

Supplement

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“Chemo- and bioinformatics resources for in silico drug discovery from medicinal plants beyond their traditional use: a critical review”

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PASS (Prediction of Activity Spectra for Substances) Approach

PASS provides simultaneous predictions of many types of biological activity (activity spectrum) based on the structure of drug-like compounds. The approach used in PASS is based on the suggestion that biological activity of any drug-like compound is a function of its structure. In PASS biological activities are described qualitatively (active or inactive).

The Biological Activity Spectrum of a chemical compound is a set of different biological activity types that reflect results of the compound's interaction with various biological entities.

The 2D structural formulae of compounds were taken as the basis for *description of a chemical structure* because this is the only information available at the early stage of research.

The molecular structure is represented by the set of unique Multilevel Neighbourhoods of Atoms (MNA) descriptors of the 1st and 2nd levels. The MNA descriptors are based on the molecular structure representation, which includes the hydrogen atoms according to the valences and partial charges of the atoms and does not specify the types of bonds. These descriptors are a linear notation of atom-centred fragments in the structure of an organic molecule (Filimonov *et al.*, 1999). MNA descriptors are generated as the recursively defined sequence:

- Zero-level MNA descriptor for each atom is the mark *A* of the atom itself;
- Any next-level MNA descriptor for the atom is the sub-structure notation $A(D_1D_2...D_i...)$, where D_i is the previous-level MNA descriptor for i -th immediate neighbor's of the atom *A*.

The mark of an atom may include not only the atomic type but also any additional information about the atom. In particular, if the atom is not included into the ring, it is marked by «-». The neighbor descriptors $D_1D_2...D_i...$ are arranged in a unique lexicographic order. Iterative process of MNA descriptors generation can be continued covering first, second, etc. neighborhoods of each atom.

An example of the structure presentation by MNA descriptors for Quercetin is shown in Fig. S1.

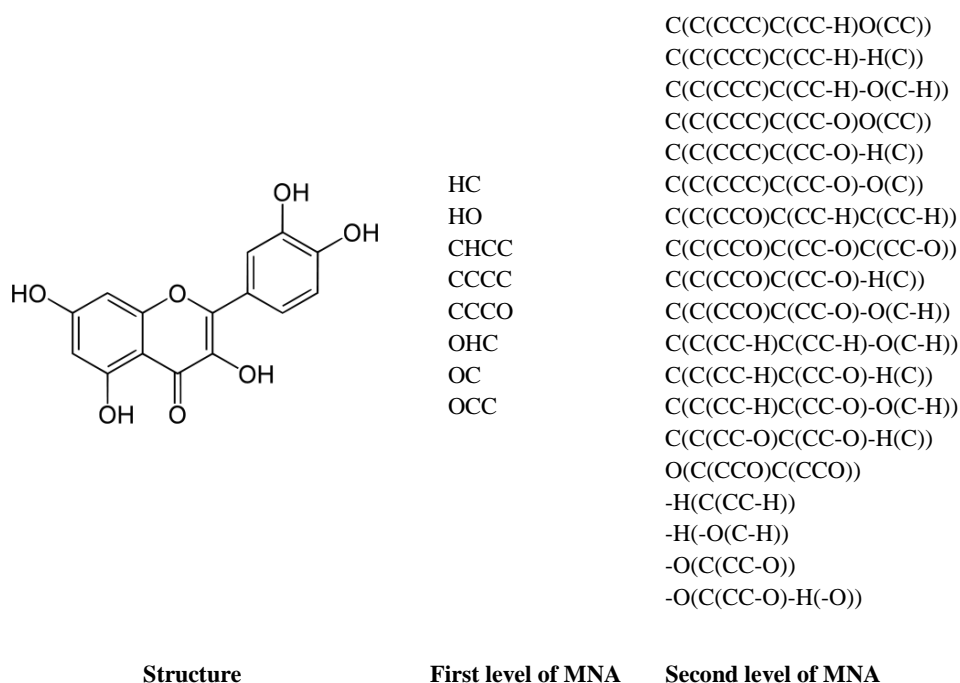


Fig. S1. Quercetin's molecule structure and its presentation by MNA descriptors.

The MNA descriptors are generated, and prediction is executed, only if molecular structure corresponds to the following criteria:

- Each atom in a molecule must be presented by an atom symbol from the periodic table. Symbols of unspecified atom A, Q, *, or R group labels are not allowed;
- Each bond in a molecule must be a covalent bond presented by single, double or triple bond types only;
- The structure must include three or more carbon atoms;

- The structure must include only one component. The second component consisted of 1-2 atoms, e.g. HCl, Cl-, OH-, Na+, etc., is excluded from MNA descriptors generation; if the second component contained more than 2 atoms, the structure is not used for prediction;
- The structure (basic part, see the previous sentence) must be neutralized;
- The absolute molecular weight of a compound must be less than 1250.

The substances are considered as being equivalent in PASS if they have the same set of MNA descriptors. Since MNA descriptors do not represent the stereochemical peculiarities of the molecule, the substances whose structures differ only stereochemically, are formally considered to be equivalent.

The PASS estimations of biological activity spectra for new compounds are based on the Structure-Activity Relationships database (SAR Base), which accumulates the results of the training set analysis.

Algorithm of the activity spectrum estimation is based on the naive Bayes approach with some significant enhancements. For each kind of activity A_k , which can be predicted by PASS, on the basis of a molecule's structure represented by the set of MNA descriptors $\{D_1, \dots, D_m\}$ the following values are calculated:

$$S_{0k} = 2P(A_k) - 1,$$

$$S_k = \text{Sin}[\sum_i \text{ArcSin}(2P(A_k|D_i) - 1)/m],$$

$$B_k = (S_k - S_{0k}) / (1 - S_k S_{0k}),$$

where $P(A_k)$ is *a priori* probability to find a compound with activity of kind A_k ; $P(A_k|D_i)$ is a conditional probability of activity of kind A_k if the descriptor D_i is present in a set of molecule's descriptors; m is a number of MNA descriptors in molecule under prediction.

The simplest frequency estimations of probabilities $P(A_k)$, $P(A_k|D_i)$ are given by:

$$P(A_k) = N_k/N, \quad P(A_k|D_i) = N_{ik}/N_i.$$

where N is the total number of compounds in the SAR Base; N_k is the number of compounds contained A_k activity in the activity spectrum; N_i is the number of compounds contained descriptor D_i in the structure description; N_{ik} is the number of compounds contained both the activity A_k and the descriptor D_i .

Leave-one-out cross-validation for all predictable types of biological activity and all substances in PASS training set provides the estimate of PASS prediction accuracy during the training procedure. The accuracy criterion ROC AUC (the Area Under the ROC Curve) is used. It is the estimate of the probability that positive and negative examples (active and inactive compounds) arbitrarily chosen from a validation set may be classified correctly by the prediction.

The predicted activity spectrum in PASS is presented by a list of activities with probabilities «to be active» Pa and «to be inactive» Pi , which are the functions of B value for a molecule under prediction. The list of predicted activities is arranged in a descending order of $Pa-Pi$ values. Thus, the more probable activity types are at the top of the list. If the user chooses rather a higher value of Pa as a cut-off for selection of probable activities, the chance to confirm the predicted activities by the experiment is also high, but many existing activities will be lost. For instance, if $Pa > 0.5$ is used as a threshold, about half of real activities will be lost; for $Pa > 0.7$, the portion of lost activities is 70%, etc.

By definition, the probabilities Pa and Pi are measures of belonging to both subsets of "active" and "inactive" compounds, and the probabilities of the 1st and 2nd types of prediction error, respectively. These two interpretations of the probabilities Pa and Pi are equivalent and can be used for interpreting the results of prediction. They can also be used for construction of different criteria for an analysis of prediction results corresponding to the specific practical tasks.

An example of prediction results for **Quercetin** is shown in Fig. S2.

Prediction results of therapeutic effects

Pa	Pi	Effect
0.962	0.001	* Antimutagenic
0.910	0.003	* Antioxidant
0.887	0.002	* Hemostatic
0.874	0.001	* Capillary fragility treatment
0.851	0.003	* Cardioprotectant
0.847	0.007	Antineurotoxic
0.832	0.017	Antiseborrheic
0.816	0.005	* Apoptosis agonist
0.810	0.005	Vasoprotector
0.778	0.007	* Anticarcinogenic
0.734	0.006	Chemopreventive
0.718	0.002	* Antihemorrhagic
0.706	0.014	* Antiinflammatory
0.704	0.018	Antineoplastic (lung cancer)
		...

Prediction results of mechanisms of action

Pa	Pi	Mechanism of action
0.987	0.001	* Chlordecone reductase inhibitor
0.972	0.001	* 2-Dehydropantoate 2-reductase inhibitor
0.971	0.002	* 1-Phosphatidylinositol-4-phosphate 5-kinase inhibitor
0.968	0.001	* Aryl-alcohol dehydrogenase (NADP+) inhibitor
0.965	0.001	* P-benzoquinone reductase (NADPH) inhibitor
0.963	0.002	* Membrane permeability inhibitor
0.956	0.001	* NADPH-ferrihemoprotein reductase inhibitor
0.944	0.001	* Glycerol dehydrogenase (NADP+) inhibitor
0.942	0.001	* 2-Dehydropantolactone reductase (A-specific) inhibitor
0.942	0.001	* Cystathionine beta-synthase inhibitor
0.938	0.002	* Alcohol dehydrogenase (NADP+) inhibitor
0.934	0.001	Quercetin 2,3-dioxygenase inhibitor
0.934	0.001	* Beta-carotene 15,15'-monooxygenase inhibitor
0.921	0.001	Chalcone isomerase inhibitor
0.919	0.002	Monophenol monooxygenase inhibitor
0.908	0.002	* Xenobiotic-transporting ATPase inhibitor
0.902	0.001	* Iodide peroxidase inhibitor
0.900	0.002	2-Enoate reductase inhibitor
0.902	0.006	Ubiquinol-cytochrome-c reductase inhibitor
0.896	0.001	* Testosterone 17beta-dehydrogenase inhibitor
0.894	0.002	Histidine kinase inhibitor
		...

Fig. S2. The part of prediction results of effects and mechanisms of action for Quercetin by PASS. * - known activity.

More detailed description of PASS can be found in our publications (Filimonov and Poroikov, 2008); description of freely available PASS web-service can be found in papers (Lagunin et al., 2000; Sadym et al., 2003; Geronikaki et al., 2008); examples of PASS application can be found in papers (Anzali et al., 2001; Poroikov et al., 2001; Poroikov et al., 2002; Borodina et al., 2003; Poroikov et al., 2003; Lagunin et al., 2003; Geronikaki et al., 2004; Dembitsky et al., 2005; Zotchev et al., 2006; Poroikov et al., 2007; Lagunin et al., 2010; Goel et al., 2011; Kryzhanovskii et al., 2012; Buchkevich et al., 2012; Lagunin et al., 2013; Filimonov et al., 2014).

References

Anzali S., Barnickel G., Cezanne B., Krug M., Filimonov D., Poroikov V. (2001). Discriminating between drugs and nondrugs by Prediction of Activity Spectra for Substances (PASS). *J. Med. Chem.*, **44** (15), 2432-2437.

- Borodina Yu., Sadym A., Filimonov D., Blinova V., Dmitriev A., Poroikov V. (2003). Predicting biotransformation potential from molecular structure. *J. Chem. Inform. Comput. Sci.*, **43** (5), 1636-1646.
- Buchkevych I., Stasevych M., Chervetsova V., Musyanovych R., Novikov V., Poroikov V., Glorizova T., Filimonov D., Zagoriy G., Ponomarenko M. (2012). Synthesis, computational and antimicrobial studies of new 1,4-naphthoquinone aminothiazole derivatives. *Cheminé Technologija*, Nr. 3 (61) 62-69.
- Dembitsky V.M., Glorizova T.A., Poroikov V.V. (2005). Novel antitumor agents: marine sponge alkaloids, their synthetic analogues and derivatives. *Mini-Reviews in Medicinal Chemistry*, **5** (3), 319-336.
- Filimonov, D. and Poroikov, V. (2008) Probabilistic approach in activity prediction. In: Alexandre Varnek and Alexander Tropsha (Eds.). *Chemoinformatics Approaches to Virtual Screening*. RSC Publishing, Cambridge, UK. pp. 182-216.
- Filimonov D.A., Lagunin A.A., Glorizova T.A., Rudik A.V., Druzhilovskii D.S., Pogodin P.V., Poroikov V.V. (2014) Prediction of the biological activity spectrum of organic compounds using the PASS Online web resource. *Chem. Heterocycl. Compd.*, **50**(3), 444-457.
- Geronikaki A., Dearden J., Filimonov D., Galaeva I., Garibova T., Glorizova T., Krajneva V., Lagunin A., Macaev F., Molodavkin G., Poroikov V., Pogrebnoi S., Shepeli F., Voronina T., Tsitlakidou M., Vlad L. (2004). Design of new cognition enhancers: from computer prediction to synthesis and biological evaluation. *J. Med. Chem.*, **47** (11), 2870-2876.
- Geronikaki A., Druzhilovsky D., Zakharov A., Poroikov V. (2008). Computer-aided predictions for medicinal chemistry via Internet. *SAR and QSAR in Environ. Res.*, **19** (1 & 2), 27-38.
- Goel R.K., Singh D., Lagunin A., Poroikov V. (2011). PASS-assisted exploration of new therapeutic potential of natural products. *Med. Chem. Res.*, **20** (9), 1509-1514.
- Kryzhanovskii S.A., Salimov R.M., Lagunin A.A., Filimonov D.A., Glorizova T.A., Poroikov V.V. (2012). Nootropic action of some antihypertensive drugs: computer predicting and experimental testing. *Pharmaceut. Chem. J.*, **45** (10), 605-611.
- Lagunin A., Stepanchikova A., Filimonov D., Poroikov V. (2000). PASS: prediction of activity spectra for biologically active substances. *Bioinformatics*, **16** (8), 747-748.
- Lagunin A., Ivanov S., Rudik A., Filimonov D., Poroikov V. (2013). DIGEP-Pred: web-service for *in silico* prediction of drug-induced gene expression profiles based on structural formula. *Bioinformatics*, **29**, 2062-2063.
- Lagunin A.A., Gomazkov O.A., Filimonov D.A., Gureeva T.A., Dilakyan E.A., Kugaevskaya E.V., Elisseeva Yu.E., Solovyeva N.I., Poroikov V.V. (2003). Computer-aided selection of potential antihypertensive compounds with dual mechanisms of action. *J. Med. Chem.*, **46** (15), 3326-3332.
- Lagunin A., Filimonov D.A., Poroikov V.V. (2010). Multi-targeted natural products evaluation based on biological activity prediction with PASS. *Cur. Phar. Des.*, **16** (15), 1703-1717.
- Poroikov V., Akimov D., Shabelnikova E., Filimonov D. (2001). Top 200 medicines: can new actions be discovered through computer-aided prediction? *SAR and QSAR in Environmental Research*, **12** (4), 327-344.
- Poroikov V.V., Filimonov D.A. (2002). How to acquire new biological activities in old compounds by computer prediction. *J. Comput. Aid. Molec. Des.*, **16** (11), 819-824.
- Poroikov V.V., Filimonov D.A., Ihlenfeldt W.-D., Glorizova T.A., Lagunin A.A., Borodina Yu.V., Stepanchikova A.V., Nicklaus M.C. (2003). PASS Biological Activity Spectrum Predictions in the Enhanced Open NCI Database Browser. *J. Chem. Inform. Comput. Sci.*, **43** (1) 228-236.
- Poroikov V., Filimonov D., Lagunin A., Glorizova T., Zakharov A. (2007). PASS: Identification of probable targets and mechanisms of toxicity. *SAR & QSAR in Environmental Research*, **18** (1-2), 101-110.
- Sadym A., Lagunin A., Filimonov D., Poroikov V. (2003). Prediction of biological activity spectra via Internet. *SAR and QSAR in Environmental Research*, **14** (5-6), 339-347.
- Zotchev S.B., Stepanchikova A.V., Sergeiko A.P., Sobolev B.N., Filimonov D.A., Poroikov V.V. (2006). Rational design of macrolides by virtual screening of combinatorial libraries generated through *in silico* manipulation of polyketide synthases. *J. Med. Chem.*, **49** (6), 2077-2087.

Table S1. The lists of 122 known therapeutic effects for 50 analyzed medicinal plants with accuracy of PASS prediction calculated by a leave-one-out cross-validation procedure during the training and number of active compounds in PASS training set.

No	Predictable Therapeutic Effect	Number of actives	AUC calculated by LOO CV, %
1	Abortion inducer	39	94.6
2	Acaricide	45	94.5
3	Allergic rhinitis treatment	494	96.6
4	Alzheimer's disease treatment	2616	89.1
5	Analgesic	8946	86.7
6	Angiogenesis inhibitor	4680	91.2
7	Anorexiant	406	80.1
8	Antialcoholic	125	90.5
9	Antiallergic	7237	88.8
10	Antiarthritic	11728	87.2
11	Antiasthmatic	8912	89.0
12	Antibacterial	7916	92.1
13	Anticarcinogenic	371	90.4
14	Anticoagulant	2655	94.8
15	Anticonvulsant	1521	87.6
16	Antidepressant	8119	91.7
17	Antidiabetic	12058	90.2
18	Antidiabetic (type 2)	3177	94.6
19	Antidiarrheal	267	89.8
20	Antidote, heavy metal	50	98.1
21	Antiepileptic	2466	92.6
22	Antifibrinolytic	18	87.3
23	Antifungal	2300	91.1
24	Antiglaucomic	1434	94.1
25	Antihelmintic	490	92.4
26	Antihelmintic (Nematodes)	59	90.1
27	Antihypercholesterolemic	289	90.2
28	Antihyperlipoproteinemic	115	93.9
29	Antihypertensive	9469	90.1
30	Antiinfective	212	87.1
31	Antiinfertility, female	88	93.2
32	Antiinflammatory	6495	84.2
33	Antiischemic, cerebral	507	77.3
34	Antileprosy	64	93.0
35	Antileukemic	377	87.8
36	Antimetastatic	24	85.0
37	Antimutagenic	36	96.1
38	Antineoplastic	39533	87.1
39	Antinociceptive	49	88.5
40	Antiobesity	7882	91.4
41	Antiosteoporotic	2863	93.2
42	Antioxidant	898	94.0
43	Antiparasitic	648	92.1

44	Antiparkinsonian	2812	89.1
45	Antiprotozoal	1765	90.3
46	Antiprotozoal (Amoeba)	95	88.6
47	Antiprotozoal (Leishmania)	169	88.6
48	Antiprotozoal (Plasmodium)	786	91.9
49	Antipruritic	290	86.2
50	Antipsoriatic	1972	90.5
51	Antipsychotic	6826	92.8
52	Antipyretic	423	92.0
53	Antithrombotic	637	86.6
54	Antitoxic	151	88.7
55	Antituberculosic	454	89.0
56	Antitussive	259	93.2
57	Antiulcerative	950	88.3
58	Antiuro lithic	145	77.6
59	Antiviral	11031	91.7
60	Antiviral (HIV)	6769	94.6
61	Antiviral (Herpes)	161	90.7
62	Anxiolytic	8237	90.7
63	Apoptosis agonist	1894	88.3
64	Bronchodilator	2095	95.5
65	Cardiodepressant	166	91.2
66	Cardioprotectant	204	86.4
67	Cardiotoxic	706	82.8
68	Cardiovascular analeptic	19	91.8
69	Chemopreventive	351	93.6
70	Chronic obstructive pulmonary disease treatment	2542	93.3
71	Cognition disorders treatment	9374	87.3
72	Constipation treatment	93	94.4
73	Contraceptive	876	95.1
74	Cytoprotectant	45	79.9
75	Cytostatic	324	90.5
76	Cytotoxic	785	92.4
77	Dementia treatment	13	84.8
78	Diabetic nephropathy treatment	66	90.0
79	Diabetic neuropathy treatment	57	82.5
80	Diuretic	777	91.9
81	Dysmenorrhea treatment	171	97.6
82	Genotoxic	146	94.8
83	Growth stimulant	78	94.2
84	Hair growth stimulant	533	96.6
85	Hepatoprotectant	322	89.8
86	Huntington's disease treatment	148	95.1
87	Hyperparathyroidism treatment	69	98.4
88	Hypoglycemic	443	90.7
89	Hypolipemic	2263	89.5
90	Immunomodulator	1702	89.0
91	Immunostimulant	1038	91.6

92	Immunosuppressant	2074	87.2
93	Insecticide	239	96.3
94	Insulin sensitizer	226	96.8
95	Lassitude treatment	18	94.0
96	Male reproductive dysfunction treatment	603	94.2
97	Metabolic disease treatment	184	90.2
98	Muscle relaxant	410	91.5
99	Myasthenia Gravis treatment	17	75.3
100	Myocardial ischemia treatment	1723	94.9
101	Neurodegenerative diseases treatment	1016	93.3
102	Neuroprotector	473	75.7
103	Neurotoxic	551	86.0
104	Nootropic	1200	75.9
105	Platelet aggregation inhibitor	3106	91.0
106	Proliferative diseases treatment	210	90.9
107	Psychosexual dysfunction treatment	63	93.4
108	Radioprotector	256	88.5
109	Renal disease treatment	1082	93.5
110	Retinoprotector	24	82.8
111	Rheumatoid arthritis treatment	1898	90.8
112	Rhinitis treatment	306	85.8
113	Sedative	1215	91.3
114	Spasmolytic	1493	89.9
115	Spermicide	58	86.8
116	Systemic lupus erythematosus treatment	142	88.7
117	Teratogen	1552	89.8
118	Ulcerative colitis treatment	3	100.0
119	Urolithiasis treatment	6	89.8
120	Uterine relaxant	48	86.8
121	Uterine stimulant	35	94.7
122	Wound healing agent	310	91.6

Table S2. The lists of 3,345 mechanisms of action that were predicted by PASS and were used in this study with accuracy of PASS prediction calculated by a leave-one-out cross-validation procedure during the training and number of active compounds in PASS training set.

No	Predictable mechanism of action	Number of actives	AUC calculated by LOO CV, %
1	(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor	6	95.1
2	(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor	24	99.6
3	(R)-6-hydroxynicotine oxidase inhibitor	3	92.8
4	(R)-Pantolactone dehydrogenase (flavin) inhibitor	8	87.2
5	(R)-aminopropanol dehydrogenase inhibitor	10	98.9
6	(R,R)-butanediol dehydrogenase inhibitor	3	99.4
7	(S)-2-Methylmalate dehydratase inhibitor	4	99.6
8	(S)-2-hydroxy-acid oxidase inhibitor	28	92.5
9	(S)-3-amino-2-methylpropionate transaminase inhibitor	8	95.1
10	(S)-3-hydroxyacid ester dehydrogenase inhibitor	3	99.0
11	(S)-6-hydroxynicotine oxidase inhibitor	4	95.1
12	(S)-carnitine 3-dehydrogenase inhibitor	7	98.6
13	(S)-methylmalonyl-CoA hydrolase inhibitor	8	100.0
14	1,2-alpha-L-fucosidase inhibitor	5	94.3
15	1,3-Beta-glucan synthase inhibitor	4	84.3
16	1,4-Alpha-glucan branching enzyme inhibitor	4	95.4
17	1,4-Lactonase inhibitor	4	80.6
18	1,5-Anhydro-D-fructose reductase inhibitor	9	99.1
19	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor	7	91.6
20	1-Alkyl-2-acetyl glycerol O-acyltransferase inhibitor	3	99.7
21	1-Alkyl-2-acetyl glycerophosphocholine esterase inhibitor	419	99.4
22	1-Alkylglycerophosphocholine O-acetyltransferase inhibitor	24	92.1
23	1-Aminocyclopropane-1-carboxylate deaminase inhibitor	11	98.5
24	1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor	3	96.4
25	1-Phosphatidylinositol-4-phosphate 5-kinase inhibitor	12	75.8
26	1-Phosphofructokinase inhibitor	9	98.9
27	1-Pyrroline-5-carboxylate dehydrogenase inhibitor	24	98.8
28	11-Beta-hydroxysteroid dehydrogenase 1 inhibitor	983	99.3
29	11-Beta-hydroxysteroid dehydrogenase inhibitor	996	99.3
30	11-Cis-retinyl-palmitate hydrolase inhibitor	4	99.5
31	12-Lipoxygenase inhibitor	46	99.2
32	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor	8	96.6
33	15-Lipoxygenase inhibitor	153	97.1
34	15-Oxoprostaglandin 13-reductase inhibitor	9	77.0
35	17-Beta-hydroxysteroid dehydrogenase 1 inhibitor	49	98.2
36	17-Beta-hydroxysteroid dehydrogenase 5 inhibitor	6	100.0
37	2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor	7	98.7
38	2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor	5	96.7
39	2,3-Dihydroxyindole 2,3-dioxygenase inhibitor	4	98.3
40	2,3-Oxidosqualene-lanosterol cyclase inhibitor	103	98.6
41	2,4-Diaminopentanoate dehydrogenase inhibitor	3	98.8
42	2,4-Dichlorophenol 6-monooxygenase inhibitor	9	97.0
43	2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor	7	98.8

44	2,6-Dihydroxypyridine 3-monooxygenase inhibitor	3	98.2
45	2-(acetamidomethylene)succinate hydrolase inhibitor	11	99.9
46	2-Acylglycerol O-acyltransferase inhibitor	18	93.4
47	2-Amino-4-hydroxy-6-hydroxymethyl-dihydropteridine diphosphokinase inhibitor	4	99.8
48	2-Amino adipate transaminase inhibitor	6	98.3
49	2-Aminoethylphosphonate-pyruvate transaminase inhibitor	9	98.9
50	2-Aminohexano-6-lactam racemase inhibitor	19	98.3
51	2-Aminohexanoate transaminase inhibitor	3	100.0
52	2-Chlorobenzoate 1,2-dioxygenase inhibitor	5	78.1
53	2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor	4	99.2
54	2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor	6	99.0
55	2-Dehydropantoate 2-reductase inhibitor	7	80.7
56	2-Dehydropantoate aldolase inhibitor	3	99.0
57	2-Dehydropantolactone reductase (A-specific) inhibitor	10	99.0
58	2-Enoate reductase inhibitor	10	96.0
59	2-Ethylmalate synthase inhibitor	3	99.9
60	2-Haloacid dehalogenase (configuration-inverting) inhibitor	6	98.3
61	2-Haloacid dehalogenase inhibitor	3	97.0
62	2-Hydroxy-3-oxoadipate synthase inhibitor	3	98.0
63	2-Hydroxy-3-oxopropionate reductase inhibitor	5	98.9
64	2-Hydroxyacylsphingosine 1-beta-galactosyltransferase inhibitor	3	100.0
65	2-Hydroxy-muconate-semialdehyde hydrolase inhibitor	7	93.1
66	2-Hydroxyquinoline 5,6-dioxygenase inhibitor	4	80.0
67	2-Hydroxyquinoline 8-monooxygenase inhibitor	6	84.2
68	2-Isopropylmalate synthase inhibitor	15	99.8
69	2-Methyl-branched-chain-enoyl-CoA reductase inhibitor	5	97.7
70	2-Methylacyl-CoA dehydrogenase inhibitor	7	98.3
71	2-Methylcitrate dehydratase inhibitor	4	99.5
72	2-Methylcitrate synthase inhibitor	3	97.6
73	2-Methyleneglutarate mutase inhibitor	9	99.0
74	2-Nitrophenol 2-monooxygenase inhibitor	3	99.0
75	2-Nitropropane dioxygenase inhibitor	21	96.6
76	2-Oxoaldehyde dehydrogenase (NAD+) inhibitor	12	98.9
77	2-Oxoaldehyde dehydrogenase (NADP+) inhibitor	3	98.2
78	2-Oxoglutarate decarboxylase inhibitor	8	98.0
79	2-Oxoisovalerate dehydrogenase (acylating) inhibitor	4	99.1
80	2-Pyrocatechuate decarboxylase inhibitor	20	99.1
81	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	6	82.8
82	3 Beta-hydroxy-delta 5-steroid dehydrogenase inhibitor	97	100.0
83	3'(2'),5'-Bisphosphate nucleotidase inhibitor	4	99.6
84	3'-Demethylstaurosporine O-methyltransferase inhibitor	4	96.6
85	3'-Nucleotidase inhibitor	8	97.5
86	3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor	9	99.2
87	3(or 17)beta-hydroxysteroid dehydrogenase inhibitor	63	97.6
88	3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor	4	98.5
89	3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor	12	99.6
90	3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor	9	100.0
91	3-Aminobutyryl-CoA ammonia-lyase inhibitor	3	99.2

92	3-Carboxyethylcatechol 2,3-dioxygenase inhibitor	4	98.6
93	3-Chloro-D-alanine dehydrochlorinase inhibitor	4	98.5
94	3-Cyanoalanine hydratase inhibitor	4	83.9
95	3-Dehydroquininate dehydratase inhibitor	14	99.3
96	3-Dehydroquininate synthase inhibitor	16	99.4
97	3-Demethylubiquinone-9 3-O-methyltransferase inhibitor	3	98.5
98	3-Deoxy-7-phosphoheptulonate synthase inhibitor	48	99.1
99	3-Deoxy-8-phosphooctulonate synthase inhibitor	8	99.4
100	3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor	3	99.2
101	3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor	6	97.8
102	3-Hydroxyacyl-CoA dehydrogenase inhibitor	4	99.3
103	3-Hydroxyanthranilate 3,4-dioxygenase inhibitor	14	94.6
104	3-Hydroxyanthranilate oxidase inhibitor	13	97.8
105	3-Hydroxybenzoate 4-monoxygenase inhibitor	7	97.9
106	3-Hydroxybenzoate 6-monoxygenase inhibitor	5	84.2
107	3-Hydroxybutyrate dehydrogenase inhibitor	25	98.8
108	3-Hydroxybutyryl-CoA dehydrogenase inhibitor	3	98.8
109	3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor	9	98.8
110	3-Hydroxyisobutyryl-CoA hydrolase inhibitor	7	100.0
111	3-Hydroxyphenylacetate 6-hydroxylase inhibitor	4	98.9
112	3-Isopropylmalate dehydratase inhibitor	8	98.4
113	3-Isopropylmalate dehydrogenase inhibitor	7	99.5
114	3-Ketoalidoxylamine C-N-lyase inhibitor	4	98.3
115	3-Mercaptopyruvate sulfurtransferase inhibitor	9	100.0
116	3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor	15	99.4
117	3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor	8	97.9
118	3-Methylbutanal reductase inhibitor	9	85.5
119	3-Oxoacid CoA-transferase inhibitor	26	99.2
120	3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor	8	100.0
121	3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor	12	95.8
122	3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor	26	97.7
123	3-Oxadipate enol-lactonase inhibitor	3	99.1
124	3-Oxosteroid 1-dehydrogenase inhibitor	6	99.3
125	3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor	41	99.7
126	3-Phytase inhibitor	9	88.6
127	3C-like protease (Human coronavirus) inhibitor	19	92.2
128	4,5-Dihydroxyphthalate decarboxylase inhibitor	16	93.0
129	4-Alpha-glucanotransferase inhibitor	8	98.9
130	4-Carboxymethyl-4-methylbutenolide mutase inhibitor	9	99.4
131	4-Chlorobenzoyl-CoA dehalogenase inhibitor	7	97.3
132	4-Chlorophenylacetate 3,4-dioxygenase inhibitor	4	98.6
133	4-Coumarate-CoA ligase inhibitor	8	85.0
134	4-Hydroxy-2-oxoglutarate aldolase inhibitor	17	99.4
135	4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor	11	99.4
136	4-Hydroxybenzoate 1-hydroxylase inhibitor	3	99.9
137	4-Hydroxybenzoate 3-monoxygenase [NAD(P)H] inhibitor	6	100.0
138	4-Hydroxybenzoate 3-monoxygenase inhibitor	28	98.5
139	4-Hydroxybenzoate decarboxylase inhibitor	7	99.7

140	4-Hydroxybenzoate nonaprenyltransferase inhibitor	15	96.1
141	4-Hydroxybenzoate-CoA ligase inhibitor	4	99.8
142	4-Hydroxyglutamate transaminase inhibitor	4	98.3
143	4-Hydroxymandelate oxidase inhibitor	10	92.4
144	4-Hydroxyphenylacetate 1-monooxygenase inhibitor	4	100.0
145	4-Hydroxyphenylacetate 3-monooxygenase inhibitor	8	87.8
146	4-Hydroxyphenylpyruvate dioxygenase inhibitor	19	99.9
147	4-Hydroxyproline epimerase inhibitor	8	87.5
148	4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor	19	89.3
149	4-Nitrophenol 2-monooxygenase inhibitor	6	82.0
150	4-Nitrophenylphosphatase inhibitor	47	89.1
151	4-Phytase inhibitor	13	98.3
152	4-Pyridoxolactonase inhibitor	6	99.4
153	4a-Hydroxytetrahydrobiopterin dehydratase inhibitor	3	99.8
154	5 Hydroxytryptamine 1 agonist	1913	98.5
155	5 Hydroxytryptamine 1 antagonist	4282	98.5
156	5 Hydroxytryptamine 1A agonist	3430	98.7
157	5 Hydroxytryptamine 1B agonist	66	99.0
158	5 Hydroxytryptamine 1B antagonist	850	99.0
159	5 Hydroxytryptamine 1D agonist	696	99.5
160	5 Hydroxytryptamine 1D antagonist	916	98.8
161	5 Hydroxytryptamine 1E antagonist	9	94.9
162	5 Hydroxytryptamine 1F agonist	117	99.9
163	5 Hydroxytryptamine 1F antagonist	76	99.8
164	5 Hydroxytryptamine 2 agonist	484	99.0
165	5 Hydroxytryptamine 2 antagonist	3623	97.6
166	5 Hydroxytryptamine 2A antagonist	2266	98.2
167	5 Hydroxytryptamine 2B antagonist	282	97.9
168	5 Hydroxytryptamine 2C agonist	416	99.5
169	5 Hydroxytryptamine 3 antagonist	1561	99.0
170	5 Hydroxytryptamine 3A antagonist	5	89.6
171	5 Hydroxytryptamine 4 agonist	345	99.4
172	5 Hydroxytryptamine 4 antagonist	534	99.5
173	5 Hydroxytryptamine 4A antagonist	7	93.5
174	5 Hydroxytryptamine 4B antagonist	6	99.9
175	5 Hydroxytryptamine 4C antagonist	4	97.6
176	5 Hydroxytryptamine 4D antagonist	4	97.6
177	5 Hydroxytryptamine 4E antagonist	27	99.5
178	5 Hydroxytryptamine 5 antagonist	106	99.0
179	5 Hydroxytryptamine 5A antagonist	104	98.9
180	5 Hydroxytryptamine 6 agonist	29	99.3
181	5 Hydroxytryptamine 6 antagonist	507	99.4
182	5 Hydroxytryptamine 7 agonist	9	94.3
183	5 Hydroxytryptamine 7 antagonist	473	98.6
184	5 Hydroxytryptamine 7B antagonist	6	77.9
185	5 Hydroxytryptamine 7L antagonist	5	95.0
186	5 Hydroxytryptamine 7S antagonist	5	94.5
187	5 Hydroxytryptamine agonist	2917	97.7

188	5 Hydroxytryptamine antagonist	9722	96.6
189	5 Hydroxytryptamine release inhibitor	33	87.5
190	5 Hydroxytryptamine release stimulant	17	91.1
191	5 Lipoxygenase activating protein inhibitor	99	99.8
192	5'-Nucleotidase inhibitor	40	99.4
193	5-Alpha-reductase 1 inhibitor	338	99.6
194	5-Alpha-reductase 2 inhibitor	267	99.1
195	5-Alpha-reductase inhibitor	1330	99.4
196	5-Aminolevulinate synthase inhibitor	25	97.6
197	5-Aminovalerate transaminase inhibitor	7	99.6
198	5-Formyltetrahydrofolate cyclo-ligase inhibitor	11	93.0
199	5-Guanidino-2-oxopentanoate decarboxylase inhibitor	8	100.0
200	5-Hydroxypentanoate CoA-transferase inhibitor	4	100.0
201	5-Lipoxygenase inhibitor	1341	98.3
202	5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor	4	99.5
203	5-O-(4-coumaroyl)-D-quininate 3'-monooxygenase inhibitor	3	87.8
204	5-Oxoprolinase (ATP-hydrolysing) inhibitor	8	99.5
205	6,7-Dihydropteridine reductase inhibitor	47	97.4
206	6-Carboxyhexanoate-CoA ligase inhibitor	3	98.8
207	6-Methylsalicylate decarboxylase inhibitor	8	98.8
208	6-Phospho-beta-glucosidase inhibitor	8	99.7
209	6-Phosphofructo-2-kinase inhibitor	11	99.2
210	6-Pyruvoyltetrahydropterin synthase inhibitor	4	98.5
211	8-Amino-7-oxononanoate synthase inhibitor	15	97.3
212	8-oxodGTPase stimulant	12	100.0
213	ACK1 kinase inhibitor	25	100.0
214	ADAM inhibitor	16	100.0
215	ADAM10 endopeptidase inhibitor	24	98.4
216	ADP-ribose diphosphatase inhibitor	7	99.8
217	ADP-ribosylarginine hydrolase inhibitor	6	92.1
218	ADP-thymidine kinase inhibitor	5	94.6
219	AICAR transformylase inhibitor	30	95.3
220	ALK inhibitor	106	98.8
221	AMP deaminase 2 inhibitor	67	100.0
222	AMP deaminase 3 inhibitor	20	100.0
223	AMP deaminase inhibitor	100	98.6
224	AMP nucleosidase inhibitor	15	99.4
225	AMPA 1 receptor antagonist	284	99.2
226	AMPA 2 receptor antagonist	12	95.1
227	AMPA 3 receptor antagonist	6	93.0
228	AMPA 4 receptor antagonist	6	100.0
229	AMPA 5 receptor antagonist	4	100.0
230	AMPA receptor agonist	73	99.4
231	AMPA receptor antagonist	964	99.0
232	ATM kinase inhibitor	25	93.9
233	ATP adenylyltransferase inhibitor	7	98.3
234	ATP citrate lysase inhibitor	47	99.6
235	ATP citrate synthase inhibitor	20	99.6

236	ATP deaminase inhibitor	5	99.6
237	ATP diphosphatase inhibitor	4	99.5
238	ATP phosphoribosyltransferase inhibitor	13	97.4
239	ATP-dependent RNA helicase inhibitor	10	100.0
240	ATPase (Mitochondrial F1F0) inhibitor	8	99.8
241	ATPase (Vacuolar H+) inhibitor	77	99.0
242	ATPase stimulant	18	87.4
243	AXL receptor tyrosine kinase inhibitor	37	97.3
244	Abl kinase inhibitor	216	96.3
245	Acetate kinase inhibitor	11	90.7
246	Acetate-CoA ligase inhibitor	23	98.4
247	Acetoacetate decarboxylase inhibitor	8	99.1
248	Acetoacetyl-CoA reductase inhibitor	10	99.8
249	Acetoin dehydrogenase inhibitor	15	98.4
250	Acetolactate decarboxylase inhibitor	15	98.0
251	Acetolactate synthase inhibitor	20	98.3
252	Acetyl-CoA C-acyltransferase inhibitor	10	96.2
253	Acetyl-CoA carboxylase 1 inhibitor	16	100.0
254	Acetyl-CoA carboxylase 2 inhibitor	16	100.0
255	Acetyl-CoA carboxylase inhibitor	21	88.2
256	Acetyl-CoA transferase 1 inhibitor	19	93.8
257	Acetyl-CoA transferase 2 inhibitor	6	84.6
258	Acetyl-CoA transferase inhibitor	1288	99.0
259	Acetylcholine M1 receptor agonist	1014	99.2
260	Acetylcholine M3 receptor agonist	16	99.6
261	Acetylcholine M3 receptor antagonist	912	99.2
262	Acetylcholine M4 receptor agonist	58	99.5
263	Acetylcholine M4 receptor antagonist	273	99.6
264	Acetylcholine M5 receptor antagonist	159	99.5
265	Acetylcholine agonist	2056	97.3
266	Acetylcholine antagonist	3388	97.3
267	Acetylcholine muscarinic agonist	1217	98.8
268	Acetylcholine muscarinic antagonist	2648	98.0
269	Acetylcholine neuromuscular blocking agent	23	86.7
270	Acetylcholine nicotinic agonist	803	97.8
271	Acetylcholine nicotinic antagonist	790	97.6
272	Acetylcholinesterase stimulant	5	100.0
273	Acetylenecarboxylate hydratase inhibitor	3	98.7
274	Acetylerase inhibitor	7	77.9
275	Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor	6	82.1
276	Acetylglutamate kinase inhibitor	4	79.5
277	Acetylorithine deacetylase inhibitor	4	98.2
278	Acetylserotonin O-methyltransferase inhibitor	11	90.8
279	Acetylspermidine deacetylase inhibitor	16	95.0
280	Acid phosphatase 1 inhibitor	5	100.0
281	Acid phosphatase inhibitor	43	95.2
282	Acid-sensing ion channel blocker	6	88.5

283	Aconitate decarboxylase inhibitor	4	99.5
284	Acrocyllindropepsin inhibitor	3	86.7
285	Acrosin inhibitor	20	96.1
286	Actin depolymerization stimulant	8	99.8
287	Actin polymerization inhibitor	5	100.0
288	Activin receptor-like kinase 4 inhibitor	23	100.0
289	Acyl-CoA dehydrogenase (NADP+) inhibitor	19	98.8
290	Acyl-CoA hydrolase inhibitor	44	97.5
291	Acyl-CoA oxidase inhibitor	11	91.1
292	Acyl-lysine deacylase inhibitor	3	99.3
293	Acylaminoacyl-peptidase inhibitor	25	95.9
294	Acylcarnitine hydrolase inhibitor	3	90.7
295	Acylglycerone-phosphate reductase inhibitor	6	98.3
296	Acyloxyacyl hydrolase inhibitor	15	98.4
297	Acylphosphatase inhibitor	13	97.6
298	Adamalysin inhibitor	8	99.6
299	Adenine deaminase inhibitor	10	98.7
300	Adenine nucleotide translocase inhibitor	23	96.2
301	Adenine phosphoribosyltransferase inhibitor	23	99.4
302	Adenomatous polyposis treatment	10	93.7
303	Adenosine A1 receptor agonist	280	99.9
304	Adenosine A1 receptor agonist enhancer	12	100.0
305	Adenosine A1 receptor antagonist	2399	99.0
306	Adenosine A2 receptor agonist	240	99.9
307	Adenosine A2 receptor antagonist	2509	99.2
308	Adenosine A2a receptor agonist	216	99.9
309	Adenosine A2a receptor antagonist	1895	99.2
310	Adenosine A2b receptor agonist	17	99.9
311	Adenosine A2b receptor antagonist	578	99.6
312	Adenosine A3 receptor agonist	90	99.8
313	Adenosine A3 receptor antagonist	1242	99.1
314	Adenosine kinase inhibitor	227	99.6
315	Adenosine receptor agonist	627	99.4
316	Adenosine receptor antagonist	3778	98.8
317	Adenosine regulator	3	89.3
318	Adenosylhomocysteine nucleosidase inhibitor	57	100.0
319	Adenosylmethionine cyclotransferase inhibitor	12	100.0
320	Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor	12	98.5
321	Adenylate cyclase I stimulant	43	100.0
322	Adenylate cyclase V inhibitor	8	97.3
323	Adenylate cyclase stimulant	89	93.4
324	Adenylosuccinate lyase inhibitor	29	99.5
325	Adenylosuccinate synthase inhibitor	60	99.0
326	Adenylyl-sulfate kinase inhibitor	20	96.9
327	Adenylyl-sulfate reductase inhibitor	5	89.5
328	Adenylylsulphatase inhibitor	17	97.9
329	Adrenaline agonist	2063	97.8
330	Adrenaline antagonist	5605	97.2

331	Adrenaline release stimulant	8	93.1
332	Adrenergic	3796	97.4
333	Adrenergic, ophthalmic	10	98.8
334	Aerobactin synthase inhibitor	3	98.9
335	Agaridine gamma-glutamyltransferase inhibitor	11	98.9
336	Aggrecanase 1 inhibitor	3	100.0
337	Aggrecanase 2 inhibitor	19	99.0
338	Aggrecanase inhibitor	236	99.5
339	Agmatinase inhibitor	7	92.4
340	AgrC-1 protein inhibitor	4	100.0
341	AgrC-2 protein inhibitor	4	100.0
342	Alanine carboxypeptidase inhibitor	10	99.4
343	Alanine dehydrogenase inhibitor	27	98.7
344	Alanine racemase inhibitor	12	97.9
345	Alanine transaminase inhibitor	18	98.4
346	Alanine-tRNA ligase inhibitor	6	96.5
347	Albendazole monooxygenase inhibitor	3	96.7
348	Alcohol O-acetyltransferase inhibitor	9	89.8
349	Alcohol dehydrogenase (NADP+) inhibitor	45	95.9
350	Alcohol dehydrogenase (acceptor) inhibitor	11	87.0
351	Alcohol dehydrogenase I inhibitor	14	100.0
352	Alcohol dehydrogenase [NAD(P)+] inhibitor	16	92.6
353	Alcohol dehydrogenase alpha inhibitor	12	100.0
354	Alcohol dehydrogenase beta 1 inhibitor	7	100.0
355	Alcohol dehydrogenase beta inhibitor	7	100.0
356	Alcohol dehydrogenase gamma 2 inhibitor	6	100.0
357	Alcohol dehydrogenase gamma inhibitor	6	100.0
358	Alcohol oxidase inhibitor	17	98.7
359	Aldehyde dehydrogenase (NAD+) inhibitor	38	95.8
360	Aldehyde dehydrogenase (NADP+) inhibitor	17	96.2
361	Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor	7	87.7
362	Aldehyde dehydrogenase 1A2 inhibitor	30	99.4
363	Aldehyde dehydrogenase [NAD(P)+] inhibitor	5	99.1
364	Aldehyde dehydrogenase inhibitor	111	96.0
365	Aldehyde ferredoxin oxidoreductase inhibitor	5	98.7
366	Aldehyde oxidase inhibitor	20	86.4
367	Aldose 1-epimerase inhibitor	31	99.2
368	Aldose reductase 2 inhibitor	88	99.6
369	Aldose reductase inhibitor	692	98.3
370	Alkanal monooxygenase (FMN-linked) inhibitor	27	95.7
371	Alkane 1-monooxygenase inhibitor	4	94.9
372	Alkene monooxygenase inhibitor	3	99.0
373	Alkenylglycerophosphocholine hydrolase inhibitor	5	90.1
374	Alkenylglycerophosphoethanolamine hydrolase inhibitor	6	92.3
375	Alkylacetyl glycerophosphatase inhibitor	4	87.3
376	Alkylator	609	94.6
377	Alkylglycerone-phosphate synthase inhibitor	6	97.8
378	Alkylglycerophosphoethanolamine phosphodiesterase inhibitor	5	96.8

379	All-trans-retinyl-palmitate hydrolase inhibitor	4	93.9
380	Allantoate deiminase inhibitor	3	99.3
381	Allantoicase inhibitor	9	98.8
382	Allantoin racemase inhibitor	4	98.9
383	Allantoinase inhibitor	4	99.1
384	Allophanate hydrolase inhibitor	5	98.4
385	Allyl-alcohol dehydrogenase inhibitor	6	98.0
386	Alpha 1 adrenoreceptor agonist	78	99.2
387	Alpha 1 adrenoreceptor antagonist	3492	98.0
388	Alpha 1L adrenoreceptor agonist	3	99.3
389	Alpha 1L adrenoreceptor antagonist	11	97.2
390	Alpha 1b adrenoreceptor antagonist	624	98.9
391	Alpha 1d adrenoreceptor antagonist	775	99.1
392	Alpha 2 adrenoreceptor agonist	338	98.5
393	Alpha 2 adrenoreceptor antagonist	1318	98.2
394	Alpha 2b adrenoreceptor agonist	45	99.9
395	Alpha 2b adrenoreceptor antagonist	153	97.0
396	Alpha 2c adrenoreceptor agonist	45	100.0
397	Alpha 2c adrenoreceptor antagonist	175	98.1
398	Alpha 2d adrenoreceptor agonist	44	99.8
399	Alpha 2d adrenoreceptor antagonist	94	98.8
400	Alpha 3 adrenoreceptor agonist	5	99.3
401	Alpha adrenoreceptor agonist	497	97.8
402	Alpha adrenoreceptor antagonist	4657	97.2
403	Alpha glucosidase I inhibitor	5	100.0
404	Alpha glucosidase II inhibitor	4	100.0
405	Alpha glucosidase inhibitor	86	97.0
406	Alpha,alpha-phosphotrehalase inhibitor	5	99.2
407	Alpha,alpha-trehalase inhibitor	20	98.3
408	Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor	11	99.3
409	Alpha,alpha-trehalose phosphorylase inhibitor	4	99.8
410	Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor	14	96.6
411	Alpha-1,3-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor	11	99.8
412	Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor	3	99.5
413	Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor	4	95.5
414	Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor	5	98.9
415	Alpha-L-fucosidase inhibitor	30	98.2
416	Alpha-L-rhamnosidase inhibitor	11	99.2
417	Alpha-Methylacyl-CoA racemase inhibitor	8	97.8
418	Alpha-N-acetylgalactosaminidase inhibitor	3	99.3
419	Alpha-N-acetylgalactosaminide alpha-2,6-sialyltransferase inhibitor	17	99.5
420	Alpha-N-acetylglucosaminidase inhibitor	4	97.6
421	Alpha-N-acetylneuraminase alpha-2,8-sialyltransferase inhibitor	15	99.7
422	Alpha-N-arabinofuranosidase inhibitor	9	98.0
423	Alpha-amino-acid esterase inhibitor	4	99.9
424	Alpha-amylase inhibitor	28	94.5
425	Alpha-glucuronidase inhibitor	4	97.6
426	Alpha-pinene-oxide decyclase inhibitor	8	98.6

427	Alternansucrase inhibitor	4	99.7
428	Altronate dehydratase inhibitor	7	99.9
429	Amidase inhibitor	129	97.4
430	Amidophosphoribosyltransferase inhibitor	25	99.7
431	Amiloride-sensitive cation channel 3 blocker	3	100.0
432	Amine dehydrogenase inhibitor	10	87.7
433	Amino-acid N-acetyltransferase inhibitor	25	99.2
434	Amino-acid racemase inhibitor	6	99.5
435	Aminoacyl-tRNA hydrolase inhibitor	5	99.4
436	Aminoacyl-tRNA synthetase inhibitor	248	97.8
437	Aminoacylase inhibitor	19	98.0
438	Aminobutyraldehyde dehydrogenase inhibitor	3	86.8
439	Aminocarboxymuconate-semialdehyde decarboxylase inhibitor	6	98.6
440	Aminoglycoside N6'-acetyltransferase inhibitor	15	100.0
441	Aminolevulinate transaminase inhibitor	26	98.9
442	Aminomuconate-semialdehyde dehydrogenase inhibitor	4	97.8
443	Aminopeptidase B inhibitor	35	92.6
444	Aminopeptidase I inhibitor	26	98.2
445	Aminopeptidase Y inhibitor	8	97.4
446	Aminopeptidase microsomal inhibitor	161	97.7
447	Amylin agonist	10	100.0
448	Amylo-alpha-1,6-glucosidase inhibitor	26	99.1
449	Amyloid beta aggregation inhibitor	39	97.4
450	Amyloid beta precursor protein antagonist	20	95.6
451	Amylosucrase inhibitor	5	99.9
452	Anaphylatoxin receptor antagonist	14	75.9
453	Androgen antagonist	733	97.2
454	Androst-4-ene-3,17-dione monooxygenase inhibitor	9	99.2
455	Angiotensin AT1 receptor antagonist	2193	99.6
456	Angiotensin AT1A receptor antagonist	7	89.8
457	Angiotensin AT2 receptor agonist	7	98.8
458	Angiotensin AT2 receptor antagonist	423	99.6
459	Angiotensin II receptor agonist	10	93.7
460	Angiotensin II receptor antagonist	2412	99.5
461	Angiotensin agonist	13	99.2
462	Angiotensin antagonist	2438	99.5
463	Anhydrotetracycline monooxygenase inhibitor	4	99.5
464	Anthranilate 3-monooxygenase (deaminating) inhibitor	11	95.8
465	Anthranilate phosphoribosyltransferase inhibitor	5	99.6
466	Anthranilate synthase inhibitor	23	98.4
467	Anthranilate-CoA ligase inhibitor	4	97.8
468	Anthrax lethal factor inhibitor	9	93.2
469	Antiadrenergic	5676	97.0
470	Antidiuretic hormone agonist	152	99.7
471	Antidiuretic hormone antagonist	1104	99.6
472	Antihistaminic	2788	95.1
473	Apolipoprotein A inhibitor	71	100.0
474	Apolipoprotein B inhibitor	225	99.6

475	Apolipoprotein B-100 inhibitor	50	99.9
476	Apyrase inhibitor	17	81.4
477	Arabinogalactan endo-1,4-beta-galactosidase inhibitor	4	99.8
478	Arabinose isomerase inhibitor	7	99.2
479	Arabinose-5-phosphate isomerase inhibitor	3	98.2
480	Arachidonate-CoA ligase inhibitor	7	99.8
481	Arachidonic acid antagonist	98	94.1
482	Aralkylamine N-acetyltransferase inhibitor	16	98.7
483	Aralkylamine dehydrogenase inhibitor	6	99.9
484	Arginine 2-monooxygenase inhibitor	4	89.0
485	Arginine N-succinyltransferase inhibitor	3	100.0
486	Arginine decarboxylase inhibitor	38	98.3
487	Arginine deiminase inhibitor	22	94.6
488	Arginine kinase inhibitor	12	99.4
489	Arginine racemase inhibitor	3	99.9
490	Arginine-tRNA ligase inhibitor	17	99.3
491	Argininosuccinate lyase inhibitor	10	99.2
492	Arginyltransferase inhibitor	6	99.3
493	Aromatase inhibitor	991	99.2
494	Aromatic-amino-acid transaminase inhibitor	14	98.8
495	Aromatic-hydroxylamine O-acetyltransferase inhibitor	7	85.1
496	Aryl hydrocarbon receptor antagonist	55	98.4
497	Aryl sulfotransferase inhibitor	30	95.0
498	Aryl-acylamidase inhibitor	35	92.0
499	Aryl-alcohol dehydrogenase (NADP+) inhibitor	7	98.5
500	Aryl-alcohol dehydrogenase inhibitor	10	98.4
501	Aryl-aldehyde dehydrogenase (NADP+) inhibitor	6	98.9
502	Arylacetonitrilase inhibitor	11	96.0
503	Arylalkyl acylamidase inhibitor	6	98.7
504	Arylamine N-acetyltransferase inhibitor	24	95.3
505	Aryldialkylphosphatase inhibitor	5	98.0
506	Arylesterase inhibitor	9	93.2
507	Arylformamidase inhibitor	28	98.2
508	Arylmalonate decarboxylase inhibitor	3	96.9
509	Arylsulfatase inhibitor	22	97.2
510	Arylsulfate sulfotransferase inhibitor	7	90.7
511	Asparaginase inhibitor	19	96.3
512	Asparagine synthase (glutamine-hydrolysing) inhibitor	81	99.2
513	Asparagine-oxo-acid transaminase inhibitor	17	99.4
514	Asparagine-tRNA ligase inhibitor	6	98.8
515	Asparaginyl endopeptidase inhibitor	12	97.7
516	Aspartate 1-decarboxylase inhibitor	7	99.5
517	Aspartate 4-decarboxylase inhibitor	19	98.2
518	Aspartate N-acetyltransferase inhibitor	3	100.0
519	Aspartate ammonia-lyase inhibitor	26	99.4
520	Aspartate carbamoyltransferase inhibitor	26	98.4
521	Aspartate kinase inhibitor	24	95.0
522	Aspartate racemase inhibitor	4	99.3

523	Aspartate transaminase inhibitor	21	98.2
524	Aspartate-ammonia ligase (ADP-forming) inhibitor	4	99.2
525	Aspartate-ammonia ligase inhibitor	3	97.2
526	Aspartate-phenylpyruvate transaminase inhibitor	4	87.0
527	Aspartate-semialdehyde dehydrogenase inhibitor	13	99.1
528	Aspartate-tRNA ligase inhibitor	6	98.3
529	Aspartoacylase inhibitor	4	98.2
530	Aspartyl aminopeptidase inhibitor	8	98.6
531	Aspartyl protease inhibitor	4	100.0
532	Aspartyltransferase inhibitor	4	84.0
533	Aspergillopepsin I inhibitor	8	92.5
534	Aspergillopepsin II inhibitor	4	94.7
535	Aspergillus nuclease S1 inhibitor	8	94.3
536	Aspulvinone dimethylallyltransferase inhibitor	3	84.2
537	Assemblin inhibitor	7	99.4
538	Astacin inhibitor	19	98.4
539	Atrolysin A inhibitor	11	94.4
540	Atrolysin C inhibitor	10	97.7
541	Aureolysin inhibitor	4	98.1
542	Aurora kinase inhibitor	737	98.5
543	Aurora-A kinase inhibitor	322	98.6
544	Aurora-B kinase inhibitor	334	98.5
545	Aurora-C kinase inhibitor	33	94.5
546	Autotaxin inhibitor	4	84.6
547	Azobenzene reductase inhibitor	5	98.5
548	Bacillus subtilis ribonuclease inhibitor	6	99.6
549	Bacterial efflux pump inhibitor	16	91.4
550	Bacterial leucyl aminopeptidase inhibitor	29	99.2
551	Baculoviral IAP repeat-containing protein 4 inhibitor	55	99.8
552	Baculoviral IAP repeat-containing protein inhibitor	106	99.6
553	Bcl-xL inhibitor	60	94.1
554	Bcl2 antagonist	121	92.4
555	Bcr-Abl kinase inhibitor	97	96.0
556	Benzaldehyde dehydrogenase (NAD+) inhibitor	8	99.3
557	Benzaldehyde dehydrogenase (NADP+) inhibitor	3	97.5
558	Benzoate 4-monooxygenase inhibitor	19	93.8
559	Benzoate-CoA ligase inhibitor	6	88.4
560	Benzodiazepine agonist	363	97.8
561	Benzodiazepine agonist partial	41	96.2
562	Benzodiazepine antagonist	400	98.9
563	Benzodiazepine inverse agonist	59	99.2
564	Benzodiazepine omega receptor agonist	7	77.9
565	Benzodiazepine receptor peripheral-type antagonist	369	99.8
566	Benzoin aldolase inhibitor	3	100.0
567	Benzoylformate decarboxylase inhibitor	9	89.4
568	Beta 3 adrenoreceptor agonist	773	99.7
569	Beta 3 adrenoreceptor antagonist	24	99.9
570	Beta adrenoreceptor agonist	1561	98.8

571	Beta adrenoreceptor antagonist	1004	98.1
572	Beta amyloid protein antagonist	125	97.1
573	Beta galactosidase inhibitor	61	98.9
574	Beta glucosidase inhibitor	15	99.3
575	Beta glucuronidase inhibitor	14	95.4
576	Beta lactamase II inhibitor	10	100.0
577	Beta lactamase Imi-1 inhibitor	5	99.9
578	Beta lactamase TEM-1 inhibitor	42	99.9
579	Beta lactamase inhibitor	261	97.5
580	Beta tubulin antagonist	5	86.6
581	Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor	13	99.2
582	Beta-D-fucosidase inhibitor	20	98.7
583	Beta-Lysine 5,6-aminomutase inhibitor	4	99.7
584	Beta-N-acetylgalactosaminidase inhibitor	3	98.2
585	Beta-N-acetylhexosaminidase inhibitor	43	97.9
586	Beta-Phosphoglucomutase inhibitor	5	99.9
587	Beta-adrenergic receptor kinase inhibitor	21	84.9
588	Beta-alanine-pyruvate transaminase inhibitor	3	98.7
589	Beta-amylase inhibitor	9	99.3
590	Beta-carotene 15,15'-monooxygenase inhibitor	17	93.8
591	Beta-cyclopiasonate dehydrogenase inhibitor	7	98.2
592	Beta-fructofuranosidase inhibitor	43	99.0
593	Beta-galactoside alpha-2,3-sialyltransferase inhibitor	10	99.8
594	Beta-glucosidase inhibitor	46	98.5
595	Beta-mannosidase inhibitor	9	98.0
596	Beta-ureidopropionase inhibitor	16	96.8
597	Betaine-aldehyde dehydrogenase inhibitor	18	99.1
598	Betaine-homocysteine S-methyltransferase inhibitor	9	99.8
599	Bile-salt sulfotransferase inhibitor	4	98.4
600	Bilirubin oxidase inhibitor	9	90.9
601	Biliverdin reductase inhibitor	11	99.3
602	Biotin carboxylase inhibitor	4	98.4
603	Biotin-CoA ligase inhibitor	3	98.8
604	Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor	4	99.9
605	Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor	3	97.6
606	Biotinidase inhibitor	8	83.4
607	Biphenyl-2,3-diol 1,2-dioxygenase inhibitor	15	99.0
608	Bis(5'-adenosyl)-triphosphatase inhibitor	4	98.9
609	Bis(5'-nucleosyl)-tetraphosphatase (asymmetrical) inhibitor	12	99.5
610	Bis(5'-nucleosyl)-tetraphosphatase (symmetrical) inhibitor	11	99.6
611	Bisphosphoglycerate mutase inhibitor	4	98.1
612	Bisphosphoglycerate phosphatase inhibitor	5	96.5
613	Bisphosphonate	68	99.9
614	Blasticidin-S deaminase inhibitor	4	97.6
615	Bombesin 1 receptor antagonist	4	81.7
616	Bombesin 2 receptor antagonist	19	98.1
617	Bombesin 3 receptor agonist	24	99.4
618	Bombesin agonist	25	99.6

619	Bombesin antagonist	141	98.6
620	Bone morphogenic protein 1 inhibitor	137	100.0
621	Bone morphogenic protein inhibitor	137	100.0
622	Bontoxilysin inhibitor	6	94.7
623	Bothrolysin inhibitor	3	98.0
624	Botulin neurotoxin A light chain inhibitor	11	87.3
625	Botulinum neurotoxin type B inhibitor	8	100.0
626	Brachyurin inhibitor	8	97.7
627	Bradykinin B1 receptor agonist	6	100.0
628	Bradykinin B1 receptor antagonist	455	99.7
629	Bradykinin B2 receptor agonist	9	100.0
630	Bradykinin B2 receptor antagonist	500	99.9
631	Bradykinin agonist	15	99.9
632	Bradykinin antagonist	1064	99.4
633	Branched-chain-amino-acid transaminase inhibitor	20	96.5
634	Breast cancer-resistant protein inhibitor	39	97.9
635	Bruton tyrosine kinase inhibitor	79	98.9
636	Butyrate-CoA ligase inhibitor	10	98.7
637	Butyryl-CoA dehydrogenase inhibitor	9	99.6
638	Butyrylcholinesterase stimulant	3	85.9
639	CC chemokine 1 receptor antagonist	156	99.5
640	CC chemokine 10 receptor antagonist	10	100.0
641	CC chemokine 2 receptor antagonist	67	94.3
642	CC chemokine 3 receptor antagonist	195	99.5
643	CC chemokine 4 receptor antagonist	8	84.5
644	CC chemokine 5 receptor agonist	14	100.0
645	CC chemokine 5 receptor antagonist	35	92.9
646	CC chemokine 9 receptor antagonist	22	100.0
647	CC chemokine receptor 2B antagonist	4	97.8
648	CC chemokine receptor agonist	15	98.5
649	CC chemokine receptor antagonist	480	97.2
650	CD45 antagonist	72	98.6
651	CD80 antagonist	81	100.0
652	CDC25 phosphatase inhibitor	36	98.7
653	CDC25A inhibitor	77	96.5
654	CDC25B inhibitor	67	96.1
655	CDC25C inhibitor	32	99.8
656	CDC7 inhibitor	46	99.5
657	CDK/Cyclin complex inhibitor	1205	97.8
658	CDK1/cyclin B inhibitor	331	98.9
659	CDK2/cyclin A inhibitor	437	96.6
660	CDK2/cyclin A3 inhibitor	30	100.0
661	CDK2/cyclin E inhibitor	475	99.4
662	CDK4/cyclin D inhibitor	427	99.5
663	CDK4/cyclin D1 inhibitor	251	98.7
664	CDK4/cyclin D3 inhibitor	7	100.0
665	CDK5/p25 inhibitor	56	98.0
666	CDK9/cyclin T1 inhibitor	11	82.0

667	CDP-4-dehydro-6-deoxyglucose reductase inhibitor	4	98.4
668	CDP-diacylglycerol diphosphatase inhibitor	6	99.9
669	CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor	3	97.4
670	CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor	15	92.1
671	CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor	6	89.9
672	CDP-glycerol diphosphatase inhibitor	6	100.0
673	CDP-glycerol glycerophosphotransferase inhibitor	4	81.1
674	CF transmembrane conductance regulator agonist	8	85.6
675	CF transmembrane conductance regulator antagonist	35	97.4
676	CMP-KDO synthase inhibitor	3	99.9
677	CMP-N-acetylneuraminate monooxygenase inhibitor	13	96.9
678	CMP-N-acylneuraminate phosphodiesterase inhibitor	23	98.4
679	CO-methylating acetyl-CoA synthase inhibitor	3	100.0
680	CPB protease inhibitor	3	99.9
681	CTP synthase inhibitor	14	98.5
682	CXC chemokine 1 receptor antagonist	7	85.4
683	CXC chemokine 2 receptor antagonist	54	98.0
684	CXC chemokine 3 receptor antagonist	20	94.6
685	CXC chemokine 4 receptor antagonist	45	99.4
686	CXC chemokine 5 receptor antagonist	328	100.0
687	CXC chemokine L1/GRO-alpha antagonist	17	100.0
688	CXC chemokine receptor antagonist	504	98.8
689	Ca(v)2.2 blocker	344	98.4
690	Ca2+/calmodulin-dependent kinase I inhibitor	9	95.6
691	Ca2+/calmodulin-dependent kinase II inhibitor	42	94.9
692	Ca2+/calmodulin-dependent protein kinase inhibitor	56	92.5
693	Cadherin antagonist	3	100.0
694	Calcineurin inhibitor	21	100.0
695	Calcitonin gene-related peptide 1 receptor antagonist	33	97.4
696	Calcitonin gene-related peptide antagonist	464	99.7
697	Calcitonin stimulant	17	96.7
698	Calcium antagonist	136	96.8
699	Calcium channel (voltage-sensitive) activator	6	80.3
700	Calcium channel (voltage-sensitive) blocker	1483	97.8
701	Calcium channel L-type blocker	985	98.6
702	Calcium channel N-type blocker	391	98.5
703	Calcium channel T-type blocker	187	98.0
704	Calcium channel activator	52	89.8
705	Calcium channel blocker	3642	96.3
706	Calcium regulator	347	85.7
707	Calcium release-activated channel blocker	51	99.7
708	Calcium-sensing receptor agonist	5	98.2
709	Calcium-sensing receptor antagonist	55	99.0
710	Calmodulin antagonist	37	79.2
711	Calpain inhibitor	79	99.3
712	Camphor 1,2-monooxygenase inhibitor	4	98.3
713	Cancer procoagulant inhibitor	11	97.2
714	Candidapepsin 2 inhibitor	10	100.0

715	Candidapepsin inhibitor	17	96.8
716	Cannabinoid CB1 receptor agonist	40	98.0
717	Cannabinoid CB1 receptor antagonist	1254	99.5
718	Cannabinoid CB2 receptor agonist	102	97.5
719	Cannabinoid CB2 receptor antagonist	246	99.6
720	Cannabinoid receptor agonist	143	98.5
721	Cannabinoid receptor antagonist	1310	99.4
722	Carbamoyl-serine ammonia-lyase inhibitor	3	99.9
723	Carbon-monoxide dehydrogenase inhibitor	3	97.3
724	Carbonic anhydrase I stimulant	56	99.9
725	Carbonic anhydrase II stimulant	59	99.2
726	Carbonic anhydrase IV inhibitor	760	100.0
727	Carbonic anhydrase IV stimulant	50	100.0
728	Carbonic anhydrase IX inhibitor	151	99.9
729	Carbonic anhydrase V inhibitor	47	99.8
730	Carbonic anhydrase VII inhibitor	8	99.5
731	Carbonic anhydrase XII inhibitor	21	99.9
732	Carbonic anhydrase XIV inhibitor	3	100.0
733	Carbonic anhydrase XV inhibitor	3	100.0
734	Carbonic anhydrase stimulant	74	99.1
735	Carboxy-cis,cis-muconate cyclase inhibitor	19	99.7
736	Carboxycyclohexadienyl dehydratase inhibitor	5	100.0
737	Carboxylate reductase inhibitor	6	99.7
738	Carboxylesterase inhibitor	36	97.9
739	Carboxymethylenebutenolidase inhibitor	3	99.3
740	Carboxypeptidase B inhibitor	17	98.9
741	Carboxypeptidase D inhibitor	9	94.8
742	Carboxypeptidase E inhibitor	21	94.2
743	Carboxypeptidase M inhibitor	5	99.6
744	Carboxypeptidase Taq inhibitor	3	92.0
745	Carboxypeptidase U inhibitor	19	99.7
746	Cardiac myosin stimulant	4	100.0
747	Carnitinamidase inhibitor	7	95.3
748	Carnitine 3-dehydrogenase inhibitor	11	98.2
749	Carnitine O-octanoyltransferase inhibitor	7	98.2
750	Carnitine dehydratase inhibitor	4	99.0
751	Carnitine palmitoyltransferase inhibitor	22	95.5
752	Carnosine synthase inhibitor	14	95.4
753	Caspase 2 inhibitor	8	99.7
754	Caspase 3 inhibitor	370	97.8
755	Caspase 3 stimulant	87	81.0
756	Caspase 6 inhibitor	46	99.9
757	Caspase 7 inhibitor	79	100.0
758	Caspase 8 inhibitor	89	98.6
759	Caspase 8 stimulant	31	83.2
760	Caspase 9 inhibitor	31	96.6
761	Catalase stimulant	113	96.0
762	Catechol 1,2-dioxygenase inhibitor	20	99.1

763	Catechol 2,3-dioxygenase inhibitor	32	99.4
764	Catechol oxidase inhibitor	15	97.3
765	Catenin beta inhibitor	9	100.0
766	Cathepsin B inhibitor	593	98.8
767	Cathepsin D inhibitor	262	97.4
768	Cathepsin E inhibitor	33	99.1
769	Cathepsin F inhibitor	30	99.5
770	Cathepsin G inhibitor	55	92.6
771	Cathepsin H inhibitor	19	93.5
772	Cathepsin K inhibitor	511	99.8
773	Cathepsin L inhibitor	433	98.2
774	Cathepsin S inhibitor	346	99.5
775	Cathepsin T inhibitor	7	94.3
776	Cathepsin V inhibitor	31	99.8
777	Cellobiose phosphorylase inhibitor	10	99.1
778	Cellulase inhibitor	12	97.0
779	Cellulose 1,4-beta-cellobiosidase inhibitor	11	89.1
780	Cellulose synthase (UDP-forming) inhibitor	14	89.9
781	Centromere associated protein inhibitor	24	98.7
782	Ceramidase inhibitor	14	95.3
783	Ceramide glucosyltransferase inhibitor	12	92.0
784	Cerebroside-sulfatase inhibitor	9	97.7
785	Cerevisin inhibitor	8	98.7
786	Chalcone isomerase inhibitor	26	99.5
787	Channel-conductance-controlling ATPase inhibitor	5	96.4
788	Chaperonin ATPase inhibitor	6	96.2
789	Check point kinase 1 inhibitor	242	99.2
790	Check point kinase 2 inhibitor	82	97.6
791	Check point kinase inhibitor	302	99.0
792	Chelator	133	97.0
793	Chelator, Iron	40	99.6
794	Chemokine receptor agonist	15	98.5
795	Chemokine receptor antagonist	986	97.7
796	Chenodeoxycholytaurine hydrolase inhibitor	3	96.0
797	Chitin deacetylase inhibitor	3	99.9
798	Chitin synthase inhibitor	32	94.9
799	Chitinase inhibitor	25	92.7
800	Chitobiosyldiphosphodolichol beta-mannosyltransferase inhibitor	5	98.2
801	Chitosanase inhibitor	8	94.2
802	Chloramphenicol O-acetyltransferase inhibitor	6	96.0
803	Chlordecone reductase inhibitor	4	90.9
804	Chloride channel activator	41	88.0
805	Chloride channel blocker	11	94.8
806	Chloride peroxidase inhibitor	3	88.4
807	Chloride/bicarbonate exchanger inhibitor	24	99.2
808	Cholate-CoA ligase inhibitor	9	98.6
809	Cholecystokinin A agonist	113	99.2
810	Cholecystokinin A antagonist	1066	99.6

811	Cholecystokinin B antagonist	1081	99.5
812	Cholecystokinin agonist	122	99.2
813	Cholecystokinin antagonist	1406	99.4
814	Cholestanetriol 26-monooxygenase inhibitor	9	91.0
815	Cholestenol delta-isomerase inhibitor	8	100.0
816	Cholestenone 5alpha-reductase inhibitor	12	91.6
817	Cholesterol antagonist	124	87.2
818	Cholesterol ester transfer protein antagonist	487	99.4
819	Cholesterol esterase inhibitor	54	99.0
820	Cholesterol monooxygenase (side-chain-cleaving) inhibitor	7	100.0
821	Cholesterol oxidase inhibitor	15	98.1
822	Choline acetyltransferase stimulant	5	93.6
823	Choline dehydrogenase inhibitor	5	99.3
824	Choline kinase inhibitor	12	92.5
825	Choline sulfotransferase inhibitor	20	98.7
826	Choline-phosphate cytidyltransferase inhibitor	15	89.6
827	Choline-sulfatase inhibitor	8	97.1
828	Cholinergic	3631	95.9
829	Cholinergic antagonist	3550	97.0
830	Choloylglycine hydrolase inhibitor	3	98.2
831	Chondroitin 6-sulfotransferase inhibitor	4	98.6
832	Chorismate mutase inhibitor	22	99.8
833	Chymase inhibitor	158	98.3
834	Chymosin inhibitor	3	86.7
835	Chymotrypsin inhibitor	194	96.5
836	Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor	3	96.7
837	Citrate (Si)-synthase inhibitor	26	99.0
838	Cl--transporting ATPase inhibitor	5	89.1
839	Clavamate synthase inhibitor	3	97.1
840	Clostripain inhibitor	22	94.0
841	Coactivator-associated arginine methyltransferase 1 inhibitor	4	83.8
842	Coccolysin inhibitor	11	90.0
843	Coenzyme-B sulfoethylthiotransferase inhibitor	3	86.6
844	Collagen inhibitor	9	76.9
845	Collagenase 3 inhibitor	1191	99.2
846	Collagenase inhibitor	1039	98.8
847	Colony stimulating factor agonist	38	94.0
848	Colony stimulating factor antagonist	171	97.9
849	Colorectum cell-derived growth factor antagonist	5	100.0
850	Complement C5a chemotactic receptor antagonist	49	97.0
851	Complement C5a convertase stimulant	3	100.0
852	Complement factor 1 inhibitor	24	95.0
853	Complement factor 1r inhibitor	22	100.0
854	Complement factor D inhibitor	3	85.2
855	Complement inhibitor	40	84.5
856	Complement stimulant	3	100.0
857	Coproporphyrinogen oxidase inhibitor	28	98.2
858	Corticosteroid antagonist	3	92.5

859	Corticosteroid side-chain-isomerase inhibitor	5	96.8
860	Corticosteroid-like	120	99.9
861	Corticotropin releasing factor 1 receptor antagonist	651	100.0
862	Corticotropin releasing factor antagonist	35	97.7
863	Corticotropin-like	3	98.9
864	Cortisol sulfotransferase inhibitor	14	99.8
865	Cortisone alpha-reductase inhibitor	4	100.0
866	Cortisone beta-reductase inhibitor	7	99.9
867	CpG-Oligodeoxynucleotides inhibitor	47	100.0
868	Creatinase inhibitor	8	99.0
869	Creatine kinase inhibitor	30	97.3
870	Creatininase inhibitor	6	90.0
871	Creatinine deaminase inhibitor	3	99.0
872	Crotonoyl-[acyl-carrier-protein] hydratase inhibitor	3	98.1
873	Cruzipain inhibitor	114	99.8
874	Cutinase inhibitor	6	96.4
875	Cyanate hydratase inhibitor	13	98.5
876	Cyanoalanine nitrilase inhibitor	5	84.3
877	Cyclamate sulfohydrolase inhibitor	4	98.9
878	Cyclic AMP agonist	15	86.4
879	Cyclic AMP antagonist	10	77.2
880	Cyclic AMP modulator	43	87.2
881	Cyclic AMP phosphodiesterase inhibitor	194	87.6
882	Cyclic GMP phosphodiesterase inhibitor	19	88.1
883	Cyclin-dependent kinase 1 inhibitor	413	98.6
884	Cyclin-dependent kinase 2 inhibitor	670	98.0
885	Cyclin-dependent kinase 4 inhibitor	353	98.6
886	Cyclin-dependent kinase 5 inhibitor	225	98.5
887	Cyclin-dependent kinase 6 inhibitor	52	95.1
888	Cyclin-dependent kinase 7 inhibitor	15	86.8
889	Cyclin-dependent kinase 9 inhibitor	14	82.9
890	Cyclin-dependent kinase inhibitor	1836	97.8
891	Cycloartenol synthase inhibitor	10	96.7
892	Cyclohexadienyl dehydrogenase inhibitor	12	99.9
893	Cyclohexanone monooxygenase inhibitor	11	84.9
894	Cyclohexyl-isocyanide hydratase inhibitor	3	97.8
895	Cyclomaltodextrin glucanotransferase inhibitor	17	99.9
896	Cyclomaltodextrinase inhibitor	6	83.4
897	Cyclooxygenase 1 inhibitor	683	97.2
898	Cyclooxygenase 2 inhibitor	2530	97.6
899	Cyclooxygenase 3 inhibitor	19	99.8
900	Cyclopentanone monooxygenase inhibitor	5	97.8
901	Cyclopropane-fatty-acyl-phospholipid synthase inhibitor	10	94.5
902	Cystathionine beta-lyase inhibitor	21	98.6
903	Cystathionine gamma-lyase inhibitor	26	98.8
904	Cysteamine dioxygenase inhibitor	9	98.1
905	Cysteine desulfurase inhibitor	5	98.9
906	Cysteine dioxygenase inhibitor	16	99.8

907	Cysteine protease B inhibitor	12	100.0
908	Cysteine synthase inhibitor	20	93.3
909	Cysteine transaminase inhibitor	3	99.6
910	Cysteine-S-conjugate beta-lyase inhibitor	3	99.3
911	Cysteine-tRNA ligase inhibitor	19	98.9
912	Cystinyl aminopeptidase inhibitor	34	94.1
913	Cytidine deaminase inhibitor	49	98.0
914	Cytidylate kinase inhibitor	19	99.6
915	Cytochrome P450 inhibitor	958	88.1
916	Cytochrome P450 stimulant	17	81.8
917	Cytochrome-b5 reductase inhibitor	21	87.1
918	Cytochrome-c3 hydrogenase inhibitor	6	99.3
919	Cytokine modulator	140	95.0
920	Cytokine production inhibitor	758	95.9
921	Cytokine production stimulant	260	98.5
922	Cytokine release inhibitor	7	98.8
923	Cytosine deaminase inhibitor	27	97.6
924	Cytosol alanyl aminopeptidase inhibitor	43	93.9
925	Cytosole dipeptidase inhibitor	5	98.9
926	Cytosolic phospholipase A2 inhibitor	26	99.7
927	D(-)-tartrate dehydratase inhibitor	5	99.9
928	D-2-hydroxy-acid dehydrogenase inhibitor	6	99.0
929	D-Ala-D-Ala ligase inhibitor	6	95.1
930	D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor	5	100.0
931	D-Alanine-poly(phosphoribitol) ligase inhibitor	5	99.9
932	D-Amino-acid oxidase inhibitor	12	99.8
933	D-Lysine 5,6-aminomutase inhibitor	22	99.4
934	D-Octopine dehydrogenase inhibitor	20	97.4
935	D-Ornithine 4,5-aminomutase inhibitor	5	99.0
936	D-Serine ammonia-lyase inhibitor	4	99.9
937	D-alanine 2-hydroxymethyltransferase inhibitor	3	98.2
938	D-alanine transaminase inhibitor	18	99.0
939	D-amino-acid dehydrogenase inhibitor	5	96.5
940	D-arabinonolactone oxidase inhibitor	5	99.0
941	D-arabinose 1-dehydrogenase inhibitor	5	78.4
942	D-aspartate oxidase inhibitor	12	99.9
943	D-benzoylarginine-4-nitroanilide amidase inhibitor	5	99.5
944	D-cysteine desulhydrase inhibitor	5	98.9
945	D-glutamate oxidase inhibitor	9	98.9
946	D-lactaldehyde dehydrogenase inhibitor	11	85.5
947	D-lactate dehydrogenase (cytochrome) inhibitor	7	98.9
948	D-lactate dehydrogenase inhibitor	7	87.6
949	D-lactate-2-sulfatase inhibitor	4	99.9
950	D-malate dehydrogenase (decarboxylating) inhibitor	10	98.9
951	D-proline reductase (dithiol) inhibitor	5	99.3
952	D-stereospecific aminopeptidase inhibitor	7	99.5
953	D-threo-aldose 1-dehydrogenase inhibitor	7	93.3
954	D-xylulose reductase inhibitor	4	98.3

955	DELTA14-sterol reductase inhibitor	13	89.0
956	DELTA24-sterol reductase inhibitor	7	87.6
957	DNA directed DNA polymerase inhibitor	184	93.3
958	DNA directed RNA polymerase inhibitor	549	93.9
959	DNA directed RNA polymerase stimulant	10	99.7
960	DNA gyrase inhibitor	310	98.3
961	DNA helicase inhibitor	31	96.8
962	DNA ligase (ATP) inhibitor	21	89.2
963	DNA methylase inhibitor	37	95.1
964	DNA methyltransferase I inhibitor	15	96.9
965	DNA nucleotidylexotransferase inhibitor	21	95.1
966	DNA polymerase I inhibitor	15	84.2
967	DNA polymerase III inhibitor	72	100.0
968	DNA repair enzyme inhibitor	123	97.6
969	DNA topoisomerase IV inhibitor	93	98.7
970	DNA-(apurinic or apyrimidinic site) lyase inhibitor	11	94.6
971	DNA-3-methyladenine glycosylase I inhibitor	5	95.7
972	DNA-3-methyladenine glycosylase II inhibitor	3	99.4
973	DNA-dependent protein kinase inhibitor	58	98.4
974	Dactylysin inhibitor	22	91.6
975	Deacetoxycephalosporin-C synthase inhibitor	10	98.9
976	Decylcitrate synthase inhibitor	4	97.4
977	Dehydro-L-gulonate decarboxylase inhibitor	3	94.3
978	Delayed rectifier potassium channel activator	162	99.2
979	Delayed rectifier potassium channel blocker	46	99.8
980	Demethylmacrococin O-methyltransferase inhibitor	10	100.0
981	Demethylsterigmatocystin 6-O-methyltransferase inhibitor	3	98.8
982	Deoxyadenosine kinase inhibitor	13	92.1
983	Deoxycytidine deaminase inhibitor	5	99.0
984	Deoxycytidine kinase inhibitor	42	98.1
985	Deoxycytidylate 5-hydroxymethyltransferase inhibitor	7	97.7
986	Deoxyguanosine kinase inhibitor	37	99.5
987	Deoxyhypusine monoxygenase inhibitor	16	99.8
988	Deoxyhypusine synthase inhibitor	28	98.3
989	Deoxynucleoside kinase inhibitor	9	100.0
990	Deoxyribonuclease (pyrimidine dimer) inhibitor	3	99.8
991	Deoxyribonuclease I inhibitor	10	94.8
992	Deoxyribonuclease X inhibitor	3	99.2
993	Deoxyribose-phosphate aldolase inhibitor	4	98.9
994	Dethiobiotin synthase inhibitor	7	98.5
995	Dextranase inhibitor	9	94.2
996	Dextranucrase inhibitor	19	99.3
997	Di-trans,poly-cis-decaprenylcistransferase inhibitor	4	97.4
998	Diacylglycerol O-acyltransferase 1 inhibitor	33	99.3
999	Diacylglycerol O-acyltransferase inhibitor	82	97.1
1000	Diacylglycerol cholinephosphotransferase inhibitor	28	97.5
1001	Diacylglycerol kinase inhibitor	23	93.7
1002	Diamine N-acetyltransferase inhibitor	12	94.2

1003	Diaminopimelate decarboxylase inhibitor	13	99.9
1004	Diaminopimelate dehydrogenase inhibitor	7	99.1
1005	Diaminopimelate epimerase inhibitor	8	99.8
1006	Diaminopropionate ammonia-lyase inhibitor	11	99.0
1007	Dichloromethane dehalogenase inhibitor	9	99.9
1008	Dichloromuconate cycloisomerase inhibitor	4	99.5
1009	Diguanidinobutanase inhibitor	6	99.3
1010	Dihydrodipicolinate reductase inhibitor	8	89.5
1011	Dihydrodipicolinate synthase inhibitor	16	99.3
1012	Dihydrofolate reductase (<i>Mycobacterium avium</i>) inhibitor	13	100.0
1013	Dihydrofolate reductase (<i>Pneumocystis carinii</i>) inhibitor	10	100.0
1014	Dihydrofolate reductase (<i>Toxoplasma gondii</i>) inhibitor	13	99.9
1015	Dihydrofolate synthase inhibitor	13	93.3
1016	Dihydrolipoamide S-acetyltransferase inhibitor	4	99.3
1017	Dihydroneopterin aldolase inhibitor	20	99.9
1018	Dihydroorotate inhibitor	16	97.1
1019	Dihydroorotate dehydrogenase inhibitor	105	97.8
1020	Dihydroorotate oxidase inhibitor	84	98.7
1021	Dihydropteroate synthase inhibitor	31	99.1
1022	Dihydropyrimidinase inhibitor	15	98.8
1023	Dihydropyrimidine dehydrogenase inhibitor	6	99.1
1024	Dihydrouracil dehydrogenase (NAD ⁺) inhibitor	5	91.5
1025	Dihydrouracil oxidase inhibitor	8	98.9
1026	Dihydroxy-acid dehydratase inhibitor	14	94.6
1027	Dihydroxyacetanilide dehydrogenase inhibitor	5	99.9
1028	Dihydroxyacetanilide epoxidase inhibitor	5	99.9
1029	Diiodophenylpyruvate reductase inhibitor	3	99.5
1030	Diiodotyrosine transaminase inhibitor	6	99.9
1031	Diisopropyl-fluorophosphatase inhibitor	5	98.9
1032	Dimethylallyltranstransferase inhibitor	34	97.4
1033	Dimethylargininase inhibitor	3	92.3
1034	Dimethylhistidine N-methyltransferase inhibitor	5	99.1
1035	Dimethylmaleate hydratase inhibitor	3	97.8
1036	Dipeptidase E inhibitor	4	92.9
1037	Dipeptidyl peptidase I inhibitor	50	97.2
1038	Dipeptidyl peptidase II inhibitor	108	97.9
1039	Dipeptidyl peptidase IX inhibitor	5	93.7
1040	Dipeptidyl peptidase VIII inhibitor	3	99.3
1041	Dipeptidyl peptidase inhibitor	1422	98.8
1042	Diphenylpicrylhydrazyl (DPPH) scavenger	3	100.0
1043	Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor	17	99.7
1044	Diphosphate-serine phosphotransferase inhibitor	8	99.9
1045	Diphosphomevalonate decarboxylase inhibitor	13	93.2
1046	Dodecenoyl-CoA Delta-isomerase inhibitor	5	78.6
1047	Dolichol kinase inhibitor	8	96.2
1048	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor	3	91.4
1049	Dolichyl-phosphatase inhibitor	6	98.4
1050	Dolichyl-phosphate beta-D-mannosyltransferase (<i>T. brucei</i>) inhibitor	3	100.0

1051	Dolichyl-phosphate beta-D-mannosyltransferase inhibitor	19	92.9
1052	Dolichyl-phosphate beta-glucosyltransferase inhibitor	5	90.5
1053	Dolichydiphosphatase inhibitor	3	100.0
1054	Dopachrome isomerase inhibitor	7	99.7
1055	Dopamine D1 agonist	54	99.5
1056	Dopamine D1 antagonist	620	98.9
1057	Dopamine D1A antagonist	25	99.9
1058	Dopamine D1B antagonist	40	99.8
1059	Dopamine D2 agonist	191	98.8
1060	Dopamine D2 agonist inducer	3	100.0
1061	Dopamine D2A antagonist	82	98.5
1062	Dopamine D2B antagonist	31	100.0
1063	Dopamine D2L antagonist	481	98.8
1064	Dopamine D2S antagonist	122	96.2
1065	Dopamine D3 agonist	29	99.4
1066	Dopamine D3 antagonist	1102	98.6
1067	Dopamine D4 agonist	558	98.9
1068	Dopamine D4 antagonist	586	98.5
1069	Dopamine D5 antagonist	33	98.9
1070	Dopamine agonist	1066	96.8
1071	Dopamine antagonist	4648	97.9
1072	Dopamine autoreceptor agonist	61	99.4
1073	Dopamine beta hydroxylase inhibitor	65	96.1
1074	Dopamine precursors	25	99.9
1075	Dopamine release inhibitor	3	100.0
1076	Dopamine release stimulant	7	95.0
1077	Dual specificity phosphatase 1 inhibitor	4	93.0
1078	Dual specificity phosphatase inhibitor	40	96.7
1079	Dual specificity protein phosphatase VHR inhibitor	9	99.9
1080	Dynamin GTPase inhibitor	4	90.9
1081	Dynein ATPase inhibitor	3	97.4
1082	Dyrk kinase inhibitor	9	96.4
1083	Ecdysone 20-monooxygenase inhibitor	15	86.0
1084	Eicosanoid agonist	6	99.7
1085	Elastase 1 inhibitor	18	99.7
1086	Elastase 2 inhibitor	7	100.0
1087	Elastase inhibitor	770	98.1
1088	Electrolyte absorption agonist	6	77.9
1089	Electrolyte absorption antagonist	54	95.4
1090	Electron-transferring-flavoprotein dehydrogenase inhibitor	3	87.8
1091	Endo-1,3(4)-beta-glucanase inhibitor	3	98.9
1092	Endo-1,4-beta-xylanase inhibitor	19	98.0
1093	Endo-beta-N-acetylglucosaminidase inhibitor	5	100.0
1094	Endoglycosylceramidase inhibitor	4	98.1
1095	Endonuclease (influenza) inhibitor	15	100.0
1096	Endopeptidase La inhibitor	39	91.5
1097	Endopeptidase So inhibitor	7	89.6
1098	Endopeptidase inhibitor	89	92.7

1099	Endothelial growth factor antagonist	13	79.1
1100	Endothelial nitric-oxide synthase inhibitor	127	99.1
1101	Endothelin A receptor antagonist	1715	99.7
1102	Endothelin B receptor antagonist	965	99.6
1103	Endothelin receptor agonist	13	100.0
1104	Endothelin receptor antagonist	2367	99.5
1105	Endothiapepsin inhibitor	6	99.6
1106	Enoyl-CoA hydratase inhibitor	9	99.4
1107	Enoyl-[acyl-carrier-protein] reductase (NADH) inhibitor	36	97.0
1108	Enteropeptidase inhibitor	6	83.2
1109	Envelysin inhibitor	18	94.7
1110	EphB4 antagonist	76	99.6
1111	Ephrin antagonist	93	99.4
1112	Epidermal growth factor antagonist	896	99.0
1113	Epidermal growth factor receptor kinase inhibitor	1152	94.8
1114	Epithelial sodium channel blocker	10	99.0
1115	Epoxide hydrolase 2 inhibitor	143	100.0
1116	Epoxide hydrolase inhibitor	284	99.0
1117	ErbB antagonist	622	98.8
1118	ErbB-1 antagonist	22	92.7
1119	ErbB-2 antagonist	422	98.7
1120	ErbB-4 antagonist	18	99.1
1121	Erythro-3-hydroxyaspartate ammonia-lyase inhibitor	4	99.9
1122	Erythropoietin receptor agonist	10	100.0
1123	Estradiol 17 beta dehydrogenase 2 inhibitor	15	99.9
1124	Estradiol 17 beta dehydrogenase 3 inhibitor	59	99.0
1125	Estradiol 17 beta dehydrogenase inhibitor	81	98.6
1126	Estradiol 17 beta dehydrogenase stimulant	19	99.8
1127	Estradiol 17alpha-dehydrogenase inhibitor	3	98.8
1128	Estrogen alpha receptor agonist	44	99.4
1129	Estrogen antagonist	1089	98.4
1130	Estrogen beta receptor agonist	185	99.7
1131	Estrogen-related receptor alpha antagonist	17	100.0
1132	Estrone sulfatase inhibitor	207	99.6
1133	Estrone sulfotransferase inhibitor	37	96.5
1134	Estrone sulfotransferase stimulant	17	99.8
1135	Ethanolamine ammonia-lyase inhibitor	10	99.9
1136	Ethanolamine kinase inhibitor	15	98.7
1137	Ethanolamine oxidase inhibitor	6	89.7
1138	Ethanolamine-phosphate cytidyltransferase inhibitor	7	92.6
1139	Ethanolaminophosphotransferase inhibitor	28	95.6
1140	Ether-a-go-go potassium channel 1 blocker	21	100.0
1141	Ether-a-go-go potassium channel blocker	21	100.0
1142	Eukaryotic elongation factor 2 kinase inhibitor	3	100.0
1143	Exoribonuclease II inhibitor	5	92.9
1144	FAD diphosphatase inhibitor	17	99.2
1145	FMN adenylyltransferase inhibitor	7	100.0
1146	FMN reductase inhibitor	22	95.0

1147	Factor IXa inhibitor	18	100.0
1148	Factor VII inhibitor	8	97.0
1149	Factor VIIa inhibitor	247	98.6
1150	Factor XIIIa inhibitor	9	92.2
1151	Factor XIIIa stimulant	3	99.7
1152	Factor XIa inhibitor	16	93.2
1153	Factor Xa inhibitor	1816	99.3
1154	Falcipain 2 inhibitor	52	95.0
1155	Falcipain 3 inhibitor	12	88.5
1156	Falcipain inhibitor	52	95.0
1157	Farnesoid X receptor agonist	96	99.4
1158	Farnesoid X receptor antagonist	18	93.6
1159	Farnesyltransferase inhibitor	2425	98.8
1160	Farnesyltranstransferase inhibitor	5	97.8
1161	Fas antagonist	5	100.0
1162	Fatty acid elongase inhibitor	6	88.3
1163	Fatty acid oxidation inhibitor	45	99.4
1164	Fatty acid synthase inhibitor	36	98.1
1165	Fatty-acyl-CoA synthase inhibitor	5	93.1
1166	Fatty-acyl-ethyl-ester synthase inhibitor	3	99.7
1167	Ferredoxin hydrogenase inhibitor	8	95.6
1168	Ferredoxin-NAD+ reductase inhibitor	3	96.5
1169	Ferredoxin-NADP+ reductase inhibitor	6	97.6
1170	Ferredoxin-nitrite reductase inhibitor	12	95.5
1171	Ferrochelataase inhibitor	5	98.8
1172	Feruloyl esterase inhibitor	6	92.2
1173	Fibrinogen receptor antagonist	35	88.5
1174	Fibroblast activation protein alpha inhibitor	8	100.0
1175	Fibroblast growth factor 1 agonist	3	95.2
1176	Fibroblast growth factor 1 antagonist	148	98.2
1177	Fibroblast growth factor 2 antagonist	12	94.1
1178	Fibroblast growth factor 3 antagonist	48	97.3
1179	Fibroblast growth factor agonist	4	91.9
1180	Fibroblast growth factor antagonist	496	98.4
1181	Fibrolase inhibitor	4	88.8
1182	Flavin-containing monooxygenase inhibitor	9	94.3
1183	Flavonoid 3'-monooxygenase inhibitor	8	75.3
1184	Focal adhesion kinase 1 inhibitor	6	100.0
1185	Focal adhesion kinase 2 inhibitor	4	100.0
1186	Focal adhesion kinase inhibitor	130	98.4
1187	Folate antagonist	24	92.5
1188	Follicle-stimulating hormone agonist	16	94.0
1189	Follicle-stimulating hormone antagonist	50	100.0
1190	Folylpolylglutamate synthase inhibitor	27	100.0
1191	Formaldehyde dehydrogenase (glutathione) inhibitor	17	97.4
1192	Formaldehyde dehydrogenase inhibitor	14	98.5
1193	Formaldehyde transketolase inhibitor	6	91.5
1194	Formate C-acetyltransferase inhibitor	5	99.7

1195	Formate dehydrogenase inhibitor	21	97.6
1196	Formate-dihydrofolate ligase inhibitor	14	89.0
1197	Formimidoylglutamase inhibitor	3	99.9
1198	Formimidoyltetrahydrofolate cyclodeaminase inhibitor	8	99.1
1199	Formyl peptide receptor antagonist	15	100.0
1200	Formyltetrahydrofolate dehydrogenase inhibitor	6	99.0
1201	Fragilysin inhibitor	6	85.5
1202	Free fatty acid receptor 1 agonist	28	100.0
1203	Free radical scavenger	253	93.3
1204	Fructan beta-fructosidase inhibitor	4	96.0
1205	Fructokinase inhibitor	13	99.6
1206	Fructose 5-dehydrogenase (NADP+) inhibitor	3	98.8
1207	Fructose 5-dehydrogenase inhibitor	4	80.3
1208	Fructose-2,6-bisphosphate 2-phosphatase inhibitor	12	96.2
1209	Fructose-2,6-bisphosphate 6-phosphatase inhibitor	4	99.6
1210	Fructuronate reductase inhibitor	3	99.3
1211	FtsZ polymerization inhibitor	3	100.0
1212	Fucokinase inhibitor	9	99.6
1213	Fucosterol-epoxide lyase inhibitor	9	92.5
1214	Fumarate reductase (NADH) inhibitor	7	89.3
1215	Fumarylacetoacetase inhibitor	14	99.3
1216	Furin inhibitor	23	98.0
1217	Fusarinine-C ornithinesterase inhibitor	3	83.7
1218	G protein-coupled receptor agonist	74	98.3
1219	G-protein-coupled bile acid receptor 1 agonist	9	95.6
1220	G-protein-coupled receptor 120 agonist	10	100.0
1221	G-protein-coupled receptor kinase inhibitor	21	84.9
1222	GABA A inverse agonist	9	88.8
1223	GABA B receptor agonist	10	91.8
1224	GABA B receptor antagonist	57	99.3
1225	GABA C receptor agonist	3	98.4
1226	GABA C receptor antagonist	6	99.1
1227	GABA inverse agonist	9	88.8
1228	GABA receptor agonist	392	93.3
1229	GABA receptor antagonist	1811	99.0
1230	GDP-L-fucose synthase inhibitor	3	99.9
1231	GDP-mannose 4,6-dehydratase inhibitor	8	100.0
1232	GDP-mannose 6-dehydrogenase inhibitor	6	89.4
1233	GHS receptor agonist	26	99.0
1234	GHS receptor antagonist	134	99.7
1235	GMP reductase inhibitor	17	99.6
1236	GMP synthase inhibitor	56	99.0
1237	GP IIb/IIIa receptor antagonist	2074	99.1
1238	GTP cyclohydrolase I inhibitor	15	99.3
1239	GTP cyclohydrolase IIa inhibitor	6	100.0
1240	Galactokinase inhibitor	6	97.9
1241	Galactolipase inhibitor	12	89.7
1242	Galactose 1-dehydrogenase (NADP+) inhibitor	3	98.7

1243	Galactose oxidase inhibitor	13	97.3
1244	Galactoside 2-alpha-L-fucosyltransferase inhibitor	12	98.3
1245	Galactoside O-acetyltransferase inhibitor	4	97.3
1246	Galactosylceramidase inhibitor	7	97.9
1247	Galactosylceramide sulfotransferase inhibitor	10	97.4
1248	Galactosylgalactosylglucosylceramidase inhibitor	5	99.4
1249	Galactosylgalactosylglucosylceramide beta-D-acetylgalactosaminyltransferase inhibitor	6	78.7
1250	Galacturan 1,4-alpha-galacturonidase inhibitor	4	98.9
1251	Galectin 3 antagonist	5	99.9
1252	Gallate decarboxylase inhibitor	5	98.0
1253	Gametolysin inhibitor	15	92.5
1254	Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor	3	97.9
1255	Gamma-butyrobetaine dioxygenase inhibitor	18	91.8
1256	Gamma-glutamyl hydrolase inhibitor	42	99.3
1257	Gamma-glutamyltransferase inhibitor	28	91.0
1258	Gamma-guanidinobutyraldehyde dehydrogenase inhibitor	5	89.0
1259	Ganglioside galactosyltransferase inhibitor	9	96.5
1260	Gastricin inhibitor	12	92.6
1261	Gastrin inhibitor	157	90.1
1262	Gastrin-releasing peptide antagonist	11	84.7
1263	Gelatinase inhibitor	19	97.0
1264	General pump inhibitor	45	83.9
1265	Gentamicin 2"-nucleotidyltransferase inhibitor	4	99.6
1266	Gentamicin 3'-N-acetyltransferase inhibitor	12	99.8
1267	Gentisate 1,2-dioxygenase inhibitor	6	98.7
1268	Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor	9	95.8
1269	Geranylgeranyltransferase I inhibitor	244	99.5
1270	Geranylgeranyltransferase inhibitor	454	99.5
1271	Geranyltranstransferase (Leishmania) inhibitor	27	100.0
1272	Geranyltranstransferase inhibitor	64	99.8
1273	Gestagen antagonist	8	96.4
1274	Gestagen-like	56	99.9
1275	Gingipain K inhibitor	6	93.5
1276	Gingipain R inhibitor	8	90.1
1277	Globoside alpha-N-acetylgalactosaminyltransferase inhibitor	13	96.1
1278	Glucagon receptor antagonist	206	98.9
1279	Glucagon-like peptide 1 agonist	9	93.7
1280	Glucagon-like peptide 1 receptor antagonist	13	100.0
1281	Glucan 1,3-alpha-glucosidase inhibitor	19	99.2
1282	Glucan 1,3-beta-glucosidase inhibitor	9	99.0
1283	Glucan 1,4-alpha-glucosidase inhibitor	19	99.5
1284	Glucan 1,4-alpha-maltotetraohydrolase inhibitor	3	97.4
1285	Glucan 1,4-alpha-maltotriohydrolase inhibitor	3	95.5
1286	Glucan 1,4-beta-glucosidase inhibitor	9	97.7
1287	Glucan 1,6-alpha-glucosidase inhibitor	6	98.6
1288	Glucan endo-1,3-alpha-glucosidase inhibitor	3	99.5
1289	Glucan endo-1,3-beta-D-glucosidase inhibitor	11	88.0
1290	Glucan endo-1,6-beta-glucosidase inhibitor	7	91.1

1291	Glucarate dehydratase inhibitor	5	98.9
1292	Glucocorticoid antagonist	429	99.1
1293	Gluconate 2-dehydrogenase (acceptor) inhibitor	4	80.6
1294	Gluconate 5-dehydrogenase inhibitor	3	95.1
1295	Gluconate dehydratase inhibitor	4	99.4
1296	Gluconokinase inhibitor	3	97.1
1297	Gluconolactonase inhibitor	3	97.5
1298	Glucosamine 6-phosphate N-acetyltransferase inhibitor	6	99.5
1299	Glucosamine N-acetyltransferase inhibitor	6	99.7
1300	Glucosamine-1-phosphate N-acetyltransferase inhibitor	4	99.3
1301	Glucosamine-6-phosphate deaminase inhibitor	12	97.9
1302	Glucose 1-dehydrogenase inhibitor	8	98.3
1303	Glucose oxidase inhibitor	7	85.2
1304	Glucose-1,6-bisphosphate synthase inhibitor	11	99.7
1305	Glucose-1-phosphatase inhibitor	3	99.0
1306	Glucose-1-phosphate adenylyltransferase inhibitor	15	99.5
1307	Glucose-1-phosphate cytidylyltransferase inhibitor	12	100.0
1308	Glucose-6-phosphate translocase inhibitor	27	99.8
1309	Glucose-dependent insulinotropic receptor agonist	62	99.9
1310	Glucosyl transferase inhibitor	37	95.0
1311	Glucosylceramidase inhibitor	18	99.5
1312	Glucuronate isomerase inhibitor	5	97.8
1313	Glucuronolactone reductase inhibitor	3	98.7
1314	Glutamate (mGluR group I) agonist	30	96.7
1315	Glutamate (mGluR group I) antagonist	180	96.8
1316	Glutamate (mGluR group II) agonist	37	98.7
1317	Glutamate (mGluR group II) antagonist	129	99.3
1318	Glutamate (mGluR group III) agonist	13	99.9
1319	Glutamate (mGluR group III) antagonist	25	97.2
1320	Glutamate (mGluR) agonist	87	98.7
1321	Glutamate (mGluR) antagonist	357	97.3
1322	Glutamate (mGluR1) agonist	10	99.8
1323	Glutamate (mGluR1) antagonist	93	95.6
1324	Glutamate (mGluR1a) agonist	4	100.0
1325	Glutamate (mGluR2) agonist	31	99.6
1326	Glutamate (mGluR2) antagonist	115	99.3
1327	Glutamate (mGluR3) agonist	11	99.4
1328	Glutamate (mGluR3) antagonist	63	98.9
1329	Glutamate (mGluR4) agonist	5	99.2
1330	Glutamate (mGluR4) antagonist	5	99.8
1331	Glutamate (mGluR5) agonist	17	94.5
1332	Glutamate (mGluR5) antagonist	92	97.4
1333	Glutamate (mGluR5a) agonist	4	100.0
1334	Glutamate (mGluR6) agonist	8	99.9
1335	Glutamate (mGluR6) antagonist	6	98.9
1336	Glutamate (mGluR8) agonist	3	99.7
1337	Glutamate (mGluR8) antagonist	13	100.0
1338	Glutamate 5-kinase inhibitor	9	88.7

1339	Glutamate N-acetyltransferase inhibitor	4	98.9
1340	Glutamate carboxypeptidase inhibitor	21	98.9
1341	Glutamate decarboxylase inhibitor	43	97.2
1342	Glutamate dehydrogenase (NADP+) inhibitor	18	99.0
1343	Glutamate dehydrogenase [NAD(P)+] inhibitor	45	98.6
1344	Glutamate formimidoyltransferase inhibitor	11	99.7
1345	Glutamate racemase inhibitor	45	99.6
1346	Glutamate receptor agonist	376	98.0
1347	Glutamate receptor antagonist	4453	97.2
1348	Glutamate release inhibitor	59	95.8
1349	Glutamate synthase (NADPH) inhibitor	54	97.6
1350	Glutamate synthase (ferredoxin) inhibitor	21	95.4
1351	Glutamate-1-semialdehyde 2,1-aminomutase inhibitor	9	95.6
1352	Glutamate-5-semialdehyde dehydrogenase inhibitor	4	87.2
1353	Glutamate-cysteine ligase inhibitor	36	99.0
1354	Glutamate-tRNA ligase inhibitor	6	82.4
1355	Glutamin-(asparagin-)ase inhibitor	13	96.4
1356	Glutaminase inhibitor	20	94.8
1357	Glutamine synthetase inhibitor	38	96.3
1358	Glutamine-fructose-6-phosphate transaminase inhibitor	4	99.3
1359	Glutamine-phenylpyruvate transaminase inhibitor	3	96.2
1360	Glutamine-pyruvate transaminase inhibitor	7	99.2
1361	Glutamine-tRNA ligase inhibitor	9	98.7
1362	Glutaminy-peptide cyclotransferase inhibitor	12	88.5
1363	Glutaminy-tRNA synthase (glutamine-hydrolysing) inhibitor	4	99.4
1364	Glutamyl endopeptidase II inhibitor	3	83.8
1365	Glutarate-semialdehyde dehydrogenase inhibitor	3	97.9
1366	Glutaryl-CoA dehydrogenase inhibitor	5	98.5
1367	Glutathione dehydrogenase (ascorbate) inhibitor	7	95.4
1368	Glutathione peroxidase inhibitor	10	94.4
1369	Glutathione reductase (NADPH) stimulant	11	97.4
1370	Glutathione reductase inhibitor	20	94.7
1371	Glutathione reductase stimulant	11	97.4
1372	Glutathione synthase inhibitor	15	98.1
1373	Glutathione thiolesterase inhibitor	3	94.3
1374	Glutathione-disulfide reductase inhibitor	46	98.3
1375	Glutathionylspermidine synthase inhibitor	15	100.0
1376	Gly-X carboxypeptidase inhibitor	6	98.4
1377	Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor	12	96.0
1378	Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor	16	98.4
1379	Glyceraldehyde-3-phosphate dehydrogenase inhibitor	3	91.9
1380	Glycerate kinase inhibitor	12	99.9
1381	Glycerol 2-dehydrogenase (NADP+) inhibitor	4	97.4
1382	Glycerol dehydratase inhibitor	6	99.4
1383	Glycerol dehydrogenase (NADP+) inhibitor	5	97.6
1384	Glycerol dehydrogenase inhibitor	34	98.3
1385	Glycerol kinase inhibitor	18	99.2
1386	Glycerol-1,2-cyclic-phosphate 2-phosphodiesterase inhibitor	7	99.9

1387	Glycerol-1-phosphatase inhibitor	3	99.0
1388	Glycerol-3-phosphate O-acyltransferase inhibitor	23	94.6
1389	Glycerol-3-phosphate dehydrogenase (NAD ⁺) inhibitor	21	97.8
1390	Glycerol-3-phosphate dehydrogenase [NAD(P) ⁺] inhibitor	6	99.9
1391	Glycerol-3-phosphate dehydrogenase inhibitor	28	90.4
1392	Glycerol-3-phosphate oxidase inhibitor	6	82.7
1393	Glycerone-phosphate O-acyltransferase inhibitor	10	98.1
1394	Glycerophosphocholine cholinephosphodiesterase inhibitor	6	99.3
1395	Glycerophosphocholine phosphodiesterase inhibitor	8	99.5
1396	Glycerophospholipid arachidonoyl-transferase (CoA-independent) inhibitor	7	79.4
1397	Glyceryl-ether monooxygenase inhibitor	11	86.0
1398	Glycine C-acetyltransferase inhibitor	12	90.6
1399	Glycine N-acyltransferase inhibitor	6	99.0
1400	Glycine N-benzoyltransferase inhibitor	6	98.9
1401	Glycine N-choloyltransferase inhibitor	10	99.3
1402	Glycine N-methyltransferase inhibitor	9	99.4
1403	Glycine amidinotransferase inhibitor	5	95.1
1404	Glycine dehydrogenase (cytochrome) inhibitor	6	79.4
1405	Glycine dehydrogenase (decarboxylating) inhibitor	3	98.3
1406	Glycine hydroxymethyltransferase inhibitor	30	96.4
1407	Glycine receptor agonist	13	93.8
1408	Glycine receptor antagonist	21	90.4
1409	Glycine transaminase inhibitor	7	99.2
1410	Glycine-tRNA ligase inhibitor	10	90.1
1411	Glycogen (starch) synthase inhibitor	26	94.2
1412	Glycogen synthase kinase-3 alpha inhibitor	101	99.4
1413	Glycogen synthase kinase-3 beta inhibitor	474	98.9
1414	Glycogen synthase kinase-3 inhibitor	858	98.9
1415	Glycogen synthase stimulant	9	87.6
1416	Glycogenin glucosyltransferase inhibitor	8	99.7
1417	Glycolaldehyde dehydrogenase inhibitor	6	99.3
1418	Glycolate dehydrogenase inhibitor	3	97.1
1419	Glycolipid 2-alpha-mannosyltransferase inhibitor	9	99.7
1420	Glycolipid 3-alpha-mannosyltransferase inhibitor	12	99.7
1421	Glycopeptide alpha-N-acetylgalactosaminidase inhibitor	8	98.3
1422	Glycoprotein 3-alpha-L-fucosyltransferase inhibitor	10	97.4
1423	Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor	9	95.5
1424	Glycosylceramidase inhibitor	14	99.1
1425	Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor	17	97.0
1426	Glycosylphosphatidylinositol phospholipase D inhibitor	4	87.7
1427	Glyoxylate oxidase inhibitor	3	97.7
1428	Glyoxylate reductase (NADP ⁺) inhibitor	12	92.7
1429	Glyoxylate reductase inhibitor	4	91.9
1430	Gonadotropin antagonist	27	87.0
1431	Granulocyte macrophage colony stimulating factor agonist	12	97.5
1432	Granulocyte stimulating factor agonist	31	99.4
1433	Granzyme A inhibitor	9	97.4
1434	Granzyme B inhibitor	23	96.6

1435	Growth factor agonist	366	93.4
1436	Growth factor antagonist	2745	97.0
1437	Growth factor receptor-bound protein 2 antagonist	70	100.0
1438	Growth hormone agonist	10	94.6
1439	Growth hormone release inhibitor	69	98.3
1440	Growth hormone release promoting	98	98.5
1441	Growth hormone releasing factor agonist	445	99.6
1442	Growth hormone releasing factor antagonist	41	99.9
1443	Guanidinoacetase inhibitor	6	97.8
1444	Guanidinoacetate N-methyltransferase inhibitor	6	97.8
1445	Guanidinoacetate kinase inhibitor	12	90.7
1446	Guanidinobutyrase inhibitor	13	99.1
1447	Guanidinodeoxy-scyllo-inositol-4-phosphatase inhibitor	3	99.3
1448	Guanidinopropionase inhibitor	5	99.4
1449	Guanine deaminase inhibitor	13	98.2
1450	Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor	4	92.0
1451	Guanylate cyclase 1 inhibitor	13	100.0
1452	Guanylate cyclase 1 stimulant	10	93.5
1453	Guanylate cyclase inhibitor	99	96.3
1454	Guanylate cyclase stimulant	76	96.0
1455	Guanylate kinase inhibitor	15	99.0
1456	H ⁺ -exporting ATPase inhibitor	12	92.4
1457	H ⁺ -transporting two-sector ATPase inhibitor	6	90.4
1458	H ⁺ /K ⁺ -transporting ATPase inhibitor	487	97.8
1459	HCV IRES inhibitor	8	83.7
1460	HCV NS3-helicase inhibitor	4	95.1
1461	HCV NS3/NS4A protease inhibitor	640	98.8
1462	HCV NS5A inhibitor	20	100.0
1463	HCV NS5B polymerase inhibitor	331	99.3
1464	HERG 1 channel blocker	38	93.8
1465	HIV attachment inhibitor	14	90.4
1466	HIV fusion inhibitor	4	100.0
1467	HIV-1 integrase (3'-Processing) inhibitor	505	98.5
1468	HIV-1 integrase (Overall Integration) inhibitor	68	98.1
1469	HIV-1 integrase (Strand Transfer) inhibitor	527	98.7
1470	HIV-1 integrase inhibitor	929	98.0
1471	HIV-1 protease inhibitor	2400	99.4
1472	HIV-1 reverse transcriptase inhibitor	1752	99.0
1473	HIV-2 retropepsin inhibitor	16	99.9
1474	HIV-2 reverse transcriptase inhibitor	3	98.4
1475	HLA-A2 antigen antagonist	188	99.9
1476	HMG CoA synthase inhibitor	5	99.4
1477	Haloacetate dehalogenase inhibitor	3	99.4
1478	Haloalkane dehalogenase inhibitor	4	99.7
1479	Heat shock protein 27 antagonist	4	97.8
1480	Heat shock protein 70 agonist	26	91.0
1481	Heat shock protein 90 antagonist	221	98.1
1482	Heat shock protein agonist	27	89.0

1483	Heat shock protein antagonist	230	97.7
1484	Hedgehog signaling activator	4	100.0
1485	Hedgehog signaling inhibitor	83	97.2
1486	Helicase E1 (Human papillomavirus) inhibitor	28	100.0
1487	Heme oxygenase inhibitor	4	88.6
1488	Heme oxygenase stimulant	10	98.7
1489	Heparan-alpha-glucosaminide N-acetyltransferase inhibitor	12	98.3
1490	Heparanase inhibitor	66	97.9
1491	Heparin epidermal growth factor antagonist	114	100.0
1492	Hepatocyte growth factor agonist	7	87.4
1493	Hepatocyte growth factor antagonist	401	99.0
1494	Hepatocyte nuclear factor 4 alpha agonist	6	100.0
1495	Hepatocyte nuclear factor 4 alpha antagonist	6	92.0
1496	Hepatocyte nuclear factor agonist	6	100.0
1497	Hepatocyte nuclear factor antagonist	6	92.0
1498	Hexokinase stimulant	119	99.1
1499	High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor	3	99.8
1500	Hippurate hydrolase inhibitor	4	99.1
1501	Histamine H1 receptor agonist	5	98.4
1502	Histamine H2 receptor agonist	45	97.0
1503	Histamine H3 receptor agonist	55	99.9
1504	Histamine H3 receptor antagonist	1371	99.5
1505	Histamine H4 receptor antagonist	97	99.8
1506	Histamine N-methyltransferase inhibitor	43	96.9
1507	Histamine agonist	127	94.0
1508	Histamine antagonist	2511	96.1
1509	Histamine release inhibitor	119	86.3
1510	Histamine release stimulant	21	88.3
1511	Histidine N-acetyltransferase inhibitor	6	81.5
1512	Histidine ammonia-lyase inhibitor	34	98.4
1513	Histidine decarboxylase inhibitor	33	97.9
1514	Histidine kinase inhibitor	4	92.8
1515	Histidine-tRNA ligase inhibitor	19	99.3
1516	Histidinol dehydrogenase inhibitor	21	93.4
1517	Histidinol-phosphatase inhibitor	6	97.0
1518	Histone acetylation inducer	19	100.0
1519	Histone acetyltransferase inhibitor	29	89.5
1520	Histone deacetylase 1 inhibitor	326	99.7
1521	Histone deacetylase 1A inhibitor	8	100.0
1522	Histone deacetylase 1B inhibitor	7	100.0
1523	Histone deacetylase 2 inhibitor	91	99.7
1524	Histone deacetylase 3 inhibitor	20	96.8
1525	Histone deacetylase 4 inhibitor	18	99.3
1526	Histone deacetylase 6 inhibitor	55	99.1
1527	Histone deacetylase 8 inhibitor	35	98.7
1528	Histone deacetylase SIRT1 inhibitor	51	96.8
1529	Histone deacetylase SIRT1 stimulant	63	99.5
1530	Histone deacetylase SIRT2 inhibitor	42	97.3

1531	Histone deacetylase SIRT2 stimulant	5	99.9
1532	Histone deacetylase class I inhibitor	383	99.7
1533	Histone deacetylase class II inhibitor	63	99.6
1534	Histone deacetylase class III inhibitor	69	97.4
1535	Histone deacetylase class IIa inhibitor	26	99.6
1536	Histone deacetylase class IIb inhibitor	55	99.1
1537	Histone deacetylase inhibitor	1551	98.6
1538	Histone deacetylase stimulant	63	99.5
1539	Histone-arginine N-methyltransferase inhibitor	9	99.3
1540	Histone-lysine N-methyltransferase inhibitor	5	99.9
1541	Homoaconitate hydratase inhibitor	3	98.8
1542	Homocitrate synthase inhibitor	18	98.0
1543	Homocysteine S-methyltransferase inhibitor	4	99.4
1544	Homocysteine desulfhydrase inhibitor	8	98.9
1545	Homogentisate 1,2-dioxygenase inhibitor	12	95.4
1546	Homoisocitrate dehydrogenase inhibitor	3	100.0
1547	Homoserine O-acetyltransferase inhibitor	11	99.7
1548	Homoserine O-succinyltransferase inhibitor	3	99.7
1549	Homoserine dehydrogenase inhibitor	14	89.0
1550	Homoserine kinase inhibitor	24	98.2
1551	Homospermidine synthase inhibitor	4	99.4
1552	Horrilysin inhibitor	3	98.2
1553	HsIV component of HsIUV peptidase inhibitor	7	78.7
1554	Hyaluronic acid agonist	4	93.8
1555	Hydrogen dehydrogenase inhibitor	3	89.4
1556	Hydrolase inhibitor	37	75.0
1557	Hydroperoxide dehydratase inhibitor	12	98.9
1558	Hydroxyacylglutathione hydrolase inhibitor	55	97.4
1559	Hydroxylamine oxidase inhibitor	6	90.4
1560	Hydroxylamine reductase (NADH) inhibitor	18	87.2
1561	Hydroxylamine reductase inhibitor	6	86.5
1562	Hydroxylysine kinase inhibitor	9	99.7
1563	Hydroxymethylbilane synthase inhibitor	11	95.9
1564	Hydroxymethylglutaryl-CoA lyase inhibitor	7	95.1
1565	Hydroxymethylglutaryl-CoA reductase inhibitor	5	99.4
1566	Hydroxypyruvate reductase inhibitor	17	99.6
1567	Hydroxyquinol 1,2-dioxygenase inhibitor	9	99.7
1568	Hydroxysteroid dehydrogenase inhibitor	3	94.0
1569	Hyponitrite reductase inhibitor	3	97.7
1570	Hypoxia inducible factor 1 alpha inhibitor	43	89.2
1571	I kappa B kinase 2 inhibitor	100	97.2
1572	I kappa B kinase inhibitor	157	96.5
1573	I(Ks) voltage-gated potassium channel blocker	38	100.0
1574	ICAM 1 antagonist	147	98.4
1575	IMP cyclohydrolase inhibitor	10	100.0
1576	Iduronate-2-sulfatase inhibitor	3	99.4
1577	IgA-specific metalloendopeptidase inhibitor	9	97.2
1578	IgA-specific serine endopeptidase inhibitor	5	95.0

1579	Imidazoleacetate 4-monooxygenase inhibitor	13	98.9
1580	Imidazoleglycerol-phosphate dehydratase inhibitor	4	99.6
1581	Imidazoline I1 receptor agonist	3	97.8
1582	Imidazoline I1 receptor antagonist	41	100.0
1583	Imidazoline I2 receptor antagonist	140	100.0
1584	Imidazoline receptor agonist	6	96.8
1585	Imidazoline receptor antagonist	148	100.0
1586	Immunoglobulin E antagonist	42	94.5
1587	Immunoglobulin Fc receptor antagonist	27	98.0
1588	Indanol dehydrogenase inhibitor	13	92.5
1589	Indole-3-acetaldehyde reductase (NADPH) inhibitor	11	99.2
1590	Indoleacetaldoxime dehydratase inhibitor	12	92.1
1591	Indoleamine-pyrrole 2,3-dioxygenase inhibitor	90	97.5
1592	Indolepyruvate C-methyltransferase inhibitor	4	97.2
1593	Inducible nitric-oxide synthase inhibitor	622	97.6
1594	Inorganic diphosphatase inhibitor	28	95.2
1595	Inosine kinase inhibitor	4	100.0
1596	Inosine monophosphate dehydrogenase 1 inhibitor	40	99.6
1597	Inosine monophosphate dehydrogenase 2 inhibitor	332	99.9
1598	Inosine monophosphate dehydrogenase inhibitor	459	99.8
1599	Inosine nucleosidase inhibitor	4	99.1
1600	Inosine-adenosine-guanosine-nucleoside hydrolase inhibitor	4	100.0
1601	Inositol 1,4,5-triphosphate receptor 1 antagonist	9	100.0
1602	Inositol 1,4,5-triphosphate receptor antagonist	10	95.4
1603	Inositol 1,4,5-trisphosphate 3-kinase B inhibitor	10	100.0
1604	Inositol 1,4,5-trisphosphate 3-kinase inhibitor	15	94.8
1605	Inositol oxygenase inhibitor	34	95.2
1606	Inositol polyphosphate-5-phosphatase D stimulant	7	100.0
1607	Inositol-3-phosphate synthase inhibitor	20	99.1
1608	Inositol-polyphosphate 5-phosphatase inhibitor	19	98.2
1609	Insulin growth factor agonist	8	79.9
1610	Insulin growth factor antagonist	281	98.6
1611	Insulin like growth factor 1 agonist	8	79.9
1612	Insulin like growth factor 1 antagonist	237	98.3
1613	Insulin like growth factor 3 antagonist	44	100.0
1614	Insulin promoter	47	84.5
1615	Insulin secretagogues	253	95.6
1616	Insulinotropin antagonist	6	82.5
1617	Insulysin inhibitor	12	90.1
1618	Integrin alpha1beta1 antagonist	42	99.4
1619	Integrin alpha2 antagonist	26	97.9
1620	Integrin alpha2beta1 antagonist	25	97.8
1621	Integrin alpha4 antagonist	1259	99.7
1622	Integrin alpha4beta1 antagonist	947	99.7
1623	Integrin alpha4beta7 antagonist	604	99.8
1624	Integrin alpha5beta1 antagonist	81	99.3
1625	Integrin alpha5beta6 antagonist	14	100.0
1626	Integrin alphaLbeta2 antagonist	38	100.0

1627	Integrin alphaVbeta1 antagonist	17	95.4
1628	Integrin alphaVbeta3 antagonist	36	99.6
1629	Integrin alphaVbeta5 antagonist	310	99.9
1630	Integrin alphaVbeta6 antagonist	79	99.9
1631	Integrin antagonist	1986	99.3
1632	Integrin-linked kinase inhibitor	13	100.0
1633	Interferon agonist	137	95.9
1634	Interferon alpha agonist	5	82.8
1635	Interferon antagonist	86	94.1
1636	Interferon gamma antagonist	85	94.5
1637	Interferon inducer	114	97.2
1638	Interleukin 1 antagonist	921	95.1
1639	Interleukin 1 beta converting enzyme inhibitor	193	98.6
1640	Interleukin 10 agonist	37	90.5
1641	Interleukin 10 antagonist	6	96.5
1642	Interleukin 12 agonist	131	96.0
1643	Interleukin 1a antagonist	17	93.9
1644	Interleukin 1b antagonist	500	96.8
1645	Interleukin 2 agonist	15	86.1
1646	Interleukin 2 antagonist	227	95.0
1647	Interleukin 4 antagonist	147	94.7
1648	Interleukin 5 antagonist	129	96.0
1649	Interleukin 6 antagonist	216	92.4
1650	Interleukin 8 antagonist	200	93.6
1651	Interleukin agonist	178	93.5
1652	Interleukin antagonist	1558	92.6
1653	Inulinase inhibitor	4	98.5
1654	Iodide peroxidase inhibitor	21	97.0
1655	Iron antagonist	9	96.1
1656	Iron-cytochrome-c reductase inhibitor	3	98.5
1657	Isoamylase inhibitor	15	98.9
1658	Isocitrate dehydrogenase (NAD+) inhibitor	28	97.4
1659	Isocitrate dehydrogenase (NADP+) inhibitor	24	99.0
1660	Isocitrate lyase inhibitor	26	98.3
1661	Isoleucine-tRNA ligase inhibitor	11	99.7
1662	Isomaltulose synthase inhibitor	6	99.3
1663	Isopenicillin-N epimerase inhibitor	9	86.4
1664	Isopenicillin-N synthase inhibitor	8	96.9
1665	Isopentenyl-diphosphate DELTA-isomerase inhibitor	22	99.8
1666	Isoquinoline 1-oxidoreductase inhibitor	4	98.4
1667	Isovaleryl-CoA dehydrogenase inhibitor	6	98.4
1668	JNK mitogen-activated protein kinase inhibitor	52	93.8
1669	Janus tyrosine kinase 1 inhibitor	17	98.7
1670	Janus tyrosine kinase 2 inhibitor	163	97.7
1671	Janus tyrosine kinase 3 inhibitor	245	98.8
1672	Janus tyrosine kinase inhibitor	454	98.0
1673	Juvenile-hormone esterase inhibitor	86	99.9
1674	K(Ca) 3.1 channel activator	4	98.6

1675	K(Ca) 3.1 channel blocker	41	98.5
1676	K(ir) 6.2 channel activator	13	95.7
1677	Kainate receptor 1 agonist	5	99.8
1678	Kainate receptor 1 antagonist	177	99.9
1679	Kainate receptor 2 antagonist	21	96.3
1680	Kainate receptor 3 antagonist	8	100.0
1681	Kainate receptor 4 antagonist	5	97.6
1682	Kainate receptor 5 antagonist	24	99.9
1683	Kainate receptor agonist	26	99.2
1684	Kainate receptor antagonist	338	99.5
1685	Kallikrein 13 inhibitor	3	99.6
1686	Kallikrein 3 inhibitor	22	96.6
1687	Kallikrein inhibitor	62	97.3
1688	Kanamycin kinase inhibitor	3	100.0
1689	Keratan sulfotransferase inhibitor	7	99.9
1690	Ketohexokinase inhibitor	14	99.2
1691	Ketol-acid reductoisomerase inhibitor	10	91.8
1692	Ketosteroid monooxygenase inhibitor	5	100.0
1693	Kexin inhibitor	16	98.1
1694	KiSS-1 receptor agonist	3	100.0
1695	Kinase inhibitor	16	75.2
1696	Kinesin antagonist	507	99.0
1697	Kynureninase inhibitor	42	98.7
1698	Kynurenine 3 monooxygenase inhibitor	55	99.9
1699	L lactate dehydrogenase A inhibitor	16	100.0
1700	L lactate dehydrogenase A4 inhibitor	15	100.0
1701	L lactate dehydrogenase B inhibitor	6	100.0
1702	L lactate dehydrogenase B4 inhibitor	6	100.0
1703	L lactate dehydrogenase C inhibitor	16	100.0
1704	L lactate dehydrogenase C4 inhibitor	16	100.0
1705	L lactate dehydrogenase inhibitor	32	96.2
1706	L lactate dehydrogenase stimulant	5	78.4
1707	L(+)-Tartrate dehydratase inhibitor	7	99.9
1708	L-3-cyanoalanine synthase inhibitor	10	99.5
1709	L-Serine ammonia-lyase inhibitor	14	99.4
1710	L-amino-acid oxidase inhibitor	20	96.7
1711	L-aminoadipate-semialdehyde dehydrogenase inhibitor	9	99.4
1712	L-ascorbate peroxidase inhibitor	16	98.5
1713	L-fuconate dehydratase inhibitor	7	99.6
1714	L-galactonolactone oxidase inhibitor	8	98.9
1715	L-glucuronate reductase inhibitor	17	95.4
1716	L-glutamate oxidase inhibitor	3	95.4
1717	L-itol 2-dehydrogenase inhibitor	100	97.6
1718	L-iduronidase inhibitor	5	98.8
1719	L-lactate dehydrogenase (cytochrome) inhibitor	6	99.8
1720	L-lysine 6-transaminase inhibitor	6	98.9
1721	L-lysine oxidase inhibitor	4	99.1
1722	L-threonine 3-dehydrogenase inhibitor	10	87.8

1723	LFA antagonist	189	99.6
1724	LFA-1 antagonist	187	99.7
1725	Laccase inhibitor	18	95.2
1726	Lactaldehyde dehydrogenase inhibitor	6	99.8
1727	Lactaldehyde reductase (NADPH) inhibitor	4	99.0
1728	Lactaldehyde reductase inhibitor	4	98.4
1729	Lactamase A inhibitor	7	99.4
1730	Lactamase C inhibitor	5	96.4
1731	Lactase inhibitor	3	85.7
1732	Lactate 2-monoxygenase inhibitor	13	92.8
1733	Lactate-malate transhydrogenase inhibitor	5	99.4
1734	Lactose synthase inhibitor	14	88.5
1735	Lactosylceramide alpha-2,3-sialyltransferase inhibitor	20	97.7
1736	Lactoylglutathione lyase inhibitor	88	98.0
1737	Laminaribiose phosphorylase inhibitor	9	97.2
1738	Lanosterol 14 alpha demethylase inhibitor	78	95.0
1739	Lck kinase inhibitor	537	98.1
1740	Leishmanolysin inhibitor	6	86.2
1741	Leucine dehydrogenase inhibitor	5	91.7
1742	Leucine transaminase inhibitor	5	99.2
1743	Leucine-tRNA ligase inhibitor	25	95.7
1744	Leucolysin inhibitor	6	98.0
1745	Leucyltransferase inhibitor	14	98.6
1746	Leukocyte elastase inhibitor	38	82.5
1747	Leukotriene A4 hydrolase inhibitor	181	99.6
1748	Leukotriene B4 antagonist	474	98.1
1749	Leukotriene B4 receptor 1 antagonist	342	99.9
1750	Leukotriene B4 receptor 2 antagonist	36	100.0
1751	Leukotriene C antagonist	24	85.0
1752	Leukotriene C4 antagonist	13	90.4
1753	Leukotriene D4 antagonist	453	99.0
1754	Leukotriene E4 antagonist	42	96.6
1755	Leukotriene agonist	6	93.9
1756	Leukotriene antagonist	1062	97.3
1757	Leukotriene-B4 20-monoxygenase inhibitor	5	95.0
1758	Leukotriene-C4 synthase inhibitor	9	87.0
1759	Levanase inhibitor	9	95.8
1760	Levansucrase inhibitor	5	94.5
1761	Licheninase inhibitor	6	97.5
1762	Ligase inhibitor	5	98.4
1763	Limulus clotting factor B inhibitor	4	83.6
1764	Limulus clotting factor C inhibitor	4	95.3
1765	Linoleate diol synthase inhibitor	15	88.6
1766	Linoleate isomerase inhibitor	22	99.5
1767	Linoleoyl-CoA desaturase inhibitor	6	95.6
1768	Lipase inhibitor	178	98.6
1769	Lipid peroxidase inhibitor	322	91.5
1770	Lipocortins synthesis agonist	79	96.5

1771	Lipocortins synthesis antagonist	11	95.4
1772	Lipoprotein lipase inhibitor	18	88.4
1773	Lipoprotein lipase stimulant	23	87.9
1774	Lipoxin receptor agonist	12	100.0
1775	Lipoxygenase inhibitor	2055	96.7
1776	Liver X receptor agonist	280	99.4
1777	Liver X receptor alpha agonist	79	99.1
1778	Liver X receptor antagonist	7	95.6
1779	Liver X receptor beta agonist	68	99.3
1780	Lombricine kinase inhibitor	6	98.2
1781	Long-chain-acyl-CoA dehydrogenase inhibitor	6	99.4
1782	Long-chain-aldehyde dehydrogenase inhibitor	4	96.6
1783	Long-chain-fatty-acid-CoA ligase inhibitor	23	99.1
1784	Luteinizing hormone-releasing hormone agonist	36	97.1
1785	Lysase inhibitor	10	83.0
1786	Lysine 2,3-aminomutase inhibitor	5	88.1
1787	Lysine 2-monooxygenase inhibitor	19	97.0
1788	Lysine 6-dehydrogenase inhibitor	3	98.8
1789	Lysine decarboxylase inhibitor	10	98.8
1790	Lysine-tRNA ligase inhibitor	16	99.7
1791	Lysophosphatidic acid receptor agonist	13	100.0
1792	Lysophosphatidic acid receptor antagonist	4	85.2
1793	Lysosomal Pro-X carboxypeptidase inhibitor	8	96.1
1794	Lysostaphin inhibitor	3	96.5
1795	Lysozyme inhibitor	13	98.2
1796	Lysyl endopeptidase inhibitor	16	98.1
1797	Lysyl oxidase inhibitor	10	84.1
1798	M7G(5')pppN diphosphatase inhibitor	4	100.0
1799	MAO B inhibitor	338	99.1
1800	MAP kinase 1 inhibitor	72	94.3
1801	MAP kinase 10 inhibitor	115	98.0
1802	MAP kinase 14 inhibitor	588	99.3
1803	MAP kinase 8 inhibitor	17	83.0
1804	MAP kinase 9 inhibitor	67	95.7
1805	MAP kinase inhibitor	1413	97.1
1806	MAP kinase kinase 1 inhibitor	11	98.4
1807	MAP kinase kinase 4 inhibitor	18	99.3
1808	MAP kinase kinase 7 inhibitor	17	98.7
1809	MAP kinase kinase inhibitor	334	99.0
1810	MAP kinase kinase kinase inhibitor	37	96.1
1811	MAP kinase stimulant	7	87.0
1812	MAP-kinase-activated kinase 1 inhibitor	17	95.8
1813	MAP-kinase-activated kinase 2 inhibitor	120	98.3
1814	MAP-kinase-activated kinase inhibitor	141	97.5
1815	MAP3K11 inhibitor	6	99.9
1816	MAP3K5 inhibitor	4	100.0
1817	MAP3K8 inhibitor	18	99.7
1818	MAP3K9 inhibitor	10	90.7

1819	MARK1 protein inhibitor	7	100.0
1820	MDM2 inhibitor	101	97.4
1821	MO15-related protein kinase Pfmrk inhibitor	14	93.2
1822	Macrococin O-methyltransferase inhibitor	9	100.0
1823	Macrophage colony stimulating factor agonist	4	81.4
1824	Macrophage colony stimulating factor antagonist	167	99.2
1825	Macrophage elastase inhibitor	151	99.0
1826	Macrophage migration inhibitory factor inhibitor	70	99.5
1827	Macrophage scavenger receptor antagonist	7	100.0
1828	Magnesium-protoporphyrin IX methyltransferase inhibitor	11	97.8
1829	Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor	10	96.4
1830	Magnolysin inhibitor	6	99.9
1831	Maillard reaction inhibitor	38	88.3
1832	Malate dehydrogenase (NADP+) inhibitor	9	99.2
1833	Malate dehydrogenase (acceptor) inhibitor	12	86.2
1834	Malate dehydrogenase (decarboxylating) inhibitor	20	99.4
1835	Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor	21	99.4
1836	Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor	16	98.4
1837	Malate dehydrogenase inhibitor	64	93.7
1838	Malate oxidase inhibitor	5	89.1
1839	Malate synthase inhibitor	18	99.1
1840	Malate-CoA ligase inhibitor	5	98.5
1841	Maleate hydratase inhibitor	11	99.5
1842	Maleate isomerase inhibitor	6	95.0
1843	Maleylacetate reductase inhibitor	4	100.0
1844	Maleylacetoacetate isomerase inhibitor	6	99.5
1845	Malonate-semialdehyde dehydrogenase inhibitor	3	99.4
1846	Malonyl-CoA decarboxylase inhibitor	19	98.5
1847	Maltose-transporting ATPase inhibitor	4	97.6
1848	Mallyl-CoA lyase inhibitor	6	98.2
1849	Mandelate 4-monooxygenase inhibitor	11	95.8
1850	Mandelate racemase inhibitor	27	99.5
1851	Manganese peroxidase inhibitor	6	91.2
1852	Mannan endo-1,4-beta-mannosidase inhibitor	3	94.0
1853	Mannan endo-1,6-alpha-mannosidase inhibitor	4	98.9
1854	Mannitol 2-dehydrogenase inhibitor	5	100.0
1855	Mannitol-1-phosphatase inhibitor	3	98.3
1856	Mannitol-1-phosphate 5-dehydrogenase inhibitor	18	99.0
1857	Mannokinase inhibitor	9	99.9
1858	Mannonate dehydratase inhibitor	9	99.0
1859	Mannose isomerase inhibitor	5	91.4
1860	Mannose-1-phosphate guanylyltransferase inhibitor	4	100.0
1861	Mannose-6-phosphate isomerase inhibitor	18	99.5
1862	Mannosidase inhibitor	59	98.3
1863	Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor	8	97.6
1864	Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor	17	99.7
1865	Mannosyl-oligosaccharide glucosidase inhibitor	18	99.6
1866	Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor	4	89.5

1867	MarA inhibitor	12	100.0
1868	Matrilysin inhibitor	187	99.3
1869	Matriptase inhibitor	6	99.8
1870	Matrix metalloproteinase (membrane-type) inhibitor	97	98.2
1871	Matrix metalloproteinase 1 (membrane-type) inhibitor	97	98.2
1872	Matrix metalloproteinase 1 inhibitor	1128	99.3
1873	Matrix metalloproteinase 2 (membrane-type) inhibitor	3	99.0
1874	Matrix metalloproteinase 3 (membrane-type) inhibitor	8	99.0
1875	Matrix metalloproteinase inhibitor	1606	98.7
1876	Mcl-1 antagonist	16	81.7
1877	Mediator release inhibitor	160	89.9
1878	Melanin inhibitor	32	93.0
1879	Melanin-concentrating hormone receptor 1 antagonist	506	99.1
1880	Melanin-concentrating hormone receptor antagonist	511	99.1
1881	Melanocortin MC-4 agonist	15	99.7
1882	Melanocortin agonist	23	99.7
1883	Melanocortin antagonist	205	98.5
1884	Melatonin 1 agonist	27	99.6
1885	Melatonin 1 antagonist	481	99.8
1886	Melatonin 1a antagonist	332	99.9
1887	Melatonin 1b antagonist	10	99.6
1888	Melatonin 2 agonist	15	100.0
1889	Melatonin 2 antagonist	233	99.9
1890	Melatonin 3 antagonist	100	99.9
1891	Melatonin 5 antagonist	68	100.0
1892	Melatonin agonist	99	99.5
1893	Melatonin antagonist	749	99.7
1894	Membrane dipeptidase inhibitor	45	95.5
1895	Membrane integrity agonist	15	82.9
1896	Membrane integrity antagonist	60	83.4
1897	Membrane permeability enhancer	47	88.0
1898	Membrane permeability inhibitor	40	82.1
1899	Membrane-oligosaccharide glycerophosphotransferase inhibitor	6	99.9
1900	Meprin A inhibitor	13	97.1
1901	Meprin B inhibitor	3	97.8
1902	Metalloproteinase D inhibitor	7	95.4
1903	Metalloproteinase inhibitor	2058	98.7
1904	Metalloproteinase-11 inhibitor	31	98.2
1905	Metalloproteinase-2 inhibitor	1208	99.1
1906	Metalloproteinase-3 inhibitor	982	99.1
1907	Metalloproteinase-9 inhibitor	1256	99.1
1908	Methane monooxygenase inhibitor	13	89.9
1909	Methanol dehydrogenase inhibitor	3	98.2
1910	Methenyltetrahydrofolate cyclohydrolase inhibitor	7	99.2
1911	Methionine adenosyltransferase inhibitor	27	99.1
1912	Methionine decarboxylase inhibitor	6	98.9
1913	Methionine-tRNA ligase inhibitor	120	99.2
1914	Methionyl aminopeptidase 1 inhibitor	62	98.4

1915	Methionyl aminopeptidase 2 inhibitor	101	99.8
1916	Methionyl aminopeptidase inhibitor	176	98.5
1917	Methionyl-tRNA formyltransferase inhibitor	7	100.0
1918	Methylamine-glutamate N-methyltransferase inhibitor	3	95.4
1919	Methylaspartate ammonia-lyase inhibitor	8	98.2
1920	Methylaspartate mutase inhibitor	8	99.9
1921	Methylcrotonoyl-CoA carboxylase inhibitor	11	98.6
1922	Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor	10	98.8
1923	Methylenetetrahydrofolate reductase (NADPH) inhibitor	10	91.7
1924	Methylglutamate dehydrogenase inhibitor	7	98.6
1925	Methylglyoxal synthase inhibitor	15	99.8
1926	Methylmalonyl-CoA carboxytransferase inhibitor	7	100.0
1927	Methylmalonyl-CoA decarboxylase inhibitor	7	98.9
1928	Methylmalonyl-CoA epimerase inhibitor	9	99.9
1929	Methylmalonyl-CoA mutase inhibitor	11	99.0
1930	Methylthioadenosine nucleosidase inhibitor	16	99.3
1931	Methyltransferase inhibitor	5	100.0
1932	Methylumbelliferyl-acetate deacetylase inhibitor	7	86.9
1933	Mevalonate kinase inhibitor	11	98.0
1934	MexAB-OprM inhibitor	3	100.0
1935	Microbial collagenase inhibitor	514	99.4
1936	Microsomal triglyceride transfer protein inhibitor	419	99.9
1937	Microtubule formation inhibitor	384	94.5
1938	Microtubule formation stimulant	14	82.5
1939	Microtubule stabilization	512	99.2
1940	Mineralocorticoid	22	100.0
1941	Mineralocorticoid antagonist	242	98.7
1942	Mitochondrial intermediate peptidase inhibitor	6	97.5
1943	Mitochondrial processing peptidase inhibitor	6	82.5
1944	Monodehydroascorbate reductase (NADH) inhibitor	17	91.7
1945	Monophenol monooxygenase inhibitor	85	96.3
1946	Morphine 6-dehydrogenase inhibitor	13	95.4
1947	Motilin receptor agonist	103	99.2
1948	Motilin receptor antagonist	70	100.0
1949	Mucinaminyserine mucinamidase inhibitor	5	82.7
1950	Mucomembranous protector	35	81.4
1951	Muconate cycloisomerase inhibitor	4	99.7
1952	Mucorpepsin inhibitor	5	96.1
1953	Multiple inositol-polyphosphate phosphatase inhibitor	5	100.0
1954	Muramoyltetrapeptide carboxypeptidase inhibitor	5	92.7
1955	Myc inhibitor	9	86.5
1956	Mycodextranase inhibitor	6	99.3
1957	Mycolysin inhibitor	3	99.7
1958	Mycothiols-S-conjugate amidase inhibitor	3	88.2
1959	Myelin associated glycoprotein antagonist	4	100.0
1960	Myeloblastin inhibitor	4	98.0
1961	Myosin ATPase inhibitor	11	87.2
1962	Myosin-light-chain-phosphatase inhibitor	6	97.2

1963	Myristoyl transferase 1 inhibitor	3	100.0
1964	Myristoyl transferase inhibitor	80	100.0
1965	Myt1 kinase inhibitor	11	98.1
1966	N-(5-amino-5-carboxypentanoyl)-L-cysteiny-D-valine synthase inhibitor	8	98.1
1967	N-(long-chain-acyl)ethanolamine deacylase inhibitor	7	96.9
1968	N-Acetylated alpha-linked acidic dipeptidase inhibitor	152	99.9
1969	N-Acyl-D-amino-acid deacylase inhibitor	4	98.7
1970	N-Acyl-D-aspartate deacylase inhibitor	3	98.2
1971	N-Carbamoyl-D-amino acid hydrolase inhibitor	5	98.4
1972	N-acetyl-gamma-glutamyl-phosphate reductase inhibitor	3	98.7
1973	N-acetylgalactosamine-4-sulfatase inhibitor	3	100.0
1974	N-acetylglucosamine kinase inhibitor	15	99.1
1975	N-acetylglucosamine-6-phosphate deacetylase inhibitor	10	99.2
1976	N-acetylglucosaminyldiphosphodolichol N-acetylglucosaminyltransferase inhibitor	6	99.7
1977	N-acetylglucosaminyldiphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor	3	93.8
1978	N-acetylactosamine synthase inhibitor	6	96.2
1979	N-acetylactosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor	5	96.5
1980	N-acetylactosaminide beta-1,6-N-acetylglucosaminyl-transferase inhibitor	7	99.6
1981	N-acetylmuramoyl-L-alanine amidase inhibitor	11	99.6
1982	N-acetylneuraminate 4-O-acetyltransferase inhibitor	3	97.5
1983	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor	6	80.9
1984	N-acetylneuraminate lyase inhibitor	14	99.1
1985	N-acetylneuraminate synthase inhibitor	4	98.9
1986	N-acylmannosamine kinase inhibitor	5	88.2
1987	N-acylneuraminate cytidyltransferase inhibitor	15	99.2
1988	N-benzyloxycarbonylglycine hydrolase inhibitor	6	88.0
1989	N-carbamoyl-L-amino-acid hydrolase inhibitor	10	98.2
1990	N-formylglutamate deformylase inhibitor	16	99.4
1991	N-formylmethionyl-peptidase inhibitor	3	96.5
1992	N-hydroxy-2-acetamidofluorene reductase inhibitor	3	97.8
1993	N-hydroxyarylamine O-acetyltransferase inhibitor	11	84.1
1994	N-methyl-2-oxoglutaramate hydrolase inhibitor	9	96.9
1995	N-methylhydantoinase (ATP-hydrolysing) inhibitor	5	96.7
1996	N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor	10	98.2
1997	N6-methyl-lysine oxidase inhibitor	4	98.2
1998	NAD(P)+ transhydrogenase (AB-specific) inhibitor	31	97.6
1999	NAD(P)+ transhydrogenase (B-specific) inhibitor	11	96.1
2000	NAD(P)+-arginine ADP-ribosyltransferase inhibitor	11	85.9
2001	NAD(P)H dehydrogenase (quinone) 1 inhibitor	3	98.4
2002	NAD(P)H dehydrogenase (quinone) inhibitor	101	97.3
2003	NAD+ diphosphatase inhibitor	11	99.1
2004	NAD+ kinase inhibitor	17	96.1
2005	NAD+ nucleosidase inhibitor	19	99.3
2006	NAD+ synthase (glutamine-hydrolysing) inhibitor	4	98.0
2007	NAD+-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor	3	99.4
2008	NADH dehydrogenase inhibitor	17	95.5
2009	NADH kinase inhibitor	3	97.1

2010	NADH oxidase inhibitor	18	100.0
2011	NADH peroxidase inhibitor	5	79.8
2012	NADPH oxidase inhibitor	16	93.7
2013	NADPH oxidoreductase inhibitor	20	98.9
2014	NADPH peroxidase inhibitor	4	90.4
2015	NADPH-cytochrome-c2 reductase inhibitor	3	87.4
2016	NADPH-ferrihemoprotein reductase inhibitor	10	86.7
2017	NF-E2-related factor 2 stimulant	10	94.8
2018	NMDA 2 receptor antagonist	941	98.9
2019	NMDA 2A receptor antagonist	568	99.4
2020	NMDA 2B receptor antagonist	396	99.0
2021	NMDA receptor agonist	164	98.1
2022	NMDA receptor antagonist	3098	98.0
2023	NMDA receptor glutamate site antagonist	3	100.0
2024	NMDA receptor glycine site B antagonist	5	99.9
2025	NMDA receptor glycine site agonist	127	98.9
2026	NMDA receptor glycine site antagonist	531	99.8
2027	NMDA receptor phencyclidine site antagonist	152	99.8
2028	NMDA receptor polyamine site agonist	3	99.9
2029	NMDA receptor polyamine site antagonist	5	94.0
2030	NMN nucleosidase inhibitor	16	99.2
2031	NTPase/helicase (JEV) inhibitor	3	100.0
2032	NTPase/helicase (WNF) inhibitor	9	100.0
2033	Na ⁺ -transporting two-sector ATPase inhibitor	7	82.7
2034	Naphthalene 1,2-dioxygenase inhibitor	3	96.5
2035	Nardilysin inhibitor	8	93.1
2036	Nav1.1 sodium channel blocker	115	97.9
2037	Nav1.2 sodium channel blocker	43	97.7
2038	Nav1.3 sodium channel blocker	15	100.0
2039	Nav1.4 sodium channel blocker	19	98.4
2040	Nav1.5 sodium channel blocker	19	87.6
2041	Nav1.7 sodium channel blocker	40	98.8
2042	Nav1.8 sodium channel blocker	9	98.3
2043	Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor	6	99.2
2044	Nerve growth factor agonist	22	78.5
2045	Nerve growth factor antagonist	40	99.3
2046	Neuraminidase (Influenza A) inhibitor	166	100.0
2047	Neuraminidase (Influenza B) inhibitor	65	100.0
2048	Neuraminidase (influenza) inhibitor	196	99.8
2049	Neuraminidase inhibitor	230	98.1
2050	Neurokinin 1 antagonist	1279	99.5
2051	Neurokinin 2 antagonist	594	99.4
2052	Neurokinin 3 antagonist	243	99.3
2053	Neurokinin antagonist	1821	99.4
2054	Neurolysin inhibitor	25	98.4
2055	Neuronal nicotinic receptor antagonist	575	99.5
2056	Neuronal nitric-oxide synthase inhibitor	342	99.4
2057	Neuropeptide FF agonist	8	88.0

2058	Neuropeptide FF antagonist	63	99.8
2059	Neuropeptide FF1 antagonist	27	99.7
2060	Neuropeptide FF2 agonist	8	88.0
2061	Neuropeptide S antagonist	3	100.0
2062	Neuropeptide Y agonist	7	95.6
2063	Neuropeptide Y antagonist	1162	98.7
2064	Neuropeptide Y1 agonist	6	100.0
2065	Neuropeptide Y1 antagonist	316	99.2
2066	Neuropeptide Y2 antagonist	41	98.5
2067	Neuropeptide Y4 antagonist	4	92.6
2068	Neuropeptide Y5 antagonist	731	99.3
2069	Neuropeptide agonist	16	91.0
2070	Neuropeptide antagonist	1228	98.8
2071	Neuropsin inhibitor	5	98.8
2072	Neurotensin 1 receptor agonist	3	99.8
2073	Neurotensin 1 receptor antagonist	31	97.7
2074	Neurotensin 2 receptor antagonist	14	100.0
2075	Neurotensin 3 receptor antagonist	13	100.0
2076	Neurotensin receptor agonist	16	99.8
2077	Neurotensin receptor antagonist	79	99.4
2078	Neurotransmitter agonist	7	78.0
2079	Neurotransmitter antagonist	9	82.8
2080	Neurotrophic factor	472	95.9
2081	Neurotrophic factor enhancer	74	92.7
2082	Neutrophil collagenase inhibitor	565	99.1
2083	Neutrophil fMLF receptor antagonist	23	100.0
2084	Nicotinamidase inhibitor	24	98.2
2085	Nicotinamide phosphoribosyltransferase inhibitor	13	96.7
2086	Nicotinamide-nucleotide adenylyltransferase inhibitor	7	99.0
2087	Nicotinamide-nucleotide amidase inhibitor	6	100.0
2088	Nicotinate dehydrogenase inhibitor	6	85.6
2089	Nicotinate phosphoribosyltransferase inhibitor	17	99.4
2090	Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor	32	99.3
2091	Nicotine dehydrogenase inhibitor	5	81.8
2092	Nicotinic acid receptor 1 agonist	102	98.8
2093	Nicotinic acid receptor 2 agonist	15	100.0
2094	Nicotinic acid receptor agonist	115	98.8
2095	Nicotinic alpha2beta2 receptor antagonist	4	88.3
2096	Nicotinic alpha2beta4 receptor agonist	4	87.0
2097	Nicotinic alpha3beta4 receptor agonist	12	99.1
2098	Nicotinic alpha3beta4 receptor antagonist	5	76.9
2099	Nicotinic alpha4 receptor agonist	16	100.0
2100	Nicotinic alpha4beta2 receptor agonist	34	99.9
2101	Nicotinic alpha4beta2 receptor antagonist	18	93.9
2102	Nicotinic alpha4beta4 receptor agonist	3	90.2
2103	Nicotinic alpha6 receptor agonist	3	99.6
2104	Nicotinic alpha6beta3beta4alpha5 receptor antagonist	3	84.2
2105	Nicotinic alpha7 receptor agonist	535	99.4

2106	Nicotinic neuronal receptor agonist	611	99.1
2107	Niemann-Pick C1-like 1 protein antagonist	14	87.3
2108	Nitrate reductase (cytochrome) inhibitor	11	87.2
2109	Nitrate reductase inhibitor	30	93.8
2110	Nitric oxide antagonist	152	94.6
2111	Nitric oxide donor	249	99.3
2112	Nitric oxide scavenger	4	94.7
2113	Nitric-oxide reductase inhibitor	9	79.7
2114	Nitric-oxide synthase inhibitor	688	97.8
2115	Nitric-oxide synthase stimulant	19	90.7
2116	Nitrilase inhibitor	18	98.2
2117	Nitrile hydratase inhibitor	22	98.6
2118	Nitrite reductase (NO-forming) inhibitor	3	95.0
2119	Nitrite reductase [NAD(P)H] inhibitor	18	87.8
2120	Nitrous-oxide reductase inhibitor	4	79.5
2121	Nociceptin (N/OFQ) receptor agonist	15	100.0
2122	Nociceptin (N/OFQ) receptor antagonist	132	98.7
2123	Nuclear receptor subfamily 4, group A, member 2 agonist	24	99.8
2124	Nuclease inhibitor	19	98.9
2125	Nucleoside deoxyribosyltransferase inhibitor	8	99.8
2126	Nucleoside oxidase (H ₂ O ₂ -forming) inhibitor	6	96.5
2127	Nucleoside phosphoacylhydrolase inhibitor	4	98.6
2128	Nucleoside-diphosphatase inhibitor	10	96.8
2129	Nucleoside-triphosphate diphosphatase inhibitor	7	100.0
2130	Nucleoside-triphosphate-adenylate kinase inhibitor	7	98.4
2131	Nucleotidase inhibitor	6	94.1
2132	Nucleotide diphosphatase inhibitor	37	97.8
2133	Nucleotide metabolism regulator	138	86.5
2134	Nucleotidyltransferase (FIV) inhibitor	15	99.6
2135	Nucleotidyltransferase inhibitor	18	99.8
2136	O-acetylhomoserine aminocarboxypropyltransferase inhibitor	15	97.6
2137	O-aminophenol oxidase inhibitor	12	91.4
2138	O ⁶ -alkylguanine-DNA alkyltransferase inhibitor	95	99.4
2139	Octadecanal decarbonylase inhibitor	6	99.3
2140	Octopamine agonist	67	99.9
2141	Octopamine antagonist	5	80.4
2142	Oleamide hydrolase inhibitor	50	100.0
2143	Oligo-1,6-glucosidase inhibitor	23	99.0
2144	Oligonucleotidase inhibitor	10	99.3
2145	Oligopeptidase B inhibitor	7	96.8
2146	Omega-amidase inhibitor	8	98.8
2147	Omptin inhibitor	4	87.4
2148	Opheline kinase inhibitor	3	97.6
2149	Opine dehydrogenase inhibitor	4	97.5
2150	Opioid agonist	489	97.7
2151	Opioid antagonist	2078	98.7
2152	Opioid delta 1 receptor antagonist	12	97.0
2153	Opioid delta 2 receptor antagonist	12	99.9

2154	Opioid delta receptor agonist	162	99.0
2155	Opioid kappa 1 receptor antagonist	90	99.1
2156	Opioid kappa 2 receptor antagonist	15	100.0
2157	Opioid kappa 2b receptor antagonist	14	100.0
2158	Opioid kappa 3 receptor antagonist	10	84.8
2159	Opioid kappa receptor agonist	134	97.6
2160	Opioid kappa receptor antagonist	1165	99.2
2161	Opioid mu 1 receptor antagonist	21	97.8
2162	Opioid mu 2 receptor antagonist	24	98.5
2163	Opioid mu receptor antagonist	1636	99.2
2164	Opioid partial agonist	8	99.7
2165	Orcinol 2-monoxygenase inhibitor	7	99.9
2166	Orexin receptor 1 antagonist	223	99.9
2167	Orexin receptor 2 antagonist	137	99.7
2168	Orexin receptor antagonist	406	99.9
2169	Ornithine cyclodeaminase inhibitor	3	98.6
2170	Ornithine decarboxylase inhibitor	94	96.7
2171	Ornithine-oxo-acid transaminase inhibitor	39	95.9
2172	Orotate phosphoribosyltransferase inhibitor	36	99.4
2173	Orotate reductase (NADH) inhibitor	8	98.5
2174	Orotate reductase (NADPH) inhibitor	5	99.7
2175	Orotidylate decarboxylase inhibitor	4	99.9
2176	Orsellinate decarboxylase inhibitor	5	100.0
2177	Oryzin inhibitor	10	91.6
2178	Oxalate oxidase inhibitor	13	94.7
2179	Oxaloacetate decarboxylase inhibitor	15	99.1
2180	Oxaloacetate tautomerase inhibitor	15	99.5
2181	Oxidizing agent	18	94.8
2182	Oxidoreductase inhibitor	82	84.2
2183	Oxoglutarate dehydrogenase (lipoamide) inhibitor	17	98.6
2184	Oxygen scavenger	14	82.5
2185	Oxytocin agonist	16	95.5
2186	Oxytocin antagonist	761	99.0
2187	P-benzoquinone reductase (NADPH) inhibitor	8	84.9
2188	P3 purinoceptor-like protein antagonist	35	100.0
2189	PRL phosphatase inhibitor	28	96.0
2190	Palmitoyl-CoA hydrolase inhibitor	44	97.5
2191	Pancreatic elastase inhibitor	11	79.6
2192	Pancreatic endopeptidase E inhibitor	6	98.8
2193	Pancreatic ribonuclease inhibitor	10	91.1
2194	Pantetheine-phosphate adenylyltransferase inhibitor	16	96.0
2195	Pantoate 4-dehydrogenase inhibitor	3	99.3
2196	Pantoate-beta-alanine ligase inhibitor	25	96.7
2197	Pantothenase inhibitor	10	98.7
2198	Pantothenate kinase inhibitor	18	99.8
2199	Pappalysin-1 inhibitor	4	96.6
2200	Para amino benzoic acid antagonist	9	92.4
2201	Parathyroid hormone antagonist	22	98.8

2202	Parathyroid hormone secretion stimulant	71	99.8
2203	Pectate lyase inhibitor	11	97.9
2204	Pectin lyase inhibitor	11	98.5
2205	Penicillin amidase inhibitor	10	95.6
2206	Penicillopepsin inhibitor	14	96.8
2207	Pepsin inhibitor	35	99.9
2208	Peptide agonist	3	93.7
2209	Peptide alpha-N-acetyltransferase inhibitor	6	93.2
2210	Peptide deformylase inhibitor	160	99.0
2211	Peptide-N4-(N-acetyl-beta-glucosaminy)asparagine amidase inhibitor	6	90.0
2212	Peptide-tryptophan 2,3-dioxygenase inhibitor	9	98.1
2213	Peptidoglycan beta-N-acetylmuramidase inhibitor	3	99.2
2214	Peptidoglycan glycosyltransferase inhibitor	4	91.0
2215	Peptidyl-Lys metalloendopeptidase inhibitor	22	94.6
2216	Peptidyl-dipeptidase B inhibitor	7	85.4
2217	Peptidyl-dipeptidase Dcp inhibitor	6	93.3
2218	Peptidyl-glycinamidase inhibitor	11	97.3
2219	Peptidylamidoglycolate lyase inhibitor	5	98.7
2220	Peptidylglycine monooxygenase inhibitor	38	98.5
2221	Peptidyltransferase inhibitor	20	88.9
2222	Peroxisome proliferator-activated receptor agonist	1962	98.9
2223	Peroxisome proliferator-activated receptor alpha agonist	1007	99.2
2224	Peroxisome proliferator-activated receptor alpha antagonist	141	99.4
2225	Peroxisome proliferator-activated receptor antagonist	388	99.2
2226	Peroxisome proliferator-activated receptor delta agonist	409	99.6
2227	Peroxisome proliferator-activated receptor delta antagonist	82	99.9
2228	Peroxisome proliferator-activated receptor gamma agonist	938	98.6
2229	Peroxisome proliferator-activated receptor gamma antagonist	375	99.1
2230	PfA-M1 aminopeptidase inhibitor	7	98.0
2231	Phenol 2-monooxygenase inhibitor	25	95.8
2232	Phenol O-methyltransferase inhibitor	3	94.8
2233	Phenylacetaldehyde dehydrogenase inhibitor	5	98.7
2234	Phenylacetate-CoA ligase inhibitor	8	97.4
2235	Phenylalanine 2-monooxygenase inhibitor	6	99.9
2236	Phenylalanine decarboxylase inhibitor	8	98.1
2237	Phenylalanine dehydrogenase inhibitor	19	98.6
2238	Phenylalanine racemase (ATP-hydrolysing) inhibitor	10	97.7
2239	Phenylalanine(histidine) transaminase inhibitor	4	98.0
2240	Phenylalanine-tRNA ligase inhibitor	13	96.7
2241	Phenylethanolamine N methyltransferase inhibitor	83	99.7
2242	Phenylpyruvate decarboxylase inhibitor	3	99.2
2243	Phenylpyruvate tautomerase inhibitor	5	100.0
2244	Phloroglucinol reductase inhibitor	13	91.6
2245	Phosphatase inhibitor	10	77.8
2246	Phosphate acetyltransferase inhibitor	14	98.2
2247	Phosphate butyryltransferase inhibitor	4	100.0
2248	Phosphatidate cytidyltransferase inhibitor	17	97.9
2249	Phosphatidate phosphatase inhibitor	24	94.1

2250	Phosphatidyl-N-methylethanolamine N-methyltransferase inhibitor	6	74.0
2251	Phosphatidylcholine-retinol O-acyltransferase inhibitor	4	82.3
2252	Phosphatidylcholine-sterol O-acyltransferase inhibitor	16	89.3
2253	Phosphatidylethanolamine N-methyltransferase inhibitor	5	79.1
2254	Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor	3	99.5
2255	Phosphatidylglycerophosphatase inhibitor	8	96.6
2256	Phosphatidylinositol 3-kinase alpha inhibitor	105	99.0
2257	Phosphatidylinositol 3-kinase beta inhibitor	25	95.9
2258	Phosphatidylinositol 3-kinase delta inhibitor	23	97.4
2259	Phosphatidylinositol 3-kinase gamma inhibitor	40	98.5
2260	Phosphatidylinositol 3-kinase inhibitor	369	98.5
2261	Phosphatidylinositol 3-kinase stimulant	6	82.0
2262	Phosphatidylinositol diacylglycerol-lyase inhibitor	12	91.9
2263	Phosphatidylinositol kinase inhibitor	439	97.0
2264	Phosphatidylserine decarboxylase inhibitor	10	93.1
2265	Phospho-N-acetylmuramoyl-pentapeptide-transferase inhibitor	124	99.3
2266	Phosphoadenylylsulfatase inhibitor	5	99.8
2267	Phosphodiesterase 10A inhibitor	64	99.9
2268	Phosphodiesterase 11A inhibitor	22	100.0
2269	Phosphodiesterase 1B inhibitor	8	100.0
2270	Phosphodiesterase 3A inhibitor	16	99.0
2271	Phosphodiesterase 4A inhibitor	195	99.6
2272	Phosphodiesterase 4B inhibitor	147	99.5
2273	Phosphodiesterase 4C inhibitor	16	99.9
2274	Phosphodiesterase 4D inhibitor	57	98.0
2275	Phosphodiesterase 5A inhibitor	106	99.3
2276	Phosphodiesterase 6A inhibitor	27	100.0
2277	Phosphodiesterase 6B inhibitor	12	94.5
2278	Phosphodiesterase 7A inhibitor	15	97.8
2279	Phosphodiesterase 9A inhibitor	12	100.0
2280	Phosphodiesterase I inhibitor	200	96.5
2281	Phosphodiesterase II inhibitor	52	96.8
2282	Phosphodiesterase III inhibitor	666	98.3
2283	Phosphodiesterase IV inhibitor	3755	98.9
2284	Phosphodiesterase IX inhibitor	15	100.0
2285	Phosphodiesterase V inhibitor	773	98.7
2286	Phosphodiesterase VI inhibitor	114	99.3
2287	Phosphodiesterase VII inhibitor	236	99.5
2288	Phosphodiesterase X inhibitor	64	99.9
2289	Phosphodiesterase XI inhibitor	22	100.0
2290	Phosphoenolpyruvate carboxykinase (ATP) inhibitor	34	94.6
2291	Phosphoenolpyruvate carboxykinase (GTP) inhibitor	25	99.6
2292	Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor	8	99.3
2293	Phosphoenolpyruvate carboxylase inhibitor	44	98.5
2294	Phosphoenolpyruvate mutase inhibitor	3	98.4
2295	Phosphoenolpyruvate-protein phosphotransferase inhibitor	4	98.8
2296	Phosphoglucomutase inhibitor	16	99.3
2297	Phosphogluconate 2-dehydrogenase inhibitor	12	99.9

2298	Phosphogluconate dehydrogenase (decarboxylating) inhibitor	56	98.9
2299	Phosphoglycerate dehydrogenase inhibitor	16	99.5
2300	Phosphoglycerate mutase inhibitor	10	98.9
2301	Phosphoglycerate phosphatase inhibitor	6	99.9
2302	Phosphoglycolate phosphatase inhibitor	12	99.1
2303	Phosphoinositide 5-phosphatase inhibitor	11	89.8
2304	Phosphoinositide dependent kinase 1 inhibitor	50	98.4
2305	Phosphoinositide phospholipase C inhibitor	9	93.7
2306	Phosphoketolase inhibitor	10	99.7
2307	Phospholipase A1 inhibitor	16	93.8
2308	Phospholipase A2 IIa inhibitor	15	97.8
2309	Phospholipase C gamma 1 inhibitor	5	100.0
2310	Phospholipase D inhibitor	25	98.0
2311	Phospholipase D1 inhibitor	3	100.0
2312	Phospholipase D2 inhibitor	5	100.0
2313	Phospholipase inhibitor	416	92.8
2314	Phospholipid-translocating ATPase inhibitor	4	87.6
2315	Phosphomannomutase inhibitor	4	99.9
2316	Phosphomevalonate kinase inhibitor	14	99.1
2317	Phosphonoacetate hydrolase inhibitor	6	99.1
2318	Phosphopantothenoylcysteine decarboxylase inhibitor	7	93.6
2319	Phosphopyruvate hydratase inhibitor	7	100.0
2320	Phosphoribosylformylglycinamide cyclo-ligase inhibitor	3	100.0
2321	Phosphoribosylformylglycinamide synthase inhibitor	7	99.8
2322	Phosphoribosylglycinamide formyltransferase inhibitor	97	100.0
2323	Phosphoribulokinase inhibitor	10	99.2
2324	Phosphorylase a inhibitor	26	99.1
2325	Phosphorylase b inhibitor	5	96.3
2326	Phosphorylase kinase inhibitor	21	95.8
2327	Phosphoserine phosphatase inhibitor	10	98.7
2328	Phosphoserine transaminase inhibitor	5	99.9
2329	Photinus-luciferin 4-monooxygenase (ATP-hydrolysing) inhibitor	11	83.4
2330	Phthalate 4,5-dioxygenase inhibitor	3	87.1
2331	Phytanoyl-CoA dioxygenase inhibitor	3	97.5
2332	Picornain 2A inhibitor	10	98.1
2333	Picornain 3C inhibitor	8	97.5
2334	Pim kinase inhibitor	48	96.9
2335	Pim-1 kinase inhibitor	29	95.9
2336	Pim-2 kinase inhibitor	14	93.5
2337	Pim-3 kinase inhibitor	9	100.0
2338	Pin1 inhibitor	5	88.5
2339	Pitrilysin inhibitor	10	93.1
2340	Plasmanyethanolamine desaturase inhibitor	8	97.8
2341	Plasmepsin I inhibitor	68	100.0
2342	Plasmepsin II inhibitor	87	99.9
2343	Plasmepsin inhibitor	97	99.8
2344	Plasmin inhibitor	135	99.3
2345	Plasminogen activator inhibitor	73	97.5

2346	Plasminogen activator inhibitor antagonist	163	98.6
2347	Plasminogen activator stimulant	14	97.1
2348	Plastoquinol-plastocyanin reductase inhibitor	7	93.7
2349	Platelet activating factor alpha antagonist	104	98.6
2350	Platelet activating factor beta antagonist	295	97.9
2351	Platelet adhesion inhibitor	17	81.6
2352	Platelet aggregation stimulant	11	86.6
2353	Platelet derived growth factor receptor kinase inhibitor	24	92.4
2354	Platelet growth factor antagonist	766	98.7
2355	Platelet growth factor beta antagonist	186	99.3
2356	Plus-end-directed kinesin ATPase inhibitor	3	98.5
2357	Polar-amino-acid-transporting ATPase inhibitor	4	96.2
2358	Polarisation inhibitor	48	93.4
2359	Polarisation stimulant	9	91.0
2360	Polo-like kinase inhibitor	276	98.4
2361	Polo-like kinase-1 inhibitor	197	98.0
2362	Poly(3-hydroxybutyrate) depolymerase inhibitor	13	98.5
2363	Poly(ADP-ribose) glycohydrolase inhibitor	19	97.3
2364	Poly(ADP-ribose) polymerase 1 inhibitor	443	99.3
2365	Poly(ADP-ribose) polymerase 2 inhibitor	12	95.9
2366	Poly(ADP-ribose) polymerase inhibitor	1054	98.9
2367	Poly(alpha-L-gulonate) lyase inhibitor	5	97.5
2368	Poly(beta-D-mannuronate) lyase inhibitor	4	96.3
2369	Polyamine biosynthesis inhibitor	18	99.0
2370	Polyamine oxidase inhibitor	14	95.6
2371	Polyamine-transporting ATPase inhibitor	3	94.7
2372	Polygalacturonase inhibitor	6	96.4
2373	Polyneuridine-aldehyde esterase inhibitor	3	98.5
2374	Polynucleotide 5'-hydroxy-kinase inhibitor	15	91.8
2375	Polynucleotide adenylyltransferase inhibitor	27	94.6
2376	Polypeptide N-acetylgalactosaminyltransferase inhibitor	16	98.7
2377	Polyphosphate kinase inhibitor	4	99.4
2378	Polyphosphate-glucose phosphotransferase inhibitor	5	100.0
2379	Polyporopepsin inhibitor	6	82.2
2380	Polyribonucleotide nucleotidyltransferase inhibitor	9	90.4
2381	Porphobilinogen synthase inhibitor	22	98.4
2382	Postsynaptic density protein 95 inhibitor	3	100.0
2383	Potassium channel (ATP-sensitive) activator	172	98.0
2384	Potassium channel (ATP-sensitive) blocker	229	98.8
2385	Potassium channel (Ca-activated) activator	186	97.2
2386	Potassium channel (Ca-activated) blocker	241	97.9
2387	Potassium channel (Inward rectifier) 1 blocker	79	99.9
2388	Potassium channel (Inward rectifier) 11 blocker	36	100.0
2389	Potassium channel (Inward rectifier) activator	172	98.0
2390	Potassium channel (Inward rectifier) blocker	380	99.0
2391	Potassium channel (Voltage-sensitive) activator	162	99.2
2392	Potassium channel (Voltage-sensitive) blocker	923	96.1
2393	Potassium channel KCNQ activator	162	99.2

2394	Potassium channel KCNQ blocker	8	99.7
2395	Potassium channel KCNQ2 activator	45	100.0
2396	Potassium channel KCNQ3 activator	6	98.4
2397	Potassium channel Kv1.1 blocker	129	98.7
2398	Potassium channel Kv1.3 blocker	199	99.0
2399	Potassium channel Kv1.5 blocker	373	98.4
2400	Potassium channel activator	1430	98.1
2401	Potassium channel blocker	1962	96.0
2402	Potassium channel intermediate-conductance Ca-activated 4 blocker	10	100.0
2403	Potassium channel intermediate-conductance Ca-activated activator	4	98.6
2404	Potassium channel intermediate-conductance Ca-activated blocker	50	98.5
2405	Potassium channel large-conductance Ca-activated activator	161	98.1
2406	Potassium channel small-conductance Ca-activated 3 activator	6	99.0
2407	Potassium channel small-conductance Ca-activated 3 blocker	36	100.0
2408	Potassium channel small-conductance Ca-activated activator	9	99.9
2409	Potassium channel small-conductance Ca-activated blocker	121	99.7
2410	Pregnane X receptor agonist	14	93.2
2411	Pregnane X receptor antagonist	27	100.0
2412	Prenyl-diphosphatase inhibitor	5	96.8
2413	Prephenate dehydratase inhibitor	23	99.3
2414	Prephenate dehydrogenase inhibitor	20	94.9
2415	Prepilin peptidase inhibitor	3	99.4
2416	Pro-opiomelanocortin converting enzyme inhibitor	5	93.1
2417	Procollagen C-endopeptidase inhibitor	17	95.8
2418	Procollagen N-endopeptidase inhibitor	7	96.8
2419	Procollagen galactosyltransferase inhibitor	13	99.7
2420	Procollagen glucosyltransferase inhibitor	13	99.3
2421	Procollagen-lysine 5-dioxygenase inhibitor	21	96.2
2422	Procollagen-proline 3-dioxygenase inhibitor	14	100.0
2423	Progesterone agonist	201	99.3
2424	Progesterone antagonist	620	99.6
2425	Progesterone receptor A antagonist	98	100.0
2426	Progesterone receptor B antagonist	66	99.9
2427	Progesterone receptor B1 antagonist	24	100.0
2428	Prokineticin receptor 1 antagonist	3	100.0
2429	Prolactin inhibitor	44	96.6
2430	Prolactin release inhibitor	64	97.4
2431	Proline dehydrogenase inhibitor	4	99.8
2432	Proline racemase inhibitor	17	99.3
2433	Prolyl aminopeptidase inhibitor	13	93.5
2434	Prolyl endopeptidase inhibitor	325	98.4
2435	Propanediol dehydratase inhibitor	17	99.3
2436	Propionate CoA-transferase inhibitor	4	99.9
2437	Propionate-CoA ligase inhibitor	7	99.3
2438	Prostacyclin agonist	65	98.5
2439	Prostacyclin antagonist	109	99.3
2440	Prostaglandin A1 agonist	3	100.0
2441	Prostaglandin D2 agonist	9	97.5

2442	Prostaglandin D2 antagonist	173	99.5
2443	Prostaglandin E1 agonist	20	99.9
2444	Prostaglandin E1 antagonist	4	95.6
2445	Prostaglandin E2 agonist	121	99.6
2446	Prostaglandin E2 antagonist	306	97.3
2447	Prostaglandin EP1 antagonist	108	99.9
2448	Prostaglandin EP12 antagonist	50	100.0
2449	Prostaglandin EP2 agonist	38	100.0
2450	Prostaglandin EP2 antagonist	150	99.9
2451	Prostaglandin EP3 antagonist	154	99.4
2452	Prostaglandin EP4 agonist	70	100.0
2453	Prostaglandin EP4 antagonist	176	99.8
2454	Prostaglandin F2 alpha antagonist	25	96.2
2455	Prostaglandin H2 antagonist	379	99.8
2456	Prostaglandin agonist	393	98.8
2457	Prostaglandin antagonist	932	97.9
2458	Prostaglandin-A1 DELTA-isomerase inhibitor	4	92.2
2459	Prostaglandin-E synthase inhibitor	32	99.6
2460	Prostaglandin-E2 9-reductase inhibitor	15	88.5
2461	Prostaglandin-E2 synthase 1 inhibitor	32	99.6
2462	Prostaglandin-I synthase inhibitor	25	99.6
2463	Protease (Human cytomegalovirus) inhibitor	149	99.9
2464	Protease 3C (Human rhinovirus) inhibitor	177	99.3
2465	Protease activated receptor 1 antagonist	145	99.0
2466	Protease activated receptor antagonist	154	97.8
2467	Protease inhibitor	576	95.9
2468	Proteasome ATPase inhibitor	3	89.6
2469	Proteasome endopeptidase complex inhibitor	32	96.4
2470	Proteasome inhibitor	200	98.4
2471	Protein 30S ribosomal subunit inhibitor	68	96.7
2472	Protein 50S ribosomal subunit inhibitor	112	98.7
2473	Protein C (activated) inhibitor	14	99.0
2474	Protein N-acetylglucosaminyltransferase inhibitor	8	99.4
2475	Protein disulfide-isomerase inhibitor	6	78.4
2476	Protein glycation inhibitor	4	100.0
2477	Protein kinase (CK1) delta inhibitor	4	100.0
2478	Protein kinase (CK1) epsilon inhibitor	5	90.3
2479	Protein kinase (CK1) inhibitor	11	81.0
2480	Protein kinase (CK2) inhibitor	65	96.5
2481	Protein kinase (CaMK, MLCK, PhK, SNF, KIN, NIM1, MAPKAP, POLO, CHK, ULK, RSK-2nd domain) inhibitor	302	99.0
2482	Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor	624	98.7
2483	Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor	93	98.7
2484	Protein kinase A inhibitor	207	98.2
2485	Protein kinase B alpha inhibitor	85	98.0
2486	Protein kinase B beta inhibitor	27	97.6
2487	Protein kinase B gamma inhibitor	10	95.4
2488	Protein kinase B inhibitor	314	96.5

2489	Protein kinase B stimulant	27	95.2
2490	Protein kinase C alpha inhibitor	290	98.9
2491	Protein kinase C beta I inhibitor	68	99.9
2492	Protein kinase C beta II inhibitor	86	99.9
2493	Protein kinase C beta inhibitor	127	98.5
2494	Protein kinase C delta inhibitor	111	99.3
2495	Protein kinase C epsilon inhibitor	77	97.8
2496	Protein kinase C eta inhibitor	61	99.9
2497	Protein kinase C gamma inhibitor	73	98.8
2498	Protein kinase C inhibitor	1107	97.6
2499	Protein kinase C mu inhibitor	8	99.9
2500	Protein kinase C nu inhibitor	5	98.4
2501	Protein kinase C theta inhibitor	93	98.4
2502	Protein kinase C zeta inhibitor	27	99.8
2503	Protein kinase inhibitor	11097	93.8
2504	Protein kinase stimulant	108	94.3
2505	Protein phosphatase 2A inhibitor	19	99.8
2506	Protein phosphatase inhibitor	1346	97.7
2507	Protein synthesis inhibitor	377	94.0
2508	Protein synthesis stimulant	9	96.1
2509	Protein-L-isoaspartate (D-aspartate) O-methyltransferase inhibitor	3	100.0
2510	Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor	12	95.5
2511	Protein-S-isoprenylcysteine O-methyltransferase inhibitor	24	95.0
2512	Protein-arginine N-methyltransferase inhibitor	6	100.0
2513	Protein-arginine deiminase inhibitor	7	92.2
2514	Protein-disulfide reductase (glutathione) inhibitor	11	79.5
2515	Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor	3	99.0
2516	Protein-glutamate O-methyltransferase inhibitor	4	98.7
2517	Protein-glutamate methylesterase inhibitor	13	95.5
2518	Protein-serine-threonine kinase inhibitor	1723	96.0
2519	Protein-synthesizing GTPase inhibitor	15	89.3
2520	Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor	219	96.1
2521	Protein-tyrosine kinase Lyn inhibitor	33	92.1
2522	Protein-tyrosine kinase p55(blk) inhibitor	6	88.0
2523	Protein-tyrosine phosphatase 1B inhibitor	981	98.3
2524	Protein-tyrosine phosphatase 2C inhibitor	51	99.8
2525	Protein-tyrosine phosphatase C inhibitor	4	100.0
2526	Protein-tyrosine phosphatase beta inhibitor	4	100.0
2527	Protein-tyrosine phosphatase epsilon inhibitor	5	100.0
2528	Protein-tyrosine phosphatase inhibitor	1283	97.8
2529	Protein-tyrosine phosphatase mu inhibitor	4	100.0
2530	Protein-tyrosine phosphatase yopH inhibitor	6	97.8
2531	Protein-tyrosine sulfotransferase inhibitor	10	97.5
2532	Proto-oncogene tyrosine-protein kinase Fgr inhibitor	6	100.0
2533	Proto-oncogene tyrosine-protein kinase Fyn inhibitor	34	95.4
2534	Proto-oncogene tyrosine-protein kinase Kit inhibitor	53	95.7
2535	Proto-oncogene tyrosine-protein kinase Yes inhibitor	13	95.5
2536	Proto-oncogene tyrosine-protein kinase c-hck inhibitor	5	100.0

2537	Protocatechuate 3,4-dioxygenase inhibitor	28	99.3
2538	Protocatechuate 4,5-dioxygenase inhibitor	11	99.9
2539	Protocollagen prolyl hydroxylase inhibitor	91	98.6
2540	Protoporphyrinogen oxidase inhibitor	17	78.1
2541	Prunasin beta-glucosidase inhibitor	6	97.0
2542	Pseudolysin inhibitor	4	79.1
2543	Pseudouridylate synthase inhibitor	4	97.5
2544	Pteridine reductase inhibitor	9	97.8
2545	Pterin deaminase inhibitor	4	92.7
2546	Pullulanase inhibitor	7	94.5
2547	Purine antagonist	19	99.8
2548	Purine biosynthesis inhibitor	14	99.3
2549	Purine nucleosidase inhibitor	26	99.6
2550	Purine nucleoside phosphorylase inhibitor	193	99.6
2551	Purinergic P2 agonist	19	96.0
2552	Purinergic P2 antagonist	583	97.7
2553	Purinergic P2T antagonist	76	98.1
2554	Purinergic P2X agonist	6	99.9
2555	Purinergic P2X antagonist	442	98.7
2556	Purinergic P2X1 antagonist	14	93.7
2557	Purinergic P2X2 antagonist	42	99.4
2558	Purinergic P2X3 antagonist	52	98.4
2559	Purinergic P2X4 antagonist	11	100.0
2560	Purinergic P2X7 antagonist	369	99.4
2561	Purinergic P2Y agonist	10	93.9
2562	Purinergic P2Y antagonist	72	95.3
2563	Purinergic P2Y1 antagonist	43	96.7
2564	Purinergic P2Y12 antagonist	9	90.1
2565	Purinergic receptor agonist	19	96.0
2566	Purinergic receptor antagonist	625	97.3
2567	Puromycin-sensitive aminopeptidase inhibitor	4	100.0
2568	Putrescine carbamoyltransferase inhibitor	6	99.9
2569	Putrescine oxidase inhibitor	14	98.4
2570	Pyridoxal 4-dehydrogenase inhibitor	9	100.0
2571	Pyridoxal kinase inhibitor	45	96.2
2572	Pyridoxamine-oxaloacetate transaminase inhibitor	13	99.8
2573	Pyridoxamine-phosphate oxidase inhibitor	9	99.6
2574	Pyridoxamine-pyruvate transaminase inhibitor	4	100.0
2575	Pyridoxine 4-oxidase inhibitor	3	97.8
2576	Pyridoxine 5-dehydrogenase inhibitor	6	99.1
2577	Pyrimidine antagonist	41	98.2
2578	Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor	6	98.9
2579	Pyroglutamyl-peptidase I inhibitor	40	95.0
2580	Pyroglutamyl-peptidase II inhibitor	14	85.8
2581	Pyroline-5-carboxylate reductase inhibitor	17	98.9
2582	Pyruvate carboxylase inhibitor	27	93.2
2583	Pyruvate decarboxylase inhibitor	7	93.1
2584	Pyruvate dehydrogenase (cytochrome) inhibitor	4	98.7

2585	Pyruvate dehydrogenase (lipoamide) inhibitor	22	97.3
2586	Pyruvate dehydrogenase inhibitor	25	95.0
2587	Pyruvate dehydrogenase kinase inhibitor	110	100.0
2588	Pyruvate dehydrogenase stimulant	48	99.8
2589	Pyruvate synthase inhibitor	5	99.9
2590	Pyruvate, phosphate dikinase inhibitor	21	99.1
2591	Pyruvate, water dikinase inhibitor	10	99.4
2592	Quercetin 2,3-dioxygenase inhibitor	11	98.3
2593	Queuine tRNA-ribosyltransferase inhibitor	37	99.6
2594	Quinate 5-dehydrogenase inhibitor	4	99.9
2595	Quinoline-4-carboxylate 2-oxidoreductase inhibitor	4	97.9
2596	Quinoprotein glucose dehydrogenase inhibitor	4	96.9
2597	Quisqualate antagonist	4	95.6
2598	RAS guanyl releasing protein antagonist	4	100.0
2599	RET inhibitor	23	87.5
2600	RNA agonist	3	99.9
2601	RNA directed DNA polymerase inhibitor	133	90.9
2602	RNA ligase (ATP) inhibitor	15	100.0
2603	RNA synthesis inhibitor	116	90.4
2604	RNA-directed RNA polymerase (Influenza A) inhibitor	13	100.0
2605	RNA-directed RNA polymerase inhibitor	26	86.0
2606	RNA-directed RNA polymerase stimulant	7	99.8
2607	Radical formation agonist	39	97.8
2608	Raf kinase B inhibitor	191	99.6
2609	Raf kinase C inhibitor	95	97.2
2610	Raf kinase inhibitor	611	98.7
2611	Reductant	69	92.7
2612	Reductase inhibitor	4	90.3
2613	Releasing hormone agonist	24	94.5
2614	Renal tissue kallikrein inhibitor	14	90.8
2615	Renilla-luciferin 2-monooxygenase inhibitor	12	99.1
2616	Renin inhibitor	2366	99.4
2617	Replication protein E1 (HPV) antagonist	3	100.0
2618	Retinal dehydrogenase inhibitor	7	90.6
2619	Retinal oxidase inhibitor	8	79.2
2620	Retinoic acid alpha receptor antagonist	227	99.9
2621	Retinoic acid beta receptor agonist	15	99.2
2622	Retinoic acid beta receptor antagonist	196	99.9
2623	Retinoic acid metabolism inhibitor	8	91.3
2624	Retinoic acid receptor agonist	172	99.5
2625	Retinoic acid receptor antagonist	372	99.8
2626	Retinoic acid receptor gamma antagonist	229	99.6
2627	Retinoid X alpha receptor agonist	23	99.5
2628	Retinoid X alpha receptor antagonist	103	100.0
2629	Retinoid X beta receptor antagonist	53	100.0
2630	Retinoid X gamma receptor antagonist	57	100.0
2631	Retinoid X receptor agonist	112	99.7
2632	Retinoid X receptor antagonist	119	100.0

2633	Retinol O-fatty-acyltransferase inhibitor	7	99.3
2634	Retinol dehydrogenase inhibitor	6	96.3
2635	Retinyl-palmitate esterase inhibitor	18	97.9
2636	Reverse transcriptase (Hepatitis B) inhibitor	36	100.0
2637	Rhamnulose-1-phosphate aldolase inhibitor	7	97.2
2638	Rhizopuspepsin inhibitor	4	93.6
2639	Rho-associated kinase I inhibitor	15	100.0
2640	Rho-associated kinase II inhibitor	33	99.6
2641	Rho-associated kinase inhibitor	121	99.8
2642	Rhodesain inhibitor	15	100.0
2643	Rhodopsin kinase inhibitor	33	96.1
2644	Rhodotorulapepsin inhibitor	9	96.4
2645	Ribitol 2-dehydrogenase inhibitor	6	99.4
2646	Riboflavin kinase inhibitor	24	99.7
2647	Riboflavin phosphotransferase inhibitor	4	98.7
2648	Riboflavin synthase inhibitor	12	99.9
2649	Ribonuclease L inhibitor	9	100.0
2650	Ribonuclease T1 inhibitor	5	77.9
2651	Ribonuclease T2 inhibitor	26	99.9
2652	Ribonuclease U2 inhibitor	5	98.8
2653	Ribonuclease inhibitor	49	95.3
2654	Ribonucleoside diphosphate reductase inhibitor	124	98.2
2655	Ribonucleoside triphosphate reductase inhibitor	18	94.4
2656	Ribonucleotide reductase inhibitor	226	98.7
2657	Ribose-5-phosphate adenylyltransferase inhibitor	7	99.0
2658	Ribose-5-phosphate isomerase inhibitor	21	99.0
2659	Ribose-5-phosphate-ammonia ligase inhibitor	7	98.5
2660	Ribose-phosphate diphosphokinase inhibitor	38	99.2
2661	Ribosomal protein S6 kinase 1, 70-kDa inhibitor	14	90.1
2662	Ribosomal protein S6 kinase inhibitor	21	88.7
2663	Ribosomal protein S6 kinase, 70-kDa inhibitor	15	83.6
2664	Ribosomal protein S6 kinase, 90-kDa inhibitor	5	82.4
2665	Ribosomal protein S6 kinase, 90kD, polypeptide 5 inhibitor	4	100.0
2666	Ribosylpyrimidine nucleosidase inhibitor	9	99.8
2667	Ribulose-bisphosphate carboxylase inhibitor	15	98.5
2668	Ribulose-phosphate 3-epimerase inhibitor	3	85.5
2669	Rotamase (FKBP) inhibitor	6	99.7
2670	Rotamase (FKBP12) inhibitor	77	99.3
2671	Rubredoxin-NAD ⁺ reductase inhibitor	14	81.8
2672	Ryanodine receptor 1 antagonist	3	100.0
2673	Ryanodine receptor antagonist	3	100.0
2674	S-adenosyl-L-methionine decarboxylase inhibitor	58	99.8
2675	S-alkylcysteine lyase inhibitor	3	97.0
2676	S-formylglutathione hydrolase inhibitor	8	88.3
2677	S-methyl-5-thioadenosine phosphorylase inhibitor	47	99.5
2678	S-methyl-5-thioribose kinase inhibitor	9	99.0
2679	Saccharolysin inhibitor	4	98.4
2680	Saccharopepsin inhibitor	3	86.7

2681	Saccharopine dehydrogenase (NAD ⁺ , L-glutamate-forming) inhibitor	4	99.2
2682	Saccharopine dehydrogenase (NAD ⁺ , L-lysine-forming) inhibitor	19	97.6
2683	Saccharopine dehydrogenase (NADP ⁺ , L-glutamate-forming) inhibitor	5	98.9
2684	Saccharopine dehydrogenase (NADP ⁺ , L-lysine-forming) inhibitor	12	99.4
2685	Salicylate 1-monoxygenase inhibitor	6	96.4
2686	Saponin-like	12	100.0
2687	Sarcosine oxidase inhibitor	14	98.2
2688	Scyllo-inosamine-4-phosphate amidinotransferase inhibitor	4	99.2
2689	Scytalone dehydratase inhibitor	21	99.1
2690	Secretase alpha stimulant	11	84.7
2691	Secretase beta 1 inhibitor	91	98.5
2692	Secretase beta 2 inhibitor	25	98.1
2693	Secretase beta inhibitor	185	98.6
2694	Secretase gamma inhibitor	147	99.3
2695	Secretase inhibitor	332	98.3
2696	Secretase stimulant	11	84.7
2697	Secretory phospholipase A2 inhibitor	8	92.4
2698	Sedoheptulose-bisphosphatase inhibitor	7	95.0
2699	Selectin E antagonist	137	98.0
2700	Selectin L antagonist	9	99.4
2701	Selectin P antagonist	20	99.9
2702	Selectin antagonist	179	97.3
2703	Selenide, water dikinase inhibitor	4	100.0
2704	Selenocysteine lyase inhibitor	3	98.7
2705	Sepiapterin deaminase inhibitor	12	99.7
2706	Sepiapterin reductase inhibitor	46	95.6
2707	Serine 3-dehydrogenase inhibitor	6	98.7
2708	Serine O-acetyltransferase inhibitor	15	95.8
2709	Serine carboxypeptidase inhibitor	34	97.9
2710	Serine protease unspecified inhibitor	25	91.6
2711	Serine-glyoxylate transaminase inhibitor	12	99.3
2712	Serine-phosphoethanolamine synthase inhibitor	10	98.5
2713	Serine-pyruvate transaminase inhibitor	4	98.1
2714	Serine-sulfate ammonia-lyase inhibitor	30	99.5
2715	Serine-tRNA ligase inhibitor	6	98.9
2716	Serine-type D-Ala-D-Ala carboxypeptidase inhibitor	27	99.5
2717	Serralysin inhibitor	22	96.1
2718	Serratia marcescens nuclease inhibitor	7	96.7
2719	Serum-glucocorticoid regulated kinase 1 inhibitor	8	93.4
2720	Serum-glucocorticoid regulated kinase inhibitor	42	97.6
2721	Shab potassium channel blocker	4	85.4
2722	Shaker potassium channel blocker	664	98.5
2723	Shal potassium channel blocker	27	96.7
2724	Shikimate 5-dehydrogenase inhibitor	6	98.3
2725	Shikimate O-hydroxycinnamoyltransferase inhibitor	4	97.0
2726	Shikimate kinase inhibitor	22	97.2
2727	Sigma 1 receptor agonist	14	96.3
2728	Sigma 1 receptor antagonist	1054	99.4

2729	Sigma 2 receptor antagonist	548	99.5
2730	Sigma 3 receptor antagonist	11	100.0
2731	Sigma receptor agonist	23	92.8
2732	Sigma receptor antagonist	1834	99.1
2733	Signal peptidase I inhibitor	12	96.6
2734	Signal peptidase IB inhibitor	3	100.0
2735	Signal peptidase II inhibitor	8	78.0
2736	Simian immunodeficiency virus proteinase inhibitor	4	85.5
2737	Sirtuin 2 inhibitor	15	100.0
2738	Sirtuin inhibitor	15	100.0
2739	Site-specific DNA-methyltransferase (adenine-specific) inhibitor	4	98.9
2740	Small monomeric GTPase inhibitor	3	99.4
2741	Smo receptor agonist	3	100.0
2742	Smo receptor antagonist	29	100.0
2743	Smooth muscle myosin light chain kinase inhibitor	10	75.2
2744	Snapalysin inhibitor	4	98.5
2745	Sodium channel (voltage-gated) blocker	241	97.7
2746	Sodium channel blocker class Ib	6	97.0
2747	Somatostatin 1 antagonist	160	99.9
2748	Somatostatin 2 agonist	12	99.8
2749	Somatostatin 2 antagonist	180	99.9
2750	Somatostatin 3 antagonist	178	99.9
2751	Somatostatin 4 antagonist	191	99.7
2752	Somatostatin 5 agonist	15	99.9
2753	Somatostatin 5 antagonist	154	99.6
2754	Somatostatin agonist	51	97.1
2755	Somatostatin antagonist	252	99.5
2756	Sorbitol-6-phosphate 2-dehydrogenase inhibitor	3	97.3
2757	Sorbose dehydrogenase inhibitor	3	99.4
2758	Spermidine dehydrogenase inhibitor	5	82.0
2759	Spermidine synthase inhibitor	35	99.5
2760	Spermine antagonist	3	100.0
2761	Spermine synthase inhibitor	23	99.5
2762	Sphinganine kinase inhibitor	6	81.8
2763	Sphinganine-1-phosphate aldolase inhibitor	6	97.6
2764	Sphingomyelinase inhibitor	15	98.3
2765	Sphingosine 1-phosphate receptor 1 agonist	107	100.0
2766	Sphingosine 1-phosphate receptor 1 antagonist	35	99.3
2767	Sphingosine 1-phosphate receptor 3 agonist	12	100.0
2768	Sphingosine 1-phosphate receptor 3 antagonist	23	99.9
2769	Sphingosine 1-phosphate receptor 4 agonist	5	100.0
2770	Sphingosine 1-phosphate receptor 4 antagonist	18	99.9
2771	Sphingosine 1-phosphate receptor 5 agonist	5	86.5
2772	Sphingosine 1-phosphate receptor 5 antagonist	21	100.0
2773	Sphingosine 1-phosphate receptor agonist	108	100.0
2774	Sphingosine 1-phosphate receptor antagonist	42	96.9
2775	Sphingosine kinase 1 inhibitor	3	99.9
2776	Sphingosine kinase inhibitor	15	95.4

2777	Sphingosine kinase stimulant	3	100.0
2778	Sporulation kinase A inhibitor	5	100.0
2779	Squalene epoxidase inhibitor	64	97.6
2780	Squalene synthetase inhibitor	486	99.4
2781	Squalene-hopene cyclase inhibitor	35	96.9
2782	Src kinase inhibitor	1773	97.7
2783	Stearoyl-CoA desaturase inhibitor	116	97.2
2784	Stem cell growth factor agonist	305	98.6
2785	Steroid 21-monooxygenase inhibitor	6	77.6
2786	Steroid 9alpha-monooxygenase inhibitor	3	99.8
2787	Steroid DELTA-isomerase inhibitor	28	97.2
2788	Steroid N-acetylglucosaminyltransferase inhibitor	4	95.4
2789	Steroid sulfotransferase inhibitor	11	92.6
2790	Steroid synthesis inhibitor	11	79.0
2791	Steroid-like	50	99.7
2792	Sterol 24-C-methyltransferase inhibitor	27	98.3
2793	Sterol 3-beta-glucosyltransferase inhibitor	12	95.3
2794	Stipitatonate decarboxylase inhibitor	5	99.8
2795	Streptogrisin A inhibitor	3	100.0
2796	Streptomycin 6-kinase inhibitor	6	99.6
2797	Streptopain inhibitor	13	98.5
2798	Strombine dehydrogenase inhibitor	5	100.0
2799	Stromelysin 2 inhibitor	4	98.8
2800	Styrene-oxide isomerase inhibitor	3	98.3
2801	Substance P antagonist	388	97.9
2802	Subtilisin inhibitor	27	95.9
2803	Succinate-CoA ligase (ADP-forming) inhibitor	16	98.0
2804	Succinate-hydroxymethylglutarate CoA-transferase inhibitor	8	99.1
2805	Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor	7	84.4
2806	Succinate-semialdehyde dehydrogenase inhibitor	20	99.1
2807	Succinic dehydrogenase inhibitor	8	96.8
2808	Sucrose alpha-glucosidase inhibitor	19	99.5
2809	Sucrose phosphorylase inhibitor	5	100.0
2810	Sucrose synthase inhibitor	16	99.1
2811	Sucrose-phosphate phosphatase inhibitor	7	99.7
2812	Sucrose-phosphate synthase inhibitor	19	97.0
2813	Sugar-phosphatase inhibitor	3	89.2
2814	Sulfate adenylyltransferase (ADP) inhibitor	8	98.4
2815	Sulfate adenylyltransferase inhibitor	14	98.1
2816	Sulfinoalanine decarboxylase inhibitor	18	99.2
2817	Sulfite dehydrogenase inhibitor	9	84.3
2818	Sulfite oxidase inhibitor	9	93.5
2819	Sulfite reductase inhibitor	6	96.7
2820	Sulfonylureas	5	98.4
2821	Sulfur dioxygenase inhibitor	6	98.5
2822	Sulfur reductase inhibitor	8	86.5
2823	Syk tyrosine kinase inhibitor	293	97.9
2824	Synaptic vesicle protein SV2, levetiracetam binding site antagonist	32	100.0

2825	T cell receptor antagonist	17	100.0
2826	T cell receptor gamma-delta antagonist	17	100.0
2827	T-cell protein-tyrosine phosphatase inhibitor	78	99.7
2828	T2-induced deoxynucleotide kinase inhibitor	3	100.0
2829	TEC kinase inhibitor	39	100.0
2830	TGF beta receptor type I kinase inhibitor	210	99.7
2831	TGF beta receptor type II kinase inhibitor	22	100.0
2832	TIE antagonist	526	98.7
2833	TIE-2 agonist	6	100.0
2834	TIE-2 antagonist	506	98.7
2835	TNF convertase inhibitor	624	99.9
2836	TRKA antagonist	86	98.0
2837	TRKB antagonist	12	100.0
2838	TRPA1 agonist	10	93.3
2839	TRPA1 antagonist	3	100.0
2840	TTK protein kinase inhibitor	5	100.0
2841	Tagaturonate reductase inhibitor	3	99.3
2842	Tankyrase 2 inhibitor	5	100.0
2843	Tankyrase inhibitor	5	100.0
2844	Tannase inhibitor	14	99.5
2845	Tardive dyskinesia treatment	41	92.7
2846	Tartrate decarboxylase inhibitor	5	100.0
2847	Tartrate dehydrogenase inhibitor	5	100.0
2848	Tau aggregation inhibitor	9	79.7
2849	Taurine dehydrogenase inhibitor	7	86.2
2850	Taurine-2-oxoglutarate transaminase inhibitor	3	97.3
2851	Taurocyamine kinase inhibitor	3	97.6
2852	Tauropine dehydrogenase inhibitor	8	95.6
2853	Telomerase inhibitor	322	97.0
2854	Telomerase stimulant	6	100.0
2855	Tentoxilysin inhibitor	4	94.0
2856	Testosterone 17beta-dehydrogenase (NADP+) inhibitor	3	85.5
2857	Testosterone 17beta-dehydrogenase inhibitor	11	96.8
2858	Testosterone agonist	5	99.6
2859	Tetanus neurotoxin inhibitor	3	100.0
2860	Tetrahydroxynaphthalene reductase inhibitor	7	98.2
2861	Theanine hydrolase inhibitor	13	99.9
2862	Thermitase inhibitor	12	90.0
2863	Thermolysin inhibitor	19	99.5
2864	Thermomycolin inhibitor	3	99.5
2865	Thiamine pyridinylase inhibitor	5	86.1
2866	Thiamine-phosphate diphosphorylase inhibitor	7	98.6
2867	Thiamine-phosphate kinase inhibitor	5	98.4
2868	Thiamine-triphosphatase inhibitor	9	87.5
2869	Thiazolidinedione	26	99.5
2870	Thimet oligopeptidase inhibitor	20	93.1
2871	Thioether S-methyltransferase inhibitor	3	99.4
2872	Thiol S-methyltransferase inhibitor	8	97.9

2873	Thiol oxidase inhibitor	13	94.6
2874	Thiol protease inhibitor	138	98.4
2875	Thiol sulfotransferase inhibitor	4	100.0
2876	Thiopurine S-methyltransferase inhibitor	17	94.2
2877	Thioredoxin inhibitor	3	93.3
2878	Thiosulfate dehydrogenase inhibitor	10	87.9
2879	Thiosulfate sulfurtransferase inhibitor	21	98.6
2880	Threonine aldolase inhibitor	5	97.2
2881	Threonine ammonia-lyase inhibitor	27	98.3
2882	Threonine synthase inhibitor	11	99.8
2883	Threonine-tRNA ligase inhibitor	5	92.6
2884	Thrombin inhibitor	2080	98.7
2885	Thrombopoietin agonist	113	100.0
2886	Thromboxane A2 antagonist	86	94.4
2887	Thromboxane B2 antagonist	18	84.2
2888	Thromboxane agonist	3	99.9
2889	Thromboxane antagonist	321	96.4
2890	Thromboxane synthase inhibitor	661	98.6
2891	Thromboxane synthase stimulant	3	98.7
2892	Thymidine kinase (Herpes simplex virus 1) inhibitor	38	100.0
2893	Thymidine kinase (Herpes simplex virus 2) inhibitor	15	100.0
2894	Thymidine kinase 1 inhibitor	12	97.4
2895	Thymidine kinase 2 inhibitor	10	100.0
2896	Thymidine kinase inhibitor	96	96.7
2897	Thymidine phosphorylase inhibitor	52	98.8
2898	Thymidine-triphosphatase inhibitor	6	99.9
2899	Thymidylate 5'-phosphatase inhibitor	5	80.6
2900	Thymidylate synthase inhibitor	816	99.4
2901	Thymine dioxygenase inhibitor	14	100.0
2902	Thyroid hormone alpha 1 antagonist	12	100.0
2903	Thyroid hormone alpha antagonist	40	100.0
2904	Thyroid hormone antagonist	88	98.7
2905	Thyroid hormone beta 1 antagonist	12	100.0
2906	Thyroid hormone beta antagonist	38	100.0
2907	Thyrotropin receptor antagonist	6	78.1
2908	Thyrotropin releasing hormone agonist	20	100.0
2909	Thyrotropin releasing hormone antagonist	6	100.0
2910	Thyroxine 5-deiodinase inhibitor	7	94.3
2911	Toll-Like receptor 2 antagonist	8	100.0
2912	Toll-Like receptor 7 agonist	86	99.8
2913	Toll-Like receptor 8 agonist	9	100.0
2914	Toll-Like receptor agonist	88	99.2
2915	Toll-Like receptor antagonist	11	88.4
2916	Topoisomerase II inhibitor	998	96.5
2917	Tpr proteinase (Porphyromonas gingivalis) inhibitor	4	85.3
2918	Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor	39	95.1
2919	Trans-2-enoyl-CoA reductase (NAD+) inhibitor	4	98.7
2920	Trans-2-enoyl-CoA reductase (NADPH) inhibitor	5	76.6

2921	Trans-acenaphthene-1,2-diol dehydrogenase inhibitor	5	80.5
2922	Trans-octaprenyltranstransferase inhibitor	6	96.4
2923	Trans-pentaprenyltranstransferase inhibitor	5	98.6
2924	Transactivator transcription protein inhibitor	29	89.9
2925	Transaldolase inhibitor	5	100.0
2926	Transcortin receptor antagonist	29	100.0
2927	Transcription factor AP-1 inhibitor	191	97.0
2928	Transcription factor NF kappa A inhibitor	17	83.2
2929	Transcription factor NF kappa B inhibitor	575	95.2
2930	Transcription factor NF kappa B stimulant	7	84.3
2931	Transcription factor STAT inhibitor	64	87.7
2932	Transcription factor STAT3 inhibitor	52	95.7
2933	Transcription factor STAT6 inhibitor	6	88.5
2934	Transcription factor inhibitor	743	94.5
2935	Transcription factor rho inhibitor	7	100.0
2936	Transcription factor stimulant	7	84.3
2937	Transferase inhibitor	33	75.9
2938	Transferase stimulant	9	78.5
2939	Transforming growth factor agonist	5	77.9
2940	Transforming growth factor antagonist	60	96.8
2941	Transforming growth factor beta 1 agonist	3	88.3
2942	Transforming growth factor beta 1 antagonist	8	80.2
2943	Transforming growth factor beta 3 antagonist	21	100.0
2944	Transforming growth factor beta agonist	5	77.9
2945	Transforming growth factor beta antagonist	46	97.5
2946	Transglutaminase 2 inhibitor	27	97.4
2947	Transketolase inhibitor	6	98.2
2948	Translation initiation factor IF-2 antagonist	5	100.0
2949	Transthyretin amyloid fibril formation inhibitor	7	99.5
2950	Trehalose-phosphatase inhibitor	3	99.4
2951	Triacetate-lactonase inhibitor	3	98.8
2952	Trimerelysin II inhibitor	7	99.1
2953	Trimethylamine dehydrogenase inhibitor	9	93.2
2954	Trimethylamine-N-oxide reductase inhibitor	11	98.9
2955	Trimethylamine-oxide aldolase inhibitor	5	80.6
2956	Trimethyllysine dioxygenase inhibitor	7	97.9
2957	Tripeptide aminopeptidase inhibitor	23	93.8
2958	Tripeptidyl peptidase II inhibitor	36	99.9
2959	Tripeptidyl-peptidase I inhibitor	22	95.9
2960	Tropinesterase inhibitor	3	85.7
2961	Trypanothione-disulfide reductase inhibitor	46	97.0
2962	Trypsin inhibitor	1134	98.9
2963	Tryptase 1 inhibitor	50	100.0
2964	Tryptase inhibitor	143	97.9
2965	Tryptophan 2,3-dioxygenase inhibitor	23	85.1
2966	Tryptophan 2-monooxygenase inhibitor	20	96.1
2967	Tryptophan 5 hydroxylase inhibitor	20	93.7
2968	Tryptophan alpha,beta-oxidase inhibitor	4	95.6

2969	Tryptophan dimethylallyltransferase inhibitor	8	97.2
2970	Tryptophan hydroxylase 1 inhibitor	11	100.0
2971	Tryptophan synthase inhibitor	14	99.5
2972	Tryptophan transaminase inhibitor	4	98.5
2973	Tryptophan-tRNA ligase inhibitor	38	98.9
2974	Tryptophanamidase inhibitor	5	98.3
2975	Tryptophanyl aminopeptidase inhibitor	3	98.9
2976	Tubulin GTPase inhibitor	6	99.6
2977	Tubulin agonist	26	100.0
2978	Tubulin antagonist	998	97.5
2979	Tubulin-tyrosine ligase inhibitor	17	98.6
2980	Tubuliny-Tyr carboxypeptidase inhibitor	6	99.8
2981	Tumour necrosis factor alpha antagonist	536	94.7
2982	Tumour necrosis factor antagonist	696	93.2
2983	Tyrosine 2,3-aminomutase inhibitor	6	99.4
2984	Tyrosine 3 hydroxylase stimulant	3	100.0
2985	Tyrosine kinase inhibitor	4768	95.7
2986	Tyrosine kinase stimulant	3	95.5
2987	Tyrosine phenol-lyase inhibitor	20	99.8
2988	Tyrosine transaminase inhibitor	34	98.5
2989	Tyrosine-ester sulfotransferase inhibitor	24	98.6
2990	Tyrosine-protein kinase EMT inhibitor	86	99.6
2991	Tyrosine-protein kinase TYRO 10 inhibitor	4	81.3
2992	Tyrosine-protein kinase receptor FLT3 inhibitor	246	98.4
2993	Tyrosine-protein kinase receptor antagonist	130	98.4
2994	UDP-3-O-acyl-N-acetylglucosamine deacetylase inhibitor	42	99.9
2995	UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor	15	99.1
2996	UDP-N-acetylglucosamine 2-epimerase inhibitor	7	99.0
2997	UDP-N-acetylglucosamine 4-epimerase inhibitor	3	89.5
2998	UDP-N-acetylglucosamine diphosphorylase inhibitor	8	99.2
2999	UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminophosphotransferase inhibitor	11	97.8
3000	UDP-N-acetylglucosamine-lysosomal-enzyme N-acetylglucosaminophosphotransferase inhibitor	9	99.6
3001	UDP-N-acetylmuramate dehydrogenase inhibitor	11	97.0
3002	UDP-N-acetylmuramate-L-alanine ligase inhibitor	18	97.4
3003	UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor	18	98.6
3004	UDP-N-acetylmuramoylalanyl-D-glutamate-2,6-diaminopimelate ligase inhibitor	8	100.0
3005	UDP-glucose 6-dehydrogenase inhibitor	8	95.0
3006	UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor	18	97.4
3007	UDP-glucuronate 4-epimerase inhibitor	13	100.0
3008	UDP-glucuronate 5'-epimerase inhibitor	3	100.0
3009	UDP-glucuronate decarboxylase inhibitor	12	99.5
3010	UDP-sugar diphosphatase inhibitor	4	99.5
3011	UTP-glucose-1-phosphate uridylyltransferase inhibitor	10	100.0
3012	Ubiquitin thiolesterase inhibitor	7	95.8
3013	Ubiquitin-protein ligase inhibitor	27	97.1
3014	Undecaprenyl-diphosphatase inhibitor	5	98.0
3015	Undecaprenyl-phosphate galactose phosphotransferase inhibitor	6	100.0

3016	Undecaprenyl-phosphate mannosyltransferase inhibitor	3	94.1
3017	Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor	3	95.0
3018	Uracil phosphoribosyltransferase inhibitor	14	99.5
3019	Urate-ribonucleotide phosphorylase inhibitor	12	92.3
3020	Urease inhibitor	18	92.4
3021	Urethanase inhibitor	10	87.1
3022	Uridine kinase inhibitor	7	99.2
3023	Uridine nucleosidase inhibitor	15	99.0
3024	Uridine phosphorylase inhibitor	95	99.8
3025	Urocanate hydratase inhibitor	16	99.3
3026	Urokinase inhibitor	330	99.5
3027	Uroporphyrinogen decarboxylase inhibitor	30	99.0
3028	Uroporphyrinogen-III synthase inhibitor	9	93.8
3029	Urotensin II agonist	36	100.0
3030	Urotensin II antagonist	15	93.8
3031	VCAM antagonist	153	97.4
3032	VCAM-1 antagonist	152	97.6
3033	VLA-4 antagonist	776	99.8
3034	Valine decarboxylase inhibitor	4	98.8
3035	Valine dehydrogenase (NADP+) inhibitor	6	99.4
3036	Valine-pyruvate transaminase inhibitor	3	100.0
3037	Valine-tRNA ligase inhibitor	10	97.6
3038	Vanilloid 1 agonist	27	91.3
3039	Vanilloid 1 antagonist	267	99.0
3040	Vanilloid 3 antagonist	6	100.0
3041	Vanilloid 4 agonist	6	100.0
3042	Vanilloid 4 antagonist	5	100.0
3043	Vanilloid agonist	34	94.6
3044	Vanilloid antagonist	306	99.0
3045	Vanillyl-alcohol oxidase inhibitor	7	99.5
3046	Vascular adhesion protein 1 inhibitor	11	90.3
3047	Vascular endothelial growth factor 1 antagonist	198	96.2
3048	Vascular endothelial growth factor 2 antagonist	1400	97.9
3049	Vascular endothelial growth factor 3 antagonist	75	95.6
3050	Vascular endothelial growth factor antagonist	2029	96.9
3051	Vasopressin 1 agonist	17	100.0
3052	Vasopressin 1 antagonist	861	99.6
3053	Vasopressin 1A agonist	9	100.0
3054	Vasopressin 1A antagonist	763	99.7
3055	Vasopressin 1B agonist	8	100.0
3056	Vasopressin 1B antagonist	115	99.9
3057	Vasopressin 2 agonist	132	99.9
3058	Vasopressin 2 antagonist	596	99.8
3059	Venom exonuclease inhibitor	8	87.1
3060	Venombin A inhibitor	9	98.1
3061	Venombin AB inhibitor	5	87.7
3062	Vibriolysin inhibitor	12	99.9

3063	Vitamin	260	98.9
3064	Vitamin D receptor agonist	102	99.9
3065	Vitamin D receptor antagonist	27	100.0
3066	Vitamin D-like	160	100.0
3067	Vitamin D3 hydroxylase inhibitor	15	99.9
3068	Vitamin K-like	20	100.0
3069	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor	7	94.4
3070	Vitronectin receptor antagonist	1166	99.7
3071	Vomilenine glucosyltransferase inhibitor	6	98.1
3072	Wee-1 tyrosine kinase inhibitor	5	99.9
3073	X-His dipeptidase inhibitor	22	97.4
3074	X-Pro dipeptidase inhibitor	21	98.4
3075	X-Trp aminopeptidase inhibitor	7	99.3
3076	X-methyl-His dipeptidase inhibitor	10	87.5
3077	Xaa-Pro dipeptidyl-peptidase inhibitor	8	98.4
3078	Xanthine dehydrogenase inhibitor	33	94.5
3079	Xanthine oxidase inhibitor	108	95.8
3080	Xanthine phosphoribosyltransferase inhibitor	39	99.7
3081	Xanthine-like	28	99.8
3082	Xanthommatin reductase inhibitor	5	98.3
3083	Xenobiotic-transporting ATPase inhibitor	13	91.4
3084	Xylan 1,4-beta-xylosidase inhibitor	14	99.2
3085	Xylan endo-1,3-beta-xylosidase inhibitor	5	96.7
3086	Xylose isomerase inhibitor	11	98.5
3087	YAK3 inhibitor	15	100.0
3088	Yeast ribonuclease inhibitor	3	95.7
3089	ZAP-70 protein tyrosine kinase inhibitor	70	98.2
3090	[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor	34	99.1
3091	[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)]-phosphatase inhibitor	12	100.0
3092	[Isocitrate dehydrogenase (NADP+)] kinase inhibitor	9	99.7
3093	[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor	5	99.7
3094	[acetyl-CoA carboxylase] kinase inhibitor	6	99.4
3095	[acyl-carrier-protein] S-acetyltransferase inhibitor	7	95.1
3096	[acyl-carrier-protein] S-malonyltransferase inhibitor	10	98.5
3097	[citrate-(pro-3S)-lyase] thiolesterase inhibitor	4	99.9
3098	[glutamate-ammonia-ligase] adenylyltransferase inhibitor	13	99.7
3099	[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor	11	95.5
3100	[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor	8	99.8
3101	[myelin basic protein]-arginine N-methyltransferase inhibitor	3	98.2
3102	[phosphorylase] phosphatase inhibitor	14	94.0
3103	[protein-PII] uridylyltransferase inhibitor	27	99.7
3104	[pyruvate dehydrogenase (lipoamide)]-phosphatase inhibitor	9	79.1
3105	c-Src kinase inhibitor	507	99.5
3106	dCMP deaminase inhibitor	19	99.6
3107	dCTP deaminase inhibitor	10	99.7
3108	dCTP diphosphatase inhibitor	3	100.0
3109	dTDP-glucose 4,6-dehydratase inhibitor	6	100.0
3110	dTMP kinase (Mycobacterium tuberculosis) inhibitor	11	100.0

3111	dTMP kinase inhibitor	28	100.0
3112	dUTP diphosphatase inhibitor	14	99.4
3113	mRNA (guanine-N7-)-methyltransferase inhibitor	18	96.2
3114	mRNA (nucleoside-2'-O-)-methyltransferase inhibitor	16	100.0
3115	mTOR inhibitor	139	98.2
3116	p21-activated kinase 1 inhibitor	6	99.5
3117	p21-activated kinase 4 inhibitor	23	98.5
3118	p21-activated kinase inhibitor	24	98.0
3119	p38 MAP kinase inhibitor	510	98.2
3120	p53 inhibitor	18	94.0
3121	pFOX inhibitor	5	100.0
3122	rRNA (adenosine-2'-O-)-methyltransferase inhibitor	12	99.8
3123	tRNA (adenine-N1-)-methyltransferase inhibitor	6	99.9
3124	tRNA (cytosine-5-)-methyltransferase inhibitor	5	98.3
3125	tRNA (guanine-N1-)-methyltransferase inhibitor	4	99.2
3126	tRNA (guanine-N2-)-methyltransferase inhibitor	5	99.3
3127	tRNA (guanine-N7-)-methyltransferase inhibitor	6	99.0
3128	tRNA (uracil-5-)-methyltransferase inhibitor	10	99.9
3129	tRNA adenylyltransferase inhibitor	9	98.4
3130	tRNA cytidyltransferase inhibitor	15	98.8
3131	tRNA methyltransferase inhibitor	22	99.4
3132	tRNA nucleotidyltransferase inhibitor	3	99.0
3133	tRNA-pseudouridine synthase I inhibitor	3	96.5
3134	11-Beta-hydroxysteroid dehydrogenase 2 inhibitor	18	99.9
3135	5 Hydroxytryptamine 1A agonist	1139	98.8
3136	5 Hydroxytryptamine 2A agonist	61	95.1
3137	5 Hydroxytryptamine 2B agonist	9	94.7
3138	5 Hydroxytryptamine 2C antagonist	1093	98.9
3139	5 Hydroxytryptamine 3 agonist	73	96.8
3140	ATPase inhibitor	145	92.8
3141	Acetylcholine M1 receptor antagonist	911	99.1
3142	Acetylcholine M2 receptor agonist	40	97.3
3143	Acetylcholine M2 receptor antagonist	852	99.2
3144	Acetylcholinesterase inhibitor	1296	96.8
3145	Aconitate hydratase inhibitor	22	99.1
3146	Acyl-CoA dehydrogenase inhibitor	15	99.2
3147	Adenosine deaminase inhibitor	164	98.3
3148	Adenylate cyclase I inhibitor	47	100.0
3149	Adenylate cyclase inhibitor	135	94.6
3150	Adenylate kinase inhibitor	23	93.3
3151	Alcohol dehydrogenase inhibitor	91	94.9
3152	Aldosterone antagonist	59	87.4
3153	Alkaline phosphatase inhibitor	27	96.8
3154	Alpha 1a adrenoreceptor agonist	48	100.0
3155	Alpha 1a adrenoreceptor antagonist	2730	98.5
3156	Alpha 2a adrenoreceptor antagonist	229	98.2
3157	Alpha galactosidase inhibitor	5	99.9
3158	Alpha-mannosidase inhibitor	47	97.9

3159	Aminopeptidase A inhibitor	38	99.9
3160	Aminopeptidase N inhibitor	130	98.1
3161	Aminopeptidase P inhibitor	8	100.0
3162	Androgen agonist	230	98.4
3163	Arginase inhibitor	34	99.2
3164	Argininosuccinate synthase inhibitor	21	98.7
3165	Aryl hydrocarbon receptor agonist	12	92.2
3166	Beta 1 adrenoreceptor agonist	50	97.5
3167	Beta 1 adrenoreceptor antagonist	304	99.3
3168	Beta 2 adrenoreceptor agonist	687	99.4
3169	Beta 2 adrenoreceptor antagonist	256	99.3
3170	Butyrylcholinesterase inhibitor	393	98.3
3171	Ca ²⁺ -transporting ATPase inhibitor	12	85.6
3172	Carbamoyl-phosphate synthase (ammonia) inhibitor	15	98.8
3173	Carbonic anhydrase I inhibitor	779	99.9
3174	Carbonic anhydrase II inhibitor	1189	99.9
3175	Carbonic anhydrase inhibitor	1291	99.9
3176	Catalase inhibitor	73	98.4
3177	Catechol O methyltransferase inhibitor	55	98.0
3178	Cyclooxygenase inhibitor	3262	96.2
3179	Cystathionine beta-synthase inhibitor	12	98.9
3180	DOPA decarboxylase inhibitor	10	98.4
3181	Diamine oxidase inhibitor	26	98.8
3182	Dihydrofolate reductase inhibitor	1568	99.4
3183	Dipeptidyl peptidase IV inhibitor	1291	99.4
3184	Dopamine D2 antagonist	3884	98.3
3185	Estrogen agonist	781	98.0
3186	Fumarate hydratase inhibitor	24	99.5
3187	GABA A receptor agonist	236	94.7
3188	GABA A receptor antagonist	1733	99.2
3189	GABA aminotransferase inhibitor	15	90.7
3190	Glucocorticoid agonist	453	99.3
3191	Glucose-6-phosphate isomerase inhibitor	22	99.8
3192	Glutamate dehydrogenase inhibitor	34	95.7
3193	HMG CoA reductase inhibitor	480	99.2
3194	Heat shock protein 70 antagonist	6	94.0
3195	Hexokinase inhibitor	21	97.2
3196	Histamine H1 receptor antagonist	712	97.6
3197	Histamine H2 receptor antagonist	315	97.5
3198	Hypoxanthine phosphoribosyltransferase inhibitor	37	98.8
3199	Insulin and insulin analogs	16	77.6
3200	Insulin antagonist	29	86.0
3201	Luteinizing hormone-releasing hormone antagonist	1104	98.8
3202	Lysine carboxypeptidase inhibitor	22	99.6
3203	MAO A inhibitor	315	97.9
3204	MAO inhibitor	775	96.6
3205	Na ⁺ K ⁺ transporting ATPase inhibitor	149	98.5
3206	Neutral endopeptidase inhibitor	545	99.5

3207	Opioid delta receptor antagonist	1399	99.4
3208	Opioid mu receptor agonist	167	96.8
3209	Ornithine carbamoyltransferase inhibitor	40	98.9
3210	Peroxidase inhibitor	15	93.0
3211	Phenylalanine 4-hydroxylase inhibitor	30	97.7
3212	Phosphodiesterase inhibitor	5565	97.1
3213	Phosphofructokinase-1 inhibitor	33	98.2
3214	Phosphoglycerate kinase inhibitor	43	99.0
3215	Phospholipase A2 inhibitor	327	93.0
3216	Phospholipase C inhibitor	77	93.8
3217	Phosphorylase inhibitor	139	97.4
3218	Platelet activating factor antagonist	1548	97.2
3219	Prostaglandin F2 alpha agonist	29	100.0
3220	Protein kinase C stimulant	67	98.8
3221	Pyruvate kinase inhibitor	38	97.1
3222	Retinoic acid alpha receptor agonist	27	99.7
3223	S-adenosyl-L-homocysteine hydrolase inhibitor	53	100.0
3224	Sodium channel blocker	701	91.9
3225	Succinate dehydrogenase inhibitor	14	95.6
3226	Superoxide dismutase inhibitor	16	89.6
3227	Thyroid hormone agonist	110	98.7
3228	Thyroid hormone alpha 1 agonist	5	100.0
3229	Thyroid hormone alpha agonist	5	100.0
3230	Thyroid hormone beta 1 agonist	5	100.0
3231	Thyroid hormone beta agonist	74	100.0
3232	Topoisomerase I inhibitor	556	96.6
3233	Triose-phosphate isomerase inhibitor	23	98.3
3234	Tyrosine 3 hydroxylase inhibitor	10	86.0
3235	UDP-glucose 4-epimerase inhibitor	25	99.3
3236	Ubiquinol-cytochrome-c reductase inhibitor	10	81.2
3237	CYP11B1 inhibitor	59	96.1
3238	CYP11B2 inhibitor	65	99.6
3239	CYP17 inhibitor	7	93.8
3240	CYP19 inhibitor	43	96.3
3241	CYP1A inhibitor	206	88.7
3242	CYP1A1 inhibitor	72	92.6
3243	CYP1B1 inhibitor	49	96.9
3244	CYP26 inhibitor	19	99.3
3245	CYP2A5 inhibitor	13	99.7
3246	CYP2B6 inhibitor	35	76.2
3247	CYP2C18 inhibitor	13	98.3
3248	CYP2C19 inhibitor	123	87.2
3249	CYP2C8 inhibitor	37	80.2
3250	CYP2E1 inhibitor	53	94.5
3251	CYP51 inhibitor	6	99.8
3252	CYP7 inhibitor	7	81.9
3253	CYP24 inhibitor	9	89.3
3254	CYP2A6 inhibitor	48	93.4

3255	CYP1A2 inhibitor	181	88.7
3256	CYP2C9 inhibitor	196	88.9
3257	CYP2D6 inhibitor	227	88.9
3258	CYP3A inhibitor	9	75.8
3259	CYP3A4 inhibitor	342	86.3
3260	APOA1 expression enhancer	9	95.6
3261	AR expression inhibitor	4	92.4
3262	CCL2 expression inhibitor	5	91.7
3263	CTGF expression inhibitor	5	100.0
3264	CYP19A1 expression inhibitor	3	100.0
3265	EIF4E expression inhibitor	3	100.0
3266	ErbB-2 expression inhibitor	6	75.7
3267	HIF1A expression inhibitor	3	86.4
3268	HMGCS2 expression enhancer	5	94.3
3269	HMOX1 expression enhancer	5	84.2
3270	ICAM1 expression inhibitor	41	98.0
3271	LECT1 expression enhancer	9	100.0
3272	MMP1 expression inhibitor	5	80.2
3273	MMP9 expression inhibitor	3	93.3
3274	NOS2 expression inhibitor	37	94.0
3275	RELA expression inhibitor	3	100.0
3276	SMN2 expression enhancer	14	93.1
3277	TH expression enhancer	9	95.0
3278	TNF expression inhibitor	23	94.2
3279	TP53 expression enhancer	5	88.8
3280	VCAM1 expression inhibitor	51	96.4
3281	VEGF expression inhibitor	44	95.1
3282	VEGFR2 expression inhibitor	5	100.0
3283	ABCA1 expression enhancer	200	99.3
3284	Gene expression stimulant	12	80.9
3285	GRP78 expression inhibitor	5	100.0
3286	ATP-binding cassette A1 stimulant	7	90.3
3287	Adenine nucleotide translocator 1 inhibitor	3	100.0
3288	Amino acid-polyamine-organocation (APC) transporter antagonist	82	100.0
3289	Apical sodium codependent bile acid transporter inhibitor	16	100.0
3290	Endocannabinoid uptake inhibitor	30	99.2
3291	Equilibrative nucleoside transport protein 1 inhibitor	74	99.7
3292	Equilibrative nucleoside transport protein inhibitor	106	99.9
3293	Excitatory amino acid transporter 1 inhibitor	6	90.7
3294	Excitatory amino acid transporter EAAC1 inhibitor	6	99.0
3295	Folate transporter 1 inhibitor	5	100.0
3296	GABA transporter 2 inhibitor	5	83.0
3297	GABA transporter 3 inhibitor	5	97.6
3298	GABA transporter inhibitor	153	99.4
3299	Glutamate uptake inhibitor	9	99.9
3300	Monoamine uptake inhibitor	41	91.4
3301	Monocarboxylic acid transporter 1 inhibitor	6	97.2
3302	Monocarboxylic acid transporter inhibitor	6	97.2

3303	Multidrug resistance-associated protein 1 inhibitor	206	98.0
3304	Multidrug resistance-associated protein inhibitor	208	97.4
3305	Nucleoside transporters inhibitor	18	99.9
3306	P2 nucleoside transporter inhibitor	11	100.0
3307	Phosphate transporter inhibitor	26	98.3
3308	Proline transporter inhibitor	23	100.0
3309	Sodium-dependent vitamin C transporter 2 inhibitor	3	100.0
3310	Sodium/calcium exchanger 1 inhibitor	25	97.1
3311	Sodium/glucose cotransporter 1 inhibitor	109	99.6
3312	Sodium/hydrogen exchanger 1 inhibitor	283	99.9
3313	Sodium/hydrogen exchanger 2 inhibitor	8	97.7
3314	Sodium/hydrogen exchanger 3 inhibitor	73	100.0
3315	Sodium/hydrogen exchanger 5 inhibitor	5	99.0
3316	Tetracycline antiport transporter antagonist	36	100.0
3317	Urate transporter 1 inhibitor	29	97.9
3318	Vesicle monoamine transporter 2 inhibitor	13	100.0
3319	Vesicle monoamine transporter inhibitor	13	100.0
3320	Vesicular acetylcholine transporter inhibitor	70	100.0
3321	Vesicular glutamate transport inhibitor	4	100.0
3322	5 Hydroxytryptamine uptake stimulant	5	81.3
3323	Adenosine uptake inhibitor	56	99.3
3324	Dopamine uptake inhibitor	1848	99.2
3325	GABA uptake inhibitor	68	99.3
3326	Glycine transporter 1 inhibitor	449	99.7
3327	Glycine transporter 2 inhibitor	44	97.8
3328	Glycine transporter inhibitor	510	99.1
3329	Ileal bile acid transport inhibitor	147	99.8
3330	Neurotransmitter uptake inhibitor	4	78.9
3331	P-glycoprotein 1 inhibitor	293	97.6
3332	P-glycoprotein inhibitor	497	96.1
3333	Sodium/bile acid cotransporter inhibitor	3	97.9
3334	Sodium/calcium exchanger inhibitor	109	98.7
3335	Sodium/glucose cotransporter 2 inhibitor	336	99.8
3336	Sodium/glucose cotransporter inhibitor	459	99.4
3337	Sodium/hydrogen exchanger inhibitor	645	99.8
3338	Electron transport complex I inhibitor	5	91.6
3339	Excitatory amino acid transporter 2 inhibitor	15	99.9
3340	GABA transporter 1 inhibitor	148	99.6
3341	5 Hydroxytryptamine uptake inhibitor	3423	98.3
3342	Adrenaline uptake inhibitor	1639	98.5

Table S3. Comparison of direct PASS prediction results of known effects for phytoconstituents of 50 TIM plants with prediction of known effects through “mechanism-effect” (column MOA) and “target-pathway-effect” (columns KEGG, NCI pathways and Reactome) relationships from PharmaExpert.

Plant	Number of PASS predicted known effects (Pa>0.5 cut-off)							All mode
	N _{emp}	N _{kn Efs}	Effects	MOA	KEGG	NCI pathways	Reactome	
Achyranthes aspera L.	18	32	17	19	25	20	27	29
Acorus calamus	44	21	11	17	19	15	19	20
Adhatoda zeylanica Medic.	2	19	0	15	15	14	16	16
Aegle marmelos.	32	31	19	21	24	18	25	31
Aerva lanata L.	9	14	6	8	10	9	10	11
Allium sativum	67	28	19	17	20	16	22	27
Aloe vera	31	16	11	9	12	10	14	16
Alpinia galanga	17	12	9	8	6	5	9	11
Alstonia scholaris L.	49	28	12	18	23	17	26	27
Andrographis paniculata	70	24	13	17	22	16	22	24
Argyreia speciosa	8	16	10	15	15	12	15	16
Asparagus racemosus	15	23	10	12	17	13	18	20
Azadirachta indica	220	21	16	16	18	15	18	21
Bacopa monnieri L.	28	28	7	12	24	18	25	25
Berberis vulgaris L.	6	19	1	5	15	11	16	16
Boerhavia diffusa L.	20	20	13	14	17	16	17	19
Cassia tora L.	29	15	11	12	12	9	14	14
Centella asiatica	26	19	13	16	17	14	18	19
Crocus sativus L.	44	20	11	16	18	14	20	20
Curcuma longa	41	18	9	12	15	14	16	16
Emblica officinalis L.	2	21	6	11	19	12	20	20
Ficus religiosa L.	5	18	7	14	16	13	17	17
Ginkgo biloba	59	19	12	14	16	17	17	17
Glycyrrhiza glabra L.	108	11	7	10	9	8	10	10
Hemidesmus indicus L.	25	9	7	5	8	6	9	9
Hibiscus sabdariffa L.	6	14	8	11	14	12	14	14
Hypericum perforatum L.	40	7	5	5	6	6	7	7
Lathyrus sativus L.	10	1	1	1	1	1	1	1
Morinda citrifolia L.	62	11	8	9	9	10	10	11
Moringa oleifera Lam.	64	20	12	15	19	15	19	20
Nardostachys jatamansi	19	10	4	8	10	8	10	10
Nigella sativa L.	36	7	6	7	7	5	7	7
Ocimum sanctum	6	19	14	10	14	9	17	18
Panax ginseng	139	21	14	17	20	18	20	20
Passiflora incarnate	9	9	2	7	8	7	8	8
Phyllanthus amarus	13	11	5	9	11	7	11	11
Piper longum L.	27	19	10	14	16	11	17	19
Psidium guajava L.	33	12	8	12	11	8	12	12
Psoralea corylifolia	48	14	10	11	11	10	12	14
Punica granatum L.	46	6	4	5	4	4	5	5
Sida cordifolia	12	4	1	2	4	3	4	4
Terminalia arjuna	35	11	10	8	9	9	9	11
Terminalia chebula	20	3	2	3	3	3	3	3

<i>Tinospora cordifolia</i>	25	15	5	8	15	13	15	15
<i>Trigonella foenum-graecum</i>	38	11	9	9	10	7	11	11
<i>Valeriana officinalis</i>	49	10	4	7	9	5	9	9
<i>Vitex negundo</i> L.	28	11	8	10	10	9	10	11
<i>Withania somnifera</i> L.	120	19	9	11	15	11	15	16
<i>Zanthoxylum armatum</i>	6	7	3	5	5	4	6	6
<i>Zingiber officinalis</i>	169	10	9	9	9	8	9	10
Average	41	16	9	11	13	10	14	15

N_{comp} – number of phytoconstituents for the appropriate plant; $N_{\text{known Efs}}$ – number of known therapeutic effects for the appropriate plant; **Effects** – number of known therapeutic effects predicted by PASS with $P_a > 0.5$; **MOA** – number of known therapeutic effects for which some mechanism of their action was predicted with $P_a > 0.5$; **All mode** - number of known therapeutic effects, which were predicted by any modes.