BT305 LAB 8

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Section 1

From the video, we can observe that the Trpcage protein at 363 K is more actively moving around the space and water molecules than the protein at 300 K.

Section 2

Exercise 1:

1)

Trpcage:

```
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

CmdLoad: "" loaded as "new_trp".

Match: read scoring matrix.

Match: assigning 19 x 20 pairwise scores.

MatchAlign: aligning residues (19 vs 20)...

MatchAlign: score 96.000

ExecutiveAlign: 19 atoms aligned.

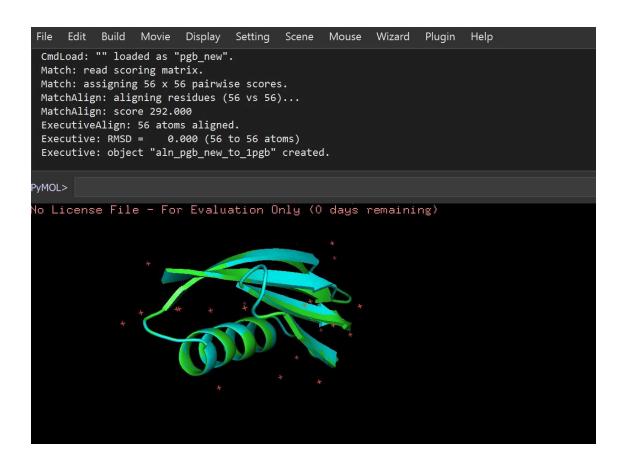
Executive: RMSD = 0.000 (19 to 19 atoms)

Executive: object "aln_new_trp_to_adityaatrp" created.

PYMOL>

No License File - For Evaluation Only (0 days remaining)
```

1PGB:



2)

ALA: N[C@H](C(=O)N[C@H](C=O)C)C

PHE: N[C@H](C=O)Cc1ccccc1
GLU: N[C@H](C=O)CCC(=O)O
LYS: N[C@H](C=O)CCCCN

Exercise 2:

Q) Convert trp.pdb to smiles format:

Ans

 $\label{eq:normalized_normalized} N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)N[C@H](C(=O)NCC(=O)NCC(=O)NCC(=O)N1[C@H](C(=O)N[C@H](C(=O)NCC(=O)N1[C@H](C(=O)N1$