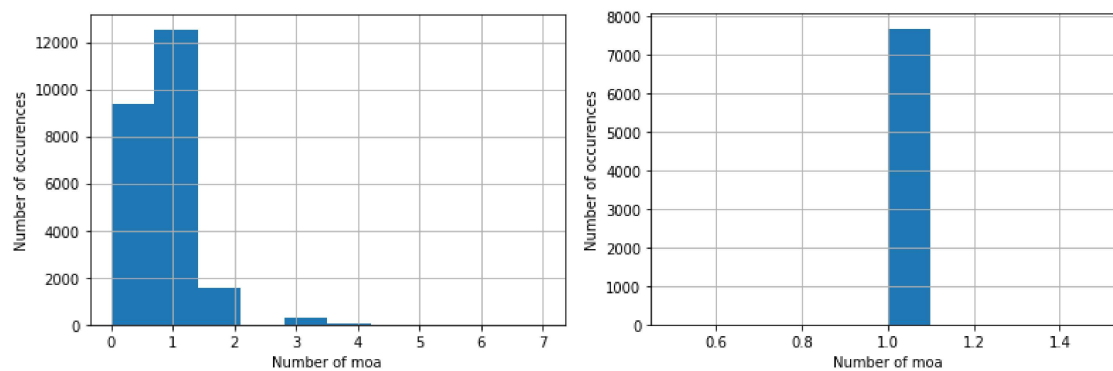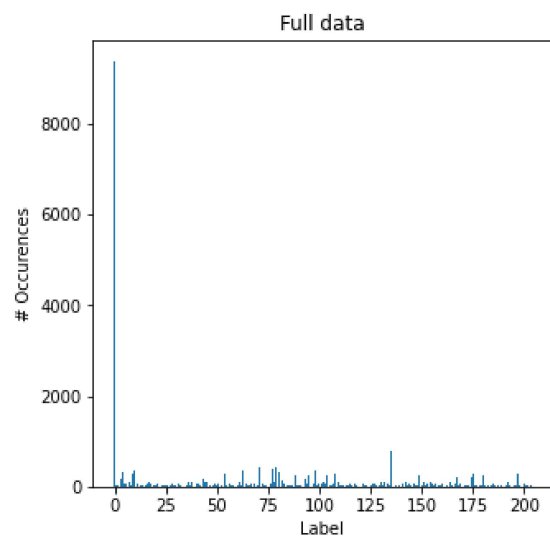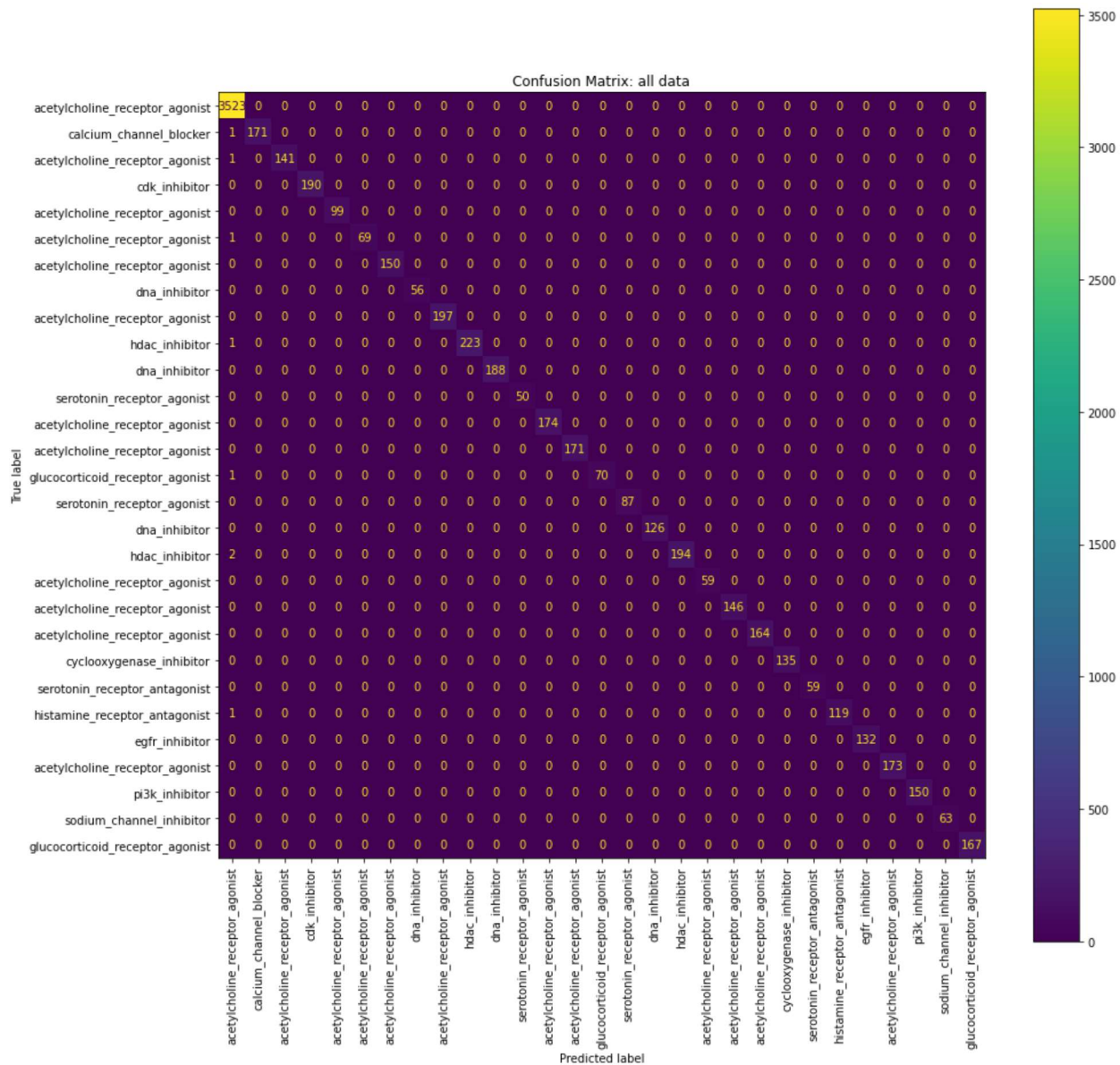# Supplemental Figures

Supp Fig. 1. Number of MoAs per sample before (left) and after (right) selection.

Supp Fig. 2. Number of occurrences by label (ordinal label).

Supp Figure 3. AutoGluon confusion matrix using all test data, with label counts.
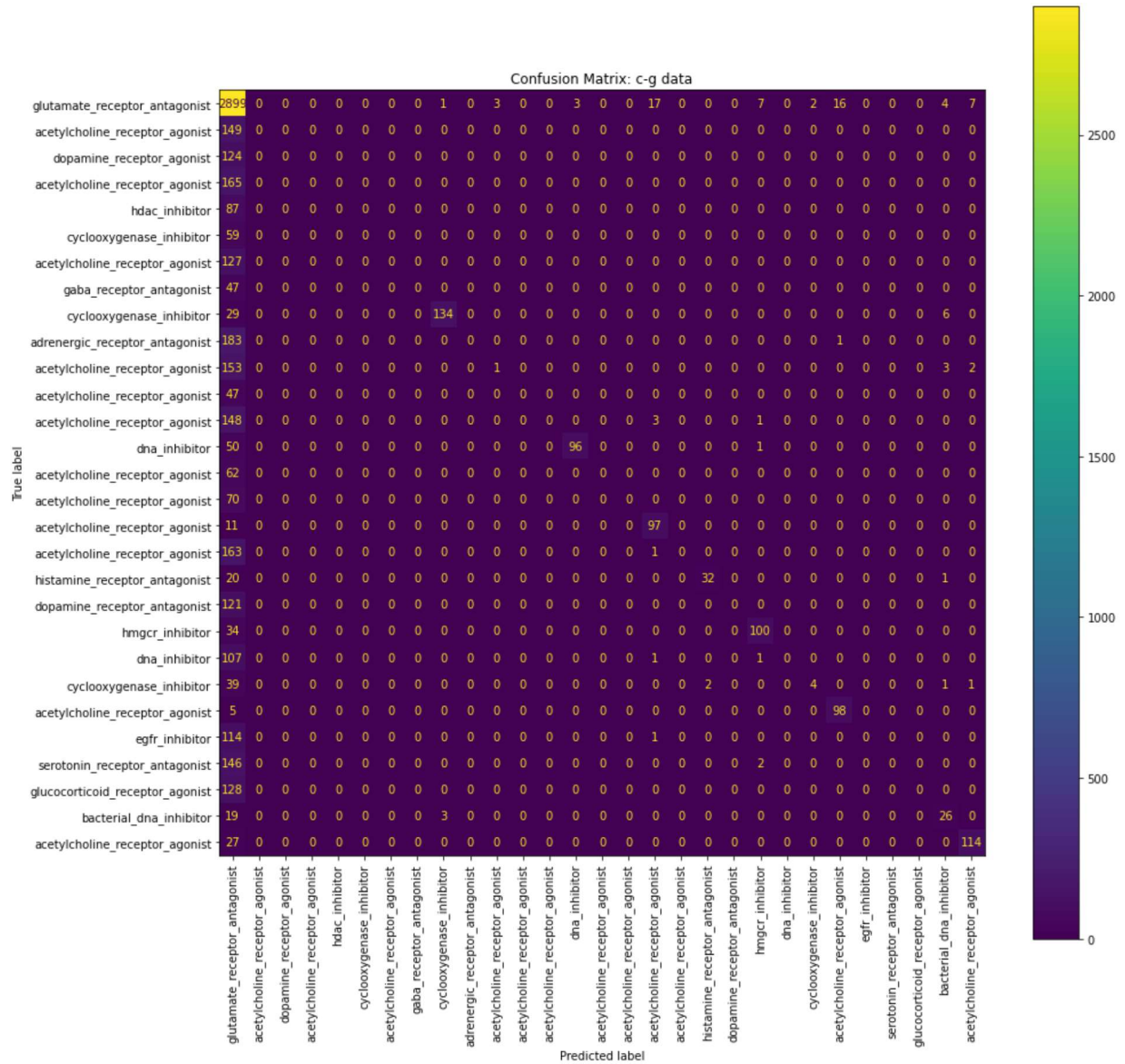
Supp Fig. 4. **AutoGluon confusion matrix using all cell viability and gene expression test data, with label counts.**

Confusion Matrix: c-g data
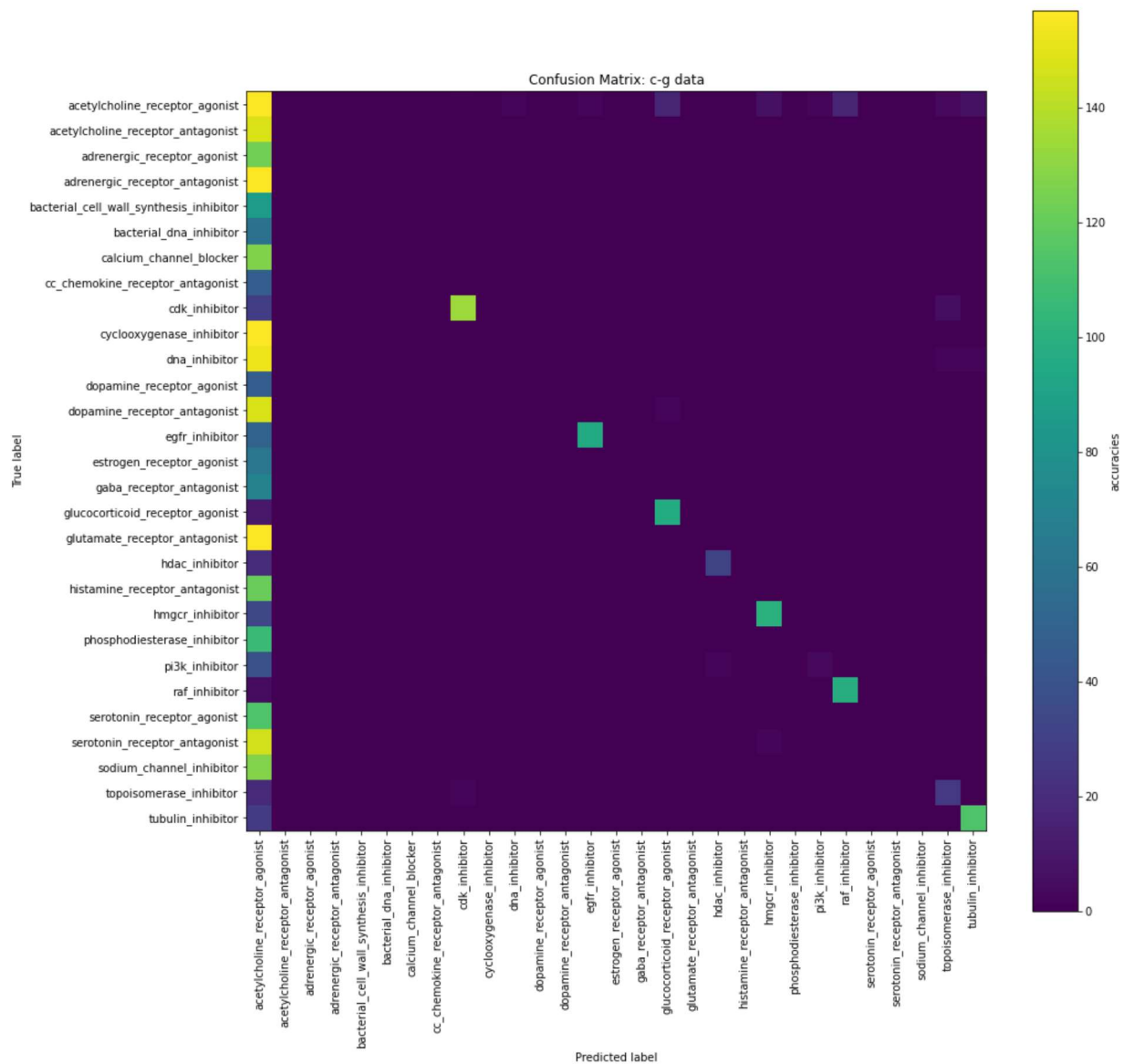
Supp Fig. 5. AutoGluon confusion matrix using all cell viability and gene expression test data, without label counts. Normalized by the smallest number of occurrences.
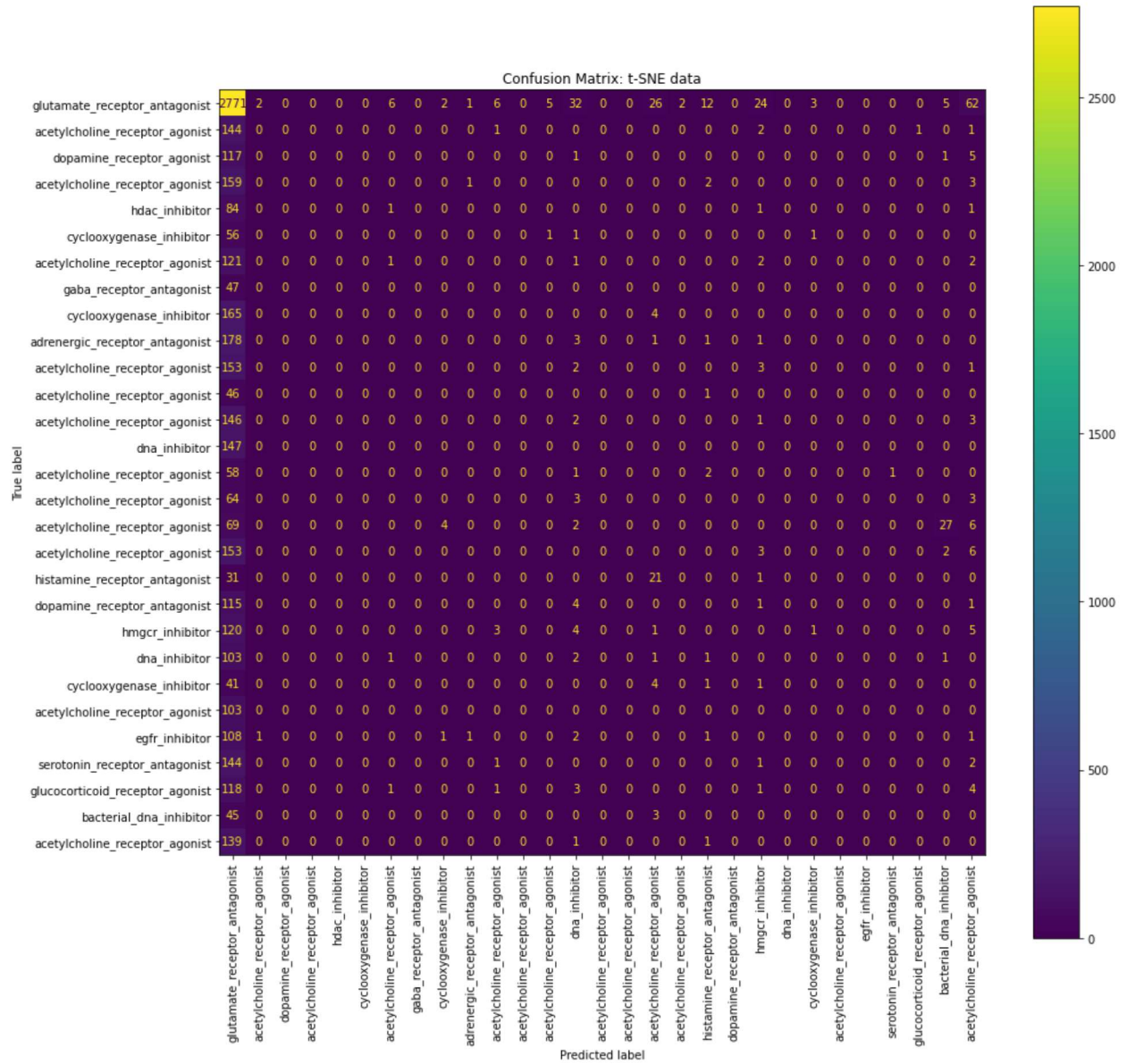
Supp Fig. 6. AutoGluon confusion matrix for t-SNE reduced test data, with label counts.
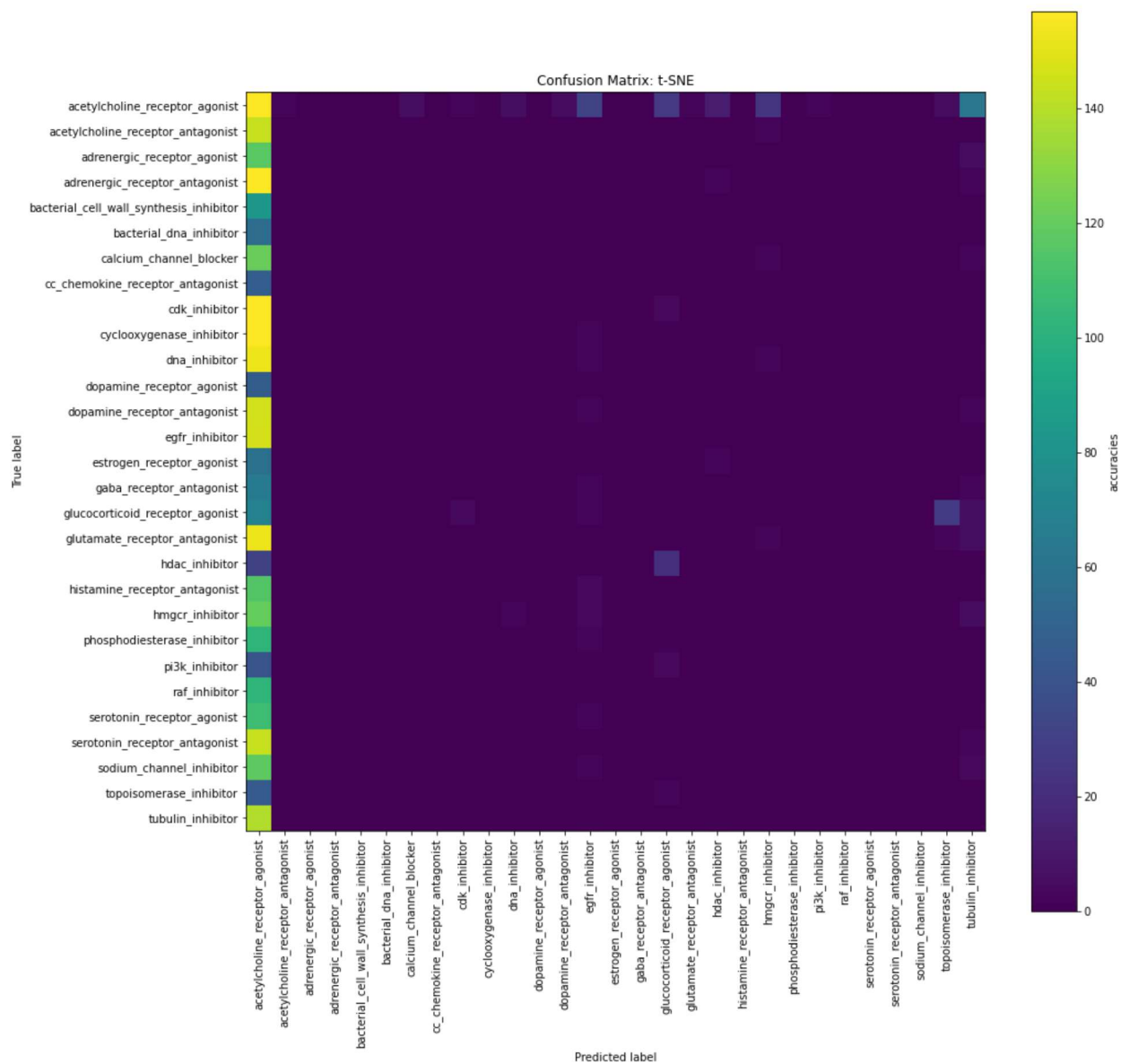
Fig. 7. AutoGluon confusion matrix for t-SNE-reduced test data, without label counts. Normalized by the smallest number of occurrences.
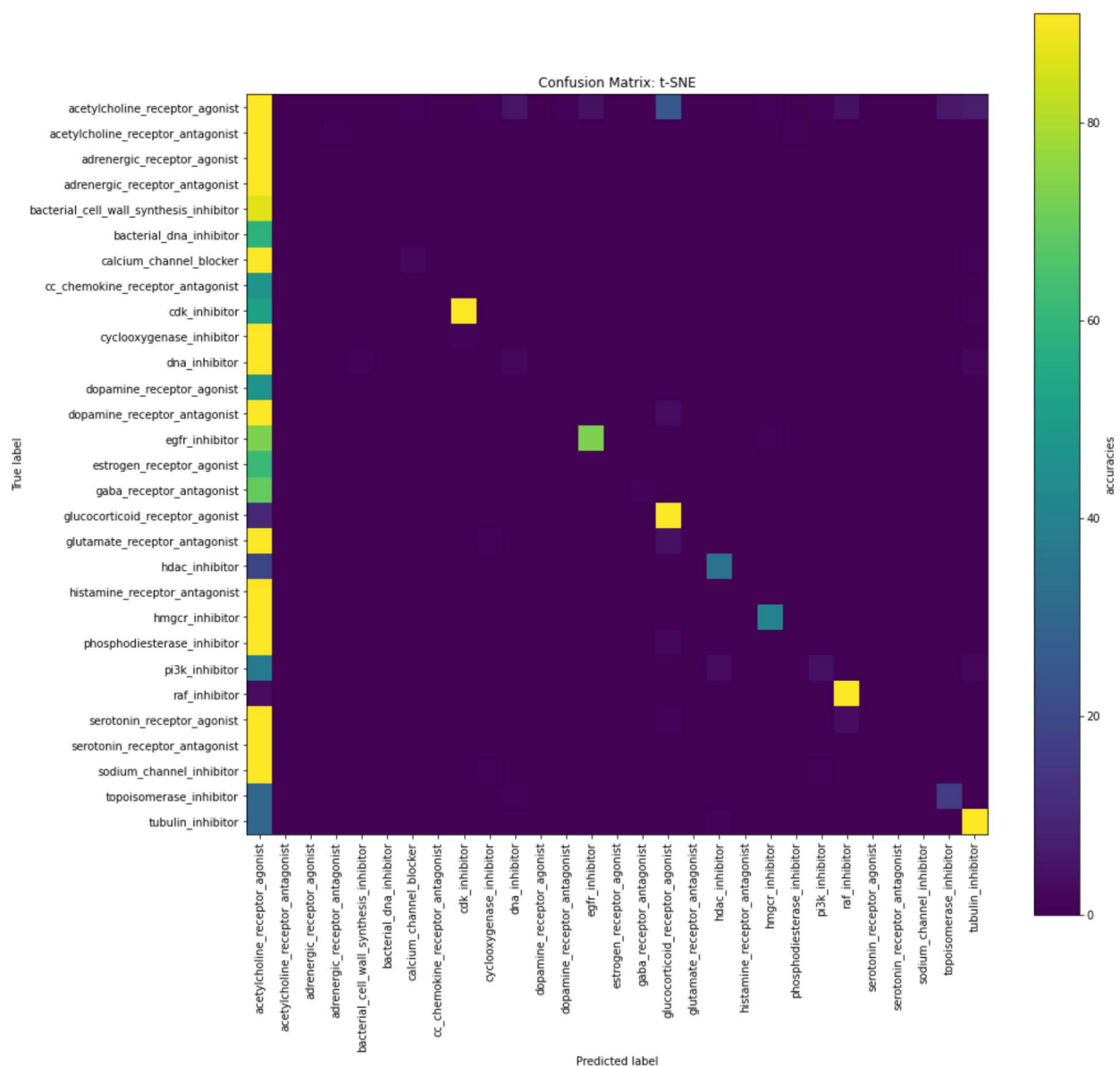
Fig. 8. AutoGluon confusion matrix for t-SNE-reduced test data, without label counts. Trained on data compensated for the most frequent (unbalanced) class, tested on original test data. Normalized by the smallest number of occurrences.

Fig. 9. AutoGluon on PHATE-reduced testing data, with label counts.

Supp Fig. 10. AutoGluon on PHATE–reduced testing data, with label counts. Normalized by the smallest number of occurrences.
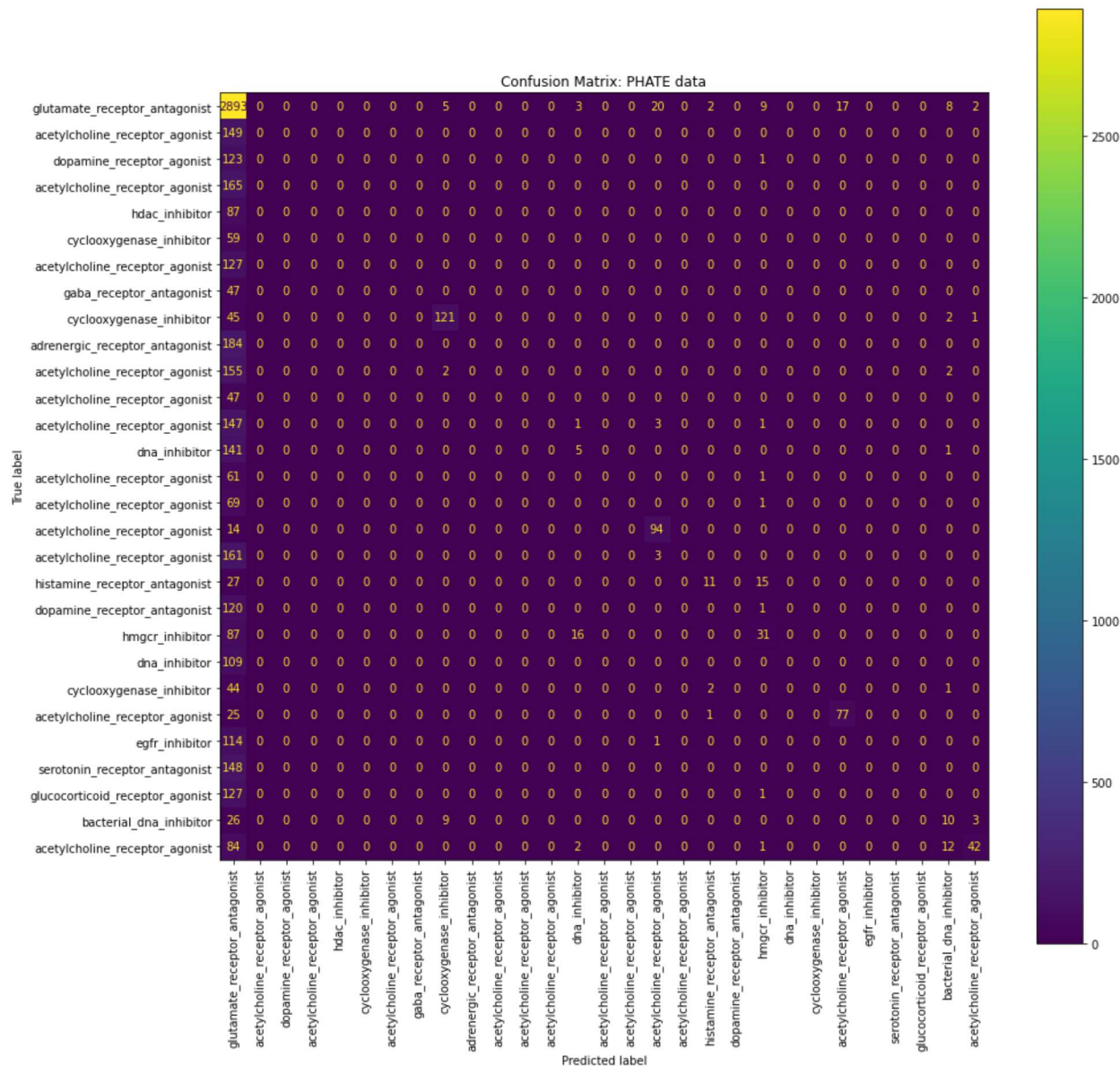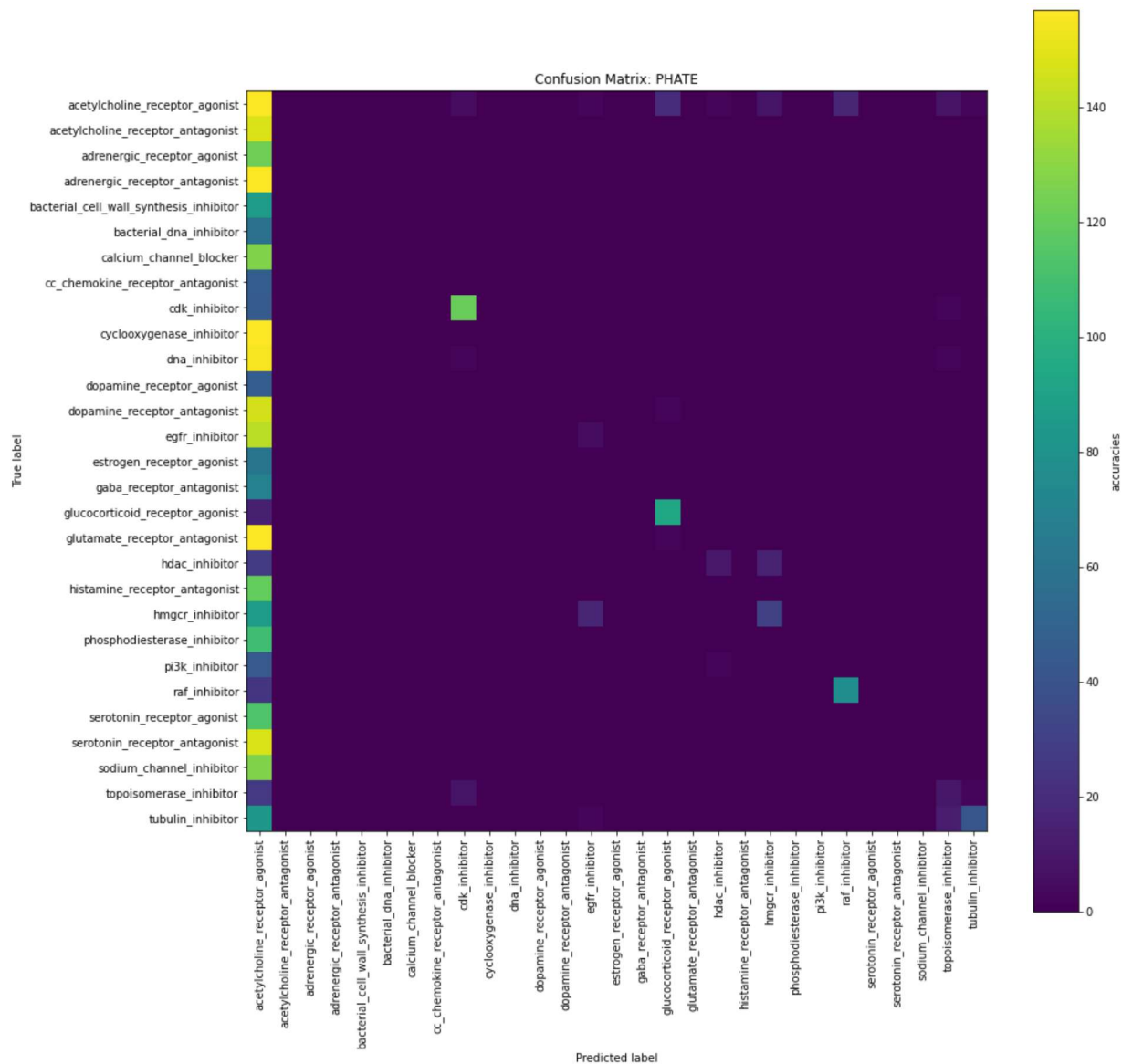
Supplemental Table 1: AutoGluon models performance on training data, for each data type.

	ALL FEATURES							
	model	score_val	pred_time_val	fit_time	pred_time_val _marginal	fit_time_margi nal	stack_level	can_infer	fit_order
0	WeightedEnsemble_L2	0.997245	0.457079	2818.764307	0.002862	0.672512	2	TRUE	13
1	CatBoost	0.990358	0.055911	2168.637975	0.055911	2168.637975	1	TRUE	8
2	NeuralNetFastAI	0.971074	0.309232	27.714371	0.309232	27.714371	1	TRUE	3
3	LightGBM	0.954545	0.243737	599.72289	0.243737	599.72289	1	TRUE	5
4	XGBoost	0.951791	0.089074	621.739449	0.089074	621.739449	1	TRUE	11
5	LightGBMLarge	0.950413	0.649085	1894.998363	0.649085	1894.998363	1	TRUE	12
6	LightGBMXT	0.896694	0.603696	606.153201	0.603696	606.153201	1	TRUE	4
7	KNeighborsUnif	0.608815	0.500135	0.522425	0.500135	0.522425	1	TRUE	1
8	KNeighborsDist	0.606061	0.499529	0.507426	0.499529	0.507426	1	TRUE	2
9	RandomForestGini	0.592287	0.210967	117.438373	0.210967	117.438373	1	TRUE	6
10	RandomForestEntr	0.586777	0.211045	387.916893	0.211045	387.916893	1	TRUE	7
11	ExtraTreesGini	0.582645	0.211138	10.422346	0.211138	10.422346	1	TRUE	9
12	ExtraTreesEntr	0.571625	0.210776	12.532067	0.210776	12.532067	1	TRUE	10

	TSNE							
	model	accuracy_val	pred_time_val	fit_time	pred_time_val _marginal	fit_time_margi nal	stack_level	can_infer	fit_order
0	WeightedEnsemble_L2	0.575663	1.048955	73.233252	0.000981	0.92158	2	TRUE	13
1	LightGBM	0.564743	0.025659	5.537528	0.025659	5.537528	1	TRUE	5
2	LightGBMLarge	0.563183	0.025512	14.022789	0.025512	14.022789	1	TRUE	12
3	XGBoost	0.563183	0.0295	6.558862	0.0295	6.558862	1	TRUE	11
4	LightGBMXT	0.563183	0.240415	33.520364	0.240415	33.520364	1	TRUE	4
5	NeuralNetFastAI	0.560062	0.031279	18.91913	0.031279	18.91913	1	TRUE	3
6	CatBoost	0.556942	0.009841	5.787583	0.009841	5.787583	1	TRUE	8
7	KNeighborsUnif	0.550702	0.109074	0.012878	0.109074	0.012878	1	TRUE	1
8	ExtraTreesGini	0.533541	0.202991	1.658499	0.202991	1.658499	1	TRUE	9
9	ExtraTreesEntr	0.533541	0.204728	2.439578	0.204728	2.439578	1	TRUE	10
10	RandomForestEntr	0.521061	0.20572	19.243975	0.20572	19.243975	1	TRUE	7
11	RandomForestGini	0.50858	0.305137	6.085887	0.305137	6.085887	1	TRUE	6
12	KNeighborsDist	0.485179	0.10392	0.018524	0.10392	0.018524	1	TRUE	2

	TSNE - improved class balance							
	model	score_val	pred_time_val	fit_time	e_val_marginal	_time_marginal	stack_level	can_infer	fit_order
0	WeightedEnsemble_L2	0.578	0.973965	23.43575	0.004835	2.021898	2	TRUE	13
1	LightGBMXT	0.576	0.241778	5.680235	0.241778	5.680235	1	TRUE	4
2	CatBoost	0.572	0.005807	5.926473	0.005807	5.926473	1	TRUE	8
3	XGBoost	0.572	0.016887	3.856479	0.016887	3.856479	1	TRUE	11
4	NeuralNetFastAI	0.566	0.023057	5.8255	0.023057	5.8255	1	TRUE	3
5	LightGBM	0.566	0.034233	3.761809	0.034233	3.761809	1	TRUE	5
6	KNeighborsUnif	0.546	0.110957	0.028606	0.110957	0.028606	1	TRUE	1
7	LightGBMLarge	0.544	0.026673	11.57406	0.026673	11.57406	1	TRUE	12
8	ExtraTreesGini	0.53	0.203764	1.764859	0.203764	1.764859	1	TRUE	9
9	ExtraTreesEntr	0.53	0.203784	1.568799	0.203784	1.568799	1	TRUE	10
10	RandomForestEntr	0.512	0.203603	6.45517	0.203603	6.45517	1	TRUE	7
11	RandomForestGini	0.51	0.203043	2.714159	0.203043	2.714159	1	TRUE	6
12	KNeighborsDist	0.48	0.110394	0.018316	0.110394	0.018316	1	TRUE	2

	PHATE							
	model	accuracy_val	pred_time_val	fit_time	pred_time_val _marginal	fit_time_margi nal	stack_level	can_infer	fit_order
0	WeightedEnsemble_L2	0.564743	0.243996	18.958103	0.000658	0.609832	2	TRUE	13
1	XGBoost	0.563183	0.020584	5.411705	0.020584	5.411705	1	TRUE	11
2	CatBoost	0.556942	0.023212	19.432676	0.023212	19.432676	1	TRUE	8
3	LightGBM	0.555382	0.013304	7.212991	0.013304	7.212991	1	TRUE	5
4	NeuralNetFastAI	0.552262	0.019787	8.972454	0.019787	8.972454	1	TRUE	3
5	LightGBMLarge	0.549142	0.02248	14.42803	0.02248	14.42803	1	TRUE	12
6	LightGBMXT	0.549142	0.381437	46.990908	0.381437	46.990908	1	TRUE	4
7	KNeighborsUnif	0.50858	0.107666	0.019777	0.107666	0.019777	1	TRUE	1
8	ExtraTreesGini	0.5039	0.202725	1.908056	0.202725	1.908056	1	TRUE	9
9	ExtraTreesEntr	0.5039	0.202943	1.961677	0.202943	1.961677	1	TRUE	10
10	RandomForestEntr	0.4883	0.203479	23.617208	0.203479	23.617208	1	TRUE	7
11	RandomForestGini	0.474259	0.202967	3.964113	0.202967	3.964113	1	TRUE	6
12	KNeighborsDist	0.429017	0.110068	0.019832	0.110068	0.019832	1	TRUE	2

c-g DATA

	model	accuracy_val	pred_time_val	fit_time	ıe_val_marginal	_time_marginal	stack_level	can_infer	fit_order
0	WeightedEnsemble_L2	0.597504	0.725556	3785.363931	0.003389	0.652876	2	TRUE	13
1	NeuralNetFastAI	0.578783	0.3336	18.753044	0.3336	18.753044	1	TRUE	3
2	LightGBMXT	0.578783	0.33843	838.631675	0.33843	838.631675	1	TRUE	4
3	XGBoost	0.577223	0.191101	1637.723604	0.191101	1637.723604	1	TRUE	11
4	LightGBM	0.575663	0.151707	956.229281	0.151707	956.229281	1	TRUE	5
5	CatBoost	0.570983	0.029472	2731.427059	0.029472	2731.427059	1	TRUE	8
6	RandomForestGini	0.570983	0.207388	78.301671	0.207388	78.301671	1	TRUE	6
7	LightGBMLarge	0.566303	0.320333	2428.539831	0.320333	2428.539831	1	TRUE	12
8	RandomForestEntr	0.560062	0.207067	345.310725	0.207067	345.310725	1	TRUE	7
9	ExtraTreesGini	0.550702	0.206985	10.433152	0.206985	10.433152	1	TRUE	9
10	ExtraTreesEntr	0.541342	0.212107	11.839658	0.212107	11.839658	1	TRUE	10
11	KNeighborsUnif	0.536661	0.398807	0.491086	0.398807	0.491086	1	TRUE	1
12	KNeighborsDist	0.513261	0.503181	0.472395	0.503181	0.472395	1	TRUE	2