

Supporting Information

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Supplement

to the paper of Alexey Lagunin, Alexey Zakharov, Dmitry Filimonov and Vladimir Poroikov
"QSAR Modelling of Rat Acute Toxicity on the Basis of PASS Prediction"

1. QSAR Modelling Using Quantitative Neighborhoods of Atoms (QNA) Descriptors by GUSAR Program

QNA descriptors are calculated based on the connectivity matrix (**C**) and the standard values of ionization potential (IP) and electron affinity (EA) of atoms in a molecule. For any given atom *i* QNA descriptors are calculated as follow:

$$P_i = B_i \sum_k \left(\text{Exp}\left(-\frac{1}{2} C\right) \right)_{ik} B_k \quad (2)$$

$$Q_i = B_i \sum_k \left(\text{Exp}\left(-\frac{1}{2} C\right) \right)_{ik} B_k A_k, \quad (3)$$

where $A_k = \frac{1}{2}(IP_k + EA_k)$, $B_k = (IP_k - EA_k)^{-\frac{1}{2}}$. The values of EA and IP collected from many different sources and used in this work are represented in Table 1. Though the value $\mu P - Q$ can be considered by convention as the partial atomic charge, where μ is the chemical potential, in general, the *P* and *Q* values are not the estimate of partial atomic charges, hardness or so forth.

Table 1. Electron affinity (EA) and first ionization potential (IP), electron volts, and atomic radius (AR), angstroms.

Atom	EA	IP	AR	Atom	EA	IP	AR	Atom	EA	IP	AR
H	0.75	13.60	0.46	Kr	-0.42	14.00	1.98	Lu	0.20	6.15	1.75
He	0.08	24.59	1.22	Rb	0.49	4.18	2.48	Hf	0.33	7.50	1.59
Li	0.62	5.39	1.55	Sr	-0.15	5.69	2.15	Ta	0.40	7.89	1.46
Be	-0.20	9.32	1.13	Y	0.31	6.22	1.81	W	0.67	7.98	1.40
B	0.28	8.30	0.91	Zr	0.33	6.84	1.60	Re	0.23	7.88	1.37
C	1.26	11.26	0.77	Nb	0.51	6.88	1.45	Os	1.44	8.73	1.35
N	0.44	14.53	0.71	Mo	0.68	7.09	1.39	Ir	1.57	9.10	1.35
O	1.46	13.62	0.73	Tc	0.54	7.23	1.36	Pt	1.10	8.96	1.38
F	3.45	17.42	0.71	Ru	1.10	7.37	1.34	Au	1.25	9.23	1.44
Ne	0.00	21.57	1.60	Rh	1.14	7.46	1.34	Hg	-0.19	10.44	1.57
Na	0.55	5.14	1.87	Pd	1.11	8.34	1.37	Tl	0.31	6.11	1.71
Mg	-0.31	7.64	1.60	Ag	1.22	7.58	1.44	Pb	1.39	7.42	1.75
Al	0.30	5.99	1.43	Cd	-0.43	8.99	1.56	Bi	0.97	7.29	1.82
Si	1.39	8.15	1.34	In	0.31	5.79	1.66	Po	1.97	8.42	1.56
P	0.75	10.49	1.30	Sn	1.39	7.34	1.58	At	2.90	9.20	1.48
S	2.00	10.36	1.04	Sb	0.90	8.64	1.61	Rn	-0.15	10.75	2.27
Cl	3.61	12.97	0.99	Te	1.97	9.01	1.70	Fr	0.48	3.98	2.80
Ar	-0.37	15.76	1.92	I	3.23	10.45	1.53	Ra	-0.15	5.28	2.35
K	0.50	4.34	2.36	Xe	-0.25	12.13	2.18	Ac	0.80	5.20	2.03
Ca	-0.19	6.11	1.97	Cs	0.47	3.89	2.66	Th	0.80	6.10	1.80
Sc	0.19	6.56	1.64	Ba	-0.15	5.21	2.23	Pa	0.84	6.00	1.62
Ti	0.33	6.82	1.46	La	0.30	5.59	1.87	U	0.82	6.19	1.53
V	0.53	6.74	1.34	Ce	0.25	5.54	1.83	Np	0.82	6.20	1.50
Cr	0.67	6.77	1.27	Pr	0.20	5.47	1.83	Pu	0.84	6.06	1.62
Mn	-0.17	7.43	1.30	Nd	0.20	5.53	1.82	Am	0.85	6.00	1.70
Fe	0.50	7.90	1.26	Pm	0.20	5.58	1.81	Cm	0.85	6.09	1.55
Co	0.66	7.86	1.25	Sm	0.20	5.64	1.80	Bk	0.82	6.23	1.49
Ni	1.16	7.64	1.24	Eu	0.20	5.67	2.04	Cf	0.84	6.27	1.42
Cu	1.23	7.72	1.28	Gd	0.20	6.15	1.80	Es	0.86	6.47	1.43
Zn	-0.44	9.39	1.39	Tb	0.20	5.86	1.78	Fm	0.86	6.60	1.38
Ga	0.30	6.00	1.39	Dy	0.20	5.94	1.77	Md	0.83	6.68	1.38
Ge	1.39	7.90	1.39	Ho	0.20	6.02	1.78	No	0.79	6.58	1.47
As	0.80	9.79	1.48	Er	0.20	6.11	1.76	Lr	0.85	6.69	1.30
Se	2.02	9.75	1.17	Tm	0.20	6.18	1.75	Db	0.46	6.43	1.14
Br	3.45	11.81	1.14	Yb	0.20	6.25	1.94	Jl	0.50	6.78	1.01

QNA describes each of the atoms in a molecule, and, at the same time, each of the P and Q values depends on the whole composition and structure of a molecule (Figure 1).

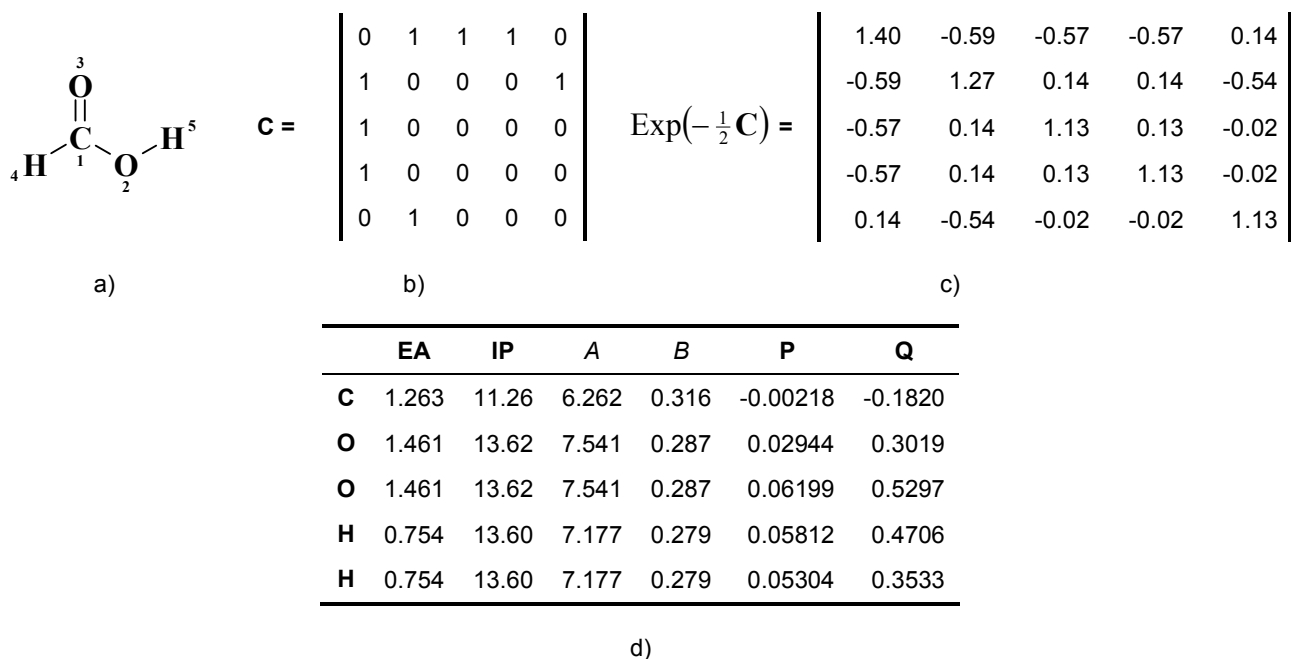


Figure 1. Example of QNA description of *formic acid*: (a) structure diagram; (b) connectivity matrix; (c) exponent of the connectivity matrix; (d) electron affinities, ionization potentials, variables of equations (2) and (3), P and Q values for each atom of *formic acid* molecule.

From Figure 1c it is clear that any atom influences the others, though the influence decreases with the increase of the distance between them; e.g. components of matrix $\text{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ for atom 1 (C) are: 1.40 for atom 1 itself, -0.59 for its immediate neighbor atom 2 (O), -0.57 for atoms 3 (O) and 4 (H), and 0.14 for atom 5 (H).

The algorithm of QNA descriptor calculation is quite simple due to uselessness of the matrix $\text{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ itself, only product of $\text{Exp}\left(-\frac{1}{2}\mathbf{C}\right)$ by vector is necessary, and that matrix $\mathbf{C}$ consists of 0 and 1 only.

QNA describe each particular atom of a molecule, at the same time, each P or Q value depends on the total molecule composition and structure. To use this molecule structure representation in equation (1) we have proposed to calculate each $f_i(S)$ function of the structure of a molecule as the average value of $g_i(P, Q)$ function of P and Q variables for those m atoms in a molecule, which have two or more immediate neighbors:

$$f_i(S) = \frac{1}{m} \sum_k g_i(P_k, Q_k) \quad (4)$$

After substitution of expression (4) into the equation (1) and interchange of summations we found:

$$y_{pred} = a_0 + \sum_i a_i \frac{1}{m} \sum_k g_i(P_k, Q_k) = \frac{1}{m} \sum_k \left(a_0 + \sum_i a_i g_i(P_k, Q_k) \right) \quad (5)$$

According to the equation (5) the estimate y_{pred} for molecule can be interpreted as an average of values predicted for particular atoms in a molecule. Formally, QNA descriptors represent a molecule structure by two descriptors only (P and Q), in contrast to numerous traditional descriptors used in QSAR.

Since P and Q values have different scales (standard deviations are 0.023 and 0.208, respectively), we made the normalization to optimize a family of functions $g_i(P, Q)$.

Normalization has been performed by calculation of the average values (E_P and E_Q), standard deviations (D_P and D_Q) and correlation between P and Q values (R_{PQ}):

$$P' = \frac{P - E_P}{D_P}, \quad Q' = \frac{Q - E_Q}{D_Q} \quad (6)$$

$$U = \frac{P' + Q'}{\sqrt{2(1 + R_{PQ})}}, \quad V = \frac{P' - Q'}{\sqrt{2(1 - R_{PQ})}} \quad (7)$$

The orthonormal U and V have zero mean, unit variance and they are uncorrelated.

Chebyshev polynomials were chosen as the family of functions $g_i(P, Q)$, and the orthonormal U and V values have been additionally transformed by using hyperbolic tangent, so, the “normalized QNA” vary from -1 to 1. After this, the functions $g_i(P, Q)$ in equation (5) are represented using Chebyshev polynomials as:

$$g_i(P, Q) = T_{uv}(P, Q) = \cos(u * \arccos(\tanh(U))) * \cos(v * \arccos(\tanh(V))), \quad (8)$$

where the integer numbers $u, v = 0, 1, 2, \dots$ define 2-dimensional Chebyshev polynomial degree. The final equation for estimate y_{pred} using QNA descriptors is:

$$y_{pred} = \frac{1}{m} \sum_k (a_0 + \sum_{uv} a_{uv} T_{uv}(P_k, Q_k)) = a_0 + \sum_{uv} a_{uv} T_{uv}, \quad T_{uv} = \frac{1}{m} \sum_k T_{uv}(P_k, Q_k). \quad (9)$$

QNA descriptors and their polynomial transformations (6)-(8) do not provide information on the shape and volume of a molecule although this information may be important for determination of the structure-activity relationships. Therefore, these parameters were added to QNA descriptors. Topological length of a molecule was calculated as the maximal distance between any two atoms and the volume of a molecule – as the sum of each atom's volume, $\frac{4}{3}\pi R^3$, where R is the atomic radius (see Table 1 (AR)).

The Chebyshev polynomials are arranged in ascending order of their degrees $u + v$. For $u + v = 1$ they are $T_{1,0}, T_{0,1}$; for $u + v = 2$ they are $T_{2,0}, T_{1,1}, T_{0,2}$; for $u + v = 3$ they are $T_{3,0}, T_{2,1}, T_{1,2}, T_{0,3}$, etc. The first, second and third power of topological length and volume of a molecule were used. The number of initial variables equals to the number of Chebyshev polynomials plus the number of the first, second and third power of topological length and volume of a molecule.

The number of initial variables depends on the number of compounds in the training set. If the number of compounds in the training set less than 25, then the initial variables are 24. If the number of compounds in the training set varied from 25 to 100, then the initial variables depends on the following equation:

$$A = (\ln(B) \times 18.755) - 36.37,$$

where A – initial variables and B – the number of compounds in the training set. If the number of compounds in the training set varied from 100 to 2000, then the number of initial variables equal to one-half of the number of compounds in the training set. If the number of compounds in the training set exceeds 2000, then the initial variables are 1000.

GUSAR algorithm uses three procedures describe below for generation of different QSAR models based on QNA descriptors.

- 1) U and V values from (8) are multiplied by value, which are randomly chosen from 0.98 to 1.09.
- 2) Coefficient before matrix $\mathbf{C}$ is randomly chosen from -0.1 to -0.9.
- 3) Calculation of QNA descriptors is randomly chosen from two cases. First case is when P and Q values are calculated for all atom types. Second case is when P and Q values are calculated for each atom, which has connection with more than one carbon.

All these procedures are used for creation of each QSAR model based on QNA descriptors. These procedures allow obtaining the different QNA models.

2. PASS (Prediction of Activity Spectra for Substances) Algorithm

In PASS biological activities are described qualitatively (active or inactive). Any property of chemical compounds, which is determined by their structural peculiarities, can be used for prediction by PASS. It is clear, that the applicability of PASS is broader than the prediction of biological activity spectra.

The Multilevel Neighbourhoods of Atoms (MNA) *descriptors* are based on the molecular structure representation, which includes the hydrogen atoms according to the valences and partial charges of other atoms and does not specify the types of bonds. MNA descriptors are generated as 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(D₁D₂...D_i...)**,

where **D_i** is the previous-level MNA descriptor for *i*-th immediate neighbor's of the atom **A**.

The mark of 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 **D₁D₂...D_i...** are arranged in unique manner, e.g., in lexicographic order. Iterative process of MNA descriptors generation can be continued covering first, second, etc. neighborhoods of each atom.

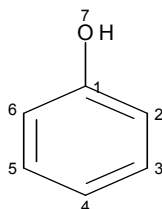
This process can be continued iteratively covering 2nd, 3rd, etc. neighbourhoods of the atom. We use 2nd level descriptors in the present version of PASS.

Multilevel Neighbourhoods of Atoms (MNA) structure descriptors of a molecule are generated on the basis of connection table (C) and table of atoms types (A) presented the substance. Connection table contains data on the [covalent](#) bonds in a molecule. Various bond types are not specified (topological approximation). All hydrogens based on valences and partial charges of atoms are taken into account. The types of atoms are specified according to the data presented in Table 1.

Table 1. Classification of different atom types used in calculation of descriptors

Class name	Elements
H	H
C	C
N	N
O	O
F	F
Si	Si
P	P
S	S
Cl	Cl
Ca	Ca
As	As
Se	Se
Br	Br
Li ⁺	Li, Na
B ⁺	B, Re
Mg ⁺	Mg, Mn
Sn ⁺	Sn, Pb
Te ⁺	Te, Po
I ⁺	I, At
Os ⁺	Os, Ir
Sc ⁺	Sc, Ti, Zr
Fe ⁺	Fe, Hf, Ta
Co ⁺	Co, Sb, W
Sr ⁺	Sr, Ba, Ra
Pd ⁺	Pd, Pt, Au
Be ⁺	Be, Zn, Cd, Hg
K ⁺	K, Rb, Cs, Fr
V ⁺	V, Cr, Nb, Mo, Tc
Ni ⁺	Ni, Cu, Ge, Ru, Rh, Ag, Bi
In ⁺	In, La, Ce, Pr, Nd, Pm, Sm, Eu
Al ⁺	Al, Ga, Y, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Tl
R ⁺	R, He, Ne, Ar, Kr, Xe, Rn, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr, Db, JI

Example of structure presentation by zero-, first- and second-levels MNA descriptors for the phenol's molecule is shown in Figure below.



Atom	MNA/0	MNA/1	MNA/2
1	C	C(CC-O)	C(C(CC-H)C(CC-H)-O(C-H))
2	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
3	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
4	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
5	C	C(CC-H)	C(C(CC-H)C(CC-H)-H(C))
6	C	C(CC-H)	C(C(CC-H)C(CC-O)-H(C))
7	-O	-O(C-H)	-O(C(CC-O)-H(-O))
8	-H	-H(C)	-H(C(CC-H))
9	-H	-H(C)	-H(C(CC-H))
10	-H	-H(C)	-H(C(CC-H))
11	-H	-H(C)	-H(C(CC-H))
12	-H	-H(C)	-H(C(CC-H))
13	-H	-H(-O)	-H(-O(C-H))

MNA descriptors for phenol.
MNA/0, MNA/1, MNA/2 - zero, first and second levels
of MNA descriptors.

It is shown that usage of the 1st & 2nd levels MNA descriptors provides the best accuracy of prediction. MNA descriptors are generated for each substance. Unique integer identifier is assigned to each particular descriptor according to the descriptors' dictionary.

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

The PASS estimations of biological activity spectra of new compounds are based on the Structure-Activity Relationships knowledge-base (SAR Base), which accumulates the results of the training set analysis. The in-house developed PASS training set includes more than 260,000 known biologically active substances (drugs, drug-candidates, leads, and toxic compounds). Since new information about biologically active compounds is discovered regularly, we perform the special informational search and analyse the new information, which is further used for updating and correcting the PASS training set.

MNA descriptors $\{D_1, \dots, D_m\}$ for each kind of activity A_k the following B_k values are calculated:

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

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

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

where $P(A_k|D_i)$ is a conditional probability of activity of kind A_k if the descriptor D_i is present in a set of molecule's descriptors; $P(A_k)$ is a priori probability to find a compound with activity of kind A_k . For any kind of activity A_k , if $P(A_k|D_i)$ is equal to 1 for all descriptors of a molecule, then $B_k = 1$; if $P(A_k|D_i)$ is equal to 0 for all descriptors of a molecule, then $B_k = -1$; if there is no relationship between the molecule's descriptors and activity of kind A_k , and, so, $P(A_k|D_i) \approx P(A_k)$, then $B_k \approx 0$.

Up to the PASS version 1.703 the algorithm of prediction was based on the following data:

n is the total number of compounds in the SAR Base;

n_i is the number of compounds containing descriptor D_i in the structure description;

n_k is the number of compounds containing the kind of activity A_k in the activity spectrum;

n_{ik} is the number of compounds containing both the kind of activity A_k and the descriptor D_i .

And the estimations of probabilities $P(A_k)$, $P(A_k|D_i)$ are given by:

$$P(A_k) = n_k/n, \quad P(A_k|D_i) = n_{ik}/n_i.$$

In PASS version 1.703 and later instead of integers n_i and n_{ik} the sums g_i and g_{ik} of descriptors weights w are used, where $w = 1/m$, and m is the number of MNA descriptors of individual molecule. This modification increases the accuracy of prediction significantly. So, right now the estimations of probabilities $P(A_k|D_i)$ are given by:

$$P(A_k|D_i) = g_{ik}/g_i.$$

The calculations are done by using $n-1$, g_i-w , and, when the kind of activity A_k is contained in its activity spectrum in the SAR Base, by using n_k-1 and $g_{ik}-w$. Here $w = 1/m$, and m is a number of MNA descriptors in molecule under prediction and its

equivalent in the SAR Base. The B_k values are calculated using MNA descriptors, which are found in SAR Base, i.e., for descriptors of a molecule under prediction with $g_i > 0$ or $g_{j-w} > 0$, in the case of structure «exclusion».

To take the «yes/no» qualitative prediction it is necessary to determine B -statistics threshold values for each kind of activity A_k . Using theory of statistical decision this can be done on the basis of risk function's minimization. But nobody can a priori specify the risk functions for all activity kinds and all possible practical tasks. Therefore, the predicted activity spectrum in PASS is presented by the rank-order list of activities with probabilities «to be active» Pa and «to be inactive» Pi , which are the results of the training procedure described below. The list is arranged in descending order of $Pa-Pi$; thus, the more probable activity kinds are at the top of the list. The list can be shortened at any desirable cutoff value, but $Pa > Pi$ is used by default. If the user chooses rather higher value of Pa as a cutoff 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 $Pa > 80\%$ is used as a threshold, about 80% of real activities will be lost; for $Pa > 70\%$, the portion of lost activities is 70%, etc.

For each compound from the training set MNA descriptors are generated and its known activity spectrum and set of descriptors are stored in the SAR Base. If this compound has the equivalent structure in SAR Base, only new activities are added to activity spectrum. After inclusion of all information from the training set(s) into SAR Base the values n , g_i , n_k , g_{ik} are calculated. For each compound in the SAR Base and for each activity kind A_k , values B_k of B -statistics are calculated. Calculations are done taking into account the described above «exclusion» of processed compound. For each activity kind A_k , the calculated values B_k are subdivided into two samples: for active and inactive compounds. These obtained samples are used for calculation the smooth estimations of B -statistics distribution functions on the following basis.

Suppose the sample $x_1, \dots, x_n$ of n values of random variable X , which has an unknown distribution function $F(x)$. Using of an empirical step-function for approximation of F often faults because of small n . To provide the smooth estimation of $F(x)$, the inverse function $x(F)$ is calculated as the conditional expectation of random variable X :

$$x(F) = \sum_i (n-1)! \cdot F^{i-1} / (i-1)! \cdot (1-F)^{n-i} / (n-i)! \cdot x'_i,$$

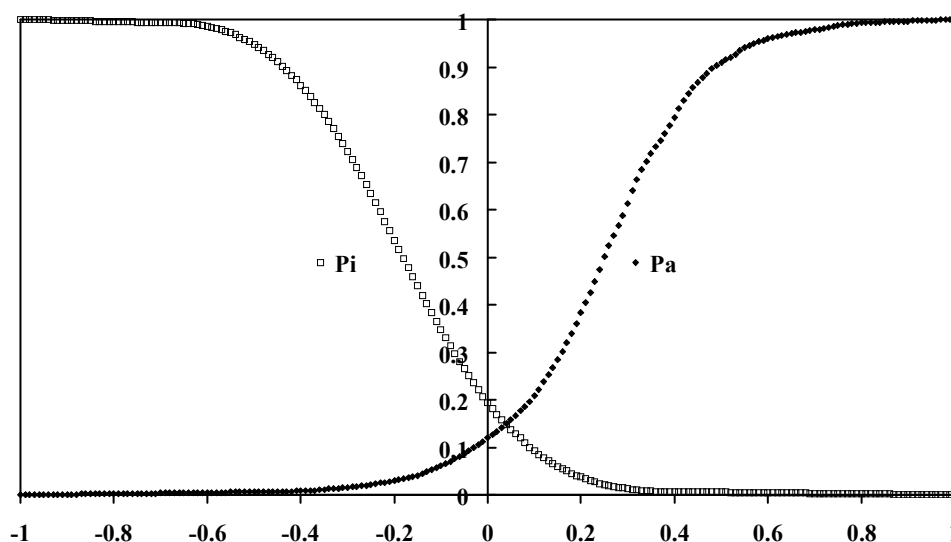
where $(n-1)! \cdot F^{i-1} / (i-1)! \cdot (1-F)^{n-i} / (n-i)!$ is the binomial distribution, and $x'_1, \dots, x'_n$ ($x'_1 < x'_2 < \dots < x'_n$) is the ranked sample $x_1, \dots, x_n$. The distribution function $F(x)$ is given reciprocal function of quantiles $x(F)$.

Each sample of B values for active compounds is arranged in the ascending order; each sample of B values for inactive compounds is arranged in descending order. The described above quantiles $b(F)$ are calculated. As a result, for each appropriate kind of activity the probabilities Pa and Pi are given by:

$$b_{active}(Pa) = B, \quad b_{inactive}(Pi) = B.$$

By definition the probabilities Pa and Pi are also the probabilities of the 1st and 2nd kinds of prediction error at the threshold B , respectively. They can be also interpreted as the measures of belonging to fuzzy subsets of «active» and «inactive» compounds. Both interpretations of 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 prediction results' analysis corresponded to specific practical problems.

The example of the probabilities $Pa(B)$ and $Pi(B)$ for activity «Alpha adrenoreceptor antagonist» as functions of B -statistics value is shown in the figure.



PASS prediction accuracy is estimated using average IEP for all predictable activity kinds. IEP is calculated for each type of activity in PASS prediction:

$$IEP = \#(B_0 > B_1) / (N_0 N_1),$$

where B_0 and B_1 are values of B -statistics for some pair of inactive and active compounds in the training set, N_0 is the number of inactive compounds in the training set,

N_1 is the number of active compounds in the training set.

If the values of B -statistics for any active compounds are higher than the values of B -statistics for all inactive compounds, then $IEP=0$. It means that all «active» and «inactive» compounds for the current type of activity from the training set were divided absolutely correct during LOO CV procedure. If the values of B -statistics for any active compounds are the same as the values of B -statistics for all inactive compounds, then $IEP=0.5$. This means that prediction is not correct.

3. Statistical parameters of QSAR models obtained for the set of LD₅₀ values of intravenous administration.

Model Name	Descriptors	Number	R ²	Q ²	Fisher	SD	V	L20%Out
Model 1	MNA	920	0.683	0.600	17.933	0.582	152	0.459
Model 2	MNA	920	0.644	0.571	19.170	0.610	127	0.439
Model 3	MNA	920	0.654	0.575	17.476	0.604	141	0.409
Model 4	MNA	920	0.663	0.579	16.638	0.599	156	0.450
Model 5	MNA	920	0.652	0.566	16.322	0.608	146	0.426
Model 6	MNA	920	0.656	0.577	17.427	0.603	145	0.439
Model 7	MNA	920	0.671	0.603	20.549	0.587	131	0.479
Model 8	MNA	920	0.656	0.570	15.786	0.606	156	0.431
Model 9	MNA	920	0.666	0.586	18.200	0.595	133	0.460
Model 10	MNA	920	0.672	0.588	17.661	0.591	145	0.433
Model 11	MNA	920	0.651	0.578	18.975	0.604	129	0.475
Model 12	MNA	920	0.633	0.554	17.162	0.621	137	0.439
Model 13	MNA	920	0.658	0.573	16.694	0.603	146	0.434
Model 14	MNA	920	0.653	0.572	17.641	0.605	143	0.425
Model 15	MNA	920	0.661	0.580	17.738	0.599	148	0.479
Model 16	MNA	920	0.665	0.590	18.922	0.594	133	0.470
Model 17	MNA	920	0.678	0.597	17.752	0.586	144	0.437
Model 18	MNA	920	0.655	0.572	16.479	0.605	146	0.421
Model 19	MNA	920	0.665	0.587	18.614	0.594	126	0.424
Model 20	MNA	920	0.680	0.605	19.747	0.581	138	0.465
Model 21	MNA	920	0.653	0.568	17.002	0.606	135	0.438
Model 22	MNA	920	0.653	0.580	18.914	0.603	125	0.446
Model 23	MNA	920	0.677	0.594	17.771	0.587	149	0.470
Model 24	MNA	920	0.663	0.579	16.694	0.599	148	0.450
Model 25	MNA	920	0.652	0.573	17.829	0.605	137	0.431
Model 26	MNA	920	0.672	0.589	17.319	0.591	150	0.434
Model 27	MNA	920	0.686	0.606	18.184	0.579	152	0.453
Model 28	MNA	920	0.653	0.572	17.729	0.605	137	0.453
Model 29	MNA	920	0.667	0.581	17.227	0.595	148	0.456
Model 30	MNA	920	0.661	0.578	16.877	0.600	146	0.434
Model 31	MNA	920	0.660	0.583	18.625	0.599	133	0.433
Model 32	MNA	920	0.673	0.591	17.992	0.589	144	0.443
Model 33	MNA	920	0.680	0.604	19.064	0.582	143	0.482
Model 34	MNA	920	0.683	0.602	18.019	0.581	151	0.482
Model 35	MNA	920	0.659	0.576	16.559	0.602	155	0.437
Model 36	MNA	920	0.678	0.595	17.270	0.587	155	0.467
Model 37	MNA	920	0.669	0.588	18.120	0.592	144	0.440
Model 38	MNA	920	0.666	0.581	17.100	0.596	151	0.427
Model 39	MNA	920	0.655	0.573	17.328	0.604	138	0.412
Model 40	MNA	920	0.645	0.570	18.937	0.609	129	0.451
Model 41	QNA	920	0.559	0.489	16.937	0.672	98	0.384

Model 42	QNA	920	0.604	0.530	17.352	0.640	113	0.425
Model 43	QNA	920	0.650	0.560	15.206	0.612	157	0.382
Model 44	QNA	920	0.626	0.550	18.116	0.624	119	0.445
Model 45	QNA	920	0.622	0.541	16.893	0.629	132	0.415
Model 46	QNA	920	0.540	0.475	18.815	0.683	83	0.421
Model 47	QNA	920	0.640	0.564	17.949	0.614	124	0.408
Model 48	QNA	920	0.637	0.553	16.549	0.618	142	0.414
Model 49	QNA	920	0.644	0.560	16.279	0.614	142	0.401
Model 50	QNA	920	0.531	0.461	15.711	0.692	103	0.408
Model 51	QNA	920	0.640	0.559	16.314	0.617	140	0.405
Model 52	QNA	920	0.587	0.518	18.321	0.651	111	0.417
Model 53	QNA	920	0.641	0.562	17.543	0.614	126	0.422
Model 54	QNA	920	0.637	0.553	16.406	0.619	140	0.414
Model 55	QNA	920	0.641	0.556	16.225	0.616	137	0.392
Model 56	QNA	920	0.640	0.566	18.526	0.613	126	0.406
Model 57	QNA	920	0.644	0.561	15.893	0.615	155	0.377
Model 58	QNA	920	0.633	0.541	16.736	0.621	133	0.383
Model 59	QNA	920	0.642	0.556	17.225	0.614	132	0.413
Model 60	QNA	920	0.595	0.523	18.224	0.646	105	0.444
Model 61	QNA	920	0.602	0.530	18.570	0.641	108	0.428
Model 62	QNA	920	0.641	0.558	16.852	0.615	133	0.423
Model 63	QNA	920	0.597	0.528	19.569	0.643	101	0.389
Model 64	QNA	920	0.593	0.527	19.135	0.646	95	0.399
Model 65	QNA	920	0.643	0.558	16.247	0.615	135	0.395
Model 66	QNA	920	0.632	0.551	16.709	0.622	132	0.380
Model 67	QNA	920	0.638	0.555	16.616	0.618	138	0.411
Model 68	QNA	920	0.634	0.546	15.591	0.623	141	0.388
Model 69	QNA	920	0.571	0.503	17.604	0.663	99	0.433
Model 70	QNA	920	0.656	0.570	17.130	0.604	146	0.395
Model 71	QNA	920	0.589	0.515	16.792	0.652	114	0.431
Model 72	QNA	920	0.545	0.478	17.677	0.681	85	0.431
Model 73	QNA	920	0.617	0.538	17.105	0.632	121	0.445
Model 74	QNA	920	0.640	0.565	18.169	0.614	120	0.408
Model 75	QNA	920	0.636	0.557	17.585	0.617	121	0.438
Model 76	QNA	920	0.640	0.559	16.672	0.616	134	0.409
Model 77	QNA	920	0.624	0.545	17.085	0.627	126	0.386
Model 78	QNA	920	0.628	0.544	17.812	0.623	120	0.420
Model 79	QNA	920	0.662	0.578	16.933	0.600	143	0.415
Model 80	QNA	920	0.654	0.573	18.016	0.604	133	0.385
Mean			0.641	0.562	17.507	0.613	133	0.428

Number – number of compounds in the training set;

Q² – average Q² of the models calculated for the training set;

Fisher – Fisher coefficient;

SD – Standard deviation;

V – number of independent variables in the model;

L20%Out – results of 20% out cross-validation procedure calculated for the appropriate training set.

4. Types of biological activities predicted by PASS (2010.1 version)

No	Activity Type	N	IAP, %
1	(-)-limonene 6-monooxygenase inhibitor	6	77.6
2	(-)-limonene 7-monooxygenase inhibitor	6	77.6
3	(N-acetylneuraminy)-galactosylglucosylceramide N-acetylgalactosaminyltransferase inhibitor	6	94.9
4	(R)-3-amino-2-methylpropionate-pyruvate transaminase inhibitor	24	99.6
5	(R)-6-hydroxynicotine oxidase inhibitor	3	92.3
6	(R)-Pantolactone dehydrogenase (flavin) inhibitor	8	86.8
7	(R)-aminopropanol dehydrogenase inhibitor	10	98.9
8	(R)-limonene 6-monooxygenase inhibitor	3	99.6
9	(R,R)-butanediol dehydrogenase inhibitor	3	99.3
10	(S)-2-Methylmalate dehydratase inhibitor	4	99.5
11	(S)-2-hydroxy-acid oxidase inhibitor	28	92.3
12	(S)-3-amino-2-methylpropionate transaminase inhibitor	8	94.8
13	(S)-3-hydroxyacid ester dehydrogenase inhibitor	3	98.9
14	(S)-6-hydroxynicotine oxidase inhibitor	4	94.7
15	(S)-carnitine 3-dehydrogenase inhibitor	10	99.4
16	(S)-methylmalonyl-CoA hydrolase inhibitor	8	100.0
17	1,2- α -L-fucosidase inhibitor	5	94.0
18	1,3-Beta-glucan synthase inhibitor	4	100.0
19	1,4-Alpha-glucan branching enzyme inhibitor	4	95.1
20	1,4-Lactonase inhibitor	5	92.8
21	1,5-Anhydro-D-fructose reductase inhibitor	9	99.0
22	1-Acylglycerol-3-phosphate O-acyltransferase inhibitor	7	91.4
23	1-Alkyl-2-acetyl glycerol O-acyltransferase inhibitor	3	99.7
24	1-Alkyl-2-acetyl glycerophosphocholine esterase inhibitor	426	99.4
25	1-Alkyl glycerophosphocholine O-acyltransferase inhibitor	24	91.7
26	1-Aminocyclopropane-1-carboxylate deaminase inhibitor	11	98.3
27	1-Deoxy-D-xylulose-5-phosphate reductoisomerase inhibitor	3	96.1
28	1-Phosphatidylinositol-4-phosphate 5-kinase inhibitor	14	84.1
29	1-Phosphofructokinase inhibitor	9	98.8
30	1-Pyrroline-5-carboxylate dehydrogenase inhibitor	24	98.6
31	11-Beta-hydroxysteroid dehydrogenase 1 inhibitor	979	99.3
32	11-Beta-hydroxysteroid dehydrogenase 2 inhibitor	18	99.9
33	11-Beta-hydroxysteroid dehydrogenase inhibitor	991	99.3
34	11-Cis-retinyl-palmitate hydrolase inhibitor	4	99.5
35	12 Lipxygenase inhibitor	46	99.2
36	15 Lipxygenase inhibitor	153	97.0
37	15-Hydroxyprostaglandin-D dehydrogenase (NADP+) inhibitor	8	96.3
38	15-Oxoprostaglandin 13-reductase inhibitor	9	76.1
39	17-Beta-hydroxysteroid dehydrogenase 1 inhibitor	49	98.2
40	17-Beta-hydroxysteroid dehydrogenase 5 inhibitor	6	100.0
41	2,2-Dialkylglycine decarboxylase (pyruvate) inhibitor	7	98.6
42	2,3,4,5-Tetrahydropyridine-2,6-dicarboxylate N-succinyltransferase inhibitor	5	96.4
43	2,3-Dihydroxyindole 2,3-dioxygenase inhibitor	4	98.2
44	2,3-Oxidosqualene-lanosterol cyclase inhibitor	103	98.5
45	2,4-Diaminopentanoate dehydrogenase inhibitor	3	98.6
46	2,4-Dichlorophenol 6-monooxygenase inhibitor	9	96.8
47	2,5-Dihydroxypyridine 5,6-dioxygenase inhibitor	7	98.7
48	2,6-Dihydroxypyridine 3-monooxygenase inhibitor	3	98.0
49	2-(acetamidomethylene)succinate hydrolase inhibitor	11	99.9
50	2-Acylglycerol O-acyltransferase inhibitor	18	93.2
51	2-Amino-4-hydroxy-6-hydroxymethyl dihydropteridine diphosphokinase inhibitor	4	99.8
52	2-Amino adipate transaminase inhibitor	6	98.2
53	2-Aminoethylphosphonate-pyruvate transaminase inhibitor	9	98.8
54	2-Aminohexano-6-lactam racemase inhibitor	19	98.1
55	2-Aminohexanoate transaminase inhibitor	3	100.0
56	2-Chlorobenzoate 1,2-dioxygenase inhibitor	5	77.8
57	2-Dehydro-3-deoxy-L-arabinonate dehydratase inhibitor	4	99.2
58	2-Dehydro-3-deoxy-phosphogluconate aldolase inhibitor	6	98.9
59	2-Dehydropantoate 2-reductase inhibitor	7	80.3
60	2-Dehydropantoate aldolase inhibitor	3	98.8
61	2-Dehydropantolactone reductase (A-specific) inhibitor	10	98.9

62	2-Enoate reductase inhibitor	11	95.9
63	2-Ethylmalate synthase inhibitor	3	99.9
64	2-Haloacid dehalogenase (configuration-inverting) inhibitor	6	97.9
65	2-Haloacid dehalogenase inhibitor	3	96.5
66	2-Hydroxy-3-oxoadipate synthase inhibitor	3	97.7
67	2-Hydroxy-3-oxopropionate reductase inhibitor	5	98.8
68	2-Hydroxyacylsphingosine 1-beta-galactosyltransferase inhibitor	3	100.0
69	2-Hydroxymuconate-semialdehyde hydrolase inhibitor	7	92.7
70	2-Hydroxyquinoline 5,6-dioxygenase inhibitor	4	79.7
71	2-Hydroxyquinoline 8-monooxygenase inhibitor	6	83.7
72	2-Isopropylmalate synthase inhibitor	15	99.8
73	2-Methyl-branched-chain-enoyl-CoA reductase inhibitor	5	97.5
74	2-Methylacyl-CoA dehydrogenase inhibitor	7	98.1
75	2-Methylcitrate dehydratase inhibitor	4	99.5
76	2-Methylcitrate synthase inhibitor	3	97.4
77	2-Methyleneglutarate mutase inhibitor	9	98.9
78	2-Nitrophenol 2-monooxygenase inhibitor	3	98.9
79	2-Nitropropane dioxygenase inhibitor	21	96.5
80	2-Oxoaldehyde dehydrogenase (NAD ⁺) inhibitor	12	98.8
81	2-Oxoaldehyde dehydrogenase (NADP ⁺) inhibitor	3	98.1
82	2-Oxoglutarate decarboxylase inhibitor	8	97.8
83	2-Oxoisovalerate dehydrogenase (acylating) inhibitor	4	99.0
84	2-Pyrocatechuate decarboxylase inhibitor	20	99.0
85	27-Hydroxycholesterol 7alpha-monooxygenase inhibitor	6	82.3
86	3 Beta-hydroxy-delta 5-steroid dehydrogenase inhibitor	97	100.0
87	3'(2'),5'-Bisphosphate nucleotidase inhibitor	4	99.5
88	3'-Demethylstaurosporine O-methyltransferase inhibitor	4	96.4
89	3'-Nucleotidase inhibitor	8	97.3
90	3(or 17)alpha-hydroxysteroid dehydrogenase inhibitor	9	99.2
91	3(or 17)beta-hydroxysteroid dehydrogenase inhibitor	63	97.6
92	3,4-Dihydroxy-9,10-secoandrosta-1,3,5(10)-triene-9,17-dione 4,5-dioxygenase inhibitor	4	98.4
93	3,4-Dihydroxyphenylacetate 2,3-dioxygenase inhibitor	13	99.5
94	3-Alpha-hydroxysteroid dehydrogenase (B-specific) inhibitor	9	100.0
95	3-Aminobutyryl-CoA ammonia-lyase inhibitor	3	99.2
96	3-Carboxyethylcatechol 2,3-dioxygenase inhibitor	4	98.3
97	3-Chloro-D-alanine dehydrochlorinase inhibitor	4	98.4
98	3-Cyanoalanine hydratase inhibitor	4	83.5
99	3-Dehydroquininate dehydratase inhibitor	14	99.2
100	3-Dehydroquininate synthase inhibitor	16	99.3
101	3-Demethylubiquinone-9 3-O-methyltransferase inhibitor	3	98.4
102	3-Deoxy-7-phosphoheptulonate synthase inhibitor	48	99.0
103	3-Deoxy-8-phosphooctulonate synthase inhibitor	8	99.3
104	3-Galactosyl-N-acetylglucosaminide 4-alpha-L-fucosyltransferase inhibitor	3	99.1
105	3-Hydroxy-4-oxoquinoline 2,4-dioxygenase inhibitor	6	97.6
106	3-Hydroxyacyl-CoA dehydrogenase inhibitor	4	99.2
107	3-Hydroxyanthranilate 3,4-dioxygenase inhibitor	14	94.6
108	3-Hydroxyanthranilate oxidase inhibitor	13	97.6
109	3-Hydroxybenzoate 4-monooxygenase inhibitor	7	97.7
110	3-Hydroxybenzoate 6-monooxygenase inhibitor	5	83.6
111	3-Hydroxybutyrate dehydrogenase inhibitor	25	98.7
112	3-Hydroxybutyryl-CoA dehydrogenase inhibitor	3	98.6
113	3-Hydroxydecanoyl-[acyl-carrier-protein] dehydratase inhibitor	9	98.7
114	3-Hydroxyisobutyryl-CoA hydrolase inhibitor	7	100.0
115	3-Hydroxyphenylacetate 6-hydroxylase inhibitor	4	98.8
116	3-Isopropylmalate dehydratase inhibitor	8	98.3
117	3-Isopropylmalate dehydrogenase inhibitor	7	99.4
118	3-Ketoalidoxylamine C-N-lyase inhibitor	4	98.0
119	3-Mercaptopyruvate sulfurtransferase inhibitor	9	100.0
120	3-Methyl-2-oxobutanoate dehydrogenase (lipoamide) inhibitor	15	99.4
121	3-Methyl-2-oxobutanoate hydroxymethyltransferase inhibitor	8	97.8
122	3-Methylbutanal reductase inhibitor	9	85.2
123	3-Oxoacid CoA-transferase inhibitor	26	99.1
124	3-Oxoacyl-[acyl-carrier-protein] synthase II inhibitor	8	100.0
125	3-Oxoacyl-[acyl-carrier-protein] synthase III inhibitor	12	95.6

126	3-Oxoacyl-[acyl-carrier-protein] synthase inhibitor	26	97.5
127	3-Oxoadipate enol-lactonase inhibitor	3	99.0
128	3-Oxosteroid 1-dehydrogenase inhibitor	6	99.3
129	3-Phosphoshikimate 1-carboxyvinyltransferase inhibitor	41	99.7
130	3-Phytase inhibitor	9	88.2
131	3C-like protease (Human coronavirus) inhibitor	19	92.0
132	4,5-Dihydroxyphthalate decarboxylase inhibitor	16	92.9
133	4-Alpha-glucanotransferase inhibitor	8	98.9
134	4-Carboxymethyl-4-methylbutenolide mutase inhibitor	9	99.3
135	4-Chlorobenzoyl-CoA dehalogenase inhibitor	7	97.0
136	4-Chlorophenylacetate 3,4-dioxygenase inhibitor	4	98.4
137	4-Coumarate-CoA ligase inhibitor	8	84.8
138	4-Hydroxy-2-oxoglutarate aldolase inhibitor	17	99.3
139	4-Hydroxy-4-methyl-2-oxoglutarate aldolase inhibitor	11	99.4
140	4-Hydroxybenzoate 1-hydroxylase inhibitor	3	99.9
141	4-Hydroxybenzoate 3-monooxygenase [NAD(P)H] inhibitor	6	100.0
142	4-Hydroxybenzoate 3-monooxygenase inhibitor	28	98.4
143	4-Hydroxybenzoate decarboxylase inhibitor	7	99.7
144	4-Hydroxybenzoate nonaprenyltransferase inhibitor	15	95.9
145	4-Hydroxybenzoate-CoA ligase inhibitor	4	99.7
146	4-Hydroxyglutamate transaminase inhibitor	4	98.1
147	4-Hydroxymandelate oxidase inhibitor	10	91.9
148	4-Hydroxyphenylacetate 1-monooxygenase inhibitor	4	100.0
149	4-Hydroxyphenylacetate 3-monooxygenase inhibitor	8	87.5
150	4-Hydroxyphenylpyruvate dioxygenase inhibitor	18	99.9
151	4-Hydroxyproline epimerase inhibitor	8	87.1
152	4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor	19	88.9
153	4-Nitrophenol 2-monooxygenase inhibitor	6	81.7
154	4-Nitrophenylphosphatase inhibitor	49	88.9
155	4-Phytase inhibitor	13	98.2
156	4-Pyridoxolactonase inhibitor	6	99.3
157	4a-Hydroxytetrahydrobiopterin dehydratase inhibitor	3	99.7
158	5 Hydroxytryptamine 1 agonist	1904	98.6
159	5 Hydroxytryptamine 1 antagonist	4266	98.5
160	5 Hydroxytryptamine 1A agonist	1132	98.8
161	5 Hydroxytryptamine 1A antagonist	3422	98.8
162	5 Hydroxytryptamine 1B agonist	65	98.9
163	5 Hydroxytryptamine 1B antagonist	847	99.0
164	5 Hydroxytryptamine 1D agonist	695	99.5
165	5 Hydroxytryptamine 1D antagonist	909	98.9
166	5 Hydroxytryptamine 1E antagonist	8	98.0
167	5 Hydroxytryptamine 1F agonist	117	99.9
168	5 Hydroxytryptamine 1F antagonist	75	99.8
169	5 Hydroxytryptamine 2 agonist	478	99.1
170	5 Hydroxytryptamine 2 antagonist	3572	97.7
171	5 Hydroxytryptamine 2A agonist	61	95.1
172	5 Hydroxytryptamine 2A antagonist	2222	98.3
173	5 Hydroxytryptamine 2B agonist	9	94.5
174	5 Hydroxytryptamine 2B antagonist	267	98.5
175	5 Hydroxytryptamine 2C agonist	415	99.5
176	5 Hydroxytryptamine 2C antagonist	1077	98.9
177	5 Hydroxytryptamine 3 agonist	74	97.2
178	5 Hydroxytryptamine 3 antagonist	1570	99.1
179	5 Hydroxytryptamine 3A antagonist	5	89.0
180	5 Hydroxytryptamine 4 agonist	345	99.4
181	5 Hydroxytryptamine 4 antagonist	533	99.5
182	5 Hydroxytryptamine 4A antagonist	303	99.8
183	5 Hydroxytryptamine 4B antagonist	4	97.5
184	5 Hydroxytryptamine 4C antagonist	4	97.5
185	5 Hydroxytryptamine 4D antagonist	4	97.5
186	5 Hydroxytryptamine 4E antagonist	27	99.5
187	5 Hydroxytryptamine 5 antagonist	103	99.3
188	5 Hydroxytryptamine 5A antagonist	103	99.3
189	5 Hydroxytryptamine 6 agonist	29	99.3

190	5 Hydroxytryptamine 6 antagonist	501	99.3
191	5 Hydroxytryptamine 7 agonist	8	93.9
192	5 Hydroxytryptamine 7 antagonist	456	98.6
193	5 Hydroxytryptamine agonist	2878	97.9
194	5 Hydroxytryptamine antagonist	9655	96.6
195	5 Hydroxytryptamine release inhibitor	33	87.4
196	5 Hydroxytryptamine release stimulant	17	90.9
197	5 Hydroxytryptamine uptake inhibitor	3417	98.4
198	5 Hydroxytryptamine uptake stimulant	5	80.6
199	5 Lipoxygenase activating protein inhibitor	99	99.8
200	5 Lipoxygenase inhibitor	1339	98.3
201	5'-Nucleotidase inhibitor	40	99.4
202	5-Alpha-reductase 1 inhibitor	338	99.6
203	5-Alpha-reductase 2 inhibitor	267	99.1
204	5-Alpha-reductase inhibitor	1324	99.4
205	5-Aminolevulinate synthase inhibitor	25	97.4
206	5-Aminovalerate transaminase inhibitor	7	99.5
207	5-Formyltetrahydrofolate cyclo-ligase inhibitor	11	92.8
208	5-Guanidino-2-oxopentanoate decarboxylase inhibitor	8	100.0
209	5-Hydroxypentanoate CoA-transferase inhibitor	4	100.0
210	5-Methyltetrahydropteroyltriglutamate-homocysteine S-methyltransferase inhibitor	4	99.5
211	5-O-(4-coumaroyl)-D-quinic 3'-monooxygenase inhibitor	3	86.9
212	5-Oxoprolinase (ATP-hydrolysing) inhibitor	8	99.4
213	6,7-Dihydropteridine reductase inhibitor	47	97.3
214	6-Carboxyhexanoate-CoA ligase inhibitor	3	98.6
215	6-Methylsalicylate decarboxylase inhibitor	8	98.6
216	6-Phospho-beta-glucosidase inhibitor	8	99.7
217	6-Phosphofructo-2-kinase inhibitor	11	99.1
218	6-Pyruvoyltetrahydropterin synthase inhibitor	4	98.3
219	8-Amino-7-oxononanoate synthase inhibitor	15	97.1
220	8-oxodGTPase stimulant	12	100.0
221	ABCA1 expression enhancer	200	99.3
222	ABCA1 expression inhibitor	5	93.5
223	ACK1 kinase inhibitor	25	100.0
224	ADAM inhibitor	16	100.0
225	ADAM10 endopeptidase inhibitor	24	98.4
226	ADP ribose polymerase 1 inhibitor	441	99.3
227	ADP ribose polymerase 2 inhibitor	10	95.0
228	ADP ribose polymerase inhibitor	757	98.8
229	ADP-ribose diphosphatase inhibitor	9	98.7
230	ADP-ribosylarginine hydrolase inhibitor	6	91.7
231	ADP-thymidine kinase inhibitor	5	94.0
232	AICAR transformylase inhibitor	30	95.1
233	ALK inhibitor	106	98.8
234	AMP deaminase 2 inhibitor	67	100.0
235	AMP deaminase 3 inhibitor	20	100.0
236	AMP deaminase inhibitor	100	98.5
237	AMP nucleosidase inhibitor	16	99.1
238	AMPA 1 receptor antagonist	284	99.1
239	AMPA 2 receptor antagonist	12	94.9
240	AMPA 3 receptor antagonist	6	92.7
241	AMPA 4 receptor antagonist	6	100.0
242	AMPA 5 receptor antagonist	4	100.0
243	AMPA receptor agonist	73	99.4
244	AMPA receptor antagonist	960	98.9
245	APOA1 expression enhancer	9	95.3
246	AR expression inhibitor	3	100.0
247	ATM kinase inhibitor	25	93.8
248	ATP adenylyltransferase inhibitor	7	98.1
249	ATP citrate lyase inhibitor	47	99.6
250	ATP citrate synthase inhibitor	20	99.5
251	ATP deaminase inhibitor	5	99.6
252	ATP diphosphatase inhibitor	4	99.4
253	ATP phosphoribosyltransferase inhibitor	13	97.2

254	ATP-binding cassette A1 stimulant	7	89.9
255	ATP-dependent RNA helicase inhibitor	10	100.0
256	ATPase (Mitochondrial F1F0) inhibitor	8	99.8
257	ATPase (Vacuolar H+) inhibitor	78	99.0
258	ATPase inhibitor	137	92.5
259	ATPase stimulant	18	87.2
260	AXL receptor tyrosine kinase inhibitor	37	97.3
261	Abl kinase inhibitor	216	96.3
262	Abortion inducer	36	89.8
263	Acaricide	38	94.0
264	Acetate kinase inhibitor	11	90.5
265	Acetate-CoA ligase inhibitor	23	98.3
266	Acetoacetate decarboxylase inhibitor	8	99.0
267	Acetoacetyl-CoA reductase inhibitor	10	99.7
268	Acetoin dehydrogenase inhibitor	15	98.2
269	Acetolactate decarboxylase inhibitor	15	97.9
270	Acetolactate synthase inhibitor	19	99.4
271	Acetyl-CoA C-acyltransferase inhibitor	10	95.9
272	Acetyl-CoA carboxylase 1 inhibitor	16	100.0
273	Acetyl-CoA carboxylase 2 inhibitor	16	100.0
274	Acetyl-CoA carboxylase inhibitor	21	88.3
275	Acetyl-CoA transferase 1 inhibitor	19	93.7
276	Acetyl-CoA transferase 2 inhibitor	6	84.6
277	Acetyl-CoA transferase inhibitor	1284	99.0
278	Acetylcholine M1 receptor agonist	1013	99.2
279	Acetylcholine M1 receptor antagonist	919	99.1
280	Acetylcholine M2 receptor agonist	41	97.6
281	Acetylcholine M2 receptor antagonist	880	99.2
282	Acetylcholine M3 receptor agonist	16	99.6
283	Acetylcholine M3 receptor antagonist	927	99.2
284	Acetylcholine M4 receptor agonist	59	99.3
285	Acetylcholine M4 receptor antagonist	269	99.7
286	Acetylcholine M5 receptor antagonist	156	99.4
287	Acetylcholine agonist	2059	97.3
288	Acetylcholine antagonist	3577	97.3
289	Acetylcholine muscarinic agonist	1220	98.8
290	Acetylcholine muscarinic antagonist	2718	98.0
291	Acetylcholine neuromuscular blocking agent	67	95.2
292	Acetylcholine nicotinic agonist	804	97.6
293	Acetylcholine nicotinic antagonist	899	97.6
294	Acetylcholine release stimulant	147	96.3
295	Acetylcholinesterase inhibitor	1324	97.0
296	Acetylcholinesterase stimulant	8	100.0
297	Acetylenecarboxylate hydratase inhibitor	3	98.6
298	Acylesterase inhibitor	7	77.5
299	Acetylgalactosaminyl-O-glycosyl-glycoprotein beta-1,3-N-acetylglucosaminyltransferase inhibitor	6	81.7
300	Acetylglutamate kinase inhibitor	4	79.5
301	Acetylmethionine deacetylase inhibitor	4	98.0
302	Acetylserotonin O-methyltransferase inhibitor	11	90.2
303	Acetylspermidine deacetylase inhibitor	16	94.7
304	Acid phosphatase 1 inhibitor	5	100.0
305	Acid phosphatase inhibitor	43	95.0
306	Acid-sensing ion channel blocker	6	88.4
307	Acidifying agent gastric	6	99.7
308	Acidifying agent non gastric	8	97.6
309	Aconitate decarboxylase inhibitor	4	99.5
310	Aconitate hydratase inhibitor	22	99.1
311	Acrocylindropepsin inhibitor	3	85.6
312	Acrosin inhibitor	20	95.8
313	Actin depolymerization inhibitor	3	99.6
314	Actin depolymerization stimulant	7	100.0
315	Actin polymerization inhibitor	4	100.0
316	Activin receptor-like kinase 4 inhibitor	23	100.0
317	Acute neurologic disorders treatment	1258	81.9

318	Acyl-CoA dehydrogenase (NADP+) inhibitor	19	98.7
319	Acyl-CoA dehydrogenase inhibitor	15	99.1
320	Acyl-CoA hydrolase inhibitor	44	97.3
321	Acyl-CoA oxidase inhibitor	11	90.8
322	Acyl-lysine deacylase inhibitor	3	99.2
323	Acylaminoacyl-peptidase inhibitor	25	95.5
324	Acylcarnitine hydrolase inhibitor	3	90.1
325	Acylglycerol lipase inhibitor	15	84.5
326	Acylglycerone-phosphate reductase inhibitor	6	98.1
327	Acyloxyacyl hydrolase inhibitor	15	98.2
328	Acylphosphatase inhibitor	13	97.4
329	Adamalysin inhibitor	8	99.6
330	Adenine deaminase inhibitor	10	98.5
331	Adenine nucleotide translocase inhibitor	23	96.1
332	Adenine nucleotide translocator 1 inhibitor	3	100.0
333	Adenine phosphoribosyltransferase inhibitor	23	99.3
334	Adenomatous polyposis treatment	10	93.5
335	Adenosine A1 receptor agonist	278	99.9
336	Adenosine A1 receptor agonist enhancer	12	100.0
337	Adenosine A1 receptor antagonist	2397	98.9
338	Adenosine A2 receptor agonist	239	99.9
339	Adenosine A2 receptor antagonist	2499	99.1
340	Adenosine A2a receptor agonist	216	99.9
341	Adenosine A2a receptor antagonist	1893	99.1
342	Adenosine A2b receptor agonist	17	99.9
343	Adenosine A2b receptor antagonist	578	99.5
344	Adenosine A3 receptor agonist	90	99.8
345	Adenosine A3 receptor antagonist	1248	99.1
346	Adenosine deaminase inhibitor	163	98.5
347	Adenosine kinase inhibitor	227	99.5
348	Adenosine receptor agonist	623	99.4
349	Adenosine receptor antagonist	3764	98.7
350	Adenosine uptake inhibitor	56	99.2
351	Adenosylhomocysteine nucleosidase inhibitor	55	100.0
352	Adenosylmethionine cyclotransferase inhibitor	12	100.0
353	Adenosylmethionine-8-amino-7-oxononanoate transaminase inhibitor	13	98.4
354	Adenylate cyclase I inhibitor	47	100.0
355	Adenylate cyclase I stimulant	43	100.0
356	Adenylate cyclase V inhibitor	8	97.2
357	Adenylate cyclase inhibitor	132	94.2
358	Adenylate cyclase stimulant	76	90.5
359	Adenylate kinase inhibitor	23	93.0
360	Adenylosuccinate lyase inhibitor	29	99.5
361	Adenylosuccinate synthase inhibitor	61	98.5
362	Adenylyl-sulfate kinase inhibitor	20	96.6
363	Adenylyl-sulfate reductase inhibitor	5	88.8
364	Adenylylsulphatase inhibitor	17	97.6
365	Adrenaline agonist	1990	97.7
366	Adrenaline antagonist	5532	97.4
367	Adrenaline release stimulant	8	92.8
368	Adrenaline uptake inhibitor	1632	98.5
369	Adrenergic	3693	97.4
370	Adrenergic, ophthalmic	10	98.8
371	Aerobactin synthase inhibitor	3	98.9
372	Agaritine gamma-glutamyltransferase inhibitor	11	98.8
373	Age-related macular degeneration treatment	116	90.3
374	Aggrecanase 1 inhibitor	3	100.0
375	Aggrecanase 2 inhibitor	19	99.0
376	Aggrecanase inhibitor	236	99.5
377	Agmatinase inhibitor	7	92.0
378	AgrC-1 protein inhibitor	4	100.0
379	AgrC-2 protein inhibitor	4	100.0
380	Alanine carboxypeptidase inhibitor	10	99.3
381	Alanine dehydrogenase inhibitor	27	98.6

382	Alanine racemase inhibitor	13	97.3
383	Alanine transaminase inhibitor	18	98.3
384	Alanine-tRNA ligase inhibitor	6	96.4
385	Albendazole monooxygenase inhibitor	3	96.4
386	Alcohol O-acetyltransferase inhibitor	9	89.5
387	Alcohol dehydrogenase (NADP+) inhibitor	45	95.4
388	Alcohol dehydrogenase (acceptor) inhibitor	11	86.6
389	Alcohol dehydrogenase I inhibitor	14	100.0
390	Alcohol dehydrogenase [NAD(P)+] inhibitor	16	92.4
391	Alcohol dehydrogenase alpha inhibitor	12	100.0
392	Alcohol dehydrogenase beta 1 inhibitor	7	100.0
393	Alcohol dehydrogenase beta inhibitor	7	100.0
394	Alcohol dehydrogenase gamma 2 inhibitor	6	100.0
395	Alcohol dehydrogenase gamma inhibitor	6	100.0
396	Alcohol dehydrogenase inhibitor	92	94.7
397	Alcohol dehydrogenase substrate	44	94.8
398	Alcohol oxidase inhibitor	17	98.6
399	Aldehyde dehydrogenase (NAD+) inhibitor	38	95.6
400	Aldehyde dehydrogenase (NADP+) inhibitor	17	96.0
401	Aldehyde dehydrogenase (pyrroloquinoline-quinone) inhibitor	7	87.5
402	Aldehyde dehydrogenase 1 substrate	5	90.5
403	Aldehyde dehydrogenase 1A2 inhibitor	30	99.4
404	Aldehyde dehydrogenase 2 substrate	5	81.9
405	Aldehyde dehydrogenase 3 substrate	3	99.9
406	Aldehyde dehydrogenase [NAD(P)+] inhibitor	6	82.5
407	Aldehyde dehydrogenase inhibitor	99	95.5
408	Aldehyde dehydrogenase substrate	31	94.2
409	Aldehyde ferredoxin oxidoreductase inhibitor	5	98.6
410	Aldehyde oxidase inhibitor	19	85.0
411	Aldehyde oxidase substrate	28	90.1
412	Aldose 1-epimerase inhibitor	31	99.2
413	Aldose reductase 2 inhibitor	88	99.5
414	Aldose reductase inhibitor	682	98.3
415	Aldosterone antagonist	36	91.2
416	Alkaline phosphatase inhibitor	27	96.5
417	Alkanal monooxygenase (FMN-linked) inhibitor	27	95.5
418	Alkane 1-monooxygenase inhibitor	4	94.5
419	Alkene monooxygenase inhibitor	3	99.0
420	Alkenylglycerophosphocholine hydrolase inhibitor	5	89.7
421	Alkenylglycerophosphoethanolamine hydrolase inhibitor	6	92.0
422	Alkylacetyl glycerophosphatase inhibitor	4	86.8
423	Alkylator	564	94.0
424	Alkylglycerone-phosphate synthase inhibitor	6	97.6
425	Alkylglycerophosphoethanolamine phosphodiesterase inhibitor	5	96.7
426	Alkylphospholipid	8	100.0
427	All-trans-retinyl-palmitate hydrolase inhibitor	4	93.5
428	Allantoate deiminase inhibitor	3	99.0
429	Allantoicase inhibitor	9	98.6
430	Allantoin racemase inhibitor	4	98.8
431	Allantoinase inhibitor	4	99.0
432	Allergic conjunctivitis treatment	21	79.2
433	Allergic rhinitis treatment	494	96.6
434	Allophanate hydrolase inhibitor	5	98.3
435	Allyl-alcohol dehydrogenase inhibitor	6	97.8
436	Alopecia treatment	7	85.6
437	Alpha 1 adrenoreceptor agonist	76	99.1
438	Alpha 1 adrenoreceptor antagonist	3468	98.1
439	Alpha 1L adrenoreceptor agonist	3	99.2
440	Alpha 1L adrenoreceptor antagonist	11	97.2
441	Alpha 1a adrenoreceptor agonist	48	99.9
442	Alpha 1a adrenoreceptor antagonist	2721	98.5
443	Alpha 1b adrenoreceptor antagonist	614	99.2
444	Alpha 1d adrenoreceptor antagonist	775	99.3
445	Alpha 2 adrenoreceptor agonist	274	98.4

446	Alpha 2 adrenoreceptor antagonist	1294	98.3
447	Alpha 2a adrenoreceptor antagonist	209	98.9
448	Alpha 2b adrenoreceptor agonist	45	99.9
449	Alpha 2b adrenoreceptor antagonist	133	98.1
450	Alpha 2c adrenoreceptor agonist	45	100.0
451	Alpha 2c adrenoreceptor antagonist	155	99.5
452	Alpha 2d adrenoreceptor agonist	44	99.8
453	Alpha 2d adrenoreceptor antagonist	90	98.8
454	Alpha 3 adrenoreceptor agonist	5	99.3
455	Alpha adrenoreceptor agonist	431	97.3
456	Alpha adrenoreceptor antagonist	4619	97.3
457	Alpha galactosidase inhibitor	5	99.9
458	Alpha glucosidase I inhibitor	5	100.0
459	Alpha glucosidase II inhibitor	4	100.0
460	Alpha glucosidase inhibitor	83	97.0
461	Alpha,alpha-phosphotrehalase inhibitor	5	99.1
462	Alpha,alpha-trehalase inhibitor	20	98.2
463	Alpha,alpha-trehalose phosphorylase (configuration-retaining) inhibitor	11	99.3
464	Alpha,alpha-trehalose phosphorylase inhibitor	4	99.8
465	Alpha,alpha-trehalose-phosphate synthase (UDP-forming) inhibitor	14	96.4
466	Alpha-1,3-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor	11	99.8
467	Alpha-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase inhibitor	3	99.5
468	Alpha-1,6-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor	4	95.1
469	Alpha-1,6-mannosyl-glycoprotein 6-beta-N-acetylglucosaminyltransferase inhibitor	5	98.8
470	Alpha-L-fucosidase inhibitor	30	98.1
471	Alpha-L-rhamnosidase inhibitor	11	99.1
472	Alpha-Methylacyl-CoA racemase inhibitor	8	97.3
473	Alpha-N-acetylgalactosaminidase inhibitor	3	99.3
474	Alpha-N-acetylgalactosaminide alpha-2,6-sialyltransferase inhibitor	17	99.4
475	Alpha-N-acetylglucosaminidase inhibitor	4	97.4
476	Alpha-N-acetylneuraminate alpha-2,8-sialyltransferase inhibitor	16	98.9
477	Alpha-N-arabinofuranosidase inhibitor	9	97.8
478	Alpha-amino-acid esterase inhibitor	4	99.9
479	Alpha-amylase inhibitor	29	94.5
480	Alpha-glucuronidase inhibitor	4	97.4
481	Alpha-mannosidase inhibitor	47	97.9
482	Alpha-pinene-oxide decyclase inhibitor	8	98.5
483	Alternansucrase inhibitor	4	99.7
484	Altronate dehydratase inhibitor	7	99.8
485	Alzheimer's disease treatment	2544	89.1
486	Amidase inhibitor	127	97.3
487	Amidophosphoribosyltransferase inhibitor	27	98.7
488	Amiloride-sensitive cation channel 3 antagonist	3	100.0
489	Amine dehydrogenase inhibitor	10	87.2
490	Amino acid-polyamine-organocation (APC) transporter antagonist	82	100.0
491	Amino-acid N-acetyltransferase inhibitor	25	99.1
492	Amino-acid racemase inhibitor	6	99.5
493	Aminoacyl-tRNA hydrolase inhibitor	5	99.4
494	Aminoacyl-tRNA synthetase inhibitor	248	97.6
495	Aminoacylase inhibitor	19	97.8
496	Aminobutyraldehyde dehydrogenase inhibitor	3	86.1
497	Aminocarboxymuconate-semialdehyde decarboxylase inhibitor	6	98.4
498	Aminoglycoside N6'-acetyltransferase inhibitor	15	100.0
499	Aminolevulinate transaminase inhibitor	26	98.8
500	Aminomuconate-semialdehyde dehydrogenase inhibitor	4	97.6
501	Aminopeptidase A inhibitor	40	99.9
502	Aminopeptidase B inhibitor	35	92.2
503	Aminopeptidase I inhibitor	26	98.1
504	Aminopeptidase N inhibitor	131	97.9
505	Aminopeptidase P inhibitor	8	100.0
506	Aminopeptidase Y inhibitor	8	97.1
507	Aminopeptidase microsomal inhibitor	162	97.6
508	Amylin agonist	15	100.0
509	Amylo-alpha-1,6-glucosidase inhibitor	27	99.1

510	Amyloid beta aggregation inhibitor	39	97.2
511	Amyloid beta precursor protein antagonist	20	95.5
512	Amylosucrase inhibitor	5	99.9
513	Amyotrophic lateral sclerosis treatment	171	89.9
514	Anabolic	122	95.5
515	Analeptic	132	92.8
516	Analgesic	8265	87.3
517	Analgesic stimulant	20	87.9
518	Analgesic, non-opioid	6278	88.8
519	Analgesic, opioid	843	96.1
520	Anaphylatoxin receptor antagonist	11	76.6
521	Androgen agonist	179	98.6
522	Androgen antagonist	717	97.3
523	Andropause treatment	85	97.3
524	Androst-4-ene-3,17-dione monooxygenase inhibitor	9	99.2
525	Anesthetic	571	94.5
526	Anesthetic general	57	92.1
527	Anesthetic inhalation	27	98.9
528	Anesthetic local	443	95.7
529	Angiogenesis inhibitor	4685	91.2
530	Angiogenesis stimulant	20	81.0
531	Angiotensin AT1 receptor antagonist	2185	99.5
532	Angiotensin AT1A receptor antagonist	4	100.0
533	Angiotensin AT2 receptor agonist	7	98.8
534	Angiotensin AT2 receptor antagonist	419	99.8
535	Angiotensin II receptor agonist	10	93.6
536	Angiotensin II receptor antagonist	2384	99.5
537	Angiotensin agonist	13	99.2
538	Angiotensin antagonist	2411	99.4
539	Angiotensin converting enzyme inhibitor	463	98.1
540	Anhydrotetracycline monooxygenase inhibitor	4	99.5
541	Ankylosing spondylitis treatment	12	78.4
542	Antacid	22	75.8
543	Anthranilate 3-monooxygenase (deaminating) inhibitor	11	95.6
544	Anthranilate phosphoribosyltransferase inhibitor	5	99.6
545	Anthranilate synthase inhibitor	23	98.3
546	Anthranilate-CoA ligase inhibitor	4	97.6
547	Anthrax lethal factor inhibitor	9	92.9
548	Anti-Helicobacter pylori	154	89.7
549	Antiacne	1247	97.0
550	Antiacromegalic	71	97.6
551	Antiadrenergic	5607	97.2
552	Antialcoholic	121	91.7
553	Antiallergic	7156	88.9
554	Antiamyloidogenic	201	90.1
555	Antianemic	173	93.3
556	Antianginal	984	83.8
557	Antianorexic	60	93.7
558	Antiarrhythmic	2275	93.4
559	Antiarthritic	11502	87.4
560	Antiasthmatic	8943	88.9
561	Antibacterial	7632	92.0
562	Antibacterial activity enhancer	25	80.5
563	Antibacterial, ophthalmic	13	75.3
564	Antibiotic	4353	96.7
565	Antibiotic Aminoglycoside-like	63	97.8
566	Antibiotic Anthracycline-like	73	99.5
567	Antibiotic Carbacephem-like	27	100.0
568	Antibiotic Carbapenem-like	270	100.0
569	Antibiotic Cephalosporin-like	535	99.8
570	Antibiotic Glycopeptide-like	106	99.0
571	Antibiotic Isocephem-like	9	100.0
572	Antibiotic Macrolide-like	730	99.8
573	Antibiotic Naphthyridine-like	49	98.0

574	Antibiotic Oxacephem-like	12	99.9
575	Antibiotic Oxazolidinone-like	156	100.0
576	Antibiotic Penem-like	50	99.9
577	Antibiotic Penicillin-like	77	100.0
578	Antibiotic Quinolone-like	428	99.4
579	Antibiotic Rifamycin-like	64	100.0
580	Antibiotic Tetracycline-like	35	99.1
581	Antibiotic Tribactam-like	20	100.0
582	Antibiotic Trimethoprim-like	11	100.0
583	Antibiotic beta Lactam-like	1137	99.6
584	Anticarcinogenic	17	93.6
585	Anticataract	57	95.5
586	Anticholelithogenic	41	97.7
587	Anticoagulant	3007	92.6
588	Anticonvulsant	1237	87.8
589	Antidepressant	7962	92.1
590	Antidepressant, Imipramin-like	87	95.5
591	Antidiabetic	11592	90.5
592	Antidiabetic (type 1)	97	93.1
593	Antidiabetic (type 2)	3144	94.6
594	Antidiabetic symptomatic	760	88.4
595	Antidiarrheal	259	89.1
596	Antidiuretic hormone agonist	152	99.7
597	Antidiuretic hormone antagonist	1099	99.6
598	Antidote	118	92.4
599	Antidote, cholinesterase reactivator	3	100.0
600	Antidote, cyanide	7	99.1
601	Antidote, heavy metal	18	98.2
602	Antidote, organophosphates	8	100.0
603	Antidyskinetic	22	79.0
604	Antieczematic	9	71.8
605	Antieczematic atopic	349	89.7
606	Antiemetic	1036	95.4
607	Antiemphysemic	230	94.7
608	Antiepileptic	2431	92.4
609	Antifibrinolytic	13	99.8
610	Antifungal	2256	91.3
611	Antifungal enhancer	19	93.2
612	Antifungal, Pneumocystis	12	89.5
613	Antiglaucomic	1374	94.5
614	Anthelmintic	493	92.8
615	Anthelmintic (Fasciola)	10	98.7
616	Anthelmintic (Nematodes)	55	87.3
617	Antihematotoxic	31	89.6
618	Antihemophilic	6	88.7
619	Antihemorrhagic	25	97.7
620	Antihistaminic	2735	95.1
621	Antihyperaldosteronism	80	100.0
622	Antihyperammonemic	3	99.7
623	Antihypercholesterolemic	256	90.5
624	Antihyperlipoproteinemic	113	93.4
625	Antihypermotility	75	97.1
626	Antihypertensive	9349	90.2
627	Antihypertriglyceridemic	143	97.2
628	Antihypoxic	39	85.1
629	Antiinfective	209	87.3
630	Antiinfertility, female	88	93.7
631	Antiinflammatory	6126	84.3
632	Antiinflammatory Leumedin-like	3	99.3
633	Antiinflammatory steroid	12	99.9
634	Antiinflammatory, intestinal	20	85.1
635	Antiinflammatory, ophthalmic	48	88.0
636	Antiinflammatory, pancreatic	5	80.4
637	Antiischemic	2241	89.5

638	Antiischemic, cerebral	468	78.7
639	Antileprosy	55	95.3
640	Antileukemic	334	87.6
641	Antimetabolite	737	98.7
642	Antimetastatic	18	83.4
643	Antimigraine	1995	94.5
644	Antimitotic	3125	95.6
645	Antimitotic Podophyllotoxin-like	42	100.0
646	Antimitotic Taxane-like	142	99.6
647	Antimutagenic	15	94.2
648	Antimycobacterial	700	89.1
649	Antimycoplasmal	39	95.1
650	Antimyopathies	8	79.1
651	Antinaupathic	17	94.4
652	Antineoplastic	38462	86.9
653	Antineoplastic (basal cell carcinoma)	15	73.7
654	Antineoplastic (bladder cancer)	63	77.6
655	Antineoplastic (bone cancer)	39	90.6
656	Antineoplastic (brain cancer)	113	75.5
657	Antineoplastic (breast cancer)	799	89.7
658	Antineoplastic (cervical cancer)	46	76.8
659	Antineoplastic (colorectal cancer)	276	85.6
660	Antineoplastic (endocrine cancer)	46	76.9
661	Antineoplastic (gastric cancer)	50	75.4
662	Antineoplastic (genitourinary cancer)	12	77.9
663	Antineoplastic (head/neck cancer)	72	70.9
664	Antineoplastic (hematological cancer)	76	73.2
665	Antineoplastic (liver cancer)	84	73.3
666	Antineoplastic (lung cancer)	73	75.8
667	Antineoplastic (lymphocytic leukemia)	72	77.5
668	Antineoplastic (lymphoma)	113	74.0
669	Antineoplastic (melanoma)	214	83.9
670	Antineoplastic (multiple myeloma)	166	84.7
671	Antineoplastic (myeloid leukemia)	119	74.6
672	Antineoplastic (non-Hodgkin's lymphoma)	79	83.0
673	Antineoplastic (non-small cell lung cancer)	160	74.0
674	Antineoplastic (ovarian cancer)	141	74.3
675	Antineoplastic (pancreatic cancer)	140	79.9
676	Antineoplastic (renal cancer)	94	77.8
677	Antineoplastic (sarcoma)	52	79.4
678	Antineoplastic (small cell lung cancer)	50	76.3
679	Antineoplastic (solid tumors)	721	86.6
680	Antineoplastic (squamous cell carcinoma)	17	79.8
681	Antineoplastic alkaloid	59	95.2
682	Antineoplastic antibiotic	1724	97.7
683	Antineoplastic antimetabolite	178	93.9
684	Antineoplastic enhancer	798	91.1
685	Antineoplastic, alkylator	143	97.0
686	Antinephritic	119	86.9
687	Antineurogenic pain	536	89.4
688	Antineurotic	48	80.6
689	Antineurotoxic	11	78.2
690	Antinociceptive	21	89.6
691	Antiobesity	7633	91.7
692	Antiosteoporotic	2808	93.4
693	Antioxidant	726	93.7
694	Antiparasitic	623	92.4
695	Antiparkinsonian	2721	89.4
696	Antiparkinsonian, rigidity relieving	37	92.1
697	Antiparkinsonian, tremor relieving	114	93.9
698	Antiperistaltic	12	95.4
699	Antiperspirant	4	99.5
700	Antiprotozoal	1638	89.8
701	Antiprotozoal (Amoeba)	92	87.3

702	Antiprotozoal (Babesia)	6	98.1
703	Antiprotozoal (Coccidial)	121	92.0
704	Antiprotozoal (Histomonas)	7	99.6
705	Antiprotozoal (Leishmania)	154	87.8
706	Antiprotozoal (Plasmodium)	670	91.4
707	Antiprotozoal (Toxoplasma)	23	92.3
708	Antiprotozoal (Trichomonas)	89	91.2
709	Antiprotozoal (Trypanosoma)	230	87.1
710	Antiprotozoal activity enhancer	5	100.0
711	Antipruritic	291	85.5
712	Antipruritic, allergic	165	82.9
713	Antipruritic, non-allergic	75	92.2
714	Antipsoriatic	1915	90.5
715	Antipsychotic	6646	93.2
716	Antipyretic	375	91.4
717	Antirickettsial	19	93.8
718	Antischistosomal	44	93.3
719	Antiseborrheic	11	89.4
720	Antisecretoric	186	90.4
721	Antiseptic	225	95.9
722	Antismoking	182	97.7
723	Antispirochetal	36	96.0
724	Antithrombocytopenic	149	97.1
725	Antithrombotic	550	85.4
726	Antithyroid	36	97.6
727	Antitoxic	152	88.4
728	Antitreponemal	12	93.5
729	Antituberculosic	414	88.7
730	Antitussive	245	92.7
731	Antitussive, narcotic	35	96.7
732	Antiulcerative	947	88.2
733	Antiuremic	39	93.0
734	Antiurolithic	72	80.8
735	Antiviral	10469	91.6
736	Antiviral (Adenovirus)	19	86.7
737	Antiviral (Arbovirus)	19	78.9
738	Antiviral (CMV)	23	89.1
739	Antiviral (HIV)	6604	94.4
740	Antiviral (Hepatitis B)	58	91.5
741	Antiviral (Hepatitis C)	1220	96.8
742	Antiviral (Hepatitis)	1362	96.2
743	Antiviral (Herpes)	149	89.6
744	Antiviral (Herpesvirus 3, Human)	7	100.0
745	Antiviral (Influenza A)	26	83.6
746	Antiviral (Influenza)	153	87.6
747	Antiviral (Papilloma)	12	80.5
748	Antiviral (Parainfluenza)	5	100.0
749	Antiviral (Picornavirus)	31	80.1
750	Antiviral (Poxvirus)	40	89.5
751	Antiviral (RSV)	19	88.6
752	Antiviral (Rhinovirus)	13	74.3
753	Antiviral (Trachoma)	12	98.5
754	Antiviral, ophthalmic	5	91.7
755	Antixerophthalmic	3	100.0
756	Anxiolytic	7995	91.3
757	Apical sodium codependent bile acid transporter inhibitor	20	100.0
758	Apolipoprotein A inhibitor	71	100.0
759	Apolipoprotein B inhibitor	225	99.6
760	Apolipoprotein B-100 inhibitor	50	99.8
761	Apoptosis agonist	1863	88.3
762	Apoptosis antagonist	423	92.3
763	Apyrase inhibitor	17	80.8
764	Arabinogalactan endo-1,4-beta-galactosidase inhibitor	4	99.7
765	Arabinose isomerase inhibitor	7	99.1

766	Arabinose-5-phosphate isomerase inhibitor	3	98.1
767	Arachidonate-CoA ligase inhibitor	7	99.8
768	Arachidonic acid antagonist	98	94.0
769	Aralkylamine N-acetyltransferase inhibitor	16	98.6
770	Aralkylamine dehydrogenase inhibitor	6	99.9
771	Arginase inhibitor	34	99.1
772	Arginine 2-monooxygenase inhibitor	4	88.0
773	Arginine N-succinyltransferase inhibitor	3	100.0
774	Arginine decarboxylase inhibitor	38	98.2
775	Arginine deiminase inhibitor	22	94.4
776	Arginine kinase inhibitor	12	99.4
777	Arginine racemase inhibitor	3	99.9
778	Arginine-tRNA ligase inhibitor	17	99.3
779	Argininosuccinate lyase inhibitor	10	99.0
780	Argininosuccinate synthase inhibitor	21	98.5
781	Arginyltransferase inhibitor	6	99.2
782	Aromatase inhibitor	971	99.2
783	Aromatic-amino-acid transaminase inhibitor	14	98.7
784	Aromatic-hydroxylamine O-acetyltransferase inhibitor	7	84.9
785	Arrhythmogenic	266	82.4
786	Aryl hydrocarbon receptor agonist	12	92.1
787	Aryl hydrocarbon receptor antagonist	55	98.4
788	Aryl sulfotransferase inhibitor	30	94.8
789	Aryl-acylamidase inhibitor	43	93.1
790	Aryl-alcohol dehydrogenase (NADP+) inhibitor	7	98.3
791	Aryl-alcohol dehydrogenase inhibitor	10	98.3
792	Aryl-aldehyde dehydrogenase (NADP+) inhibitor	6	98.8
793	Arylacetonitrilase inhibitor	11	95.7
794	Arylalkyl acylamidase inhibitor	6	98.5
795	Arylamine N-Acetyltransferase substrate	29	96.0
796	Arylamine N-acetyltransferase inhibitor	24	95.0
797	Aryldialkylphosphatase inhibitor	5	97.8
798	Arylesterase inhibitor	9	92.8
799	Arylformamidase inhibitor	28	98.0
800	Arylmalonate decarboxylase inhibitor	3	96.7
801	Arylsulfatase inhibitor	23	97.1
802	Arylsulfate sulfotransferase inhibitor	7	90.1
803	Asparaginase inhibitor	19	96.1
804	Asparagine synthase (glutamine-hydrolysing) inhibitor	81	99.2
805	Asparagine synthetase inhibitor	3	99.8
806	Asparagine-oxo-acid transaminase inhibitor	17	99.3
807	Asparagine-tRNA ligase inhibitor	6	98.7
808	Asparaginyl endopeptidase inhibitor	12	97.5
809	Aspartate 1-decarboxylase inhibitor	7	99.5
810	Aspartate 4-decarboxylase inhibitor	19	98.1
811	Aspartate N-acetyltransferase inhibitor	3	100.0
812	Aspartate ammonia-lyase inhibitor	26	99.3
813	Aspartate carbamoyltransferase inhibitor	26	98.3
814	Aspartate kinase inhibitor	24	94.8
815	Aspartate racemase inhibitor	4	99.3
816	Aspartate transaminase inhibitor	21	98.0
817	Aspartate-ammonia ligase (ADP-forming) inhibitor	4	99.1
818	Aspartate-ammonia ligase inhibitor	3	96.9
819	Aspartate-phenylpyruvate transaminase inhibitor	4	86.4
820	Aspartate-semialdehyde dehydrogenase inhibitor	14	91.9
821	Aspartate-tRNA ligase inhibitor	6	98.0
822	Aspartic protease inhibitor	3	98.9
823	Aspartoacylase inhibitor	4	98.0
824	Aspartyl aminopeptidase inhibitor	8	98.5
825	Aspartyl protease inhibitor	4	100.0
826	Aspartyltransferase inhibitor	4	83.6
827	Aspergillopepsin I inhibitor	8	92.0
828	Aspergillopepsin II inhibitor	4	94.3
829	Aspergillus nuclease S1 inhibitor	8	93.8

830	Assemblin inhibitor	7	99.3
831	Astacin inhibitor	19	98.2
832	Astringent	15	97.7
833	Atherosclerosis treatment	3671	89.0
834	Atrial natriuretic peptide agonist	9	96.2
835	Atrolysin A inhibitor	11	94.1
836	Atrolysin C inhibitor	10	97.5
837	Attention deficit/hyperactivity disorder treatment	666	97.5
838	Aureolysin inhibitor	4	98.0
839	Aurora kinase inhibitor	736	98.7
840	Aurora-A kinase inhibitor	322	98.6
841	Aurora-B kinase inhibitor	333	98.7
842	Aurora-C kinase inhibitor	33	94.6
843	Autism spectrum disorders treatment	9	79.0
844	Autoimmune disorders treatment	4287	88.4
845	Autophagy inducer	3	93.0
846	Autotaxin inhibitor	4	84.4
847	Azobenzene reductase inhibitor	5	98.4
848	Bacillus subtilis ribonuclease inhibitor	6	99.5
849	Bacterial efflux pump inhibitor	16	91.2
850	Bacterial leucyl aminopeptidase inhibitor	29	99.2
851	Baculoviral IAP repeat-containing protein 4 inhibitor	55	99.8
852	Baculoviral IAP repeat-containing protein inhibitor	106	99.6
853	Bax channel antagonist	8	100.0
854	Bcl-xL inhibitor	61	94.1
855	Bcl2 antagonist	120	92.2
856	Bcr-Abl kinase inhibitor	97	96.0
857	Benzaldehyde dehydrogenase (NAD+) inhibitor	8	99.3
858	Benzaldehyde dehydrogenase (NADP+) inhibitor	3	97.2
859	Benzoate 4-monooxygenase inhibitor	19	93.6
860	Benzoate-CoA ligase inhibitor	6	87.9
861	Benzodiazepine agonist	359	97.8
862	Benzodiazepine agonist partial	39	96.1
863	Benzodiazepine antagonist	394	98.9
864	Benzodiazepine inverse agonist	59	99.2
865	Benzodiazepine omega receptor agonist	7	77.5
866	Benzodiazepine receptor peripheral-type antagonist	369	99.8
867	Benzoylformate decarboxylase inhibitor	9	89.3
868	Beta 1 adrenoreceptor agonist	49	97.4
869	Beta 1 adrenoreceptor antagonist	297	99.3
870	Beta 2 adrenoreceptor agonist	684	99.4
871	Beta 2 adrenoreceptor antagonist	248	99.5
872	Beta 3 adrenoreceptor agonist	772	99.7
873	Beta 3 adrenoreceptor antagonist	24	99.9
874	Beta adrenoreceptor agonist	1555	98.8
875	Beta adrenoreceptor antagonist	968	98.2
876	Beta amyloid protein antagonist	126	96.7
877	Beta galactosidase inhibitor	62	98.8
878	Beta glucosidase inhibitor	15	99.3
879	Beta glucuronidase inhibitor	14	95.4
880	Beta lactamase II inhibitor	10	100.0
881	Beta lactamase Imi-1 inhibitor	5	99.9
882	Beta lactamase TEM-1 inhibitor	42	99.9
883	Beta lactamase inhibitor	260	97.4
884	Beta tubulin antagonist	5	86.6
885	Beta-1,4-mannosyl-glycoprotein 4-beta-N-acetylglucosaminyltransferase inhibitor	13	99.1
886	Beta-D-fucosidase inhibitor	20	98.6
887	Beta-Lysine 5,6-aminomutase inhibitor	4	99.7
888	Beta-N-acetylgalactosaminidase inhibitor	3	98.0
889	Beta-N-acetylhexosaminidase inhibitor	43	97.8
890	Beta-Phosphoglucomutase inhibitor	5	99.8
891	Beta-adrenergic receptor kinase inhibitor	22	83.1
892	Beta-alanine-pyruvate transaminase inhibitor	3	98.6
893	Beta-amylase inhibitor	9	99.2

894	Beta-carotene 15,15'-monooxygenase inhibitor	17	93.5
895	Beta-cyclopiasonate dehydrogenase inhibitor	7	97.9
896	Beta-fructofuranosidase inhibitor	43	98.9
897	Beta-galactoside alpha-2,3-sialyltransferase inhibitor	10	99.8
898	Beta-glucosidase inhibitor	46	98.4
899	Beta-mannosidase inhibitor	9	97.9
900	Beta-ureidopropionase inhibitor	16	96.6
901	Betaine-aldehyde dehydrogenase inhibitor	23	99.1
902	Betaine-homocysteine S-methyltransferase inhibitor	11	99.8
903	Bile-salt sulfotransferase inhibitor	4	98.3
904	Biliary tract disorders treatment	93	88.2
905	Bilirubin oxidase inhibitor	9	90.8
906	Biliverdin reductase inhibitor	11	99.2
907	Biotin carboxylase inhibitor	4	98.3
908	Biotin-CoA ligase inhibitor	3	98.6
909	Biotin-[methylmalonyl-CoA-carboxytransferase] ligase inhibitor	4	99.9
910	Biotin-[propionyl-CoA-carboxylase (ATP-hydrolysing)] ligase inhibitor	3	97.4
911	Biotinidase inhibitor	8	82.9
912	Biphenyl-2,3-diol 1,2-dioxygenase inhibitor	15	99.0
913	Bipolar disorder treatment	193	96.3
914	Bis(5'-adenosyl)-triphosphatase inhibitor	4	98.8
915	Bis(5'-nucleosyl)-tetrphosphatase (asymmetrical) inhibitor	12	99.5
916	Bis(5'-nucleosyl)-tetrphosphatase (symmetrical) inhibitor	11	99.5
917	Bisphosphoglycerate mutase inhibitor	4	98.0
918	Bisphosphoglycerate phosphatase inhibitor	5	96.2
919	Bisphosphonate	72	100.0
920	Blasticidin-S deaminase inhibitor	4	97.5
921	Bombesin 1 receptor antagonist	3	89.3
922	Bombesin 2 receptor antagonist	19	98.0
923	Bombesin 3 receptor agonist	24	99.4
924	Bombesin agonist	25	99.5
925	Bombesin antagonist	138	98.6
926	Bone diseases treatment	3485	92.8
927	Bone formation stimulant	539	92.3
928	Bone morphogenic protein 1 inhibitor	136	100.0
929	Bone morphogenic protein inhibitor	136	100.0
930	Bontoxilysin inhibitor	6	94.4
931	Bothrolysin inhibitor	3	97.7
932	Botulin neurotoxin A light chain inhibitor	11	86.8
933	Botulinum neurotoxin type B inhibitor	8	100.0
934	Brachyurin inhibitor	8	97.5
935	Bradykinin B1 receptor agonist	6	100.0
936	Bradykinin B1 receptor antagonist	448	99.7
937	Bradykinin B2 receptor agonist	9	100.0
938	Bradykinin B2 receptor antagonist	506	99.9
939	Bradykinin agonist	15	99.9
940	Bradykinin antagonist	1068	99.5
941	Branched-chain-amino-acid transaminase inhibitor	20	96.3
942	Breast cancer-resistant protein inhibitor	37	98.7
943	Bronchoconstrictor	53	77.2
944	Bronchodilator	2095	95.5
945	Bruton tyrosine kinase inhibitor	79	98.9
946	Bulimia treatment	103	99.7
947	Butyrate-CoA ligase inhibitor	10	98.6
948	Butyryl-CoA dehydrogenase inhibitor	9	99.5
949	Butyrylcholinesterase inhibitor	376	98.6
950	CC chemokine 1 receptor antagonist	167	99.5
951	CC chemokine 10 receptor antagonist	10	100.0
952	CC chemokine 2 receptor antagonist	68	94.5
953	CC chemokine 3 receptor antagonist	198	99.4
954	CC chemokine 4 receptor antagonist	8	84.7
955	CC chemokine 5 receptor agonist	14	100.0
956	CC chemokine 5 receptor antagonist	38	91.7
957	CC chemokine 9 receptor antagonist	5	100.0

958	CC chemokine receptor 2B antagonist	5	87.8
959	CC chemokine receptor agonist	15	98.4
960	CC chemokine receptor antagonist	479	97.0
961	CCL2 expression inhibitor	5	91.3
962	CD45 antagonist	72	98.6
963	CD80 antagonist	81	100.0
964	CDC25 phosphatase inhibitor	36	98.7
965	CDC25A inhibitor	77	96.4
966	CDC25B inhibitor	67	96.1
967	CDC25C inhibitor	32	99.7
968	CDC7 inhibitor	46	99.5
969	CDK/Cyclin complex inhibitor	1205	97.8
970	CDK1/cyclin B inhibitor	331	98.9
971	CDK2/cyclin A inhibitor	437	96.5
972	CDK2/cyclin A3 inhibitor	30	100.0
973	CDK2/cyclin E inhibitor	475	99.4
974	CDK2/cyclin E2 inhibitor	5	100.0
975	CDK4/cyclin D inhibitor	427	99.5
976	CDK4/cyclin D1 inhibitor	251	98.6
977	CDK4/cyclin D3 inhibitor	7	100.0
978	CDK5/p25 inhibitor	56	97.9
979	CDK9/cyclin T1 inhibitor	11	81.9
980	CDP-4-dehydro-6-deoxyglucose reductase inhibitor	4	98.2
981	CDP-diacylglycerol diphosphatase inhibitor	6	99.9
982	CDP-diacylglycerol-glycerol-3-phosphate 3-phosphatidyltransferase inhibitor	3	97.2
983	CDP-diacylglycerol-inositol 3-phosphatidyltransferase inhibitor	17	92.4
984	CDP-diacylglycerol-serine O-phosphatidyltransferase inhibitor	6	89.7
985	CDP-glycerol diphosphatase inhibitor	6	100.0
986	CDP-glycerol glycerophosphotransferase inhibitor	6	84.7
987	CDP-ribitol ribitolphosphotransferase inhibitor	5	77.5
988	CF transmembrane conductance regulator agonist	8	85.6
989	CF transmembrane conductance regulator antagonist	35	97.3
990	CMP-KDO synthase inhibitor	3	99.9
991	CMP-N-acetylneuraminate monooxygenase inhibitor	13	96.7
992	CMP-N-acylneuraminate phosphodiesterase inhibitor	23	98.2
993	CNS active muscle relaxant	140	96.4
994	CO-methylating acetyl-CoA synthase inhibitor	3	100.0
995	CPB protease inhibitor	3	99.9
996	CTGF expression inhibitor	5	100.0
997	CTP synthase inhibitor	12	98.0
998	CXC chemokine 1 receptor antagonist	6	76.4
999	CXC chemokine 2 receptor antagonist	52	98.0
1000	CXC chemokine 3 receptor antagonist	19	92.8
1001	CXC chemokine 4 receptor antagonist	43	99.4
1002	CXC chemokine 5 receptor antagonist	336	100.0
1003	CXC chemokine L1/GRO-alpha antagonist	17	100.0
1004	CXC chemokine receptor antagonist	507	98.7
1005	CYP1 substrate	667	87.7
1006	CYP11B substrate	7	100.0
1007	CYP11B1 inhibitor	59	96.1
1008	CYP11B1 substrate	3	100.0
1009	CYP11B2 inhibitor	65	99.6
1010	CYP11B2 substrate	6	100.0
1011	CYP17 inhibitor	7	93.8
1012	CYP17 substrate	10	98.4
1013	CYP17A substrate	4	100.0
1014	CYP19 inducer	3	100.0
1015	CYP19 inhibitor	43	96.3
1016	CYP19 substrate	23	97.1
1017	CYP19A1 expression inhibitor	3	100.0
1018	CYP19A1 substrate	12	100.0
1019	CYP1A inducer	45	91.3
1020	CYP1A inhibitor	209	88.8
1021	CYP1A substrate	654	87.7

1022	CYP1A1 inducer	30	96.0
1023	CYP1A1 inhibitor	75	92.6
1024	CYP1A1 substrate	348	90.7
1025	CYP1A1* substrate	10	100.0
1026	CYP1A2 inducer	24	88.5
1027	CYP1A2 inhibitor	182	88.7
1028	CYP1A2 substrate	505	86.9
1029	CYP1A3 substrate	5	99.5
1030	CYP1B substrate	86	92.6
1031	CYP1B1 inducer	9	99.9
1032	CYP1B1 inhibitor	50	96.8
1033	CYP1B1 substrate	84	93.6
1034	CYP2 substrate	1232	87.0
1035	CYP24 inhibitor	9	89.3
1036	CYP24 substrate	24	94.7
1037	CYP24A1 substrate	5	99.8
1038	CYP26 inhibitor	19	99.3
1039	CYP26 substrate	5	94.5
1040	CYP26A substrate	4	93.0
1041	CYP27 substrate	15	98.3
1042	CYP27A substrate	12	97.8
1043	CYP27A1 substrate	8	100.0
1044	CYP2A substrate	255	85.6
1045	CYP2A1 substrate	18	81.3
1046	CYP2A10 substrate	4	97.8
1047	CYP2A11 substrate	3	97.4
1048	CYP2A13 substrate	3	99.9
1049	CYP2A2 substrate	8	95.3
1050	CYP2A3 substrate	14	95.4
1051	CYP2A4 substrate	3	90.1
1052	CYP2A5 inhibitor	13	99.7
1053	CYP2A5 substrate	8	93.2
1054	CYP2A6 inhibitor	50	93.2
1055	CYP2A6 substrate	226	84.9
1056	CYP2A8 substrate	3	95.1
1057	CYP2B substrate	469	90.2
1058	CYP2B1 substrate	182	93.9
1059	CYP2B10 substrate	3	85.6
1060	CYP2B11 substrate	10	92.2
1061	CYP2B18 substrate	4	86.0
1062	CYP2B2 substrate	78	90.1
1063	CYP2B4 substrate	37	98.3
1064	CYP2B5 substrate	3	94.8
1065	CYP2B6 inhibitor	38	77.2
1066	CYP2B6 substrate	237	87.2
1067	CYP2C substrate	623	85.0
1068	CYP2C10 substrate	18	92.6
1069	CYP2C11 substrate	92	88.9
1070	CYP2C12 substrate	11	76.1
1071	CYP2C18 inhibitor	13	98.2
1072	CYP2C18 substrate	38	90.6
1073	CYP2C19 inducer	6	78.9
1074	CYP2C19 inhibitor	126	87.9
1075	CYP2C19 substrate	296	86.0
1076	CYP2C2 substrate	5	95.3
1077	CYP2C29 substrate	5	82.6
1078	CYP2C3 substrate	6	85.9
1079	CYP2C6 substrate	55	89.2
1080	CYP2C8 inducer	9	97.1
1081	CYP2C8 inhibitor	39	80.8
1082	CYP2C8 substrate	198	83.4
1083	CYP2C9 inducer	24	79.6
1084	CYP2C9 inhibitor	197	89.1
1085	CYP2C9 substrate	384	84.2

1086	CYP2C9-Arg substrate	10	89.4
1087	CYP2C9-Cys substrate	6	88.5
1088	CYP2C9-Cys144 substrate	6	80.2
1089	CYP2D substrate	504	86.3
1090	CYP2D1 substrate	38	93.5
1091	CYP2D15 substrate	5	81.0
1092	CYP2D16 substrate	3	90.9
1093	CYP2D2 inhibitor	5	89.3
1094	CYP2D6 inhibitor	228	88.7
1095	CYP2D6 substrate	478	86.1
1096	CYP2D6-Val substrate	10	80.6
1097	CYP2E substrate	422	90.0
1098	CYP2E1 inducer	13	87.6
1099	CYP2E1 inhibitor	61	94.8
1100	CYP2E1 substrate	413	90.0
1101	CYP2F1 substrate	8	94.0
1102	CYP2G1 substrate	11	95.8
1103	CYP2J substrate	5	84.9
1104	CYP2J2 substrate	4	84.7
1105	CYP3A inducer	75	87.9
1106	CYP3A inhibitor	8	87.2
1107	CYP3A substrate	1097	85.0
1108	CYP3A1 substrate	52	81.9
1109	CYP3A11 substrate	4	99.9
1110	CYP3A2 substrate	63	79.6
1111	CYP3A3 substrate	36	84.7
1112	CYP3A4 inducer	71	87.4
1113	CYP3A4 inhibitor	334	87.2
1114	CYP3A4 substrate	915	84.5
1115	CYP3A5 inducer	4	97.2
1116	CYP3A5 substrate	143	84.0
1117	CYP3A7 substrate	48	86.3
1118	CYP3A9 substrate	3	83.4
1119	CYP3C substrate	7	98.4
1120	CYP4 substrate	76	91.8
1121	CYP4A substrate	39	86.8
1122	CYP4A1 substrate	8	99.0
1123	CYP4A11 substrate	17	86.4
1124	CYP4A2 substrate	4	96.9
1125	CYP4B substrate	16	94.3
1126	CYP4B1 substrate	15	94.3
1127	CYP4F substrate	25	98.1
1128	CYP4F12 substrate	7	96.1
1129	CYP4F2 inhibitor	33	99.5
1130	CYP4F2 substrate	13	96.0
1131	CYP4F3 substrate	10	100.0
1132	CYP4F8 substrate	4	100.0
1133	CYP51 inhibitor	6	99.8
1134	CYP7 inhibitor	7	81.8
1135	CYP7 substrate	8	100.0
1136	CYP7A1 inhibitor	3	100.0
1137	CYP7A1 substrate	5	100.0
1138	CYP7B substrate	4	100.0
1139	CYP7B1 substrate	4	100.0
1140	Ca(v)2.2 antagonist	344	98.4
1141	Ca2+-transporting ATPase inhibitor	12	85.4
1142	Ca2+/calmodulin-dependent kinase I inhibitor	9	95.7
1143	Ca2+/calmodulin-dependent kinase II inhibitor	41	94.6
1144	Ca2+/calmodulin-dependent protein kinase inhibitor	54	93.2
1145	Cachexia treatment	131	96.0
1146	Cadherin antagonist	3	100.0
1147	Calcineurin inhibitor	21	100.0
1148	Calcitonin gene-related peptide 1 receptor antagonist	33	97.3
1149	Calcitonin gene-related peptide antagonist	465	99.7

1150	Calcitonin stimulant	23	96.2
1151	Calcium antagonist	115	96.6
1152	Calcium channel (voltage-sensitive) agonist	6	79.6
1153	Calcium channel (voltage-sensitive) antagonist	1487	97.8
1154	Calcium channel L-type antagonist	989	98.6
1155	Calcium channel N-type antagonist	391	98.5
1156	Calcium channel T-type antagonist	187	97.9
1157	Calcium channel agonist	51	89.0
1158	Calcium channel antagonist	3632	96.2
1159	Calcium regulator	301	87.8
1160	Calcium release-activated channel antagonist	51	99.7
1161	Calcium-sensing receptor agonist	5	98.0
1162	Calcium-sensing receptor antagonist	55	99.0
1163	Calmodulin antagonist	37	77.0
1164	Calpain I inhibitor	253	99.6
1165	Calpain II inhibitor	177	100.0
1166	Calpain inhibitor	77	99.5
1167	Camphor 1,2-monooxygenase inhibitor	4	98.1
1168	Cancer associated disorders treatment	51	84.5
1169	Cancer procoagulant inhibitor	11	97.0
1170	Candidapepsin 2 inhibitor	10	100.0
1171	Candidapepsin inhibitor	17	96.6
1172	Cannabinoid CB1 receptor agonist	40	98.1
1173	Cannabinoid CB1 receptor antagonist	1252	99.5
1174	Cannabinoid CB2 receptor agonist	102	97.5
1175	Cannabinoid CB2 receptor antagonist	245	99.7
1176	Cannabinoid receptor agonist	138	98.5
1177	Cannabinoid receptor antagonist	1306	99.4
1178	Capillary fragility treatment	23	87.7
1179	Carbamoyl-phosphate synthase (ammonia) inhibitor	15	98.7
1180	Carbamoyl-serine ammonia-lyase inhibitor	3	99.9
1181	Carbon-monoxide dehydrogenase inhibitor	3	97.1
1182	Carbonic anhydrase I inhibitor	833	99.9
1183	Carbonic anhydrase I stimulant	68	100.0
1184	Carbonic anhydrase II inhibitor	1248	99.9
1185	Carbonic anhydrase II stimulant	71	99.2
1186	Carbonic anhydrase IV inhibitor	819	100.0
1187	Carbonic anhydrase IV stimulant	65	100.0
1188	Carbonic anhydrase IX inhibitor	161	99.9
1189	Carbonic anhydrase V inhibitor	47	99.8
1190	Carbonic anhydrase VII inhibitor	8	99.5
1191	Carbonic anhydrase XII inhibitor	21	99.9
1192	Carbonic anhydrase XIV inhibitor	3	100.0
1193	Carbonic anhydrase XV inhibitor	3	100.0
1194	Carbonic anhydrase inhibitor	1350	99.9
1195	Carbonic anhydrase stimulant	85	99.1
1196	Carbonyl reductase (NADPH) inhibitor	38	90.5
1197	Carboxy-cis,cis-muconate cyclase inhibitor	19	99.7
1198	Carboxycyclohexadienyl dehydratase inhibitor	5	100.0
1199	Carboxylate reductase inhibitor	7	99.7
1200	Carboxylesterase inhibitor	34	97.3
1201	Carboxymethylenebutenolidase inhibitor	3	99.2
1202	Carboxypeptidase B inhibitor	17	98.8
1203	Carboxypeptidase D inhibitor	9	94.3
1204	Carboxypeptidase E inhibitor	20	92.8
1205	Carboxypeptidase M inhibitor	5	99.5
1206	Carboxypeptidase Taq inhibitor	3	91.4
1207	Carboxypeptidase U inhibitor	19	99.7
1208	Carcinogenic	1555	93.7
1209	Carcinogenic, group 1	23	86.5
1210	Carcinogenic, group 2A	36	95.0
1211	Carcinogenic, group 2B	195	95.8
1212	Carcinogenic, group 3	392	94.5
1213	Carcinogenic, mouse	471	91.8

1214	Carcinogenic, mouse, female	399	91.3
1215	Carcinogenic, mouse, male	374	92.6
1216	Carcinogenic, rat	622	92.9
1217	Carcinogenic, rat, female	463	92.2
1218	Carcinogenic, rat, male	520	92.8
1219	Cardiac myosin stimulant	4	100.0
1220	Cardiodepressant	166	91.2
1221	Cardioprotectant	164	84.6
1222	Cardiotonic	3291	89.1
1223	Cardiotoxic	101	81.6
1224	Cardiovascular analeptic	19	91.7
1225	Carminative	3	98.2
1226	Carnitinamidase inhibitor	8	97.1
1227	Carnitine 3-dehydrogenase inhibitor	12	98.4
1228	Carnitine O-octanoyltransferase inhibitor	8	96.1
1229	Carnitine acetyltransferase stimulant	4	100.0
1230	Carnitine dehydratase inhibitor	5	99.3
1231	Carnitine palmitoyltransferase 1 inhibitor	9	93.1
1232	Carnitine palmitoyltransferase inhibitor	28	97.5
1233	Carnosine synthase inhibitor	14	95.1
1234	Caspase 2 inhibitor	8	99.7
1235	Caspase 3 inhibitor	366	97.8
1236	Caspase 3 stimulant	71	82.8
1237	Caspase 6 inhibitor	45	99.9
1238	Caspase 7 inhibitor	78	100.0
1239	Caspase 8 inhibitor	70	98.2
1240	Caspase 8 stimulant	23	79.3
1241	Caspase 9 inhibitor	12	89.8
1242	Caspase 9 stimulant	27	77.7
1243	Catalase inhibitor	73	98.3
1244	Catalase stimulant	113	95.9
1245	Catechol 1,2-dioxygenase inhibitor	20	99.0
1246	Catechol 2,3-dioxygenase inhibitor	32	99.4
1247	Catechol O methyltransferase inhibitor	40	97.3
1248	Catechol oxidase inhibitor	15	97.1
1249	Catenin beta inhibitor	9	100.0
1250	Cathepsin B inhibitor	592	98.8
1251	Cathepsin D inhibitor	262	97.3
1252	Cathepsin E inhibitor	33	99.0
1253	Cathepsin F inhibitor	30	99.4
1254	Cathepsin G inhibitor	55	92.4
1255	Cathepsin H inhibitor	20	90.2
1256	Cathepsin K inhibitor	510	99.8
1257	Cathepsin L inhibitor	434	98.1
1258	Cathepsin S inhibitor	346	99.5
1259	Cathepsin T inhibitor	7	93.8
1260	Cathepsin V inhibitor	31	99.8
1261	Celiac disease treatment	32	97.1
1262	Cell adhesion inhibitor	670	96.2
1263	Cell adhesion molecule inhibitor	97	87.6
1264	Cell wall biosynthesis inhibitor	20	88.4
1265	Cell wall synthesis inhibitor	533	96.4
1266	Cellobiose phosphorylase inhibitor	10	99.1
1267	Cellulase inhibitor	12	96.8
1268	Cellulose 1,4-beta-cellobiosidase inhibitor	11	89.0
1269	Cellulose synthase (UDP-forming) inhibitor	13	96.0
1270	Centromere associated protein inhibitor	24	98.7
1271	Cephalosporin-C deacetylase inhibitor	7	73.0
1272	Ceramidase inhibitor	14	95.1
1273	Ceramide glucosyltransferase inhibitor	12	91.3
1274	Cerebroside-sulfatase inhibitor	9	97.5
1275	Cerebrovascular disorders treatment	506	92.2
1276	Cerevisin inhibitor	8	98.5
1277	Chalcone isomerase inhibitor	26	99.5

1278	Channel-conductance-controlling ATPase inhibitor	5	96.2
1279	Chaperonin ATPase inhibitor	6	96.2
1280	Check point kinase 1 inhibitor	241	99.2
1281	Check point kinase 2 inhibitor	82	97.6
1282	Check point kinase inhibitor	301	99.0
1283	Chelator	102	96.2
1284	Chelator, Iron	10	98.7
1285	Chemokine receptor agonist	15	98.4
1286	Chemokine receptor antagonist	988	97.5
1287	Chemopreventive	348	93.5
1288	Chemoprotective	165	89.0
1289	Chemosensitizer	205	83.3
1290	Chenodeoxycholytaurine hydrolase inhibitor	3	95.6
1291	Chitin deacetylase inhibitor	3	99.9
1292	Chitin synthase inhibitor	32	94.6
1293	Chitinase inhibitor	25	92.1
1294	Chitobiosyldiphosphodolichol beta-mannosyltransferase inhibitor	5	98.0
1295	Chitosanase inhibitor	8	93.8
1296	Chloramphenicol O-acetyltransferase inhibitor	7	99.6
1297	Chlordecone reductase inhibitor	4	90.3
1298	Chloride channel agonist	41	88.0
1299	Chloride channel antagonist	11	94.8
1300	Chloride peroxidase inhibitor	3	87.8
1301	Chloride/bicarbonate exchanger inhibitor	24	99.1
1302	Cholate-CoA ligase inhibitor	9	98.5
1303	Cholecystokinin A agonist	113	99.2
1304	Cholecystokinin A antagonist	1072	99.6
1305	Cholecystokinin B agonist	3	99.9
1306	Cholecystokinin B antagonist	1084	99.5
1307	Cholecystokinin agonist	123	99.2
1308	Cholecystokinin antagonist	1408	99.3
1309	Choleretic	120	92.7
1310	Cholestanetriol 26-monooxygenase inhibitor	9	90.7
1311	Cholestenol delta-isomerase inhibitor	8	100.0
1312	Cholestenone 5alpha-reductase inhibitor	12	91.6
1313	Cholesterol absorption inhibitor	54	93.4
1314	Cholesterol antagonist	127	86.8
1315	Cholesterol ester transfer protein antagonist	487	99.4
1316	Cholesterol esterase inhibitor	54	98.9
1317	Cholesterol monooxygenase (side-chain-cleaving) inhibitor	7	100.0
1318	Cholesterol oxidase inhibitor	15	98.1
1319	Cholesterol synthesis inhibitor	74	95.3
1320	Choline acetyltransferase stimulant	5	93.3
1321	Choline dehydrogenase inhibitor	15	99.7
1322	Choline kinase inhibitor	36	97.4
1323	Choline sulfotransferase inhibitor	28	98.8
1324	Choline-phosphate cytidyltransferase inhibitor	15	89.1
1325	Choline-sulfatase inhibitor	12	97.9
1326	Cholinergic	3666	96.0
1327	Cholinergic antagonist	3791	97.1
1328	Choloylglycine hydrolase inhibitor	3	98.2
1329	Chondroitin 6-sulfotransferase inhibitor	4	98.5
1330	Chorismate mutase inhibitor	22	99.7
1331	Chronic obstructive pulmonary disease treatment	2431	94.0
1332	Chymase inhibitor	158	98.2
1333	Chymosin inhibitor	3	85.6
1334	Chymotrypsin inhibitor	195	96.4
1335	Cis-1,2-dihydro-1,2-dihydroxynaphthalene dehydrogenase inhibitor	3	96.4
1336	Citrate (Si)-synthase inhibitor	26	98.9
1337	Cl-transporting ATPase inhibitor	5	88.6
1338	Clavamate synthase inhibitor	3	96.9
1339	Clostripain inhibitor	22	93.7
1340	Coactivator-associated arginine methyltransferase 1 inhibitor	4	83.4
1341	Coagulant	22	97.4

1342	Cocain dependency treatment	203	95.7
1343	Coccolysin inhibitor	11	89.6
1344	Coenzyme-B sulfoethylthiotransferase inhibitor	3	86.3
1345	Cognition disorders treatment	9230	87.6
1346	Collagen inhibitor	9	76.3
1347	Collagenase 3 inhibitor	1191	99.2
1348	Collagenase inhibitor	1039	98.8
1349	Colony stimulating factor agonist	38	93.8
1350	Colony stimulating factor antagonist	171	97.9
1351	Colorectum cell-derived growth factor antagonist	5	100.0
1352	Complement C5a chemotactic receptor antagonist	49	96.9
1353	Complement C5a convertase stimulant	3	100.0
1354	Complement factor 1 inhibitor	24	94.9
1355	Complement factor 1r inhibitor	22	100.0
1356	Complement factor D inhibitor	3	84.6
1357	Complement inhibitor	43	86.4
1358	Complement stimulant	3	100.0
1359	Constipation treatment	94	94.9
1360	Contraceptive	867	94.2
1361	Contraceptive female	131	94.2
1362	Contraceptive male	179	97.0
1363	Convulsant	255	82.2
1364	Coproporphyrinogen oxidase inhibitor	29	97.9
1365	Corneal wound healing stimulator	13	99.0
1366	Corticosteroid antagonist	3	92.5
1367	Corticosteroid side-chain-isomerase inhibitor	5	96.5
1368	Corticosteroid-like	110	99.6
1369	Corticotropin releasing factor 1 receptor antagonist	651	100.0
1370	Corticotropin releasing factor antagonist	35	97.7
1371	Corticotropin-like	4	99.7
1372	Cortisol sulfotransferase inhibitor	14	99.8
1373	Cortisone alpha-reductase inhibitor	4	100.0
1374	Cortisone beta-reductase inhibitor	7	99.9
1375	CpG-Oligodeoxynucleotides inhibitor	47	100.0
1376	Creatinase inhibitor	8	98.9
1377	Creatine kinase inhibitor	30	97.2
1378	Creatine kinase stimulant	37	89.1
1379	Creatininase inhibitor	6	89.3
1380	Creatinine deaminase inhibitor	3	98.8
1381	Crotonoyl-[acyl-carrier-protein] hydratase inhibitor	3	97.9
1382	Cruzipain inhibitor	114	99.8
1383	Cushing's syndrome treatment	77	96.6
1384	Cutinase inhibitor	6	96.1
1385	Cyanate hydratase inhibitor	13	98.4
1386	Cyanoalanine nitrilase inhibitor	5	84.0
1387	Cyclamate sulfohydrolase inhibitor	4	98.7
1388	Cyclic AMP agonist	16	82.2
1389	Cyclic AMP antagonist	10	76.8
1390	Cyclic AMP modulator	44	85.9
1391	Cyclic AMP phosphodiesterase inhibitor	190	87.2
1392	Cyclic GMP phosphodiesterase inhibitor	18	86.6
1393	Cyclin-dependent kinase 1 inhibitor	413	98.6
1394	Cyclin-dependent kinase 2 inhibitor	670	98.0
1395	Cyclin-dependent kinase 4 inhibitor	354	98.6
1396	Cyclin-dependent kinase 5 inhibitor	225	98.5
1397	Cyclin-dependent kinase 6 inhibitor	52	95.2
1398	Cyclin-dependent kinase 7 inhibitor	15	86.8
1399	Cyclin-dependent kinase 9 inhibitor	14	82.9
1400	Cyclin-dependent kinase inhibitor	1837	97.8
1401	Cycloartenol synthase inhibitor	10	96.6
1402	Cyclohexadienyl dehydrogenase inhibitor	12	99.9
1403	Cyclohexanone monooxygenase inhibitor	11	84.4
1404	Cyclohexyl-isocyanide hydratase inhibitor	3	97.6
1405	Cyclomaltodextrin glucanotransferase inhibitor	17	99.9

1406	Cyclomaltodextrinase inhibitor	6	83.1
1407	Cyclooxygenase 1 inhibitor	681	97.1
1408	Cyclooxygenase 2 inhibitor	2521	97.5
1409	Cyclooxygenase 3 inhibitor	19	99.8
1410	Cyclooxygenase inhibitor	3245	96.1
1411	Cyclooxygenase substrate	4	85.0
1412	Cyclopentanone monooxygenase inhibitor	5	97.5
1413	Cyclopropane-fatty-acyl-phospholipid synthase inhibitor	11	94.3
1414	Cystathionine beta-lyase inhibitor	21	98.4
1415	Cystathionine beta-synthase inhibitor	12	98.9
1416	Cystathionine gamma-lyase inhibitor	26	98.7
1417	Cysteamine dioxygenase inhibitor	9	98.0
1418	Cysteine desulfurase inhibitor	5	98.8
1419	Cysteine dioxygenase inhibitor	16	99.8
1420	Cysteine protease B inhibitor	12	100.0
1421	Cysteine synthase inhibitor	20	93.1
1422	Cysteine transaminase inhibitor	3	99.6
1423	Cysteine-S-conjugate beta-lyase inhibitor	3	99.2
1424	Cysteine-tRNA ligase inhibitor	19	98.8
1425	Cystic fibrosis treatment	228	86.3
1426	Cystinyl aminopeptidase inhibitor	34	93.9
1427	Cytidine deaminase inhibitor	49	97.9
1428	Cytidylate kinase inhibitor	19	99.5
1429	Cytochrome P450 inhibitor	938	88.6
1430	Cytochrome-b5 reductase inhibitor	21	86.7
1431	Cytochrome-c release inhibitor	8	100.0
1432	Cytochrome-c3 hydrogenase inhibitor	6	99.2
1433	Cytokine modulator	140	95.0
1434	Cytokine production inhibitor	758	95.9
1435	Cytokine production stimulant	260	98.4
1436	Cytokine release inhibitor	6	97.7
1437	Cytoprotectant	26	79.3
1438	Cytosine deaminase inhibitor	27	97.3
1439	Cytosol alanyl aminopeptidase inhibitor	43	93.5
1440	Cytosole dipeptidase inhibitor	5	98.8
1441	Cytosolic phospholipase A2 inhibitor	25	99.8
1442	Cytostatic	265	89.5
1443	Cytotoxic	308	94.8
1444	D(-)-tartrate dehydratase inhibitor	5	99.9
1445	D-2-hydroxy-acid dehydrogenase inhibitor	6	99.0
1446	D-Ala-D-Ala ligase inhibitor	7	92.4
1447	D-Alanine-alanyl-poly(glycerolphosphate) ligase inhibitor	5	100.0
1448	D-Alanine-poly(phosphoribitol) ligase inhibitor	5	99.9
1449	D-Amino-acid oxidase inhibitor	12	99.8
1450	D-Lysine 5,6-aminomutase inhibitor	22	99.3
1451	D-Octopine dehydrogenase inhibitor	20	97.1
1452	D-Ornithine 4,5-aminomutase inhibitor	5	98.8
1453	D-Serine ammonia-lyase inhibitor	4	99.9
1454	D-alanine 2-hydroxymethyltransferase inhibitor	3	97.9
1455	D-alanine transaminase inhibitor	18	98.9
1456	D-amino-acid dehydrogenase inhibitor	5	96.2
1457	D-arabinonolactone oxidase inhibitor	5	98.9
1458	D-arabinose 1-dehydrogenase inhibitor	5	78.1
1459	D-aspartate oxidase inhibitor	12	99.9
1460	D-benzoylarginine-4-nitroanilide amidase inhibitor	5	99.4
1461	D-cysteine desulphydrase inhibitor	5	98.8
1462	D-glutamate oxidase inhibitor	9	98.8
1463	D-lactaldehyde dehydrogenase inhibitor	11	85.2
1464	D-lactate dehydrogenase (cytochrome) inhibitor	7	98.8
1465	D-lactate dehydrogenase inhibitor	7	87.5
1466	D-lactate-2-sulfatase inhibitor	4	99.9
1467	D-malate dehydrogenase (decarboxylating) inhibitor	10	98.8
1468	D-proline reductase (dithiol) inhibitor	5	99.2
1469	D-stereospecific aminopeptidase inhibitor	7	99.4

1470	D-threo-aldose 1-dehydrogenase inhibitor	7	93.0
1471	D-xylulose reductase inhibitor	4	98.1
1472	DELTA14-sterol reductase inhibitor	13	88.9
1473	DELTA24-sterol reductase inhibitor	8	89.0
1474	DNA damaging	474	96.6
1475	DNA directed DNA polymerase inhibitor	175	93.4
1476	DNA directed RNA polymerase inhibitor	451	92.8
1477	DNA directed RNA polymerase stimulant	10	99.7
1478	DNA gyrase inhibitor	310	98.3
1479	DNA helicase inhibitor	31	96.8
1480	DNA intercalator	597	98.2
1481	DNA ligase (ATP) inhibitor	24	93.9
1482	DNA methylase inhibitor	36	94.7
1483	DNA methyltransferase I inhibitor	15	96.8
1484	DNA nucleotidylexotransferase inhibitor	21	94.9
1485	DNA polymerase I inhibitor	13	83.0
1486	DNA polymerase III inhibitor	72	100.0
1487	DNA repair enzyme inhibitor	126	97.4
1488	DNA synthesis inhibitor	294	88.1
1489	DNA topoisomerase IV inhibitor	93	98.7
1490	DNA-(apurinic or apyrimidinic site) lyase inhibitor	11	94.1
1491	DNA-3-methyladenine glycosylase I inhibitor	5	95.3
1492	DNA-3-methyladenine glycosylase II inhibitor	3	99.4
1493	DNA-dependent protein kinase inhibitor	59	97.1
1494	DOPA decarboxylase inhibitor	9	98.9
1495	Dactylisin inhibitor	22	91.1
1496	Deacetoxycephalosporin-C synthase inhibitor	10	98.8
1497	Decylcitrate synthase inhibitor	4	97.2
1498	Dehydro-L-gulonate decarboxylase inhibitor	3	93.9
1499	Delayed rectifier potassium channel activator	162	99.2
1500	Delayed rectifier potassium channel antagonist	46	99.7
1501	Dementia treatment	13	84.6
1502	Demethylmacrocin O-methyltransferase inhibitor	10	100.0
1503	Demethylsterigmatocystin 6-O-methyltransferase inhibitor	3	98.7
1504	Deoxyadenosine kinase inhibitor	13	92.0
1505	Deoxycytidine deaminase inhibitor	5	98.9
1506	Deoxycytidine kinase inhibitor	42	98.0
1507	Deoxycytidylate 5-hydroxymethyltransferase inhibitor	7	97.5
1508	Deoxyguanosine kinase inhibitor	37	99.5
1509	Deoxyhypusine monooxygenase inhibitor	16	99.8
1510	Deoxyhypusine synthase inhibitor	28	98.2
1511	Deoxynucleoside kinase inhibitor	9	100.0
1512	Deoxyribonuclease (pyrimidine dimer) inhibitor	3	99.8
1513	Deoxyribonuclease I inhibitor	10	94.5
1514	Deoxyribonuclease II inhibitor	3	95.0
1515	Deoxyribonuclease X inhibitor	3	99.0
1516	Deoxyribose-phosphate aldolase inhibitor	4	98.8
1517	Dependence treatment	1225	93.8
1518	Depression	70	74.9
1519	Dethiobiotin synthase inhibitor	7	98.3
1520	Dextranase inhibitor	9	93.9
1521	Dextranucrase inhibitor	19	99.2
1522	Di-trans,poly-cis-decaprenylcistransferase inhibitor	4	97.3
1523	Diabetes insipidus treatment	31	98.0
1524	Diabetic nephropathy treatment	66	89.8
1525	Diabetic neuropathy treatment	55	81.1
1526	Diabetic retinopathy treatment	276	93.2
1527	Diacylglycerol O-acyltransferase 1 inhibitor	33	99.3
1528	Diacylglycerol O-acyltransferase inhibitor	82	97.1
1529	Diacylglycerol cholinephosphotransferase inhibitor	29	97.4
1530	Diacylglycerol kinase inhibitor	23	93.6
1531	Diamine N-acetyltransferase inhibitor	12	93.8
1532	Diamine oxidase inhibitor	25	98.7
1533	Diaminopimelate decarboxylase inhibitor	13	99.9

1534	Diaminopimelate dehydrogenase inhibitor	7	99.0
1535	Diaminopimelate epimerase inhibitor	8	99.8
1536	Diaminopropionate ammonia-lyase inhibitor	11	98.9
1537	Dichloromethane dehalogenase inhibitor	9	99.9
1538	Dichloromuconate cycloisomerase inhibitor	4	99.5
1539	Digestive functional disorders treatment	51	72.3
1540	Diguanidinobutanase inhibitor	6	99.2
1541	Dihydrodipicolinate reductase inhibitor	8	89.3
1542	Dihydrodipicolinate synthase inhibitor	16	99.3
1543	Dihydrofolate reductase (<i>Mycobacterium avium</i>) inhibitor	13	100.0
1544	Dihydrofolate reductase (<i>Pneumocystis carinii</i>) inhibitor	10	100.0
1545	Dihydrofolate reductase (<i>Toxoplasma gondii</i>) inhibitor	13	99.9
1546	Dihydrofolate reductase inhibitor	1566	99.3
1547	Dihydrofolate synthase inhibitor	13	93.3
1548	Dihydrolipoamide S-acetyltransferase inhibitor	4	99.2
1549	Dihydroneopterin aldolase inhibitor	20	99.9
1550	Dihydroorotate inhibitor	9	98.8
1551	Dihydroorotate dehydrogenase inhibitor	105	97.7
1552	Dihydroorotate oxidase inhibitor	84	98.6
1553	Dihydroopterate synthase inhibitor	31	99.1
1554	Dihydropyrimidinase inhibitor	15	98.7
1555	Dihydropyrimidine dehydrogenase inhibitor	5	98.6
1556	Dihydouracil oxidase inhibitor	8	98.8
1557	Dihydroxy-acid dehydratase inhibitor	15	94.4
1558	Dihydroxyacetanilide dehydrogenase inhibitor	5	100.0
1559	Dihydroxyacetanilide epoxidase inhibitor	5	100.0
1560	Diiodophenylpyruvate reductase inhibitor	3	99.5
1561	Diiodotyrosine transaminase inhibitor	6	99.9
1562	Diisopropyl-fluorophosphatase inhibitor	7	98.9
1563	Dimethylallyltranstransferase inhibitor	34	97.3
1564	Dimethylargininase inhibitor	3	91.6
1565	Dimethylhistidine N-methyltransferase inhibitor	5	99.0
1566	Dimethylmaleate hydratase inhibitor	3	97.6
1567	Dipeptidase E inhibitor	4	92.4
1568	Dipeptidyl peptidase I inhibitor	50	97.1
1569	Dipeptidyl peptidase II inhibitor	109	97.2
1570	Dipeptidyl peptidase IV inhibitor	1279	99.3
1571	Dipeptidyl peptidase IX inhibitor	5	93.7
1572	Dipeptidyl peptidase VIII inhibitor	3	99.3
1573	Dipeptidyl peptidase inhibitor	1411	98.7
1574	Diphenylpicrylhydrazyl (DPPH) scavenger	3	100.0
1575	Diphosphate-fructose-6-phosphate 1-phosphotransferase inhibitor	17	99.6
1576	Diphosphate-serine phosphotransferase inhibitor	8	99.9
1577	Diphosphomevalonate decarboxylase inhibitor	13	93.0
1578	Diuretic	733	92.6
1579	Diuretic inhibitor	87	89.1
1580	Dodecenoyl-CoA Delta-isomerase inhibitor	5	78.4
1581	Dolichol kinase inhibitor	8	95.9
1582	Dolichyl-diphosphooligosaccharide-protein glycotransferase inhibitor	3	91.0
1583	Dolichyl-phosphatase inhibitor	6	98.3
1584	Dolichyl-phosphate beta-D-mannosyltransferase (<i>T. brucei</i>) inhibitor	3	100.0
1585	Dolichyl-phosphate beta-D-mannosyltransferase inhibitor	18	97.8
1586	Dolichyl-phosphate beta-glucosyltransferase inhibitor	4	96.9
1587	Dolichyldiphosphatase inhibitor	3	100.0
1588	Dopachrome isomerase inhibitor	7	99.7
1589	Dopamine D1 agonist	51	99.5
1590	Dopamine D1 antagonist	614	98.9
1591	Dopamine D1A antagonist	22	100.0
1592	Dopamine D1B antagonist	37	100.0
1593	Dopamine D2 agonist	181	98.9
1594	Dopamine D2 agonist inducer	3	100.0
1595	Dopamine D2 antagonist	3850	98.4
1596	Dopamine D2A antagonist	80	99.3
1597	Dopamine D2B antagonist	31	100.0

1598	Dopamine D2L antagonist	458	99.3
1599	Dopamine D2S antagonist	103	98.1
1600	Dopamine D3 agonist	28	99.4
1601	Dopamine D3 antagonist	1071	98.7
1602	Dopamine D4 agonist	558	98.9
1603	Dopamine D4 antagonist	568	98.7
1604	Dopamine D5 antagonist	28	99.8
1605	Dopamine agonist	1032	96.8
1606	Dopamine antagonist	4601	98.0
1607	Dopamine autoreceptor agonist	61	99.4
1608	Dopamine beta hydroxylase inhibitor	64	96.0
1609	Dopamine precursors	25	99.9
1610	Dopamine release inhibitor	3	100.0
1611	Dopamine release stimulant	7	94.8
1612	Dopamine transporter antagonist	128	97.9
1613	Dopamine uptake inhibitor	1845	99.2
1614	Dry eye syndrome treatment	46	91.6
1615	Dual specificity phosphatase 1 inhibitor	4	92.6
1616	Dual specificity phosphatase inhibitor	40	96.6
1617	Dual specificity protein phosphatase VHR inhibitor	9	99.9
1618	Dynamin GTPase inhibitor	4	90.4
1619	Dynein ATPase inhibitor	3	97.2
1620	Dyrk kinase inhibitor	9	96.4
1621	Dysmenorrhea treatment	171	97.6
1622	Dyspepsia treatment	74	93.4
1623	EIF4E expression inhibitor	3	100.0
1624	ERK inhibitor	75	93.7
1625	ERK2 inhibitor	71	94.1
1626	Ecdysone 20-monooxygenase inhibitor	15	85.6
1627	Eicosanoid agonist	6	99.7
1628	Elastase 1 inhibitor	18	99.7
1629	Elastase 2 inhibitor	7	100.0
1630	Elastase inhibitor	770	98.1
1631	Electrolyte absorption agonist	6	77.4
1632	Electrolyte absorption antagonist	54	95.3
1633	Electron transport complex I inhibitor	5	91.5
1634	Electron-transferring-flavoprotein dehydrogenase inhibitor	3	87.1
1635	Embryotoxic	1743	89.8
1636	Emetic	293	76.6
1637	Endo-1,3(4)-beta-glucanase inhibitor	3	98.8
1638	Endo-1,4-beta-xylanase inhibitor	19	97.8
1639	Endo-beta-N-acetylglucosaminidase inhibitor	5	100.0
1640	Endocannabinoid uptake inhibitor	30	99.2
1641	Endocrine disorders treatment	16	84.2
1642	Endoglycosylceramidase inhibitor	4	97.8
1643	Endometriosis treatment	297	97.2
1644	Endonuclease (influenza) inhibitor	15	100.0
1645	Endopeptidase La inhibitor	39	91.1
1646	Endopeptidase So inhibitor	7	89.1
1647	Endopeptidase inhibitor	64	91.4
1648	Endothelial growth factor antagonist	13	79.4
1649	Endothelial nitric oxide synthase inhibitor	127	99.0
1650	Endothelin A receptor antagonist	1714	99.6
1651	Endothelin B receptor antagonist	968	99.6
1652	Endothelin converting enzyme inhibitor	229	98.0
1653	Endothelin receptor agonist	14	93.3
1654	Endothelin receptor antagonist	2371	99.4
1655	Endothiapepsin inhibitor	6	99.6
1656	Enoyl-CoA hydratase inhibitor	9	99.3
1657	Enoyl-[acyl-carrier-protein] reductase (NADH) inhibitor	36	96.8
1658	Enteropeptidase inhibitor	6	82.8
1659	Envelysin inhibitor	18	94.3
1660	EphB4 antagonist	76	99.6
1661	Ephrin antagonist	93	99.4

1662	Epidermal growth factor antagonist	894	99.0
1663	Epidermal growth factor receptor kinase inhibitor	1152	94.7
1664	Epithelial sodium channel antagonist	10	99.0
1665	Epoxide hydrolase 2 inhibitor	143	100.0
1666	Epoxide hydrolase inhibitor	283	99.0
1667	Epoxide hydrolase substrate	71	93.9
1668	Equilibrative nucleoside transport protein 1 inhibitor	74	99.7
1669	Equilibrative nucleoside transport protein inhibitor	106	99.8
1670	ErbB antagonist	623	98.6
1671	ErbB-1 antagonist	22	92.7
1672	ErbB-2 antagonist	421	98.7
1673	ErbB-2 expression inhibitor	6	75.8
1674	ErbB-4 antagonist	18	99.1
1675	Erectile dysfunction treatment	315	95.4
1676	Erythro-3-hydroxyaspartate ammonia-lyase inhibitor	4	99.9
1677	Erythropoiesis stimulant	6	84.0
1678	Erythropoietin receptor agonist	10	100.0
1679	Estradiol 17 beta dehydrogenase 2 inhibitor	15	99.9
1680	Estradiol 17 beta dehydrogenase 3 inhibitor	59	99.0
1681	Estradiol 17 beta dehydrogenase inhibitor	81	98.5
1682	Estradiol 17 beta dehydrogenase stimulant	19	99.9
1683	Estradiol 17alpha-dehydrogenase inhibitor	3	98.8
1684	Estrogen agonist	637	98.5
1685	Estrogen alpha receptor agonist	44	99.4
1686	Estrogen alpha receptor antagonist	530	99.5
1687	Estrogen antagonist	1063	98.4
1688	Estrogen beta receptor agonist	185	99.7
1689	Estrogen beta receptor antagonist	530	99.7
1690	Estrogen-related receptor alpha antagonist	17	100.0
1691	Estrone sulfatase inhibitor	205	99.6
1692	Estrone sulfotransferase inhibitor	37	96.4
1693	Estrone sulfotransferase stimulant	17	99.9
1694	Ethanolamine ammonia-lyase inhibitor	10	99.9
1695	Ethanolamine kinase inhibitor	26	98.8
1696	Ethanolamine oxidase inhibitor	6	89.4
1697	Ethanolamine-phosphate cytidyltransferase inhibitor	8	93.3
1698	Ethanolaminephosphotransferase inhibitor	29	95.5
1699	Ether-a-go-go potassium channel 1 antagonist	21	100.0
1700	Ether-a-go-go potassium channel antagonist	21	100.0
1701	Euglycemic	3	99.9
1702	Eukaryotic elongation factor 2 kinase inhibitor	3	100.0
1703	Excitatory amino acid transporter 1 inhibitor	6	90.5
1704	Excitatory amino acid transporter 2 inhibitor	15	99.9
1705	Excitatory amino acid transporter EAAC1 inhibitor	6	98.9
1706	Exoribonuclease II inhibitor	5	92.4
1707	Expectorant	134	93.5
1708	Extrapyramidal disorders treatment	119	96.6
1709	Eye irritation, high	461	96.5
1710	Eye irritation, inactive	91	89.2
1711	Eye irritation, moderate	232	96.3
1712	Eye irritation, weak	349	96.4
1713	FAD diphosphatase inhibitor	18	98.7
1714	FMN adenyltransferase inhibitor	7	100.0
1715	FMN reductase inhibitor	22	94.7
1716	FMO1 substrate	13	76.5
1717	FMO3 substrate	36	85.5
1718	FRZB protein inhibitor	4	99.8
1719	Factor IXa inhibitor	18	100.0
1720	Factor VII inhibitor	8	96.9
1721	Factor VIIa inhibitor	244	98.9
1722	Factor XIIIa inhibitor	14	94.0
1723	Factor XIIIa stimulant	3	99.7
1724	Factor XIa inhibitor	16	93.0
1725	Factor Xa inhibitor	1807	99.2

1726	Falcpain 2 inhibitor	46	95.3
1727	Falcpain 3 inhibitor	6	82.1
1728	Falcpain inhibitor	46	95.3
1729	Farnesoid X receptor agonist	96	99.4
1730	Farnesoid X receptor antagonist	18	93.6
1731	Farnesyltransferase inhibitor	2426	98.8
1732	Farnesyltranstransferase inhibitor	5	97.7
1733	Fas antagonist	5	100.0
1734	Fatty acid elongase inhibitor	6	89.8
1735	Fatty acid oxidation inhibitor	45	99.4
1736	Fatty acid synthase inhibitor	36	98.0
1737	Fatty-acyl-CoA synthase inhibitor	5	92.6
1738	Fatty-acyl-ethyl-ester synthase inhibitor	3	99.7
1739	Female sexual dysfunction treatment	128	96.5
1740	Ferredoxin hydrogenase inhibitor	7	95.0
1741	Ferredoxin-NAD ⁺ reductase inhibitor	3	96.1
1742	Ferredoxin-NADP ⁺ reductase inhibitor	6	97.3
1743	Ferredoxin-nitrite reductase inhibitor	12	95.3
1744	Ferrochelataase inhibitor	5	98.8
1745	Fertility enhancer	15	77.1
1746	Feruloyl esterase inhibitor	6	91.7
1747	Fibrinogen receptor antagonist	26	81.6
1748	Fibrinolytic	41	83.3
1749	Fibroblast activation protein alpha inhibitor	8	100.0
1750	Fibroblast growth factor 1 antagonist	148	98.2
1751	Fibroblast growth factor 2 antagonist	12	94.2
1752	Fibroblast growth factor 3 antagonist	48	97.3
1753	Fibroblast growth factor antagonist	498	98.4
1754	Fibrolase inhibitor	4	88.1
1755	Fibromyalgia syndrome treatment	54	92.4
1756	Fibrosis treatment	93	95.6
1757	Flavin-containing monooxygenase inhibitor	9	93.9
1758	Flavin-containing monooxygenase substrate	50	86.8
1759	Flavonoid 3'-monooxygenase inhibitor	8	74.7
1760	Focal adhesion kinase 1 inhibitor	6	100.0
1761	Focal adhesion kinase 2 inhibitor	4	100.0
1762	Focal adhesion kinase inhibitor	130	98.5
1763	Folate antagonist	21	90.1
1764	Folate transporter 1 inhibitor	5	100.0
1765	Follicle-stimulating hormone agonist	13	91.8
1766	Follicle-stimulating hormone antagonist	50	100.0
1767	Folylpolyglutamate synthase inhibitor	27	100.0
1768	Formaldehyde dehydrogenase (glutathione) inhibitor	17	97.2
1769	Formaldehyde dehydrogenase inhibitor	14	98.4
1770	Formaldehyde transketolase inhibitor	6	90.9
1771	Formate C-acetyltransferase inhibitor	5	99.7
1772	Formate dehydrogenase inhibitor	21	97.4
1773	Formate-dihydrofolate ligase inhibitor	14	88.5
1774	Formimidoylglutamase inhibitor	3	99.8
1775	Formimidoyltetrahydrofolate cyclodeaminase inhibitor	8	99.0
1776	Formyl peptide receptor antagonist	15	100.0
1777	Formyltetrahydrofolate dehydrogenase inhibitor	6	98.9
1778	Fragilysin inhibitor	6	84.8
1779	Free fatty acid receptor 1 agonist	28	100.0
1780	Free radical scavenger	227	92.9
1781	Fructan beta-fructosidase inhibitor	4	95.7
1782	Fructokinase inhibitor	13	99.6
1783	Fructose 5-dehydrogenase (NADP ⁺) inhibitor	3	98.7
1784	Fructose 5-dehydrogenase inhibitor	4	79.9
1785	Fructose bisphosphatase inhibitor	82	99.9
1786	Fructose bisphosphate aldolase inhibitor	4	84.4
1787	Fructose-2,6-bisphosphate 2-phosphatase inhibitor	12	95.9
1788	Fructose-2,6-bisphosphate 6-phosphatase inhibitor	4	99.6
1789	Fructuronate reductase inhibitor	3	99.3

1790	FtsZ polymerization inhibitor	3	100.0
1791	Fucokinase inhibitor	9	99.5
1792	Fucosterol-epoxide lyase inhibitor	9	92.0
1793	Fumarate hydratase inhibitor	24	99.4
1794	Fumarate reductase (NADH) inhibitor	7	89.1
1795	Fumarylacetoacetase inhibitor	14	99.3
1796	Furin inhibitor	23	97.8
1797	G protein-coupled receptor agonist	74	98.3
1798	G-Quadruplex telomerase inhibitor	3	91.3
1799	G-protein coupled bile acid receptor 1 agonist	9	95.8
1800	G-protein coupled receptor 120 agonist	10	100.0
1801	G-protein-coupled receptor kinase inhibitor	22	83.1
1802	GABA A inverse agonist	9	88.6
1803	GABA A receptor agonist	227	94.6
1804	GABA A receptor antagonist	1736	99.2
1805	GABA B receptor agonist	9	90.9
1806	GABA B receptor antagonist	57	99.3
1807	GABA C receptor agonist	3	98.2
1808	GABA C receptor antagonist	6	99.0
1809	GABA aminotransferase inhibitor	15	90.3
1810	GABA inverse agonist	9	88.6
1811	GABA receptor agonist	375	92.8
1812	GABA receptor antagonist	1804	98.9
1813	GABA transporter 1 inhibitor	148	99.6
1814	GABA transporter 2 inhibitor	5	82.7
1815	GABA transporter 3 inhibitor	5	97.4
1816	GABA transporter inhibitor	153	99.4
1817	GABA uptake inhibitor	67	99.2
1818	GDP-L-fucose synthase inhibitor	3	99.9
1819	GDP-mannose 4,6-dehydratase inhibitor	8	99.9
1820	GDP-mannose 6-dehydrogenase inhibitor	6	89.2
1821	GHS receptor agonist	26	99.0
1822	GHS receptor antagonist	134	99.7
1823	GMP reductase inhibitor	17	99.6
1824	GMP synthase inhibitor	56	98.9
1825	GP IIb/IIIa receptor antagonist	2081	99.1
1826	GRP78 expression inhibitor	5	100.0
1827	GST A substrate	9	78.1
1828	GST A1-1 substrate	7	72.3
1829	GST M substrate	16	81.8
1830	GST M1-1 substrate	10	81.4
1831	GST P substrate	16	97.6
1832	GST P1-1 substrate	15	97.7
1833	GST T substrate	15	92.6
1834	GST T1-1 substrate	15	92.6
1835	GTP cyclohydrolase I inhibitor	15	99.2
1836	GTP cyclohydrolase IIa inhibitor	6	100.0
1837	Galactokinase inhibitor	6	97.7
1838	Galactolipase inhibitor	13	90.5
1839	Galactose 1-dehydrogenase (NADP+) inhibitor	3	98.6
1840	Galactose oxidase inhibitor	13	97.1
1841	Galactoside 2-alpha-L-fucosyltransferase inhibitor	12	98.2
1842	Galactoside O-acetyltransferase inhibitor	4	97.1
1843	Galactosylceramidase inhibitor	7	97.9
1844	Galactosylceramide sulfotransferase inhibitor	9	96.6
1845	Galactosylgalactosylglucosylceramidase inhibitor	5	99.4
1846	Galactosylgalactosylglucosylceramide beta-D-acetylgalactosaminyltransferase inhibitor	6	78.0
1847	Galacturan 1,4-alpha-galacturonidase inhibitor	4	98.8
1848	Galectin 3 antagonist	5	99.9
1849	Gallate decarboxylase inhibitor	5	97.7
1850	Gametolysin inhibitor	15	92.2
1851	Gamma-D-Glutamyl-meso-diaminopimelate peptidase inhibitor	3	97.7
1852	Gamma-butyrobetaine dioxygenase inhibitor	19	92.1
1853	Gamma-glutamyl hydrolase inhibitor	42	99.3

1854	Gamma-glutamyltransferase inhibitor	28	90.7
1855	Gamma-guanidinobutyraldehyde dehydrogenase inhibitor	5	88.4
1856	Ganglioside galactosyltransferase inhibitor	9	96.2
1857	Gastric antisecretory	503	91.9
1858	Gastric emptying disorders treatment	103	97.4
1859	Gastric secretion stimulant	21	78.9
1860	Gastricsin inhibitor	12	92.1
1861	Gastrin inhibitor	158	89.4
1862	Gastrin-releasing peptide antagonist	8	80.3
1863	Gastritis treatment	14	92.1
1864	Gastroesophageal reflux disease treatment	220	96.5
1865	Gastrointestinal disorders treatment	292	94.7
1866	Gastrointestinal motility stimulant	82	90.5
1867	Gaucher disease treatment	10	96.2
1868	Gelatinase inhibitor	19	96.9
1869	Gene expression stimulant	12	80.1
1870	Gentamicin 2"-nucleotidyltransferase inhibitor	4	99.6
1871	Gentamicin 3'-N-acetyltransferase inhibitor	12	99.7
1872	Gentisate 1,2-dioxygenase inhibitor	6	98.5
1873	Geranylgeranyl-diphosphate geranylgeranyltransferase inhibitor	9	95.5
1874	Geranylgeranyltransferase I inhibitor	245	99.5
1875	Geranylgeranyltransferase inhibitor	454	99.6
1876	Geranyltranstransferase (Leishmania) inhibitor	28	100.0
1877	Geranyltranstransferase inhibitor	65	99.8
1878	Gestagen antagonist	8	96.4
1879	Gestagen-like	38	99.9
1880	Gingipain K inhibitor	6	93.1
1881	Gingipain R inhibitor	8	89.7
1882	Globoside alpha-N-acetylgalactosaminyltransferase inhibitor	13	95.8
1883	Glucagon receptor antagonist	194	98.3
1884	Glucagon-like peptide 1 agonist	12	96.5
1885	Glucagon-like peptide 1 receptor antagonist	13	100.0
1886	Glucan 1,3-alpha-glucosidase inhibitor	19	99.2
1887	Glucan 1,3-beta-glucosidase inhibitor	9	98.9
1888	Glucan 1,4-alpha-glucosidase inhibitor	19	99.5
1889	Glucan 1,4-alpha-maltotetrahydrolase inhibitor	3	97.2
1890	Glucan 1,4-alpha-maltotriohydrolase inhibitor	3	95.3
1891	Glucan 1,4-beta-glucosidase inhibitor	9	97.5
1892	Glucan 1,6-alpha-glucosidase inhibitor	6	98.5
1893	Glucan endo-1,3-alpha-glucosidase inhibitor	3	99.4
1894	Glucan endo-1,3-beta-D-glucosidase inhibitor	13	89.5
1895	Glucan endo-1,6-beta-glucosidase inhibitor	7	90.5
1896	Glucarate dehydratase inhibitor	5	98.8
1897	Glucocorticoid agonist	428	99.4
1898	Glucocorticoid antagonist	421	99.3
1899	Gluconate 2-dehydrogenase (acceptor) inhibitor	4	80.2
1900	Gluconate 5-dehydrogenase inhibitor	3	94.7
1901	Gluconate dehydratase inhibitor	4	99.3
1902	Gluconokinase inhibitor	3	96.8
1903	Gluconolactonase inhibitor	3	97.3
1904	Glucosamine 6-phosphate N-acetyltransferase inhibitor	6	99.4
1905	Glucosamine N-acetyltransferase inhibitor	6	99.6
1906	Glucosamine-1-phosphate N-acetyltransferase inhibitor	4	99.2
1907	Glucosamine-6-phosphate deaminase inhibitor	12	97.7
1908	Glucose 1-dehydrogenase inhibitor	8	98.1
1909	Glucose oxidase inhibitor	7	84.6
1910	Glucose-1,6-bisphosphate synthase inhibitor	11	99.6
1911	Glucose-1-phosphatase inhibitor	3	98.9
1912	Glucose-1-phosphate adenyltransferase inhibitor	15	99.4
1913	Glucose-1-phosphate cytidyltransferase inhibitor	12	100.0
1914	Glucose-6-phosphate isomerase inhibitor	22	99.8
1915	Glucose-6-phosphate translocase inhibitor	27	99.7
1916	Glucose-dependent insulinotropic receptor agonist	62	99.9
1917	Glucosyl transferase inhibitor	37	94.6

1918	Glucosylceramidase inhibitor	18	99.5
1919	Glucuronate isomerase inhibitor	5	97.5
1920	Glucuronolactone reductase inhibitor	3	98.6
1921	Glucuronosyltransferase inhibitor	47	97.9
1922	Glutamate (mGluR group I) agonist	30	96.7
1923	Glutamate (mGluR group I) antagonist	169	96.7
1924	Glutamate (mGluR group II) agonist	36	98.6
1925	Glutamate (mGluR group II) antagonist	125	99.3
1926	Glutamate (mGluR group III) agonist	13	99.9
1927	Glutamate (mGluR group III) antagonist	25	97.1
1928	Glutamate (mGluR) agonist	86	98.7
1929	Glutamate (mGluR) antagonist	343	97.5
1930	Glutamate (mGluR1) agonist	10	99.8
1931	Glutamate (mGluR1) antagonist	82	95.1
1932	Glutamate (mGluR1a) agonist	4	100.0
1933	Glutamate (mGluR2) agonist	31	99.6
1934	Glutamate (mGluR2) antagonist	112	99.3
1935	Glutamate (mGluR3) agonist	11	99.4
1936	Glutamate (mGluR3) antagonist	59	98.8
1937	Glutamate (mGluR4) agonist	5	99.1
1938	Glutamate (mGluR4) antagonist	5	99.8
1939	Glutamate (mGluR5) agonist	17	94.4
1940	Glutamate (mGluR5) antagonist	92	97.4
1941	Glutamate (mGluR5a) agonist	4	100.0
1942	Glutamate (mGluR6) agonist	8	99.9
1943	Glutamate (mGluR6) antagonist	6	98.9
1944	Glutamate (mGluR8) agonist	3	99.7
1945	Glutamate (mGluR8) antagonist	13	100.0
1946	Glutamate 5-kinase inhibitor	9	88.6
1947	Glutamate N-acetyltransferase inhibitor	4	98.8
1948	Glutamate carboxypeptidase inhibitor	21	98.8
1949	Glutamate decarboxylase inhibitor	43	97.1
1950	Glutamate dehydrogenase (NADP+) inhibitor	18	98.9
1951	Glutamate dehydrogenase [NAD(P)+] inhibitor	45	98.5
1952	Glutamate dehydrogenase inhibitor	34	95.6
1953	Glutamate formimidoyltransferase inhibitor	11	99.6
1954	Glutamate racemase inhibitor	45	99.6
1955	Glutamate receptor agonist	374	97.9
1956	Glutamate receptor antagonist	4477	97.1
1957	Glutamate release inhibitor	60	94.2
1958	Glutamate synthase (NADPH) inhibitor	55	97.4
1959	Glutamate synthase (ferredoxin) inhibitor	21	95.1
1960	Glutamate uptake inhibitor	9	99.9
1961	Glutamate-1-semialdehyde 2,1-aminomutase inhibitor	9	95.4
1962	Glutamate-5-semialdehyde dehydrogenase inhibitor	4	86.1
1963	Glutamate-cysteine ligase inhibitor	37	99.0
1964	Glutamate-tRNA ligase inhibitor	6	82.2
1965	Glutamin-(asparagin-)-ase inhibitor	14	96.5
1966	Glutaminase inhibitor	21	94.4
1967	Glutamine synthetase inhibitor	38	96.1
1968	Glutamine-fructose-6-phosphate transaminase inhibitor	4	99.3
1969	Glutamine-phenylpyruvate transaminase inhibitor	3	95.8
1970	Glutamine-pyruvate transaminase inhibitor	7	99.1
1971	Glutamine-tRNA ligase inhibitor	9	98.6
1972	Glutaminy-peptide cyclotransferase inhibitor	12	88.2
1973	Glutaminy-tRNA synthase (glutamine-hydrolysing) inhibitor	4	99.3
1974	Glutarate-semialdehyde dehydrogenase inhibitor	3	97.7
1975	Glutaryl-CoA dehydrogenase inhibitor	5	98.4
1976	Glutathione S transferase P1 inhibitor	11	97.8
1977	Glutathione S transferase inhibitor	32	99.0
1978	Glutathione S transferase substrate	94	92.1
1979	Glutathione dehydrogenase (ascorbate) inhibitor	7	95.0
1980	Glutathione peroxidase inhibitor	10	94.0
1981	Glutathione peroxidase stimulant	3	99.8

1982	Glutathione reductase (NADPH) stimulant	11	97.3
1983	Glutathione reductase inhibitor	21	94.2
1984	Glutathione reductase stimulant	11	97.3
1985	Glutathione synthase inhibitor	15	97.8
1986	Glutathione thioesterase inhibitor	3	93.8
1987	Glutathione-disulfide reductase inhibitor	47	98.2
1988	Glutathionylspermidine synthase inhibitor	15	100.0
1989	Gly-X carboxypeptidase inhibitor	6	98.2
1990	Glyceraldehyde-3-phosphate dehydrogenase (NADP+) inhibitor	12	95.8
1991	Glyceraldehyde-3-phosphate dehydrogenase (phosphorylating) inhibitor	17	97.6
1992	Glyceraldehyde-3-phosphate dehydrogenase inhibitor	3	91.4
1993	Glycerate kinase inhibitor	12	99.9
1994	Glycerol 2-dehydrogenase (NADP+) inhibitor	4	97.2
1995	Glycerol dehydratase inhibitor	8	99.1
1996	Glycerol dehydrogenase (NADP+) inhibitor	5	97.4
1997	Glycerol dehydrogenase inhibitor	36	98.1
1998	Glycerol kinase inhibitor	18	99.1
1999	Glycerol-1,2-cyclic-phosphate 2-phosphodiesterase inhibitor	7	99.9
2000	Glycerol-1-phosphatase inhibitor	3	98.9
2001	Glycerol-3-phosphate O-acyltransferase inhibitor	23	94.5
2002	Glycerol-3-phosphate dehydrogenase (NAD+) inhibitor	22	97.5
2003	Glycerol-3-phosphate dehydrogenase [NAD(P)+] inhibitor	6	99.8
2004	Glycerol-3-phosphate dehydrogenase inhibitor	29	90.1
2005	Glycerol-3-phosphate oxidase inhibitor	6	82.2
2006	Glycerone-phosphate O-acyltransferase inhibitor	11	97.9
2007	Glycerophosphocholine cholinephosphodiesterase inhibitor	10	99.7
2008	Glycerophosphocholine phosphodiesterase inhibitor	10	99.6
2009	Glycerophospholipid arachidonoyl-transferase (CoA-independent) inhibitor	7	78.8
2010	Glyceryl-ether monooxygenase inhibitor	11	85.7
2011	Glycine C-acetyltransferase inhibitor	12	90.5
2012	Glycine N-acyltransferase inhibitor	6	98.8
2013	Glycine N-benzoyltransferase inhibitor	6	98.7
2014	Glycine N-choloyltransferase inhibitor	10	99.3
2015	Glycine N-methyltransferase inhibitor	9	99.3
2016	Glycine amidinotransferase inhibitor	5	94.7
2017	Glycine dehydrogenase (cytochrome) inhibitor	6	78.5
2018	Glycine dehydrogenase (decarboxylating) inhibitor	3	98.1
2019	Glycine hydroxymethyltransferase inhibitor	30	96.2
2020	Glycine receptor agonist	13	93.7
2021	Glycine receptor antagonist	20	90.1
2022	Glycine transaminase inhibitor	7	99.2
2023	Glycine transporter 1 inhibitor	449	99.7
2024	Glycine transporter 2 inhibitor	44	97.7
2025	Glycine transporter inhibitor	510	99.1
2026	Glycine-tRNA ligase inhibitor	10	89.8
2027	Glycogen (starch) synthase inhibitor	26	94.1
2028	Glycogen synthase kinase-3 alpha inhibitor	101	99.4
2029	Glycogen synthase kinase-3 beta inhibitor	473	98.9
2030	Glycogen synthase kinase-3 inhibitor	857	98.9
2031	Glycogenin glucosyltransferase inhibitor	8	99.6
2032	Glycolaldehyde dehydrogenase inhibitor	6	99.3
2033	Glycolate dehydrogenase inhibitor	3	96.9
2034	Glycolipid 2-alpha-mannosyltransferase inhibitor	9	99.7
2035	Glycolipid 3-alpha-mannosyltransferase inhibitor	12	99.6
2036	Glycopeptide alpha-N-acetylgalactosaminidase inhibitor	8	98.2
2037	Glycoprotein 3-alpha-L-fucosyltransferase inhibitor	10	97.2
2038	Glycoprotein-fucosylgalactoside alpha-N-acetylgalactosaminyltransferase inhibitor	9	95.3
2039	Glycosylceramidase inhibitor	14	99.1
2040	Glycosylphosphatidylinositol diacylglycerol-lyase inhibitor	18	96.8
2041	Glycosylphosphatidylinositol phospholipase D inhibitor	4	86.9
2042	Glyoxylate oxidase inhibitor	3	97.4
2043	Glyoxylate reductase (NADP+) inhibitor	12	92.4
2044	Glyoxylate reductase inhibitor	4	91.4
2045	Gonadotropin antagonist	24	88.3

2046	Gonadotropin-releasing hormone	4	96.4
2047	Gout treatment	108	93.8
2048	Granulocyte macrophage colony stimulating factor agonist	12	97.3
2049	Granulocyte stimulating factor agonist	31	99.4
2050	Granzyme A inhibitor	9	97.2
2051	Granzyme B inhibitor	23	96.4
2052	Growth factor agonist	358	93.5
2053	Growth factor antagonist	2746	97.0
2054	Growth factor receptor-bound protein 2 antagonist	70	100.0
2055	Growth hormone agonist	11	95.1
2056	Growth hormone antagonist	8	75.9
2057	Growth hormone release inhibitor	70	99.6
2058	Growth hormone release promoting	93	99.0
2059	Growth hormone releasing factor agonist	446	99.5
2060	Growth hormone releasing factor antagonist	45	99.9
2061	Growth stimulant	64	93.8
2062	Guanidinoacetase inhibitor	6	97.6
2063	Guanidinoacetate N-methyltransferase inhibitor	6	97.5
2064	Guanidinoacetate kinase inhibitor	12	90.5
2065	Guanidinobutyrase inhibitor	13	99.0
2066	Guanidinodeoxy-scyllo-inositol-4-phosphatase inhibitor	3	99.2
2067	Guanidinopropionase inhibitor	5	99.3
2068	Guanine deaminase inhibitor	13	98.1
2069	Guanosine-3',5'-bis(diphosphate) 3'-diphosphatase inhibitor	4	91.7
2070	Guanylate cyclase 1 inhibitor	13	100.0
2071	Guanylate cyclase 1 stimulant	10	93.6
2072	Guanylate cyclase inhibitor	58	97.1
2073	Guanylate cyclase stimulant	66	95.8
2074	Guanylate kinase inhibitor	15	98.8
2075	Gynecological disorders treatment	1082	98.1
2076	H ⁺ -exporting ATPase inhibitor	12	92.1
2077	H ⁺ -transporting two-sector ATPase inhibitor	7	94.0
2078	H ⁺ /K ⁺ -transporting ATPase inhibitor	474	97.8
2079	HCV IRES inhibitor	8	83.3
2080	HCV NS3-helicase inhibitor	5	94.9
2081	HCV NS3/NS4A protease inhibitor	641	98.8
2082	HCV NS5A inhibitor	20	100.0
2083	HCV NS5B polymerase inhibitor	331	99.4
2084	HDL-cholesterol increasing	174	95.4
2085	HERG 1 channel antagonist	38	93.9
2086	HERG channel antagonist	140	92.1
2087	HIV attachment inhibitor	14	90.5
2088	HIV fusion inhibitor	4	100.0
2089	HIV-1 integrase (3'-Processing) inhibitor	510	98.3
2090	HIV-1 integrase (Overall Integration) inhibitor	69	96.5
2091	HIV-1 integrase (Strand Transfer) inhibitor	532	98.5
2092	HIV-1 integrase inhibitor	898	97.8
2093	HIV-1 protease inhibitor	2365	99.4
2094	HIV-1 reverse transcriptase inhibitor	1747	98.9
2095	HIV-2 retropepsin inhibitor	16	99.9
2096	HIV-2 reverse transcriptase inhibitor	3	98.2
2097	HLA-A2 antigen antagonist	188	99.9
2098	HMG CoA reductase inhibitor	453	99.3
2099	HMG CoA synthase inhibitor	5	99.4
2100	HMGCS2 expression enhancer	5	93.5
2101	HMOX1 expression enhancer	5	83.5
2102	Hair growth stimulant	478	96.9
2103	Hallucinogen	159	84.1
2104	Haloacetate dehalogenase inhibitor	3	99.3
2105	Haloalkane dehalogenase inhibitor	4	99.7
2106	Heart failure treatment	1568	94.3
2107	Heat shock protein 27 antagonist	3	93.5
2108	Heat shock protein 70 agonist	26	90.9
2109	Heat shock protein 70 antagonist	6	93.8

2110	Heat shock protein 90 antagonist	216	98.0
2111	Heat shock protein agonist	27	88.9
2112	Heat shock protein antagonist	225	97.7
2113	Hedgehog signaling activator	4	100.0
2114	Hedgehog signaling inhibitor	83	97.3
2115	Helicase E1 (Human papillomavirus) inhibitor	28	100.0
2116	Hematinic	19	92.8
2117	Hematopoietic	89	91.7
2118	Hematopoietic inhibitor	18	90.4
2119	Heme oxygenase inhibitor	5	100.0
2120	Heme oxygenase stimulant	4	99.9
2121	Hemostatic	107	90.5
2122	Heparan-alpha-glucosaminide N-acetyltransferase inhibitor	12	98.1
2123	Heparanase inhibitor	72	99.2
2124	Heparin and LMW heparins	3	90.6
2125	Heparin epidermal growth factor antagonist	114	100.0
2126	Hepatic disorders treatment	745	90.2
2127	Hepatocyte growth factor agonist	7	87.4
2128	Hepatocyte growth factor antagonist	401	99.0
2129	Hepatocyte nuclear factor 4 alpha agonist	6	100.0
2130	Hepatocyte nuclear factor 4 alpha antagonist	6	91.7
2131	Hepatocyte nuclear factor agonist	6	100.0
2132	Hepatocyte nuclear factor antagonist	6	91.7
2133	Hepatoprotectant	308	89.7
2134	Hepatotoxic	460	82.0
2135	Hexokinase inhibitor	21	97.0
2136	Hexokinase stimulant	115	99.1
2137	High-mannose-oligosaccharide beta-1,4-N-acetylglucosaminyltransferase inhibitor	3	99.7
2138	Hippurate hydrolase inhibitor	4	99.0
2139	Hirsutism treatment	82	98.5
2140	Histamine H1 receptor agonist	4	99.2
2141	Histamine H1 receptor antagonist	684	97.5
2142	Histamine H2 receptor agonist	30	96.6
2143	Histamine H2 receptor antagonist	311	97.3
2144	Histamine H3 receptor agonist	55	99.9
2145	Histamine H3 receptor antagonist	1350	99.6
2146	Histamine H4 receptor antagonist	97	99.8
2147	Histamine N-methyltransferase inhibitor	44	95.4
2148	Histamine agonist	99	97.4
2149	Histamine antagonist	2471	96.1
2150	Histamine release inhibitor	121	86.1
2151	Histamine release stimulant	32	89.7
2152	Histidine N-acetyltransferase inhibitor	6	81.3
2153	Histidine ammonia-lyase inhibitor	34	98.3
2154	Histidine decarboxylase inhibitor	33	97.7
2155	Histidine kinase inhibitor	4	92.6
2156	Histidine-tRNA ligase inhibitor	19	99.2
2157	Histidinol dehydrogenase inhibitor	21	93.2
2158	Histidinol-phosphatase inhibitor	6	96.8
2159	Histone acetylation inducer	19	100.0
2160	Histone acetyltransferase inhibitor	26	88.1
2161	Histone deacetylase 1 inhibitor	325	99.6
2162	Histone deacetylase 1A inhibitor	8	100.0
2163	Histone deacetylase 1B inhibitor	7	100.0
2164	Histone deacetylase 2 inhibitor	91	99.7
2165	Histone deacetylase 3 inhibitor	20	96.7
2166	Histone deacetylase 4 inhibitor	18	99.3
2167	Histone deacetylase 6 inhibitor	55	99.1
2168	Histone deacetylase 8 inhibitor	35	98.6
2169	Histone deacetylase SIRT1 inhibitor	39	96.1
2170	Histone deacetylase SIRT1 stimulant	30	99.3
2171	Histone deacetylase SIRT2 inhibitor	20	97.8
2172	Histone deacetylase SIRT2 stimulant	5	99.9
2173	Histone deacetylase class I inhibitor	382	99.7

2174	Histone deacetylase class II inhibitor	63	99.6
2175	Histone deacetylase class III inhibitor	47	96.6
2176	Histone deacetylase class IIa inhibitor	26	99.6
2177	Histone deacetylase class IIb inhibitor	55	99.1
2178	Histone deacetylase inhibitor	1523	98.7
2179	Histone deacetylase stimulant	31	99.5
2180	Histone-arginine N-methyltransferase inhibitor	9	99.3
2181	Histone-lysine N-methyltransferase inhibitor	5	99.8
2182	Homoaconitate hydratase inhibitor	3	98.6
2183	Homocitrate synthase inhibitor	18	97.8
2184	Homocysteine S-methyltransferase inhibitor	4	99.4
2185	Homocysteine desulfhydrase inhibitor	8	98.8
2186	Homogentisate 1,2-dioxygenase inhibitor	12	95.2
2187	Homoisocitrate dehydrogenase inhibitor	3	100.0
2188	Homoserine O-acetyltransferase inhibitor	11	99.7
2189	Homoserine O-succinyltransferase inhibitor	3	99.7
2190	Homoserine dehydrogenase inhibitor	14	88.9
2191	Homoserine kinase inhibitor	24	98.0
2192	Homospermidine synthase inhibitor	4	99.3
2193	Horriylsin inhibitor	3	98.0
2194	Hot flush treatment	91	98.3
2195	HslIV component of HslUV peptidase inhibitor	7	78.2
2196	Huntington's disease treatment	134	95.0
2197	Hyaluronic acid agonist	4	93.5
2198	Hyaluronidase inhibitor	3	94.3
2199	Hydrogen dehydrogenase inhibitor	3	88.7
2200	Hydrolase inhibitor	37	74.2
2201	Hydroperoxide dehydratase inhibitor	12	98.8
2202	Hydroxyacylglutathione hydrolase inhibitor	55	97.2
2203	Hydroxylamine oxidase inhibitor	6	90.0
2204	Hydroxylamine reductase (NADH) inhibitor	18	86.9
2205	Hydroxylamine reductase inhibitor	6	86.4
2206	Hydroxylysine kinase inhibitor	10	99.6
2207	Hydroxymethylbilane synthase inhibitor	11	95.6
2208	Hydroxymethylglutaryl-CoA lyase inhibitor	7	94.8
2209	Hydroxymethylglutaryl-CoA reductase inhibitor	5	99.4
2210	Hydroxypyruvate reductase inhibitor	17	99.5
2211	Hydroxyquinol 1,2-dioxygenase inhibitor	9	99.6
2212	Hydroxysteroid dehydrogenase inhibitor	3	93.8
2213	Hypercalcaemic	20	80.6
2214	Hypercalcemia treatment	44	94.7
2215	Hypercholesterolemic	10	83.8
2216	Hyperglycemic	49	74.6
2217	Hyperparathyroidism treatment	59	98.9
2218	Hyperprolactinemia treatment	9	97.5
2219	Hypertensive	332	84.8
2220	Hypertensive, ophthalmic	11	95.7
2221	Hyperthermic	179	75.2
2222	Hypnotic	711	91.7
2223	Hypocalcaemic	38	85.3
2224	Hypogonadism treatment	125	99.9
2225	Hypokalemia	27	79.7
2226	Hypolipemic	1892	90.5
2227	Hyponitrite reductase inhibitor	3	97.5
2228	Hypothermic	125	87.2
2229	Hypoxanthine phosphoribosyltransferase inhibitor	37	98.7
2230	Hypoxia inducible factor 1 alpha inhibitor	42	87.8
2231	I kappa B kinase 2 inhibitor	100	97.2
2232	I kappa B kinase inhibitor	157	96.6
2233	I(Ks) voltage-gated potassium channel antagonist	38	100.0
2234	IAP inhibitor	73	99.8
2235	IAP1 inhibitor	13	98.8
2236	IAP2 inhibitor	12	100.0
2237	ICAM 1 antagonist	147	98.4

2238	ICAM1 expression inhibitor	40	98.0
2239	IMP cyclohydrolase inhibitor	10	100.0
2240	Iduronate-2-sulfatase inhibitor	3	99.4
2241	IgA-specific metalloendopeptidase inhibitor	9	96.9
2242	IgA-specific serine endopeptidase inhibitor	6	96.9
2243	Ileal bile acid transport inhibitor	152	99.9
2244	Imidazoleacetate 4-monooxygenase inhibitor	13	98.8
2245	Imidazoleglycerol-phosphate dehydratase inhibitor	4	99.6
2246	Imidazoline I1 receptor agonist	3	97.8
2247	Imidazoline I1 receptor antagonist	41	100.0
2248	Imidazoline I2 receptor antagonist	140	100.0
2249	Imidazoline receptor agonist	6	96.7
2250	Imidazoline receptor antagonist	148	100.0
2251	Immunoglobulin E antagonist	42	94.5
2252	Immunoglobulin Fc receptor antagonist	27	97.9
2253	Immunomodulator	1653	88.9
2254	Immunomodulator (HIV)	32	70.2
2255	Immunostimulant	998	91.8
2256	Immunostimulant (HIV)	18	70.0
2257	Immunosuppressant	1911	87.5
2258	Immunosuppressant Cyclosporine-like	19	100.0
2259	Indanol dehydrogenase inhibitor	13	92.2
2260	Indole-3-acetaldehyde reductase (NADPH) inhibitor	11	99.1
2261	Indoleacetaldoxime dehydratase inhibitor	12	91.9
2262	Indoleamine-pyrrole 2,3-dioxygenase inhibitor	90	98.5
2263	Indolepyruvate C-methyltransferase inhibitor	4	97.0
2264	Inducible nitric oxide synthase inhibitor	623	97.6
2265	Inflammatory Bowel disease treatment	1307	89.2
2266	Inorganic diphosphatase inhibitor	28	94.9
2267	Inosine kinase inhibitor	4	100.0
2268	Inosine monophosphate dehydrogenase 1 inhibitor	40	99.6
2269	Inosine monophosphate dehydrogenase 2 inhibitor	332	99.9
2270	Inosine monophosphate dehydrogenase inhibitor	458	99.8
2271	Inosine nucleosidase inhibitor	4	99.0
2272	Inosine-adenosine-guanosine-nucleoside hydrolase inhibitor	4	100.0
2273	Inositol 1,4,5-triphosphate receptor 1 antagonist	9	100.0
2274	Inositol 1,4,5-triphosphate receptor antagonist	10	95.2
2275	Inositol 1,4,5-trisphosphate 3-kinase B inhibitor	10	100.0
2276	Inositol 1,4,5-trisphosphate 3-kinase inhibitor	10	100.0
2277	Inositol oxygenase inhibitor	34	94.9
2278	Inositol polyphosphate-5-phosphatase D stimulant	6	100.0
2279	Inositol-1(or 4)-monophosphatase inhibitor	22	98.1
2280	Inositol-3-phosphate synthase inhibitor	20	99.0
2281	Inositol-polyphosphate 5-phosphatase inhibitor	19	98.1
2282	Inositol-trisphosphate 3-kinase inhibitor	5	92.6
2283	Inotropic	44	92.4
2284	Insecticide	129	93.9
2285	Insulin and insulin analogs	16	77.5
2286	Insulin antagonist	28	86.1
2287	Insulin growth factor agonist	9	74.1
2288	Insulin growth factor antagonist	281	98.6
2289	Insulin like growth factor 1 agonist	8	79.5
2290	Insulin like growth factor 1 antagonist	237	98.3
2291	Insulin like growth factor 3 antagonist	44	100.0
2292	Insulin promoter	43	82.6
2293	Insulin secretagogues	254	95.5
2294	Insulin sensitizer	226	96.7
2295	Insulinotropin antagonist	7	89.6
2296	Insulysin inhibitor	12	89.5
2297	Integrin alpha1beta1 antagonist	42	99.4
2298	Integrin alpha2 antagonist	26	97.8
2299	Integrin alpha2beta1 antagonist	25	97.8
2300	Integrin alpha4 antagonist	1255	99.7
2301	Integrin alpha4beta1 antagonist	947	99.7

2302	Integrin alpha4beta7 antagonist	604	99.8
2303	Integrin alpha5beta1 antagonist	81	99.3
2304	Integrin alpha5beta6 antagonist	14	100.0
2305	Integrin alphaLbeta2 antagonist	38	100.0
2306	Integrin alphaVbeta1 antagonist	17	95.3
2307	Integrin alphaVbeta3 antagonist	34	99.3
2308	Integrin alphaVbeta5 antagonist	311	99.9
2309	Integrin alphaVbeta6 antagonist	79	99.9
2310	Integrin antagonist	1982	99.3
2311	Integrin-linked kinase inhibitor	13	100.0
2312	Interferon agonist	138	95.7
2313	Interferon alpha agonist	5	82.2
2314	Interferon antagonist	86	94.0
2315	Interferon gamma antagonist	85	94.4
2316	Interferon inducer	113	97.1
2317	Interleukin 1 antagonist	924	95.0
2318	Interleukin 1 beta converting enzyme inhibitor	190	98.5
2319	Interleukin 10 agonist	37	90.3
2320	Interleukin 10 antagonist	6	96.6
2321	Interleukin 12 agonist	131	96.0
2322	Interleukin 1a antagonist	17	93.8
2323	Interleukin 1b antagonist	500	96.8
2324	Interleukin 2 agonist	15	86.0
2325	Interleukin 2 antagonist	228	94.9
2326	Interleukin 4 antagonist	148	94.8
2327	Interleukin 5 antagonist	130	95.7
2328	Interleukin 6 antagonist	216	92.4
2329	Interleukin 8 antagonist	204	93.6
2330	Interleukin agonist	179	93.5
2331	Interleukin antagonist	1565	92.4
2332	Intermittent claudication treatment	12	79.4
2333	Inulinase inhibitor	4	98.3
2334	Iodide peroxidase inhibitor	21	96.8
2335	Iron antagonist	10	95.0
2336	Iron-cytochrome-c reductase inhibitor	3	98.3
2337	Irritable Bowel syndrome treatment	1412	94.5
2338	Isoamylase inhibitor	15	98.8
2339	Isocitrate dehydrogenase (NAD+) inhibitor	28	97.2
2340	Isocitrate dehydrogenase (NADP+) inhibitor	25	98.9
2341	Isocitrate lyase inhibitor	26	98.1
2342	Isoleucine-tRNA ligase inhibitor	11	99.7
2343	Isomaltulose synthase inhibitor	6	99.2
2344	Isopenicillin-N epimerase inhibitor	9	86.2
2345	Isopenicillin-N synthase inhibitor	8	96.6
2346	Isopentenyl-diphosphate DELTA-isomerase inhibitor	22	99.8
2347	Isoquinoline 1-oxidoreductase inhibitor	4	98.3
2348	Isovaleryl-CoA dehydrogenase inhibitor	6	98.3
2349	JNK mitogen-activated protein kinase inhibitor	52	93.6
2350	Janus tyrosine kinase 1 inhibitor	16	99.8
2351	Janus tyrosine kinase 2 inhibitor	163	97.7
2352	Janus tyrosine kinase 3 inhibitor	245	98.8
2353	Janus tyrosine kinase inhibitor	453	98.1
2354	Juvenile-hormone esterase inhibitor	86	99.9
2355	K(Ca) 3.1 channel activator	4	98.5
2356	K(Ca) 3.1 channel antagonist	41	98.5
2357	K(ir) 6.2 channel stimulant	13	95.7
2358	K(v) 2.1 channel antagonist	4	85.1
2359	K(v) 4.3 channel antagonist	27	96.7
2360	Kainate receptor 1 agonist	5	99.8
2361	Kainate receptor 1 antagonist	177	99.8
2362	Kainate receptor 2 antagonist	21	96.1
2363	Kainate receptor 3 antagonist	8	100.0
2364	Kainate receptor 4 antagonist	5	97.3
2365	Kainate receptor 5 antagonist	24	99.9

2366	Kainate receptor agonist	26	99.1
2367	Kainate receptor antagonist	335	99.4
2368	Kallikrein 13 inhibitor	3	99.6
2369	Kallikrein 3 inhibitor	22	96.4
2370	Kallikrein inhibitor	62	97.2
2371	Kanamycin kinase inhibitor	3	100.0
2372	Keratan sulfotransferase inhibitor	7	99.9
2373	Keratolytic	36	94.0
2374	Keratosis actinic (solar) treatment	71	95.6
2375	Ketohexokinase inhibitor	14	99.2
2376	Ketol-acid reductoisomerase inhibitor	10	91.6
2377	Ketosteroid monooxygenase inhibitor	5	100.0
2378	Kexin inhibitor	16	97.9
2379	KISS-1 receptor agonist	3	100.0
2380	Kidney function stimulant	9	71.2
2381	Kinase inhibitor	14	82.8
2382	Kinesin antagonist	507	99.0
2383	Kinesin-like spindle protein (Eg5) antagonist	507	99.0
2384	Kynureninase inhibitor	42	98.6
2385	Kynurenine 3 monooxygenase inhibitor	55	99.9
2386	L lactate dehydrogenase A inhibitor	16	100.0
2387	L lactate dehydrogenase A4 inhibitor	15	100.0
2388	L lactate dehydrogenase B inhibitor	6	100.0
2389	L lactate dehydrogenase B4 inhibitor	6	100.0
2390	L lactate dehydrogenase C inhibitor	16	100.0
2391	L lactate dehydrogenase C4 inhibitor	16	100.0
2392	L lactate dehydrogenase inhibitor	32	96.2
2393	L lactate dehydrogenase stimulant	5	78.2
2394	L(+)-Tartrate dehydratase inhibitor	7	99.9
2395	L-3-cyanoalanine synthase inhibitor	10	99.5
2396	L-Serine ammonia-lyase inhibitor	14	99.3
2397	L-amino-acid oxidase inhibitor	20	96.5
2398	L-aminoadipate-semialdehyde dehydrogenase inhibitor	9	99.3
2399	L-ascorbate peroxidase inhibitor	16	98.3
2400	L-fuconate dehydratase inhibitor	7	99.5
2401	L-galactonolactone oxidase inhibitor	8	98.8
2402	L-glucuronate reductase inhibitor	17	95.0
2403	L-glutamate oxidase inhibitor	3	95.0
2404	L-iditol 2-dehydrogenase inhibitor	100	97.5
2405	L-iduronidase inhibitor	5	98.7
2406	L-lactate dehydrogenase (cytochrome) inhibitor	6	99.8
2407	L-lysine 6-transaminase inhibitor	6	98.8
2408	L-lysine oxidase inhibitor	4	99.0
2409	L-threonine 3-dehydrogenase inhibitor	10	87.5
2410	LDL receptor expression enhancer	99	97.3
2411	LECT1 expression enhancer	9	100.0
2412	LFA antagonist	188	99.5
2413	LFA-1 antagonist	186	99.7
2414	Laccase inhibitor	19	95.2
2415	Lactaldehyde dehydrogenase inhibitor	6	99.8
2416	Lactaldehyde reductase (NADPH) inhibitor	4	98.8
2417	Lactaldehyde reductase inhibitor	4	98.4
2418	Lactamase A inhibitor	7	99.4
2419	Lactamase C inhibitor	5	96.2
2420	Lactase inhibitor	3	85.5
2421	Lactate 2-monooxygenase inhibitor	13	92.6
2422	Lactate-malate transhydrogenase inhibitor	5	99.4
2423	Lactose synthase inhibitor	14	88.2
2424	Lactosylceramide alpha-2,3-sialyltransferase inhibitor	20	97.4
2425	Lactoylglutathione lyase inhibitor	89	97.8
2426	Laminaribiose phosphorylase inhibitor	9	97.0
2427	Lanosterol 14 alpha demethylase inhibitor	77	94.8
2428	Lassitude treatment	18	94.0
2429	Lathosterol oxidase inhibitor	3	98.6

2430	Laxative	49	94.3
2431	Lck kinase inhibitor	537	98.0
2432	Leishmanolysin inhibitor	6	86.1
2433	Leucine dehydrogenase inhibitor	5	91.3
2434	Leucine transaminase inhibitor	5	99.1
2435	Leucine-tRNA ligase inhibitor	25	95.6
2436	Leucolysin inhibitor	6	97.8
2437	Leucyltransferase inhibitor	14	98.5
2438	Leukocyte elastase inhibitor	35	83.3
2439	Leukopoiesis inhibitor	23	83.6
2440	Leukopoiesis stimulant	9	82.0
2441	Leukotriene A4 hydrolase inhibitor	177	99.6
2442	Leukotriene B4 antagonist	476	98.1
2443	Leukotriene B4 receptor 1 antagonist	348	99.9
2444	Leukotriene B4 receptor 2 antagonist	34	100.0
2445	Leukotriene C antagonist	24	84.5
2446	Leukotriene C4 antagonist	13	90.2
2447	Leukotriene D4 antagonist	447	99.0
2448	Leukotriene E4 antagonist	42	96.6
2449	Leukotriene agonist	6	93.7
2450	Leukotriene antagonist	1057	97.3
2451	Leukotriene synthesis inhibitor	210	95.9
2452	Leukotriene-B4 20-monooxygenase inhibitor	5	94.6
2453	Leukotriene-C4 synthase inhibitor	9	86.9
2454	Levanase inhibitor	9	95.4
2455	Levansucrase inhibitor	5	94.4
2456	Licheninase inhibitor	6	97.3
2457	Ligase inhibitor	5	98.5
2458	Limulus clotting factor B inhibitor	4	82.9
2459	Limulus clotting factor C inhibitor	4	94.9
2460	Linoleate diol synthase inhibitor	15	88.1
2461	Linoleate isomerase inhibitor	22	99.4
2462	Linoleoyl-CoA desaturase inhibitor	6	95.3
2463	Lipase inhibitor	181	98.6
2464	Lipid metabolism regulator	133	86.6
2465	Lipid peroxidase inhibitor	304	91.5
2466	Lipocortins synthesis agonist	80	96.3
2467	Lipocortins synthesis antagonist	11	95.5
2468	Lipoprotein disorders treatment	4528	95.4
2469	Lipoprotein lipase inhibitor	18	87.8
2470	Lipoprotein lipase stimulant	23	87.8
2471	Lipotropic	15	97.8
2472	Lipoxin receptor agonist	12	100.0
2473	Lipoxygenase inhibitor	2039	96.6
2474	Lipoxygenase substrate	11	92.3
2475	Liver X receptor agonist	280	99.4
2476	Liver X receptor alpha agonist	79	99.1
2477	Liver X receptor antagonist	7	95.4
2478	Liver X receptor beta agonist	68	99.3
2479	Liver cirrhosis treatment	52	92.9
2480	Liver fibrosis treatment	281	95.1
2481	Lombricine kinase inhibitor	6	98.0
2482	Long-chain-acyl-CoA dehydrogenase inhibitor	6	99.3
2483	Long-chain-aldehyde dehydrogenase inhibitor	4	96.3
2484	Long-chain-fatty-acid-CoA ligase inhibitor	23	99.1
2485	Loop diuretic	8	86.6
2486	Luteinizing hormone-releasing hormone agonist	40	97.4
2487	Luteinizing hormone-releasing hormone antagonist	1145	98.8
2488	Luteolytic	8	99.8
2489	Lymphocyte kinase inhibitor	35	90.7
2490	Lymphocytopoiesis inhibitor	10	95.5
2491	Lysase inhibitor	10	82.6
2492	Lysine 2,3-aminomutase inhibitor	5	87.3
2493	Lysine 2-monooxygenase inhibitor	19	96.8

2494	Lysine 6-dehydrogenase inhibitor	3	98.6
2495	Lysine carboxypeptidase inhibitor	22	99.5
2496	Lysine decarboxylase inhibitor	10	98.7
2497	Lysine-tRNA ligase inhibitor	16	99.6
2498	Lysophosphatidic acid receptor 3 agonist	5	100.0
2499	Lysophosphatidic acid receptor agonist	13	100.0
2500	Lysophosphatidic acid receptor antagonist	4	84.9
2501	Lysosomal Pro-X carboxypeptidase inhibitor	8	95.7
2502	Lysostaphin inhibitor	3	96.0
2503	Lysozyme inhibitor	13	98.1
2504	Lysyl endopeptidase inhibitor	16	97.9
2505	Lysyl oxidase inhibitor	10	83.7
2506	M7G(5')pppN diphosphatase inhibitor	4	100.0
2507	MAO A inhibitor	312	98.0
2508	MAO B inhibitor	334	99.2
2509	MAO inhibitor	745	96.5
2510	MAO-A substrate	16	90.2
2511	MAO-B substrate	8	99.9
2512	MAP kinase 10 inhibitor	115	98.1
2513	MAP kinase 14 inhibitor	584	99.4
2514	MAP kinase 8 inhibitor	17	83.0
2515	MAP kinase 9 inhibitor	66	96.7
2516	MAP kinase inhibitor	1410	97.2
2517	MAP kinase kinase 1 inhibitor	11	98.4
2518	MAP kinase kinase 4 inhibitor	18	99.3
2519	MAP kinase kinase 7 inhibitor	17	98.7
2520	MAP kinase kinase inhibitor	334	98.9
2521	MAP kinase kinase kinase inhibitor	37	96.1
2522	MAP kinase stimulant	5	83.7
2523	MAP-kinase-activated kinase 1 inhibitor	17	95.7
2524	MAP-kinase-activated kinase 2 inhibitor	120	98.4
2525	MAP-kinase-activated kinase inhibitor	141	97.5
2526	MAP3K11 inhibitor	6	99.9
2527	MAP3K5 inhibitor	4	100.0
2528	MAP3K8 inhibitor	18	99.7
2529	MAP3K9 inhibitor	10	90.7
2530	MARK1 protein inhibitor	7	100.0
2531	MDM2 inhibitor	101	97.3
2532	MEK inhibitor	165	98.6
2533	MEK1 inhibitor	73	98.1
2534	MEK2 inhibitor	28	98.9
2535	MET tyrosine kinase inhibitor	17	94.1
2536	MMP1 expression inhibitor	5	80.1
2537	MMP9 expression inhibitor	3	93.3
2538	MO15-related protein kinase Pfmrk inhibitor	14	93.1
2539	Macrocin O-methyltransferase inhibitor	9	100.0
2540	Macrophage colony stimulating factor agonist	4	80.7
2541	Macrophage colony stimulating factor antagonist	167	99.2
2542	Macrophage elastase inhibitor	151	99.0
2543	Macrophage migration inhibitory factor inhibitor	70	99.4
2544	Macrophage scavenger receptor antagonist	7	100.0
2545	Macrophage stimulant	5	96.6
2546	Macular degeneration treatment	255	93.7
2547	Magnesium-protoporphyrin IX methyltransferase inhibitor	11	97.6
2548	Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor	11	96.7
2549	Magnolysin inhibitor	6	99.9
2550	Maillard reaction inhibitor	34	88.0
2551	Malate dehydrogenase (NADP+) inhibitor	9	99.1
2552	Malate dehydrogenase (acceptor) inhibitor	12	85.7
2553	Malate dehydrogenase (decarboxylating) inhibitor	20	99.4
2554	Malate dehydrogenase (oxaloacetate-decarboxylating) (NADP+) inhibitor	21	99.4
2555	Malate dehydrogenase (oxaloacetate-decarboxylating) inhibitor	16	98.2
2556	Malate dehydrogenase inhibitor	66	93.5
2557	Malate oxidase inhibitor	5	88.4

2558	Malate synthase inhibitor	18	99.0
2559	Malate-CoA ligase inhibitor	5	98.3
2560	Male reproductive dysfunction treatment	569	94.7
2561	Maleate hydratase inhibitor	11	99.4
2562	Maleate isomerase inhibitor	6	94.8
2563	Maleylacetate reductase inhibitor	4	100.0
2564	Maleylacetoacetate isomerase inhibitor	6	99.5
2565	Malonate-semialdehyde dehydrogenase inhibitor	3	99.3
2566	Malonyl-CoA decarboxylase inhibitor	19	98.3
2567	Maltose-transporting ATPase inhibitor	4	97.5
2568	Malyl-CoA lyase inhibitor	6	98.0
2569	Mandelate 4-monooxygenase inhibitor	11	95.5
2570	Mandelate racemase inhibitor	27	99.5
2571	Manganese peroxidase inhibitor	6	90.7
2572	Mannan endo-1,4-beta-mannosidase inhibitor	3	93.6
2573	Mannan endo-1,6-alpha-mannosidase inhibitor	4	98.8
2574	Mannitol 2-dehydrogenase inhibitor	5	100.0
2575	Mannitol-1-phosphatase inhibitor	3	98.0
2576	Mannitol-1-phosphate 5-dehydrogenase inhibitor	18	98.9
2577	Mannokinase inhibitor	9	99.9
2578	Mannonate dehydratase inhibitor	9	98.9
2579	Mannose isomerase inhibitor	6	92.6
2580	Mannose-1-phosphate guanylyltransferase inhibitor	4	100.0
2581	Mannose-6-phosphate isomerase inhibitor	18	99.5
2582	Mannosidase inhibitor	59	98.3
2583	Mannosyl-glycoprotein endo-beta-N-acetylglucosaminidase inhibitor	9	98.1
2584	Mannosyl-oligosaccharide 1,2-alpha-mannosidase inhibitor	17	99.6
2585	Mannosyl-oligosaccharide glucosidase inhibitor	18	99.6
2586	Mannotetraose 2-alpha-N-acetylglucosaminyltransferase inhibitor	4	89.3
2587	MarA inhibitor	12	100.0
2588	Matrilysin inhibitor	187	99.3
2589	Matriptase inhibitor	6	99.8
2590	Matrix metalloproteinase (membrane-type) inhibitor	97	98.2
2591	Matrix metalloproteinase 1 (membrane-type) inhibitor	97	98.2
2592	Matrix metalloproteinase 1 inhibitor	1128	99.3
2593	Matrix metalloproteinase 2 (membrane-type) inhibitor	3	99.0
2594	Matrix metalloproteinase 3 (membrane-type) inhibitor	8	99.0
2595	Matrix metalloproteinase inhibitor	1601	98.7
2596	Mcl-1 antagonist	16	81.6
2597	Mediator release inhibitor	164	89.6
2598	Melanin inhibitor	32	92.9
2599	Melanin-concentrating hormone receptor 1 antagonist	509	98.9
2600	Melanin-concentrating hormone receptor antagonist	514	98.9
2601	Melanocortin MC-1 agonist	8	99.7
2602	Melanocortin MC-1 antagonist	71	99.7
2603	Melanocortin MC-4 agonist	15	99.6
2604	Melanocortin MC-4 antagonist	178	99.7
2605	Melanocortin agonist	23	99.5
2606	Melanocortin antagonist	234	98.8
2607	Melatonin 1 agonist	27	99.6
2608	Melatonin 1 antagonist	479	99.8
2609	Melatonin 1a antagonist	330	99.9
2610	Melatonin 1b antagonist	3	99.9
2611	Melatonin 2 agonist	15	100.0
2612	Melatonin 2 antagonist	233	99.9
2613	Melatonin 3 antagonist	100	99.9
2614	Melatonin 5 antagonist	68	99.9
2615	Melatonin agonist	99	99.4
2616	Melatonin antagonist	748	99.7
2617	Membrane dipeptidase inhibitor	44	95.3
2618	Membrane integrity agonist	16	83.1
2619	Membrane integrity antagonist	66	84.5
2620	Membrane permeability enhancer	47	88.3
2621	Membrane permeability inhibitor	43	78.7

2622	Membrane-oligosaccharide glycerophosphotransferase inhibitor	6	99.8
2623	Menopausal disorders treatment	79	86.6
2624	Menstruation disorders treatment	255	93.4
2625	Mental retardation treatment	7	99.0
2626	Meprin A inhibitor	13	96.8
2627	Meprin B inhibitor	3	97.6
2628	Metabolic disease treatment	170	89.8
2629	Metallocarboxypeptidase D inhibitor	7	95.1
2630	Metalloproteinase inhibitor	2054	98.6
2631	Metalloproteinase-11 inhibitor	31	98.1
2632	Metalloproteinase-2 inhibitor	1206	99.0
2633	Metalloproteinase-3 inhibitor	979	99.1
2634	Metalloproteinase-9 inhibitor	1256	99.1
2635	Methane monooxygenase inhibitor	13	89.6
2636	Methanol dehydrogenase inhibitor	3	98.0
2637	Methenyltetrahydrofolate cyclohydrolase inhibitor	7	99.1
2638	Methionine adenosyltransferase inhibitor	27	99.0
2639	Methionine decarboxylase inhibitor	6	98.8
2640	Methionine-tRNA ligase inhibitor	120	99.1
2641	Methionyl aminopeptidase 1 inhibitor	62	98.4
2642	Methionyl aminopeptidase 2 inhibitor	101	99.8
2643	Methionyl aminopeptidase inhibitor	176	98.5
2644	Methionyl-tRNA formyltransferase inhibitor	7	100.0
2645	Methylamine-glutamate N-methyltransferase inhibitor	3	94.9
2646	Methylaspartate ammonia-lyase inhibitor	8	98.1
2647	Methylaspartate mutase inhibitor	8	99.9
2648	Methylcrotonoyl-CoA carboxylase inhibitor	11	98.5
2649	Methylenetetrahydrofolate dehydrogenase (NADP+) inhibitor	10	98.6
2650	Methylenetetrahydrofolate reductase (NADPH) inhibitor	10	90.8
2651	Methylglutamate dehydrogenase inhibitor	7	98.5
2652	Methylglyoxal synthase inhibitor	15	99.8
2653	Methylmalonyl-CoA carboxytransferase inhibitor	7	100.0
2654	Methylmalonyl-CoA decarboxylase inhibitor	7	98.8
2655	Methylmalonyl-CoA epimerase inhibitor	9	99.9
2656	Methylmalonyl-CoA mutase inhibitor	11	98.9
2657	Methylthioadenosine nucleosidase inhibitor	16	99.3
2658	Methylumbelliferyl-acetate deacetylase inhibitor	7	86.4
2659	Mevalonate kinase inhibitor	11	97.8
2660	MexAB-OprM inhibitor	3	100.0
2661	Microbial collagenase inhibitor	514	99.4
2662	Microsomal triglyceride transfer protein inhibitor	419	99.9
2663	Microtubule formation inhibitor	378	94.4
2664	Microtubule formation stimulant	14	82.1
2665	Microtubule stabilization	513	99.2
2666	Mineralocorticoid	17	100.0
2667	Mineralocorticoid antagonist	242	98.7
2668	Mitochondrial electron transport inhibitor	4	90.0
2669	Mitochondrial intermediate peptidase inhibitor	6	97.2
2670	Mitochondrial processing peptidase inhibitor	6	82.2
2671	Monoamine oxidase substrate	24	92.2
2672	Monoamine uptake inhibitor	39	90.8
2673	Monocarboxylic acid transporter 1 inhibitor	6	97.0
2674	Monocarboxylic acid transporter inhibitor	6	97.0
2675	Monodehydroascorbate reductase (NADH) inhibitor	18	91.6
2676	Monophenol monooxygenase inhibitor	75	96.6
2677	Mood disorders treatment	8267	92.0
2678	Morphine 6-dehydrogenase inhibitor	13	95.3
2679	Motilin receptor agonist	105	99.1
2680	Motilin receptor antagonist	70	100.0
2681	Movement disorders treatment	43	93.9
2682	Mucinaminylserine mucinaminidase inhibitor	5	82.3
2683	Mucolytic	107	93.0
2684	Mucomembranous protector	36	81.8
2685	Muconate cycloisomerase inhibitor	4	99.7

2686	Mucorpepsin inhibitor	5	95.9
2687	Mucositis treatment	14	82.6
2688	Multidrug resistance-associated protein 1 inhibitor	204	97.9
2689	Multidrug resistance-associated protein inhibitor	206	97.3
2690	Multiple inositol-polyphosphate phosphatase inhibitor	5	100.0
2691	Multiple sclerosis treatment	943	90.2
2692	Muramoyltetrapeptide carboxypeptidase inhibitor	5	92.6
2693	Muscle relaxant	461	92.0
2694	Muscular dystrophy treatment	73	92.3
2695	Mutagenic	3650	97.0
2696	Mutagenic, Salmonella	3489	97.2
2697	Myasthenia Gravis treatment	22	78.5
2698	Myc inhibitor	9	86.6
2699	Mycodextranase inhibitor	6	99.3
2700	Mycolysin inhibitor	3	99.7
2701	Mycothiols-S-conjugate amidase inhibitor	3	87.9
2702	Myelin associated glycoprotein antagonist	4	100.0
2703	Myeloblastin inhibitor	4	97.9
2704	Myeloperoxidase inhibitor	4	81.4
2705	Myocardial infarction treatment	486	93.6
2706	Myocardial ischemia treatment	1698	94.9
2707	Myosin ATPase inhibitor	11	86.9
2708	Myosin-light-chain-phosphatase inhibitor	6	97.1
2709	Myristoyl transferase 1 inhibitor	3	100.0
2710	Myristoyl transferase inhibitor	80	100.0
2711	Myt1 kinase inhibitor	11	98.0
2712	N-(5-amino-5-carboxypentanoyl)-L-cysteinyl-D-valine synthase inhibitor	8	97.9
2713	N-(long-chain-acyl)ethanolamine deacylase inhibitor	7	96.8
2714	N-Acetylated alpha-linked acidic dipeptidase inhibitor	152	99.9
2715	N-Acyl-D-amino-acid deacylase inhibitor	4	98.5
2716	N-Acyl-D-aspartate deacylase inhibitor	3	98.0
2717	N-Carbamoyl-D-amino acid hydrolase inhibitor	5	98.2
2718	N-acetyl-gamma-glutamyl-phosphate reductase inhibitor	3	98.6
2719	N-acetylgalactosamine-4-sulfatase inhibitor	3	100.0
2720	N-acetylglucosamine kinase inhibitor	15	99.1
2721	N-acetylglucosamine-6-phosphate deacetylase inhibitor	10	99.2
2722	N-acetylglucosaminylidiphosphodolichol N-acetylglucosaminyltransferase inhibitor	6	99.7
2723	N-acetylglucosaminylidiphosphoundecaprenol N-acetyl-beta-D-mannosaminyltransferase inhibitor	3	93.4
2724	N-acetylglucosamine synthase inhibitor	6	95.9
2725	N-acetylglucosaminide beta-1,3-N-acetylglucosaminyltransferase inhibitor	5	96.2
2726	N-acetylglucosaminide beta-1,6-N-acetylglucosaminyl-transferase inhibitor	7	99.6
2727	N-acetylmuramoyl-L-alanine amidase inhibitor	12	99.2
2728	N-acetylneuraminate 4-O-acetyltransferase inhibitor	3	97.3
2729	N-acetylneuraminate 7-O(or 9-O)-acetyltransferase inhibitor	6	80.7
2730	N-acetylneuraminate lyase inhibitor	14	99.0
2731	N-acetylneuraminate synthase inhibitor	4	98.8
2732	N-acylmannosamine kinase inhibitor	5	87.8
2733	N-acylneuraminate cytidyltransferase inhibitor	15	99.1
2734	N-benzyloxycarbonylglycine hydrolase inhibitor	6	87.6
2735	N-carbamoyl-L-amino-acid hydrolase inhibitor	10	98.0
2736	N-formylglutamate deformylase inhibitor	16	99.3
2737	N-formylmethionyl-peptidase inhibitor	3	96.2
2738	N-hydroxy-2-acetamidofluorene reductase inhibitor	3	97.6
2739	N-hydroxyarylamine O-acetyltransferase inhibitor	11	83.7
2740	N-methyl-2-oxoglutaramate hydrolase inhibitor	9	96.7
2741	N-methylhydantoinase (ATP-hydrolysing) inhibitor	5	96.4
2742	N4-(beta-N-acetylglucosaminyl)-L-asparaginase inhibitor	10	98.0
2743	N6-methyl-lysine oxidase inhibitor	4	98.0
2744	NAD(P)+ transhydrogenase (AB-specific) inhibitor	32	97.4
2745	NAD(P)+ transhydrogenase (B-specific) inhibitor	11	95.9
2746	NAD(P)+-arginine ADP-ribosyltransferase inhibitor	11	85.5
2747	NAD(P)H dehydrogenase (quinone) 1 inhibitor	3	98.3
2748	NAD(P)H dehydrogenase (quinone) inhibitor	86	98.0
2749	NAD+ diphosphatase inhibitor	11	99.0

2750	NAD+ kinase inhibitor	20	96.4
2751	NAD+ nucleosidase inhibitor	22	99.4
2752	NAD+ synthase (glutamine-hydrolysing) inhibitor	4	97.8
2753	NAD+-dinitrogen-reductase ADP-D-ribosyltransferase inhibitor	3	99.3
2754	NADH dehydrogenase (ubiquinone) inhibitor	14	71.0
2755	NADH dehydrogenase inhibitor	17	95.3
2756	NADH kinase inhibitor	3	97.1
2757	NADH oxidase inhibitor	18	100.0
2758	NADH peroxidase inhibitor	5	79.7
2759	NADPH oxidase inhibitor	16	93.4
2760	NADPH oxidoreductase inhibitor	20	98.8
2761	NADPH peroxidase inhibitor	4	89.7
2762	NADPH-cytochrome-c2 reductase inhibitor	3	86.6
2763	NADPH-ferrihemoprotein reductase inhibitor	10	86.4
2764	NADPH:quinone reductase inhibitor	17	97.1
2765	NAT1 substrate	13	99.7
2766	NAT2 substrate	24	94.0
2767	NF-E2-related factor 2 stimulant	9	93.6
2768	NMDA 2 receptor antagonist	941	98.9
2769	NMDA 2A receptor antagonist	568	99.4
2770	NMDA 2B receptor antagonist	396	99.0
2771	NMDA receptor agonist	164	98.0
2772	NMDA receptor antagonist	3137	97.8
2773	NMDA receptor glutamate site antagonist	3	100.0
2774	NMDA receptor glycine site B antagonist	5	99.9
2775	NMDA receptor glycine site agonist	127	98.8
2776	NMDA receptor glycine site antagonist	532	99.7
2777	NMDA receptor phencyclidine site antagonist	185	99.8
2778	NMDA receptor polyamine site agonist	3	99.9
2779	NMDA receptor polyamine site antagonist	5	93.7
2780	NMN nucleosidase inhibitor	17	99.3
2781	NOS2 expression inhibitor	37	93.7
2782	NOS3 expression stimulant	58	99.5
2783	NTPase/helicase (JEV) inhibitor	3	100.0
2784	NTPase/helicase (WNF) inhibitor	9	100.0
2785	Na+ K+ transporting ATPase inhibitor	147	98.4
2786	Na+-transporting two-sector ATPase inhibitor	7	82.6
2787	Naphthalene 1,2-dioxygenase inhibitor	3	96.1
2788	Narcolepsy treatment	12	96.0
2789	Narcotic	106	94.5
2790	Narcotic antagonist	74	95.5
2791	Nardilysin inhibitor	8	92.7
2792	Nav1.1 sodium channel antagonist	115	97.8
2793	Nav1.2 sodium channel antagonist	43	97.7
2794	Nav1.3 sodium channel antagonist	15	100.0
2795	Nav1.4 sodium channel antagonist	19	98.4
2796	Nav1.5 sodium channel antagonist	19	87.4
2797	Nav1.7 sodium channel antagonist	40	98.8
2798	Nav1.8 sodium channel antagonist	9	98.4
2799	Necroptosis inhibitor	6	94.1
2800	Necrosis treatment	6	100.0
2801	Neolactotetraosylceramide alpha-2,3-sialyltransferase inhibitor	6	99.1
2802	Nephrotoxic	422	84.5
2803	Nerve growth factor agonist	24	77.7
2804	Nerve growth factor antagonist	41	99.0
2805	Neuraminidase (Influenza A) inhibitor	168	100.0
2806	Neuraminidase (Influenza B) inhibitor	65	100.0
2807	Neuraminidase (influenza) inhibitor	198	99.8
2808	Neuraminidase inhibitor	232	98.0
2809	Neurodegenerative diseases treatment	942	93.5
2810	Neurokinin 1 antagonist	1296	99.5
2811	Neurokinin 2 antagonist	591	99.4
2812	Neurokinin 3 antagonist	232	99.5
2813	Neurokinin agonist	4	84.8

2814	Neurokinin antagonist	1824	99.3
2815	Neurolysin inhibitor	23	98.1
2816	Neuronal nicotinic receptor antagonist	597	99.4
2817	Neuronal nitric oxide synthase inhibitor	343	99.4
2818	Neuropathy treatment	22	98.1
2819	Neuropeptide FF agonist	8	88.0
2820	Neuropeptide FF antagonist	60	99.8
2821	Neuropeptide FF1 antagonist	27	99.7
2822	Neuropeptide FF2 agonist	8	88.0
2823	Neuropeptide S antagonist	3	100.0
2824	Neuropeptide Y agonist	9	99.7
2825	Neuropeptide Y antagonist	1160	98.7
2826	Neuropeptide Y1 agonist	6	100.0
2827	Neuropeptide Y1 antagonist	315	99.1
2828	Neuropeptide Y2 antagonist	40	98.3
2829	Neuropeptide Y4 antagonist	3	100.0
2830	Neuropeptide Y5 antagonist	730	99.3
2831	Neuropeptide agonist	18	93.2
2832	Neuropeptide antagonist	1223	98.8
2833	Neuroprotector	425	73.7
2834	Neuropsin inhibitor	5	98.6
2835	Neurotensin 1 receptor agonist	3	99.7
2836	Neurotensin 1 receptor antagonist	33	97.9
2837	Neurotensin 2 receptor antagonist	16	100.0
2838	Neurotensin 3 receptor antagonist	15	100.0
2839	Neurotensin receptor agonist	17	99.7
2840	Neurotensin receptor antagonist	81	99.4
2841	Neurotoxic	163	74.4
2842	Neurotransmitter agonist	7	77.7
2843	Neurotransmitter antagonist	9	82.4
2844	Neurotransmitter uptake inhibitor	3	89.9
2845	Neurotrophic factor	471	95.8
2846	Neurotrophic factor enhancer	72	93.5
2847	Neutral endopeptidase inhibitor	547	99.6
2848	Neutropenia treatment	48	100.0
2849	Neutrophil collagenase inhibitor	565	99.1
2850	Neutrophil fMLF receptor antagonist	23	100.0
2851	Nicotinamidase inhibitor	24	98.1
2852	Nicotinamide phosphoribosyltransferase inhibitor	17	97.2
2853	Nicotinamide-nucleotide adenylyltransferase inhibitor	8	99.0
2854	Nicotinamide-nucleotide amidase inhibitor	6	100.0
2855	Nicotinate dehydrogenase inhibitor	6	85.4
2856	Nicotinate phosphoribosyltransferase inhibitor	18	99.4
2857	Nicotinate-nucleotide diphosphorylase (carboxylating) inhibitor	33	99.2
2858	Nicotine dehydrogenase inhibitor	6	80.9
2859	Nicotinic acid receptor 1 agonist	102	98.8
2860	Nicotinic acid receptor 2 agonist	15	99.9
2861	Nicotinic acid receptor agonist	115	98.8
2862	Nicotinic alpha2beta4 receptor agonist	4	87.0
2863	Nicotinic alpha3beta4 receptor agonist	12	99.1
2864	Nicotinic alpha3beta4 receptor antagonist	4	89.9
2865	Nicotinic alpha4 receptor agonist	16	100.0
2866	Nicotinic alpha4beta2 receptor agonist	33	99.8
2867	Nicotinic alpha4beta2 receptor antagonist	10	87.6
2868	Nicotinic alpha4beta4 receptor agonist	3	90.5
2869	Nicotinic alpha6 receptor agonist	3	99.6
2870	Nicotinic alpha7 receptor agonist	535	99.4
2871	Nicotinic alpha7 receptor antagonist	19	99.8
2872	Nicotinic neuronal receptor agonist	611	98.9
2873	Niemann-Pick C1-like 1 protein antagonist	11	86.4
2874	Nitrate reductase (cytochrome) inhibitor	11	86.6
2875	Nitrate reductase inhibitor	31	93.7
2876	Nitric oxide antagonist	150	93.9
2877	Nitric oxide donor	244	98.8

2878	Nitric oxide scavenger	4	94.7
2879	Nitric oxide synthase inhibitor	1353	97.4
2880	Nitric-oxide reductase inhibitor	9	79.4
2881	Nitrilase inhibitor	18	98.0
2882	Nitrile hydratase inhibitor	22	98.4
2883	Nitrite reductase (NO-forming) inhibitor	3	94.6
2884	Nitrite reductase [NAD(P)H] inhibitor	18	87.3
2885	Nitrous-oxide reductase inhibitor	4	79.3
2886	Nociceptin (N/OFQ) receptor agonist	15	100.0
2887	Nociceptin (N/OFQ) receptor antagonist	133	98.7
2888	Non-steroidal antiinflammatory agent	1255	91.8
2889	Nootropic	842	76.2
2890	Nuclear receptor subfamily 4, group A, member 2 agonist	24	99.8
2891	Nuclease inhibitor	19	98.9
2892	Nucleoside deoxyribosyltransferase inhibitor	8	99.7
2893	Nucleoside oxidase (H2O2-forming) inhibitor	6	96.2
2894	Nucleoside phosphoacylhydrolase inhibitor	4	98.4
2895	Nucleoside transporters inhibitor	18	99.9
2896	Nucleoside-diphosphatase inhibitor	10	96.5
2897	Nucleoside-triphosphatase inhibitor	8	71.5
2898	Nucleoside-triphosphate diphosphatase inhibitor	7	100.0
2899	Nucleoside-triphosphate-adenylate kinase inhibitor	7	98.2
2900	Nucleotidase inhibitor	6	94.0
2901	Nucleotide diphosphatase inhibitor	39	97.6
2902	Nucleotide metabolism regulator	138	86.1
2903	Nucleotidyltransferase (FIV) inhibitor	15	99.5
2904	Nucleotidyltransferase inhibitor	18	99.8
2905	O-acetylhomoserine aminocarboxypropyltransferase inhibitor	15	97.4
2906	O-aminophenol oxidase inhibitor	12	91.0
2907	O6-alkylguanine-DNA alkyltransferase inhibitor	88	99.3
2908	Obsessive-compulsive disorder treatment	68	94.6
2909	Octadecanal decarbonylase inhibitor	6	99.2
2910	Octopamine agonist	67	99.9
2911	Octopamine antagonist	5	80.0
2912	Oleamide hydrolase inhibitor	50	100.0
2913	Oligo-1,6-glucosidase inhibitor	23	99.0
2914	Oligonucleotidase inhibitor	10	99.2
2915	Oligopeptidase B inhibitor	7	96.6
2916	Omega-amidase inhibitor	8	98.7
2917	Ompin inhibitor	4	86.7
2918	Opheline kinase inhibitor	3	97.4
2919	Ophthalmic drug	1903	89.5
2920	Opine dehydrogenase inhibitor	4	97.2
2921	Opioid agonist	459	97.7
2922	Opioid antagonist	2067	98.8
2923	Opioid delta 1 receptor antagonist	12	96.9
2924	Opioid delta 2 receptor antagonist	12	99.9
2925	Opioid delta receptor agonist	153	99.0
2926	Opioid delta receptor antagonist	1395	99.4
2927	Opioid dependency treatment	33	91.1
2928	Opioid kappa 1 receptor antagonist	90	99.1
2929	Opioid kappa 2 receptor antagonist	15	100.0
2930	Opioid kappa 2b receptor antagonist	14	100.0
2931	Opioid kappa 3 receptor antagonist	6	94.1
2932	Opioid kappa receptor agonist	130	97.7
2933	Opioid kappa receptor antagonist	1162	99.3
2934	Opioid mu 1 receptor antagonist	21	97.8
2935	Opioid mu 2 receptor antagonist	21	97.8
2936	Opioid mu receptor agonist	157	96.9
2937	Opioid mu receptor antagonist	1619	99.3
2938	Opioid partial agonist	8	99.7
2939	Orcinol 2-monooxygenase inhibitor	7	99.9
2940	Orexin receptor 1 antagonist	223	99.9
2941	Orexin receptor 2 antagonist	137	99.7

2942	Orexin receptor antagonist	406	99.9
2943	Ornithine carbamoyltransferase inhibitor	40	98.7
2944	Ornithine cyclodeaminase inhibitor	3	98.4
2945	Ornithine decarboxylase inhibitor	91	96.4
2946	Ornithine-oxo-acid transaminase inhibitor	39	95.7
2947	Orotate phosphoribosyltransferase inhibitor	36	99.3
2948	Orotate reductase (NADH) inhibitor	8	98.3
2949	Orotate reductase (NADPH) inhibitor	5	99.7
2950	Orotidylate decarboxylase inhibitor	4	99.9
2951	Orsellinate decarboxylase inhibitor	5	100.0
2952	Oryzin inhibitor	10	91.3
2953	Osmosis stimulant non-diuretic	3	87.5
2954	Osmotic diuretic	7	99.8
2955	Osteoarthritis treatment	339	95.3
2956	Osteoclast antagonist	23	96.4
2957	Ovulation inhibitor	16	86.5
2958	Oxalate oxidase inhibitor	13	94.5
2959	Oxaloacetate decarboxylase inhibitor	15	99.0
2960	Oxaloacetate tautomerase inhibitor	15	99.5
2961	Oxidizing agent	17	94.6
2962	Oxidoreductase inhibitor	82	83.7
2963	Oxoglutarate dehydrogenase (lipoamide) inhibitor	18	98.5
2964	Oxygen scavenger	14	82.0
2965	Oxytocic	26	95.7
2966	Oxytocin agonist	16	95.3
2967	Oxytocin antagonist	758	99.1
2968	P-benzoquinone reductase (NADPH) inhibitor	8	84.6
2969	P-glycoprotein 1 inhibitor	293	97.6
2970	P-glycoprotein inhibitor	469	96.3
2971	P-glycoprotein substrate	59	84.5
2972	P2 nucleoside transporter inhibitor	11	100.0
2973	P3 purinoceptor-like protein antagonist	35	100.0
2974	PRL phosphatase inhibitor	28	95.8
2975	Paget's disease treatment	45	97.0
2976	Palmitoyl-CoA hydrolase inhibitor	44	97.3
2977	Pancreatic disorders treatment	159	91.4
2978	Pancreatic elastase inhibitor	11	79.0
2979	Pancreatic endopeptidase E inhibitor	6	98.7
2980	Pancreatic ribonuclease inhibitor	10	90.8
2981	Pantetheine-phosphate adenylyltransferase inhibitor	16	95.8
2982	Pantoate 4-dehydrogenase inhibitor	3	99.2
2983	Pantoate-beta-alanine ligase inhibitor	25	96.6
2984	Pantothenase inhibitor	11	94.0
2985	Pantothenate kinase inhibitor	18	99.8
2986	Pappalysin-1 inhibitor	4	96.4
2987	Para amino benzoic acid antagonist	9	92.2
2988	Paraoxonase substrate	5	83.2
2989	Parathyroid hormone	5	84.2
2990	Parathyroid hormone antagonist	22	98.9
2991	Parathyroid hormone secretion stimulant	71	99.8
2992	Pectate lyase inhibitor	11	97.7
2993	Pectin lyase inhibitor	11	98.3
2994	Pediculicide	8	93.4
2995	Penicillin amidase inhibitor	10	95.3
2996	Penicillopepsin inhibitor	15	96.7
2997	Pepsin inhibitor	35	99.9
2998	Peptide alpha-N-acetyltransferase inhibitor	6	92.7
2999	Peptide deformylase inhibitor	160	99.0
3000	Peptide-N4-(N-acetyl-beta-glucosaminyl)asparagine amidase inhibitor	6	89.5
3001	Peptide-tryptophan 2,3-dioxygenase inhibitor	9	97.9
3002	Peptidoglycan beta-N-acetylmuramidase inhibitor	3	99.2
3003	Peptidoglycan glycosyltransferase inhibitor	4	90.6
3004	Peptidyl-Lys metalloendopeptidase inhibitor	22	94.3
3005	Peptidyl-dipeptidase B inhibitor	7	85.2

3006	Peptidyl-dipeptidase Dcp inhibitor	6	92.6
3007	Peptidyl-glycinamidase inhibitor	11	97.0
3008	Peptidylamidoglycolate lyase inhibitor	5	98.5
3009	Peptidylglycine monooxygenase inhibitor	38	98.3
3010	Peptidylprolyl isomerase inhibitor	328	99.0
3011	Peptidyltransferase inhibitor	20	88.8
3012	Periodontitis treatment	23	94.2
3013	Peristaltic stimulant	189	94.4
3014	Peroxidase inhibitor	15	92.7
3015	Peroxidase substrate	6	97.1
3016	Peroxisome proliferator-activated receptor agonist	1957	98.9
3017	Peroxisome proliferator-activated receptor alpha agonist	1005	99.2
3018	Peroxisome proliferator-activated receptor alpha antagonist	141	99.4
3019	Peroxisome proliferator-activated receptor antagonist	388	99.1
3020	Peroxisome proliferator-activated receptor delta agonist	409	99.6
3021	Peroxisome proliferator-activated receptor delta antagonist	82	99.9
3022	Peroxisome proliferator-activated receptor gamma agonist	938	98.6
3023	Peroxisome proliferator-activated receptor gamma antagonist	375	99.1
3024	PfA-M1 aminopeptidase inhibitor	7	97.9
3025	Phenol 2-monooxygenase inhibitor	25	95.6
3026	Phenol O-methyltransferase inhibitor	3	94.4
3027	Phenylacetaldehyde dehydrogenase inhibitor	5	98.7
3028	Phenylacetate-CoA ligase inhibitor	8	97.2
3029	Phenylalanine 2-monooxygenase inhibitor	6	99.9
3030	Phenylalanine 4-hydroxylase inhibitor	30	97.6
3031	Phenylalanine decarboxylase inhibitor	8	97.9
3032	Phenylalanine dehydrogenase inhibitor	19	98.4
3033	Phenylalanine racemase (ATP-hydrolysing) inhibitor	10	97.5
3034	Phenylalanine(histidine) transaminase inhibitor	4	97.7
3035	Phenylalanine-tRNA ligase inhibitor	13	96.5
3036	Phenylethanolamine N methyltransferase inhibitor	82	99.9
3037	Phenylpyruvate decarboxylase inhibitor	3	99.2
3038	Phenylpyruvate tautomerase inhibitor	5	100.0
3039	Phloroglucinol reductase inhibitor	13	91.5
3040	Phobic disorders treatment	4	79.9
3041	Phosphatase inhibitor	9	84.2
3042	Phosphate acetyltransferase inhibitor	14	98.0
3043	Phosphate butyryltransferase inhibitor	4	100.0
3044	Phosphate transporter inhibitor	19	97.2
3045	Phosphatidate cytidyltransferase inhibitor	17	97.8
3046	Phosphatidate phosphatase inhibitor	25	94.0
3047	Phosphatidylcholine-retinol O-acyltransferase inhibitor	4	81.8
3048	Phosphatidylcholine-sterol O-acyltransferase inhibitor	17	89.5
3049	Phosphatidylethanolamine N-methyltransferase inhibitor	5	78.8
3050	Phosphatidylglycerol-membrane-oligosaccharide glycerophosphotransferase inhibitor	3	99.5
3051	Phosphatidylglycerophosphatase inhibitor	8	96.4
3052	Phosphatidylinositol 3-kinase alpha inhibitor	105	99.0
3053	Phosphatidylinositol 3-kinase beta inhibitor	25	95.9
3054	Phosphatidylinositol 3-kinase delta inhibitor	23	97.4
3055	Phosphatidylinositol 3-kinase gamma inhibitor	40	98.5
3056	Phosphatidylinositol 3-kinase inhibitor	369	98.5
3057	Phosphatidylinositol 3-kinase p110alpha inhibitor	12	100.0
3058	Phosphatidylinositol 3-kinase p110beta inhibitor	3	99.8
3059	Phosphatidylinositol 3-kinase p110gamma inhibitor	3	99.8
3060	Phosphatidylinositol diacylglycerol-lyase inhibitor	14	93.0
3061	Phosphatidylinositol kinase inhibitor	418	96.8
3062	Phosphatidylserine decarboxylase inhibitor	10	92.6
3063	Phospho-N-acetylmuramoyl-pentapeptide-transferase inhibitor	123	99.9
3064	Phosphoadenylylsulfatase inhibitor	5	99.7
3065	Phosphodiesterase 10A inhibitor	64	99.9
3066	Phosphodiesterase 11A inhibitor	22	100.0
3067	Phosphodiesterase 1B inhibitor	8	100.0
3068	Phosphodiesterase 3A inhibitor	16	99.0
3069	Phosphodiesterase 4A inhibitor	195	99.6

3070	Phosphodiesterase 4B inhibitor	147	99.6
3071	Phosphodiesterase 4C inhibitor	16	99.9
3072	Phosphodiesterase 4D inhibitor	57	98.0
3073	Phosphodiesterase 5A inhibitor	105	99.3
3074	Phosphodiesterase 6A inhibitor	27	100.0
3075	Phosphodiesterase 6B inhibitor	12	94.4
3076	Phosphodiesterase 7A inhibitor	15	97.8
3077	Phosphodiesterase 9A inhibitor	12	100.0
3078	Phosphodiesterase I inhibitor	201	96.1
3079	Phosphodiesterase II inhibitor	50	96.8
3080	Phosphodiesterase III inhibitor	661	98.3
3081	Phosphodiesterase IV inhibitor	3739	98.9
3082	Phosphodiesterase IV stimulant	57	99.1
3083	Phosphodiesterase IX inhibitor	15	100.0
3084	Phosphodiesterase V inhibitor	758	98.8
3085	Phosphodiesterase V stimulant	51	100.0
3086	Phosphodiesterase VI inhibitor	114	99.3
3087	Phosphodiesterase VII inhibitor	236	99.5
3088	Phosphodiesterase X inhibitor	64	99.9
3089	Phosphodiesterase XI inhibitor	22	100.0
3090	Phosphodiesterase inhibitor	5519	97.1
3091	Phosphodiesterase stimulant	109	99.2
3092	Phosphoenolpyruvate carboxykinase (ATP) inhibitor	34	94.5
3093	Phosphoenolpyruvate carboxykinase (GTP) inhibitor	25	99.6
3094	Phosphoenolpyruvate carboxykinase (diphosphate) inhibitor	8	99.3
3095	Phosphoenolpyruvate carboxylase inhibitor	44	98.4
3096	Phosphoenolpyruvate mutase inhibitor	3	98.3
3097	Phosphoenolpyruvate-protein phosphotransferase inhibitor	4	98.7
3098	Phosphofructokinase-1 inhibitor	33	98.0
3099	Phosphoglucomutase inhibitor	16	99.3
3100	Phosphogluconate 2-dehydrogenase inhibitor	12	99.9
3101	Phosphogluconate dehydrogenase (decarboxylating) inhibitor	57	98.6
3102	Phosphoglycerate dehydrogenase inhibitor	16	99.5
3103	Phosphoglycerate kinase inhibitor	43	98.9
3104	Phosphoglycerate mutase inhibitor	10	98.8
3105	Phosphoglycerate phosphatase inhibitor	6	99.9
3106	Phosphoglycolate phosphatase inhibitor	12	99.0
3107	Phosphoinositide 5-phosphatase inhibitor	12	89.0
3108	Phosphoinositide dependent kinase 1 inhibitor	50	98.4
3109	Phosphoinositide phospholipase C inhibitor	9	93.4
3110	Phosphoketolase inhibitor	10	99.6
3111	Phosphokinase stimulant	3	99.4
3112	Phospholipase A1 inhibitor	17	93.2
3113	Phospholipase A2 IIa inhibitor	15	97.8
3114	Phospholipase A2 inhibitor	326	92.7
3115	Phospholipase C inhibitor	78	92.8
3116	Phospholipase D inhibitor	27	97.7
3117	Phospholipase D1 inhibitor	3	100.0
3118	Phospholipase D2 inhibitor	5	100.0
3119	Phospholipase inhibitor	418	92.5
3120	Phospholipid-translocating ATPase inhibitor	4	86.8
3121	Phosphomannomutase inhibitor	4	99.9
3122	Phosphomevalonate kinase inhibitor	14	99.0
3123	Phosphonoacetate hydrolase inhibitor	6	99.0
3124	Phosphopantothenoylcysteine decarboxylase inhibitor	7	93.1
3125	Phosphopyruvate hydratase inhibitor	7	100.0
3126	Phosphoribosylformylglycinamide cyclo-ligase inhibitor	3	100.0
3127	Phosphoribosylformylglycinamide synthase inhibitor	7	99.7
3128	Phosphoribosylglycinamide formyltransferase inhibitor	97	100.0
3129	Phosphoribulokinase inhibitor	10	99.1
3130	Phosphorylase a inhibitor	26	99.0
3131	Phosphorylase b inhibitor	5	96.3
3132	Phosphorylase inhibitor	140	97.1
3133	Phosphorylase kinase inhibitor	21	95.5

3134	Phosphoserine phosphatase inhibitor	12	98.8
3135	Phosphoserine transaminase inhibitor	5	99.9
3136	Photinus-luciferin 4-monooxygenase (ATP-hydrolysing) inhibitor	11	83.0
3137	Photosensitizer	63	94.8
3138	Phthalate 4,5-dioxygenase inhibitor	3	86.4
3139	Phytanoyl-CoA dioxygenase inhibitor	3	97.3
3140	Picornain 2A inhibitor	10	97.9
3141	Picornain 3C inhibitor	8	97.2
3142	Pim kinase inhibitor	47	96.7
3143	Pim-1 kinase inhibitor	29	95.8
3144	Pim-2 kinase inhibitor	13	92.2
3145	Pim-3 kinase inhibitor	9	100.0
3146	Pin1 inhibitor	5	87.9
3147	Pitriylsin inhibitor	10	92.6
3148	Plasmanylethanolamine desaturase inhibitor	8	97.6
3149	Plasmeprin I inhibitor	68	100.0
3150	Plasmeprin II inhibitor	87	99.9
3151	Plasmeprin inhibitor	97	99.8
3152	Plasmin inhibitor	135	99.2
3153	Plasminogen activator inhibitor	73	97.4
3154	Plasminogen activator inhibitor antagonist	155	98.9
3155	Plasminogen activator stimulant	14	96.9
3156	Plastoquinol-plastocyanin reductase inhibitor	7	93.4
3157	Platelet activating factor agonist	3	100.0
3158	Platelet activating factor alpha antagonist	104	98.6
3159	Platelet activating factor antagonist	1661	97.4
3160	Platelet activating factor beta antagonist	294	97.9
3161	Platelet adhesion inhibitor	16	85.5
3162	Platelet aggregation inhibitor	3086	91.2
3163	Platelet aggregation stimulant	12	91.7
3164	Platelet antagonist	1964	95.1
3165	Platelet derived growth factor receptor kinase inhibitor	25	88.8
3166	Platelet growth factor antagonist	766	98.7
3167	Platelet growth factor beta antagonist	186	99.3
3168	Plus-end-directed kinesin ATPase inhibitor	3	98.4
3169	Polar-amino-acid-transporting ATPase inhibitor	5	97.2
3170	Polarisation inhibitor	55	93.3
3171	Polarisation stimulant	9	91.1
3172	Polo-like kinase inhibitor	276	98.4
3173	Polo-like kinase-1 inhibitor	197	97.9
3174	Poly(3-hydroxybutyrate) depolymerase inhibitor	14	97.6
3175	Poly(ADP-ribose) glycohydrolase inhibitor	19	97.1
3176	Poly(alpha-L-gulonate) lyase inhibitor	5	97.3
3177	Poly(beta-D-mannuronate) lyase inhibitor	4	96.0
3178	Polyamine biosynthesis inhibitor	17	98.8
3179	Polyamine oxidase inhibitor	14	95.4
3180	Polyamine-transporting ATPase inhibitor	3	94.2
3181	Polygalacturonase inhibitor	6	96.0
3182	Polyneuridine-aldehyde esterase inhibitor	3	98.2
3183	Polynucleotide 5'-hydroxy-kinase inhibitor	15	91.5
3184	Polynucleotide adenylyltransferase inhibitor	27	94.5
3185	Polypeptide N-acetylgalactosaminyltransferase inhibitor	16	98.6
3186	Polyphosphate kinase inhibitor	4	99.4
3187	Polyphosphate-glucose phosphotransferase inhibitor	5	99.9
3188	Polyporopepsin inhibitor	6	81.1
3189	Polyribonucleotide nucleotidyltransferase inhibitor	9	90.3
3190	Porphobilinogen synthase inhibitor	22	98.3
3191	Postcoital contraceptive	42	99.0
3192	Postmenopausal disorders treatment	239	98.4
3193	Postsynaptic density protein 95 inhibitor	3	100.0
3194	Posttraumatic stress disorder treatment	30	94.4
3195	Potassium channel (ATP-sensitive) activator	172	97.9
3196	Potassium channel (ATP-sensitive) antagonist	229	98.8
3197	Potassium channel (Ca-activated) activator	186	97.2

3198	Potassium channel (Ca-activated) antagonist	275	97.9
3199	Potassium channel (Inward rectifier) 1 antagonist	79	99.9
3200	Potassium channel (Inward rectifier) 11 antagonist	36	100.0
3201	Potassium channel (Inward rectifier) activator	172	97.9
3202	Potassium channel (Inward rectifier) antagonist	380	98.9
3203	Potassium channel (Voltage-sensitive) activator	162	99.2
3204	Potassium channel (Voltage-sensitive) antagonist	923	96.1
3205	Potassium channel KCNQ activator	162	99.2
3206	Potassium channel KCNQ antagonist	8	99.7
3207	Potassium channel KCNQ2 activator	45	100.0
3208	Potassium channel KCNQ3 activator	6	98.4
3209	Potassium channel Kv1.1 antagonist	129	98.7
3210	Potassium channel Kv1.3 antagonist	199	99.0
3211	Potassium channel Kv1.5 antagonist	373	98.4
3212	Potassium channel activator	1426	98.0
3213	Potassium channel antagonist	1993	96.0
3214	Potassium channel intermediate-conductance Ca-activated 4 antagonist	10	100.0
3215	Potassium channel intermediate-conductance Ca-activated activator	4	98.5
3216	Potassium channel intermediate-conductance Ca-activated antagonist	50	98.5
3217	Potassium channel large-conductance Ca-activated activator	161	98.1
3218	Potassium channel small-conductance Ca-activated 3 activator	6	98.9
3219	Potassium channel small-conductance Ca-activated 3 antagonist	36	100.0
3220	Potassium channel small-conductance Ca-activated activator	9	99.9
3221	Potassium channel small-conductance Ca-activated antagonist	155	99.6
3222	Potassium sparing diuretic	21	73.3
3223	Pregnane X receptor agonist	11	88.1
3224	Pregnane X receptor antagonist	27	100.0
3225	Premature ejaculation treatment	112	98.0
3226	Premenstrual syndrome treatment	26	95.6
3227	Preneoplastic conditions treatment	8	85.8
3228	Prenyl-diphosphatase inhibitor	5	96.5
3229	Prephenate dehydratase inhibitor	23	99.3
3230	Prephenate dehydrogenase inhibitor	20	94.7
3231	Prepilin peptidase inhibitor	3	99.3
3232	Preterm labor treatment	87	97.3
3233	Prion diseases treatment	42	94.0
3234	Pro-opiomelanocortin converting enzyme inhibitor	5	92.4
3235	Procollagen C-endopeptidase inhibitor	17	95.5
3236	Procollagen N-endopeptidase inhibitor	7	96.6
3237	Procollagen galactosyltransferase inhibitor	13	99.6
3238	Procollagen glucosyltransferase inhibitor	13	99.2
3239	Procollagen-lysine 5-dioxygenase inhibitor	21	96.0
3240	Procollagen-proline 3-dioxygenase inhibitor	14	100.0
3241	Progesterone agonist	183	99.3
3242	Progesterone antagonist	614	99.6
3243	Progesterone receptor A antagonist	98	100.0
3244	Progesterone receptor B antagonist	66	99.9
3245	Progesterone receptor B1 antagonist	24	100.0
3246	Prokinetic	513	97.9
3247	Prokineticin receptor 1 antagonist	3	100.0
3248	Prolactin inhibitor	44	96.5
3249	Prolactin release inhibitor	63	98.1
3250	Prolactin stimulant	5	78.4
3251	Proliferative diseases treatment	13	83.5
3252	Proline dehydrogenase inhibitor	4	99.7
3253	Proline racemase inhibitor	17	99.2
3254	Proline transporter inhibitor	23	100.0
3255	Prolyl aminopeptidase inhibitor	13	93.1
3256	Prolyl endopeptidase inhibitor	324	98.1
3257	Propanediol dehydratase inhibitor	17	99.2
3258	Propionate CoA-transferase inhibitor	4	99.9
3259	Propionate-CoA ligase inhibitor	7	99.3
3260	Prostacyclin agonist	62	98.3
3261	Prostacyclin antagonist	109	99.2

3262	Prostaglandin A1 agonist	3	100.0
3263	Prostaglandin D2 agonist	9	97.4
3264	Prostaglandin D2 antagonist	167	99.5
3265	Prostaglandin E1 agonist	20	99.9
3266	Prostaglandin E1 antagonist	3	96.3
3267	Prostaglandin E2 agonist	120	99.6
3268	Prostaglandin E2 antagonist	303	97.4
3269	Prostaglandin EP1 antagonist	108	99.9
3270	Prostaglandin EP12 antagonist	50	100.0
3271	Prostaglandin EP2 agonist	37	100.0
3272	Prostaglandin EP2 antagonist	150	99.9
3273	Prostaglandin EP3 antagonist	154	99.4
3274	Prostaglandin EP4 agonist	70	100.0
3275	Prostaglandin EP4 antagonist	176	99.8
3276	Prostaglandin F2 alpha agonist	28	100.0
3277	Prostaglandin F2 alpha antagonist	25	96.2
3278	Prostaglandin H2 antagonist	380	99.8
3279	Prostaglandin agonist	393	98.8
3280	Prostaglandin antagonist	923	97.8
3281	Prostaglandin-A1 DELTA-isomerase inhibitor	4	91.6
3282	Prostaglandin-E2 9-reductase inhibitor	14	95.4
3283	Prostaglandin-E2 synthase 1 inhibitor	32	99.6
3284	Prostaglandin-I synthase inhibitor	25	99.6
3285	Prostate cancer treatment	752	90.5
3286	Prostate disorders treatment	416	90.1
3287	Prostatic (benign) hyperplasia treatment	2149	96.4
3288	Protease (Human cytomegalovirus) inhibitor	149	99.9
3289	Protease 3C (Human rhinovirus) inhibitor	177	99.3
3290	Protease 3C (Human rhinovirus) stimulant	15	100.0
3291	Protease activated receptor 1 antagonist	145	99.0
3292	Protease activated receptor antagonist	154	97.7
3293	Protease inhibitor	562	95.8
3294	Proteasome ATPase inhibitor	3	89.2
3295	Proteasome endopeptidase complex inhibitor	33	96.0
3296	Proteasome inhibitor	200	98.4
3297	Protein 23S ribosomal subunit inhibitor	3	90.2
3298	Protein 30S ribosomal subunit inhibitor	71	96.8
3299	Protein 50S ribosomal subunit inhibitor	112	98.7
3300	Protein C (activated) inhibitor	14	98.9
3301	Protein N-acetylglucosaminyltransferase inhibitor	8	99.4
3302	Protein disulfide-isomerase inhibitor	7	80.0
3303	Protein glycation inhibitor	4	100.0
3304	Protein kinase (CK1) delta inhibitor	4	100.0
3305	Protein kinase (CK1) epsilon inhibitor	5	90.5
3306	Protein kinase (CK1) inhibitor	11	80.7
3307	Protein kinase (CK2) inhibitor	65	96.4
3308	Protein kinase (CaMK, MLCK, PhK, SNF, KIN, NIM1, MAPKAP, POLO, CHK, ULK, RSK-2nd domain) inhibitor	301	99.0
3309	Protein kinase (Mos, Mil/Raf, MEKK, RIPK, TESK, LIMK, IRAK, ILK, Activin/TGF-beta) inhibitor	624	98.7
3310	Protein kinase (PKA, PKC, AKT, GRK, AGC-related, RSK, DBF2, SGK) inhibitor	93	98.7
3311	Protein kinase A inhibitor	194	98.1
3312	Protein kinase B alpha inhibitor	85	98.0
3313	Protein kinase B beta inhibitor	27	97.6
3314	Protein kinase B gamma inhibitor	10	95.3
3315	Protein kinase B inhibitor	313	96.5
3316	Protein kinase B stimulant	6	100.0
3317	Protein kinase C alpha inhibitor	289	98.8
3318	Protein kinase C alpha stimulant	9	100.0
3319	Protein kinase C beta I inhibitor	68	99.9
3320	Protein kinase C beta II inhibitor	86	99.9
3321	Protein kinase C beta inhibitor	127	98.4
3322	Protein kinase C delta inhibitor	109	99.0
3323	Protein kinase C epsilon inhibitor	77	97.8
3324	Protein kinase C eta inhibitor	61	99.9

3325	Protein kinase C gamma inhibitor	73	98.8
3326	Protein kinase C inhibitor	1121	97.5
3327	Protein kinase C mu inhibitor	8	99.9
3328	Protein kinase C nu inhibitor	5	98.4
3329	Protein kinase C stimulant	57	98.9
3330	Protein kinase C theta inhibitor	93	98.4
3331	Protein kinase C zeta inhibitor	27	99.8
3332	Protein kinase inhibitor	11091	93.6
3333	Protein kinase stimulant	73	94.0
3334	Protein phosphatase 1 inhibitor	19	99.9
3335	Protein phosphatase 2A inhibitor	19	99.8
3336	Protein phosphatase inhibitor	1349	97.5
3337	Protein synthesis inhibitor	396	94.0
3338	Protein synthesis stimulant	9	95.9
3339	Protein-L-isoaspartate (D-aspartate) O-methyltransferase inhibitor	3	100.0
3340	Protein-Npi-phosphohistidine-sugar phosphotransferase inhibitor	12	95.3
3341	Protein-S-isoprenylcysteine O-methyltransferase inhibitor	24	94.7
3342	Protein-arginine N-methyltransferase inhibitor	3	100.0
3343	Protein-arginine deiminase inhibitor	7	92.0
3344	Protein-disulfide reductase (glutathione) inhibitor	11	78.9
3345	Protein-glucosylgalactosylhydroxylysine glucosidase inhibitor	3	98.9
3346	Protein-glutamate O-methyltransferase inhibitor	4	98.6
3347	Protein-glutamate methylesterase inhibitor	13	94.9
3348	Protein-serine-threonine kinase inhibitor	1720	96.1
3349	Protein-synthesizing GTPase inhibitor	15	89.1
3350	Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor	219	96.1
3351	Protein-tyrosine kinase Lyn inhibitor	33	92.2
3352	Protein-tyrosine kinase p55(blk) inhibitor	6	87.9
3353	Protein-tyrosine phosphatase 1B inhibitor	984	98.2
3354	Protein-tyrosine phosphatase 2C inhibitor	51	99.7
3355	Protein-tyrosine phosphatase C inhibitor	4	100.0
3356	Protein-tyrosine phosphatase beta inhibitor	4	100.0
3357	Protein-tyrosine phosphatase epsilon inhibitor	5	100.0
3358	Protein-tyrosine phosphatase inhibitor	1286	97.6
3359	Protein-tyrosine phosphatase mu inhibitor	4	100.0
3360	Protein-tyrosine phosphatase yopH inhibitor	6	97.6
3361	Protein-tyrosine sulfotransferase inhibitor	10	97.3
3362	Proto-oncogene tyrosine-protein kinase Fgr inhibitor	6	100.0
3363	Proto-oncogene tyrosine-protein kinase Fyn inhibitor	34	95.3
3364	Proto-oncogene tyrosine-protein kinase Kit inhibitor	53	95.8
3365	Proto-oncogene tyrosine-protein kinase Yes inhibitor	13	95.5
3366	Proto-oncogene tyrosine-protein kinase c-hck inhibitor	5	100.0
3367	Protocatechuate 3,4-dioxygenase inhibitor	28	99.2
3368	Protocatechuate 4,5-dioxygenase inhibitor	11	99.9
3369	Protecollagen prolyl hydroxylase inhibitor	90	98.6
3370	Protoporphyrinogen oxidase inhibitor	15	79.3
3371	Prunasin beta-glucosidase inhibitor	6	96.8
3372	Pseudouridylyl synthase inhibitor	4	97.3
3373	Psychosexual dysfunction treatment	60	93.3
3374	Psychostimulant	261	89.5
3375	Psychotropic	19463	87.7
3376	Pteridine reductase inhibitor	9	97.6
3377	Pterin deaminase inhibitor	4	92.2
3378	Pullulanase inhibitor	7	94.1
3379	Pulmonary hypertension treatment	133	91.6
3380	Purine antagonist	19	99.8
3381	Purine biosynthesis inhibitor	8	98.9
3382	Purine nucleosidase inhibitor	26	99.6
3383	Purine nucleoside phosphorylase inhibitor	193	99.6
3384	Purinergic P2 agonist	20	96.0
3385	Purinergic P2 antagonist	565	97.6
3386	Purinergic P2T antagonist	59	97.7
3387	Purinergic P2X agonist	6	99.9
3388	Purinergic P2X antagonist	440	98.4

3389	Purinergic P2X1 antagonist	15	94.2
3390	Purinergic P2X2 antagonist	40	99.1
3391	Purinergic P2X3 antagonist	48	98.3
3392	Purinergic P2X4 antagonist	11	100.0
3393	Purinergic P2X7 antagonist	370	99.3
3394	Purinergic P2Y agonist	11	94.2
3395	Purinergic P2Y antagonist	73	94.6
3396	Purinergic P2Y1 antagonist	43	96.7
3397	Purinergic P2Y12 antagonist	10	88.3
3398	Purinergic receptor agonist	20	96.0
3399	Purinergic receptor antagonist	603	97.4
3400	Puromycin-sensitive aminopeptidase inhibitor	4	100.0
3401	Putrescine carbamoyltransferase inhibitor	6	99.8
3402	Putrescine oxidase inhibitor	14	98.2
3403	Pyridoxal 4-dehydrogenase inhibitor	9	100.0
3404	Pyridoxal kinase inhibitor	45	96.1
3405	Pyridoxamine-oxaloacetate transaminase inhibitor	13	99.8
3406	Pyridoxamine-phosphate oxidase inhibitor	9	99.5
3407	Pyridoxamine-pyruvate transaminase inhibitor	5	100.0
3408	Pyridoxine 4-oxidase inhibitor	3	97.6
3409	Pyridoxine 5-dehydrogenase inhibitor	6	99.0
3410	Pyrimidine antagonist	41	98.2
3411	Pyrimidine-deoxynucleoside 2'-dioxygenase inhibitor	6	98.9
3412	Pyroglutamyl-peptidase I inhibitor	39	94.7
3413	Pyroglutamyl-peptidase II inhibitor	13	90.7
3414	Pyrroline-5-carboxylate reductase inhibitor	17	98.7
3415	Pyruvate carboxylase inhibitor	27	93.0
3416	Pyruvate decarboxylase inhibitor	7	92.7
3417	Pyruvate dehydrogenase (cytochrome) inhibitor	4	98.6
3418	Pyruvate dehydrogenase (lipoamide) inhibitor	22	97.0
3419	Pyruvate dehydrogenase inhibitor	25	94.8
3420	Pyruvate dehydrogenase kinase inhibitor	110	100.0
3421	Pyruvate dehydrogenase kinase stimulant	11	99.5
3422	Pyruvate kinase inhibitor	38	97.0
3423	Pyruvate synthase inhibitor	5	99.9
3424	Pyruvate, phosphate dikinase inhibitor	21	99.0
3425	Pyruvate, water dikinase inhibitor	10	99.3
3426	QT interval prolongation	129	87.3
3427	Quercetin 2,3-dioxygenase inhibitor	11	98.1
3428	Queueine tRNA-ribosyltransferase inhibitor	37	99.6
3429	Quinate 5-dehydrogenase inhibitor	4	99.9
3430	Quinoline-4-carboxylate 2-oxidoreductase inhibitor	4	97.7
3431	Quinoprotein glucose dehydrogenase inhibitor	4	96.6
3432	Quisqualate antagonist	4	95.3
3433	RAS guanyl releasing protein antagonist	4	100.0
3434	RELA expression inhibitor	3	100.0
3435	RET inhibitor	23	87.5
3436	RNA agonist	3	99.9
3437	RNA directed DNA polymerase inhibitor	139	89.2
3438	RNA ligase (ATP) inhibitor	15	100.0
3439	RNA synthesis inhibitor	118	89.7
3440	RNA-directed RNA polymerase (Influenza A) inhibitor	13	100.0
3441	RNA-directed RNA polymerase inhibitor	26	85.6
3442	RNA-directed RNA polymerase stimulant	7	99.8
3443	Radical formation agonist	41	96.6
3444	Radioprotector	257	88.4
3445	Radiosensitizer	224	85.5
3446	Raf kinase B inhibitor	191	99.6
3447	Raf kinase C inhibitor	95	97.2
3448	Raf kinase inhibitor	611	98.7
3449	Raynaud's phenomenon treatment	11	87.1
3450	Reductant	70	92.6
3451	Releasing hormone agonist	25	94.4
3452	Renal disease treatment	1054	93.6

3453	Renal failure treatment	502	94.8
3454	Renal tissue kallikrein inhibitor	14	90.4
3455	Renilla-luciferin 2-monooxygenase inhibitor	12	99.0
3456	Renin inhibitor	2359	99.5
3457	Replication protein E1 (HPV) antagonist	3	100.0
3458	Respiratory analeptic	85	92.1
3459	Respiratory distress syndrome treatment	260	90.2
3460	Restenosis treatment	933	94.2
3461	Restless leg syndrome treatment	21	94.3
3462	Retinal dehydrogenase inhibitor	7	90.4
3463	Retinal oxidase inhibitor	8	78.7
3464	Retinoic acid alpha receptor agonist	27	99.7
3465	Retinoic acid alpha receptor antagonist	227	99.9
3466	Retinoic acid beta receptor agonist	15	99.2
3467	Retinoic acid beta receptor antagonist	196	99.9
3468	Retinoic acid metabolism inhibitor	8	90.8
3469	Retinoic acid receptor agonist	169	99.5
3470	Retinoic acid receptor antagonist	372	99.8
3471	Retinoic acid receptor gamma antagonist	229	99.6
3472	Retinoid X alpha receptor agonist	23	99.5
3473	Retinoid X alpha receptor antagonist	103	100.0
3474	Retinoid X beta receptor antagonist	53	100.0
3475	Retinoid X gamma receptor antagonist	57	100.0
3476	Retinoid X receptor agonist	112	99.6
3477	Retinoid X receptor antagonist	119	100.0
3478	Retinol O-fatty-acyltransferase inhibitor	7	99.3
3479	Retinol dehydrogenase inhibitor	6	96.3
3480	Retinopathy treatment	22	92.1
3481	Retinoprotector	20	89.7
3482	Retinyl-palmitate esterase inhibitor	18	97.8
3483	Reverse transcriptase (Hepatitis B) inhibitor	36	100.0
3484	Rhamnulose-1-phosphate aldolase inhibitor	7	97.0
3485	Rheumatoid arthritis treatment	1821	90.9
3486	Rhinitis treatment	219	85.7
3487	Rhizopuspepsin inhibitor	4	93.1
3488	Rho-associated kinase I inhibitor	15	100.0
3489	Rho-associated kinase II inhibitor	33	99.6
3490	Rho-associated kinase inhibitor	121	99.8
3491	Rhodesain inhibitor	15	100.0
3492	Rhodopsin kinase inhibitor	33	95.9
3493	Rhodotorulapepsin inhibitor	9	96.0
3494	Ribitol 2-dehydrogenase inhibitor	6	99.4
3495	Riboflavin kinase inhibitor	24	99.7
3496	Riboflavin phosphotransferase inhibitor	4	98.6
3497	Riboflavin synthase inhibitor	12	99.8
3498	Ribonuclease L inhibitor	9	100.0
3499	Ribonuclease T1 inhibitor	5	77.4
3500	Ribonuclease T2 inhibitor	26	99.8
3501	Ribonuclease U2 inhibitor	5	98.5
3502	Ribonuclease inhibitor	50	94.7
3503	Ribonucleoside diphosphate reductase inhibitor	125	98.5
3504	Ribonucleoside triphosphate reductase inhibitor	18	94.2
3505	Ribonucleotide reductase inhibitor	220	98.9
3506	Ribose-5-phosphate adenylyltransferase inhibitor	7	98.9
3507	Ribose-5-phosphate isomerase inhibitor	21	98.9
3508	Ribose-5-phosphate-ammonia ligase inhibitor	7	98.3
3509	Ribose-phosphate diphosphokinase inhibitor	37	99.2
3510	Ribosomal protein S6 kinase 1, 70-kDa inhibitor	14	90.1
3511	Ribosomal protein S6 kinase inhibitor	21	88.7
3512	Ribosomal protein S6 kinase, 70-kDa inhibitor	15	83.6
3513	Ribosomal protein S6 kinase, 90-kDa inhibitor	5	82.4
3514	Ribosomal protein S6 kinase, 90kD, polypeptide 5 inhibitor	4	100.0
3515	Ribosylpyrimidine nucleosidase inhibitor	9	99.8
3516	Ribulose-bisphosphate carboxylase inhibitor	15	98.4

3517	Ribulose-phosphate 3-epimerase inhibitor	3	84.8
3518	Rotamase (FKBP) inhibitor	6	99.7
3519	Rotamase (FKBP12) inhibitor	77	99.3
3520	Rubefacient	7	96.7
3521	Rubredoxin-NAD+ reductase inhibitor	14	81.3
3522	Ryanodine receptor 1 antagonist	3	100.0
3523	Ryanodine receptor antagonist	3	100.0
3524	S-adenosyl-L-homocysteine hydrolase inhibitor	53	100.0
3525	S-adenosyl-L-methionine decarboxylase inhibitor	58	99.6
3526	S-alkylcysteine lyase inhibitor	3	96.7
3527	S-formylglutathione hydrolase inhibitor	8	87.5
3528	S-methyl-5-thioadenosine phosphorylase inhibitor	47	99.4
3529	S-methyl-5-thioribose kinase inhibitor	9	98.9
3530	SMN2 expression enhancer	14	93.1
3531	SULT1A1 substrate	42	96.1
3532	SULT1A2 substrate	25	98.5
3533	SULT1A3 substrate	18	94.9
3534	SULT1E1 substrate	6	97.7
3535	SULT2A1 substrate	4	87.4
3536	Saccharolysin inhibitor	4	98.2
3537	Saccharopepsin inhibitor	3	85.6
3538	Saccharopine dehydrogenase (NAD+, L-glutamate-forming) inhibitor	4	99.1
3539	Saccharopine dehydrogenase (NAD+, L-lysine-forming) inhibitor	19	97.4
3540	Saccharopine dehydrogenase (NADP+, L-glutamate-forming) inhibitor	5	98.8
3541	Saccharopine dehydrogenase (NADP+, L-lysine-forming) inhibitor	13	93.6
3542	Salicylate 1-monooxygenase inhibitor	6	96.1
3543	Saluretic	86	90.6
3544	Saponin-like	12	99.9
3545	Sarcopenia treatment	25	97.9
3546	Sarcosine oxidase inhibitor	14	98.0
3547	Scleroderma treatment	21	86.6
3548	Sclerosant	4	93.4
3549	Scyllo-inosamine-4-phosphate amidinotransferase inhibitor	4	99.2
3550	Scytalone dehydratase inhibitor	21	99.1
3551	Secretase alpha stimulant	5	77.4
3552	Secretase beta 1 inhibitor	91	98.5
3553	Secretase beta 2 inhibitor	25	98.1
3554	Secretase beta inhibitor	186	98.6
3555	Secretase gamma inhibitor	147	99.3
3556	Secretase inhibitor	333	98.4
3557	Secretase stimulant	5	77.4
3558	Secretory phospholipase A2 inhibitor	8	92.1
3559	Sedative	1130	91.1
3560	Sedoheptulose-bisphosphatase inhibitor	7	94.7
3561	Selectin E antagonist	137	98.0
3562	Selectin L antagonist	9	99.4
3563	Selectin P antagonist	20	99.9
3564	Selectin antagonist	175	97.7
3565	Selenide, water dikinase inhibitor	4	100.0
3566	Selenocysteine lyase inhibitor	3	98.6
3567	Sensitization	158	92.0
3568	Sepiapterin deaminase inhibitor	12	99.6
3569	Sepiapterin reductase inhibitor	46	95.4
3570	Sepsis treatment	151	93.2
3571	Septic shock treatment	1030	92.0
3572	Serine 3-dehydrogenase inhibitor	6	98.6
3573	Serine O-acetyltransferase inhibitor	15	95.6
3574	Serine carboxypeptidase inhibitor	34	97.8
3575	Serine protease unspecified inhibitor	26	91.7
3576	Serine-glyoxylate transaminase inhibitor	12	99.2
3577	Serine-phosphoethanolamine synthase inhibitor	11	97.5
3578	Serine-pyruvate transaminase inhibitor	4	97.9
3579	Serine-sulfate ammonia-lyase inhibitor	30	99.4
3580	Serine-tRNA ligase inhibitor	6	98.8

3581	Serine-type D-Ala-D-Ala carboxypeptidase inhibitor	28	98.9
3582	Serralysin inhibitor	23	95.4
3583	Serratia marcescens nuclease inhibitor	7	96.4
3584	Serum-glucocorticoid regulated kinase 1 inhibitor	8	93.5
3585	Serum-glucocorticoid regulated kinase inhibitor	42	97.6
3586	Severe acute respiratory syndrome treatment	29	89.8
3587	Shab potassium channel antagonist	4	85.1
3588	Shaker potassium channel antagonist	664	98.5
3589	Shal potassium channel antagonist	27	96.7
3590	Shikimate 5-dehydrogenase inhibitor	6	98.2
3591	Shikimate O-hydroxycinnamoyltransferase inhibitor	4	96.7
3592	Shikimate kinase inhibitor	8	89.7
3593	Shock treatment	69	96.1
3594	Sialagogue	10	75.6
3595	Sickle-cell anemia treatment	53	91.9
3596	Sigma 1 receptor agonist	14	96.3
3597	Sigma 1 receptor antagonist	1053	99.4
3598	Sigma 2 receptor antagonist	548	99.5
3599	Sigma 3 receptor antagonist	12	100.0
3600	Sigma receptor agonist	23	92.6
3601	Sigma receptor antagonist	1833	99.1
3602	Signal peptidase I inhibitor	12	96.1
3603	Signal peptidase IB inhibitor	3	100.0
3604	Signal peptidase II inhibitor	8	77.0
3605	Signal transduction pathways inhibitor	7179	93.3
3606	Simian immunodeficiency virus proteinase inhibitor	4	84.6
3607	Sirtuin 2 inhibitor	15	100.0
3608	Sirtuin inhibitor	15	100.0
3609	Site-specific DNA-methyltransferase (adenine-specific) inhibitor	4	98.8
3610	Skeletal muscle relaxant	247	91.4
3611	Skin irritation, high	303	97.9
3612	Skin irritation, inactive	188	93.0
3613	Skin irritation, moderate	270	97.3
3614	Skin irritation, weak	469	96.5
3615	Skin irritative effect	1032	96.6
3616	Skin-whitener	42	97.0
3617	Sleep apnea treatment	79	96.0
3618	Sleep disorders treatment	1235	96.2
3619	Small monomeric GTPase inhibitor	3	99.3
3620	Smo receptor agonist	3	100.0
3621	Smo receptor antagonist	28	100.0
3622	Smooth muscle myosin light chain kinase inhibitor	10	74.9
3623	Snalysin inhibitor	4	98.3
3624	Sodium channel blocker	681	92.5
3625	Sodium channel blocker class Ib	6	96.8
3626	Sodium channel, voltage-gated antagonist	241	97.7
3627	Sodium-dependent vitamin C transporter 2 inhibitor	3	100.0
3628	Sodium/bile acid cotransporter inhibitor	3	97.8
3629	Sodium/calcium exchanger 1 inhibitor	25	97.1
3630	Sodium/calcium exchanger inhibitor	109	98.7
3631	Sodium/glucose cotransporter 1 inhibitor	109	99.5
3632	Sodium/glucose cotransporter 2 inhibitor	336	99.8
3633	Sodium/glucose cotransporter inhibitor	459	99.4
3634	Sodium/hydrogen exchanger 1 inhibitor	283	99.9
3635	Sodium/hydrogen exchanger 2 inhibitor	8	97.8
3636	Sodium/hydrogen exchanger 3 inhibitor	73	100.0
3637	Sodium/hydrogen exchanger 5 inhibitor	5	99.0
3638	Sodium/hydrogen exchanger inhibitor	645	99.8
3639	Somatostatin 1 agonist	3	95.1
3640	Somatostatin 1 antagonist	159	99.9
3641	Somatostatin 2 agonist	12	99.8
3642	Somatostatin 2 antagonist	178	99.9
3643	Somatostatin 3 antagonist	178	99.9
3644	Somatostatin 4 antagonist	190	99.8

3645	Somatostatin 5 agonist	15	99.9
3646	Somatostatin 5 antagonist	153	99.6
3647	Somatostatin agonist	59	97.2
3648	Somatostatin antagonist	248	99.6
3649	Sorbitol accumulation inhibitor	7	100.0
3650	Sorbitol-6-phosphate 2-dehydrogenase inhibitor	3	97.0
3651	Sorbose dehydrogenase inhibitor	3	99.3
3652	Spasmogenic	253	91.1
3653	Spasmolytic	1532	90.2
3654	Spasmolytic, Papaverin-like	188	92.8
3655	Spasmolytic, urinary	28	85.6
3656	Spermicide	24	84.8
3657	Spermidine dehydrogenase inhibitor	5	81.7
3658	Spermidine synthase inhibitor	36	99.4
3659	Spermine antagonist	3	100.0
3660	Spermine synthase inhibitor	24	99.4
3661	Sphinganine kinase inhibitor	6	81.4
3662	Sphinganine-1-phosphate aldolase inhibitor	6	97.3
3663	Sphingomyelinase inhibitor	16	98.3
3664	Sphingosine 1-phosphate receptor 1 agonist	107	100.0
3665	Sphingosine 1-phosphate receptor 1 antagonist	35	99.3
3666	Sphingosine 1-phosphate receptor 3 agonist	12	100.0
3667	Sphingosine 1-phosphate receptor 3 antagonist	23	99.9
3668	Sphingosine 1-phosphate receptor 4 agonist	5	100.0
3669	Sphingosine 1-phosphate receptor 4 antagonist	18	99.9
3670	Sphingosine 1-phosphate receptor 5 agonist	5	86.2
3671	Sphingosine 1-phosphate receptor 5 antagonist	21	100.0
3672	Sphingosine 1-phosphate receptor agonist	108	100.0
3673	Sphingosine 1-phosphate receptor antagonist	42	96.9
3674	Sphingosine kinase 1 inhibitor	3	99.9
3675	Sphingosine kinase inhibitor	14	95.0
3676	Sporulation kinase A inhibitor	5	100.0
3677	Squalene epoxidase inhibitor	64	97.6
3678	Squalene synthetase inhibitor	470	99.4
3679	Squalene-hopene cyclase inhibitor	35	96.8
3680	Src kinase inhibitor	1773	97.6
3681	Stearoyl-CoA desaturase inhibitor	116	97.2
3682	Stem cell growth factor agonist	305	98.6
3683	Steroid 17alpha-monooxygenase inhibitor	246	99.7
3684	Steroid 21-monooxygenase inhibitor	6	76.8
3685	Steroid 9alpha-monooxygenase inhibitor	3	99.7
3686	Steroid DELTA-isomerase inhibitor	28	97.2
3687	Steroid N-acetylglucosaminyltransferase inhibitor	4	95.2
3688	Steroid sulfotransferase inhibitor	11	92.5
3689	Steroid synthesis inhibitor	11	79.1
3690	Steroid-like	50	99.7
3691	Sterol 24-C-methyltransferase inhibitor	31	98.4
3692	Sterol 3-beta-glucosyltransferase inhibitor	13	94.1
3693	Stipitatonate decarboxylase inhibitor	5	99.8
3694	Streptogrisin A inhibitor	3	100.0
3695	Streptomycin 6-kinase inhibitor	6	99.6
3696	Streptopain inhibitor	14	98.4
3697	Stroke treatment	4815	92.1
3698	Strombine dehydrogenase inhibitor	5	99.9
3699	Stromelysin 2 inhibitor	4	98.7
3700	Styrene-oxide isomerase inhibitor	3	98.2
3701	Substance P antagonist	358	97.8
3702	Subtilisin inhibitor	27	95.6
3703	Succinate dehydrogenase inhibitor	12	94.5
3704	Succinate-CoA ligase (ADP-forming) inhibitor	16	97.7
3705	Succinate-hydroxymethylglutarate CoA-transferase inhibitor	8	99.0
3706	Succinate-semialdehyde dehydrogenase [NAD(P)+] inhibitor	7	84.2
3707	Succinate-semialdehyde dehydrogenase inhibitor	20	99.1
3708	Succinic dehydrogenase inhibitor	8	96.6

3709	Sucrose 1F-fructosyltransferase inhibitor	4	80.1
3710	Sucrose alpha-glucosidase inhibitor	19	99.5
3711	Sucrose phosphorylase inhibitor	5	100.0
3712	Sucrose synthase inhibitor	16	99.0
3713	Sucrose-phosphatase inhibitor	7	99.7
3714	Sucrose-phosphate synthase inhibitor	19	96.9
3715	Sugar-phosphatase inhibitor	3	88.5
3716	Sulfate adenyltransferase (ADP) inhibitor	8	98.2
3717	Sulfate adenyltransferase inhibitor	14	97.9
3718	Sulfinolalanine decarboxylase inhibitor	18	99.2
3719	Sulfite dehydrogenase inhibitor	9	83.9
3720	Sulfite oxidase inhibitor	9	93.1
3721	Sulfite reductase inhibitor	6	96.4
3722	Sulfonylureas	5	98.3
3723	Sulfotransferase substrate	111	93.7
3724	Sulfur dioxygenase inhibitor	6	98.3
3725	Sulfur reductase inhibitor	8	85.9
3726	Superoxide dismutase inhibitor	17	90.0
3727	Superoxide dismutase stimulant	12	88.0
3728	Sweetener	30	96.3
3729	Syk tyrosine kinase inhibitor	292	98.1
3730	Synaptic vesicle protein SV2, levetiracetam binding site antagonist	32	100.0
3731	Systemic lupus erythematosus treatment	135	90.2
3732	T cell inhibitor	24	88.5
3733	T cell receptor antagonist	17	100.0
3734	T cell receptor gamma-delta antagonist	17	100.0
3735	T-cell protein-tyrosine phosphatase inhibitor	78	99.7
3736	T2-induced deoxynucleotide kinase inhibitor	3	100.0
3737	TEC kinase inhibitor	39	100.0
3738	TERT expression inhibitor	3	97.6
3739	TGF beta receptor type I kinase inhibitor	210	99.7
3740	TGF beta receptor type II kinase inhibitor	22	100.0
3741	TH expression enhancer	9	94.9
3742	TIE antagonist	526	98.7
3743	TIE-2 agonist	6	100.0
3744	TIE-2 antagonist	506	98.7
3745	TNF convertase inhibitor	624	99.9
3746	TNF expression inhibitor	23	94.1
3747	TP53 expression enhancer	5	88.2
3748	TRKA antagonist	86	98.0
3749	TRKB antagonist	12	100.0
3750	TRPA1 agonist	9	91.6
3751	TRPA1 antagonist	3	100.0
3752	TTK protein kinase inhibitor	5	100.0
3753	Tagaturonate reductase inhibitor	3	99.3
3754	Tankyrase 2 inhibitor	5	100.0
3755	Tankyrase inhibitor	5	100.0
3756	Tannase inhibitor	14	99.5
3757	Tardive dyskinesia treatment	41	92.8
3758	Tartrate decarboxylase inhibitor	5	100.0
3759	Tartrate dehydrogenase inhibitor	5	100.0
3760	Tau aggregation inhibitor	9	79.5
3761	Taurine dehydrogenase inhibitor	7	85.5
3762	Taurine-2-oxoglutarate transaminase inhibitor	3	97.1
3763	Taurocyamine kinase inhibitor	3	97.4
3764	Tauropine dehydrogenase inhibitor	8	95.3
3765	Telomerase inhibitor	332	97.2
3766	Tentoxilysin inhibitor	4	93.6
3767	Teratogen	1548	89.7
3768	Testosterone 17beta-dehydrogenase (NADP+) inhibitor	3	84.8
3769	Testosterone 17beta-dehydrogenase inhibitor	11	96.7
3770	Testosterone agonist	5	99.6
3771	Tetanus neurotoxin inhibitor	3	100.0
3772	Tetracycline antiport transporter antagonist	36	100.0

3773	Tetrahydroxynaphthalene reductase inhibitor	7	98.0
3774	Theanine hydrolase inhibitor	13	99.9
3775	Thermitase inhibitor	11	94.0
3776	Thermolysin inhibitor	19	99.5
3777	Thermomycolin inhibitor	3	99.4
3778	Thermopsin inhibitor	4	87.2
3779	Thiamine diphosphokinase inhibitor	9	97.7
3780	Thiamine pyridinylase inhibitor	9	91.7
3781	Thiamine-phosphate diphosphorylase inhibitor	7	98.4
3782	Thiamine-phosphate kinase inhibitor	9	98.9
3783	Thiamine-triphosphatase inhibitor	13	90.4
3784	Thiazolidinedione	24	99.5
3785	Thimet oligopeptidase inhibitor	20	92.7
3786	Thioether S-methyltransferase inhibitor	3	99.3
3787	Thiol S-methyltransferase inhibitor	8	97.7
3788	Thiol oxidase inhibitor	13	94.4
3789	Thiol protease inhibitor	131	98.1
3790	Thiol sulfotransferase inhibitor	4	100.0
3791	Thiopurine S-methyltransferase inhibitor	17	93.8
3792	Thioredoxin inhibitor	3	92.8
3793	Thioredoxin-disulfide reductase inhibitor	27	89.5
3794	Thiosulfate dehydrogenase inhibitor	10	87.5
3795	Thiosulfate sulfurtransferase inhibitor	21	98.4
3796	Threonine aldolase inhibitor	5	97.0
3797	Threonine ammonia-lyase inhibitor	27	98.2
3798	Threonine synthase inhibitor	11	99.8
3799	Threonine-tRNA ligase inhibitor	5	92.6
3800	Thrombin inhibitor	2091	98.7
3801	Thrombocytopoiesis inhibitor	11	83.2
3802	Thrombolytic	140	93.6
3803	Thrombopoietin agonist	111	99.9
3804	Thromboxane A2 antagonist	85	94.2
3805	Thromboxane B2 antagonist	17	83.6
3806	Thromboxane agonist	3	99.9
3807	Thromboxane antagonist	312	96.3
3808	Thromboxane synthase inhibitor	659	98.5
3809	Thromboxane synthase stimulant	3	98.6
3810	Thymidine kinase (Herpes simplex virus 1) inhibitor	38	100.0
3811	Thymidine kinase (Herpes simplex virus 2) inhibitor	15	100.0
3812	Thymidine kinase 1 inhibitor	12	97.3
3813	Thymidine kinase 2 inhibitor	10	100.0
3814	Thymidine kinase inhibitor	95	96.3
3815	Thymidine phosphorylase inhibitor	59	98.8
3816	Thymidine-triphosphatase inhibitor	6	99.9
3817	Thymidylate 5'-phosphatase inhibitor	5	80.3
3818	Thymidylate synthase inhibitor	814	99.3
3819	Thymine dioxygenase inhibitor	14	100.0
3820	Thyroid hormone agonist	106	98.6
3821	Thyroid hormone alpha 1 agonist	5	100.0
3822	Thyroid hormone alpha 1 antagonist	12	100.0
3823	Thyroid hormone alpha agonist	5	100.0
3824	Thyroid hormone alpha antagonist	40	100.0
3825	Thyroid hormone antagonist	90	97.6
3826	Thyroid hormone beta 1 agonist	5	100.0
3827	Thyroid hormone beta 1 antagonist	12	100.0
3828	Thyroid hormone beta agonist	74	100.0
3829	Thyroid hormone beta antagonist	38	100.0
3830	Thyrotropin receptor antagonist	6	77.8
3831	Thyrotropin releasing hormone agonist	20	99.9
3832	Thyrotropin releasing hormone antagonist	7	93.9
3833	Thyroxine 5-deiodinase inhibitor	7	94.3
3834	Tissue kallikrein inhibitor	6	84.1
3835	Tocolytic	138	98.1
3836	Toll-Like receptor 2 antagonist	8	100.0

3837	Toll-Like receptor 4 agonist	4	100.0
3838	Toll-Like receptor 7 agonist	86	99.7
3839	Toll-Like receptor 8 agonist	9	100.0
3840	Toll-Like receptor agonist	92	99.6
3841	Toll-Like receptor antagonist	11	88.1
3842	Topoisomerase I inhibitor	540	96.9
3843	Topoisomerase II inhibitor	998	96.5
3844	Torsades de pointes	65	85.4
3845	Toxic	2881	87.0
3846	Toxic, respiratory center	15	92.5
3847	Tpr proteinase (Porphyromonas gingivalis) inhibitor	4	84.8
3848	Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor	39	95.0
3849	Trans-2-enoyl-CoA reductase (NAD+) inhibitor	4	98.6
3850	Trans-2-enoyl-CoA reductase (NADPH) inhibitor	5	76.2
3851	Trans-acenaphthene-1,2-diol dehydrogenase inhibitor	5	80.3
3852	Trans-octaprenyltranstransferase inhibitor	6	96.2
3853	Trans-pentaprenyltranstransferase inhibitor	5	98.5
3854	Transactivator transcription protein inhibitor	29	89.9
3855	Transaldolase inhibitor	5	100.0
3856	Transcortin receptor antagonist	29	100.0
3857	Transcription factor AP-1 inhibitor	191	97.0
3858	Transcription factor NF kappa A inhibitor	17	82.8
3859	Transcription factor NF kappa B inhibitor	574	95.1
3860	Transcription factor NF kappa B stimulant	8	94.8
3861	Transcription factor STAT inhibitor	64	87.4
3862	Transcription factor STAT3 inhibitor	52	95.5
3863	Transcription factor STAT6 inhibitor	6	88.4
3864	Transcription factor inhibitor	742	94.3
3865	Transcription factor rho inhibitor	7	100.0
3866	Transcription factor stimulant	8	94.8
3867	Transferase inhibitor	28	72.9
3868	Transferase stimulant	9	77.4
3869	Transforming growth factor agonist	6	81.5
3870	Transforming growth factor antagonist	60	96.8
3871	Transforming growth factor beta 1 agonist	4	90.9
3872	Transforming growth factor beta 1 antagonist	8	79.7
3873	Transforming growth factor beta 3 antagonist	21	100.0
3874	Transforming growth factor beta agonist	6	81.5
3875	Transforming growth factor beta antagonist	46	97.5
3876	Transglutaminase 2 inhibitor	13	94.2
3877	Transketolase inhibitor	7	93.6
3878	Translation initiation factor IF-2 antagonist	5	100.0
3879	Transplant rejection treatment	822	92.9
3880	Transthyretin amyloid fibril formation inhibitor	7	99.5
3881	Trehalose-phosphatase inhibitor	3	99.4
3882	Triacetate-lactonase inhibitor	3	98.6
3883	Trimerelysin II inhibitor	7	99.0
3884	Trimethylamine dehydrogenase inhibitor	12	95.1
3885	Trimethylamine-N-oxide reductase inhibitor	11	98.7
3886	Trimethylamine-oxide aldolase inhibitor	5	80.3
3887	Trimethyllysine dioxygenase inhibitor	8	99.4
3888	Triose-phosphate isomerase inhibitor	23	98.2
3889	Tripeptide aminopeptidase inhibitor	23	93.5
3890	Tripeptidyl peptidase II inhibitor	36	99.9
3891	Tripeptidyl-peptidase I inhibitor	22	95.5
3892	Tropinesterase inhibitor	3	85.1
3893	Trypanothione-disulfide reductase inhibitor	58	97.0
3894	Trypsin inhibitor	1140	98.8
3895	Tryptase 1 inhibitor	50	100.0
3896	Tryptase inhibitor	140	98.5
3897	Tryptophan 2,3-dioxygenase inhibitor	22	91.8
3898	Tryptophan 2-monooxygenase inhibitor	21	95.9
3899	Tryptophan 5 hydroxylase inhibitor	20	93.5
3900	Tryptophan alpha,beta-oxidase inhibitor	4	95.3

3901	Tryptophan dimethylallyltransferase inhibitor	8	97.0
3902	Tryptophan hydroxylase 1 inhibitor	11	100.0
3903	Tryptophan synthase inhibitor	14	99.4
3904	Tryptophan transaminase inhibitor	4	98.4
3905	Tryptophan-tRNA ligase inhibitor	38	98.7
3906	Tryptophanamidase inhibitor	5	98.1
3907	Tryptophanyl aminopeptidase inhibitor	3	98.9
3908	Tubulin GTPase inhibitor	6	99.5
3909	Tubulin agonist	26	100.0
3910	Tubulin antagonist	998	97.5
3911	Tubulin-tyrosine ligase inhibitor	17	98.5
3912	Tubuliny-Tyr carboxypeptidase inhibitor	6	99.8
3913	Tumour necrosis factor agonist	11	78.5
3914	Tumour necrosis factor alpha antagonist	538	94.5
3915	Tumour necrosis factor alpha release inhibitor	2434	94.4
3916	Tumour necrosis factor antagonist	700	93.0
3917	Tyrosine 2,3-aminomutase inhibitor	6	99.3
3918	Tyrosine 3 hydroxylase inhibitor	10	85.5
3919	Tyrosine 3 hydroxylase stimulant	3	100.0
3920	Tyrosine kinase inhibitor	4765	95.5
3921	Tyrosine phenol-lyase inhibitor	20	99.8
3922	Tyrosine transaminase inhibitor	34	98.4
3923	Tyrosine-ester sulfotransferase inhibitor	24	98.5
3924	Tyrosine-protein kinase EMT inhibitor	86	99.6
3925	Tyrosine-protein kinase TYRO 10 inhibitor	4	81.1
3926	Tyrosine-protein kinase receptor FLT3 inhibitor	245	98.4
3927	Tyrosine-protein kinase receptor antagonist	130	98.4
3928	UDP-3-O-acyl-N-acetylglucosamine deacetylase inhibitor	42	99.9
3929	UDP-N-acetylglucosamine 1-carboxyvinyltransferase inhibitor	15	99.0
3930	UDP-N-acetylglucosamine 2-epimerase inhibitor	7	98.9
3931	UDP-N-acetylglucosamine 4-epimerase inhibitor	3	88.9
3932	UDP-N-acetylglucosamine diphosphorylase inhibitor	8	99.1
3933	UDP-N-acetylglucosamine-dolichyl-phosphate N-acetylglucosaminephosphotransferase inhibitor	11	97.6
3934	UDP-N-acetylglucosamine-lysosomal-enzyme N-acetylglucosaminephosphotransferase inhibitor	9	99.5
3935	UDP-N-acetylmuramate dehydrogenase inhibitor	11	96.8
3936	UDP-N-acetylmuramate-L-alanine ligase inhibitor	18	97.3
3937	UDP-N-acetylmuramoylalanine-D-glutamate ligase inhibitor	18	98.5
3938	UDP-N-acetylmuramoylalanine-D-glutamate-2,6-diaminopimelate ligase inhibitor	8	99.9
3939	UDP-glucose 4-epimerase inhibitor	25	99.2
3940	UDP-glucose 6-dehydrogenase inhibitor	8	94.8
3941	UDP-glucose-hexose-1-phosphate uridylyltransferase inhibitor	18	97.2
3942	UDP-glucuronate 4-epimerase inhibitor	13	100.0
3943	UDP-glucuronate 5'-epimerase inhibitor	3	100.0
3944	UDP-glucuronate decarboxylase inhibitor	12	99.4
3945	UDP-glucuronosyltransferase substrate	592	91.2
3946	UDP-sugar diphosphatase inhibitor	4	99.4
3947	UGT1A substrate	320	91.2
3948	UGT1A1 substrate	120	91.8
3949	UGT1A10 substrate	96	92.4
3950	UGT1A3 substrate	117	92.5
3951	UGT1A4 substrate	126	93.0
3952	UGT1A5 substrate	17	97.6
3953	UGT1A6 substrate	80	88.7
3954	UGT1A7 substrate	55	90.7
3955	UGT1A8 substrate	96	94.5
3956	UGT1A9 substrate	107	87.0
3957	UGT2B substrate	218	92.8
3958	UGT2B1 substrate	30	93.2
3959	UGT2B10 substrate	20	90.6
3960	UGT2B11 substrate	37	95.3
3961	UGT2B15 substrate	86	93.7
3962	UGT2B17 substrate	17	86.6
3963	UGT2B18 substrate	7	83.1
3964	UGT2B19 substrate	6	86.0

3965	UGT2B20 substrate	19	95.3
3966	UGT2B23 substrate	6	86.0
3967	UGT2B28 substrate	8	95.6
3968	UGT2B30 substrate	5	99.1
3969	UGT2B33 substrate	3	99.1
3970	UGT2B4 substrate	38	86.4
3971	UGT2B4D substrate	5	99.1
3972	UGT2B4E substrate	5	99.1
3973	UGT2B7 substrate	143	92.4
3974	UGT2B7H substrate	26	97.6
3975	UGT2B7Y substrate	28	97.8
3976	UGT2B9 substrate	36	94.1
3977	UTP-glucose-1-phosphate uridylyltransferase inhibitor	10	100.0
3978	Ubiquinol-cytochrome-c reductase inhibitor	10	80.4
3979	Ubiquitin thiolesterase inhibitor	7	95.5
3980	Ubiquitin-protein ligase inhibitor	27	97.1
3981	Ulcerative colitis treatment	3	100.0
3982	Undecaprenyl-diphosphatase inhibitor	5	97.8
3983	Undecaprenyl-phosphate galactose phosphotransferase inhibitor	7	99.8
3984	Undecaprenyl-phosphate mannosyltransferase inhibitor	3	93.9
3985	Undecaprenyldiphospho-muramoylpentapeptide beta-N-acetylglucosaminyltransferase inhibitor	3	94.6
3986	Uracil phosphoribosyltransferase inhibitor	14	99.4
3987	Urate transporter 1 inhibitor	28	99.0
3988	Urate-ribonucleotide phosphorylase inhibitor	12	92.0
3989	Urease inhibitor	18	91.8
3990	Urethanase inhibitor	10	86.8
3991	Uric acid excretion stimulant	116	94.2
3992	Uridine kinase inhibitor	7	99.1
3993	Uridine nucleosidase inhibitor	15	98.9
3994	Uridine phosphorylase inhibitor	95	99.7
3995	Urinary incontinence treatment	1946	95.5
3996	Urocanate hydratase inhibitor	16	99.2
3997	Urokinase inhibitor	329	99.5
3998	Urolithiasis treatment	6	89.6
3999	Urologic disorders treatment	176	72.0
4000	Uroporphyrinogen decarboxylase inhibitor	30	98.9
4001	Uroporphyrinogen-III synthase inhibitor	9	93.3
4002	Urotensin II agonist	36	100.0
4003	Urotensin II antagonist	15	93.8
4004	Urticaria treatment	8	95.0
4005	Uterine relaxant	45	90.8
4006	Uterine stimulant	34	95.2
4007	VCAM antagonist	153	97.4
4008	VCAM-1 antagonist	152	97.6
4009	VCAM1 expression inhibitor	51	96.3
4010	VEGF expression inhibitor	38	96.7
4011	VEGFR2 expression inhibitor	5	100.0
4012	VLA-4 antagonist	776	99.8
4013	Valine decarboxylase inhibitor	4	98.7
4014	Valine dehydrogenase (NADP+) inhibitor	6	99.2
4015	Valine-pyruvate transaminase inhibitor	3	100.0
4016	Valine-tRNA ligase inhibitor	10	97.3
4017	Vanilloid 1 agonist	27	91.2
4018	Vanilloid 1 antagonist	267	99.0
4019	Vanilloid 3 antagonist	6	100.0
4020	Vanilloid 4 agonist	6	100.0
4021	Vanilloid 4 antagonist	5	100.0
4022	Vanilloid agonist	34	94.5
4023	Vanilloid antagonist	306	98.9
4024	Vanillyl-alcohol oxidase inhibitor	7	99.4
4025	Vascular (periferal) disease treatment	807	91.0
4026	Vascular dementia treatment	10	88.0
4027	Vascular endothelial growth factor 1 antagonist	198	96.2
4028	Vascular endothelial growth factor 2 antagonist	1399	98.0

4029	Vascular endothelial growth factor 3 antagonist	75	95.7
4030	Vascular endothelial growth factor antagonist	2029	97.0
4031	Vasculitis treatment	6	85.7
4032	Vasodilator	1079	87.9
4033	Vasodilator, cerebral	34	83.1
4034	Vasodilator, coronary	278	87.0
4035	Vasodilator, peripheral	217	84.3
4036	Vasodilator, renal	35	74.5
4037	Vasopressin 1 agonist	17	100.0
4038	Vasopressin 1 antagonist	856	99.6
4039	Vasopressin 1A agonist	9	100.0
4040	Vasopressin 1A antagonist	761	99.7
4041	Vasopressin 1B agonist	8	100.0
4042	Vasopressin 1B antagonist	115	99.9
4043	Vasopressin 2 agonist	132	99.9
4044	Vasopressin 2 antagonist	595	99.8
4045	Vasopressor	109	89.3
4046	Vasoprotector	28	76.9
4047	Venom exonuclease inhibitor	8	86.7
4048	Venombin A inhibitor	9	97.9
4049	Venombin AB inhibitor	5	87.0
4050	Vesicle monoamine transporter 2 inhibitor	13	100.0
4051	Vesicle monoamine transporter inhibitor	13	100.0
4052	Vesicular acetylcholine transporter inhibitor	73	100.0
4053	Vesicular glutamate transport inhibitor	4	100.0
4054	Vibriolysin inhibitor	12	99.8
4055	Viral entry inhibitor	6	78.3
4056	Viral fusion inhibitor	3	100.0
4057	Vitamin D receptor agonist	94	100.0
4058	Vitamin D receptor antagonist	27	100.0
4059	Vitamin D-like	159	100.0
4060	Vitamin D3 hydroxylase inhibitor	12	94.0
4061	Vitamin D3-like	12	100.0
4062	Vitamin K-like	20	100.0
4063	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor	7	94.2
4064	Vitronectin receptor antagonist	1167	99.7
4065	Vomilenine glucosyltransferase inhibitor	6	98.0
4066	Wee-1 tyrosine kinase inhibitor	5	99.9
4067	Wound healing agent	309	91.2
4068	X-His dipeptidase inhibitor	22	97.2
4069	X-Pro dipeptidase inhibitor	21	98.2
4070	X-Trp aminopeptidase inhibitor	7	99.3
4071	X-methyl-His dipeptidase inhibitor	10	87.2
4072	Xaa-Pro dipeptidyl-peptidase inhibitor	8	98.3
4073	Xanthine dehydrogenase inhibitor	32	94.3
4074	Xanthine oxidase inhibitor	97	95.4
4075	Xanthine oxidase substrate	17	93.4
4076	Xanthine phosphoribosyltransferase inhibitor	39	99.6
4077	Xanthine-like	27	99.8
4078	Xanthommatin reductase inhibitor	5	98.2
4079	Xenobiotic-transporting ATPase inhibitor	12	85.4
4080	Xylan 1,4-beta-xylosidase inhibitor	14	99.1
4081	Xylan endo-1,3-beta-xylosidase inhibitor	5	96.4
4082	Xylose isomerase inhibitor	11	98.4
4083	YAK3 inhibitor	15	100.0
4084	Yeast ribonuclease inhibitor	3	95.3
4085	ZAP-70 protein tyrosine kinase inhibitor	70	98.1
4086	[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)] kinase inhibitor	36	99.0
4087	[3-methyl-2-oxobutanoate dehydrogenase (lipoamide)]-phosphatase inhibitor	12	100.0
4088	[Isocitrate dehydrogenase (NADP+)] kinase inhibitor	9	99.7
4089	[Skp1-protein]-hydroxyproline N-acetylglucosaminyltransferase inhibitor	5	99.6
4090	[acetyl-CoA carboxylase] kinase inhibitor	6	99.4
4091	[acyl-carrier-protein] S-acetyltransferase inhibitor	7	94.7
4092	[acyl-carrier-protein] S-malonyltransferase inhibitor	10	98.3

4093	[citrate-(pro-3S)-lyase] thiolesterase inhibitor	4	99.9
4094	[glutamate-ammonia-ligase] adenylyltransferase inhibitor	13	99.6
4095	[hydroxymethylglutaryl-CoA reductase (NADPH)] kinase inhibitor	11	95.3
4096	[hydroxymethylglutaryl-CoA reductase (NADPH)]-phosphatase inhibitor	8	99.7
4097	[myelin basic protein]-arginine N-methyltransferase inhibitor	3	98.0
4098	[phosphorylase] phosphatase inhibitor	14	93.9
4099	[protein-PII] uridylyltransferase inhibitor	28	99.3
4100	[pyruvate dehydrogenase (lipoamide)]-phosphatase inhibitor	9	78.6
4101	c-Src kinase inhibitor	507	99.5
4102	dCMP deaminase inhibitor	20	99.1
4103	dCTP deaminase inhibitor	10	99.6
4104	dCTP diphosphatase inhibitor	3	100.0
4105	dTDP-glucose 4,6-dehydratase inhibitor	7	99.6
4106	dTMP kinase (Mycobacterium tuberculosis) inhibitor	11	100.0
4107	dTMP kinase inhibitor	28	100.0
4108	dUTP diphosphatase inhibitor	14	99.4
4109	mRNA (guanine-N7-)-methyltransferase inhibitor	18	96.1
4110	mRNA (nucleoside-2'-O-)-methyltransferase inhibitor	16	100.0
4111	mTOR inhibitor	134	98.1
4112	p21-activated kinase 1 inhibitor	6	99.5
4113	p21-activated kinase 4 inhibitor	22	100.0
4114	p21-activated kinase inhibitor	23	99.6
4115	p38 MAP kinase inhibitor	510	98.3
4116	p53 inhibitor	18	93.8
4117	pFOX inhibitor	5	100.0
4118	rRNA (adenosine-2'-O-)-methyltransferase inhibitor	12	99.8
4119	sAPP-alpha secretion enhancer	8	100.0
4120	tRNA (adenine-N1-)-methyltransferase inhibitor	6	99.9
4121	tRNA (cytosine-5-)-methyltransferase inhibitor	5	98.2
4122	tRNA (guanine-N1-)-methyltransferase inhibitor	4	99.2
4123	tRNA (guanine-N2-)-methyltransferase inhibitor	5	99.2
4124	tRNA (guanine-N7-)-methyltransferase inhibitor	6	98.9
4125	tRNA (uracil-5-)-methyltransferase inhibitor	10	99.9
4126	tRNA adenylyltransferase inhibitor	9	98.3
4127	tRNA cytidylyltransferase inhibitor	16	98.9
4128	tRNA methyltransferase inhibitor	22	99.4
4129	tRNA nucleotidyltransferase inhibitor	3	98.9
4130	tRNA-pseudouridine synthase I inhibitor	3	96.0

N is the number of compounds with the appropriate activity in the PASS training set;

IAP is the Invariant Accuracy of Prediction (%) estimated in leave one out cross-validation for the whole training set.

$$IAP = \frac{N\{p_1 > p_0\}}{n_1 \cdot n_0} * 100\%$$

where, $N\{p_1 > p_0\}$ is the number of cases when the predicted probability to be active for an active compound (p_1) is higher than that for an inactive compound (p_0); n_1 and n_0 are the numbers of active and inactive compounds, respectively.