Dataset	Target	$R^2 \uparrow$	$\rho \uparrow$	UER-AUC$_{mean} \uparrow$	UER-AUC$_{max} \uparrow$	RLL $\uparrow$
logp	0	$0.98\pm_{0.02}$	$0.59\pm_{0.13}$	$0.28\pm_{0.05}$	$0.67\pm_{0.22}$	$0.75\pm_{0.04}$
aqsoldb	0	$0.87\pm_{0.01}$	$0.36\pm_{0.03}$	$0.26\pm_{0.01}$	$0.33\pm_{0.05}$	$0.42\pm_{0.06}$
lipophilicity	0	$0.72\pm_{0.03}$	$0.21\pm_{0.05}$	$0.10\pm_{0.02}$	$0.20\pm_{0.14}$	$0.28\pm_{0.03}$
compas	0	$0.74\pm_{0.25}$	$0.55\pm_{0.16}$	$0.31\pm_{0.10}$	$0.41\pm_{0.12}$	$0.59\pm_{0.12}$
compas	1	$0.96\pm_{0.02}$	$0.41\pm_{0.06}$	$0.28\pm_{0.05}$	$0.62\pm_{0.15}$	$0.70\pm_{0.01}$
qm9	3	$0.78\pm_{0.01}$	$0.57\pm_{0.02}$	$0.48\pm_{0.01}$	$0.78\pm_{0.08}$	$0.53\pm_{0.00}$
qm9	5	$0.93\pm_{0.00}$	$0.55\pm_{0.01}$	$0.27\pm_{0.01}$	$0.60\pm_{0.17}$	$0.63\pm_{0.01}$
qm9	6	$0.99\pm_{0.00}$	$0.50\pm_{0.03}$	$0.25\pm_{0.01}$	$0.71\pm_{0.08}$	$0.73\pm_{0.00}$
qm9	7	$0.97\pm_{0.00}$	$0.53\pm_{0.01}$	$0.28\pm_{0.01}$	$0.72\pm_{0.05}$	$0.69\pm_{0.00}$