

Table S1. Oligonucleotides used in this study. Blue and red denote nucleotides involved in Watson-Crick and reverse Hoogsteen base pairing, respectively.

Name	Sequence (5' - 3')	ϵ ($\times 10^3$, $M^{-1}cm^{-1}$)
R2	CCCCTCCC TTTT GGGAGGGG CGCTTAT GGGGAGGG	366.0
R2FQ	CCCCTCCC TT-FAMdT-TT GGGAGGGG CGCTTAT GGGGAGGG-BHQ1	404.1
MCRa2	CCCTCCCC ATAAGCG CCCCTCCC AAAAA	282.1
GT	GGGG TTTT GGGG TTTT GGGG AAAA GGGG TTTT CCCC TTTT CCCC	446.4

Table S2-1. List of 320 chemical compounds. Purity data was obtained using an HPLC equipped with UV detector from the specific batch indicated. NA indicated data was not available because they do not absorb UV. Further details can be found at <https://www.selleckchem.com/>.

Compound ID	CAS Number	Targets	Selleck Cat No	Batch	Purity, %
ABT-263 (Navitoclax)	923564-51-6	Bcl-2	S1001	S100101	99.33
Entinostat (MS-275)	209783-80-2	HDAC	S1053	S105301	99.11
PCI-24781 (Abexinostat)	783355-60-2	HDAC	S1090	S109001	92.77
Mocetinostat (MGCD0103)	726169-73-9	HDAC	S1122	S112202	99.04
S31-201	501919-59-1	STAT	S1155	S115501	94.4
MK-2866 (GTX-024)	841205-47-8	Androgen Receptor	S1174	S117401	99.36
Finasteride	98319-26-7	5-alpha Reductase	S1197	S119701	99.27
Epothilone A	152044-53-6	Microtubule Associated	S1297	S129701	99.1
Pirarubicin	72496-41-4	Topoisomerase	S1393	S139301	99.09
Calcitriol	32222-06-3	Others	S1466	S146601	99.1
Veliparib (ABT-888)	912444-00-9	PARP	S1004	S100401	99.74
Obatoclox Mesylate	803712-79-0	Bcl-2, Autophagy	S1057	S105701	99.25
LAQ824 (Dacinostat)	404951-53-7	HDAC	S1095	S109501	95.4
BMS-754807	1001350-96-4	IGF-1R, Trk receptor, c-Met	S1124	S112401	99.58
CEP-18770 (Delanzomib)	847499-27-8	Proteasome	S1157	S115701	99.25
BIB021	848695-25-0	HSP (e.g. HSP90)	S1175	S117501	99.54
Dimesna	16208-51-8	Others	S1201	S120101	100
Ki16425	355025-24-0	LPA Receptor	S1315	S131501	91.73
Tenofovir Disoproxil Fumarate	202138-50-9	Reverse Transcriptase	S1400	S140001	99.03
Safinamide Mesylate	202825-46-5	MAO	S1472	S147201	99.85
FG-4592	808118-40-3	HIF	S1007	S100701	99.01
Olaparib	763113-22-0	PARP	S1060	S106003	99
Quisinosat	875320-29-9	HDAC	S1096	S109601	99.62
SRT1720	1001645-58-4	Sirtuin	S1129	S112901	99.3
MK-8245	1030612-90-8	Dehydrogenase	S1158	S115801	99.1
XAV-939	284028-89-3	Wnt/beta-catenin	S1180	S118001	99.17
Doxorubicin (Adriamycin)	25316-40-9	Autophagy, Topoisomerase	S1208	S120802	99.1
Costunolide	553-21-9	Telomerase	S1319	S131901	99.08
Elaiophylin	37318-06-2	Others	S1448	S144801	99.42
Oligomycin A	579-13-5	ATPase	S1478	S147801	97.33
Panobinostat (LBH589)	404950-80-7	HDAC	S1030	S103002	97.17
Nutlin-3	890090-75-2	E3 Ligase, Mdm2	S1061	S106101	97.64
BTZ043 Racemate	957217-65-1	Others	S1097	S109702	99.14
YM155	781661-94-7	Survivin	S1130	S113001	99.38
Ganetespib (STA-9090)	888216-25-9	HSP (e.g. HSP90)	S1159	S115901	99.69
Danoprevir (ITMN-191)	850876-88-9	HCV Protease	S1183	S118301	95.4
PFI-1 (PF-6405761)	1403764-72-6	Epigenetic Reader Domain	S1216	S121601	99
Dexamethasone (DHAP)	50-02-2	Autophagy, IL Receptor	S1322	S132201	99.02
Nanchangmycin	65101-87-3	Others	S1450	S145001	92.77
VX-222 (VCH-222, Lomibuvir)	1026785-59-0	HCV Protease	S1480	S148001	99.66
NVP-AEW541	475489-16-8	IGF-1R	S1034	S103401	99.43
AUY922 (NVP-AUY922)	747412-49-3	HSP (e.g. HSP90)	S1069	S106902	95.06
Rucaparib	459868-92-9	PARP	S1098	S109802	99.63
ADL5859 HCl	850173-95-4	Opioid Receptor	S1139	S113901	99.18
PA-824	187235-37-6	Others	S1162	S116201	99.91
BIBR 1532	321674-73-1	Telomerase	S1186	S118601	99.75
Idarubicin HCl	57852-57-0	Topoisomerase	S1228	S122801	99.06
Ginkgolide B	15291-77-7	PAFR	S1343	S134302	99.63
Ispinesib (SB-715992)	336113-53-2	Kinesin	S1452	S145201	99.04
Zosuquidar (LY335979)3HCl	167465-36-3	P-gp	S1481	S148101	99.14
STF-62247	315702-99-9	Others	S1041	S104101	99.68
HA14-1	65673-63-4	Bcl-2	S1071	S107102	97
Varespladib (LY315920)	172732-68-2	Phospholipase (e.g. PLA)	S1110	S111002	99.38
Andarine	401900-40-1	Androgen Receptor	S1140	S114001	99.19
AT13387	912999-49-6	HSP (e.g. HSP90)	S1163	S116301	99.01
CUDC-101	1012054-59-9	HDAC, HER2, EGFR	S1194	S119401	99.02
2-Methoxyestradiol	362-07-2	HIF	S1233	S123301	99.31
Losartan Potassium	124750-99-8	RAAS	S1359	S135901	99.39
Tipifarnib	192185-72-1	Transferase	S1453	S145301	96.3
Daclatasvir (BMS-790052)	1009119-64-5	HCV Protease	S1482	S148202	99.7

Table S2-2. List of 320 chemical compounds (cont'd).

Compound ID	CAS Number	Targets	Selleck Cat No	Batch	Purity, %
Trichostatin A (TSA)	58880-19-6	HDAC	S1045	S104502	99.33
Belinostat (PXD101)	414864-00-9	HDAC	S1085	S108501	99.16
Odanacatib (MK-0822)	603139-19-1	Cathepsin K	S1115	S111501	99.18
17-AAG (Tanespimycin)	75747-14-7	HSP (e.g. HSP90)	S1141	S114101	99.6
ABT-751 (E7010)	141430-65-1	Microtubule Associated	S1165	S116501	99.23
TAK-700 (Orteronel)	426219-18-3	P450 (e.g. CYP17)	S1195	S119501	99.16
Vinblastine	865-21-4	Microtubule Associated	S1248	S124801	93.05
Epothilone B	152044-54-7	Microtubule Associated	S1364	S136401	99.22
Cilomilast	153259-65-5	PDE	S1455	S145501	95.52
MC1568	852475-26-4	HDAC	S1484	S148401	95.04
Elesclomol (STA-4783)	488832-69-5	HSP (e.g. HSP90)	S1052	S105202	99.06
Iniparib (BSI-201)	160003-66-7	PARP	S1087	S108701	99.59
TW-37	877877-35-5	Bcl-2	S1121	S112101	99.78
Alvespimycin, HCl	467214-21-7	HSP (e.g. HSP90)	S1142	S114201	99.72
Serdemetan	881202-45-5	p53, E3 Ligase	S1172	S117201	99.03
Exemestane	107868-30-4	Aromatase	S1196	S119601	99.31
Avagacestat	1146699-66-2	Gamma-secretase, Beta Amyloid	S1262	S126201	96.92
BMS-707035	729607-74-3	Integrase	S1366	S136601	99.3
Zibotentan (ZD4054)	186497-07-4	Endothelin Receptor	S1456	S145601	99.15
Alprostadil	745-65-3	Others	S1508	S150801	100
Pracinostat (SB939)	929016-96-6	HDAC	S1515	S151501	99
SB408124	288150-92-5	OX Receptor	S1545	S154501	99.74
Gemcitabine	95058-81-4	Autophagy, DNA/RNA Synthesis	S1714	S171401	99.26
Albendazole Oxide	54029-12-8	Others	S1836	S183601	99.73
Adenine HCl	2922-28-3	DNA/RNA Synthesis	S1983	S198301	99.1
Imidapril HCl	89396-94-1	RAAS	S2109	S210901	99.23
LY2608204	1234703-40-2	Others	S2155	S215501	99.74
SB505124	694433-59-5	TGF-beta/Smad	S2186	S218601	99.25
AR-42	935881-37-1	HDAC	S2244	S224401	99.03
Andrographolide	5508-58-7	Others	S2261	S226101	99.1
Tosedostat (CHR2797)	238750-77-1	Aminopeptidase	S1522	S152201	83.58
Dapagliflozin	461432-26-8	SGLT	S1548	S154803	96.52
Terbinafine	91161-71-6	Others	S1725	S172501	100
Chenodeoxycholic Acid	474-25-9	Others	S1843	S184301	99.3
Fluticasone propionate	80474-14-2	Others	S1992	S199201	97.93
Licofelone	156897-06-2	COX	S2121	S212101	95.02
LY2886721	1262036-50-9	Others	S2156	S215601	99.63
Avasimibe	166518-60-1	P450 (e.g. CYP17)	S2187	S218701	97.84
Abiraterone Acetate	154229-18-2	P450 (e.g. CYP17)	S2246	S224601	99.64
Artesunate	88495-63-0	Others	S2265	S226502	99.15
MK-1775	955365-80-7	Wee1	S1525	S152501	99.38
VX-809 (Lumacaftor)	936727-05-8	CFTR	S1565	S156501	99.02
Levonorgestrel	797-63-7	Others	S1727	S172701	100
Talc	14807-96-6	Others	S1900	NA	NA
PCI-34051	950762-95-5	HDAC	S2012	S201201	99.01
S- (+)-Rolipram	85416-73-5	PDE	S2127	S212701	100
PD128907 HCl	112960-16-4	Dopamine Receptor	S2168	S216801	99.44
SGL-1776 free base	1025065-69-3	Pim	S2198	S219801	96.99
(-)-Huperzine A (HupA)	102518-79-6	GluR	S2251	S225101	98.19
Azomycin	527-73-1	Others	S2267	S226701	99.99
LY2811376	1194044-20-6	Beta Amyloid, Gamma-secretase	S1528	S152801	99.55
Semagacestat (LY450139)	425386-60-3	Gamma-secretase	S1594	S159401	97.66
Suprofen	40828-46-4	Others	S1761	S176101	99.25
Amlodipine	88150-42-9	Calcium Channel	S1905	S190501	95.65
Benidipine HCl	91599-74-5	Calcium Channel	S2017	S201701	99.64
Bazedoxifene HCl	198480-56-7	Estrogen/progesterone Receptor	S2128	S212801	99.06
Givinostat (ITF2357)	732302-99-7	HDAC	S2170	S217001	99.07
Irinotecan HCl Trihydrate	136572-09-3	Topoisomerase	S2217	S221701	99.45
(+)-Usniacin	7562-61-0	Others	S2252	NA	NA
Baicalin	21967-41-9	Others	S2269	NA	NA
Org 27569	868273-06-7	Cannabinoid Receptor	S1534	S153401	99.72
Cefoperazone	62893-19-0	Others	S1611	S161101	99.71
Quetiapine Fumarate	111974-72-2	Dopamine Receptor	S1763	S176301	99
Nystatin (Fungicidin)	1400-61-9	Others	S1934	NA	NA
Doxifluridine	3094-09-5	Others	S2045	S204502	99.73

Table S2-3. List of 320 chemical compounds (cont'd).

Compound ID	CAS Number	Targets	Selleck Cat No	Batch	Purity, %
Atropine	5908-99-6	AChR	S2130	S213001	99.78
AG-14361	328543-09-5	PARP	S2178	S217801	99.13
UK 383367	348622-88-8	Procollagen C Proteinase	S2224	S222402	99.92
3-Indolebutyric acid (IBA)	133-32-4	Others	S2253	S225301	99.23
Bilobalide	33570-04-6	Others	S2276	S227602	95.92
DMXAA (Vadimezan)	117570-53-3	VDA	S1537	S153701	99.04
Pilocaine	721-50-6	Others	S1619	S161901	100
Chlorprothixene	113-59-7	Dopamine Receptor	S1771	S177101	97.25
Cyclocytidine HCl	10212-25-6	Others	S1973	S197301	95.04
Terazosin HCl	70024-40-7	Adrenergic Receptor	S2059	S205901	99.38
GSK1292263	1032823-75-8	GPR	S2149	S214901	99.03
MLN2238	1072833-77-2	Proteasome	S2180	S218001	99.05
VX-765	273404-37-8	Caspase	S2228	S222801	91.06
Esculin	531-75-9	Others	S2258	S225801	97.38
Dihydroartemisinin (DHA)	71939-50-9	Others	S2290	NA	NA
EX 527 (Selisistat)	49843-98-3	Sirtuin	S1541	S154101	94.54
Loteprednol etabonate	82034-46-6	Others	S1669	S166901	100
Oxytetracycline	79-57-2	Others	S1773	S177301	97
Meglumine	6284-40-8	Others	S1974	S197401	100
Trimebutine	39133-31-8	Opioid Receptor	S2085	S208501	99.05
Erismodegib	956697-53-3	Hedgehog/Smoothed	S2151	S215101	99.6
MLN9708	1201902-80-8	Proteasome	S2181	S218101	99.62
LY2157299	700874-72-2	TGF-beta/Smad	S2230	S223001	99
Aloe-emodin	481-72-1	Others	S2259	S225901	99.09
Glycyrrhizic Acid	1405-86-3	Others	S2302	S230202	99.8
AM1241	444912-48-5	Cannabinoid Receptor	S1544	S154401	99.73
Lubiprostone	136790-76-6	Others	S1675	S167501	91.85
Fenoprofen Calcium	34597-40-5	Others	S1823	S182301	99.01
Methscopolamine	155-41-9	AChR	S1978	S197801	95.12
Betaxolol	659-18-7	Adrenergic Receptor	S2091	S209101	96.01
CGS 21680 HCl	124431-80-7	5-alpha Reductase	S2153	S215301	99.04
SB743921	940929-33-9	Kinesin	S2182	S218201	95.24
Ketanserin	74050-98-9	5-HT Receptor	S2232	S223201	97.87
Laetrile	29883-15-6	Others	S2260	S226002	97.54
Gramine	87-52-5	Others	S2304	S230401	97.83
Gynostemma Extract	80321-63-7	Others	S2306	NA	NA
Morin Hydrate	6202-27-3	Others	S2325	S232501	90.5
(-)-Parthenolide	20554-84-1	E3 Ligase	S2341	S234102	99.7
Tetrahydropapaverine HCl	6429-04-5	Others	S2367	NA	NA
Hematoxylin	517-28-2	Others	S2384	NA	NA
Curcuminol	4871-97-0	Others	S2407	S240702	99.01
Equl	531-95-3	Estrogen/progestogen Receptor	S2450	S245001	99.04
Scopolamine HBr	114-49-8	AChR	S2508	S250802	99.08
Ceftiofur HCl	103980-44-5	Others	S2543	S254301	95.68
GSK256066	801312-28-7	PDE	S2620	S262001	97.59
Hyodeoxycholic acid (HDCA)	83-49-8	Others	S2311	S231102	95
Myricitrin	17912-87-7	Others	S2327	S232701	99.06
Phlorizin	60-81-1	Others	S2343	S234302	99.48
Vanillylacetone	122-48-5	Others	S2371	NA	NA
Hordenine	539-15-1	Others	S2385	S238501	97.44
Astragaloside A	83207-58-3	TGF-beta/Smad	S2415	S241501	98.78
Clindamycin HCl	21462-39-5	Others	S2457	S245701	97
Spectinomycin HCl	21736-83-4	Others	S2510	S251002	99
Scopine HCl	85700-55-6	Others	S2548	NA	NA
CK-1827452	873697-71-3	ATPase	S2623	S262301	99.66
Kaempferol	520-18-3	Others	S2314	S231401	99.21
Neohesperidin	13241-33-3	Others	S2332	S233203	99.01
Rutin	153-18-4	Others	S2350	S235002	97.09
5-hydroxytryptophan (5-HTP)	56-69-9	Others	S2374	S237401	99.67
Lappaconite HBr	97792-45-5	Others	S2387	S238701	95.83
20-Hydroxyecdysone	5289-74-7	Others	S2417	S241701	99.25
Hexestrol	84-16-2	Estrogen/progestogen Receptor	S2473	S247301	99
Vardenafil HCl Trihydrate	224785-90-4	PDE	S2515	S251501	99.45
Sulbactam sodium	69388-84-7	Others	S2551	S255101	98.35
Fostamatinib (R788)	901119-35-5	Syk	S2625	S262501	99.03

Table S2-4. List of 320 chemical compounds (cont'd).

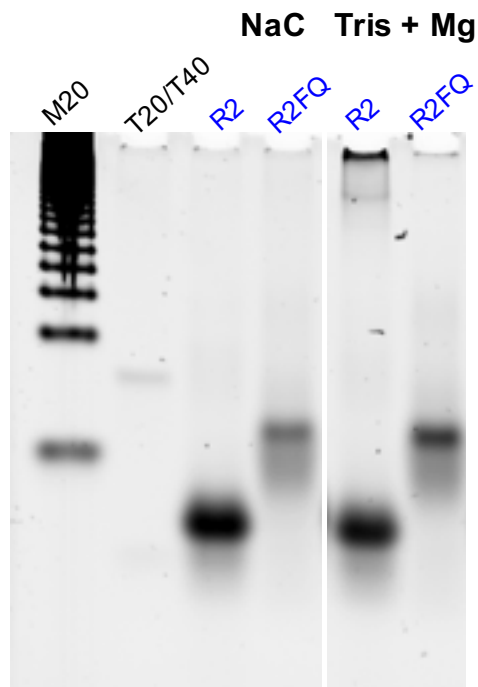
Compound ID	CAS Number	Targets	Selleck Cat No	Batch	Purity, %
L-(+)-Rhamnose Monohydrate	10030-85-0	Others	S2317	NA	NA
Oleanolic Acid	508-02-1	Others	S2334	S233401	99.02
Salinomycin	53003-10-4	Others	S2352	NA	NA
Butylscopolamine Bromide	149-64-4	Others	S2378	S237802	98.92
Naringin Dihydrochalcone	18916-17-1	Others	S2389	NA	NA
Aloperine	56293-29-9	Others	S2420	S242001	100
Lincomycin HCl	859-18-7	Others	S2479	S247901	95.04
Epinephrine Bitartrate	51-42-3	Adrenergic Receptor	S2521	S252102	99.11
Amoxicillin Sodium	34642-77-8	Others	S2565	S256501	99.11
Tubastatin A HCl	1310693-92-5	HDAC	S2627	s262701	99.05
Luteolin	491-70-3	PDE	S2320	S232002	97.89
Oridonin	28957-04-2	Others	S2335	S233501	92.9
Sclareol	515-03-7	Others	S2354	S235402	95
Dioscin	19057-60-4	Others	S2379	S237902	97
Sesamin	607-80-7	Others	S2392	S239201	99.07
Apocynin	498-02-2	Others	S2425	S242501	99.81
Manidipine 2HCl	89226-75-5	Calcium Channel	S2482	S248201	99.09
L-Adrenaline	51-43-4	Adrenergic Receptor	S2522	S252201	96.7
Pioglitazone	111025-46-8	Others	S2590	s259002	98.97
PNU-120596	501925-31-1	AChR	S2629	S262901	99.01
Magnolol	528-43-8	Others	S2321	S232101	99.35
6-Carboxyuracil	65-86-1	Others	S2336	S233601	99.8
Sclareolide	564-20-5	Others	S2355	NA	NA
D-Mannitol	69-65-8	Others	S2381	NA	NA
Dihydromyricetin	27200-12-0	Others	S2399	S239901	99.09
Rotundine	483-14-7	Dopamine Receptor	S2437	S243701	99.36
Olopatadine HCl	140462-76-6	Histamine Receptor	S2494	NA	NA
Methacycline HCl	3963-95-9	Others	S2527	S252701	100
Clindamycin palmitate HCl	25507-04-4	Others	S2596	S259601	99.96
GW3965 HCl	405911-17-3	Liver X Receptor	S2630	S263001	99.02
(+)-Matrine	519-02-8	Opioid Receptor	S2322	S232201	99.34
Osthole	484-12-8	Others	S2337	S233701	99.01
Silymarin	65666-07-1	Others	S2358	NA	NA
Evodiamine	518-17-2	Others	S2382	S238202	99.76
Sodium Danshensu	67920-52-9	Others,P450 (e.g. CYP17)	S2401	S240101	97.58
Synephrine HCl	5985-28-4	Adrenergic Receptor	S2438	S243801	99.14
Pancuronium dibromide	15500-66-0	AChR	S2497	S249702	99.97
L-Ascorbyl 6-palmitate	137-66-6	Others	S2532	S253201	100
DHEA	53-43-0	Androgen Receptor	S2604	S260401	100
URB597	546141-08-6	FAAH	S2631	S263101	99.73
Methyl-Hesperidin	11013-97-1	Others	S2323	NA	NA
Oxymatrine	16837-52-8	Others	S2338	S233801	99.52
Tanshinone I	568-73-0	Others	S2364	S236402	95.97
Gastrodin	62499-27-8	Others	S2383	S238301	99.7
Sophocarpine	6483-15-4	Others	S2405	S240502	99.8
Guanosine	118-00-3	Others	S2439	S243901	99.05
Quinine HCl Dihydrate	6119-47-7	Others	S2502	S250201	99.98
Isoconazole nitrate	24168-96-5	Others	S2534	S253401	100
MG-132	133407-82-6	Proteasome	S2619	S261903	93.43
BMS-378806	357263-13-9	gp120/CD4	S2632	S263201	99
NPS-2143	284035-33-2	CaSR	S2633	S263302	97.61
PF-3845	1196109-52-0	FAAH	S2666	S266601	99.09
Resminostat	864814-88-0	HDAC	S2693	S269301	99.04
JTC-801	244218-51-7	Opioid Receptor	S2722	S272201	99.05
Dalcetrapib	211513-37-0	CETP	S2772	S277201	97.03
A-803467	944261-79-4	Sodium Channel	S2785	S278501	99.05
Sirtinol	410536-97-9	Sirtuin	S2804	S280401	97
ARN-509	956104-40-8	Androgen Receptor	S2840	S284001	99.29
StemRegenin 1 (SR1)	1227633-49-9	Others	S2858	S285801	99.51
Camostat Mesilate	59721-29-8	Others	S2874	S287401	99.79
TAK-875	1374598-80-7	GPR	S2637	S263702	97.63
Dolutegravir	1051375-16-6	Integrase	S2667	S266701	99.06
XL335	629664-81-9	FXR	S2694	S269401	99.27
AZ 3146	1124329-14-1	Kinesin	S2731	S273101	99.46
SB705498	501951-42-4	TRPV	S2773	S277301	99.9

Table S2-5. List of 320 chemical compounds (cont'd).

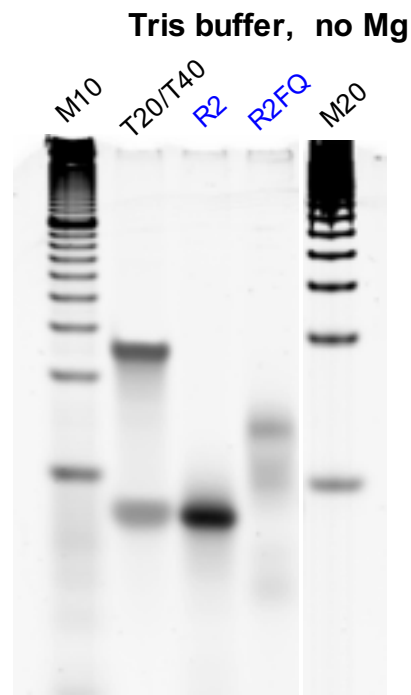
Compound ID	CAS Number	Targets	Selleck Cat No	Batch	Purity, %
Laquinimod	248281-84-7	Others	S2787	S278701	99.26
MPEP	96206-92-7	GluR	S2809	S280901	99.16
Cathepsin Inhibitor 1	225120-65-0	Others	S2847	S284701	99.87
IEM 1754 dihydrobroMide	162831-31-4	GluR,5-HT Receptor	S2860	S286001	100
Prucalopride	179474-81-8	5-HT Receptor	S2875	S287501	99.96
SNX-2112 (PF-04928473)	908112-43-6	HSP (e.g. HSP90)	S2639	S263901	99.58
A922500	959122-11-3	Transferase	S2674	S267401	99.08
RS-127445	199864-87-3	5-HT Receptor	S2698	S269801	97.08
Anacetrapib (MK-0859)	875446-37-0	CETP	S2748	S274801	99.38
CPI-613	95809-78-2	Dehydrogenase	S2776	S277601	98.55
Istradefylline	155270-99-8	Others	S2790	S279001	98.65
Ciproxifan	184025-18-1	Histamine Receptor	S2813	S281301	100
BRL-54443	57477-39-1	5-HT Receptor	S2852	S285201	99.05
CTEP (RO4956371)	871362-31-1	GluR	S2861	S286101	99.04
(-)-MK 801 Maleate	121917-57-5	GluR	S2857	S285701	99.83
PF-04929113 (SNX-5422)	908115-27-5	HSP (e.g. HSP90)	S2656	S265601	97.43
BRL-15572	193611-72-2	5-HT Receptor	S2677	S267701	99.7
CH5132799	1007207-67-1	mTOR,PI3K	S2699	S269901	99.03
GW788388	452342-67-5	TGF-beta/Smad	S2750	S275001	99.02
PF-5274857	1373615-35-0	Hedgehog/Smoothened	S2777	S277701	97.74
Sotrastaurin	425637-18-9	PKC	S2791	S279101	98.65
CI994 (Tacedinaline)	112522-64-2	HDAC	S2818	S281801	99.74
Carfilzomib (PR-171)	868540-17-4	Proteasome	S2853	S285301	94.38
VU 0364770	61350-00-3	GluR	S2862	S286201	99.02
Acesulfame Potassium	55589-62-3	Others	S2884	S288401	99.97
PNU 200577	207679-81-0	AChR	S2659	S265901	99.01
Flavopiridol HCl	131740-09-5	CDK	S2679	S267901	99.07
LY2109761	700874-71-1	TGF-beta/Smad	S2704	S270401	99.18
CUDC-907	1339928-25-4	PI3K,HDAC	S2759	S275901	99.38
GW842166X	666260-75-9	Cannabinoid Receptor	S2778	S277801	99.09
Torcetrapib	262352-17-0	CETP	S2792	S279202	99.46
RG108	48208-26-0	Transferase,DNA Methyltransferase	S2821	S282101	99.69
BML-190	2854-32-2	Cannabinoid Receptor	S2854	S285401	99.01
ML130 (Nodinitib-1)	799264-47-4	NOD1	S2863	S286301	99.8
A-205804	251992-66-2	Others	S2885	S288501	99.66
MK-0752	471905-41-6	Gamma-secretase,Beta Amyloid	S2660	S266001	99.1
KW-2478	819812-04-9	HSP (e.g. HSP90)	S2685	S268501	99.01
YO-01027	209984-56-5	Gamma-secretase	S2711	S271101	97.83
Canagliflozin	842133-18-0	SGLT	S2760	S276001	99.82
M344	251456-60-7	HDAC	S2779	S277901	99.36
VU 0357121	433967-28-3	GluR	S2795	S279501	99.47
OC000459	851723-84-7	GPR	S2822	S282201	99.36
MRS 2578	711019-86-2	P2 Receptor	S2855	S285501	99.02
VUF 10166	155584-74-0	5-HT Receptor	S2865	S286501	99.77
PJ34	344458-19-1	PARP	S2886	S288601	99.05
ICG-001	780757-88-2	Wnt/beta-catenin	S2662	S266201	100
R547	741713-40-6	CDK	S2688	S268801	100
Geldanamycin	30562-34-6	HSP (e.g. HSP90),Autophagy	S2713	S271302	97.62
MK-2048	869901-69-9	Integrase	S2765	S276501	99.01
I-BET151 (GSK1210151A)	1300031-49-5	Epigenetic Reader Domain	S2780	S278001	99.2
Lonafarnib	193275-84-2	Transferase	S2797	S279701	99.48
ML133 HCl	1222781-70-5	Potassium Channel	S2825	S282501	99.77
SB271046	209481-20-9	5-HT Receptor	S2856	S285601	99.06
U-104	178606-66-1	Carbonic Anhydrase	S2866	S286601	99.05
VU 0361737	1161205-04-4	GluR	S2892	S289201	100
Clinofibrate	30299-08-2	RAAS	S2664	S266401	99.68
ADX-47273	851881-60-2	GluR	S2690	S269001	99.01
LY411575	209984-57-6	Gamma-secretase	S2714	S271401	99.44
TKI-258, Dilactic Acid	852433-84-2	PDGFR,FGFR,c-Kit,FLT3,VEGFR	S2769	S276903	99.56
GW4064	278779-30-9	FXR	S2782	S278202	99.52
Galeterone	851983-85-2	P450 (e.g. CYP17),Androgen Receptor	S2803	S280301	99.03
Clindamycin	18323-44-9	Others	S2830	S283050	100
MK-801 (Dizocilpine)	77086-21-6	GluR	S8227	NA	NA
Alogliptin	850649-61-5	DPP-4	S5365	NA	NA
SB742457	607742-69-8	5-HT Receptor	S2894	S289401	97.8

S1. Characterization of non-B DNA structure formation by native PAGE and CD spectroscopy. Native gel electrophoresis results showing folded mobilities under **A) Sodium cacodylate (NaC) and Tris + Mg²⁺ buffers, B) Tris buffer alone (no Mg²⁺).** *M10=10-bp marker; M20=20-bp marker.* Samples in panel A were electrophoresed on a single gel containing 10 mM Mg²⁺, while samples in panel B were electrophoresed on a single gel in the absence of Mg²⁺. Circular dichroism (CD) spectroscopy results showing a negative peak in the 210-220 nm region indicates triplex formation under **C) NaC and Tris + Mg²⁺ buffers, D) Tris, no Mg²⁺ buffer.**

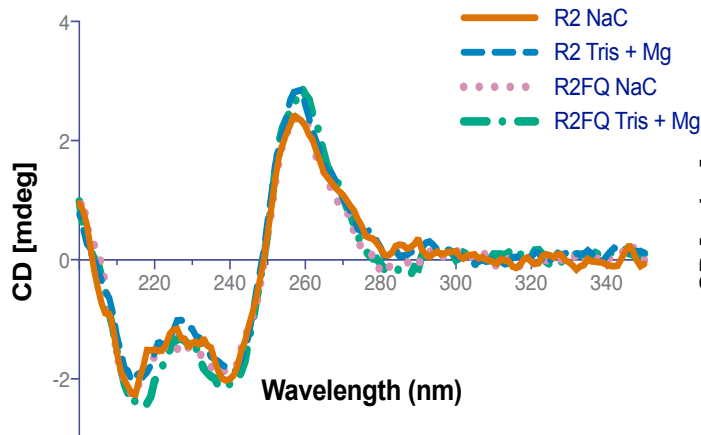
A



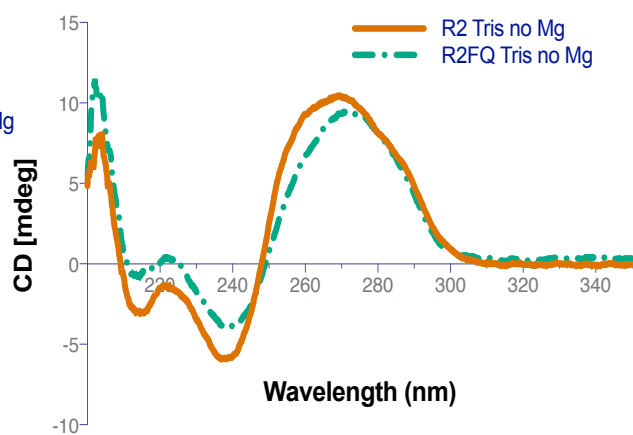
B



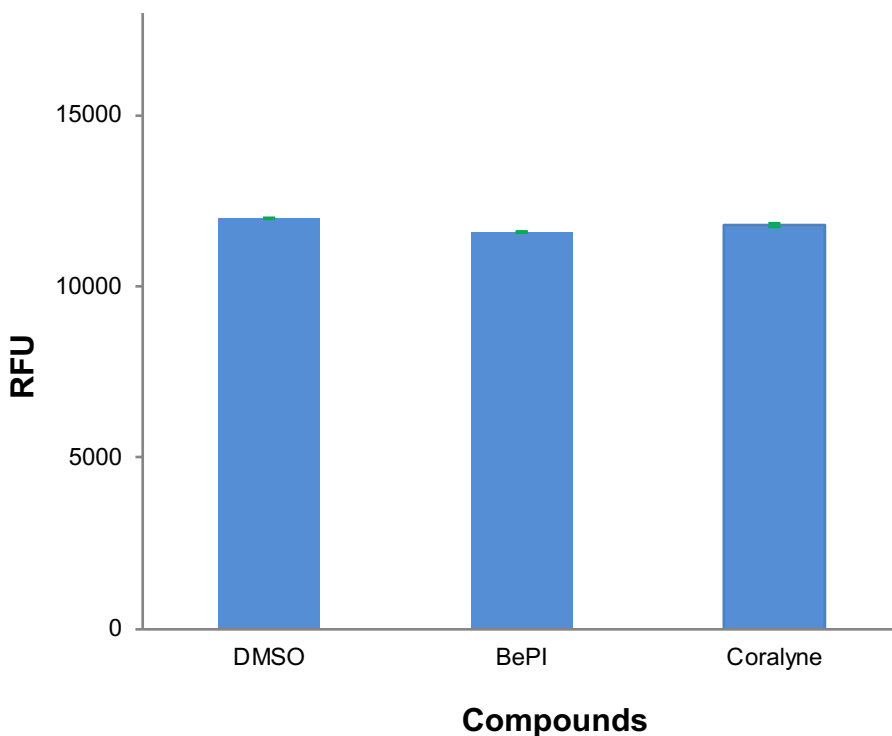
C



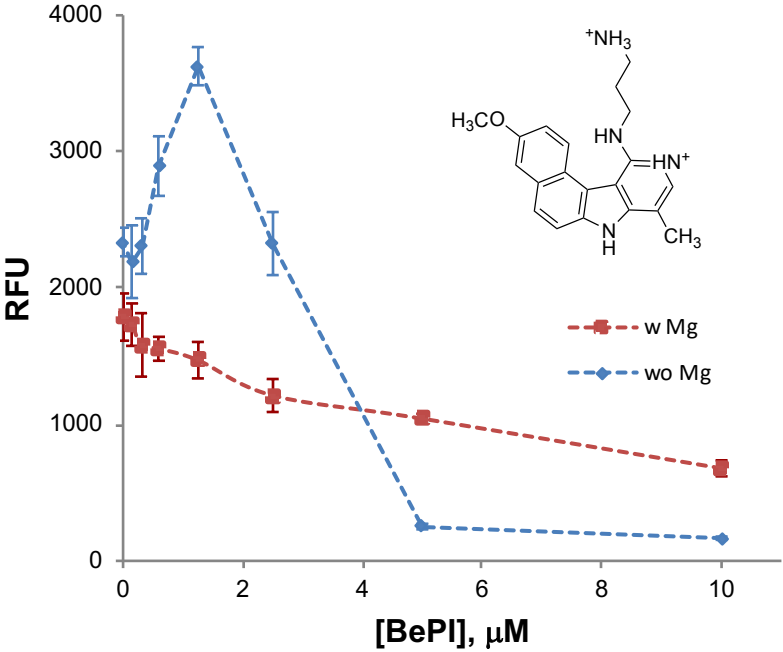
D



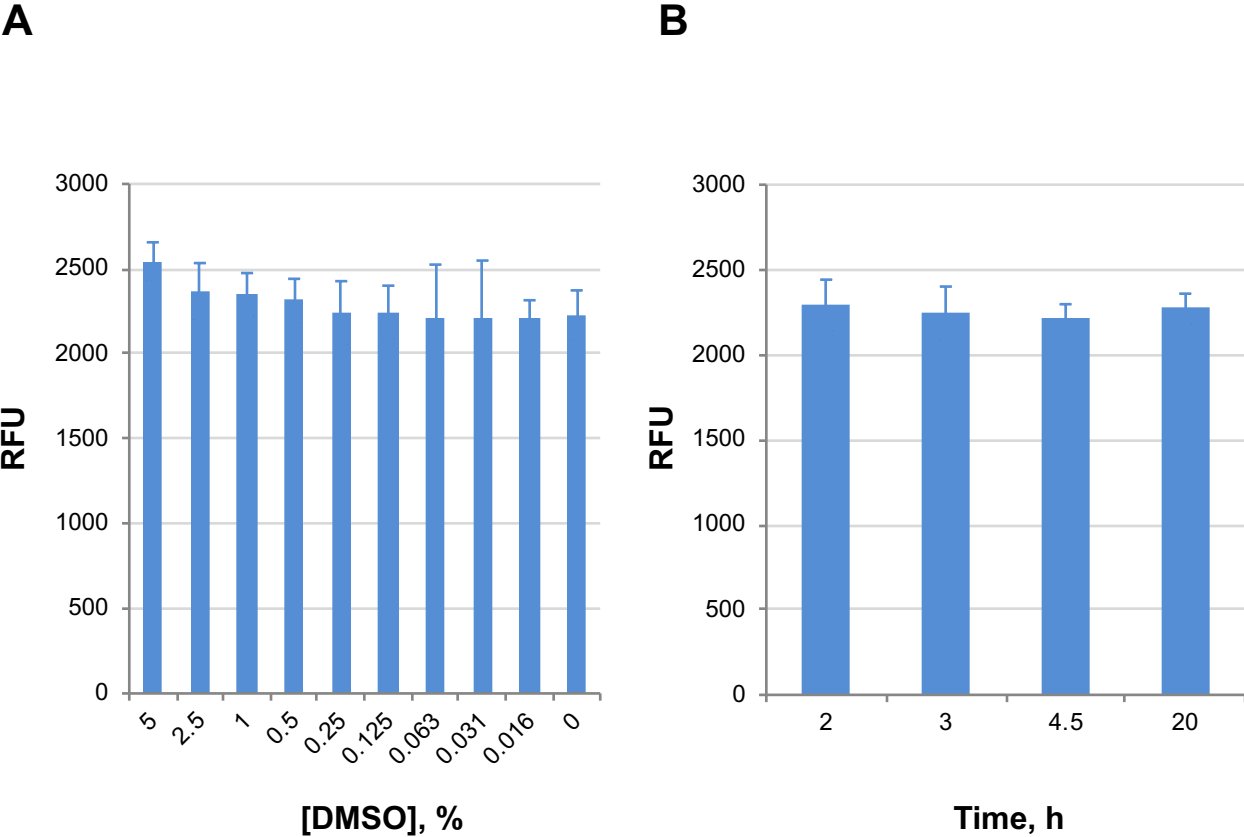
S2. FAM fluorescence is not substantially quenched by the presence of ligands used. Using Tris buffer, 5 μL of 40 nM FAM solution was added to compounds in an assay plate ($[\text{FAM}]_{\text{final}} = 20 \text{ nM}$) containing 5 μL of 2x compound solution. Final $[\text{Coralyne}]$ and $[\text{BePI}] = 7.5 \mu\text{M}$. Excitation: 495/13.5, Emission: 520/9.0



S3. Dose-dependent signal change in the presence of BePI in Tris buffer.

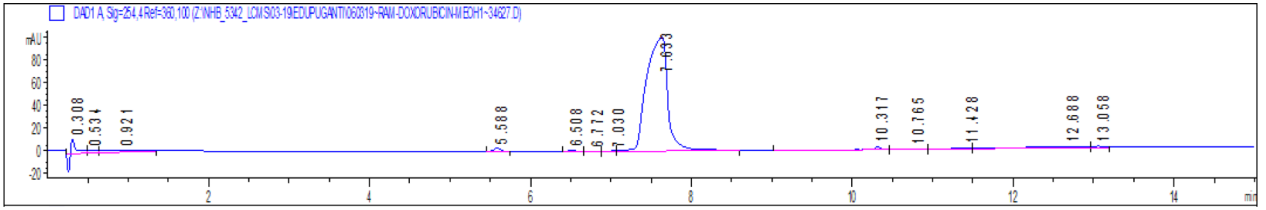


S4. R2FQ assay with regard to A) tolerance to DMSO, and B) stability at room temperature in Tris buffer.



S5. HPLC (A) and MS (B) data of Doxorubicin showing its purity over 99% and corresponding mass (M+H⁺) of m/z 544.

A



B

