CNMR_Predict

https://github.com/nuzillard/KnapsackSearch/tree/master/CNMR_Predict

Start with file “small.txt” from directory CNMR_predict

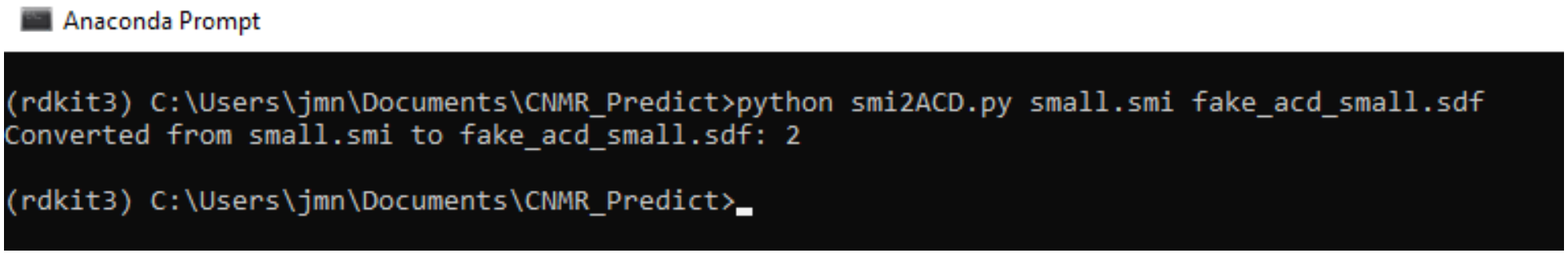
```
1  C1=CC(=CC=C1/C=C/C2=CC(=CC(=C2)O)O)O resveratrol
2  C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O quercetin
```

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*



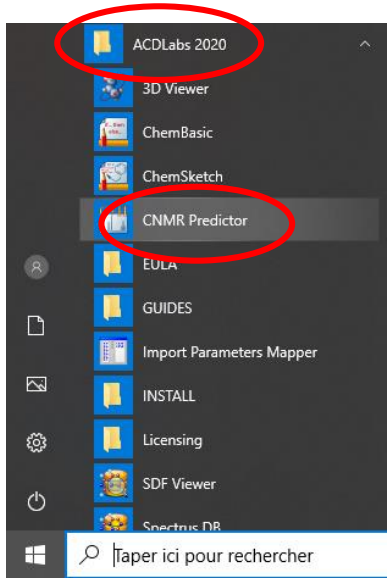
File *fake_acd_small.sdf* was created.
It contains a MOL block with 2D coordinates and '99.99' as ^{13}C NMR chemical shift values.

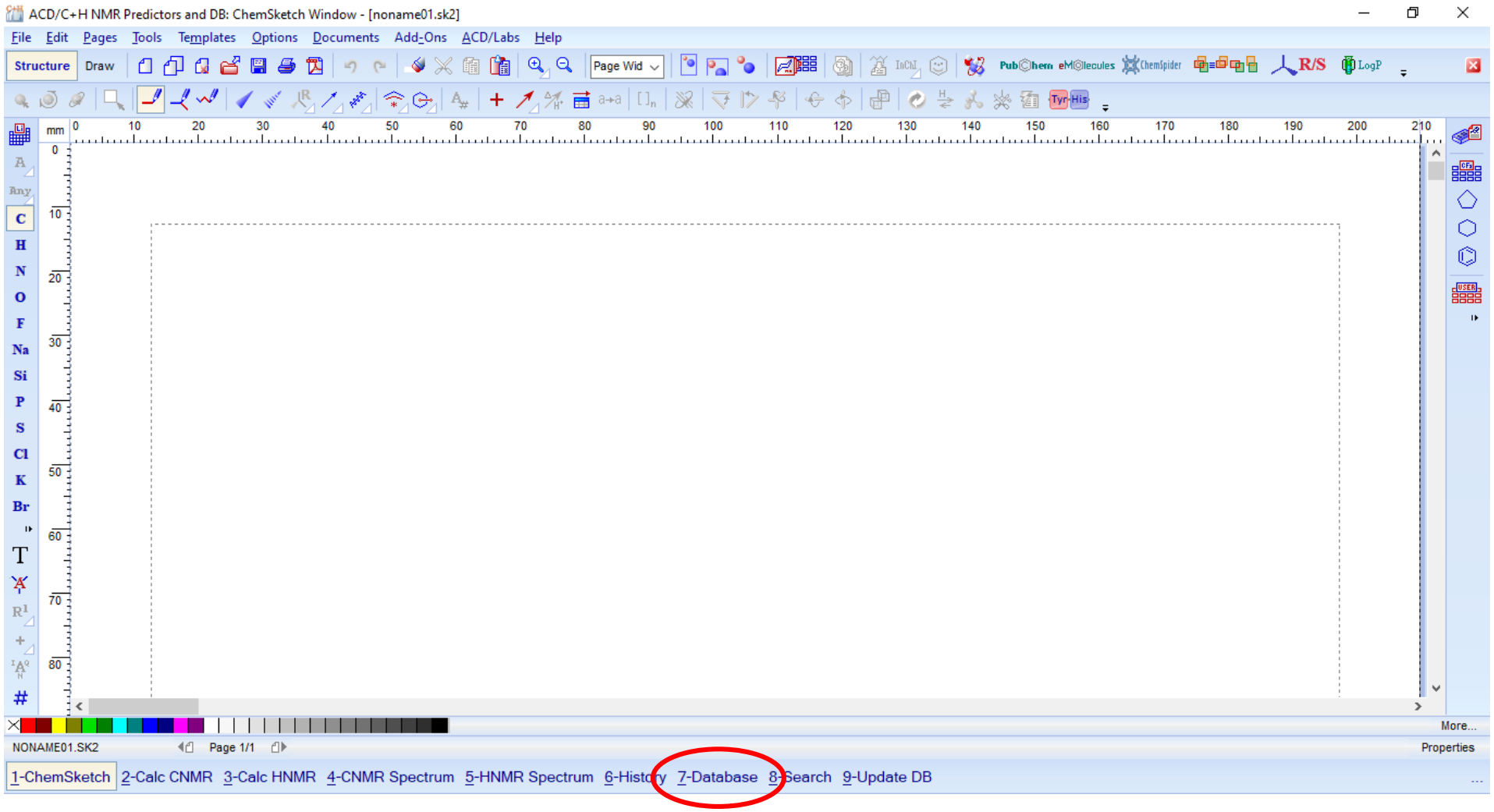
```
    1.9912   -0.5478    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.9876    0.4522    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1198    0.9490    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    0.2556    0.4460    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    1.1162    1.9490    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
    2.8590   -1.0448    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
   -4.9298   -2.5726    0.0000 O   0  0  0  0  0  0  0  0  0  0  0  0
  1  2  2  0
  2  3  1  0
  3  4  2  0
  4  5  1  0
  5  6  2  0
  6  7  1  0
  7  8  2  0
  8  9  1  0
  9 10  2  0
 10 11  1  0
 11 12  2  0
 12 13  1  0
 13 14  2  0
 13 15  1  0
 11 16  1  0
  3 17  1  0
  6  1  1  0
 14  9  1  0
M  END
>  <CNMR_SHIFTS>  (1)
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

$$$$
quercetin
     RDKit          2D

 22 24  0  0  0  0  0  0  0  0999 V2000
    1.3160   -3.0544    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    2.1816   -3.5550    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
    3.0480   -3.0558    0.0000 C   0  0  0  0  0  0  0  0  0  0  0  0
```

2D coordinates

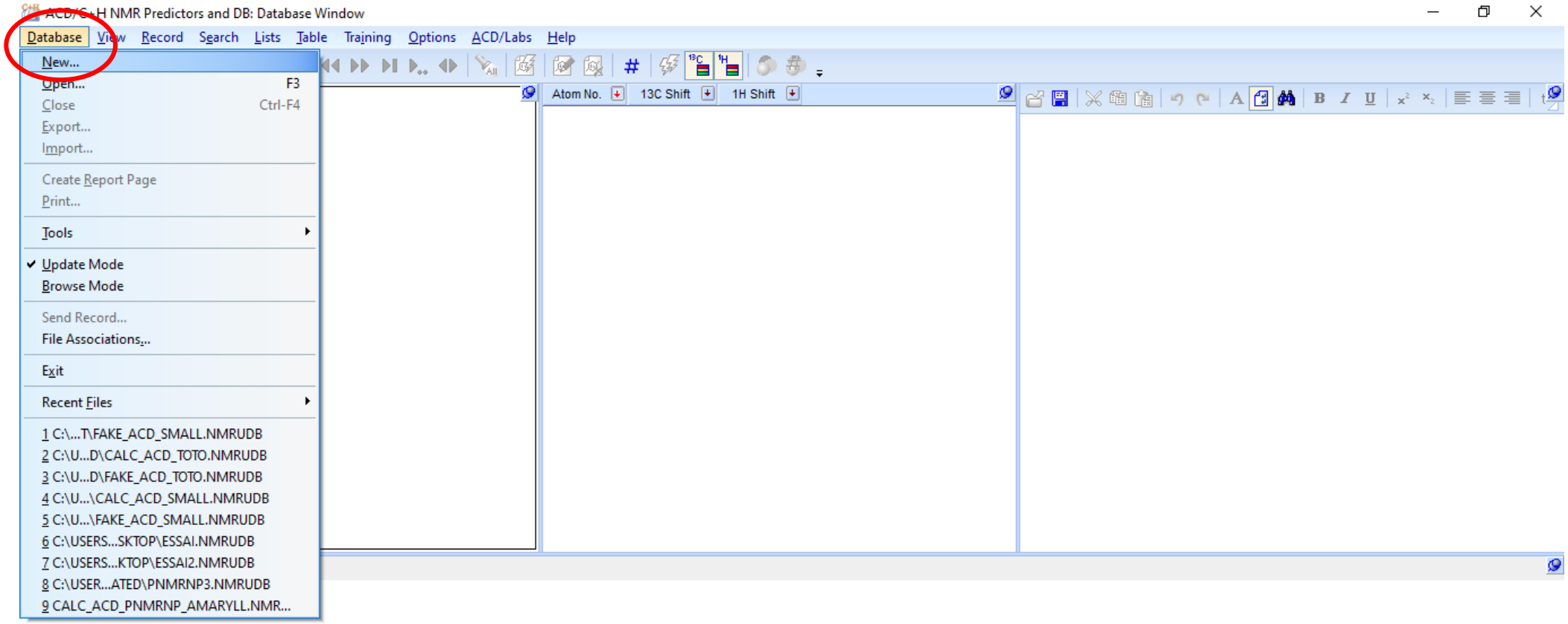
Temporary ^{13}C NMR data

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

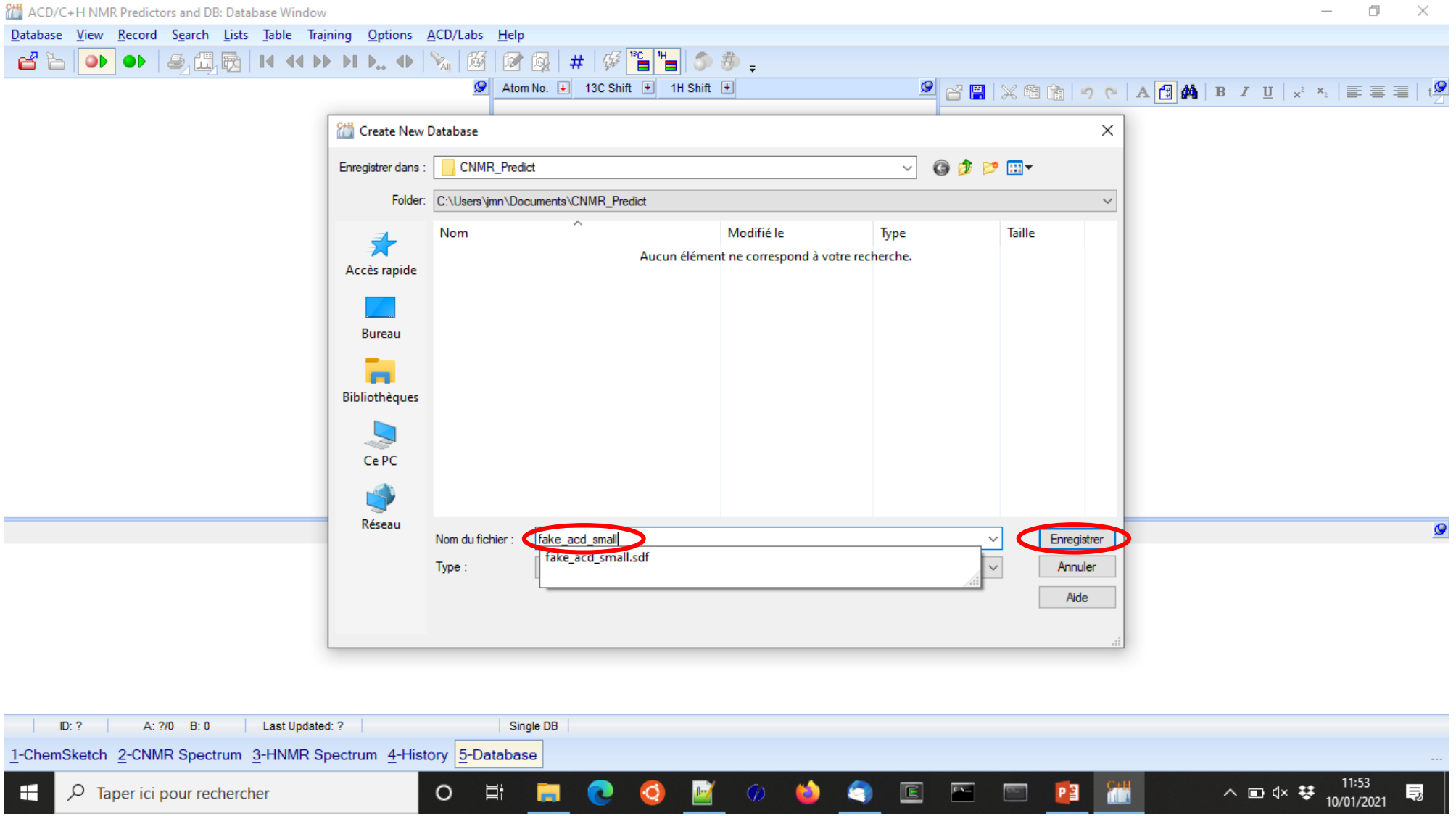




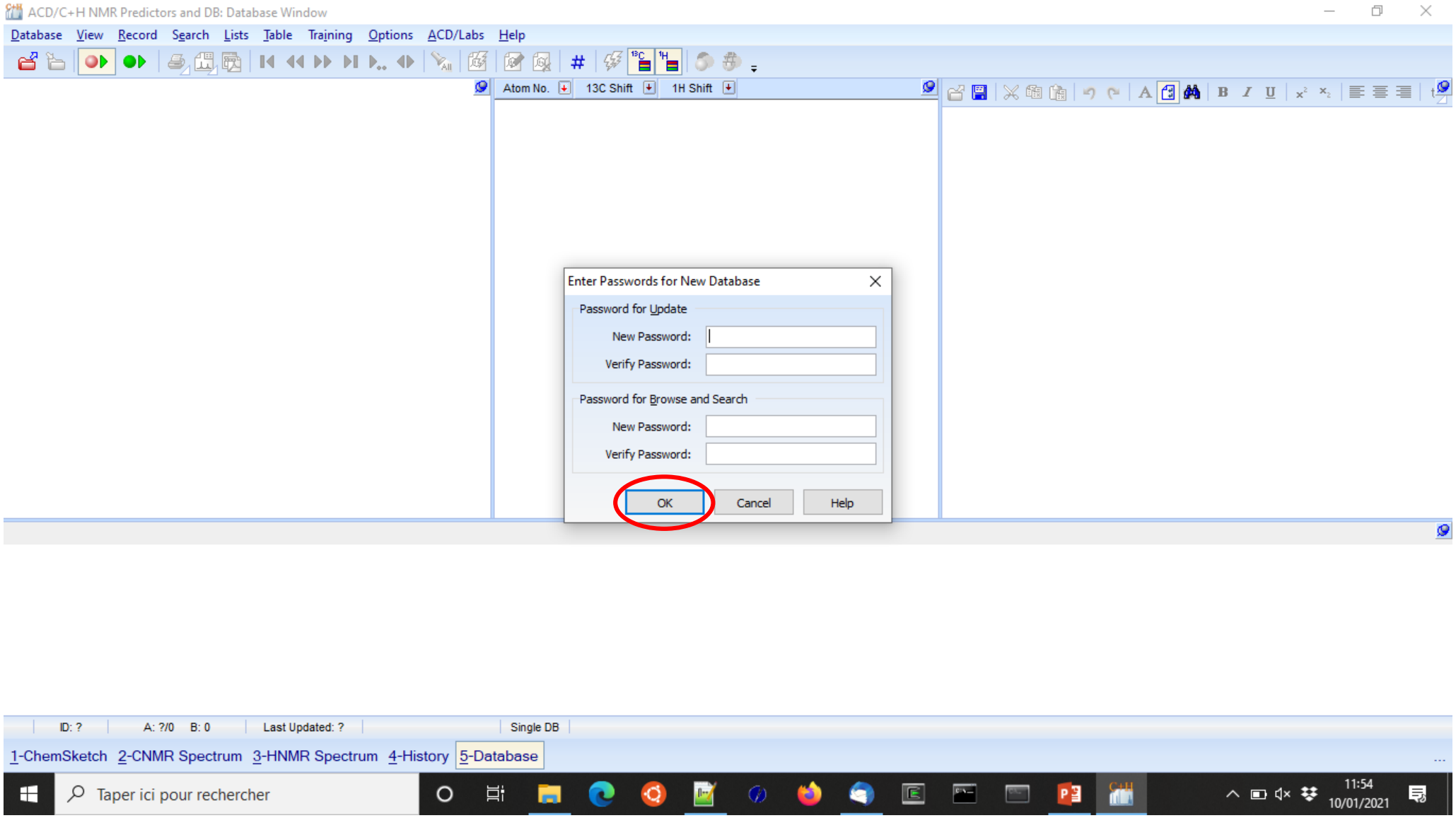
Create a new ACD/Labs Database: Database→New…



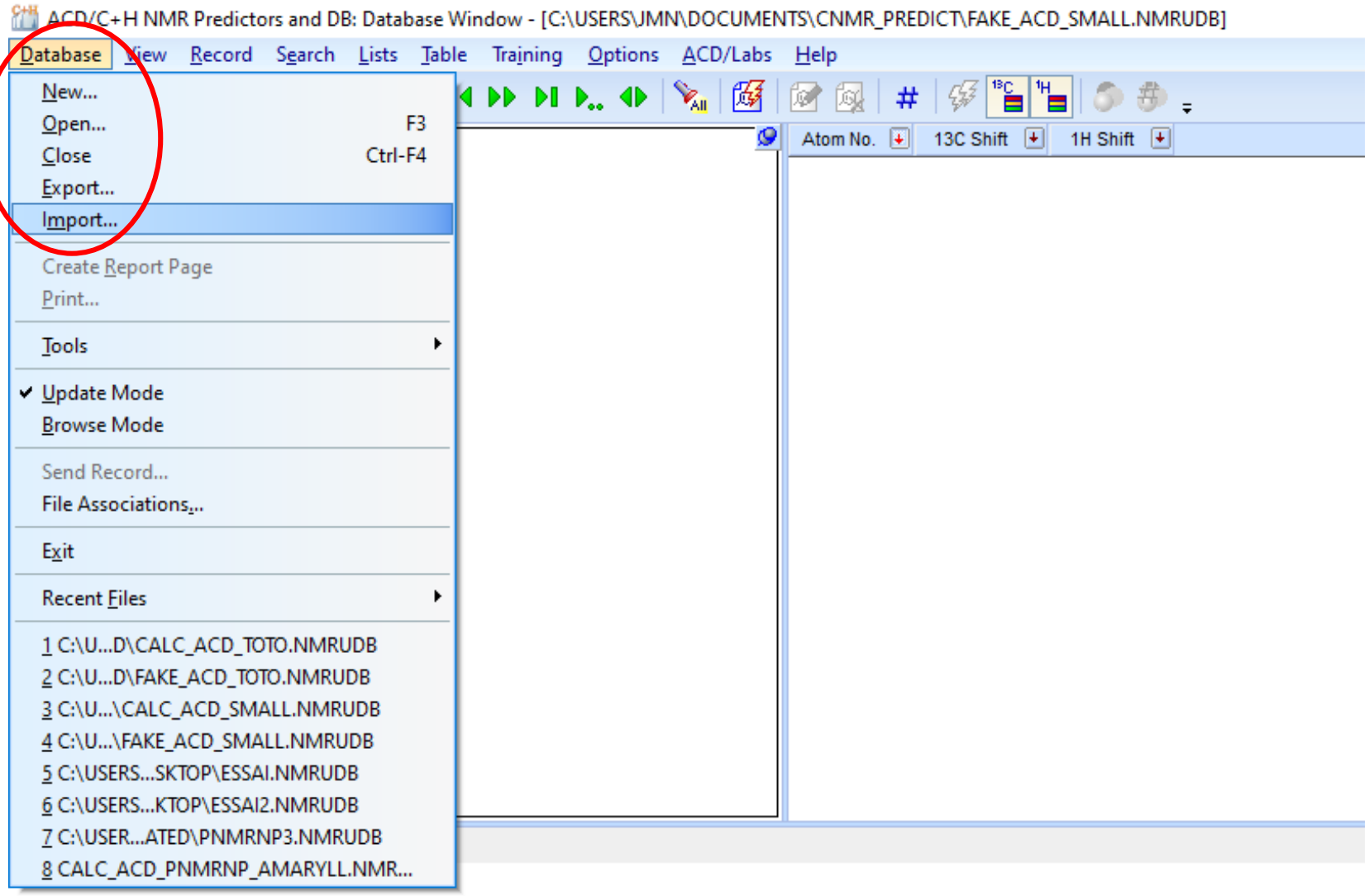
Name this ACD/Labs Database *fake_acd_small.NMRUDB*



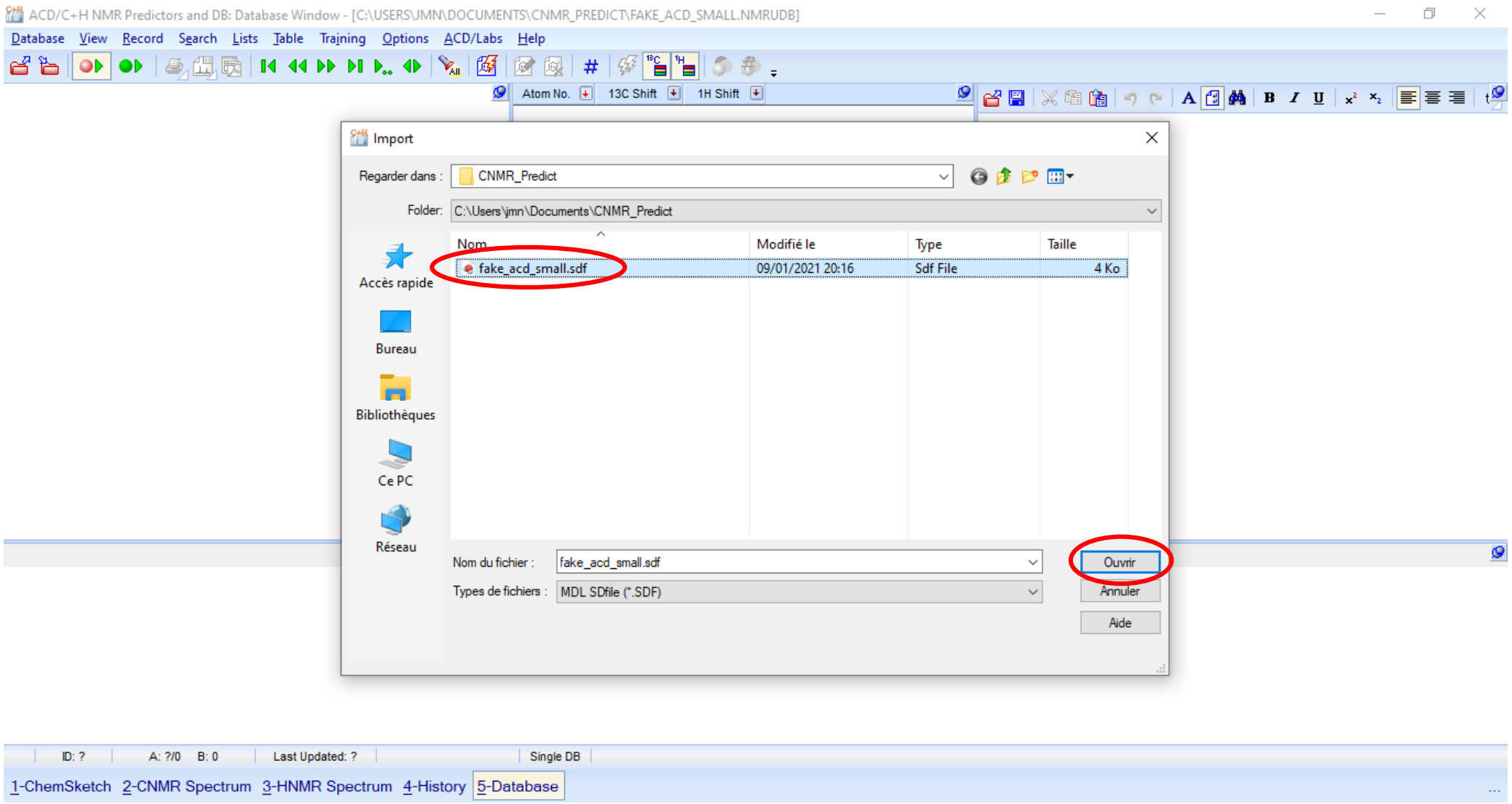
Leave password fields blank



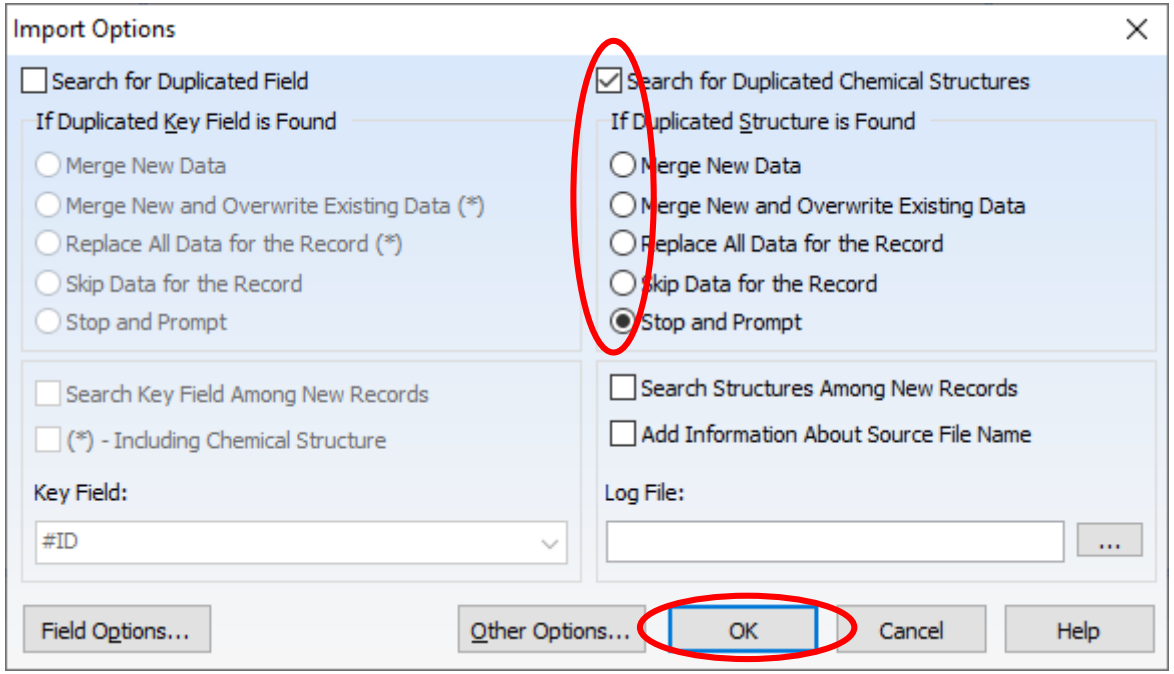
Import *fake_acd_small.sdf*: Database→Import…



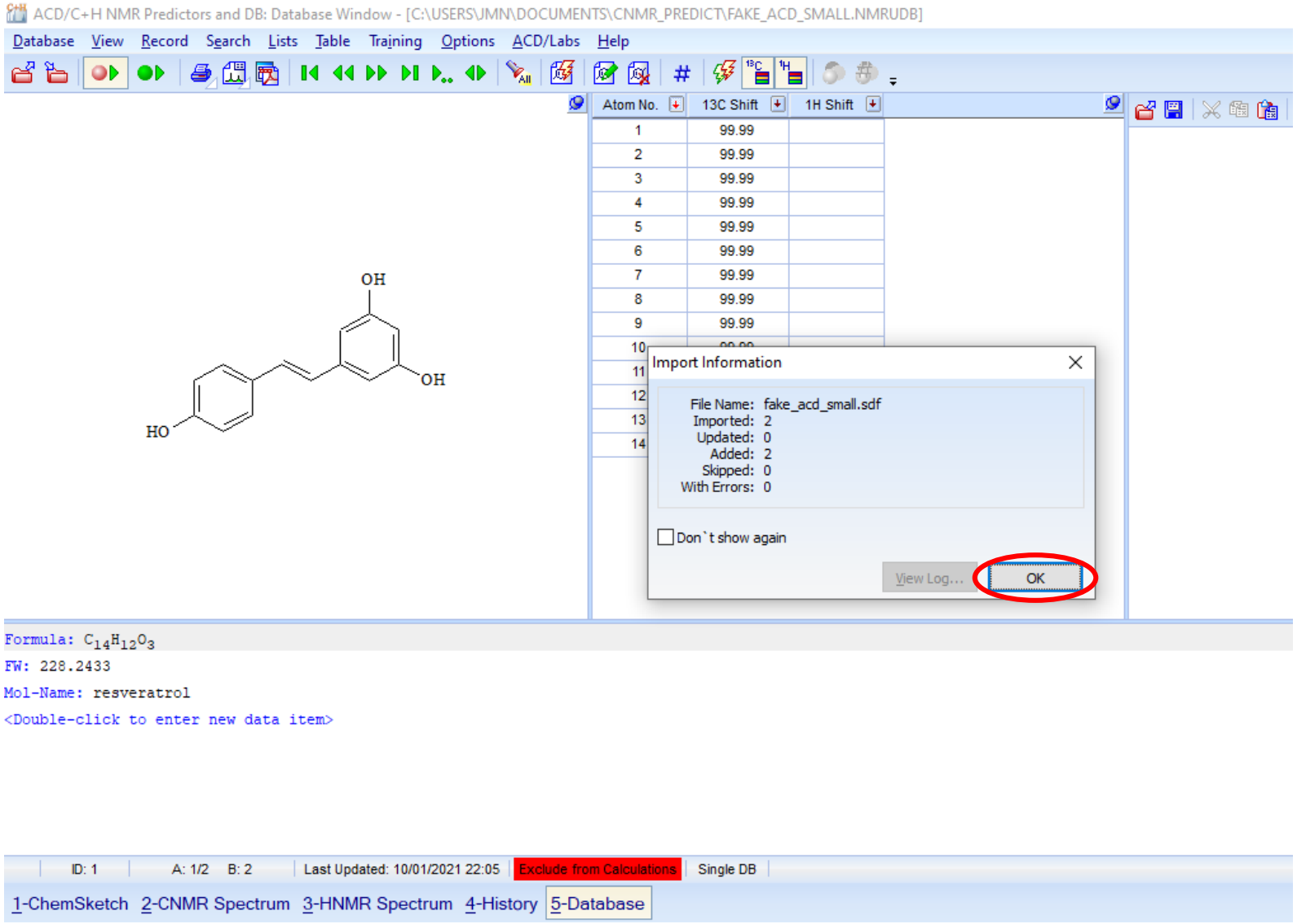
Import *fake_acd_small.sdf*



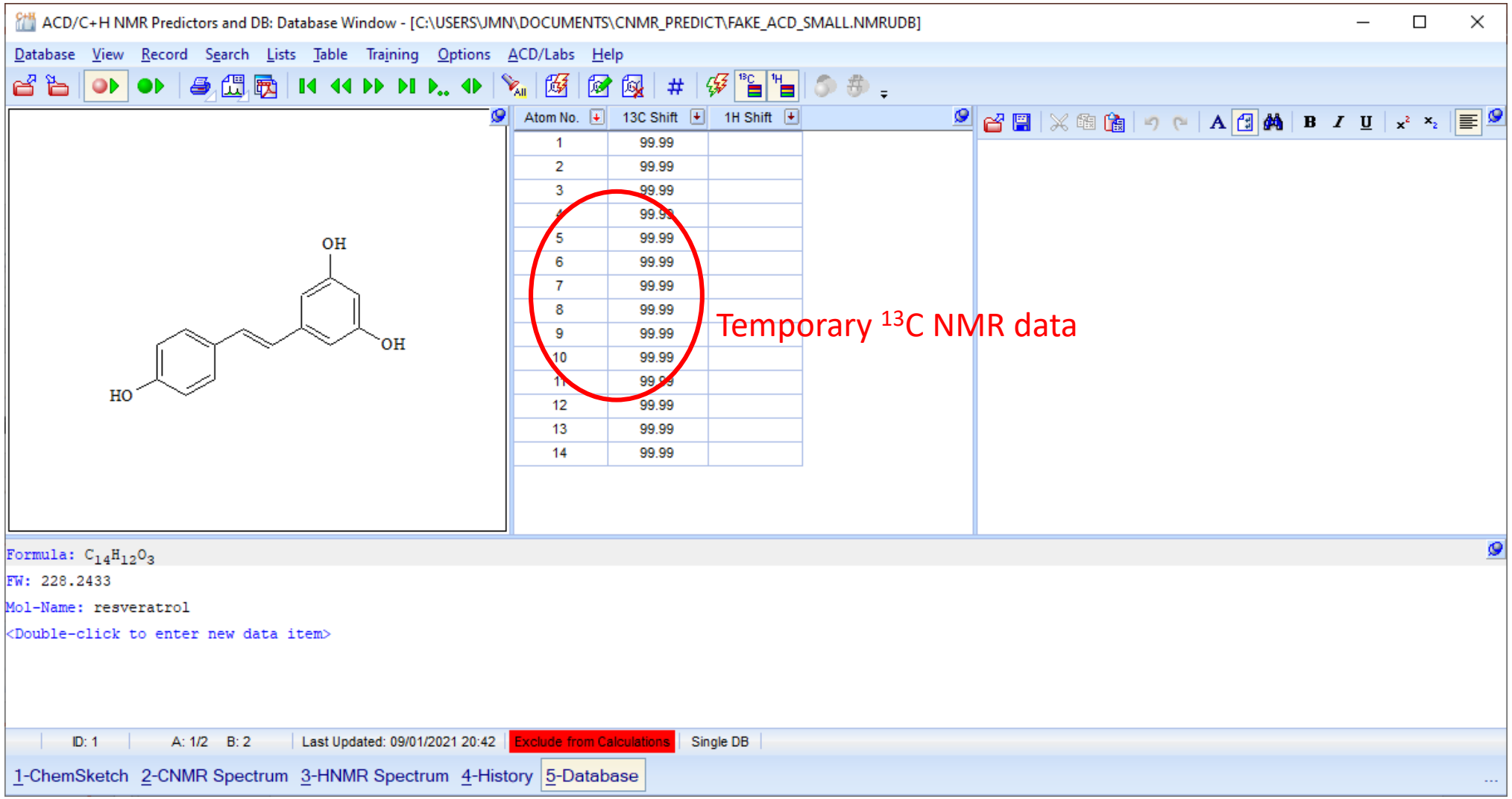
Select options for importation



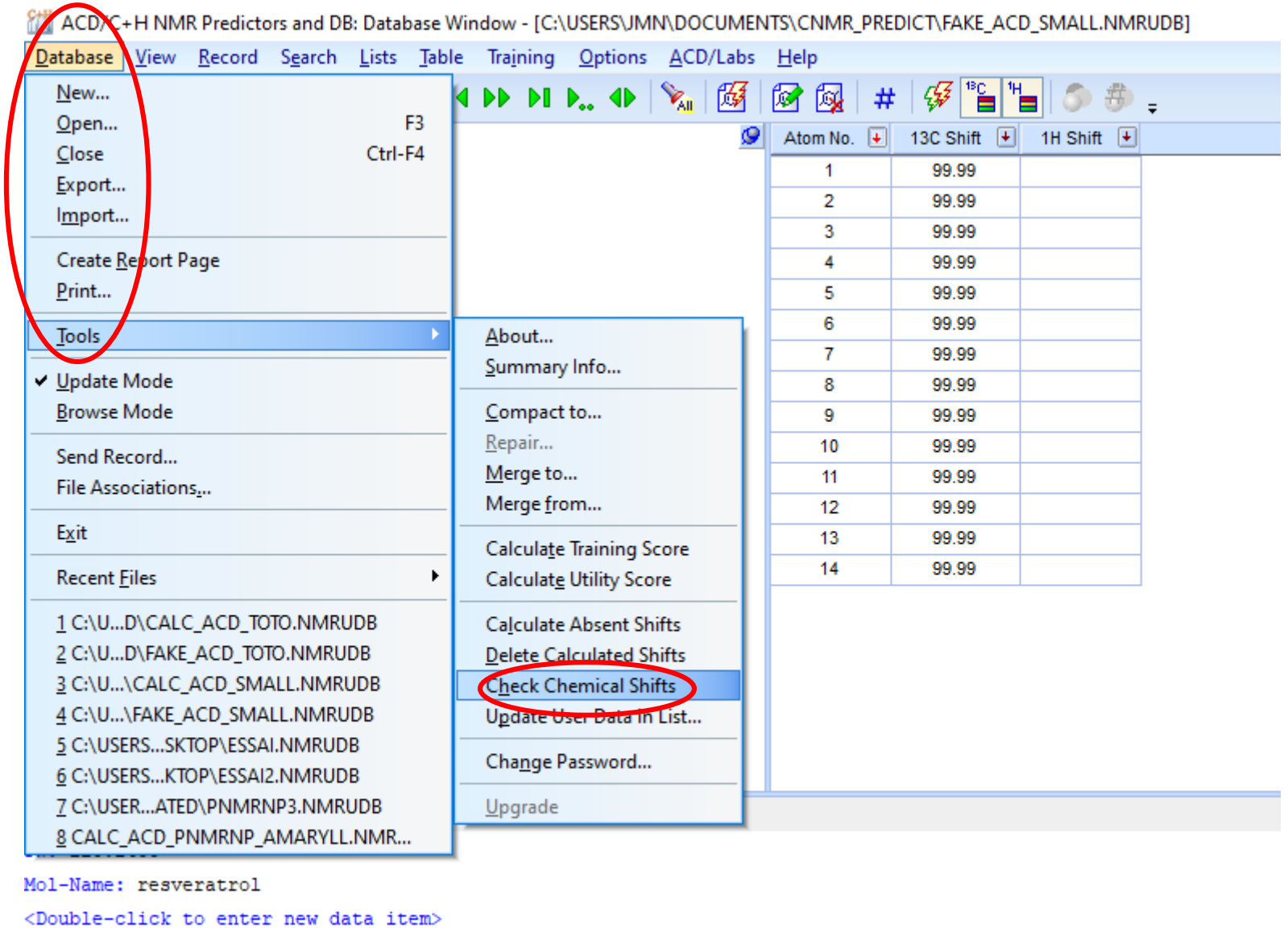
Importation finished



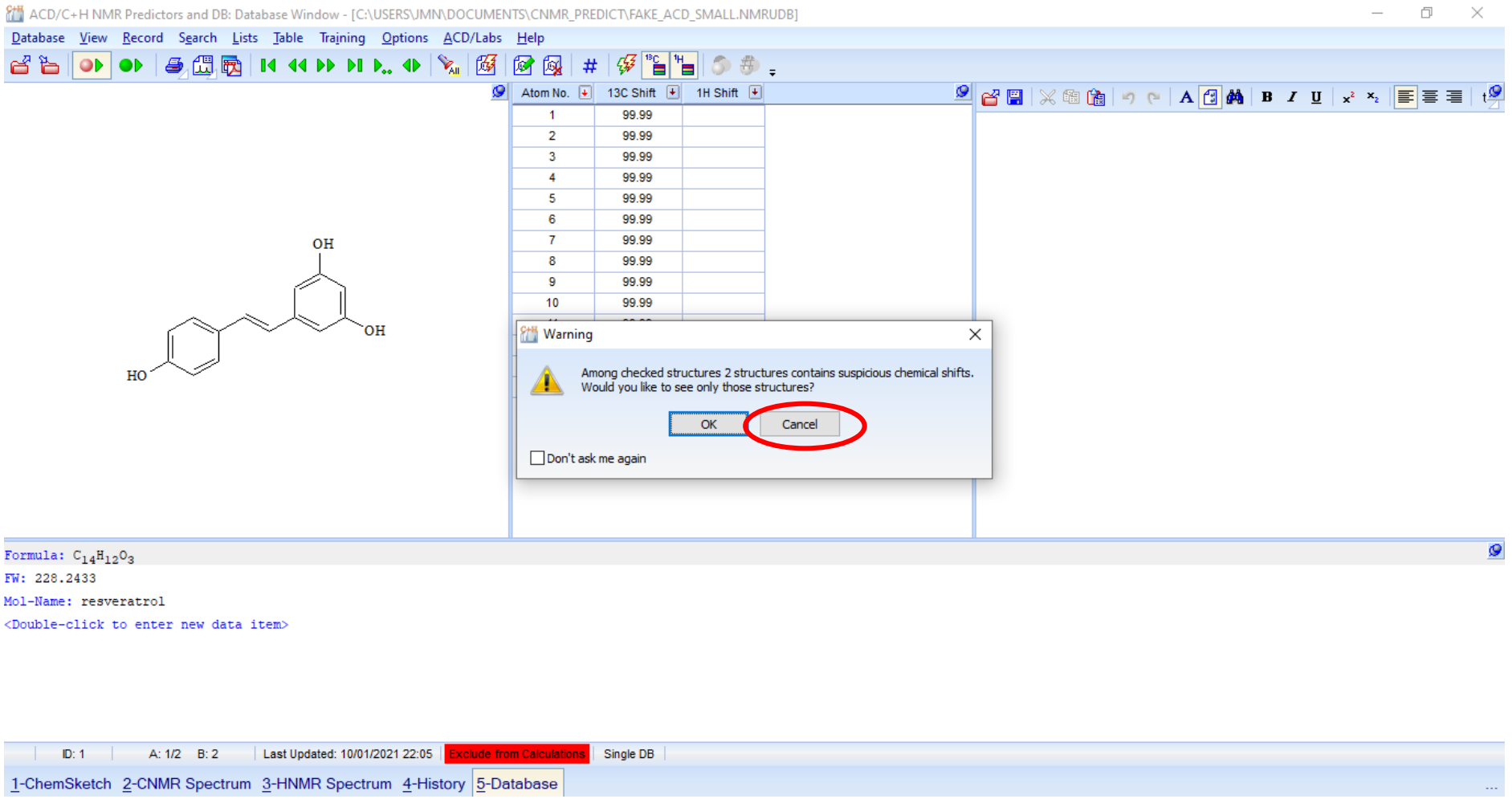
Fake_acd_small.NMRUDB and *fake_acd_small.sdf* inside



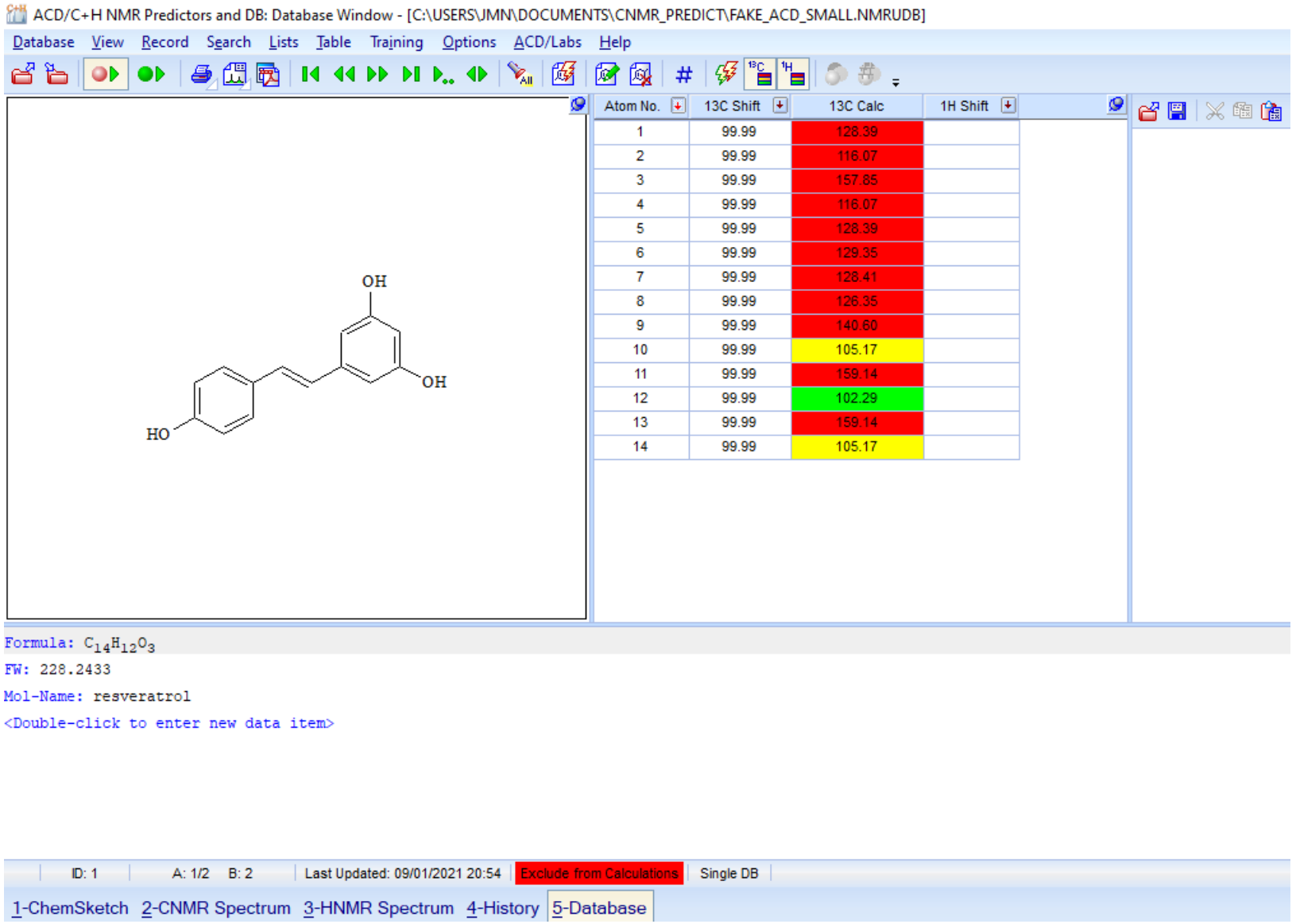
Calculate Chemical Shifts: Database→Tools →Check Chemical Shifts



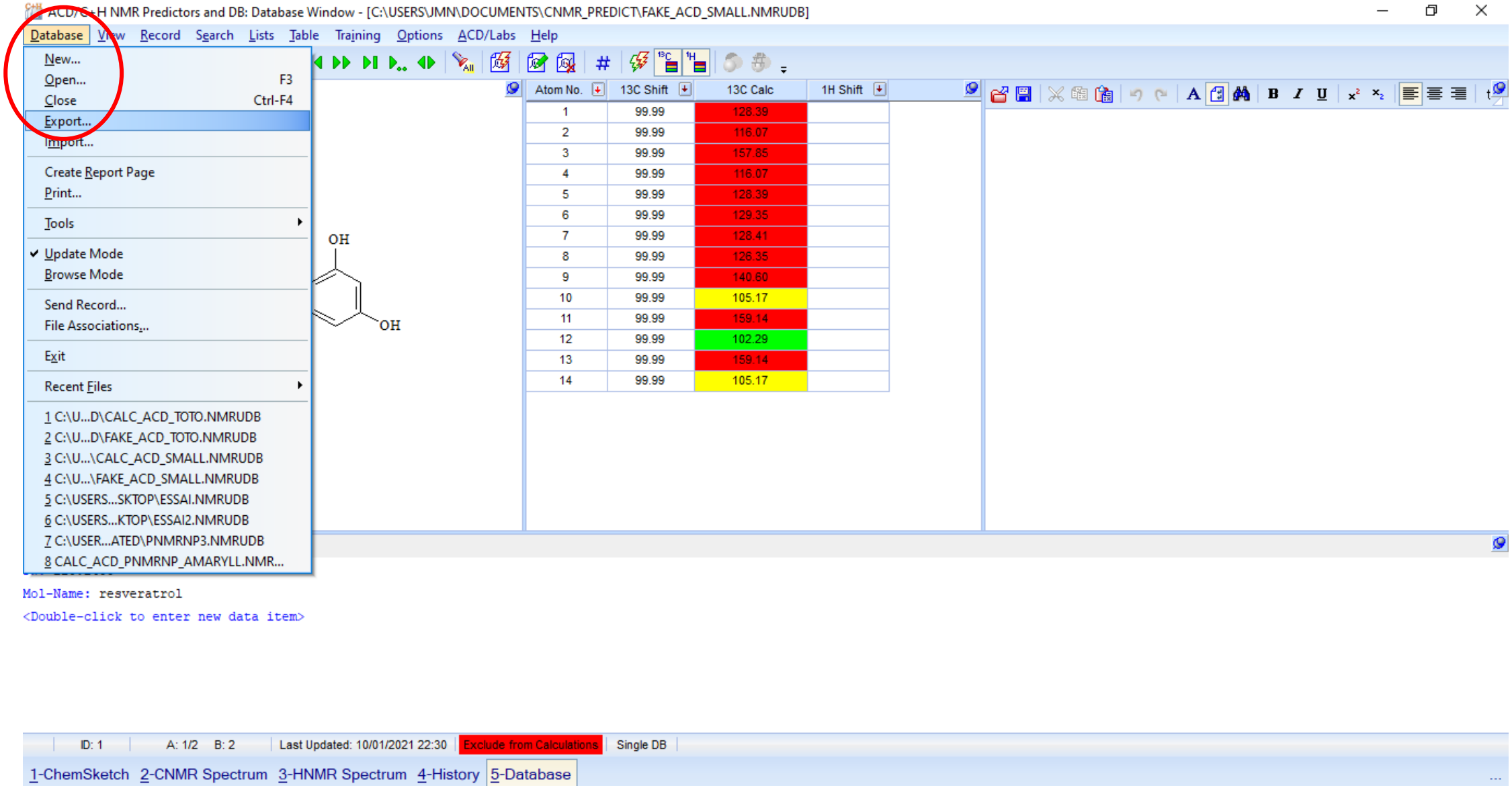
Ignore the warning message



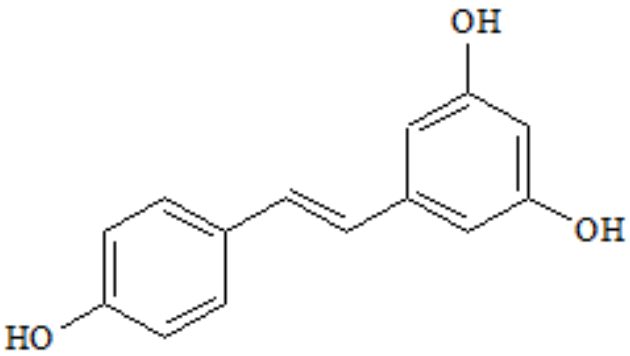
Disastrous checking, but this is not a problem…



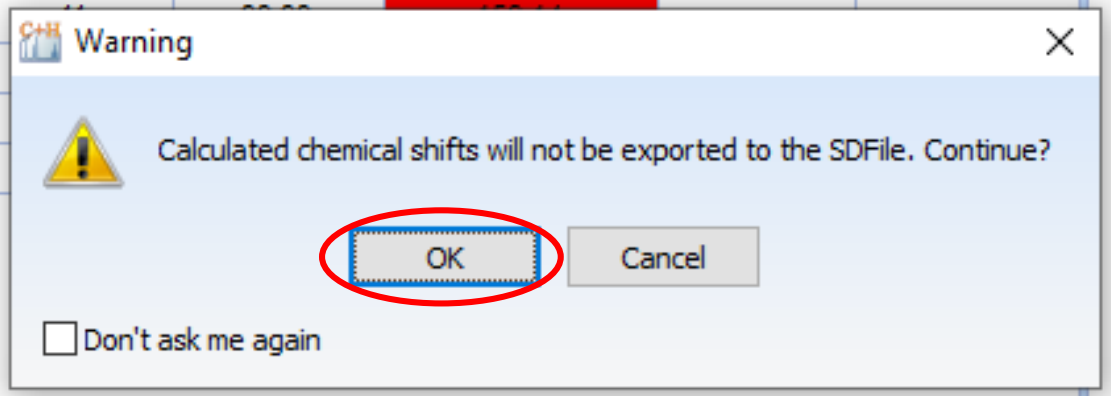
Export database: Database→Export



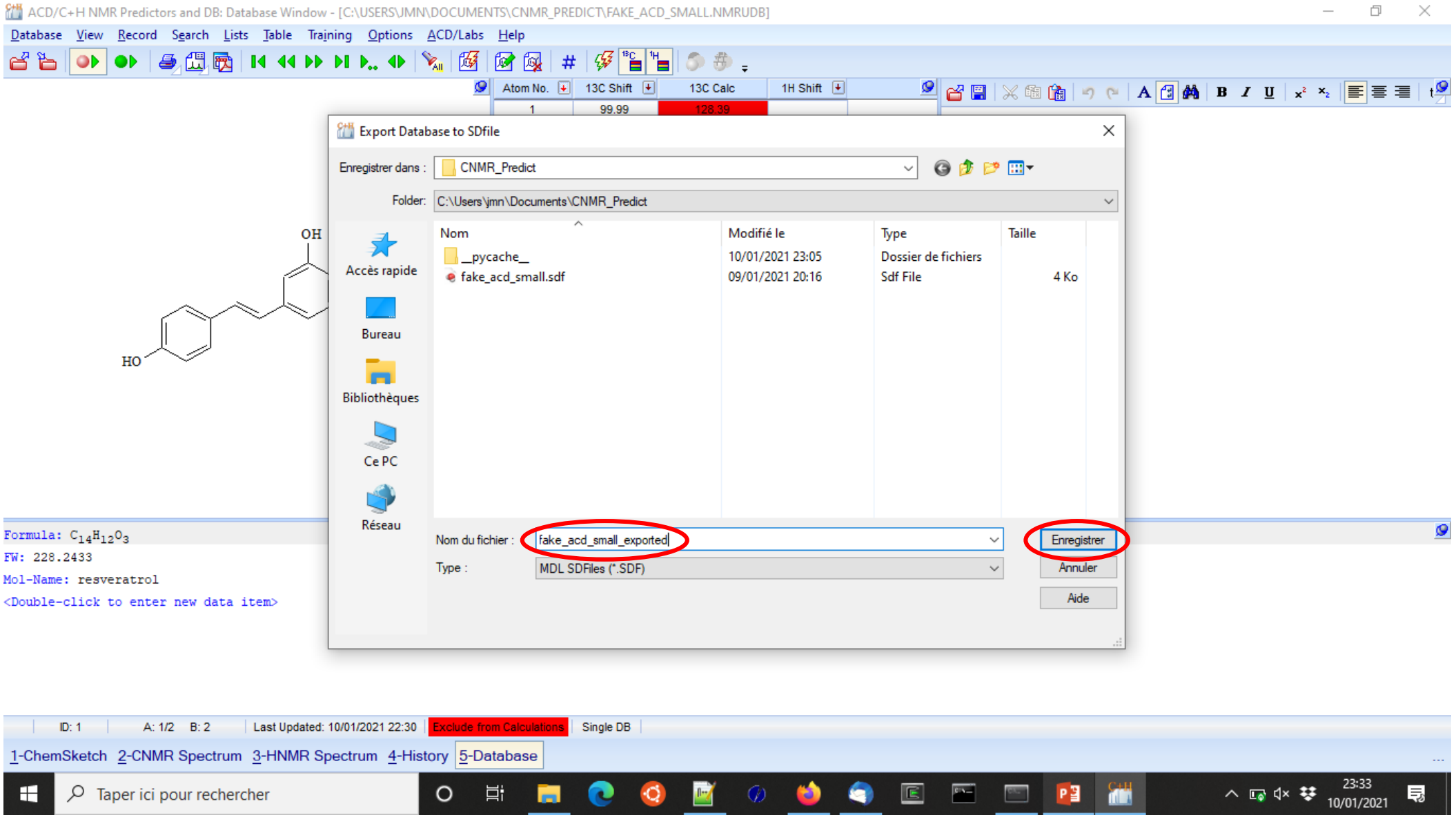
Calculated chemical shifts **will be** exported, anyway…



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



Export database as *fake_acd_small_exported.sdf*



fake_acd_small_exported.sdf. Calculated chemical shifts were copied into the exported file.

```
M  END
>  <ID>
1

>  <Formula>
C14H12O3

>  <FW>
228.2433

>  <CNMR_SHIFTS>
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

>  <HNMR_SHIFTS>

>  <CNMR_CALC_SHIFTS>
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,
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
 = 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 =
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:Exac
t = 105.17,ExactErr = 0.97,NN = 106.22,Increm = 107.99

>  <HNMR_CALC_SHIFTS>

>  <NMR_CONSTANTS>

>  <CHEMICAL_SHIFTS.13C>
1,99.99
2,99.99
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

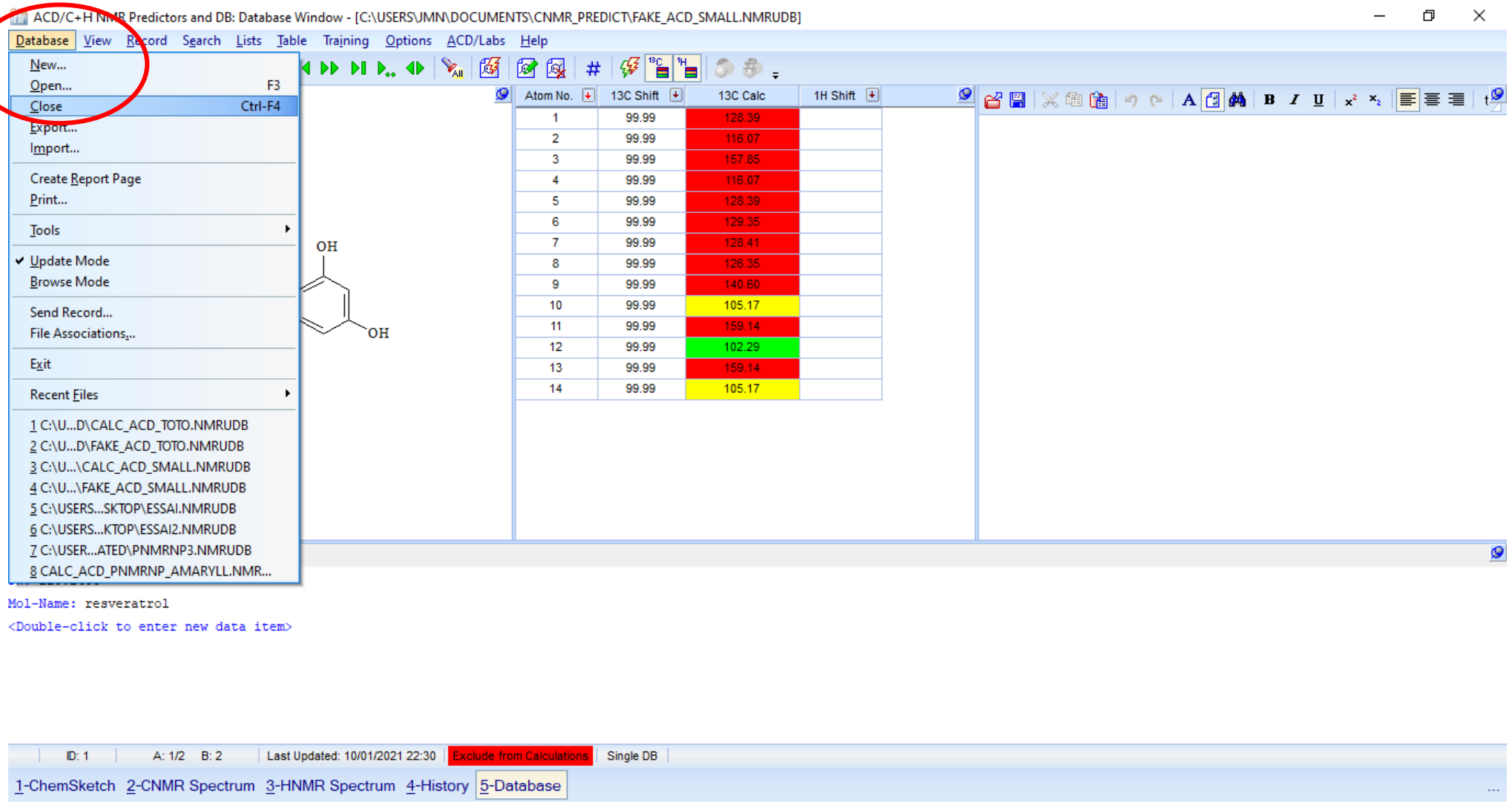
```
(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>python CNMR_predict.py fake_acd_small_exported.sdf calc_acd_small.sdf

(rdkit3) C:\Users\jmn\Documents\CNMR_Predict>
```

Calc_acd_small.sdf

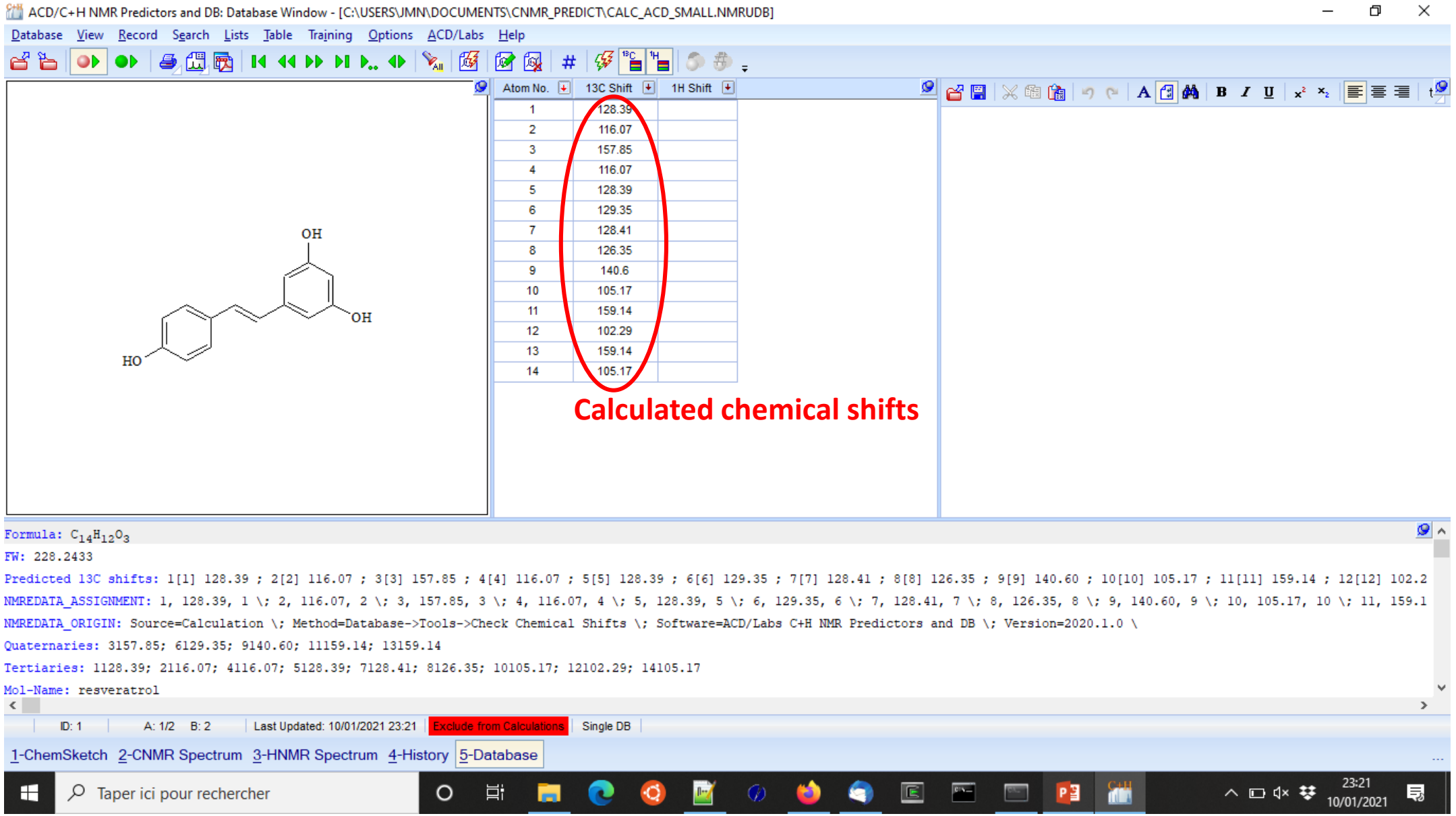
```
 9 14  1  0  0  0  0
10 11  1  0  0  0  0
11 12  2  0  0  0  0
11 16  1  0  0  0  0
12 13  1  0  0  0  0
13 14  2  0  0  0  0
13 15  1  0  0  0  0
M  END
>  <ID>
1

>  <Formula>
C14H12O3

>  <FW>
228.2433

>  <CNMR_SHIFTS>
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

```

Temporary chemical shifts have been replaced by calculated ones

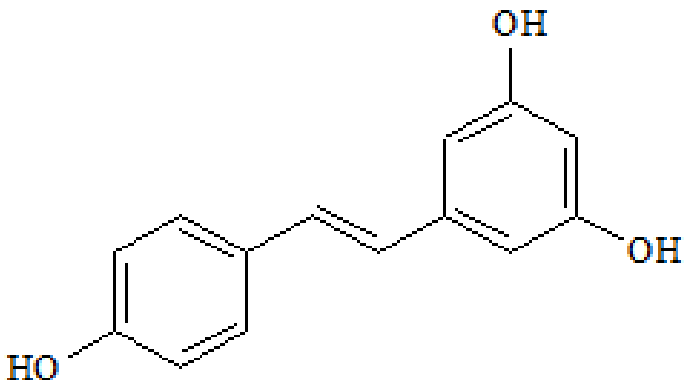
Close current database: Database→Close



Create new database *calc_acd_small.NMRUDB* and import *calc_acd_small.sdf* (see pages 5 to 13)



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*