Table S1. Detailed information of literature data sources of compounds with experimental hERG blocking bioactivities value used in this study.

	source	number of blockers	number of decoys	threshold of decoy	source of experimental data
1	Doddareddy *et al*. (2010)[1]	1112	1532	30 μM	patch clamp or radioligand binding assays; literature
2	Wang *et al.* (2016)[2]	587	176	40 μM	mammalian and non-mammalian cell lines; PubChem's BioAssay database
3	Didziapetris *et al*. (2016)[3]	3908	2782	10 μM	ChEMBL bioactivity database; previously published collections of patch-clamp measurements and competitive displacement assays
4	Chemi *et al*. (2017)[4]	730	7250	NA	literature (blockers); DUE-E (decoys)

Table S2. Detailed description of literature-derived hERG blockers used in this study.

No.	source	number of adopted hERG blockers
1	Doddareddy *et al*. (2010)[1]	1354
2	Wang *et al.* (2016)[2]	323
3	Didziapetris *et al*. (2016)[3]	3741
4	Chemi *et al*. (2017)[4]	666
	Merge	4355

Table S5. The area under the receiver operating characteristic curve (AUC) values of multi-task deep neural network (DNN), single-task DNN, support vector machine, naïve Bayes, random forest, and graph convolutional neural network (GCNN) models across different decoy thresholds on training set and validation set.

Approach	Training set						Validation set					
	10μM	20μM	40μM	60μM	80μM	100μM	10μM	20μM	40μM	60μM	80μM	100μM
Multi-task DNN	0.792	0.847	0.911	0.931	0.944	0.943	0.883	0.899	0.950	0.962	0.967	0.958
Single-task DNN	0.778	0.834	0.896	0.910	0.930	0.933	0.845	0.875	0.931	0.955	0.957	0.943
Support vector machine	0.617	0.732	0.821	0.827	0.893	0.936	0.641	0.773	0.871	0.879	0.908	0.913
Naïve Bayes	0.740	0.777	0.828	0.852	0.834	0.843	0.818	0.845	0.894	0.926	0.922	0.929
Random forest	0.770	0.820	0.879	0.903	0.928	0.929	0.829	0.867	0.930	0.939	0.950	0.943
GCNN	0.822	0.871	0.925	0.943	0.957	0.959	0.902	0.911	0.938	0.936	0.959	0.947

Table S8. Detailed descriptions and PubMed ID (PMID) of the 15 deephERG-predicted antineoplastic drugs whose hERG inhibitory activities have been validated by clinical case report or reported pre-clinical data.

Drug name	PMID	Summarized effect	Category
Cyclosporine	22128262	CsA inhibited the hERG channel in a concentration-dependent manner	Immunosuppressants
Fingolimod	25223691	Fingolimod significantly inhibited hERG current	Immunosuppressants
Imatinib	23196655	IM inhibited hERG in a concentration-dependent manner in HEK-293 cells and Xenopus oocytes	Protein kinase inhibitors
Erlotinib	23707608	Erlotinib inhibited 35% (mean) of hERG current at the concentration of 10 μM	Protein kinase inhibitors
Sunitinib	23707608	Sunitinib potently blocked the hERG channel, resulting in IC_{50} values of 0.5 μM	Protein kinase inhibitors
Lapatinib	20406211	In ion channel studies, lapatinib inhibited the hERG current in a concentration-dependent manner	Protein kinase inhibitors
Nilotinib	23707608	Nilotinib potently blocked the hERG channel, resulting in IC_{50} values of 0.7 μM	Protein kinase inhibitors
Vandetanib	29630634	Vandetanib at concentrations of 1 and 3 μM inhibited the hERG currents	Protein kinase inhibitors
Crizotinib	23707608	Crizotinib potently blocked the hERG channel, resulting in IC_{50} values of 1.7 μM	Protein kinase inhibitors
Ponatinib	23609479	ponatinib inhibits hERG current at concentrations above 1μM	Protein kinase inhibitors
Ibrutinib	29324347	Ibrutinib moderate inhibit against hERG current (IC_{50} = 0.97 μM)	Protein kinase inhibitors
Dactinomycin	22613764	Actinomycin-D markedly reduced the hERG mRNA levels in both control and cAMP-stimulated cells	Cytotoxic antibiotics and related substances
Tamoxifen	12827215	Tamoxifen blocked hERG potassium channels with an IC_{50} value of 45.3 microM	Endocrine therapy
Amsacrine	15148258	Amsacrine blocked hERG currents in HEK 293 cells and Xenopus oocytes	Other antineoplastic agents
Celecoxib	22039467	Celecoxib inhibited the hERG channels in HEK-293 cells with IC_{50} of 6 μM	Other antineoplastic agents

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