Probe-Mesh tutorial around QM Cluster model

To run this tutorial, you need to have followed files:

probe_mesh_rin.py, 4urh_CS_A_h.pdb, 4urh_CS_A_h.probe, template_8.pdb & template44.pdb

Files can be found: https://github.com/MiloCheng17/RINRUS/tree/master/examples/mesh

Probe- The contact dot algorithm rolls a spherical probe of radius 0.25 Å (default) around the van der Waals surface of each atom and documents a series of "dots" when the probe touches another non-covalently bound atom. (radius can be change while generating probe using `(-Radius1.0)` keyword). Probe file and model file is already generated and given here.

Run following command using Python:

```
probe_mesh_rin.py -model template44.pdb -data 4urh_CS_A_h.probe
```

probemesh_rin.xyz and probemesh_rin.dat (and other .dat & .xyz) file will be created.

probemesh_rin.xyz is xyz file containing co-ordinates in H = hb (hydrogen bond), N = so,bo (big overlap), o = others form.

probemesh_rin.dat file contains xyz coordinates, type of contact, Atom it contact with and score. Example of probemesh_rin.dat is given below.

O 3.696 12.776 64.467 @ cc S:83:SER:CA S:481:HIS:HE2 0.000 0.0605

Once we have the XYZ file generated, we can open it in pymol with template PDB given in command.

```
Open probemesh_rin.xyz (OR any other .xyz file) and
template44.pdb in pymol
```

Colour, Atom, File info

probe_mesh000.dat probe_mesh000.xyz (Contains contacts where any one score is 0.000)

probe_meshXXX.dat probe_meshXXX.xyz (Contains contacts where both score is NOT 0.000)

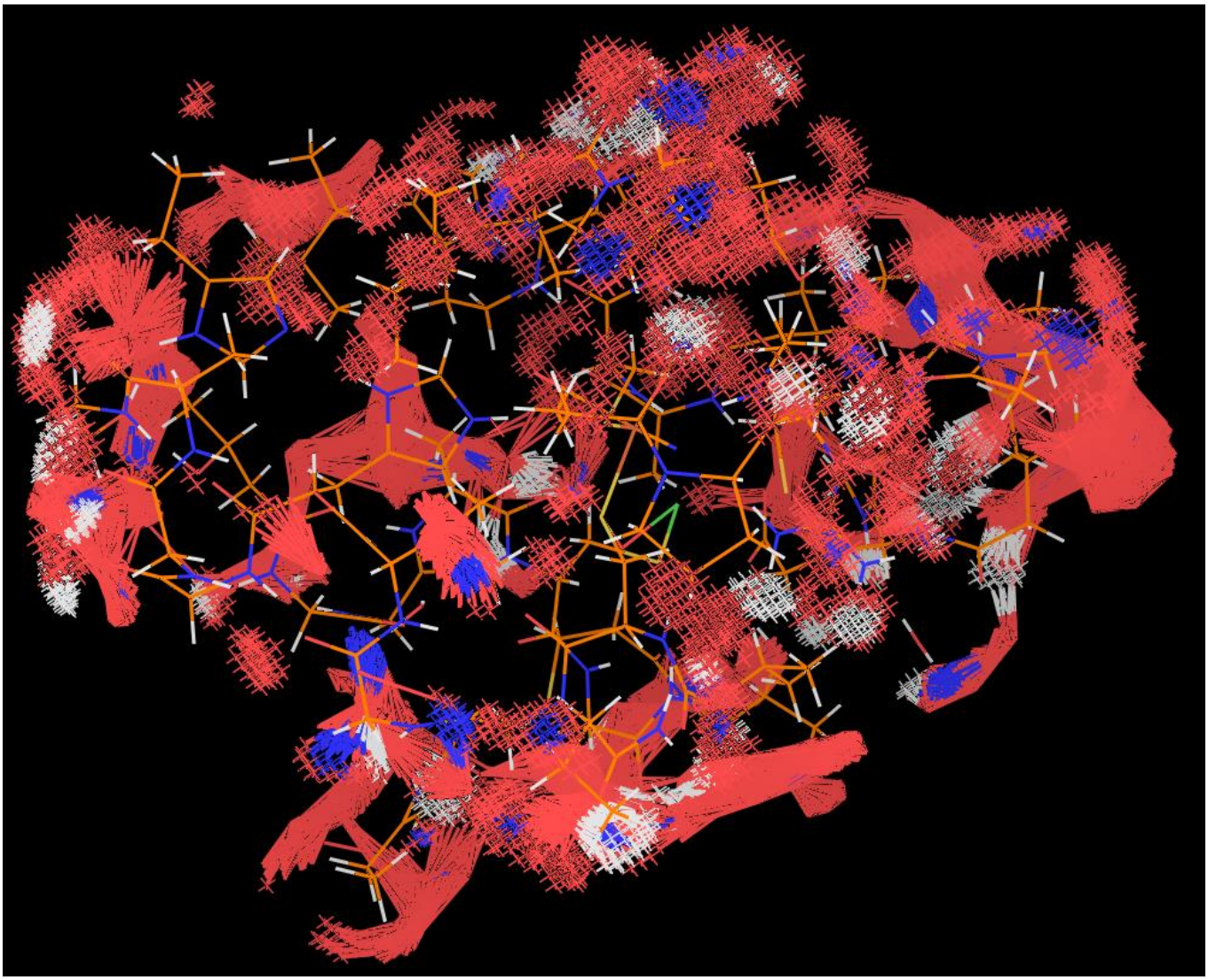
probe_meshCA.dat probe_meshCA.xyz (Contains contacts of CA atoms with other atoms)

probe_meshH.dat probe_meshH.xyz (Contains contacts with H= hb (hydrogen bond)) (White color)

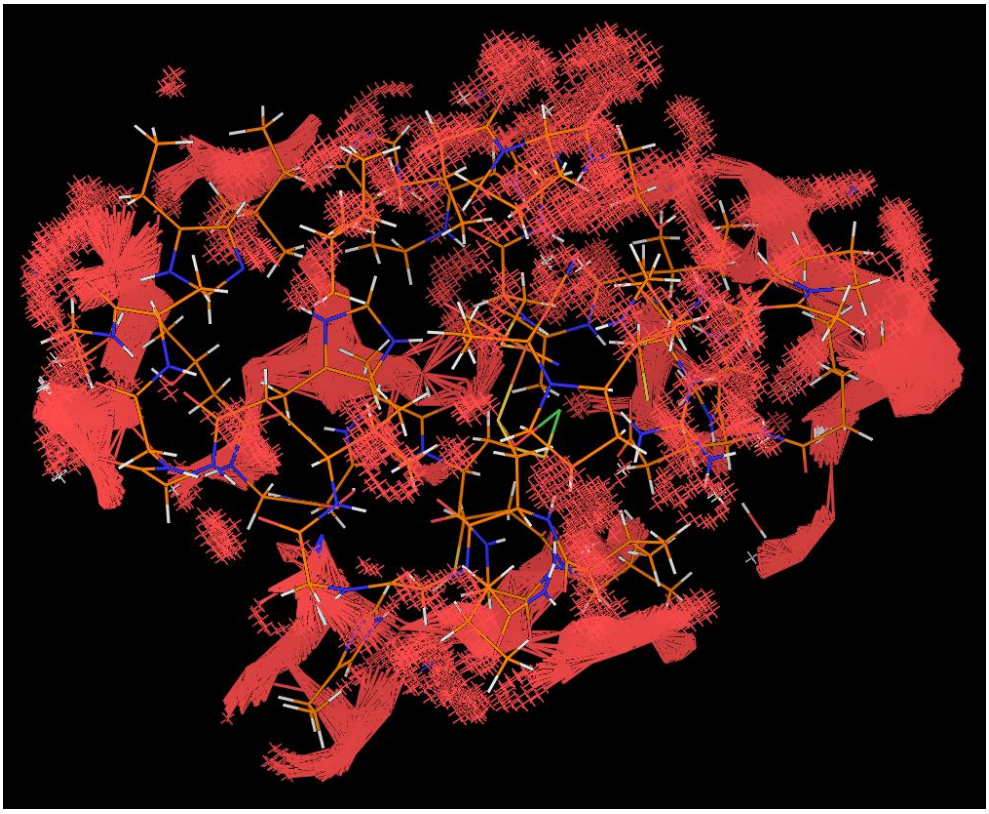
probe_meshN.dat probe_meshN.xyz (Contains contacts with N = so,bo (big overlap)(Blue Color)

probe_mesho.dat probe_mesho.xyz (Contains contacts with o = other than hb,so,bo)(Red color)

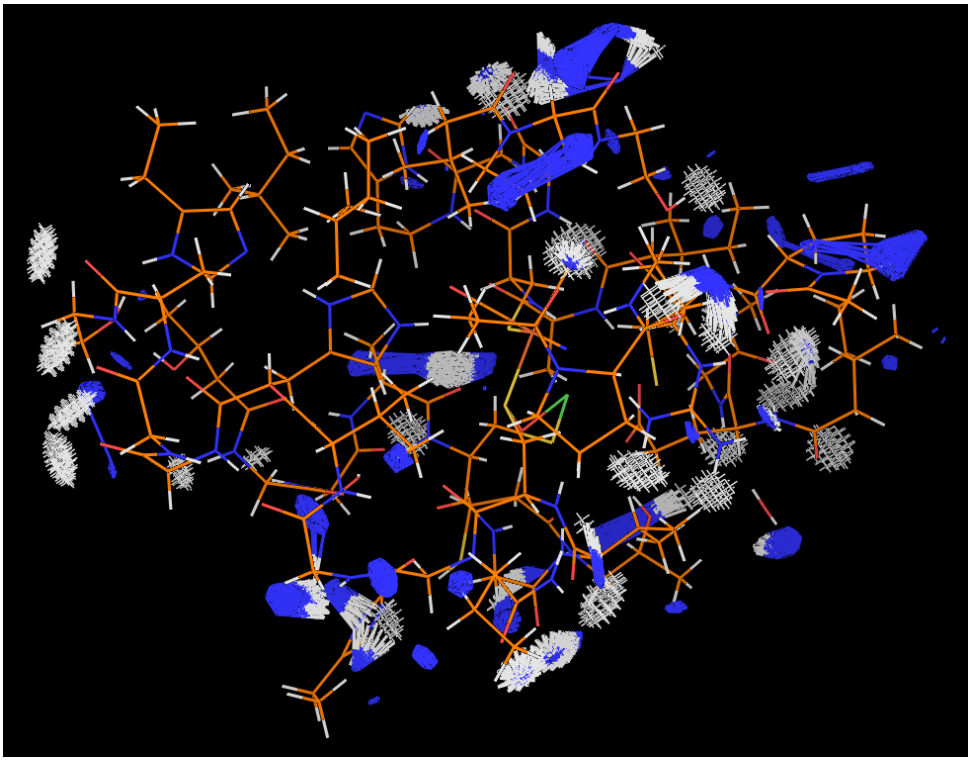
H(White) = hb (hydrogen bond), N(Blue) = so,bo (big overlap), o(Red) = others form.



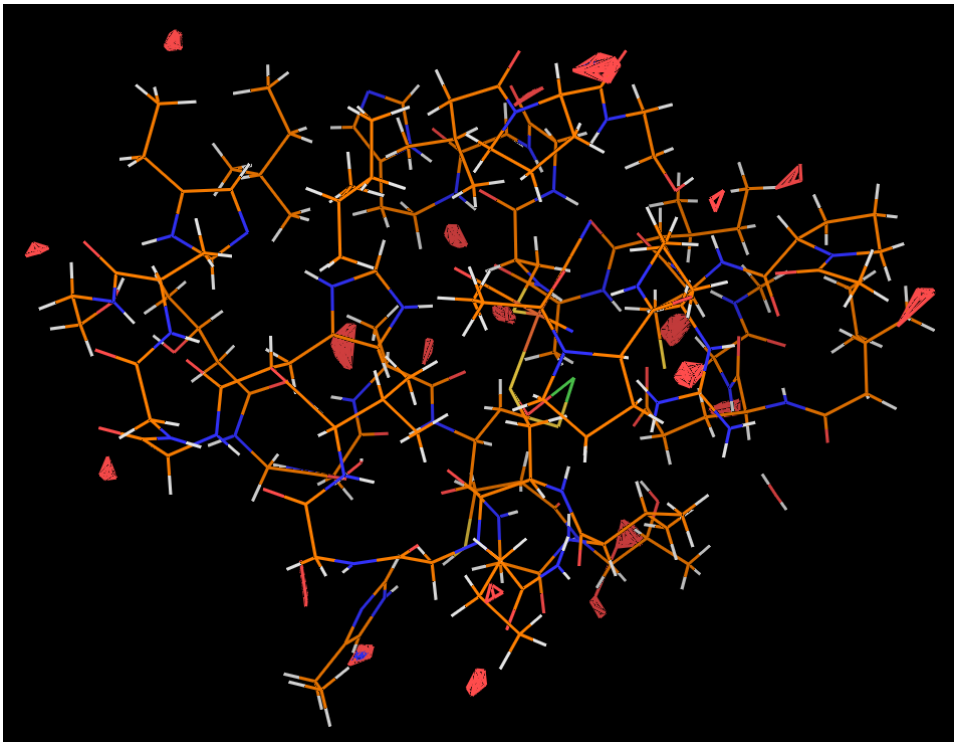
probemesh_rin.xyz



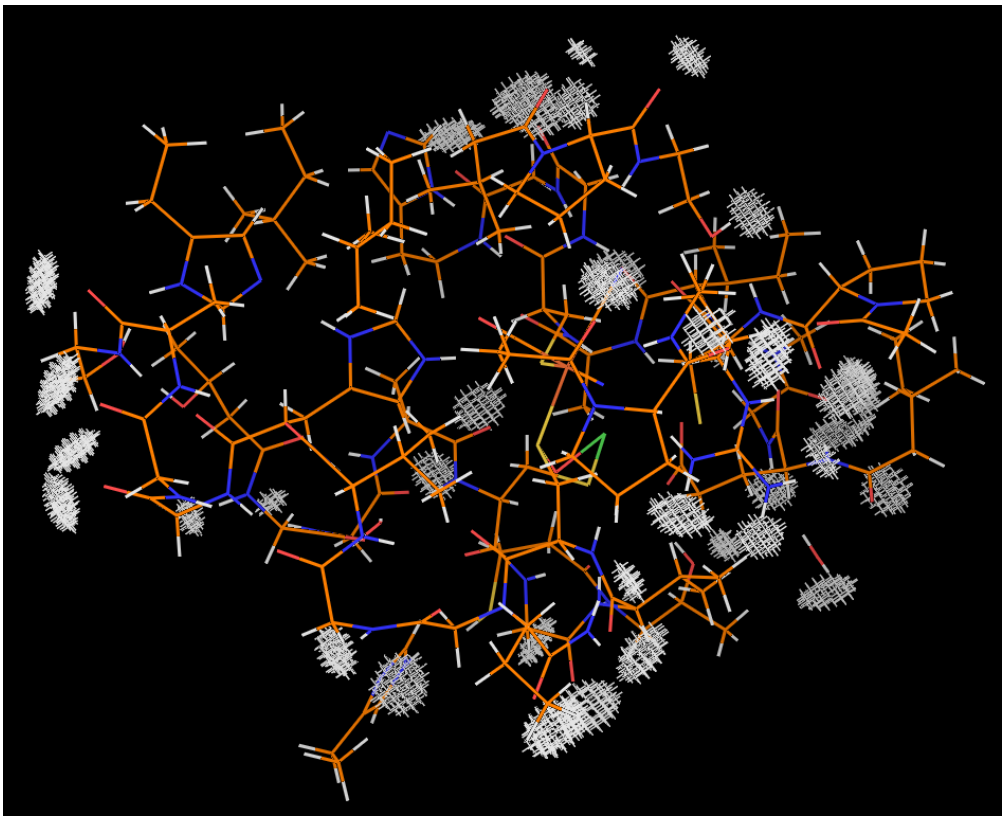
probe_mesh000.xyz



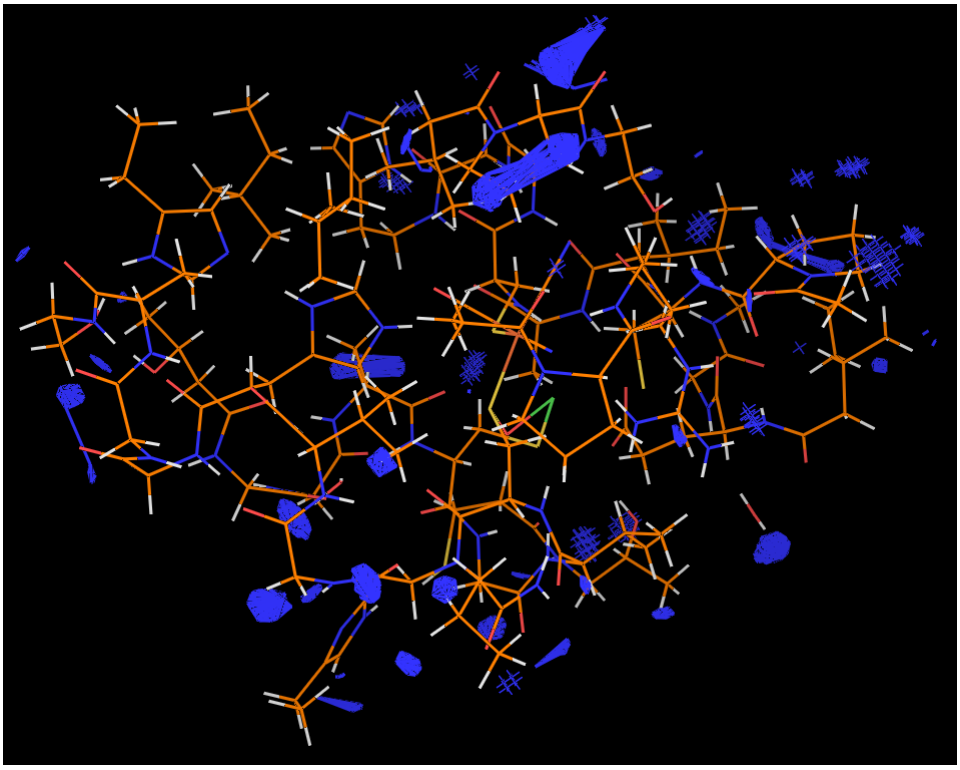
probe_meshXXX.xyz



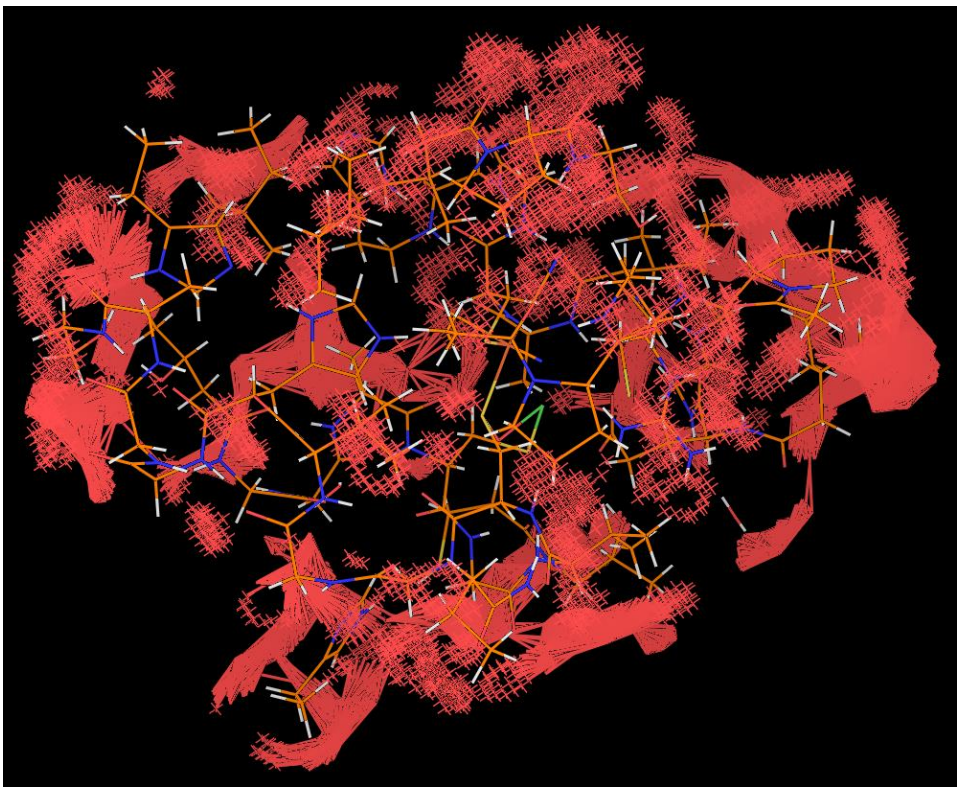
probe_meshCA.xyz



probe_meshH.xyz



probe_meshN.xyz



probe_mesho.xyz