Files

1. Indole\_-\_cytoprotekcja\_.xlsx
2. Training\_data\_preparation.ipynb
3. test\_training\_data\_smiles.parquet
4. Neural\_network.ipynb
5. Prediction\_1\_0.1\_tensor\_noise.ipynb
6. Prediction\_1\_0.2\_tensor\_noise.ipynb
7. Molecules\_generated\_tensor\_scaling\_0\_1.xlsx
8. Molecules\_generated\_tensor\_scaling\_0\_2.xlsx
9. Predictive\_model-Decision\_Tree-Train.ipynb
10. Predictive\_model-KNeighbors.ipynb
11. Predictive\_model-Random\_forest.ipynb
12. Predictive\_model-SVM.ipynb
13. Predictive\_model.ipynb
14. create\_whole\_report.py
15. Whole\_report.xlsx
16. gramina\_tiouracyle\_pred\_pic.xlsx
17. Generated\_structures\_PubChem\_search.ipynb
18. new\_structures\_indole.xlsx
19. Tanimoto\_similarity\_report.ipynb
20. Proposed\_structures\_with\_AI\_indole\_tanimoto\_similarity\_.xlsx
21. Tanimoto\_similarity\_pictures.ipynb
22. SYBA\_selected\_structures\_similarity.xlsx
23. t-SNE\_chemical\_space.ipynb