Supporting information

NPClassifier: A deep neural network-based structural classification tool for natural products

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1.1. Website

NPClassifier webpage (https://npclassifier.ucsd.edu) was designed to provide easy-to-use classification for a single queried molecule.

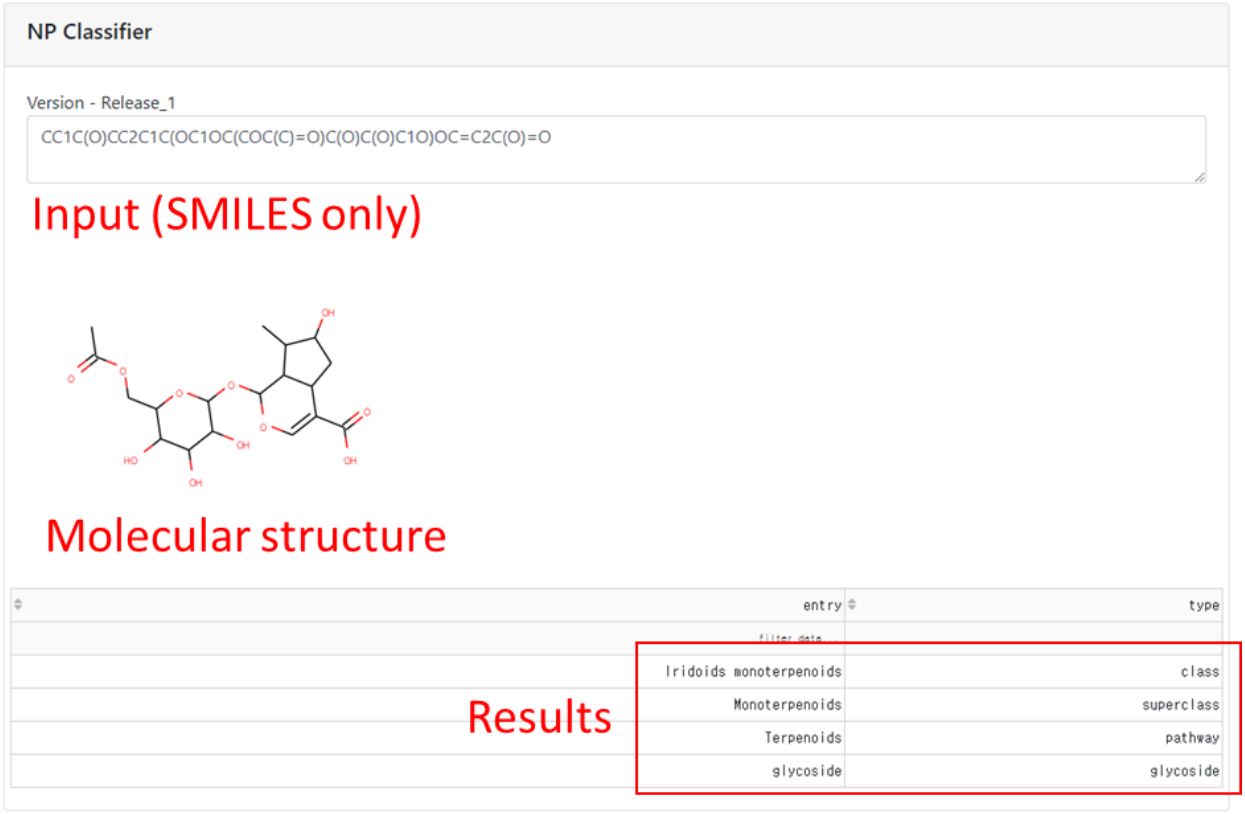


Figure S1 Webpage of NPClassifier

Input: Paste the SMILES into the blank. Only isomeric or canonical SMILES strings are supported as input format.

Molecular structure: The structure of a queried molecule. It will be shown when the SMILES is submitted.

Results: Three hierarchical classes (Pathway, Superclass, and Class) and glycoside information are provided. The glycoside results are shown when the queried molecule contains sugar moiety. If the queried molecule isn't classified (probability is under threshold, 0.5), the results section remains empty.

***Note**: If the queried SMILES is invalid, the molecular structure may not be shown. Then please visit https://cactus.nci.nih.gov/translate/, get a unique SMILES, and try again with NPClassifier.

1.2. Application programming interface (API) for NPClassifier

The API for NPClassifier was built for classifying massive data easily by scripts.

Link: https://npclassifier.ucsd.edu/classify?smiles=<SMILES>

Output: dictionary

Key list:

"class_results": Class results

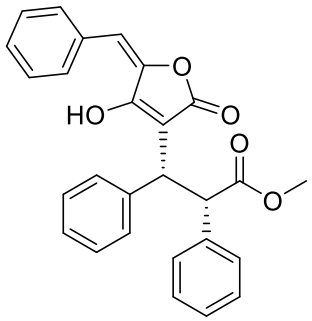
"superclass_results": Superclass results

"pathway_results": Pathway results

"isglycoside": Whether the queried molecule is a glycoside or not (true/false)

"fp1": Counted Morgan fingerprints

1.3. An example of using API (Isoravenelone)



SMILES:
COC(=O)[C@H](C1=CC=CC=C1)[C@H](C2=CC=CC=C2)C3=C(/C(=C\C4=CC=CC=C4)/OC3=O)O

Link:

https://npclassifier.ucsd.edu/classify?smiles=COC([C@@H]([C@@H](C1=C(O)/C(OC1=O)=C\C2=CC=CC=C2)C3=CC=CC=C3)C4=CC=CC=C4)=O

Result:

{"class_results": ["Pulvinones"], "superclass_results": ["Diazotetronic acids and derivatives"], "pathway_results": ["Shikimates and Phenylpropanoids"], "isglycoside": false, "fp1": [0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,
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Figure S2 A result from application programming interface (API) for NPClassifier.

An example code for Python.

```
import requests
import json

url = "https://npclassifier.ucsd.edu"
smiles = 'COC(=O)[C@H](C1=CC=CC=C1)[C@H](C2=CC=CC=C2)C3=C(/C(=C#C4=CC=CC=C4)/OC3=O)O'

r = requests.get(f"{url}/classify?smiles={smiles}")
print(r.json()['pathway_results'],r.json()['superclass_results'],r.json()['class_results'])
```

```
['Shikimates and Phenylpropanoids'] ['Diazotetronic acids and derivatives'] ['Pulvinones']
```

2. Experimental Methods

Dataset for training. The dataset for training the neural network was prepared using Class, Superclass and Pathway designations as indicated in SI Section 3. Compounds with these same category descriptions were manually collected from hundreds of research papers, review papers, titles, books, and abstracts.[1-49] These collected keywords were converted to structures using the Pubchem identifier exchange service and Chemspider. Additional compounds from the ChEBI database[50] were integrated to make the dataset balanced between different classes of NPs. The structures of unconverted keywords via Pubchem or Chemspider were manually curated by searching the UNPD database[51] or by drawing the structures from primary literature sources. Duplicates were removed by comparing the InChIKey representations; these in turn were produced by conversion from the SMILES.[52] In total, 73,607 natural products were labeled and established as a dataset for training NPClassifier (Figure S3, high-resolution image is available on https://zenodo.org/record/5068687#.YPm57ehKiUl).

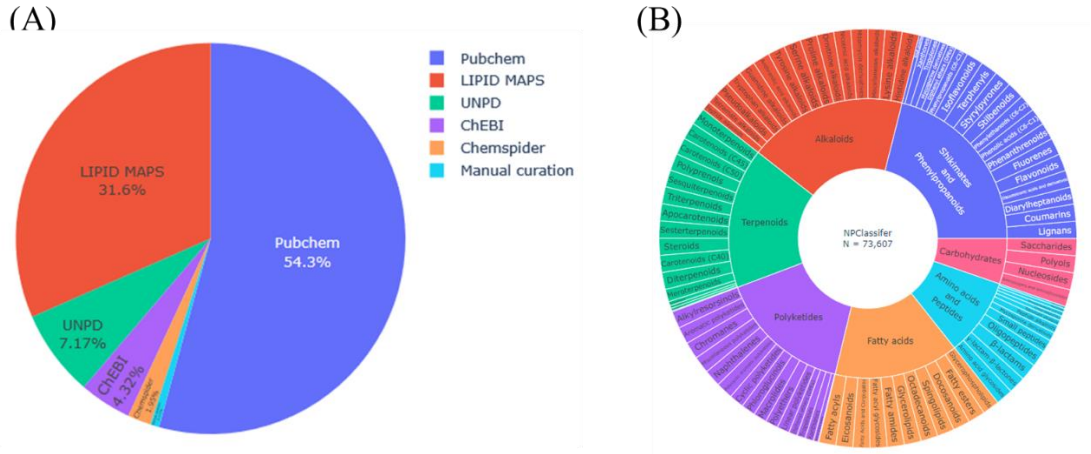
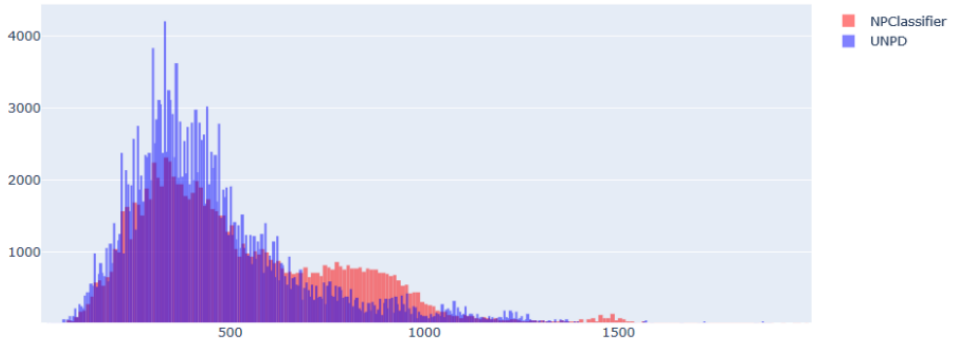


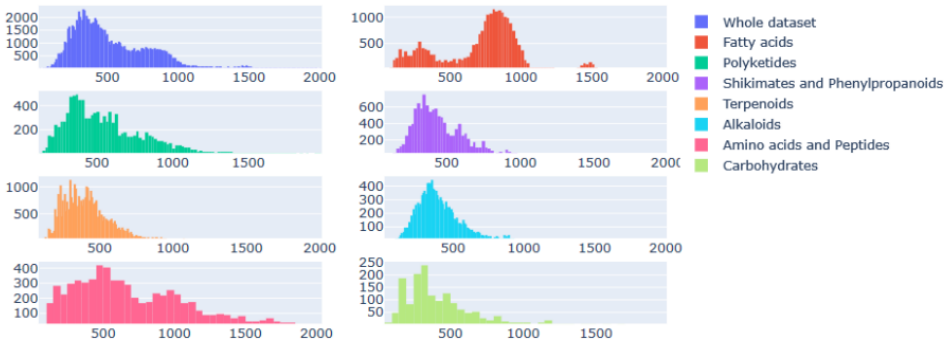
Figure S3 Overview of the NPClassifier dataset. (A) The public database source for the dataset: Pubchem (n=39,549), LIPID MAPS (n=23,506), UNPD (n=5,337), ChEBI (n=3,219), Chemspider (n=1,453), and manual curation (n=534). (B) Pathways and Superclasses in the data set.

The distribution of the molecular weights from the dataset is shown in Figure S4. Over all classes, the molecular weights were mostly distributed in the range 100 to 2000, which is similar to those in the Dictionary of Natural Products and UNPD, two representative natural product databases.[51, 53] The minimum molecular weight was 58 Da for pentane, a representative of the hydrocarbon Class. The maximum molecular weight NP was 5031 Da for polytheonamide A, a ribosomally synthesized and post-translationally modified peptides (RiPPs). This dataset was split in a stratified fashion using the Class labels; 64% were assigned to the training set, 16% to validation set, and 20% to the test set.

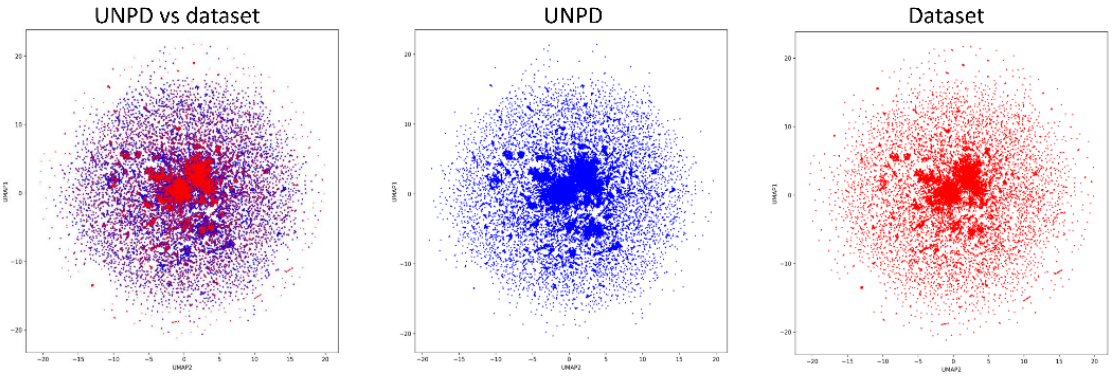
(A)


NPClassifier
UNPD
4000
3000
2000
1000
500
1000
1500

(B)


Whole dataset
Fatty acids
Polyketides
Shikimates and Phenylpropanoids
Terpenoids
Alkaloids
Amino acids and Peptides
Carbohydrates

(C)


UNPD vs dataset
UNPD
Dataset

(D)

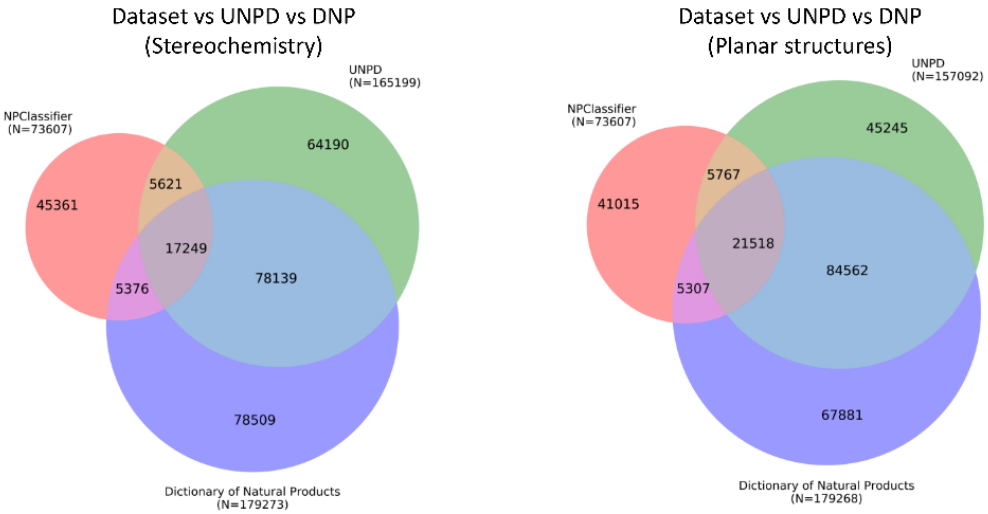

Dataset vs UNPD vs DNP
(Stereochemistry)
NPClassifier
(N=73607)
UNPD
(N=165199)
Dictionary of Natural Products
(N=179273)
45361
5621
64190
17249
78139
5376
78509
Dataset vs UNPD vs DNP
(Planar structures)
NPClassifier
(N=73607)
UNPD
(N=157092)
Dictionary of Natural Products
(N=179268)
41015
5767
45245
21518
84562
5307
67881

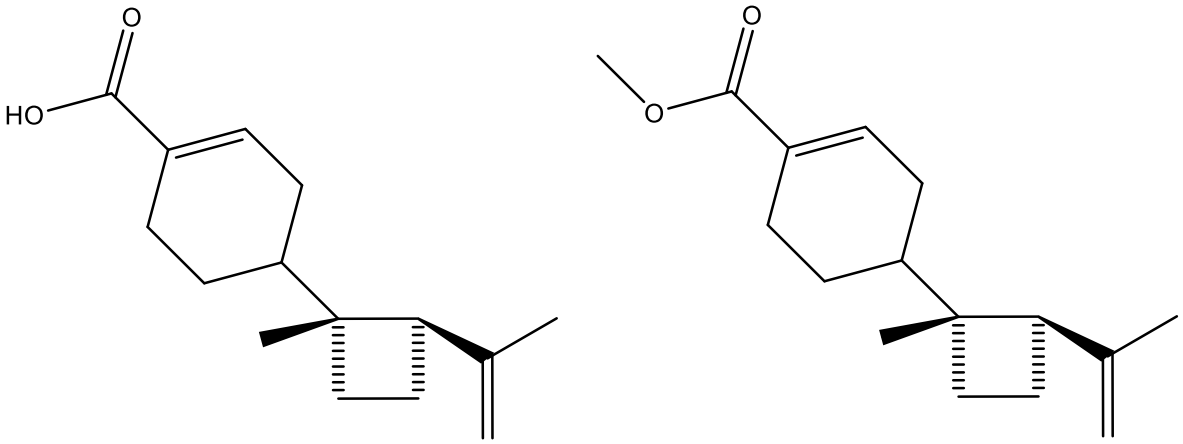
Figure S4 The distribution of molecular weights in the NPClassifier dataset. (A) The overlapped histogram of molecular weights from the NPClassifier dataset and UNPD database. (B) The distribution of molecular weights from each Pathway of the data set. Note that the y-axes are different in each case. (C) Mapping chemical spaces of UNPD database (Blue) and NPClassifier dataset (Red) with UMAP. Molecular structures in the analysis were represented by 2048-bit Morgan fingerprints. (D) Venn diagrams of the chemical entities from NPClassifier dataset, UNPD database, and Dictionary of Natural Products with/without stereochemistry.

Data augmentation. The number of NP examples in the training set for each of the Classes was unbalanced because some of the reported scaffolds are quite rare. For example, there are only two examples of dunniane-type sesquiterpenoids, (-)-dunniane and (-)-cumacrene. Because there were several other poorly populated classes of NPs in the dataset, we artificially built biosynthetically possible structures based on actual structures in these classes, and then integrated them into the training set (Figure S5). The biosynthetically plausible analogs were created as follows:

1. Addition of methyl groups to hydroxy groups to generate methoxy groups

2. Replacement of methoxy groups with hydroxy groups

All duplicate structures that were generated during the data augmentation process were filtered and removed by comparing their InChIKeys. Augmentation was done for 47,108 structures resulting in 125,580 chemical entities in the training set.



(-)-dunniane

(-)-dunniane methyl ester
(Not real compound)

Figure S5 (-)-Dunniane (left) and its artificially modified methyl ester structure (right) as an illustration of data augmentation.

Preparing an external evaluation test set. To evaluate and compare the performance between different platforms, compound Classes that were included in both the NPClassifier and ClassyFire platforms were chosen from the Dictionary of Natural Products (http://dnp.chemnetbase.com/). In the external test set, 3,000 chemical entities for three Pathways (amino acid-peptides, polyketides, and terpenoids), 3,000 compounds for three Superclasses (flavonoids, lignans, and steroids), and 6,200 compounds for sixty-two Classes were included. As these structures are from a commercial library, this data was only used for testing, and were not included in the training set of NPClassifier.

Data labelling and Evaluation metric. For the output of NPClassifier, each unique category from the three classification levels were encoded by the binary encoding method. For the Pathway designation, "*Polyketides"* was defined as [0,0,0,0,1,0,0], and *"Amino acids and Peptides"* were defined as [0,1,0,0,0,0,0]. If the molecules were biosynthesized from a hybrid of *"Polyketides"* and *"Amino acids and Peptides"*, they were defined as [0,1,0,0,1,0,0]. We used cosine scores to measure the similarity between these binarized vectors, and this allowed comparison between the predicted results and the ground truth results during training.

To compare the performance between each model, average precision, mean average precision, and F1 scores were computed from the results. In the precision recall curves, the tradeoff between precision and recall was shown for different thresholds. A high area under the curve represents both high recall and high precision, where high precision relates to a low false positive rate, and high recall relates to a low false negative rate. Thus, high scores for both demonstrate that the classifier is returning accurate results. Average precision (AP) summarizes a precision-recall curve as the weighted mean of precisions achieved at each threshold, with the increase in recall from the

previous threshold used as the weight:

$$AP = \sum_{k=1}^{n} (R_k - R_{k-1}) P_k$$

where P_k and R_k are the precision and recall at the k^{th} threshold.

Mean average precision (mAP) is the average AP from k classes in order to measure the performance of multi-label classification problems.[54]

$$mAP = \frac{1}{k} \sum_{i=1}^{k} AP_i$$

F1 score is defined as the harmonic mean of precision and recall. This score is often used in the field of information retrieval for measuring search, document classification, and query classification performance.

$$F1\ score = 2 \times \frac{Precision \times Recall}{Precision + Recall}$$

Deep Neural Network Architectures. The DNN for the NPClassifier was composed of three different networks that classified the molecular structure at the three levels noted (Pathway, Superclass, Class) with feed-forward neural network architecture. (We tested and compared random forest (RF) and deep neural network (DNN) architectures in preliminary studies. We found, using a small dataset that was available at the time, that the DNN gave the best performance; average precision, 0.95 using DNN, and 0.81 using RF). For each network, there is an input layer, representing the counted fingerprints, followed by three hidden layers and a fully-connected layer

to the output. Dropout was applied to the fully-connected layers to improve generalization. The activation function for the hidden layers used the ReLu function and all hidden layers were normalized by batch normalization to avoid problems of overfitting and vanishing gradient.[55]

In natural products classification, many multi-labelled cases are encountered. For example, the plant alkaloid, halfordinol, contains two chemical moieties (Figure S6). One moiety is a pyridine ring from nicotinic acid, and the other is an oxazole deriving from tyrosine.[56, 57] Thus, this molecule derives from two amino acids and can be classified as both a pyridine alkaloid and an oxazole alkaloid.

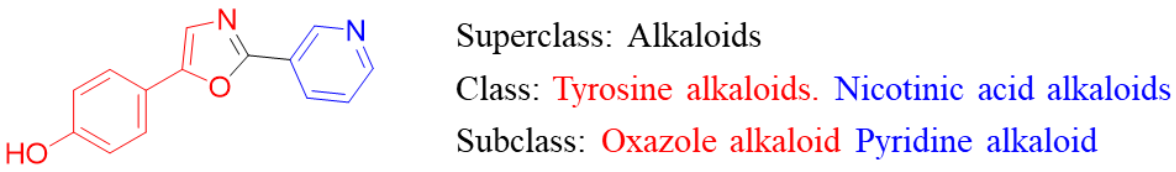


Figure S6 An example of a molecule possessing multi-components. The halfordinol contains oxazole and pyridine moieties that derive from tyrosine and nicotinic acid, respectively.

Following from this example, the classification of natural products was considered as a multiclass and multilabel situation, and thus a sigmoid function and a binary cross-entropy objective function was used for the output layers.[58]

Hyperparameters. The training of DNNs is affected by independent adjustable parameters known as 'hyperparameters', which include the learning rate, optimizer, batch size, the number of hidden layers, epochs, and others.[59] The numbers of hidden layers, neurons, and regularization rates are also considered as hyperparameters. Accordingly, the performance of neural networks depends on how the hyperparameters are tuned, which can only be done by repeated experimentation (Figure S7). Hyperparameters were optimized by the Hyperband algorithm in

Keras Tuner. 254 combinations of hyperparameters were tried and the hyperparameters with the lowest validation loss was chosen. The optimized hyperparameter set used for NPClassifier is shown in Table S1. The source code for NPClassifier is available on GitHub at https://github.com/mwang87/NP-Classifier.

Table S1. Hyperparameters for training the deep neural networks for NPClassifier

Optimizer	Adam
Activation functions	ReLu (hidden layers), sigmoid (top layer)
Hidden layer units	3072, 2304, 1152
Loss function	Binary cross-entropy
Learning rate	0.00001 (decay = $1*e^{-6}$)
Batch normalization	Used
Dropout rate	0.1
Batch size	128
Regularization	Early stopping (patience = 5)

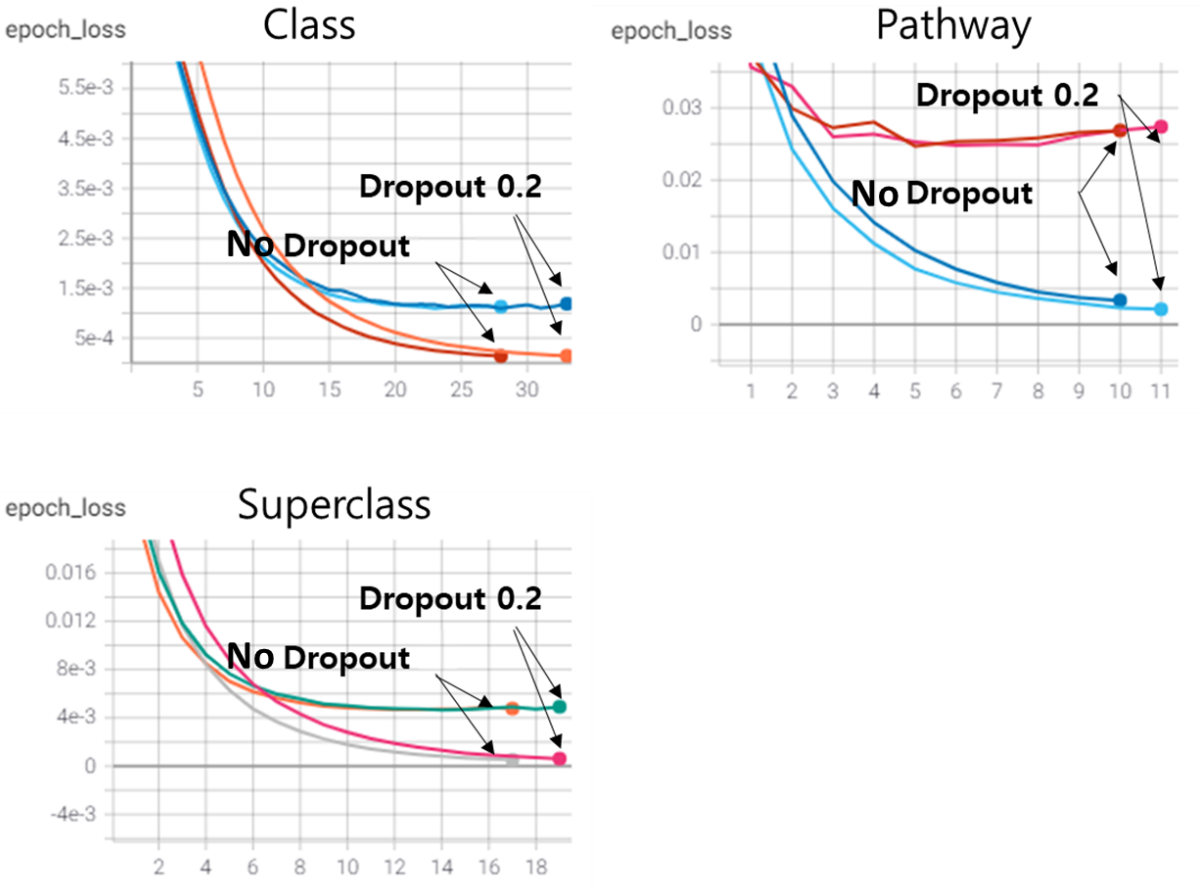


Figure S7 Effect of dropout regularization in the training of NPClassifier (logscale).

3. Classification schema and evaluation of NPClassifier

Pathway	Superclass	Class	Precision and Recall of Class			Population
			Precision	Recall	F1 score	
Alkaloids	Ornithine alkaloids	Stemona alkaloids	1.000	1.000	1.000	112
Alkaloids	Tyrosine alkaloids	Acutumine alkaloids	1.000	1.000	1.000	12
Alkaloids	Tyrosine alkaloids	Betalain alkaloids	0.909	0.833	1.000	19
Alkaloids	Tyrosine alkaloids	Cephalotaxus alkaloids	1.000	1.000	1.000	10
Alkaloids	Tryptophan alkaloids	Hapalindole alkaloids	1.000	1.000	1.000	18
Alkaloids	Tryptophan alkaloids	Pyrroloindole alkaloids	1.000	1.000	1.000	66
Alkaloids	Anthranilic acid alkaloids	Phenoxazine alkaloids	1.000	1.000	1.000	26
Alkaloids	Guanidine alkaloids	Saxitoxins	1.000	1.000	1.000	9
Alkaloids	Guanidine alkaloids	Tetrodotoxins	1.000	1.000	1.000	26
Alkaloids	Guanidine alkaloids	Acyclic guanidine alkaloids	1.000	1.000	1.000	4
Alkaloids	Guanidine alkaloids	Bicyclic guanidine alkaloids	1.000	1.000	1.000	17
Alkaloids	Guanidine alkaloids	Monocyclic guanidine alkaloids	1.000	1.000	1.000	6
Alkaloids	Pseudoalkaloids	Cytochalasan alkaloids	1.000	1.000	1.000	125
Alkaloids	Pseudoalkaloids	Capsaicins and Capsaicinoids	0.833	0.714	1.000	17
Alkaloids	Pseudoalkaloids	Isariotin alkaloids	1.000	1.000	1.000	10
Alkaloids	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Pro)	1.000	1.000	1.000	47
Alkaloids	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Trp)	1.000	1.000	1.000	13
Alkaloids	Peptide alkaloids	Other indole diketopiperazine alkaloids	0.966	0.933	1.000	43
Alkaloids	Tetramate alkaloids	Pyrrocidine tetramate alkaloids	1.000	1.000	1.000	25
Alkaloids	Tetramate alkaloids	Cyclopiazonic acid-tpye tetramate alkaloids	1.000	1.000	1.000	24
Alkaloids	Tetramate alkaloids	Simple tetramate alkaloids	0.917	0.846	1.000	18
Alkaloids	Mitomycin derivatives	Mitomycins	1.000	1.000	1.000	12
Alkaloids	Proline alkaloids	Prodigiosins	1.000	1.000	1.000	26
Alkaloids	Tryptophan alkaloids	Carbazole alkaloids	0.994	1.000	0.988	406
Alkaloids	Peptide alkaloids	Ansa peptide alkaloids	0.980	1.000	0.960	128

Alkaloids	Tryptophan alkaloids	Aspidosperma type	0.946	0.936	0.957	241
Alkaloids	Tryptophan alkaloids	Indole-Diterpenoid alkaloids (Penitrems)	0.971	1.000	0.944	90
Alkaloids	Tyrosine alkaloids	Morphinan alkaloids	0.959	0.986	0.934	408
Alkaloids	Guanidine alkaloids	Pentacyclic guanidine alkaloids	0.966	1.000	0.933	36
Alkaloids	Tyrosine alkaloids	Hasubanan alkaloids	0.929	0.929	0.929	37
Alkaloids	Tryptophan alkaloids	Ergot alkaloids	0.963	1.000	0.929	72
Alkaloids	Tryptophan alkaloids	Carboline alkaloids	0.951	0.978	0.925	734
Alkaloids	Tryptophan alkaloids	Iboga type	0.960	1.000	0.923	135
Alkaloids	Ornithine alkaloids	Tropane alkaloids	0.958	1.000	0.920	292
Alkaloids	Pseudoalkaloids	Steroidal alkaloids	0.948	0.986	0.913	405
Alkaloids	Anthranilic acid alkaloids	Acridone alkaloids	0.954	1.000	0.912	285
Alkaloids	Tryptophan alkaloids	Corynanthe type	0.838	0.775	0.912	177
Alkaloids	Tyrosine alkaloids	Protoberberine alkaloids	0.949	1.000	0.903	170
Alkaloids	Lysine alkaloids	Quinolizidine alkaloids	0.925	0.949	0.902	216
Alkaloids	Tyrosine alkaloids	Phenethylisoquinoline alkaloids	0.947	1.000	0.900	102
Alkaloids	Tryptophan alkaloids	Pyrroloquinoline alkaloids	0.918	0.966	0.875	178
Alkaloids	Serine alkaloids	Thiazole alkaloids	0.933	1.000	0.875	32
Alkaloids	Pseudoalkaloids	Purine alkaloids	0.876	0.886	0.867	235
Alkaloids	Tyrosine alkaloids	Isoquinoline alkaloids	0.806	0.757	0.862	903
Alkaloids	Ornithine alkaloids	Polyamines	0.918	0.986	0.859	434
Alkaloids	Tryptophan alkaloids	Strychnos type	0.906	0.960	0.857	146
Alkaloids	Pseudoalkaloids	Phenylalanine-derived alkaloids	0.889	0.923	0.857	143
Alkaloids	Miscellaneous alkaloids	Miscellaneous alkaloids	0.923	1.000	0.857	18
Alkaloids	Pseudoalkaloids	Terpenoid alkaloids	0.902	0.965	0.846	335
Alkaloids	Anthranilic acid alkaloids	Anthranillic acid derivatives	0.889	0.941	0.842	43
Alkaloids	Ornithine alkaloids	Pyrrolizidine alkaloids	0.897	0.972	0.833	218
Alkaloids	Tyrosine alkaloids	Protopine alkaloids	0.909	1.000	0.833	28
Alkaloids	Tyrosine alkaloids	Aporphine alkaloids	0.907	1.000	0.830	237
Alkaloids	Pseudoalkaloids	pteridine alkaloids	0.905	1.000	0.826	115
Alkaloids	Anthranilic acid alkaloids	Phenazine alkaloids	0.903	1.000	0.824	86

Alkaloids	Anthranilic acid alkaloids	Benzodiazepine alkaloids	0.903	1.000	0.824	49
Alkaloids	Tyrosine alkaloids	Phenylethylamines	0.901	1.000	0.821	215
Alkaloids	Tryptophan alkaloids	Simple oxindole alkaloids	0.889	1.000	0.800	21
Alkaloids	Tryptophan alkaloids	Aspidosperma-Iboga hybrid type (Vinca alkaloids)	0.667	0.571	0.800	56
Alkaloids	Pseudoalkaloids	Isoindole alkaloids	0.889	1.000	0.800	72
Alkaloids	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Ala)	0.880	1.000	0.786	39
Alkaloids	Tyrosine alkaloids	Amarylidaceae alkaloids	0.833	0.889	0.784	253
Alkaloids	Anthranilic acid alkaloids	Quinazoline alkaloids	0.839	0.929	0.765	88
Alkaloids	Peptide alkaloids	Thiodiketopiperazine alkaloids	0.839	0.929	0.765	87
Alkaloids	Peptide alkaloids	Simple diketopiperazine alkaloids	0.857	1.000	0.750	28
Alkaloids	Tryptophan alkaloids	Yohimbine-like alkaloids	0.842	1.000	0.727	63
Alkaloids	Nicotinic acid alkaloids	Pyridine alkaloids	0.802	0.901	0.722	623
Alkaloids	Pseudoalkaloids	Azo and Azoxy alkaloids	0.818	1.000	0.692	71
Alkaloids	Lysine alkaloids	Piperidine alkaloids	0.771	0.914	0.667	259
Alkaloids	Tyrosine alkaloids	Terpenoid tetrahydroisoquinoline alkaloids	0.800	1.000	0.667	57
Alkaloids	Tyrosine alkaloids	Homoerythrina alkaloids	0.667	0.667	0.667	10
Alkaloids	Tryptophan alkaloids	Quinoline alkaloids	0.791	1.000	0.654	132
Alkaloids	Anthranilic acid alkaloids	Quinoline alkaloids	0.791	1.000	0.654	132
Alkaloids	Histidine alkaloids	Imidazole alkaloids	0.744	0.879	0.644	236
Alkaloids	Peptide alkaloids	Pyrazine and Piperazine alkaloids	0.682	0.938	0.536	142
Alkaloids	Tetramate alkaloids	Pyrazine and Piperazine alkaloids	0.682	0.938	0.536	142
Alkaloids	Peptide alkaloids	Simple amide alkaloids	0.667	0.920	0.523	199
Alkaloids	Tyrosine alkaloids	Tetrahydroisoquinoline alkaloids	0.683	1.000	0.519	156
Alkaloids	Tyrosine alkaloids	Oxazole alkaloids	0.667	1.000	0.500	10
Alkaloids	Ornithine alkaloids	Pyrrolidine alkaloids	0.636	0.933	0.483	150
Alkaloids	Proline alkaloids	Pyrrole alkaloids	0.632	1.000	0.462	66
Alkaloids	Lysine alkaloids	Indolizidine alkaloids	0.615	0.941	0.457	187
Alkaloids	Guanidine alkaloids	Tricyclic guanidine alkaloids	0.545	1.000	0.375	27
Alkaloids	Tryptophan alkaloids	Simple indole alkaloids	0.526	1.000	0.357	144
Alkaloids	Pseudoalkaloids	Acetate-derived alkaloids	0.400	0.500	0.333	19

Amino acids and Peptides	Macrolides	Epothilones	1.000	1.000	1.000	63
Amino acids and Peptides	Macrolides	Rhizoxins	1.000	1.000	1.000	8
Amino acids and Peptides	Macrolides	Macrolide lactams	1.000	1.000	1.000	35
Amino acids and Peptides	Macrolides	Lactam bearing macrolide lactones	0.976	0.952	1.000	24
Amino acids and Peptides	Macrolides	Antimycins	1.000	1.000	1.000	48
Amino acids and Peptides	Macrolides	Macrocyclic tetramic acids	1.000	1.000	1.000	46
Amino acids and Peptides	Linear polyketides	Elfamycins	1.000	1.000	1.000	10
Amino acids and Peptides	Linear polyketides	DKXanthenes and derivatives	1.000	1.000	1.000	13
Amino acids and Peptides	Cyclic polyketides	3-Spirotetramic acids	1.000	1.000	1.000	22
Amino acids and Peptides	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Pro)	1.000	1.000	1.000	47
Amino acids and Peptides	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Trp)	1.000	1.000	1.000	13
Amino acids and Peptides	Peptide alkaloids	Other indole diketopiperazine alkaloids	0.966	0.933	1.000	43
Amino acids and Peptides	Tetramate alkaloids	Pyrrocidine tetramate alkaloids	1.000	1.000	1.000	25
Amino acids and Peptides	Tetramate alkaloids	Cyclopiazonic acid-type tetramate alkaloids	1.000	1.000	1.000	24
Amino acids and Peptides	Mycosporine derivatives	Mycosporine and Mycosporine-like amino acids	1.000	1.000	1.000	27
Amino acids and Peptides	Oligopeptides	Aeruginosins	1.000	1.000	1.000	46
Amino acids and Peptides	Oligopeptides	Microginins	1.000	1.000	1.000	41
Amino acids and Peptides	Oligopeptides	Anabaenopeptins	0.976	0.952	1.000	38
Amino acids and Peptides	Oligopeptides	Microcystins	1.000	1.000	1.000	59
Amino acids and Peptides	Oligopeptides	Microcolins and mirabimides	1.000	1.000	1.000	16
Amino acids and Peptides	Oligopeptides	Tantazoles and mirabazoles	1.000	1.000	1.000	7
Amino acids and Peptides	Oligopeptides	Vancomycins and Teicoplanins	1.000	1.000	1.000	283
Amino acids and Peptides	Oligopeptides	Streptogramins	1.000	1.000	1.000	14
Amino acids and Peptides	Oligopeptides	Actinomycins	1.000	1.000	1.000	99
Amino acids and Peptides	β-lactams	Penicillins	1.000	1.000	1.000	101
Amino acids and Peptides	β-lactams	Cephalosporins	0.973	0.947	1.000	90
Amino acids and Peptides	β-lactams	Cephamycins	1.000	1.000	1.000	19
Amino acids and Peptides	β-lactams	Clavams	1.000	1.000	1.000	13
Amino acids and Peptides	β-lactams	Carbapenems	1.000	1.000	1.000	30
Amino acids and Peptides	β-lactams	Monocyclic β-lactams	1.000	1.000	1.000	3

Amino acids and Peptides	γ-lactam-β-lactones	Salinosporamides	1.000	1.000	1.000	8
Amino acids and Peptides	Oligopeptides	RiPPs-Amatoxins and Phallotoxins	1.000	1.000	1.000	8
Amino acids and Peptides	Oligopeptides	RiPPs-Bottromycins	1.000	1.000	1.000	4
Amino acids and Peptides	Oligopeptides	RiPPs-Lasso peptides	1.000	1.000	1.000	6
Amino acids and Peptides	Oligopeptides	RiPPs-Microcins	1.000	1.000	1.000	4
Amino acids and Peptides	Peptide alkaloids	Ansa peptide alkaloids	0.980	1.000	0.960	128
Amino acids and Peptides	Oligopeptides	Cyclic peptides	0.967	0.984	0.951	1232
Amino acids and Peptides	Oligopeptides	RiPPs-Thiopeptides	0.968	1.000	0.938	22
Amino acids and Peptides	Oligopeptides	Depsipeptides	0.960	0.985	0.937	671
Amino acids and Peptides	Amino acid glycosides	Glucosinolates	0.966	1.000	0.933	74
Amino acids and Peptides	Oligopeptides	Lipopeptides	0.929	0.929	0.929	284
Amino acids and Peptides	Oligopeptides	RiPPs-Lanthipeptides	0.962	1.000	0.926	17
Amino acids and Peptides	Cyclic polyketides	3-Decalinoyltetramic acids	0.960	1.000	0.923	67
Amino acids and Peptides	Oligopeptides	Linear peptides	0.927	0.935	0.918	247
Amino acids and Peptides	Phenylpropanoids (C6-C3)	Cinnamic acid amides	0.952	1.000	0.909	24
Amino acids and Peptides	Oligopeptides	Bleomycins	0.900	0.900	0.900	47
Amino acids and Peptides	Oligopeptides	Cryptophycins	0.917	1.000	0.846	36
Amino acids and Peptides	Oligopeptides	Peptaibols	0.917	1.000	0.846	66
Amino acids and Peptides	Small peptides	Dipeptides	0.859	0.880	0.838	531
Amino acids and Peptides	Small peptides	Aminoacids	0.883	0.935	0.837	486
Amino acids and Peptides	Linear polyketides	Melithiazole and Myxothiazole derivatives	0.909	1.000	0.833	23
Amino acids and Peptides	Linear polyketides	3-acyl tetramic acids	0.897	1.000	0.813	74
Amino acids and Peptides	Peptide alkaloids	Indole diketopiperazine alkaloids (L-Trp, L-Ala)	0.880	1.000	0.786	39
Amino acids and Peptides	Peptide alkaloids	Thiodiketopiperazine alkaloids	0.839	0.929	0.765	87
Amino acids and Peptides	Peptide alkaloids	Simple diketopiperazine alkaloids	0.857	1.000	0.750	28
Amino acids and Peptides	Small peptides	Tripeptides	0.819	0.919	0.739	231
Amino acids and Peptides	Amino acid glycosides	Cyanogenic glycosides	0.800	1.000	0.667	34
Amino acids and Peptides	Peptide alkaloids	Pyrazine and Piperazine alkaloids	0.682	0.938	0.536	142
Amino acids and Peptides	Oligopeptides	RiPPs-Cyanobactins	0.400	1.000	0.250	15
Carbohydrates	Polyols	Cyclitols	1.000	1.000	1.000	42

Carbohydrates	Nucleosides	Streptothricins and derivatives	1.000	1.000	1.000	16
Carbohydrates	Nucleosides	Purine nucleos(t)ides	0.955	1.000	0.913	114
Carbohydrates	Nucleosides	Pyrimidine nucleos(t)ides	0.947	1.000	0.900	99
Carbohydrates	Saccharides	Disaccharides	0.842	0.889	0.800	32
Carbohydrates	Saccharides	Orthosomycins	0.889	1.000	0.800	18
Carbohydrates	Saccharides	Monosaccharides	0.848	0.933	0.778	92
Carbohydrates	Aminosugars and aminoglycosides	Aminoglycosides	0.714	0.667	0.769	58
Carbohydrates	Polyols	Amino cyclitols	0.851	1.000	0.741	121
Carbohydrates	Aminosugars and aminoglycosides	Aminosugars	0.776	0.864	0.704	127
Carbohydrates	Saccharides	Paulomycins and derivatives	0.800	1.000	0.667	16
Carbohydrates	Saccharides	Polysaccharides	0.714	1.000	0.556	51
Fatty acids	Fatty Acids and Conjugates	Methoxy fatty acids	0.966	0.933	1.000	32
Fatty acids	Fatty Acids and Conjugates	Nitro fatty acids	1.000	1.000	1.000	14
Fatty acids	Fatty Acids and Conjugates	Mycolic acids	1.000	1.000	1.000	130
Fatty acids	Octadecanoids	12-oxophytodienoic acid metabolites	1.000	1.000	1.000	9
Fatty acids	Octadecanoids	Phytoprostanes	1.000	1.000	1.000	14
Fatty acids	Octadecanoids	Phytofurans	1.000	1.000	1.000	4
Fatty acids	Eicosanoids	Leukotrienes	0.988	0.976	1.000	49
Fatty acids	Eicosanoids	Thromboxanes	1.000	1.000	1.000	11
Fatty acids	Eicosanoids	Lipoxins	1.000	1.000	1.000	7
Fatty acids	Eicosanoids	Hydroxy-hydroperoxyeicosatrienoic acids	0.923	0.857	1.000	17
Fatty acids	Eicosanoids	Epoxyeicosatrienoic acids	1.000	1.000	1.000	8
Fatty acids	Eicosanoids	Hepoxilins	0.800	0.667	1.000	11
Fatty acids	Eicosanoids	Levuglandins	1.000	1.000	1.000	9
Fatty acids	Eicosanoids	Isofurans	1.000	1.000	1.000	8
Fatty acids	Eicosanoids	Eicosa-1,2-dioxolanes	1.000	1.000	1.000	2
Fatty acids	Eicosanoids	Resolvin Es	0.941	0.889	1.000	9
Fatty acids	Eicosanoids	Clavulones	1.000	1.000	1.000	33
Fatty acids	Docosanoids	Neuroprostanes	1.000	1.000	1.000	40

Fatty acids	Docosanoids	Neurofurans	1.000	1.000	1.000	16
Fatty acids	Docosanoids	Docosa-1,2-dioxolanes	1.000	1.000	1.000	2
Fatty acids	Docosanoids	Resolvin Ds	1.000	1.000	1.000	8
Fatty acids	Fatty esters	Fatty acyl CoAs	1.000	1.000	1.000	265
Fatty acids	Fatty esters	Fatty acyl carnitines	1.000	1.000	1.000	90
Fatty acids	Fatty amides	Fatty acyl homoserine lactones	1.000	1.000	1.000	37
Fatty acids	Fatty acyls	Fatty ethers	1.000	1.000	1.000	3
Fatty acids	Fatty acyl glycosides	Sophorolipids	1.000	1.000	1.000	4
Fatty acids	Fatty acyl glycosides	Rhamnolipids	0.971	0.944	1.000	16
Fatty acids	Glycerolipids	Monoacylglycerols	1.000	1.000	1.000	53
Fatty acids	Glycerolipids	Glycosylmonoacylglycerols	1.000	1.000	1.000	7
Fatty acids	Glycerophospholipids	Glycerophosphocholines	1.000	1.000	1.000	1724
Fatty acids	Glycerophospholipids	Glycerophosphoserines	1.000	1.000	1.000	1219
Fatty acids	Glycerophospholipids	Glycerophosphoglycerophosphates	1.000	1.000	1.000	3
Fatty acids	Glycerophospholipids	Glycerophosphoinositols	1.000	1.000	1.000	1188
Fatty acids	Glycerophospholipids	Glycerophosphoinositol phosphates	1.000	1.000	1.000	7
Fatty acids	Glycerophospholipids	Glycerophosphates	1.000	1.000	1.000	1198
Fatty acids	Glycerophospholipids	Glycerophosphoglycerophosphoglycerols	1.000	1.000	1.000	666
Fatty acids	Glycerophospholipids	CDP-Glycerols	1.000	1.000	1.000	36
Fatty acids	Glycerophospholipids	Glycosylglycerophospholipids	1.000	1.000	1.000	5
Fatty acids	Glycerophospholipids	Glycerophosphoinositolglycans	1.000	1.000	1.000	113
Fatty acids	Glycerophospholipids	Oxidized glycerophospholipids	1.000	1.000	1.000	245
Fatty acids	Glycerophospholipids	Long-Chain Bicyclic Phosphotriester	1.000	1.000	1.000	30
Fatty acids	Sphingolipids	Acidic glycosphingolipids	1.000	1.000	1.000	13
Fatty acids	Fatty acyls	Resin glycosides	0.983	0.967	1.000	145
Fatty acids	Fatty acyls	Paraconic acids and derivatives	1.000	1.000	1.000	18
Fatty acids	Fatty acyls	Halogenated hydrocarbons	1.000	1.000	1.000	43
Fatty acids	Glycerolipids	Triacylglycerols	1.000	1.000	0.999	6889
Fatty acids	Glycerophospholipids	Glycerophosphoethanolamines	0.996	0.996	0.996	1336
Fatty acids	Glycerophospholipids	Glycerophosphoglycerols	0.998	1.000	0.996	1209

Fatty acids	Fatty acyls	Hydrocarbons	0.989	0.985	0.992	654
Fatty acids	Sphingolipids	Phosphosphingolipids	0.992	1.000	0.985	326
Fatty acids	Sphingolipids	Ceramides	0.987	1.000	0.975	200
Fatty acids	Glycerolipids	Diacylglycerols	0.987	1.000	0.974	570
Fatty acids	Fatty acyl glycosides	Ascarosides	0.983	1.000	0.967	152
Fatty acids	Sphingolipids	Neutral glycosphingolipids	0.982	1.000	0.966	143
Fatty acids	Fatty esters	Fatty acid estolides	0.981	1.000	0.963	123
Fatty acids	Fatty acyls	Fatty aldehydes	0.938	0.927	0.950	201
Fatty acids	Fatty Acids and Conjugates	Branched fatty acids	0.902	0.871	0.937	395
Fatty acids	Eicosanoids	Isoprostanes	0.900	0.871	0.931	38
Fatty acids	Fatty esters	Wax monoesters	0.952	0.977	0.929	905
Fatty acids	Glycerolipids	Glycosyldiacylglycerols	0.960	1.000	0.923	35
Fatty acids	Fatty Acids and Conjugates	Hydroperoxy fatty acids	0.957	1.000	0.917	27
Fatty acids	Fatty Acids and Conjugates	Heterocyclic fatty acids	0.957	1.000	0.917	60
Fatty acids	Fatty acyls	Oxygenated hydrocarbons	0.955	1.000	0.914	289
Fatty acids	Fatty amides	N-acyl ethanolamines (endocannabinoids)	0.952	1.000	0.909	56
Fatty acids	Fatty Acids and Conjugates	Unsaturated fatty acids	0.901	0.895	0.906	794
Fatty acids	Fatty Acids and Conjugates	Epoxy fatty acids	0.800	0.727	0.889	32
Fatty acids	Fatty Acids and Conjugates	Carbocyclic fatty acids	0.909	0.938	0.882	85
Fatty acids	Fatty amides	N-acyl amines	0.928	0.978	0.882	255
Fatty acids	Eicosanoids	Prostaglandins	0.900	0.947	0.857	167
Fatty acids	Fatty Acids and Conjugates	Amino fatty acids	0.882	0.938	0.833	40
Fatty acids	Fatty Acids and Conjugates	Oxo fatty acids	0.778	0.757	0.800	173
Fatty acids	Fatty Acids and Conjugates	Oxo fatty acids	0.778	0.757	0.800	173
Fatty acids	Fatty Acids and Conjugates	Dicarboxylic acids	0.851	0.909	0.800	121
Fatty acids	Octadecanoids	Jasmonic acids	0.889	1.000	0.800	11
Fatty acids	Eicosanoids	Hydroxy-hydroperoxyeicosatetraenoic acids	0.842	0.889	0.800	52
Fatty acids	Eicosanoids	Hydroxy-hydroperoxyeicosapentaenoic acids	0.857	0.923	0.800	26
Fatty acids	Fatty esters	Cyano esters	0.889	1.000	0.800	24
Fatty acids	Sphingolipids	Sphingoid bases	0.889	1.000	0.800	77

Fatty acids	Fatty acyls	Fatty alcohols	0.866	0.951	0.795	366
Fatty acids	Fatty esters	Lactones	0.850	1.000	0.739	114
Fatty acids	Octadecanoids	Other Octadecanoids	0.795	0.917	0.702	238
Fatty acids	Docosanoids	Other Docosanoids	0.706	0.750	0.667	51
Fatty acids	Fatty acyl glycosides	Fatty acyl glycosides of mono- and disaccharides	0.778	1.000	0.636	56
Fatty acids	Fatty Acids and Conjugates	Hydroxy fatty acids	0.772	1.000	0.629	291
Fatty acids	Fatty Acids and Conjugates	Hydroxy fatty acids	0.772	1.000	0.629	291
Fatty acids	Eicosanoids	Other Eicosanoids	0.667	0.800	0.571	16
Fatty acids	Fatty amides	Primary amides	0.600	0.750	0.500	27
Fatty acids	Fatty acyls	Fatty nitriles	0.667	1.000	0.500	5
Fatty acids	Fatty esters	Wax diesters	0.500	1.000	0.333	19
Polyketides	Macrolides	Tylosins	0.923	0.857	1.000	60
Polyketides	Macrolides	Avermectins	1.000	1.000	1.000	169
Polyketides	Macrolides	Ascomycins and Rapamycins	1.000	1.000	1.000	88
Polyketides	Macrolides	Ascomycins and Rapamycins	1.000	1.000	1.000	88
Polyketides	Macrolides	Epothilones	1.000	1.000	1.000	63
Polyketides	Macrolides	Rhizoxins	1.000	1.000	1.000	8
Polyketides	Macrolides	Oligomycins	1.000	1.000	1.000	18
Polyketides	Macrolides	Bafilomycins	1.000	1.000	1.000	24
Polyketides	Macrolides	Macrolide lactams	1.000	1.000	1.000	35
Polyketides	Macrolides	Lactam bearing macrolide lactones	0.976	0.952	1.000	24
Polyketides	Macrolides	Enediynes	1.000	1.000	1.000	40
Polyketides	Macrolides	Bryostatins	1.000	1.000	1.000	18
Polyketides	Macrolides	Antimycins	1.000	1.000	1.000	48
Polyketides	Macrolides	Oxa-Bridged Macrolides	1.000	1.000	1.000	17
Polyketides	Macrolides	Macrocyclic tetramic acids	1.000	1.000	1.000	46
Polyketides	Linear polyketides	Linear tetronates	1.000	1.000	1.000	7
Polyketides	Linear polyketides	Elfamycins	1.000	1.000	1.000	10
Polyketides	Linear polyketides	3-oligoenoyltetramic acids	1.000	1.000	1.000	58
Polyketides	Linear polyketides	Linear polyenes	0.980	0.960	1.000	47

Polyketides	Linear polyketides	Polyesters	1.000	1.000	1.000	6
Polyketides	Linear polyketides	DKXanthenes and derivatives	1.000	1.000	1.000	13
Polyketides	Chromanes	Cytosporins	1.000	1.000	1.000	12
Polyketides	Cyclic polyketides	Decalins with 2-pyrones	1.000	1.000	1.000	14
Polyketides	Cyclic polyketides	3-Spirotetramic acids	1.000	1.000	1.000	22
Polyketides	Cyclic polyketides	Nonadrides	1.000	1.000	1.000	28
Polyketides	Alkylresorcinols	Monoalkylresorcinols	0.889	0.800	1.000	8
Polyketides	Alkylresorcinols	Dialkylresorcinols	1.000	1.000	1.000	47
Polyketides	Chromanes	Aflatoxins	1.000	1.000	1.000	68
Polyketides	Aromatic polyketides	Griseofulvins	1.000	1.000	1.000	36
Polyketides	Aromatic polyketides	Catechols with side chains	1.000	1.000	1.000	237
Polyketides	Aromatic polyketides	Aromatic polyketides with side chains	1.000	1.000	1.000	25
Polyketides	Aromatic polyketides	Simple aromatic polyketides	1.000	1.000	1.000	46
Polyketides	Aromatic polyketides	Luminacins and derivatives	1.000	1.000	1.000	12
Polyketides	Meroterpenoids	Cannabinoids	1.000	1.000	1.000	136
Polyketides	Polycyclic aromatic polyketides	Pradimicins	1.000	1.000	1.000	7
Polyketides	Polycyclic aromatic polyketides	Fasamycins and derivatives	1.000	1.000	1.000	35
Polyketides	Polycyclic aromatic polyketides	Benastatins and derivatives	1.000	1.000	1.000	9
Polyketides	Phloroglucinols	Phloroglucinol-terpene hybrids	1.000	1.000	1.000	35
Polyketides	Phloroglucinols	Prenylated,geranylated phloroglucinols	1.000	1.000	1.000	34
Polyketides	Naphthalenes	Spirodioxynaphthalenes	1.000	1.000	1.000	70
Polyketides	Polyethers	Macrotetrolides	1.000	1.000	1.000	26
Polyketides	Tropolones	Tropolones and derivatives (PKS)	1.000	1.000	1.000	31
Polyketides	Diphenyl ethers (DPEs)	Fungal DPEs	0.964	0.931	1.000	48
Polyketides	Meroterpenoids	Triketide meroterpenoids	1.000	1.000	1.000	73
Polyketides	Meroterpenoids	Other polyketide meroterpenoids	1.000	1.000	1.000	24
Polyketides	Linear polyketides	Phoslactomycins or Phosphazomycins	1.000	1.000	1.000	28

Polyketides	Polycyclic aromatic polyketides	Phenalens	1.000	1.000	1.000	9
Polyketides	Naphthalenes	Naphthalenones	1.000	1.000	1.000	30
Polyketides	Polycyclic aromatic polyketides	Ericamycins	1.000	1.000	1.000	28
Polyketides	Aromatic polyketides	Benzophenones	0.966	0.933	1.000	18
Polyketides	Macrolides	Boromycins	0.923	0.857	1.000	13
Polyketides	Macrolides	Aplysiatoxins	1.000	1.000	1.000	17
Polyketides	Polycyclic aromatic polyketides	Duclauxin and derivatives	1.000	1.000	1.000	23
Polyketides	Macrolides	Ansa macrolides	0.992	1.000	0.984	608
Polyketides	Meroterpenoids	Polyprenylated cyclic polyketides (Hop meroterpenoids)	0.992	1.000	0.984	303
Polyketides	Macrolides	Erythromycins	0.986	1.000	0.971	532
Polyketides	Aromatic polyketides	Depsides	0.985	1.000	0.971	342
Polyketides	Linear polyketides	Acetogenins	0.976	0.984	0.968	314
Polyketides	Aromatic polyketides	Depsidones	0.983	1.000	0.967	154
Polyketides	Polycyclic aromatic polyketides	Tetracyclines	0.978	1.000	0.957	124
Polyketides	Phloroglucinols	Acyl phloroglucinols	0.977	1.000	0.955	107
Polyketides	Phloroglucinols	Oligomeric phloroglucinols (phlorotannins)	0.950	0.950	0.950	103
Polyketides	Macrolides	Spirotetronate macrolides	0.970	1.000	0.941	83
Polyketides	Aromatic polyketides	Sorbicilinoids	0.970	1.000	0.941	83
Polyketides	Polycyclic aromatic polyketides	Anthracyclines	0.970	1.000	0.941	186
Polyketides	Oligopeptides	Depsipeptides	0.960	0.985	0.937	671
Polyketides	Cyclic polyketides	2-pyrone derivatives	0.951	0.967	0.935	311
Polyketides	Aromatic polyketides	Usnic acid and derivatives	0.964	1.000	0.931	39
Polyketides	Cyclic polyketides	3-Decalinoyltetramic acids	0.960	1.000	0.923	67
Polyketides	Cyclic polyketides	4-pyrone derivatives	0.917	0.917	0.917	41
Polyketides	Polyethers	Ladder polyethers	0.957	1.000	0.917	58
Polyketides	Cyclic polyketides	Fungal cyclic polyketides (Miscellaneous)	0.957	1.000	0.917	26

Polyketides	Polycyclic aromatic polyketides	Anthraquinones and anthrones	0.918	0.929	0.907	639
Polyketides	Macrolides	Polyene macrolides	0.947	1.000	0.900	154
Polyketides	Polyethers	Polyether ionophores	0.941	1.000	0.889	97
Polyketides	Chromanes	Azaphilones	0.929	1.000	0.867	305
Polyketides	Linear polyketides	Melithiazole and Myxothiazole derivatives	0.909	1.000	0.833	23
Polyketides	Polycyclic aromatic polyketides	Angucyclines	0.899	0.976	0.833	244
Polyketides	Aromatic polyketides	Strobilurins and derivatives	0.909	1.000	0.833	23
Polyketides	Aromatic polyketides	Benzoquinones	0.909	1.000	0.833	17
Polyketides	Xanthones	Methyl xanthones	0.900	1.000	0.818	163
Polyketides	Linear polyketides	3-acyl tetramic acids	0.897	1.000	0.813	74
Polyketides	Meroterpenoids	Tetraketide meroterpenoids	0.882	0.968	0.811	184
Polyketides	Linear polyketides	Open-chain polyketides	0.864	0.961	0.785	453
Polyketides	Cyclic polyketides	Phthalide derivatives	0.878	1.000	0.783	114
Polyketides	Phloroglucinols	Dimeric phloroglucinols	0.857	0.947	0.783	121
Polyketides	Cyclic polyketides	Monacolins and Monacolin derivatives	0.741	0.769	0.714	69
Polyketides	Macrolides	Macrolide lactones	0.821	1.000	0.696	116
Polyketides	Chromanes	Chromones	0.791	0.944	0.680	241
Polyketides	Naphthalenes	Bisnaphthalenes	0.800	1.000	0.667	142
Polyketides	Cyclic polyketides	Decalins with side chains	0.788	1.000	0.650	93
Polyketides	Naphthalenes	Naphthoquinones	0.752	0.898	0.646	419
Polyketides	Macrolides	Zearalenones	0.783	1.000	0.643	72
Polyketides	Cyclic polyketides	Oblogolides	0.778	1.000	0.636	24
Polyketides	Cyclic polyketides	Furans	0.737	0.875	0.636	56
Polyketides	Naphthalenes	Naphthalenes and derivatives	0.629	0.786	0.524	108
Polyketides	Cyclic polyketides	Simple cyclic polyketides	0.632	0.857	0.500	61
Polyketides	Miscellaneous polyketides	Miscellaneous polyketides	0.667	1.000	0.500	79
Shikimates and Phenylpropanoids	Phenolic acids (C6-C1)	Bagremycins	1.000	1.000	1.000	7

Shikimates and Phenylpropanoids	Diphenyl ethers (DPEs)	Marine-bacterial DPEs	1.000	1.000	1.000	18
Shikimates and Phenylpropanoids	Phenylpropanoids (C6-C3)	Cinnamoyl phenols	1.000	1.000	1.000	18
Shikimates and Phenylpropanoids	Mycosporine derivatives	Mycosporine and Mycosporine-like amino acids	1.000	1.000	1.000	27
Shikimates and Phenylpropanoids	Lignans	Dibenzylbutyrolactone lignans	1.000	1.000	1.000	53
Shikimates and Phenylpropanoids	Lignans	Furofuranoid lignans	1.000	1.000	1.000	63
Shikimates and Phenylpropanoids	Lignans	Dibenzocyclooctadienes lignans	1.000	1.000	1.000	127
Shikimates and Phenylpropanoids	Lignans	Coumarinolignans	0.933	0.875	1.000	28
Shikimates and Phenylpropanoids	Coumarins	Coumarinolignans	0.933	0.875	1.000	28
Shikimates and Phenylpropanoids	Diarylheptanoids	Biaryl type diarylheptanoids	1.000	1.000	1.000	56
Shikimates and Phenylpropanoids	Fluorenes	Selaginellins	1.000	1.000	1.000	42
Shikimates and Phenylpropanoids	Flavonoids	Flavans	1.000	1.000	1.000	20
Shikimates and Phenylpropanoids	Flavonoids	Aurones	1.000	1.000	1.000	43
Shikimates and Phenylpropanoids	Flavonoids	Isoaurones	1.000	1.000	1.000	12
Shikimates and Phenylpropanoids	Flavonoids	Flavonostilbenes	1.000	1.000	1.000	14
Shikimates and Phenylpropanoids	Stilbenoids	Flavonostilbenes	1.000	1.000	1.000	14
Shikimates and Phenylpropanoids	Stilbenoids	Stilbenolignans	1.000	1.000	1.000	15
Shikimates and Phenylpropanoids	Lignans	Stilbenolignans	1.000	1.000	1.000	15
Shikimates and Phenylpropanoids	Isoflavonoids	Coumaronochromones	0.971	0.944	1.000	49

Shikimates and Phenylpropanoids	Flavonoids	Open-chained neoflavonoids	1.000	1.000	1.000	9
Shikimates and Phenylpropanoids	Phenanthrenoids	Phenanthrenes	0.988	0.977	1.000	421
Shikimates and Phenylpropanoids	Flavonoids	Flavonols	0.993	0.995	0.991	1097
Shikimates and Phenylpropanoids	Flavonoids	Flavones	0.987	0.987	0.987	1148
Shikimates and Phenylpropanoids	Flavonoids	Flavan-3-ols	0.925	0.886	0.969	147
Shikimates and Phenylpropanoids	Styrylpyrones	Kavalactones and derivatives	0.926	0.893	0.962	129
Shikimates and Phenylpropanoids	Flavonoids	Chalcones	0.969	0.978	0.960	1386
Shikimates and Phenylpropanoids	Lignans	Furanoid lignans	0.950	0.950	0.950	40
Shikimates and Phenylpropanoids	Diarylheptanoids	Diarylether type diarylheptanoids	0.974	1.000	0.950	47
Shikimates and Phenylpropanoids	Flavonoids	Anthocyanidins	0.972	1.000	0.946	597
Shikimates and Phenylpropanoids	Flavonoids	Dihydroflavonols	0.889	0.842	0.941	84
Shikimates and Phenylpropanoids	Xanthones	Plant xanthones	0.968	1.000	0.938	162
Shikimates and Phenylpropanoids	Coumarins	Furocoumarins	0.955	0.981	0.930	263
Shikimates and Phenylpropanoids	Diarylheptanoids	Linear diarylheptanoids	0.912	0.897	0.929	138
Shikimates and Phenylpropanoids	Flavonoids	Proanthocyanins	0.963	1.000	0.929	71
Shikimates and Phenylpropanoids	Flavonoids	Flavanones	0.944	0.962	0.927	516
Shikimates and Phenylpropanoids	Stilbenoids	Oligomeric stibenes	0.945	0.977	0.915	225
Shikimates and Phenylpropanoids	Isoflavonoids	Isoflavones	0.944	0.977	0.913	233

Shikimates and Phenylpropanoids	Phenylpropanoids (C6-C3)	Cinnamic acid amides	0.952	1.000	0.909	24
Shikimates and Phenylpropanoids	Isoflavonoids	Coumestan	0.947	1.000	0.900	54
Shikimates and Phenylpropanoids	Isoflavonoids	Rotenoids	0.944	1.000	0.895	90
Shikimates and Phenylpropanoids	Phenylpropanoids (C6-C3)	Cinnamic acids and derivatives	0.926	0.962	0.893	142
Shikimates and Phenylpropanoids	Terphenyls	m-Terphenyls	0.842	0.800	0.889	11
Shikimates and Phenylpropanoids	Phenolic acids (C6-C1)	Gallotannins	0.923	0.973	0.878	200
Shikimates and Phenylpropanoids	Phenylethanoids (C6-C2)	Phenylethanoids	0.903	0.933	0.875	85
Shikimates and Phenylpropanoids	Coumarins	Isocoumarins	0.909	0.950	0.872	544
Shikimates and Phenylpropanoids	Isoflavonoids	Pterocarpan	0.915	0.964	0.871	159
Shikimates and Phenylpropanoids	Flavonoids	Neoflavonoids	0.897	0.929	0.867	75
Shikimates and Phenylpropanoids	Terphenyls	p-Terphenyls	0.923	1.000	0.857	138
Shikimates and Phenylpropanoids	Diazotetronic acids and derivatives	Pulvinones	0.923	1.000	0.857	75
Shikimates and Phenylpropanoids	Coumarins	Pyranocoumarins	0.896	0.956	0.843	200
Shikimates and Phenylpropanoids	Small peptides	Aminoacids	0.883	0.935	0.837	3
Shikimates and Phenylpropanoids	Coumarins	Simple coumarins	0.865	0.906	0.828	817
Shikimates and Phenylpropanoids	Isoflavonoids	Isoflavanones	0.848	0.875	0.824	86
Shikimates and Phenylpropanoids	Isoflavonoids	2-arylbenzofurans	0.900	1.000	0.818	99
Shikimates and Phenylpropanoids	Tropolones	Tropolones and derivatives (Shikimate)	0.889	1.000	0.800	15

Shikimates and Phenylpropanoids	Lignans	Neolignans	0.870	0.952	0.800	230
Shikimates and Phenylpropanoids	Lignans	Arylnaphthalene and aryltetralin lignans	0.884	1.000	0.792	118
Shikimates and Phenylpropanoids	Stilbenoids	Monomeric stilbenes	0.857	0.955	0.778	114
Shikimates and Phenylpropanoids	Flavonoids	Flavonolignans	0.857	1.000	0.750	64
Shikimates and Phenylpropanoids	Lignans	Flavonolignans	0.857	1.000	0.750	64
Shikimates and Phenylpropanoids	Flavonoids	Flavandiols (Leucoanthocyanidins)	0.815	1.000	0.688	81
Shikimates and Phenylpropanoids	Lignans	Dibenzylbutane lignans	0.750	1.000	0.600	54
Shikimates and Phenylpropanoids	Phenolic acids (C6-C1)	Simple phenolic acids	0.704	0.962	0.556	219
Shikimates and Phenylpropanoids	Phenolic acids (C6-C1)	Shikimic acids and derivatives	0.444	0.571	0.364	62
Shikimates and Phenylpropanoids	Lignans	Minor lignans	0.364	1.000	0.222	50
Terpenoids	Diterpenoids	Platensimycin and Platencins	1.000	1.000	1.000	35
Terpenoids	Meroterpenoids	Cannabinoids	1.000	1.000	1.000	136
Terpenoids	Phloroglucinols	Phloroglucinol-terpene hybrids	1.000	1.000	1.000	35
Terpenoids	Polyethers	Oxasqualenoids	1.000	1.000	1.000	26
Terpenoids	Sesquiterpenoids	Alliacane sesquiterpenoids	1.000	1.000	1.000	30
Terpenoids	Sesquiterpenoids	Allohimachalane sesquiterpenoids	1.000	1.000	1.000	10
Terpenoids	Sesquiterpenoids	Bicyclogermacrane sesquiterpenoids	1.000	1.000	1.000	36
Terpenoids	Sesquiterpenoids	Bicyclohumulane sesquiterpenoids	1.000	1.000	1.000	8
Terpenoids	Sesquiterpenoids	Chiloscyphane sesquiterpenoids	1.000	1.000	1.000	6
Terpenoids	Sesquiterpenoids	Coloratane sesquiterpenoids	1.000	1.000	1.000	15
Terpenoids	Sesquiterpenoids	Cyclobisabolane sesquiterpenoids	1.000	1.000	1.000	12
Terpenoids	Sesquiterpenoids	Cyclonerane sesquiterpenoids	1.000	1.000	1.000	10
Terpenoids	Sesquiterpenoids	Elemane sesquiterpenoids	1.000	1.000	1.000	129

Terpenoids	Sesquiterpenoids	Fukinane sesquiterpenoids	1.000	1.000	1.000	49
Terpenoids	Sesquiterpenoids	Herbertane sesquiterpenoids	0.952	0.909	1.000	19
Terpenoids	Sesquiterpenoids	Iphionane sesquiterpenoids	1.000	1.000	1.000	15
Terpenoids	Sesquiterpenoids	Isocomane sesquiterpenoids	1.000	1.000	1.000	15
Terpenoids	Sesquiterpenoids	Ivaxillarane sesquiterpenoids	1.000	1.000	1.000	7
Terpenoids	Sesquiterpenoids	Longipinane sesquiterpenoids	1.000	1.000	1.000	53
Terpenoids	Sesquiterpenoids	Marasmane sesquiterpenoids	1.000	1.000	1.000	19
Terpenoids	Sesquiterpenoids	Noreremophilane sesquiterpenoids	0.933	0.875	1.000	20
Terpenoids	Sesquiterpenoids	Oplopane sesquiterpenoids	1.000	1.000	1.000	52
Terpenoids	Sesquiterpenoids	Pinguisane sesquiterpenoids	1.000	1.000	1.000	31
Terpenoids	Sesquiterpenoids	Quadrane sesquiterpenoids	1.000	1.000	1.000	13
Terpenoids	Sesquiterpenoids	Rotundane sesquiterpenoids	1.000	1.000	1.000	12
Terpenoids	Sesquiterpenoids	Santalane sesquiterpenoids	1.000	1.000	1.000	41
Terpenoids	Sesquiterpenoids	Sativane sesquiterpenoids	1.000	1.000	1.000	21
Terpenoids	Sesquiterpenoids	Silphinane sesquiterpenoids	1.000	1.000	1.000	28
Terpenoids	Sesquiterpenoids	Silphiperfolane sesquiterpenoids	1.000	1.000	1.000	21
Terpenoids	Sesquiterpenoids	Sinularane sesquiterpenoids	1.000	1.000	1.000	10
Terpenoids	Sesquiterpenoids	Spiroaxane sesquiterpenoids	1.000	1.000	1.000	25
Terpenoids	Sesquiterpenoids	Sterpurane sesquiterpenoids	1.000	1.000	1.000	15
Terpenoids	Sesquiterpenoids	Arteminisin	1.000	1.000	1.000	61
Terpenoids	Sesquiterpenoids	Hamigerane sesquiterpenoids	1.000	1.000	1.000	11
Terpenoids	Diterpenoids	Prenylbisabolane diterpenoids	1.000	1.000	1.000	15
Terpenoids	Diterpenoids	Dactylomelane diterpenoids	1.000	1.000	1.000	14
Terpenoids	Diterpenoids	Cycloabietane diterpenoids	1.000	1.000	1.000	26
Terpenoids	Diterpenoids	Parguerane diterpenoids	1.000	1.000	1.000	20
Terpenoids	Diterpenoids	Devadarane diterpenoids	1.000	1.000	1.000	9
Terpenoids	Diterpenoids	Villanovane diterpenoids	1.000	1.000	1.000	13
Terpenoids	Diterpenoids	Aphidicolane diterpenoids	1.000	1.000	1.000	91
Terpenoids	Diterpenoids	Gibberellins	1.000	1.000	1.000	140
Terpenoids	Diterpenoids	Norcembrane diterpenoids	1.000	1.000	1.000	10

Terpenoids	Diterpenoids	Gersemiane diterpenoids	1.000	1.000	1.000	5
Terpenoids	Diterpenoids	Asbestinane diterpenoids	1.000	1.000	1.000	21
Terpenoids	Diterpenoids	Sphaerane diterpenoids	1.000	1.000	1.000	24
Terpenoids	Diterpenoids	Dolastane diterpenoids	1.000	1.000	1.000	39
Terpenoids	Diterpenoids	Verrucosane diterpenoids	1.000	1.000	1.000	27
Terpenoids	Diterpenoids	Casbane diterpenoids	1.000	1.000	1.000	19
Terpenoids	Diterpenoids	Segetane diterpenoids	1.000	1.000	1.000	14
Terpenoids	Diterpenoids	Pepluane diterpenoids	1.000	1.000	1.000	10
Terpenoids	Diterpenoids	Paraliane diterpenoids	1.000	1.000	1.000	9
Terpenoids	Diterpenoids	Lathyrane diterpenoids	1.000	1.000	1.000	39
Terpenoids	Diterpenoids	Premyrsinane diterpenoids	1.000	1.000	1.000	12
Terpenoids	Diterpenoids	Myrsinane diterpenoids	0.909	0.833	1.000	51
Terpenoids	Diterpenoids	Tigliane diterpenoids	0.968	0.938	1.000	149
Terpenoids	Diterpenoids	Jatropholane diterpenoids	1.000	1.000	1.000	21
Terpenoids	Diterpenoids	Abeotaxane diterpenoids	1.000	1.000	1.000	22
Terpenoids	Diterpenoids	Trinervitane diterpenoids	1.000	1.000	1.000	39
Terpenoids	Diterpenoids	Kempane diterpenoids	1.000	1.000	1.000	3
Terpenoids	Diterpenoids	Amphilectane diterpenoids	1.000	1.000	1.000	38
Terpenoids	Diterpenoids	Eremane diterpenoids	1.000	1.000	1.000	4
Terpenoids	Diterpenoids	Lobane diterpenoids	0.968	0.938	1.000	37
Terpenoids	Diterpenoids	Decipiane diterpenoids	1.000	1.000	1.000	2
Terpenoids	Diterpenoids	Sacculatane diterpenoids	1.000	1.000	1.000	34
Terpenoids	Diterpenoids	Obtusane diterpenoids	1.000	1.000	1.000	4
Terpenoids	Diterpenoids	Breviane diterpenoids	1.000	1.000	1.000	13
Terpenoids	Diterpenoids	Cyclopiane diterpenoids	1.000	1.000	1.000	13
Terpenoids	Sesterterpenoids	Asperane sesterterpenoids	1.000	1.000	1.000	7
Terpenoids	Sesterterpenoids	Cericerane sesterterpenoids	1.000	1.000	1.000	14
Terpenoids	Sesterterpenoids	Ophiobolane sesterterpenoids	1.000	1.000	1.000	30
Terpenoids	Sesterterpenoids	Betaestacin-type sesterterpenoids	1.000	1.000	1.000	6
Terpenoids	Sesterterpenoids	Mangicol-type sesterterpenoids	1.000	1.000	1.000	9

Terpenoids	Triterpenoids	Cycloapotirucallane triterpenoids	1.000	1.000	1.000	37
Terpenoids	Triterpenoids	Baccharane triterpenoids	1.000	1.000	1.000	18
Terpenoids	Triterpenoids	Shionane triterpenoids	1.000	1.000	1.000	21
Terpenoids	Triterpenoids	Pachysanane triterpenoids	1.000	1.000	1.000	12
Terpenoids	Triterpenoids	Bauerane triterpenoids	1.000	1.000	1.000	21
Terpenoids	Triterpenoids	Adianane triterpenoids	1.000	1.000	1.000	12
Terpenoids	Triterpenoids	Filicane triterpenoids	1.000	1.000	1.000	16
Terpenoids	Triterpenoids	Malabaricane triterpenoids	1.000	1.000	1.000	44
Terpenoids	Triterpenoids	Saponaceolide triterpenoids	1.000	1.000	1.000	20
Terpenoids	Steroids	Bufadienolides	1.000	1.000	1.000	42
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-Ψ)	1.000	1.000	1.000	97
Terpenoids	Carotenoids (C40)	Carotenoids (C40, ε-Ψ)	1.000	1.000	1.000	13
Terpenoids	Carotenoids (C40)	Carotenoids (C40, π-Ψ)	1.000	1.000	1.000	8
Terpenoids	Carotenoids (C40)	Carotenoids (C40, X-Ψ)	0.667	0.500	1.000	3
Terpenoids	Carotenoids (C40)	Carotenoids (C40, γ-ε)	1.000	1.000	1.000	3
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-π)	0.667	0.500	1.000	6
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-X)	1.000	1.000	1.000	8
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-κ)	0.978	0.957	1.000	35
Terpenoids	Carotenoids (C40)	Carotenoids (C40, κ-X)	1.000	1.000	1.000	2
Terpenoids	Carotenoids (C40)	Carotenoids (C40, π-π)	0.800	0.667	1.000	6
Terpenoids	Carotenoids (C40)	Carotenoids (C40, π-X)	0.667	0.500	1.000	3
Terpenoids	Carotenoids (C45)	Carotenoids (C45, β-Ψ)	1.000	1.000	1.000	2
Terpenoids	Carotenoids (C45)	Carotenoids (C45, ε-Ψ)	1.000	1.000	1.000	5
Terpenoids	Carotenoids (C50)	Carotenoids (C50, β-β)	1.000	1.000	1.000	2
Terpenoids	Carotenoids (C50)	Carotenoids (C50, ε-ε)	1.000	1.000	1.000	7
Terpenoids	Carotenoids (C50)	Carotenoids (C50, γ-γ)	1.000	1.000	1.000	3
Terpenoids	Apocarotenoids	Apocarotenoids (C30, Ψ-Ψ)	0.842	0.727	1.000	33
Terpenoids	Polyprenols	Bactoprenols	0.952	0.909	1.000	15
Terpenoids	Polyprenols	Dolichols	1.000	1.000	1.000	14
Terpenoids	Polyprenols	Polyprenol derivatives	1.000	1.000	1.000	33

Terpenoids	Meroterpenoids	Triketide meroterpenoids	1.000	1.000	1.000	73
Terpenoids	Meroterpenoids	Other polyketide meroterpenoids	1.000	1.000	1.000	24
Terpenoids	Meroterpenoids	Merosesquiterpenoids	1.000	1.000	1.000	34
Terpenoids	Meroterpenoids	Meroterpenoids with 5- or 6-membered ring	1.000	1.000	1.000	15
Terpenoids	Meroterpenoids	Meroterpenoids with bridged ring	1.000	1.000	1.000	23
Terpenoids	Diterpenoids	Platensimycin and Platencins	1.000	1.000	1.000	35
Terpenoids	Meroterpenoids	Merohemiterpenoids	0.933	0.875	1.000	14
Terpenoids	Sesquiterpenoids	Agarofuran sesquiterpenoids	0.980	0.974	0.987	385
Terpenoids	Meroterpenoids	Polyprenylated cyclic polyketides (Hop meroterpenoids)	0.992	1.000	0.984	303
Terpenoids	Steroids	Vitamin D3 and derivatives	0.984	0.989	0.978	457
Terpenoids	Triterpenoids	Limonoids	0.983	0.989	0.977	438
Terpenoids	Triterpenoids	Lupane triterpenoids	0.978	0.985	0.971	689
Terpenoids	Triterpenoids	Ursane and Taraxastane triterpenoids	0.984	1.000	0.969	162
Terpenoids	Steroids	Cardenolides	0.969	0.969	0.969	39
Terpenoids	Diterpenoids	Briarane diterpenoids	0.976	1.000	0.952	211
Terpenoids	Diterpenoids	Grayanotoxane diterpenoids	0.974	1.000	0.950	100
Terpenoids	Triterpenoids	Oleanane triterpenoids	0.946	0.946	0.946	373
Terpenoids	Sesquiterpenoids	Lactarane sesquiterpenoids	0.971	1.000	0.944	33
Terpenoids	Tryptophan alkaloids	Indole-Diterpenoid alkaloids (Penitrems)	0.971	1.000	0.944	90
Terpenoids	Meroterpenoids	Prenyl quinone meroterpenoids	0.949	0.959	0.940	251
Terpenoids	Diterpenoids	Mulinane diterpenoids	0.968	1.000	0.938	43
Terpenoids	Sesterterpenoids	Norsesterterpenoids	0.968	1.000	0.938	39
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-β)	0.946	0.957	0.936	237
Terpenoids	Sesquiterpenoids	Laurane sesquiterpenoids	0.903	0.875	0.933	68
Terpenoids	Triterpenoids	Dammarane and Protostane triterpenoids	0.938	0.950	0.927	207
Terpenoids	Sesquiterpenoids	Cedrane and Isocedrane sesquiterpenoids	0.960	1.000	0.923	39
Terpenoids	Sesterterpenoids	Monocarbocyclic sesterterpenoids	0.923	0.923	0.923	29
Terpenoids	Carotenoids (C40)	Carotenoids (C40, Ψ-Ψ)	0.923	0.923	0.923	131
Terpenoids	Diterpenoids	Cembrane diterpenoids	0.953	0.989	0.919	493

Terpenoids	Sesquiterpenoids	Aristolane sesquiterpenoids	0.917	0.917	0.917	61
Terpenoids	Sesquiterpenoids	Cyclofarnesane sesquiterpenoids	0.957	1.000	0.917	25
Terpenoids	Meroterpenoids	Spriromeroterpenoids	0.917	0.917	0.917	57
Terpenoids	Sesquiterpenoids	Trichothecane sesquiterpenoids	0.955	1.000	0.914	177
Terpenoids	Pseudoalkaloids	Steroidal alkaloids	0.948	0.986	0.913	405
Terpenoids	Triterpenoids	Quassinoids	0.954	1.000	0.912	169
Terpenoids	Triterpenoids	Cycloartane triterpenoids	0.935	0.960	0.911	388
Terpenoids	Triterpenoids	Multiflorane triterpenoids	0.952	1.000	0.909	54
Terpenoids	Triterpenoids	Serratane triterpenoids	0.952	1.000	0.909	52
Terpenoids	Diterpenoids	Kaurane and Phyllocladane diterpenoids	0.940	0.975	0.907	228
Terpenoids	Sesquiterpenoids	Chamigrane sesquiterpenoids	0.950	1.000	0.905	107
Terpenoids	Diterpenoids	Nagilactone diterpenoids	0.950	1.000	0.905	41
Terpenoids	Sesquiterpenoids	Africanane sesquiterpenoids	0.947	1.000	0.900	34
Terpenoids	Sesquiterpenoids	Asteriscane sesquiterpenoids	0.947	1.000	0.900	24
Terpenoids	Diterpenoids	Guanacastane diterpenoids	0.947	1.000	0.900	52
Terpenoids	Diterpenoids	Pachydictyane diterpenoids	0.900	0.900	0.900	52
Terpenoids	Sesterterpenoids	Linear sesterterpenoids	0.947	1.000	0.900	46
Terpenoids	Steroids	Ecdysteroids	0.947	1.000	0.900	99
Terpenoids	Steroids	Vitamin D2 and derivatives	0.947	1.000	0.900	31
Terpenoids	Triterpenoids	Cucurbitane triterpenoids	0.933	0.972	0.897	198
Terpenoids	Diterpenoids	Taxane diterpenoids	0.904	0.917	0.892	202
Terpenoids	Sesquiterpenoids	Oppositane sesquiterpenoids	0.941	1.000	0.889	25
Terpenoids	Diterpenoids	Furanoabietane diterpenoids	0.842	0.800	0.889	19
Terpenoids	Diterpenoids	Tetracyclic diterpenoids	0.867	0.847	0.889	390
Terpenoids	Steroids	Furostane steroids	0.923	0.973	0.878	204
Terpenoids	Sesquiterpenoids	Germacrane sesquiterpenoids	0.917	0.961	0.876	562
Terpenoids	Sesquiterpenoids	Gymnomitrane sesquiterpenoids	0.933	1.000	0.875	32
Terpenoids	Sesquiterpenoids	Presilphiperfolane and Probotryane sesquiterpenoids	0.933	1.000	0.875	18
Terpenoids	Diterpenoids	Pseudopterane diterpenoids	0.933	1.000	0.875	46

Terpenoids	Diterpenoids	Daphnane diterpenoids	0.933	1.000	0.875	82
Terpenoids	Diterpenoids	Xenicane diterpenoids	0.933	1.000	0.875	36
Terpenoids	Diterpenoids	Serrulatane and Biflorane diterpenoids	0.933	1.000	0.875	83
Terpenoids	Triterpenoids	Abeolupane triterpenoids	0.933	1.000	0.875	14
Terpenoids	Triterpenoids	Acyclic triterpenoids	0.897	0.929	0.867	37
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-ε)	0.897	0.929	0.867	74
Terpenoids	Diterpenoids	Dolabellane diterpenoids	0.927	1.000	0.864	101
Terpenoids	Triterpenoids	Apotirucallane triterpenoids	0.905	0.950	0.864	109
Terpenoids	Steroids	Pregnane steroids	0.918	0.982	0.862	311
Terpenoids	Sesquiterpenoids	Tremulane sesquiterpenoids	0.923	1.000	0.857	42
Terpenoids	Sesquiterpenoids	Pentalenane sesquiterpenoids	0.923	1.000	0.857	14
Terpenoids	Diterpenoids	Totarane diterpenoids	0.923	1.000	0.857	46
Terpenoids	Triterpenoids	Onocerane triterpenoids	0.923	1.000	0.857	19
Terpenoids	Triterpenoids	Polypodane triterpenoids	0.923	1.000	0.857	14
Terpenoids	Carotenoids (C50)	Carotenoids (C50, Ψ-Ψ)	0.923	1.000	0.857	14
Terpenoids	Monoterpenoids	Thujane monoterpenoids	0.880	0.917	0.846	63
Terpenoids	Diterpenoids	Erythroxylane diterpenoids	0.917	1.000	0.846	29
Terpenoids	Diterpenoids	Xeniaphyllane diterpenoids	0.917	1.000	0.846	35
Terpenoids	Pseudoalkaloids	Terpenoid alkaloids	0.902	0.965	0.846	335
Terpenoids	Triterpenoids	Hopane and Moretane triterpenoids	0.905	0.974	0.844	227
Terpenoids	Monoterpenoids	Iridoids monoterpenoids	0.897	0.956	0.844	396
Terpenoids	Steroids	Androstane steroids	0.897	0.963	0.839	164
Terpenoids	Steroids	Cholestane steroids	0.833	0.829	0.836	550
Terpenoids	Monoterpenoids	Carane monoterpenoids	0.893	0.962	0.833	152
Terpenoids	Sesquiterpenoids	Picrotoxane sesquiterpenoids	0.909	1.000	0.833	83
Terpenoids	Sesquiterpenoids	Thujopsane sesquiterpenoids	0.909	1.000	0.833	21
Terpenoids	Sesquiterpenoids	Valerenane sesquiterpenoids	0.909	1.000	0.833	18
Terpenoids	Diterpenoids	Halimane diterpenoids	0.882	0.938	0.833	92
Terpenoids	Diterpenoids	Rhamnofolane diterpenoids	0.909	1.000	0.833	17
Terpenoids	Steroids	Cholane steroids	0.909	1.000	0.833	59

Terpenoids	Monoterpenoids	Acyclic monoterpenoids	0.789	0.754	0.827	266
Terpenoids	Sesquiterpenoids	Spirovetivane sesquiterpenoids	0.903	1.000	0.824	48
Terpenoids	Apocarotenoids	Apocarotenoids(ε-)	0.875	0.933	0.824	47
Terpenoids	Diterpenoids	Colensane and Clerodane diterpenoids	0.868	0.920	0.821	150
Terpenoids	Sesquiterpenoids	Himachalane sesquiterpenoids	0.900	1.000	0.818	37
Terpenoids	Sesquiterpenoids	Nardosinane sesquiterpenoids	0.900	1.000	0.818	56
Terpenoids	Diterpenoids	Fusicoccane diterpenoids	0.900	1.000	0.818	57
Terpenoids	Sesterterpenoids	Cheilanthane sesterterpenoids	0.857	0.900	0.818	26
Terpenoids	Triterpenoids	Fusidane triterpenoids	0.857	0.900	0.818	55
Terpenoids	Sesquiterpenoids	Guaiane sesquiterpenoids	0.890	0.985	0.813	404
Terpenoids	Sesquiterpenoids	Pseudoguaiane sesquiterpenoids	0.897	1.000	0.813	38
Terpenoids	Diterpenoids	Cassane diterpenoids	0.867	0.929	0.813	166
Terpenoids	Meroterpenoids	Tetraketide meroterpenoids	0.882	0.968	0.811	184
Terpenoids	Sesquiterpenoids	Eremophilane sesquiterpenoids	0.873	0.948	0.809	337
Terpenoids	Diterpenoids	Eunicellane diterpenoids	0.893	1.000	0.806	150
Terpenoids	Sesterterpenoids	Scalarane sesterterpenoids	0.893	1.000	0.806	152
Terpenoids	Sesquiterpenoids	Caryolane sesquiterpenoids	0.889	1.000	0.800	12
Terpenoids	Sesquiterpenoids	Illudalane sesquiterpenoids	0.762	0.727	0.800	55
Terpenoids	Diterpenoids	Viscidane diterpenoids	0.889	1.000	0.800	10
Terpenoids	Steroids	Ergostane steroids	0.831	0.873	0.793	596
Terpenoids	Sesquiterpenoids	Patchoulane sesquiterpenoids	0.880	1.000	0.786	43
Terpenoids	Diterpenoids	Norkaurane diterpenoids	0.846	0.917	0.786	211
Terpenoids	Diterpenoids	Beyerane diterpenoids	0.880	1.000	0.786	69
Terpenoids	Triterpenoids	Fernane and Arborinane triterpenoids	0.880	1.000	0.786	63
Terpenoids	Diterpenoids	Jatrophane diterpenoids	0.878	1.000	0.783	119
Terpenoids	Sesquiterpenoids	Bergamotane sesquiterpenoids	0.875	1.000	0.778	26
Terpenoids	Sesquiterpenoids	Illudane sesquiterpenoids	0.875	1.000	0.778	50
Terpenoids	Triterpenoids	Glutinane triterpenoids	0.875	1.000	0.778	27
Terpenoids	Sesquiterpenoids	Aromadendrane sesquiterpenoids	0.850	0.944	0.773	109
Terpenoids	Diterpenoids	Ingenane diterpenoids	0.870	1.000	0.769	52

Terpenoids	Sesquiterpenoids	Bisabolane sesquiterpenoids	0.848	0.955	0.764	281
Terpenoids	Diterpenoids	Labdane diterpenoids	0.857	0.977	0.764	277
Terpenoids	Diterpenoids	Secolabdane diterpenoids	0.865	1.000	0.762	46
Terpenoids	Steroids	Spirostane steroids	0.842	0.941	0.762	107
Terpenoids	Steroids	Stigmastane steroids	0.846	0.957	0.759	145
Terpenoids	Monoterpenoids	Menthane monoterpenoids	0.829	0.920	0.754	308
Terpenoids	Monoterpenoids	Irregular monoterpenoids	0.857	1.000	0.750	29
Terpenoids	Sesquiterpenoids	Capnellane sesquiterpenoids	0.857	1.000	0.750	29
Terpenoids	Sesquiterpenoids	Carabrane sesquiterpenoids	0.857	1.000	0.750	15
Terpenoids	Sesquiterpenoids	Clovane sesquiterpenoids	0.857	1.000	0.750	20
Terpenoids	Diterpenoids	Abietane diterpenoids	0.800	0.857	0.750	162
Terpenoids	Diterpenoids	Spongiane diterpenoids	0.833	0.938	0.750	103
Terpenoids	Diterpenoids	Trachylobane diterpenoids	0.857	1.000	0.750	62
Terpenoids	Diterpenoids	Cyathane diterpenoids	0.857	1.000	0.750	59
Terpenoids	Diterpenoids	Prenyleudesmane diterpenoids	0.857	1.000	0.750	9
Terpenoids	Triterpenoids	Neohopane triterpenoids	0.857	1.000	0.750	11
Terpenoids	Monoterpenoids	Monocyclic monoterpenoids	0.844	0.974	0.745	253
Terpenoids	Monoterpenoids	Secoiridoid monoterpenoids	0.853	1.000	0.744	194
Terpenoids	Triterpenoids	Lanostane, Tirucallane and Euphane triterpenoids	0.820	0.934	0.731	387
Terpenoids	Sesquiterpenoids	Brasilane sesquiterpenoids	0.842	1.000	0.727	25
Terpenoids	Monoterpenoids	Pinane monoterpenoids	0.814	0.923	0.727	167
Terpenoids	Diterpenoids	Verticillane diterpenoids	0.842	1.000	0.727	53
Terpenoids	Diterpenoids	Atisane diterpenoids	0.839	1.000	0.722	88
Terpenoids	Sesquiterpenoids	Cuparane sesquiterpenoids	0.833	1.000	0.714	70
Terpenoids	Sesquiterpenoids	Eudesmane sesquiterpenoids	0.800	0.909	0.714	343
Terpenoids	Sesquiterpenoids	Zizaane sesquiterpenoids	0.833	1.000	0.714	26
Terpenoids	Diterpenoids	Sphenolobane diterpenoids	0.833	1.000	0.714	20
Terpenoids	Meroterpenoids	Meromonoterpenoids	0.833	1.000	0.714	65
Terpenoids	Sesquiterpenoids	Daucane sesquiterpenoids	0.829	1.000	0.708	121
Terpenoids	Diterpenoids	Secokaurane diterpenoids	0.828	1.000	0.706	86

Terpenoids	Triterpenoids	Taraxerane triterpenoids	0.828	1.000	0.706	85
Terpenoids	Apocarotenoids	Apocarotenoids (β-)	0.809	0.950	0.704	131
Terpenoids	Sesquiterpenoids	Cycloeudesmane sesquiterpenoids	0.824	1.000	0.700	95
Terpenoids	Steroids	Estrane steroids	0.824	1.000	0.700	52
Terpenoids	Sesquiterpenoids	Botryane sesquiterpenoids	0.818	1.000	0.692	25
Terpenoids	Sesquiterpenoids	Humulane sesquiterpenoids	0.815	1.000	0.688	83
Terpenoids	Diterpenoids	Podocarpane diterpenoids	0.774	0.889	0.686	174
Terpenoids	Sesquiterpenoids	Campherenane sesquiterpenoids	0.800	1.000	0.667	16
Terpenoids	Sesquiterpenoids	Copacamphane sesquiterpenoids	0.800	1.000	0.667	6
Terpenoids	Sesquiterpenoids	Dunniane sesquiterpenoids	0.800	1.000	0.667	8
Terpenoids	Sesquiterpenoids	Gorgonane sesquiterpenoids	0.800	1.000	0.667	16
Terpenoids	Sesquiterpenoids	Ishwarane sesquiterpenoids	0.800	1.000	0.667	10
Terpenoids	Sesquiterpenoids	Isolactarane sesquiterpenoids	0.800	1.000	0.667	21
Terpenoids	Diterpenoids	Pimarane and Isopimarane diterpenoids	0.784	0.952	0.667	148
Terpenoids	Triterpenoids	Friedelane triterpenoids	0.800	1.000	0.667	48
Terpenoids	Triterpenoids	Stictane triterpenoids	0.800	1.000	0.667	15
Terpenoids	Sesquiterpenoids	Cadinane sesquiterpenoids	0.779	0.957	0.657	338
Terpenoids	Sesquiterpenoids	Noreudesmane sesquiterpenoids	0.783	1.000	0.643	36
Terpenoids	Diterpenoids	Cleistanthane diterpenoids	0.778	1.000	0.636	58
Terpenoids	Sesquiterpenoids	Copaane sesquiterpenoids	0.769	1.000	0.625	24
Terpenoids	Sesquiterpenoids	Secoeudesmane sesquiterpenoids	0.769	1.000	0.625	21
Terpenoids	Sesquiterpenoids	Acorane sesquiterpenoids	0.750	1.000	0.600	50
Terpenoids	Sesquiterpenoids	Cubebane sesquiterpenoids	0.750	1.000	0.600	16
Terpenoids	Sesquiterpenoids	Cyclolaurane sesquiterpenoids	0.750	1.000	0.600	14
Terpenoids	Sesquiterpenoids	Humbertiane sesquiterpenoids	0.750	1.000	0.600	16
Terpenoids	Sesquiterpenoids	Isodaucane sesquiterpenoids	0.750	1.000	0.600	17
Terpenoids	Diterpenoids	Icetexane diterpenoids	0.750	1.000	0.600	50
Terpenoids	Triterpenoids	Gammacerane triterpenoids	0.750	1.000	0.600	20
Terpenoids	Apocarotenoids	Megastigmanes	0.714	0.882	0.600	122
Terpenoids	Diterpenoids	Phytane diterpenoids	0.714	0.909	0.588	83

Terpenoids	Meroterpenoids	Miscellaneous meroterpenoids	0.720	0.947	0.581	157
Terpenoids	Apocarotenoids	Miscellaneous apocarotenoids	0.667	0.800	0.571	30
Terpenoids	Diterpenoids	Secoabietane diterpenoids	0.710	1.000	0.550	96
Terpenoids	Sesquiterpenoids	Caryophyllane sesquiterpenoids	0.667	1.000	0.500	107
Terpenoids	Sesquiterpenoids	Homofarnesane sesquiterpenoids	0.667	1.000	0.500	7
Terpenoids	Sesquiterpenoids	Longibornane sesquiterpenoids	0.667	1.000	0.500	6
Terpenoids	Sesquiterpenoids	Pacifigorgiane sesquiterpenoids	0.667	1.000	0.500	9
Terpenoids	Sesquiterpenoids	Valerane sesquiterpenoids	0.667	1.000	0.500	14
Terpenoids	Diterpenoids	Abeoabietane diterpenoids	0.638	0.882	0.500	146
Terpenoids	Diterpenoids	Sphaeroane diterpenoids	0.667	1.000	0.500	6
Terpenoids	Carotenoids (C40)	Carotenoids (C40, β-γ)	0.667	1.000	0.500	4
Terpenoids	Carotenoids (C40)	Carotenoids (C40, ε-ε)	0.667	1.000	0.500	7
Terpenoids	Sesquiterpenoids	Drimane sesquiterpenoids	0.649	1.000	0.480	138
Terpenoids	Monoterpenoids	Camphane monoterpenoids	0.621	0.900	0.474	101
Terpenoids	Sesquiterpenoids	Longifolane sesquiterpenoids	0.600	1.000	0.429	30
Terpenoids	Sesquiterpenoids	Farnesane sesquiterpenoids	0.596	1.000	0.424	162
Terpenoids	Monoterpenoids	Fenchane monoterpenoids	0.571	1.000	0.400	21
Terpenoids	Sesquiterpenoids	Prezizaane sesquiterpenoids	0.571	1.000	0.400	52
Terpenoids	Sesquiterpenoids	Protoilludane sesquiterpenoids	0.545	0.857	0.400	75
Terpenoids	Diterpenoids	Valparane diterpenoids	0.571	1.000	0.400	21
Terpenoids	Diterpenoids	Norpimarane and Norisopimarane diterpenoids	0.522	0.857	0.375	76
Terpenoids	Sesquiterpenoids	Hirsutane sesquiterpenoids	0.526	1.000	0.357	67
Terpenoids	Diterpenoids	Norlabdane diterpenoids	0.516	1.000	0.348	84
Terpenoids	Sesquiterpenoids	Bourbonane sesquiterpenoids	0.500	1.000	0.333	19
Terpenoids	Sesquiterpenoids	Thapsane sesquiterpenoids	0.500	1.000	0.333	16
Terpenoids	Diterpenoids	Cyclophytane diterpenoids	0.455	0.714	0.333	82
Terpenoids	Sesquiterpenoids	Secogermacrane sesquiterpenoids	0.400	1.000	0.250	15
Terpenoids	Diterpenoids	Cycloamphilectane diterpenoids	0.400	1.000	0.250	18

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