

Supplementary data

Exploration of potential Ewing's sarcoma drugs from FDA approved pharmaceuticals through computational drug repositioning, pharmacogenomics, molecular docking, and MD simulation studies

Mubashir Hassan^{1,3*}, Muhammad Yasir¹, Saba Shahzadi², Andrzej Kloczkowski^{3,4*}

¹Institute of Molecular Biology and Biotechnology, The University of Lahore (Defense Road Campus), Lahore, Pakistan.

²Institute of Molecular Sciences and Bioinformatics (IMSB), Nisbet Road, Lahore, Pakistan

³The Steve and Cindy Rasmussen Institute for Genomic Medicine at Nationwide Children's Hospital, Columbus, OH 43205, USA

⁴Department of Pediatrics, The [Ohio State University](http://www.ohio-state.edu), Columbus, Ohio 43205, USA

Correspondence

Dr. Mubashir Hassan

¹Institute of Molecular Biology and Biotechnology, The University of Lahore (Defense Road Campus), Lahore, Pakistan. The Steve and Cindy Rasmussen Institute for Genomic Medicine, Nationwide Children Hospital, Columbus, Ohio 43205, USA

Emails: mubashirhassan_gcul@yahoo.com & Mubasher.Hassan@nationwidechildrens.org

Prof. Andrzej Kloczkowski

The Steve and Cindy Rasmussen Institute for Genomic Medicine, Nationwide Children Hospital & Department of Pediatrics, The Ohio State University, Columbus, Ohio 43205, USA

Email: Andrzej.Kloczkowski@nationwidechildrens.org

Table S1. Screened drug and their FDA status

Accession No	Generic name	Score	Approved	Investigational	Experimental
DB06589	Pazopanib	0.998	+	-	-
DB01394	Colchicine	0.022	+	-	-
DB00806	Pentoxifylline	0.018	+	+	-
DB00862	Vardenafil	0.018	+	-	-
DB01113	Papaverine	0.016	+	+	-
DB08911	Trametinib	0.016	+	-	-
DB08873	Boceprevir	0.015	+	-	-
DB00450	Droperidol	0.015	+	-	-
DB00338	Omeprazole	0.014	+	+	-
DB00869	Dorzolamide	0.014	+		-
DB01029	Irbesartan	0.014	+	+	-
DB08822	Azilsartan medoxomil	0.013	+	+	-
DB00203	Sildenafil	0.013	+	+	-
DB01349	Tasosartan	0.013			+
DB00736	Esomeprazole	0.012	+	+	-
DB00820	Tadalafil	0.011	+	+	-
DB01336	Metocurine	0.010	+	-	-
DB00757	Dolasetron	0.010	+	+	-
DB08965	Fusafungine	0.010	+	-	-
DB06802	Nepafenac	0.010	+	+	-
DB06605	Apixaban	0.010	+	-	-
DB06751	Drotaverine	0.010	+	+	-
DB01247	socarboxazid	0.010	+	-	-
DB00705	Delavirdine	0.010	+	-	-
DB01298	Sulfacytine	0.009	+	-	-
DB01342	Forasartan	0.009	-	-	+
DB01482	Fenethylline	0.009	-	-	+
DB01039	Fenofibrate	0.009	+	-	-
DB00421	Spirolactone	0.008	+	-	-
DB00589	Lisuride	0.008	+	+	-
DB00490	Buspirone	0.008	+	+	-
DB00202	Succinylcholine	0.008	+	-	-
DB08828	Vismodegib	0.008	+	+	-
DB01122	Ambenonium	0.008	+	-	-
DB06288	Amisulpride	0.008	+	+	-
DB00527	Cinchocaine	0.008	+	-	-
DB08811	Tofisopam	0.008	-	-	+
DB00808	Indapamide	0.008	+	-	-
DB06414	Etravirine	0.008	+	-	-
DB08983	Etofibrate	0.008	-	-	+
DB09020	Bisacodyl	0.008	+	-	-

DB06209	Prasugrel	0.008	+	-	-
DB01026	Ketoconazole	0.008	+	+	-
DB01138	Sulfinpyrazone	0.007	+	-	-
DB01411	Pranlukast	0.007	-	+	-
DB00745	Modafinil	0.007	+	+	-
DB01065	Melatonin	0.007	+	-	-
DB00343	Diltiazem	0.007	+	+	-
DB00843	Donepezil	0.007	+	-	-
DB00662	Trimethobenzamide	0.007	+	+	-
DB08974	Flubendazole	0.007	-	-	+
DB01168	Procarbazine	0.007	+	+	-
DB00546,	Adinazolam	0.007	-	-	+
DB00706	Tamsulosin	0.007	+	+	-
DB01035	Procainamide	0.007	+	-	-
DB01233	Metoclopramide	0.007	+	+	-
DB00962	Zaleplon	0.007	+	+	-
DB01325	Quinethazone	0.007	+	-	-
DB00980	Ramelteon	0.007	+	+	-
DB00214	Torasemide	0.007	+	-	-
DB00280	Disopyramide	0.007	+	-	-
DB00426	Famciclovir	0.007	+	+	-
DB08982	Etozoline	0.006	-	-	+
DB00981	Physostigmine	0.006	+	+	-
DB01337	Pancuronium	0.006	+		-
DB01420	Testosterone Propionate	0.006	+	+	-
DB00486	Nabilone	0.006	+	+	-
DB00480	Lenalidomide	0.006	+	-	-
DB06729	Sulfaphenazole	0.006	+	-	-
DB09003	Clocapramine	0.006	-	-	+
DB00496	Darifenacin	0.006	+	+	-
DB01238	Aripiprazole	0.006	+	+	-
DB01153	Sertaconazole	0.006	+	+	-
DB06691	Mepyramine	0.006	+	-	-
DB00637	Astemizole	0.006	+	-	-
DB00643	Mebendazole	0.006	+	-	-
DB00972	Azelastine	0.006	+	-	-
DB08810	Cinitapride	0.006	-	+	-
DB00391	Sulpiride	0.006	+	+	-
DB00721	Procaine	0.006	+	+	-
DB01161	Chloroprocaine	0.006	+	-	-
DB00613	Amodiaquine	0.006	+	+	-
DB00807	Proparacaine	0.006	+	-	-
DB00892	Oxybuprocaine	0.006	+	+	-
DB00812	Phenylbutazone	0.006	+	-	-

DB00395	Carisoprodol	0.006	+	-	-
DB01339	Vecuronium	0.005	+	+	-
DB00603	Medroxyprogesterone Acetate	0.005	+	+	-
DB00984	Nandrolone phenpropionate	0.005	+	+	-
DB00758	Clopidogrel	0.005	+	-	-
DB00637	Astemizole	0.006	+	+	-
DB00562	Benzthiazide	0.005	+	-	-
DB00310	Chlorthalidone	0.005	+	-	-
DB00837	Progabide	0.005	-	-	+
DB00656	Trazodone	0.005	+	+	-
DB01127	Econazole	0.005	+	-	-
DB01110	Miconazole	0.005	+	+	-
DB08943	Isoconazole	0.005	+	-	-
DB04880	Enoximone	0.005	+	+	-
DB06150	Sulfadimethoxine	0.005	+	-	-
DB06594	Agomelatine	0.005	+	+	-

Table S2. Virtual screening of drugs using PyRx

Docking Complexes	Drugs	Binding Affinity (Kcal/mol)	Docking Complexes	Drugs	Binding Affinity (Kcal/mol)
DB00395	Carisoprodol	-4.5	DB00862	Vardenafil	-6.5
DB00721	Procaine	-4.7	DB09020	Bisacodyl	-6.6
DB01161	Chlorprocaine	-4.8	DB06594	Agomelatine	-6.6
DB00807	Proparacaine	-4.9	DB06414	Etravirine	-6.6
DB00202	Succinylcholine	-4.9	DB00613	Amodiaquine	-6.6
DB01035	Procainamide	-5	DB00214	Torasemide	-6.6
DB00892	Oxybuprocaine	-5.3	DB00203	Sildenafil	-6.6
DB00662	Trimethobenzamide	-5.3	DB08810	Cinitapride	-6.7
DB01233	Metoclopramide	-5.4	DB00984	Nandrolone phenpropionate	-6.7
DB00426	Famciclovir	-5.4	DB00656	Trazodone	-6.7
DB04880	Enoximone	-5.5	DB00962	Zaleplon	-6.8
DB00745	Modafinil	-5.5	DB00843	Donepezil	-6.8
DB01298	Sulfacytine	-5.6	DB01238	Aripiprazole	-6.9
DB01065	Melatonin	-5.6	DB01127	Econazole	-6.9
DB00806	Pentoxifylline	-5.6	DB01110	Miconazole	-6.9
DB00706	Tamsulosin	-5.6	DB01138	Sulfinpyrazone	-7
DB08943	Isoconazole	-5.8	DB00808	Indapamide	-7
DB06729	Sulfaphenazole	-5.8	DB08974	Flubendazole	-7.1
DB06751	Drotaverine	-5.9	DB00280	Disopyramide	-7.1

DB06288	Amisulpride	-5.9	DB01122	Ambenonium	-7.2
DB01325	Quinethazone	-5.9	DB01029	Irbesartan	-7.2
DB00812	Phenylbutazone	-5.9	DB00837	Progabide	-7.2
DB00391	Sulpiride	-5.9	DB00450	Droperidol	-7.2
DB06150	Sulfadimethoxine	-6	DB00643	Mebendazole	-7.4
DB01247	Isocarboxazid	-6	DB00579	Mazindol	-7.4
DB01113	Papaverine	-6	DB00705	Delavirdine	-7.5
DB00480	Lenalidomide	-6	DB06605	Apixaban	-7.6
DB06802	Nepafenac	-6.1	DB06589	Pazopanib	-7.6
DB01394	Colchicine	-6.1	DB08828	Vismodegib	-7.7
DB08811	Tofisopam	-6.2	DB01026	Ketoconazole	-7.7
DB01168	Procarbazine	-6.2	DB00546	Adinazolam	-7.7
DB01153	Sertaconazole	-6.2	DB01342	Forasartan	-7.8
DB00527	Cinchocaine	-6.2	DB00310	Chlorthalidone	-7.8
DB06209	Prasugrel	-6.3	DB01411	Pranlukast	-8
DB06691	Mepyramine	-6.4	DB09003	Clocapramine	-8.1
DB00736	Esomeprazole	-6.4	DB00637	Astemizole	-8.3
DB00338	Omeprazole	-6.4	DB00972	Azelastine	-8.7
DB00496	Darifenacin	-9.2	DB01349	Tasosartan	-8.9