

**Table S8:** The comprehensive performance evaluation (including accuracy, AUC, AUPR, F1, precision, recall and kappa) of ImageMol on molecular property prediction task with random scaffold split.

	accuracy	auc	aupr	f1	precision	recall	kappa
BACE	$0.861 \pm 0.005$	$0.939 \pm 0.011$	$0.936 \pm 0.011$	$0.859 \pm 0.001$	$0.845 \pm 0.035$	$0.877 \pm 0.040$	$0.722 \pm 0.010$
BBBP	$0.916 \pm 0.007$	$0.952 \pm 0.002$	$0.983 \pm 0.001$	$0.946 \pm 0.005$	$0.929 \pm 0.014$	$0.963 \pm 0.016$	$0.762 \pm 0.023$
ClinTox	$0.982 \pm 0.004$	$0.975 \pm 0.007$	$0.582 \pm 0.023$	$0.495 \pm 0.001$	$0.497 \pm 0.000$	$0.494 \pm 0.002$	$-0.006 \pm 0.004$
SIDER	$0.769 \pm 0.007$	$0.708 \pm 0.010$	$0.698 \pm 0.008$	$0.633 \pm 0.018$	$0.648 \pm 0.013$	$0.659 \pm 0.031$	$0.160 \pm 0.016$
Tox21	$0.923 \pm 0.003$	$0.847 \pm 0.003$	$0.437 \pm 0.008$	$0.340 \pm 0.016$	$0.503 \pm 0.046$	$0.287 \pm 0.033$	$0.306 \pm 0.014$
ToxCast	$0.843 \pm 0.001$	$0.751 \pm 0.001$	$0.415 \pm 0.003$	$0.296 \pm 0.015$	$0.392 \pm 0.010$	$0.276 \pm 0.019$	$0.176 \pm 0.013$