**Python codes and input files**

1. TSR key generation code for proteins using C alpha atoms
2. TSR key generation code for pigments using all atoms except hydrogen atoms
3. TSR key generation code for tryptophan using all atoms except hydrogen atoms
4. USR code for proteins using C alpha atoms
5. USR code for pigments using all atoms except hydrogen atoms
6. USR code for tryptophan using all atoms except hydrogen atoms
7. RMSD code for pigments using all atoms except hydrogen atoms
8. RMSD code for tryptophan using all atoms except hydrogen atoms
9. aminoAcidCode\_lexicographic\_new.txt
10. drug\_atom\_lexical\_txt.csv
11. sample\_details\_psi\_ab\_mix1.csv
12. sample\_details\_et\_mix5\_name\_id\_atom.csv

The 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 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 for the ten scientists who want to use the TSR method at the same time.