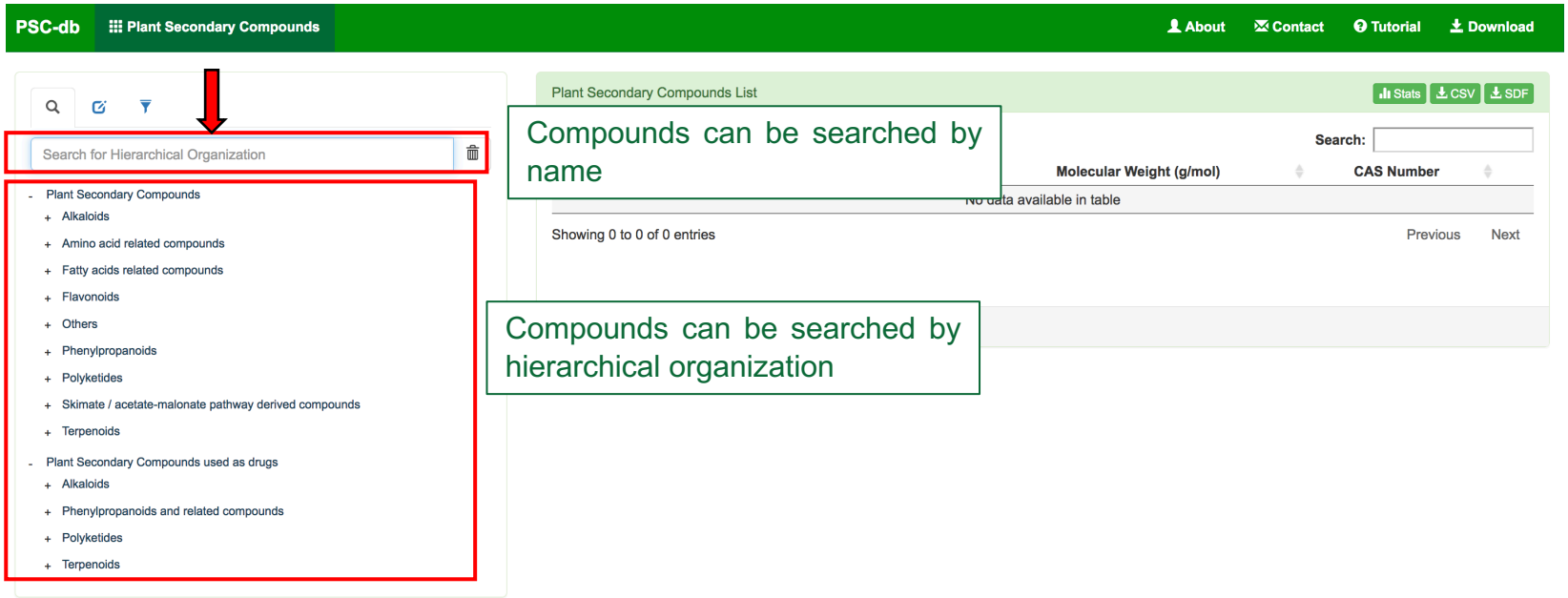
PSC-db Tutorial

PSC-db is a free accessible database containing the 3D-structures of several Plant Secondary Compounds along with its physicochemical and pharmaceutical properties. It has been developed by the Center for Bioinformatics, Simulations and Modelling (CBSM) and the School of Bioinformatics Engineering at Universidad de Talca, the Ramirez Lab at Universidad Autónoma de Chile, in collaboration with the DynaMo Center at University of Copenhagen.

1. Searching molecules for hierarchical organization


PSC-db
Plant Secondary Compounds
About
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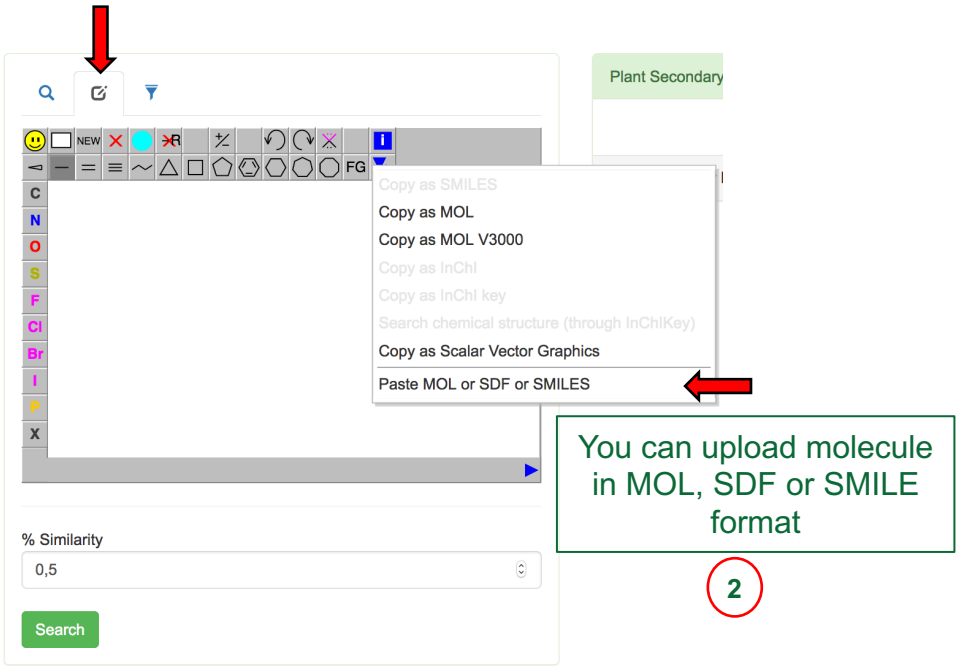
Tutorial
Download
Search for Hierarchical Organization
Plant Secondary Compounds
Alkaloids
Amino acid related compounds
Fatty acids related compounds
Flavonoids
Others
Phenylpropanoids
Polyketides
Skimate / acetate-malonate pathway derived compounds
Terpenoids
Plant Secondary Compounds used as drugs
Alkaloids
Phenylpropanoids and related compounds
Polyketides
Terpenoids
Plant Secondary Compounds List
Stats
CSV
SDF
Search:
Molecular Weight (g/mol)
CAS Number
No data available in table
Showing 0 to 0 of 0 entries
Previous
Next
Compounds can be searched by name
Compounds can be searched by hierarchical organization

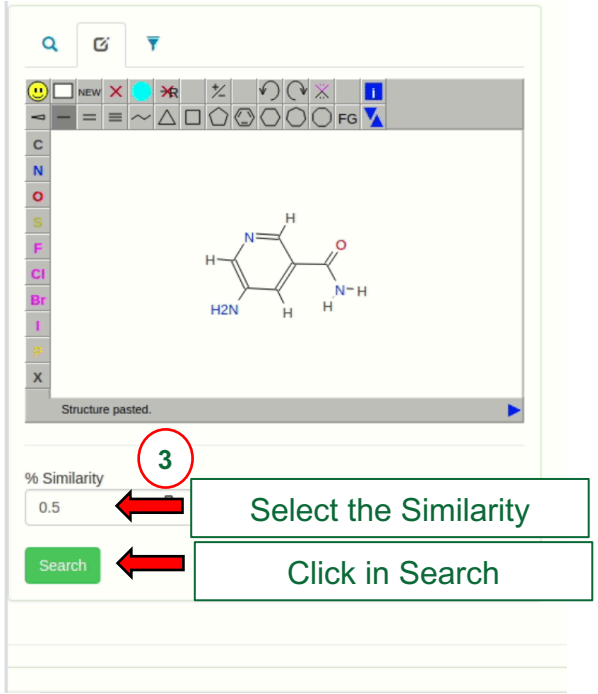
2. Searching molecules by Similarity

1 Select search by similarity



You can upload molecule in MOL, SDF or SMILE format

2



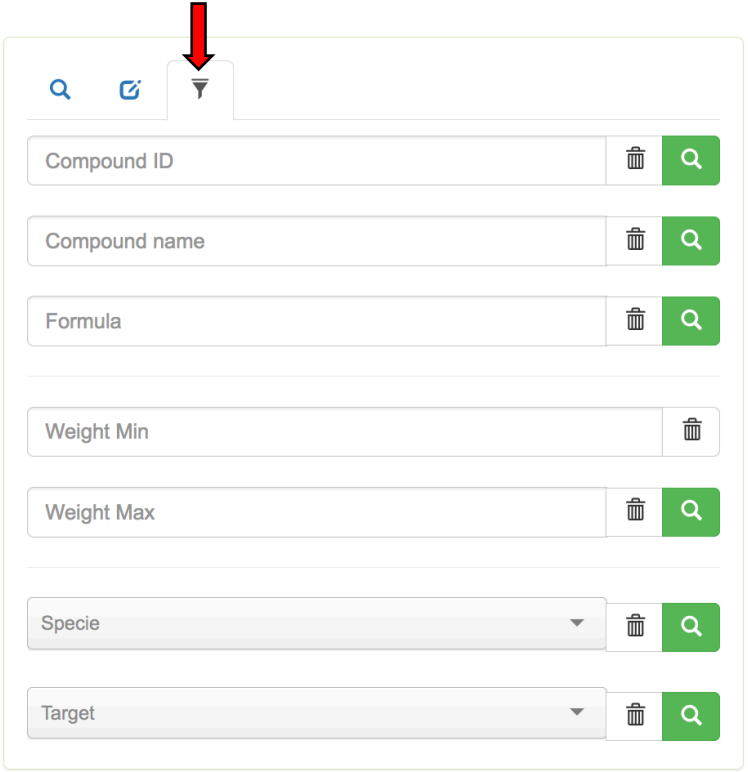
Select the Similarity

Click in Search

3. Searching by other filter

PSC-db Plant Secondary Compounds

Click here for seach molecules by other filters



Filter molecule by:
Compound ID **OR**
Compound name **OR**
Formula **OR**
Weight Min – Weight Max **OR**
Specie **OR**
Target

4. Visualizating molecules

Click in this icon to visualizate the molecules

Search for Hierarchical Organization

- Plant Secondary Compounds
  - + Alkaloids
  - + Amino acid related compounds
  - + Fatty acids related compounds
  - + Flavonoids
  - + Others
  - + Phenylpropanoids
  - + Polyketides
  - + Skimate / acetate-malonate pathway derived compounds
  - + Terpenoids
- Plant Secondary Compounds used as drugs
  - + Alkaloids
  - + Phenylpropanoids and related compounds
  - + Polyketides
  - + Terpenoids

Plant Secondary Compounds List Stats CSV SDF

Show 10 entries Search:

ID	Names	Chemical Formula	Molecular Weight (g/mol)	CAS Number
0	Nicotinamide Nicotinic acid amide Niacinamide Vitamin PP	$C_6H_6N_2O$	122.12	98-92-0
6	Nicotinate Nicotinic acid Niacin 3-Pyridinecarboxylic acid	$C_6H_5NO_2$	123.11	59-67-6
7	Hypoxanthine Purine-6-ol	$C_5H_4N_4O$	136.11	68-94-0
12	Xanthine	$C_5H_4N_4O_2$	152.11	69-89-6
14	Tryptamine 3-(2-Aminoethyl)indole	$C_{10}H_{12}N_2$	160.22	61-54-1
17	L-Pipecolate Pipecolinic acid Pipecolic acid 2-Piperidinecarboxylic acid (S)-Piperidine-2-carboxylic acid	$C_6H_{11}NO_2$	129.16	3105-95-1
25	Tyramine	$C_8H_{11}NO$	137.18	51-67-2

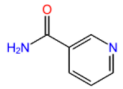
Molecules can be dowload in mol2 format.

In this section you can see ADME/Tos properties

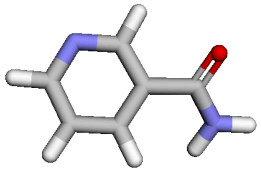
Molecules can be visualized in 2D and 3D.

Nicotinamide
Nicotinic acid amide
Niacinamide
Vitamin PP

2D Image

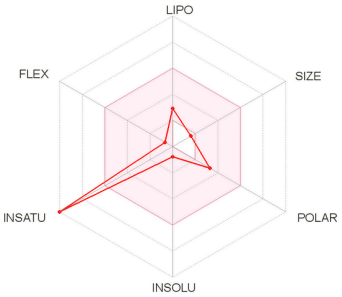


3D MOL2



Rotation: Hold down the primary mouse button.
Translation: Hold down the Ctrl button and the primary mouse button or the middle mouse button.
Zoom: Scroll the mouse wheel or hold down the second mouse button or hold down the button Shift and the primary mouse button.

Radar ADME/Tox Image



The colored zone is the suitable physicochemical space for oral bioavailability.

LIPO (Lipophility): -0.7 < XLogP3 < +5.0
SIZE (mg/mol): 150 < MW < 500
POLAR (Polarity): 20 Å^2 < TPSA < 130 Å^2
INSOLU (Insolubility): 0 < Log S < 6
INSATU (Insaturation): 0.25 < fraction C-sp3 < 1
FLEX (Flexibility): 0 < # rotable bonds < 9

Calculated with SWISSADME (http://www.swissadme.ch/)

5. Visualizating compound details

Click in this icon to see compound datails

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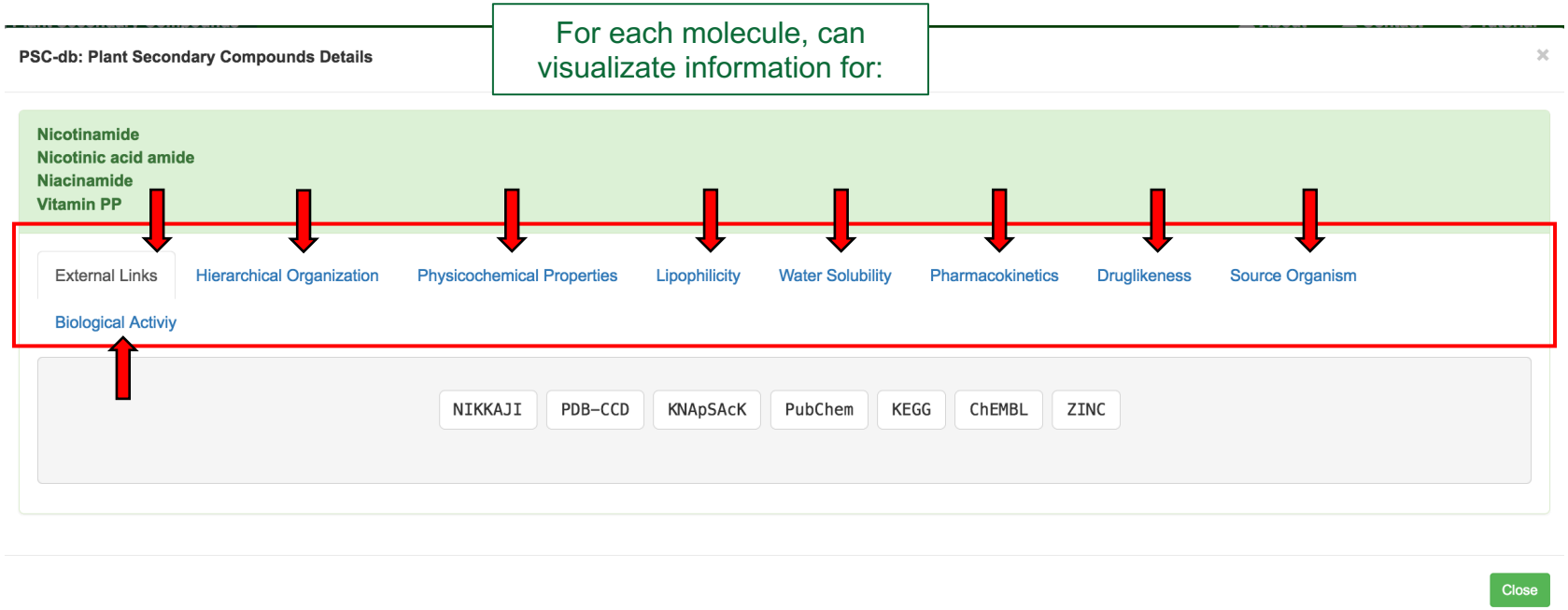
For each molecule, can visualizate information for:
PSC-db: Plant Secondary Compounds Details
Nicotinamide
Nicotinic acid amide
Niacinamide
Vitamin PP
External Links
Hierarchical Organization
Physicochemical Properties
Lipophilicity
Water Solubility
Pharmacokinetics
Druglikeness
Source Organism
Biological Activiy
NIKKAJI
PDB-CCD
KNApSAcK
PubChem
KEGG
ChEMBL
ZINC
Close

6. Visualizating Statistics

Click here for see statistics

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Plant Secondary Compounds List

Stats CSV SDF

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Adicionally, the information can be download in CSV format and molecules can be dowloades in SDF format

PSC-db: Statistics

Statistics | Properties correlations

Select the proprety to plot

Physicochemical Properties
Molecular Weight

Lipophilicity
iLOGP

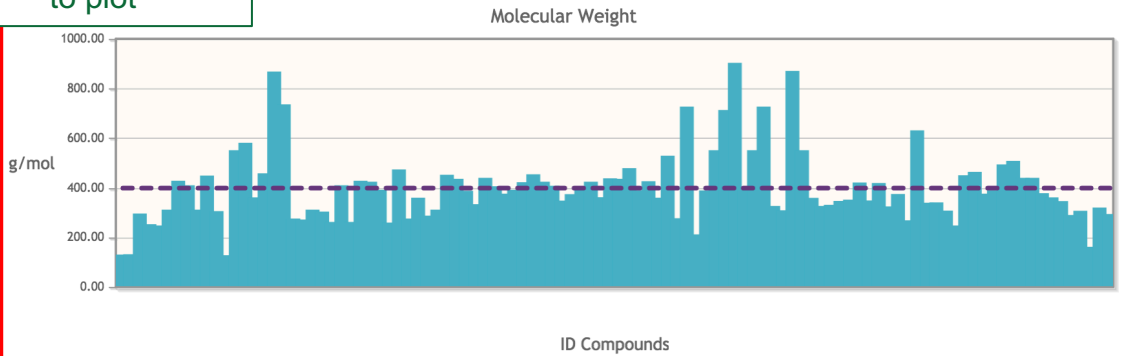
Water Solubility
ESOL Log S

Pharmacokinetics
Skin permeation

Druglikeness
Lipinski (Pfizer) filter violations

Point Labels Xaxis Labels Generate

Click here for generate plot



Download

Download plot

# Compounds	104
Average	397.82 g/mol
Max value	902.76 g/mol
Min value	127.19 g/mol

Details of the data

PSC-db Plant Secondary Compounds

PSC-db: Statistics

Statistics | Properties correlations

Select the proprety correlation to plot

Physicochemical Properties
Molecular Weight

Lipophilicity
iLOGP

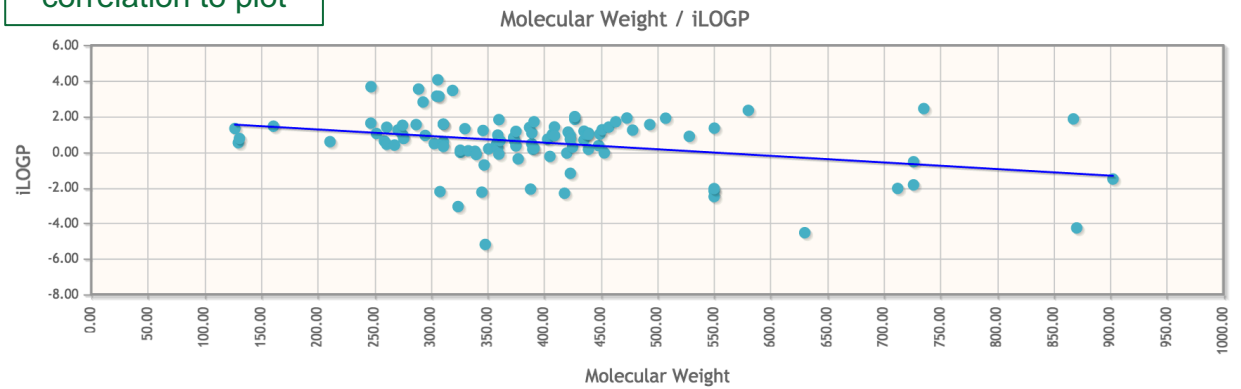
Water Solubility
ESOL Log S

Pharmacokinetics
Skin permeation

Druglikeness
Lipinski (Pfizer) filter violations

Generate

Click here for generate plot



Download

Download plot

R^2 = 0.105
y = -0.004x + 2.021

Details of the data