BCB 569: Assignment 2
(100 pts)
Due date: 5pm, Monday, Oct 10, 2011

Purpose:
Learn to compute solvent accessible surface area (SASA)

References:
[1] Internal cavities and buried waters in globular proteins, Biochemistry 25:3619-25, 1986.

Assignment Description:

In this assignment, you are to construct the solvent accessible surface of a protein (2GB1.pdb) and compute solvent accessible surface area (SASA) for each atom in the protein. You may use the same algorithm as described in [1] to approximate the surface by 500 uniformly distributed dots. Choose a probe sphere of size 1.4 Angstrom. Use Bondi's van der Waals radii for the sizes of atoms (H: 1.20, C: 1.70, O: 1.52, N: 1.55 etc.)

Compute the solvent accessible surface area for each atom, then for each residue, and the total surface areas of the protein. Output the results in a text file called 2GB1-SASA.txt.

(Optional) Save protein structure and the dots that represent the protein surface into one file 2GB1-surface.pdb, and visualize the protein surface in a visualization software (e.g., Pymol).

Question to ponder: can you find analytical solutions to SASA?

Submission:
when you are finished and ready to submit, put your program, and the output files for each protein into a folder called hw2*yourLastName*. Zip up the folder into hw2*yourLastName*.zip. *Don't use other archivers than zip.*, and then upload it to the HW2 assignment in WebCT. Remember to hit the submit button, or your assignment will not be turned in; uploading is not enough. After submitting, double check that it went through by looking under the Submitted instead of the Inbox tab in the Assignment tool in WebCT.