

Small Molecular Drug Screening Based on Clinical Therapeutic Effect

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Supplementary Table S1.

Table S1. Molecules information included in four molecular sets.

No.	Name	Category	No.	Name	Category
1	Aceclofenac ¹²³⁴	Analgesic	511	Ceftaroline fosamil ¹²³⁴	Antibacterial
2	Acemetacin ¹²³⁴	Analgesic	512	Ceftazidime ¹²³⁴	Antibacterial
3	Acetaminophen ¹²³⁴	Analgesic	513	Cefteram ¹²³⁴	Antibacterial
4	Acetanilide ¹²³⁴	Analgesic	514	Ceftezole ¹²³⁴	Antibacterial
5	Acetyldihydrocodeine ¹²³⁴	Analgesic	515	Ceftibuten ¹²³⁴	Antibacterial
6	Alclofenac ¹²³⁴	Analgesic	516	Ceftiofur ¹²³	Antibacterial
7	Alfentanil ¹²³⁴	Analgesic	517	Ceftiolene ¹²³⁴	Antibacterial
8	Allobarbitol ¹²	Analgesic	518	Ceftizoxime ¹²³⁴	Antibacterial
9	Alminoprofen ¹²³⁴	Analgesic	519	Ceftobiprole ¹²³⁴	Antibacterial
10	Almotriptan ¹²³⁴	Analgesic	520	Unii-yxv28V1B07 ¹²³⁴	Antibacterial
11	Alphaprodine ¹²³⁴	Analgesic	521	Ceftolozane ¹²³⁴	Antibacterial
12	Aminophenazone ¹²³⁴	Analgesic	522	Ceftriaxone ¹²³⁴	Antibacterial
13	Amitriptyline ¹²³⁴	Analgesic	523	Cefuroxime ¹²³⁴	Antibacterial
14	Ampiroxicam ¹²³⁴	Analgesic	524	Ceftin ¹²³⁴	Antibacterial
15	Ampyrone ¹²³⁴	Analgesic	525	Cefuzonam ¹²³⁴	Antibacterial
16	Anileridine ¹²³⁴	Analgesic	526	Cephalosporin C ¹²³⁴	Antibacterial
17	Antipyrine ¹²³⁴	Analgesic	527	Cethromycin ¹²³⁴	Antibacterial
18	Articaine ¹²	Analgesic	528	Chloramphenicol ¹²³⁴	Antibacterial
19	Aspirin ¹²³⁴	Analgesic	529	Chlortetracycline ¹²³⁴	Antibacterial
20	Azapropazone ¹²³⁴	Analgesic	530	Cinoxacin ¹²³⁴	Antibacterial
21	Bendazac ¹²³⁴	Analgesic	531	Ciprofloxacin ¹²³⁴	Antibacterial
22	Benorilate ¹²³⁴	Analgesic	532	Clarithromycin ¹²³⁴	Antibacterial
23	Benoxaprofen ¹²³⁴	Analgesic	533	Clavulanic acid ¹²³⁴	Antibacterial
24	Benzocaine ¹	Analgesic	534	Clinafloxacin ¹²³⁴	Antibacterial
25	Benzydamine ¹²³⁴	Analgesic	535	Clindamycin ¹²³⁴	Antibacterial
26	Benzylmorphine ¹²³⁴	Analgesic	536	Clofoctol ¹²³⁴	Antibacterial
27	Bezitramide ¹²³⁴	Analgesic	537	Clometocillin ¹²³⁴	Antibacterial
28	Bromfenac ¹²³⁴	Analgesic	538	Clomocycline ¹²³⁴	Antibacterial
29	Bucetin ¹²³⁴	Analgesic	539	Cloxacillin ¹²³⁴	Antibacterial
30	Bufexamac ¹²³⁴	Analgesic	540	Colistin ¹²³⁴	Antibacterial
31	Bumadizone ¹²³⁴	Analgesic	541	Cycloserine ¹²³⁴	Antibacterial
32	Buprenorphine ¹²³⁴	Analgesic	542	Dalfopristin ¹²³	Antibacterial
33	Butanilcaine ¹	Analgesic	543	Danofloxacin ¹²³	Antibacterial
34	Butorphanol ¹²³⁴	Analgesic	544	Dapsone ¹²	Antibacterial
35	Camphor ¹²³⁴	Analgesic	545	Daptomycin ¹²³⁴	Antibacterial
36	Cannabidiol ¹²³⁴	Analgesic	546	Deacetoxycephalosporin C ¹²³	Antibacterial
37	Capsaicin ¹²³	Analgesic	547	Delafloxacin ¹²³⁴	Antibacterial
38	Carbamazepine	Analgesic	548	Demeclocycline ¹²³⁴	Antibacterial
39	Carfentanil ¹²³	Analgesic	549	Dibekacin ¹²³⁴	Antibacterial
40	Carisoprodol ¹	Analgesic	550	Dicloxacin ¹²³⁴	Antibacterial
41	Chloroprocaine ¹²	Analgesic	551	Difloxacin ¹²³	Antibacterial
42	Chlorzoxazone ¹	Analgesic	552	Dihydrostreptomycin ¹²³⁴	Antibacterial

43	Cinchocaine ¹²	Analgesic	553	Dirithromycin ¹²³⁴	Antibacterial
44	Clonidine ¹²³⁴	Analgesic	554	Doripenem ¹²³⁴	Antibacterial
45	Cocaine ¹	Analgesic	555	Doxycycline ¹²³⁴	Antibacterial
46	Codeine ¹²³⁴	Analgesic	556	Enoxacin ¹²³⁴	Antibacterial
47	Cyclobenzaprine ¹	Analgesic	557	Enrofloxacin ¹²	Antibacterial
48	Cyclomethycaine ¹	Analgesic	558	Eperezolid ¹²³	Antibacterial
49	Desomorphine ¹²³⁴	Analgesic	559	Epicillin ¹²³⁴	Antibacterial
50	Dexmedetomidine ¹²	Analgesic	560	Eravacycline ¹²³⁴	Antibacterial
51	Dextromoramide ¹²³⁴	Analgesic	561	Ertapenem ¹²³⁴	Antibacterial
52	Dextropropoxyphene ¹²³⁴	Analgesic	562	Erythromycin ¹²³⁴	Antibacterial
53	Dezocine ¹²³⁴	Analgesic	563	Faropenem ¹²³⁴	Antibacterial
54	Diacerein ¹²³⁴	Analgesic	564	Finafloxacin ¹²³⁴	Antibacterial
55	Diamorphine ¹²³⁴	Analgesic	565	Fleroxacin ¹²³⁴	Antibacterial
56	Diclofenac ¹²³⁴	Analgesic	566	Flomoxef ¹²³⁴	Antibacterial
57	Diflunisal ¹²³⁴	Analgesic	567	Florfenicol ¹²³	Antibacterial
58	Dihydrocodeine ¹²³⁴	Analgesic	568	Flucloxacillin ¹²³⁴	Antibacterial
59	Dihydroergotamine ¹²³⁴	Analgesic	569	Flumequine ¹²³⁴	Antibacterial
60	Dihydromorphine ¹²³⁴	Analgesic	570	Flurithromycin ¹²³⁴	Antibacterial
61	Dimenoxadol ¹²³⁴	Analgesic	571	Fosfomycin ¹²³⁴	Antibacterial
62	Dimethocaine ¹	Analgesic	572	Framycetin ¹²³⁴	Antibacterial
63	Dimetotiazine ¹²³⁴	Analgesic	573	Furazidin ¹²³⁴	Antibacterial
64	Dipipanone ¹²³⁴	Analgesic	574	Furazolidone ¹²³	Antibacterial
65	Dipyrocetyl ¹²³⁴	Analgesic	575	Fusidic acid ¹²³⁴	Antibacterial
66	Dronabinol ¹²³⁴	Analgesic	576	Garenoxacin ¹²	Antibacterial
67	Droxicam ¹²³⁴	Analgesic	577	Gatifloxacin ¹²³⁴	Antibacterial
68	DSP-2230 ¹²	Analgesic	578	Gemifloxacin ¹²³⁴	Antibacterial
69	Dyclonine ¹	Analgesic	579	Gentamicin ¹²³⁴	Antibacterial
70	Eletriptan ¹²³⁴	Analgesic	580	Grepafloxacin ¹²³⁴	Antibacterial
71	Ergotamine ¹²³⁴	Analgesic	581	Hetacillin ¹²³⁴	Antibacterial
72	Ethenzamide ¹²³⁴	Analgesic	582	Hygromycin B ¹²³	Antibacterial
73	Ethoheptazine ¹²³⁴	Analgesic	583	Ibafloxacin ¹²³⁴	Antibacterial
74	Ethylmorphine ¹²³⁴	Analgesic	584	Iclaprim ¹²³⁴	Antibacterial
75	Etidocaine ¹	Analgesic	585	Imipenem ¹²³⁴	Antibacterial
76	Etodolac ¹²³⁴	Analgesic	586	Isepamicin ¹²³⁴	Antibacterial
77	Etofenamate ¹²³⁴	Analgesic	587	Isoniazid ¹²³⁴	Antibacterial
78	Etoricoxib ¹²³⁴	Analgesic	588	Josamycin ¹²³⁴	Antibacterial
79	Eugenol ¹²	Analgesic	589	Kanamycin ¹²³⁴	Antibacterial
80	Fenbufen ¹²³⁴	Analgesic	590	Latamoxef ¹²³⁴	Antibacterial
81	Fenoprofen ¹²³⁴	Analgesic	591	Lefamulin ¹²³⁴	Antibacterial
82	Fentanyl ¹²	Analgesic	592	Lincomycin ¹²³⁴	Antibacterial
83	Fentiazac ¹²³⁴	Analgesic	593	Linezolid ¹²³⁴	Antibacterial
84	Feprazone ¹²³⁴	Analgesic	594	Lomefloxacin ¹²³⁴	Antibacterial
85	Floctafenine ¹²³⁴	Analgesic	595	Loracarbef ¹²³⁴	Antibacterial
86	Flufenamic acid ¹²³⁴	Analgesic	596	Lymecycline ¹²³⁴	Antibacterial
87	Flumetroxone ¹²³⁴	Analgesic	597	Mandelic acid ¹²³⁴	Antibacterial
88	Flunoxaprofen ¹²³⁴	Analgesic	598	Marbofloxacin ¹²³	Antibacterial
89	Flupirtine ¹²³⁴	Analgesic	599	Meclocycline ¹²³⁴	Antibacterial
90	Fluproquazone ¹²³	Analgesic	600	Meropenem ¹²³⁴	Antibacterial
91	Flurbiprofen ¹²³⁴	Analgesic	601	Metacycline ¹²³⁴	Antibacterial
92	Frovatriptan ¹²³⁴	Analgesic	602	Metampicillin ¹²³⁴	Antibacterial
93	Funapide ¹²	Analgesic	603	Methenamine ¹²³	Antibacterial
94	Gabapentin ¹²³⁴	Analgesic	604	Methicillin ¹²³⁴	Antibacterial
95	Gabapentin enacarbil ¹²³⁴	Analgesic	605	Metronidazole ¹²³⁴	Antibacterial
96	Glafenine ¹²³⁴	Analgesic	606	Mezlocillin ¹²³⁴	Antibacterial
97	Guacetisal ¹²³⁴	Analgesic	607	Midecamycin ¹²³⁴	Antibacterial
98	Halothane ¹	Analgesic	608	Minocycline ¹²³⁴	Antibacterial
99	Hydrocodone ¹²³⁴	Analgesic	609	Miocamycin ¹²³⁴	Antibacterial

100	Hydromorphinol ¹²³⁴	Analgesic	610	Moxifloxacin ¹²³⁴	Antibacterial
101	Hydromorphone ¹²³⁴	Analgesic	611	Mupirocin ¹²³⁴	Antibacterial
102	Ibuprofen ¹²³⁴	Analgesic	612	Nadifloxacin ¹²³⁴	Antibacterial
103	Indometacin ¹²³⁴	Analgesic	613	Nafcillin ¹²³⁴	Antibacterial
104	Indomethacin farnesil ¹²³	Analgesic	614	Nalidixic acid ¹²³⁴	Antibacterial
105	Indoprofen ¹²³⁴	Analgesic	615	Nemonoxacin ¹²³⁴	Antibacterial
106	Iprazochrome ¹²³⁴	Analgesic	616	Netilmicin ¹²³⁴	Antibacterial
107	Isoflurane ¹²	Analgesic	617	Nifurtinol ¹²³⁴	Antibacterial
108	Kebuzone ¹²³⁴	Analgesic	618	Nitrofurantoin ¹²³⁴	Antibacterial
109	Ketamine ¹²	Analgesic	619	Nitroxoline ¹²³⁴	Antibacterial
110	Ketobemidone ¹²³⁴	Analgesic	620	Nocardin A ¹²³⁴	Antibacterial
111	Ketorolac ¹²³⁴	Analgesic	621	Norfloxacin ¹²³⁴	Antibacterial
112	Lacosamide ¹	Analgesic	622	Nourseothricin ¹²	Antibacterial
113	Levorphanol ¹²³⁴	Analgesic	623	Novobiocin ¹²³⁴	Antibacterial
114	Lisuride ¹²	Analgesic	624	Oleandomycin ¹²³	Antibacterial
115	Lofentanil ¹²³⁴	Analgesic	625	Omadacycline ¹²³⁴	Antibacterial
116	Lonazolac ¹²³⁴	Analgesic	626	Orbifloxacin ¹²³	Antibacterial
117	Lornoxicam ¹²³⁴	Analgesic	627	Oritavancin ¹²³⁴	Antibacterial
118	Loxoprofen ¹²³⁴	Analgesic	628	Ornidazole ¹²³⁴	Antibacterial
119	Lumiracoxib ¹²³⁴	Analgesic	629	Oxacillin ¹²³⁴	Antibacterial
120	Meclofenamic acid ¹²³⁴	Analgesic	630	Oxolinic acid ¹²	Antibacterial
121	Mefenamic acid ¹²³⁴	Analgesic	631	Oxytetracycline ¹²³⁴	Antibacterial
122	Meloxicam ¹²³⁴	Analgesic	632	Ozenoxacin ¹²³⁴	Antibacterial
123	Menthol ¹²³	Analgesic	633	Panipenem ¹²³⁴	Antibacterial
124	Meperidine ¹²³⁴	Analgesic	634	Paromomycin ¹²³⁴	Antibacterial
125	Mephenoxalone ¹²	Analgesic	635	Pazufloxacin ¹²³⁴	Antibacterial
126	Mepivacaine ¹	Analgesic	636	Pefloxacin ¹²³⁴	Antibacterial
127	Meptazinol ¹²³⁴	Analgesic	637	Penamocillin ¹²³⁴	Antibacterial
128	Metabutethamine ¹	Analgesic	638	Pheneticillin ¹²³⁴	Antibacterial
129	Metamizole ¹²³⁴	Analgesic	639	Phenoxymethylpenicillin ¹²³⁴	Antibacterial
130	Metethoheptazine ¹²³⁴	Analgesic	640	Pipemidic acid ¹²	Antibacterial
131	Methadone ¹²³⁴	Analgesic	641	Piperacillin ¹²³⁴	Antibacterial
132	Metheptazine ¹²³⁴	Analgesic	642	Pirlimycin ¹²³	Antibacterial
133	Methocarbamol ¹²³	Analgesic	643	Piromidic acid ¹²³⁴	Antibacterial
134	Methoxyflurane ¹²³	Analgesic	644	Pivampicillin ¹²³⁴	Antibacterial
135	Methyl salicylate ¹²³⁴	Analgesic	645	Pivmecillinam ¹²³⁴	Antibacterial
136	Methysergide ¹²³	Analgesic	646	Plazomicin ¹²³⁴	Antibacterial
137	Metopon ¹²³⁴	Analgesic	647	Polymyxin B ¹²³⁴	Antibacterial
138	Mirogabalin ¹²³⁴	Analgesic	648	Posizolid ¹²³⁴	Antibacterial
139	Mioprofen ¹²³⁴	Analgesic	649	Pradofloxacin ¹²³	Antibacterial
140	Mofebutazone ¹²³⁴	Analgesic	650	Prontosil ¹²³⁴	Antibacterial
141	Morniflumate ¹²³⁴	Analgesic	651	Propicillin ¹²³⁴	Antibacterial
142	Morphine ¹²³⁴	Analgesic	652	Prulifloxacin ¹²³⁴	Antibacterial
143	Morpholine ¹²	Analgesic	653	Puromycin ¹²	Antibacterial
144	Nabilone ¹²	Analgesic	654	Quinupristin ¹²³	Antibacterial
145	Nabumetone ¹²³⁴	Analgesic	655	Radezolid ¹²³⁴	Antibacterial
146	Nalbuphine ¹²³⁴	Analgesic	656	Ranbezolid ¹²³	Antibacterial
147	Naproxen ¹²³⁴	Analgesic	657	Relebactam ¹²³⁴	Antibacterial
148	Naratriptan ¹²³⁴	Analgesic	658	Retapamulin ¹²³⁴	Antibacterial
149	Nefopam ¹²³⁴	Analgesic	659	Ribostamycin ¹²³⁴	Antibacterial
150	Nefopam ¹²³⁴	Analgesic	660	Rifabutin ¹²³⁴	Antibacterial
151	NFEPP ¹²³⁴	Analgesic	661	Rifalazil ¹²³⁴	Antibacterial
152	Nicocodeine ¹²³⁴	Analgesic	662	Rifamycin ¹²³⁴	Antibacterial
153	Nicodicodine ¹²³⁴	Analgesic	663	Rifapentine ¹²³⁴	Antibacterial
154	Nicomorphine ¹²³⁴	Analgesic	664	Rifaximin ¹²³⁴	Antibacterial
155	Nifenazone ¹²³⁴	Analgesic	665	Ritipenem ¹²³⁴	Antibacterial
156	Niflumic acid ¹²³⁴	Analgesic	666	Rokitamycin ¹²³⁴	Antibacterial

157	Nimesulide ¹²³⁴	Analgesic	667	Rolitetracycline ¹²³⁴	Antibacterial
158	Nitrous Oxide ¹²	Analgesic	668	Rosoxacin ¹²³⁴	Antibacterial
159	Norpipanone ¹²³⁴	Analgesic	669	Roxithromycin ¹²³⁴	Antibacterial
160	Nortilidine ¹²³⁴	Analgesic	670	Rufloxacin ¹²³⁴	Antibacterial
161	Orphenadrine ¹²³	Analgesic	671	Sarafloxacin ¹²³	Antibacterial
162	Oxametacin ¹²³	Analgesic	672	Sarecycline ¹²³⁴	Antibacterial
163	Oxaprozin ¹²³⁴	Analgesic	673	Sisomicin ¹²³⁴	Antibacterial
164	Oxetorone ¹²³⁴	Analgesic	674	Sitafloxacin ¹²³⁴	Antibacterial
165	Oxycodone ¹²³⁴	Analgesic	675	Solithromycin ¹²³⁴	Antibacterial
166	Oxymorphone ¹²³⁴	Analgesic	676	Sparfloxacin ¹²³⁴	Antibacterial
167	Oxyphenbutazone ¹²³⁴	Analgesic	677	Spectinomycin ¹²³⁴	Antibacterial
168	Parecoxib ¹²³⁴	Analgesic	678	Spiramycin ¹²³⁴	Antibacterial
169	Pentazocine ¹²³	Analgesic	679	Streptomycin ¹²³⁴	Antibacterial
170	PF-05089771 ¹²³⁴	Analgesic	680	Sulbactam ¹²³⁴	Antibacterial
171	Phenacetin ¹²³⁴	Analgesic	681	Sulbenicillin ¹²³⁴	Antibacterial
172	Phenadoxone ¹²³⁴	Analgesic	682	Sulfacetamide ¹²³⁴	Antibacterial
173	Phenazocine ¹²³⁴	Analgesic	683	Sulfadiazine ¹²³⁴	Antibacterial
174	Phenazopyridine ¹²³	Analgesic	684	Sulfadicramide ¹²³	Antibacterial
175	Phenol ¹²	Analgesic	685	Sulfadimethoxine ¹²³⁴	Antibacterial
176	Phenoperidine ¹²³⁴	Analgesic	686	Sulfadimidine ¹²³⁴	Antibacterial
177	Phenylbutazone ¹²³⁴	Analgesic	687	Sulfadoxine ¹²³⁴	Antibacterial
178	Piminodine ¹²³⁴	Analgesic	688	Sulfafurazole ¹²³⁴	Antibacterial
179	Piperocaine ¹	Analgesic	689	Sulfaisodimidine ¹²³⁴	Antibacterial
180	Piritramide ¹²³⁴	Analgesic	690	Sulfalene ¹²³⁴	Antibacterial
181	Piroxicam ¹²³⁴	Analgesic	691	Sulfamazone ¹²	Antibacterial
182	Pirprofen ¹²³⁴	Analgesic	692	Sulfamerazine ¹²³⁴	Antibacterial
183	Pizotifen ¹²³	Analgesic	693	Sulfameter ¹²³⁴	Antibacterial
184	Pregabalin ¹²³	Analgesic	694	Sulfamethizole ¹²³⁴	Antibacterial
185	Prilocaine ¹²	Analgesic	695	Sulfamethoxazole ¹²³⁴	Antibacterial
186	Procaine ¹²	Analgesic	696	Sulfamethoxypyridazine ¹²³⁴	Antibacterial
187	Proglumetacin ¹²³⁴	Analgesic	697	Sulfametomidine ¹²³⁴	Antibacterial
188	Proglumide ¹²³	Analgesic	698	Sulfametrole ¹²³⁴	Antibacterial
189	Proheptazine ¹²³⁴	Analgesic	699	Sulfamoxole ¹²³⁴	Antibacterial
190	Propacetamol ¹²³⁴	Analgesic	700	Sulfanilamide ¹²³⁴	Antibacterial
191	Proparacaine ¹	Analgesic	701	Sulfanitran ¹²³	Antibacterial
192	Propiram ¹²³⁴	Analgesic	702	Sulfaperin ¹²³⁴	Antibacterial
193	Propoxycaine ¹	Analgesic	703	Sulfaphenazole ¹²³⁴	Antibacterial
194	Propyphenazone ¹²³⁴	Analgesic	704	Sulfapyridine ¹²³⁴	Antibacterial
195	Proquazone ¹²³⁴	Analgesic	705	Sulfathiazole ¹²³⁴	Antibacterial
196	Proxibarbal ¹²³	Analgesic	706	Sulfathiourea ¹²³⁴	Antibacterial
197	Remifentanil ¹	Analgesic	707	Sultamicillin ¹²³⁴	Antibacterial
198	Rimazolium ¹²³⁴	Analgesic	708	Sutezolid ¹²³⁴	Antibacterial
199	Rizatriptan ¹²³	Analgesic	709	Talampicillin ¹²³⁴	Antibacterial
200	Rofecoxib ¹²³⁴	Analgesic	710	Tazobactam ¹²³⁴	Antibacterial
201	Ropivacaine ¹²³	Analgesic	711	Tebipenem pivoxil ¹²³⁴	Antibacterial
202	Salicin ¹²³⁴	Analgesic	712	Tedizolid ¹²³⁴	Antibacterial
203	Salicylamide ¹²³⁴	Analgesic	713	Telavancin ¹²³⁴	Antibacterial
204	Salsalate ¹²³⁴	Analgesic	714	Telithromycin ¹²³⁴	Antibacterial
205	Saxitoxin ¹	Analgesic	715	Temafloxacin ¹²³⁴	Antibacterial
206	Sevoflurane ¹²	Analgesic	716	Temocillin ¹²³⁴	Antibacterial
207	Spilanthol ¹²	Analgesic	717	Tetracycline ¹²³⁴	Antibacterial
208	Sufentanil ¹²	Analgesic	718	Tetroxoprim ¹²³⁴	Antibacterial
209	Sulindac ¹²³⁴	Analgesic	719	Thiamphenicol ¹²³⁴	Antibacterial
210	Sumatriptan ¹²³⁴	Analgesic	720	Tiamulin ¹²³	Antibacterial
211	Suprofen ¹²³⁴	Analgesic	721	Ticarcillin ¹²³⁴	Antibacterial
212	Tapentadol ¹²³⁴	Analgesic	722	Tigecycline ¹²³⁴	Antibacterial
213	Tenoxicam ¹²³⁴	Analgesic	723	Tigemonam ¹²³⁴	Antibacterial

214	Tetracaine ¹²	Analgesic	724	Tinidazole ¹²³⁴	Antibacterial
215	Tetrodotoxin ¹²³	Analgesic	725	Tobramycin ¹²³⁴	Antibacterial
216	Thebacon ¹²³⁴	Analgesic	726	Tosufloxacin ¹²³⁴	Antibacterial
217	Thiopental ¹²	Analgesic	727	Trimethoprim ¹²³⁴	Antibacterial
218	Tiaprofenic acid ¹²³⁴	Analgesic	728	Troleandomycin ¹²³⁴	Antibacterial
219	Tilidine ¹²³⁴	Analgesic	729	Trovaflaxacin ¹²³⁴	Antibacterial
220	Tolfenamic acid ¹²³⁴	Analgesic	730	Tyrothricin ¹²³⁴	Antibacterial
221	Tolmetin ¹²³⁴	Analgesic	731	Vaborbactam ¹²³⁴	Antibacterial
222	Tramadol ¹²³⁴	Analgesic	732	Valnemulin ¹²³⁴	Antibacterial
223	Trichloroethylene ¹²	Analgesic	733	Vancomycin ¹²³⁴	Antibacterial
224	Trimecaine ¹²	Analgesic	734	Verdamicin ¹²³⁴	Antibacterial
225	Valdecobix ¹²³⁴	Analgesic	735	Xibornol ¹²³	Antibacterial
226	Viminol ¹²³⁴	Analgesic	736	Abacavir ¹²³⁴	Antiviral
227	Zolmitriptan ¹²³⁴	Analgesic	737	Aciclovir ¹²³⁴	Antiviral
228	Zomepirac ¹²³⁴	Analgesic	738	Adefovir ¹²	Antiviral
229	Abemaciclib ¹²³⁴	Antineoplastic	739	Adefovir dipivoxil ¹²³⁴	Antiviral
230	Acalabrutinib ¹²³⁴	Antineoplastic	740	Amdoxovir ¹²³⁴	Antiviral
231	Aclarubicin ¹²	Antineoplastic	741	Amenamavir ¹²³⁴	Antiviral
232	Afatinib ¹²³⁴	Antineoplastic	742	Amprenavir ¹²³⁴	Antiviral
233	Alectinib ¹²³⁴	Antineoplastic	743	Apricitabine ¹²³⁴	Antiviral
234	Alpelisib ¹²³⁴	Antineoplastic	744	Asunaprevir ¹²³⁴	Antiviral
235	Altretamine ¹²³⁴	Antineoplastic	745	Atazanavir ¹²³⁴	Antiviral
236	Alvocidib ¹²³	Antineoplastic	746	Baloxavir marboxil ¹²³⁴	Antiviral
237	Aminolevulinic acid ¹²³⁴	Antineoplastic	747	Bevirimat ¹²³⁴	Antiviral
238	Aminopropionitrile ¹²³⁴	Antineoplastic	748	BI 224436 ¹²³⁴	Antiviral
239	Aminopterin ¹²³⁴	Antineoplastic	749	Bictegravir ¹²³⁴	Antiviral
240	Amrubicin ¹²	Antineoplastic	750	BIT225 ¹²³⁴	Antiviral
241	Amsacrine ¹²³⁴	Antineoplastic	751	BMS-955176 ¹²³⁴	Antiviral
242	Anagrelide ¹²³⁴	Antineoplastic	752	Boceprevir ¹²³⁴	Antiviral
243	Asparagine ¹	Antineoplastic	753	Brivudine ¹²³⁴	Antiviral
244	Atrasentan ¹²	Antineoplastic	754	Cabotegravir ¹²³⁴	Antiviral
245	Axitinib ¹²³⁴	Antineoplastic	755	Calanolide A ¹²³⁴	Antiviral
246	Azacitidine ¹²³⁴	Antineoplastic	756	Cenicriviroc ¹²	Antiviral
247	Baricitinib ¹²³⁴	Antineoplastic	757	Censavudine ¹²³⁴	Antiviral
248	Belinostat ¹²³⁴	Antineoplastic	758	Cidofovir ¹²³⁴	Antiviral
249	Belotecan ¹²³⁴	Antineoplastic	759	Clevudine ¹²³⁴	Antiviral
250	Bendamustine ¹²³⁴	Antineoplastic	760	Daclatasvir ¹²³⁴	Antiviral
251	Bexarotene ¹²³⁴	Antineoplastic	761	Darunavir ¹²³⁴	Antiviral
252	Binimetinib ¹²³⁴	Antineoplastic	762	Dasabuvir ¹²³⁴	Antiviral
253	Bleomycin ¹²	Antineoplastic	763	Delavirdine ¹²³⁴	Antiviral
254	Bortezomib ¹²³⁴	Antineoplastic	764	Didanosine ¹²³⁴	Antiviral
255	Bosutinib ¹²³⁴	Antineoplastic	765	Docosanol ¹²³⁴	Antiviral
256	Brigatinib ¹²³⁴	Antineoplastic	766	Dolutegravir ¹²³⁴	Antiviral
257	Busulfan ¹²³⁴	Antineoplastic	767	Doravirine ¹²³⁴	Antiviral
258	Cabazitaxel ¹²³⁴	Antineoplastic	768	Edoxudine ¹²³⁴	Antiviral
259	Cabozantinib ¹²³⁴	Antineoplastic	769	Efavirenz ¹²³⁴	Antiviral
260	Camptothecin ¹²³⁴	Antineoplastic	770	Elbasvir ¹²³⁴	Antiviral
261	Capecitabine ¹²³⁴	Antineoplastic	771	Elvitegravir ¹²³⁴	Antiviral
262	Carboquone ¹²³	Antineoplastic	772	Elvucitabine ¹²³⁴	Antiviral
263	Carfilzomib ¹²³⁴	Antineoplastic	773	Emtricitabine ¹²³⁴	Antiviral
264	Carmofur ¹²³⁴	Antineoplastic	774	Entecavir ¹²³⁴	Antiviral
265	Carmustine ¹²³⁴	Antineoplastic	775	Epigallocatechin gallate ¹²³	Antiviral
266	Cediranib ¹²³⁴	Antineoplastic	776	Etravirine ¹²³⁴	Antiviral
267	Ceritinib ¹²³⁴	Antineoplastic	777	Faldaprevir ¹²³⁴	Antiviral
268	Chlorambucil ¹²³⁴	Antineoplastic	778	Famciclovir ¹²³⁴	Antiviral
269	Chlormethine ¹²³⁴	Antineoplastic	779	Favipiravir ¹²³⁴	Antiviral
270	Cladribine ¹²³⁴	Antineoplastic	780	Filiciclovir ¹²³⁴	Antiviral

271	Clofarabine ¹²³⁴	Antineoplastic	781	Fosamprenavir ¹²³⁴	Antiviral
272	Cobimetinib ¹²³⁴	Antineoplastic	782	Foscarnet ¹²³⁴	Antiviral
273	Copanlisib ¹²³⁴	Antineoplastic	783	Fosdevirine ¹²³⁴	Antiviral
274	Cositecan ¹²³⁴	Antineoplastic	784	Fostemsavir ¹²³⁴	Antiviral
275	Crizotinib ¹²³⁴	Antineoplastic	785	Ganciclovir ¹²³⁴	Antiviral
276	Cyclophosphamide ¹²³⁴	Antineoplastic	786	Grazoprevir ¹²³⁴	Antiviral
277	Dabrafenib ¹²³⁴	Antineoplastic	787	Idoxuridine ¹²³⁴	Antiviral
278	Dacarbazine ¹²³⁴	Antineoplastic	788	Imiquimod ¹²³⁴	Antiviral
279	Dacomitinib ¹²³⁴	Antineoplastic	789	Indinavir ¹²³⁴	Antiviral
280	Dactinomycin ¹²	Antineoplastic	790	Islatravir ¹²³⁴	Antiviral
281	Dasatinib ¹²³⁴	Antineoplastic	791	KP-1461 ¹²³⁴	Antiviral
282	Daunorubicin ¹²³	Antineoplastic	792	Lamivudine ¹²³⁴	Antiviral
283	Decitabine ¹²³⁴	Antineoplastic	793	Laninamivir ¹²³⁴	Antiviral
284	Demecolcine ¹²	Antineoplastic	794	Letermovir ¹²³⁴	Antiviral
285	Docetaxel ¹²³⁴	Antineoplastic	795	Lobucavir ¹²³⁴	Antiviral
286	Doxifluridine ¹²³⁴	Antineoplastic	796	Lopinavir ¹²³⁴	Antiviral
287	Elesclomol ¹²³⁴	Antineoplastic	797	Maraviroc ¹²³⁴	Antiviral
288	Elsamitucin ¹²	Antineoplastic	798	Maribavir ¹²³⁴	Antiviral
289	Enasidenib ¹²³⁴	Antineoplastic	799	Methisazone ¹²³⁴	Antiviral
290	Encorafenib ¹²³⁴	Antineoplastic	800	Miltefosine ¹²	Antiviral
291	Entinostat ¹²³⁴	Antineoplastic	801	MK-2048 ¹²³⁴	Antiviral
292	Entrectinib ¹²³⁴	Antineoplastic	802	Moroxydine ¹²³⁴	Antiviral
293	Epacadostat ¹²³⁴	Antineoplastic	803	Nelfinavir ¹²³⁴	Antiviral
294	Erdafitinib ¹²³⁴	Antineoplastic	804	Nevirapine ¹²³⁴	Antiviral
295	Eribulin ¹²³⁴	Antineoplastic	805	Oseltamivir ¹²³⁴	Antiviral
296	Erlotinib ¹²³⁴	Antineoplastic	806	Penciclovir ¹²³⁴	Antiviral
297	Estramustine ¹²³⁴	Antineoplastic	807	Ingavirin ¹²³⁴	Antiviral
298	Estramustine phosphate ¹²³⁴	Antineoplastic	808	Peramivir ¹²³⁴	Antiviral
299	Etoglucid ¹²³	Antineoplastic	809	Phosphonoacetate ¹²³⁴	Antiviral
300	Etoposide ¹²³⁴	Antineoplastic	810	Pleconaril ¹²³⁴	Antiviral
301	Everolimus ¹²³⁴	Antineoplastic	811	Podophyllotoxin ¹²	Antiviral
302	Exatecan ¹²³⁴	Antineoplastic	812	Raltegravir ¹²³⁴	Antiviral
303	Fedratinib ¹²³⁴	Antineoplastic	813	Remdesivir ¹²³⁴	Antiviral
304	Filgotinib ¹²³⁴	Antineoplastic	814	Resiquimod ¹²	Antiviral
305	Floxuridine ¹²³⁴	Antineoplastic	815	Ribavirin ¹²³⁴	Antiviral
306	Fludarabine ¹²³⁴	Antineoplastic	816	Rilpivirine ¹²³⁴	Antiviral
307	Fluorouracil ¹²³⁴	Antineoplastic	817	Rimantadine ¹²³⁴	Antiviral
308	Fotemustine ¹²³⁴	Antineoplastic	818	Ritonavir ¹²³⁴	Antiviral
309	Gefitinib ¹²³⁴	Antineoplastic	819	Saquinavir ¹²³⁴	Antiviral
310	Gemcitabine ¹²³⁴	Antineoplastic	820	Simeprevir ¹²³⁴	Antiviral
311	Gilteritinib ¹²³⁴	Antineoplastic	821	Sofosbuvir ¹²³⁴	Antiviral
312	Gimatecan ¹²³	Antineoplastic	822	Sorivudine ¹²³⁴	Antiviral
313	Hydroxyurea ¹²³⁴	Antineoplastic	823	Stampidine ¹²³	Antiviral
314	Ibrutinib ¹²³⁴	Antineoplastic	824	Stavudine ¹²³⁴	Antiviral
315	Icotinib ¹²³⁴	Antineoplastic	825	Taribavirin ¹²³⁴	Antiviral
316	Idarubicin ¹²	Antineoplastic	826	Tecovirimat ¹²³⁴	Antiviral
317	Idelalisib ¹²³⁴	Antineoplastic	827	Telaprevir ¹²³⁴	Antiviral
318	Ifosfamide ¹²³⁴	Antineoplastic	828	Telbivudine ¹²³⁴	Antiviral
319	Imatinib ¹²³⁴	Antineoplastic	829	Tenofovir ¹²³⁴	Antiviral
320	Infigratinib ¹²³⁴	Antineoplastic	830	Tenofovir alafenamide ¹²³⁴	Antiviral
321	Irinotecan ¹²³⁴	Antineoplastic	831	Tenofovir disoproxil ¹²³⁴	Antiviral
322	Ivosidenib ¹²³⁴	Antineoplastic	832	Tilorone ¹²	Antiviral
323	Ixabepilone ¹²	Antineoplastic	833	Tipranavir ¹²³⁴	Antiviral
324	Ixazomib ¹²³⁴	Antineoplastic	834	TMC-310911 ¹²³⁴	Antiviral
325	Lapatinib ¹²³⁴	Antineoplastic	835	Trifluridine ¹²³⁴	Antiviral
326	Larotaxel ¹²³	Antineoplastic	836	Tromantadine ¹²³⁴	Antiviral
327	Larotrectinib ¹²³⁴	Antineoplastic	837	Umifenovir ¹²³⁴	Antiviral

328	Lenvatinib ¹²³⁴	Antineoplastic	838	Valaciclovir ¹²³⁴	Antiviral
329	Lestaurtinib ¹²³⁴	Antineoplastic	839	Valganciclovir ¹²³⁴	Antiviral
330	Lomustine ¹²³⁴	Antineoplastic	840	Vicriviroc ¹²³	Antiviral
331	Lonidamine ¹²³⁴	Antineoplastic	841	Zalcitabine ¹²³⁴	Antiviral
332	Lorlatinib ¹²³⁴	Antineoplastic	842	Zanamivir ¹²³⁴	Antiviral
333	Losoxantrone ¹²	Antineoplastic	843	Zidovudine ¹²³⁴	Antiviral
334	Lucanthone ¹	Antineoplastic	844	Abafungin ¹²³⁴	Antifungal
335	Lurtotecan ¹²³⁴	Antineoplastic	845	Albaconazole ¹²³⁴	Antifungal
336	Mannosulfan ¹²³	Antineoplastic	846	Amorolfine ¹²³⁴	Antifungal
337	Masitinib ¹²³	Antineoplastic	847	Amphotericin B ¹²³⁴	Antifungal
338	Masoprocol ¹²³⁴	Antineoplastic	848	Anidulafungin ¹²³⁴	Antifungal
339	Melphalan ¹²³⁴	Antineoplastic	849	Atovaquone ¹²³⁴	Antifungal
340	Mercaptopurine ¹²³⁴	Antineoplastic	850	Bifonazole ¹²³⁴	Antifungal
341	Methotrexate ¹²³	Antineoplastic	851	Bromochlorosalicylanilide ¹²³⁴	Antifungal
342	Midostaurin ¹²³⁴	Antineoplastic	852	Butenafine ¹²³⁴	Antifungal
343	Mitobronitol ¹²³	Antineoplastic	853	Butoconazole ¹²³⁴	Antifungal
344	Mitoguazone ¹²³⁴	Antineoplastic	854	Caspofungin ¹²³⁴	Antifungal
345	Mitomycin ¹²	Antineoplastic	855	Chlormidazole ¹²³⁴	Antifungal
346	Mitotane ¹²³⁴	Antineoplastic	856	Chlorophetanol ¹²³⁴	Antifungal
347	Mitoxantrone ¹²	Antineoplastic	857	Chlorphenesin ¹²	Antifungal
348	Momelotinib ¹²³	Antineoplastic	858	Ciclopirox ¹²³⁴	Antifungal
349	Nelarabine ¹²³⁴	Antineoplastic	859	Clotrimazole ¹²	Antifungal
350	Neratinib ¹²³⁴	Antineoplastic	860	Croconazole ¹²³	Antifungal
351	Nilotinib ¹²³⁴	Antineoplastic	861	Dimazole ¹²³⁴	Antifungal
352	Nimustine ¹²³⁴	Antineoplastic	862	Eberconazole ¹²³⁴	Antifungal
353	Nintedanib ¹²³⁴	Antineoplastic	863	Econazole ¹²³⁴	Antifungal
354	Niraparib ¹²³⁴	Antineoplastic	864	Efinaconazole ¹²³⁴	Antifungal
355	Olaparib ¹²³⁴	Antineoplastic	865	Ethylparaben ¹²³⁴	Antifungal
356	Olmotinib ¹²³⁴	Antineoplastic	866	Fenticonazole ¹²³⁴	Antifungal
357	Omacetaxine ¹²³⁴	Antineoplastic	867	Fluconazole ¹²³⁴	Antifungal
358	Oprozomib ¹²³	Antineoplastic	868	Flucytosine ¹²³⁴	Antifungal
359	Ortataxel ¹²³	Antineoplastic	869	Flutrimazole ¹²³⁴	Antifungal
360	Osimertinib ¹²³⁴	Antineoplastic	870	Fosfluconazole ¹²³⁴	Antifungal
361	Paclitaxel ¹²³⁴	Antineoplastic	871	Griseofulvin ¹²	Antifungal
362	Pacritinib ¹²³	Antineoplastic	872	Haloprogin ¹²³⁴	Antifungal
363	Palbociclib ¹²³⁴	Antineoplastic	873	Hexaconazole ¹²³	Antifungal
364	Panobinostat ¹²³⁴	Antineoplastic	874	Isavuconazole ¹²³⁴	Antifungal
365	Pazopanib ¹²³	Antineoplastic	875	Isoconazole ¹²³⁴	Antifungal
366	Pemetrexed ¹²³⁴	Antineoplastic	876	Itraconazole ¹²³⁴	Antifungal
367	Pemigatinib ¹²³⁴	Antineoplastic	877	Ketoconazole ¹²³⁴	Antifungal
368	Pentostatin ¹²³⁴	Antineoplastic	878	Luliconazole ¹²³⁴	Antifungal
369	Pipobroman ¹²³⁴	Antineoplastic	879	Mepartricin ¹²	Antifungal
370	Pirarubicin ¹²	Antineoplastic	880	Micafungin ¹²³⁴	Antifungal
371	Pixantrone ¹²	Antineoplastic	881	Miconazole ¹²³⁴	Antifungal
372	Plicamycin ¹²	Antineoplastic	882	Naftifine ¹²³⁴	Antifungal
373	Plitidepsin ¹²³⁴	Antineoplastic	883	Natamycin ¹²	Antifungal
374	Ponatinib ¹²³⁴	Antineoplastic	884	Neticonazole ¹²³⁴	Antifungal
375	Pralatrexate ¹²³⁴	Antineoplastic	885	Nystatin ¹²³⁴	Antifungal
376	Pralsetinib ¹²³⁴	Antineoplastic	886	Omoconazole ¹²³⁴	Antifungal
377	Prednimustine ¹²³⁴	Antineoplastic	887	Oxiconazole ¹²³⁴	Antifungal
378	Procarbazine ¹²³⁴	Antineoplastic	888	Pecilocin ¹²	Antifungal
379	Quizartinib ¹²³⁴	Antineoplastic	889	Pentamidine ¹²³⁴	Antifungal
380	Radotinib ¹²³⁴	Antineoplastic	890	Posaconazole ¹²³⁴	Antifungal
381	Raltitrexed ¹²³⁴	Antineoplastic	891	Pyrrolnitrin ¹²³	Antifungal
382	Ranimustine ¹²³⁴	Antineoplastic	892	Ravuconazole ¹²³⁴	Antifungal
383	Regorafenib ¹²³⁴	Antineoplastic	893	Sertaconazole ¹²³⁴	Antifungal
384	Ribociclib ¹²³⁴	Antineoplastic	894	Sulbentine ¹²³⁴	Antifungal

385	Ridaforolimus ¹²³	Antineoplastic	895	Sulconazole ¹²³⁴	Antifungal
386	Ripretinib ¹²³⁴	Antineoplastic	896	Taurolidine ¹²	Antifungal
387	Rociletinib ¹²³	Antineoplastic	897	Tavaborole ¹²³⁴	Antifungal
388	Romidepsin ¹²³⁴	Antineoplastic	898	Terbinafine ¹²³⁴	Antifungal
389	Rubitecan ¹²	Antineoplastic	899	Terconazole ¹²³⁴	Antifungal
390	Rucaparib ¹²	Antineoplastic	900	Thiabendazole ¹²³⁴	Antifungal
391	Ruxolitinib ¹²³⁴	Antineoplastic	901	Ticlatone ¹²³⁴	Antifungal
392	Selinexor ¹²³⁴	Antineoplastic	902	Tioconazole ¹²³⁴	Antifungal
393	Selpercatinib ¹²³⁴	Antineoplastic	903	Tolciclate ¹²³⁴	Antifungal
394	Selumetinib ¹²³⁴	Antineoplastic	904	Tolnaftate ¹²³⁴	Antifungal
395	Semaxanib ¹²³	Antineoplastic	905	Tribromometacresol ¹²³⁴	Antifungal
396	Semustine ¹²³⁴	Antineoplastic	906	Undecylenic acid ¹²³⁴	Antifungal
397	Silatecan ¹²³	Antineoplastic	907	Voriconazole ¹²³⁴	Antifungal
398	Sonidegib ¹²³⁴	Antineoplastic	908	Acarbose ¹²³⁴	Antidiabetic
399	Sorafenib ¹²³⁴	Antineoplastic	909	Acetohexamide ¹²³⁴	Antidiabetic
400	Streptozocin ¹²	Antineoplastic	910	Aleglitazar ¹²³⁴	Antidiabetic
401	Sunitinib ¹²³⁴	Antineoplastic	911	Alogliptin ¹²³⁴	Antidiabetic
402	Talazoparib ¹²³⁴	Antineoplastic	912	Anagliptin ¹²³⁴	Antidiabetic
403	Tegafur ¹²³⁴	Antineoplastic	913	Benfluorex ¹²³⁴	Antidiabetic
404	Temozolomide ¹²³⁴	Antineoplastic	914	Bexagliflozin ¹²³⁴	Antidiabetic
405	Temsirolimus ¹²³⁴	Antineoplastic	915	Bromocriptine ¹²³⁴	Antidiabetic
406	Teniposide ¹²³⁴	Antineoplastic	916	Buformin ¹²³⁴	Antidiabetic
407	Tepotinib ¹²³⁴	Antineoplastic	917	Canagliflozin ¹²³⁴	Antidiabetic
408	Tesetaxel ¹²³	Antineoplastic	918	Carbutamide ¹²³⁴	Antidiabetic
409	Testolactone ¹²³⁴	Antineoplastic	919	Chlorpropamide ¹²³⁴	Antidiabetic
410	Tezacitabine ¹²³	Antineoplastic	920	Ciglitazone ¹²	Antidiabetic
411	Thiotepa ¹²³⁴	Antineoplastic	921	Dapagliflozin ¹²³⁴	Antidiabetic
412	Tiazofurine ¹²³	Antineoplastic	922	Darglitazone ¹²	Antidiabetic
413	Tioguanine ¹²	Antineoplastic	923	Empagliflozin ¹²³⁴	Antidiabetic
414	Tipifarnib ¹²³⁴	Antineoplastic	924	Englitazone ¹²³⁴	Antidiabetic
415	Tivozanib ¹²³⁴	Antineoplastic	925	Epalrestat ¹²	Antidiabetic
416	Toceranib ¹²³	Antineoplastic	926	Ertugliflozin ¹²³⁴	Antidiabetic
417	Topotecan ¹²³⁴	Antineoplastic	927	Evogliptin ¹²³⁴	Antidiabetic
418	Trabectedin ¹²³⁴	Antineoplastic	928	Fasiglifam ¹²³⁴	Antidiabetic
419	Trametinib ¹²³⁴	Antineoplastic	929	Fidarestat ¹²³	Antidiabetic
420	Treosulfan ¹²³⁴	Antineoplastic	930	Gemigliptin ¹²	Antidiabetic
421	Triapine ¹²³⁴	Antineoplastic	931	Glibenclamide ¹²³⁴	Antidiabetic
422	Triaziquone ¹²³⁴	Antineoplastic	932	Glibornuride ¹²³⁴	Antidiabetic
423	Triethylenemelamine ¹²³	Antineoplastic	933	Glicaramide ¹²³⁴	Antidiabetic
424	Trofosfamide ¹²³⁴	Antineoplastic	934	Gliclazide ¹²³⁴	Antidiabetic
425	Tucatinib ¹²³⁴	Antineoplastic	935	Glimepiride ¹²³⁴	Antidiabetic
426	Uramustine ¹²³⁴	Antineoplastic	936	Glipizide ¹²³⁴	Antidiabetic
427	Valrubicin ¹²	Antineoplastic	937	Gliquidone ¹²³⁴	Antidiabetic
428	Vandetanib ¹²³⁴	Antineoplastic	938	Glisoxepide ¹²³⁴	Antidiabetic
429	Vemurafenib ¹²³⁴	Antineoplastic	939	Glycopyramide ¹²³⁴	Antidiabetic
430	Venetoclax ¹²³⁴	Antineoplastic	940	Glymidine ¹²³⁴	Antidiabetic
431	Vinblastine ¹²³⁴	Antineoplastic	941	Gosogliptin ¹²³⁴	Antidiabetic
432	Vincristine ¹²³⁴	Antineoplastic	942	Ipragliflozin ¹²³⁴	Antidiabetic
433	Vindesine ¹²³⁴	Antineoplastic	943	Linagliptin ¹²³⁴	Antidiabetic
434	Vinflunine ¹²³⁴	Antineoplastic	944	Lobeglitazone ¹²³⁴	Antidiabetic
435	Vinorelbine ¹²³⁴	Antineoplastic	945	Luseogliflozin ¹²³⁴	Antidiabetic
436	Vismodegib ¹²³⁴	Antineoplastic	946	Metahexamide ¹²³⁴	Antidiabetic
437	Vorinostat ¹²³⁴	Antineoplastic	947	Metformin ¹²³⁴	Antidiabetic
438	Vosaroxin ¹²³⁴	Antineoplastic	948	Miglitol ¹²³⁴	Antidiabetic
439	Zorubicin ¹²	Antineoplastic	949	Mitiglinide ¹²³⁴	Antidiabetic
440	2,4-Diaminopyrimidine ¹	Antibacterial	950	Muraglitazar ¹²³⁴	Antidiabetic
441	Alatrofloxacin ¹²³⁴	Antibacterial	951	Nateglinide ¹²³⁴	Antidiabetic

442	Amdinocillin ¹²³⁴	Antibacterial	952	Netoglitazone ¹²³⁴	Antidiabetic
443	Amikacin ¹²³⁴	Antibacterial	953	Omarigliptin ¹²³⁴	Antidiabetic
444	Amoxicillin ¹²³⁴	Antibacterial	954	Phenformin ¹²³⁴	Antidiabetic
445	Ampicillin ¹²³⁴	Antibacterial	955	Pioglitazone ¹²³⁴	Antidiabetic
446	Apramycin ¹²³	Antibacterial	956	Ranirestat ¹²³⁴	Antidiabetic
447	Arbekacin ¹²³⁴	Antibacterial	957	Remogliflozin etabonate ¹²³⁴	Antidiabetic
448	Aspoxicillin ¹²³⁴	Antibacterial	958	Repaglinide ¹²³⁴	Antidiabetic
449	Astomicin ¹²³⁴	Antibacterial	959	Rivoglitazone ¹²³⁴	Antidiabetic
450	Avibactam ¹²³⁴	Antibacterial	960	Rosiglitazone ¹²³⁴	Antidiabetic
451	Azidamfenicol ¹	Antibacterial	961	Saroglitazar ¹²³⁴	Antidiabetic
452	Azidocillin ¹²³⁴	Antibacterial	962	Saxagliptin ¹²³⁴	Antidiabetic
453	Azithromycin ¹²³⁴	Antibacterial	963	Sergliflozin etabonate ¹²³⁴	Antidiabetic
454	Azlocillin ¹²³⁴	Antibacterial	964	Sitagliptin ¹²³⁴	Antidiabetic
455	Aztreonam ¹²³⁴	Antibacterial	965	Sotagliflozin ¹²³⁴	Antidiabetic
456	Bacampicillin ¹²³⁴	Antibacterial	966	Teneligliptin ¹²³⁴	Antidiabetic
457	Bacitracin ¹²³⁴	Antibacterial	967	Tesaglitazar ¹²³⁴	Antidiabetic
458	Balofloxacin ¹²³⁴	Antibacterial	968	Thiazolidinedione ¹²³	Antidiabetic
459	Bekanamycin ¹²³⁴	Antibacterial	969	Tofogliflozin ¹²³⁴	Antidiabetic
460	Benzylpenicillin ¹²³⁴	Antibacterial	970	Tolazamide ¹²³⁴	Antidiabetic
461	Besifloxacin ¹²³⁴	Antibacterial	971	Tolbutamide ¹²³⁴	Antidiabetic
462	Biapenem ¹²³⁴	Antibacterial	972	Tolrestat ¹²³⁴	Antidiabetic
463	Boromycin ¹²	Antibacterial	973	Trelagliptin ¹²³⁴	Antidiabetic
464	Brodinoprim ¹²³⁴	Antibacterial	974	Troglitazone ¹²³⁴	Antidiabetic
465	Carbenicillin ¹²³⁴	Antibacterial	975	Vildagliptin ¹²³⁴	Antidiabetic
466	Carindacillin ¹²³⁴	Antibacterial	976	Voglibose ¹²³⁴	Antidiabetic
467	Carumonam ¹²³⁴	Antibacterial	977	Zenarestat ¹²³	Antidiabetic
468	Cefacetrile ¹²³⁴	Antibacterial	978	Acebutolol ¹²³⁴	Anti-arrhythmic
469	Cefaclor ¹²³⁴	Antibacterial	979	Ajmaline ¹²³⁴	Anti-arrhythmic
470	Cefadroxil ¹²³⁴	Antibacterial	980	Amiodarone ¹²³⁴	Anti-arrhythmic
471	Cefalexin	Antibacterial	981	Aprindine ¹²³⁴	Anti-arrhythmic
472	Cefaloglycin ¹²³⁴	Antibacterial	982	Atenolol ¹²³⁴	Anti-arrhythmic
473	Cefalonium ¹²³⁴	Antibacterial	983	Atropine ¹²³	Anti-arrhythmic
474	Cefaloridine ¹²³⁴	Antibacterial	984	Bretylum ¹²³⁴	Anti-arrhythmic
475	Cefalotin ¹²³⁴	Antibacterial	985	Bunaftine ¹²³⁴	Anti-arrhythmic
476	Cefamandole ¹²³⁴	Antibacterial	986	Celivarone ¹²³⁴	Anti-arrhythmic
477	Cefapirin ¹²³⁴	Antibacterial	987	Cibenzoline ¹²³⁴	Anti-arrhythmic
478	Cefatrizine ¹²³⁴	Antibacterial	988	Digitoxin ¹²³⁴	Anti-arrhythmic
479	Cefazaflur ¹²³⁴	Antibacterial	989	Digoxin ¹²³⁴	Anti-arrhythmic
480	Cefazedone ¹²³⁴	Antibacterial	990	Diltiazem ¹²³⁴	Anti-arrhythmic
481	Cefazolin ¹²³⁴	Antibacterial	991	Disopyramide ¹²	Anti-arrhythmic
482	Cefbuperazone ¹²³⁴	Antibacterial	992	Dofetilide ¹²³⁴	Anti-arrhythmic
483	Cefcapene ¹²³⁴	Antibacterial	993	Dronedarone ¹²³⁴	Anti-arrhythmic
484	Cefdaloxime ¹²³⁴	Antibacterial	994	Encainide ¹²³⁴	Anti-arrhythmic
485	Cefdinir ¹²³⁴	Antibacterial	995	Esmolol ¹²³⁴	Anti-arrhythmic
486	Cefditoren ¹²³⁴	Antibacterial	996	Ethacizine ¹²³⁴	Anti-arrhythmic
487	Cefepime ¹²³⁴	Antibacterial	997	Flecainide ¹²³⁴	Anti-arrhythmic
488	Cefetamet ¹²³⁴	Antibacterial	998	Hydroquinidine ¹²³⁴	Anti-arrhythmic
489	Cefixime ¹²³⁴	Antibacterial	999	Ibutilide ¹²³⁴	Anti-arrhythmic
490	Cefmenoxime ¹²³⁴	Antibacterial	1000	Indecainide ¹²	Anti-arrhythmic
491	Cefmetazole ¹²³⁴	Antibacterial	1001	Lorajmine ¹²³⁴	Anti-arrhythmic
492	Cefminox ¹²³⁴	Antibacterial	1002	Lorcainide ¹²³⁴	Anti-arrhythmic
493	Cefodizime ¹²³⁴	Antibacterial	1003	Metoprolol ¹²³⁴	Anti-arrhythmic
494	Cefonicid ¹²³⁴	Antibacterial	1004	Moracizine ¹²³⁴	Anti-arrhythmic
495	Cefoperazone ¹²³⁴	Antibacterial	1005	Nadolol ¹²³⁴	Anti-arrhythmic
496	Ceforanide ¹²³⁴	Antibacterial	1006	Nifekalant ¹²³⁴	Anti-arrhythmic
497	Cefotaxime ¹²³⁴	Antibacterial	1007	Ouabain ¹²³⁴	Anti-arrhythmic
498	Cefotetan ¹²³⁴	Antibacterial	1008	Pindolol ¹²³⁴	Anti-arrhythmic

499	Cefotiam ¹²³⁴	Antibacterial	1009	Prajaline ¹²³⁴	Anti-arrhythmic
500	Cefovecin ¹²³	Antibacterial	1010	Procainamide ¹²³⁴	Anti-arrhythmic
501	Cefoxitin ¹²³⁴	Antibacterial	1011	Propafenone ¹²³⁴	Anti-arrhythmic
502	Cefozopran ¹²³⁴	Antibacterial	1012	Propranolol ¹²	Anti-arrhythmic
503	Cefpimizole ¹²³⁴	Antibacterial	1013	Quinidine ¹²³⁴	Anti-arrhythmic
504	Cefpiramide ¹²³⁴	Antibacterial	1014	Sotalol ¹²³⁴	Anti-arrhythmic
505	Cefpirome ¹²³⁴	Antibacterial	1015	Sparteine ¹²³⁴	Anti-arrhythmic
506	Cefpodoxime ¹²³⁴	Antibacterial	1016	Tedisamil ¹²³⁴	Anti-arrhythmic
507	Cefprozil ¹²³⁴	Antibacterial	1017	Tocainide ¹²³⁴	Anti-arrhythmic
508	Cefradine ¹²³⁴	Antibacterial	1018	Verapamil ¹²³⁴	Anti-arrhythmic
509	Cefroxadine ¹²³⁴	Antibacterial	1019	Vernakalant ¹²³⁴	Anti-arrhythmic
510	Cefsulodin ¹²³⁴	Antibacterial			

1. Molecule is in molecular set S₁. 2. Molecule is in molecular set S₂. 3. Molecule is in molecular set S₃. 4. Molecule is in molecular set S₄.

Table S2. Molecules in external validation set.

No.	Name	Category
1	Abiraterone acetate	Antineoplastic
2	Acetylcysteine	Analgesic, antineoplastic, antiviral
3	Anastrozole	Antineoplastic
4	Apalutamide	Antineoplastic
5	Avapritinib	Antineoplastic
6	Berzosertib	Antineoplastic
7	Capmatinib	Antineoplastic
8	Celecoxib	Analgesic, antineoplastic
9	Cyproheptadine	Analgesic
10	Cytarabine	Antineoplastic, antiviral
11	Darolutamide	Antineoplastic
12	Dextromethorphan	Analgesic, antiviral
13	Duvelisib	Antineoplastic
14	Enzalutamide	Antineoplastic
15	Exemestane	Antineoplastic
16	Fulvestrant	Antineoplastic
17	Glasdegib	Antineoplastic
18	Lasmiditan	Analgesic
19	Letrozole	Antineoplastic
20	Lurbinectedin	Antineoplastic
21	Methylethylgometriner	Analgesic
22	Mobocertinib	Antineoplastic
23	Oliceridine	Analgesic
24	Pomalidomide	Analgesic, antineoplastic
25	Promethazine	Analgesic, antiviral
26	Rifampicin	Antibacterial, antiviral
27	Salicylic acid	Analgesic, antibacterial, antifungal
28	Seliciclib	Antineoplastic, antiviral
29	Sotorasib	Antineoplastic
30	Suxibuzone	Analgesic, antineoplastic
31	Talaporfin	Antineoplastic
32	Tamoxifen	Antineoplastic
33	Tazemetostat	Antineoplastic
34	Tofacitinib	Antineoplastic
35	Ubrogepant	Analgesic
36	Vebicorvir	Antiviral
37	Zanubrutinib	Antineoplastic