

Exercise 12.1 Filling the void

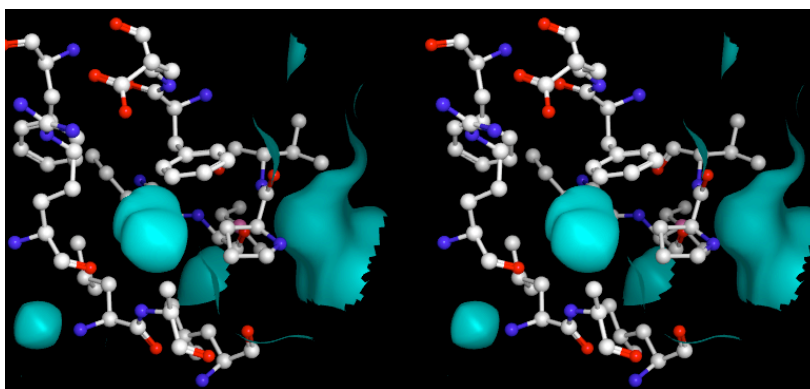
1. Open the MOE file for homework 6
2. <http://www.bioinfo.rpi.edu/bystrc/courses/biol4550/homework6.moe>
3. Delete the SWISS model and the template leaving only the MOE model.
4. Calculate the molecular surface. Select a few core residues (**shift-ctrl-left mouse**) to draw the surface around. Select origin of rotation (**middle-mouse click** on atom). Then,

Compute | Surfaces | molecular surface , (Name: surf1, Surface: receptor atoms, Near: selected, constant color.)

- Make the front surface transparent.
 - Hide all atoms and ribbons.
 - Locate the largest void (buried cavity).
 - Show all atoms. Keeping your eye on the void.
 - Select atoms around the void. **Hide | unselected.**
 - Turn 90°. Select atoms around the void. **Hide | unselected.**
 - **Select | extend | residue. Show | selected.**
 - Now you have just the atoms around the void.
5. Re-calculate the molecular surface.

Compute | Surfaces.. , (Name: surf1, Surface: receptor atoms, Near: selected, Within: 4.5, constant color.)

6. Show complete amino acid residues.
Select | Extend | Residue, Show | Selected, Atoms | ball-and-stick.



7. Select one of the side chains to rotate.
Protein | Rotamer Explorer, (get from MOE, Explore, select rotamer, Mutate... etc.)

8. Energy minimize side chains, not backbone.
Hide | backbone
Left-mouse select all visible atoms, which are sidechains
Isolate (see footnote)
Selection | Extend | Residue puts back backbone atoms.
Minimize.
9. Re-calculate the molecular surface. Select atoms, then
Compute | Surfaces.. , (Name: surf1, Surface: receptor atoms, Near: selected, Within: 4.5, constant color.)
10. What happened to the void? Is it better? Smaller? Did other buried cavities appear? Did pockets appear?
11. Repeat from step 7. Try to eliminate all voids. Is it possible?
12. Set up a stereo image (**Render | stereo | stereo**).
Display extended as thin lines with residue labels. (**Select | extend | near residues, Show | selected, Select | clear, Atoms | thin line, Atoms | residue, Hydrogens** (all off))
Save the image (**File | Save | Picture**) as png format.
13. Upload png file as Exercise 12.1

Isolate =

**Edit | Potential | Unfix
Selection | Invert
Edit | Potential | Fix
Selection | Clear.**

Make this a function key!