

Bioinformatics: Life Sciences on Your Computer

Week 3 Practice Problems - Part 3

These are two practice problems for the PDB database. If you're feeling adventurous, try the structure database at NCBI with these two proteins and see what you find.

1. Search for 2C4A in the PDB database (<http://www.pdb.org/>).
 - a. What is its release date?
 - b. What is the EC number of the enzyme?
 - c. What enzyme does that EC number represent?
 - d. What is the resolution of the crystal structure?
 - e. List all five ligand chemical components (by identifier).
 - f. What is the SCOP class?
 - g. How many beta-sheets are shown in the graphic?
2. Go to the PDB homepage (<http://www.pdb.org/pdb/home/home.do>). Click Browse (upper right).
 - a. Click the CATH tab at the top. Under Mainly Alpha (click the triangle to the left of Mainly Alpha), click the link that reads Alpha Horseshoe. How many Structure Hits?
 - b. In the lower right of the box, by "Show only representatives...," flip the Pull-Down to 50% Identity. Now how many Structure Hits?
 - c. Scroll down to the results. List the PDB number and the date of the most recent submission.
 - d. What is the resolution of the structure?
 - e. The expression system is the organism into which the genes for these proteins were cloned. What is the expression system in this record?
 - f. The structure validation graphic helps provide evidence, based on bond angles and other factors, that the structure is one that normally occurs in proteins. What percent is listed for "Ramachandran outliers?"

Answers

- 1.a. 2007-03-27 (March 27, 2007)
 - b. 3.2.1.18
 - c. Exo-alpha-sialidase (hover your mouse over the number without clicking)
 - d. 2.15 angstroms
 - e. beta-D-mannose, calcium ion, alpha-D-mannose, n-acetyl-D-glucosamine, o-sialic acid
 - f. All beta proteins
 - g. 25
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2. a. 460 hits (as of June 23, 2014)
 - b. 141 hits
 - c. 3SFX, 2011-08-03 (August 3, 2011)
 - d. 2.00 angstroms
 - e. *Escherichia coli* (*E. coli*)
 - f. 0.1%

Note: The Ramachandran outliers should be very low if the protein structure is "correct."

