

Table SI. Specifications and experimental conditions and concentrations of tested compounds

TdP risk	Compound	ETPC, μM	Concentration, μM	Solvent	Manufacturer
H	Azimilide	7.0×10^{-2}	0.05/0.5/5/50	DMSO	Sigma
H	Bepiridil	3.2×10^{-2}	0.03/0.3/3/10	DMSO	Sigma
H	Disopyramide	7.0×10^{-1}	0.1/1/10/30	DMSO	Sigma
H	Dofetilide	2.0×10^{-3}	0.03/0.1/0.3	DMSO	Sigma
H	Ibutilide	1.0×10^{-1}	0.0001/0.001/0.01/0.1	DMSO	Sigma
H	Quinidine	3.0×10	0.01/0.1/1/10	DMSO	Med chem Express
H	Sotalol	1.5×10^1	1/3/10/30	DMSO	NIFDC
H	Vandetanib	3.0×10^{-1}	0.01/0.1/1/10	DMSO	Selleckchem
I	Astemizole	3.0×10^{-4}	0.001/0.01/0.1/1	DMSO	NIFDC
I	Chlorpromazine	3.5×10^{-2}	0.03/0.3/3/10	DMSO	NIFDC
I	Cisapride	2.6×10^{-3}	3/10/30/	DMSO	NIFDC
I	Clarithromycin	1.2×10	0.1/1/10/100	DMSO	NIFDC
I	Clozapine	7.1×10^{-2}	0.03/0.3/3/10	DMSO	NIFDC
I	Domperidone	2.0×10^{-2}	0.003/0.03/0.3/3	DMSO	NIFDC
I	Droperidol	1.6×10^{-2}	0.01/0.03/0.1/0.3	DMSO	Sigma
I	Ondansetron	3.7×10^{-1}	0.1/0.3/1/3	DMSO	Sigma
I	Pimozide	4.3×10^{-4}	0.001/0.01/0.1/1	DMSO	Sigma
I	Risperidone	1.8×10^{-3}	0.001/0.01/0.1/1	DMSO	NIFDC
I	Terfenadine	2.9×10^{-4}	0.3/1/3	DMSO	Sigma
L	Diltiazem	1.3×10^{-1}	0.03/0.3/3/10	DMSO	Sigma
L	Loratadine	4.5×10^{-4}	0.003/0.03/0.3/1	DMSO	NIFDC
L	Ranolazine	1.9×10	1/3/10/30	DMSO	Sigma
L	Metoprolol	1.8×10	0.1/1/10/30	DMSO	NIFDC
L	Mexiletine	2.5×10	3/10/30	DMSO	Sigma
L	Nifedipine	7.7×10^{-3}	0.1/0.3/1	DMSO	Sigma
L	Nitrendipine	3.0×10^{-3}	0.003/0.03/0.3/1	DMSO	NIFDC
L	Tamoxifen	2.1×10^{-2}	0.3/1/3/10	DMSO	NIFDC
L	Verapamil	4.5×10^{-2}	0.1/0.3/1	DMSO	Sigma
Non	Amiodarone	7.0×10^{-4}	0.03/0.3/1/10	DMSO	Sigma
Non	Flecainide	7.5×10^{-1}	0.1/1/3/10	DMSO	NIFDC
Non	Moxifloxacin	3.6×10	3/10/100/300	DMSO	Sigma
Non	E4031	8.4×10^{-3}	0.001/0.01/0.3/0.9	H2O	Sigma

Non	Methadone	9.9×10^{-1}	0.02/0.2/2/20	DMSO	NIFDC
Non	Nicotinamide	1.2×10^3	0.005/0.05/0.5/5	H2O	NIFDC
Non	Mannitol	2.4×10^3	0.005/0.05/0.5/5	H2O	NIFDC

TdP, torsades de pointes; H, high; I, intermediate; L, low; Non, non-Comprehensive *in vitro* Proarrhythmia Assay; ETPC, effective therapeutic plasma concentration.

Table SII. Changes in AMPL and BPM

TdP risk	Compounds	AMPL	BMP
H	Azimilide	↓	↓
H	Bepidil	↑	↑
H	Disopyramide	↑	↑
H	Dofetilide	↓	↓
H	Ibutilide	↓	↓
H	Quinidine	↓	↓
H	Sotalol	↑	↓
H	Vandetanib	↑	↓
I	Astemizole	↓	↓
I	Chlorpromazine	↓	↓
I	Cisapride	↓	↓
I	Clarithromycin	↓	↓
I	Clozapine	↑	↑
I	Domperidone	↑	↑
I	Droperidol	↓	↓
I	Ondansetron	↓	↓
I	Pimozide	↓	↓
I	Risperidone	↓	↓
I	Terfenadine	↓	↓
L	Diltiazem	↓	↓
L	Loratadine	↓	↑
L	Ranolazine	↑	↑
L	Metoprolol	↓	↓
L	Mexiletine	↓	↓
L	Nifedipine	↓	↑
L	Nitrendipine	↓	↑
L	Tamoxifen	↓	↓
L	Verapamil	↓	↑
Non	Amiodarone	↓	↓

Non	Flecainide	↑	↑
Non	Moxifloxacin	↑	↓
Non	E4031	↑	↑
Non	Methadone	↓	↓
Non	Nicotinamide	↓	↓
Non	Mannitol	↑	↑

TdP risk: H,high; I,intermediate; L,low; Non,non-CiPA compounds; “↑” indicates an increase, “↓” indicates a decrease.

Table SIII. Model output based on the training set

A, LR					
Risk	Precision	Recall	N	Accuracy	AUC
Low	0.78	0.78	9	0.86	0.84
High&Intermediate	0.89	0.89	19		
B, AdaBoost					
Risk	Precision	Recall	N	Accuracy	AUC
Low	1.00	1.00	9	1.00	1.00
High&Intermediate	1.00	1.00	19		
C, SVM					
Risk	Precision	Recall	N	Accuracy	AUC
Low	0.62	0.89	9	0.79	0.81
High&Intermediate	0.93	0.74	19		
D, CatBoost					
Risk	Precision	Recall	N	Accuracy	AUC
Low	1.00	1.00	9	1.00	1.00
High&Intermediate	1.00	1.00	19		
E, KNN					
Risk	Precision	Recall	N	Accuracy	AUC
Low	1.00	1.00	9	1.00	1.00
High&Intermediate	1.00	1.00	19		
F, RF					
Risk	Precision	Recall	N	Accuracy	AUC
Low	1.00	1.00	9	1.00	1.00
High&Intermediate	1.00	1.00	19		

G, DT					
Risk	Precision	Recall	N	Accuracy	AUC
Low	0.82	1.00	9	0.93	0.95
High&Intermediate	1.00	0.89	19		

Low, Low TdP risk Compounds; High&Intermediate, high- and intermediate TdP risk compounds.