EXPERIMENT 8: MEMBRANE PROTEIN ANALYSIS

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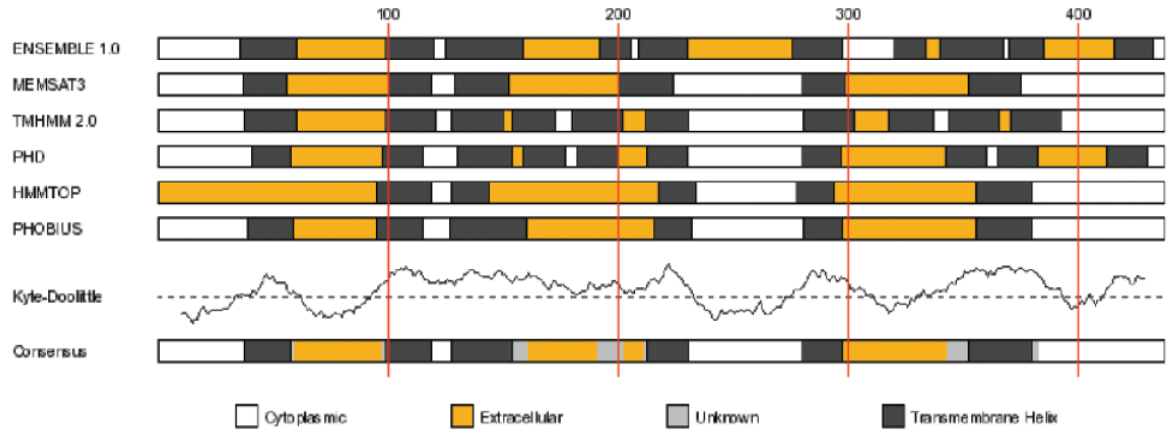
SUSTC

Methods

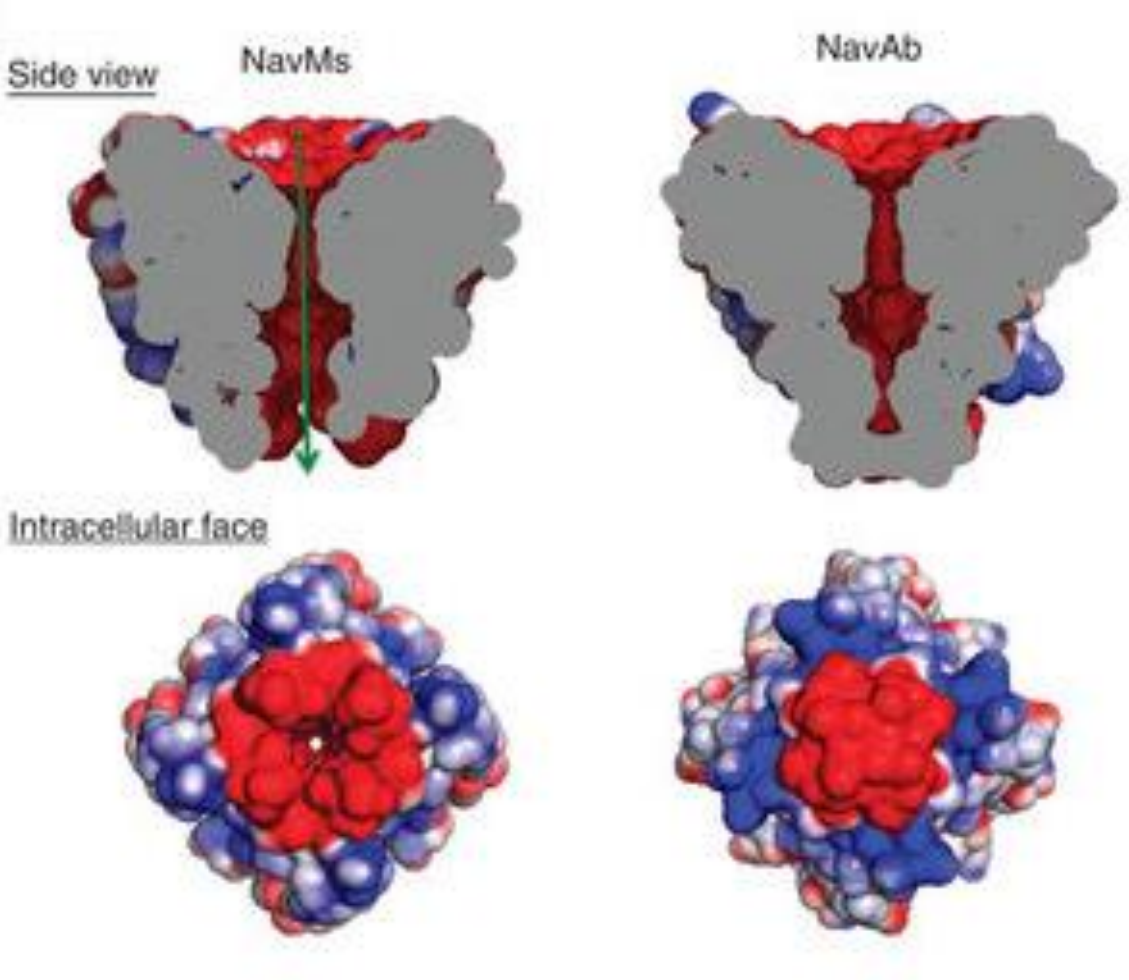
- Sequence based analysis
  - Prediction of transmembrane helices and topology
- Structure based analysis
  - Cross-section
  - Tunnel analysis

Prediction of transmembrane helices and topology

- TMHMM
  - http://www.cbs.dtu.dk/services/TMHMM/
- SCAMPI
  - http://scampi.cbr.su.se/
- HMMTOP
  - http://www.enzim.hu/hmmtop/index.php
- Phobius
  - http://phobius.sbc.su.se/



Cross-section



PyMOL tips and tricks

http://www-cryst.bioc.cam.ac.uk/members/zbyszek/figures_pymol

- **I would like to cut my protein in half**

It is sometimes useful to have cross section of your protein, especially in case of pockets, tunnels etc.
First issue following commands:

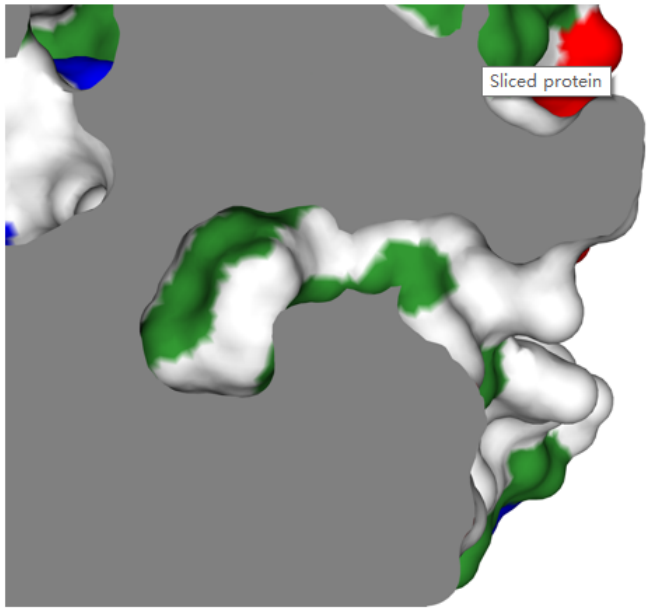
```
hide all
show surface
set ray_trace_mode, 0
set two_sided_lighting, off
set ray_interior_color, grey50
```

Of course you can set up ray_interior_color to any colour you want. This colour is used to display the clipping plane.

Then you will have to adjust the 'near' clipping plane so that it will cut you protein in desired place:

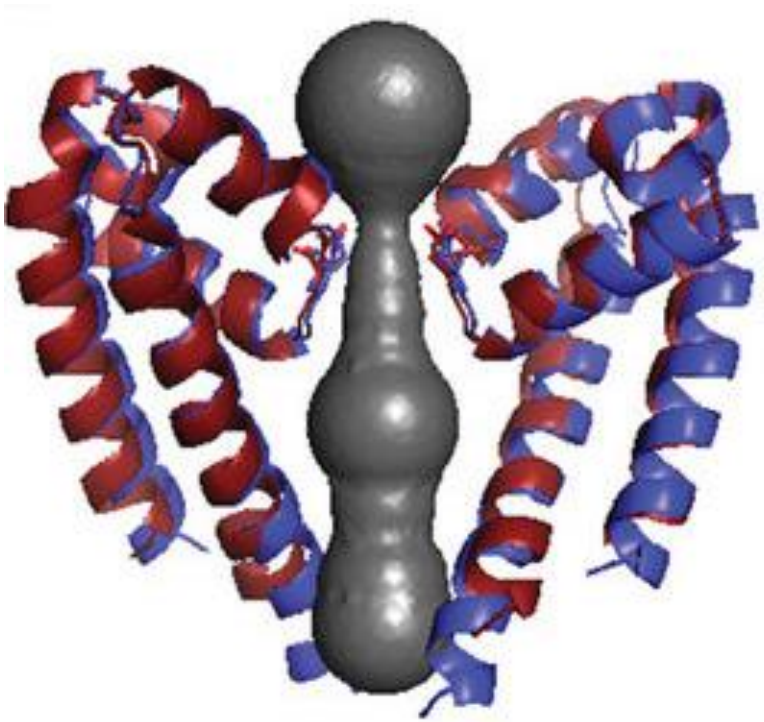
```
cmd.clip("near", x)
```

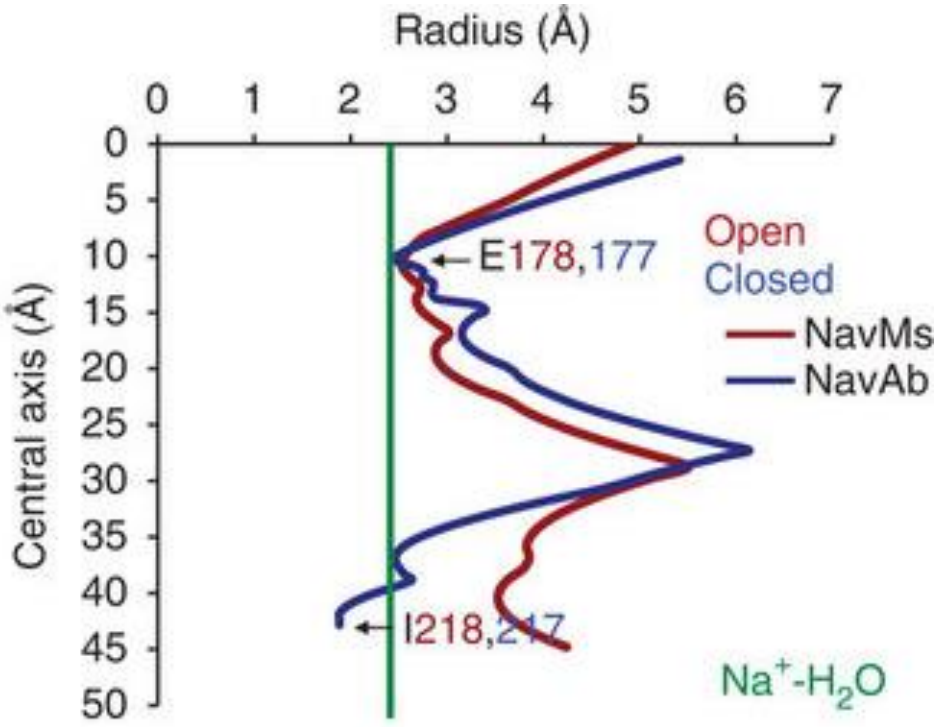
Where **x** can be positive or negative value (e.g -15 , +10, -90, +100 etc.).
Negative values will move clipping plane towards the molecule and positive values will move it towards you. You will have to start from negative values to move the clipping plane into the molecule.
You will have to ray trace image to see final result.



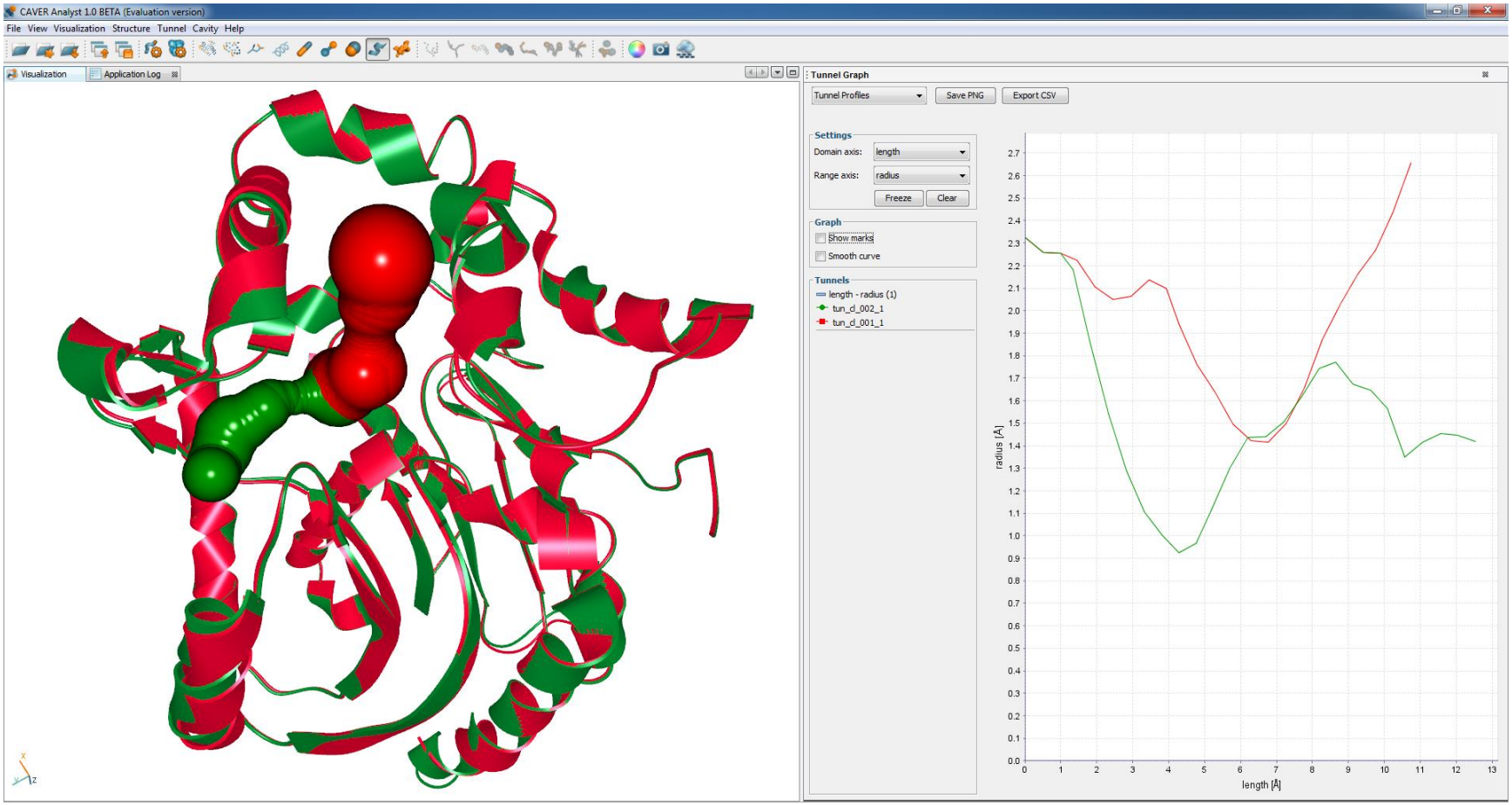
Example of protein sliced using method described above

Tunnel analysis





Caver (http://caver.cz/)



Tasks

1. Predict the transmembrane helices and topology of human voltage-gated potassium channel
   - Compare your predicted results from one or more servers with solved potassium channel structure
2. Load the potassium channel structure (PDB id: 1BL8) to PyMOL and show its surface with electrostatic potential
   - Analyze its charge distribution features
3. Make cross-section of the structure to show its internal channel
   - Is this channel at its open or close state?
4. Use your previous results by CAVER for the potassium channel structure (PDB id: 1BL8) to further analysis the channel radius versus distance along the channel direction
   - What is the residue(s) at the narrowest place? Why?

Lab report format

- Title
- Your name and student No.
- Introduction
- Methods
- Results
- Conclusions