CS612 Homework Assignment 2

Due Wed. October 18, 2017

1. **Protein structure, multiple sequence alignment:** The Protein Data Bank (PDB) has a Molecule of the Month section to feature examples of molecules archived in the PDB. To find an entry about ABO blood types, point your browser to http://www.rcsb.org/pdb/101/motm.do?momID=156

   (a) From the Molecule of the Month article, identify the name of the enzyme that determines blood type A. Identify the name of the related enzyme that determines that blood type B.

   (b) Based on the two enzymes identified in part A, explain how the two enzymes function to determine blood type B.

   (c) Use the sequences shown below. Perform a ClustalO run with the three sequences. The server can be found at https://www.ebi.ac.uk/Tools/msa/clustalo/ . Paste the three sequences to the input windows, leave the default parameters and hit "submit" Include the letter-by-letter sequence comparison results in your answer. This is found on the results page under the Alignment heading. You can use the download tab in the ClustalO alignment or cut and paste from the web browser into a text program, such as Notepad, that you can submit as a separate file. You may have to adjust the text formatting, such as using Courier New font, to keep the sequences aligned.

   >blood_type1
   MVYPQPKVLTPCRKDVLVVTPWLAPIVWEGTFNIDILNEQFRLQNTTIGLTVFAIKKY
   VAFLKLFLETAEKHFMVGHRVHYYVFTDQPAAVPRVTLGTGRQLSVLEVRAYKRWQDV
   SMRRMEMISDFCERRFLSEVDYLVCVDVDMEFRDHVGVEILTPLFGTLHPGFYGSSRE
   AFTYERRPQSQAYIPKDEGDFYYLGGFFGGSVQEVQRLTRACHQAMMVDQANGIEAVW
   HDESHLNKYLLRHKPTKVLSPEYLWDQQLLGWPAVLRKLRFTAVPKNHQAVRNP

   >blood_type2
   MVYPQPKVLTPSRKDVLVVTPWLAPIVWEGTFNIDILNEQFRLQNTTIGLTVFAIKKY
   VAFLKLFLETAEKHFMVGHRVHYYVFTDQPAAVPRVTLGTGRQLSVLEVGAYKRWQDV
   SMRRMEMISDFSERRFLSEVDYLVCVDVDMEFRDHVGVEILTPLFGTLHPSFYGSSRE
   AFTYERRPQSQAYIPKDEGDFYYMGAFFGGSVQEVQRLTRACHQAMMVDQANGIEAVW
   HDESHLNKYLLRHKPTKVLSPEYLWDQQLLGWPAVLRKLRFTAVPKNHQAVRNP

   >blood_type3
   MVYPQPKVLTPCRKDVLVVTPWLAPIVWEGTFNIDILNEQFRLQNTTIGLTVFAIKKY
   VAFLKLFLETAEKHFMVGHRVHYYVFTDQPAAVPRVTLGTGRQLSVLEVRAYKRWQDV
   SMRRMEMISDFCQRRFLSEVDYLVCVDVDMEFRDHVGVEILTPLFGTLHPGFYGSSRE
   AFTYERRPQSQAYIPKDEGDFYYLGGFFGGSVQEVQRLTRACHQAMMVDQANGIEAVW
   HDESHLNKYLLRHKPTKVLSPEYLWDQQLLGWPSVLRKLRFTAVPKNHQAVRNP

   (d) Based on the sequence alignment, which two sequences (blood type 1, 2, or 3) are the most similar? Explain how you arrived at your answer. Note: for ClustalO a * indicates an amino acid match. Any other symbol indicates an amino acid difference.

2. **Protein structure search and classification:** Search the PDB with the entry 2BAA. Download the pdb file as text, and download FASTA sequence as text.

a. How many atoms are there in the .pdb file?
b. What atom type is atom 289?
c. What is its amino acid 3 letter code?
d. What are the x,y,z coordinates of this atom?
e. Search for 2BAA in SCOPe (at http://scop.berkeley.edu) – what is the class, fold and family of this protein?

3. **Protein visualization:** Install VMD and Chimera, both available for free in the links given in class (handouts for this HW). Upload 2BAA.pdb (from the last question) in each viewer.

   a. On vmd – upload 2BAA.pdb (from last question), display the protein in New Cartoon and color by secondary structure. How many helices do you see? (refer only to those colored in purple). How many beta strands? You can now render the display using File→Render. This will create a .tga file in your working directory. Print this file and submit it with the homework. You may want to change the color of the background from black to white to save ink. This can be done under the Graphics option of the menu, under Background. If the .tga doesn't work out you can print out a screenshot. b. On chimera – upload the protein with the PDB code 1BWW (using File→fetch by id). Select all the beta strands (Select → structure → secondary structure → strand), and color them yellow by action → color and select yellow. Attach a printout by either saving a screenshot or File → save image. To save ink you can change the background color to white by selecting favorites → preferences and change "categories" to background. Click on color and change from black to white.