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Basics of Using Grasp, Molscript, Raster3D, and Render to Generate Pictures

1. Start from 4 if you don't need surface

2. Generate electrostatic potential surface using Grasp

***Input**: test.pdb* ***Output**: test2.pdb & test2.surf*

1) Under SGI, type "grasp", this will open up the program.
2) Click right button of the mouse, choose "Read", then "PDB file", then "show list", then choose **test.pdb**.
3) If we suppose in **test.pdb**, the ligand name is LIG, then type "r=LIG,c=5". The ligand will be colored by purple, you can then rotate the whole molecule to the desirable orientation (click left button of the mouse and drag).
4) Click right button of the mouse, choose "Build", then "Molecular Surface", then "Enter String", then type "r=-LIG".
5) Click right button of the mouse, choose "Read", then "Radius/Charge File(+Assign)", then choose "full.crg".
6) Click right button of the mouse, choose "Calculate", then "New Potential Map".
7) Click right button of the mouse, choose "Calculate", then ""Pot. Via Map at Surfaces/Atoms", then "All atoms", then "All surfaces".
8) Click right button of the mouse, choose "Panels", then "Surfaces", then "Rendered", then quit "Panel".
9) Click right button of the mouse, choose "write", then "Grasp Surface file", then "Let me enter it", then type "test2.surf", then "Box and Rotated", then "All surfaces".
10) Click right button of the mouse, choose "write", then "Atom (PDB file)", then "Let me enter it", then type "test2.pdb", then "Box and Rotated", then "All atoms".
11) Click right button of the mouse and quit Grasp.

3. Convert the Grasp output surface file into Molscript input surface file

***Input**: test2.surf* ***Output**: surf*

Under SGI, type "convsurf", then following:
Input file format: **G** or **g**
Input file: **test2.surf**
Color by potential? **y**
How did GRASP say the max potential was? **10**
Clipping bounds: **y**
Output grid rather than surface? **n**
Invert normals? (**Hit Return**)
Raster3D or Molscript? **m**
Output file: **surf**

4. Generate Molscript file

Input: test2.surf surf Output: test2.input

1) Under Linux or SGI, type "molauto test2.pdb > test2.input".
2) If you want to incorporate surface, type "vi test2.input", before "end_plot", add "object surf;".
3) You can view, rotate, room in or out the picture by typing "molscript –gl –in test2.input".

5. Generate Raster3D file

Input: test2.input Output: test2.r3d

Under Linux or SGI, type "molscript –r <test2.input> test2.r3d".

6. Generate picture file

Input: test2.r3d Output: test2.tif

Under Linux or SGI, type "render –tiff test2.tif < test2.r3d". **test2.tif** can be displayed directly by typing "display test2.tif", or you can open it with programs like Photoshop on your PC or Mac.

Notes:

1) **test2.input** and **test2.r3d** are text files that can be modified directly.
2) For different renderings for protein or ligands, etc. modify **test2.input**.
3) For high resolution, different background, add light, shade, etc, modify **test2.r3d**.
4) For more details, you can go to the website (google search, key words are "grasp", "molscript", and "raster3d") or ask Xiyun.