

ELECTROSTATIC POTENTIAL MAP

Steps

1. preparing the molecule by assigning partial charges and adding hydrogens and other missing atoms
2. calculating the electrostatic map
3. visualization of the charged molecular surface

1) Go to the PDB2PQR server ->

<http://server.poissonboltzmann.org/pdb2pqr>

Upload the pdb file—download the PQR file

2) Pymol->file->open pdb

Pymol--> Plugin--> APBS tools

(Under the "Main" tab of the PyMOL APBS Tools window)

Select RUN

3) Charmm GUI-

a) Register

2) <https://charmm-gui.org/?doc=input/pbeqsolver&step=2>

b) Upload pdb

c) Generate pdb2pqr

To view the PBEQ electrostatic map in PyMOL, please use the following steps:

d) download 'step2_pbeq.dx' and 'step2_pbeq.pdb'

e) open step2_pbeq.pdb in PyMOL

f) type following commands in PyMOL

PyMOL> load step2_pbeq.dx, map

PyMOL> show surface, step2_pbeq

PyMOL> ramp_new elvl, map,[-2,0,2]

PyMOL> set surface_color, elvl, step2_pbeq

g) if you want to draw solvent accessible surface, use following command:

PyMOL> set surface_solvent, 1

- h) if you want to change the electrostatic level in the map, adjust the value in 'ramp_new' command