

Supporting Information

Few-Shot Learning for Low-Data Drug Discovery

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1 Few-Shot Learning on Tox21

1.1 SR-HSE (372 Actives and 6,095 Inactives)

Table S1: ROC-AUC and PR-AUC Scores for ML Models on TOX21 SR-HSE Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

TOX21 SR-HSE	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.563 \pm 0.030	0.572 \pm 0.049	0.780 \pm 0.028	0.793 \pm 0.002	0.782 \pm 0.017	0.774 \pm 0.004
	PR-AUC	0.078 \pm 0.014	0.080 \pm 0.022	0.133 \pm 0.020	0.272 \pm 0.015	0.271 \pm 0.055	0.271 \pm 0.021
5+/10-	ROC-AUC	0.546 \pm 0.035	0.565 \pm 0.047	0.777 \pm 0.067	0.778 \pm 0.002	0.772 \pm 0.013	0.791 \pm 0.003
	PR-AUC	0.074 \pm 0.013	0.085 \pm 0.020	0.117 \pm 0.034	0.266 \pm 0.012	0.278 \pm 0.045	0.280 \pm 0.031
1+/10-	ROC-AUC	0.518 \pm 0.036	0.540 \pm 0.058	0.778 \pm 0.168	0.788 \pm 0.001	0.780 \pm 0.003	0.776 \pm 0.001
	PR-AUC	0.064 \pm 0.009	0.075 \pm 0.019	0.052 \pm 0.047	0.208 \pm 0.007	0.283 \pm 0.016	0.243 \pm 0.007
1+/5-	ROC-AUC	0.515 \pm 0.044	0.503 \pm 0.061	0.801 \pm 0.162	0.775 \pm 0.002	0.773 \pm 0.005	0.789 \pm 0.001
	PR-AUC	0.064 \pm 0.010	0.064 \pm 0.013	0.064 \pm 0.041	0.235 \pm 0.017	0.270 \pm 0.018	0.229 \pm 0.005
1+/1-	ROC-AUC	0.521 \pm 0.045	0.520 \pm 0.066	0.769 \pm 0.084	0.770 \pm 0.006	0.779 \pm 0.007	0.772 \pm 0.001
	PR-AUC	0.066 \pm 0.009	0.066 \pm 0.015	0.125 \pm 0.059	0.230 \pm 0.024	0.266 \pm 0.029	0.274 \pm 0.008

1.2 SR-MMP (918 Actives and 4,892 Inactives)

Table S2: ROC-AUC and PR-AUC Scores for ML Models on TOX21 SR-MMP Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

TOX21 SR-MMP	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.679 \pm 0.047	0.654 \pm 0.068	0.860 \pm 0.025	0.844 \pm 0.005	0.845 \pm 0.015	0.842 \pm 0.007
	PR-AUC	0.296 \pm 0.052	0.270 \pm 0.066	0.371 \pm 0.029	0.511 \pm 0.017	0.510 \pm 0.032	0.496 \pm 0.023
5+/10-	ROC-AUC	0.647 \pm 0.055	0.652 \pm 0.056	0.858 \pm 0.055	0.853 \pm 0.007	0.846 \pm 0.014	0.842 \pm 0.007
	PR-AUC	0.268 \pm 0.044	0.273 \pm 0.059	0.303 \pm 0.064	0.519 \pm 0.031	0.527 \pm 0.029	0.494 \pm 0.038
1+/10-	ROC-AUC	0.613 \pm 0.063	0.587 \pm 0.081	0.876 \pm 0.068	0.842 \pm 0.002	0.849 \pm 0.005	0.844 \pm 0.002
	PR-AUC	0.236 \pm 0.054	0.221 \pm 0.050	0.158 \pm 0.124	0.444 \pm 0.005	0.508 \pm 0.025	0.470 \pm 0.011
1+/5-	ROC-AUC	0.539 \pm 0.078	0.592 \pm 0.095	0.815 \pm 0.172	0.853 \pm 0.001	0.846 \pm 0.005	0.846 \pm 0.001
	PR-AUC	0.188 \pm 0.035	0.226 \pm 0.059	0.179 \pm 0.099	0.499 \pm 0.011	0.508 \pm 0.025	0.470 \pm 0.007
1+/1-	ROC-AUC	0.580 \pm 0.060	0.572 \pm 0.128	0.845 \pm 0.055	0.851 \pm 0.008	0.847 \pm 0.003	0.840 \pm 0.004
	PR-AUC	0.209 \pm 0.034	0.219 \pm 0.075	0.311 \pm 0.084	0.511 \pm 0.037	0.506 \pm 0.018	0.471 \pm 0.022

1.3 SR-p53 (423 Actives and 6,351 Inactives)

Table S3: ROC-AUC and PR-AUC Scores for ML Models on TOX21 SR-p53 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

TOX21 SR-p53	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.610 \pm 0.033	0.635 \pm 0.048	0.835 \pm 0.029	0.834 \pm 0.003	0.850 \pm 0.004	0.826 \pm 0.011
	PR-AUC	0.101 \pm 0.011	0.101 \pm 0.022	0.172 \pm 0.027	0.317 \pm 0.007	0.369 \pm 0.027	0.313 \pm 0.039
5+/10-	ROC-AUC	0.614 \pm 0.033	0.614 \pm 0.054	0.848 \pm 0.060	0.842 \pm 0.003	0.852 \pm 0.009	0.834 \pm 0.002
	PR-AUC	0.102 \pm 0.014	0.098 \pm 0.023	0.151 \pm 0.045	0.323 \pm 0.014	0.358 \pm 0.042	0.291 \pm 0.028
1+/10-	ROC-AUC	0.558 \pm 0.069	0.548 \pm 0.083	0.855 \pm 0.148	0.837 \pm 0.001	0.848 \pm 0.005	0.824 \pm 0.001
	PR-AUC	0.084 \pm 0.019	0.081 \pm 0.023	0.088 \pm 0.061	0.249 \pm 0.004	0.361 \pm 0.030	0.262 \pm 0.007
1+/5-	ROC-AUC	0.548 \pm 0.070	0.582 \pm 0.088	0.805 \pm 0.154	0.833 \pm 0.001	0.840 \pm 0.005	0.822 \pm 0.001
	PR-AUC	0.083 \pm 0.022	0.093 \pm 0.028	0.076 \pm 0.057	0.283 \pm 0.012	0.310 \pm 0.023	0.257 \pm 0.003
1+/1-	ROC-AUC	0.549 \pm 0.064	0.553 \pm 0.103	0.840 \pm 0.061	0.838 \pm 0.004	0.834 \pm 0.003	0.827 \pm 0.001
	PR-AUC	0.079 \pm 0.016	0.085 \pm 0.027	0.160 \pm 0.046	0.316 \pm 0.022	0.346 \pm 0.021	0.279 \pm 0.015

2 Few-Shot Learning on MUV

2.1 MUV-832 (30 Actives and 14,637 Decoys)

Table S4: ROC-AUC and PR-AUC Scores for ML Models on MUV MUV-832 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

MUV MUV-832	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.824 \pm 0.068	0.753 \pm 0.073	0.608 \pm 0.019	0.720 \pm 0.043	0.585 \pm 0.041	0.566 \pm 0.050
	PR-AUC	0.069 \pm 0.047	0.006 \pm 0.004	0.001 \pm 0.000	0.005 \pm 0.001	0.004 \pm 0.003	0.003 \pm 0.001
5+/10-	ROC-AUC	0.747 \pm 0.072	0.683 \pm 0.080	0.561 \pm 0.039	0.651 \pm 0.031	0.656 \pm 0.021	0.561 \pm 0.105
	PR-AUC	0.122 \pm 0.058	0.012 \pm 0.017	0.001 \pm 0.002	0.008 \pm 0.001	0.007 \pm 0.001	0.003 \pm 0.001
1+/10-	ROC-AUC	0.601 \pm 0.060	0.556 \pm 0.076	0.722 \pm 0.136	0.615 \pm 0.026	0.607 \pm 0.014	0.683 \pm 0.010
	PR-AUC	0.035 \pm 0.034	0.007 \pm 0.009	0.003 \pm 0.004	0.004 \pm 0.001	0.006 \pm 0.000	0.007 \pm 0.000
1+/5-	ROC-AUC	0.579 \pm 0.071	0.551 \pm 0.115	0.773 \pm 0.084	0.514 \pm 0.012	0.570 \pm 0.021	0.500 \pm 0.000
	PR-AUC	0.036 \pm 0.033	0.005 \pm 0.003	0.003 \pm 0.003	0.003 \pm 0.000	0.004 \pm 0.001	0.002 \pm 0.000
1+/1-	ROC-AUC	0.582 \pm 0.089	0.567 \pm 0.155	0.768 \pm 0.079	0.496 \pm 0.028	0.517 \pm 0.010	0.577 \pm 0.011
	PR-AUC	0.039 \pm 0.038	0.006 \pm 0.009	0.005 \pm 0.003	0.003 \pm 0.000	0.005 \pm 0.001	0.004 \pm 0.000

2.2 MUV-846 (30 Actives and 14,681 Decoys)

Table S5: ROC-AUC and PR-AUC Scores for ML Models on MUV MUV-846 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

MUV MUV-846	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.876 \pm 0.048	0.849 \pm 0.045	0.594 \pm 0.024	0.715 \pm 0.048	0.719 \pm 0.036	0.482 \pm 0.035
	PR-AUC	0.115 \pm 0.053	0.025 \pm 0.019	0.001 \pm 0.000	0.022 \pm 0.012	0.003 \pm 0.001	0.001 \pm 0.000
5+/10-	ROC-AUC	0.833 \pm 0.042	0.754 \pm 0.065	0.555 \pm 0.056	0.453 \pm 0.024	0.560 \pm 0.033	0.549 \pm 0.047
	PR-AUC	0.088 \pm 0.055	0.038 \pm 0.029	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/10-	ROC-AUC	0.676 \pm 0.104	0.656 \pm 0.123	0.711 \pm 0.104	0.437 \pm 0.026	0.490 \pm 0.017	0.556 \pm 0.008
	PR-AUC	0.024 \pm 0.031	0.012 \pm 0.012	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/5-	ROC-AUC	0.661 \pm 0.093	0.690 \pm 0.124	0.688 \pm 0.171	0.388 \pm 0.011	0.441 \pm 0.012	0.500 \pm 0.000
	PR-AUC	0.039 \pm 0.034	0.014 \pm 0.013	0.001 \pm 0.001	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/1-	ROC-AUC	0.624 \pm 0.123	0.642 \pm 0.159	0.647 \pm 0.094	0.518 \pm 0.029	0.456 \pm 0.025	0.490 \pm 0.008
	PR-AUC	0.031 \pm 0.040	0.011 \pm 0.010	0.009 \pm 0.021	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000

2.3 MUV-852 (29 Actives and 14,622 Decoys)

Table S6: ROC-AUC and PR-AUC Scores for ML Models on MUV MUV-852 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

MUV MUV-852	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.790 \pm 0.048	0.803 \pm 0.054	0.574 \pm 0.019	0.647 \pm 0.035	0.639 \pm 0.052	0.515 \pm 0.042
	PR-AUC	0.137 \pm 0.086	0.010 \pm 0.004	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.001
5+/10-	ROC-AUC	0.787 \pm 0.041	0.779 \pm 0.031	0.612 \pm 0.031	0.564 \pm 0.033	0.592 \pm 0.032	0.453 \pm 0.026
	PR-AUC	0.130 \pm 0.093	0.021 \pm 0.023	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/10-	ROC-AUC	0.665 \pm 0.103	0.654 \pm 0.156	0.741 \pm 0.129	0.556 \pm 0.020	0.591 \pm 0.022	0.594 \pm 0.008
	PR-AUC	0.036 \pm 0.044	0.007 \pm 0.005	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.003 \pm 0.000
1+/5-	ROC-AUC	0.639 \pm 0.145	0.607 \pm 0.168	0.665 \pm 0.126	0.485 \pm 0.020	0.523 \pm 0.017	0.500 \pm 0.000
	PR-AUC	0.052 \pm 0.062	0.007 \pm 0.006	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/1-	ROC-AUC	0.621 \pm 0.114	0.674 \pm 0.174	0.673 \pm 0.099	0.462 \pm 0.014	0.506 \pm 0.020	0.510 \pm 0.008
	PR-AUC	0.034 \pm 0.050	0.007 \pm 0.005	0.006 \pm 0.011	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000

2.4 MUV-858 (29 Actives and 14,745 Decoys)

Table S7: ROC-AUC and PR-AUC Scores for ML Models on MUV MUV-858 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

MUV MUV-858	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.609 \pm 0.079	0.644 \pm 0.071	0.533 \pm 0.031	0.545 \pm 0.057	0.539 \pm 0.041	0.489 \pm 0.052
	PR-AUC	0.004 \pm 0.003	0.003 \pm 0.001	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.001 \pm 0.000
5+/10-	ROC-AUC	0.573 \pm 0.070	0.598 \pm 0.054	0.529 \pm 0.036	0.446 \pm 0.036	0.562 \pm 0.026	0.469 \pm 0.026
	PR-AUC	0.011 \pm 0.013	0.003 \pm 0.002	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/10-	ROC-AUC	0.537 \pm 0.058	0.556 \pm 0.052	0.527 \pm 0.162	0.405 \pm 0.009	0.488 \pm 0.014	0.477 \pm 0.008
	PR-AUC	0.005 \pm 0.008	0.003 \pm 0.001	0.000 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/5-	ROC-AUC	0.534 \pm 0.065	0.550 \pm 0.071	0.514 \pm 0.140	0.440 \pm 0.016	0.482 \pm 0.014	0.500 \pm 0.000
	PR-AUC	0.005 \pm 0.008	0.003 \pm 0.002	0.001 \pm 0.001	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000
1+/1-	ROC-AUC	0.521 \pm 0.065	0.505 \pm 0.069	0.558 \pm 0.103	0.554 \pm 0.017	0.526 \pm 0.014	0.437 \pm 0.014
	PR-AUC	0.002 \pm 0.001	0.003 \pm 0.001	0.002 \pm 0.001	0.002 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000

2.5 MUV-859 (24 Actives and 14,722 Decoys)

Table S8: ROC-AUC and PR-AUC Scores for ML Models on MUV MUV-859 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

MUV MUV-859	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.539 \pm 0.077	0.517 \pm 0.057	0.499 \pm 0.018	0.516 \pm 0.042	0.513 \pm 0.041	0.398 \pm 0.053
	PR-AUC	0.003 \pm 0.005	0.001 \pm 0.000	0.001 \pm 0.000	0.001 \pm 0.000	0.001 \pm 0.000	0.001 \pm 0.000
5+/10-	ROC-AUC	0.538 \pm 0.066	0.515 \pm 0.067	0.492 \pm 0.020	0.464 \pm 0.023	0.510 \pm 0.024	0.481 \pm 0.052
	PR-AUC	0.002 \pm 0.001	0.002 \pm 0.001	0.000 \pm 0.000	0.001 \pm 0.000	0.001 \pm 0.000	0.005 \pm 0.004
1+/10-	ROC-AUC	0.517 \pm 0.081	0.504 \pm 0.060	0.539 \pm 0.109	0.446 \pm 0.015	0.522 \pm 0.011	0.427 \pm 0.014
	PR-AUC	0.002 \pm 0.001	0.002 \pm 0.000	0.000 \pm 0.000	0.001 \pm 0.000	0.002 \pm 0.000	0.001 \pm 0.000
1+/5-	ROC-AUC	0.524 \pm 0.064	0.527 \pm 0.057	0.426 \pm 0.121	0.480 \pm 0.013	0.453 \pm 0.013	0.500 \pm 0.000
	PR-AUC	0.002 \pm 0.001	0.002 \pm 0.002	0.000 \pm 0.000	0.002 \pm 0.000	0.001 \pm 0.000	0.002 \pm 0.000
1+/1-	ROC-AUC	0.517 \pm 0.064	0.499 \pm 0.061	0.455 \pm 0.072	0.504 \pm 0.016	0.522 \pm 0.009	0.406 \pm 0.014
	PR-AUC	0.002 \pm 0.001	0.002 \pm 0.001	0.001 \pm 0.000	0.002 \pm 0.000	0.002 \pm 0.000	0.001 \pm 0.000

3 Few-Shot Learning on DUD-E GPCR Subset

3.1 ADRB2 (231 Actives and 15,000 Decoys)

Table S9: ROC-AUC and PR-AUC Scores for ML Models on DUD-E GPCR adrb2 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

DUD-E GPCR adrb2	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.969 \pm 0.018	0.914 \pm 0.038	0.998 \pm 0.000	1.000 \pm 0.000	1.000 \pm 0.000	0.998 \pm 0.001
	PR-AUC	0.806 \pm 0.103	0.311 \pm 0.099	0.963 \pm 0.014	0.986 \pm 0.002	0.997 \pm 0.001	0.991 \pm 0.002
5+/10-	ROC-AUC	0.948 \pm 0.022	0.875 \pm 0.043	0.998 \pm 0.005	0.996 \pm 0.000	1.000 \pm 0.000	0.998 \pm 0.001
	PR-AUC	0.729 \pm 0.088	0.230 \pm 0.102	0.959 \pm 0.047	0.982 \pm 0.003	0.996 \pm 0.001	0.985 \pm 0.001
1+/10-	ROC-AUC	0.842 \pm 0.055	0.748 \pm 0.072	0.998 \pm 0.001	0.999 \pm 0.000	0.998 \pm 0.000	0.998 \pm 0.000
	PR-AUC	0.339 \pm 0.135	0.099 \pm 0.056	0.909 \pm 0.117	0.975 \pm 0.002	0.966 \pm 0.009	0.974 \pm 0.000
1+/5-	ROC-AUC	0.842 \pm 0.088	0.744 \pm 0.080	0.998 \pm 0.000	0.995 \pm 0.000	0.996 \pm 0.000	0.997 \pm 0.000
	PR-AUC	0.339 \pm 0.142	0.095 \pm 0.059	0.913 \pm 0.131	0.953 \pm 0.005	0.993 \pm 0.001	0.917 \pm 0.005
1+/1-	ROC-AUC	0.776 \pm 0.122	0.731 \pm 0.088	0.998 \pm 0.001	0.996 \pm 0.000	0.997 \pm 0.000	0.998 \pm 0.000
	PR-AUC	0.227 \pm 0.180	0.058 \pm 0.032	0.909 \pm 0.052	0.981 \pm 0.003	0.982 \pm 0.006	0.964 \pm 0.002

3.2 CXCR4 (40 Actives and 3,406 Decoys)

Table S10: ROC-AUC and PR-AUC Scores for ML Models on DUD-E GPCR cxcr4 Target. Values are mean values with standard deviation over 20 rounds of testing. Best values are highlighted in bold text. The first column shows the composition of the support set as explained in text.

DUD-E GPCR cxcr4	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC-AUC	0.994 \pm 0.005	0.965 \pm 0.020	0.570 \pm 0.028	0.801 \pm 0.030	0.631 \pm 0.045	0.858 \pm 0.014
	PR-AUC	0.938 \pm 0.043	0.697 \pm 0.134	0.014 \pm 0.002	0.085 \pm 0.022	0.107 \pm 0.020	0.133 \pm 0.038
5+/10-	ROC-AUC	0.968 \pm 0.019	0.927 \pm 0.062	0.525 \pm 0.038	0.693 \pm 0.025	0.685 \pm 0.130	0.679 \pm 0.019
	PR-AUC	0.794 \pm 0.141	0.626 \pm 0.188	0.031 \pm 0.012	0.029 \pm 0.003	0.122 \pm 0.054	0.096 \pm 0.010
1+/10-	ROC-AUC	0.866 \pm 0.086	0.828 \pm 0.108	0.520 \pm 0.087	0.764 \pm 0.021	0.684 \pm 0.032	0.734 \pm 0.018
	PR-AUC	0.380 \pm 0.140	0.361 \pm 0.162	0.039 \pm 0.066	0.066 \pm 0.027	0.041 \pm 0.009	0.108 \pm 0.009
1+/5-	ROC-AUC	0.874 \pm 0.081	0.781 \pm 0.094	0.520 \pm 0.084	0.707 \pm 0.082	0.590 \pm 0.087	0.700 \pm 0.007
	PR-AUC	0.417 \pm 0.092	0.347 \pm 0.111	0.050 \pm 0.082	0.079 \pm 0.037	0.045 \pm 0.017	0.063 \pm 0.005
1+/1-	ROC-AUC	0.833 \pm 0.088	0.689 \pm 0.150	0.545 \pm 0.040	0.593 \pm 0.034	0.732 \pm 0.022	0.496 \pm 0.010
	PR-AUC	0.375 \pm 0.124	0.174 \pm 0.151	0.091 \pm 0.102	0.041 \pm 0.008	0.104 \pm 0.012	0.035 \pm 0.005

4 ECFP vs GCN Learned Embeddings on Tox21

Table S11: ROC-AUC and PR-AUC Scores for Prototypical Networks on Tox21 with ECFP or GCN embeddings. Values are mean values with standard deviation over 20 runs. Best values are highlighted in bold text. A Mann-Whitney U Rank p-value less than 0.05 indicates significant difference of the GCN Embeddings over ECFPs.

Tox21 Target	Support Set	Metric	ECFP	Graphs	p-value
SR-HSE	10+/10-	ROC-AUC	0.751 \pm 0.017	0.782 \pm 0.017	0.000
		PR-AUC	0.227 \pm 0.042	0.271 \pm 0.055	0.004
SR-HSE	5+/10-	ROC-AUC	0.741 \pm 0.016	0.772 \pm 0.013	0.000
		PR-AUC	0.202 \pm 0.045	0.278 \pm 0.045	0.000
SR-HSE	1+/10-	ROC-AUC	0.665 \pm 0.156	0.780 \pm 0.003	0.000
		PR-AUC	0.148 \pm 0.062	0.283 \pm 0.016	0.000
SR-HSE	1+/5-	ROC-AUC	0.715 \pm 0.102	0.773 \pm 0.005	0.000
		PR-AUC	0.181 \pm 0.060	0.270 \pm 0.018	0.000
SR-HSE	1+/1-	ROC-AUC	0.641 \pm 0.168	0.779 \pm 0.007	0.000
		PR-AUC	0.163 \pm 0.081	0.266 \pm 0.029	0.000
SR-MMP	10+/10-	ROC-AUC	0.793 \pm 0.022	0.845 \pm 0.015	0.000
		PR-AUC	0.477 \pm 0.044	0.510 \pm 0.032	0.015
SR-MMP	5+/10-	ROC-AUC	0.765 \pm 0.046	0.846 \pm 0.014	0.000
		PR-AUC	0.425 \pm 0.049	0.527 \pm 0.029	0.000
SR-MMP	1+/10-	ROC-AUC	0.763 \pm 0.080	0.849 \pm 0.005	0.000
		PR-AUC	0.444 \pm 0.109	0.508 \pm 0.025	0.021
SR-MMP	1+/5-	ROC-AUC	0.736 \pm 0.156	0.846 \pm 0.005	0.000
		PR-AUC	0.445 \pm 0.121	0.508 \pm 0.025	0.002
SR-MMP	1+/1-	ROC-AUC	0.647 \pm 0.219	0.847 \pm 0.003	0.000
		PR-AUC	0.355 \pm 0.151	0.506 \pm 0.018	0.000
SR-p53	10+/10-	ROC-AUC	0.793 \pm 0.013	0.850 \pm 0.004	0.000
		PR-AUC	0.309 \pm 0.051	0.369 \pm 0.027	0.000
SR-p53	5+/10-	ROC-AUC	0.782 \pm 0.022	0.852 \pm 0.009	0.000
		PR-AUC	0.278 \pm 0.068	0.358 \pm 0.042	0.000
SR-p53	1+/10-	ROC-AUC	0.780 \pm 0.087	0.848 \pm 0.005	0.000
		PR-AUC	0.279 \pm 0.086	0.361 \pm 0.030	0.000
SR-p53	1+/5-	ROC-AUC	0.770 \pm 0.036	0.840 \pm 0.005	0.000
		PR-AUC	0.273 \pm 0.087	0.310 \pm 0.023	0.323
SR-p53	1+/1-	ROC-AUC	0.753 \pm 0.116	0.834 \pm 0.003	0.000
		PR-AUC	0.274 \pm 0.089	0.346 \pm 0.021	0.001