Dataset	Property	R^2	ρ	UER-AUC$_{\text{mean}}$	UER-AUC$_{\text{max}}$
AqSolDB	logS	$0.88\pm_{0.02}$	$0.40\pm_{0.02}$	$0.26\pm_{0.02}$	$0.39\pm_{0.15}$
Lipop	logD	$0.75\pm_{0.01}$	$0.24\pm_{0.05}$	$0.12\pm_{0.02}$	$0.15\pm_{0.05}$
COMPAS	Gap	$0.96\pm_{0.04}$	$0.54\pm_{0.07}$	$0.31\pm_{0.02}$	$0.43\pm_{0.12}$
QM9	Energy	$1.00\pm_{0.00}$	$0.66\pm_{0.25}$	$0.23\pm_{0.09}$	$0.51\pm_{0.26}$
QM9	Dipole Moment	$0.80\pm_{0.02}$	$0.61\pm_{0.05}$	$0.48\pm_{0.02}$	$0.69\pm_{0.10}$