

Table 1: ROC-AUC (%) scores on eight MoleculeNet datasets. Bold indicates the best performance under the same encoder. \* denotes result borrowed from original paper. Other results are reproduced using their source codes. Blue denotes newly added result. Some baselines are omitted to save space.

Dataset	BBBP	Tox21	ToxCast	SIDER	ClinTox	MUV	HIV	BACE	Avg. GAIN
<b>GINE</b>									
No Pre-train	67.8±1.6	73.9±0.9	62.4±0.4	58.3±1.5	62.6±4.4	73.4±2.7	76.5±1.7	76.8±2.8	69.0 -
JOAO	71.8±1.0	74.1±0.6	63.9±0.3	60.8±0.9	79.6±1.4	74.2±1.3	76.2±1.6	77.2±2.1	72.2 3.2
ADGCL	70.5±1.8	74.5±0.7	63.0±0.5	59.1±0.9	78.5±3.7	71.5±2.2	75.9±1.4	74.0±2.2	70.9 1.9
BGRL	67.0±0.6	74.5±0.4	62.3±0.2	58.9±0.7	65.5±2.3	76.6±0.8	76.8±0.5	75.6±2.2	69.6 0.6
GraphLOG	71.0±1.1	74.9±0.4	62.8±0.5	59.7±0.9	76.9±1.9	70.8±2.0	75.8±1.4	82.9±0.9	71.8 2.8
RGCL	71.2±0.9	75.3±0.5	63.1±0.3	61.2±0.6	<b>85.0±0.8</b>	73.1±1.2	77.3±0.8	75.7±1.3	72.7 3.7
GraphMAE	72.0±0.9	75.1±0.4	63.0±0.3	58.5±0.7	80.5±2.0	75.7±1.2	76.4±0.8	81.3±1.0	72.8 3.8
GraphMAE*	72.0±0.6	75.5±0.6	64.1±0.3	60.3±1.1	82.3±1.2	76.3±2.4	77.2±1.0	83.1±0.9	73.8 4.8
Mole-BERT	70.5±0.8	75.2±0.9	63.9±0.3	61.0±0.8	79.9±2.8	77.3±1.9	77.2±0.9	81.3±1.2	73.3 4.3
Mole-BERT*	71.9±1.6	<b>76.8±0.5</b>	<b>64.3±0.2</b>	<b>62.8±1.1</b>	78.9±3.0	78.6±1.8	<b>78.2±0.8</b>	80.8±1.4	74.0 5.0
SimSGT	<b>72.3±0.7</b>	75.7±0.5	64.1±0.4	60.6±0.5	82.0±2.6	<b>79.5±0.6</b>	77.7±0.8	<b>83.6±0.8</b>	<b>74.4</b> 5.4
<b>GraphTrans</b>									
No Pre-train	68.7±1.3	75.5±0.5	64.5±0.8	58.0±1.0	71.2±4.9	69.7±1.5	74.2±2.2	77.2±1.6	69.9 -
JOAO	70.8±0.6	75.2±1.5	63.8±0.8	61.0±0.9	78.7±3.0	75.7±2.6	77.0±1.2	77.5±1.2	72.5 2.6
ADGCL	67.9±1.0	73.0±1.2	63.2±0.4	60.2±1.0	78.8±1.6	75.6±2.5	75.5±1.3	73.4±1.6	71.0 1.1
BGRL	<b>72.7±0.9</b>	75.8±1.0	65.1±0.5	60.4±1.2	77.6±4.1	76.7±2.8	77.1±1.2	74.7±2.6	72.5 2.6
GraphLOG	67.6±1.6	76.0±0.8	63.6±0.6	59.8±2.1	79.1±3.2	72.8±1.8	72.5±1.6	83.6±2.0	71.9 2.0
RGCL	71.4±0.8	75.7±0.4	63.9±0.3	60.9±0.6	80.0±1.6	75.9±1.2	77.8±0.6	79.9±1.0	73.2 3.3
S2GAE	67.6±2.0	69.6±1.0	58.7±0.8	55.4±1.3	59.6±1.1	60.1±2.4	68.0±3.7	68.6±2.1	63.5 -6.5
Mole-BERT	70.8±0.5	76.6±0.7	63.7±0.5	59.2±1.1	77.2±1.4	77.2±1.1	76.5±0.8	82.8±1.4	73.0 3.1
GraphMAE	71.7±0.8	76.0±0.9	65.8±0.6	60.0±1.0	79.2±2.2	76.3±1.9	75.9±1.8	81.7±1.6	73.3 3.4
GraphMAE2	71.6±1.6	75.9±0.8	65.6±0.7	59.6±0.6	78.8±3.0	78.5±1.1	76.1±2.2	81.0±1.4	73.4 3.5
SimSGT	72.2±0.9	<b>76.8±0.9</b>	<b>65.9±0.8</b>	<b>61.7±0.8</b>	<b>85.7±1.8</b>	<b>81.4±1.4</b>	<b>78.0±1.9</b>	<b>84.3±0.6</b>	<b>75.8</b> 5.9

Table 2: Time spent for pretraining 100 epochs on ZINC15 when using the GTS encoder.

Model	GraphMAE	Mole-BERT	S2GAE	GraphMAE2	SimSGT
Pretrain Time	527 min	2199 min	1763 min	1195 min	645 min

Table 3: Mean Average Error (MAE) performance on the QM9 dataset. We report average performances and standard deviations across 10 random seeds. GTS encoder is used for compared models.

#Tasks	QM7	QM8	QM9
	1	12	12
GraphCL	80.4±3.3	0.0200±0.0004	5.76±0.37
GraphMAE	78.4±2.3	0.0190±0.0003	5.84±0.16
Mole-BERT	79.8±2.6	0.0190±0.0003	5.75±0.16
SimSGT	<b>75.4±0.7</b>	<b>0.0183±0.0003</b>	<b>5.53±0.25</b>

Table 4: ROC-AUC (%) scores on eight MoleculeNet datasets. Compared methods use GTS encoder and GTS-Small decoder with remask-v2 decoding. Blue denotes newly added result.

Dataset	BBBP	Tox21	ToxCast	SIDER	ClinTox	MUV	HIV	BACE	Avg. GAIN
Motif, MGSSL, Mean	72.5±0.9	77.5±0.4	65.2±0.6	60.7±0.9	85.0±3.5	79.9±1.5	78.0±1.5	83.0±1.0	75.2 5.3
Motif, MGSSL, Max	71.5±0.9	75.8±1.2	66.2±0.7	60.7±1.3	82.6±2.3	78.9±1.8	76.5±1.4	83.8±1.6	74.5 4.6
Motif, MGSSL, Sum	71.7±1.4	75.9±0.6	66.1±0.7	60.4±1.4	83.4±1.5	79.5±1.0	76.8±1.2	84.2±1.1	74.8 4.8
SimSGT	72.2±0.9	76.8±0.9	65.9±0.8	61.7±0.8	85.7±1.8	81.4±1.4	78.0±1.9	84.3±0.6	<b>75.8</b> 5.9