Supplementary materials for:

In Silico Prediction of hERG Potassium Channel Blockage by Chemical Category Approaches

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Table S1. Performance of binary classification models for training set and test set using different modeling methods based on molecular descriptors

threshold	modeling methods	training set					test set				
		Q	SE	SP	AUC	C	Q	SE	SP	AUC	C
1	NB	0.7346	0.4592	0.8271	0.7132	0.2888	0.6992	0.4833	0.7727	0.7002	0.2451
	SVM	0.8123	0.3991	0.9510	0.8215	0.4417	0.8093	0.4333	0.9375	0.7623	0.4441
	kNN	0.7940	0.4764	0.9006	0.7773	0.4134	0.7797	0.5500	0.8580	0.7420	0.4126
	RF	0.7519	0.0644	0.9827	0.6932	0.1215	0.7627	0.0667	1.000	0.6885	0.2249
	CT	0.7400	0.4635	0.8329	0.6892	0.3003	0.7288	0.5167	0.8011	0.7100	0.3083
5	NB	0.6461	0.6130	0.6771	0.6954	0.2907	0.6102	0.6000	0.6207	0.6455	0.2207
	SVM	0.7314	0.7136	0.7479	0.7929	0.4619	0.7161	0.6583	0.7759	0.7727	0.4368
	*k*NN	0.7055	0.6711	0.7375	0.7518	0.4097	0.6737	0.6833	0.6638	0.7483	0.3472
	RF	0.5480	0.0694	0.9938	0.7126	0.1677	0.5254	0.0750	0.9914	0.6363	0.1647
	CT	0.6300	0.6018	0.6562	0.6420	0.2584	0.6695	0.6833	0.6552	0.7001	0.3387
10	NB	0.6461	0.6566	0.6301	0.7005	0.2812	0.6737	0.6993	0.6265	0.6917	0.3158
	SVM	0.6926	0.7687	0.5753	0.7388	0.3488	0.6864	0.7843	0.5060	0.7243	0.2977
	*k*NN	0.7174	0.8434	0.5233	0.7723	0.3906	0.7034	0.7974	0.5301	0.7196	0.3359
	RF	0.6256	0.9537	0.1205	0.7231	0.1374	0.6653	0.9869	0.0723	0.6247	0.1563
	CT	0.6569	0.7206	0.5589	0.6423	0.2801	0.6695	0.7516	0.5181	0.6562	0.2712
30	NB	0.7573	0.8363	0.4806	0.7325	0.3112	0.7627	0.8413	0.4468	0.7370	0.2795
	SVM	0.7713	0.8779	0.3981	0.7025	0.2965	0.7839	0.8889	0.3617	0.7369	0.2795
	*k*NN	0.8069	0.9695	0.2379	0.7862	0.3241	0.8347	0.9683	0.2979	0.7651	0.3816
	RF	0.8026	0.9681	0.2233	0.7738	0.3032	0.8220	0.9788	0.1915	0.6904	0.2982
	CT	0.7713	0.8474	0.5049	0.6846	0.3476	0.7881	0.8995	0.3404	0.6436	0.2696

Table S2. Performance of binary classification models for the training set and test set using different fingerprints and modeling methods

threshold	modeling method	training set					test set				
		Q	SE	SP	AUC	C	Q	SE	SP	AUC	C
1	Estate-NB	0.7195	0.1588	0.9078	0.6597	0.0927	0.7669	0.2667	0.9375	0.6925	0.2793
	Estate-*k*NN	0.7831	0.5365	0.8660	0.7742	0.4117	0.7627	0.5500	0.8352	0.7333	0.3811
	Estate-SVM	0.7843	0.3348	0.9352	0.7640	0.3452	0.8008	0.3500	0.9545	0.8086	0.4039
	Estate-RF	0.7519	0.0558	0.9856	0.7180	0.1154	0.7458	0.0167	0.9943	0.7866	0.0522
	Estate-CT	0.7346	0.4077	0.8444	0.6871	0.2644	0.7542	0.4833	0.8466	0.7251	0.3377
	FP-NB	0.6839	0.5751	0.7205	0.7472	0.2681	0.7203	0.6667	0.7386	0.7868	0.3667
	FP-*k*NN	0.8176	0.5794	0.8977	0.8328	0.4978	0.8008	0.6667	0.8466	0.8370	0.4957
	FP-SVM	0.8339	0.5193	0.9395	0.8584	0.5228	0.8347	0.6333	0.9034	0.8389	0.5528
	FP-RF	0.7821	0.2489	0.9611	0.8139	0.3157	0.8305	0.5167	0.9375	0.8382	0.5170
	FP-CT	0.7454	0.4678	0.8386	0.6715	0.312	0.7712	0.5167	0.8580	0.6742	0.3834
	FP4-NB	0.7324	0.3734	0.8530	0.7099	0.2438	0.7161	0.2833	0.8636	0.7384	0.1689
	FP4-*k*NN	0.7940	0.5236	0.8847	0.7919	0.4291	0.8051	0.6333	0.8636	0.7912	0.4917
	FP4-SVM	0.8198	0.4249	0.9524	0.8059	0.4684	0.8051	0.4667	0.9205	0.8333	0.4407
	FP4-RF	0.7616	0.0730	0.9928	0.7627	0.1874	0.7797	0.2000	0.9773	0.7828	0.3070
	FP4-CT	0.7529	0.4592	0.8516	0.7053	0.3221	0.7542	0.4333	0.8636	0.7101	0.3164
	MACCS-NB	0.6936	0.4850	0.7637	0.6763	0.2357	0.7161	0.6333	0.7443	0.7239	0.3444
	MACCS-*k*NN	0.8036	0.5579	0.8862	0.8094	0.4610	0.7924	0.6500	0.8409	0.8165	0.4741
	MACCS-SVM	0.8198	0.4893	0.9308	0.8211	0.4799	0.8220	0.5333	0.9205	0.8406	0.4988
	MACC-RF	0.7778	0.2232	0.9640	0.7586	0.2942	0.7924	0.2667	0.9716	0.8278	0.3644
	MACCS-CT	0.7712	0.5193	0.8559	0.7123	0.3669	0.7881	0.5833	0.8580	0.7357	0.4413
	PubChem-NB	0.6558	0.5365	0.6960	0.6796	0.2098	0.6398	0.6667	0.6307	0.6737	0.2605
	PubChem-*k*NN	0.8090	0.5880	0.8833	0.8244	0.4820	0.7924	0.6500	0.8409	0.8326	0.4741
	PubChem-SVM	0.8296	0.4635	0.9524	0.8481	0.5025	0.8136	0.5667	0.8977	0.8400	0.4879
	PubChem-RF	0.7885	0.2747	0.9611	0.8146	0.3437	0.7797	0.4000	0.9091	0.8034	0.3587
	PubChem-CT	0.7777	0.5408	0.8573	0.7443	0.4028	0.7669	0.6167	0.8182	0.7051	0.4163
5	Estate-NB	0.6311	0.6286	0.6333	0.6686	0.2618	0.7034	0.6833	0.7241	0.7091	0.4076

	Estate-*k*NN	0.7066	0.7226	0.6917	0.7606	0.4141	0.7076	0.7333	0.6810	0.7542	0.4150
	Estate-SVM	0.7012	0.6532	0.7458	0.7505	0.4011	0.7034	0.7083	0.6983	0.7517	0.4066
	Estate-RF	0.6797	0.5593	0.7917	0.7307	0.3617	0.6737	0.6500	0.6983	0.7352	0.3485
	Estate-CT	0.6688	0.6353	0.7000	0.7153	0.3361	0.6864	0.6750	0.6983	0.6605	0.3733
	FP-NB	0.6257	0.6197	0.6312	0.6779	0.2508	0.6356	0.6250	0.6466	0.6989	0.2716
	FP-*k*NN	0.7185	0.7204	0.7167	0.7898	0.4368	0.7415	0.7667	0.7155	0.8259	0.4830
	FP-SVM	0.7206	0.6868	0.7521	0.7757	0.4400	0.7712	0.7750	0.7672	0.8260	0.5422
	FP-RF	0.6667	0.5503	0.7750	0.7374	0.3346	0.7331	0.6167	0.8534	0.8052	0.4829
	FP-CT	0.6764	0.6890	0.6646	0.6855	0.3534	0.6525	0.6583	0.6466	0.6700	0.3049
	FP4-NB	0.6354	0.6913	0.5833	0.6706	0.2758	0.6229	0.7333	0.5086	0.6483	0.2485
	FP4-*k*NN	0.6915	0.6846	0.6979	0.7811	0.3824	0.5508	0.5167	0.5862	0.5436	0.1031
	FP4-SVM	0.7141	0.6532	0.7708	0.7671	0.4276	0.7415	0.7417	0.7414	0.7990	0.4830
	FP4-RF	0.6688	0.5414	0.7875	0.7436	0.3402	0.5890	0.3583	0.8276	0.6725	0.2101
	FP4-CT	0.6602	0.6532	0.6667	0.7049	0.3198	0.5593	0.5667	0.5517	0.6075	0.1184
	MACCS-NB	0.6224	0.6711	0.5771	0.6780	0.2490	0.6949	0.7417	0.6466	0.7250	0.3902
	MACCS-*k*NN	0.7541	0.7472	0.7604	0.8032	0.5075	0.7203	0.7750	0.6638	0.8026	0.4419
	MACCS-SVM	0.7627	0.7204	0.8021	0.8217	0.5248	0.7500	0.7500	0.7500	0.8236	0.4999
	MACC-RF	0.7131	0.5727	0.8438	0.7927	0.4335	0.7203	0.6250	0.8190	0.8185	0.4518
	MACCS-CT	0.7055	0.6868	0.7229	0.7136	0.4100	0.6907	0.6750	0.7069	0.6917	0.3820
	PubChem-NB	0.6397	0.6756	0.6062	0.6812	0.2822	0.6949	0.7167	0.6724	0.7224	0.3895
	PubChem-*k*NN	0.7347	0.7539	0.7167	0.8009	0.4704	0.7542	0.7667	0.7414	0.8123	0.5083
	PubChem-SVM	0.7530	0.7293	0.7750	0.8022	0.5050	0.7754	0.7833	0.7672	0.8408	0.5507
	PubChem-RF	0.7001	0.5615	0.8292	0.7884	0.4069	0.7246	0.6333	0.8190	0.8084	0.4596
	PubChem-CT	0.7034	0.6913	0.7146	0.6998	0.4059	0.7034	0.7583	0.6466	0.7376	0.4077
10	Estate-NB	0.6462	0.7954	0.4164	0.6458	0.2285	0.6949	0.7974	0.5060	0.7051	0.3134
	Estate-*k*NN	0.6937	0.7847	0.5534	0.7437	0.3467	0.7585	0.8497	0.5904	0.7618	0.4563
	Estate-SVM	0.7206	0.8505	0.5205	0.7557	0.3973	0.6907	0.8170	0.4578	0.7247	0.2924
	Estate-RF	0.6645	0.7687	0.5041	0.7280	0.2816	0.7034	0.7908	0.5422	0.7399	0.3392
	Estate-CT	0.6731	0.7527	0.5507	0.6970	0.3075	0.6949	0.7843	0.5301	0.6685	0.3202
	FP-NB	0.6203	0.6530	0.5699	0.6585	0.2197	0.6568	0.6601	0.6506	0.7319	0.2983

	FP-*k*NN	0.7433	0.8096	0.6411	0.8071	0.4566	0.7542	0.8039	0.6627	0.8344	0.4641
	FP-SVM	0.7346	0.8203	0.6027	0.8011	0.4344	0.7881	0.8693	0.6386	0.8102	0.5246
	FP-RF	0.6958	0.7278	0.6466	0.7738	0.3706	0.7246	0.7908	0.6024	0.8107	0.3944
	FP-CT	0.6796	0.7384	0.5890	0.6640	0.3280	0.7288	0.8105	0.5783	0.7086	0.3959
	FP4-NB	0.6548	0.8114	0.4137	0.6770	0.2457	0.6992	0.8431	0.4337	0.7455	0.3036
	FP4-*k*NN	0.7013	0.7829	0.5753	0.7781	0.3651	0.7712	0.8431	0.6386	0.8096	0.4906
	FP4-SVM	0.7217	0.8096	0.5863	0.7809	0.4066	0.7627	0.8366	0.6265	0.7692	0.4717
	FP4-RF	0.6797	0.8452	0.4247	0.7615	0.3002	0.6822	0.7582	0.5422	0.7627	0.3012
	FP4-CT	0.7044	0.7794	0.5890	0.7037	0.3737	0.7288	0.7778	0.6386	0.6976	0.4121
	MACCS-NB	0.6343	0.7082	0.5205	0.6707	0.2300	0.6737	0.7917	0.5517	0.7130	0.3542
	MACCS-*k*NN	0.7282	0.7954	0.6247	0.7815	0.4251	0.6992	0.9000	0.4914	0.8050	0.4302
	MACCS-SVM	0.7443	0.8310	0.6110	0.8029	0.4578	0.6907	0.9167	0.4569	0.7946	0.4222
	MACC-RF	0.6894	0.7367	0.6164	0.7724	0.3518	0.7288	0.8917	0.5603	0.8119	0.4804
	MACCS-CT	0.7109	0.7705	0.6192	0.7021	0.3916	0.6864	0.8417	0.5259	0.7324	0.3882
	PubChem-NB	0.6408	0.6762	0.5863	0.6639	0.2592	0.7203	0.7190	0.7229	0.7667	0.4254
	PubChem-*k*NN	0.7465	0.8238	0.6274	0.8105	0.4611	0.7500	0.8366	0.5904	0.7901	0.4394
	PubChem-SVM	0.7638	0.8274	0.6658	0.8246	0.5000	0.7839	0.8824	0.6024	0.8185	0.5111
	PubChem-RF	0.7012	0.7580	0.6137	0.7852	0.3726	0.7203	0.7386	0.6867	0.8184	0.4128
	PubChem-CT	0.6991	0.7669	0.5945	0.7166	0.3647	0.7415	0.8170	0.6024	0.7427	0.4257
30	Estate-NB	0.7756	0.9528	0.1553	0.6271	0.1749	0.8093	0.9630	0.1915	0.7257	0.2454
	Estate-*k*NN	0.7594	0.8779	0.3447	0.6827	0.2455	0.7966	0.9259	0.2766	0.7160	0.2541
	Estate-SVM	0.7756	0.9695	0.0971	0.6283	0.1331	0.8093	0.9841	0.1064	0.7084	0.1997
	Estate-RF	0.7713	0.9667	0.0874	0.6806	0.1081	0.8263	0.9788	0.2128	0.8033	0.3239
	Estate-CT	0.7379	0.8571	0.3204	0.6048	0.1912	0.7924	0.8995	0.3617	0.6457	0.2901
	FP-NB	0.7163	0.7809	0.4903	0.6846	0.2512	0.7203	0.7725	0.5106	0.7693	0.2508
	FP-*k*NN	0.7821	0.8904	0.4029	0.7582	0.3211	0.7881	0.8730	0.4468	0.7762	0.3251
	FP-SVM	0.8080	0.9501	0.3107	0.7784	0.3494	0.8475	0.9894	0.2766	0.7988	0.4355
	FP-RF	0.7950	0.9209	0.3544	0.7683	0.3296	0.8263	0.9577	0.2979	0.7964	0.3510
	FP-CT	0.7401	0.8308	0.4223	0.6663	0.2518	0.8093	0.8889	0.4894	0.7137	0.3879
	FP4-NB	0.7864	0.9348	0.2670	0.6851	0.2681	0.8008	0.9365	0.2553	0.6897	0.2535

FP4-*k*NN	0.7789	0.8946	0.3738	0.7283	0.3006	0.8136	0.9153	0.4043	0.7510	0.3591
FP4-SVM	0.7972	0.9709	0.1893	0.7068	0.2707	0.8220	0.9577	0.2766	0.7636	0.3286
FP4-RF	0.7983	0.9612	0.2282	0.7303	0.2886	0.8305	0.9471	0.3617	0.7914	0.3874
FP4-CT	0.7552	0.8599	0.3883	0.6350	0.2604	0.7669	0.8889	0.2766	0.6689	0.1882
MACCS-NB	0.7228	0.8031	0.4417	0.6980	0.2346	0.7669	0.8519	0.4255	0.7200	0.2752
MACCS-*k*NN	0.7896	0.8904	0.4369	0.7482	0.3525	0.8390	0.9418	0.4255	0.7670	0.4343
MACCS-SVM	0.8004	0.9515	0.2718	0.7869	0.3120	0.8347	0.9683	0.2979	0.7675	0.3816
MACC-RF	0.7961	0.9112	0.3932	0.7751	0.3484	0.8305	0.9418	0.3830	0.8134	0.3951
MACCS-CT	0.7551	0.8488	0.4272	0.6256	0.2805	0.8008	0.9206	0.3191	0.5873	0.2875
PubChem-NB	0.7087	0.7906	0.4223	0.6532	0.2026	0.7500	0.8042	0.5319	0.7243	0.3050
PubChem-*k*NN	0.7951	0.8988	0.4320	0.7746	0.3621	0.7966	0.8942	0.4043	0.7559	0.3209
PubChem-SVM	0.8080	0.9612	0.2718	0.7640	0.3375	0.8220	0.9683	0.2340	0.7953	0.3125
PubChem-RF	0.8080	0.9279	0.3883	0.7770	0.3762	0.8390	0.9524	0.3830	0.7798	0.4208
PubChem-CT	0.7789	0.8696	0.4612	0.6949	0.3413	0.8093	0.9101	0.4043	0.6385	0.3491

Table S3. Performance of classification models for the taining set and test set using different modeling methods based on molecular descriptors (MD) combining fingerprints

thresholds (μM)	modeling methods	training set					test set				
		Q	SE	SP	AUC	C	Q	SE	SP	AUC	C
1	(Estate+MD)-NB	0.7454	0.5107	0.8242	0.7394	0.3312	0.7161	0.5500	0.7727	0.7472	0.3040
	(Estate+MD)-*k*NN	0.7993	0.5622	0.8790	0.8144	0.4534	0.7712	0.6000	0.8295	0.8326	0.4167
	(Estate+MD)-SVM	0.8091	0.4721	0.9222	0.8306	0.4482	0.7881	0.4167	0.9148	0.8389	0.3847
	(Estate+MD)-RF	0.7778	0.2275	0.9625	0.7889	0.2952	0.8051	0.4000	0.9432	0.8295	0.4255
	(Estate+MD)-CT	0.7367	0.4592	0.8300	0.6813	0.2926	0.7415	0.5500	0.8068	0.7326	0.3446
	(FP+MD)-NB	0.7173	0.5837	0.7622	0.7741	0.3205	0.7331	0.6833	0.7500	0.7987	0.3931
	(FP+MD)-*k*NN	0.8220	0.5837	0.9020	0.8402	0.5086	0.8008	0.6667	0.8466	0.8366	0.4957
	(FP+MD)-SVM	0.8177	0.4807	0.9308	0.8529	0.4724	0.8305	0.6333	0.8977	0.8414	0.5436
	(FP+MD)-RF	0.7972	0.3219	0.9568	0.8372	0.3814	0.8093	0.3833	0.9545	0.8369	0.4355
	(FP+MD)-CT	0.7573	0.4635	0.8559	0.6677	0.3321	0.7712	0.5833	0.8352	0.7370	0.4100
	(FP4+MD)-NB	0.7583	0.5536	0.8271	0.7461	0.3726	0.7076	0.5667	0.7557	0.7343	0.2994
	(FP4+MD)-*k*NN	0.8004	0.5279	0.8919	0.8065	0.4444	0.8136	0.6167	0.8807	0.8312	0.5030
	(FP4+MD)-SVM	0.8393	0.4893	0.9568	0.8680	0.5342	0.8263	0.5500	0.9205	0.8472	0.5129
	(FP4+MD)-RF	0.7940	0.2618	0.9726	0.7986	0.3621	0.8051	0.3167	0.9716	0.7807	0.4153
	(FP4+MD)-CT	0.7454	0.4549	0.8429	0.6876	0.3061	0.7246	0.5000	0.8011	0.6964	0.2935
	(MACCS+MD)-NB	0.7248	0.5708	0.7767	0.7343	0.3257	0.7246	0.6500	0.7500	0.7563	0.3648
	(MACCS+MD)-*k*NN	0.8058	0.5579	0.889	0.8177	0.4656	0.8051	0.6500	0.8580	0.8255	0.4975
	(MACCS+MD)-SVM	0.8123	0.4592	0.9308	0.8264	0.4534	0.8220	0.5500	0.9148	0.8511	0.5028
	(MACCS+MD)-RF	0.7961	0.2747	0.9712	0.8025	0.3715	0.8178	0.3833	0.9659	0.8148	0.4632
	(MACCS+MD)-CT	0.7508	0.4678	0.8458	0.7096	0.3218	0.7458	0.5833	0.8011	0.6909	0.3665
	(PubChem+MD)-NB	0.6784	0.5708	0.7147	0.7111	0.2585	0.6356	0.6500	0.6307	0.7071	0.2462
	(PubChem+MD)-*k*NN	0.8079	0.5837	0.8833	0.8314	0.4784	0.7754	0.6500	0.8182	0.8397	0.4445
	(PubChem+MD)-SVM	0.8350	0.5150	0.9424	0.8570	0.5250	0.8136	0.5667	0.8977	0.8416	0.4879
	(PubChem+MD)-RF	0.8058	0.3305	0.9654	0.8214	0.4119	0.7881	0.4000	0.9205	0.8089	0.3796
	(PubChem+MD)-CT	0.7594	0.4721	0.8559	0.7092	0.3399	0.7161	0.4833	0.7955	0.6920	0.2717
5	(Estate+MD)-NB	0.6526	0.6130	0.6896	0.7103	0.3035	0.6483	0.6583	0.6379	0.6797	0.2963
	(Estate+MD)-*k*NN	0.7422	0.7427	0.7417	0.8152	0.4842	0.7288	0.7750	0.6810	0.7955	0.4583
	(Estate+MD)-SVM	0.7131	0.6913	0.7333	0.7771	0.4250	0.7331	0.7250	0.7414	0.7691	0.4663
	(Estate+MD)-RF	0.7044	0.5682	0.8313	0.7826	0.4155	0.6695	0.5250	0.8190	0.7643	0.3591
	(Estate+MD)-CT	0.6505	0.6286	0.6708	0.6602	0.2997	0.6525	0.6750	0.6293	0.6619	0.3047
	(FP+MD)-NB	0.6430	0.6488	0.6375	0.6960	0.2861	0.6441	0.6583	0.6293	0.6989	0.2878

	(FP+MD)-*k*NN	0.7249	0.7271	0.7229	0.7927	0.4497	0.7500	0.7667	0.7328	0.8243	0.4998
	(FP+MD)-SVM	0.7400	0.7025	0.7750	0.8120	0.4791	0.7627	0.7750	0.7500	0.8349	0.5252
	(FP+MD)-RF	0.6969	0.5705	0.8146	0.7860	0.3983	0.7161	0.6750	0.7586	0.8015	0.4348
	(FP+MD)-CT	0.6666	0.6779	0.6562	0.6868	0.3339	0.6864	0.7250	0.6466	0.6799	0.3728
	(FP4+MD)-NB	0.6559	0.6376	0.6729	0.7153	0.3106	0.6059	0.6167	0.5948	0.6595	0.2115
	(FP4+MD)-*k*NN	0.7368	0.7315	0.7417	0.7950	0.4731	0.6102	0.7167	0.5000	0.6546	0.2221
	(FP4+MD)-SVM	0.7389	0.7047	0.7708	0.8079	0.4769	0.7415	0.7333	0.7500	0.8004	0.4833
	(FP4+MD)-RF	0.6947	0.5436	0.8354	0.7984	0.3978	0.5551	0.1833	0.9397	0.6994	0.1873
	(FP4+MD)-CT	0.6537	0.6309	0.675	0.6676	0.3061	0.6314	0.6917	0.5690	0.6647	0.2627
	(MACCS+MD)-NB	0.6536	0.6667	0.6417	0.7096	0.3082	0.6653	0.6750	0.6552	0.7116	0.3302
	(MACCS+MD)-*k*NN	0.7586	0.7539	0.7625	0.8095	0.5163	0.7288	0.7500	0.7069	0.8062	0.4574
	(MACCS+MD)-SVM	0.7691	0.7293	0.8063	0.8286	0.5377	0.7585	0.7583	0.7586	0.8261	0.5169
	(MACCS+MD)-RF	0.7184	0.613	0.8167	0.7947	0.4401	0.7076	0.6000	0.8190	0.7795	0.4286
	(MACCS+MD)-CT	0.6440	0.6085	0.6771	0.6570	0.2863	0.6483	0.7083	0.5862	0.6849	0.2969
	(PubChem+MD)-NB	0.6526	0.6711	0.6354	0.7051	0.3065	0.6610	0.6750	0.6466	0.7261	0.3217
	(PubChem+MD)-*k*NN	0.7487	0.7517	0.7458	0.8032	0.4972	0.7627	0.7833	0.7414	0.8243	0.5253
	(PubChem+MD)-SVM	0.7605	0.8416	0.6356	0.8270	0.4901	0.7712	0.7750	0.7672	0.8425	0.5422
	(PubChem+MD)-RF	0.7153	0.5973	0.8250	0.7983	0.4351	0.7246	0.6583	0.7931	0.8191	0.4551
	(PubChem+MD)-CT	0.6612	0.6443	0.6771	0.6805	0.3215	0.7203	0.8000	0.6379	0.7258	0.4443
10	(Estate+MD)-NB	0.6526	0.6601	0.6411	0.7137	0.2954	0.6695	0.6928	0.6265	0.7219	0.3090
	(Estate+MD)-*k*NN	0.7304	0.7989	0.6247	0.7817	0.4292	0.7542	0.8627	0.5542	0.8030	0.4416
	(Estate+MD)-SVM	0.7152	0.7972	0.5890	0.7867	0.3943	0.7627	0.8497	0.6024	0.7947	0.4670
	(Estate+MD)-RF	0.7281	0.7794	0.6493	0.7852	0.4295	0.6949	0.8039	0.4940	0.7096	0.3102
	(Estate+MD)-CT	0.6666	0.7189	0.5863	0.6704	0.3042	0.6737	0.7451	0.5422	0.6745	0.2865
	(FP+MD)-NB	0.6257	0.6726	0.5534	0.6750	0.2240	0.6992	0.7255	0.6506	0.7454	0.3656
	(FP+MD)-*k*NN	0.7433	0.8096	0.6411	0.8109	0.4566	0.7542	0.8039	0.6627	0.8335	0.4641
	(FP+MD)-SVM	0.7411	0.8327	0.6000	0.7876	0.4400	0.7924	0.8693	0.6506	0.8122	0.5351
	(FP+MD)-RF	0.7250	0.7776	0.6438	0.7974	0.4225	0.7585	0.7974	0.6867	0.8210	0.4781
	(FP+MD)-CT	0.6742	0.7456	0.5644	0.6748	0.3125	0.7246	0.7843	0.6145	0.6777	0.3977
	(FP4+MD)-NB	0.6559	0.7100	0.5726	0.7200	0.2817	0.6992	0.7582	0.5904	0.7211	0.3458
	(FP4+MD)-*k*NN	0.7336	0.8185	0.6027	0.8039	0.4323	0.7331	0.8301	0.5542	0.8147	0.3985
	(FP4+MD)-SVM	0.7476	0.8345	0.6137	0.8215	0.4616	0.7500	0.8301	0.6024	0.7729	0.4420
	(FP4+MD)-RF	0.7001	0.7651	0.6000	0.7790	0.3678	0.6864	0.7647	0.5422	0.7490	0.3086
	(FP4+MD)-CT	0.6689	0.7135	0.6000	0.6754	0.3115	0.7034	0.7647	0.5904	0.7123	0.3532
	(MACCS+MD)-NB	0.6526	0.6904	0.5945	0.7104	0.2819	0.6441	0.7250	0.5603	0.7030	0.2895
	(MACCS+MD)-*k*NN	0.7325	0.806	0.6192	0.7960	0.4325	0.7203	0.9000	0.5345	0.8052	0.4682

	(MACCS+MD)-SVM	0.7584	0.8310	0.6466	0.8268	0.4869	0.6737	0.9000	0.4397	0.8063	0.3839
	(MACCS+MD)-RF	0.7238	0.7473	0.6877	0.7954	0.4301	0.6949	0.8083	0.5776	0.7847	0.3972
	(MACCS+MD)-CT	0.6591	0.7278	0.5534	0.6468	0.2826	0.6525	0.7833	0.5172	0.7047	0.3122
	(PubChem+MD)-NB	0.6559	0.6975	0.5918	0.6884	0.2867	0.7288	0.7386	0.7108	0.7700	0.4349
	(PubChem+MD)-*k*NN	0.7498	0.8167	0.6466	0.8160	0.4700	0.7415	0.8366	0.5663	0.7935	0.4178
	(PubChem+MD)-SVM	0.7605	0.8416	0.6356	0.8270	0.4901	0.7797	0.8693	0.6145	0.8197	0.5036
	(PubChem+MD)-RF	0.7281	0.7562	0.6849	0.7977	0.4371	0.7669	0.8431	0.6265	0.8092	0.4799
	(PubChem+MD)-CT	0.6968	0.7544	0.6082	0.7003	0.3636	0.7203	0.8170	0.5422	0.6971	0.3710
30	(Estate+MD)-NB	0.7692	0.8419	0.5146	0.7442	0.3483	0.7669	0.8360	0.4894	0.7524	0.3093
	(Estate+MD)-*k*NN	0.7843	0.8821	0.4417	0.7522	0.3433	0.8347	0.9365	0.4255	0.7638	0.4223
	(Estate+MD)-SVM	0.7961	0.9570	0.2330	0.7334	0.2829	0.8347	0.9735	0.2766	0.7554	0.3764
	(Estate+MD)-RF	0.8069	0.9029	0.4709	0.7933	0.4044	0.8178	0.9524	0.2766	0.7604	0.3145
	(Estate+MD)-CT	0.7594	0.8363	0.4903	0.6785	0.3197	0.7373	0.8466	0.2979	0.5830	0.1494
	(FP+MD)-NB	0.7346	0.7989	0.5097	0.7005	0.2891	0.7500	0.8042	0.5319	0.7831	0.3050
	(FP+MD)-*k*NN	0.7875	0.8946	0.4126	0.7540	0.3371	0.7881	0.8730	0.4468	0.7579	0.3251
	(FP+MD)-SVM	0.7832	0.9501	0.1990	0.7325	0.2246	0.8475	0.9894	0.2766	0.7988	0.4355
	(FP+MD)-RF	0.8123	0.9140	0.4563	0.8049	0.4115	0.8305	0.9524	0.3404	0.7943	0.3800
	(FP+MD)-CT	0.7768	0.8682	0.4563	0.6730	0.3296	0.7627	0.8624	0.3617	0.6070	0.2319
	(FP4+MD)-NB	0.7778	0.8627	0.4806	0.7456	0.3482	0.7839	0.8624	0.4681	0.7107	0.3279
	(FP4+MD)-*k*NN	0.7918	0.8877	0.4563	0.7418	0.3654	0.7966	0.9048	0.3617	0.7469	0.2994
	(FP4+MD)-SVM	0.7994	0.9612	0.2330	0.8002	0.2943	0.839	0.9471	0.4043	0.7631	0.4274
	(FP4+MD)-RF	0.8037	0.9140	0.4175	0.7901	0.3762	0.8263	0.9259	0.4255	0.7427	0.3997
	(FP4+MD)-CT	0.7724	0.8599	0.4660	0.6805	0.3312	0.7669	0.8783	0.3191	0.6364	0.2145
	(MACCS+MD)-NB	0.7412	0.8003	0.5340	0.7476	0.3116	0.7712	0.8360	0.5106	0.7552	0.3274
	(MACCS+MD)-*k*NN	0.8015	0.9015	0.4515	0.7607	0.3846	0.8220	0.9259	0.4043	0.7899	0.3802
	(MACCS+MD)-SVM	0.7853	0.9417	0.2379	0.7842	0.2510	0.8347	0.9577	0.3404	0.7855	0.3939
	(MACCS+MD)-RF	0.8156	0.9182	0.4563	0.8157	0.4194	0.8178	0.9206	0.4043	0.7705	0.3695
	(MACCS+MD)-CT	0.7519	0.828	0.4854	0.6756	0.3044	0.7627	0.8519	0.4043	0.6666	0.2561
	(PubChem+MD)-NB	0.7271	0.8072	0.4466	0.6742	0.2440	0.7627	0.836	0.4681	0.7510	0.2910
	(PubChem+MD)-*k*NN	0.7972	0.896	0.4515	0.7821	0.3750	0.8051	0.9101	0.3830	0.7562	0.3293
	(PubChem+MD)-SVM	0.7853	0.932	0.2718	0.7421	0.2675	0.8432	0.9577	0.3830	0.8338	0.4345
	(PubChem+MD)-RF	0.7983	0.9029	0.4320	0.8028	0.3694	0.8347	0.9312	0.4468	0.7953	0.4299
	(PubChem+MD)-CT	0.7670	0.8502	0.4757	0.6966	0.3259	0.7797	0.8889	0.3404	0.6119	0.2519