Supplementary Material

Didactic strategy based on molecular modeling tools for teaching about the chemistry present in food

MINI-COURSE TUTORIAL: Is there Chemistry in Food?

WATER
Guiding questions: • How is the structure of a water molecule? • How are charges distributed in a water molecule? • Is water a polar or a non-polar molecule? • What type of interaction occurs to form the water molecule and between one water molecule and another? • Why is water such an important solvent? • Which atoms are responsible for the most positive region? And negative?
Procedures: 1. Open the Molview program at www.molview.org 2. Click on close and in the trash Symbol to initiate. 3. Use the tool on the left to draw a water molecule. First draw one oxygen, then two single bonds and complete with hydrogen. Click on 2D to 3D. 4. Use the left mouse button to rotate the molecule. Observe what the water molecule looks like in three dimensions and which atoms form it. 5. Click on Jmol and Charge to observe the charges of each atom of the water. 6. Click on Jmol and Bond dipoles to calculate the bond dipole vector. Observe the resulting dipole vector by clicking on Jmol and on overall dipole. 7. Click on Jmol and MEP surface Lucent and observe in red the most negative regions and in blue the most positive regions.

SALT - SODIUM CHLORIDE
Guiding questions: • Is table salt soluble in water? • How is its structure? • Which is the negatively charged and which is the positively charged ion? • What do you expect to happen to this structure in water?
Procedures: 1. In the molview program write NaCl in the search bar and hit enter.

2. Click on Jmol MEP surface opaque and observe the colors and sizes of each ion. In red the most negative regions and in blue the most positive regions.

AMINO ACIDS AND PEPTIDES
Guiding questions: • What is the structure of an amino acid like? • How does one amino acid link to another? • How important is chirality in biological systems? • Can you identify the differences between aspartame and its isomer?
Procedures: 1. In the molview program, open the structure of the amino acid phenylalanine. To do this, type Phe in the search bar and hit enter. Observe the structure. 2. Type L-Asp-L-Phe in the search bar to open the structure of the peptide L-aspartic and L-phenylalanine and hit enter. Observe how the structure of this peptide and the peptide bond is. 3. Open aspartame structure by writing “aspartame” in the search box. Aspartame is a commonly used sweetener. Observe its amino acid composition. 4. Open another window of the Molview program and write L-aspartyl-D-Phenylalanine methyl Ester and click enter. Try to rotate the structures to put them in the same position and compare.

PROTEINS
Guiding questions: • Does the structure of a protein relate to its function? • What is the role of hemoglobin in the body? • How many chains are present in hemoglobin? • How is oxygen transported? • What happens with a person that lacks iron in the body? • What is gelatin made of? • How does it solidify? • How is the structure of collagen and what is the relationship to its function? • Why is gelatin made with hot water? • Pepper is formed by the capsaicin molecule, which is responsible for burning. • What is the structure of capsaicin and its receptor like? • How many chains are there? • How does it bind to the receptor? • Why does drinking water not alleviate the burning sensation of pepper?
Procedures: 1. In the Molview program, click on the search box, type hemoglobin and hit enter.

2. Click on Protein and ribbon in the chain representation option. Afterwards, click on the chain in the color scheme chain option.
3. Observe its structure and the heme group attached to each chain.
4. Open the Mol* Viewer program for 3D visualization in RCSB protein data bank at www.rcsb.org
5. In the search box, write the code 1GZX and hit enter.
6. Select 3D View to open the structure.
7. Note that iron is a central atom of heme, necessary for the binding of oxygen to hemoglobin.
8. Note that each type of atom is represented with a different color.
9. In the Molview program, type Collagen and hit enter.
10. Click on Protein, check Ribbon, Bonds and Chain and observe the triple helix structure of collagen. Note the shape of the protein. In hot water, the triple helix separates. These collagen helices interact with others and form the collagen fibers that are present in the skin.
11. Open the TrpV1 receptor structure at www.rcsb.org. The capsaicin binds to this receptor.
12. In the search rectangle write the code 5is0 and click on the magnifying glass.
13. Select Predict membrane below the figure. Observe the structure of this receptor and the predominant colors inside the lipid bilayer and outside. Capsazepine is a ligand for this receptor, as binds in the same site as capsaicin.

CARBOHYDRATES
Guiding questions: • What is mono, disaccharide, and polysaccharide? • What sugars make up lactose? • And amylopectin? • The hydrolysis (breakdown) of lactose normally occurs in the body by an enzyme (lactase), forming glucose and galactose. • What happens in case of people with lactose intolerance? • Knowing the role of glucose in organisms, what should be the function of amylopectin? • What happens when you eat too much sugar? • How is the structure of sucrose? • What sugars form it? • Is the sucrose molecule soluble in water? • Does the sucrose molecule have more hydrophilic or hydrophobic regions?
Procedures: 1. in the Molview program open the structure of glucose, writing D-glucose in the search box. Glucose is a very important sugar for providing energy to the body. 2. Next, open the lactose structure by writing lactose in the rectangle. Observe the glucose molecules that bind to form lactose.

Write amylopectin in the rectangle and hit enter. Amylopectin is a polysaccharide of glucose and is the main starch molecule. It can have up to 100,000 glucose molecules.

3. Observe how the glucose molecules bound to each other's. Find a glucose molecule linked to 3 others.

4. Open the Molinspiration program http://www.molinspiration.com/cgi-bin/properties

5. Paste the sucrose smile code in the search box and hit enter.

C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)O[C@]2([C@H]([C@@H]([C@H](O2)CO)O)O)CO)O)O)O)O

6. Click on the pink rectangle "Galaxy 3D Generator".

7. Calculate the lipophilicity map of the molecule (MLP). In this map the color varies according to the scale from the most hydrophobic to the most hydrophilic in this order (Purple, blue, green, yellow, orange, and red).

LIPIDS
Guiding questions: • How is the structure of the stearic acid? • Does the stearic acid molecule have more hydrophilic or hydrophobic regions? • Compare the structures of fatty acids. What are the differences in relation to the number of carbons and double bonds? Compare the spatial organization (or possible conformations)? • Based on the structures of the molecules and the possible intermolecular interactions, propose explanations for the different melting points of some fatty acids. Which one is solid, and which one is liquid at room temperature? • Why is butter solid at room temperature and canola oil liquid?
Procedures: 1. Open the Molinspiration program http://www.molinspiration.com/cgi-bin/properties 2. Paste the stearic acid smile code in the search box and hit enter. CCCCCCCCCCCCCCCCCC(=O)O 3. Click on the pink rectangle "Galaxy 3D Generator". Calculate the lipophilicity map of the molecule (MLP). 4. Click on dotted to see which atoms are responsible for making some parts of the molecule more hydrophilic or lipophilic. 5. Open the structure of the stearic acid in the Molview program www.molview.com To do this, type Stearic acid in the search box and press the enter button. 6. In the Molview write Oleic acid in the search box and hit the enter button. 7. The melting points of fatty acids are: stearic acid 69.3ºC and oleic acid 13.4ºC. Note the composition of the canola oil and butter below:

In canola oil ~6% is saturated fatty acids and the rest is unsaturated. In butter ~65% are saturated fatty acids (mostly long chain) and the rest is unsaturated. Observe how the conformation of fatty acids and how the presence of unsaturated fatty acids interferes with the physical state. The differences are due to the intermolecular interactions.

DNA AND THE TOXIC AGENT AFLATOXIN
Guiding questions: How is DNA structure? Wha tis the basic unit of DNA and which atoms are present? How does the pairing between the nitrogen bases occur? How does aflatoxin bind to DNA? What is the effect of a mutation in DNA? How does the presence of this toxin in food occur?
Procedures: 1. In the Molview write DNA in the search box and hit the enter button. 4. Click on Protein and leave it in ribbon, and bonds. 5. Open the RCSB program at www.rcsb.org and in the search box type the code 1MK6 and hit enter. Select the 3D View to open the structure. 7. Observe the first and second nucleotides and how they link together. Note the pairing between the nitrogenous bases. 9. Aflatoxin is a toxin produced by a fungus that contaminates grains such as peanuts. It binds to the nitrogenous base of DNA and leads to incorrect pairing. DNA has the code for protein synthesis and, in case of p53, a mutation can lead to hepatic cancer, since this protein is involved in the regulation in the cell cycle and tumor formation.