

**Table S28:** Ablation results of data augmentation on benchmark datasets with ROC-AUC metric and random scaffold split. None means not to use any data augmentation. RandomHorizontalFlip, RandomGrayscale and RandomRotation represent data augmentation methods. All means using these three data augmentation methods. All results are reported as mean  $\pm$  standard deviation. Bold font indicates best result.

Classification (Higher is better)						
	BBBP	SIDER	clintox	BACE	Tox21	toxcast
None	0.903 $\pm$ 0.025	0.618 $\pm$ 0.023	0.488 $\pm$ 0.161	0.838 $\pm$ 0.047	0.809 $\pm$ 0.004	0.692 $\pm$ 0.007
RandomHorizontalFlip	0.903 $\pm$ 0.015	0.605 $\pm$ 0.027	0.409 $\pm$ 0.093	0.820 $\pm$ 0.029	0.819 $\pm$ 0.006	0.697 $\pm$ 0.017
RandomGrayscale	0.897 $\pm$ 0.027	0.605 $\pm$ 0.011	0.517 $\pm$ 0.155	0.784 $\pm$ 0.021	0.795 $\pm$ 0.009	0.687 $\pm$ 0.009
RandomRotation	<b>0.954<math>\pm</math>0.010</b>	0.706 $\pm$ 0.008	0.904 $\pm$ 0.013	0.930 $\pm$ 0.016	0.823 $\pm$ 0.002	0.739 $\pm$ 0.009
RandomHorizontalFlip+RandomGrayscale	0.913 $\pm$ 0.016	0.617 $\pm$ 0.010	0.484 $\pm$ 0.102	0.834 $\pm$ 0.028	0.801 $\pm$ 0.010	0.680 $\pm$ 0.004
RandomHorizontalFlip+RandomRotation	0.951 $\pm$ 0.006	0.706 $\pm$ 0.010	0.894 $\pm$ 0.019	0.931 $\pm$ 0.012	0.830 $\pm$ 0.008	0.742 $\pm$ 0.011
RandomGrayscale+RandomRotation	0.942 $\pm$ 0.010	0.706 $\pm$ 0.009	0.936 $\pm$ 0.030	0.933 $\pm$ 0.009	0.828 $\pm$ 0.019	0.740 $\pm$ 0.009
All	0.952 $\pm$ 0.002	<b>0.708<math>\pm</math>0.010</b>	<b>0.975<math>\pm</math>0.007</b>	<b>0.939<math>\pm</math>0.010</b>	<b>0.847<math>\pm</math>0.003</b>	<b>0.751<math>\pm</math>0.002</b>
Regression (Lower is better)						
	FreeSolv	ESOL	Lipo	QM7		
None	1.741 $\pm$ 0.117	0.925 $\pm$ 0.050	0.908 $\pm$ 0.015	88.237 $\pm$ 1.600		
RandomHorizontalFlip	1.551 $\pm$ 0.101	0.766 $\pm$ 0.033	0.907 $\pm$ 0.058	87.547 $\pm$ 9.531		
RandomGrayscale	1.592 $\pm$ 0.113	1.005 $\pm$ 0.026	0.943 $\pm$ 0.013	93.779 $\pm$ 2.121		
RandomRotation	1.655 $\pm$ 0.296	0.722 $\pm$ 0.017	0.630 $\pm$ 0.003	73.567 $\pm$ 5.157		
RandomHorizontalFlip+RandomGrayscale	2.140 $\pm$ 0.181	1.001 $\pm$ 0.161	0.895 $\pm$ 0.025	84.998 $\pm$ 4.017		
RandomHorizontalFlip+RandomRotation	1.594 $\pm$ 0.242	0.776 $\pm$ 0.030	0.629 $\pm$ 0.008	66.412 $\pm$ 6.028		
RandomGrayscale+RandomRotation	1.513 $\pm$ 0.306	<b>0.670<math>\pm</math>0.002</b>	0.631 $\pm$ 0.010	77.853 $\pm$ 6.500		
All	<b>1.149<math>\pm</math>0.004</b>	0.690 $\pm$ 0.003	<b>0.625<math>\pm</math>0.009</b>	<b>65.9<math>\pm</math>2.6</b>		