

# Putting molecules from the computer screen into students' hands using 3D printing



ALEXANDRU IOAN CUZA UNIVERSITY of IAȘI

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

<https://modeleleculare.ro/>

# A bit about us and our work in Iași



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## Department of Biology



Bulevardul Carol I nr. 20A,  
Iași, Romania, 700505  
Tel.: +40(0)232201072  
Fax: 40(0)232201472

[www.bio.uaic.ro](http://www.bio.uaic.ro)

Founded in 1948

### BioActive research group

- Isolation
  - Identification
  - Characterization
  - Biological effects (neurological effects, cytotoxicity, oxidative stress, antimicrobial activity)
- of biological active molecules with potential applications in biotechnology.



22.10.2024

3D printed macromolecular models

Slide 2 / 46

# A bit about us and our work in Iași

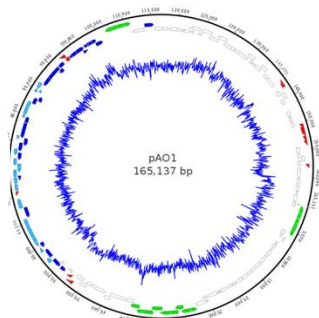
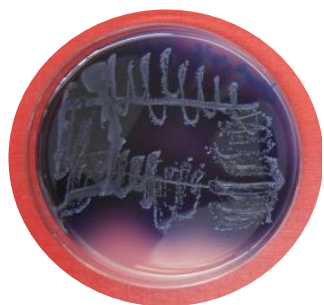


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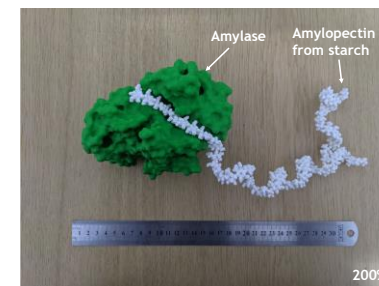
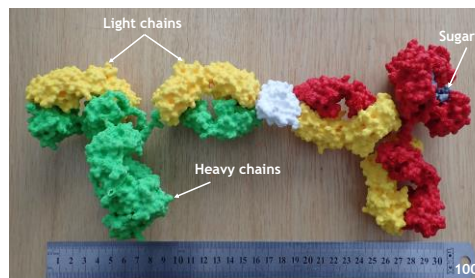
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## Main research subjects:

- 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:

El-Sabeh et al. BMC Genomics (2023) 24:516  
<https://doi.org/10.1186/s12864-023-09644-3>

BMC Genomics

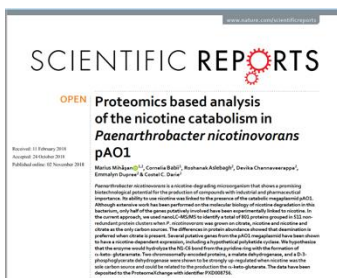
RESEARCH

Open Access

Characterisation of the *Paenarthrobacter nicotinovorans* ATCC 49919 genome and identification of several strains harbouring a highly syntenic *nic*-genes cluster

Amada El-Sabeh<sup>1</sup>, Andreea-Mihaela Miesnita<sup>1</sup>, Iustin-Tiberiu Munteanu<sup>1</sup>, Iasmina Honceriu<sup>1</sup>, Fakhri Kallabi<sup>1,2</sup>, Razvan-Stefan Boiangiu<sup>1</sup> and Marius Mihasan<sup>1\*</sup>

## Most Important paper:



Received: 23 July 2020 | Revised: 4 January 2021 | Accepted: 17 February 2021  
DOI: 10.1002/bmb.21493

ARTICLE

WILEY

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

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Abstract

The structure and function of biomolecules relationship is the hallmark of biochemistry, molecular biology, and life sciences in general. Physical models of macromolecules give students the possibility to manipulate these structures in three dimensions, developing a sense of spatiality and a better understanding of key aspects such as atom size and shape, bond lengths and symmetry. Several molecular model systems were developed specifically to represent particular classes or groups of molecules and hence lack the flexibility of a universal solution. Three-dimensional printing could nevertheless provide such a universal solution, as it can be used to create physical models of biomolecular structures based on the teacher's or demonstrator's needs and requirements. Here, insulin was used as a model molecule and several depiction and printing parameters were tested in order to highlight the technical limitations of the approach. In the end, a set of settings that worked is provided which could serve as a starting point for anyone wishing to print his or her own custom macromolecular model on the cheap.

KEYWORDS

3D printing; general public; insulin; molecular models

## Developed educational resources:



<https://www.nature.com/articles/s41598-018-34687-y>

<https://doi.org/10.1002/bmb.21493>

<https://modele-moleculare.ro/>





## Theoretical part:

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

## Hands-on part:

- .pdb to .stl file - software and steps
- Practical considerations when 3D printing molecular models

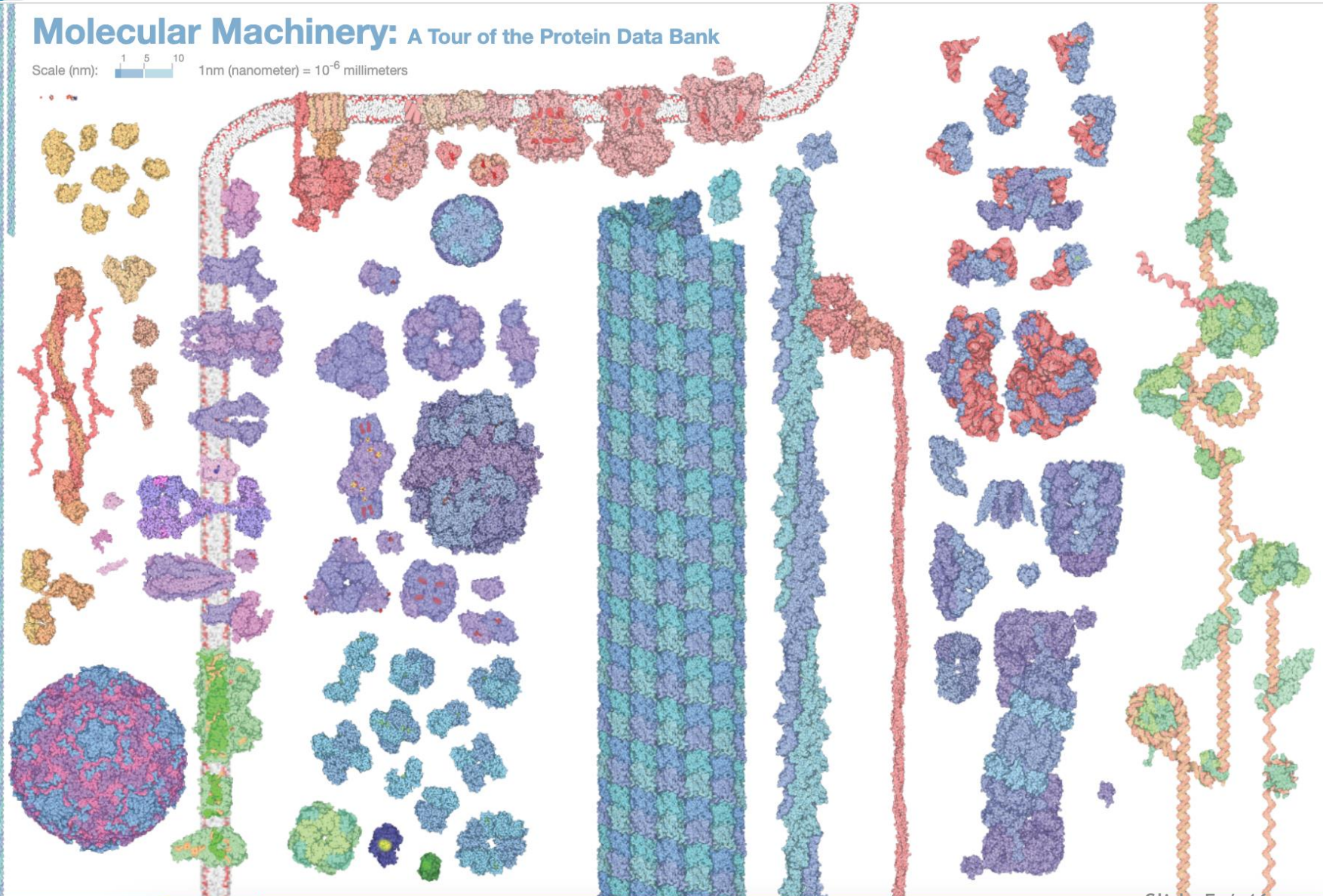


# Understanding Life Sciences relies on understanding Structural Biology



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

Scale (nm): 1 5 10 1nm (nanometer) = 10<sup>-6</sup> millimeters



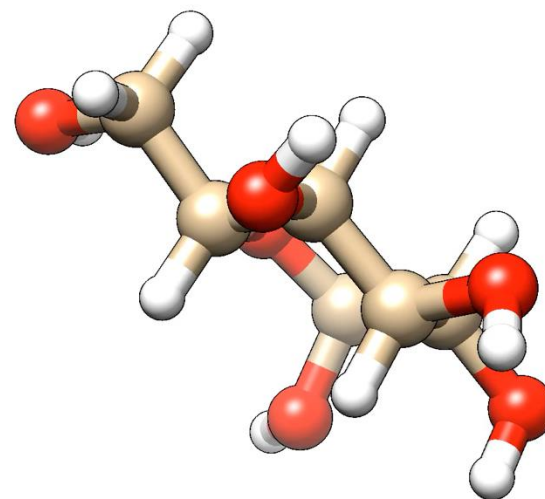
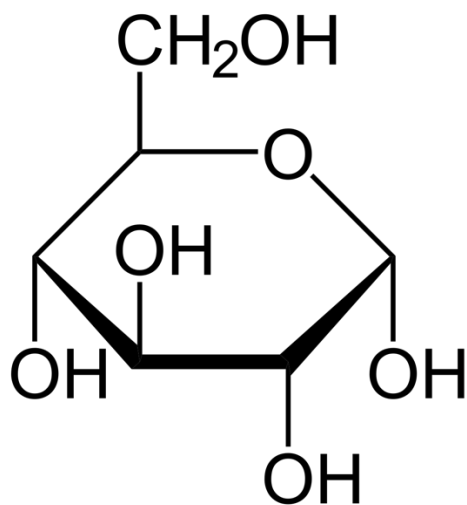
Extracellular

Membrane

Intracellular/Cytosol

Slide 5 / 41  
Intracellular/Nucleus

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



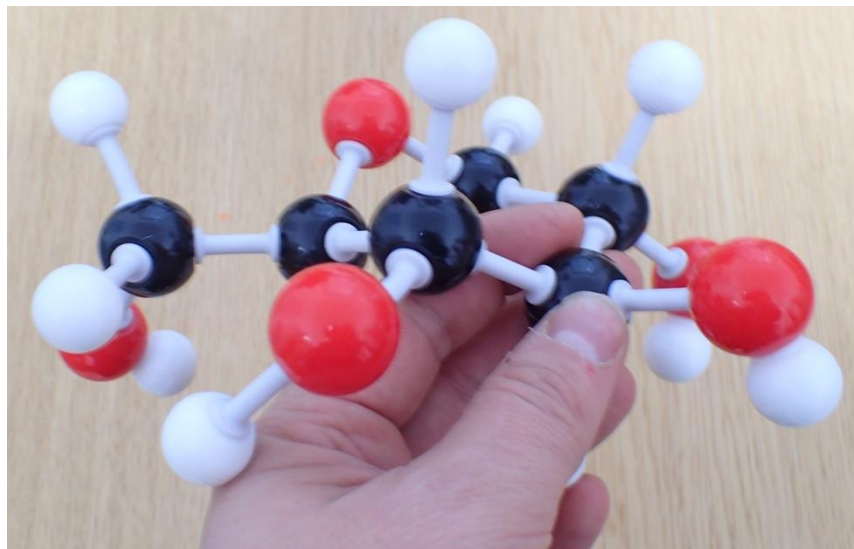
$\alpha$ -D-glucopyranose

# Molecular models to aid teaching - Molymod



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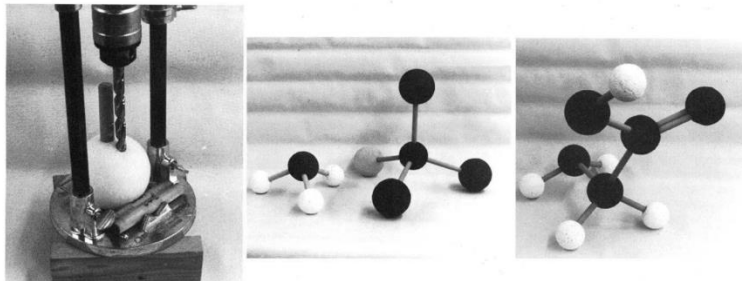


[http://www.molymod.com/MMS-004\\_Inorganic\\_\\_Organic\\_Teacher\\_Set.jpg](http://www.molymod.com/MMS-004_Inorganic__Organic_Teacher_Set.jpg)

**molymod**<sup>®</sup>

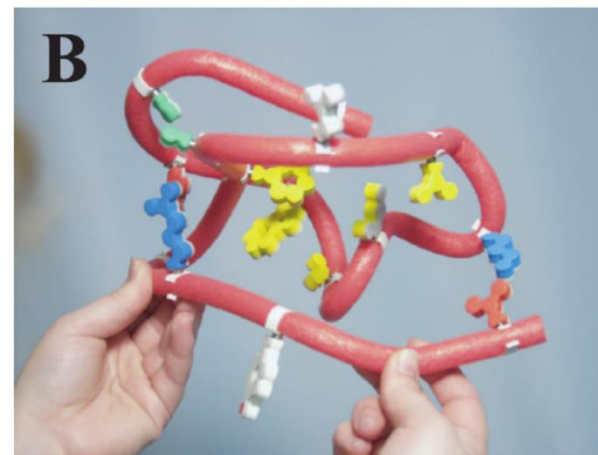
The *original* dual-scale system of molecular models





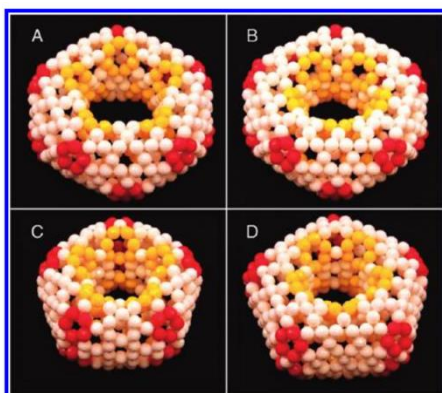
## Styrofoam balls and copper wires

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



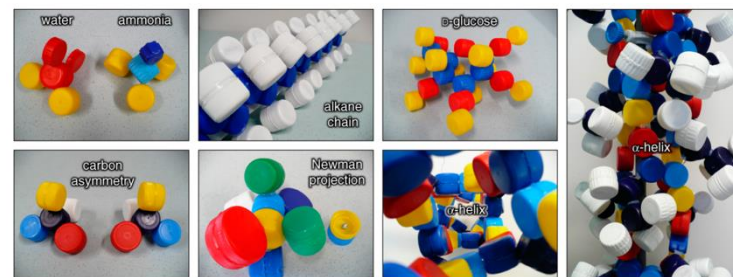
## Flexible foam, wires and foam cut-outs

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 - Paper models



Antibody  
(Paper Model)



DNA  
(Paper Model)



Dengue Virus  
(Paper Model)



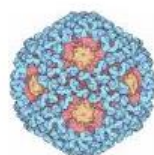
Green and Red  
Fluorescent Proteins  
(Paper Model)



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)

## Build a Paper Model of DNA



1 Cut out the model.



2 Fold the paper in half so that the backbone (with '5' written at the top) pops out.



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



4 Fold the paper in half so that the backbone (with '5' written at the top) pops out.



5 Turn the other backbone flags (with '3' at the top) one over the other, so your model looks like the one 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.



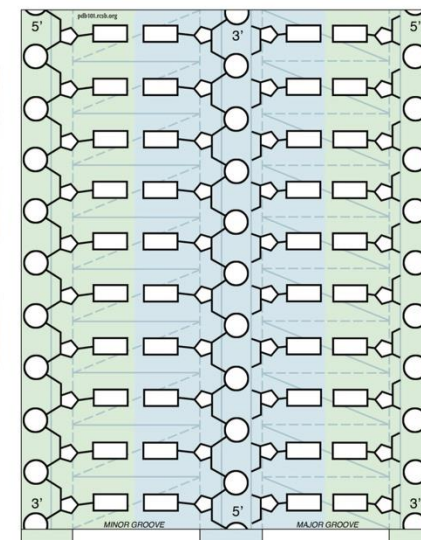
8 Pull the model open, and pop out the backbones on the sides.



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

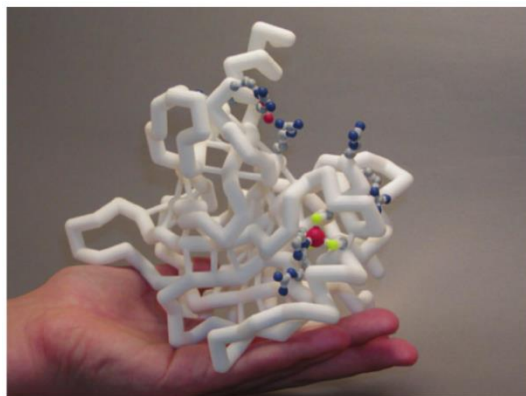
**About DNA**  
DNA is perfect for the storage and readout of genetic information, which is stored in the way the bases match one another on opposite sides of the double helix. Adenine (A) pairs with thymine (T), and guanine (G) with cytosine (C), with each pair forming a set of complementary hydrogen bonds.  
The all-atom model (shown on the second side) has the sequence C-G-C-T-T-A-A-G-C-G-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 Molecular 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 - 3D printed models



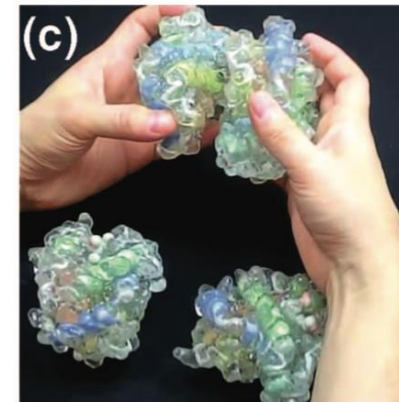
**p53 tumor suppressor protein**

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



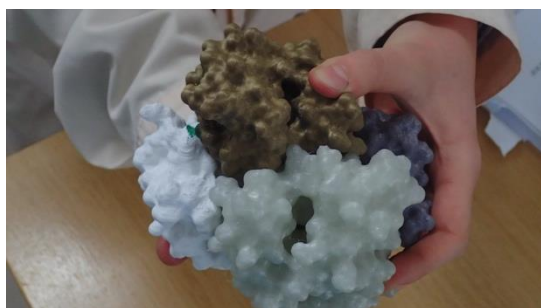
**Leucine zipper**

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

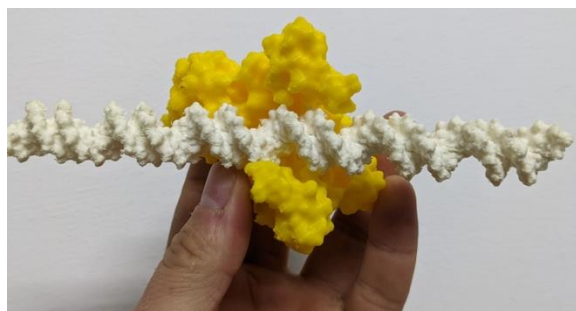


**Human haemoglobin**

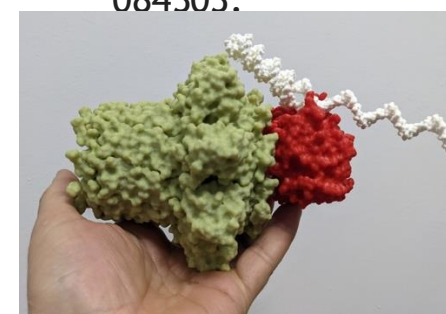
Kawakami M. A soft and transparent handleable protein model. *Rev Sci Instrum.* 2012; 83(8): 084303.



**Human deoxyhaemoglobin**



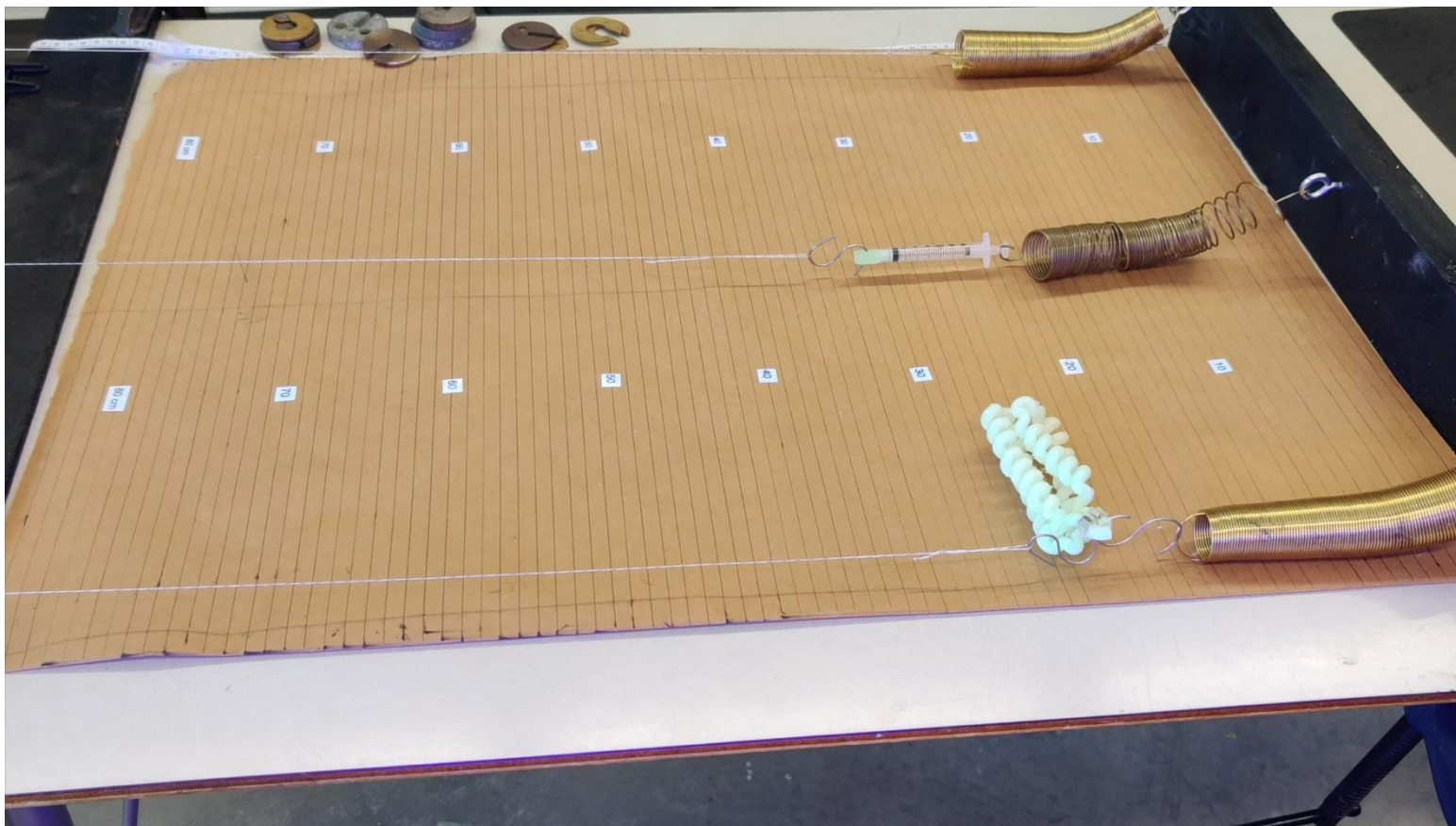
**EcoRI endonuclease and DNA**



**Nanopore sequencing complex**



# Molecular models to aid teaching - 3D printed models



Ionel Popa and Florin Saitis, *Journal of Chemical Education* 2022 99 (8), 3074-3082, DOI: 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



molecular visualization software  
**Chimera, Jmol, PyMol**

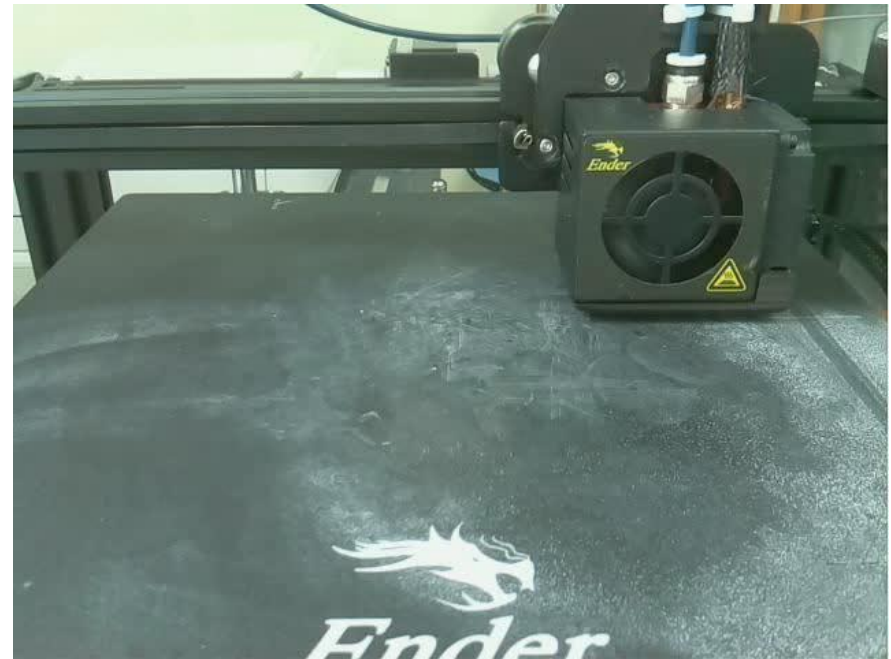
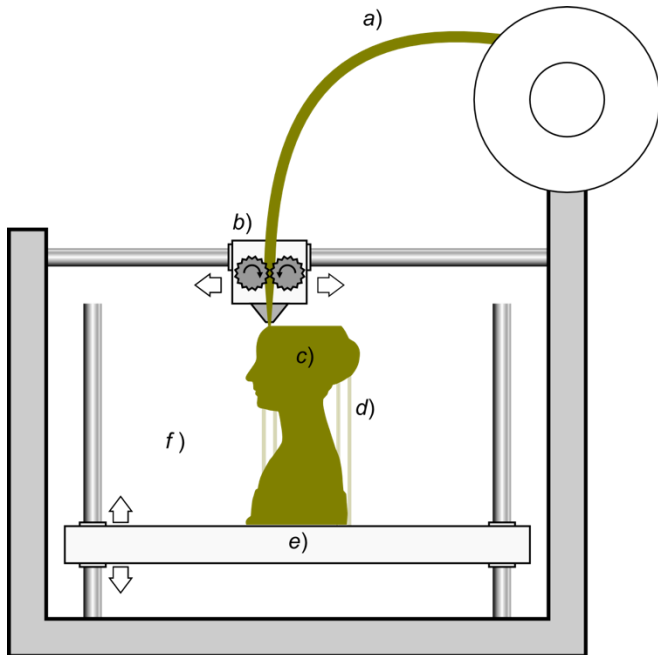
3D printing can do that

# 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

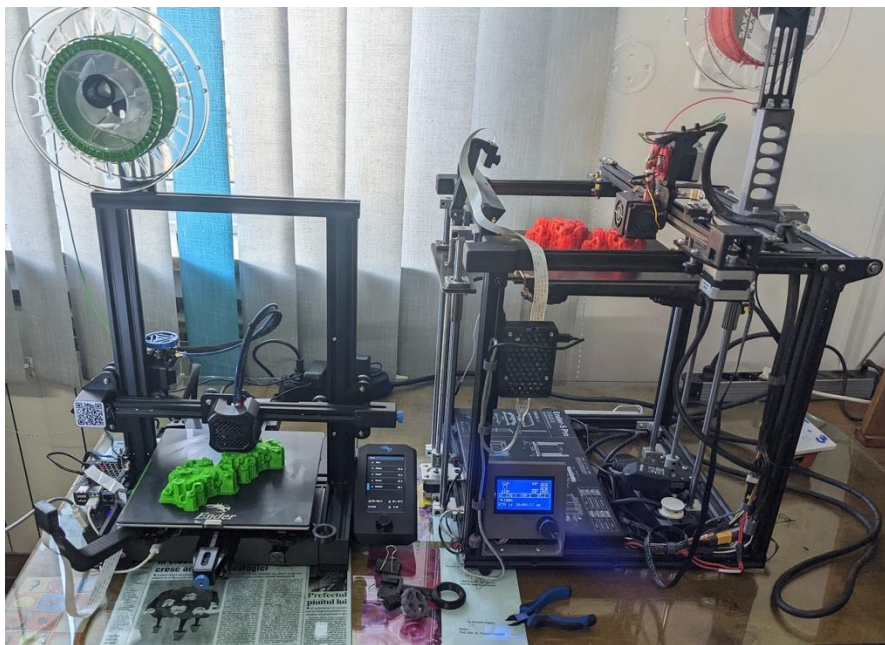


# 3D printing using FFF is accessible



Under 500\$ printers

20\$ - 40\$ Kg of plastic



amazon Deliver to Marius last 700440 All pla Hello, Ma... Returns Account & Orders

All Today's Deals Customer Service Marius's Amazon.com Buy Again Browsing History Gift Cards Amazon's response to COVID-19

1-16 of over 1,000 results for "pla" Sort by: Featured

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Movies & TV  
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Prime Video  
TV Shows  
See All 6 Departments

Avg. Customer Review  
★★★★★ & Up  
★★★★☆ & Up  
★★★☆☆ & Up  
★★☆☆☆ & Up

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 HATCHBOX  
 SUNLU  
 OVERTURE  
 TECBEARS  
 3D Solutech  
 MIKASD  
 eSUN  
See more

3D Printing Materials  
 ABS  
 HIPS  
 PETG  
 PLA  
 PVA  
 Wood-Plastic Composite

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

From Our Brands  
 Our Brands

Packaging Option  
 Frustration-Free Packaging

Sponsored  
TECBEARS PLA 3D Printer Filament 1.75mm Black, Dimensional Accuracy +/- 0.02 mm, 1 Kg Spool, Pack of 1  
★★★★★ ~ 4,769  
\$19<sup>99</sup>  
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Sponsored  
OVERTURE PLA Filament 1.75mm with 3D Build Surface 200mm x 200mm 3D Printer Consumables, 1kg Spool...  
★★★★★ ~ 6,128  
\$20<sup>99</sup> (\$1.05/10 Items)  
Save more with Subscribe & Save  
Ships to Romania

Best Seller  
HATCHBOX PLA 3D Printer Filament, Dimensional Accuracy +/- 0.03 mm, 1 kg Spool, 1.75 mm, Black, Pack...  
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\$21.50 (9 used & new offers)

OVERTURE PLA Filament 1.75mm with 3D Build Surface 200mm x 200mm 3D Printer Consumables, 1kg Spool...  
★★★★★ ~ 6,129  
\$22<sup>99</sup> (\$1.15/10 Items) \$25-59  
Save more with Subscribe & Save  
Ships to Romania  
More Buying Choices  
\$18.99 (17 new offers)

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

# 3D printed models - how to get them



The easy, but not necessarily the cheap 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).

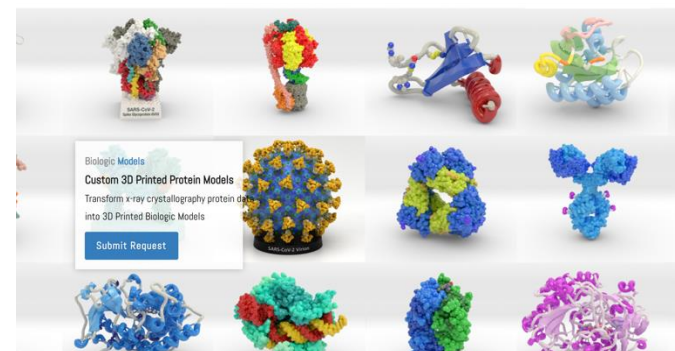
Copies of the model have been gifted to the vaccine development teams at Oxford University and

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

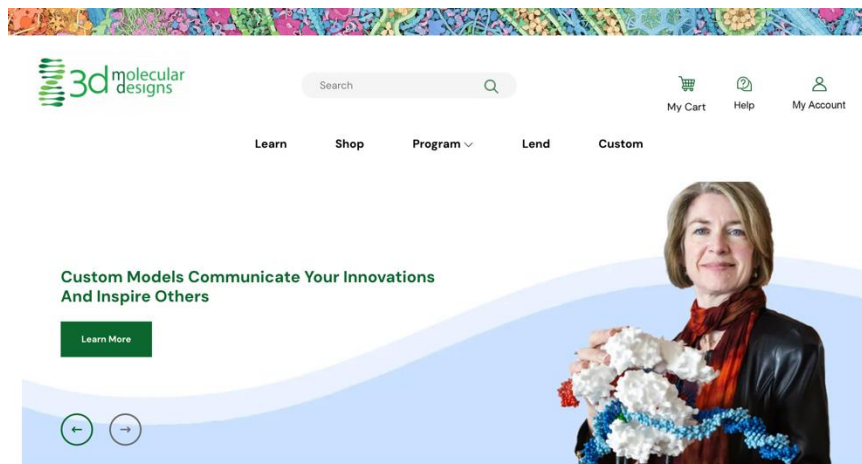
## BIOLOGIC MODELS

Home Explore 3D Print Shop Contact

0 items



<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://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/>

AND

**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

Get the latest research information from NIH:  
<https://www.nih.gov/coronavirus>

**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

The NIH 3D Print Exchange

EXPLOREAZĂ UNIVERSUL MOLECULAR CU AJUTORUL MODELELOR IMPRIMATE 3D!

Despre noi Cum obținem modelele ▼ Modele noi Modele gratuite

**Modele fizice ale moleculelor pentru o mai bună educație în științele vieții**

Un concept de bază în științele vieții este legătura dintre structura unei molecule și funcția acesteia. Formulele chimice nu pot reda eficient complexitatea structurală a moleculelor biologice și sunt cel mai frecvent recepționate de studenți și elevi ca simple imagini. Modelele fizice permit manipularea moleculelor în spațiu tridimensional, oferind o experiență de învățare multisensorială și o mai bună înțelegere a unor aspecte cheie precum dimensiunea atomilor, unghiurile dintre legăturile chimice și relațiile dimensionale dintre diverse molecule.

[MAI MULTE DESPRE MODELELE FIZICE ALE MOLECULELOR →](#)



# Do these models make a difference in teaching?



## A compensatory research study

	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	<b>Intervention</b>	2 days after lecture, 30 minutes, 10 questions	Intervention and Feedback form
Group B			<b>Intervention</b>			No intervention		

The project was approved by the ethics committee at the Department of Psychology 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?



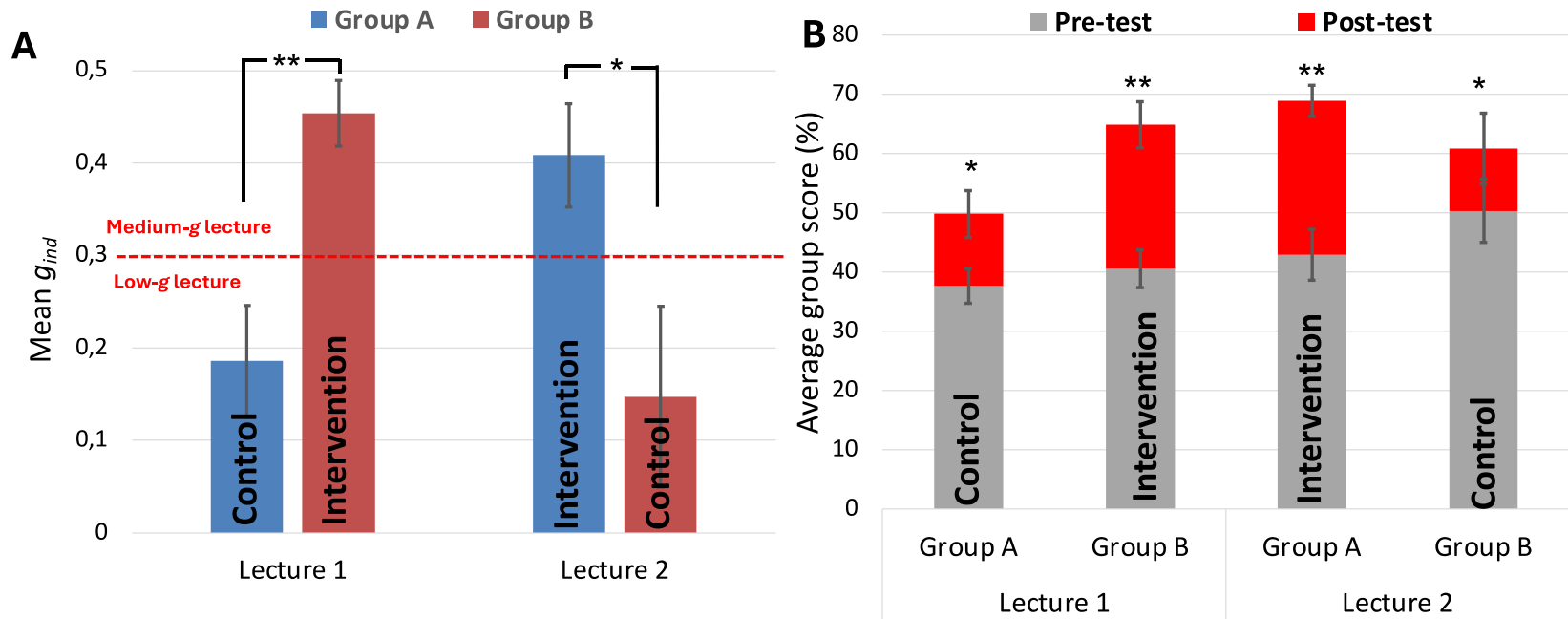
## Evaluation of impact is key

Models	NIH 3D DOI:	Assessment questions	Learning objective	Biomolecular visualization learning goals
<b>Amino acids, peptides and proteins</b>				
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)
<b>Nucleotides and nucleic acids</b>				
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 rotatable 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



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







Received: 13 July 2019 | Revised: 1 April 2020 | Accepted: 27 April 2020  
DOI: 10.1002/bmb.21362

ARTICLE



## Interactive learning modules with 3D printed models improve student understanding of protein structure–function relationships

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Funding information

National Science Foundation, Grant/Award Number: DUE-1625804

### 1 | INTRODUCTION

Protein structure and function is fundamental to biochemistry. Biochemistry textbooks and classes begin with a unit on protein structure and function because of their role in nearly all biochemical processes. Because of the versatility of these macromolecules (including enzymes and structural, transport, motility, and signaling proteins), undergraduate life science students must develop proficiency in foundational intramolecular structure–

Abstract

Ensuring undergraduate students become proficient in relating protein structure to biological function has important implications. With current two-dimensional (2D) methods of teaching, students frequently develop misconceptions, including that proteins contain a lot of empty space, that bond angles for different amino acids can rotate equally, and that product inhibition is equivalent to allostery. To help students translate 2D images to 3D molecules and assign biochemical meaning to physical structures, we designed three 3D learning modules consisting of interactive activities with 3D printed models for amino acids, proteins, and allosteric regulation with coordinating pre- and post-assessments. Module implementation resulted in normalized learning gains on module-based assessments of 30% compared to 17% in a no-module course and normalized learning gains on a comprehensive assessment of 19% compared to 3% in a no-module course. This suggests that interacting with these modules helps students develop an improved ability to visualize and retain molecular structure and function.

KEYWORDS

3D printing, allosteric regulation, amino acids, model-based learning, molecular visualization, protein structure–function, student misconceptions, undergraduate

function relationships in order to understand complex macromolecular interactions and higher-order processes. Moreover, designing drugs, antibiotics, or pesticides and responding to disease-causing mutations represent practical applications that rely on comprehending how protein structure directly drives biochemical function.

Unfortunately, teaching protein structure and function with traditional two-dimensional (2D) methods results in crucial misunderstandings (Table ) identified from the literature and polling instructors.<sup>1–8</sup> From chemical or stick representations of amino acids and peptides, biochemistry undergraduates develop inaccurate

Roston and Couch contributed equally to this manuscript.

356 | © 2020 International Union of Biochemistry and Molecular Biology wileyonlinelibrary.com/journal/bmb Biochem Mol Biol Educ. 2020;48:356–368.

<https://doi.org/10.1002/bmb.21362>

Article

## Student Understanding of DNA Structure–Function Relationships Improves from Using 3D Learning Modules with Dynamic 3D Printed Models<sup>§</sup>

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From the <sup>1</sup>Department of Biochemistry, University of Nebraska, Lincoln, Nebraska, 68588-0664, <sup>†</sup>School of Biological Sciences, University of Nebraska, Lincoln, Nebraska, 68588-0118, <sup>§</sup>Department of Chemistry, Doane University, Crete, Nebraska, 68333

Abstract

Understanding the relationship between molecular structure and function represents an important goal of undergraduate life sciences. Although evidence suggests that handling physical models supports gains in student understanding of structure–function relationships, such models have not been widely implemented in biochemistry classrooms. Three-dimensional (3D) printing represents an emerging cost-effective means of producing molecular models to help students investigate structure–function concepts. We developed three interactive learning modules with dynamic 3D printed models to help biochemistry students visualize biomolecular structures and address particular misconceptions. These modules targeted specific learning objectives related to

DNA and RNA structure, transcription factor–DNA interactions, and DNA supercoiling dynamics. We also designed accompanying assessments to gauge student learning. Students responded favorably to the modules and showed normalized learning gains of 49% with respect to their ability to understand and relate molecular structures to biochemical functions. By incorporating accurate 3D printed structures, these modules represent a novel advance in instructional design for biomolecular visualization. We provide instructors with the materials necessary to incorporate each module in the classroom, including instructions for acquiring and distributing the models, activities, and assessments. © 2019 International Union of Biochemistry and Molecular Biology, 47(3):303–317, 2019.

**Keywords:** DNA; RNA; student misconceptions; 3D printing; model-based learning; nucleic acid structure and function; molecular visualization

### Introduction

Understanding the complex interdependence of macromolecular structure and function represents a central goal of undergraduate life science education, particularly within

biochemistry [1–3]. However, life science students frequently struggle to visualize and translate between the static two-dimensional (2D) images displayed in textbooks and the dynamic three-dimensional (3D) concepts they represent [4–8]. Hence, many students leave life sciences classrooms with misconceptions about structure–function relationships [8]. One fundamental biological concept with which students struggle is the relationship of DNA structure to its functions. For example, students have misconceptions about the way DNA bases are stacked and accessible to DNA binding proteins, the continuity of and information presented in DNA grooves, the flexibility and dynamic nature of DNA molecules, and the enzymes that cleave and repair DNA [9–12]. For example, students fail to realize that although DNA bases lie between the DNA backbones, they are accessible to proteins [9]. As a result, students do not realize that the presented chemical information varies between the major and minor grooves of a specific DNA segment. Moreover, many students do not realize that transcription factors can interact with a

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§Additional Supporting Information may be found in the online version of this article.

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Biochemistry and Molecular Biology Education

303

<https://doi.org/10.1002/bmb.21234>



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

**Let's walk through the process together, and judge yourself**

# Overview of the steps involved in fabricating a macromolecular model



Download structure from



PDB or CIF file

Visualize and prepare the model in

UCSF ChimeraX

STL file

Prepare the file for printing using

PrusaSlicer

GCODE file

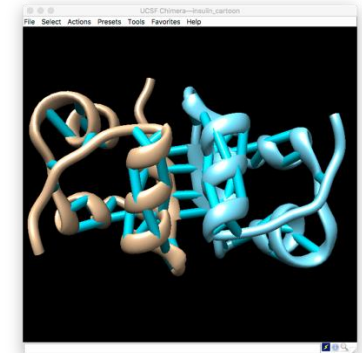
Print



Support material removal

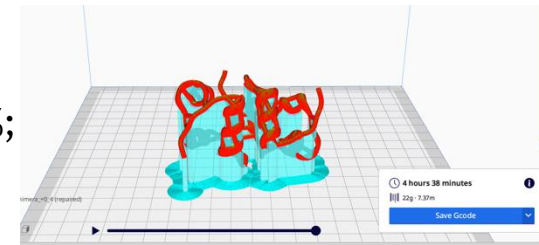


1. Chose or combine **visualization styles**;
2. Add **H bonds** or **create struts** to make the model more sturdy (mandatory for cartoon and balls and sticks models, not required for surface);
3. Increase the **thickness** of each printed element and/or **improve the smoothness** for molecular surfaces.



## 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

## C. Clean up and finalize the physical model



# A. Generation of the computer model (or stl file)



## 1. Download and install UCSF ChimeraX;

<https://www.cgl.ucsf.edu/chimerax/>

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

1. Jmol - <https://jmol.sourceforge.net/>
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

## 2. Open the .pdb file of your choice via File > Fetch by ID... > Select PDB and Enter PDB ID

If unsure, use one these PDB IDs:

- 1BDNA
- 1TRA
- 2HHB
- 4INS
- 1AON
- 6VYB
- 2FG4
- 3KXU
- 1EMA
- 1LYD

# A. Generation of the computer model (or stl file)



## 3. Edit/apply a visualization style to make the molecule 3D printable

Default visualization styles in all molecular visualization software are not compatible with 3D printing

Specific visualization styles need to be applied via

## 1. Buttons and menus

The screenshot displays the ChimeraX software interface. The main window shows a 3D ribbon model of a protein structure. The interface includes a menu bar (File, Edit, Select, Actions, Tools, Favorites, Presets, Help) and a toolbar with various visualization options. A 'Log' window is open on the right, displaying chain information for 2hhb #1 and non-standard residues. The 'Models' window at the bottom right shows the current model (2hhb) with its ID (1) and visibility options.

Chain information for 2hhb #1		
Chain	Description	UniProt
<a href="#">A C</a>	<a href="#">HEMOGLOBIN (DEOXY) (ALPHA CHAIN)</a>	<a href="#">HBA_HUMAN 1-141</a>
<a href="#">B D</a>	<a href="#">HEMOGLOBIN (DEOXY) (BETA CHAIN)</a>	<a href="#">HBB_HUMAN 1-146</a>

Non-standard residues in 2hhb #1	
<a href="#">HEM</a>	<a href="#">— protoporphyrin IX containing Fe</a> (HEME)
<a href="#">PO4</a>	<a href="#">— phosphate ion</a>

Name	ID	Shown	Select	Close
> 2hhb	1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	Hide Show View Info

## 2. CLI

# A. Generation of the computer model (or stl file)



The fastest and easiest way to have good-enough printable models:  
**NIHPresets** from the ChimeraX Toolshed

In ChimeraX install via **Tools > More tools... >** In the new window, search for **NIHPresets**, Click on it and hit **Install**

ChimeraX Toolshed

https://cxtoolshed.rvbi.ucsf.edu/

Submit a Bundle Search the Toolshed Sign In

**All Bundles**

**Categories**

- EM
- User Interface
- Structure Analysis
- Input/Output
- Structure Editing
- external program
- MD
- augmented reality
- atomic structure
- Sequence
- Model validation
- Light microscopy
- Fitting
- developer

**Newest Releases**

- ArtiaX**  
Visualization and editing of cryo-ET particle lists.
- TetraScope**  
Automatically create tetrahedral protein
- copick**  
Collaborative annotation of cryo-electron tomograms.
- SchoIAR**  
Create augmented reality and web browser data
- NIHPresets**  
Presets useful for 3D printing
- clix**  
A powerful and intelligent ChimeraX command line

[more newest releases >](#)

ChimeraX Toolshed - NIHPresets

https://jcsf.edu/apps/chimeraxnihpresets?platform=Windows&version=1.8

Submit a Bundle Search the Toolshed Sign In

← Go back to home

**NIHPresets**  
Presets useful for 3D printing

★★★★★ (1) 6057 downloads

Details **Release History**

Categories: [presets](#)

This bundle adds presets useful for 3D printing. The user should be aware that these presets are "destructive" in that they delete solvent.

**Installed**

Version 1.2.5  
Released 22 Aug 2024  
Works with ChimeraX  
~1.3

RESOURCES

- Ask a question

New visualization style presets are available in ChimeraX via the menu **Presets > NIH3D>**



# A. Generation of the computer model (or stl file)

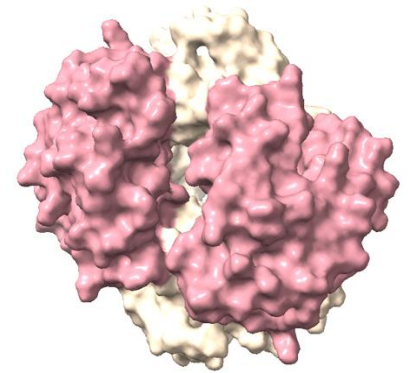


## Frequently used visualization styles

In ChimeraX Menu **Presets > NIH3D>**

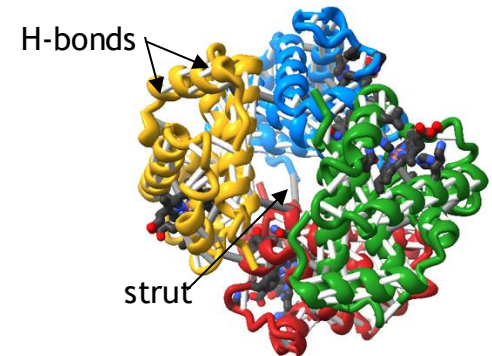
### Surface by chains (Printable)

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



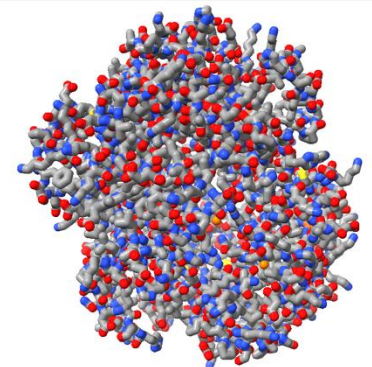
### Ribbon by chains (Printable)

H-bonds and struts have been added  
All elements are thicker  
Works for small proteins (one chain of hemoglobine)  
Can be difficult to print at times



### Sticks (Printable)

Applicable **only** to small molecules or ligands



# A. Generation of the computer model (or stl file)



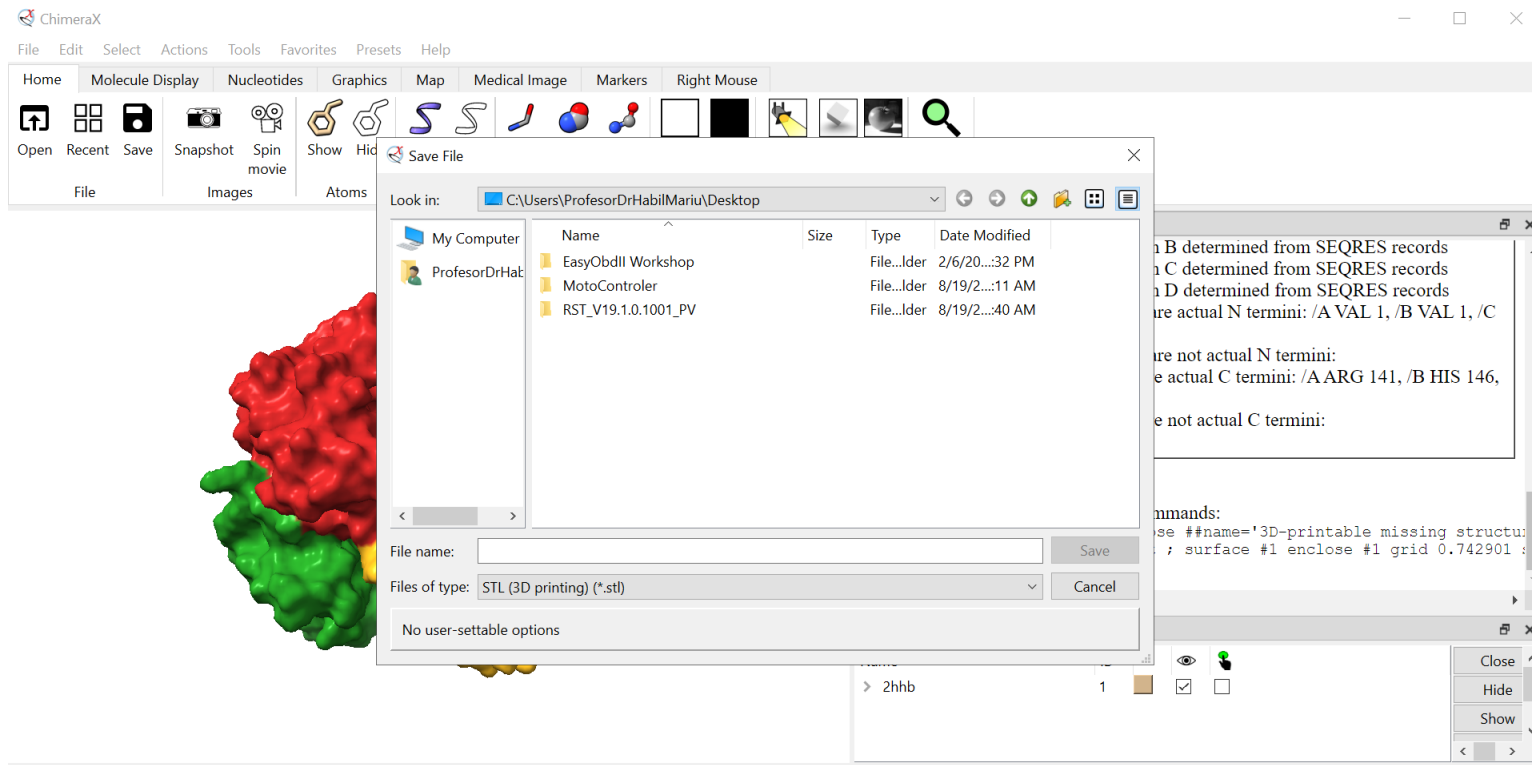
## 4. Final step

In ChimeraX Menu **File > Save ...**

In the new window under File name: **type your preferred name**

under Files of type: **STL (3D printing) (\*.stl)**

And hit **Save**



## B. 3D Printing the computer generated model



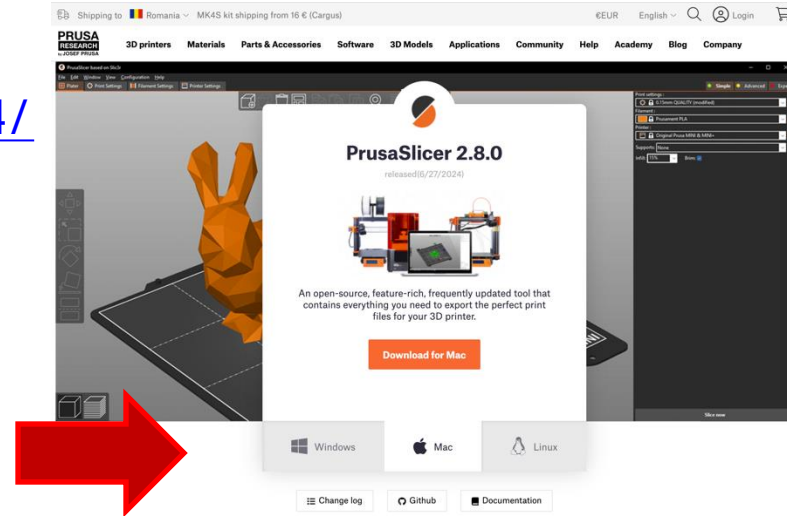
### 1. Download and install **PrusaSlicer**;

[https://www.prusa3d.com/page/prusaslicer\\_424/](https://www.prusa3d.com/page/prusaslicer_424/)

Alternative slicer programs used to control 3D printers:

1. **Ultimaker Cura** - <https://ultimaker.com/software/ultimaker-cura/>
2. **Slic3r** - <https://slic3r.org/>
3. **Simplify3D** - <https://www.simplify3d.com/> not free

Choosing one or another depends on the printer one has available



### 2. Open **PrusaSlicer** and **Cancel the configuration Wizard**.

### 3. Download the configuration bundle. Link on the event website.

<https://drive.google.com/file/d/1YM3sqMOEYSa7XxrpmzS5EqOsNFwNfaT8/view>

### 4. In **PrusaSlicer** navigate to **Menu > File > Import > Import Config Bundle...** Point to the newly downloaded file 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 **PrusaSlicer** navigate to **Menu > File > Import > Import STL/3MF/STEP...** Point to the .stl file and hit **Open**

Set

3. Print settings

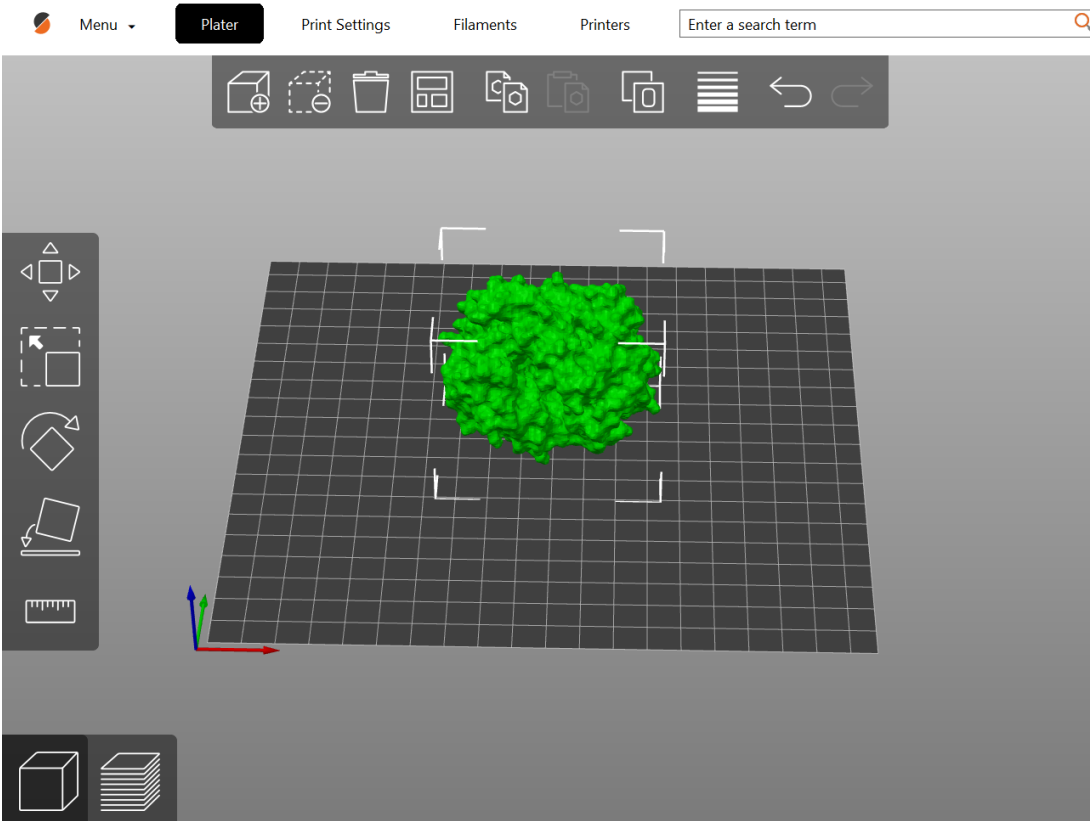
2. Material

1. Printer

4. Scale

5. Hit Slice

\*Untitled - PrusaSlicer-2.8.0 based on Slic3r



Print settings:

MM\_0.20mm-surface

Filament: Sakata 3DIngeo850 PLA

Printer: MM\_Kingroon KP3S-Pro BLTouch

Supports: Everywhere

Infill: 5% Brim:

**Object manipulation**

Name: 2hhb.stl

	X	Y	Z	
Position:	102	102	30.73	mm
Rotate (relative):	0	0	0	°
Scale factors:	100	100	100	%
Size [World]:	70.31	60.17	61.46	mm

Inches

Slice now

# B. 3D Printing the computer generated model



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

\*Untitled - PrusaSlicer-2.8.0 based on Slic3r

The screenshot shows the PrusaSlicer software interface. The main window displays a 3D model of a printed object on a grid. The interface includes a menu bar at the top with options like 'Menu', 'Plater', 'Print Settings', 'Filaments', and 'Printers'. A search bar is located in the top right. The left sidebar contains a 'Legend' panel with a table of feature types and their associated printing metrics. The right sidebar contains several panels: 'Print settings', 'Object manipulation', and 'Sliced Info'. The 'Print settings' panel shows the current printer and filament. The 'Object manipulation' panel shows the object name and position. The 'Sliced Info' panel shows the total printing time and filament usage. The 'Export G-code' button is highlighted with a red circle.

Feature type	Time	Percentage	Used filament
Perimeter	1h37m	14.2%	2.95 m 8.81 g
External perimeter	1h41m	14.8%	2.96 m 8.83 g
Overhang perimeter	3m	0.5%	0.08 m 0.25 g
Internal Infill	41m	6.1%	1.85 m 5.52 g
Solid infill	1h27m	12.7%	2.49 m 7.42 g
Top solid infill	4m	0.6%	0.12 m 0.36 g
Bridge infill	9m	1.3%	0.47 m 1.39 g
Skirt/Brim	35s	0.1%	0.02 m 0.05 g
Support material	2h10m	19.1%	4.49 m 13.40 g
Support material interface	22m	3.2%	0.40 m 1.21 g
Custom	12s	0.0%	0.02 m 0.06 g

Estimated printing times:  
First layer: 9m  
Total: 11h22m

Print settings:  
MM\_0.20mm-surface  
Filament: Sakata 3DIngeo850 PLA  
Printer: MM\_Kingroon KP3S-Pro BLTouch  
Supports: Everywhere  
Infill: 5% Brim:

Object manipulation  
Name: 2hhb.stl  
Position: x: 102, y: 102, z: 30.73 mm  
Rotate (relative): 0, 0, 0 °  
Scale factors: 100, 100, 100 %  
Size [World]: 70.31, 60.17, 61.46 mm  
 Inches

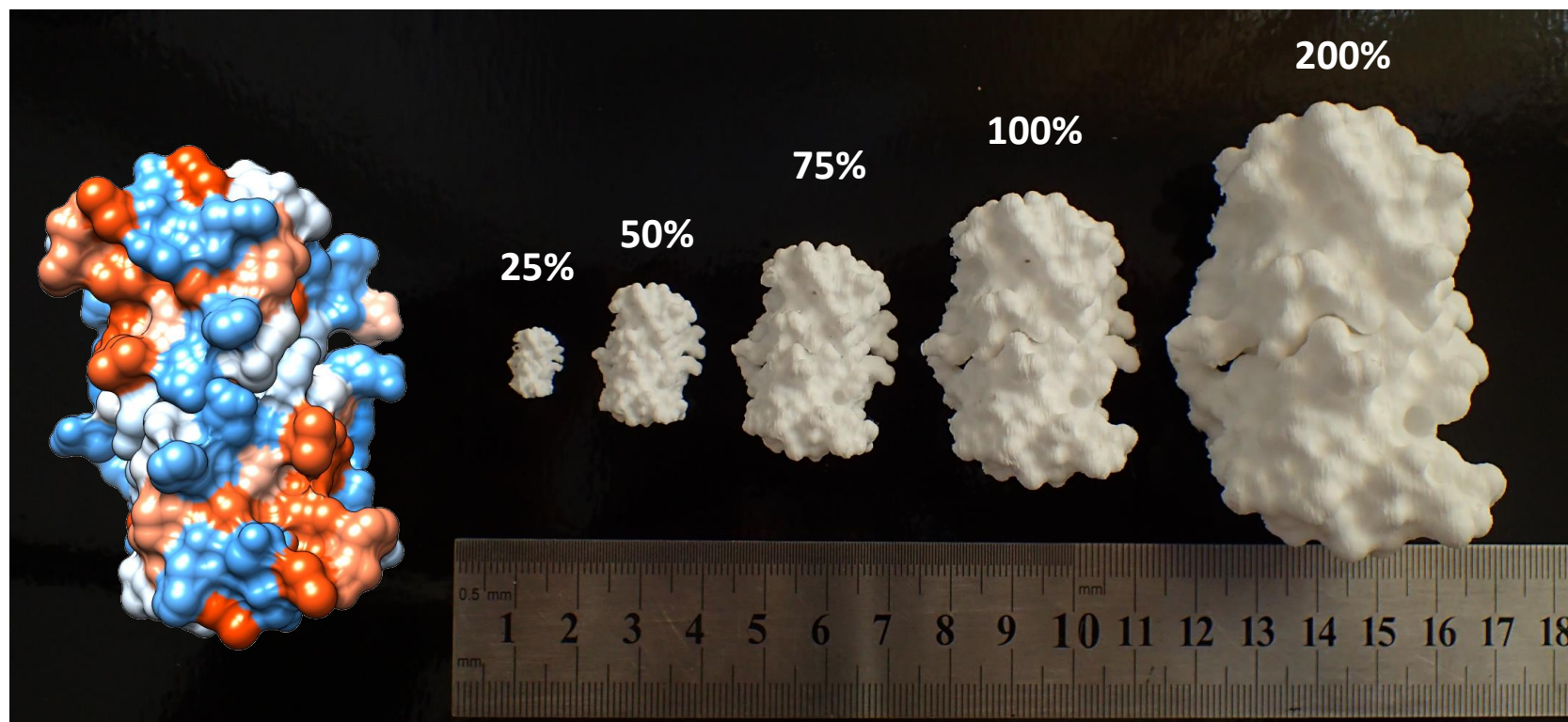
Sliced Info  
Used Filament (g) 47.29 (1047.29) (including spool)  
Used Filament (m) 15.85  
Used Filament (mm<sup>3</sup>) 38134.51  
Cost 3.45  
Estimated printing time: - normal mode 11h22m

**Export G-code**



## A. Models printed as molecular surface

- Can be printed at scales as low as 50% with good details on atoms;
- Wall thickness of 0.8 mm (2 layers for walls, 4 mm nozzle) is suffice



Insulin model in Chimera

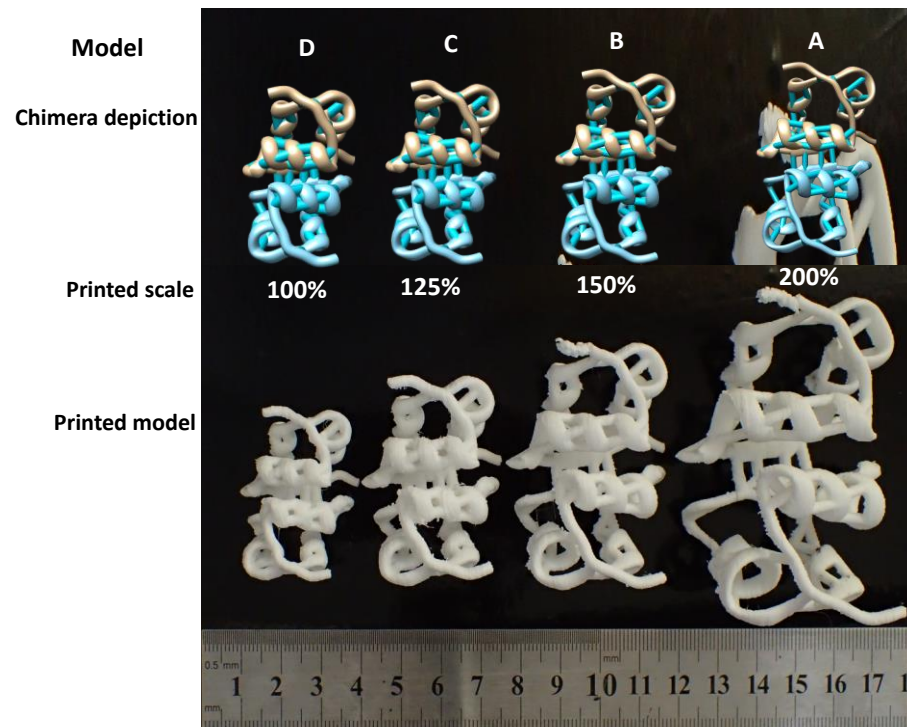
Physical models of insulin printed at various scales





## B. Models printed as cartoons

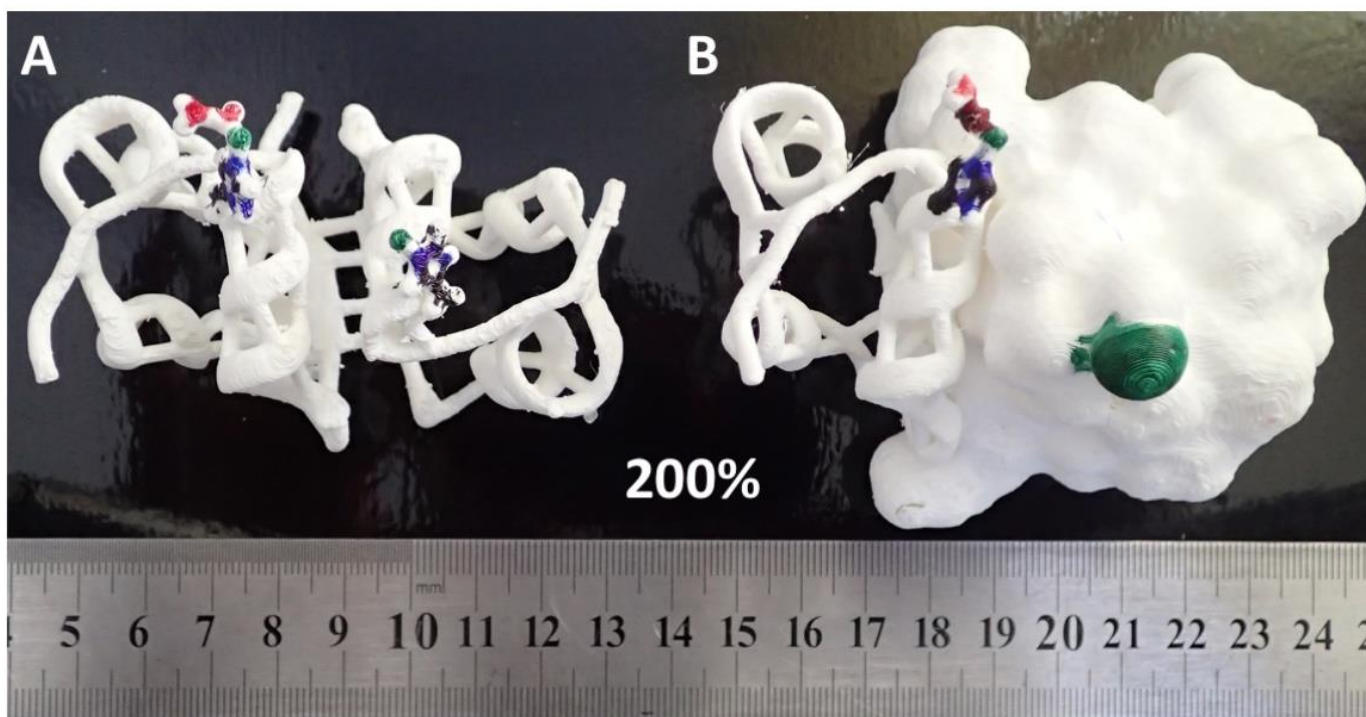
- H bonds and struts need to be added to increase rigidity of the model;
- Chimera default rendering parameters are not suitable for generating printable models. Rendering parameters need to be tinkered so that the thinnest elements (coils and H bonds) are printed at at least **2.6 mm in diameter**;
- Wall thickness of 1.6 mm (**4 layers for walls, 4 mm nozzle**) provides enough rigidity;
- Minimum recommended scale is **200x**





## C. Models printed as balls and sticks

- Macromolecular models are complicated and difficult to print;
- Extensive support material is required and sometimes impossible to remove;
- Chimera rendering parameters need to be tinkered so that the thinnest elements (bonds) are printed at at least **2.6 mm in diameter**;
- Wall thickness of 1.6 mm (**4 layers for walls, 4 mm nozzle**) provides enough rigidity;
- Unusable for proteins, but can be combined with other visualization modes.





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**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/NIAID/OD/OSSMO/OCICB

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

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

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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 (2017).

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**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. Tailor,<sup>‡</sup> Vincent F. Scalfani,<sup>§</sup> and Nabyl Merbouch<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

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**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

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**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>







## Secondary structure of lysozyme

Relevant Chimera model depiction settings\*

Scaling Cross Section Residue Class

Ribbon Scaling

3D\_printing\_proteins

Save Save As... Delete

	Width	Height
Coil	0.7	0.7
Helix	1.4	0.7
Sheet	1.4	0.7
Arrow (base)	2.8	0.7
Arrow (tip)	0.7	0.7
Nucleic	1	0.7

Number of grid divisions: 10 Erase All

Changing grid division erases drawn cross section.

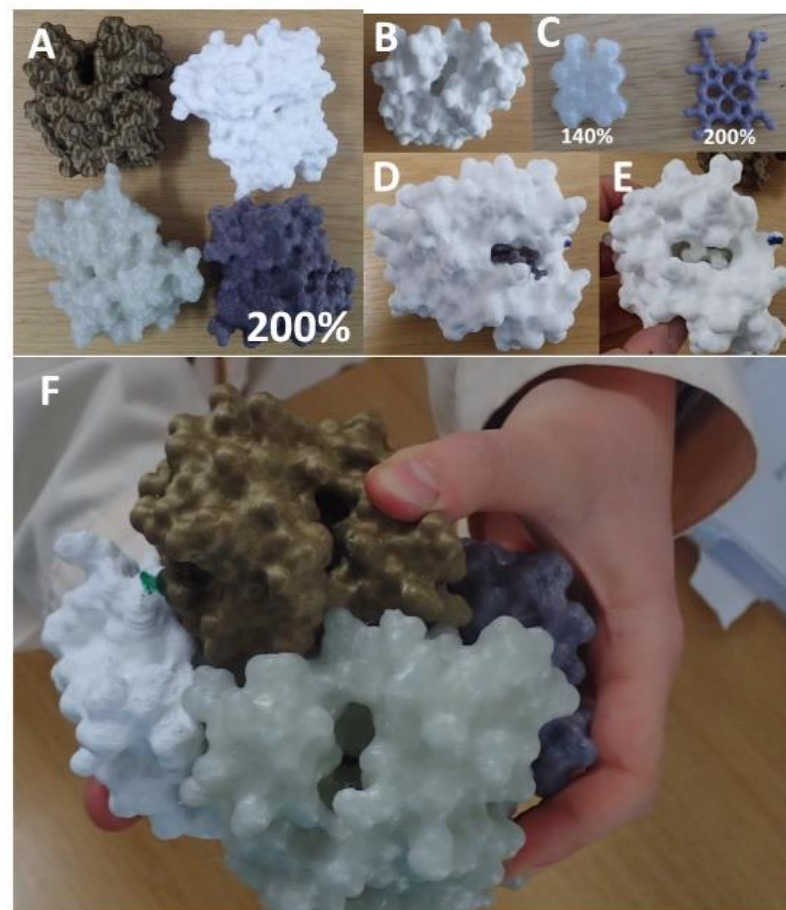
<https://3dprint.nih.gov/discover/3dpx-014894>

Printed scale and physical model



## Quaternary structure of human deoxyhemoglobin

Printed scale and physical models

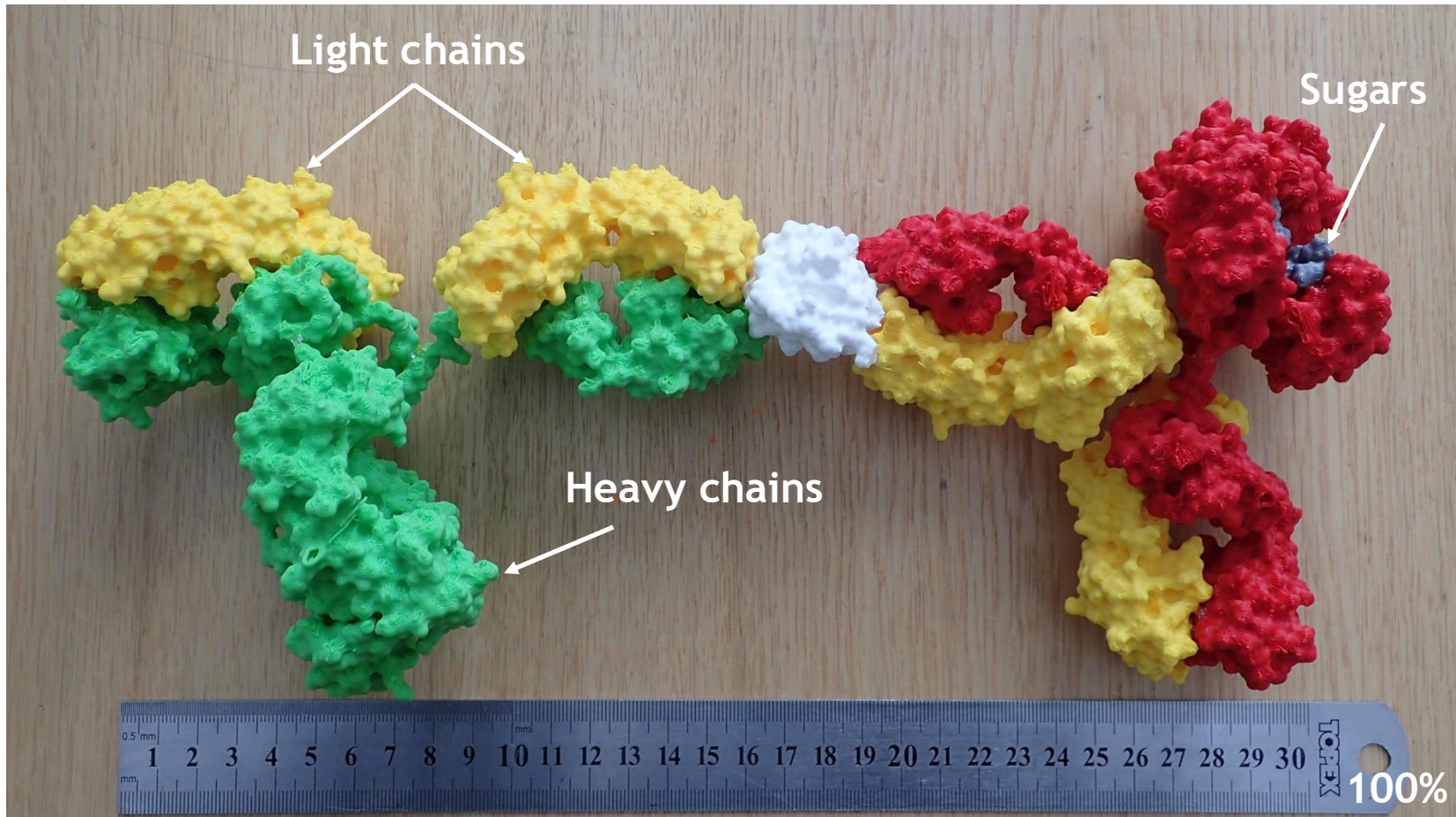


<https://3dprint.nih.gov/discover/3dpx-014895>





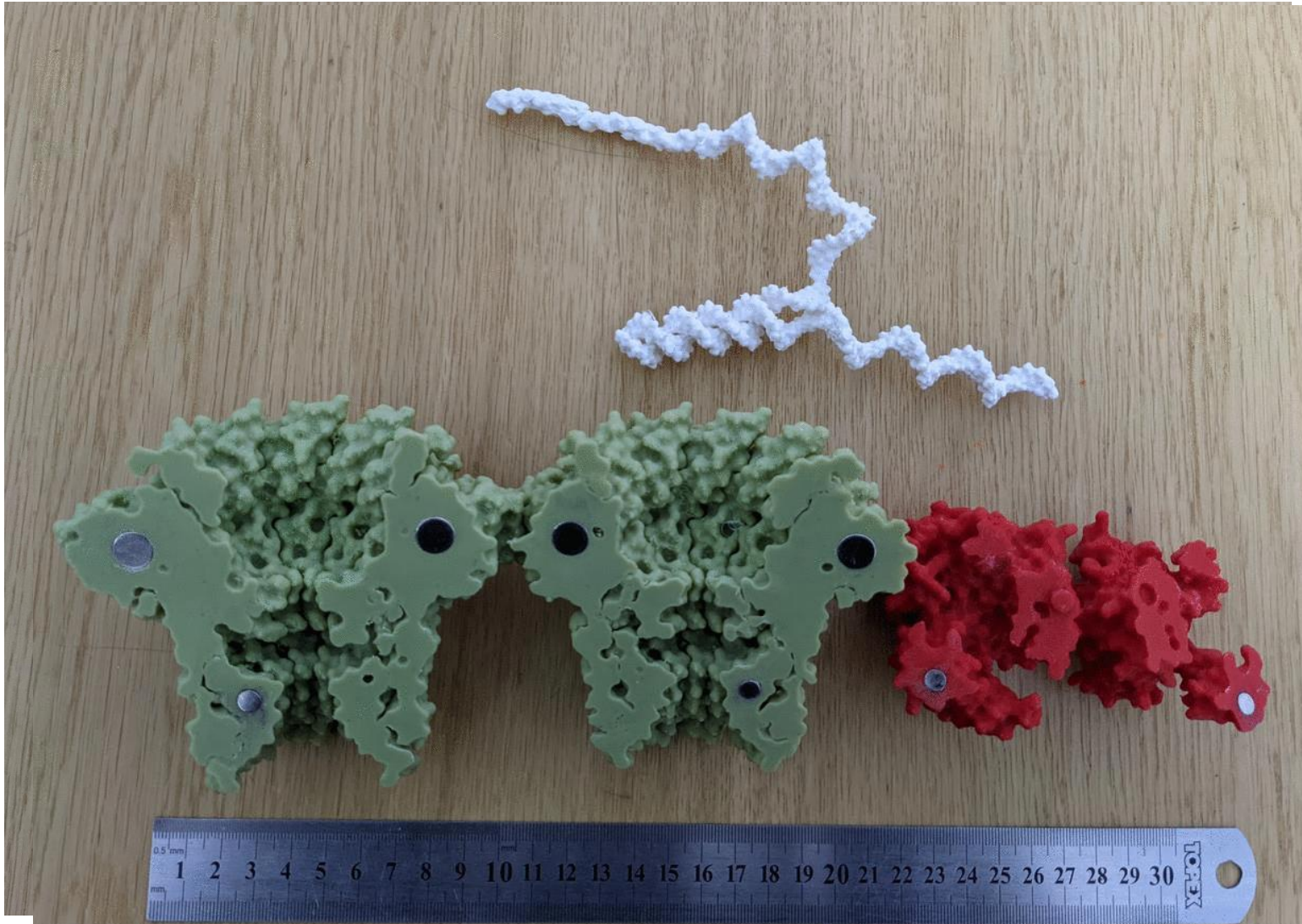
## Antibodies interacting with an antigen (lysozyme)



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



## A protein nanopore sequencing DNA

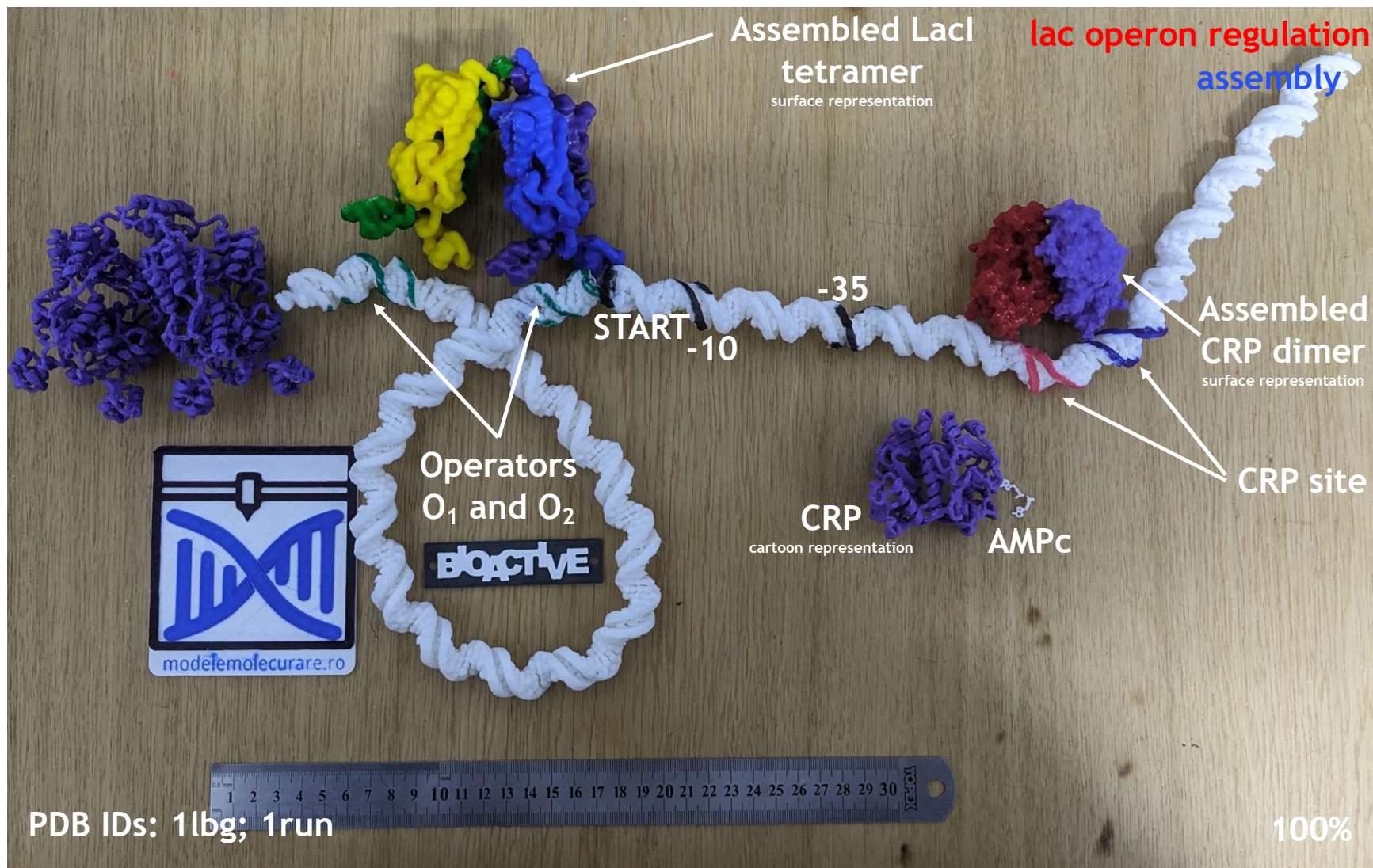




# Examples of printed models currently used for teaching



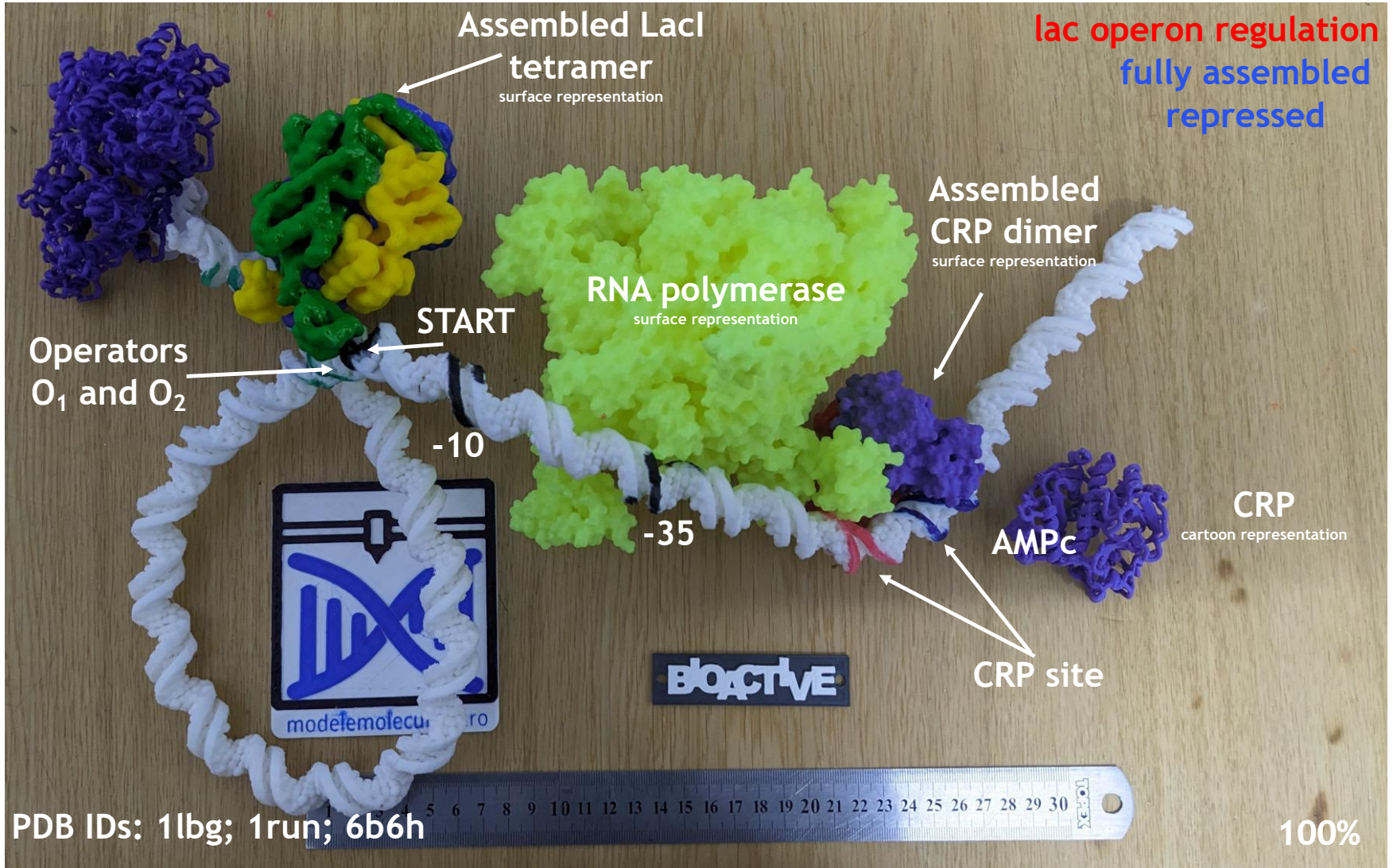
## Physical model for teaching lac operon regulation







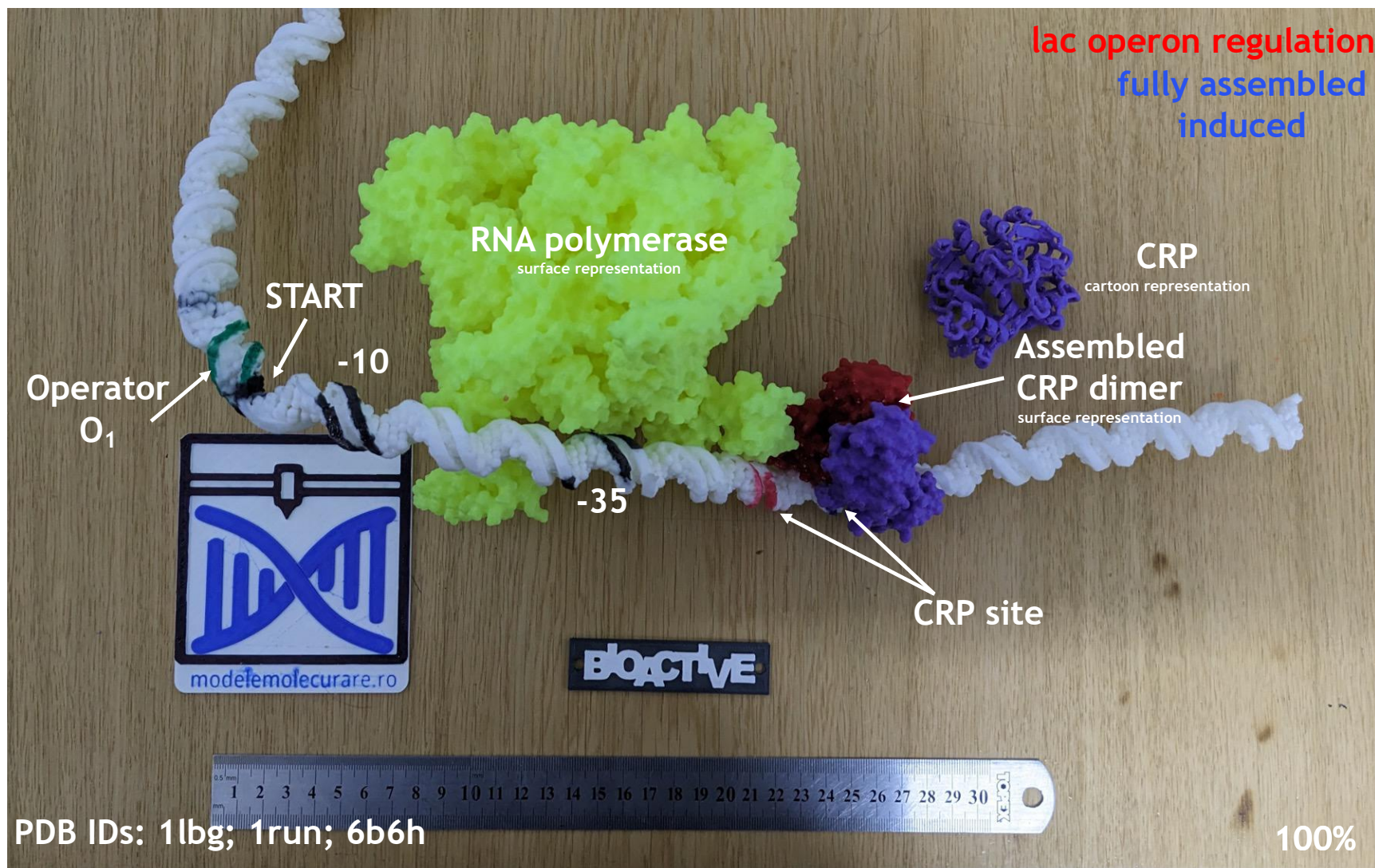
## Physical model for teaching lac operon regulation







## Physical model for teaching lac operon regulation





# Alternative ways of using the models for teaching



## Asking students to paint the models in order to recognize different structures



# 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

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

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.**

# Updates and new printed models



ALEXANDRU IOAN CUZA UNIVERSITY of IAȘI

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## Identification and Characterization of Biological Active Molecules

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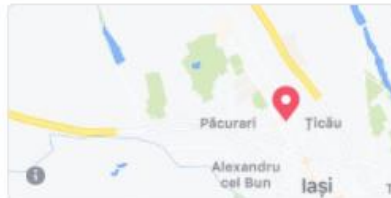
Liked

Message



### About

See All



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

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### PINNED POST



#### 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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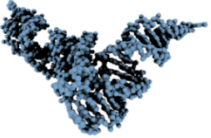
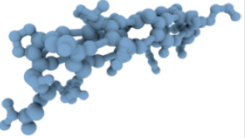
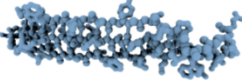
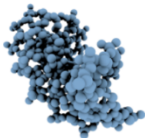
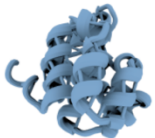




# Most models and instructions on how to print are available under CC BY license



U.S. Department of Health and Human Services — National Institutes of Health

**NIH** NIH 3D Print Exchange

 <p><b>3DPX-014890</b> tRNA in various represent...</p> <p><i>tRNA, teaching</i></p>	 <p><b>3DPX-014891</b> An protein alpha helix in...</p> <p><i>ALFA HELIX, teaching tools</i></p>	 <p><b>3DPX-014892</b> A beta-sheet from a sucro...</p> <p><i>beta-sheet, teaching</i></p>
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Submitted by:  **mariusmihasan**

Tue, 2021-03-09 06:48

Remix It Add New Version I Printed This

Printer Technology/Material  
Polylactic Acid (PLA)

Printer Make/Model  
Creality Ender 5 Pro

Print Units mm

Scale At Given Print Units 100x


Pre- and Postprocessing Instructions

Printed at 0.2 resolution with 2 wall lines and 5% infill. Extensive supports are required but were rather easy to remove. Models are really fragile in the hinge region broke during handling, but were easy to glue back together.

DOWNLOAD

RATING  
Average: 5 (2 votes)

LICENSING  
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<https://3dprint.nih.gov/users/mariusmihasan/model>