**Python codes and input files for the PS I-TSR project**

1. TSR key generation code for proteins using C alpha atoms (KeyGen\_CA\_Tarikul.py)
2. TSR key generation code for pigments using all atoms except hydrogen atoms (Drug\_Triplets\_Keys\_Cal\_Atom\_Selection\_in\_Sample.py)
3. TSR key generation code for tryptophan using all atoms except hydrogen atoms (aa\_Triplets\_key\_cal\_trp\_dist58.py)
4. USR code for proteins using C alpha atoms (usr\_similarity\_atomic\_distance\_psi\_a\_b\_ca.py)
5. USR code for pigments using all atoms except hydrogen atoms (usr\_similarity\_atomic\_distance\_psi\_chl\_atom\_selection.py)
6. USR code for tryptophan using all atoms except hydrogen atoms (usr\_similarity\_atomic\_distance\_psi\_a\_b\_trp.py)
7. RMSD code for pigments using all atoms except hydrogen atoms (rmsd\_modified\_atom.py)
8. RMSD code for tryptophan using all atoms except hydrogen atoms (rmsd\_modified\_trp\_a\_b.py)
9. aminoAcidCode\_lexicographic\_new.txt (input file for TSR key generation code for proteins using C alpha atoms)
10. drug\_atom\_lexical\_txt.csv (input file for TSR key generation code for pigments using all atoms except hydrogen atoms and for TSR key generation code for tryptophan using all atoms except hydrogen atoms)
11. sample\_details\_psi\_ab\_mix1.csv (input file for TSR key generation code for proteins using C alpha atoms and for TSR key generation code for tryptophan using all atoms except hydrogen atoms)
12. sample\_details\_et\_mix5\_name\_id\_atom.csv (input file for TSR key generation code for pigments using all atoms except hydrogen atoms)
13. Supplementary File 1 (Supplementary\_File1\_Sample\_Details.csv for protein global analyses)

All other TSR-method related source code is available for academic users on GitHub: https://github.com/tarikulislammilon/TSR and <https://github.com/WuXu26/Protein-3D-TSR>. If you have any questions about the Python codes, please contact Dr. Wu Xu at [wxx6941@louisiana.edu](mailto:wxx6941@louisiana.edu). If you need supercomputer access to run any of the Python codes, please contact us. We can provide access to the supercomputers up to ten scientists and for them to use the TSR method at a time.