


Breast Cancer	RMSE	MAE	MSE	R2
Transcriptomics + gdsc1	2.474	1.939	6.119	0.029
Transcriptomics + gdsc1 + isoSMILES	1.482	1.147	2.196	0.709
Transcriptomics + gdsc1 + Proteomics	2.412	1.901	5.81	0.037
Transcriptomics + gdsc1 + Proteomics + isoSMILES	1.447	1.123	2.096	0.7227
Transcriptomics + gdsc1 + Geonomics	ERROR			
Transcriptomics + gdsc1 + Geonomics + isosmiles	2.546	2.087	6.482	0.206

Best Performance: Transcriptomics + Proteomics + GDSC + isosmiles

Next step:

- Recheck the training code   Produced better one
- Train with cancer (Colon cancer) into Transcriptomic + Proteomics + GDSC + isosmiles   Used gdsc2 and achieved better results

RE-RUNNING PREVIOUS GROUP CODE using the same dataset

Previous group (Transcript + GDSC2 + isoSMILES)

- Root Mean Squared Error (RMSE): 1.470
- Mean Absolute Error (MAE): 1.118
- Mean Squared Error (MSE): 2.162
- Pearson Correlation: 0.8533
- R-squared (R2): 0.7266

GDSC1

- GDSC1 uses older pharmacological profiling protocols
- Drugs tested: Fewer drugs (~138 compounds)
- Cell lines: ~1000 human cancer cell lines

GDSC2:

- Uses more advanced high-throughput screening methods and updated protocols
- Drugs tested: Over 500 compounds, including more targeted therapies
- Cell lines: ~800–900 overlapping with GDSC1, but tested with new assays

Re-worked preprocessing & DNN model to → 1) finding best patience, 2) increase epoch size, 3) squeezing y_pred for mean_sqr_error dimension

Breast Cancer	RMSE	MAE	MSE	R2
<ul style="list-style-type: none">• Transcriptomics• gdsc2• isoSMILES	1.378	1.067	1.898	0.765
<ul style="list-style-type: none">• Transcriptomics• Proteomics• gdsc2• isoSMILES	1.22	0.952	1.488	0.804
<ul style="list-style-type: none">• Transcriptomics• Geonomics• gdsc2• isoSMILES	1.636	1.276	2.678	0.671
<ul style="list-style-type: none">• Transcriptomics• Proteomics• Genomics• gdsc2• isoSMILES	1.780	1.416	3.171	0.633

Colon & Breast cancer	RMSE	MAE	MSE	R2
<ul style="list-style-type: none"> • Transcriptomics • gdsc2 • isoSMILES 	1.292	1.001	1.67	0.793
<ul style="list-style-type: none"> • Transcriptomics • Proteomics • gdsc2 • isoSMILES 	1.2702			0.8047

Head n Neck & Lung & Colon & Breast cancer	RMSE	MAE	MSE	R2
<ul style="list-style-type: none"> • Transcriptomics • Proteomics • gdsc2 • isoSMILES 	1.118	0.868	1.28	0.8420

Previous group

Previous group Breast cancer	RMSE	MAE	MSE	R2
<ul style="list-style-type: none"> • Transcriptomics • gdsc2 • isoSMILES 	1.304	0.9829	1.700	0.7850