How to create a custom database for SIRIUS with the compounds already identified for family/genus/species ?

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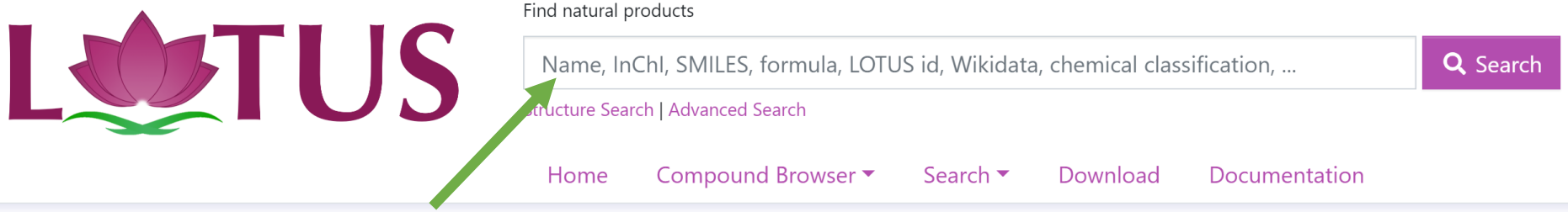
06/06/2022

Open LOTUS



Natural Products Online is an open source project for Natural Products (NPs) storage, search and analysis. This page hosts LOTUS, the naturaL prOducTs occUrrence databaSe, one of the biggest and best annotated resources for NPs occurrences available free of charge and without any restriction. LOTUS is a living database which is hosted in parallel at Wikidata and here. The Wikidata version allows for community curation and addition of novel data. The current version allows a more user friendly experience (such as structural search, taxonomy oriented query, flat table and structures exports).

Component Browser

Cards | Table

There are 276 518 natural products in the database

« ‹ 1 2 3 4 5 6 7 8 9 10 ... 11521 › »

Specify the genus or species and download SDF

LOTUS

Find natural products

Inula montana

Search

Structure Search | Advanced Search

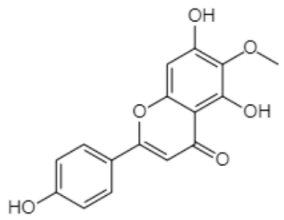
Home Compound Browser Search Download Documentation

Search Results

Your search for "Inula montana" returned 9 natural products.

Download SDF

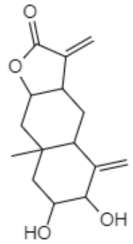
Not what you were searching for? Try our structure or advanced search for more results



Q15410994

Hispidulin

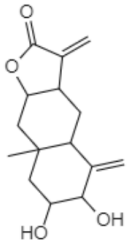
Mol. formula	C16H12O6
Mol. weight	300.26
Tmp. LOTUS id	LTS0135598



Q105113085

(3ar,4ar,6r,7r,8ar,9ar)-6,7-dihydroxy-8a-methyl-3,5-dimethylidene-octahydronaphtho[2,3-b]furan-2-one

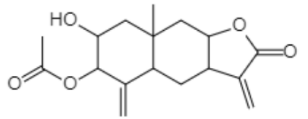
Mol. formula	C15H20O4
Mol. weight	264.32



Q82060062

6,7-dihydroxy-8a-methyl-3,5-dimethylidene-octahydronaphtho[2,3-b]furan-2-one

Mol. formula	C15H20O4
Mol. weight	264.32
Tmp. LOTUS id	LTS0087074



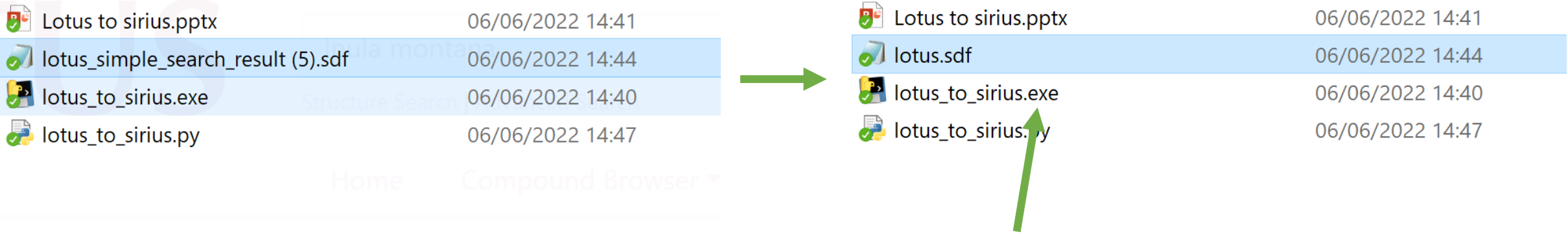
Q105255497

(3ar,4ar,6r,7r,8ar,9ar)-7-hydroxy-8a-methyl-3,5-dimethylidene-2-oxo-octahydronaphtho[2,3-b]furan-6-yl acetate

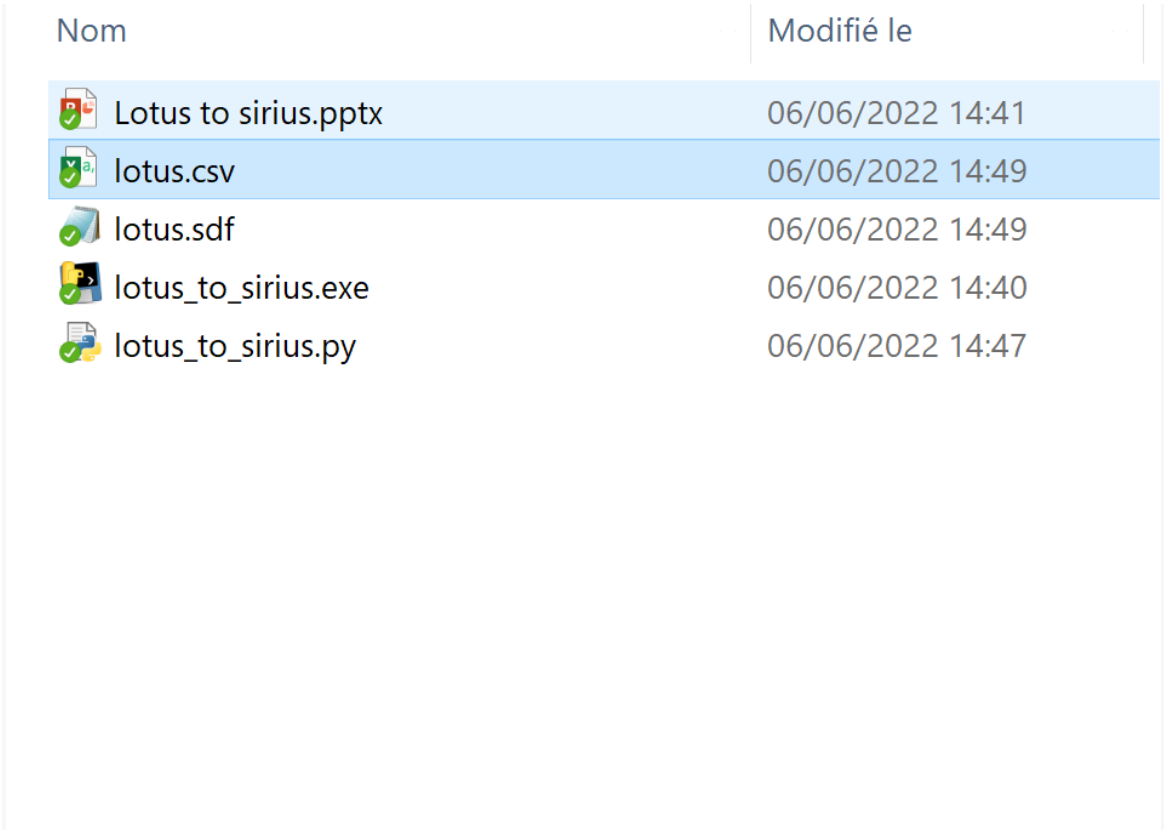
Mol. formula	C17H22O5
Mol. weight	306.35

lotus_simple_searc....sdf

Rename the sdf file to lotus.sdf and open exe file

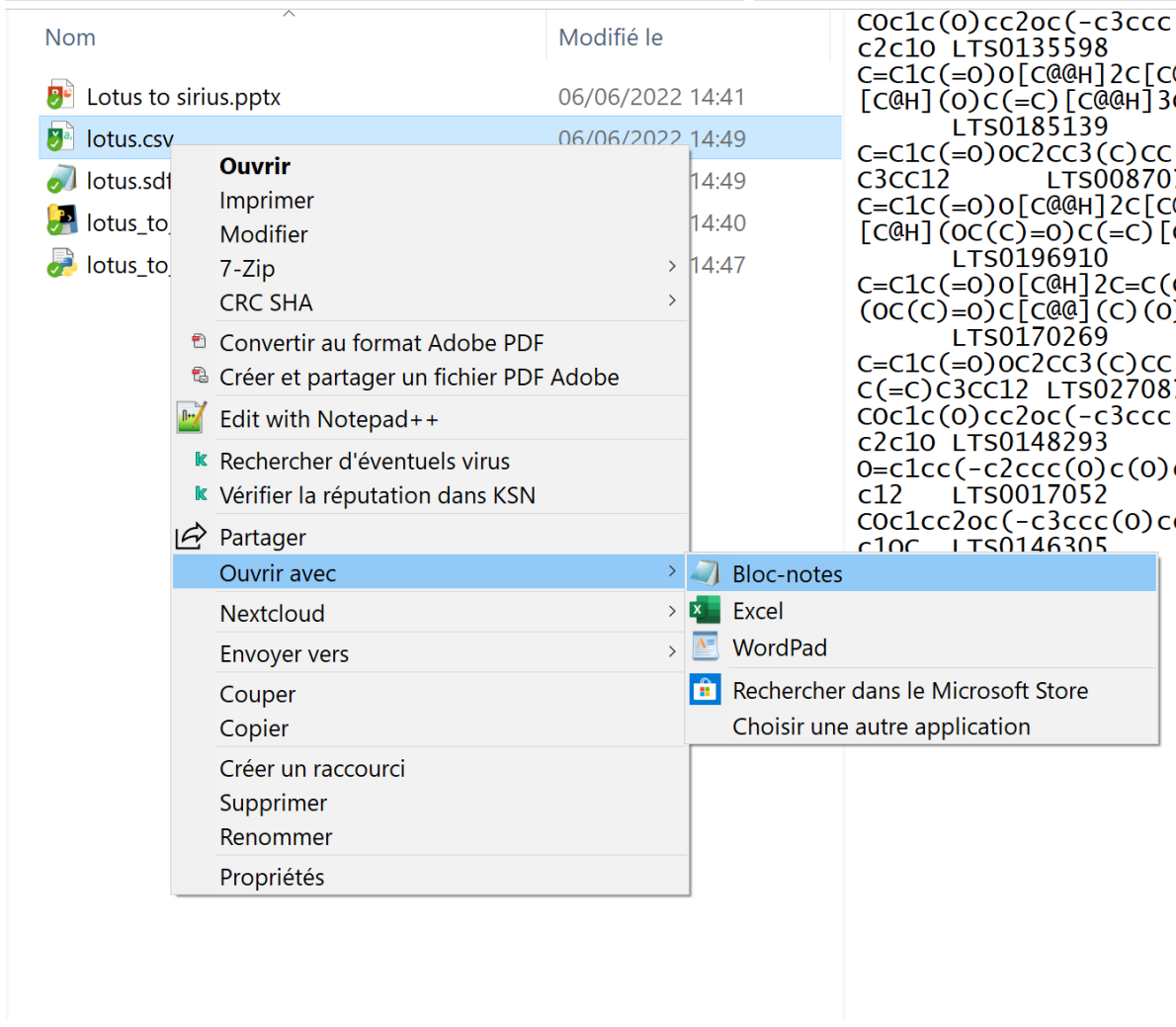


csv file with SMILES and lotus ID is generated

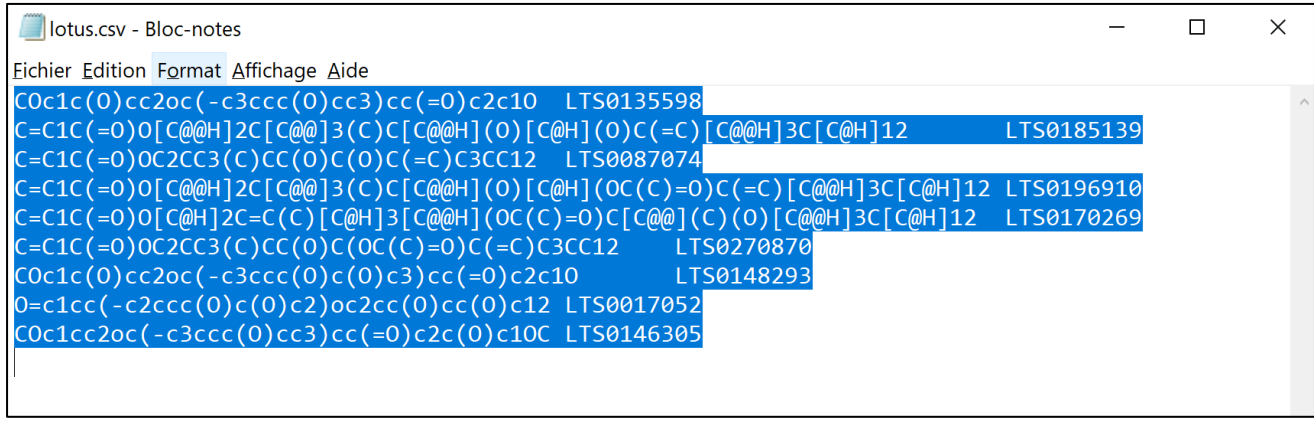



```
COc1c(O)cc2oc(-c3ccc(O)cc3)cc(=O)
c2c1O LTS0135598
C=C1C(=O)O[C@@H]2C[C@@]3(C)C[C@@H]
[C@H](O)C(=C)[C@@H]3C[C@H]12
      LTS0185139
C=C1C(=O)OC2CC3(C)CC(O)C(O)C(=C)
C3CC12      LTS0087074
C=C1C(=O)O[C@@H]2C[C@@]3(C)C[C@@H]
[C@H](OC(C)=O)C(=C)[C@@H]3C[C@H]12
      LTS0196910
C=C1C(=O)O[C@H]2C=C(C)[C@H]3[C@@H]
(OC(C)=O)C[C@@](C)(O)[C@@H]3C[C@H]
      LTS0170269
C=C1C(=O)OC2CC3(C)CC(O)C(OC(C)=O)
C(=C)C3CC12 LTS0270870
COc1c(O)cc2oc(-c3ccc(O)c(O)c3)cc(=
c2c1O LTS0148293
O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(
c12   LTS0017052
COc1cc2oc(-c3ccc(O)cc3)cc(=O)c2c(O
c1OC  LTS0146305
```

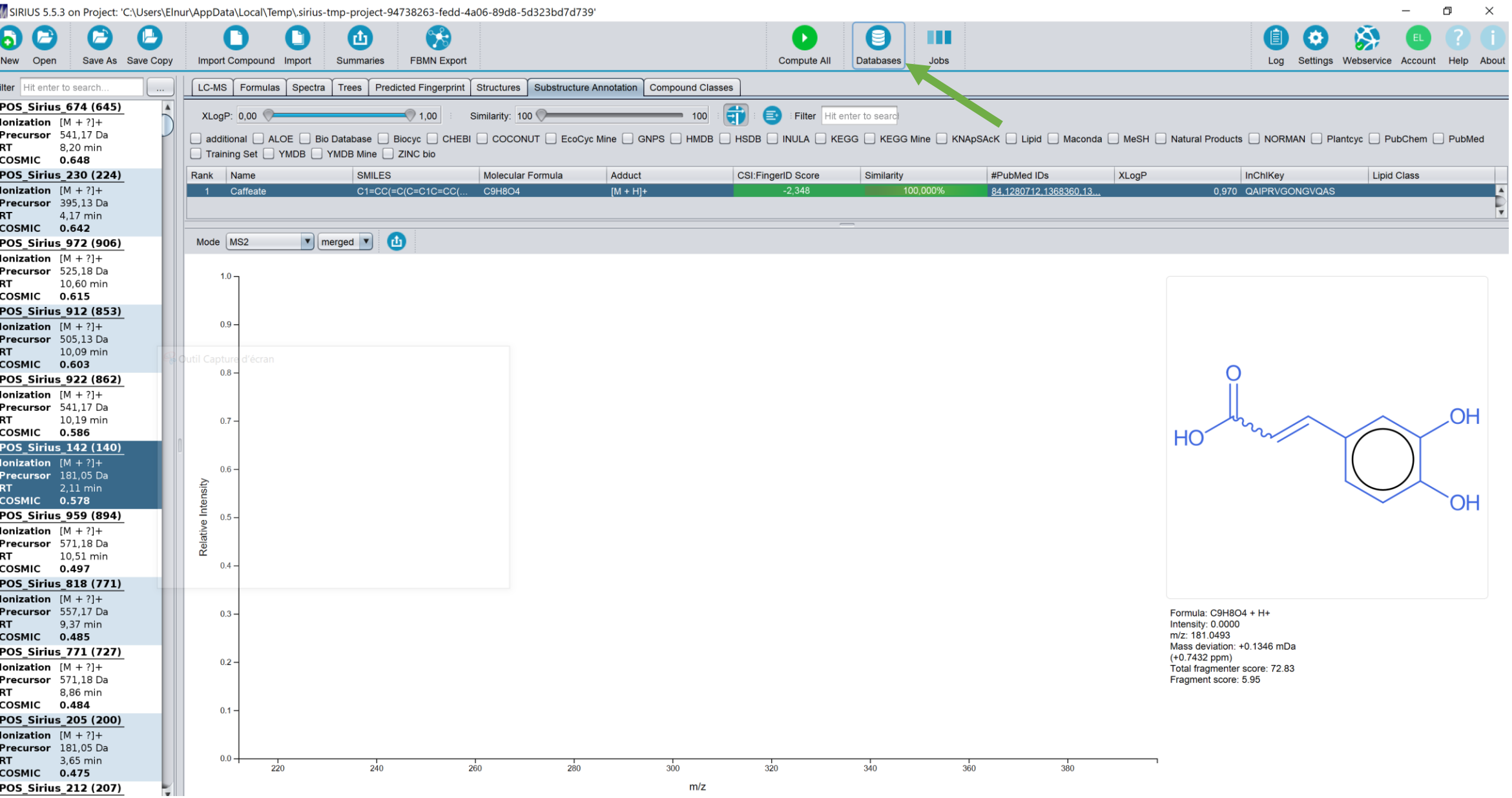
Open csv file with bloc-note and copy the content




```
COc1c(O)cc2oc(-c3ccc(O)cc3)cc(=O)
c2c1O LTS0135598
C=C1C(=O)O[C@@H]2C[C@@]3(C)C[C@@H](O)
[C@H](O)C(=C)[C@@H]3C[C@H]12
      LTS0185139
C=C1C(=O)OC2CC3(C)CC(O)C(O)C(=C)
C3CC12      LTS0087074
C=C1C(=O)O[C@@H]2C[C@@]3(C)C[C@@H](O)
[C@H](OC(C)=O)C(=C)[C@@H]3C[C@H]12
      LTS0196910
C=C1C(=O)O[C@H]2C=C(C)[C@H]3[C@@H]
(OC(C)=O)C[C@@](C)(O)[C@@H]3C[C@H]12
      LTS0170269
C=C1C(=O)OC2CC3(C)CC(O)C(OC(C)=O)
C(=C)C3CC12 LTS0270870
COc1c(O)cc2oc(-c3ccc(O)c(O)c3)cc(=O)
c2c1O LTS0148293
O=c1cc(-c2ccc(O)c(O)c2)oc2cc(O)cc(O)
c12   LTS0017052
COc1cc2oc(-c3ccc(O)cc3)cc(=O)c2c(O)
c1OC   LTS0146305
```

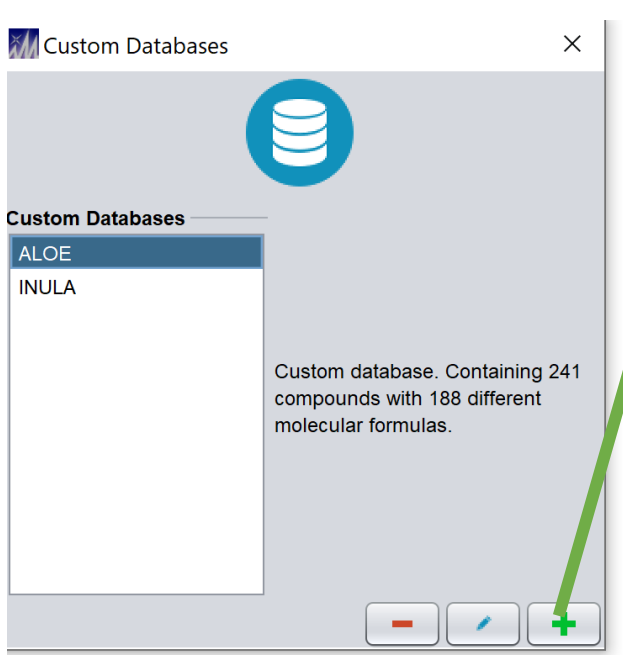


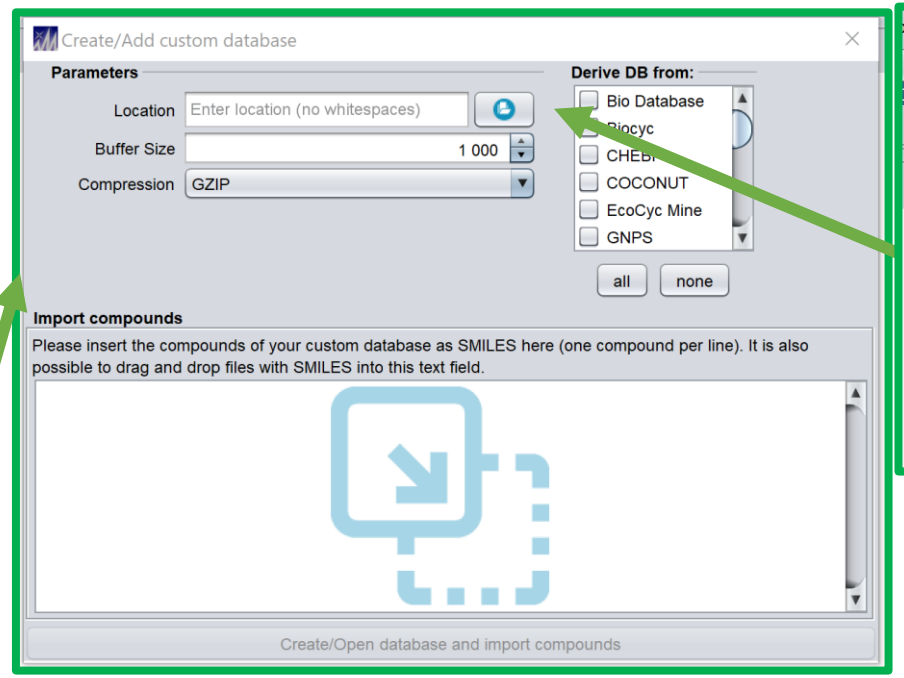
Open SIRIUS and click on Databases

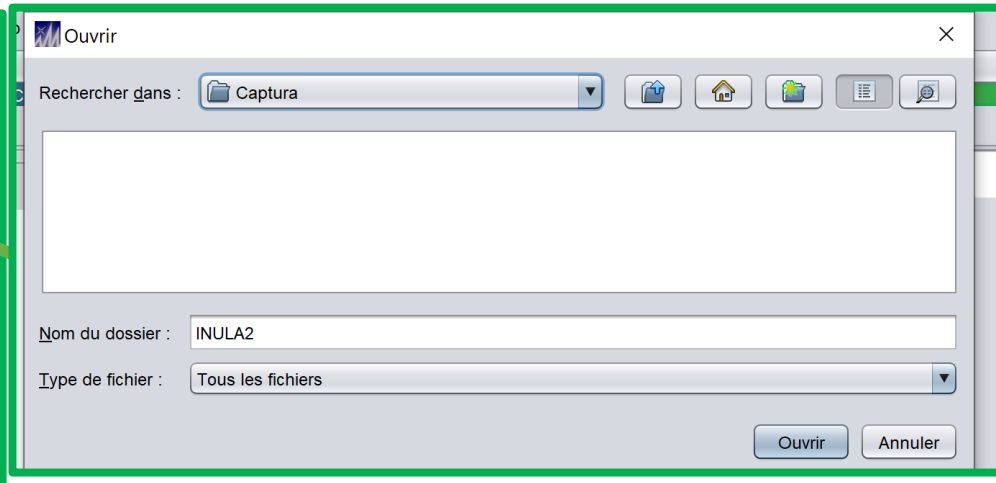


1. Add new database

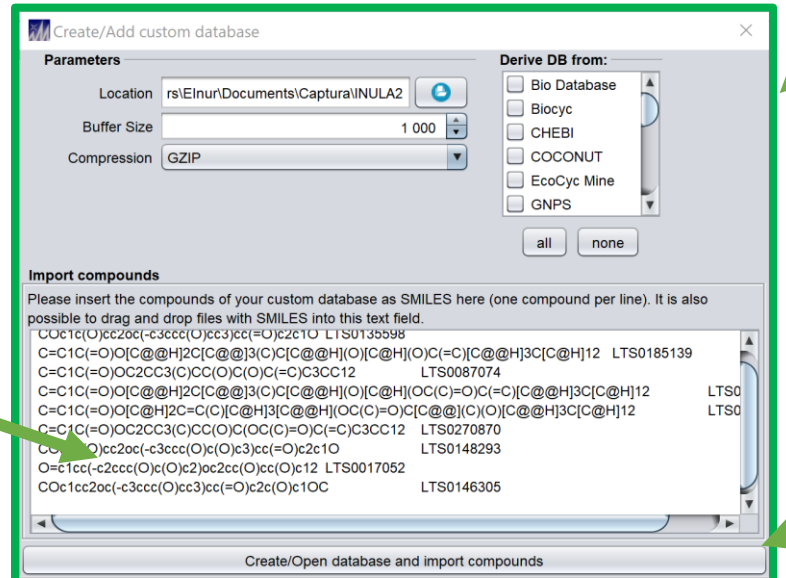
2.Specify the location without spaces in the filename







3. Paste the content of csv file into the window



4. Click on Create

Database is created. Enjoy ;)