

**Table S12:** The performance of different methods on 10 G protein coupled receptors (GPCRs) datasets with balanced scaffold split.

	1. 5HT1A		2. 5HT2A		3. AA1R	
	RMSE	MAE	RMSE	MAE	RMSE	MAE
MoCLR <sub>GIN</sub>	0.850±0.021	0.670±0.012	0.853±0.019	0.642±0.014	0.786±0.015	0.588±0.009
MoCLR <sub>GCN</sub>	0.949±0.027	0.764±0.014	0.875±0.008	0.681±0.024	0.856±0.026	0.662±0.026
RNN LR	1.574±0.091	0.937±0.019	1.602±0.245	1.103±0.151	1.073±0.087	0.762±0.057
TRFM LR	1.636±0.004	1.109±0.001	1.389±0.000	0.999±0.001	1.060±0.003	0.810±0.001
RNN MLP	0.957±0.013	0.768±0.010	1.167±0.010	0.890±0.003	0.848±0.004	0.662±0.008
TRFM MLP	0.939±0.034	0.730±0.025	1.013±0.026	0.728±0.021	0.878±0.051	0.657±0.031
RNN RF	0.788±0.004	<b>0.617±0.004</b>	1.001±0.001	0.747±0.001	0.717±0.003	0.554±0.002
TRFM RF	0.855±0.001	0.672±0.001	1.011±0.002	0.777±0.002	0.740±0.001	0.568±0.001
CHEM-BERT	0.876±0.018	0.706±0.012	0.909±0.057	0.682±0.056	0.734±0.038	<b>0.544±0.027</b>
ImageMol	<b>0.776±0.012</b>	0.620±0.014	<b>0.780±0.017</b>	<b>0.578±0.022</b>	<b>0.711±0.012</b>	0.554±0.009
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	4. AA2AR		5. AA3R		6. CNR2	
	RMSE	MAE	RMSE	MAE	RMSE	MAE
MoCLR <sub>GIN</sub>	0.748±0.012	0.588±0.008	0.840±0.014	0.692±0.010	0.926±0.047	0.758±0.036
MoCLR <sub>GCN</sub>	0.819±0.011	0.651±0.008	0.855±0.010	0.700±0.011	0.978±0.023	0.803±0.021
RNN LR	1.801±0.600	1.193±0.335	2.295±0.463	1.190±0.155	5.505±0.093	1.611±0.032
TRFM LR	1.130±0.000	0.906±0.000	1.155±0.001	0.919±0.001	1.700±0.001	1.213±0.000
RNN MLP	0.967±0.002	0.773±0.005	0.883±0.010	0.707±0.012	1.091±0.015	0.881±0.013
TRFM MLP	0.948±0.013	0.744±0.005	0.945±0.010	0.749±0.014	1.144±0.055	0.903±0.038
RNN RF	0.887±0.002	0.692±0.001	0.796±0.009	<b>0.624±0.007</b>	0.965±0.002	0.766±0.001
TRFM RF	0.926±0.003	0.735±0.004	0.856±0.001	0.701±0.002	0.965±0.002	0.800±0.002
CHEM-BERT	0.862±0.071	0.674±0.058	0.861±0.058	0.684±0.047	0.925±0.051	0.727±0.041
ImageMol	<b>0.734±0.015</b>	<b>0.573±0.009</b>	<b>0.793±0.008</b>	0.634±0.001	<b>0.905±0.004</b>	<b>0.717±0.015</b>
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	7. DRD2		8. DRD3		9. HRH3	
	RMSE	MAE	RMSE	MAE	RMSE	MAE
MoCLR <sub>GIN</sub>	0.814±0.009	0.591±0.007	0.858±0.017	0.673±0.022	0.734±0.006	0.581±0.004
MoCLR <sub>GCN</sub>	0.855±0.022	0.634±0.017	0.914±0.024	0.725±0.025	0.740±0.016	0.576±0.006
RNN LR	1.142±0.077	0.839±0.038	1.316±0.011	0.942±0.005	1.616±0.236	0.943±0.070
TRFM LR	1.000±0.000	0.719±0.000	1.219±0.000	0.914±0.000	1.169±0.002	0.911±0.002
RNN MLP	0.895±0.006	0.694±0.005	1.021±0.007	0.819±0.007	0.871±0.015	0.702±0.011
TRFM MLP	0.919±0.016	0.686±0.016	1.012±0.041	0.790±0.023	0.863±0.011	0.676±0.009
RNN RF	0.837±0.001	0.612±0.001	0.861±0.001	0.685±0.001	0.771±0.002	0.613±0.002
TRFM RF	0.864±0.001	0.636±0.002	0.904±0.001	0.717±0.001	0.770±0.002	0.602±0.001
CHEM-BERT	0.816±0.011	0.587±0.013	0.803±0.029	0.631±0.026	0.770±0.033	0.594±0.022
ImageMol	<b>0.772±0.014</b>	<b>0.573±0.009</b>	<b>0.735±0.018</b>	<b>0.576±0.014</b>	<b>0.710±0.006</b>	<b>0.561±0.006</b>
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	10. OPRM					
	RMSE	MAE				
MoCLR <sub>GIN</sub>	0.856±0.008	0.664±0.016				
MoCLR <sub>GCN</sub>	0.853±0.009	0.653±0.020				
RNN LR	2.649±1.024	1.744±0.614				
TRFM LR	1.694±0.001	1.282±0.000				
RNN MLP	1.022±0.014	0.781±0.008				
TRFM MLP	1.084±0.009	0.849±0.007				
RNN RF	0.876±0.010	0.671±0.009				
TRFM RF	0.852±0.002	0.660±0.003				
CHEM-BERT	0.893±0.024	0.672±0.019				
ImageMol	<b>0.849±0.018</b>	<b>0.645±0.015</b>				