

**Table S5:** The ROC-AUC (%) performance of different methods on benchmark datasets with scaffold. All results are reported as mean  $\pm$  standard deviation. The yellow and blue backgrounds represent methods without and with pretraining, respectively. The light green background represents the results of our method. Rank represents the ranking of ImageMol in the comparison. Grover-10M and MPG-10M are our reproduced results based on the 10M pre-training data used by ImageMol.

Classification (Higher is better)								
	BBBP	Tox21	ClinTox	HIV	BACE	SIDER	MUV	ToxCast
GCN	71.8 $\pm$ 0.9	70.9 $\pm$ 2.6	62.5 $\pm$ 2.8	74.0 $\pm$ 3.0	71.6 $\pm$ 2.0	53.6 $\pm$ 3.2	71.6 $\pm$ 4.0	-
GIN	65.8 $\pm$ 4.5	74.0 $\pm$ 0.8	58.0 $\pm$ 4.4	75.3 $\pm$ 1.9	70.1 $\pm$ 5.4	57.3 $\pm$ 1.6	71.8 $\pm$ 2.5	-
GCC	66.9 $\pm$ 0.7	76.6 $\pm$ 0.5	73.2 $\pm$ 2.6	75.5 $\pm$ 0.8	75.0 $\pm$ 1.5	58.0 $\pm$ 0.9	74.1 $\pm$ 1.4	63.5 $\pm$ 0.4
GPT-GNN	67.5 $\pm$ 1.3	76.1 $\pm$ 0.4	74.9 $\pm$ 2.7	77.0 $\pm$ 1.7	78.5 $\pm$ 0.9	59.3 $\pm$ 0.8	75.0 $\pm$ 2.5	63.1 $\pm$ 0.5
Grover	68.0 $\pm$ 1.5	76.3 $\pm$ 0.6	76.9 $\pm$ 1.9	77.8 $\pm$ 1.4	79.5 $\pm$ 1.1	60.7 $\pm$ 0.5	75.8 $\pm$ 1.7	63.4 $\pm$ 0.6
MGSSL*	70.5 $\pm$ 1.1	76.5 $\pm$ 0.3	80.7 $\pm$ 2.1	79.5 $\pm$ 1.1	79.7 $\pm$ 0.8	61.8 $\pm$ 0.8	78.7 $\pm$ 1.5	64.1 $\pm$ 0.7
3D InfoMax	69.1 $\pm$ 1.1	74.5 $\pm$ 0.7	59.4 $\pm$ 3.2	76.1 $\pm$ 1.3	79.4 $\pm$ 1.9	53.4 $\pm$ 3.3	-	64.4 $\pm$ 0.9
G-Motif	66.4 $\pm$ 3.4	73.2 $\pm$ 0.8	77.8 $\pm$ 2.0	73.8 $\pm$ 1.4	73.4 $\pm$ 4.0	60.6 $\pm$ 1.1	73.3 $\pm$ 2.0	62.6 $\pm$ 0.5
GraphLoG	67.8 $\pm$ 1.7	73.0 $\pm$ 0.3	62.0 $\pm$ 1.8	73.4 $\pm$ 0.6	78.8 $\pm$ 0.7	57.4 $\pm$ 2.3	73.1 $\pm$ 1.7	62.2 $\pm$ 0.4
GraphCL	67.5 $\pm$ 3.3	74.4 $\pm$ 0.7	78.9 $\pm$ 4.2	75.0 $\pm$ 0.4	68.7 $\pm$ 7.8	60.1 $\pm$ 1.3	77.1 $\pm$ 1.0	62.8 $\pm$ 0.2
GraphMVP*	72.4 $\pm$ 1.6	75.9 $\pm$ 0.5	79.1 $\pm$ 2.8	77.0 $\pm$ 1.2	81.2 $\pm$ 0.9	63.9 $\pm$ 1.2	77.7 $\pm$ 0.6	63.1 $\pm$ 0.2
X-MOL	71.6 $\pm$ 1.1	75.1 $\pm$ 0.8	79.6 $\pm$ 1.6	74.1 $\pm$ 0.5	78.1 $\pm$ 1.2	61.3 $\pm$ 0.6	78.1 $\pm$ 0.5	62.1 $\pm$ 0.2
MolCLR	71.6 $\pm$ 0.7	75.0 $\pm$ 0.4	<b>91.9<math>\pm</math>1.2</b>	78.3 $\pm$ 0.4	81.9 $\pm$ 1.5	59.9 $\pm$ 0.9	79.7 $\pm$ 1.2	-
Grover-10M	71.8 $\pm$ 0.5	76.5 $\pm$ 0.7	84.3 $\pm$ 2.1	78.6 $\pm$ 0.6	82.2 $\pm$ 0.7	63.7 $\pm$ 0.5	76.9 $\pm$ 1.4	63.5 $\pm$ 0.8
MPG-10M	72.8 $\pm$ 0.6	77.1 $\pm$ 0.8	90.1 $\pm$ 3.0	78.5 $\pm$ 0.9	83.8 $\pm$ 1.3	64.4 $\pm$ 0.2	79.1 $\pm$ 1.2	63.4 $\pm$ 0.3
ImageMol	<b>73.9<math>\pm</math>0.2</b>	<b>77.3<math>\pm</math>0.1</b>	85.1 $\pm$ 1.4	<b>79.7<math>\pm</math>0.2</b>	<b>83.9<math>\pm</math>0.5</b>	<b>66.0<math>\pm</math>0.1</b>	<b>82.5<math>\pm</math>0.8</b>	<b>65.3<math>\pm</math>0.2</b>
Rank	1	1	3	1	1	1	1	1
Regression (Lower is better)								
	FreeSolv	ESOL	Lipo	QM9				
GCN	2.87 $\pm$ 0.14	1.43 $\pm$ 0.05	0.85 $\pm$ 0.08	5.796 $\pm$ 1.969				
GIN	2.76 $\pm$ 0.18	1.45 $\pm$ 0.02	0.85 $\pm$ 0.07	4.741 $\pm$ 0.912				
Hu et al.	2.83 $\pm$ 0.12	1.22 $\pm$ 0.02	0.74 $\pm$ 0.00	4.349 $\pm$ 0.061				
N-Gram	2.51 $\pm$ 0.19	1.10 $\pm$ 0.03	0.88 $\pm$ 0.12	7.636 $\pm$ 0.027				
MolCLR	2.47 $\pm$ 0.13	1.21 $\pm$ 0.01	0.69 $\pm$ 0.02	3.916 $\pm$ 0.124				
Grover-10M	2.48 $\pm$ 0.05	0.99 $\pm$ 0.03	<b>0.66<math>\pm</math>0.01</b>	4.983 $\pm$ 0.256				
MPG-10M	2.05 $\pm$ 0.10	1.02 $\pm$ 0.11	0.69 $\pm$ 0.02	4.827 $\pm$ 0.132				
ImageMol	<b>2.02<math>\pm</math>0.07</b>	<b>0.97<math>\pm</math>0.07</b>	0.72 $\pm$ 0.01	<b>3.724<math>\pm</math>0.025</b>				
Rank	1	1	4	1				