

Table S7: The comprehensive performance evaluation (including accuracy, auc, aupr, f1, precision, recall and kappa) of ImageMol on molecular property prediction task with scaffold split.

	accuracy	auc	aupr	f1	precision	recall	kappa
BACE	0.708 ± 0.049	0.839 ± 0.005	0.824 ± 0.016	0.663 ± 0.092	0.842 ± 0.024	0.564 ± 0.136	0.428 ± 0.088
BBBP	0.605 ± 0.006	0.739 ± 0.002	0.776 ± 0.006	0.698 ± 0.004	0.586 ± 0.008	0.864 ± 0.029	0.182 ± 0.016
ClinTox	0.922 ± 0.012	0.851 ± 0.014	0.719 ± 0.026	0.700 ± 0.015	0.710 ± 0.039	0.697 ± 0.026	0.322 ± 0.027
SIDER	0.766 ± 0.006	0.660 ± 0.001	0.647 ± 0.002	0.636 ± 0.020	0.627 ± 0.005	0.661 ± 0.036	0.163 ± 0.012
Tox21	0.906 ± 0.002	0.773 ± 0.001	0.386 ± 0.006	0.327 ± 0.038	0.545 ± 0.038	0.254 ± 0.044	0.286 ± 0.031
ToxCast	0.802 ± 0.004	0.653 ± 0.001	0.332 ± 0.002	0.259 ± 0.014	0.331 ± 0.011	0.256 ± 0.018	0.102 ± 0.006
HIV	0.964 ± 0.011	0.797 ± 0.002	0.325 ± 0.026	0.315 ± 0.018	0.538 ± 0.182	0.267 ± 0.095	0.299 ± 0.015
MUV	0.997 ± 0.000	0.825 ± 0.007	0.108 ± 0.037	0.033 ± 0.047	0.044 ± 0.063	0.030 ± 0.042	0.033 ± 0.047