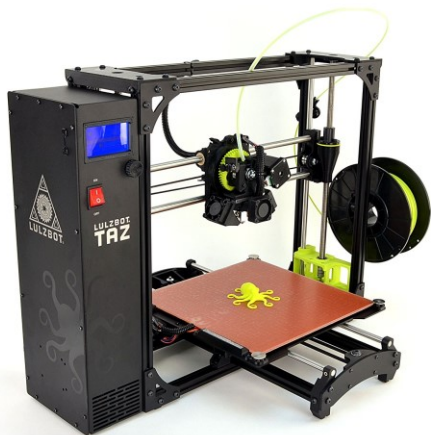




+

6 12.0107 C CARBON	2 4.0026 He HELIUM	74 183.84 M TUNGSTEN	53 126.90 I IODINE	6 12.0107 C CARBON	13 26.982 Al ALUMINIUM
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ENGINEERING

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3D Printing & Arduino in the ChE Classroom:

Protein Structures, Heat Exchangers, and Spectrophotometers

Jacob Elmer & Daniel Kraut

Villanova University

6/25/18

Goals

ChE students may complete several design simulations/projects, but they rarely get a chance to design and build prototypes.

3D Printing & Arduino/Pi make it easy & cheap to build prototypes.

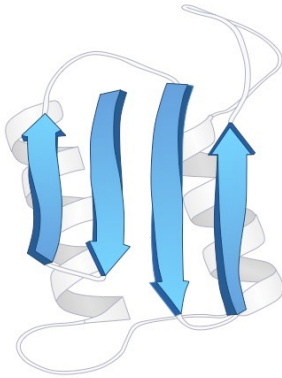
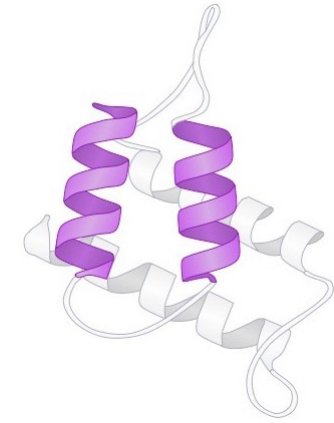
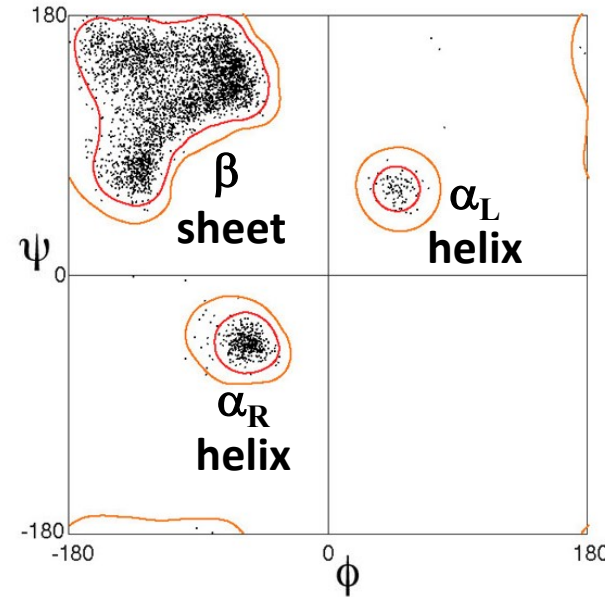
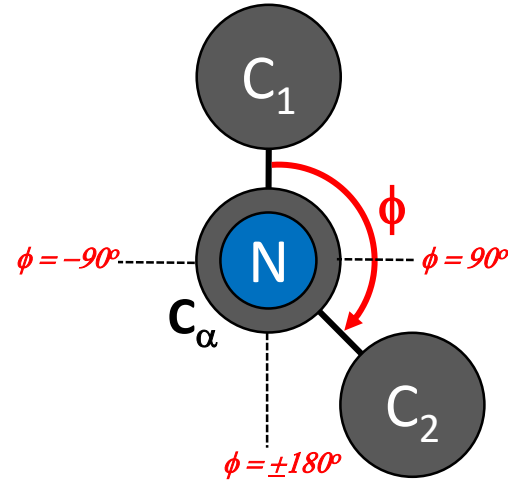
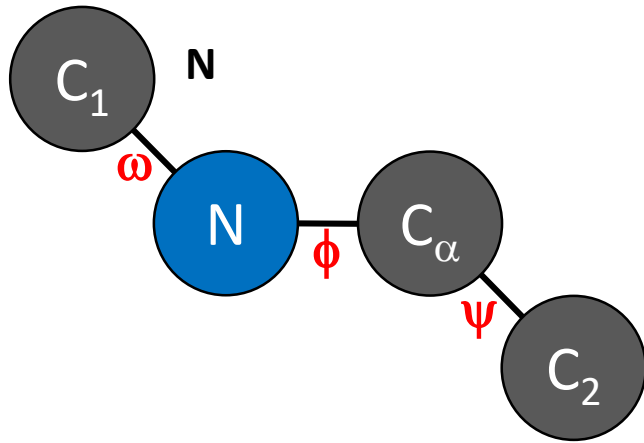
Goal 1: Enhance student learning.

Goal 2: Introduce students to drafting, coding, etc.

Goal 3: Give the students an opportunity to be creative!

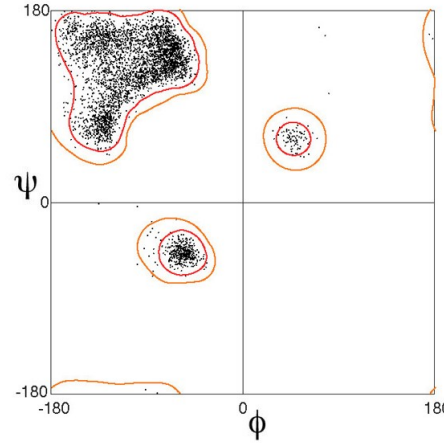
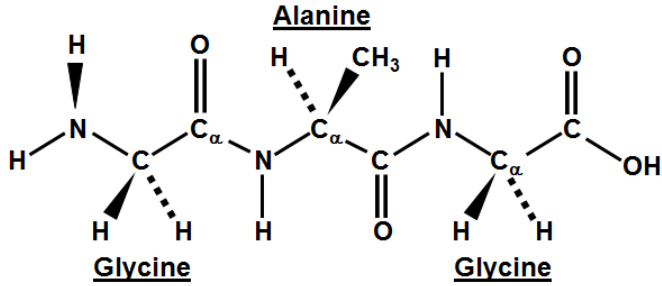
Module 1: Dihedral Angles in Proteins

Students do not need to know CAD or coding for this module - they just play with 3D printed parts!



- The peptide backbone in a protein has 3 unique dihedral angles: ω , ψ , and ϕ
- ω is fixed, but ψ and ϕ can rotate between 0-180°
- Steric hindrance makes some angles more favorable
- Some angles provide unique 2' structures – α helices + β strands

3D Printing Proteins

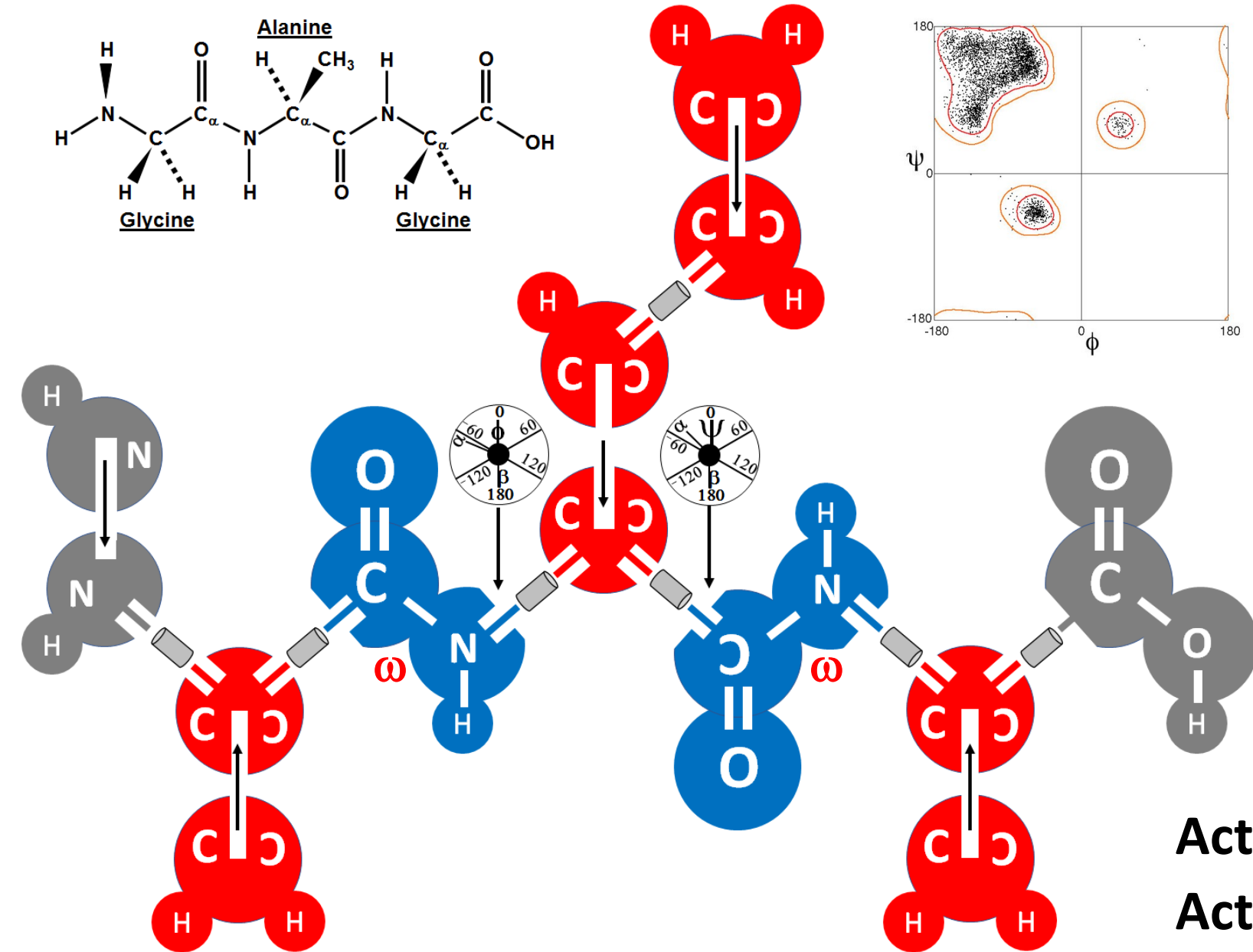


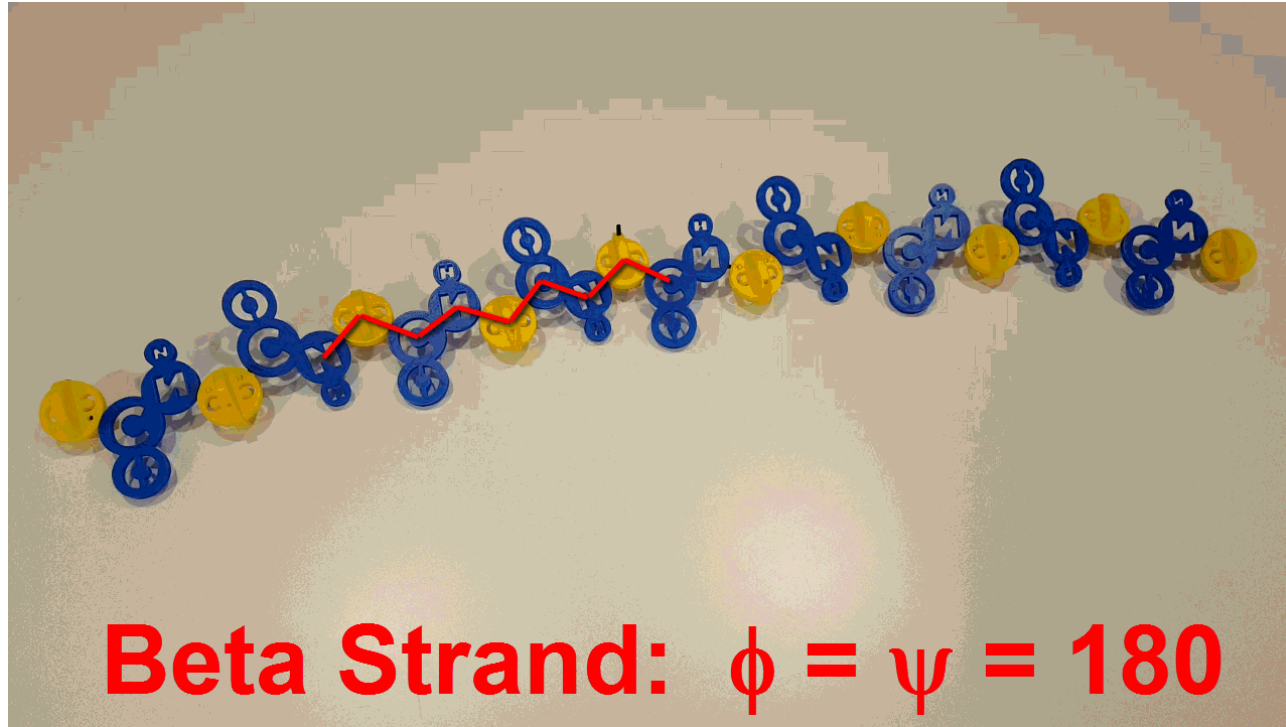
- Tripeptide = Gly-Ala-Gly
- 26 atoms
- 7 unique pieces
- 14 parts
- Parts connected by tubing
- Dials show dihedral angles
- 2 pieces for tetrahedrons
- Peptide bond is planar

Note: Additional side chains can also be included.

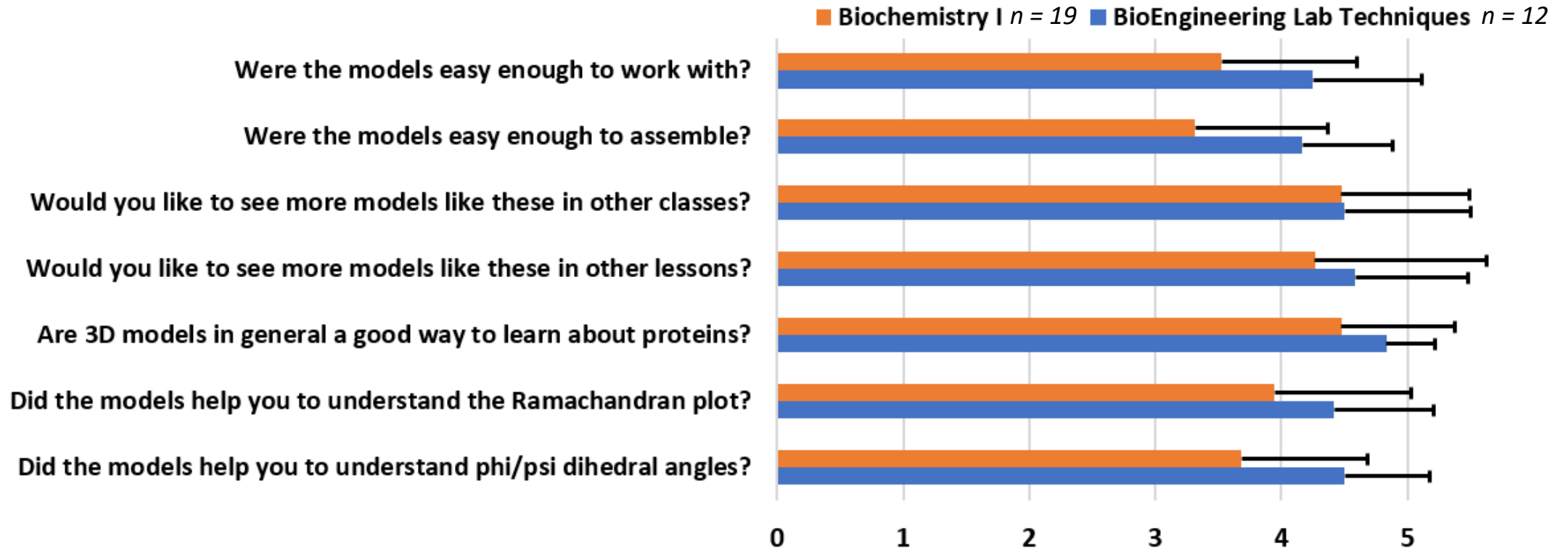
Activity 1: Ramachandran Plot

Activity 2: α helices + β sheets





Student Feedback



Likert scale, 1 = Strongly Disagree/No, 2 = Disagree/No, 3 = Neutral, 4 = Somewhat Agree/Yes 5 = Strongly Agree/Yes

Student Comments:

- Assembly
 - Joints were a little hard to work with, models could be assembled incorrectly
- Timing
 - Need more time for assembly, maybe send a kit home for review?

Module 3: DIY Spectrophotometer (Colorimeter)

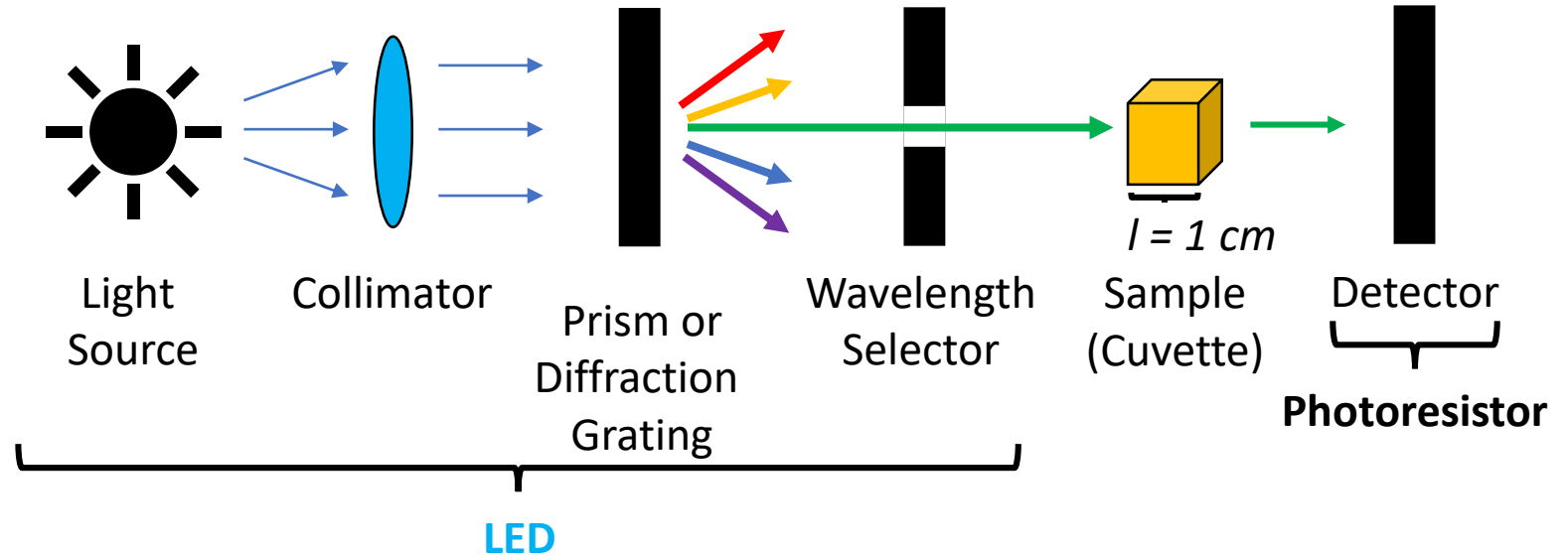
Freshman Interdisciplinary Engineering Design Course (EGR 1200)



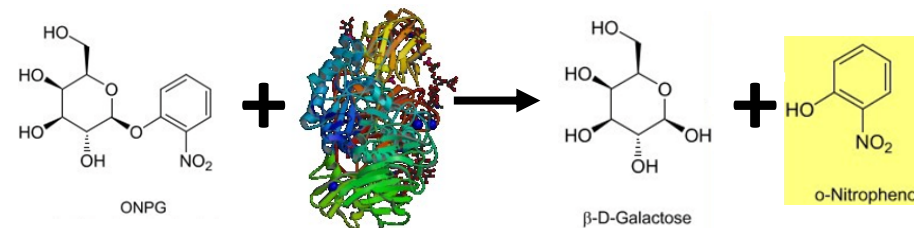
Spectrophotometers are commonly used to measure concentrations, enzymatic reaction rates, etc.

Unfortunately, they can also be quite expensive ($\geq \$1,000$).....

However, spectrophotometers are based on a relatively simple principle:



If you only need to measure a specific wavelength (e.g. 420 nm for ONP), then this design can be simplified by just using a (blue) LED as a light source and photoresistor as a detector.

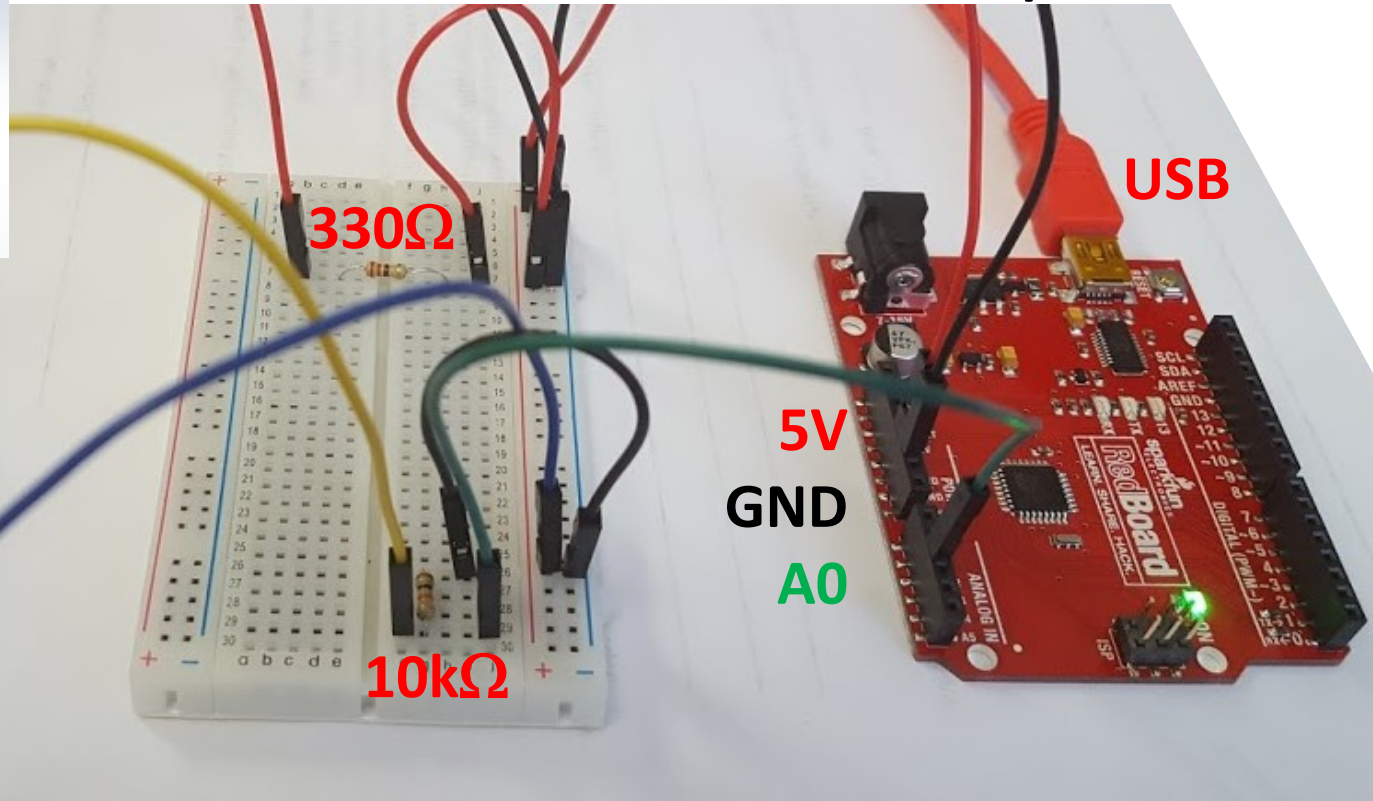
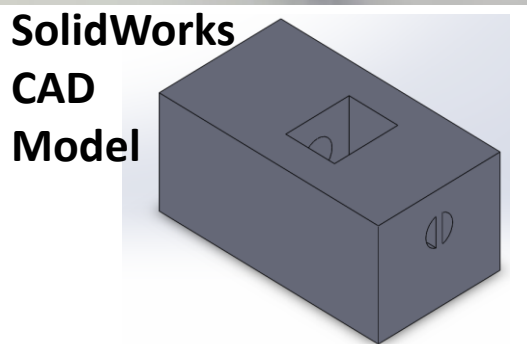
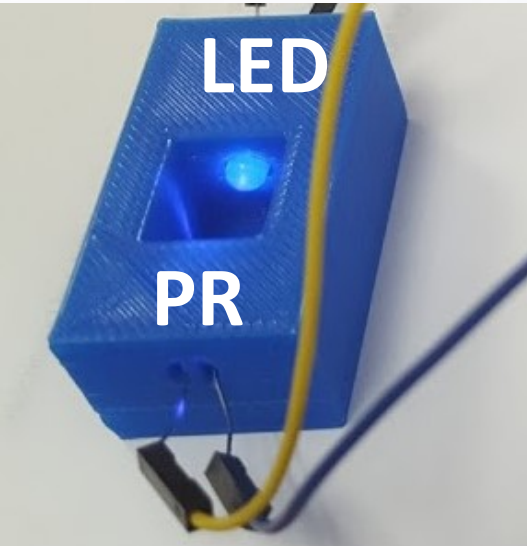
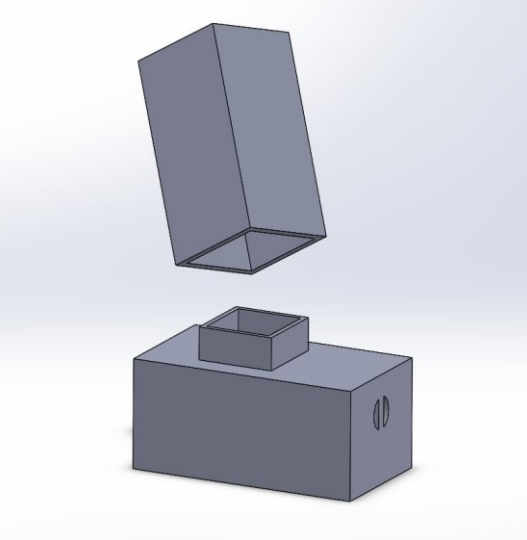


Device Design

Breadboard Circuit

Arduino/RedBoard

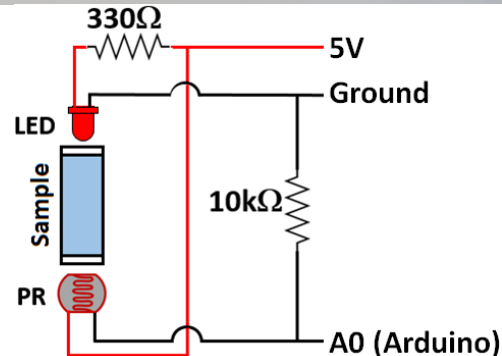
Arduino IDE Code



```
PLX-DAQ | Arduino 1.8.4
File Edit Sketch Tools Help

PLX-DAQ

int bits;
int runtime;
void setup() {
  Serial.begin(9600);
  Serial.println("CLEARDATA");
  Serial.println("LABEL,Elapsed time (s),Reading (bits)");
}
void loop() {
  runtime++;
  bits = analogRead(A0);
  Serial.print("DATA,");
  Serial.print(runtime);
  Serial.print(",");
  Serial.println(bits);
  delay(1000);
}
```



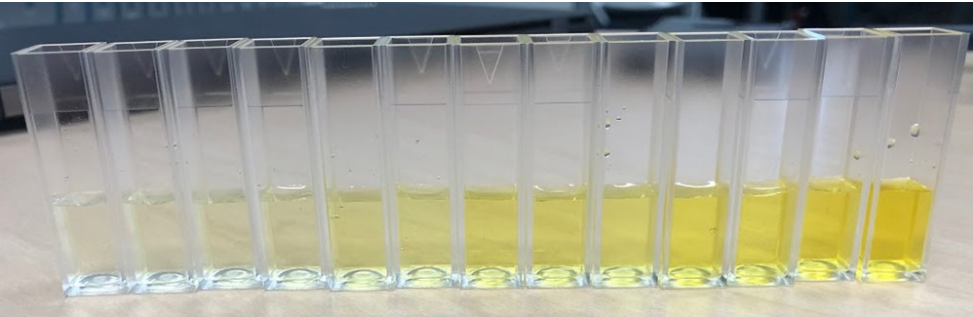
This is a minimal design that students are allowed to modify.

Most groups add covers for the cuvette

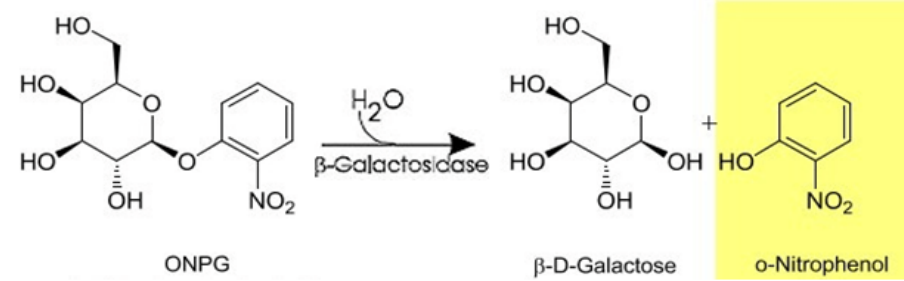
Some groups make enclosures for the circuit

One group designed a device that could monitor 2 cuvettes!

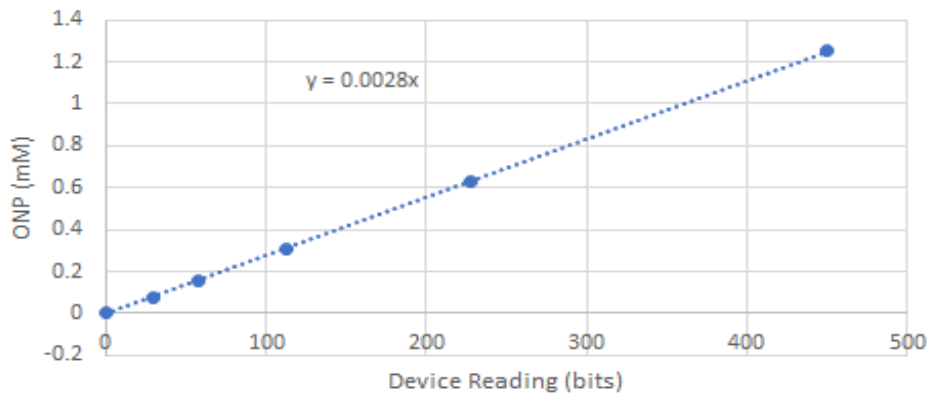
Standard Curve: O-nitrophenol (ONP)



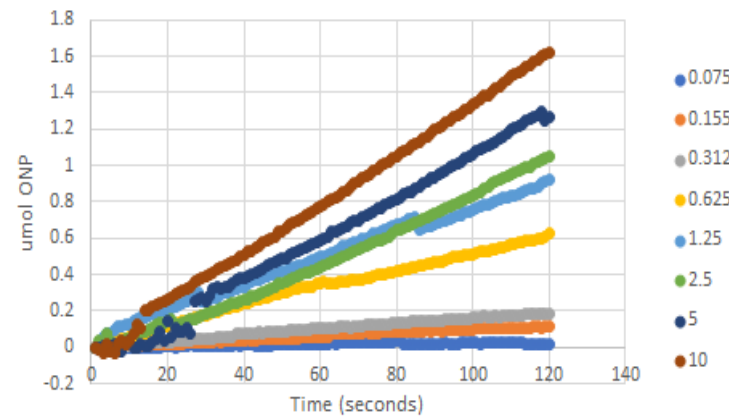
β -galactosidase Reaction: Enzymatic conversion of ONPG $\rightarrow$ ONP



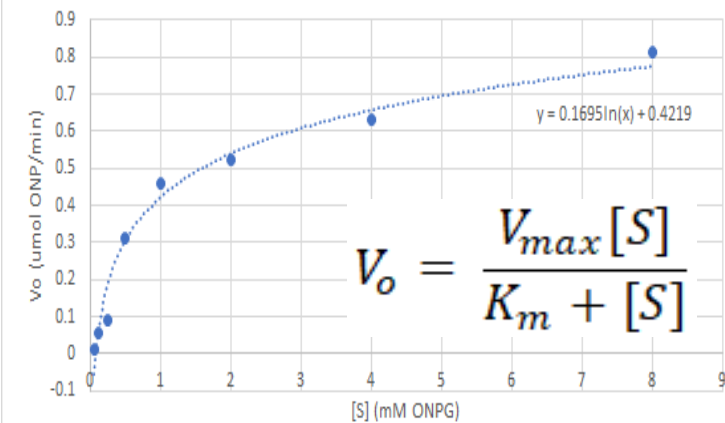
Standard Curve



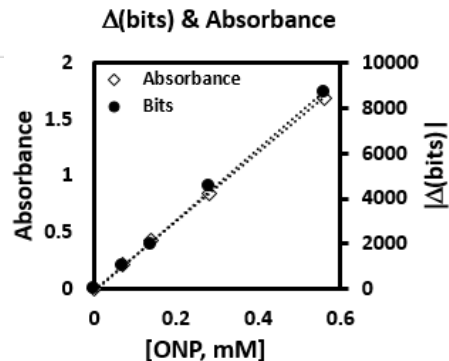
umol ONP VS Time



Michaelis-Menten: [S] VS V_o



Trends obtained with the devices are identical to a commercial spectrophotometer



The device detects changes in reaction rates (V_o) from varying substrate concentrations, which can then be used to prepare a Michaelis-Menten plot

$$V_{max} = 138 \pm 25.1 \frac{\mu\text{mol ONP}}{\text{min} \cdot \text{mg } \beta\text{gal}}$$

$$V_{max} = 134 \frac{\mu\text{mol ONP}}{\text{min} \cdot \text{mg } \beta\text{gal}}$$

$$K_m = 0.92 \pm 0.12 \text{ mM}$$

$$K_m = 0.95 \text{ mM}$$

Summary

Module	3D Printed Parts (Thingiverse IDs)	Arduino?	Available Materials	Cost/Student
Peptides	2758246 (Tubing) 2509708 (Screws)	No	Videos PPT Slides Activities Stickers	\$1.50
Plate & Frame	2452341	Optional	PPT Slides	\$5-50 + pumps, baths
Colorimeter	2760937 (Cuvette) 2456868 (Flow Cell)	Yes	Lab Manual PPT Slides Example Data Arduino Code	\$50/device \$500 for reagents

Please contact me (jacob.elmer@villanova.edu) if you have any interest in using these modules.

Thank you for coming!



Acknowledgements:

Villanova University - Freshman Design Miniproject Grant

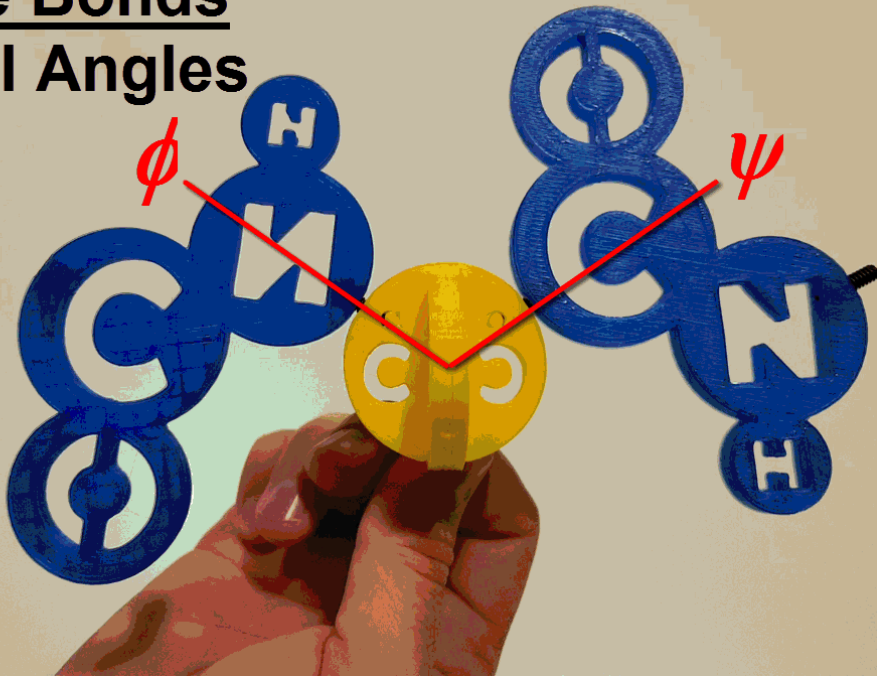
George Simmons - Director of the Multi-Disciplinary Lab @ Villanova

Students – William Landis, Brianna Conte, Neill Boyce, Jeffrey Neuhaus

Links + GIFs

- Amino acids with screws: <https://www.thingiverse.com/thing:2758246>
- Amino acids with tubing: <https://www.thingiverse.com/thing:2509708>
- Dihedral Demo: https://www.youtube.com/watch?v=1usemtIYe_s (3213 views!)
- α/β Demo: <https://www.youtube.com/watch?v=4x61Je8UWsE> (314 views...)
- 3D CAD Protein models: <https://biologicmodels.com/> <https://3dprint.nih.gov/create>
- Magnetic models: <https://makezine.com/projects/peppytides/>

Peptide Bonds Dihedral Angles



Beta Strand: $\phi = \psi = 180$

Parts + Links

- **CAD + STL files:**

- Cuvette holders: <https://www.thingiverse.com/thing:2760937>
- Flow cell: <https://www.thingiverse.com/thing:2456868>

- **Other colorimeter designs:**

de L. M. de Morais C, Carvalho JC, Sant'Anna C, Eugênio M, Gasparotto LHS, Lima KMG. A low-cost microcontrolled photometer with one color recognition sensor for selective detection of Pb²⁺ using gold nanoparticles. *Anal Methods*. 2015;7(18):7917-7922.

Davis EJ, Jones M, Thiel DA, Pauls S. Using Open-Source, 3D Printable Optical Hardware To Enhance Student Learning in the Instrumental Analysis Laboratory. *J Chem Educ*. 2018;95(4):672-677.

Kelley C, Krolick A, Brunner L, et al. An Affordable Open-Source Turbidimeter. *Sensors*. 2014;14(4):7142-7155.

Kitson PJ, Rosnes MH, Sans V, Dragone V, Cronin L. Configurable 3D-Printed millifluidic and microfluidic “lab on a chip” reactionware devices. *Lab Chip*. 2012;12(18):3267.

Anzalone G, Glover A, Pearce J. Open-Source Colorimeter. *Sensors*. 2013;13(12):5338-5346.

Wittbrodt BT, Squires DA, Walbeck J, Campbell E, Campbell WH, Pearce JM. Open-Source Photometric System for Enzymatic Nitrate Quantification. Hong Y, ed. *PLoS One*. 2015;10(8):e0134989.

Porter LA, Chapman CA, Alaniz JA. Simple and Inexpensive 3D Printed Filter Fluorometer Designs: User-Friendly Instrument Models for Laboratory Learning and Outreach Activities. *J Chem Educ*. 2017;94(1):105-111.

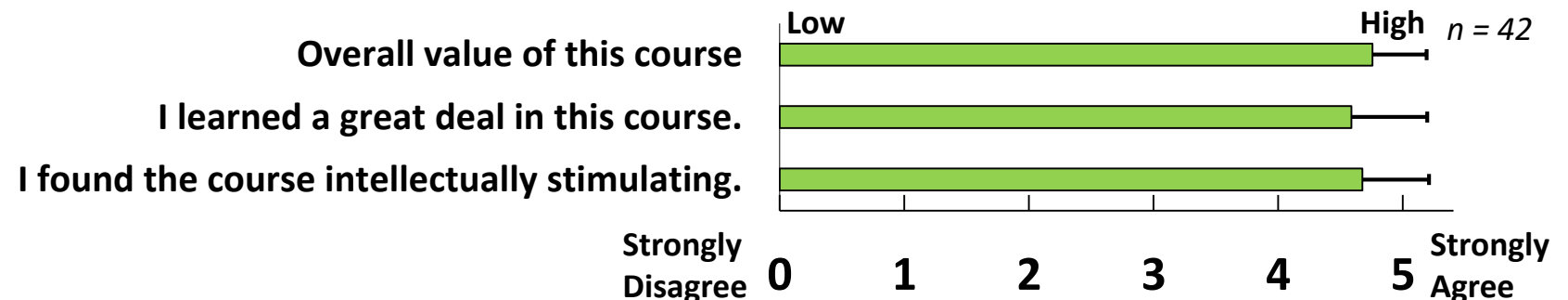
Grasse EK, Torcasio MH, Smith AW. Teaching UV–Vis Spectroscopy with a 3D-Printable Smartphone Spectrophotometer. *J Chem Educ*. 2016;93(1):146-151.

- **Student Survey Results**

0-5 scale

0 = strongly disagree

5 = strongly agree



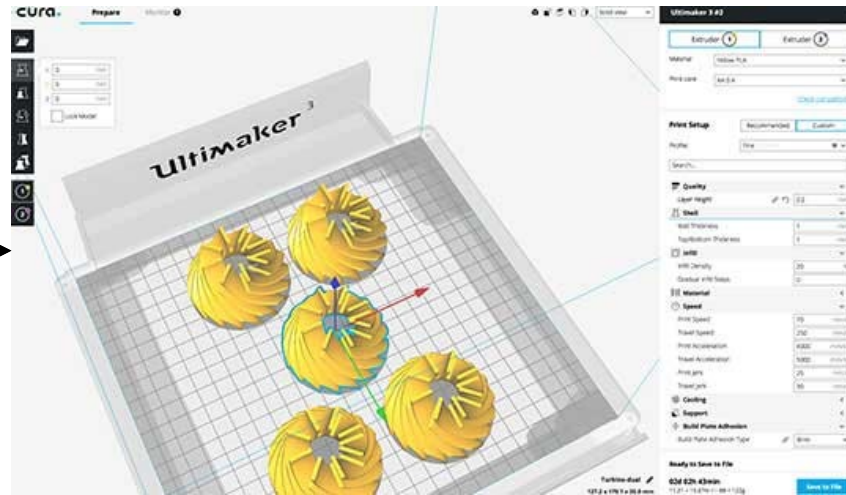
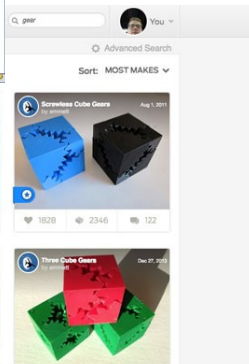
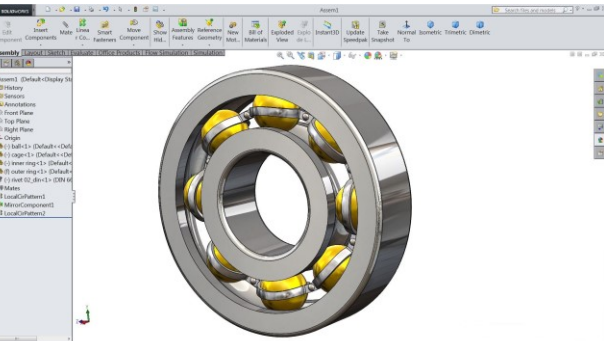
3D Printing Primer

- 3D Printing is now easier, cheaper, and faster than ever
- Make/download a part, convert it into G-Code, and print it yourself/online
- Online tutorials are available for every step
- Parts can be hollow, metal, flexible, etc.

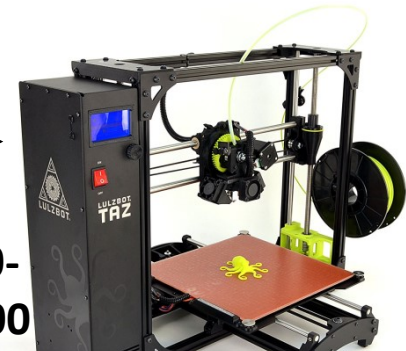
Design part(s) in CAD Program (Solidworks) or download (www.thingiverse.com)

Convert .STL file into .gcode (Cura)

Print! Use a 3D printer (Taz 6) or order online.



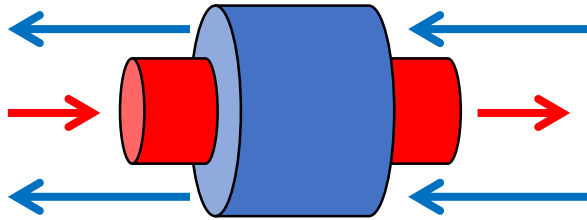
\$1,250-
\$50,000



www.shapeways.com

Module 2: Plate & Frame Heat Exchanger

Double-Pipe



Shell & Tube

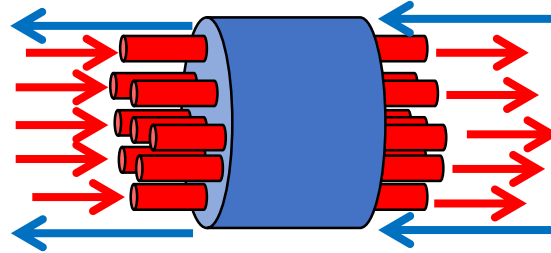
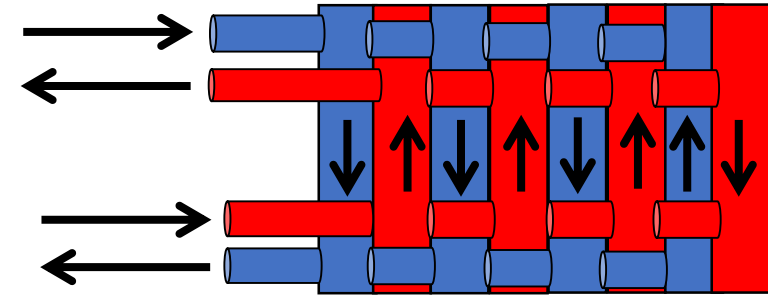
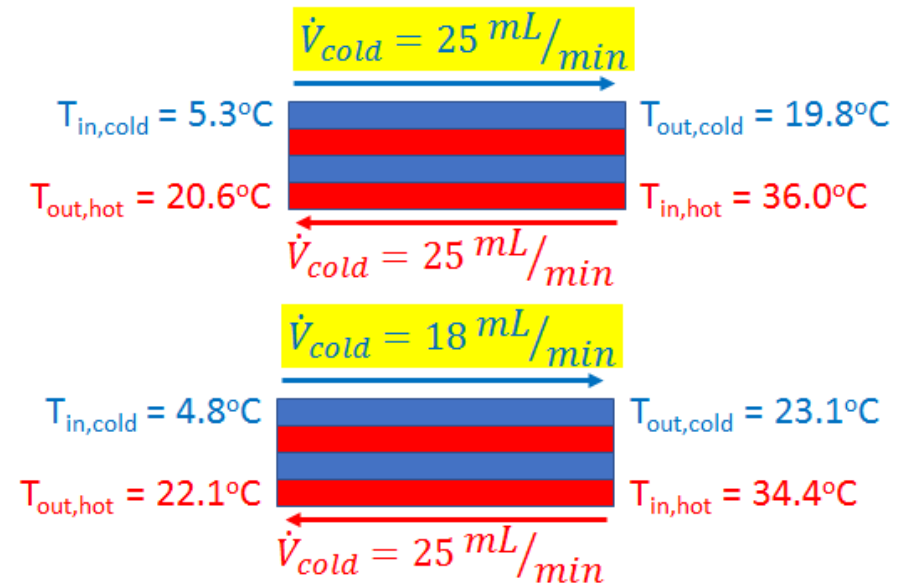
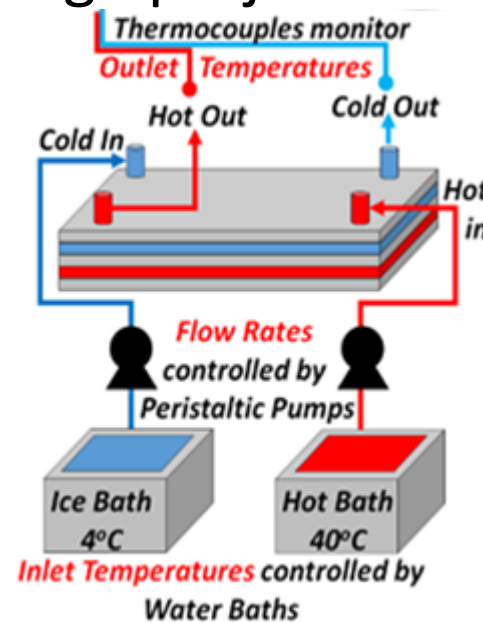
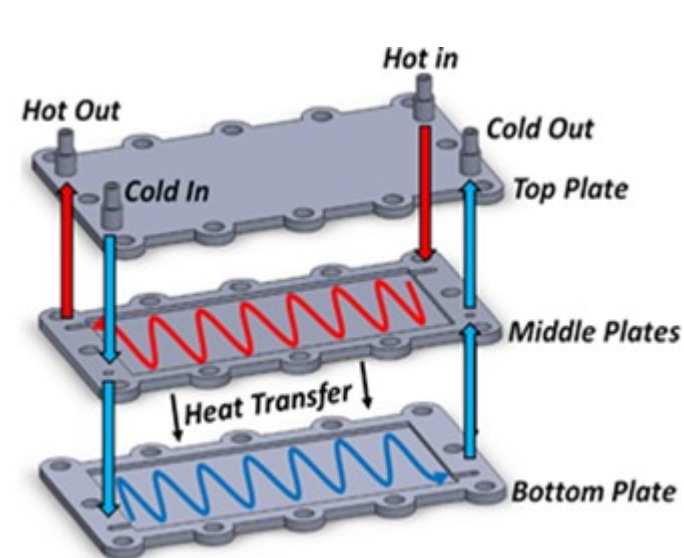


Plate & Frame



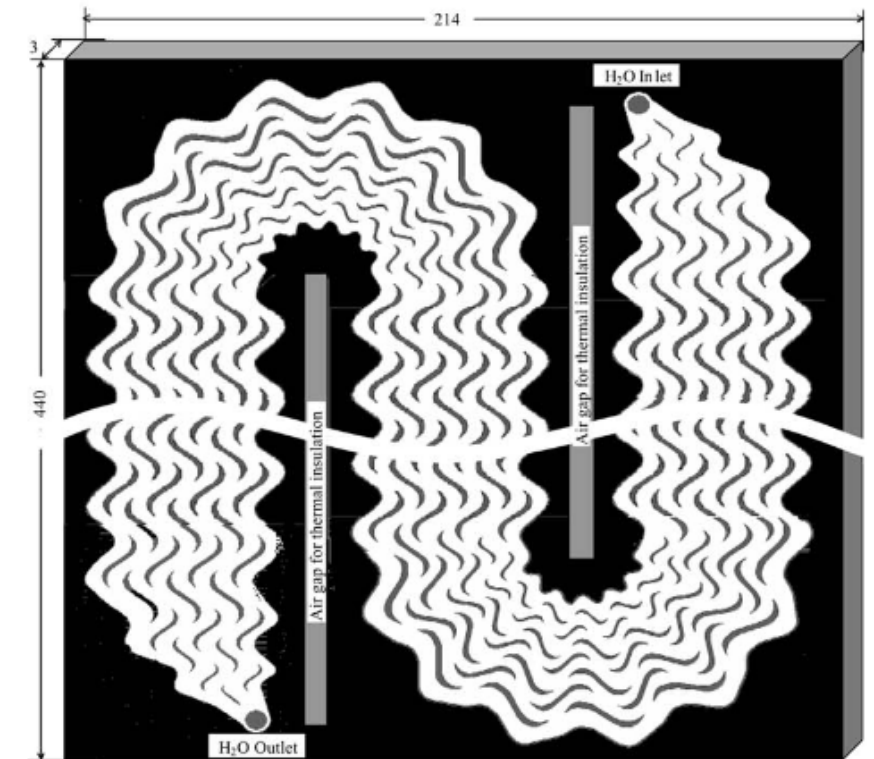
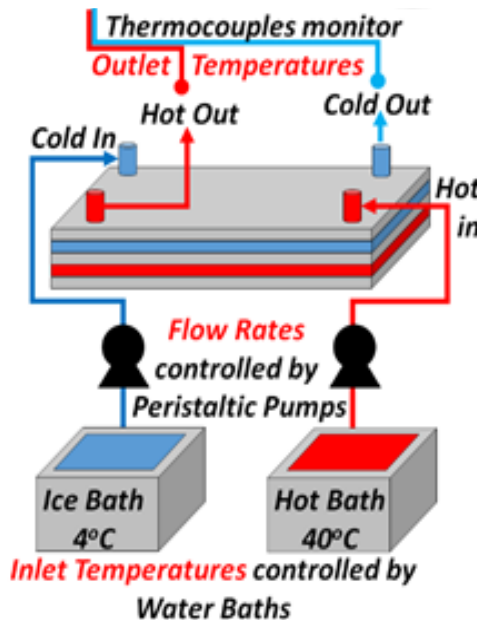
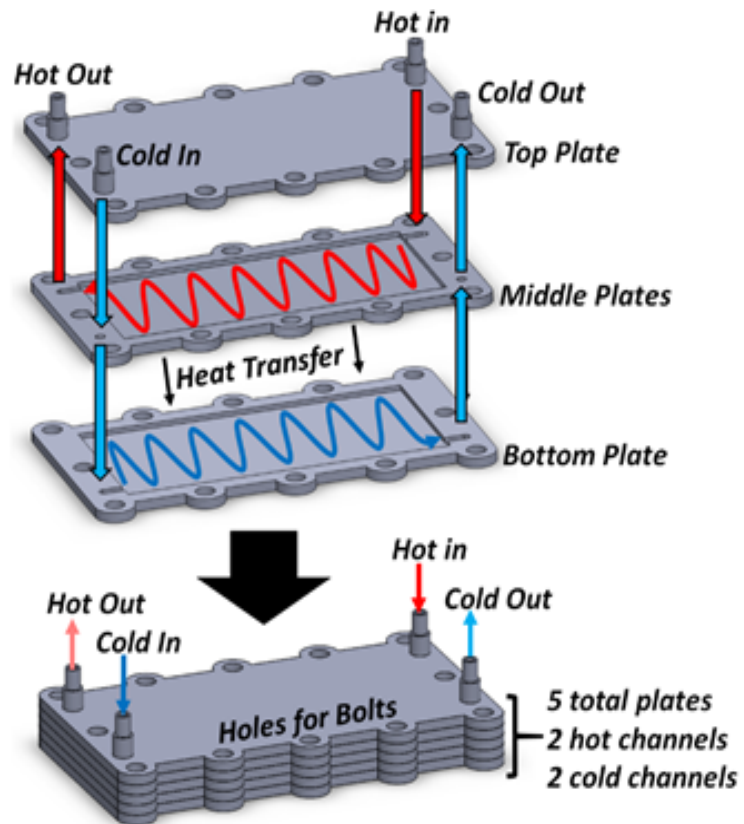
Our Heat Transfer course had a heat exchanger design project, but no lab component...

..so I introduced an Honors design project on 3D printing a Plate & Frame heat exchanger:



Parts + Links

- Plates (top, middle, bottom): <https://www.thingiverse.com/thing:2452341>
- Vacuum-formed Heat Exchanger
 - https://www.ijee.ie/latestissues/Vol33-2A/22_ijee3409ns.pdf



Ngo TL, Kato Y, Nikitin K, Tsuzuki N. New printed circuit heat exchanger with S-shaped fins for hot water supplier. Exp Therm Fluid Sci [Internet]. 2006 Aug 1 [cited 2018 Jan 17];30(8):811–9.