Molecular Analysis Scripts Collection

1. select_pose

This script automates the extraction of a specific pose from a molecular dynamics trajectory using cpptraj.**Functionality:**

- Allows user to select a specific pose
- Centers the pose based on a specified residue range
- Saves the pose as a PDB file

Usage:

1. Run the script
2. Provide the following inputs when prompted:
    - Pose number to extract
    - Parm file (*.prmtop)
    - Trajectory file (*.mdcrd or *.dcd)
    - Residue range for centering

Output: A PDB file with the pose number as filename (e.g., 1.pdb for pose 1)

2. clustering

This script automates the clustering of molecular dynamics snapshots using cpptraj.**Functionality:**

- Performs k-means clustering on molecular trajectories
- Allows specification of parameters such as number of clusters and sieve value

Usage:

1. Run the script
2. Provide the following inputs:
    - Topology file (*.prmtop)
    - Trajectory file (*.dcd or *.mdcrd)
    - Snapshot range to analyze
    - Residue range for RMSD calculations
    - Number of clusters
    - Sieve value for clustering
    - Maximum iterations for k-means algorithm
    - Inclusion of hydrogens in RMSD calculation

Output:

- cnumvtime.dat: Cluster assignment for each frame
- summary.dat: Clustering process summary
- info.dat: Detailed clustering information
- rep/avg.pdb: Representative and average structures in PDB format
- singlerep.nc: Representative structures in NetCDF format

3. trajectory_to_rmsd

This script automates the calculation of Root Mean Square Deviation (RMSD) for a specific range of residues in a molecular dynamics trajectory.**Functionality:**

- Calculates RMSD of specified residues relative to the first frame of the trajectory

Usage:

1. Run the script
2. Provide the following inputs:
    - Topology file (*.prmtop)
    - Trajectory file (*.mdcrd or *.dcd)
    - Residue range to analyze
    - Base name for output file

Output: An RMSD plot file (*.agr) containing RMSD data

4. rmsd_columns

This script processes multiple RMSD data files (*.agr format), extracts the data, and combines them into a single CSV file.**Functionality:**

- Combines RMSD data for receptor, ligand, and ligand-receptor system
- Aligns datasets and fills with empty cells where data is missing

Usage:

1. Run the script
2. Provide names of three RMSD files:
    - Receptor RMSD file
    - Ligand RMSD file
    - Ligand+receptor RMSD file

Output: A CSV file (rmsd_columns.csv) with combined RMSD data

5. hbond_average

This script performs hydrogen bond analysis on a molecular dynamics trajectory using cpptraj.**Functionality:**

- Calculates hydrogen bond contacts within a specified residue range
- Option to include intramolecular hydrogen bonds

Usage:

1. Run the script
2. Provide the following inputs:
    - Parameter file (*.prmtop)
    - Trajectory file (*.dcd or *.mdcrd)
    - Residue range to analyze
    - Inclusion of intramolecular hydrogen bonds

Output: A file (avg_hbond.dat) with average hydrogen bond contact data

6. total_hbond_interactions

This script performs detailed hydrogen bond analysis on a molecular dynamics trajectory for a specified residue range.**Functionality:**

- Calculates number of hydrogen bond interactions for each frame
- Generates CSV files with detailed data and summaries

Usage:

1. Run the script
2. Provide the following inputs:
    - Parameter file (*.prmtop)
    - Trajectory file (*.dcd or *.mdcrd)
    - Number of frames in trajectory
    - Residue range to analyze
    - Inclusion of intramolecular hydrogen bonds

Output:

- hbond_summary.csv: Summary of hydrogen bond interactions
- interactions_per_frame.csv: Number of interactions per frame

7. watershell

This script performs water shell analysis on a molecular dynamics trajectory using cpptraj.**Functionality:**

- Analyzes water molecule interaction within a specified residue range

Usage:

1. Run the script
2. Provide the following inputs:
    - Parameter file (*.prmtop)
    - Trajectory file (*.dcd or *.mdcrd)
    - Residue range to analyze

Output: A file (watershell.out.dat) with water shell analysis results

8. solvation_spheres_average

This script calculates average solvation shell values based on data from a watershell.out.dat file.**Functionality:**

- Calculates average for first and second solvation shells

Usage:

1. Run the script (requires a pre-existing watershell.out.dat file)

Output: A file (solvation_average.txt) with solvation shell averages

9. lie

This script automates Linear Interaction Energy (LIE) analysis using cpptraj.**Functionality:**

- Calculates interaction energy between a ligand and receptor for each frame of a trajectory

Usage:

1. Run the script
2. Provide the following inputs:
    - Parameter file (*.prmtop)
    - Trajectory file (*.dcd or *.mdcrd)
    - Ligand residue range
    - Receptor residue range

Output: A file (lie.dat) with LIE analysis results