Model	AUROC	AUPRC	p-value
ChemAP (student)	**0.782 ±0.025**	**0.842 ±0.026**	-
MLP	0.749 ±0.020	0.819 ±0.015	1.3×10^{-3}
ChemBERT	0.726 ±0.027	0.795 ±0.040	1.7×10^{-4}
MolCLR	0.646 ±0.043	0.746 ±0.040	3.9×10^{-5}
MoLFormer	0.694 ±0.034	0.781 ±0.031	3.5×10^{-4}
MAT	0.666 ±0.033	0.746 ±0.041	3.5×10^{-5}
Graph Transformer	0.574 ±0.053	0.743 ±0.047	6.1×10^{-7}
GraphMVP	0.688 ±0.028	0.785 ±0.020	9.1×10^{-5}
Uni-Mol	0.696 ±0.029	0.779 ±0.029	1.7×10^{-4}
Random forest	<u>0.750 ±0.023</u>	0.819 ±0.023	5.9×10^{-4}
Catboost	0.748 ±0.021	<u>0.820 ±0.020</u>	5.6×10^{-4}
XGBRF	0.692 ±0.016	0.773 ±0.022	5.9×10^{-7}
XGBoost	0.672 ±0.016	0.748 ±0.032	5.3×10^{-7}
SVM	0.705 ±0.028	0.765 ±0.039	4.8×10^{-7}

Table S1. The prediction performances for drug approval under the drug split setting. Bold is best and underline is second best. The p-value indicates a statistically significant difference between ChemAP and the baseline model based on the paired t-test.

Model	AUROC	AUPRC	p-value
ChemAP (student)	**0.702 ±0.055**	**0.791 ±0.033**	-
MLP	0.663 ±0.063	0.753 ±0.052	3.1×10^{-3}
ChemBERT	0.659 ±0.059	0.756 ±0.043	5.6×10^{-3}
MolCLR	0.590 ±0.030	0.756 ±0.043	1.2×10^{-4}
MoLFormer	0.641 ±0.059	0.741 ±0.044	1.0×10^{-3}
MAT	0.636 ±0.061	0.740 ±0.043	1.1×10^{-3}
Graph Transformer	0.587 ±0.074	0.719 ±0.052	2.8×10^{-4}
GraphMVP	0.611 ±0.055	0.729 ±0.049	3.6×10^{-4}
Uni-Mol	0.635 ±0.066	0.734 ±0.048	4.5×10^{-4}
Random forest	0.661 ±0.063	0.760 ±0.044	1.3×10^{-2}
Catboost	<u>0.674 ±0.052</u>	<u>0.768 ±0.047</u>	3.0×10^{-2}
XGBRF	0.648 ±0.044	0.746 ±0.046	3.6×10^{-3}
XGBoost	0.636 ±0.042	0.728 ±0.043	2.3×10^{-3}
SVM	0.600 ±0.056	0.713 ±0.047	3.5×10^{-4}

Table S2. The prediction performances for drug approval under the scaffold split setting. Bold is best and underline is second best. The p-value indicates a statistically significant difference between ChemAP and the baseline model based on the paired t-test.