Teaching with Schrödinger

DNA_RNA_worksheet

Warm-Up Questions:

Read the Khan Academy article on Nucleic Acids and answer the following questions:

1) What is the basic subunit of DNA and RNA called? What is this subunit made of?

Name: _ Class: _

2) What is the difference between a purine and pyrimidine?

3) What is the central dogma of molecular biology?

Computational Exercise #1: Creating DNA and RNA

Question #1: Roughly how many Hydrogen Bonds can you count in the DNA and RNA molecules? *Remember, the Hydrogen Bonds appear as yellow dotted lines on the Maestro interface*



Question #2: Take a screenshot of your short_DNA and short_RNA structures side-by-side in the tile view. Paste your screenshot in the table below. Compare and contrast the structures of the DNA and RNA. What similarities can you observe? What differences are noticeable? Note them down in the table below.

DNA and RNA side-by-side screenshot:	
Similarities	Differences

Question #3: Read the following two articles on <u>DNA</u> and the <u>sugar-phosphate backbone</u>. Why is the sugar-phosphate backbone of DNA negatively charged? What function does this serve?



Question #4: List what hydrogen bond distances (in units of Ångstroms) you see between the DNA base pairs.

Question #5: Other than hydrogen bonds, what are other non covalent interactions that you see within the DNA?

Individual Exercises:

Part A: Calculate the distance between bases in your short_RNA structure. You can follow the same steps from Part 4 of the computational exercise.

1) List a few of the hydrogen bond distances (in units of Angstroms) between the RNA bases. What do you notice about the lengths of the hydrogen bonds in RNA?

2) What overall conclusion or trend can you draw about hydrogen bond lengths in the structures of DNA and RNA?



Part B: Identifying base pairs in DNA.

1) Zoom into your short_DNA structure and identify an instance where A is paired with T and where G is paired with C. Take screenshots of each base pair.

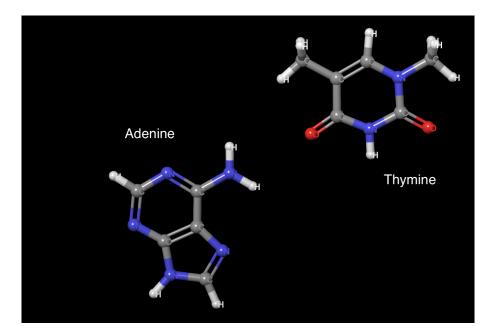
A - T screenshot:	G - C screenshot:

2) How did you identify which base pair was which?



Part C: Oxygen and nitrogen are electronegative atoms found in nitrogenous bases. They are represented in models by the color conventions: red for oxygen, and blue for nitrogen. Electronegative O and N atoms with free lone pairs are potential **hydrogen bond acceptors**. Hydrogen atoms attached to very electronegative atoms like O and N have strong partial positive charge and are potential **hydrogen bond donors**.

1) In the structures of adenine and thymine below, where are the hydrogen bond acceptors and donors? Draw an arrow pointing outwards to indicate a hydrogen bond donor, and draw an arrow pointing inwards to indicate a hydrogen bond acceptor.





2) In the structures of guanine and cytosine below, where are the hydrogen bond acceptors and donors? Draw an arrow pointing outwards to indicate a hydrogen bond donor, and draw an arrow pointing inwards to indicate a hydrogen bond acceptor.

