

Table 1: Model Comparison Results

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

Table 2: Ablation Study Results

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