Table 1: Linear probing: molecular property prediction; binary classification, ROC-AUC (%). **Clear improvements (i.e., considering standard deviation) are in bold face.**

	Tox21	ToxCast	Sider	ClinTox	MUV	HIV	BBBP	Bace	Average
AD-GCL	67.6 (0.5)	58.2 (0.3)	56.9 (1.2)	60.8 (1.2)	66.0 (1.6)	67.4 (0.6)	58.9 (0.7)	68.3 (0.7)	63.01
GraphCL	64.4 (0.5)	59.4 (0.2)	54.6 (0.3)	59.8 (1.2)	70.2 (1.0)	63.7 (2.3)	62.4 (0.7)	71.1 (0.7)	63.20
GraphCL + TDL	**72.0** (0.4)	**61.1** (0.2)	**59.7** (0.6)	**65.3** (1.3)	**76.1** (0.9)	**68.2** (1.1)	**65.4** (0.9)	**76.4** (1.1)	**68.02**
GraphCL + TDL (ToDD)	**72.7** (0.5)	60.8 (0.4)	58.9 (0.8)	64.1 (1.7)	72.7 (1.4)	69.7 (1.2)	64.5 (0.8)	76.1 (1.3)	67.44
JOAO	70.6 (0.4)	60.5 (0.3)	57.4 (0.6)	54.1 (2.6)	69.8 (1.9)	68.1 (0.9)	63.7 (0.3)	71.2 (1.0)	64.42
JOAO + TDL	70.5 (0.3)	60.4 (0.2)	57.8 (1.5)	54.6 (1.3)	**74.2** (1.6)	68.2 (0.6)	**65.2** (0.3)	72.7 (3.1)	65.41
JOAO + TDL (ToDD)	**71.7** (0.4)	**61.3** (0.3)	**58.9** (0.7)	52.4 (1.7)	69.6 (1.7)	69.9 (0.6)	64.1 (0.5)	72.6 (0.9)	65.06
SimGRACE	64.6 (0.4)	59.1 (0.2)	54.9 (0.6)	63.4 (2.6)	67.4 (1.2)	66.3 (1.5)	65.4 (1.2)	67.8 (1.3)	63.61
SimGRACE + TDL	**68.6** (0.3)	**61.1** (0.2)	**59.5** (0.4)	62.2 (1.7)	**69.7** (2.0)	**69.5** (1.8)	60.6 (0.5)	**72.1** (0.7)	65.41
SimGRACE + TDL (ToDD)	**70.1** (0.3)	**60.3** (0.3)	**59.1** (0.3)	65.1 (1.4)	**71.4** (1.1)	**71.1** (0.7)	64.9 (0.6)	**73.4** (0.8)	66.93
GraphLoG	67.2 (0.2)	57.9 (0.2)	57.9 (0.3)	57.8 (0.9)	64.2 (1.1)	65.0 (1.3)	54.3 (0.7)	72.3 (0.9)	62.08
GraphLoG + TDL	**72.1** (0.3)	**62.0** (0.2)	**60.7** (0.2)	56.6 (0.8)	**73.0** (0.9)	**70.4** (0.9)	**61.2** (0.4)	**76.8** (0.7)	66.59
GraphLoG + TDL (ToDD)	**70.7** (0.2)	**60.7** (0.3)	**61.5** (0.3)	59.5 (0.5)	**72.9** (1.8)	**71.6** (0.8)	**62.1** (0.3)	**80.1** (0.4)	67.39

Table 2: Transfer results: binary classification over MoleculeNet; ROC-AUC (%).

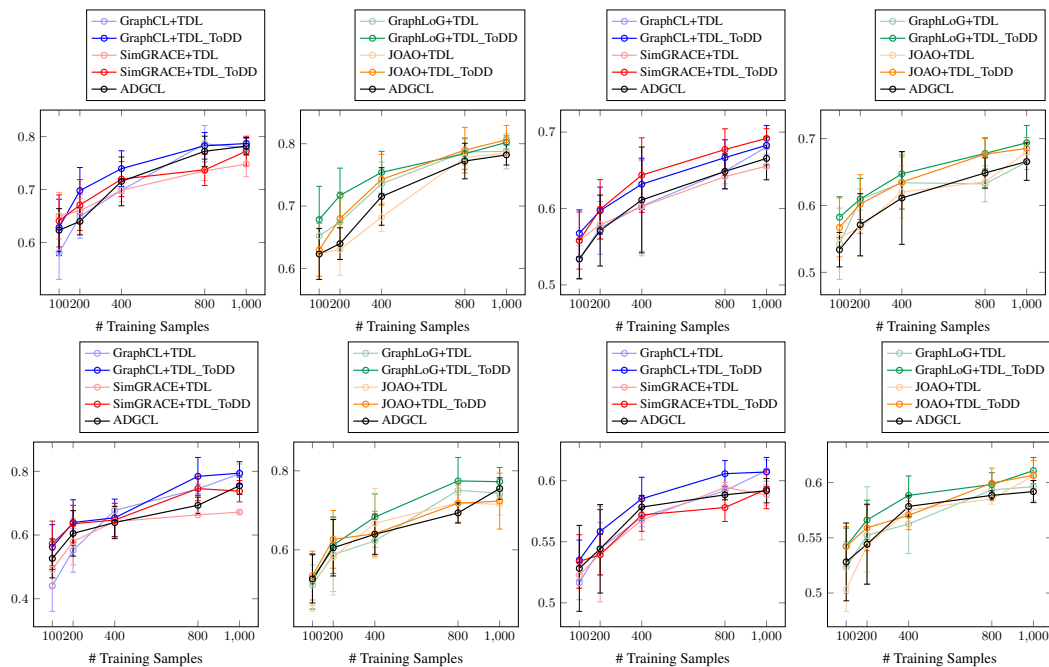|	Tox21	ToxCast	Sider	ClinTox	MUV	HIV	BBBP	Bace	Average
AD-GCL (Original paper)	76.5 (0.8)	63.0 (0.7)	63.2 (0.7)	79.7 (3.5)	72.3 (1.6)	78.2 (0.9)	70.0 (1.0)	78.5 (0.8)	72.67
AD-GCL	74.8 (0.4)	63.8 (0.9)	61.1 (0.9)	78.2 (2.7)	76.3 (1.4)	76.7 (1.2)	71.0 (0.8)	76.2 (1.6)	72.24
AD-GCL + TDL	75.1 (0.5)	64.5 (0.6)	60.9 (1.3)	79.4 (2.8)	74.4 (1.7)	77.4 (0.9)	**71.9** (1.1)	**82.1** (1.4)	73.21
TAE	75.2 (0.8)	63.1 (0.3)	61.9 (0.8)	80.6 (1.9)	74.6 (1.8)	73.5 (2.1)	67.5 (1.1)	82.5 (1.1)	72.36
TAE (ToDD filtration)	**76.8** (0.9)	**64.0** (0.5)	61.9 (0.8)	79.3 (3.6)	75.8 (3.2)	**75.9** (1.1)	**70.4** (0.8)	81.6 (1.4)	73.22
GraphCL	73.9 (0.7)	62.4 (0.6)	60.5 (0.9)	76.0 (2.7)	69.8 (2.7)	78.5 (1.2)	69.7 (0.7)	75.4 (1.4)	70.78
GraphCL + TDL	**75.3** (0.4)	**64.4** (0.3)	61.2 (0.6)	**83.7** (2.7)	**75.7** (0.8)	78.0 (0.9)	**70.9** (0.6)	**80.5** (0.8)	73.71
GraphCL + TDL (ToDD)	**75.2** (0.7)	**64.2** (0.3)	**61.5** (0.2)	**85.2** (1.4)	**75.9** (2.1)	77.9 (0.8)	69.9 (0.9)	**81.2** (1.9)	73.88
JOAO	75.0 (0.3)	62.9 (0.5)	60.0 (0.8)	81.3 (2.5)	71.7 (1.4)	76.7 (1.2)	70.2 (1.0)	77.3 (0.5)	71.89
JOAO + TDL	**75.5** (0.3)	**63.8** (0.2)	60.6 (0.5)	76.8 (1.5)	**73.8** (1.9)	**78.3** (1.2)	70.3 (0.5)	**78.7** (0.6)	72.22
JOAO + TDL (ToDD)	75.2 (0.3)	**63.6** (0.2)	**61.6** (0.6)	80.7 (3.3)	**74.6** (1.6)	77.4 (0.9)	**71.3** (0.8)	**81.0** (2.2)	73.18
SimGRACE	74.4 (0.3)	62.6 (0.7)	60.2 (0.9)	75.5 (2.0)	75.4 (1.3)	75.0 (0.6)	71.2 (1.1)	74.9 (2.0)	71.15
SimGRACE + TDL	74.7 (0.5)	63.0 (0.3)	59.5 (0.4)	73.7 (1.5)	**75.9** (1.6)	**77.3** (1.1)	69.5 (0.9)	**79.1** (0.5)	71.59
SimGRACE + TDL (ToDD)	**75.6** (0.4)	63.3 (0.5)	59.9 (0.8)	**82.4** (2.5)	75.6 (2.0)	**76.1** (1.3)	69.9 (0.8)	78.9 (1.6)	72.71
GraphLoG	75.0 (0.6)	63.4 (0.6)	59.3 (0.8)	70.1 (4.6)	75.5 (1.6)	76.1 (0.8)	69.6 (1.6)	82.1 (1.0)	71.43
GraphLoG + TDL	**76.1** (0.7)	63.7 (0.4)	59.9 (1.0)	**75.7** (3.5)	75.7 (1.2)	76.2 (1.8)	69.6 (1.2)	82.2 (1.5)	72.39
GraphLoG + TDL (ToDD)	**75.9** (0.8)	63.5 (0.7)	**63.4** (0.3)	**79.8** (1.9)	75.6 (1.1)	76.2 (1.6)	70.7 (0.9)	82.1 (1.9)	73.39

Figure 1: Performance over smaller datasets. Each datapoint is the mean ROC-AUC of 10 different splits while keeping scaffolds, with standard deviations shown as error bars. From the upper left to the lower right: Bace, BBBP, Clintox, Sider.