



Molecular Modeling Database and Cn3D Investigation II

1.) SOD

Open NCBI: <http://www.ncbi.nlm.nih.gov/>

Choose Structure → Type “Superoxide Dismutase”

Of the more than 200 structures, find:

MMDB ID: 54363 PDB ID: 2V0A Atomic Resolution Crystal

Click on “2V0A” link above the picture.

Click on the reference (title of paper) and determine in which year the article was published:

_____. What disease is described in the text? _____

Use the back arrow to return to the MMDB Structure Summary. Choose “Structure View in Cn3D,” found under the picture. Using A Beginner’s Guide to Molecular Structures¹, by Sandra Porter, PhD., complete the following manipulations. Get a teacher’s signature for each activity.

Control Key (size) _____

Left Mouse to drag _____

Shift key down to move _____

Style Menu → Coloring Shortcuts → Rainbow _____

Style Menu → Rendering Shortcuts → Ball and Stick _____

Style Menu → Rendering Shortcuts → Space Fill _____

RETURN to Rendering Shortcuts → Worms AND Coloring Shortcuts → Secondary Structure

Click part of Sequence → Open Show/Hide Menu → Show Selected Residues

Return by “Show All Residues.”

Style Menu → Coloring Shortcuts → Domain _____

Describe why this molecule is described as a dimer _____

What two metals are an integral part of SOD? _____

2.) Hemoglobin

Open NCBI: <http://www.ncbi.nlm.nih.gov/>

Choose Structure → Type “Solution Structure of Human Normal Adult Hemoglobin”

MMDB ID: 42825 PDB ID: 2H35

¹ Porter, Sandra. A Beginner’s Guide to Molecular Structure. Seattle, WA: CafePress.com (ISBN 0-0763846-3-9) and Geospiza <http://www.geospiza.com/education/>

Click on the reference (PMID: 1706917) and complete the first sentence of the abstract. “So far high-resolution structure determination by _____ (NMR) spectroscopy has been limited to proteins < _____, although global fold determination is possible for substantially larger proteins.”

Use the back arrow to return to the MMDB Structure Summary. Choose “Structure View in Cn3D,” found under the picture. Using A Beginner’s Guide to Molecular Structures², by Sandra Porter, PhD., complete the following manipulations. Get a teacher’s signature for each activity.

Look at the protein sequences on the bottom of your screen. There are four rows of sequences. Click on the 2H35_B. Where does that link send you?

Select the entire row of letters on 2H35_B (you will need to use the Ctrl key to select the entire row). Open Show/Hide Menu → Show Selected Residues (“residue” is a synonym for amino acid) Toggle between Show Selected Residues and Show All. Teacher Signature _____
Using this information, hemoglobin is made of how many globular protein chains? _____

3.) DNA and Proteins Interact

Open NCBI: <http://www.ncbi.nlm.nih.gov/>
Choose Structure→Type “NMR Study of Trp Repressor-Operator DNA Complex”
NMDA ID: 51146 PDB ID 1RCS

Click on the reference (PMID 8176748) and complete this statement. The solution structures of the complex between _____ trp holorepressor and a _____ base-pair consensus operator DNA were determined. This describes an interaction between protein and DNA.

Use the back arrow to return to the MMDB Structure Summary. Choose “Structure View in Cn3D,” found under the picture. Using A Beginner’s Guide to Molecular Structures³, by Sandra Porter, PhD., complete the following manipulations.

On the Sequence Alignment Viewer (below) what do the purple and blue lines represent?

Why are the sequence letters in the last two printed lines different from the first two lines of print?

Select Style→Rendering Shortcuts→Ball and Stick
Select Style→Coloring Shortcuts→Molecule
On your computer screen, what colors represent the two DNA strands? _____
Teacher signature: _____

4.) Nucleosomes: Packed Eukaryotic DNA

² Porter, Sandra. A Beginner’s Guide to Molecular Structure. Seattle, WA: CafePress.com (ISBN 0-0763846-3-9) and Geospiza <http://www.geospiza.com/education/>

³ Porter, Sandra. A Beginner’s Guide to Molecular Structure. Seattle, WA: CafePress.com (ISBN 0-0763846-3-9) and Geospiza <http://www.geospiza.com/education/>

Open NCBI: <http://www.ncbi.nlm.nih.gov/>

Choose Structure → Type “Structure of the Drosophila nucleosome core particle and H2A-H2B histone dimer

NMDB ID: 60536 PDB ID: 2PYO

Click on the reference (PMID: 17957772) and read the introductory sentences. Using Google, what organism is:

Drosophila _____

Xenopus _____

Use the back arrow to return to the MMDB Structure Summary. Choose “Structure View in Cn3D,” found under the picture. Using A Beginner’s Guide to Molecular Structures⁴, by Sandra Porter, PhD., complete the following manipulations.

In Cn3D, how many of the sequences from the structure are protein sequences? _____

How many are nucleic acid sequences? _____

Choose Style → Rendering Shortcuts → Space fill

Also choose Style → Coloring Shortcuts → Molecule

Great your professor’s signature _____

5.) Your Own Discovery

Open NCBI: <http://www.ncbi.nlm.nih.gov/>

Choose Structure → Type the name of a molecule that you have studied in class. Name that molecule, find an interesting fact in the reference section and create in Cn3D.

Name of molecule: _____

Interesting fact: _____

Professor signature of Cn3D manipulation: _____

⁴ Porter, Sandra. A Beginner’s Guide to Molecular Structure. Seattle, WA: CafePress.com (ISBN 0-0763846-3-9) and Geospiza <http://www.geospiza.com/education/>