Table 1: Model Comparison Results

Dataset Name	Split type	GC	WEAVE	AttentiveFP	XGBoost	FP-GNN	Ours
BACE	Random			0.876	0.889	0.881	**0.903**±0.007
	Scaffold	0.783	0.806			**0.860**	0.828±0.009
HIV	Random			0.824	0.816	0.825	**0.835**±0.016
	Scaffold	0.763	0.703			0.824	**0.825**±0.008
Tox21	Random	0.829	0.820	**0.852**	0.836	0.815	0.823±0.005
BBBP	Random			0.887	0.926	**0.935**	0.907±0.008
	Scaffold	0.690	0.671			0.916	**0.931**±0.012
Clintox	Random	0.807	0.832	0.904	**0.911**	0.840	0.870±0.011
SIDER	Random	0.638	0.581	0.623	0.642	0.661	**0.674**±0.005

Table 2: Ablation Study Results

Dataset Name	Split type	FP-GNN	Ours	Bond$^-$	CrossAttn$^-$	SelfAttn$^+$
BACE	Random	0.881	**0.903**±0.007	0.889±0.031	0.886±0.027	0.640±0.033
BBBP	Scaffold	0.916	0.931±0.012	0.901±0.023	0.911±0.025	0.816±0.085
SIDER	Random	0.661	0.674±0.005	0.672±0.013	0.679±0.008	0.584±0.014