Chem 352 - Spring 2018

Hand-in Problem Set 2 (Due Wednesday, 11. April)

The goal of this exercise is to analyze both the 3-dimensional structures of enzymes and the reactions they catalyze. On the last page there is a table where I have assigned each of you a different enzyme using one of their Protein Data Bank ID’s. These are ID’s for structure files that can be found in the Protein Data Bank, and all are for enzymes that catalyze reactions found in some of the metabolic pathways we will be discussing this semester: *glycolysis*, *gluconeogenesis*, *the citric acid cycle*, *alcohol fermentation*, *lactic acid fermentation*, *glycogen synthesis* and *amino acid synthesis*. Before starting, please enter your assigned PDB ID on the line provided above.

For this problem set, you will retrieve information about your enzyme from its entry in the [Protein Data Bank](https://www.rcsb.org), The [IUBMB Enzyme Nomenclature Database](http://www.sbcs.qmul.ac.uk/iubmb/enzyme/), and [BRENDA](http://www.brenda-enzymes.org/index.php), The Comprehensive Enzyme System.

1. Start by navigating to the [home page of the Protein Data Bank](http://www.rcsb.org/pdb/home/home.do).

**Questions:**

* 1. While on the PDB home page,
		1. As of today, how many biological macromolecular structures are entered in the Protein Data Bank?
		\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		2. Near the bottom of the homepage there is a section labeled “PDB at a Glance”. Go there and note how many of the protein structures out of the number cited above are distinct and how are derived from human origins?
		Distinct Structures \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_ Human Derived Structures \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
1. What is the current (March) *Molecule of the Month*? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
 (If it is now April, you may need to click on the *Molecule of the Month* and select March, 2018 from the *By Date* tab.)
	* 1. Click on the March Molecule of the Month and read the description. In a couple of sentences, describe the function of this macromolecular structure?

(insert here)

1. Navigate to the entry for your assigned enzyme. Do this first going to the [PDB home page](http://www.rcsb.org/pdb/home/home.do), and then entering the PDB ID into the search pill at the top of the home page.

**Questions:**

* 1. Looking at the description summary at the top of the page,
		1. What is the title for this entry?
		\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		2. Which of the six enzyme classes does your enzyme belong to? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		3. What organism produces this version of your enzyme? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
1. Scroll down to the Literature section for this entry.

**Questions:**

* 1. Give the citation for the article that first reported on this structure

(insert citation here here)

* 1. First read, and then copy and paste the PubMed Abstract for this article.

(insert abstract here)

1. Scroll down to the Macromolecules section for this entry

**Questions:**

* 1. Under the Molecule column, you should be able to find the common name for your enzyme. What is the common name for you enemy? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
	2. Under the Details column, you should be able to find the Enzyme Commission number (EC) for your enzyme. What is this number? EC: \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
1. Go to the [IUBMB (International Union of Biochemistry and Molecular Biology) Nomenclature site](http://www.sbcs.qmul.ac.uk/iubmb/enzyme/). Scroll down and click through the EC links until you find the entry for your enzyme’s EC number

**Questions:**

* 1. Once you have found the entry for your enzyme. What is the Accepted name for your enzyme? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		1. Does it agree the one you obtained above from the Protein Data Bank? \_\_\_\_\_\_\_\_\_\_\_\_\_\_
	2. Look at the Reaction entry and copy the reaction equation below,

(insert here)

1. In the line labeled Links to other data based:, click on the link for BRENDA. This will take you to the entry for you enzyme in The Comprehensive Enzyme Information System.

**Questions:**

* 1. Scroll down to the Recommended Name section. What is the Recommended name for your enzyme? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		1. Does it agree the one you obtained above from the Protein Data Bank and from the IUBMB database? \_\_\_\_\_\_\_\_\_\_\_\_\_\_
	2. Scroll down to the Reaction section. Click on the  icon under the Reaction Diagram column heading. This will bring up an image of the chemical equation for the balanced chemical reaction using structural formulas. Take a screen shot of this image, or reproduce in some other way using a chemical drawing program such as MarvinSketch or ChemDraw. Substitute your image for the example shown below or print it and attach it to this worksheet.



* 1. Scroll down to the Pathway section. Look for one of the metabolic pathways mentioned at the top of the first page and enter it below:
		1. \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
	2. Scroll down to to the kcat/KMsection. If you see a + shown above the table, click on it to reveal all of the entries, 
		1. Based on the largest value reported for the catalytic efficiency, is your enzyme capable of demonstrating catalytic perfection? Be sure to convert to units of 1/(M•s.) \_\_\_\_\_\_\_\_\_\_\_\_\_\_
		Explain:
1. Return to the [Protein Data Bank](http://www.rcsb.org/pdb/home/home.do) entry for your enzyme. Scroll down to the the Small Molecules section. This section lists any small molecules (ligands) that were found bound to your enzyme when its structure was determined. These can include *substrates*, *products*, *coenzymes*, *metallic cofactors*, *substrate analogues*, and other *ions and small organic molecules* that are present in the *solvent*. List below what you find and try and ascertain which of these roles they represent. If you need help identifying coenzymes, refer to Chapter 7 in Moran *et al*.

| **Ligand Name** | **Proposed Role** |
| --- | --- |
|  |  |
|  |  |
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|  |  |
|  |  |
|  |  |

1. At the top of the PDB entry for your enzyme are a series of tabs. Click on the 3D View tab. This will take you to a 3D, interactive model for your enzyme. To the right side of this model are a number of selectable options. Be sure the Bioassembly option for the Assembly setting is chosen; this represents the biologically relevant form for your enzyme. Practice spinning and zooming the model. If you need instructions on how to do this, click on the [Mouse controls documentation](https://www.rcsb.org/pages/help/3dview#mouse-controls) link.

**Questions:**

* 1. Select the Cartoon option for the Style setting, the By Secondary Structure option for the Color option, and the Spacefill option for the Ligand setting.
		1. Is your enzyme composed primarily of α-helices, primarily β-sheets, or a mixture of the two.
		\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		2. Rotate and orient your 3-D model to reveal any ligands that are bound to your enzyme and then click on the button below the model labeled “Screenshot”. This will download an image file. Print and attache to this worksheet.
	2. Select the Surface option for the Style setting, the Chain option for the Color option, and the Spacefill option for the Ligand setting.
		1. Do you see any evidence that this enzyme has a quaternary structure? \_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_\_
		Explain:
		2. Rotate and orient your 3-D model to reveal multiple chains, if they exist, and at the same time show any ligands that might still be visible, then click on the button below the model labeled “Screenshot”. This will download an image file. Print and attache to this worksheet

**After completing this worksheet, print it, attach printed 3-D images, and hand in during class on Wednesday, 11. April, 2018**

| Name | PDB ID |
| --- | --- |
| Bayer | Rachel | 1bdg |
| Berry | Kendra | 1bg3 |
| Bierman | Gina | 1e0u |
| Breuer | Matt | 1u0e |
| Brunner | Lucas | 1a59 |
| Cantu | Corey | 1hox |
| Chernyaev | Michael | 1n8t |
| Close | Miranda | 1kfi |
| Dickenson | Abe | 1khb |
| Egbert | Kelsey | 1kq7 |
| Egdorf | John | 1pfk |
| Fischer | Kourtney | 1pkn |
| Flanagan | Rachel | 4ply |
| Gorres | Kaci | 1x29 |
| Heck | Keelie | 1yfe |
| Hicks | Matthew | 1yxi |
| Kompsie | Mark | 1b7g |
| Kurth | Maranda | 2fp4 |
| Lemke | Alana | 2al1 |
| Marcus | Katie | 4dbc |
| Neuman | Victoria | 2e3d |
| Plautz | Tessa | 1cqi |
| Puls | Isabella | 2jjk |
| Reetz | Eric | 2oeg |
| Reffke | Weston | 5euj |
| Schara | Breanna | 2xe8 |
| Schroeder | Dan | 3abv |
| Schwoerer | Guenter | 3blv |
| Smith | Jenna | 3bv4 |
| Spatz | Marissa | 3dfn |
| Stratman | Bobbie | 3hb9 |
| Thompson | Chris | 3tcm |
| Treacy | Patrick | 3pfk |
| Tsolak | David | 2akm |
| Voss | Max | 3vpg |
| Wenzel | Michael | 4csc |
| Zedler | Alex | 1qpg |