Calculating surface electrostatic potential on a pre-computed molecular (Connolly) surface of a protein

How to run:

Check that you have all the input files: 2haq.pdb, amber.siz, amber.crg, 2haq_surf.pdb

To run it, type:

<path>/delphi param_conolly_protein.prm > connolly_prot.log

Press enter key, and you should get the results.

Output files: 2haq_surf.pot

*Note: <path> is the full path where the delphi executable file is located.

Details of the run:

This example is used to calculate the electrostatic potential on the molecular (Connolly) surface of a protein (PDB ID: 2haq, Cyclophilin of *Leishmania donovanii*, a beta-barrel protein). The pre-computed molecular surface (**Figure 1**) is fed to the program as a PDB file (2haq_surf.pdb) using the frc input option.

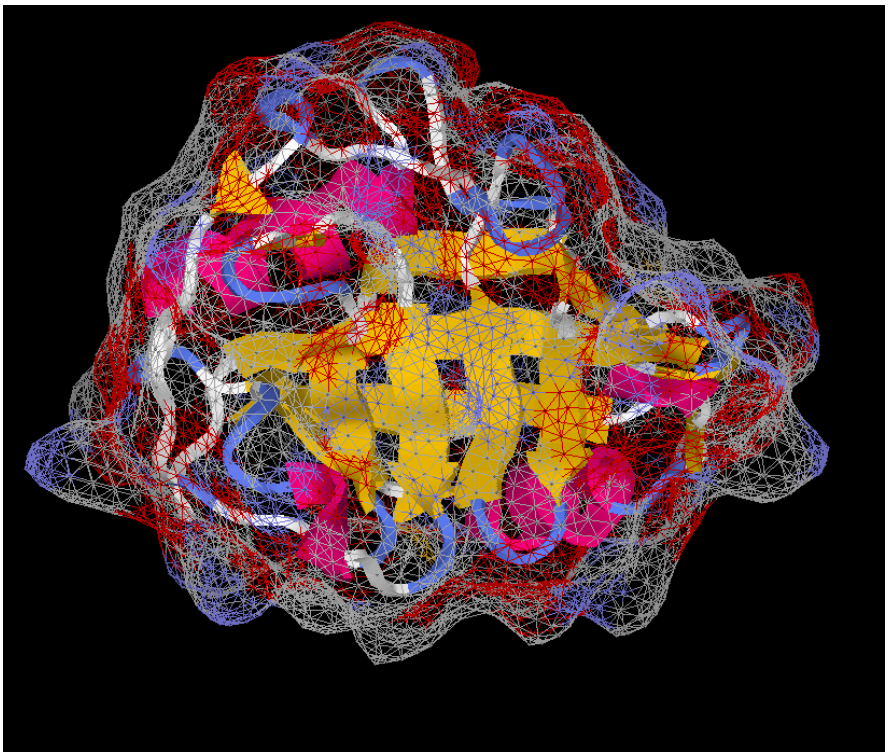

Figure 1. The molecular surface (represented as a colored mesh) of a protein, 2haq. The protein molecule is represented as a cartoon.

The outfile is written in ‘2haq_surf.pot’ which lists the surface potentials (as in the last column) against the dot surface points (x,y,z).

ATOM	DESCRIPTOR	ATOM COORDINATES (X,Y,Z)			GRID PT.
OE2	GLU X 24	-15.9830	14.6140	62.6810	-0.6038
NZ	LYS X 50	-16.1200	14.5880	63.7170	0.3311
CD	LYS X 50	-16.1600	15.7840	63.2490	0.3835
NZ	LYS X 50	-15.8870	14.7510	64.6580	-1.0425
CD	LYS X 50	-16.2650	15.6170	64.4630	-0.3934
CD	LYS X 50	-16.4140	16.5070	64.2580	1.3682
CD	LYS X 50	-16.0550	16.8770	63.5190	6.3464
CD	LYS X 50	-15.9610	16.6690	65.2220	6.2783
CD	LYS X 50	-15.9630	17.4500	64.4270	1.7405
OE2	GLU X 24	-15.0060	12.6750	61.5090	-2.0561
OE2	GLU X 24	-15.5670	13.7770	61.1920	-1.2264
OE2	GLU X 24	-14.9450	13.6050	60.3170	-1.4011
OE1	GLU X 24	-15.0440	12.7090	62.6120	-0.2108
OE2	GLU X 24	-15.6900	13.5840	62.1260	-1.2517
NZ	LYS X 50	-15.3800	13.4230	63.3290	-2.2103
OE2	GLU X 24	-15.2430	14.6740	60.6130	-22.9873
OE2	GLU X 24	-15.6920	14.6550	61.6480	3.3172
NZ	LYS X 50	-15.3610	13.7870	64.6020	11.5541
NZ	LYS X 50	-15.0550	13.8240	65.2230	59.1307
…	…	…			

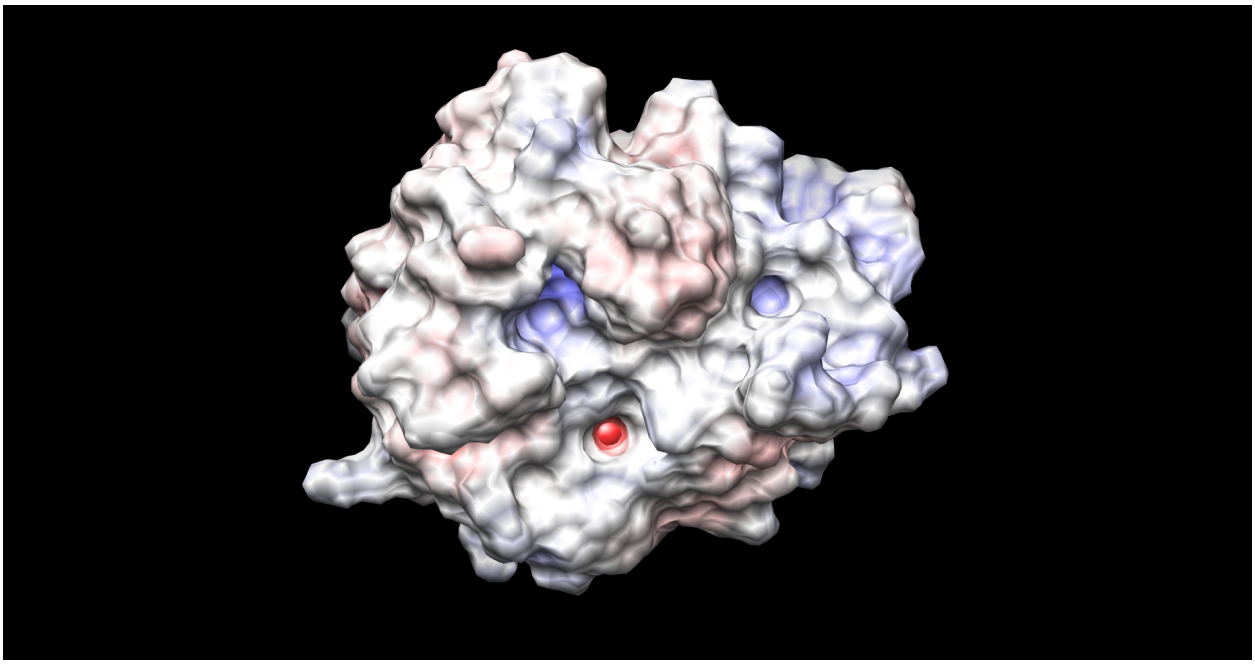

Figure 2. The electrostatic surface potential map of the protein 2haq drawn in chimera, using the output phimap option.

The molecular surface is computed by: https://zhanglab.ccmb.med.umich.edu/EDTSurf/

Ref: Xu, D.; Zhang, Y. Generating Triangulated Macromolecular Surfaces by Euclidean Distance Transform. *PLoS ONE* **2009**, *4* (12), e8140.