

Supplementary Data 1. Compounds in the FDA-approved library used in our screening.

Compound numbers used in Fig. 2c, name, category of target molecule, and obtained MSD ratios are indicated for every compound.

#	Name	Target	Relative MSD ratio (fold)
1	Phenoxybenzamine	membrane receptor	0.75
2	Pramipexole	membrane receptor	0.6
3	Formoterol	membrane receptor	0.63
4	Mirtazapine	membrane receptor	0.83
5	Fesoterodine	membrane receptor	0.81
6	Ritodrine	membrane receptor	0.72
7	Conivaptan	membrane receptor	0.71
8	Dronedarone	membrane receptor	0.86
9	Dopamine	membrane receptor	0.87
10	Clemastine	membrane receptor	0.86
11	Xylazine	membrane receptor	0.88
12	Valsartan	membrane receptor	0.7
13	Erlotinib	membrane receptor	3.86
14	Epinephrine Bitartrate	membrane receptor	0.91
15	Atropine	membrane receptor	0.79
16	Ketotifen Fumarate	membrane receptor	0.82
17	Diphenhydramine	membrane receptor	0.41
18	Adrenaline	membrane receptor	0.91
19	Naftopidil	membrane receptor	0.73
20	Metoprolol	membrane receptor	0.55
21	Sotalol	membrane receptor	0.79
22	Nizatidine	membrane receptor	0.82
23	Aspartame	membrane receptor	0.87
24	Maraviroc	membrane receptor	0.79
25	Salbutamol	membrane receptor	0.75
26	Candesartan	membrane receptor	ND
27	Adrenaline	membrane receptor	0.74
28	Phentolamine	membrane receptor	0.82
29	Naphazoline	membrane receptor	0.83
30	Urapidil	membrane receptor	0.91
31	Scopolamine	membrane receptor	0.89
32	Levobetaxolol	membrane receptor	1.01
33	Tiotropium	membrane receptor	1.08
34	Misoprostol	membrane receptor	1.12
35	Metaproterenol Sulfate	membrane receptor	0.92
36	Mesoridazine	membrane receptor	0.66
37	Isoetharine	membrane receptor	0.45
38	Prochlorperazine	membrane receptor	0.84

39	Pindolol	membrane receptor	0.74
40	Diphenylpyraline	membrane receptor	0.85
41	Lofexidine	membrane receptor	0.9
42	Eltrombopag	membrane receptor	1.8
43	Citrate	membrane receptor	0.7
44	Anisotropine	membrane receptor	0.8
45	Pimozide	membrane receptor	0.88
46	Azelastine	membrane receptor	0.87
47	Pyrilamine	membrane receptor	0.85
48	Serotonin	membrane receptor	0.8
49	Doxylamine	membrane receptor	0.83
50	Pipenzolate	membrane receptor	0.85
51	Pilocarpine	membrane receptor	0.87
52	Bromocriptine	membrane receptor	0.91
53	Plerixafor	membrane receptor	0.9
54	Methoxamine	membrane receptor	0.98
55	Nalmefene	membrane receptor	0.9
56	Otilonium	membrane receptor	1.27
57	Aceclidine	membrane receptor	1.04
58	Mepenzolate	membrane receptor	0.97
59	Thioridazine	membrane receptor	0.87
60	Dicyclomine	membrane receptor	1.01
61	Triflupromazine	membrane receptor	0.92
62	Metaraminol	membrane receptor	0.86
63	Pheniramine	membrane receptor	1.03
64	Tolvaptan	membrane receptor	1.06
65	Moxonidine	membrane receptor	1.32
66	Carbachol	membrane receptor	0.99
67	Bismuth	membrane receptor	0.93
68	Benztropine	membrane receptor	0.92
69	Terfenadine	membrane receptor	1.08
70	Ractopamine	membrane receptor	1.06
71	Apomorphine	membrane receptor	1.21
72	Procyclidine	membrane receptor	1.07
73	Almotriptan	membrane receptor	0.85
74	Oxprenolol	membrane receptor	0.95
75	Hyoscyamine	membrane receptor	0.98
76	Desloratadine	membrane receptor	0.65
77	Acebutolol	membrane receptor	0.91
78	Mirabegron	membrane receptor	0.79
79	Rimonabant	membrane receptor	1.06
80	Cimetidine	membrane receptor	0.67
81	Betahistine	membrane receptor	0.88
82	Pazopanib	membrane receptor	1.06
83	Ticagrelor	membrane receptor	1.71
84	Propranolol	membrane receptor	0.81

85	Ipratropium	membrane receptor	0.94
86	Guanabenz Acetate	membrane receptor	0.9
87	Noradrenaline	membrane receptor	0.6
88	Tripelennamine	membrane receptor	1.1
89	Choline Chloride	membrane receptor	1.0
90	Darifenacin	membrane receptor	1.0
91	Doxofylline	membrane receptor	1.25
92	Orphenadrine	membrane receptor	1.0
93	Haloperidol	membrane receptor	0.94
94	Tropicamide	membrane receptor	1.11
95	Tolterodine	membrane receptor	0.95
96	Trospium	membrane receptor	0.96
97	Alfuzosin	membrane receptor	1.31
98	Loxapine Succinate	membrane receptor	1.03
99	Cyproheptadine	membrane receptor	0.9
100	Bismuth	membrane receptor	1.05
101	Azatadine	membrane receptor	1.25
102	Medetomidine	membrane receptor	1.12
103	Histamine	membrane receptor	0.94
104	Azilsartan	membrane receptor	0.91
105	Solifenacin	membrane receptor	1.05
106	Pergolide	membrane receptor	1.15
107	Montelukast	membrane receptor	1.23
108	Fexofenadine	membrane receptor	1.03
109	Meptazinol	membrane receptor	0.97
110	Azilsartan	membrane receptor	1.07
111	Lurasidone	membrane receptor	0.86
112	Eprosartan	membrane receptor	1.14
113	Droxidopa	membrane receptor	1.29
114	Esmolol	membrane receptor	1.01
115	Fosaprepitant	membrane receptor	0.86
116	Bepotastine	membrane receptor	1.12
117	Droperidol	membrane receptor	1.19
118	Trifluoperazine	membrane receptor	0.86
119	Ropinirole	membrane receptor	0.93
120	Antazoline	membrane receptor	0.9
121	Adrenalone	membrane receptor	0.91
122	Blonanserin	membrane receptor	0.6
123	Afatinib	membrane receptor	2.63
124	Lapatinib	membrane receptor	3.8
125	Oxybutynin	membrane receptor	0.87
126	Imatinib	membrane receptor	1.21
127	Aminophylline	membrane receptor	1.01
128	Famotidine	membrane receptor	0.91
129	Losartan	membrane receptor	0.98
130	Ramelteon	membrane receptor	0.86

131	Biperiden	membrane receptor	0.93
132	Loperamide	membrane receptor	1.03
133	Methyldopa	membrane receptor	0.67
134	Gallamine	membrane receptor	0.93
135	Cinacalcet	membrane receptor	0.54
136	Asenapine	membrane receptor	0.91
137	Aripiprazole	membrane receptor	1.06
138	Ambrisentan	membrane receptor	1.03
139	Naratriptan	membrane receptor	1.09
140	Cetirizine	membrane receptor	1.12
141	Zolmitriptan	membrane receptor	0.79
142	Pranlukast	membrane receptor	1.37
143	Nebivolol	membrane receptor	1.02
144	Carvedilol	membrane receptor	1.25
145	Meglumine	membrane receptor	0.95
146	Bethanechol	membrane receptor	0.76
147	Prasugrel	membrane receptor	1.12
148	Chlorpromazine	membrane receptor	0.69
149	Pramipexole	membrane receptor	0.88
150	Masitinib	membrane receptor	1.07
151	Iloperidone	membrane receptor	0.85
152	Vandetanib	membrane receptor	1.67
153	Ranitidine	membrane receptor	0.63
154	Crizotinib	membrane receptor	1.08
155	Clozapine	membrane receptor	0.71
156	Vismodegib	membrane receptor	0.55
157	Sunitinib	membrane receptor	ND
158	Cabozantinib	membrane receptor	1.22
159	Bimatoprost	membrane receptor	1.0
160	Acetylcholine	membrane receptor	0.76
161	Clonidine	membrane receptor	0.65
162	Trimebutine	membrane receptor	0.89
163	Axitinib	membrane receptor	1.16
164	Cilostazol	membrane receptor	0.96
165	Dexmedetomidine	membrane receptor	1.03
166	Betaxolol	membrane receptor	0.85
167	Chlorpheniramine	membrane receptor	0.79
168	Detomidine	membrane receptor	0.97
169	Aprepitant	membrane receptor	1.03
170	Naltrexone	membrane receptor	1.03
171	Levosulpiride	membrane receptor	0.97
172	Betaxolol hydrochloride	membrane receptor	1.1
173	Prazosin	membrane receptor	1.38
174	Lapatinib	membrane receptor	2.67
175	Imatinib Mesylate	membrane receptor	0.99
176	Adenine	membrane receptor	1.06

177	Quetiapine	membrane receptor	0.91
178	Ziprasidone	membrane receptor	1.03
179	Gefitinib	membrane receptor	2.82
180	Ticlopidine	membrane receptor	1.01
181	Erlotinib	membrane receptor	2.44
182	Olanzapine	membrane receptor	1.07
183	Adenine	membrane receptor	1.14
184	Olopatadine	membrane receptor	0.65
185	Dasatinib	membrane receptor	2.4
186	Zafirlukast	membrane receptor	0.85
187	Doxazosin	membrane receptor	1.29
188	Sumatriptan	membrane receptor	0.96
189	Meclizine	membrane receptor	0.67
190	Agomelatine	membrane receptor	0.96
191	Oxymetazoline	membrane receptor	0.8
192	Chlorprothixene	membrane receptor	0.96
193	Alprostadil	membrane receptor	0.84
194	Irbesartan	membrane receptor	0.82
195	Adenine	membrane receptor	1.08
196	Domperidone	membrane receptor	0.97
197	Mizolastine	membrane receptor	1.05
198	Dyphylline	membrane receptor	0.95
199	Pazopanib	membrane receptor	1.02
200	Amisulpride	membrane receptor	0.98
201	Amiodarone	membrane receptor	1.31
202	Tizanidine	membrane receptor	0.98
203	Clopidogrel	membrane receptor	0.81
204	Rocuronium	membrane receptor	0.87
205	Methscopolamine	membrane receptor	0.86
206	Nilotinib	membrane receptor	1.86
207	Adenosine	membrane receptor	0.89
208	Lonidamine	enzyme	1.42
209	Uridine	enzyme	0.59
210	Methimazole	enzyme	0.81
211	Diclofenac	enzyme	0.97
212	Ibandronate	enzyme	0.93
213	Ketorolac	enzyme	0.7
214	Acarbose	enzyme	0.7
215	Ketoprofen	enzyme	0.64
216	Uracil	enzyme	0.84
217	Celecoxib	enzyme	0.78
218	Moclobemide	enzyme	1.03
219	Ibuprofen	enzyme	1.02
220	Carfilzomib	enzyme	0.94
221	Cobicistat	enzyme	0.76
222	Diclofenac	enzyme	0.8

223	Etodolac	enzyme	0.88
224	Ampiroxicam	enzyme	0.94
225	Rosuvastatin	enzyme	1.03
226	Dichlorphenamide	enzyme	1.14
227	Rasagiline	enzyme	1.43
228	Benzydamine	enzyme	1.01
229	Anisindione	enzyme	0.85
230	Perindopril	enzyme	0.85
231	Gemcitabine	enzyme	0.93
232	Sulindac	enzyme	0.9
233	Temocapril	enzyme	0.99
234	Sildenafil	enzyme	0.76
235	Capecitabine	enzyme	1.0
236	Tenoxicam	enzyme	0.77
237	Sodium salicylate	enzyme	1.01
238	Tadalafil	enzyme	0.92
239	Rolipram	enzyme	0.83
240	Cyclosporine	enzyme	0.86
241	Vardenafil	enzyme	0.92
242	Oxaprozin	enzyme	1.0
243	Methylthiouracil	enzyme	1.03
244	Mitoxantrone	enzyme	0.9
245	Risedronate	enzyme	0.84
246	Rofecoxib	enzyme	1.14
247	Roflumilast	enzyme	0.45
248	Leflunomide	enzyme	0.92
249	Allopurinol	enzyme	0.92
250	Zaltoprofen	enzyme	0.82
251	Irinotecan	enzyme	0.87
252	Dipyridamole	enzyme	ND
253	Linagliptin	enzyme	0.89
254	Topotecan	enzyme	0.97
255	Orlistat	enzyme	0.84
256	Fenoprofen	enzyme	0.97
257	Ibuprofen	enzyme	1.0
258	Nepafenac	enzyme	1.0
259	Bufexamac	enzyme	0.86
260	Rivastigmine	enzyme	0.85
261	Pitavastatin	enzyme	1.19
262	Hydroxyurea	enzyme	0.88
263	Anagrelide	enzyme	1.1
264	Esomeprazole	enzyme	1.02
265	Carbidopa	enzyme	0.84
266	Fosinopril	enzyme	0.81
267	Triflusal	enzyme	0.88
268	Finasteride	enzyme	1.22

269	Pimobendan	enzyme	1.55
270	Irinotecan	enzyme	0.91
271	Cladribine	enzyme	0.99
272	Voglibose	enzyme	0.94
273	Dabigatran	enzyme	0.82
274	Rivaroxaban	enzyme	0.89
275	Aliskiren	enzyme	0.73
276	TAME	enzyme	0.92
277	Dexlansoprazole	enzyme	1.09
278	Alendronate	enzyme	0.93
279	Pranoprofen	enzyme	0.8
280	Pravastatin	enzyme	0.95
281	Mefenamic	enzyme	0.65
282	Naproxen	enzyme	0.95
283	Daunorubicin	enzyme	1.99
284	Tolfenamic	enzyme	0.77
285	Exemestane	enzyme	1.0
286	Tranexamic	enzyme	0.81
287	Gabexate	enzyme	0.9
288	Mofetil	enzyme	0.84
289	Aspirin	enzyme	1.01
290	Benazepril	enzyme	0.86
291	Phenylbutazone	enzyme	0.66
292	Imidapril	enzyme	0.93
293	Cytidine	enzyme	1.05
294	Enalaprilat	enzyme	0.91
295	Tacrine	enzyme	1.0
296	Simvastatin	enzyme	0.98
297	Racecadotril	enzyme	0.7
298	Atorvastatin	enzyme	1.14
299	Carmofur	enzyme	0.99
300	Lisinopril	enzyme	0.82
301	Phenindione	enzyme	1.13
302	Neostigmine	enzyme	0.83
303	Avanafil	enzyme	1.05
304	Pemetrexed	enzyme	1.06
305	Nimesulide	enzyme	0.76
306	Ramipril	enzyme	0.71
307	Physostigmine	enzyme	0.91
308	Moexipril	enzyme	0.74
309	Captopril	enzyme	0.86
310	Bortezomib	enzyme	1.41
311	Glycyrrhizinate	enzyme	0.88
312	Dabigatran	enzyme	1.24
313	Cilazapril	enzyme	0.93
314	Enalapril	enzyme	0.65

315	Fluvastatin	enzyme	1.16
316	Propylthiouracil	enzyme	0.62
317	Zileuton	enzyme	0.97
318	Ozagrel	enzyme	0.64
319	Abiraterone	enzyme	0.89
320	Doxifluridine	enzyme	0.91
321	Lornoxicam	enzyme	0.93
322	Donepezil	enzyme	0.75
323	Esomeprazole	enzyme	0.83
324	Carbenoxolone	enzyme	0.92
325	Tolmetin	enzyme	1.0
326	Physostigmine	enzyme	0.88
327	Amfenac	enzyme	0.95
328	Benserazide	enzyme	0.91
329	Teniposide	enzyme	0.83
330	Floxuridine	enzyme	0.74
331	Valdecixib	enzyme	1.01
332	Nabumetone	enzyme	1.04
333	Aminocaproic	enzyme	0.91
334	Tegafur	enzyme	0.77
335	Aminoglutethimide	enzyme	1.06
336	Ethoxzolamide	enzyme	0.8
337	Diclofenac	enzyme	0.75
338	Thioguanine	enzyme	0.82
339	Risedronic	enzyme	0.84
340	Mercaptopurine	enzyme	0.66
341	Acemetacin	enzyme	1.02
342	Pamidronate	enzyme	0.94
343	Flurbiprofen	enzyme	1.02
344	Disulfiram	enzyme	0.61
345	Zoledronic	enzyme	0.87
346	Epalrestat	enzyme	1.12
347	Abiraterone	enzyme	0.67
348	Rolipram	enzyme	0.93
349	Carbimazole	enzyme	1.0
350	Brinzolamide	enzyme	0.92
351	Ozagrel	enzyme	0.83
352	Vorinostat	enzyme	1.01
353	Thiouracil	enzyme	0.85
354	Argatroban	enzyme	0.93
355	Pimecrolimus	enzyme	0.78
356	Gimeracil	enzyme	1.06
357	Fludarabine	enzyme	0.79
358	Mycophenolic	enzyme	0.96
359	Tacrolimus	enzyme	0.88
360	Pralatrexate	enzyme	0.82

361	Azacitidine	enzyme	0.79
362	Nialamide	enzyme	0.98
363	Benzoic	ion channel	1.03
364	Amantadine	ion channel	0.94
365	Triamterene	ion channel	0.8
366	Vecuronium	ion channel	0.98
367	Amlodipine	ion channel	0.92
368	Nifedipine	ion channel	0.74
369	Memantine	ion channel	0.83
370	Rufinamide	ion channel	0.99
371	Articaine	ion channel	0.81
372	Flunarizine	ion channel	0.91
373	Gluconate	ion channel	0.88
374	Clevidipine	ion channel	0.75
375	Hexamethonium	ion channel	0.82
376	Nicardipine	ion channel	1.08
377	Phenytoin	ion channel	0.9
378	Tropisetron	ion channel	0.77
379	Ivabradine	ion channel	0.85
380	Mepivacaine	ion channel	0.91
381	Gabapentin	ion channel	0.99
382	Niflumic	ion channel	0.72
383	Oxybuprocaine	ion channel	0.94
384	Valproic	ion channel	1.03
385	Proparacaine	ion channel	1.01
386	Topiramate	ion channel	0.81
387	Atracurium	ion channel	0.96
388	Disopyramide	ion channel	0.72
389	Quipazine	ion channel	0.81
390	Azasetron	ion channel	0.84
391	Cilnidipine	ion channel	0.91
392	Diltiazem	ion channel	0.62
393	Oxethazaine	ion channel	0.95
394	Nitrendipine	ion channel	1.27
395	Isradipine	ion channel	0.89
396	Dofetilide	ion channel	0.82
397	Bupivacaine	ion channel	1.01
398	Ondansetron	ion channel	0.75
399	Propafenone	ion channel	0.77
400	ATP	ion channel	0.8
401	Phenytoin	ion channel	1.05
402	Lacidipine	ion channel	1.04
403	Ibutilide	ion channel	0.7
404	Zonisamide	ion channel	0.69
405	Pancuronium	ion channel	0.77
406	Varenicline	ion channel	1.45

407	Cisatracurium	ion channel	0.78
408	Etomidate	ion channel	0.94
409	Mexiletine	ion channel	1.03
410	Gabapentin	ion channel	0.86
411	Benidipine	ion channel	1
412	Lomerizine	ion channel	0.93
413	Amiloride	ion channel	0.68
414	Nisoldipine	ion channel	0.88
415	Amlodipine	ion channel	0.76
416	Nimodipine	ion channel	0.96
417	Nicotinic	ion channel	0.88
418	Lamotrigine	ion channel	1.04
419	Pramoxine	ion channel	0.92
420	Divalproex	ion channel	1.04
421	Felodipine	ion channel	1.15
422	Felbamate	ion channel	0.96
423	Benzocaine	ion channel	1.14
424	Ropivacaine	ion channel	0.99
425	Manidipine	ion channel	1.07
426	Carbamazepine	ion channel	1.02
427	Palonosetron	ion channel	0.99
428	Azelinidipine	ion channel	0.72
429	Flumazenil	ion channel	1.02
430	Vitamin D3	nuclear receptor	1.03
431	Dichlorisone	nuclear receptor	0.73
432	Toremifene	nuclear receptor	0.82
433	Fluorometholone	nuclear receptor	0.65
434	Ethisterone	nuclear receptor	1.13
435	Fluocinonide	nuclear receptor	0.98
436	Adapalene	nuclear receptor	0.87
437	Flutamide	nuclear receptor	0.97
438	Hydrocortisone	nuclear receptor	0.91
439	Medrysone	nuclear receptor	0.73
440	Betamethasone	nuclear receptor	1.07
441	Ursodiol	nuclear receptor	0.63
442	Desonide	nuclear receptor	0.97
443	Loteprednol	nuclear receptor	0.91
444	Rosiglitazone	nuclear receptor	0.95
445	Ethinodiol	nuclear receptor	0.95
446	Pioglitazone	nuclear receptor	0.86
447	Estradiol valerate	nuclear receptor	1.09
448	Mifepristone	nuclear receptor	1.1
449	Spirolactone	nuclear receptor	1.03
450	Fenofibrate	nuclear receptor	0.83
451	Betamethasone	nuclear receptor	0.93
452	Megestrol	nuclear receptor	0.88

453	Meprednisone	nuclear receptor	0.93
454	Canrenoate	nuclear receptor	1.08
455	Liothyronine	nuclear receptor	0.96
456	Tiratricol	nuclear receptor	0.8
457	Estrone	nuclear receptor	0.89
458	Fluticasone	nuclear receptor	1.76
459	Budesonide	nuclear receptor	0.92
460	Fulvestrant	nuclear receptor	0.97
461	Tamoxifen	nuclear receptor	0.88
462	Bexarotene	nuclear receptor	1.08
463	Dexamethasone	nuclear receptor	0.86
464	Oxymetholone	nuclear receptor	0.98
465	Tazarotene	nuclear receptor	1.19
466	Flumethasone	nuclear receptor	1.04
467	Bazedoxifene	nuclear receptor	0.95
468	Halobetasol Propionate	nuclear receptor	1.09
469	Diethylstilbestrol	nuclear receptor	0.82
470	Mestranol	nuclear receptor	0.85
471	Dydrogesterone	nuclear receptor	0.79
472	Estradiol	nuclear receptor	0.85
473	Rosiglitazone	nuclear receptor	0.91
474	butyrate	nuclear receptor	0.71
475	Difluprednate	nuclear receptor	1.02
476	Mometasone	nuclear receptor	0.73
477	Triamcinolone	nuclear receptor	0.89
478	Deflazacort	nuclear receptor	0.7
479	Fluocinolone	nuclear receptor	0.96
480	Tretinoin	nuclear receptor	0.95
481	Calcitriol	nuclear receptor	1.39
482	Dexamethasone	nuclear receptor	1.01
483	Doxercalciferol	nuclear receptor	1.45
484	Estriol	nuclear receptor	0.75
485	Altrenogest	nuclear receptor	0.8
486	Betamethasone	nuclear receptor	0.9
487	Calcifediol	nuclear receptor	1.17
488	Alfacalcidol	nuclear receptor	0.87
489	Clofibrate	nuclear receptor	0.87
490	Triamcinolone	nuclear receptor	0.9
491	Nateglinide	transporter	1.03
492	Reboxetine	transporter	0.81
493	Imipramine	transporter	1.06
494	Gliclazide	transporter	0.91
495	Bendroflumethiazide	transporter	0.86
496	Amitriptyline	transporter	1.04
497	Benzthiazide	transporter	1.06
498	Ivacaftor	transporter	ND

499	Methyclothiazide	transporter	0.94
500	Indapamide	transporter	0.84
501	Venlafaxine	transporter	1.04
502	Sertraline	transporter	1.06
503	Tolbutamide	transporter	1.01
504	Mitiglinide	transporter	0.91
505	Repaglinide	transporter	1.02
506	Dapoxetine	transporter	0.83
507	Gliquidone	transporter	1.26
508	Duloxetine	transporter	0.74
509	Torsemide	transporter	0.96
510	Chlorothiazide	transporter	0.96
511	Paroxetine	transporter	0.55
512	Trimipramine	transporter	0.44
513	Fluvoxamine	transporter	0.96
514	Trichlormethiazide	transporter	0.9
515	Glipizide	transporter	0.88
516	Benzbromarone	transporter	1.0
517	Clomipramine	transporter	0.9
518	Tolazamide	transporter	0.96
519	Bumetanide	transporter	0.92
520	Amoxapine	transporter	0.86
521	Ezetimibe	transporter	1.17
522	Guanethidine	transporter	0.84
523	Nicorandil	transporter	1.09
524	Nomifensine	transporter	0.89
525	Maprotiline	transporter	0.78
526	Meticrane	transporter	0.8
527	Atomoxetine	transporter	0.89
528	Milnacipran	transporter	1.01
529	Pinacidil	transporter	0.94
530	Chlorpropamide	transporter	1.07
531	Fluoxetine	transporter	0.93
532	Everolimus	non-receptor kinase	1.07
533	Sorafenib	non-receptor kinase	1.48
534	Vemurafenib	non-receptor kinase	1.0
535	Phenformin	non-receptor kinase	0.94
536	Ponatinib	non-receptor kinase	1.78
537	Ibrutinib	non-receptor kinase	2.17
538	Regorafenib	non-receptor kinase	1.68
539	Metformin	non-receptor kinase	0.75
540	Dabrafenib	non-receptor kinase	0.77
541	Temsirolimus	non-receptor kinase	0.7
542	Thalidomide	cytokine	0.98
543	Pomalidomide	cytokine	1.12
544	Lenalidomide	cytokine	0.76

545	Bindarit	cytokine	1.0
546	Sulfanilamide	other	0.86
547	Edaravone	other	0.88
548	Methoxyestradiol	other	0.94
549	Cyclamic	other	1.07
550	Lithocholic	other	0.87
551	Emtricitabine	other	1.26
552	Genistein	other	0.97
553	Valnemulin	other	1.08
554	Monofluorophosphate	other	0.82
555	Ethambutol	other	1.0
556	Leucovorin	other	0.79
557	Gatifloxacin	other	1.07
558	Temozolomide	other	0.96
559	Sulfasalazine	other	1.29
560	Ouabain	other	0.64
561	Clofibrilic	other	0.91
562	Nitazoxanide	other	1
563	Azaperone	other	0.61
564	Nithiamide	other	0.65
565	Allylthiourea	other	0.86
566	Cysteamine	other	0.85
567	Zoxazolamine	other	0.93
568	Phenazopyridine	other	0.72
569	Penciclovir	other	0.95
570	Vincristine	other	0.94
571	Clinafloxacin	other	0.67
572	Natamycin	other	0.93
573	Ritonavir	other	1.04
574	Alverine Citrate	other	0.72
575	Didanosine	other	1.04
576	Besifloxacin	other	0.98
577	Amidopyrine	other	1.28
578	Triclabendazole	other	0.61
579	Dicloxacillin	other	0.98
580	Vinorelbine	other	1.15
581	Chlorocresol	other	1.13
582	Telaprevir	other	0.99
583	Isovaleramide	other	1.04
584	Danofloxacin	other	0.68
585	Sulconazole	other	0.7
586	Enrofloxacin	other	0.68
587	Tilmicosin	other	0.92
588	Ethionamide	other	0.95
589	Thiamine	other	0.91
590	Troxipide	other	0.96

591	Fluconazole	other	1.03
592	Ellagic	other	1.08
593	Fidaxomicin	other	0.97
594	Clodronate	other	1.04
595	Minocycline	other	0.9
596	Diminazene	other	1.19
597	Cinepazide	other	1.11
598	Sucralose	other	0.99
599	Praziquantel	other	1.01
600	Mevastatin	other	0.64
601	Suprofen	other	1.01
602	Doxycycline	other	0.77
603	Dirithromycin	other	1.03
604	Pemirolast	other	0.63
605	Ranolazine	other	0.91
606	Busulfan	other	0.97
607	Cisplatin	other	0.83
608	Dibenzepine	other	0.78
609	Cepharanthine	other	0.83
610	Phenacetin	other	0.87
611	Spectinomycin	other	0.94
612	Thonzonium	other	1.05
613	Thiostrepton	other	0.97
614	Camptothecin	other	1.07
615	Rolitetracycline	other	0.96
616	Rapamycin	other	0.94
617	Oxeladin	other	0.99
618	Carbadox	other	1.04
619	Piromidic	other	1.06
620	Deoxyarbutin	other	0.9
621	Monobenzene	other	0.78
622	Clindamycin	other	0.99
623	Pantothenic acid	other	0.95
624	Cephalomannine	other	0.95
625	Sarafloxacin	other	0.95
626	Pentoxifylline	other	0.95
627	Moxalactam	other	1.05
628	Camylofin	other	0.9
629	Benfotiamine	other	0.65
630	Methapyrilene	other	0.43
631	Clofazimine	other	1.1
632	Pentamidine	other	1.13
633	Cefaclor	other	0.84
634	Amoxicillin	other	1.05
635	Artemisinin	other	0.92
636	Telbivudine	other	0.93

637	Aniracetam	other	0.79
638	Catharanthine	other	0.99
639	Tranilast	other	1.76
640	Buflomedil	other	1.14
641	Lomefloxacin	other	1.01
642	Moroxydine	other	0.88
643	Ginkgolide	other	1.05
644	Metrizamide	other	1.06
645	Methylhydantoin	other	1.1
646	Voriconazole	other	0.99
647	Pridinol Methanesulfonate	other	1.01
648	Tioconazole	other	0.96
649	Penicillin	other	0.91
650	Flumequine	other	1.08
651	Atazanavir	other	0.83
652	Ofloxacin	other	0.85
653	Fenbendazole	other	1.14
654	Dextrose	other	0.92
655	Marbofloxacin	other	0.82
656	Pyrimethamine	other	0.93
657	Suxibuzone	other	0.87
658	Phthalylsulfacetamide	other	0.92
659	Phenothrin	other	0.91
660	Noscapine	other	0.94
661	Glafenine	other	1.5
662	Cinoxacin	other	0.86
663	aminohippurate Hydrate	other	0.87
664	Primaquine	other	0.91
665	Mepiroxol	other	0.94
666	Hemicholinium	other	0.86
667	Clofocetol	other	1.09
668	Cephapirin	other	0.89
669	Glucaptate	other	0.89
670	Butacaine	other	0.71
671	Auranofin	other	2.62
672	Aztreonam	other	0.85
673	Aminoacridine	other	0.93
674	Docetaxel	other	0.66
675	Alexidine	other	ND
676	Ethacridine	other	0.99
677	Potassium Iodide	other	0.86
678	Digoxigenin	other	0.89
679	Guanidine	other	0.88
680	Bentiromide	other	0.85
681	Fosfomycin	other	0.64
682	Difloxacin	other	0.89

683	Bekanamycin	other	0.83
684	Paclitaxel	other	0.85
685	Proadifen	other	0.81
686	ascorbate	other	0.99
687	Deoxycorticosterone	other	0.81
688	Cetrimonium Bromide	other	1.89
689	Norfloxacin	other	0.97
690	Bergapten	other	0.98
691	Bephenium	other	0.79
692	Diperodon	other	0.77
693	Isoxicam	other	0.72
694	Malotilate	other	0.87
695	Famprofazone	other	0.82
696	Piperacillin	other	0.98
697	Ifosfamide	other	0.77
698	Spiramycin	other	0.75
699	Phosphatidylcholine	other	0.51
700	Procodazole	other	0.94
701	Amorolfine	other	0.85
702	Chloramphenicol	other	0.83
703	Picrotoxinin	other	0.72
704	Pasiniazid	other	0.96
705	Sulbactam	other	0.48
706	Emetine	other	0.67
707	Streptozotocin	other	0.66
708	Mesalamine	other	0.76
709	Dimaprit	other	0.81
710	Dibenzothiophene	other	0.95
711	Colistimethate	other	0.79
712	Clorgyline	other	0.86
713	Clopamide	other	0.56
714	Hydrastinine	other	0.99
715	Clinafoxacin	other	0.95
716	Chromocarb	other	0.93
717	Ceftazidime	other	0.83
718	Nifenazone	other	1.02
719	Cephalexin	other	0.93
720	Meclocycline	other	0.65
721	Isosorbide	other	0.86
722	Azaguanine	other	1.12
723	Furaltadone	other	0.82
724	Ceftiofur	other	1.03
725	Resveratrol	other	0.72
726	Clindamycin	other	0.71
727	Levofloxacin	other	0.75
728	Riboflavin	other	ND

729	Dyclonine	other	0.92
730	Sorbitol	other	0.92
731	carnitine	other	1.07
732	Mannitol	other	0.72
733	Metronidazole	other	0.92
734	Menadione	other	0.82
735	Nalidixic acid	other	0.97
736	Cefprozil	other	0.93
737	Avobenzone	other	1.03
738	Artemether	other	1.15
739	Talc	other	0.97
740	Methoxsalen	other	0.76
741	Nicotinamide	other	0.88
742	Miconazole	other	0.73
743	Acetanilide	other	0.79
744	Sulfamethizole	other	0.87
745	Secnidazole	other	0.84
746	Famciclovir	other	0.95
747	Miconazole	other	0.65
748	Econazole nitrate	other	0.73
749	Adiphenine	other	0.86
750	Carnitine	other	0.78
751	Isoconazole	other	0.75
752	Scopine	other	1.0
753	Isoniazid	other	0.69
754	Clindamycin	other	1.06
755	Bisacodyl	other	0.97
756	Pramiracetam	other	1.03
757	Clarithromycin	other	1.09
758	Vidarabine	other	0.78
759	Aminolevulinic	other	1.48
760	Azacyclonol	other	0.81
761	Irsogladine	other	1.23
762	Amfebutamone	other	1.18
763	Alibendol	other	1.12
764	Mecarbinat	other	1.14
765	Moxifloxacin	other	0.98
766	Clindamycin	other	0.83
767	Rifaximin	other	0.98
768	Geniposidic	other	0.93
769	Sulfisoxazole	other	1.15
770	Genipin	other	1.07
771	Sulfamethoxazole	other	0.99
772	Geniposide	other	1.0
773	Pregnenolone	other	0.99
774	Paeoniflorin	other	0.9

775	Deacetylbaecatin	other	0.85
776	Cromoglycate	other	0.94
777	Sulbactam	other	0.81
778	Oxytetracycline	other	1.07
779	Nystatin	other	0.88
780	Crystal Violet	other	ND
781	Rebamipide	other	0.77
782	Acadesine	other	0.82
783	Fenticonazole	other	0.63
784	Azithromycin	other	1.72
785	Albendazole	other	0.99
786	Flunixin	other	0.99
787	Etidronate	other	0.73
788	Xylose	other	0.71
789	Raltegravir	other	0.79
790	Elvitegravir	other	0.87
791	Roxithromycin	other	0.8
792	orthovanadate	other	0.91
793	Ribavirin	other	0.78
794	Cycloserine	other	0.68
795	Liranaftate	other	0.68
796	Fudosteine	other	0.7
797	Quinine	other	0.66
798	Procarbazine	other	0.79
799	Licofelone	other	0.78
800	Bifonazole	other	0.61
801	Arbidol	other	1.07
802	Penicillamine	other	0.83
803	Probucol	other	0.71
804	Oxibendazole	other	0.9
805	Daidzein	other	0.71
806	Curcumin	other	1.76
807	Chloroxine	other	1.16
808	Vinpocetine	other	0.67
809	Lomustine	other	0.69
810	Novobiocin	other	1.1
811	Butoconazole	other	0.7
812	Valaciclovir	other	0.5
813	Oxfendazole	other	1.25
814	Ciclopirox	other	0.81
815	Methacycline	other	0.8
816	Lopinavir	other	1.06
817	Acipimox	other	0.92
818	Ciprofloxacin	other	0.84
819	Aciclovir	other	0.81
820	DAPT	other	0.73

821	Fleroxacin	other	0.87
822	Sulphadimethoxine	other	0.83
823	Rimantadine	other	1.2
824	Sparfloxacin	other	1.01
825	Primidone	other	0.87
826	Idoxuridine	other	1.1
827	Pivoxil	other	0.96
828	Protionamide	other	0.71
829	Itraconazole	other	1.21
830	Nefiracetam	other	0.92
831	Lincomycin	other	0.85
832	Chlormezanone	other	1.0
833	Cidofovir	other	0.89
834	Erdosteine	other	0.96
835	Suplatast	other	0.84
836	Tobramycin	other	0.79
837	Taurine	other	1.29
838	Sulfadoxine	other	1.16
839	Sitafloracin	other	0.77
840	Ganciclovir	other	0.83
841	Trifluridine	other	0.68
842	Oseltamivir	other	1.02
843	Verteporfin	other	ND
844	Valganciclovir	other	0.88
845	Cyclandelate	other	1.01
846	Antipyrine	other	0.84
847	Sasapyrine	other	0.96
848	Enoxacin	other	0.89
849	Salicylanilide	other	0.87
850	Ampicillin	other	0.91
851	Domiphen	other	1.22
852	Abacavir	other	0.68
853	Sulfacetamide	other	0.9
854	Amoxicillin	other	0.91
855	Linezolid	other	0.93
856	Rifapentine	other	1.2
857	L-Arginine	other	1.02
858	Amprenavir	other	0.99
859	Zanamivir	other	0.59
860	Mequinol	other	0.64
861	Albendazole	other	1.12
862	L-Thyroxine	other	1.11
863	Carbazochrome	other	0.93
864	Flucytosine	other	0.62
865	Hygromycin	other	0.71
866	Aminosaliclate	other	0.7

867	Decamethonium	other	0.87
868	Paromomycin Sulfate	other	0.88
869	Tylosin tartrate	other	0.98
870	Nifuroxazide	other	0.85
871	Posaconazole	other	1.21
872	Sertaconazole	other	0.62
873	Cinchophen	other	0.96
874	Chlorquinaldol	other	0.97
875	Azlocillin	other	0.88
876	Florfenicol	other	0.73
877	Tolperisone	other	0.85
878	Octopamine	other	0.72
879	Vinblastine	other	1.13
880	Aminothiazole	other	0.91
881	Bemegride	other	1.05
882	Carboplatin	other	0.98
883	Erythromycin	other	1.04
884	Amphotericin	other	0.96
885	Niclosamide	other	0.91
886	Fenspiride	other	1.04
887	Betamipron	other	1.0
888	PMSF	other	1.0
889	Teicoplanin	other	0.88
890	Cabazitaxel	other	1.0
891	Tenofovir	other	0.83
892	Tenofovir	other	1.02
893	Glutamine	other	0.85
894	Ciclopirox	other	0.78
895	Tigecycline	other	0.88
896	Gadodiamide	other	0.95
897	Broxyquinoline	other	1.44
898	Carbenicillin	other	0.98
899	Chenodeoxycholic	other	0.74
900	Entecavir Hydrate	other	0.86
901	Stavudine	other	0.98
902	Nefopam	other	0.86
903	Hexadecanol	other	0.97
904	Naftifine	other	1.0
905	Sulfadiazine	other	0.76
906	Dehydroepiandrosterone	other	1.04
907	Idebenone	other	1.2
908	Erythromycin	other	1.06
909	Retapamulin	other	1.0
910	Trimethoprim	other	1.01
911	Oxytetracycline	other	0.99
912	Ranolazine	other	0.81

913	Cytarabine	other	1.14
914	Ronidazole	other	1.13
915	Cetylpyridinium	other	1.41
916	Carotene	other	0.87
917	Coumarin	other	0.97
918	Biotin	other	1.0
919	Pefloxacin Mesylate	other	0.96
920	Methenamine	other	1.03
921	Cyromazine	other	0.96
922	Benzethonium	other	1.82
923	Cefditoren	other	0.84
924	Sulfamerazine	other	1.02
925	Rifampin	other	0.84
926	Clorsulon	other	1.1
927	Sulfamethazine	other	0.96
928	Nitrofur	other	0.69
929	Sulfaguanidine	other	1.08
930	Trometamol	other	1.0
931	Tianeptine	other	0.82
932	Deferiprone	other	0.8
933	Netilmicin	other	0.99
934	Pyrazinamide	other	0.93
935	Tinidazole	other	0.8
936	Peramivir	other	1.23
937	Climbazole	other	0.92
938	Dequalinium	other	1.29
939	Tioxolone	other	1.08
940	Mezlocillin	other	0.95
941	Arecoline	other	1.0
942	Butenafine	other	1.16

Compounds in plates with the Z'-factor below the threshold.

#	Name	Target
1	Sildenafil	membrane receptor
2	Pizotifen	membrane receptor
3	Fumarate	membrane receptor
4	Clorprenaline	membrane receptor
5	Naloxone	membrane receptor
6	Brompheniramine	membrane receptor
7	Mianserin	membrane receptor
8	Telmisartan	membrane receptor
9	Mosapride	membrane receptor
10	Risperidone	membrane receptor
11	Methylsulfate	membrane receptor
12	Trazodone	membrane receptor

13	Homatropine	membrane receptor
14	Melatonin	membrane receptor
15	Bisoprolol fumarate	membrane receptor
16	Olmesartan	membrane receptor
17	Imiquimod	membrane receptor
18	Hydroxyzine	membrane receptor
19	Indacaterol	membrane receptor
20	Dexmedetomidine	membrane receptor
21	Rizatriptan	membrane receptor
22	Phenylephrine	membrane receptor
23	Candesartan	membrane receptor
24	Oxybutynin	membrane receptor
25	Isoprenaline	membrane receptor
26	Lafutidine	membrane receptor
27	Acidinium	membrane receptor
28	baclofen	membrane receptor
29	Paliperidone	membrane receptor
30	Tetrahydrozoline	membrane receptor
31	Levodopa	membrane receptor
32	Roxatidine	membrane receptor
33	Terazosin	membrane receptor
34	Xylometazoline	membrane receptor
35	Loratadine	membrane receptor
36	Fludarabine	enzyme
37	Doxorubicin	enzyme
38	Indomethacin	enzyme
39	Fluorouracil	enzyme
40	Methotrexate	enzyme
41	Clofarabine	enzyme
42	Methazolamide	enzyme
43	Idarubicin	enzyme
44	Apixaban	enzyme
45	Quinapril	enzyme
46	Pyridostigmine	enzyme
47	Lovastatin	enzyme
48	Tolcapone	enzyme
49	Decitabine	enzyme
50	Epirubicin	enzyme
51	Hydralazine	enzyme
52	Dexrazoxane	enzyme
53	Etoposide	enzyme
54	Ubenimex	enzyme
55	Flavoxate	enzyme
56	Dorzolamide	enzyme
57	Mitotane	enzyme
58	Dutasteride	enzyme

59	Gemcitabine	enzyme
60	Fenoprofen	enzyme
61	Piroxicam	enzyme
62	Miglitol	enzyme
63	Omeprazole	enzyme
64	Carprofen	enzyme
65	Mizoribine	enzyme
66	Ketoconazole	enzyme
67	Lansoprazole	enzyme
68	Meloxicam	enzyme
69	Riluzole	ion channel
70	Granisetron	ion channel
71	Penfluridol	ion channel
72	Oxcarbazepine	ion channel
73	Procaine	ion channel
74	Prilocaine	ion channel
75	Dibucaine	ion channel
76	Lidocaine	ion channel
77	Tetracaine	ion channel
78	Amiloride	ion channel
79	Ondansetron	ion channel
80	Rosiglitazone	nuclear receptor
81	Beclomethasone	nuclear receptor
82	Medroxyprogesterone	nuclear receptor
83	Prednisolone	nuclear receptor
84	Clomifene	nuclear receptor
85	Cortisone	nuclear receptor
86	Prednisolone	nuclear receptor
87	Ulipristal	nuclear receptor
88	Bezafibrate	nuclear receptor
89	Norethindrone	nuclear receptor
90	Vitamin C	nuclear receptor
91	Pioglitazone	nuclear receptor
92	Gestodene	nuclear receptor
93	Drospirenone	nuclear receptor
94	Isotretinoin	nuclear receptor
95	Gemfibrozil	nuclear receptor
96	Estradiol	nuclear receptor
97	Levonorgestrel	nuclear receptor
98	Eplerenone	nuclear receptor
99	Methylprednisolone	nuclear receptor
100	Clobetasol	nuclear receptor
101	Progesterone	nuclear receptor
102	Prednisone	nuclear receptor
103	Acitretin	nuclear receptor
104	Raloxifene	nuclear receptor

105	Levetiracetam	transporter
106	Hydrochlorothiazide	transporter
107	Minoxidil	transporter
108	Furosemide	transporter
109	Glyburide	transporter
110	Metolazone	transporter
111	Reserpine	transporter
112	Glimepiride	transporter
113	Pidotimod	other
114	Ornidazole	other
115	Chloroquine	other
116	Sulfathiazole	other
117	Chlorzoxazone	other
118	Caspofungin	other
119	Dropropizine	other
120	Flubendazole	other
121	Pyridoxine	other
122	D-Phenylalanine	other
123	Eprazinone	other
124	Chlortetracycline	other
125	Thiamphenicol	other
126	Ethamsylate	other
127	Vitamin D2	other
128	Olsalazine	other
129	levofolinate	other
130	Zidovudine	other
131	Nafcillin	other
132	Ampicillin	other
133	Azithromycin	other
134	Amprolium	other
135	Toltrazuril	other
136	Bacitracin	other
137	Acetylcysteine	other
138	Orbifloxacin	other
139	Doxapram	other
140	Moguisteine	other
141	Atovaquone	other
142	Nadifloxacin	other
143	Creatinine	other
144	Decoquinat	other
145	Rifabutin	other
146	Nevirapine	other
147	Sulfapyridine	other
148	Amikacin	other
149	Cefoperazone	other
150	Clafen	other

151	Altretamine	other
152	Terbinafine	other
153	Doripenem	other
154	Azathioprine	other
155	Daptomycin	other
156	Zalcitabine	other
157	Cefoselis	other
158	Adefovir	other
159	Biapenem	other
160	Bleomycin	other
161	Nelarabine	other
162	Clotrimazole	other
163	Bendamustine	other
164	Cefdinir	other
165	Deferasirox	other
166	Ivermectin	other
167	Lamivudine	other
168	Sulfameter	other
169	Darunavir	other
170	Dacarbazine	other
171	Oxacillin	other
172	Streptomycin	other
173	Probenecid	other
174	Neomycin	other
175	Picosulfate	other
176	Cloxacillin	other
177	Colistin	other
178	Meropenem	other
179	Balofloxacin	other
180	Tiopronin	other
181	Bromhexine	other
182	Tolnaftate	other
183	Cyclophosphamide	other
184	Docosanol	other
185	Guaifenesin	other
186	Thiabendazole	other
187	Vancomycin	other
188	Nafamostat	other
189	Methocarbamol	other
190	Mesna	other
191	Terbinafine	other
192	Tetracycline	other