Impact of 3D-printed molecular models on teaching protein and DNA structure

ALEXANDRU IOAN CUZA UNIVERSITY of IAŞI www.uaic.ro

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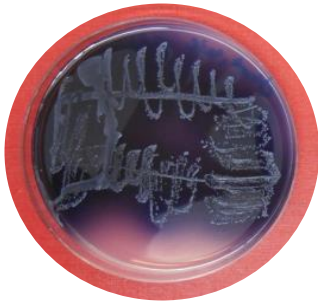
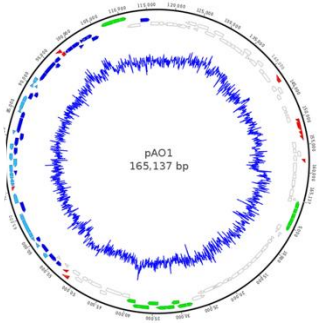
https://3dprint.nih.gov/users/mariusmihasan

A bit about us and our work in Iași

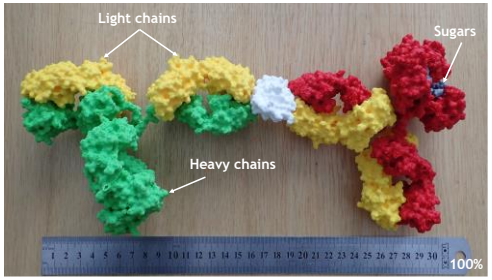
Main research subjects:

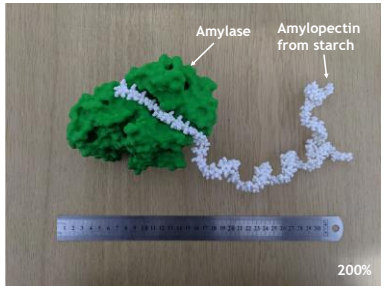
- molecular biology of pAO1 megaplasmid related to nicotine catabolism, stress induced by nicotine degradation and biotechnological applications..



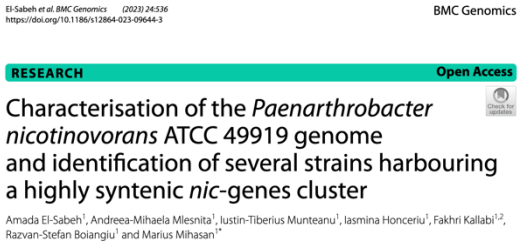


- using 3D printing for creating teaching materials to support molecular bioscience education.





Latest paper:


El-Sabeh et al. BMC Genomics (2023) 24:536
https://doi.org/10.1186/s12864-023-09644-3

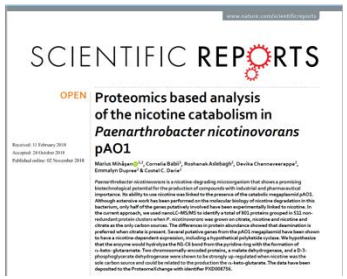
BMC Genomics

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[1], Andreea-Mihaela Mlesnita[1], Iustin-Tiberius Munteanu[1], Iasmina Honceriu[1], Fakhri Kallabi[1,2], Razvan-Stefan Boiangiu[1] and Marius Mihasan[1*]

Most Important paper:


SCIENTIFIC REPORTS

OPEN

Proteomics based analysis of the nicotine catabolism in *Paenarthrobacter nicotinovorans* pAO1

Marius Mihasan, Cornelia Babii, Roshanak Aslebagh, Devika Channaveerappa, Emmalyn Dupree & Costel C. Darie

Developed educational resources: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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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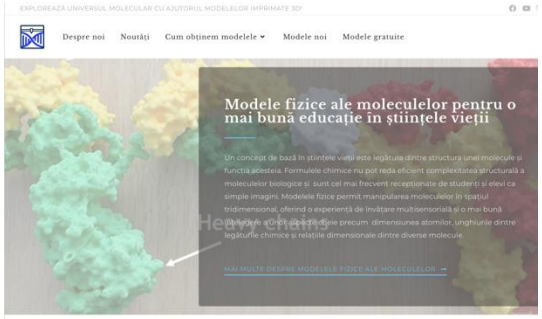
Abstract

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



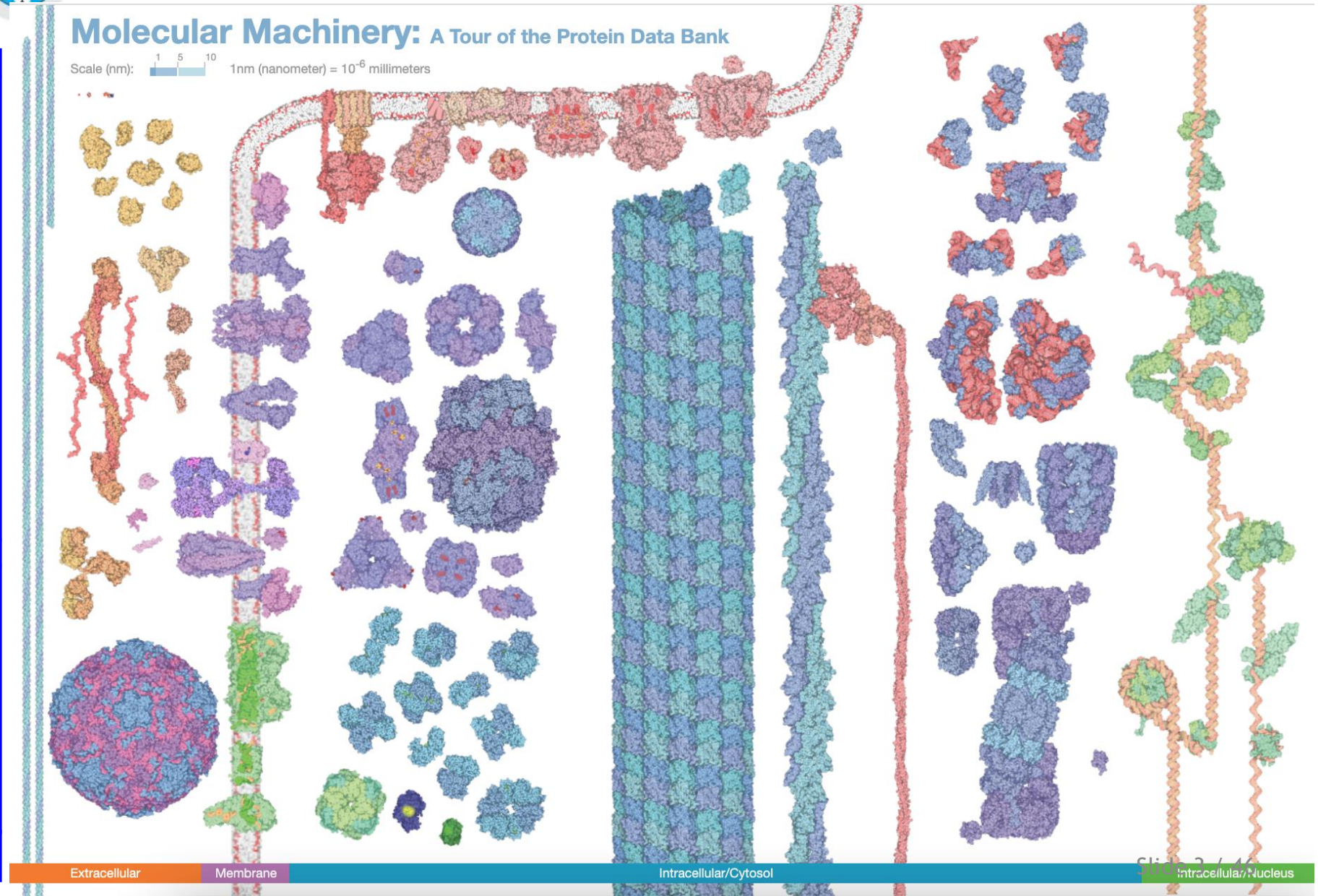
https://www.nature.com/articles/s41598-018-34687-y

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

https://modelemoleculare.ro/

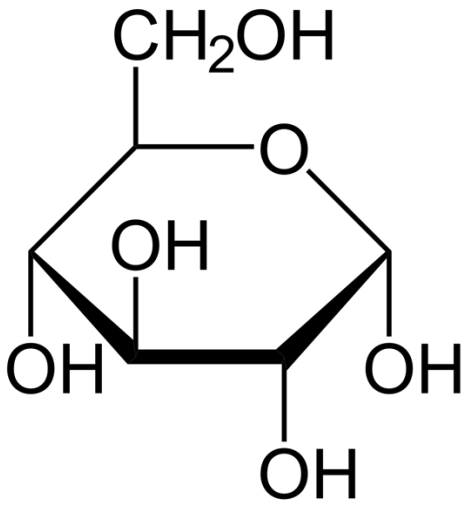
https://bmcgenomics.biomedcentral.com/articles/10.1186/s12864-023-09644-3

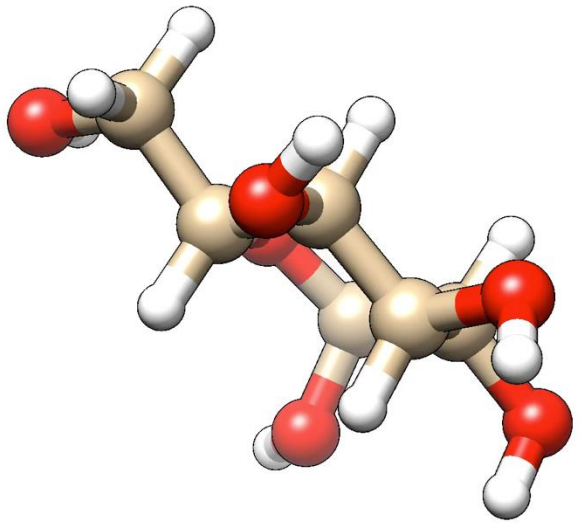
Understanding Life Sciences relies on understanding Structural Biology



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

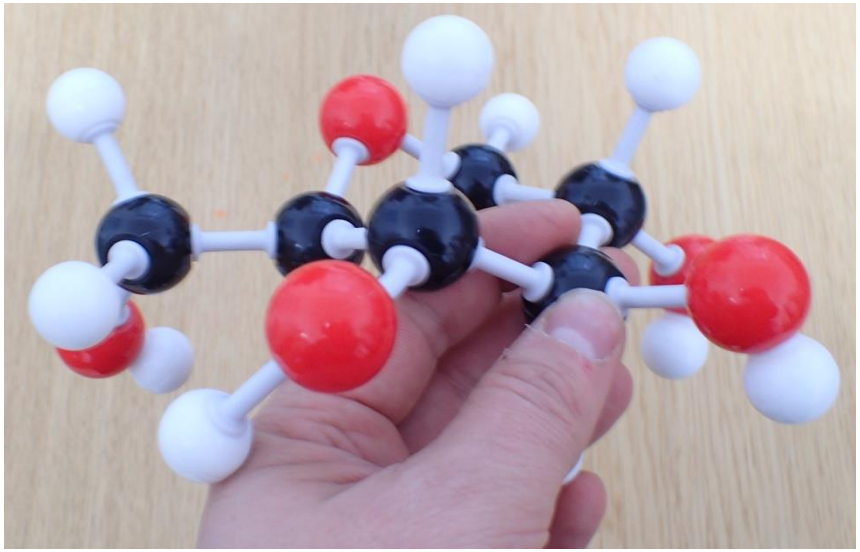
Teaching Chemistry and Biochemistry relies on structural formulae





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

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

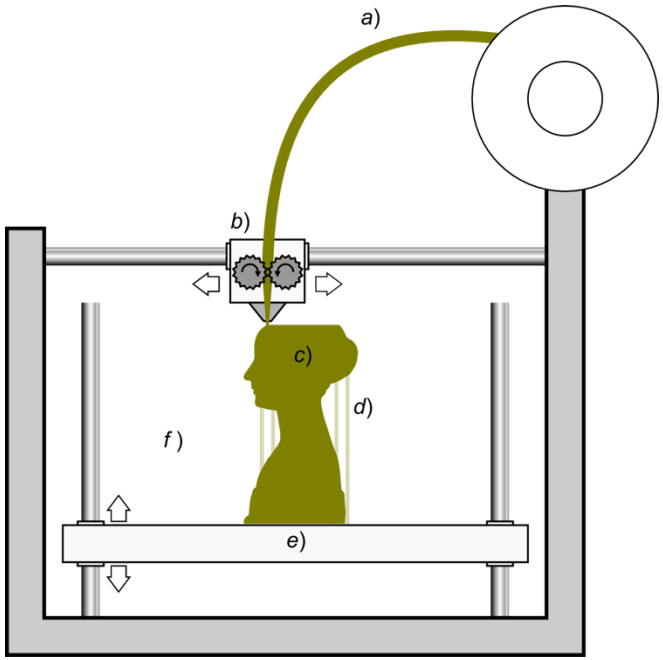
molecular visualization software
Chimera, PyMol

3D printing can do that

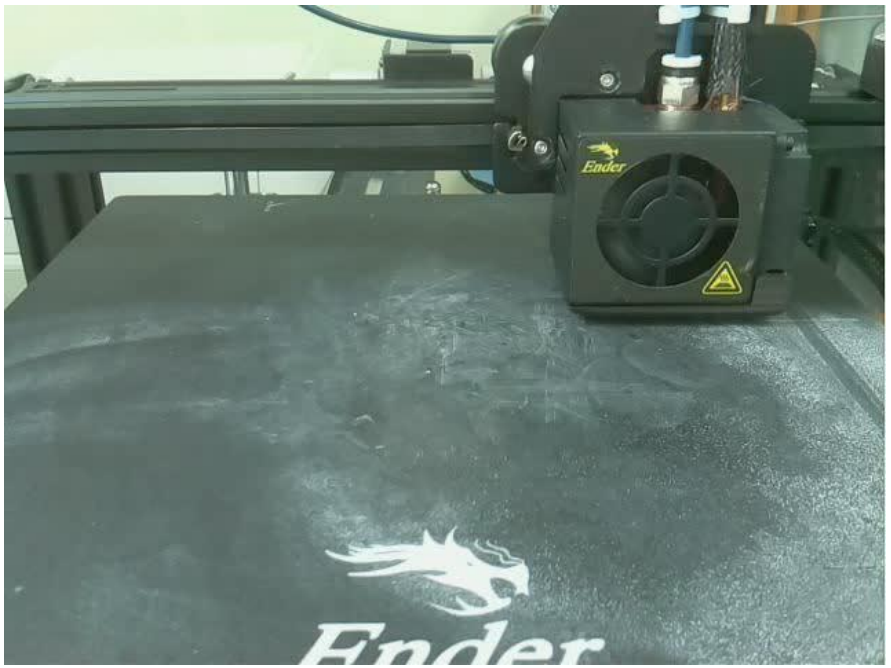
What is 3D printing?

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



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 Chimera

STL file

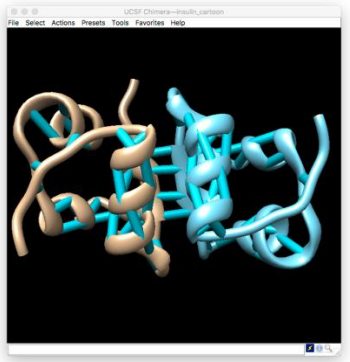
Prepare the file for printing using

Ultimaker Cura

GCODE file

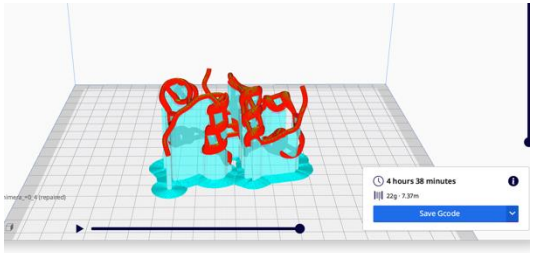
Print

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.

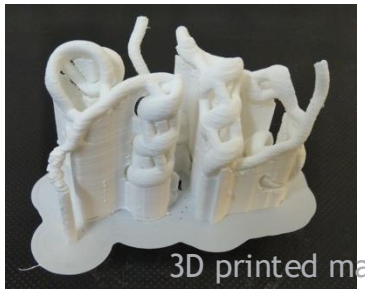


A. Generate the computer model

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



3D printed macromolecular models

Support material removal

C. Clean up and finalize the physical model

Others guides and more details are available

jove Journal of Visualized Experiments www.jove.com

Video Article

3D Printing of Biomolecular Models for Research and Pedagogy

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

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

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

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

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

Date Published: 3/13/2017

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

JOURNAL OF CHEMICAL EDUCATION Communication pubs.acs.org/jchemeduc

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

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

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

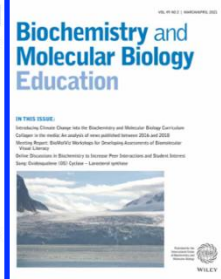
Supporting Information

JOURNAL OF CHEMICAL EDUCATION Article pubs.acs.org/jchemeduc

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

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

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



Biochemistry and Molecular Biology Education

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

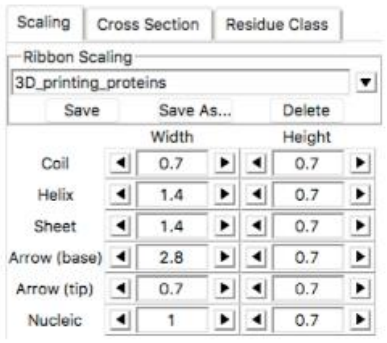
Marius Mihasan

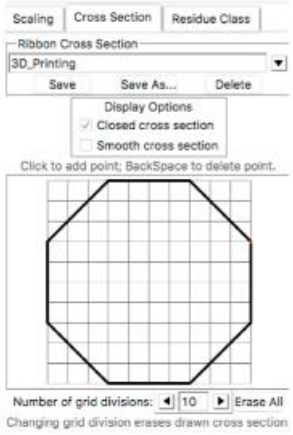
First published: 23 March 2021 | https://doi.org/10.1002/bmb.21493

Examples of printed models currently used for teaching

Secondary structure of lysozyme

Relevant Chimera model depiction settings*



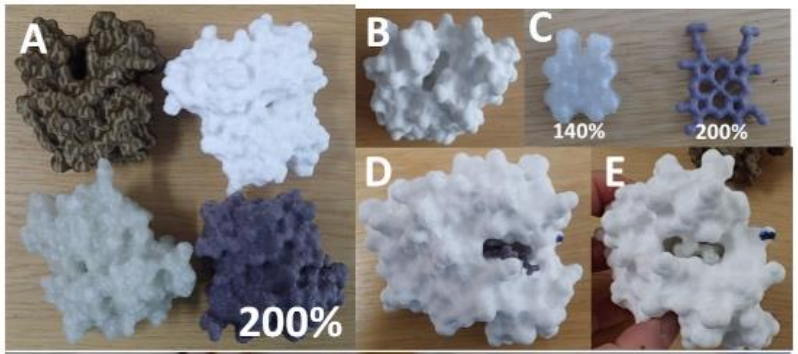


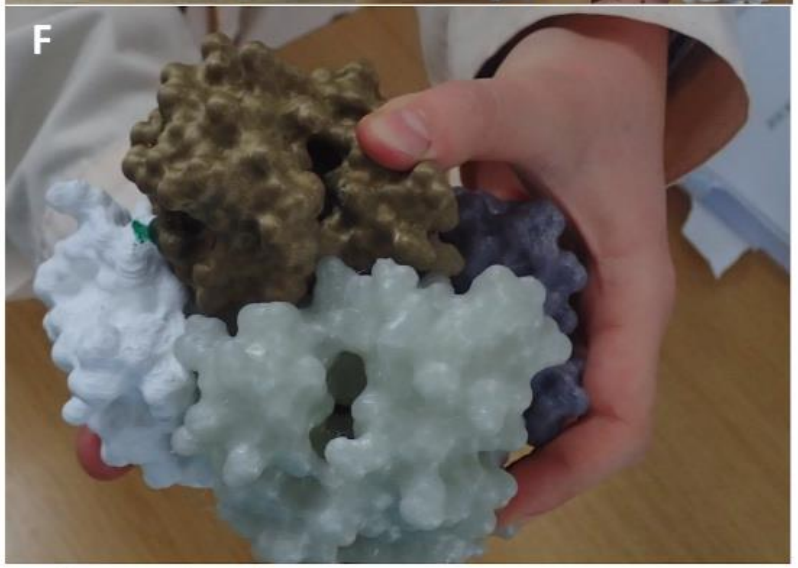
https://3dprint.nih.gov/discover/3dpx-014894

Printed scale and physical model

Quaternary structure of human deoxyhemoglobin

Printed scale and physical models

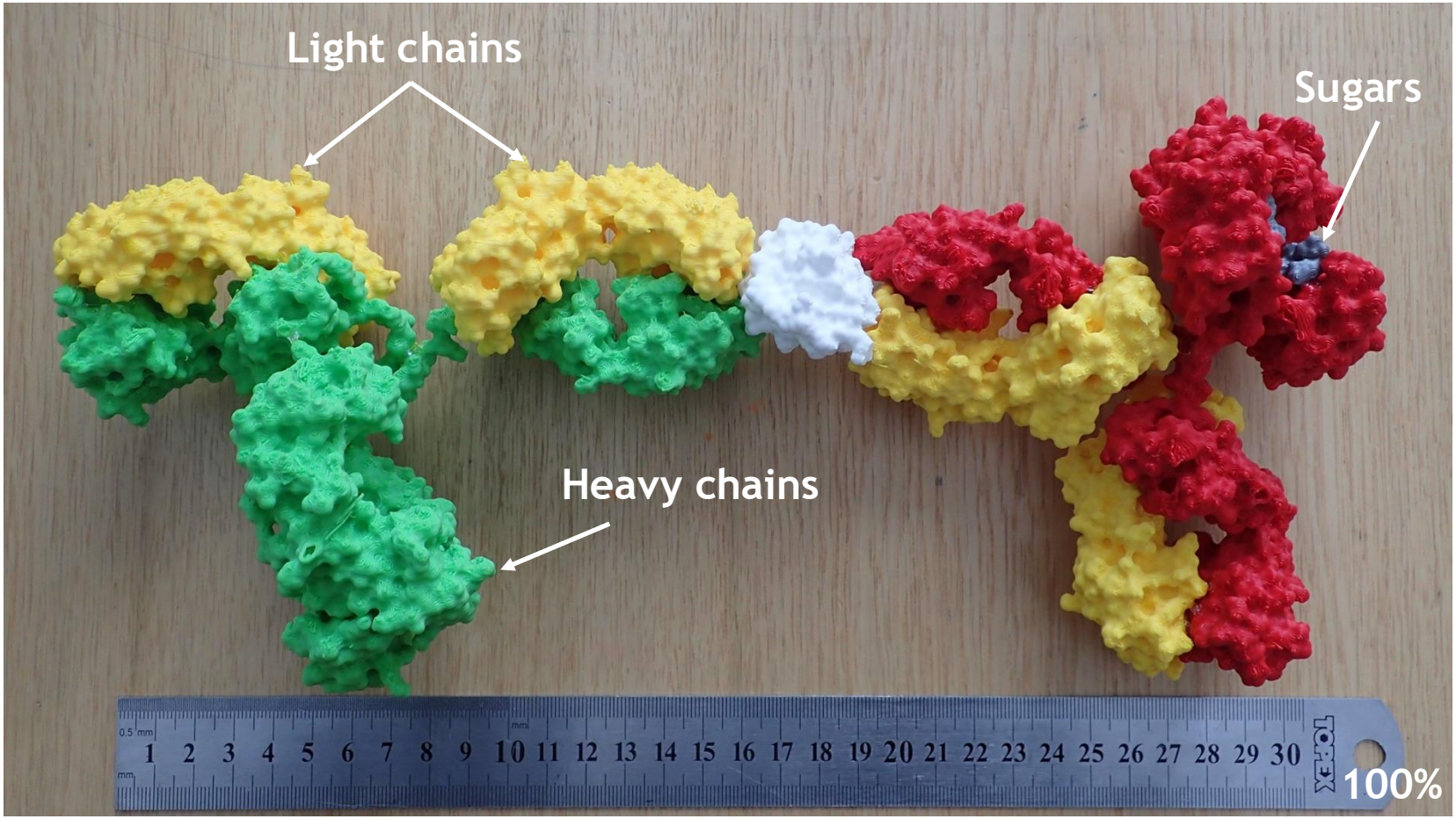




https://3dprint.nih.gov/discover/3dpx-014895

Examples of printed models currently used for teaching

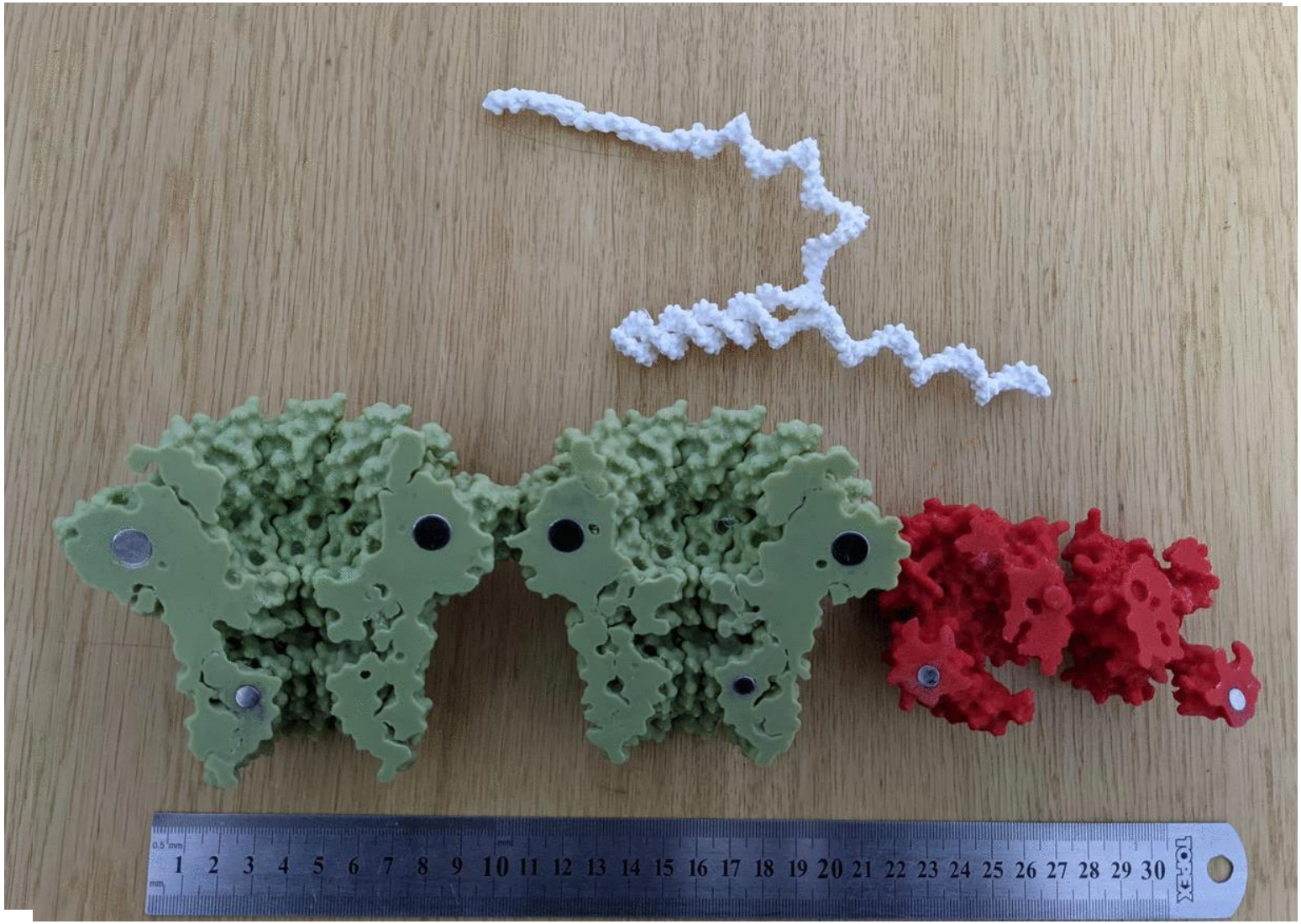
Antibodies interacting with an antigen (lysozyme)



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

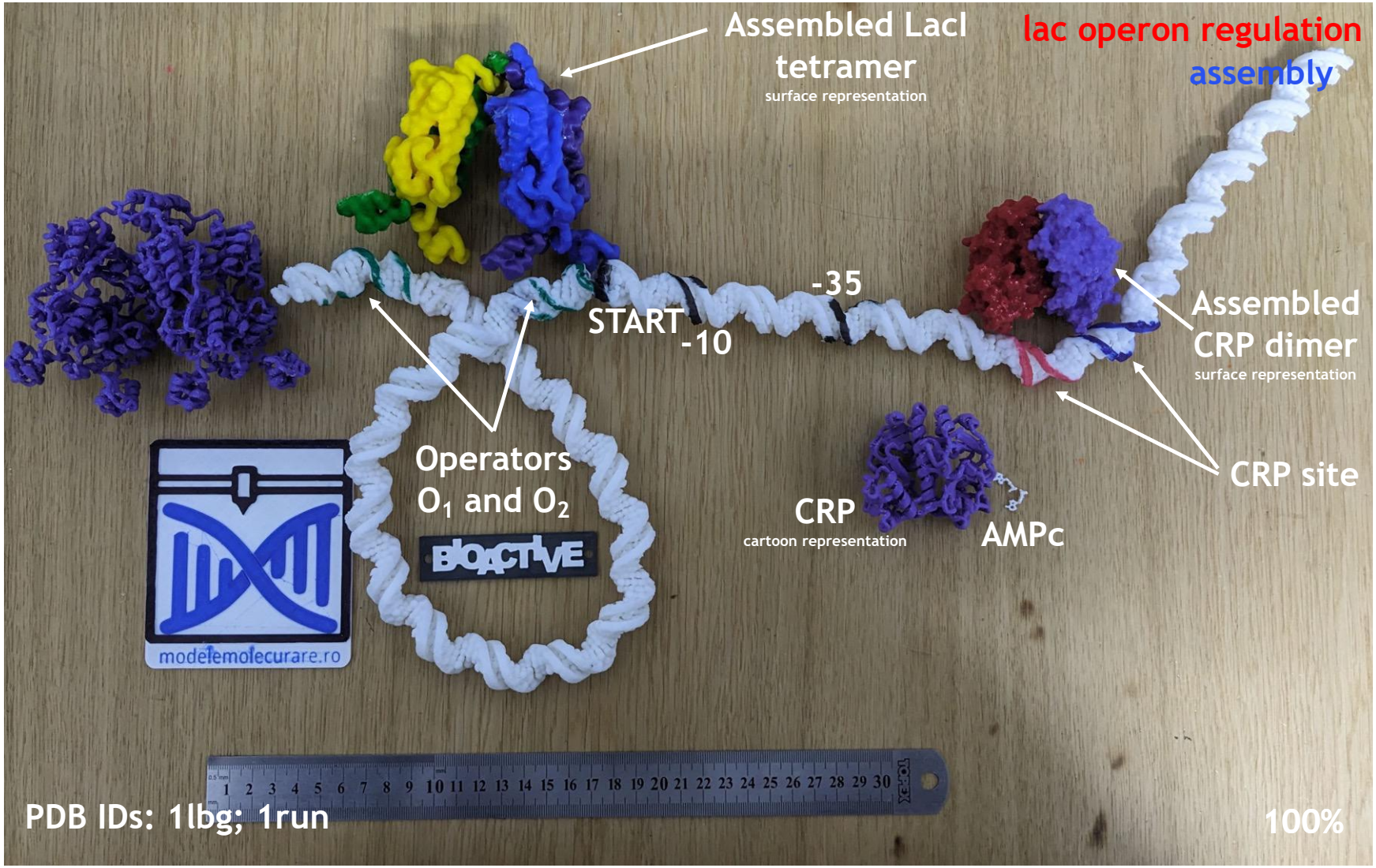
Examples of printed models currently used for teaching

A protein nanopore sequencing DNA



Examples of printed models currently used for teaching

Physical model for teaching lac operon regulation



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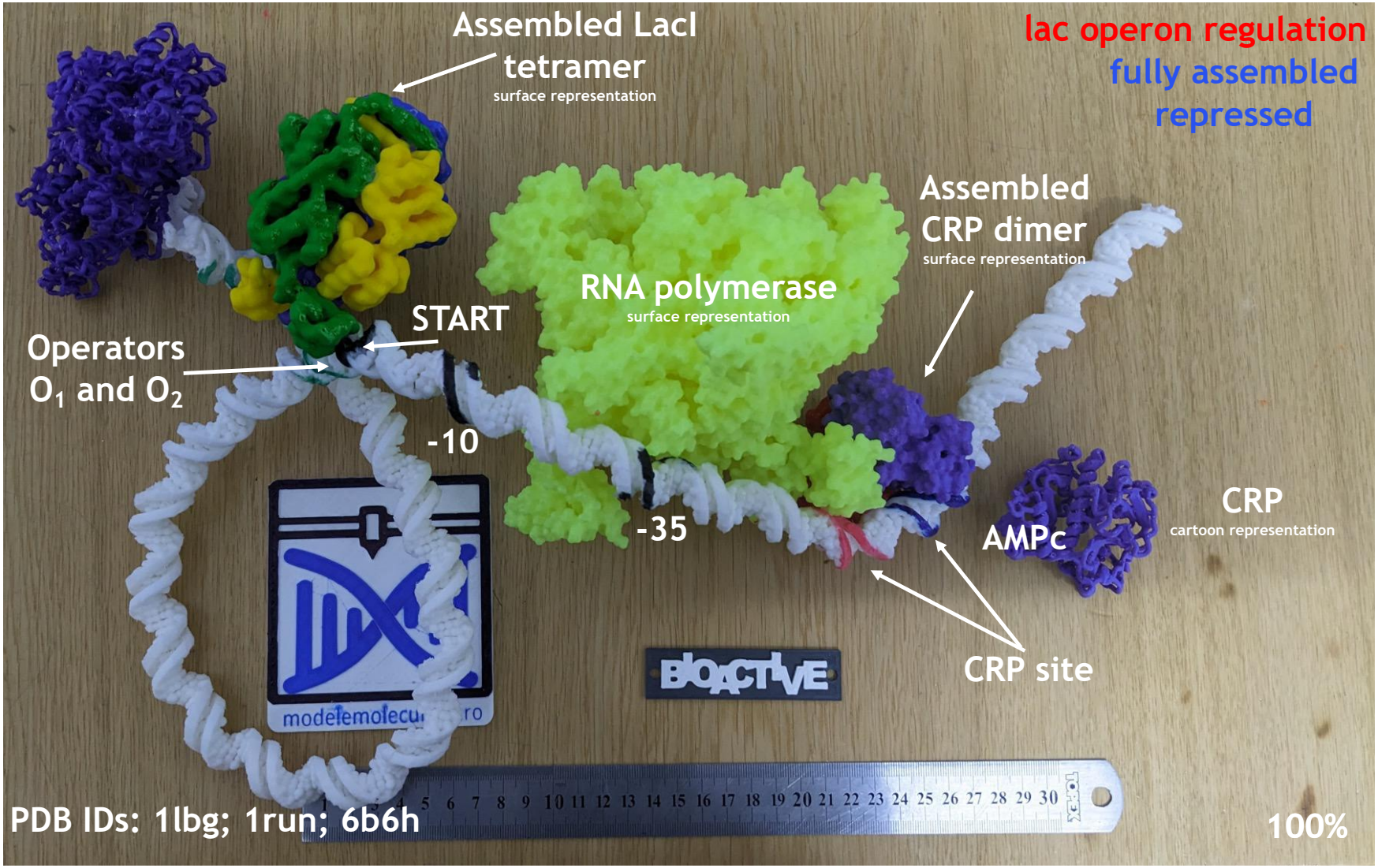
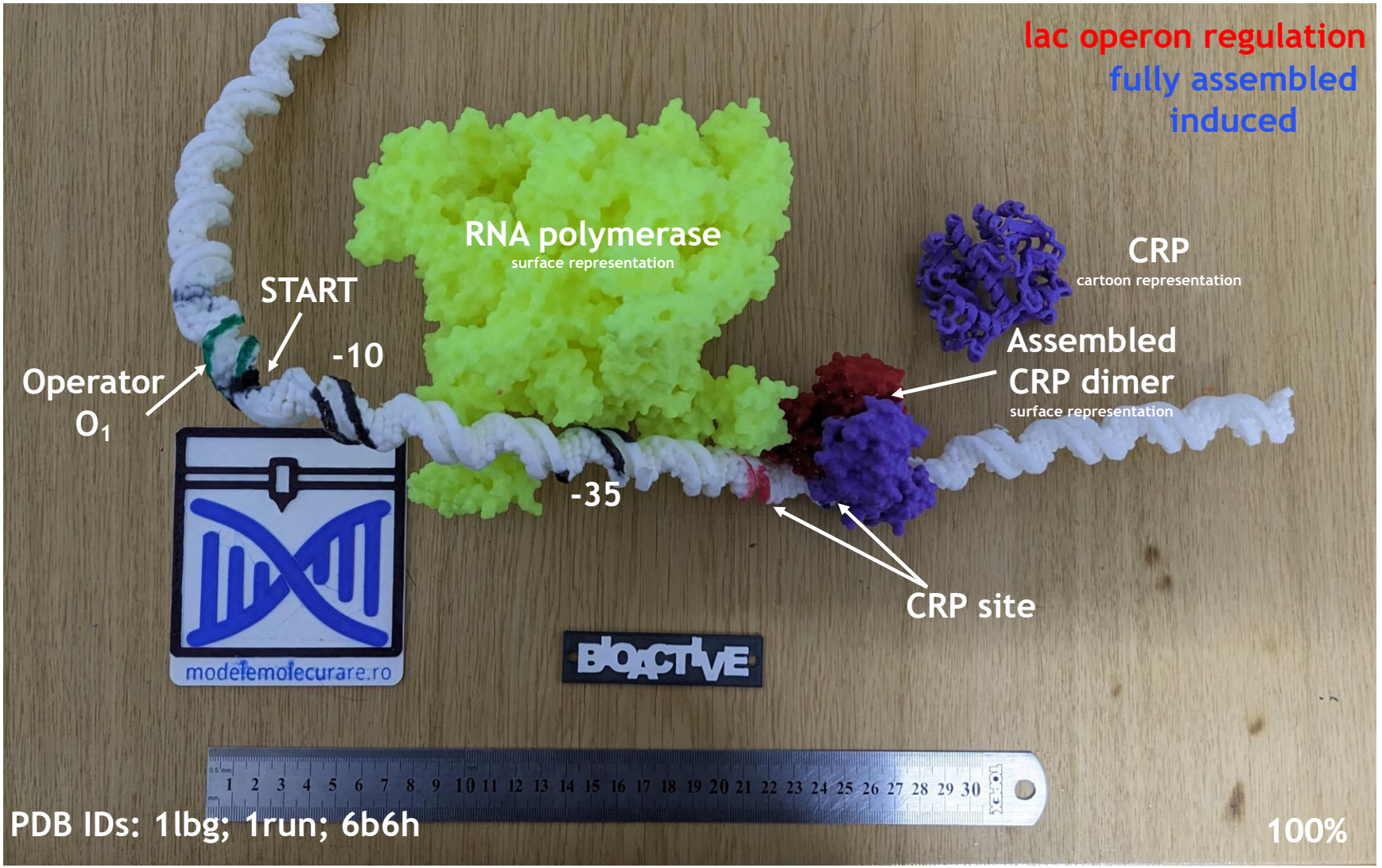


Examples of printed models currently used for teaching

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

But are these models efficient?

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.

But are these models efficient?

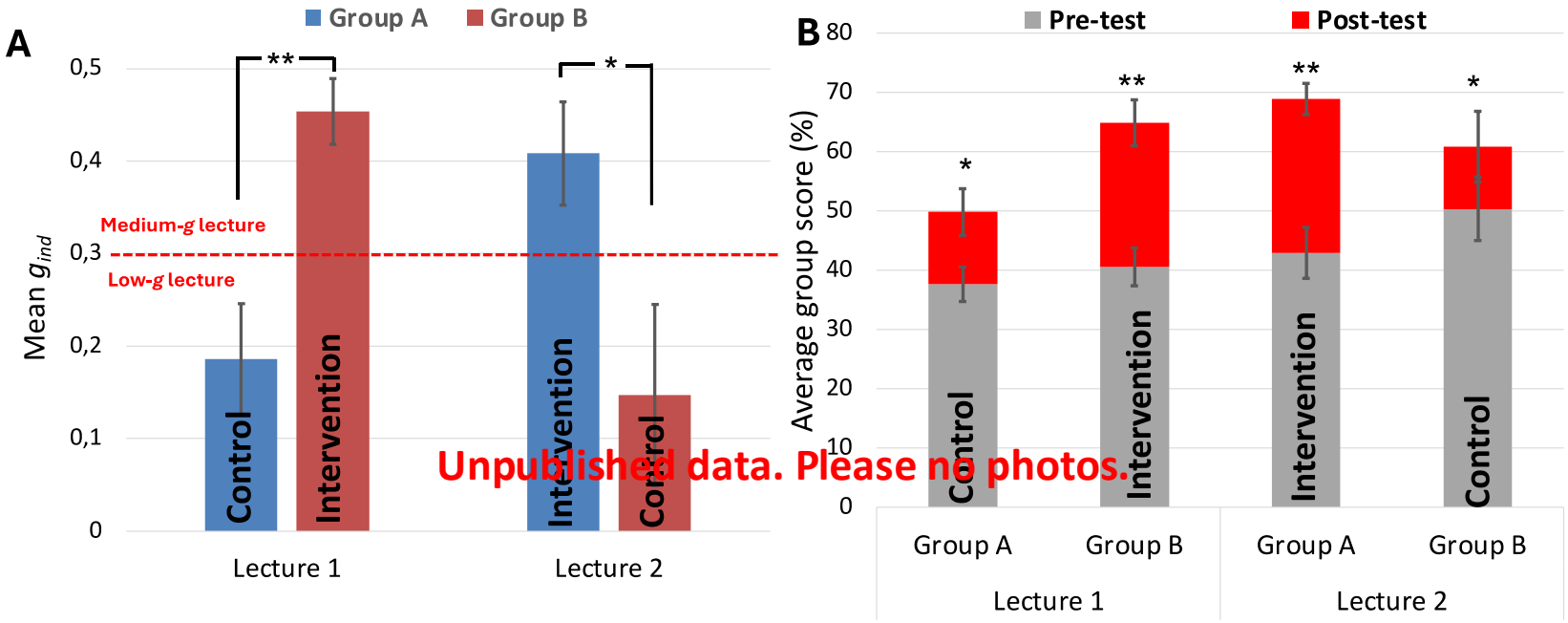
A compensatory research study

	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	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.

Results

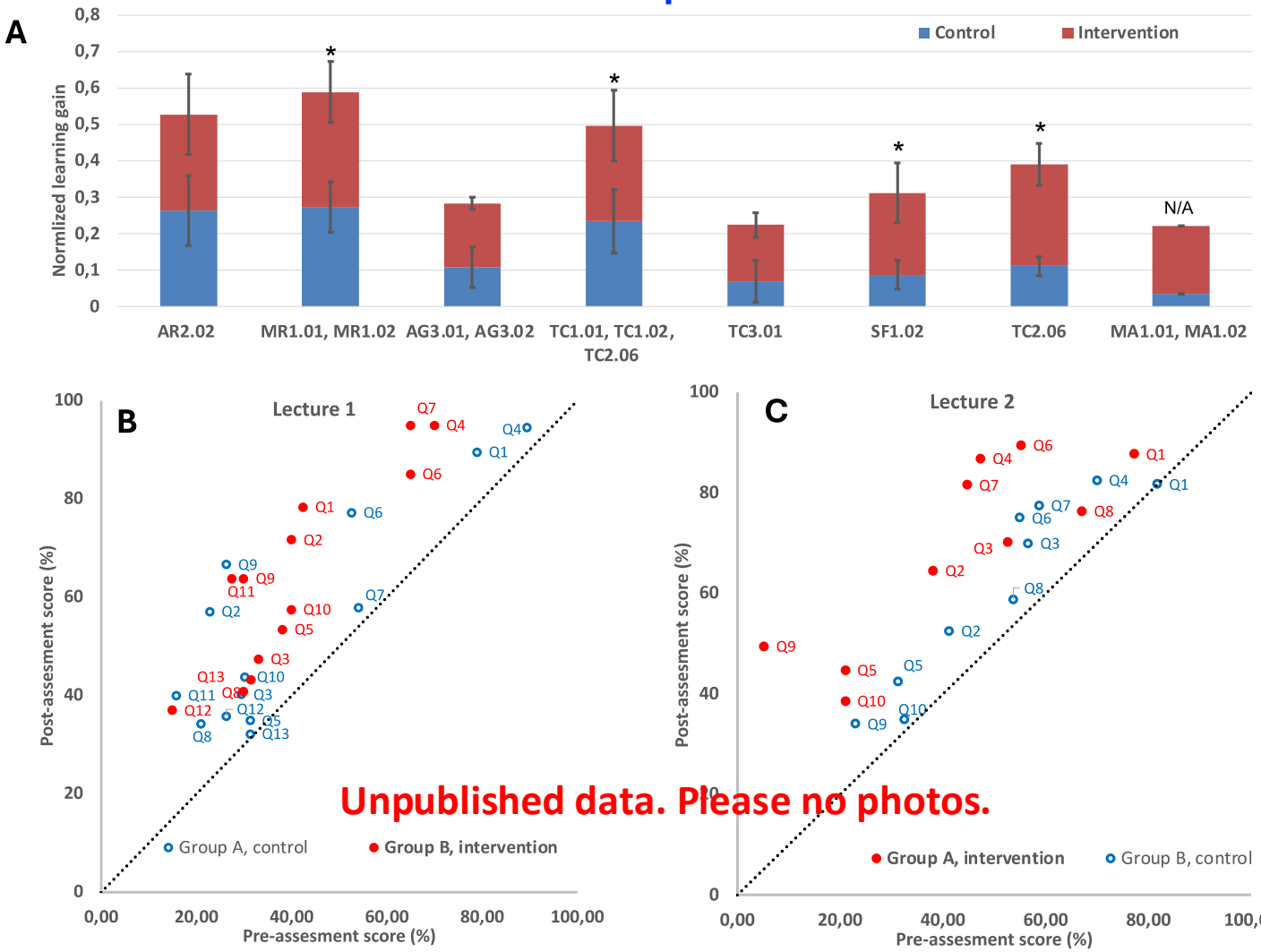
Individual learning gain



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

Results

Individual questions

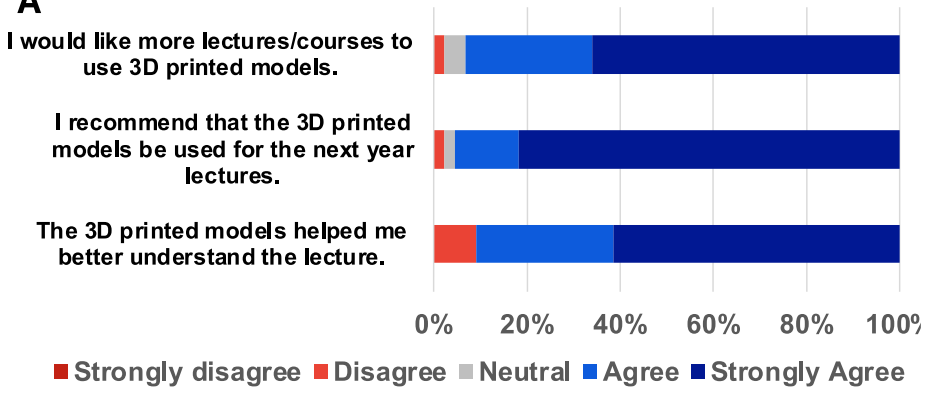


Unpublished data. Please no photos.

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

Free-form assessment

A



B

Unpublished data. Please no photos.

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

"The 3D models were **verry 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**".

Summary

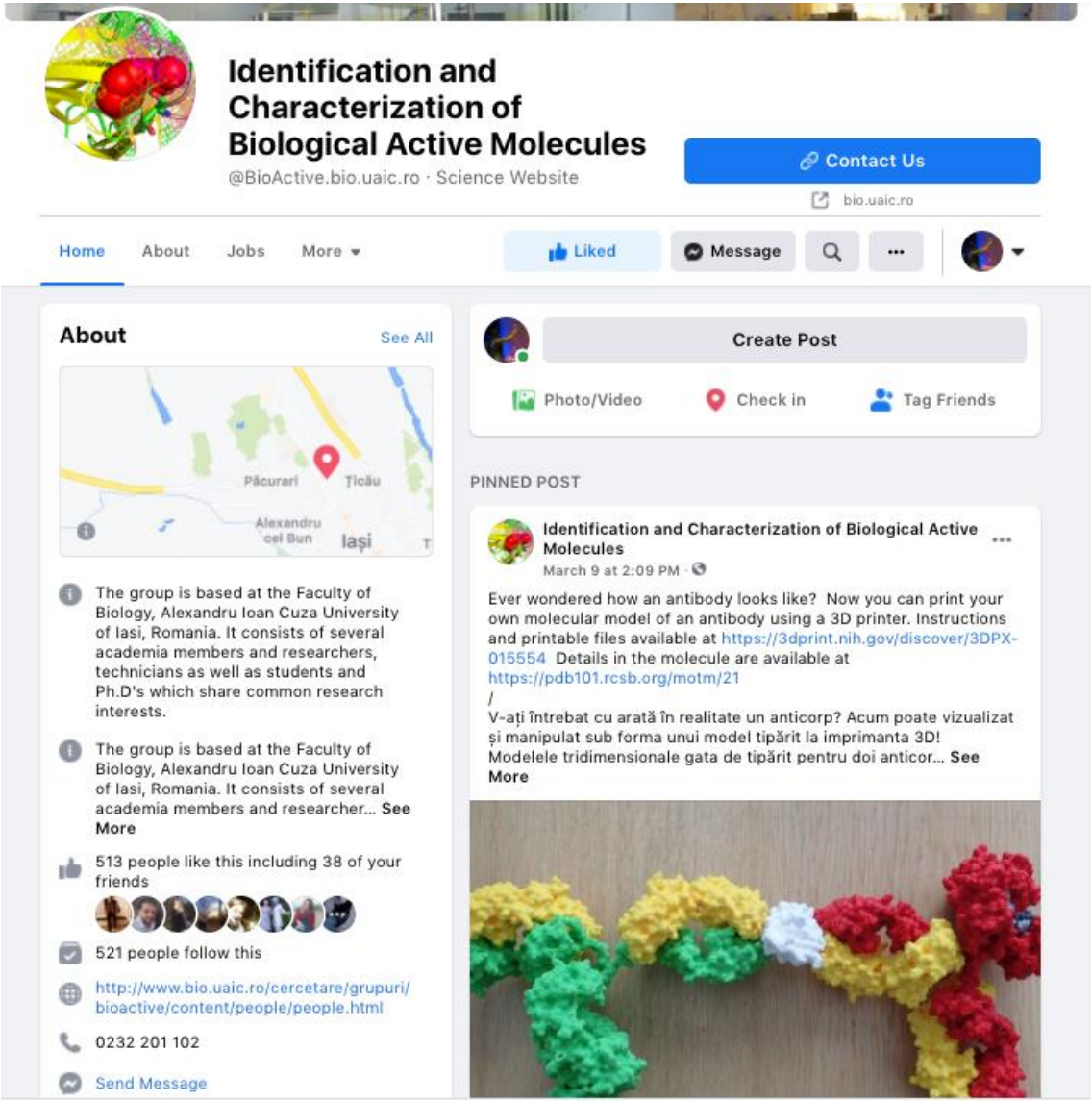
Usage of physical models of (macro)molecules improves learning outcomes, but need to be tailored to teachers needs

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



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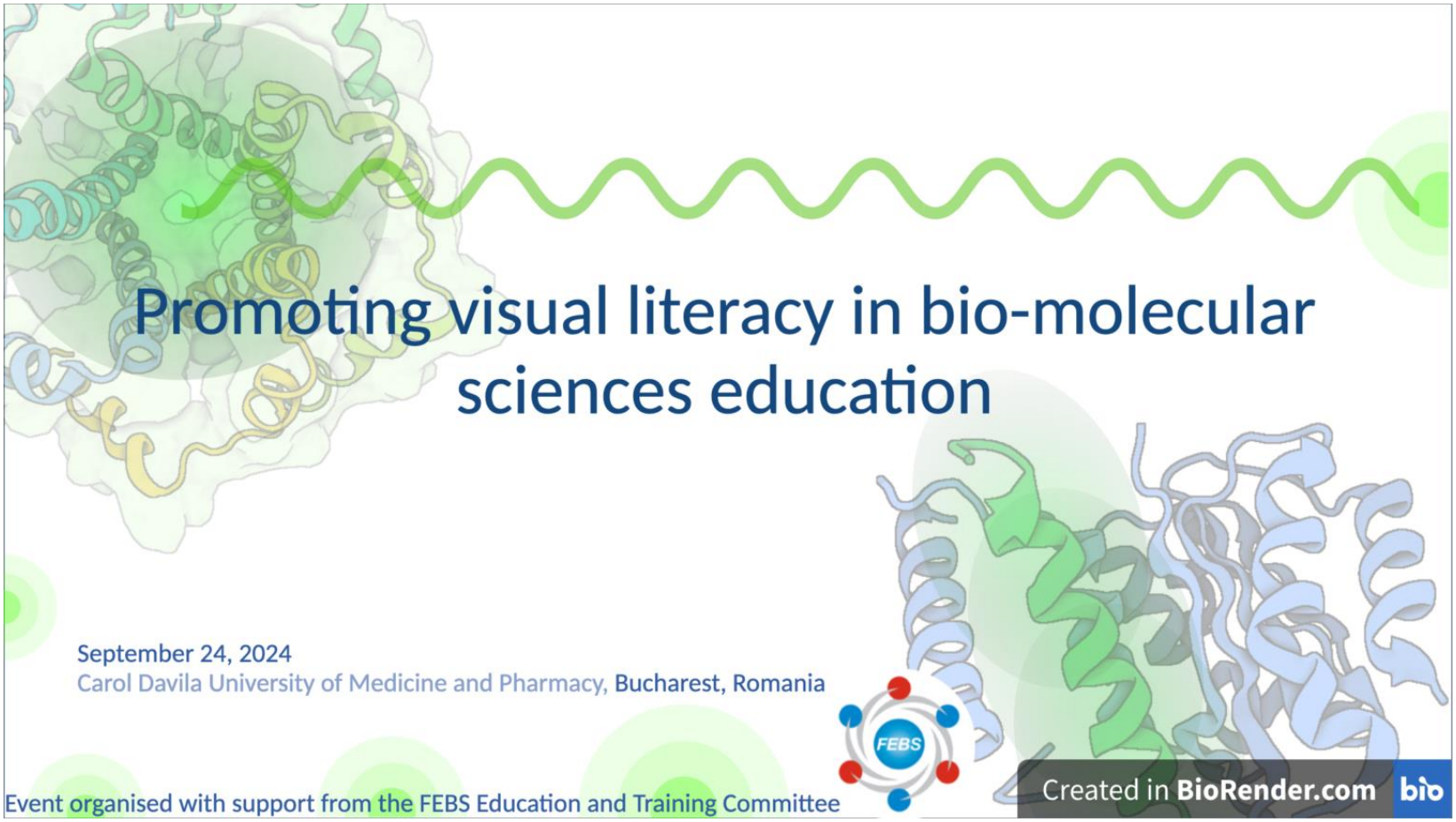
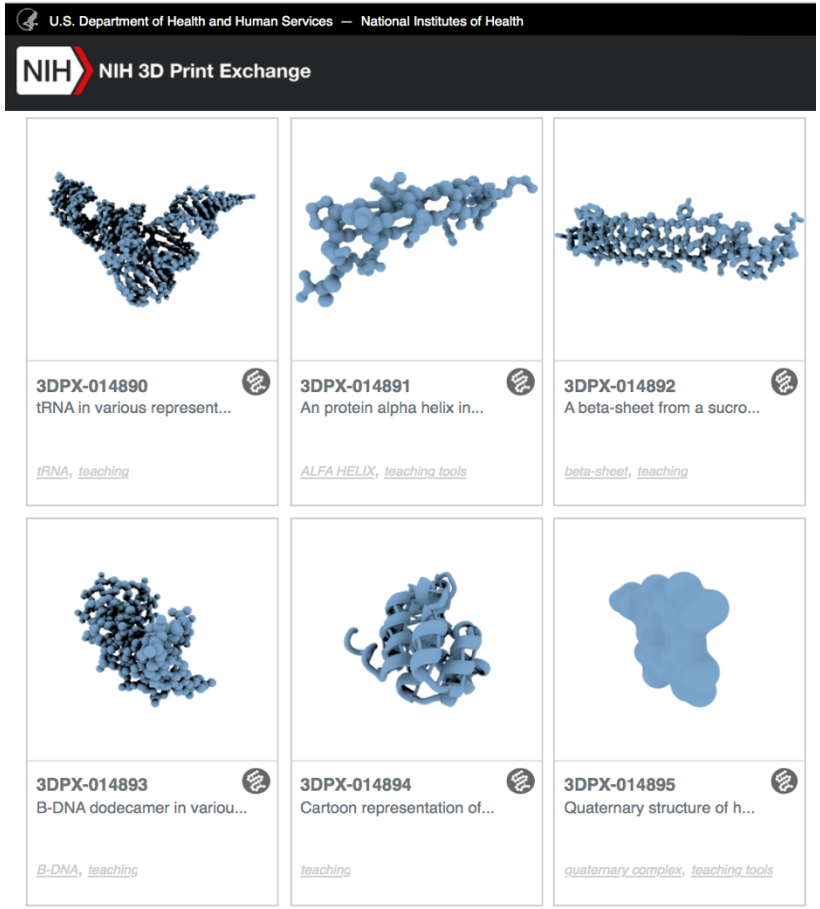
Event coming soon. Few places still available.

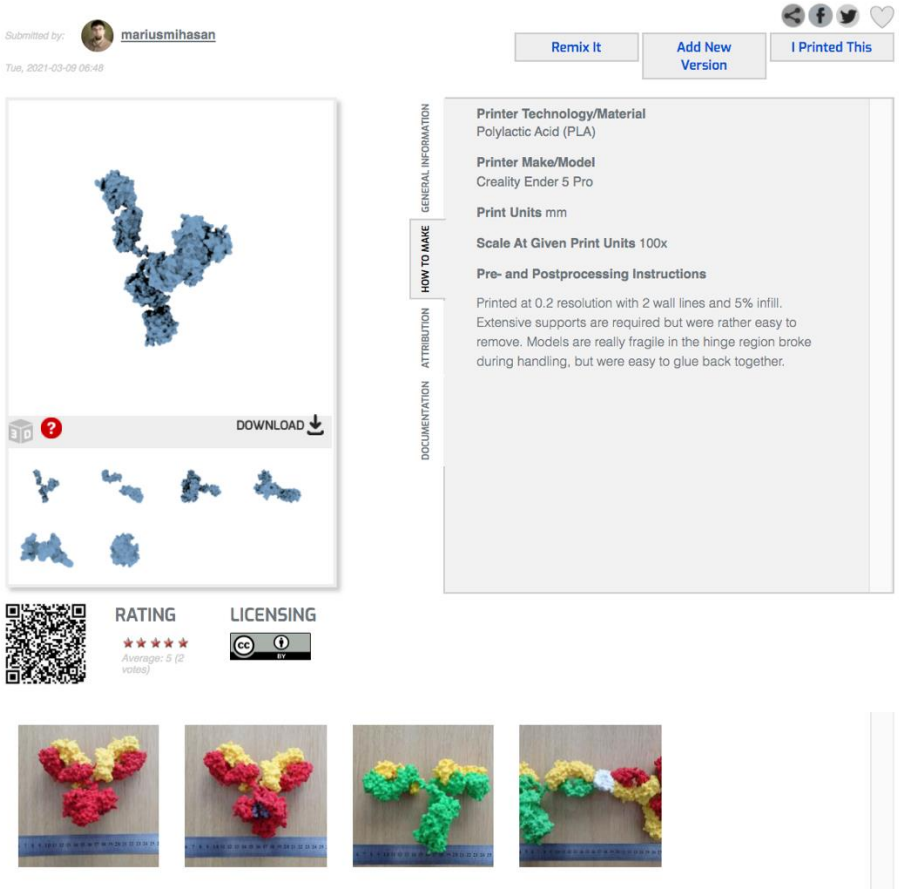


https://srbbm.biochim.ro/event/promoting-visual-literacy-in-bio-molecular-sciences-education/

In person participation recommended, on-line participation possible
Interested - drop me an e-mail at: marius.mihasan@uaic.ro

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

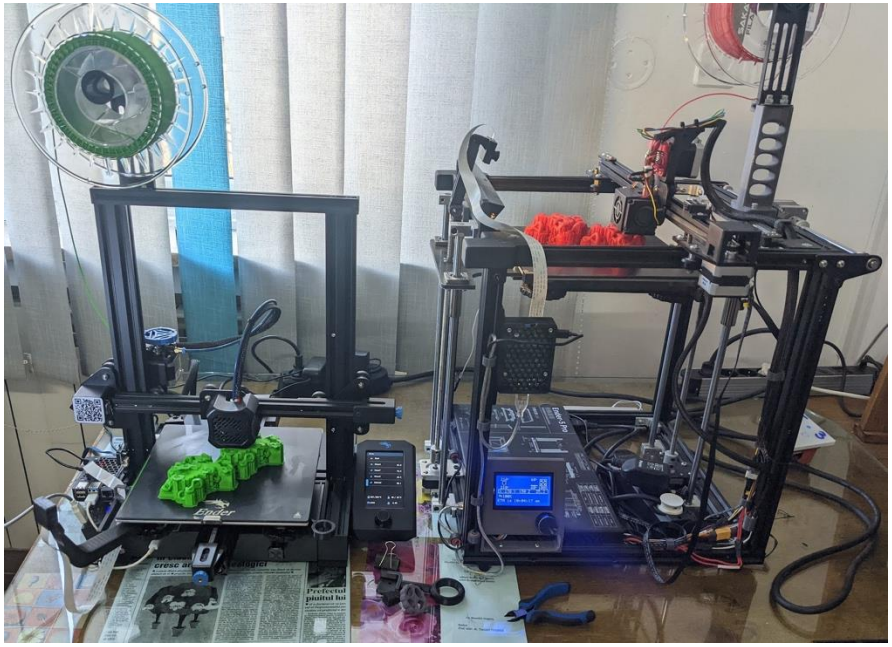




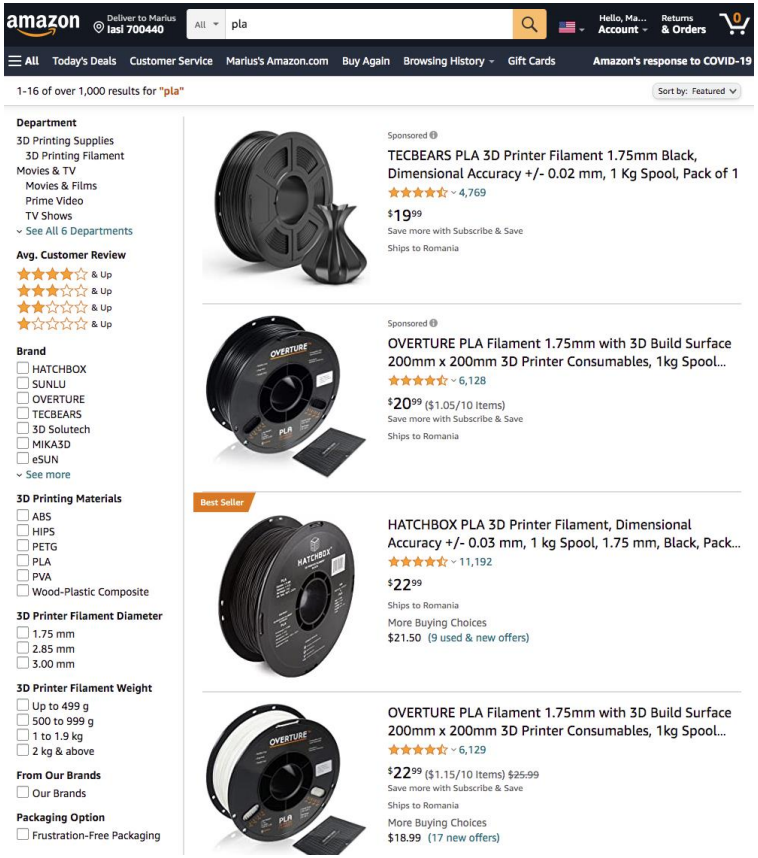
https://3dprint.nih.gov/users/mariusmihasan/model

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