

Supporting Documents

1.1 | Few-Shot Learning on Tox21

1.1.1 | SR-HSE - 372 Actives - 6,095 Inactives

TOX21 SR-HSE	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.1: 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.

1.1.2 | SR-MMP - 918 Actives - 4,892 Inactives

TOX21 SR-MMP	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.2: 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.

1.1.3 | SR-p53 - 423 Actives - 6,351 Inactives

TOX21 SR-p53	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.3: 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.

1.2 | Few-Shot Learning on MUV

1.2.1 | MUV-832 - 30 Actives - 14,637 Decoys

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

Table 1.4: 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.

1.2.2 | MUV-846 - 30 Actives - 14,681 Decoys

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

Table 1.5: 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.

1.2.3 | MUV-852 - 29 Actives - 14,622 Decoys

MUV MUV-852	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.6: 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.

1.2.4 | MUV-858 - 29 Actives - 14,745 Decoys

MUV MUV-858	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.7: 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.

1.2.5 | MUV-859 - 24 Actives - 14,722 Decoys

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

Table 1.8: 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.

1.3 | Few-Shot Learning on DUD-E GPCR Subset

DUD-E GPCR adrb2	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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	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
	PRC	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

Table 1.9: 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 cxcr4	Metric	RF	Graph Conv	SiameseNet	MatchingNet	ProtoNet	RelationNet
10+/10-	ROC	0.994 ± 0.005	0.965 ± 0.020	0.570 ± 0.028	0.801 ± 0.030	0.631 ± 0.045	0.858 ± 0.014
	PRC	0.938 ± 0.043	0.697 ± 0.134	0.014 ± 0.002	0.085 ± 0.022	0.107 ± 0.020	0.133 ± 0.038
5+/10-	ROC	0.968 ± 0.019	0.927 ± 0.062	0.525 ± 0.038	0.693 ± 0.025	0.685 ± 0.130	0.679 ± 0.019
	PRC	0.794 ± 0.141	0.626 ± 0.188	0.031 ± 0.012	0.029 ± 0.003	0.122 ± 0.054	0.096 ± 0.010
1+/10-	ROC	0.866 ± 0.086	0.828 ± 0.108	0.520 ± 0.087	0.764 ± 0.021	0.684 ± 0.032	0.734 ± 0.018
	PRC	0.380 ± 0.140	0.361 ± 0.162	0.039 ± 0.066	0.066 ± 0.027	0.041 ± 0.009	0.108 ± 0.009
1+/5-	ROC	0.874 ± 0.081	0.781 ± 0.094	0.520 ± 0.084	0.707 ± 0.082	0.590 ± 0.087	0.700 ± 0.007
	PRC	0.417 ± 0.092	0.347 ± 0.111	0.050 ± 0.082	0.079 ± 0.037	0.045 ± 0.017	0.063 ± 0.005
1+/1-	ROC	0.833 ± 0.088	0.689 ± 0.150	0.545 ± 0.040	0.593 ± 0.034	0.732 ± 0.022	0.496 ± 0.010
	PRC	0.375 ± 0.124	0.174 ± 0.151	0.091 ± 0.102	0.041 ± 0.008	0.104 ± 0.012	0.035 ± 0.005

Table 1.10: 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.

1.3.1 | ECFP vs GCN Learned Embeddings on Tox21

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

Table 1.11: 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.