## **Files**

1. ZINC-downloader-2D-smi.wget
2. Data\_preparation.ipynb
3. zinc20\_selected\_to\_create\_model\_processed.parquet
4. RORgamma\_active\_compounds.xlsx
5. ROR\_gamma\_active\_QED\_Lipinski.ipynb
6. ROR\_gamma\_active\_QED\_Lipinski.xlsx
7. SYBA\_class\_ROR\_gamma\_activ\_AFTER\_QED\_LIPINSKI.ipynb
8. Prediction\_initializers\_ROR\_activ.xlsx
9. SELFIES\_coder.py
10. UniCode\_char.csv
11. Molecule\_generator-Generative\_neural\_network.py
12. SELFIES\_to\_mol\_seq.json
13. mol\_seq\_to\_SELFIES.json
14. mol\_seq\_to\_int.json
15. int\_to\_mol\_seq.json
16. mol\_seq2lat\_ZINC.h5
17. lat2state\_ZINC.h5
18. samplemodel\_ZINC.h5
19. Prediction\_1\_0.1\_tensor\_scaling.ipynb
20. Prediction\_2\_0.2\_tensor\_scaling.ipynb
21. Molecules\_generated\_tensor\_scaling\_0\_1.xlsx
22. Molecules\_generated\_tensor\_scaling\_0\_2.xlsx
23. Selection\_from\_0\_1\_tensor\_scaling.ipynb
24. Selection\_from\_0\_2\_tensor\_scaling.ipynb
25. Selected\_molecules\_from\_0\_1\_tensor\_scaling.xlsx
26. Selected\_molecules\_from\_0\_2\_tensor\_scaling.xlsx
27. Combine\_Generated\_and\_Selected\_structures.ipynb
28. Assigning\_prediction\_mode\_to\_selected\_SMILES.ipynb
29. All\_generated\_SMILES\_QED\_Lipinski.xlsx
30. SYBA\_classifier\_additional\_filter.ipynb
31. All\_generated\_SMILES\_SYBA\_filtration.xlsx
32. All\_generated\_SMILES\_visualization.ipynb
33. Python\_molecular\_docking.py
34. Tanimoto\_similarity-SYBA\_selection.ipynb
35. Tanimoto\_similarity\_All\_generated\_and\_selected.ipynb
36. Checking\_if\_ROR\_gamma\_activ\_are\_in\_ZINC\_db.ipynb
37. dockingResults\_ROR\_gamma\_SYBA\_selected.xlsx
38. Clean\_results.ipynb
39. Selection\_of\_most\_prominent\_structures.ipynb
40. SMILES\_to\_3D\_PDB.ipynb
41. My\_score\_to\_final\_structures.ipynb
42. dockingResults\_ROR\_gamma\_SYBA\_CLEAN.xlsx
43. Reference\_dockings folder
44. 7npc\_structure\_of\_native\_ligand.dlg
45. 7NP5\_structure\_of\_native\_ligand.dlg
46. 7KXD\_structure\_of\_native\_ligand.dlg
47. master\_thesis\_calculations.xlsx