Directions to download and use Cn3D structure modeling program

Go to the Cn3D home page: http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml
There are links for a tutorial, frequently asked questions and installation guide on this page.

Program can be downloaded for PC or MAC computers using the "Download" link on the top. (You must download the program in order to view downloaded HLA structures later on your own computer).

To get HLA structures, click on the MMDB link on the left side (Molecular Modeling DataBase).

In the search engine, select "Structure" and type "HLA" in the "for" box to view all HLA structures. Click on "GO". If you prefer a subset, e.g., HLA-DQ or HLA-A only, type the desired subset in the "for" box.

Click on the picture of the peptide for the selected structure. To view the structure, set the formats on the right side as:
File format: Cn3D
Display as: 3D structure
Data set: Single 3D structure
Press the "View Structure" button. On the File Download box that appears, press "Open".

To save the structure to your computer, under the "File" tab, select "Save As", pick the location, name the structure and select "All files" under "Select file type".

Structures are displayed as ribbon models. To see them as 3-dimensional globular models, make the following changes under the "Style" tab along the menu on the top:
Under "Rendering Shortcuts", select "Space Fill".
Under "Coloring Shortcuts", select "Molecule".
Under "Edit Global Style", click on the Background color square, then select White, click "OK", then click "Done".

To zoom in or out, go to the "View" tab, or press "z" to enlarge, "x" to make smaller.

For class I, the "A" chain (pink) is the polymorphic α chain, "B" (blue) is β2 microglobulin, and "C" (brown) is the peptide. For HLA-DR, the "A" chain is DRα, "B" (blue) is DR β and "C" (brown) is peptide. For HLA-DQ, the "A" chain (pink) is DQA, "B" (blue) is DQB and "C" (brown) is peptide. **The sequences shown below the model do NOT always start at position 1; always check the sequence shown with a published sequence to confirm the starting point.**

If more structures appear than you want (such as proteins the molecule is bound to), go to the "Select" menu tab, and click on "Pick Structure". All structures that appear are highlighted. You may have to deselect all and then highlight the ones you want to appear.

To highlight a single amino acid position, find the position in the sequences below the model and click on it; it will appear highlighted in yellow. To highlight multiple positions, select one, then hold the Ctrl key down while highlighting the others. Individual positions can be removed from a group of highlighted ones in the same way; hold down the Ctrl key while clicking on the position to remove. **There is a position**

counter along the very bottom of the screen that indicates your position as you move along the sequence with your mouse. The PDB number should be the correct amino acid position, but again, remember to check the position numbers with a known sequence.

To rotate the molecule, hold down the mouse button while the cursor is on the molecule, then rotate the mouse.

To select residues within a specific radius of an amino acid position, select the position in the middle of the patch. Under the “Select” menu tab, choose “Select by distance”. Indicate the desired radius (in Ångstroms) and click “OK”. All the positions within the selected radius of the center position will be highlighted in yellow.

To save a reconfigured molecule on your computer, go to “File” and select “Export PNG”. Name the file and select a location. Save as file type “PNG”. To add labels or copy the figure, use the “Open with” function and open the PNG file with Paint. Lines, arrows and text can be added here. Select a region and it can then be copied to a Word or Powerpoint file.

THESE ARE ONLY THE MOST BASIC INSTRUCTIONS; YOU CAN DO A LOT MORE WITH THE Cn3D PROGRAM. SEE THE TUTORIAL AND WEBPAGE TO LEARN MORE.

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