



Deep View Course Exercises

Version 1.0 (public)



Licence

This manual is © 2007-8, Simon Andrews.

This manual is distributed under the creative commons Attribution-Non-Commercial-Share Alike 2.0 licence. This means that you are free:

- to copy, distribute, display, and perform the work
- to make derivative works

Under the following conditions:

- Attribution. You must give the original author credit.
- Non-Commercial. You may not use this work for commercial purposes.
- Share Alike. If you alter, transform, or build upon this work, you may distribute the resulting work only under a licence identical to this one.

Please note that:

- For any reuse or distribution, you must make clear to others the licence terms of this work.
- Any of these conditions can be waived if you get permission from the copyright holder.
- Nothing in this license impairs or restricts the author's moral rights.

Full details of this licence can be found at

<http://creativecommons.org/licenses/by-nc-sa/2.0/uk/legalcode>



Exercise 1: Searching for Structures

- Use the text search tool in Deep View to search for structures for “Acrosin”.
 - How many structures do you find?
 - Are they all single chains?
- Make a note of the accession number for the full structure of Ram Acrosin.
- Search for thrombin structures.
- Since the list you get is so large, reduce it by searching for epsilon thrombin
- To narrow the search further add the term “complex” to your search to find structures which have a substrate bound to them
- Make a note of the thrombin structure which is complexed with MQPA

Exercise 2: Basic Molecule Manipulations

- Load in the Ram Acrosin structure you identified in the first section
- Spend a few minutes familiarising yourself with the basic movement controls. Make sure you are happy you know how to:
 - Rotate, Translate and Zoom just using the mouse
 - Rotate the molecule about the Z-axis using the keyboard modifier
 - Add a slab to the view, change its thickness and drag the molecule through it

Exercise 3: Different Structural Representations

- Create the following views of the Ram Acrosin molecule. See how they look in the various OpenGL modes.
 - A view of the backbone atoms coloured by their type
 - A ribbon view coloured by secondary structure
 - A Backbone and sidechain view of residues 16-20 only, coloured by CPK, and with residue 18 being spacefilled
 - A ribbon view of the whole structure, coloured grey, with the following residues shown as backbone and sidechains coloured red, and labelled.
 - His 57
 - Ser 195



Exercise 4: Making Selections

- Use the selection mechanisms to create the following views of the acrosin molecule
 - A grey ribbon, with residues $\geq 40\%$ solvent accessible highlighted in blue
 - A backbone view of everything except solvent molecules
 - A backbone view, (coloured green) with sidechains added (coloured by type) for all aromatic amino acids (Tyrosine, Tryptophan and Phenylalanine)
 - A backbone and sidechains view, coloured by CPK, with labels of all residues within 5\AA of Trp 215

Exercise 5: Adding Surfaces

- Add a surface to the acrosin molecule which excludes chains L and S
- Add the L chain back to the molecule with a Van de Waals surface showing
- Once the surface is added make sure you can then add and remove it interactively using the control panel
- Try taking a slab through your surface so you can see the interior of your protein.

Exercise 6: Finding Regions of Interest

- Close the acrosin structure and open the thrombin structure you previously identified
- What is the reference for the original paper which published this structure
- Does this structure contain Prosite Motifs?
- Do any of them indicate the position of the active site?

Exercise 7: Working with Multiple Structures

- Open the acrosin structure as well as the thrombin
- Fit the two structures together using just the CA atoms
- What is the RMS of the fit?



-
- Colour the alignment by alignment diversity . Are the residues more conserved in the interior of the protein or the exterior?
 - Select Residues in both structures which are within 5Å of the substrate M chain in the thrombin structure. Show these residues as backbone and sidechains coloured by layer. How similar are the two structures in this region?

Exercise 8: Creating Publication Quality Graphics

- Change your view of the Thrombin/Acrosin overlay by adding a Van der Waals surface to chain M in the thrombin structures
- Rotate the view to get a nice angle then create a rendered version of this scene using POV-Ray