

## Files

The files pertaining to the conducted study have been consolidated on GitHub's platform and are accessible through this link: [https://github.com/XDamianX-coder/Colchicine\\_ML](https://github.com/XDamianX-coder/Colchicine_ML)

File 1. Kolchicyna\_prepared\_data.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/Kolchicyna\\_prepared\\_data.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/Kolchicyna_prepared_data.xlsx)

File 2. training\_data\_preparation.py

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/training\\_data\\_preparation.py](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/training_data_preparation.py)

File 3. training\_smiles.parquet

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/training\\_smiles.parquet](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/training_smiles.parquet)

File 4. neural\_network.py

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/neural\\_network.py](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/neural_network.py)

File 5. mol\_seq2lat.h5

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/mol\\_seq2lat.h5](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/mol_seq2lat.h5)

File 6. lat2state.h5

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/lat2state.h5](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/lat2state.h5)

File 7. samplemodel.h5

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/samplemodel.h5](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/samplemodel.h5)

File 8. Neural\_network\_log.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/Neural\\_network\\_log.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/Neural_network_log.ipynb)

File 9. do\_predictions.py

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/do\\_predictions.py](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/do_predictions.py)

File 10. AI\_generated\_Molecules\_0\_1\_.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/AI\\_generated\\_Molecules\\_0\\_1\\_.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/AI_generated_Molecules_0_1_.xlsx)

File 11. AI\_generated\_Molecules\_0\_2\_.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/AI\\_generated\\_Molecules\\_0\\_2\\_.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/AI_generated_Molecules_0_2_.xlsx)

File 12. Data\_transformation.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Data\\_transformation.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Data_transformation.ipynb)

File 13. Kolchicyna\_machine\_learning.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/Kolchicyna\\_machine\\_learning.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/Kolchicyna_machine_learning.xlsx)

File 14. Correlation\_to\_targets.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Correlation\\_to\\_targets.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Correlation_to_targets.ipynb)

File 15. Models\_A549\_rs\_15.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_A549\\_rs\\_15.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_A549_rs_15.ipynb)

File 16. Models\_A549\_rs\_28.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_A549\\_rs\\_28.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_A549_rs_28.ipynb)

File 17. Models\_A549\_rs\_42.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_A549\\_rs\\_42.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_A549_rs_42.ipynb)

File 18. Models\_BALB\_3T3\_rs\_15.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_BALB\\_3T3\\_rs\\_15.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_BALB_3T3_rs_15.ipynb)

File 19. Models\_BALB\_3T3\_rs\_28.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_BALB\\_3T3\\_rs\\_28.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_BALB_3T3_rs_28.ipynb)

File 20. Models\_BALB\_3T3\_rs\_42.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_BALB\\_3T3\\_rs\\_42.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_BALB_3T3_rs_42.ipynb)

File 21. Models\_LoVo\_DX\_rs\_15.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_DX\\_rs\\_15.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_DX_rs_15.ipynb)

File 22. Models\_LoVo\_DX\_rs\_28.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_DX\\_rs\\_28.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_DX_rs_28.ipynb)

File 23. Models\_LoVo\_DX\_rs\_42.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_DX\\_rs\\_42.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_DX_rs_42.ipynb)

File 24. Models\_LoVo\_rs\_15.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_rs\\_15.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_rs_15.ipynb)

File 25. Models\_LoVo\_rs\_28.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_rs\\_28.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_rs_28.ipynb)

File 26. Models\_LoVo\_rs\_42.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_LoVo\\_rs\\_42.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_LoVo_rs_42.ipynb)

File 27. Models\_MCF-7\_rs\_15.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_MCF-7\\_rs\\_15.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_MCF-7_rs_15.ipynb)

File 28. Models\_MCF-7\_rs\_28.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_MCF-7\\_rs\\_28.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_MCF-7_rs_28.ipynb)

File 29. Models\_MCF-7\_rs\_42.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Models\\_MCF-7\\_rs\\_42.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Models_MCF-7_rs_42.ipynb)

File 30. Load data and analyze results.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Load%20data%20and%20analyze%20results.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Load%20data%20and%20analyze%20results.ipynb)

a. Load data and analyze results-RMSE.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Load%20data%20and%20analyze%20results-RMSE.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Load%20data%20and%20analyze%20results-RMSE.ipynb)

File 31. Activity\_prediction.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Activity\\_prediction.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Activity_prediction.ipynb)

File 32. random\_forest\_model\_17\_estimators\_A549.joblib

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_forest/random\\_forest\\_model\\_17\\_estimators\\_A549.joblib](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_forest/random_forest_model_17_estimators_A549.joblib)

File 33. random\_forest\_model\_19\_estimators\_BALB\_3T3.joblib

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_forest/random\\_forest\\_model\\_19\\_estimators\\_BALB\\_3T3.joblib](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_forest/random_forest_model_19_estimators_BALB_3T3.joblib)

File 34. random\_forest\_model\_14\_estimators\_LoVo\_DX.joblib

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_forest/random\\_forest\\_model\\_14\\_estimators\\_LoVo\\_DX.joblib](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_forest/random_forest_model_14_estimators_LoVo_DX.joblib)

File 35. random\_forest\_model\_18\_estimators\_LoVo.joblib

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_forest/random\\_forest\\_model\\_18\\_estimators\\_LoVo.joblib](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_forest/random_forest_model_18_estimators_LoVo.joblib)

File 36. random\_forest\_model\_3\_estimators\_MCF-7.joblib

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_forest/random\\_forest\\_model\\_3\\_estimators\\_MCF-7.joblib](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_forest/random_forest_model_3_estimators_MCF-7.joblib)

File 37. Structures\_comparision.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/Structures\\_comparision.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/Structures_comparision.ipynb)

File 38. Preserve\_colchicine\_similar\_structures.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/Preserve\\_colchicine\\_similar\\_structures.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/Preserve_colchicine_similar_structures.ipynb)

File 39. Proposed\_structures\_with\_AI\_colchicyne\_tanimoto\_similarity\_.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/Proposed\\_structures\\_with\\_AI\\_colchicyne\\_tanimoto\\_similarity\\_.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/Proposed_structures_with_AI_colchicyne_tanimoto_similarity_.xlsx)

File 40. SYBA\_selection.py

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/SYBA\\_selection.py](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/SYBA_selection.py)

File 41. Whole\_report.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/Whole\\_report.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/Whole_report.xlsx)

File 42. Stereochemistry\_selection.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/Stereochemistry\\_selection.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/Stereochemistry_selection.ipynb)

File 43. t-SNE.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/t-SNE.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/t-SNE.ipynb)

File 44. PubChemPy\_search.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/PubChemPy\\_search.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/PubChemPy_search.ipynb)

File 45. PubChemSearch\_colchicyne.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/PubChemSearch\\_colchicyne.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/PubChemSearch_colchicyne.xlsx)

File 46. PubChemPy\_search-selected\_structures.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/New\\_structures/PubChemPy\\_search-selected\\_structures.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/New_structures/PubChemPy_search-selected_structures.ipynb)

File 47. PubChemSearch\_colchicyne\_selected.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/PubChemSearch\\_colchicyne\\_selected.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/PubChemSearch_colchicyne_selected.xlsx)

File 48. Colchicine PDB.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/Colchicine%20PDB.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/Colchicine%20PDB.ipynb)

File 49. Create folders for structures, 3D structures, distribute files and read results.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/Create%20folders%20for%20structures%2C%203D%20structures%2C%20distribute%20files%20and%20read%20results.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/Create%20folders%20for%20structures%2C%203D%20structures%2C%20distribute%20files%20and%20read%20results.ipynb)

File 50. Prepare\_pdbqt\_from\_pdb.txt

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/Prepare\\_pdbqt\\_from\\_pdb.txt](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/Prepare_pdbqt_from_pdb.txt)

File 51. to\_be\_executed.txt

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/to\\_be\\_executed.txt](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/to_be_executed.txt)

File 52. docking\_results\_1SA0\_chain\_AB.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/docking\\_results\\_1SA0\\_chain\\_AB.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/docking_results_1SA0_chain_AB.xlsx)

File 53. Save\_docking\_results.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Molecular\\_docking/Save\\_docking\\_results.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Molecular_docking/Save_docking_results.ipynb)

File 54. molecular\_docking\_chirality.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/molecular\\_docking\\_chirality.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/molecular_docking_chirality.xlsx)

File 55. Random\_state\_explanation.ipynb

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Activity/Random\\_state\\_explanation.ipynb](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Activity/Random_state_explanation.ipynb)

File 56. A549\_random\_state\_15.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/A549\\_random\\_state\\_15.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/A549_random_state_15.xlsx)

File 57. A549\_random\_state\_28.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/A549\\_random\\_state\\_28.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/A549_random_state_28.xlsx)

File 58. A549\_random\_state\_42.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/A549\\_random\\_state\\_42.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/A549_random_state_42.xlsx)

File 59. BALB\_3T3\_random\_state\_15.xlsx

[https://github.com/XDamianX-coder/Colchicine\\_ML/blob/main/Data/BALB\\_3T3\\_random\\_state\\_15.xlsx](https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/BALB_3T3_random_state_15.xlsx)

File 60. BALB_3T3_random_state_28.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/BALB_3T3_random_state_28.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/BALB_3T3_random_state_28.xlsx</a>
File 61. BALB_3T3_random_state_42.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/BALB_3T3_random_state_42.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/BALB_3T3_random_state_42.xlsx</a>
File 62. LoVo_random_state_15.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_15.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_15.xlsx</a>
File 63. LoVo_random_state_28.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_28.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_28.xlsx</a>
File 64. LoVo_random_state_42.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_42.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_random_state_42.xlsx</a>
File 65. LoVo_DX_random_state_15.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_15.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_15.xlsx</a>
File 66. LoVo_DX_random_state_28.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_28.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_28.xlsx</a>
File 67. LoVo_DX_random_state_42.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_42.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/LoVo_DX_random_state_42.xlsx</a>
File 68. MCF-7_random_state_15.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_15.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_15.xlsx</a>
File 69. MCF-7_random_state_28.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_28.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_28.xlsx</a>
File 70. MCF-7_random_state_42.xlsx
<a href="https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_42.xlsx">https://github.com/XDamianX-coder/Colchicine_ML/blob/main/Data/MCF-7_random_state_42.xlsx</a>