Description: Here I am sharing a package containing scripts for SIFt analysis. These tools enable the user to compare the SIFts of docked ligands with a averaged reference SIFt by calculating the Tanimoto coefficients. Additionally, the script analyzes all input SIFts values of docked ligands to find and characterize (by numbering) amino acids involved in interactions with the ligand in the active center of target protein.

Manual: To run the tool, paste "python sequence\_analysis.py" in the terminal. The script requires a file containing SIFts of the docked ligands, ending with "fp.dat", in the same directory. To save the output to some file, paste "python sequence\_analysis.py > filename.txt" in the terminal. It is worth mentioning that the reference\_sift\_map list in the main() function in the sift\_parser.py script can be freely edited to adjust the number of SIFts references to specific tasks.

Comment: The regex pattern contained in these scripts may not be suitable for another user, so you may need to define the regular expression pattern yourself.