

# PCMD tutorial

## Home

Plant comparative metabolome database (PCMD) is a comprehensive multi-level comparison database encompassing intra- and cross-species metabolic profiling in 530 plants. The predicted metabolites provided in PCMD are mainly based on the Genome Scale Metabolism Model (GEM), which has been proven to be effective in predicting the presence of metabolites in organisms based on the genome (Mendoza, Olivier, Molenaar,&Teusink, 2019). PCMD contains 213,264 metabolites, 8,384 enzymes, 8,678 reactions, 30,669 experimentally-supported metabolites, 33,397 literature references. Moreover, PCMD also provides a range of user-friendly online tools, such as Species-comparison, Metabolites-enrichment, and ID conversion. The Species-comparison tool allows users to compare the specificity and commonness of metabolites between two different groups of plants at multiple taxonomic levels. The Metabolites-enrichment tool enables users to analyze the enrichment of metabolites. The ID conversion tool allows for efficient conversion of metabolite IDs across multiple published metabolomics databases.

**Plant Comparative Metabolome Database**  
—A multi-level comparison of metabolic profiles in 530 plant species

Navigation bar: Home, Species, Metabolites, Reactions, Literature, Download, Help

**Introduction of PCMD**  
Welcome to PCMD!  
Plant comparative metabolome database (PCMD) is a comprehensive multi-level comparison database encompassing intra- and cross-species metabolic profiling in 530 plants. The predicted metabolites provided in PCMD are mainly based on the Genome Scale Metabolism Model (GEM), which has been proven to be effective in predicting the presence of metabolites in organisms based on the genomes (Mendoza, Oliver, Molenaar, & Teusink, 2016). PCMD contains 230,017 metabolites, 8,384 enzymes, 8,678 reactions, 14,521 experimentally-supported reactions and metabolites, 33,397 literature references. Moreover, PCMD also provides a range of user-friendly online tools, such as Species-comparison, Metabolites-enrichment, and ID conversion. The Species-comparison tool allows users to compare the specificity and commonness of metabolites between two different groups of plants at multiple taxonomic levels. The Metabolites-enrichment tool enables users to analyze the enrichment of metabolites. The ID conversion tool allows for efficient conversion of metabolite IDs across multiple published metabolomics databases.

**News & Events**  

- PCMD has expanded the experimental metabolite data of *Arabidopsis* and annotated whether the predicted metabolites have experimental support. (2024/11/22)
- PCMD has added a precise search functionality for metabolites in the literature module. (2024/10/19)
- The methods and tutorial videos for PCMD have been updated in the database. (2023/12/12)
- ID conversion tool has been developed and available in the Metabolite ports. (2023/07/19)
- The basic information of 31,227 metabolites has been added to PCMD. (2023/04/01)

**Global search**  
 e.g. Species or Taxonomy: *Arabidopsis thaliana*, *Aly*, maize, Grassia, Prunose  
 Metabolite or Enzyme: alpha-selenine, CPD-921, PMR00026, EG\_5.2.1.13, succinate semialdehyde reductase  
 Reaction or Pathway: RXN-15489, PMRX0001, glycyrhettinate biosynthesis

**The statistics of various data in PCMD**

530 Species	230,017 Metabolites	8,384 Enzymes	8,678 Reactions	25,785 Experiments	33,397 Literature
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**The classification of 530 species in PCMD**

Taxonomy	6 Kingdom and Phylum	72 Class and Order	114 Family	283 Genus
Seed and leaf characteristics	397 Eudicot	102 Monocot	22 Spore plants	9 Gymnosperms
Reproductive characteristics	502 Flowering	28 Non-flowering		
Domestication information	151 Domesticated	186 Wild and wild relative	78 Cultivated and bred	

**Functional modules in PCMD**

**The workflow of PCMD**

Data Collection: Protein sequences, Enzymes, Compounds, Classifications, 530 species, GEM modeling, Plant metabolite network

Data Analysis: Multi-level comparison (Taxonomic level and leaf characteristics), Metabolites, Enrichment

Data Application: Species A, Species B, Metabolites, Enrichment

Logos: hmdb, PMN, Plant Reactome

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## Search species

The “Search species” module provides metabolite information of 530 species in PCMD. In this page, users can enter scientific name, abbreviation, or common name of the interested species to get the related information. For example, if users enter ‘*Arabidopsis thaliana*’ in box 1, results in boxes 2 to 15 will be obtained.

Search species

1 Input species:

e.g. *Arabidopsis thaliana* or *Aly* or rice

Submit Reset

Firstly, box 2 provides an overview of the entered species, including information such as the number and ranking of metabolites, the number of predicted metabolites

supported by experiments and metabolites experimentally measured, the top 10 plants with the closest and farthest metabolite similarity in PCMD, the top 5 enriched metabolite categories, the top 10 enriched metabolites, the pairs of predicted protein-metabolites, related literature, and the metabolic network. User can get a table of the genes associated with metabolites in the entered species (box 3) by clicking on the number of predicted protein-metabolite pairs. Clicking the “Go” button obtain the metabolic network of the entered species (box 4).

2

Overview

### Arabidopsis thaliana

Number of metabolites	4416 (Ranking 146 in 530 species)
Number of predicted metabolites supported by experiments	78
Number of metabolites experimentally measured	816


**Comparison of metabolite similarities between *Arabidopsis thaliana* and other plants:**

The top 10 plants with the **closest** metabolite similarity (Jaccard similarity coefficient):

1. *Brassica rapa* (0.97022)
2. *Brassica carinata* (0.96723)
3. *Arabidopsis lyrata* (0.93425)
4. *Raphanus sativus* (0.93336)
5. *Eutrema salsugineum* (0.93180)
6. *Microthlaspi erraticum* (0.92868)
7. *Descurainia sophioides* (0.92787)
8. *Capsella rubella* (0.92603)
9. *Brassica oleracea* (0.92323)
10. *Cardamine hirsuta* (0.92249)

The top 10 plants with the **farthest** metabolite similarity (Jaccard similarity coefficient):

1. *Picea glauca* (0.15868)
2. *Populus simonii* (0.23183)
3. *Apium graveolens* (0.25501)
4. *Passiflora edulis* (0.29079)
5. *Nelumbo nucifera* (0.30393)
6. *Anthoceros agrestis* (0.58859)
7. *Chondrus crispus* (0.58863)
8. *Cyanidioschyzon merolae* (0.60408)
9. *Doroceras hygrometricum* (0.60803)
10. *Ostreococcus lucimarinus* (0.61618)



Scientific name	<i>Arabidopsis thaliana</i>
Common name	mouse-ear cress;thale-cress
Class	Eukaryota;Viridiplantae;Streptophyta;Magnoliopsida;Brassicales;Brassicaceae;Arabidopsis
Taxonomy	Eudicot
Characteristic	Flowering
Domestication	Wild

**The most enriched metabolite category**    **Top 5: (P-value)**

1. Other (5.55e-16)
2. plant hormone (2.46e-11)
3. ribonucleic acid (3.31e-9)
4. glycoconjugate (3.25e-6)
5. aliphatic aldoxime (5.05e-6)

**The most enriched metabolite**    **Top 10: (P-value)**

1. 3'-Keto-3'-deoxy-AMP (0.00586)
2. N-acetylpuromycin (0.00586)
3. 3'-amino-3'-deoxyAMP (0.00586)
4. puromycin (0.00586)
5. Histidyltryptophyldiketopiperazine (0.0245)
6. Roquefortine D (0.0245)
7. Delhydrohistidyltryptophyldiketopiperazine (0.0245)
8. Roquefortine C (0.0245)
9. (2S)-3-sulfolactate (0.0284)
10. 24-epi-campesterol (0.0321)

Pairs of predicted protein-metabolites: 39933

Number of literature: 1194

Network: GO

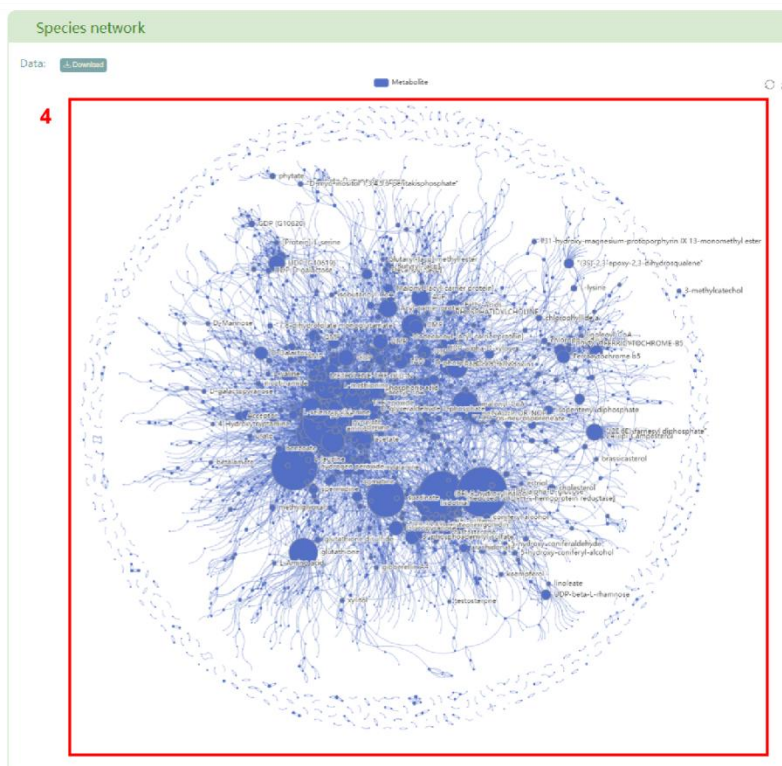
Browse pairs of predicted protein-metabolites

3 Search:  Download

Chr	Start	End	Strand	Gene name	Protein id	Number of metabolites
Chr1	31170	33153	-	AT1G01050	AT1G01050.1	4
Chr1	47485	49286	-	AT1G01090	AT1G01090.1	11
Chr1	57269	59167	-	AT1G01120	AT1G01120.1	12
Chr1	83045	84864	-	AT1G01190	AT1G01190.1	27
Chr1	91376	95651	+	AT1G01220	AT1G01220.1	5
Chr1	112263	113947	+	AT1G01280	AT1G01280.1	28
Chr1	114286	115549	+	AT1G01290	AT1G01290.1	3
Chr1	148120	149806	-	AT1G01390	AT1G01390.1	22
Chr1	154492	156011	-	AT1G01420	AT1G01420.1	22
Chr1	168723	171165	+	AT1G01460	AT1G01460.1	6

Showing 1 to 10 of 4,528 entries

Previous 1 2 3 4 5 ... 453 Next



Secondly, users will obtain a basic information table of metabolites in the entered species (box 5) and a bar chart of metabolite classification (box 6). By clicking the metabolite ID, users can access the corresponding metabolite page in PCMD (box 7) and gather detailed information on the metabolite (box 8), accessed by clicking the metabolite name. Additionally, users can click on the reaction to access the related details page (box 9) for that specific reaction. Furthermore, users can access the basic information table of predicted metabolites supported by experiments (box 10) and metabolites experimentally measured (box 11) in the entered species. Sources of

experimental support for the metabolites are also shown in the table.

7

**Basic information of metabolite**

**5-dehydroavenasterol**

Abbreviation: CPD-1128  
 Molecular formula: C<sub>29</sub>H<sub>48</sub>O  
 Synonyms: 5-Dehydroavenasterol; 5-Dihydro-avenasterol; 24Z-47-ethylcholesta-5,7-dien-3beta-ol; SCHEMBL4623291; LIGAND184185; glxglsigmaalk7\_24Zcyclohexyl; (24Z)-Sigma-5,7,24(28)-trien-3beta-ol  
 Molecular weight: 410.7  
 Monoisotopic masses: 410.355



8

**Detailed information of the metabolite (Information in PCMD)**

Jump to: [Basic information](#) | [Chemical status](#) | [Isotopes](#) | [Literature deposits](#) | [Reactions](#) | [Libraries](#)

**Basic information**

Abbreviation: CPD-1128  
 Name: 5-dehydroavenasterol  
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5

**Browse metabolites**

Search:

Download

Id	Name	Formula	Molecular weight	Monoisotopic mass	Species	Reaction
PMIR00028	5-dehydroavenasterol	C <sub>29</sub> H <sub>48</sub> O	410.7	410.355	Arabidopsis thaliana	RXN-4210;RXN-4209
PMIR00028	ergosta-5,7-dienol	C <sub>28</sub> H <sub>46</sub> O	398.7	398.355	Arabidopsis thaliana	RXN-13883
PMIR00030	porifersta-5,7-dienol	C <sub>28</sub> H <sub>46</sub> O	412.7	412.371	Arabidopsis thaliana	RXN-13892
PMIR00031	ergosta-5,7,24(28)-trien-3beta-ol	C <sub>28</sub> H <sub>44</sub> O	396.6	396.339	Arabidopsis thaliana	R07492;RXN-707;RXN30-227;R074
PMIR00036	porifersta-7-enol	C <sub>29</sub> H <sub>50</sub> O	414.7	414.386	Arabidopsis thaliana	RXN-13892
PMIR00038	ergosta-7-enol	C <sub>28</sub> H <sub>48</sub> O	400.7	400.371	Arabidopsis thaliana	RXN-13883
PMIR00040	episterol	C <sub>28</sub> H <sub>46</sub> O	398.7	398.355	Arabidopsis thaliana	R07491;RXN30-218;RXN-11934
PMIR00041	choloyl-CoA	C <sub>45</sub> H <sub>70</sub> N <sub>7</sub> O <sub>20</sub> P <sub>3</sub> S <sub>1</sub>	1154.1	1153.36	Arabidopsis thaliana	3.1.2.27-RXN
PMIR00042	HCl	H <sub>1</sub> Cl <sub>1</sub>	36.46	35.9767	Arabidopsis thaliana	R04500;R07092
PMIR00043	TRIBOA-beta-D-glucoside	C <sub>14</sub> H <sub>17</sub> N <sub>1</sub> O <sub>10</sub>	359.28	359.085	Arabidopsis thaliana	RXN-6685

Showing 1 to 10 of 4,416 entries

Previous 1 2 3 4 5 ... 442 Next



9


**Browse reaction**

**2-oxoglutarate + DIBOA-beta-D-glucoside + oxygen -> CO<sub>2</sub> + TRIBOA-beta-D-glucoside + succinate**

Name: **DIMBOA-glucoside dioxygenase**

Enzymes: "2,4-dihydroxy-1,4-benzoxazin-3-one-glucoside dioxygenase; BX6 (gene name); DIBOA-Glc dioxygenase"

Reaction:



Pathway: **DIMBOA-glucoside biosynthesis**

External database link: [RXN-6685](#)

### Browse predicted metabolites supported by experiments

10

Search:

[Download](#)

Id	Name	Formula	Molecular weight	Monoisotopic mass	Reactions
PMIR00262	L-xyllo-hex-3-ulono-1,4-lactone	C6H8O6	176.1200	176.0321	RXN-8784
PMIR00271	3,4-dihydroxy-2-methyl-4-farnesyl-3H-quinolin-1-ium-1-olate	C25H35N1O3	397.5000	397.2617	R11148
PMIR00412	L-phenylalanine	C9H11N1O2	165.1900	165.0790	CARBOXYCYCLOHEXADIENYL-DEH <sup>+</sup>
PMIR00445	kaempferol-3-O-rutinoside	C27H30O15	594.5000	594.1585	R12046
PMIR00713	3-O-beta-D-glucosyl-daphnetin	C15H16O9	340.2800	340.0794	RXN-13452
PMIR00851	pheophorbide a	C35H34N4O5	590.7000	590.2529	3.1.1.82-RXN;RXN-17252;RXN-7739,R
PMIR00861	10,16-dihydroxypalmitate	C16H31O4	287.4100	287.2222	R09460
PMIR01748	1-18.3.2-16.3-monogalactosyldiacylglycerol	C43H70O10	747.0000	746.4969	RXN-8301
PMIR01907	13(S)-HOT	C18H29O3	293.4000	293.2117	RXN-13945
PMIR02469	Feruloylputrescine	C14H20N2O3	264.3202	264.1474	R09257

Showing 1 to 10 of 78 entries

Previous [1](#) [2](#) [3](#) [4](#) [5](#) ... [8](#) [Next](#)

### Browse metabolites experimentally measured

11

Search:

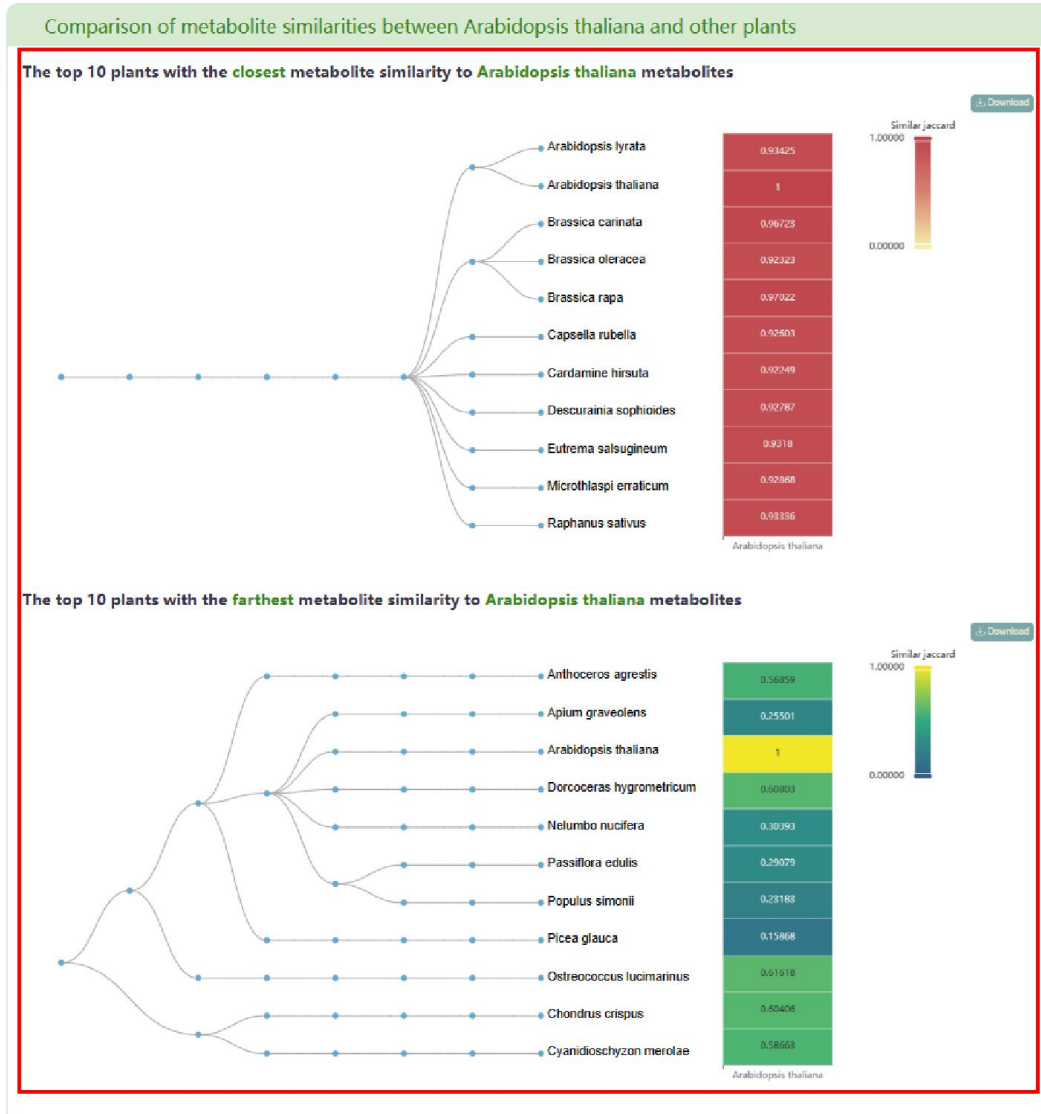
[Download](#)

Name	PCMD	Formula	Molecular weight	Source of support	Other database
Choline	PMIR06774	C5H13NO	104.1700	Mid000001	KEGG:C00114 CAS:62-49-7
(E)-1-butenesulfonate	PMIR17949	C4H8OS	104.1700	Mid000002	PubChem:87828817
o-Cresol	PMIR11575; PMIR27040	C7H8O	108.1400	Mid000003	KEGG:C01542 PubChem:335 KNAPSAcK:C00030878
4-Vinylcyclohexene	PMIR39348	C8H12	108.1800	Mid000004	KEGG:C19310
4-Hydroxyaniline	PMIR12137; PMIR34385	C6H7NO	109.1300	Mid000005	KEGG:C02372 PubChem:3
Cyclohexyl isocyanide	PMIR04739; PMIR13644	C7H11N	109.1700	Mid000006	KEGG:C11520 PubChem:79129
Cytosine	PMIR25803	C4H5N3O	111.1000	Mid000007	KEGG:C00380 CAS:71-30-7
epsilon-Caprolactam	PMIR12575; PMIR35826	C6H11NO	113.1600	Mid000008	KEGG:C06593 PubChem:7768 KNAPSAcK:C00000318
Proline	-	C5H9NO2	115.1300	Mid000009	-
Indole	PMIR25513	C8H7N	117.1500	Mid000010	KEGG:C00463 KNAPSAcK:C00001418

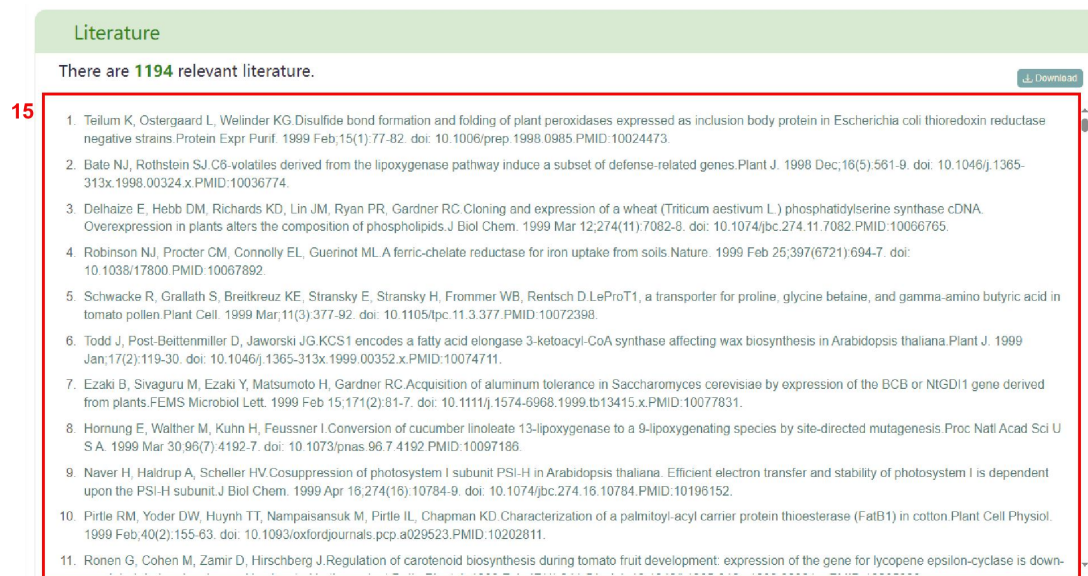
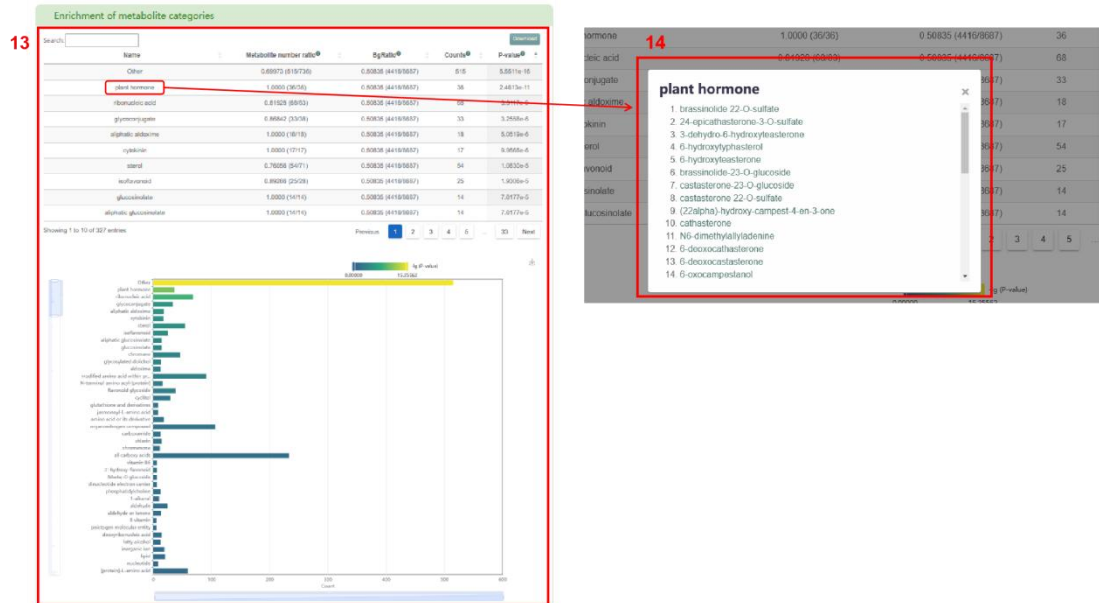
Showing 1 to 10 of 818 entries

Previous [1](#) [2](#) [3](#) [4](#) [5](#) ... [82](#) [Next](#)

Next, a visualization is provided that compares the metabolite similarity between the entered species and other plants. The result primarily display the top 10 plants with the highest and lowest metabolite similarities in PCMD (box 12).



In addition, users can obtain the enrichment of metabolite categories in the entered species (box 13) and view the metabolites belonging to a specific category, such as ‘plant hormone’ (box 14). Finally, users can access a list of literature related to their search in box 15.



## Species-comparison

The “Species-comparison” module allows users to compare metabolite differences between plants. To begin, users can select whether to enter species by stratification (box 1). If users choose “Yes”, PCMD offers three classification types: Class,



Taxonomy, and Characteristic (box 2). Users can select plants according to family by choosing “Class”, monocotyledonous, wild or domesticated types by selecting “Taxonomy”, and flowering and non-flowering classifications by selecting “Characteristic”. Users can enter two different groups of species based on the corresponding classification criteria (box 3). Alternatively, if users choose “No” in the stratification, they can freely enter or upload two different groups of species, provided the species are among the 530 species in PCMD (box 4). After entering the species, users click the “Submit” button to obtain the related information.

The image displays two screenshots of a web application interface titled "Comparison of metabolite differences between plants".

The top screenshot shows the input form with three red boxes highlighting specific elements:

- Box 1:** Stratification:  Yes  No
- Box 2:** Choose type:  Class  Taxonomy  Characteristic
- Box 3:** A taxonomic tree dropdown menu showing a hierarchy: Virdiplantae > Streptophyta > Pinopsida > Pinales > Pinaceae > Abies > Abies alba, Aal (checked).

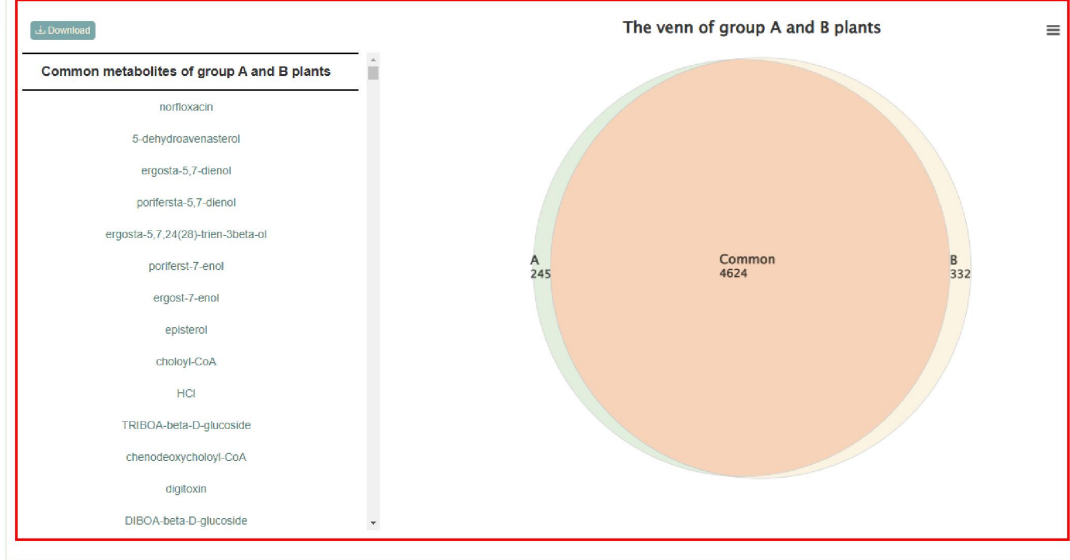
The bottom screenshot shows the same form with "Stratification" set to "No" and two large text input fields for "Species A" and "Species B".

- Box 4:** A red box highlighting the "Species A" and "Species B" input fields. Below "Species A" is the text "e.g. Abies alba or Solanum aethiopicum, Solanum chacoense" and a "选择文件" (Select file) button. Below "Species B" is the text "e.g. Zea mays or Brassica napus, Brassica juncea" and a "选择文件" (Select file) button.

The first page of results displays the distribution of metabolite difference between group A and group B (box 5). Subsequently, the enrichment table of common or specific metabolites in group A and group B is displayed (box 6). Clicking the “Pathway” button enables users to obtain a list of pathways (box 7). If users click on the pathway name, the corresponding pathway page in the MetaCyc database will be retrieved. Users can also view the enrichment of common or specific metabolites in group A and group B. Moving the mouse over the bubble in the bubble diagram allow users to view the corresponding metabolite information (box 8). Clicking on the metabolite name in the table or the bubble in the bubble diagram provides access the reaction related to the metabolite (box 9).

## Distribution of metabolite difference between group A and group B plants

5



6

### Enrichment of group A and B plants common metabolites

Name	Species number ratio <sup>®</sup>	Significance <sup>®</sup>	Counts <sup>®</sup>	P-value <sup>®</sup>	Pathway
(+)-2-carene	0.26846 (15/52)	0.03025 (1/1500)	15	1.696e-14	Pathway
(2E)-4-cyclohex-5-yl-N-hydroxy-omega-pentylbutylacetate 1-amine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
(E)-1-(4-cyclohex-5-yl)-N-hydroxy-omega-pentylbutylacetate 1-amine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
L-ornithine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
(E)-1-(4-cyclohex-5-yl)-N-hydroxy-omega-methylbutylacetate 1-amine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
(E)-1-(4-cyclohex-5-yl)-N-hydroxy-omega-pentylbutylacetate 1-amine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
(E)-1-(4-cyclohex-5-yl)-N-hydroxy-omega-methylbutylacetate 1-amine	0.17647 (15/86)	0.03025 (1/1500)	12	2.9439e-8	Pathway
1-epinephrine	0.091429 (16/175)	0.03025 (1/1500)	16	1.4916e-7	Pathway
1-phenethyl-2-ethyl-1-methyl-4-propylpiperazine	0.091429 (16/175)	0.03025 (1/1500)	16	1.4916e-7	Pathway

Showing 1 to 10 of 209 entries

7



9



8



Furthermore, users can obtain a heat map of metabolite similarities between group A and group B plants (box 10), and a list of literature related to all plants in groups A and B (box 11).



Literature

There are 6 relevant literature. [Download](#)

11

1. Flinkers-Tomczak A, Bakker E, de Boer J, van der Vossen E, Achenbach U, Golas T, Suryaningrat S, Smant G, Bakker J, Govers A Comparative sequence analysis of the potato cyst nematode resistance locus H1 reveals a major lack of co-linearity between three haplotypes in potato (*Solanum tuberosum* spp.). *Theor Appl Genet.* 2011 Feb;122(3):595-608. doi: 10.1007/s00122-010-1472-9. Epub 2010 Nov 4. PMID:21049265.
2. Felcher KJ, Coombs JJ, Massa AN, Hansey CN, Hamilton JP, Velleux RE, Buell CR, Douches DS. Integration of two diploid potato linkage maps with the potato genome sequence. *PLoS One.* 2012;7(4):e36347. doi: 10.1371/journal.pone.0036347. Epub 2012 Apr 27. PMID:22558443.
3. de Boer JM, Datema E, Tang X, Borm TJ, Bakker EH, van Eck HJ, van Ham RC, de Jong H, Visser RG, Bachem CW. Homologues of potato chromosome 5 show variable collinearity in the euchromatin, but dramatic absence of sequence similarity in the pericentromeric heterochromatin. *BMC Genomics.* 2015 May 10;16(1):374. doi: 10.1186/s12864-015-1578-1. PMID:25958312.
4. Lemke P, Moersbacher BM, Singh R. Transcriptome Analysis of *Solanum Tuberosum* Genotype RH89-039-16 in Response to Chitosan. *Front Plant Sci.* 2020 Aug 5;11:1193. doi: 10.3389/fpls.2020.01193. eCollection 2020. PMID:32903855.
5. Lomin SN, Myakushina YA, Kolachevskaya OO, Getman IA, Savelieva EM, Arhipov DV, Delgraf SV, Romanov GA. Global View on the Cytokinin Regulatory System in Potato. *Front Plant Sci.* 2020 Dec 21;11:613624. doi: 10.3389/fpls.2020.613624. eCollection 2020. PMID:33408733.
6. Lomin SN, Kolachevskaya OO, Arhipov DV, Romanov GA. Canonical and Alternative Auxin Signaling Systems in Mono-, Di-, and Tetraploid Potatoes. *Int J Mol Sci.* 2023 Jul 13;24(14):11408. doi: 10.3390/ijms241411408. PMID:37511169.

## Species list

In the “Species list” module, PCMD has collected extensive species classification information (e.g. taxonomy, reproductive characteristics, seed and leaf characteristics, domesticated information) of 530 species, allowing for comparison of metabolite characteristics of intra- and cross-species or multiple taxonomic levels. Taxonomy includes 283 genera, 114 families, 57 orders, 15 classes and 4 phyla. Reproductive characteristics include 502 species of flowering plants, 28 species of non-flowering

plants. Seed and leaf characteristics include 397 species of dicotyledons, 102 species of monocotyledons, 9 species of gymnosperms, and 22 species of spore plants. Domesticated information includes 151 domesticated, 186 wild and wild relative, 78 cultivated and feral, 58 natural commodity (box 1). By clicking on a species, users can access its position in the tree diagram (box 2). Additionally, users can access the corresponding species details page by clicking on the species branch in the tree diagram or the corresponding bar chart (box 3).

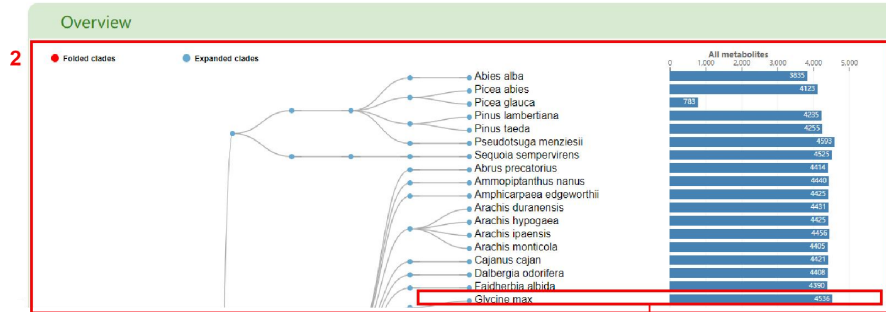
**Species list**

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Search:  Download

Species	Number of metabolites	Ranking	Number of exogenous metabolites	Ranking	Number of enzymes	Ranking	Num
<i>Abies alba</i> (Aal)	3835	504	706	513	1651	505	
<i>Abrus precatorius</i> (Apr)	4414	150	835	32	1905	238	
<i>Acer truncatum</i> (Atr)	4229	406	803	155	1813	441	
<i>Acer yangbiense</i> (Aya)	4434	108	814	94	1939	81	
<i>Actinidia chinensis</i> (Ach)	4364	248	827	47	1889	290	
<i>Actinidia eriantha</i> (Aer)	4344	272	777	357	1898	262	
<i>Actinidia rufa</i> (Aru)	4361	253	792	229	1865	300	
<i>Aegilops tauschii</i> (Afa)	4539	24	850	19	1939	81	
<i>Aetrovanda vesiculosa</i> (Ava)	4126	454	733	498	1825	426	
<i>Allium sativum</i> (Asa)	4391	201	785	292	1912	204	

Showing 1 to 10 of 530 entries Previous 1 2 3 4 5 ... 53 Next



**Overview**

***Glycine max***

Number of metabolites: 4538 (Ranking 26 in 530 species)


Number of predicted metabolites supported by experiments: 77

Number of metabolites experimentally measured: 744

Comparison of metabolite similarities between *Glycine max* and other plants:

The top 10 plants with the closest metabolite similarity (Jaccard similarity coefficient):

- Glycine soja* (0.93506)
- Ammopiptanthus nanus* (0.91713)
- Papaver somniferum* (0.91527)
- Amphicarpaea edgeworthii* (0.91393)
- Arachis ipaensis* (0.91075)
- Arachis duranensis* (0.90909)
- Vigna unguiculata* (0.90725)
- Phaseolus lunatus* (0.90703)
- Cicer arietinum* (0.90625)
- Arachis monticola* (0.90558)



Scientific name: *Glycine max*

Common name: soybeans

Class: Eukaryota;Viridiplantae;Streptophyta;Magnoliopsida;Fabales;Fabaceae;Glycine

Taxonomy: Eudicot

Characteristic: Flowering

Domestication: Domesticated

# Search metabolites

The “Search metabolites” module is mainly divided into two parts: “Search metabolite” and “Browse metabolites”. In the “Search metabolite” section, users can input the name or ID in PCMD of a metabolite (box 1), and then click the “Submit” button to retrieve the related information of the metabolite.

Search metabolite

1

e.g. gamma-solanine or PMIR00026

Submit
Reset

The first page of results is basic information about the metabolite (box 2), the distribution of metabolite in 530 species (box 3) and the classification of the species containing this metabolite (box 4). Users can also access the enrichment table (box 5) and bar chart (box 6) of species by family.

Basic information of metabolite

2

### 5-dehydroavenasterol

**SMILES:** CC1=C(C)C2=C(C1)C3=C(C=C2)C(=C)C(C=C3)C

**PubChem ID:** 111111

**Molecular weight:** 254.36

**Number of species containing this metabolite:** 525

**Top 10 (descending) species:**

1. *Abies alba* (0.81%)
2. *Pinus taeda* (0.75%)
3. *Pinus strobus* (0.72%)
4. *Pinus resinosa* (0.68%)
5. *Pinus contorta* (0.64%)
6. *Pinus strobus* (0.61%)
7. *Pinus strobus* (0.58%)
8. *Pinus strobus* (0.55%)
9. *Pinus strobus* (0.52%)
10. *Pinus strobus* (0.49%)

Distribution of metabolite in 530 species

3

The input metabolite is contained in **525** species, accounting for **99.06%** of all species.

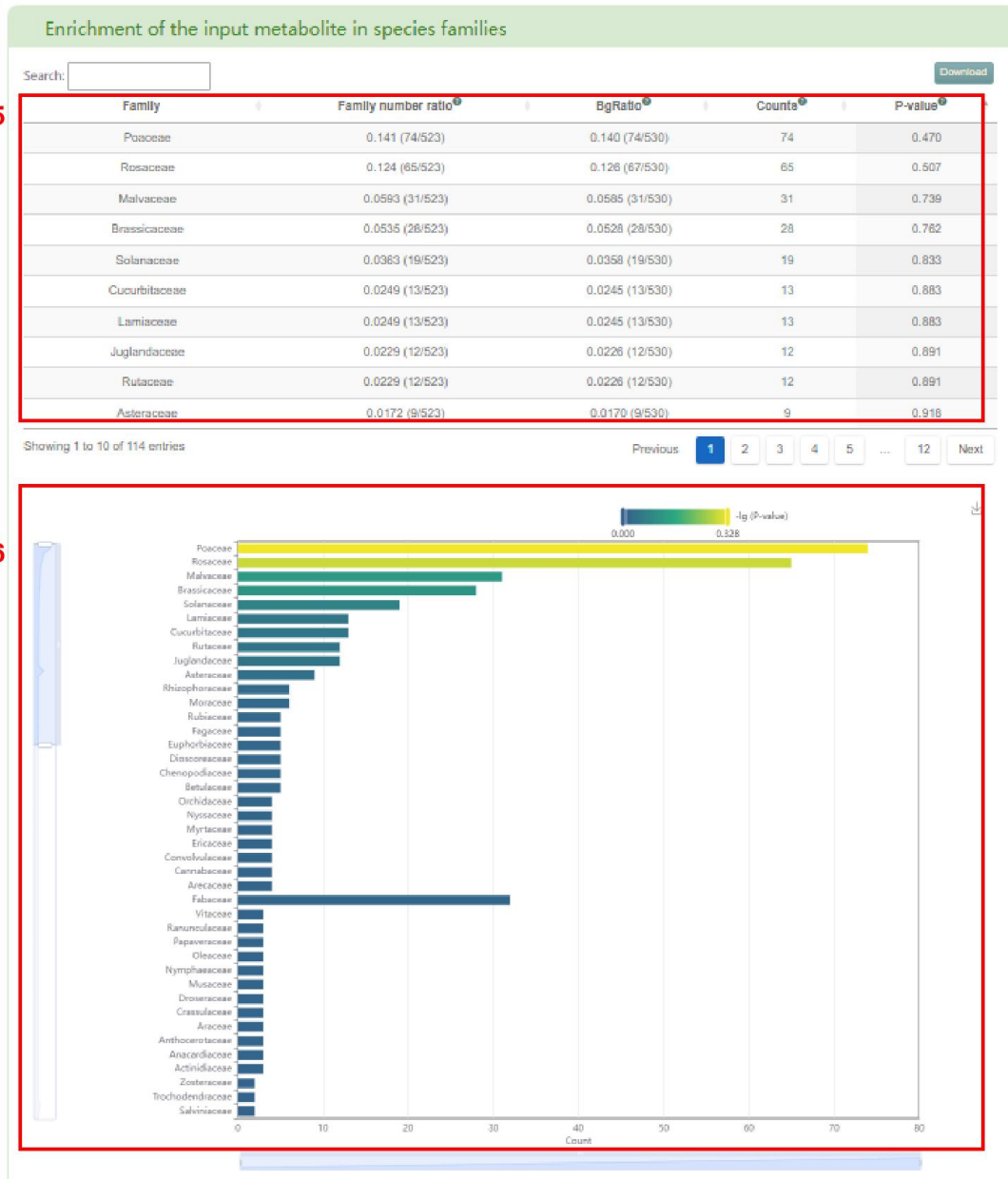
Species with the input metabolite

Classification of species containing this metabolite:

4

Choose classification level:  Class  Order  Family  Genus

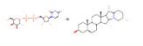
Class	Order	Family	Genus	Percentage
Pinales	Fagales	Fagaceae	<i>Abies alba</i>	0.81%
			<i>Pinus taeda</i>	0.75%
			<i>Pinus strobus</i>	0.72%
			<i>Pinus resinosa</i>	0.68%
Sapindales	Rosales	Rosaceae	<i>Rubus idaeus</i>	14.82%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
			<i>Rubus fruticosus</i>	1.25%
Ericales	Ericales	Ericaceae	<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%
			<i>Calluna vulgaris</i>	1.25%



Additionally, users can obtain reactions associated with the metabolite (box 7). Clicking on the “details” button allow users to access the detailed information page of the reaction (box 8). The list of literature based on metabolite category can be obtained in box 9.

**Reactions**

7 **UDP-alpha-D-galactose + solanidine -> gamma-solanine + H+ + UDP**



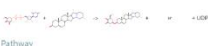
8 **Browse reaction**

**UDP-alpha-D-galactose + solanidine -> gamma-solanine + H+ + UDP**

Name  
**solanine UDP-galactose galactosyltransferase**

Enzymes  
Hexosyltransferases

Reaction



Pathway  
**alpha-solanine/solanoside biosynthesis**

External database link  
RXN-8875

**Literature based on metabolite category**

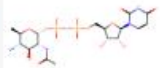
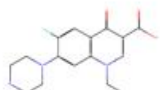
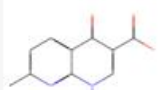
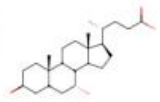
There are 57 relevant literature

9

1. Callero M, D'Amico F, Schialler H, Audenverre L, Vitell S, Giampieri Norcini S, Sangalli R. "Biosynthesis, metabolism and cell storage in Arabidopsis thaliana. I. Molecular, cellular and physiological characterization of the Arabidopsis thaliana mutant defective in the delta7-sterol C5 desaturation step leading to brassinosteroid biosynthesis." *Planta*. 2001 Apr;212(4):689-72. doi: 10.1007/s004250050468.PMID:11349638.
2. Darnet S, Bard M, Poirier A. Functional identification of sterol alpha-methyl oxidase cDNAs from Arabidopsis thaliana by complementation of a yeast erg25 mutant lacking sterol alpha-methyl oxidase (SME) activity. *Plant Physiol*. 2001 Nov;148(5):159-61. doi: 10.1104/pp.148.5.159.PMID:11707284.
3. Schialler H, Giacomini S, Benveniste P, Chy M, Xu C, Song YH, Chua NH. Expression of the Nevoa brassinolein (B.B.K.) Mut. Arg. 3-Hydroxy-3-Methylglutaryl Coenzyme A Reductase 1 in Tobacco Results in Sterol Overproduction. *Plant Physiol*. 1998 Nov;119(3):781-770. doi: 10.1104/pp.119.3.781.PMID:12229630.
4. Burger C, Parnis S, Benveniste P, Schialler H. Virus-induced silencing of sterol biosynthesis genes: identification of a Nicotiana glauca L. sterol methyl-10alpha-demethylase (CYP703) by genetic manipulation of the sterol biosynthetic pathway in Nicotiana glauca L. *Exp Bot*. 2003 Jul;54(10):1273-83. doi: 10.1093/aob/54.10.1273.PMID:13811885.
5. NICOLOSID (Determination of sterol and sterene content of Quercus ilex and Quercus agrifolia at various stages of growth). *J Pharm Sci*. 1967 Aug;56:840-7. doi: 10.1002/jps.2600560804.PMID:13720754.
6. Azevedo JS, Canal S, Pereira JA, Soares RM, Oliveira SP. Determination of sterol and fatty acid composition, oxidative stability, and nutritional value of six wheat (Triticum aestivum L.) cultivars grown in Portugal. *J Agric Food Chem*. 2002 Dec;15(12):1688-702. doi: 10.1021/jf020441u.PMID:14864231.
7. Pujol-Monada N, Rosenberg H, Delacour DL, Peltreux G, Delcroyer A, Barcelo C, Monquero C, Delacour MM, Mounier M, Habib-Jaouh J, Quin-Ledezma J. Sterol (Triticum aestivum L.) and ester wheat (Triticum aestivum L.) waxes from similar sterol profiles, as determined by quantitative liquid chromatography and mass spectrometry analysis. *J Agric Food Chem*. 2004 Jul;52(15):4602-7. doi: 10.1021/jf04172u.PMID:15048919.
8. Bush PJ, Grunwald C. Sterol Changes during Germination of Nicotiana glauca Seeds. *Plant Physiol*. 1972 Jul;50(1):69-72. doi: 10.1104/pp.50.1.69.PMID:16858136.
9. Davis DL, Fritzsche VC. Influence of Temperature on Sterol Biosynthesis in Triticum aestivum. *Plant Physiol*. 1973 Oct;52(4):524-6. doi: 10.1104/pp.52.4.524.PMID:16858856.
10. Davis DL, Fritzsche VC. Sterol Accumulation and Composition in Developing Zea mays L. Kernels. *Plant Physiol*. 1974 Nov;54(5):794-6. doi: 10.1104/pp.54.5.794.PMID:16859976.

In the “Browse metabolites” section, basic information about metabolites in PCMD is displayed. By clicking the metabolite ID, users can access the metabolite page in PCMD. Clicking the metabolite name allows users to access the metabolite’s detail information page.

**Browse metabolites**

Id	Name	Structure	Formula	Molecular weight	Monoisotopic mass
PMIR00013	UDP-N-acetylbacillosamine		C17H27N4O15P2	589.4000	589.0948
PMIR00014	norfloxacin		C16H18N3O3F1	319.3300	319.1332
PMIR00016	nalidixate		C12H11N2O3	231.2300	231.0770
PMIR00017	7alpha-hydroxy-3-oxo-5beta-cholanate		C24H37O4	389.5000	389.2692

### Search structure

The “Search structure” module offers two search modes (box 1): Input the structure and Draw the structure. When selecting “Input the structure”, users need to input the

structural formula of metabolites and species of metabolites (box 2). On the other hand, when selecting "Draw the structure", users need to draw the structural formula diagram of the metabolite (box 3) using the plug-in, generate the mol formula of the metabolite, and input the supported similarity, molecular weight, maximum output result and species (box 4). Afterward, users can click the "Submit" button to obtain the list of metabolites that meet their requirements (box 5). Moreover, in search results (box 5), users can access the metabolite page in PCMD by clicking on the metabolite ID and the metabolite's details page by clicking on the metabolite name.

The screenshot shows the 'Search by structure' interface with four numbered boxes highlighting specific features:

- 1**: A radio button group labeled 'Choose type' with options 'Input the structure' (selected) and 'Draw the structure'.
- 2**: Two input fields. The first is 'Input sturcture' with a placeholder 'e.g. C29H46O1'. The second is 'filter by species' with a placeholder 'e.g. Actinidia chinensis'.
- 3**: A chemical drawing tool window showing the structure 'H—OH'.
- 4**: A 'Display options' panel with checkboxes for 'Carbon labels', 'Atom maps visible' (checked), and 'CPK coloring' (checked). Below it is a text area containing a MOL file for 'MJ212000' with atom coordinates and bond orders. Further down are input fields for 'Similarity' (placeholder 'e.g. 0.7'), 'Molecular Weight' (placeholder 'e.g. 0 to 20'), 'Maximum Results' (dropdown menu set to '100', placeholder 'e.g. 100'), and 'Species' (placeholder 'e.g. Actinidia chinensis').



Search result:

Search:  report

5

Id	Name	Structure	Formula	Molecular weight	Monoisotopic mass	Species	Reaction
PMIR00026	5-dehydroavenasterol		C <sub>29</sub> H <sub>46</sub> O <sub>1</sub>	410.7	410.355	Actinidia chinensis	RXN-4210;RXN-4209
PMIR00228	avenasterone		C <sub>29</sub> H <sub>46</sub> O <sub>1</sub>	410.7	410.355	Actinidia chinensis	RXN-11939;RXN-11938
PMIR01695	4,4-dimethyl-5-alpha-cholesta-8,14,24-trien-3-beta-ol		C <sub>29</sub> H <sub>46</sub> O <sub>1</sub>	410.7	410.355	Actinidia chinensis	RXN66-306;R12323
PMIR01696	4alpha-methyl-5alpha-ergosta-8,14,24(28)-trien-3beta-ol		C <sub>29</sub> H <sub>46</sub> O <sub>1</sub>	410.7	410.355	Actinidia chinensis	RXN-4144;1.14.13.70-RXN

Showing 1 to 4 of 4 entries Previous 1 Next

## Search molecular weight

In the "Search molecular weight" module, users can search for metabolites by molecular weight. Users enter the range of molecular weight and species in box 1, and then click the "Submit" button to obtain the list of metabolites that meet their requirements (box 2). Similarly, in the search results, users can access the metabolite page in PCMD by clicking on the metabolite ID and the metabolite's details page by clicking on the metabolite name.

Search by molecular weight

1 Choose molecular weight:  to    
 e.g. 0 to 20

Filter by species:    
 e.g. Actinidia chinensis

Search results:

Search:  Download

2

Id	Name	Structure	Formula	Molecular weight	Monoisotopic mass	Species	Reaction
PMIR00683	ammonia		H <sub>3</sub> N <sub>1</sub>	17.031	17.0265	Actinidia chinensis	R04930;R04770;R11918;R00571;R00919275;RXN-19274;R06221
PMIR01344	H <sub>2</sub> O		H <sub>2</sub> O <sub>1</sub>	18.015	18.0106	Actinidia chinensis	RXN30-227;R07491;RXN-20979;RXN-15526;R04936;RXN-17335;R04770;R0413811;RXN-9847;R11978;FORMAMIDA DEHYDRATASE-RXN;GLUTDEHYD-R DEHYDROGENASE-RXN;RXN0-3962.f
PMIR01481	OH-		H <sub>1</sub> O <sub>1</sub>	17.007	17.0027	Actinidia chinensis	RXN-16805
PMIR01609	ammonium		H <sub>4</sub> N <sub>1</sub>	18.039	18.0344	Actinidia chinensis	FORMAMIDASE-RXN;RXN-8990;PHEN DEHYDROGENASE-RXN;RXN-10032;16809;AMINEPHEN-RXN;AMINEOXID-UREIDOPROPIONASE-RXN;UREIDOC RXN;L-CYSDESULF-RXN;GLUTAMATE 13997;CYSTATHIONINE-BETA-LYASE-RXN;RIBOFLAVINSYNDEAM-RXN

Showing 1 to 4 of 4 entries Previous 1 Next

## Metabolites-enrichment

The “Metabolites-enrichment” module allows users to perform an enrichment analysis of a group of metabolites. In this page, users can input a group of metabolite names or upload a metabolite file (box 1) and click the "Submit" button to obtain the related results.

### Input metabolites

Tips: Please input metabolite names or id in PCMD. Metabolites are separated by ";" or "," if uploading file, be aware that only metabolites should be in the file.

eg. alpha-solanine;beta-solanine;gamma-solanine or example\_1




1 选择文件 | 未选择文件

The first page of results displays the basic information of metabolites (box 2) and the classification of metabolite (box 3), which is defined by PCMD. Users can also access the metabolite page in PCMD by clicking on the metabolite ID and the metabolite’s detail information page by clicking on the metabolite name.

3 item(s) detected as input.  
3 result(s) found in PCMD.

### Basic information of metabolites

Search:

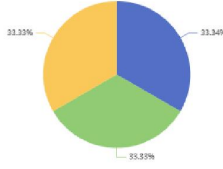
Id	Name	Structure	Formula	Molecular weight	Monoisotopic mass	Species
PMIR04525	all-trans-lycopene		C40H56	536.882	536.438	Abies alba, Abrus precatorius A...
PMIR05429	solanidine		C27H44N1O1	398.651	397.334	Actinidia chinensis, Artemisia ...
PMIR06965	Flavones			0	0	Abies alba, Abrus precatorius A...

Showing 1 to 3 of 3 entries Previous **1** Next

### Classification of metabolites

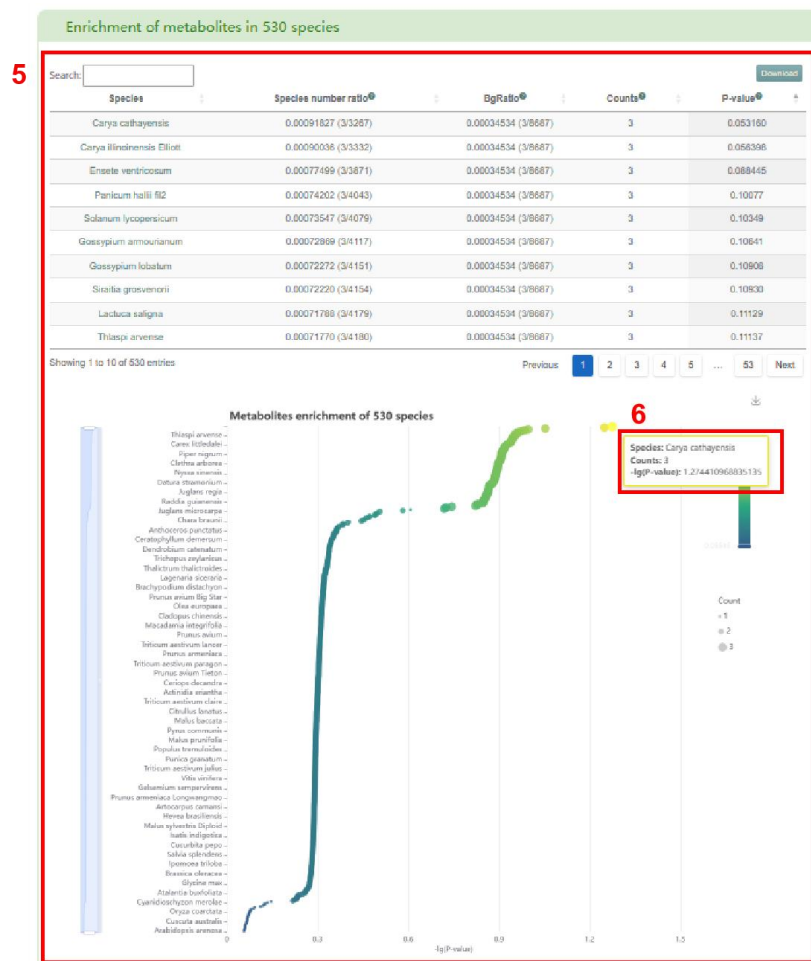
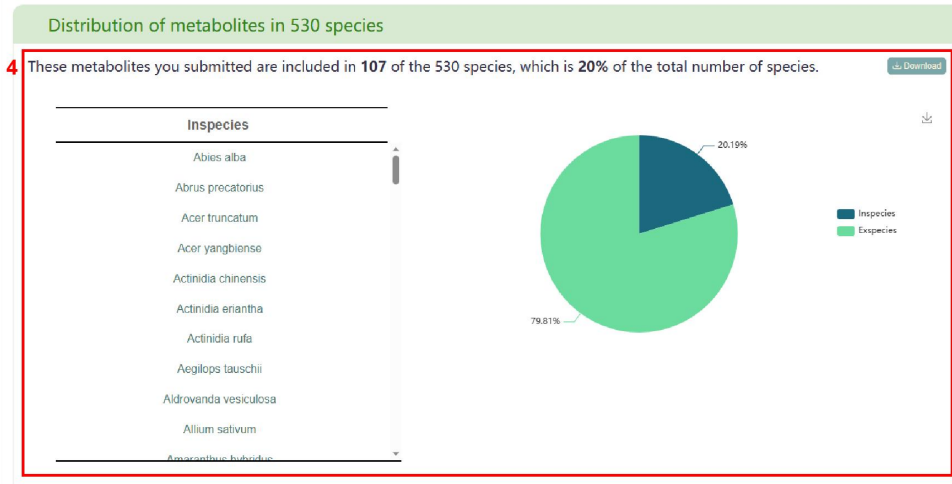
3 PCMD roughly classifies metabolites, and the specific classification of metabolites is as follows:

isoprenoid	secondary metabolite	organic heterobicyclic compound
all-trans-lycopene	solanidine	Flavones



- isoprenoid
- secondary metabolite
- organic heterobicyclic compound

Next, users can view the distribution of the input metabolites in 530 species (box 4). In box 5, users can access the enrichment of metabolites in 530 species. By clicking the species name in the table, users can obtain the detailed page of species and hover the mouse on the bubble to display the name of the enriched species, the number of the enriched metabolites and the corresponding P-value (box 6). Finally, users can obtain the list of literature related to the input metabolites in box 7.



**Literature**

There are **100** relevant literature. Download

7

1. Mauri PL, Iemoli L, Gardana C, Riso P, Simonetti P, Porrini M, Pietta PG. Liquid chromatography/electrospray ionization mass spectrometric characterization of flavonol glycosides in tomato extracts and human plasma. *Rapid Commun Mass Spectrom.* 1999;13(10):924-31. doi: 10.1002/(SICI)1097-0231(19990530)13:10<924::AID-RCM588>3.0.CO;2-G. PMID:10353226.
2. Sue M, Ishihara A, Iwamura H. Purification and characterization of a hydroxamic acid glucosidase beta-glucosidase from wheat (*Triticum aestivum* L.) seedlings. *Planta.* 2000 Feb;210(3):432-8. doi: 10.1007/s004250050029. PMID:10750901.
3. Shobana S, Naidu KA. Antioxidant activity of selected Indian spices. *Prostaglandins Leukot Essent Fatty Acids.* 2000 Feb;62(2):107-10. doi: 10.1054/plef.1999.0128. PMID:10780875.
4. Norbaek R, Brandt K, Kondo T. Identification of flavone C-glycosides including a new flavonoid chromophore from barley leaves (*Hordeum vulgare* L.) by improved NMR techniques. *J Agric Food Chem.* 2000 May;48(5):1703-7. doi: 10.1021/jf9910640. PMID:10820082.
5. Rauha JP, Remes S, Heinonen M, Hopia A, Kahkonen M, Kujala T, Pihlaja K, Vuorela H, Vuorela P. Antimicrobial effects of Finnish plant extracts containing flavonoids and other phenolic compounds. *Int J Food Microbiol.* 2000 May 25;56(1):3-12. doi: 10.1016/s0168-1605(00)00218-x. PMID:10857921.
6. Castro O, Gutierrez JM, Barrios M, Castro I, Romero M, Umama E. [Neutralization of the hemorrhagic effect induced by *Bothrops asper* (Serpentes: Viperidae) venom with tropical plant extracts]. *Rev Biol Trop.* 1999 Sep;47(3):605-16. PMID:10883329.
7. Mauri P, Pietta P. Electro spray characterization of selected medicinal plant extracts. *J Pharm Biomed Anal.* 2000 Aug 1;23(1):61-8. doi: 10.1016/s0731-7085(00)00264-8. PMID:10898155.
8. Harder LH, Christensen LPA. A new flavone O-glycoside and other constituents from wheat leaves (*Triticum aestivum* L.). *Z Naturforsch C J Biosci.* 2000 May-Jun;55(5-6):337-40. doi: 10.1515/znc-2000-5-807. PMID:10928543.
9. Leuzzi U, Caristi C, Panzera V, Licandro G. Flavonoids in pigmented orange juice and second-pressure extracts. *J Agric Food Chem.* 2000 Nov;48(11):5501-6. doi: 10.1021/jf000538o. PMID:11087509.
10. Bednarek P, Franski R, Kerhoas L, Einhorn J, Wojtaszek P, Stobiecki M. Profiling changes in metabolism of isoflavonoids and their conjugates in *Lupinus albus* treated with biotic elicitor. *Phytochemistry.* 2001 Jan 56(1):77-85. doi: 10.1016/s0031-9422(00)00366-6. PMID:11198822.

## ID conversion

The "ID conversion" module supports 17 databases for id conversion, including Biocyc, PubChem, CHEBI, KEGG, CAS, ChEMBL, MetanetX, NIKKAJI, KNApSACk, 3DMET, ChemSpider, SEED, PDB-CCD, HMDB, BiGG, Metabolights, PMhub database. Users first select the database of the input ID (box 1), enter the ID, or upload the file containing the ID (box 2), then select the target database for ID conversion (box 3) and click the "Submit" button to obtain the related result.

Firstly, PCMD displays the number of items entered, the number of results in PCMD, and the number of results that meet the requirements in PCMD (box 4). Secondly, users can obtain the list of ID conversion (box 5).

**ID conversion**

Tips: The ID conversion tool supports the conversion of metabolite IDs between PCMD and 17 published metabolomics databases. The databases involved are Biocyc, PubChem, CHEBI, KEGG, CAS, ChEMBL, MetanetX, NIKKAJI, KNApSACk, 3DMET, ChemSpider, SEED, PDB-CCD, HMDB, BiGG, Metabolights, PMhub. Please choose the entered ID type, input the ID, and select the target type for the ID conversion. Please upload the file according to the format of the example.

1 Input type:

2 Input id:   
e.g. PMIR02337, PMIR02338, PMIR02339  
 未选择文件

3 Target type:

4

3 item(s) detected as input.  
 3 result(s) found in PCMD.  
 3 result(s) found for the target type in PCMD.

Results:

Search:  Download

5

PCMD	Convertible database
PMIR01334	Biocyc: CARNITINE PubChem: 10917 CHEBI: 16347 CAS: 44985-71-9
PMIR01344	Biocyc: WATER PubChem: 962 CHEBI: 15377 CAS: 7732-18-5
PMIR02338	PubChem: 3385 CHEBI: 15946; 61553 KEGG: C00085 CAS: 643-13-0 ChEMBL: CHEMBL604196 NIKKAJ: J92.807K KNApSack: C00007305 3DMET: B04628 PDB-CCD: F6P, P6P

Showing 1 to 3 of 3 entries Previous **1** Next

## Metabolites-comparison

The "Metabolites-comparison" page supports comparison of metabolite data with data in PCMD to annotate metabolite data. Users can enter a set of metabolite names or upload a file containing metabolite names (box 1). After clicking submit, the page will display the basic information of the metabolites (ID, name, formula, molecular weight, monoisotopic mass, classification, number of participating reactions), distribution among 530 plant species and support from other databases (box 2). Among them, click on the number of plants to get all the plants containing the metabolite, and click on the plant name to jump to the corresponding plant details page (box 3). Click on any other database ID corresponding to the metabolite to jump to the corresponding page (box 4).

## Metabolites-comparison

Tips: Users can upload or input metabolites to compare them with the metabolite data in PCMD. It is worth noting that the file content should consist of the metabolite names, and the metabolites should be separated by ';', 'n', or ','.

1

Input metabolites :

```
alpha-solanine  
beta-solanine  
gamma-solanine
```

e.g. example data

未选择文件

3 item(s) detected as input.  
3 result(s) found in PCMD.

## Results:

Search:

2

Id	Name	Formula	Molecular weight	Monoisotopic mass	Class	Reaction	Species	Other database
PMIR00304	gamma-solanine	C33H54N1O6	560.8000	560.3951	chemical entity;molecular entity;secondary metabolite;alkaloid;gamma-solanine	1	36	PubChem: 25245074 KNApSACk: C00034521 HMDB: HMDB0033678 pmhub_id: MS000172850
PMIR02301	beta-solanine	C39H63N1O11	722.9000	722.4479	chemical entity;molecular entity;secondary metabolite;alkaloid;glycoalkaloid;beta-solanine	1	12	PubChem: 45479590 HMDB: HMDB33696 pmhub_id: MS000015094
PMIR02310	alpha-solanine	C45H74N1O15	869.1000	868.5059	chemical entity;molecular entity;secondary metabolite;alkaloid;glycoalkaloid;alpha-solanine	1	12	Blocyc: CPD-9211 PubChem: 25245960 CHEBI: 9188 KEGG: C10820 KNApSACk: C00002262 HMDB: HMDB34202 pmhub_id: MS000098594

Showing 1 to 3 of 3 entries

Previous  Next

4

3

**Species**

- Actinidia chinensis
- Artemisia annua
- Artocarpus altilis
- Camellia sinensis
- Capsicum chinense
- Chiococca alba
- Citrus medica
- Clethra arborea
- Coriandrum sativum
- Cynara cardunculus
- Daemonorops jenkinsiana
- Datura stramonium
- Daucus carota
- Ensete ventricosum
- Ficus microcarpa
- Hellianthus annuus
- Lactuca saligna
- Lactuca sativa

## Reactions

In the “Reactions” module, the page is mainly divided into two parts. In the “Search reactions” section, users can input the metabolite name (box 1), select the input metabolite as a reactant or product (box 2), and then click the "Submit" button to obtain reactions that meet their requirements (box 3). Furthermore, users can access the reaction’s detail page by clicking the “details” button.

Search reactions

1 Input metabolite: all-trans-lycopen  
e.g. all-trans-lycopen or solanidine or Flavones

2 Choose type:  reactant  product

Submit Reset

Search results:

3 Reactions [Download](#)

all-trans-lycopen + 2 oxygen -> 2 pseudoionone + 4,9-dimethyldodeca-2,4,6,8,10-pentaene-1,12-dial	<a href="#">details</a>
all-trans-lycopen + 2 oxygen -> bixin aldehyde + 2 sulcatone	<a href="#">details</a>
Acceptor + all-trans-lycopen -> all-trans-3,4-didehydrolycopen + Donor-H2	<a href="#">details</a>
all-trans-lycopen -> delta-carotene	<a href="#">details</a>
all-trans-lycopen -> gamma-carotene	<a href="#">details</a>
all-trans-lycopen + 2 oxygen -> pseudoionone + 8',10'-diapocartene-8',10'-dial + geranial	<a href="#">details</a>
all-trans-lycopen + 2 oxygen -> pseudoionone + 10',6'-diapocartene-10',6'-dial + sulcatone	<a href="#">details</a>
7',9'-cis-lycopen <=> all-trans-lycopen	<a href="#">details</a>
ETR-Quinones + all-trans neurosporene -> all-trans-lycopen + ETR-Quinols	<a href="#">details</a>
prolycopen -> all-trans-lycopen	<a href="#">details</a>
Acceptor + all-trans neurosporene -> all-trans-lycopen + Donor-H2	<a href="#">details</a>
4 Acceptor + 15-cis-phytoene -> all-trans-lycopen + 4 Donor-H2	<a href="#">details</a>

The second section is “Browse reaction” (box4), which displays all the reactions in PCMD. Users can click on the metabolite in the reaction to jump to the detailed page. By clicking the "details" button, users can access the basic information of the reaction, including the equation name, enzyme, pathway, and links to the equation in other databases (box 5). Additionally, users can click on the enzyme name to jump to the corresponding enzyme details page (box 6) and click on the link of pathway and other databases to jump to the corresponding page.

The image shows two parts of the KEGG database interface. On the left, a 'Browse reactions' page lists various metabolic reactions with their respective enzymes and cofactors. A red box labeled '4' highlights the search results. On the right, a 'Browse reaction' page shows the details for the reaction 'prolycopene -> all-trans-lycopene'. A red box labeled '5' highlights the reaction details, including the enzyme name 'prolycopene isomerase' and its EC number 'EC 1.1.1.19'. Below this, a 'Detailed information of the enzyme' page is shown, with a red box labeled '6' highlighting the 'Identification' section, which lists the enzyme's name, EC number, and class.

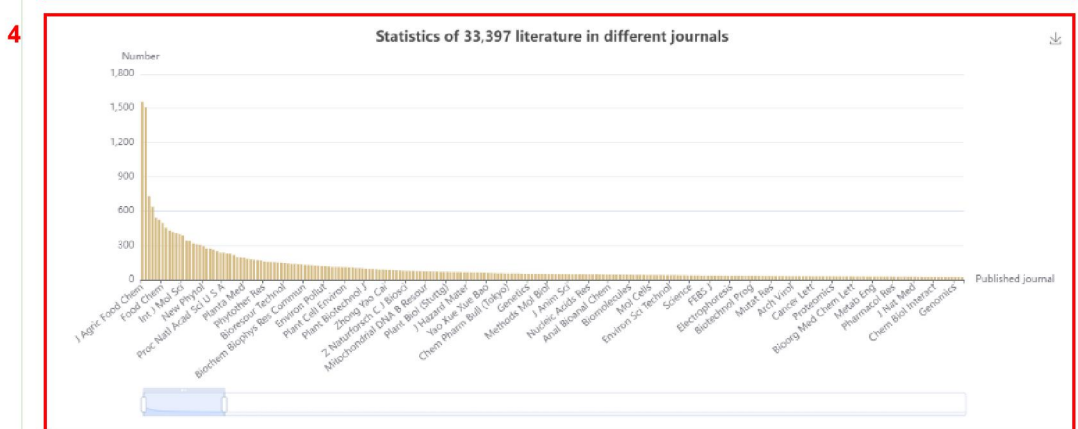
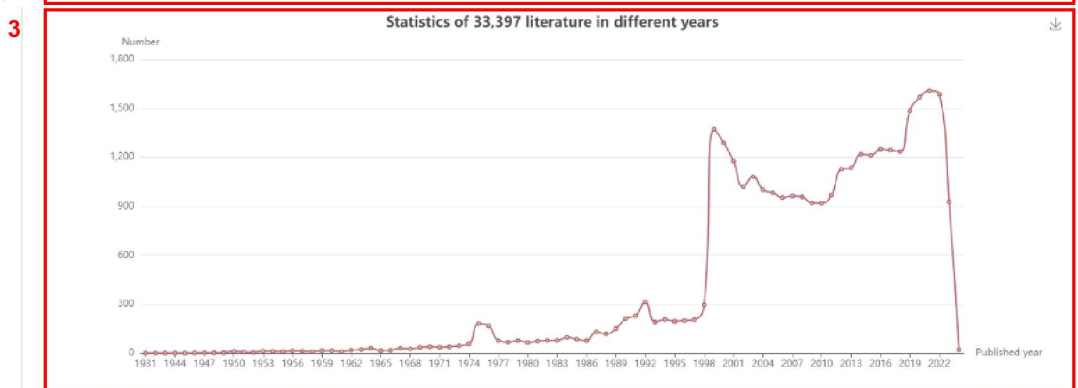
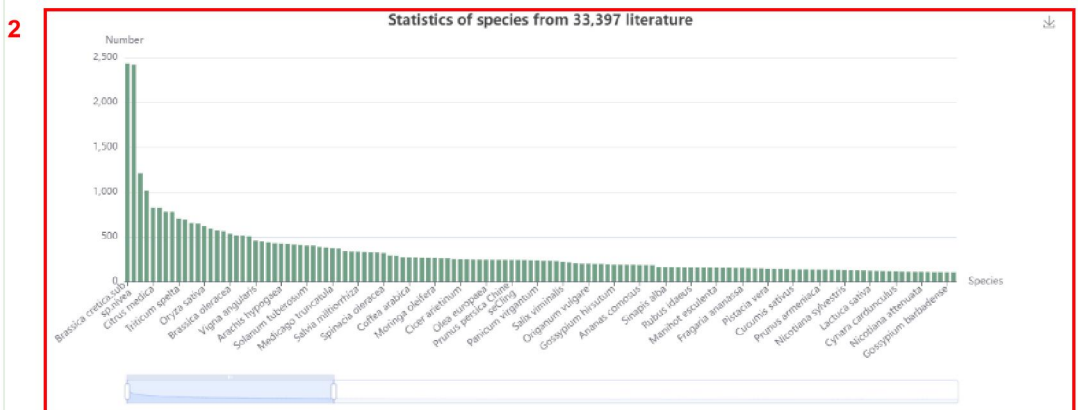
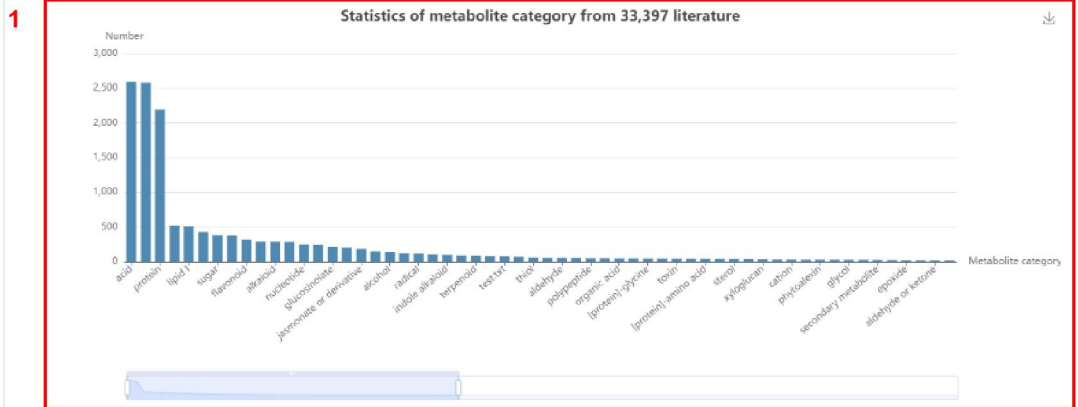
## Literature

In the “Literature” module, this page is divided into two parts: Statistics of literature and Literature search. In the “Statistics of literature” section, users can obtain the statistics of all literature about metabolites category (box 1), 530 species (box 2), published year (box 3) and published journals (box 4). By clicking on the bar chart and line chart, a list of the related literature information will be displayed.

In the “Search literature” section, users can select an option: “Metabolite category”, “Species”, “Published year” or “Published journal”, after that click the "Submit" button to obtain the related result. The search result is a list of the literature information in PCMD that meets user’s requirements (box 5). Additionally, users can access the PubMed page of literature by clicking on the title of the literature.



Statistics of literature



Search literature

Metabolite category flavonoid

e.g. flavonoid or alpha-solanine or Arabidopsis thaliana or 2022 or Plant Physiol

Submit Reset

5 Search:  Download

Metabolite	
4,4-dimethyl-5alpha-cholesta-8-en-3beta-ol;3,4-dihydroxy-2-methyl-4-farnesyl-3H-quinolin-1-ium-1-olate;2,4-dihydroxycinnamoyl-CoA;3,5,7-trioxododecanoyl-CoA;H+	C
beta-D-Glucoside	Ti
Flavones;Beta-D-glucosides	H
(E)-2-methylpropanal-oxime;D-Glucose;all-trans-18-Hydroxyretinoic acid;UDP (G10619);wogonin 7-O-beta-D-glucuronate	S
FLAVANONES	G
UDP	V
kaempferol 3-O-beta-D-glucosylgalactoside	G
kaempferol 3-O-beta-D-glucosylgalactoside	G
intermediate I; 1,16-hexadecane-diol; 1,18-octadecane-diol;6-dehydroguadinomine B;2,3-Dehydroacyl-CoA	P
3,4-dihydroxy-2-methyl-4-farnesyl-3H-quinolin-1-ium-1-olate;2,4-dihydroxycinnamoyl-CoA;2,4-dihydroxyhept-2-enedioate;all-trans-18-Hydroxyretinoic acid;Jasmonoyl-L-amino acid	P

Showing 1 to 10 of 304 entries

Previous **1** 2 3 4 5 ... 31 Next

## Download

The “Download” module currently supports three types of data download: metabolites and metabolic network. To access the data, users can input the species (box 1) and click the "Download" button.

Metabolites

1 Input species:

Download Reset

Metabolic network

Input species:

Download Reset