale, your model will be approximately (x,y,z) **203 x 108 x 184 mm**.

Make printer files

Note: Before processing, we removed from the structure solvent (UREA, SO4, PO4, HOH, DOD, WAT), NA,K,CL,BR,GOL,DIO,DOX,NO,NO3,EDO,DMS,FMT,ACT,IPA, and they **will not appear** on the printed model.

- What, How and other tips at Print3D Help
- Browse our Gallery of 3DPrinted Models

A. How to generate of the computer model (or .STL/.OBJ file)

Step one:

Please choose the parameters to tailor the aspect of the resulting printed model on page *Ribose-5-phosphate_isomerase*

Scheme: Ribbon

Hydrogen atoms: OFF — Recommended to be off unless you have particular reasons to have the hydrogen atoms shown in the model. H atoms might be required when the model is represented as ball and sticks, or when ligands are present. If not H atoms are not mandatory, keep in mind that keeping this option on will increase the minimum scale at which the model can be printed.

Nuclear struts: ON — If nucleic acids are to be connected with the macromolecule.

Ligand struts: ON — If ligands are to be connected with the macromolecule.

Printer: Multimaterial/Multicolor

Printer scale: 25 % — You may set from 17% to 25%. With the current scale, your model will be approximately (x,y,z) **203 x 108 x 184 mm**.

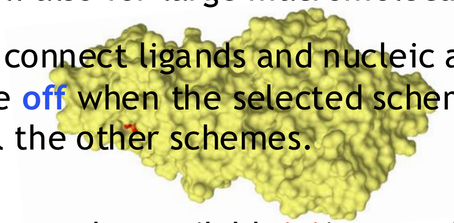
Make printer files

Note: Before processing, we removed from the structure solvent (UREA, SO4, PO4, HOH, DOD, WAT), NA,K,CL,BR,GOL,DIO,DOX,NO,NO3,EDO,DMS,FMT,ACT,IPA, and they **will not appear** on the printed model.

- What, How and other tips at Print3D Help
- Browse our Gallery of 3DPrinted Models

Surface

Great for arguing the complementary of molecular shapes
Extremely easy to print without any processing
Works well also for large macromolecular complexes



Struts to connect ligands and nucleic acids to the models. Should be off when the selected scheme is Surface. Can be on for all the other schemes.

Backbone, Trace, Ribbon, Cartoon

Struts have been added; All elements are thicker; Works for small proteins; Can be difficult to print at times

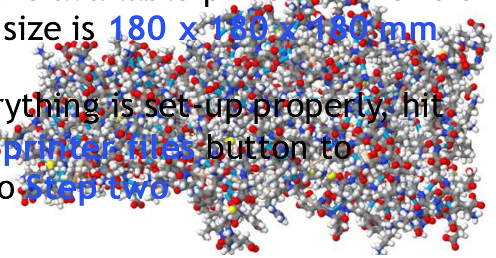
Depending on the available printer, color models can also be generated. Generation of Multicolor/Multimaterial models takes a lot of computational time, so please leave it to Single Color/Material for this exercise.

Size of your final printed model. Usually, larger is better but takes more time and material. Smaller is faster, but fine details might be lost and is always more difficult to print.

Ball & Stick

Applicable only to small molecules or ligands

The tool automatically select the largest possible size for you and calculates the final dimensions in mm. Adjust based on the available printer. For this exercise, the maximum size is 180 x 180 x 180 mm

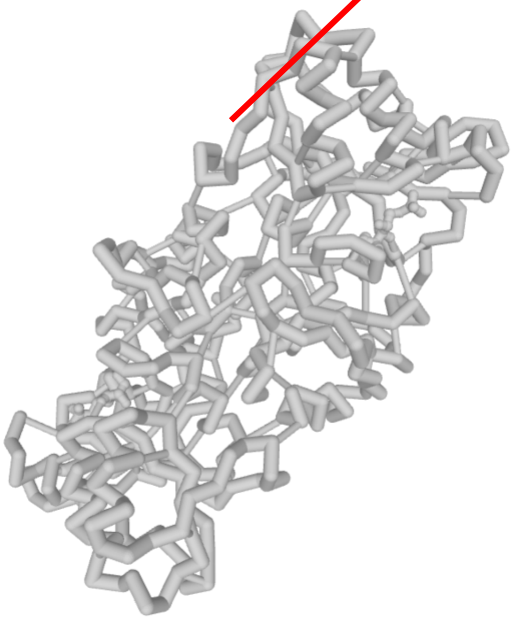


Once everything is set-up properly, hit the Make printer files button to proceed to Step two

A. How to generate of the computer model (or .STL/.OBJ file)

Step two:

Preview of the rendered model. Can be be rotated for a closer examination.



Drag the model with the mouse to rotate

Page:

Ribose-5-phosphate_isomerase

Scheme: backbone
Scale: 25%
Ligand struts: true
Nucleic acids struts: true

Applied setting for rendering the model. Please note the scale in %. It is going to be needed in downstream steps.

Download Files

Download SCRIPT

Finally download the files in your computer

With this STL file, your printer will generate a **Backbone** model of the **Biological Assembly** of **Ribose-5-phosphate_isomerase**

The size of your model will be approximately (x,y,z) **203 x 108 x 184 mm**.

Generate files for the Same structure with different parameters.

If the model is not as expected, hit this button to get back to Step One

Programming and implementation by Jaime Prilusky. STL/OBJ/MTL files generated with Jmol and 3DP-Jmol. Model preview powered with Online 3D viewer

- What, How and other tips at Print3D Help
- Browse our Gallery of 3DPrinted Models

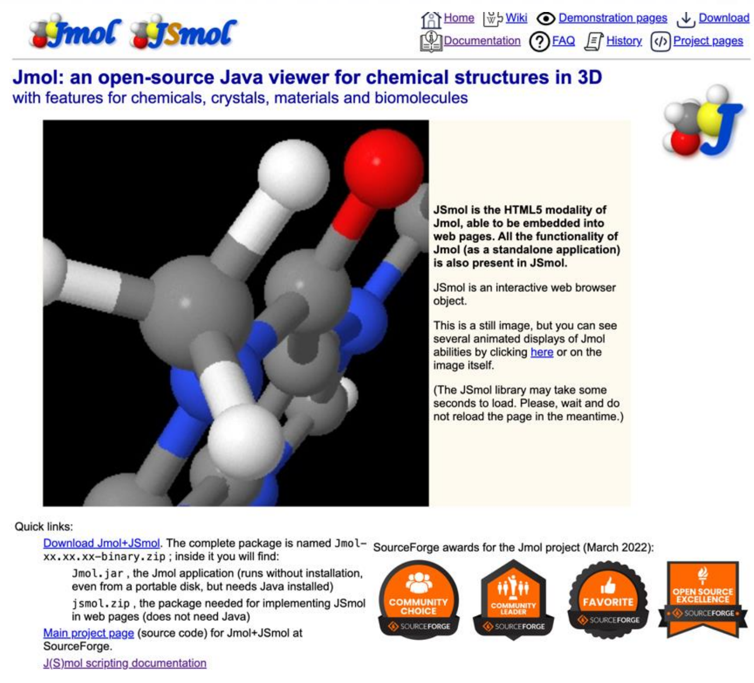
A2. Using 3DP-Jmol and Jmol offline;

1. Download and unpack Jmol;

https://jmol.sourceforge.net/

Alternative molecular visualization programs that will work but are not covered here:

1. **ChimeraX** - https://www.rbvi.ucsf.edu/chimerax/
2. **PyMOL** – https://www.pymol.org/ some extra steps in CAD software are required
3. **Molecular Maya** -https://clarafi.com/tools/mmaya/ - the plugin is free, but the Maya software is not
4. **Mol*** - https://molstar.org/



2. Access and copy 3DP-Jmol code by:

- Access the 3DP-Jmol Hithub at https://github.com/mariusmihasan/3DP-Jmol
- Click on the file 3DP-Jmol.v.alfa1.public
- Select the whole text and copy it.

3. Open a text editor of your choice (**Microsoft word works also**) and paste the code. Edit the first lines as indicated to select your molecule of interest and other relevant parameters. Read carefully and only edit the lines indicated. Do not close the text editor window!!

4. Open the previously unzipped Jmol application and navigate in the menu to **File**>**Console**…. A new window entitled **Console** will open;

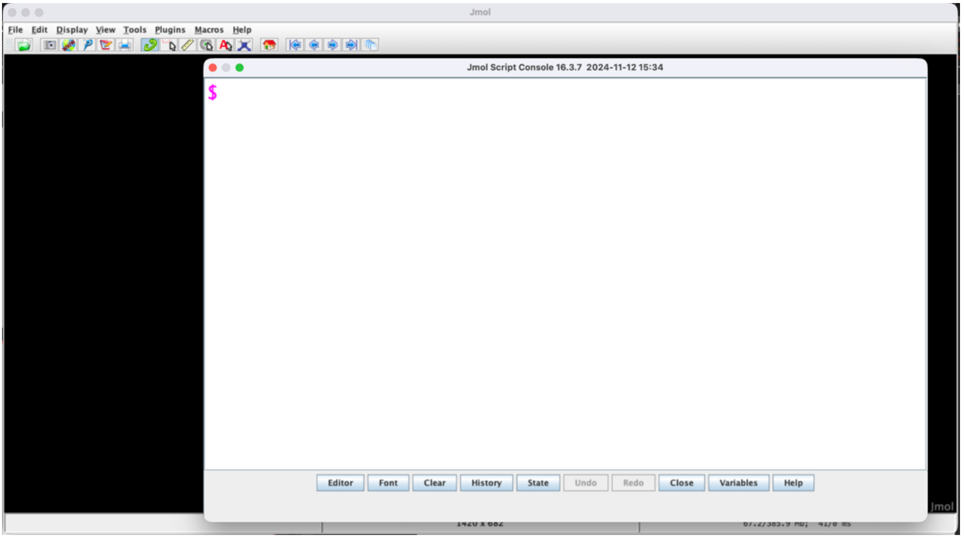
4. Copy the entire content of the text file edited in step 3 and paste it in the **Console** window using the **Ctrl-V** keyboard combination (or **Cmd+V** for Mac);

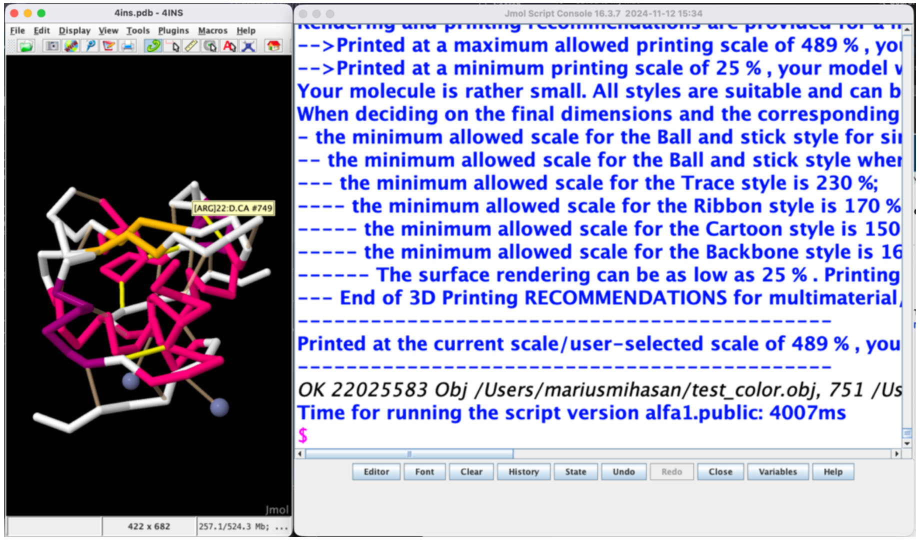
5. Wait patiently until JMol generates your printable file. This should be signaled by the appearance of a text similar to:

OK 20527284 Stl /Users/mariusmihasan/test.stl

Time for running the script version alfa1.public is: 4956ms

6. Check the instructions in the **Console** and, if required, based on the indications and your choice, come back to step 3 and repeat. The path for the **test.stl** file generated is indicated before the last line in the **Console**. Print it and enjoy!





B. 3D Printing the computer generated model

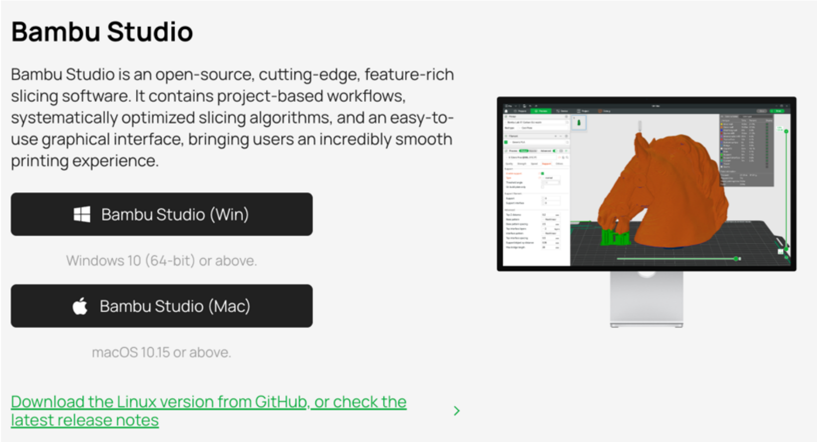
1. Download and install BambuStudio;

https://bambulab.com/en/download/studio

Alternative slicer programs used to control 3D printers:

1. **Prusa Slicer -** https://www.prusa3d.com/page/prusaslicer_424/
2. **Ultimaker Cura -** https://ultimaker.com/software/ultimaker-cura/
3. **Slic3r** – https://slic3r.org/
4. **Simplify3D -** https://www.simplify3d.com/ not free

Choosing one or another depends on the printer one has available



2. Open BambuStudio and run the Configuration Wizard. Accept all the defaults, except for the printer selection screen. Here make sure that only the BambuLab A1 mini printer is selected (not critical, but helps).

3. Download the configuration bundle. Link in the e-mail from the organisers
https://drive.google.com/file/d/1YM3sqMOEYSa7XxrpmzS5EqOsNFwNfaT8/view

4. In BambuStudio navigate to Menu > File > Import > Import Configigs…
Point to the newly downloaded file .BBSCFG and hit Open

What we just did is to install the printer control software and configs required to run my printer

B. 3D Printing the computer generated model

4. Load the created .stl file - In BambuStudio navigate to Menu > File > Import > Import STL/3MF/STEP… Point to the .stl file and hit Open

Set

1. Printer

2. Material

3. Print/process settings

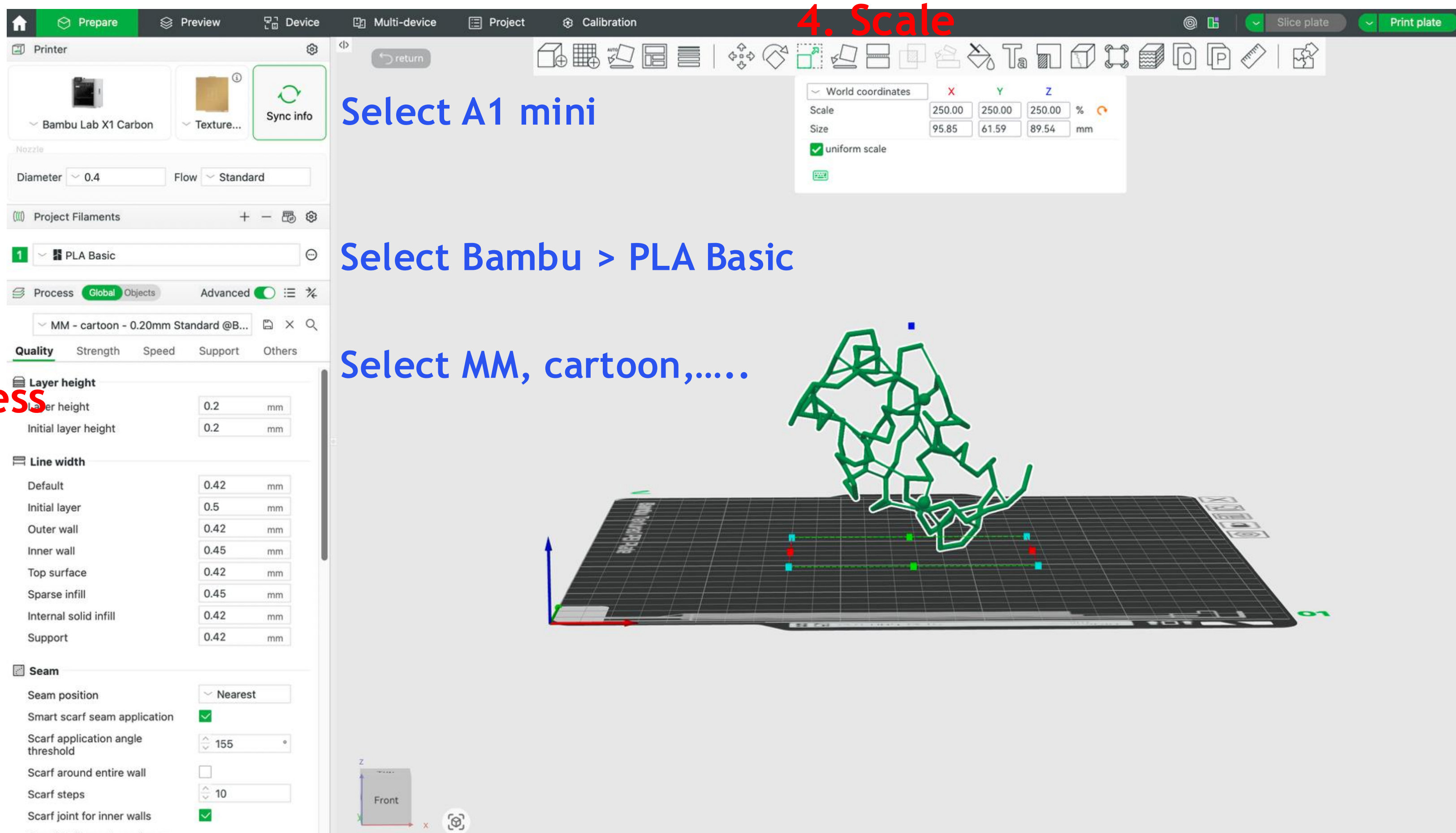
4. Scale

5. Hit Slice

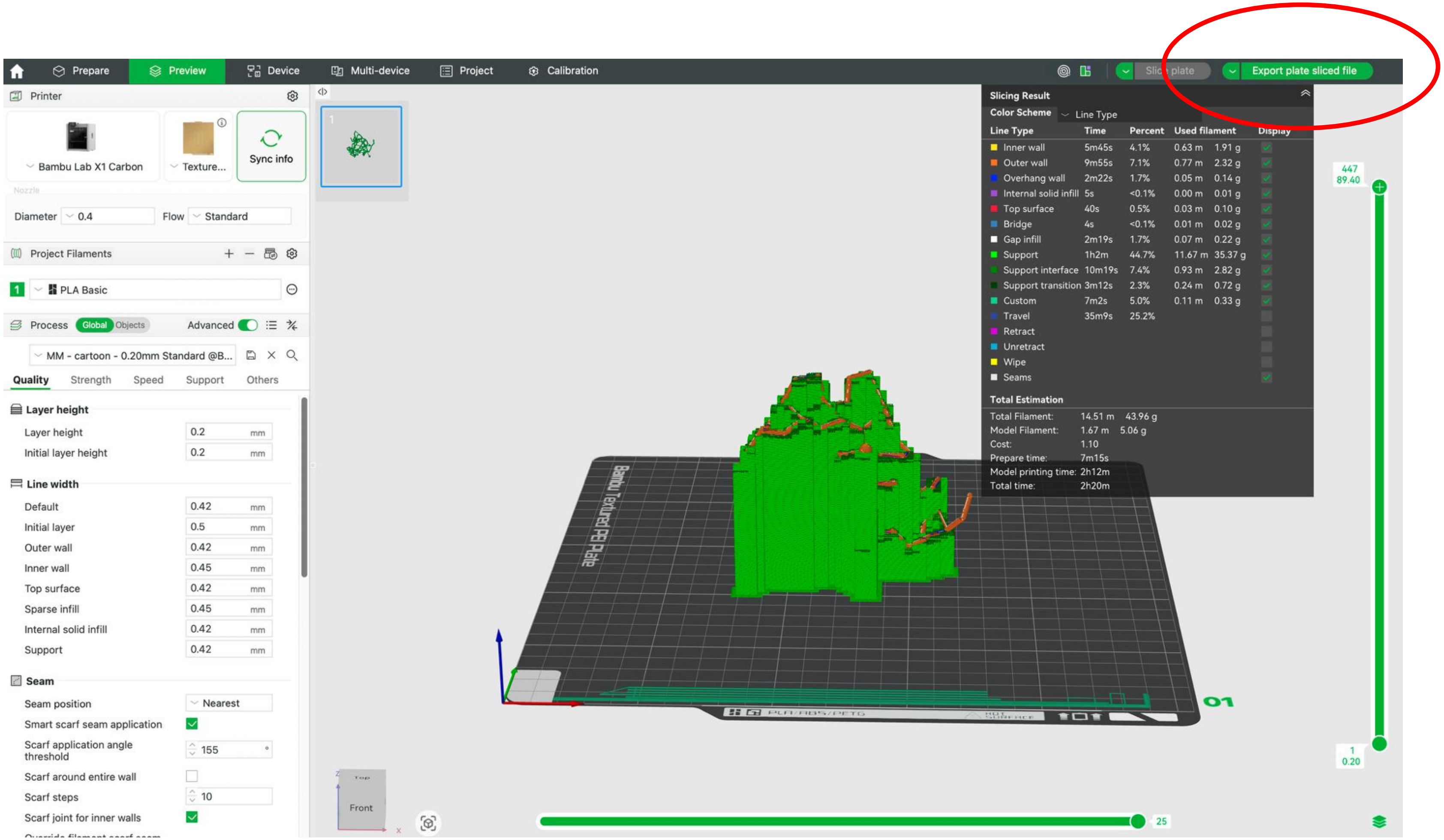
Select A1 mini

Select Bambu > PLA Basic

Select MM, cartoon,…..



5. Export .gcode file and transfer it to the printer via a SD-Card



Guidelines and more details are available

Visit the Main Page [ctrl-z]

User:Marius Mihasan/Print3D help

< User:Marius Mihasan

Contents [hide]

1 Proteopedia and 3D Printing
2 «3D Printing 101»: an introduction to 3D printing
  2.1 Printer Types: FDM vs. SLA/DLP
  2.2 Single- vs. Multi-Material Printers
  2.3 File Formats Used in 3D Printing
3 Overview of the 3D printing process
  3.1 Preparing the structure and generating a printable File
  3.2 Slicing the Model
  3.3 3D Printing the Model
  3.4 Post-Processing
4 Generating printable files on Proteopedia
5 Step-by-step guide for automatic generation of printable files on Proteopedia
  5.1 Open a structure and access the Print3D tool
  5.2 Select a molecular representation and a printing scale
  5.3 Download the .STL or .OBJ files
6 Printing files from Proteopedia
  6.1 Using 3D printing services
  6.2 Using a desktop 3D printer
    6.2.1 Note on multi-color printing
7 Other relevant resources
8 References

Proteopedia and 3D Printing

Physical molecular models, by engaging both visual and tactile senses, provide an effective means of deepening the understanding of complex concepts in molecular biology and biochemistry. They allow students to perceive the three-dimensional organization of macromolecules, thereby enhancing comprehension of the relationship between structure and function [1] [2]. Numerous studies have demonstrated that the use of tangible models in science education improves learning outcomes, fosters conceptual reasoning, and increases student engagement [3] [4] [5]. The rapid development of 3D-printing technologies has made it possible to create customized and affordable molecular models [6] [7] [8].

Affordable desktop 3D printers can now be used to fabricate physical models from virtually any structure or scene on Proteopedia. This page provides an introduction to 3D printing, a step-by-step guide to generating printable files directly from Proteopedia, and several tested printing profiles for common printers (e.g., Prusa Research, Bambu Lab, Creality, or Elegoo).

Let's 3D-print the whole Proteopedia!

«3D Printing 101»: an introduction to 3D printing

3D printing, also known as *additive manufacturing*, builds physical objects layer by layer from digital designs. For more technical details please head for the excellent introductory article on All3DP. In structural biology education, 3D printing provides an affordable and accessible way to transform atomic coordinate data (e.g., from PDB, MOL or SDF files) into tangible molecular models that can be observed, handled, and discussed in class or laboratory settings.

Printer Types: FDM vs. SLA/DLP

The two most accessible 3D-printing technologies that can be used to create molecular models are:

- **FDM (Fused Deposition Modeling)**

This method extrudes a heated thermoplastic filament (such as PLA, PETG or TPU) through a fine nozzle, depositing successive layers that form the model. FDM printers have the advantages of low cost, easy maintenance, wide availability, and being capable of printing large and colorful molecular models. This technology has a few limitations, such as: visible layer lines, lower surface resolution, and less suited for very small or intricate molecular details.

- **SLA/DLP (Resin Printing)**

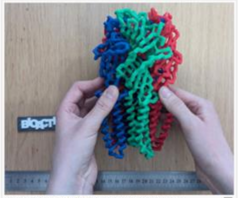
This technique uses liquid photopolymer resin, cured layer by layer with ultraviolet light. SLA/DLP printers have the advantages of a very high resolution, smooth surfaces and are ideal for compact and detailed models (e.g., small proteins rendered as surface, ligands, or symmetric assemblies). This technology has its own limitations, such as higher material cost, post-processing requirements (washing and UV-curing), and the need for careful handling of resin.

When choosing between FDM and SLA printers, model size and resolution are the key criteria: **FDM** is preferred for *large, educational display models*; **SLA/DLP** is optimal for *small, precise structures.*

While FDM and SLA/DLP are the most widely used technologies in educational and research contexts due to their accessibility, other additive manufacturing methods also exist — such as *Selective Laser Sintering* (SLS), *PolyJet*, and *Binder Jetting*— each employing different materials and curing mechanisms. These industrial-grade techniques can produce highly detailed or multi-material parts but are generally more expensive and less accessible for classroom use. For an overview of major 3D-printing technologies, see All3DP: Complete Overview of the Types of 3D Printers

Single- vs. Multi-Material Printers

Most entry-level desktop 3D printers use a single filament or resin, producing models in one color or material. However, multi-material systems (such as Bambu Lab AMS and its variants or Prusa MMU3) can simultaneously print multiple filaments, enabling color-coded domains, subunits, or ligands directly in one print. For complex color information, users can also apply post-print color coding (painting or labeling) or print separate parts and assemble them manually.

A large FDM-printed model	A multi-material FDM-printed model	Small resin-printed models
 GABAA receptor, 6x3x, scale at the bottom in cm	 Bacterial 70S ribosome, 4v5d, scale at the bottom in cm	 DNA (left) and insulin (right) models, 4bna and 4ins, scale at the bottom in cm

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User:Marius Mihasan/Print3D models gallery

< User:Marius Mihasan

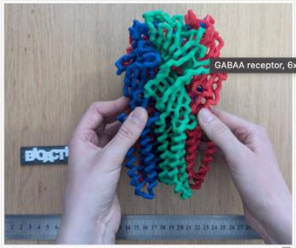
Welcome to the Proteopedia gallery of 3D printed models

Did you use the **Print3D** tool in Proteopedia to create a printable model?

Do you have pictures of the final 3D printed model of a molecule?

Or better, do you have a picture of the model put to good use?

We would love to know more about it. Please feel free to contribute to this page and share your prints! Note: If editing this page it's not for you and you would prefer to focus on 3D printing, drop us an e-mail at marius.mihasan(@)uaic.ro and we would love to hear your story and share it on this page.

Model	Picture	Details (including link to Proteopedia page if possible)
A simplified model of SV40 Capsid	 SV40 Capsid, SV40_Capsid_Simplified	Model of SV40 Capsid printed on multi-material printer (Bambulab A1 Mini). Printable files available on Printables.com. Generated with the Proteopedia Print3D tool from SV40_Capsid_Simplified. Printed by Marius Mihasan 12:27, 8 October 2025 (UTC).
GABBA receptor	 GABAA receptor, 6x3x	Trace Model of the GABAA receptor 6x3x printed on a single material FDM-Printer (Prusa MK3S+). Each of the 5 subunits was printed separately and can be assembled. Printable files available on Printables.com. Printed by Marius Mihasan 12:27, 8 October 2025 (UTC)
Model 3	Image with model 3	Description of model 3

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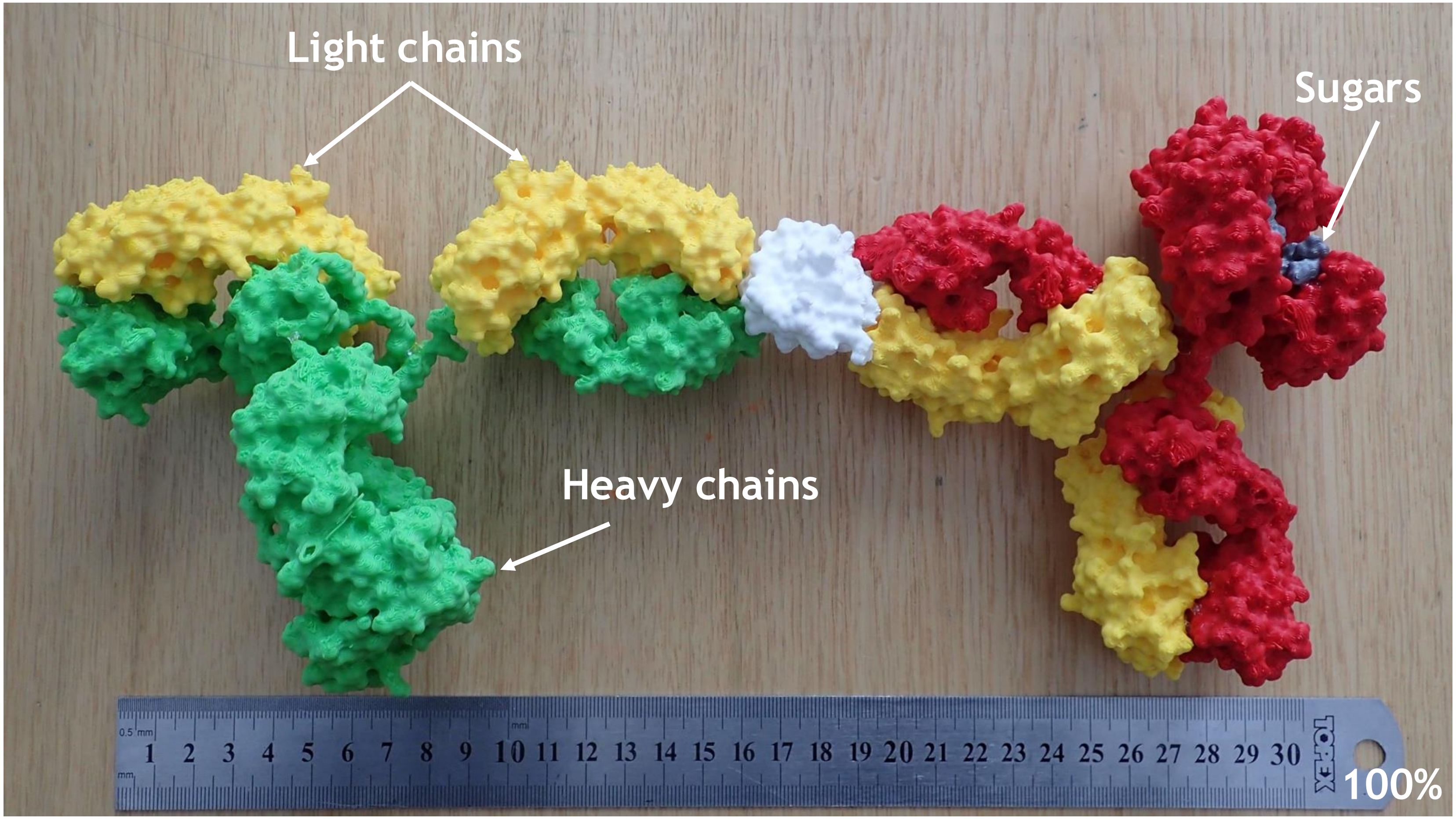
Proteopedia Page Contributors and Editors (what is this?)

Marius Mihasan

Category: 3D printer files

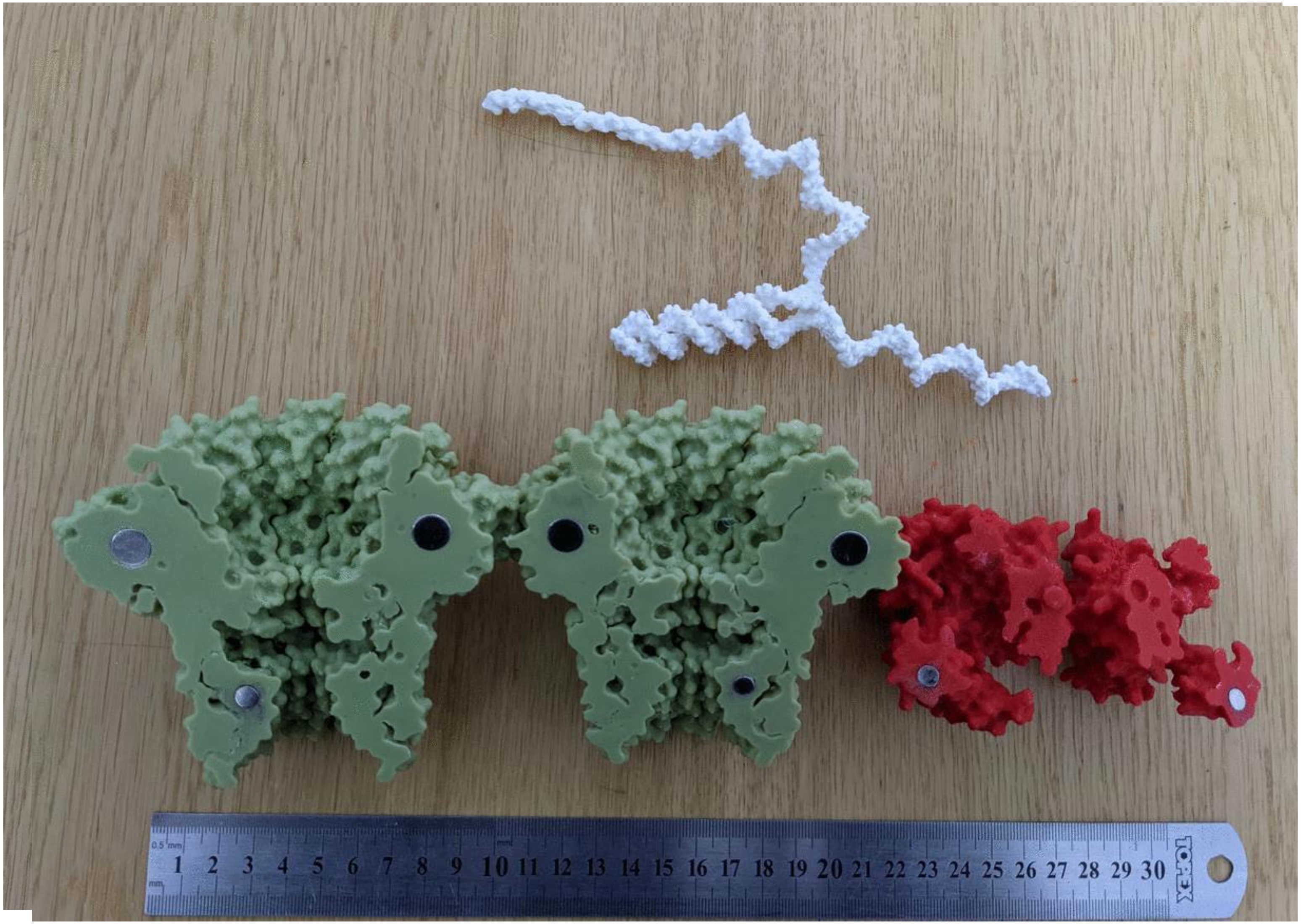
Examples of printed models currently used for teaching

Antibodies interacting with an antigen (lysozyme)

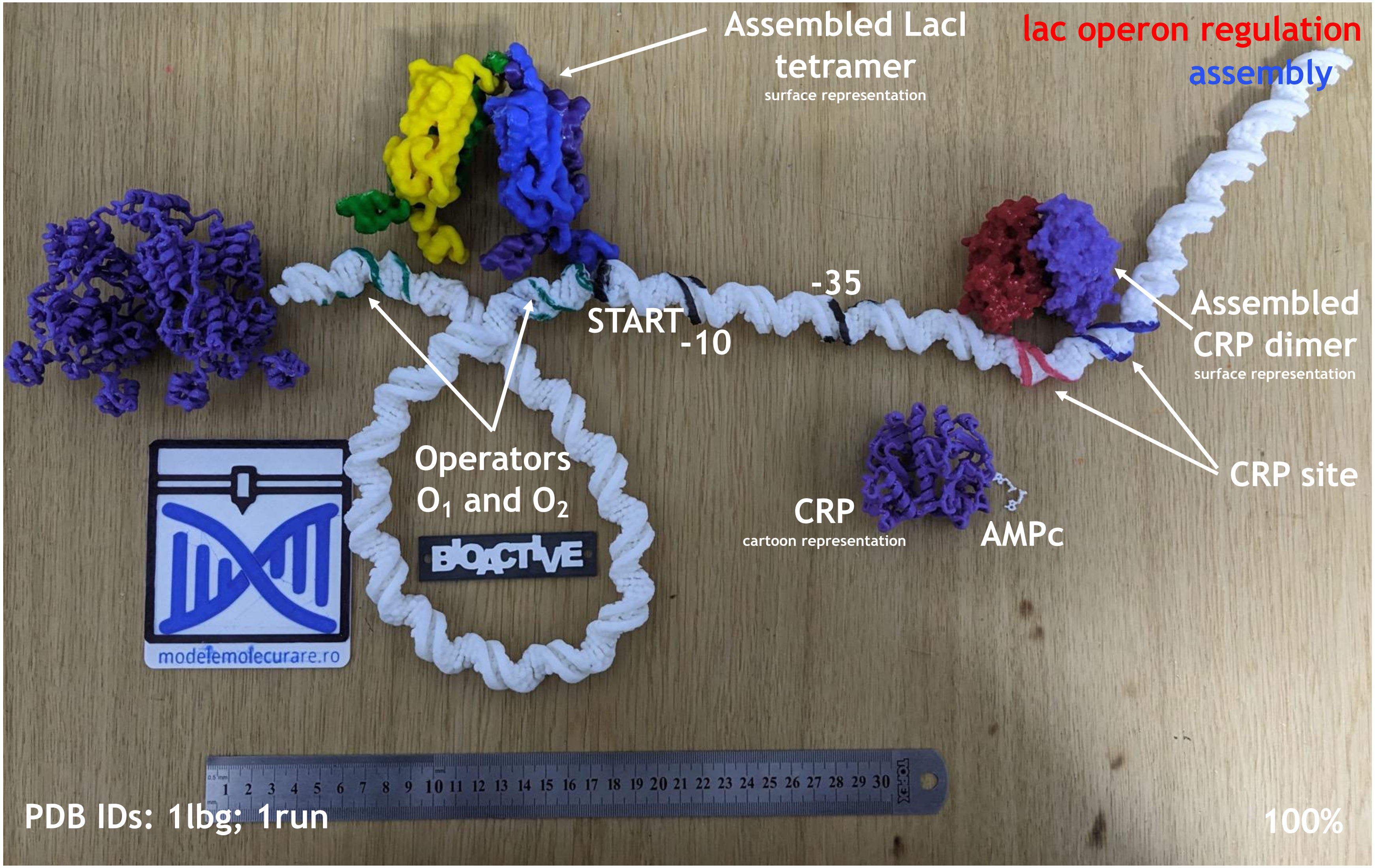


https://3dprint.nih.gov/discover/3dpx-015554

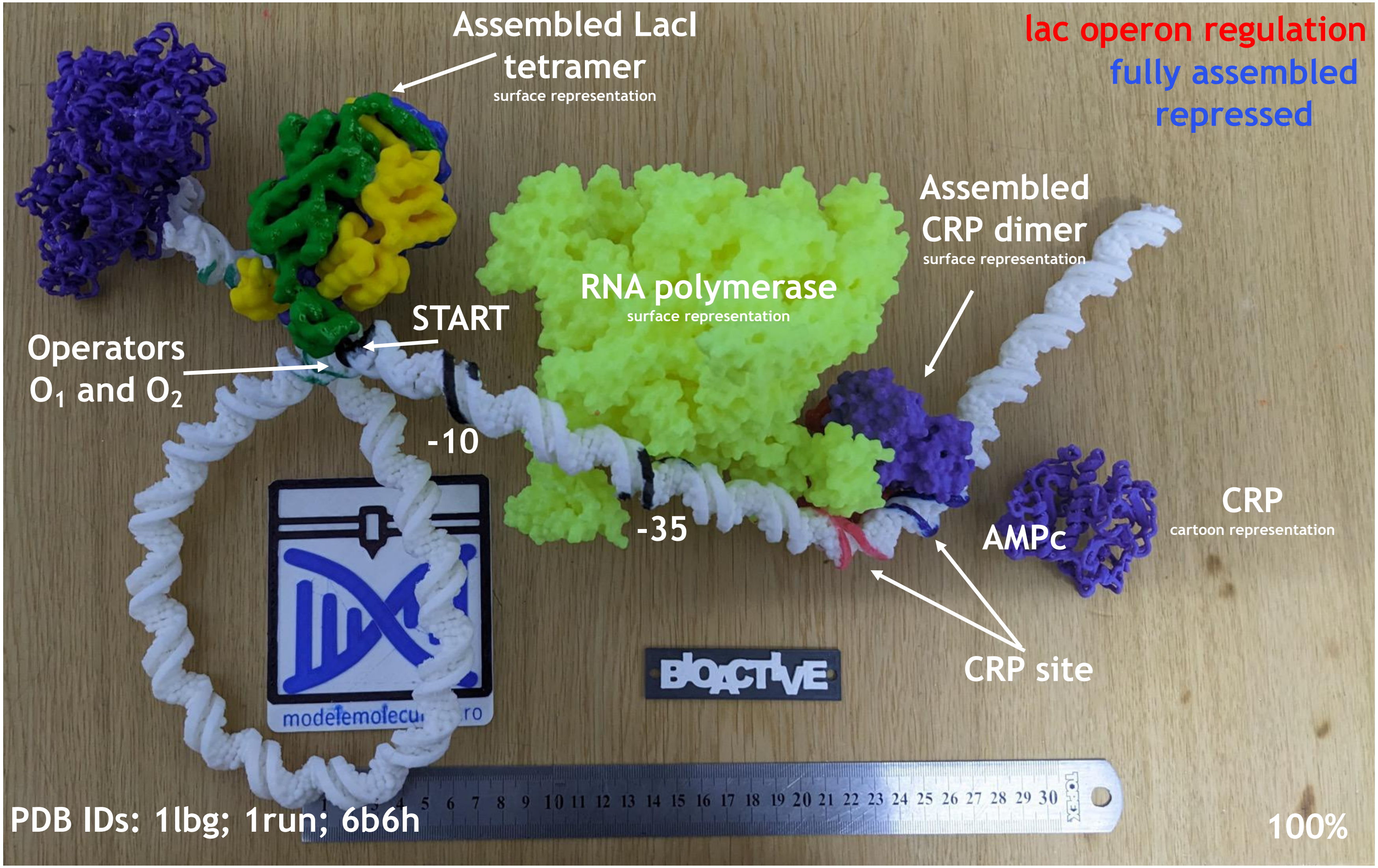
A protein nanopore sequencing DNA



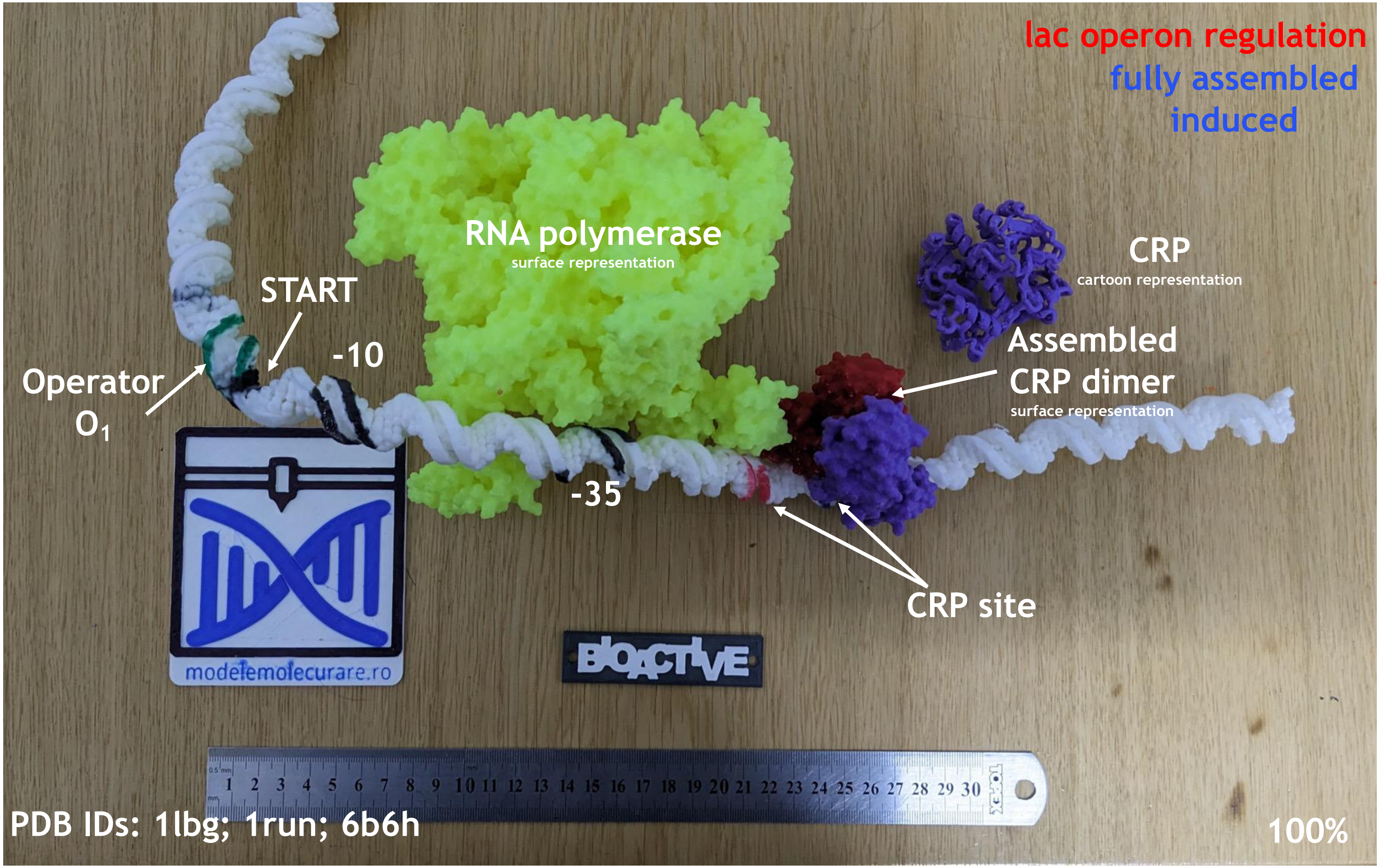
Physical model for teaching lac operon regulation



Physical model for teaching lac operon regulation



Physical model for teaching lac operon regulation



Feedback and Follow-Up

Your feedback is extremely valuable in improving future workshops and ensuring that the 3DP-Jmol resources continue to evolve to best serve the educational community.

Please take 2–3 minutes after the session to complete a short, anonymous feedback form:

📋 Feedback Form: https://forms.gle/zUAG9ChebcJdkedP8

🕒 Estimated time: 2–3 minutes

You may also access the form by scanning the QR code: