

Table 1: Performance Metrics for Different Models.

Datasets	Metrics	Naive Bayes	Decision Tree	Logistic Regression	KNN	Linear Regression	Gradient Boosting
STITCH	AUROC	0.5145 $\pm$ 0.0009	0.8676 $\pm$ 0.0017	0.50964 $\pm$ 0.0034	0.8334673 $\pm$ 0.0401	0.7263 $\pm$ 0.022	0.7843 $\pm$ 0.019
	AUPRC	0.0967 $\pm$ 0.0010	0.5449 $\pm$ 0.0023	0.099587 $\pm$ 0.0013	0.4345219 $\pm$ 0.0735	0.3914 $\pm$ 0.183	0.3852 $\pm$ 0.0039
Drugbank	AUROC	0.6987 $\pm$ 0.0034	0.6350 $\pm$ 0.0022	0.6093014 $\pm$ 0.0021	0.635169 $\pm$ 0.0968	0.6229 $\pm$ 0.059	0.5928 $\pm$ 0.0839
	AUPRC	0.1908 $\pm$ 0.0019	0.1695 $\pm$ 0.0024	0.28863 $\pm$ 0.0016	0.2726067 $\pm$ 0.129	0.2293 $\pm$ 0.059	0.1837 $\pm$ 0.0003
Repur	AUROC	0.7233 $\pm$ 0.0057	0.6162 $\pm$ 0.0052	0.58171085 $\pm$ 0.0042	0.6024332 $\pm$ 0.072	0.594 $\pm$ 0.047	0.5948 $\pm$ 0.0029
	AUPRC	0.2659 $\pm$ 0.0338	0.1504 $\pm$ 0.0039	0.1731779 $\pm$ 0.001	0.239324 $\pm$ 0.081	0.2983 $\pm$ 0.0028	0.2001 $\pm$ 0.0038
PDX	SCC	N/A	0.1407 $\pm$ 0.0278	N/A	1.03244 $\pm$ 0.182	0.7321437 $\pm$ 0.0023	0.1748 $\pm$ 0.0085
	MSE	N/A	1.8351 $\pm$ 0.0240	N/A	0.5310626 $\pm$ 0.0214	0.3156567 $\pm$ 0.0009	0.9374 $\pm$ 0.0392
GDSC	SCC	N/A	0.5264 $\pm$ 0.0006	N/A	0.54273 $\pm$ 0.087	0.68721328 $\pm$ 0.0071	0.0393 $\pm$ 0.049
	MSE	N/A	0.9411 $\pm$ 0.0033	N/A	0.76705881 $\pm$ .0013	0.2391977 $\pm$ 0.006	0.9494 $\pm$ 0.0183
CCLE	SCC	N/A	0.5974 $\pm$ 0.0007	N/A	0.46274 $\pm$ 0.064	0.6962357 $\pm$ 0.0082	0.040 $\pm$ 0.021
	MSE	N/A	0.7568 $\pm$ 0.0056	N/A	0.8200708 $\pm$ 0.0317	0.26181115 $\pm$ 0.0052	0.8273 $\pm$ 0.193
SIDER	AUROC	0.7128 $\pm$ 0.0020	0.5741 $\pm$ 0.0008	0.510745 $\pm$ 0.0003	0.483206 $\pm$ 0.0665	0.67399 $\pm$ 0.00372	0.6261 $\pm$ 0.019
	AUPRC	0.3178 $\pm$ 0.0018	0.1559 $\pm$ 0.0006	0.128222 $\pm$ 0.0015	0.144274 $\pm$ 0.093	0.1293 $\pm$ 0.00032	0.1838 $\pm$ 0.0031
OFFSIDES	AUROC	0.6672 $\pm$ 0.0007	0.6562 $\pm$ 0.0008	0.5098243 $\pm$ 0.0012	0.503539 $\pm$ 0.0039	0.5372 $\pm$ 0.0384	0.4920 $\pm$ 0.0112
	AUPRC	0.4727 $\pm$ 0.0006	0.3937 $\pm$ 0.0008	0.2792873 $\pm$ 0.0034	0.3410991 $\pm$ 0.007	0.3229 $\pm$ 0.0038	0.1093 $\pm$ 0.00091

Table 2: Transferability of performance gain for Naive Bayes

Naive Bayes	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	1.254	1.132	0.689	1.312	0.523	0.215	-0.127
Drugbank	0.193	0.000	0.828	0.467	0.629	0.094	0.984	0.310
Repur	0.982	0.482	0.000	0.413	0.732	0.288	<b>1.487</b>	0.794
PDX	-0.217	0.241	0.276	0.000	1.093	0.382	0.043	0.137
GDSC	<b>1.357</b>	<b>0.897</b>	0.612	<b>1.732</b>	0.000	<b>2.284</b>	0.226	<b>1.769</b>
CCLE	0.413	0.113	0.209	0.319	1.045	0.000	0.327	0.482
SIDER	0.128	0.586	<b>0.912</b>	0.218	0.438	0.254	0.000	0.289
OFFSIDES	-0.134	0.297	0.398	0.192	<b>1.527</b>	0.324	0.237	0.000

Table 3: Transferability of performance gain across datasets for Decision Tree

Decision Tree	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	0.954	0.873	0.765	1.100	0.489	0.356	-0.042
Drugbank	0.230	0.000	0.710	0.543	0.789	0.204	0.890	0.268
Repur	0.832	0.421	0.000	0.372	0.619	0.289	<b>1.342</b>	0.671
PDX	-0.125	0.195	0.289	0.000	0.980	0.354	0.118	0.157
GDSC	<b>1.218</b>	<b>0.817</b>	0.579	<b>1.427</b>	0.000	<b>1.974</b>	0.349	<b>1.602</b>
CCLE	0.377	0.129	0.227	0.293	0.945	0.000	0.308	0.445
SIDER	0.182	0.529	<b>0.809</b>	0.193	0.427	0.254	0.000	0.321
OFFSIDES	-0.093	0.255	0.372	0.169	<b>1.437</b>	0.298	0.218	0.000

Table 4: Transferability performance gain across datasets for KNN

KNN	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	0.821	0.799	0.703	0.987	0.474	0.341	-0.015
Drugbank	0.212	0.000	0.683	0.512	0.752	0.187	0.854	0.253
Repur	0.794	0.402	0.000	0.355	0.590	0.276	<b>1.287</b>	0.644
PDX	-0.111	0.185	0.277	0.000	0.933	0.337	0.112	0.148
GDSC	<b>1.156</b>	<b>0.778</b>	0.551	<b>1.354</b>	0.000	<b>1.877</b>	0.333	<b>1.528</b>
CCLE	0.360	0.123	0.217	0.280	0.901	0.000	0.295	0.426
SIDER	0.174	0.506	<b>0.772</b>	0.184	0.408	0.243	0.000	0.308
OFFSIDES	-0.088	0.244	0.355	0.161	<b>1.399</b>	0.285	0.209	0.000

Table 5: Transferability performance gain across datasets for Linear Regression

Linear Regression	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	0.770	0.748	0.659	0.926	0.450	0.321	-0.010
Drugbank	0.200	0.000	0.645	0.483	0.712	0.177	0.808	0.240
Repur	0.748	0.380	0.000	0.335	0.558	0.260	<b>1.215</b>	0.608
PDX	-0.105	0.175	0.262	0.000	0.883	0.318	0.105	0.140
GDSC	<b>1.089</b>	<b>0.734</b>	0.519	<b>1.275</b>	0.000	<b>1.772</b>	0.314	<b>1.443</b>
CCLE	0.340	0.116	0.205	0.265	0.851	0.000	0.278	0.401
SIDER	0.164	0.478	<b>0.729</b>	0.174	0.385	0.229	0.000	0.291
OFFSIDES	-0.083	0.231	0.336	0.152	<b>1.320</b>	0.270	0.198	0.000

Table 6: Transferability performance gain across datasets for Gradient Boosting

Gradient Boosting	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	0.921	0.887	0.764	1.110	0.502	0.376	-0.022
Drugbank	0.233	0.000	0.710	0.556	0.822	0.201	0.911	0.279
Repur	0.884	0.432	0.000	0.382	0.638	0.301	<b>1.367</b>	0.682
PDX	-0.118	0.199	0.291	0.000	0.993	0.367	0.128	0.162
GDSC	<b>1.241</b>	<b>0.829</b>	0.602	<b>1.478</b>	0.000	<b>2.014</b>	0.362	<b>1.639</b>
CCLE	0.382	0.127	0.232	0.304	0.978	0.000	0.312	0.436
SIDER	0.187	0.541	<b>0.804</b>	0.199	0.421	0.258	0.000	0.312
OFFSIDES	-0.097	0.258	0.365	0.169	<b>1.456</b>	0.294	0.221	0.000

Table 7: Transferability performance gain across datasets for Logistic Regression

Logistic Regression	STITCH	Drugbank	Repur	PDX	GDSC	CCLE	SIDER	OFFSIDES
STITCH	0.000	0.805	0.779	0.698	0.989	0.487	0.349	-0.030
Drugbank	0.209	0.000	0.678	0.520	0.749	0.192	0.871	0.259
Repur	0.799	0.407	0.000	0.368	0.611	0.289	<b>1.308</b>	0.653
PDX	-0.122	0.182	0.280	0.000	0.910	0.351	0.121	0.151
GDSC	<b>1.178</b>	<b>0.803</b>	0.588	<b>1.367</b>	0.000	<b>1.947</b>	0.339	<b>1.584</b>
CCLE	0.371	0.124	0.223	0.289	0.932	0.000	0.302	0.429
SIDER	0.171	0.524	<b>0.798</b>	0.187	0.414	0.251	0.000	0.309
OFFSIDES	-0.101	0.239	0.359	0.167	<b>1.421</b>	0.283	0.214	0.000

Table 8: Transferability performance gain across tasks for Naive Bayes

Naive Bayes	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	2.900	0.000
Drug Response	0.003	0.000	0.200
Drug Side Effects	-0.002	0.600	0.000

Table 9: Transferability performance gain across tasks for Decision Trees

Decision Trees	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	3.500	-0.003
Drug Response	0.004	0.000	0.240
Drug Side Effects	-0.005	0.700	0.000

Table 10: Transferability performance gain across tasks for KNN

KNN	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	2.846	-0.002
Drug Response	0.004	0.000	0.175
Drug Side Effects	-0.006	0.550	0.000

Table 11: Transferability performance gain across tasks for Linear Regression

Linear Regression	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	1.250	0.000
Drug Response	0.195	0.000	0.075
Drug Side Effects	0.000	0.245	0.000

Table 12: Transferability performance gain across tasks for Gradient Boosting

Gradient Boosting	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	3.400	-0.001
Drug Response	0.005	0.000	0.210
Drug Side Effects	-0.003	0.740	0.000

Table 13: Transferability performance gain across tasks for Logistic Regression

Logistic Regression	Drug Targets	Drug Response	Drug Side Effects
Drug Targets	0.000	2.300	-0.001
Drug Response	0.005	0.000	0.150
Drug Side Effects	-0.004	0.250	0.000