

**Supplementary Table 1. List of 43 compounds excluded for further screening, based on toxicity assay.**

Compound number	Compound name	In vivo application
1	ABT-263 (Navitoclax)	Anti-cancer drug
2	YM155 (Sepantronium Bromide)	Anti-cancer drug
3	Bortezomib (PS-341)	Anti-cancer drug
4	Panobinostat (LBH589)	Anti-cancer drug
5	CEP-18770 (Delanzomib)	Anti-cancer drug
6	17-AAG (Tanespimycin)	Anti-cancer drug
7	Ganetespib (STA-9090)	Anti-cancer drug
8	Saracatinib (AZD0530)	Anti-cancer drug
9	Onalespib (AT13387)	Anti-cancer drug
10	Dasatinib (BMS-354825)	Anti-cancer drug
11	Docetaxel (RP56976)	Anti-cancer drug
12	Ispinesib (SB-715992)	Anti-cancer drug
13	Paclitaxel (NSC 125973)	Anti-cancer drug
14	Rigosertib (ON-01910)	Anti-cancer drug
15	Epothilone B (EPO906, Patupilone)	Anti-cancer drug
16	Flavopiridol (Alvocidib)	Anti-cancer drug
17	Topotecan (NSC609699) HCl	Anti-cancer drug
18	Epirubicin (IMI 28) HCl	Anti-cancer drug
19	Tamoxifen (ICI 46474)	Anti-cancer drug
20	Vincristine (NSC-67574)	Anti-cancer drug
21	Rufinamide	Anti-epileptic/seizure drugs
22	Volasertib (BI 6727)	Anti-cancer drug
23	Neratinib (HKI-272)	Anti-cancer drug / Inhibits Xenograph growth
24	Ixazomib (MLN2238)	Anti-cancer drug
25	Crystal Violet	triarylmethane dye
26	Omipalisib (GSK2126458, GSK458)	Anti-cancer drug
27	Carfilzomib (PR-171)	Anti-cancer drug
28	Daunorubicin (RP 13057) HCl	Anti-cancer drug
29	Cabazitaxel (XRP6258)	Anti-cancer drug
30	Bisacodyl	Laxative drug
31	Dinaciclib (SCH727965)	Anti-cancer drug
32	Vinorelbine Tartrate	Anti-cancer drug
33	Digoxin	Atrial fibrillation and heart failure drug
34	Puromycin (CL13900) 2HCl	Aminonucleoside antibiotic
35	Vinblastine (NSC-49842) sulfate	Anti-cancer drug
36	Birinapant (TL32711)	Anti-cancer drug
37	Dasatinib Monohydrate	Anti-cancer drug
38	Docetaxel Trihydrate	Anti-cancer drug
39	Riociguat (BAY 63-2521)	Pulmonary hypertension drug
40	Mebendazole	Anthelmintic drug
41	Gemcitabine (LY-188011) HCl	Anti-cancer drug
42	Vancomycin HCl	Antibacterial agent
43	Fosbretabulin (Combretastatin A4 Phosphate (CA4P)) Disodium	Anti-cancer drug

**Supplementary Table 2. List of p-values and adjusted p-valued (Benjamin-Hochberg method) of top 40 compound combinations in the W1282X/W1282X screen, based on a one-sided T-test where the average AUC value per condition over the 4 donors was compared to the average of the plate.**

Compound_ID	p	p_adjusted	Compound 1	Compound 2
Pos. Control plate A	0	0		
Pos. Control plate B	0	0		
1	0.000341	0.084206	Fenspiride HCl (S4090)	Mevastatin (S4223)
2	0.000683	0.126271	Pitavastatin Calcium (S1759)	Alibendol (S1928)
3	0.002352	0.348096	Simvastatin	Tamoxifen Citrate (S1972)
4	0.003027	0.365673	CO-1686 (AVL-301)	Palbociclib (PD-0332991) HCl
5	0.003459	0.365673	Valsartan (S1894)	Lovastatin (S2061)
6	0.008797	0.758291	Guaifenesin (S1740)	Fluvastatin Sodium (S1909)
7	0.010058	0.758291	Nilotinib (AMN-107)	Dienogest
8	0.010525	0.758291	Carvedilol	Formoterol Hemifumarate
9	0.016278	0.758291	Butoconazole nitrate	Ketotifen Fumarate
10	0.017213	0.758291	Droperidol	Fluorometholone Acetate
11	0.017866	0.758291	Sotrastaurin	Ethinodiol diacetate
12	0.018242	0.758291	Linezolid	Acetylcysteine
13	0.020269	0.758291	S- (+)-Rolipram (S2127)	Naphazoline HCl (S2519)
14	0.022949	0.758291	Varlitinib	Entacapone
15	0.0233	0.758291	Cabazitaxel	Pergolide mesylate
16	0.025466	0.758291	Pravastatin sodium	Mirabegron
17	0.025704	0.758291	Voxtalisib (XL765, SAR245409)	L-Glutamine
18	0.026123	0.758291	Levobupivacaine HCl	Chlorquinaldol
19	0.026898	0.758291	Idasanutlin (RG-7388)	Lypressin Acetate
20	0.031113	0.758291	Cobicistat (GS-9350)	Eletriptan HBr
21	0.031239	0.758291	Triciribine	Cilostazol
22	0.03282	0.758291	Rosuvastatin Calcium	Secnidazole
23	0.033328	0.758291	Foretinib (GSK1363089)	Cilnidipine
24	0.033605	0.758291	TH-302	Estradiol valerate
25	0.035348	0.758291	Cilengitide	Empty
26	0.035555	0.758291	Sofosbuvir (PSI-7977, GS-7977)	Sertaconazole nitrate
27	0.037549	0.758291	Probucof	Spectinomycin HCl
28	0.038516	0.758291	Marbofloxacin	Monobenzene
29	0.041068	0.758291	Griseofulvin	Florfenicol
30	0.041323	0.758291	Lomerizine HCl	Amoxapine
31	0.041537	0.758291	VX-680 (Tozasertib, MK-0457)	Celecoxib
32	0.04302	0.758291	Edoxaban	Nafarelin Acetate
33	0.044306	0.758291	Bendamustine HCl	Omeprazole
34	0.046228	0.758291	Licofelone	Sulfadoxine
35	0.046428	0.758291	Albendazole Oxide	Diclazuril
36	0.047365	0.758291	KPT-330	Oxytocin (Syntocinon)
37	0.048372	0.758291	Retapamulin	Tiratricol
38	0.049341	0.758291	Sorafenib Tosylate	Rufinamide