GDNF Alignment with Bicyclic CLIPS

Rohit Shankar

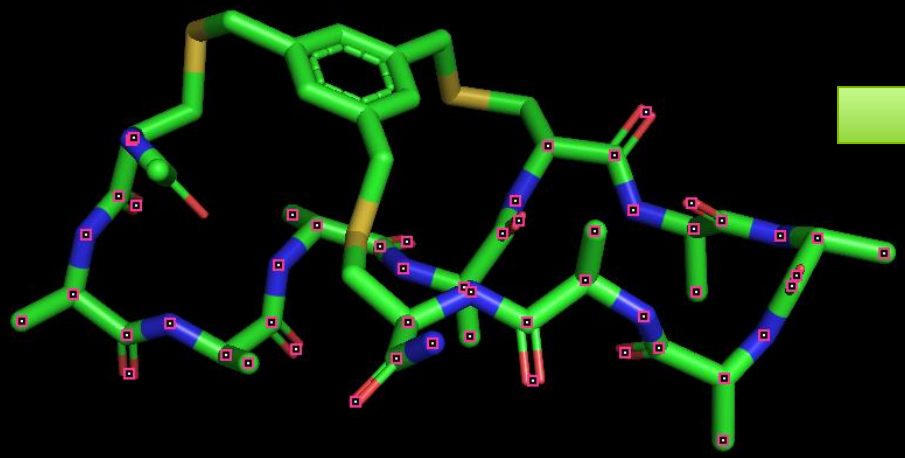
GDNF Alignment Procedure

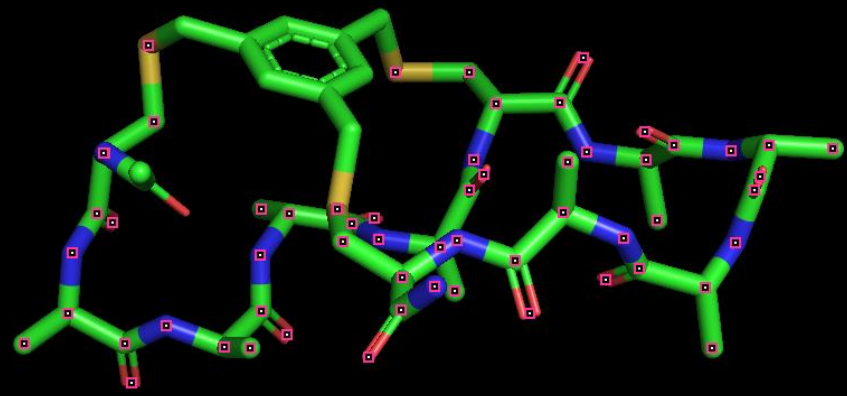
Python Commands for Alignment

- Procedure:
- Open bicyclic CLIPS file.
- Select residues of both rings in bicyclic
- Open GDNF single loop file.
- Align GDNF with selection of bicyclic.

- Commands:
- Cmd.load(“Bicyclic”)
- Cmd.Select(“Residue numbers”)
- Cmd.load(“GDNF”)
- Cmd.align(“GDNF i. residue numbers”, “Bicyclic”)

Procedure Visualized





```
/4A-4A2_2932///      1                   6                  11
               UNK 0 UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
    /gdnfpdb//F/ 209     211                 216                 221
               UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK UNK
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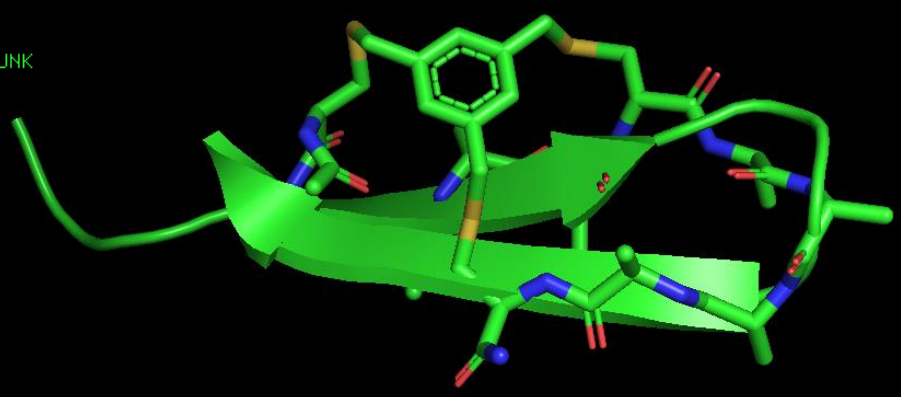


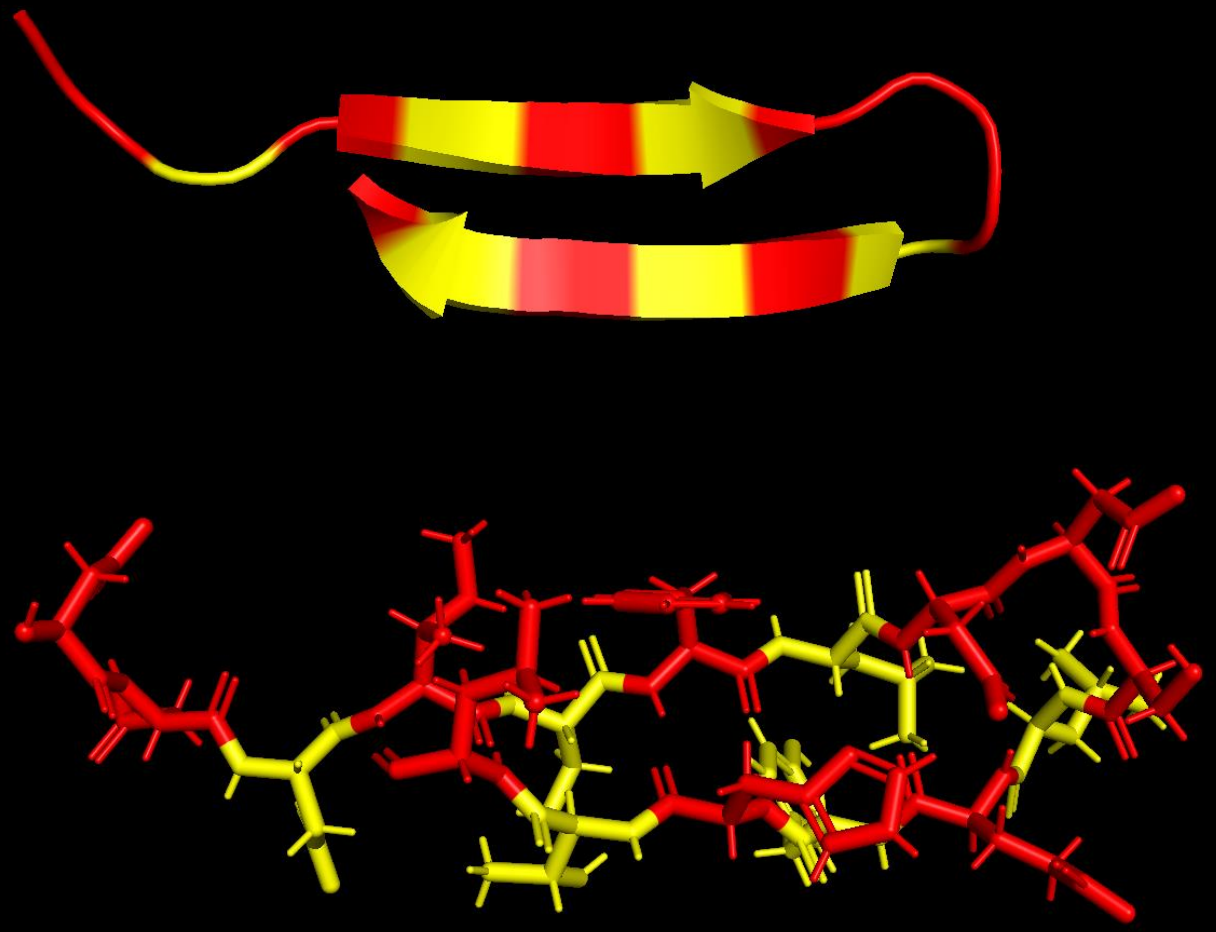
Selecting GDNF Residues for Alignment

GDNF Alignment Residues

- Residue available for mutation had to be upward facing for cysteine. Red portions of next picture.

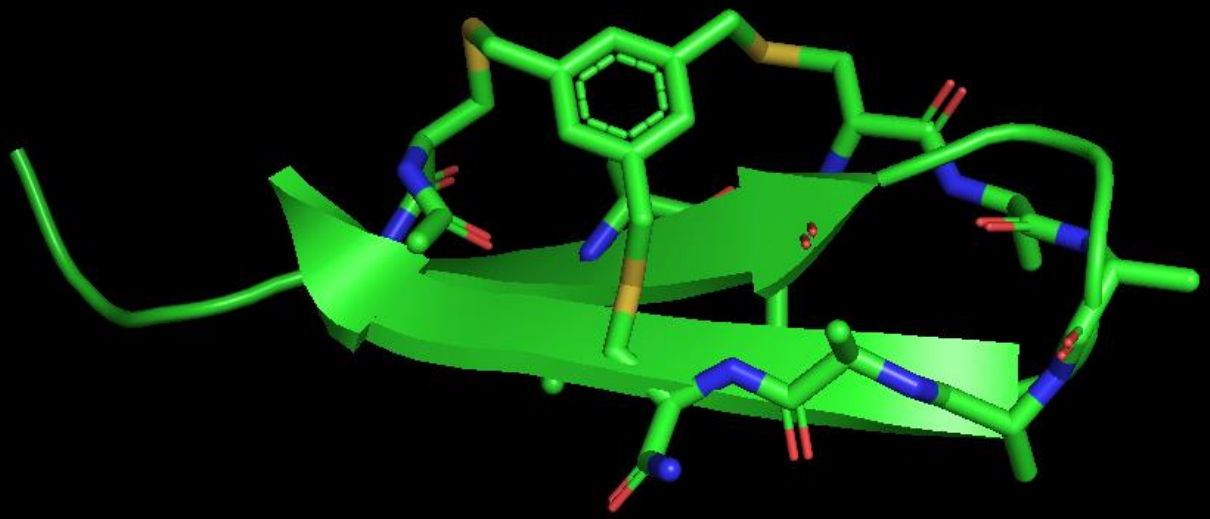
- Alignment residues starts with right ring cysteine finding starting mutating point such that middle cysteine and left ring cysteine are also on mutation points. Right ring cysteine tests GDNF residue id 220,222, and 224.

GDNF Loop



GDNF Alignment Results/Pictures

Alignment Length 4 Example



Alignment 4A-4A2_2932
RMSD: 2.025

Alignment Results

RMSD	File Name	GDNF Selection
2.025034	4A-4A2_2932.mol2	2 1 2 - 2 2 2
2.832149	5A-5A1_3384.mol2	2 1 0 - 2 2 2
2.956409	4A-6A7_3538.mol2	2 1 0 - 2 2 2
3.199573	6A-7A5_4007.mol2	2 0 9 - 2 2 4
3.251551	3A-8A1_5918.mol2	2 0 9 - 2 2 2
3.823663	3A-9A8_2662.mol2	2 1 0 - 2 2 4
4.103341	3A-10A4_1984.mol2	2 0 9 - 2 2 4