Prof. Dr. Daniel Huson
Zentrum für Bioinformatik
Fachbereich Informatik
Mathematisch-Naturwissenschaftliche Fakultät

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

Grundlagen der Bioinformatik — SoSe 2018

Assignment 10 — **Submit electronically in Ilias by 9.7.2018, 10h**

This assignment sheet is based on the "RCSB PDB Molecule of the Month"
(source `http://cdn.rcsb.org/pdb101/teach/files/Molecule-of-the-Month-1.docx`)

Go to the Molecule of the Month Article at the PDB-101 website `www.rcsb.org/pdb-101/`. Read the article and respond to the following questions. ∗If there are 3 or more different proteins discussed in the article–e.g. as in the case of the Glycolytic Enzymes– choose any one of the molecules to answer the starred (∗) questions.

1 Which Molecule of the Month?

Which Molecule of the Month article did you read?

2 About the Featured Molecule(s) (4 points)

1. *Function*: What is the main biological function discussed in the article?
2. ∗*Players*: Name the key molecule(s) (proteins, nucleic acid, etc.) performing the function(s) listed above. Are there any other molecules mentioned in the article that interact with the molecule being studied – either facilitating or regulating the discussed function? Name the molecule(s).
3. *Big picture*: Describe in 3–4 sentences how reading this article helps you understand the function of a living organism or the world around you?

3 Structure-function relationship (6 points)

∗Explore the structure-function relationship of the molecule(s) discussed in the article

1. *Overview*: Describe how the shape, size and interaction of relevant molecules discussed in the article help in performing the function
2. *Details*: Go to "Exploring the Structure" section in the article and analyze the structures shown in detail.
   (a) Basic level: Examine the static images, and JSmol interactive views, where available. If only static images are available, take a screen shot of the image, include it in your answer and explain in 1-2 sentences the structural and functional detail highlighted in it. In articles where the JSmol interactive views are available, take screenshots of at least two different views, and include them in your answer. Explain in 1-2 sentences the structural and functional details that these images highlight.
   (b) Advanced level: Click on any one of the 4-character accession code (PDB ID) discussed in the "Exploring the Structure" section of the article. This should lead you to the Structure Summary page of that PDB structure. Click on the "3D View" tab and open a JSmol image that can be manipulated. Select from the various visualization/customization options available. Take screenshots of at least two different views highlighting structural details that are important for its function, and include them in your answer. Include the PDB ID that you use, in your answer. Explain in 1-2 sentences the structural and functional details that each of these images highlight.