rar file contains 5 .py files

1. FMO+Eg
2. FMO+Eg+Descriptor
3. FMO+Eg+Fingerprints
4. Generating Similarity Scores
5. Mordred Descriptor Generation

For 1, 2 and 3 requirements.txt should be used for creating the environment.

For 4 and 5 saperated environment should be used by installing RDKit and Mordred package.

 and 9 .csv files

1. FMO+Eg
2. FMO+Eg+RDKIT
3. FMO+Eg+Mordred
4. FMO+Eg+Extended
5. FMO+Eg+MACCS
6. FMO+Eg+Pubchem
7. FMO+Eg+Morgan
8. Molecular Similarity
9. Mordred Descriptior Generation

While running .py files .csv files are used as input. In .py files all the file input commands are written in comments. Uncomment the desired file and leave all other input files in comment only.