

The 3dRPC web server

User Manual

3dRPC is an automatic program of building three-dimensional RNA-protein complex structures by docking RNA and protein structure. The input of the 3dRPC server is the structure of protein and RNA in PDB format. You can upload the structures by clicking the corresponding buttons. Here are some instructions before you upload your pdb structures:

- 1, Only 20 standard amino acids and 4 nucleic acids (ACGU) are accepted, other residues are ignored during the calculation.

- 2, Hydrogens are ignored.

- 3, Structures with missing atoms/residues are accepted.

Then, you can input the number of predictions. The 3dRPC server can generate corresponding number of complexes. Optionally, you can set interface residues or distance constraint in the advanced settings. Finally, submit your job by clicking the "Submit" button. Once a job is submitted to the 3dRPC server, a web page is displayed to show the rate of progress and the predicted result if the job is finished. A parameter file is also supplied. You can run 3dRPC with the parameter file if you have a local version of 3dRPC.

RPDock.receptor = 1DFU_r_u.pdb	file name of protein structure
RPDock.receptor.chain = V	chain id of protein
RPDock.ligand = 1DFU_l_u.pdb	file name of RNA structure
RPDock.ligand.chain = CB	chain id of RNA
RPDock.outfile = 1DFU.out	output file name of RPDOCK
RPDock.grid_step = 1	grid step of RPDOCK, 1 is recommended
RPDock.out_pdb = 10	number of complexes generated
RPDock.dc = 1.dc	distance constraint file
RPDock.li = 1.li	interface residues file
