PRIME Tutorial

The PRIME (Protein-RNA Interaction ModEling) approach to prediction of the 3D structure of protein-RNA complexes involves two steps: (1) search for a template from the template library, and (2) generating the model of the complex based on the selected template. Example with target protein-RNA complex 2I82, chains A and E, is in the directory “example” of the PRIME package.

Template search

Identifying a template from the library of 439 structures requires a parameter file *parameter_searching_model* (the example is for the 2I82 target structure):

```
native.receptor_pdb_filename = 2I82.pdb
native.receptor.chainid =  A
native.ligand_pdb_filename = 2I82.pdb
native.ligand.chainid  =  E
sort_by = complex_structure_score
out_model_pdb_number = 0
model_outfile = 2I82_AE
#LIB 1SER.pdb B 1SER.pdb T
...
#LIB 4OOG.pdb C 4OOG.pdb D
#LIB 2AB4.pdb A 2AB4.pdb B
...
```

The lines starting with #LIB are 439 template structures. The format: #LIB <protein pdb file> <protein chain id> <RNA pdb file> <RNA chain id>

PRIME is executed by running the following command in linux:

PRIME –mode 15 –system 3 –par parameter_searching_model

The output files:

**.TMalign* - protein alignments

**SARAalign.pdb* - RNA alignments

**normalized_file* - normalization value for the complex structure score

2I82_AE_sort_tmscore.transform - rank, TM-score, complex structure score, translation vector, rotation angles, and template ID.

In the example, the complex structure score and the TM-score are both 0.50, which is larger than the cutoff 0.45, thus 2AB4_AB is chosen as the template.

Generating model

Parameter file *parameter_building_model*:

```
native.receptor_pdb_filename = 2I82.pdb
native.receptor.chainid = A
native.ligand_pdb_filename = 2I82.pdb
native.ligand.chainid = E
sort_by = tmscore
out_model_pdb_number = 1
#LIB 2AB4.pdb A 2AB4.pdb B
```

Compared with the template search, this file has a single selected template (2AB4_AB), the *out_model_pdb_number* is 1, and the value of *sort_by* is changed to *tmscore*.

PRIME is executed by running the following command:

PRIME –mode 15 –system 3 –par parameter_building_model

The output files:

2I82.pdb_A_2AB4.pdb_A.TMalign - protein alignment

2I82.pdb_E_2AB4.pdb_B.SARAalign.pdb - RNA alignment

2I82_AE_sort_tmscore.transform - rank, TM-score, complex structure score, translation vector, rotation angles, and template ID.

2I82_E.normalized_file.pdb - normalization value

2I82_model_on_2AB4.pdb - model in PDB format

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