Peptide Co-Assembly Design Code User Manual

Running the code:

1. Prepare input structure

To run the Peptide Self Assembly (PepCAD) code the first step is to build the initial coordinate file (PDB fortmat) of the desired structure. The structure can be constructed in a molecule design package like Discovery Studio 3.5. Once the desired structure is built, it should be relaxed by running a short molecular dynamics simulation using a moleucular dynamics package to eliminate unfavourable atomic overlaps.

Save the PDB file as comp.pdb. Add N and C to the terminal amino acids of each peptide (for example, NHIE). Delete TER lines.

2. Edit the input file

The input file looks like the following. The input file can be edited as per the requirements of the project

filename
Name of the initial input structure file, (e.g. : comp.pdb)

recalcu_switch
Equal to zero if starting from the original pdb file (eg: comp.pdb); equal to 1 if restarting from another file

nstep_start
The starting step number

nstep_terminal
The final step number (typically 10000)

idum
The seed for the random number

ekt
A value determined empirically determined (typically ≤ 1) for each project. It is referred to as $kT_{sequence}$.

num4category(i)
Sheet number for a β sheet type structure

peptideID(i)
Peptide number on the sheet (i)

peptideID(i+1)
Peptide number on the sheet (i)

peptideID(i+2)
Peptide number on the sheet (i)

peptideID(i+3)
Peptide number on the sheet (i)

fpho_peptide(i)
No. of hydrophobic residues in peptide(i)

fpos_peptide(i)
No. of charged residues in peptide(i)

fneg_pepide(i)
No. of charged residues in peptide(i)

fpol_peptide(i)
No. of hydrophilic residues in peptide(i)

foth_peptide(i)
No. of charged residues in peptide(i)

3. Submitting the job

To be able to submit a PepCAD join the following files should be present in the directory:

a. main.f90 (Main code file)
b. comp.pdb (starting input structure file)
c. lib folder (directory containing the amber forcefield data)

d. pdbfiles (an empty directory where the PDB files from the design will be stored)
e. input.txt (the input file)

Once all the above files are present in the directory the main.f90 code can be compiled using a fortran compiler and the job can be submitted. An example of a command that can be used to compile the code using the ifort compiler:
ifort -O3 -r8 -o main main.f90

Details of PepCAD output files

energydetails.txt

step	attempt	score	binding energy	entropy	score4hydration	$P_{aggregation}$	Type of move: Not SCMF: Residue mutation Intra SCMF: Intra chain residue exchange

energyprofile.txt

step	score	binding energy	entropy	score4hydration	$P_{aggregation}$

minimumenergy.txt

step	attempt	score