

# CNMR\_Predict

[https://github.com/nuzillard/KnapsackSearch/tree/master/CNMR\\_Predict](https://github.com/nuzillard/KnapsackSearch/tree/master/CNMR_Predict)


Start with file “small.txt” from directory CNMR\_predict

```
1 C1=CC(=CC=C1/C=C/C2=CC(=CC(=C2)O)O)O resveratrol
2 C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O quercetin
```

Each line contains a SMILES chain, a space, and a compound name

**Goal:** Create an ACD/Labs Database file with predicted chemical shifts for these two compounds

- Open an Anaconda prompt window
- Navigate to the CNMR\_Predict directory
- Activate an environment with Python3 and RDKit
- Run command *python smi2ACD.py small.smi fake\_acd\_small.sdf*

 Anaconda Prompt

```
(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>python smi2ACD.py small.smi fake_acd_small.sdf
Converted from small.smi to fake_acd_small.sdf: 2
(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>_
```

File *fake\_acd\_small.sdf* was created.

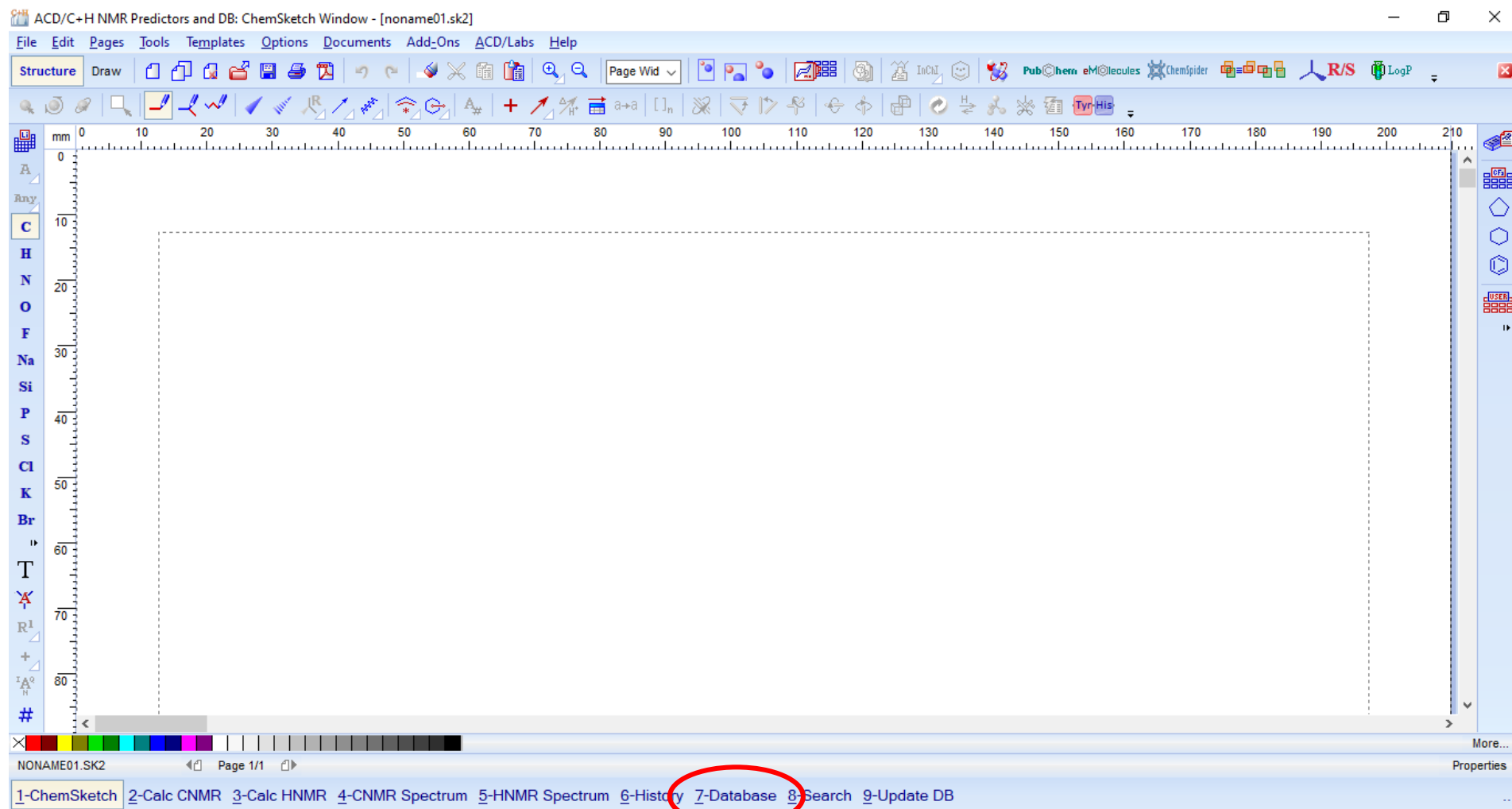
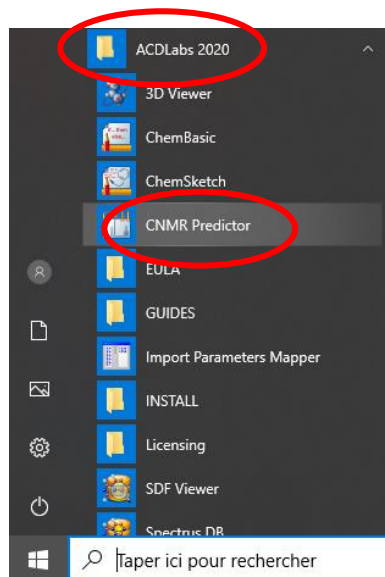
It contains a MOL block with 2D coordinates and '99.99' as  $^{13}\text{C}$  NMR chemical shift values.

```
15 1.9912 -0.5478 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
16 1.9876 0.4522 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
17 1.1198 0.9490 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
18 0.2556 0.4460 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
19 1.1162 1.9490 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
20 2.8590 -1.0448 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
21 -4.9298 -2.5726 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
22 1 2 2 0
23 2 3 1 0
24 3 4 2 0
25 4 5 1 0
26 5 6 2 0
27 6 7 1 0
28 7 8 2 0
29 8 9 1 0
30 9 10 2 0
31 10 11 1 0
32 11 12 2 0
33 12 13 1 0
34 13 14 2 0
35 13 15 1 0
36 11 16 1 0
37 3 17 1 0
38 6 1 1 0
39 14 9 1 0
40 M END
41 > <CNMR_SHIFTS> (1)
42 0:1|99.99;1:2|99.99;2:3|99.99;3:4|99.99;4:5|99.99;5:6|99.99;6:7|99.99;7:8|99.99;8:9|99.99;9:10|99.99;10:11|99.99;11:12|99.99;12:13|99.99;13:14|99.99
43
44 $$$
45 quercetin
46 RDKit 2D
47
48 22 24 0 0 0 0 0 0 0 0 0999 V2000
49 1.3160 -3.0544 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
50 2.1816 -3.5550 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
51 3.0480 -3.0558 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
```

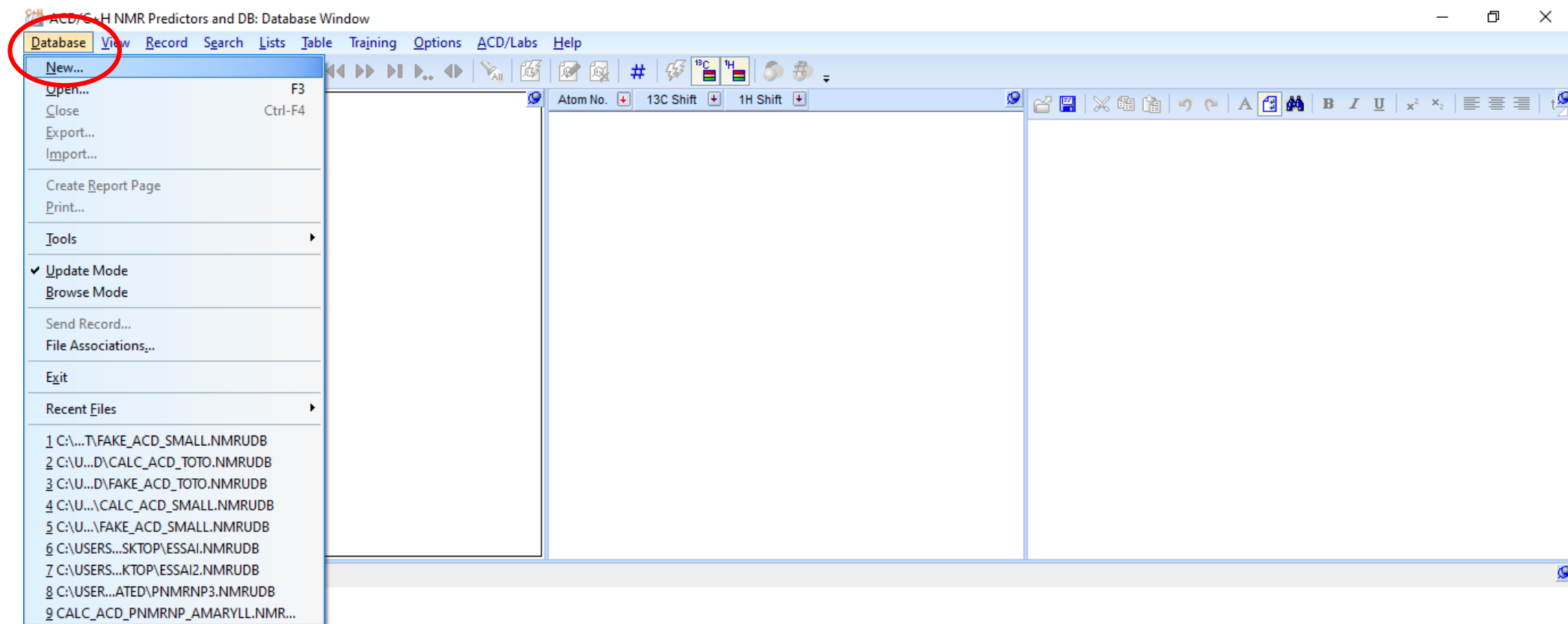
2D coordinates

Temporary  $^{13}\text{C}$  NMR data

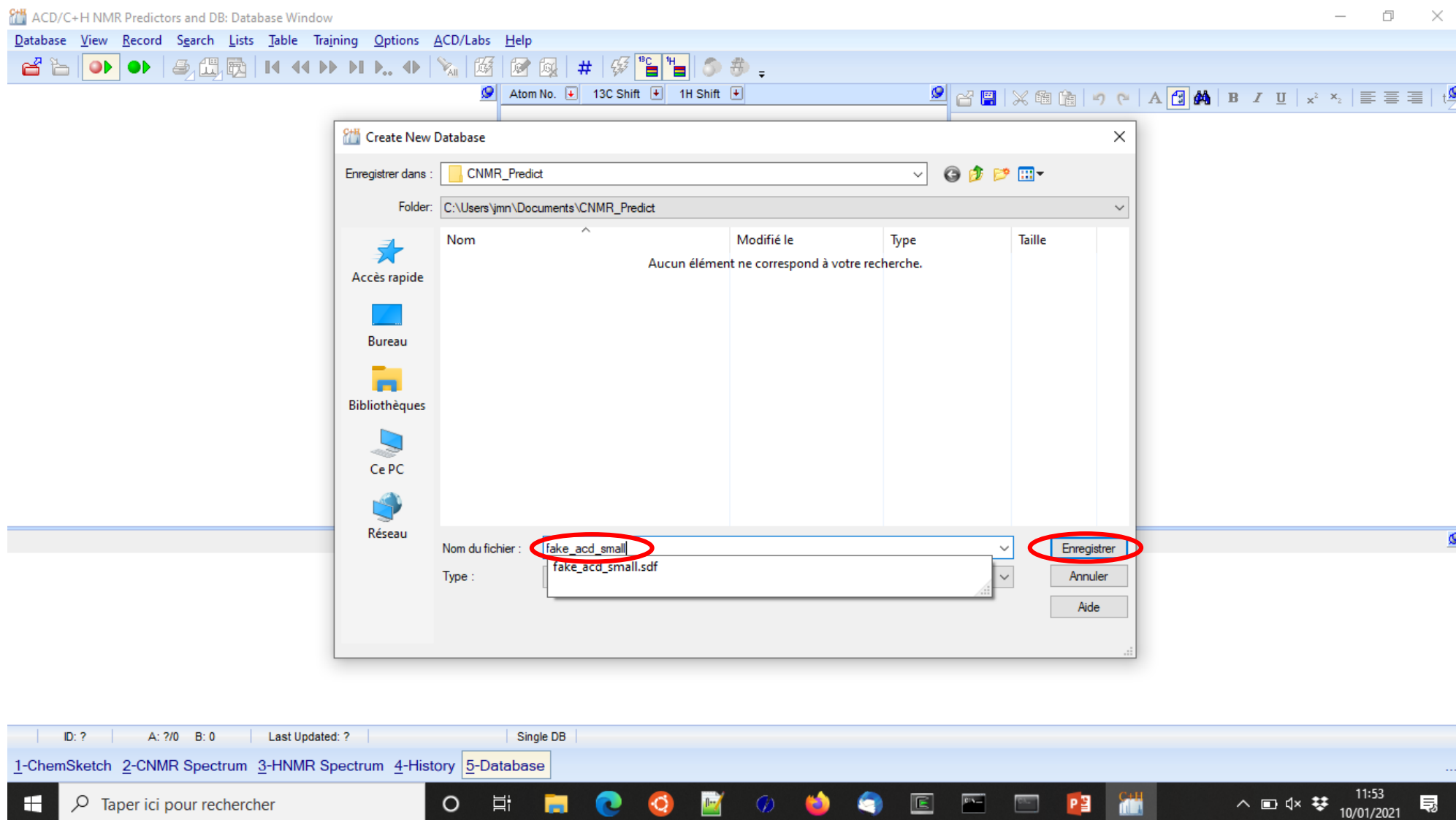
Launch ACD/Labs CNMR Predictor and switch to the Database window



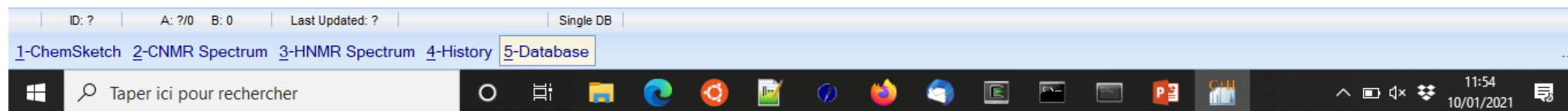
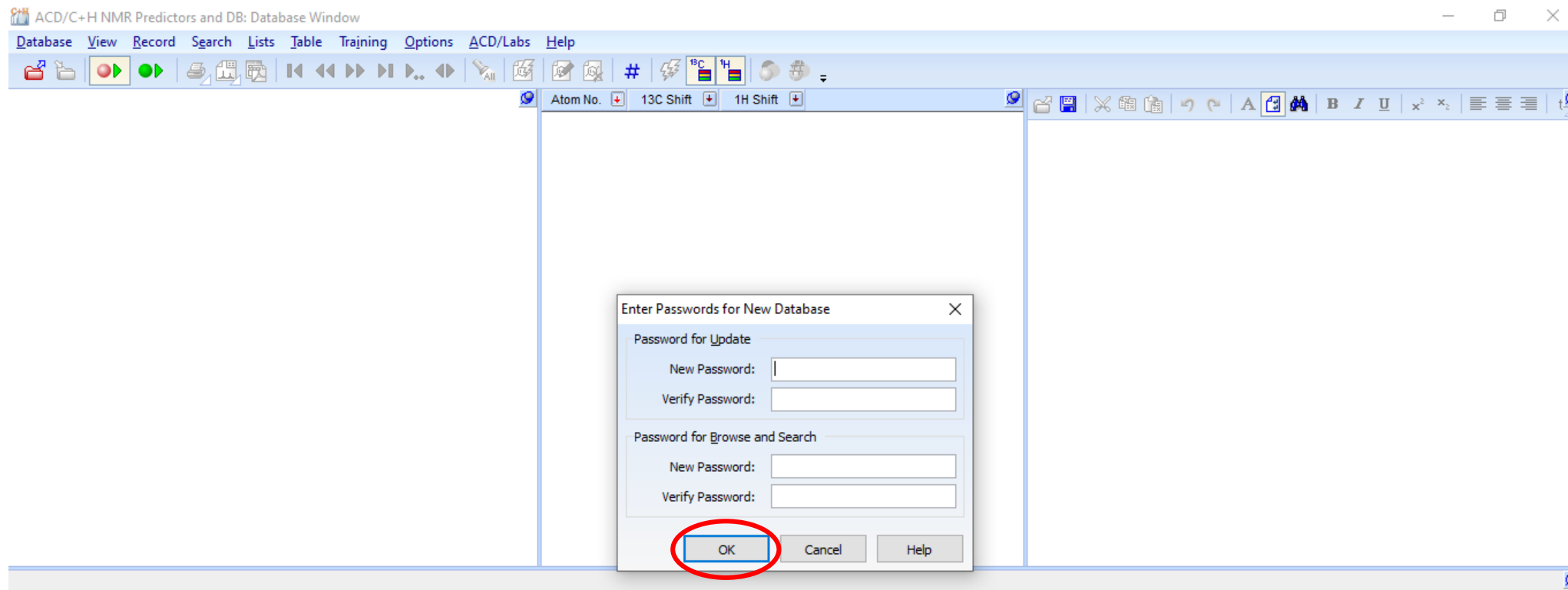
Create a new ACD/Labs Database: Database→New...



Name this ACD/Labs Database *fake\_acd\_small.NMRUDB*

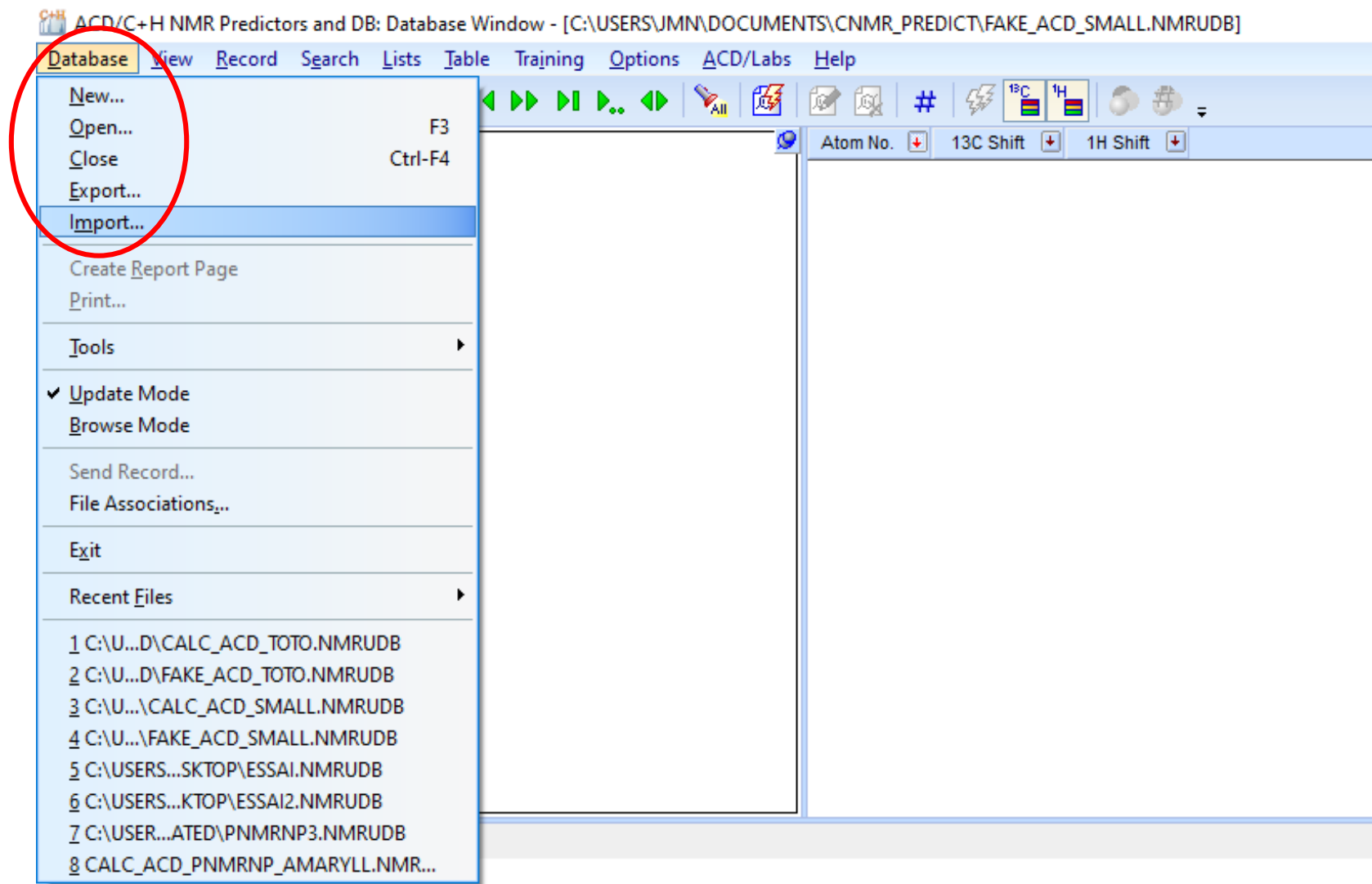


## Leave password fields blank





Import *fake\_acd\_small.sdf*: Database→Import...



## Import *fake\_acd\_small.sdf*

ACD/C-H NMR Predictors and DB: Database Window - [C:\USERS\jmn\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help

Atom No. 13C Shift 1H Shift

Import

Regarder dans : CNMR\_Predict

Folder: C:\Users\jmn\Documents\CNMR\_Predict

Nom	Modifié le	Type	Taille
fake_acd_small.sdf	09/01/2021 20:16	Sdf File	4 Ko

Nom du fichier : fake\_acd\_small.sdf

Types de fichiers : MDL SDFfile (\*.SDF)

Ouvrir Annuler Aide

ID: ? A: ?/0 B: 0 Last Updated: ? Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

Select options for importation

The image shows a software dialog box titled "Import Options" with a close button (X) in the top right corner. The dialog is divided into two main sections. The left section is titled "Search for Duplicated Field" and contains a checkbox for "Search for Duplicated Field" (which is unchecked). Below it, under the heading "If Duplicated Key Field is Found", are five radio button options: "Merge New Data", "Merge New and Overwrite Existing Data (\*)", "Replace All Data for the Record (\*)", "Skip Data for the Record", and "Stop and Prompt". Below these is a checkbox for "Search Key Field Among New Records" (unchecked), a checkbox for " (\*) - Including Chemical Structure" (unchecked), and a "Key Field:" label followed by a dropdown menu currently showing "#ID". The right section is titled "Search for Duplicated Chemical Structures" and contains a checked checkbox for "Search for Duplicated Chemical Structures". Below it, under the heading "If Duplicated Structure is Found", are five radio button options: "Merge New Data", "Merge New and Overwrite Existing Data", "Replace All Data for the Record", "Skip Data for the Record", and "Stop and Prompt" (which is selected). Below these are checkboxes for "Search Structures Among New Records" (unchecked) and "Add Information About Source File Name" (unchecked). At the bottom of the right section is a "Log File:" label followed by a text input field and a browse button "...". At the very bottom of the dialog are five buttons: "Field Options...", "Other Options...", "OK", "Cancel", and "Help". Two red circles are drawn on the image: one around the "Search for Duplicated Chemical Structures" checkbox and its associated radio button options, and another around the "OK" button.

Import Options

☐ Search for Duplicated Field

If Duplicated Key Field is Found

☐ Merge New Data

☐ Merge New and Overwrite Existing Data (\*)

☐ Replace All Data for the Record (\*)

☐ Skip Data for the Record

☐ Stop and Prompt

☐ Search Key Field Among New Records

☐ (\*) - Including Chemical Structure

Key Field:

#ID

☒ Search for Duplicated Chemical Structures

If Duplicated Structure is Found

☐ Merge New Data

☐ Merge New and Overwrite Existing Data

☐ Replace All Data for the Record

☐ Skip Data for the Record

☒ Stop and Prompt

☐ Search Structures Among New Records

☐ Add Information About Source File Name

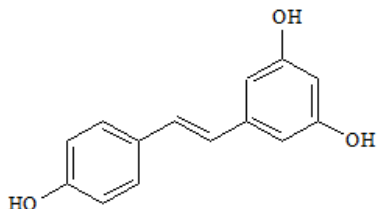
Log File:

Field Options... Other Options... OK Cancel Help

# Importation finished

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help



Atom No.	13C Shift	1H Shift
1	99.99	
2	99.99	
3	99.99	
4	99.99	
5	99.99	
6	99.99	
7	99.99	
8	99.99	
9	99.99	
10	99.99	
11	99.99	
12	99.99	
13	99.99	
14	99.99	

Import Information

File Name: fake\_acd\_small.sdf  
Imported: 2  
Updated: 0  
Added: 2  
Skipped: 0  
With Errors: 0

☐ Don't show again

View Log... OK

Formula:  $C_{14}H_{12}O_3$   
FW: 228.2433  
Mol-Name: resveratrol  
<Double-click to enter new data item>

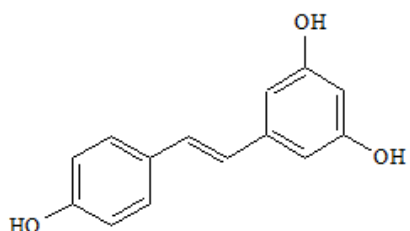
ID: 1 | A: 1/2 B: 2 | Last Updated: 10/01/2021 22:05 | Exclude from Calculations | Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

*Fake\_acd\_small.NMRUDb* and *fake\_acd\_small.sdf* inside

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help



Chemical structure of resveratrol (3,5,4'-trihydroxy-stilben-2-ol) is displayed.

Atom No.	13C Shift	1H Shift
1	99.99	
2	99.99	
3	99.99	
4	99.99	
5	99.99	
6	99.99	
7	99.99	
8	99.99	
9	99.99	
10	99.99	
11	99.99	
12	99.99	
13	99.99	
14	99.99	

Temporary <sup>13</sup>C NMR data

Formula: C<sub>14</sub>H<sub>12</sub>O<sub>3</sub>  
FW: 228.2433  
Mol-Name: resveratrol  
<Double-click to enter new data item>

ID: 1 | A: 1/2 B: 2 | Last Updated: 09/01/2021 20:42 | Exclude from Calculations | Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

## Calculate Chemical Shifts: Database→Tools →Check Chemical Shifts

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help

New...  
Open... F3  
Close Ctrl-F4  
Export...  
Import...  
Create Report Page  
Print...  
Tools  
Update Mode  
Browse Mode  
Send Record...  
File Associations...  
Exit  
Recent Files  
1 C:\U...D\CALC\_ACD\_TOTO.NMRUDB  
2 C:\U...D\FAKE\_ACD\_TOTO.NMRUDB  
3 C:\U...D\CALC\_ACD\_SMALL.NMRUDB  
4 C:\U...D\FAKE\_ACD\_SMALL.NMRUDB  
5 C:\USERS...SKTOP\ESSAI.NMRUDB  
6 C:\USERS...KTOP\ESSAI2.NMRUDB  
7 C:\USER...ATED\PNMRNP3.NMRUDB  
8 CALC\_ACD\_PNMRNP\_AMARYLL.NMR...

About...  
Summary Info...  
Compact to...  
Repair...  
Merge to...  
Merge from...  
Calculate Training Score  
Calculate Utility Score  
Calculate Absent Shifts  
Delete Calculated Shifts  
Check Chemical Shifts  
Update User Data in List...  
Change Password...  
Upgrade

Atom No.	13C Shift	1H Shift
1	99.99	
2	99.99	
3	99.99	
4	99.99	
5	99.99	
6	99.99	
7	99.99	
8	99.99	
9	99.99	
10	99.99	
11	99.99	
12	99.99	
13	99.99	
14	99.99	

Mol-Name: resveratrol

<Double-click to enter new data item>

## Ignore the warning message

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help

Atom No. 13C Shift 1H Shift

1	99.99	
2	99.99	
3	99.99	
4	99.99	
5	99.99	
6	99.99	
7	99.99	
8	99.99	
9	99.99	
10	99.99	

Warning

Among checked structures 2 structures contains suspicious chemical shifts.  
Would you like to see only those structures?

OK Cancel

☐ Don't ask me again

Formula:  $C_{14}H_{12}O_3$   
FW: 228.2433  
Mol-Name: resveratrol  
<Double-click to enter new data item>

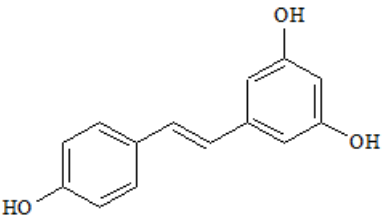
ID: 1 A: 1/2 B: 2 Last Updated: 10/01/2021 22:05 Exclude from Calculations Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

## Disastrous checking, but this is not a problem...

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help



Chemical structure of resveratrol is displayed.

Atom No.	13C Shift	13C Calc	1H Shift
1	99.99	128.39	
2	99.99	116.07	
3	99.99	157.85	
4	99.99	116.07	
5	99.99	128.39	
6	99.99	129.35	
7	99.99	128.41	
8	99.99	126.35	
9	99.99	140.60	
10	99.99	105.17	
11	99.99	159.14	
12	99.99	102.29	
13	99.99	159.14	
14	99.99	105.17	

Formula:  $C_{14}H_{12}O_3$   
FW: 228.2433  
Mol-Name: resveratrol  
<Double-click to enter new data item>

ID: 1 A: 1/2 B: 2 Last Updated: 09/01/2021 20:54 Exclude from Calculations Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database



## Export database: Database→Export

ACD/CD NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help

New... F3  
Open... Ctrl-F4  
Close  
Export...  
Import...  
Create Report Page  
Print...  
Tools  
Update Mode  
Browse Mode  
Send Record...  
File Associations...  
Exit  
Recent Files

1 C:\U...D\CALC\_ACD\_TOTO.NMRUDB  
2 C:\U...D\FAKE\_ACD\_TOTO.NMRUDB  
3 C:\U...D\CALC\_ACD\_SMALL.NMRUDB  
4 C:\U...D\FAKE\_ACD\_SMALL.NMRUDB  
5 C:\USERS...SKTOP\ESSAI.NMRUDB  
6 C:\USERS...KTOP\ESSAI2.NMRUDB  
7 C:\USER...ATED\PNMRNP3.NMRUDB  
8 CALC\_ACD\_PNMRNP\_AMARYLL.NMR...

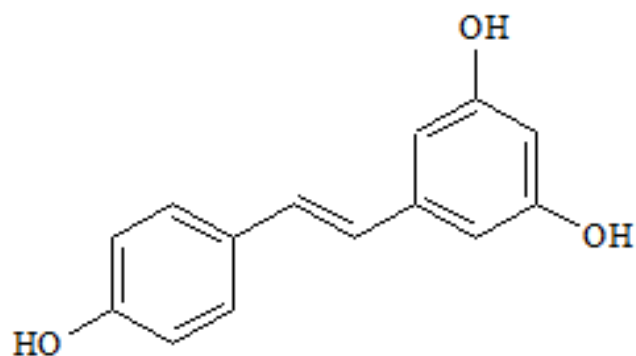
Chemical structure: Oc1ccc(O)cc1

Atom No.	13C Shift	13C Calc	1H Shift
1	99.99	128.39	
2	99.99	116.07	
3	99.99	157.85	
4	99.99	116.07	
5	99.99	128.39	
6	99.99	129.35	
7	99.99	128.41	
8	99.99	126.35	
9	99.99	140.60	
10	99.99	105.17	
11	99.99	159.14	
12	99.99	102.29	
13	99.99	159.14	
14	99.99	105.17	

Mol-Name: resveratrol


<Double-click to enter new data item>

Calculated chemical shifts **will be** exported, anyway...



5	99.99	128.39
6	99.99	129.35
7	99.99	128.41
8	99.99	126.35
9	99.99	140.60
10	99.99	105.17

Warning

 Calculated chemical shifts will not be exported to the SDFFile. Continue?

OK

Cancel

☐ Don't ask me again

## Export database as *fake\_acd\_small\_exported.sdf*

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]

Database View Record Search Lists Table Training Options ACD/Labs Help

Atom No. 13C Shift 13C Calc 1H Shift

1 99.99 128.39

OH

HO

Formula:  $C_{14}H_{12}O_3$   
FW: 228.2433  
Mol-Name: resveratrol  
<Double-click to enter new data item>

Export Database to Sdf file

Enregistrer dans : CNMR\_Predict

Folder: C:\Users\jmn\Documents\CNMR\_Predict

Nom	Modifié le	Type	Taille
__pycache__	10/01/2021 23:05	Dossier de fichiers	
fake_acd_small.sdf	09/01/2021 20:16	Sdf File	4 Ko

Nom du fichier : fake\_acd\_small\_exported

Type : MDL SDFFiles (\*.SDF)

Enregistrer Annuler Aide

ID: 1 A: 1/2 B: 2 Last Updated: 10/01/2021 22:30 Exclude from Calculations Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

Taper ici pour rechercher

23:33 10/01/2021

*fake\_acd\_small\_exported.sdf*. Calculated chemical shifts were copied into the exported file.

```
40 M END
41 > <ID>
42 1
43
44 > <Formula>
45 C14H12O3
46
47 > <FW>
48 228.2433
49
50 > <CNMR_SHIFTS>
51 0:1|99.99;1:2|99.99;2:3|99.99;3:4|99.99;4:5|99.99;5:6|99.99;6:7|99.99;7:8|99.99;8:9|99.99;9:10|99.99;10:11|99.99;11:12|99.99;12:13|99.99;13:14|99.99
52
53 > <HNMR_SHIFTS>
54
55 > <CNMR_CALC_SHIFTS>
56 0:Exact = 128.39,ExactErr = 0.69,NN = 129.13,Increm = 129.35;1:Exact = 116.07,ExactErr = 0.67,NN = 115.81,Increm = 116.21;2:Exact = 157.85,ExactErr = 0.75,NN = 157.95,Increm =
158.57;3:Exact = 116.07,
57 ExactErr = 0.67,NN = 115.81,Increm = 116.21;4:Exact = 128.39,ExactErr = 0.69,NN = 129.13,Increm = 129.35;5:Exact = 129.35,ExactErr = 1.35,NN = 130.03,Increm = 129.4;6:Exact =
128.41,ExactErr = 0.99,NN
58 = 130.21,Increm = 131.06;7:Exact = 126.35,ExactErr = 1.06,NN = 127.07,Increm = 130.71;8:Exact = 140.6,ExactErr = 1.7,NN = 141.67,Increm = 139.63;9:Exact = 105.17,ExactErr = 0.97,NN
= 106.22,Increm =
59 107.99;10:Exact = 159.14,ExactErr = 0.86,NN = 159.19,Increm = 158.51;11:Exact = 102.29,ExactErr = 0.62,NN = 103.14,Increm = 103.52;12:Exact = 159.14,ExactErr = 0.86,NN =
159.19,Increm = 158.51;13:Exact
60 = 105.17,ExactErr = 0.97,NN = 106.22,Increm = 107.99
61
62 > <HNMR_CALC_SHIFTS>
63
64 > <NMR_CONSTANTS>
65
66 > <CHEMICAL_SHIFTS.13C>
67 1,99.99
68 2,99.99
69 3,99.99
```

Temporary chemical shifts

Exported calculated chemical shifts

Temporary chemical shifts

Copy the calculated chemical shifts in the new file *calc\_acd\_small.sdf*, as if they were experimental ones:

*python CNMR\_predict fake\_acd\_small\_exported.sdf calc\_acd\_small.sdf*

Anaconda Prompt

```
(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>python CNMR_predict.py fake_acd_small_exported.sdf calc_acd_small.sdf  
(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>
```

Calc\_acd\_small.sdf

```
33      9 14  1  0  0  0  0  
34     10 11  1  0  0  0  0  
35     11 12  2  0  0  0  0  
36     11 16  1  0  0  0  0  
37     12 13  1  0  0  0  0  
38     13 14  2  0  0  0  0  
39     13 15  1  0  0  0  0  
40 M  END  
41 > <ID>  
42 1  
43  
44 > <Formula>  
45 C14H12O3  
46  
47 > <FW>  
48 228.2433  
49  
50 > <CNMR_SHIFTS>  
51 0:1|128.39;1:2|116.07;2:3|157.85;3:4|116.07;4:5|128.39;5:6|129.35;6:7|128.41;7:8|126.35;8:9|140.60;9:10|105.17;10:11|159.14;11:12|102.29;12:13|159.14;13:14|105.17  
52
```

Temporary chemical shifts have been replaced by calculated ones

## Close current database: Database→Close

The screenshot shows the ACD/ChemSketch Database Window. The 'Database' menu is open, and the 'Close' option is highlighted with a red circle. The window title is 'ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\FAKE\_ACD\_SMALL.NMRUDB]'. The menu options include New..., Open..., Close (Ctrl-F4), Export..., Import..., Create Report Page, Print..., Tools, Update Mode (checked), Browse Mode, Send Record..., File Associations..., Exit, and Recent Files. The Recent Files list includes several database files. The main window displays a table with columns: Atom No., 13C Shift, 13C Calc, and 1H Shift. The table contains 14 rows of data. A chemical structure of resveratrol is shown on the left. The status bar at the bottom indicates 'Mol-Name: resveratrol' and '<Double-click to enter new data item>'. The bottom of the window shows a tabbed interface with '1-ChemSketch', '2-CNMR Spectrum', '3-HNMR Spectrum', '4-History', and '5-Database' (selected).

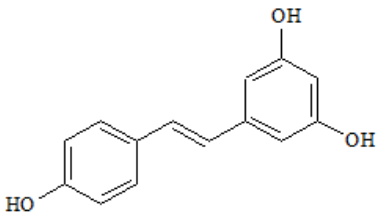
Atom No.	13C Shift	13C Calc	1H Shift
1	99.99	128.39	
2	99.99	116.07	
3	99.99	157.85	
4	99.99	116.07	
5	99.99	128.39	
6	99.99	129.35	
7	99.99	128.41	
8	99.99	126.35	
9	99.99	140.60	
10	99.99	105.17	
11	99.99	159.14	
12	99.99	102.29	
13	99.99	159.14	
14	99.99	105.17	

Mol-Name: resveratrol  
<Double-click to enter new data item>

Create new database *calc\_acd\_small.NMRUDb* and import *calc\_acd\_small.sdf* (see pages 5 to 13)

ACD/C+H NMR Predictors and DB: Database Window - [C:\USERS\JMN\DOCUMENTS\CNMR\_PREDICT\CALC\_ACD\_SMALL.NMRUDb]

Database View Record Search Lists Table Training Options ACD/Labs Help



Atom No.	13C Shift	1H Shift
1	128.39	
2	116.07	
3	157.85	
4	116.07	
5	128.39	
6	129.35	
7	128.41	
8	126.35	
9	140.6	
10	105.17	
11	159.14	
12	102.29	
13	159.14	
14	105.17	

**Calculated chemical shifts**

Formula:  $C_{14}H_{12}O_3$   
FW: 228.2433  
Predicted 13C shifts: 1[1] 128.39 ; 2[2] 116.07 ; 3[3] 157.85 ; 4[4] 116.07 ; 5[5] 128.39 ; 6[6] 129.35 ; 7[7] 128.41 ; 8[8] 126.35 ; 9[9] 140.60 ; 10[10] 105.17 ; 11[11] 159.14 ; 12[12] 102.2  
NMREDATA\_ASSIGNMENT: 1, 128.39, 1 \; 2, 116.07, 2 \; 3, 157.85, 3 \; 4, 116.07, 4 \; 5, 128.39, 5 \; 6, 129.35, 6 \; 7, 128.41, 7 \; 8, 126.35, 8 \; 9, 140.60, 9 \; 10, 105.17, 10 \; 11, 159.1  
NMREDATA\_ORIGIN: Source=Calculation \; Method=Database->Tools->Check Chemical Shifts \; Software=ACD/Labs C+H NMR Predictors and DB \; Version=2020.1.0 \

Quaternaries: 3157.85; 6129.35; 9140.60; 11159.14; 13159.14  
Tertiaries: 1128.39; 2116.07; 4116.07; 5128.39; 7128.41; 8126.35; 10105.17; 12102.29; 14105.17  
Mol-Name: resveratrol

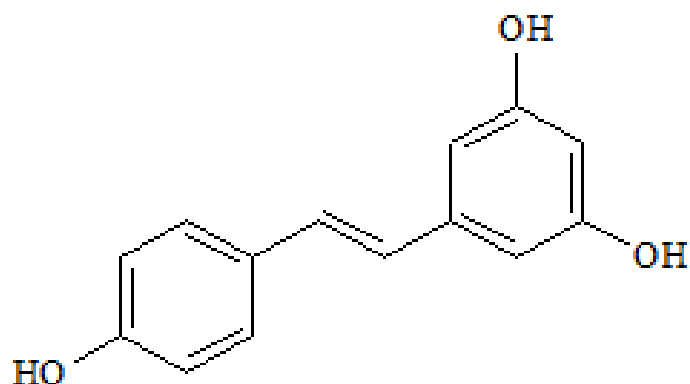
ID: 1 | A: 1/2 | B: 2 | Last Updated: 10/01/2021 23:21 | Exclude from Calculations | Single DB

1-ChemSketch 2-CNMR Spectrum 3-HNMR Spectrum 4-History 5-Database

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23:21  
10/01/2021

Calculate Chemical Shifts in the new database *calc\_acd\_small.NMRUDb* (see page 14)



Atom No.	13C Shift	13C Calc	1H
1	128.39	128.39	
2	116.07	116.07	
3	157.85	157.85	
4	116.07	116.07	
5	128.39	128.39	
6	129.35	129.35	
7	128.41	128.41	
8	126.35	126.35	
9	140.6	140.60	
10	105.17	105.17	
11	159.14	159.14	
12	102.29	102.29	
13	159.14	159.14	
14	105.17	105.17	

The experimental and calculated shifts are the identical

The whole process was carried out on all (2) molecules of the initial file *small.smi*