

Table S10: The performance of different methods on CYP450 datasets with balanced scaffold split.

CYP1A2							
	accuracy	auc	aupr	f1	precision	recall	kappa
Mo1CLR _{GIN}	0.831±0.005	0.900±0.003	0.893±0.007	0.829±0.004	0.818±0.008	0.841±0.006	0.661±0.009
Mo1CLR _{RGN}	0.814±0.007	0.885±0.001	0.871±0.002	0.803±0.009	0.825±0.004	0.782±0.018	0.626±0.014
RNN LR	0.722±0.000	0.790±0.000	0.759±0.000	0.707±0.000	0.724±0.000	0.691±0.000	0.443±0.000
TRFM LR	0.791±0.000	0.868±0.000	0.869±0.000	0.778±0.000	0.804±0.000	0.754±0.000	0.581±0.000
RNN MLP	0.681±0.023	0.771±0.007	0.739±0.007	0.631±0.061	0.715±0.017	0.576±0.115	0.357±0.050
TRFM MLP	0.774±0.004	0.850±0.002	0.857±0.003	0.754±0.011	0.803±0.022	0.712±0.037	0.546±0.008
RNN RF	0.780±0.003	0.855±0.002	0.856±0.002	0.764±0.004	0.797±0.003	0.733±0.004	0.558±0.006
TRFM RF	0.790±0.004	0.871±0.000	0.871±0.000	0.778±0.004	0.799±0.005	0.758±0.004	0.578±0.007
CHEM-BERT	0.794±0.006	0.874±0.004	0.871±0.007	0.772±0.008	0.834±0.021	0.720±0.022	0.586±0.013
GROVER	0.809±0.001	0.884±0.000	0.882±0.000	0.798±0.002	0.823±0.006	0.774±0.007	0.618±0.002
ImageMol	0.834±0.006	0.905±0.002	0.903±0.002	0.834±0.004	0.811±0.015	0.859±0.010	0.668±0.011
CYP2C9							
	accuracy	auc	aupr	f1	precision	recall	kappa
Mo1CLR _{GIN}	0.779±0.007	0.838±0.008	0.724±0.016	0.706±0.012	0.694±0.016	0.719±0.031	0.529±0.016
Mo1CLR _{RGN}	0.757±0.003	0.818±0.002	0.714±0.002	0.651±0.016	0.690±0.012	0.617±0.036	0.465±0.013
RNN LR	0.698±0.000	0.743±0.000	0.615±0.000	0.522±0.000	0.627±0.000	0.447±0.000	0.310±0.000
TRFM LR	0.720±0.000	0.780±0.000	0.682±0.000	0.603±0.000	0.630±0.000	0.579±0.000	0.387±0.000
RNN MLP	0.653±0.012	0.729±0.007	0.578±0.009	0.401±0.157	0.587±0.058	0.393±0.285	0.199±0.078
TRFM MLP	0.727±0.008	0.776±0.006	0.668±0.004	0.625±0.012	0.634±0.014	0.616±0.019	0.411±0.017
RNN RF	0.719±0.001	0.763±0.000	0.623±0.002	0.603±0.003	0.628±0.001	0.580±0.005	0.386±0.003
TRFM RF	0.735±0.001	0.798±0.001	0.691±0.002	0.614±0.001	0.664±0.003	0.571±0.001	0.414±0.002
CHEM-BERT	0.752±0.006	0.822±0.003	0.711±0.002	0.649±0.019	0.681±0.033	0.627±0.065	0.458±0.009
GROVER	0.745±0.005	0.814±0.002	0.725±0.003	0.595±0.024	0.719±0.013	0.509±0.039	0.417±0.019
ImageMol	0.785±0.001	0.859±0.001	0.776±0.004	0.711±0.001	0.703±0.005	0.719±0.006	0.539±0.002
CYP2C19							
	accuracy	auc	aupr	f1	precision	recall	kappa
Mo1CLR _{GIN}	0.789±0.010	0.865±0.000	0.833±0.002	0.787±0.006	0.741±0.019	0.840±0.012	0.579±0.020
Mo1CLR _{RGN}	0.792±0.001	0.862±0.001	0.837±0.002	0.785±0.002	0.755±0.009	0.819±0.015	0.584±0.002
RNN LR	0.692±0.000	0.751±0.000	0.692±0.000	0.662±0.000	0.677±0.000	0.648±0.000	0.380±0.000
TRFM LR	0.729±0.000	0.816±0.000	0.785±0.000	0.708±0.000	0.709±0.000	0.708±0.000	0.455±0.000
RNN MLP	0.667±0.014	0.739±0.006	0.684±0.002	0.624±0.058	0.660±0.039	0.613±0.124	0.327±0.033
TRFM MLP	0.725±0.010	0.789±0.005	0.755±0.004	0.696±0.016	0.716±0.007	0.678±0.026	0.445±0.022
RNN RF	0.715±0.003	0.790±0.001	0.734±0.001	0.696±0.002	0.691±0.004	0.701±0.002	0.428±0.005
TRFM RF	0.747±0.003	0.824±0.001	0.792±0.001	0.728±0.003	0.728±0.005	0.727±0.006	0.491±0.006
CHEM-BERT	0.780±0.006	0.855±0.001	0.821±0.007	0.771±0.011	0.747±0.012	0.798±0.031	0.560±0.014
GROVER	0.759±0.001	0.838±0.000	0.798±0.001	0.737±0.001	0.749±0.002	0.725±0.004	0.514±0.002
ImageMol	0.793±0.001	0.871±0.001	0.847±0.002	0.791±0.004	0.749±0.008	0.838±0.020	0.588±0.002
CYP2D6							
	accuracy	auc	aupr	f1	precision	recall	kappa
Mo1CLR _{GIN}	0.812±0.004	0.823±0.001	0.621±0.002	0.583±0.003	0.576±0.012	0.591±0.016	0.452±0.003
Mo1CLR _{RGN}	0.816±0.003	0.819±0.001	0.623±0.004	0.505±0.015	0.680±0.023	0.403±0.024	0.408±0.014
RNN LR	0.787±0.000	0.670±0.000	0.387±0.000	0.206±0.000	0.582±0.000	0.125±0.000	0.139±0.000
TRFM LR	0.798±0.000	0.754±0.000	0.504±0.000	0.392±0.000	0.586±0.000	0.294±0.000	0.286±0.000
RNN MLP	0.780±0.004	0.670±0.007	0.369±0.016	0.204±0.014	0.515±0.046	0.128±0.013	0.127±0.006
TRFM MLP	0.782±0.007	0.721±0.003	0.465±0.010	0.448±0.002	0.511±0.021	0.400±0.012	0.316±0.008
RNN RF	0.803±0.002	0.727±0.001	0.478±0.002	0.398±0.002	0.611±0.010	0.295±0.002	0.297±0.003
TRFM RF	0.806±0.002	0.769±0.001	0.531±0.002	0.315±0.011	0.719±0.014	0.201±0.008	0.241±0.011
CHEM-BERT	0.813±0.011	0.780±0.014	0.550±0.032	0.483±0.012	0.632±0.064	0.395±0.030	0.376±0.016
GROVER	0.807±0.003	0.789±0.003	0.534±0.012	0.331±0.031	0.706±0.006	0.217±0.027	0.254±0.027
ImageMol	0.818±0.009	0.827±0.002	0.626±0.002	0.568±0.015	0.603±0.036	0.544±0.06	0.454±0.008
CYP3A4							
	accuracy	auc	aupr	f1	precision	recall	kappa
Mo1CLR _{GIN}	0.833±0.003	0.898±0.001	0.821±0.006	0.746±0.010	0.749±0.015	0.745±0.033	0.622±0.009
Mo1CLR _{RGN}	0.810±0.004	0.874±0.001	0.770±0.003	0.686±0.011	0.755±0.001	0.629±0.018	0.551±0.012
RNN LR	0.775±0.000	0.826±0.000	0.674±0.000	0.635±0.000	0.685±0.000	0.591±0.000	0.474±0.000
TRFM LR	0.806±0.000	0.867±0.000	0.782±0.000	0.707±0.000	0.704±0.000	0.711±0.000	0.562±0.000
RNN MLP	0.757±0.003	0.812±0.006	0.655±0.007	0.610±0.035	0.652±0.028	0.582±0.090	0.436±0.026
TRFM MLP	0.782±0.005	0.844±0.004	0.713±0.015	0.667±0.004	0.673±0.014	0.662±0.010	0.506±0.009
RNN RF	0.779±0.004	0.837±0.000	0.713±0.001	0.654±0.007	0.675±0.004	0.635±0.010	0.492±0.010
TRFM RF	0.810±0.004	0.862±0.001	0.773±0.004	0.697±0.007	0.732±0.007	0.666±0.007	0.559±0.010
CHEM-BERT	0.827±0.004	0.892±0.004	0.808±0.009	0.745±0.014	0.729±0.025	0.766±0.053	0.615±0.013
GROVER	0.826±0.003	0.891±0.001	0.817±0.002	0.720±0.004	0.768±0.013	0.678±0.013	0.594±0.005
ImageMol	0.845±0.004	0.903±0.001	0.833±0.001	0.765±0.002	0.769±0.025	0.763±0.029	0.65±0.003