

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	0.903 \pm 0.007
	Scaffold					0.860	0.828 \pm 0.009
HIV	Random	0.763	0.703	0.824	0.816	0.825	0.835 \pm 0.016
	Scaffold					0.824	0.825 \pm 0.008
Tox21	Random	0.829	0.820	0.852	0.836	0.815	0.823 \pm 0.005
BBBP	Random	0.690	0.671	0.887	0.926	0.935	0.907 \pm 0.008
	Scaffold					0.916	0.931 \pm 0.012
Clintox	Random	0.807	0.832	0.904	0.911	0.840	0.870 \pm 0.011
SIDER	Random	0.638	0.581	0.623	0.642	0.661	0.674 \pm 0.005

Table 2: Ablation Study Results

Dataset Name	Split type	FP-GNN	Ours	Bond ⁻	CrossAttn ⁻	SelfAttn	GraphSAGE
BACE	Random	0.881	0.903 \pm 0.007	0.889 \pm 0.031	0.886 \pm 0.027	0.640 \pm 0.033	0.871 \pm 0.017
BBBP	Scaffold	0.916	0.931 \pm 0.012	0.901 \pm 0.023	0.911 \pm 0.025	0.816 \pm 0.085	0.871 \pm 0.011
SIDER	Random	0.661	0.674 \pm 0.005	0.672 \pm 0.013	0.679 \pm 0.008	0.584 \pm 0.014	0.627 \pm 0.021