Using YASARA View to look at molecular structure

YASARA is a computer graphics program designed for looking at and manipulating the structure of proteins and nucleic acids. There is a free version called YASARA view, available for both Mac and Pc computers which this worksheet uses.

Download YASARA View from here http://www.yasara.org.

You should also download the files that accompany this worksheet.

1. Using YASARA View: GFP video tutorial.

As part of the video presentation that accompanies this worksheet, there is a short video on using some of the basic features of YASARA – watch the video, but here are the instructions for doing it yourself.

OPEN YASARA View

On the top menu select:

File, Load, Yasara scene

Locate the files you downloaded to accompany this worksheet, then select

GFP4EUL.sce

This opens the GFP protein in a simplified cartoon view where you can see the basic skeleton of the protein. The types of secondary structure are represented and coloured differently – alpha helices are blue cylinders, beta-strands red arrows and loops green and cyan. You can see the structure is mostly formed of red beta-strands which hydrogen bond together to form a barrel. The chromophore (which fluoresces) is in the centre of the barrel and shown in a space filled representation.

Basic instructions for moving and rotating the molecule:

The following tables are taken from the Yasara User manual which is available under HELP on the top menu. This manual is good to use, and there are also some tutorial videos built into Yasara if you are interested.

Keyboard controls:

Zoom in	T
Zoom out	Y
Move Left, right, up down	Cursor keys
Rotate ⬇⬆	A and S
Rotate ⬅➡	D and F
Rotate ↻↺	G and H

Mouse controls:

Move Left, right, up down	Left and right button and move mouse
Rotate	Left button and mouse movement

Remember you have 3 dimensions to move your molecule in, including front to back, so it can be easy to get confused.

If (when!) you want to re-centre and reset everything:

From the top menu click:

EFFECTS, POSITION, SET FOR SCENE

This sets the x, y and z coordintates to 0 as default (i.e. back in the centre of the screen!), so click OK

Everything is now back in the middle of the screen – reduce the zoom by holding down Y on the keyboard until you are happy.

Loading a file from the Protein Data Bank https://www.rcsb.org

The Protein Data Bank (PDB) is a fantastic resource containing all of the structures for biological molecules which have been currently determined. Each structure has a unique code (for example the GFP you have just looked at has the code 4EUL), and Yasara allows you to download directly from this. A search of the PDB will give you a code for any protein you are interested in.

The GFP you have been looking at in the Yasara scene file GFP4EUL.sce was already edited to show a simplified, more useful view. However, if you download a file from the PDB it will usually display all atoms, including water molecules and other small molecules that were present when the structure was determined.

In Yasara, select:

FILE, NEW, OK – this clears away the previous session

Now you can download the same GFP structure 4EUL directly from the PDB as follows:

FILE, LOAD, PDB file from internet

In the PDB ID box enter 4EUL, then click OK

You can see this is the same structure, but now all atoms are visible, including lots of red dots which are water molecules.

Click: VIEW, STYLE SCENE, CARTOON

Now you are back with the simple representation, but including some small molecules which have interacted with the protein during the structure determination experiment.

On the right hand side of the screen is a SCENE CONTENT panel.

Click on 4EUL in this panel, and it shows the different molecules that are in the 4EUL file. One of the columns is headed Vis (for visible). Try clicking this to No for the molecules and you will find the first molecule is the protein, and the others are the small molecules.

Sometimes there may be more than one copy of the protein in the file, and you can hide one of them in the same way.

You are now able to use the basic features of Yasara to look at proteins.

The software also allows you to colour all or part of a protein, measure angles and distances, build small molecules, display molecular surfaces and many other things, some of which will be explored in the other sections of this worksheet.

This is the end of the video tutorial, but below are some projects on proteins and DNA you can explore, or if you prefer, use some of the instructions to look at a protein which interests you!

2. Structure of the nucleosome

In this section you can explore the structure of the nucleosome. This contains double-stranded DNA wound round a complex of proteins that you will investigate further. More information on the nucleosome can be found here https://pdb101.rcsb.org/motm/7

First you will load the file into YASARA:

Select: FILE, LOAD, YASARA scene, then choose the file NUCLEOSOME.SCE.

This has opened the file containing the nucleosome. You can move this using the mouse, or the touch screen of the monitor – try rotating it, and zooming in to see more detail. The DNA is coloured cyan, and the protein is displayed as a cartoon showing the secondary structure – you should be able to see a lot of blue alpha-helices.

Everything looks very complicated and it is not possible to identify the different protein subunits inside the DNA. There are actually 8 proteins, 2 copies each of histones H3, H4, H2A and H2B. You can begin by colouring each of the histones a separate colour:

On the right hand side of the screen is a SCREEN CONTENT table, which has the whole assembly listed as 1aoi, then all of the individual subunits listed under this.

Move your mouse to Mol H3, and right hand click.

This brings up a box with things you can do to molecule H3.

Click on COLOR, select a colour, select OK

You have now coloured one of the copies of histone H3, and you can see how this is positioned in the nucleosome.

Repeat for the other histone molecules – you could colour all 8 proteins separate colours, but it is simpler to view if you colour the two copies of the same protein the same colour. If you want to change the colour of the DNA, you can also click on the Mol DNA in the same way.

You can now see more clearly how the histones are packed together inside the DNA. You can also see the long tails protruding outside the core particle, and identify which of these belong to which histone.

This view means you can still see the secondary structure detail of the individual proteins, but it does show you how closely everything is packed together. You can now put a molecular surface on each of the subunits as follows:

As before, right hand click on H3

Select SHOW, SURFACE

This brings up another box with lots of options for creating a molecular surface.

Select SET SURFACE COLOUR FOR THE ENTIRE OBJECT

Then in the box on the right:

Select AtomCol

This will make sure the surface is the same colour as the underlying protein. If you select a different colour, all of the surfaces you apply to this protein will be that colour, so you won't be able to see the different histones.

Enter a value in the Alpha Box (default 100)

This is the transparency of the surface you are adding (0 is totally transparent and 100 is solid). You might like to experiment with this value – a solid surface gives you a better feel for how tightly the proteins pack together, but transparency allows you to still see the secondary structure beneath.

Repeat this process for all the protein subunits and the DNA. If you want to apply the same surface parameters to all of the molecules within the nucleosome assembly you can right hand click on the 1aoi above the individual molecules and apply the surface.

Now it is easy to see the path of the DNA winding around the protein complex, and clear where the nucleosome protein tails are protruding.