Progress report for week #2

Since last Thursday was working on the following things:
1. Got ConSurf evaluations on across-species conservations for morph pairs from MMDB database;
2. Combined the torsion angle fluctuation of a protein with its conservation score;
3. Finished reading Sam's articles on hinge analysis.
4. Currently working on cutting the target proteins pool to only the hinge region and analyzing the torsion angle change of the hinge regions.

For the past week I was able to get the across-species conservation evaluation via ConSurf server with the guide from Declan. The proteins we submitted onto the ConSurf server were morph pairs from MolMovDB, where a ~400 protein morph candidates were available. For those PDBs from the database, around 1/2 were trackable (the PDB ID could be tracked), and around ~80 morphs were covered on ConSurf. There are "holes" in the ConSurf scoring output due to the inaccessibility of certain residues of that PDB stored in ConSurf served, and thus we obtained 76 complete ConSurf analysis for the morphs for analysis.

In order to combine the conservation information to the dihedral angle calculation, a python script was developed that would align the two. Starting from the 4th residue in each PDB file, the conservation information, torsion angle for the two structures for that residue was aligned in the same row. This made the information easier to process in R. In the figure below is what the file looks like. "Resname" is also listed after "resid" for easier tracking.

```
resid   resname score   ini_torsion     fin_torsion     difference
4       SER     -0.088  257.605602114   271.771793868   14.1661917537
5       ILE     -0.153  204.364700705   213.358016706   8.99331600043
6       ASN     0.631   261.595428401   250.418749822   11.1766785795
7       GLU     -0.132  66.3618750971   71.1878607284   4.82598563121
8       CYS     0.984   50.8057137392   50.3443192349   0.461394504371
9       ASP     0.030   100.45180765    94.258061506    6.19374614393
10      LEU     0.462   234.178516646   232.859352256   1.31916438993
11      LYS     1.435   158.960504324   163.163308119   4.20280379512
12      GLY     0.196   116.456335108   123.119790743   6.66345563461
13      LYS     -0.829  0.502611666139  351.164207152   350.661595486
14      LYS     -0.324  130.91463748    128.205996295   2.70864118515
15      VAL     -0.925  224.365955067   235.731653818   11.3656987514
16      LEU     -0.393  207.545400507   205.004136938   2.54126356861
17      ILE     -0.417  207.310958755   210.873870759   3.56291200365
```

For analyzing the correlation between dihedral angle changes and conservation, a simple plot was made for quick observation. From the plot below, we could not observe obvious signal o trend simply upon the scattering plot, and further analysis was called for for more insights. One thing I am working on right now is to focus only on the hinge region, taking from the candidate morphs from *Hinge Atlas* database by S. Flores, and analyzing the relationship of torsion angle change with the conversation scores. In this way the noise from the "non-flexible" regions would be reduced.

relationship btw conservation and conformation change

conservation score

difference of CA torsion angel from initial to final structure