

Batchwise Selection of Chromatographic Methods Based on Resolution from Impurities

Version 8.0

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1. Advanced Chemistry Development, Inc.
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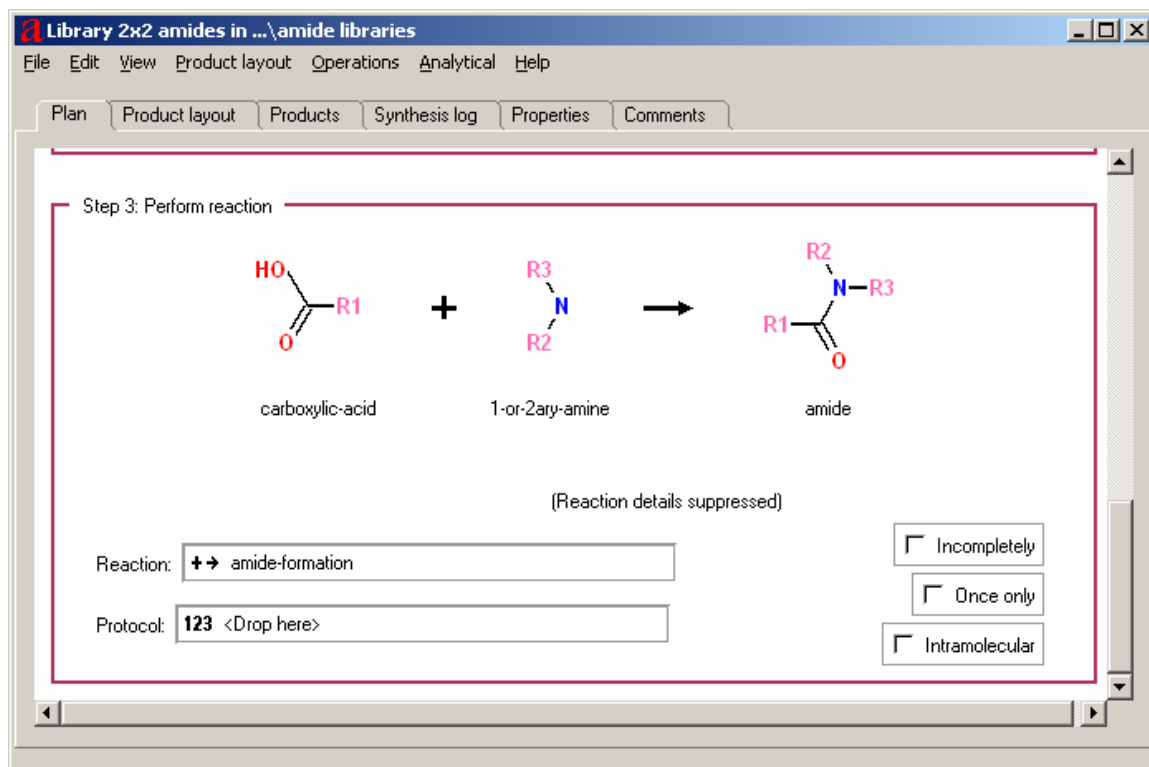
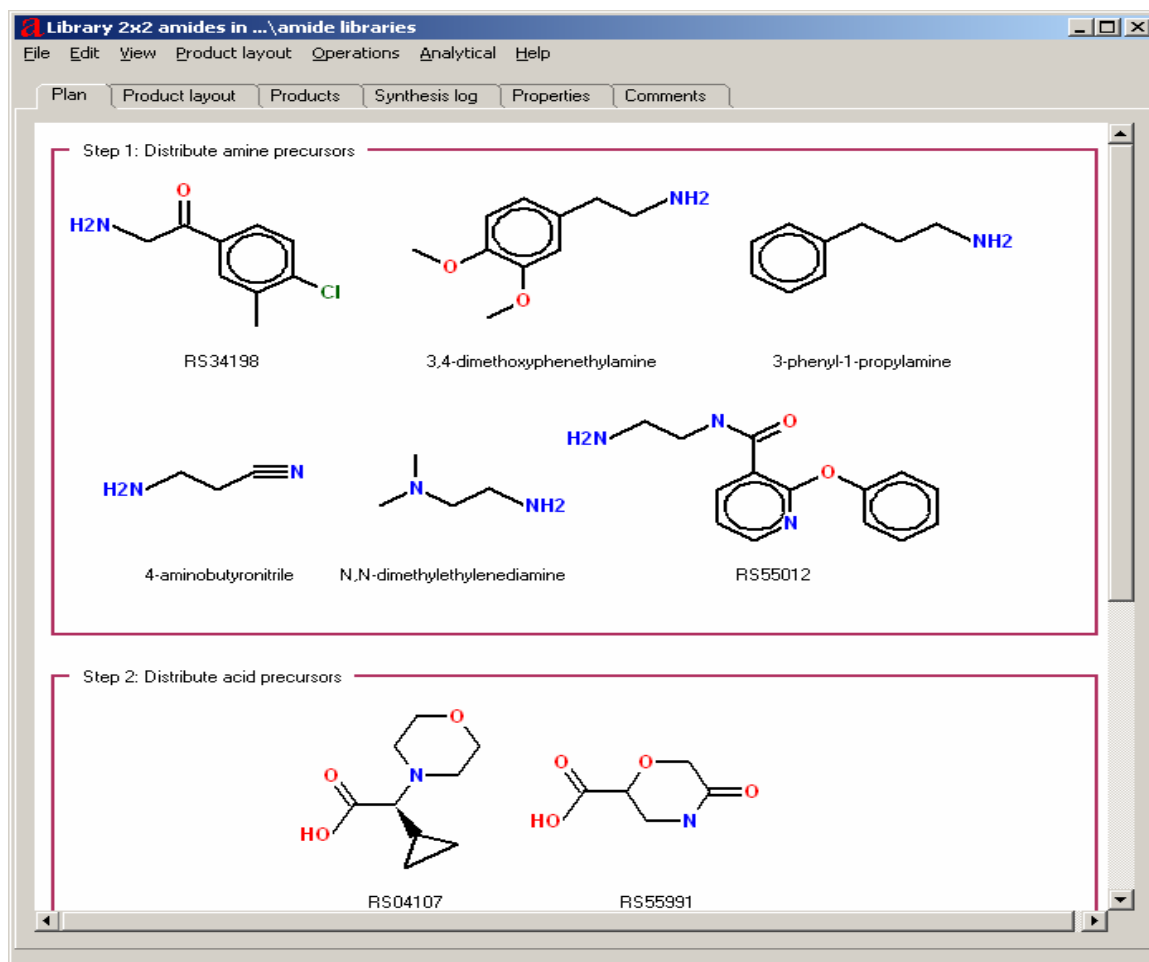
2. Elsevier MDL
San Leandro, Switzerland
www.MDL.com

With the help of this Technical Note we will demonstrate how to create an SDfile that will list specific information about products created using an MDL® Afferent™ library. Then, we will calculate retention times and show the suggested method within [ACD/ChromGenius Batch](#) [1] for all the structures from an SDfile.

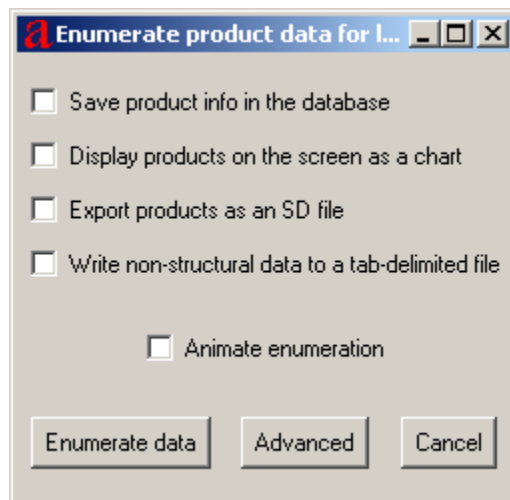
Preparing an SDfile

Note You must use the latest version of MDL Afferent, 3.0 SP2, in order to successfully complete this procedure.

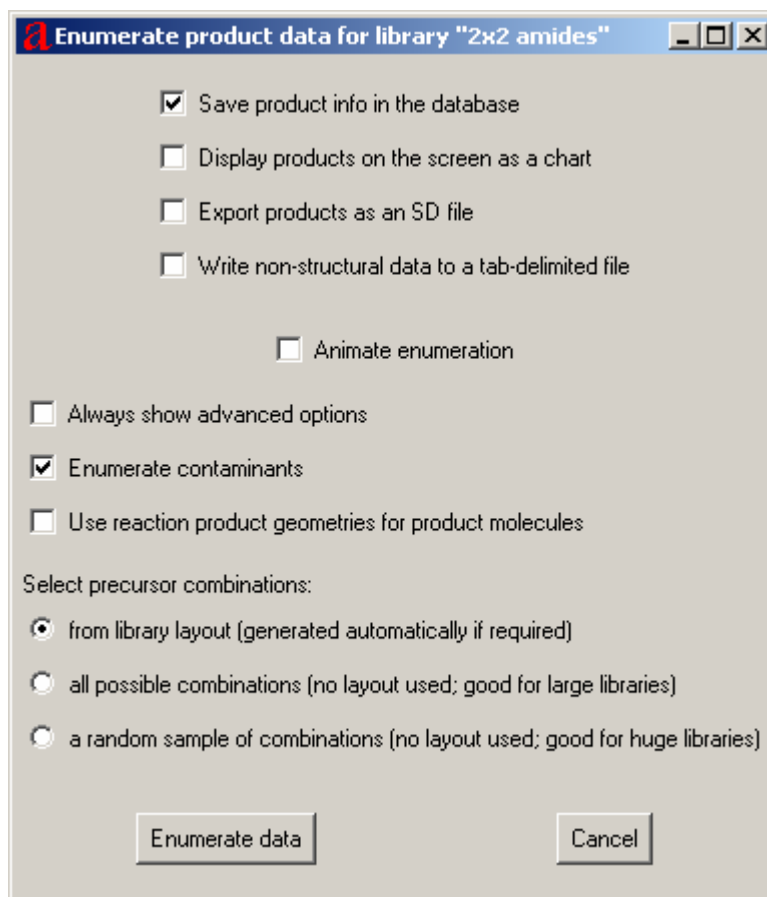
1. Open your **MDL Afferent Database** and create a **Library** that contains precursors and a reaction.



- Click the **Products** tab. From the **Operations** menu, choose **Enumerate product data**. A new dialog box appears:

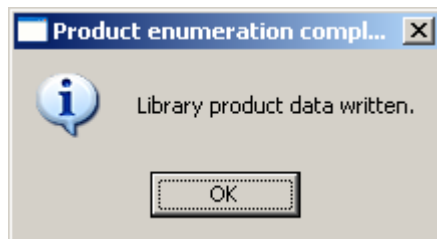


- Select the **Save product info in the database** check box and click **Advanced**. After the dialog box is expanded, select the **Enumerate contaminants** check box:

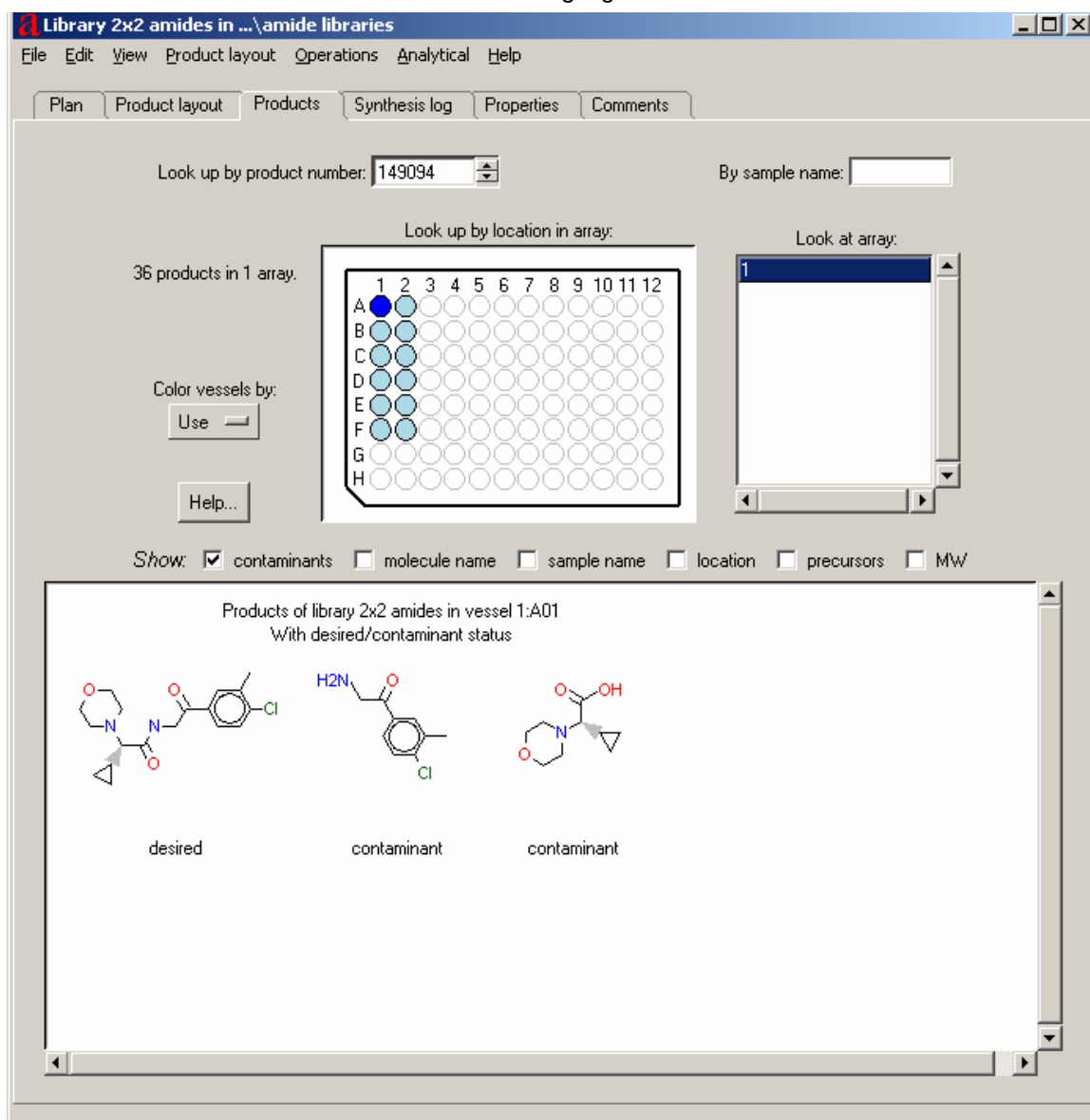


Note Doing the SDfile export during enumeration will not provide the desired information. Instead, the samples must be exported AFTER enumeration is completed.

4. Click **Enumerate data**. Click **OK** when the enumeration is done:



5. To view the contaminant status, on the **Products** tab, select the **Show contaminants** check box. Make sure the well of interest is highlighted:



Library 2x2 amides in ...\amide libraries

File Edit View Product layout Operations Analytical Help

Plan Product layout Products Synthesis log Properties Comments

Look up by product number: 149094 By sample name:

Look up by location in array:

36 products in 1 array.

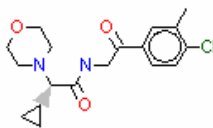
	1	2	3	4	5	6	7	8	9	10	11	12
A	●	○	○	○	○	○	○	○	○	○	○	○
B	○	○	○	○	○	○	○	○	○	○	○	○
C	○	○	○	○	○	○	○	○	○	○	○	○
D	○	○	○	○	○	○	○	○	○	○	○	○
E	○	○	○	○	○	○	○	○	○	○	○	○
F	○	○	○	○	○	○	○	○	○	○	○	○
G	○	○	○	○	○	○	○	○	○	○	○	○
H	○	○	○	○	○	○	○	○	○	○	○	○

Color vessels by:

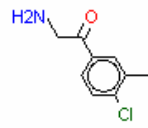
Look at array:

Show: contaminants molecule name sample name location precursors MW

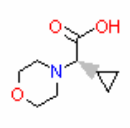
Products of library 2x2 amides in vessel 1:A01
With desired/contaminant status



desired



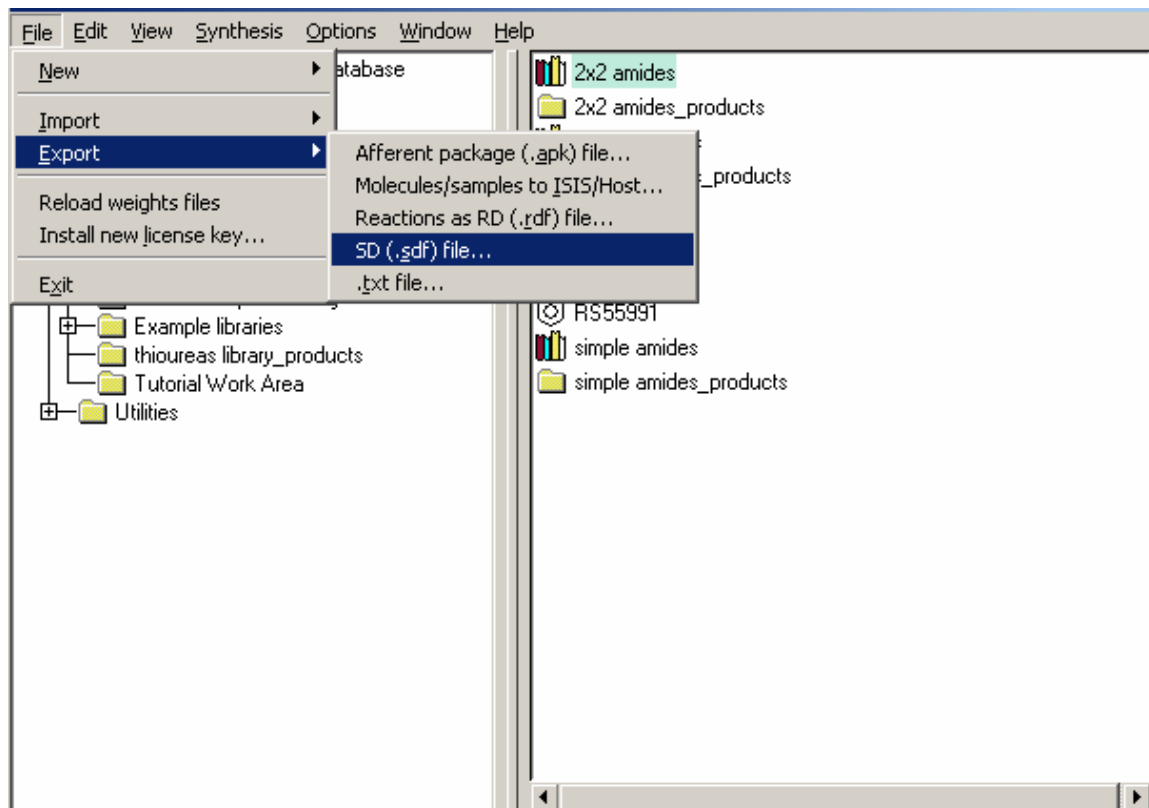
contaminant



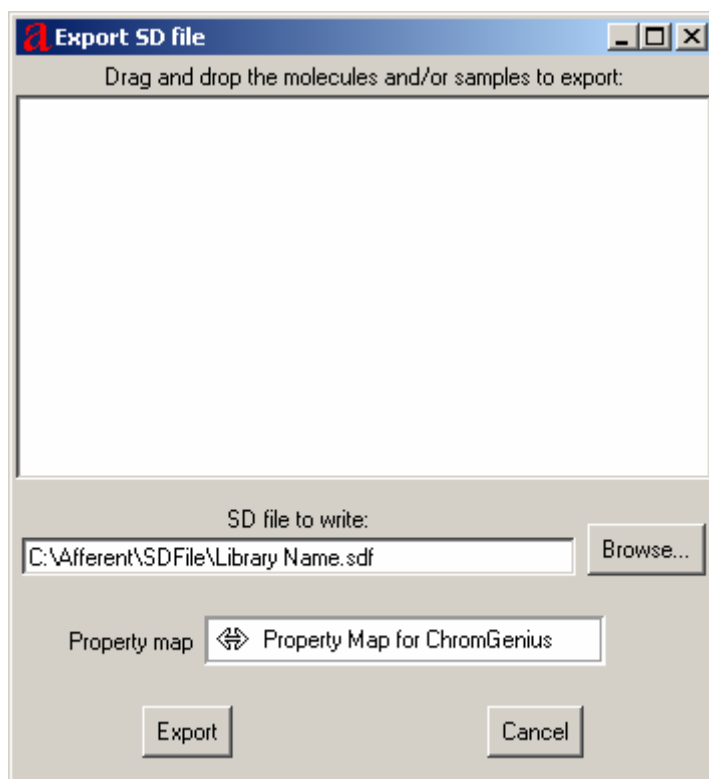
contaminant

6. Close the library.

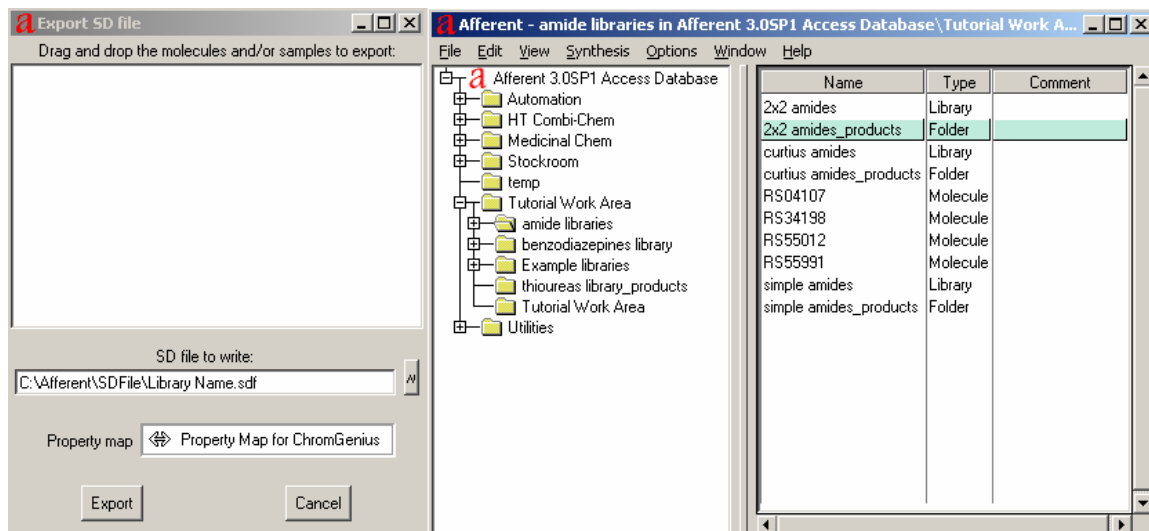
- In the **Afferent Explorer** dialog box, on the **File** menu, point to **Export**, and then choose **SD (.sdf) file**.



- You will see a new **Export SD file** dialog box. Click **Browse** and specify the name and location of your SDfile:

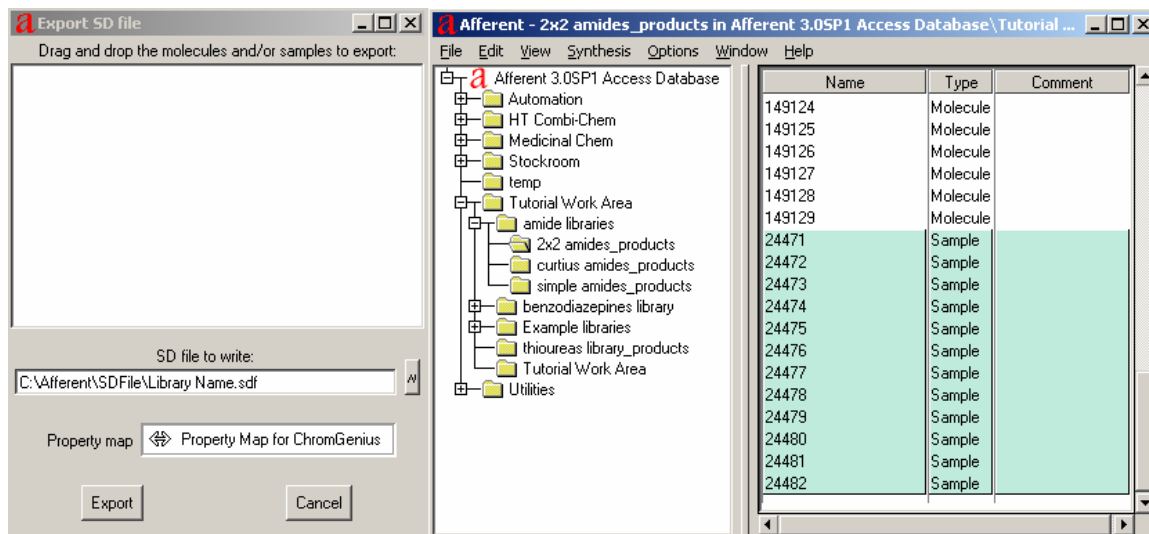


9. Place both dialog boxes, **Export SD file** and **Afferent Explorer**, next to each other for convenience:

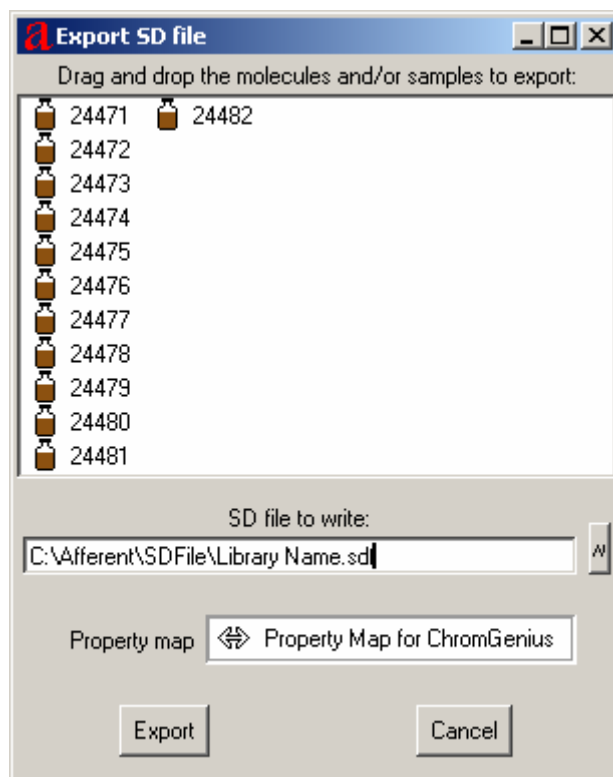


10. Using the **Afferent Explorer** dialog box, navigate to the library products folder, which was automatically generated during enumeration and can be found in the same folder as the library itself.

11. From the **View** menu, choose **Detail** and then sort data by type:



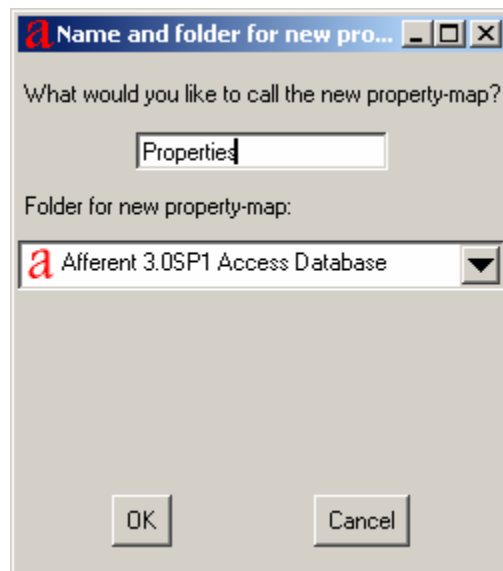
12. Select all of the samples in the folder, and either drag and drop, or cut and paste them into the **Export SD file** dialog box. Do NOT include any molecule or mixture objects that may also be in the folder.



13. Right click the inside of the **Property map** field and choose **[New]**.

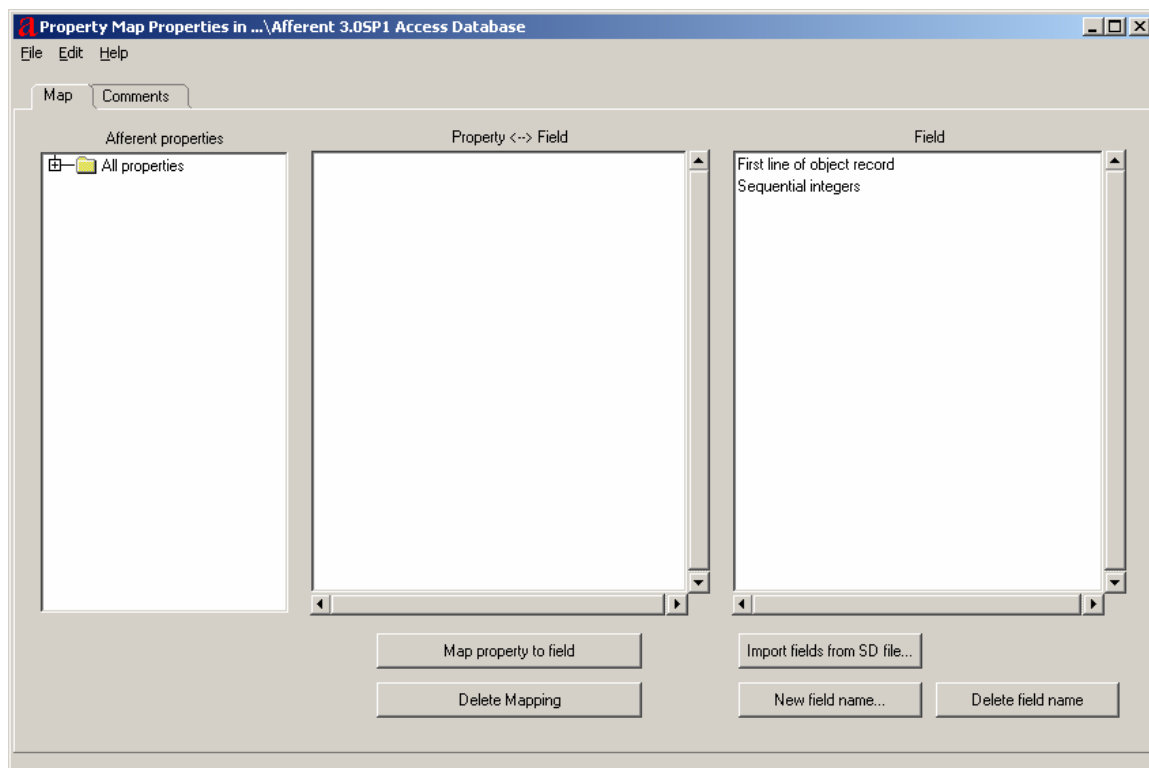
Note A property map is used to relate fields in external files (such as SDfiles, RFiles, and tab delimited files) with Afferent properties. When you import or export such files, you can specify a property map to indicate how data in the Afferent database is to be associated with the file data.

14. In a new window, specify a name for the map.

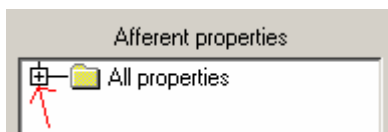


15. Click **OK**.

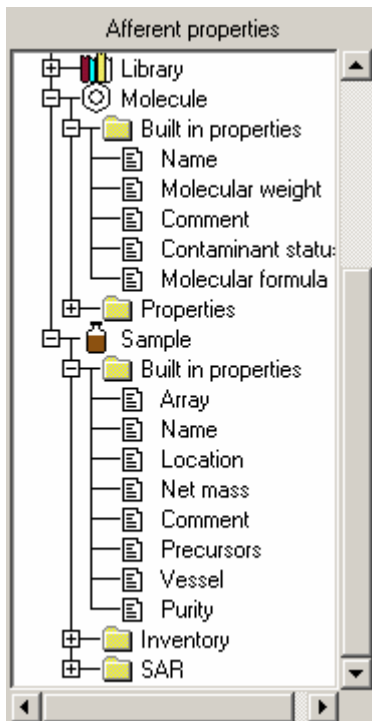
16. A blank **Property map** dialog box appears:



17. Click + to expand the **All properties** folder:



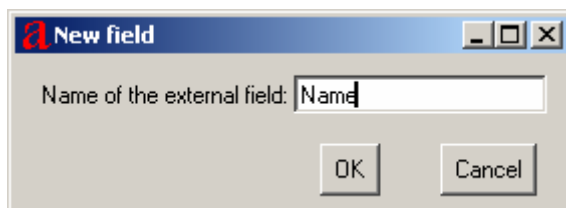
18. Then expand the **Built in properties** folder under the **Molecule** and **Sample** objects:



19. For this example, we want to extract the **Name** and **Contaminant Status** fields from the **Molecule** object and the **Array**, **Location**, **Precursors**, and **Vessel** fields from the **Sample** object.

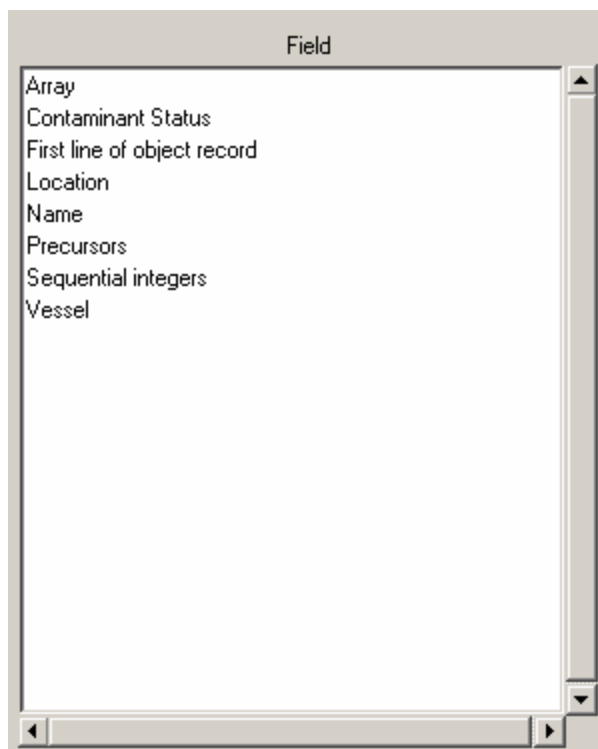
Note This property map shows the mappings necessary for creating an SDfile in MDL Afferent that ACD/ChromGenius Batch will accept.

20. Click **New field name** . In the new dialog box that appears, type the Name and click **OK** to close this window:

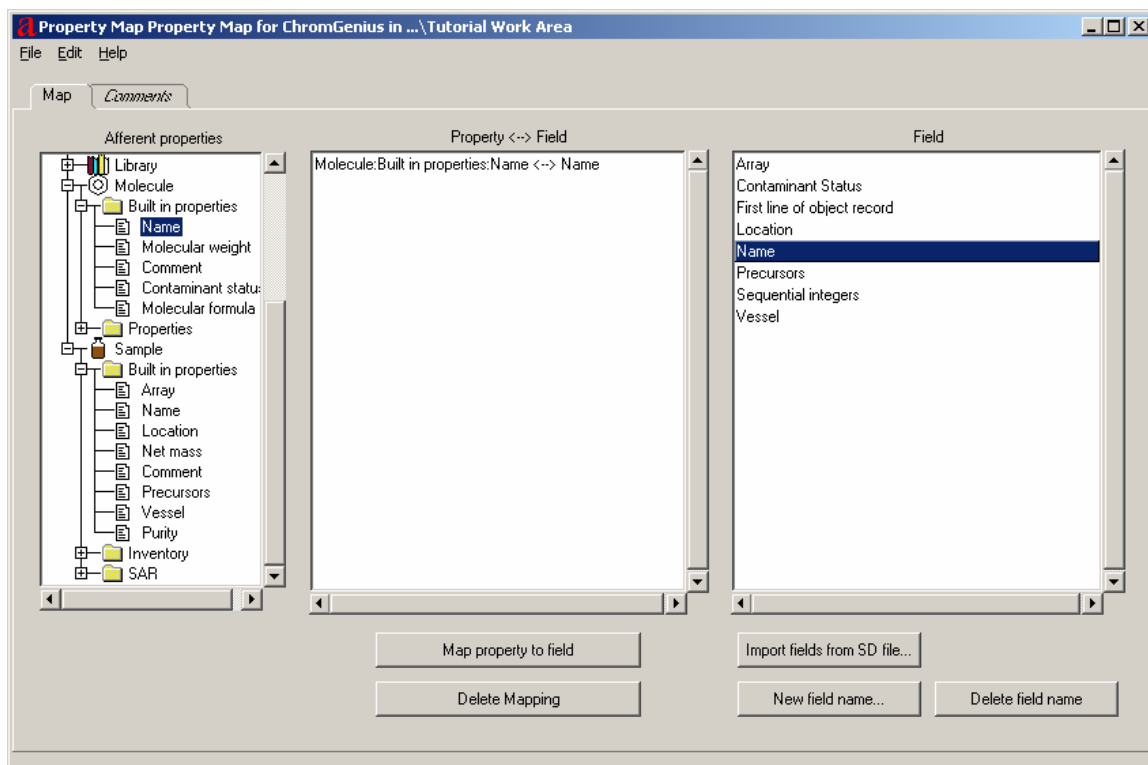


21. Click **New field name** again and create **Contaminant status**, **Array**, **Precursors**, **Vessel**, and **Location** fields in the same manner.

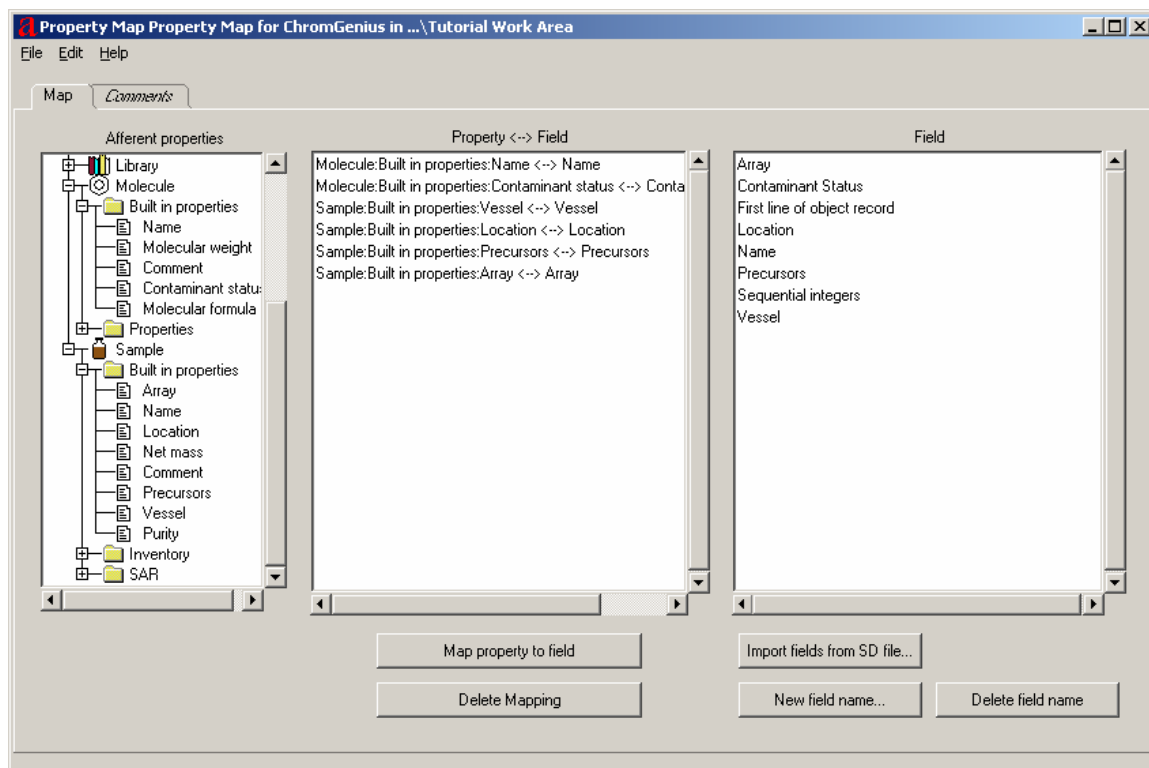
22. You will see all new fields appear in the **Field** section:




23. Highlight **Molecule > Name** in the Afferent properties section and **Name** in the Field section and click **Map property to field**  to see the following connection:




24. Follow the same procedure for the rest of the created fields to complete the connection:



25. From the **File** menu, choose **Save** to save all the changes to the property map.

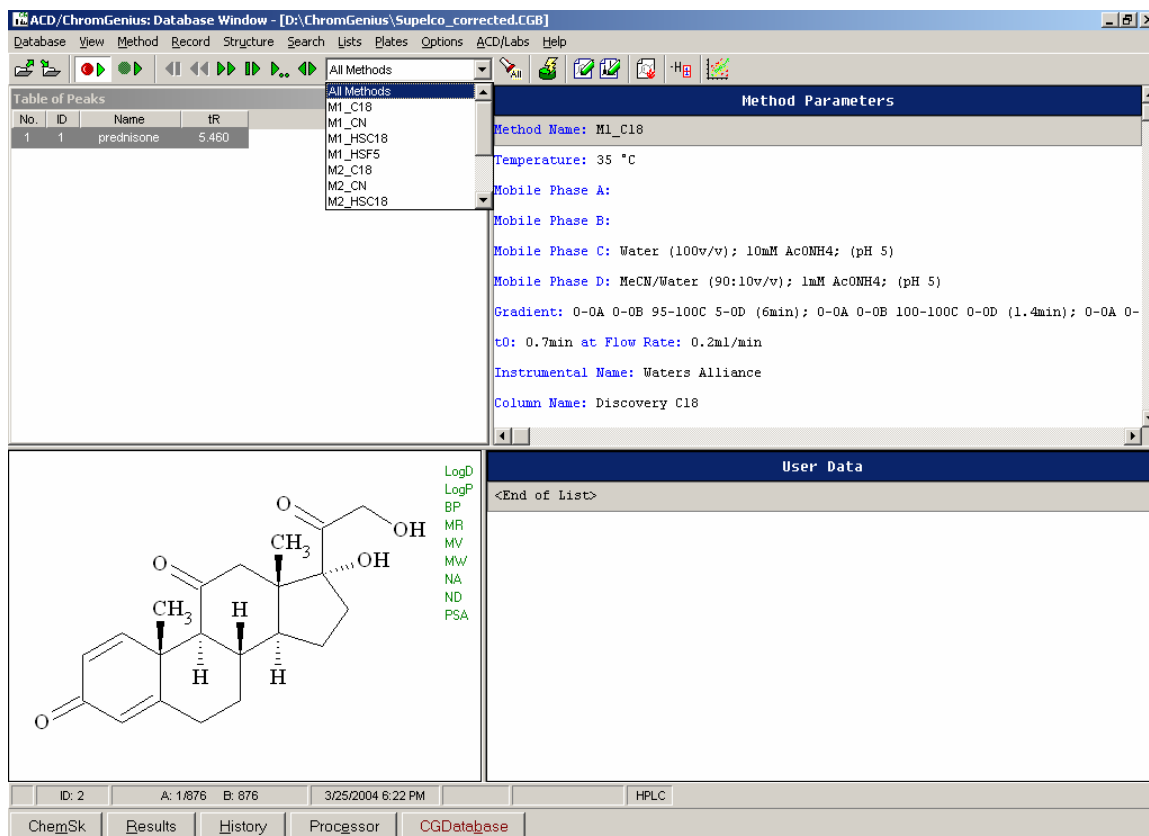
26. Close the property map by clicking **Close** .

27. Return to the **Export SD file** dialog box and click **Export** .

Importing an SDfile

1. We are now ready to predict retention times and suggest the best method for the structures in SDfile.

2. Start **ACD/ChromGenius Batch** and open a database with a few methods:



The screenshot shows the ACD/ChromGenius Database Window with the following components:

- Table of Peaks:**

No.	ID	Name	tR
1	1	prednisone	5.460
- Method Parameters:**

Method Name: M1_C18
Temperature: 35 °C
Mobile Phase A:
Mobile Phase B:
Mobile Phase C: Water (100v/v); 10mM AcONH4; (pH 5)
Mobile Phase D: MeCN/Water (90:10v/v); 1mM AcONH4; (pH 5)
Gradient: 0-0A 0-0B 95-100C 5-0D (6min); 0-0A 0-0B 100-100C 0-0D (1.4min); 0-0A 0-
t0: 0.7min at Flow Rate: 0.2ml/min
Instrumental Name: Waters Alliance
Column Name: Discovery C18
- Chemical Structure:**

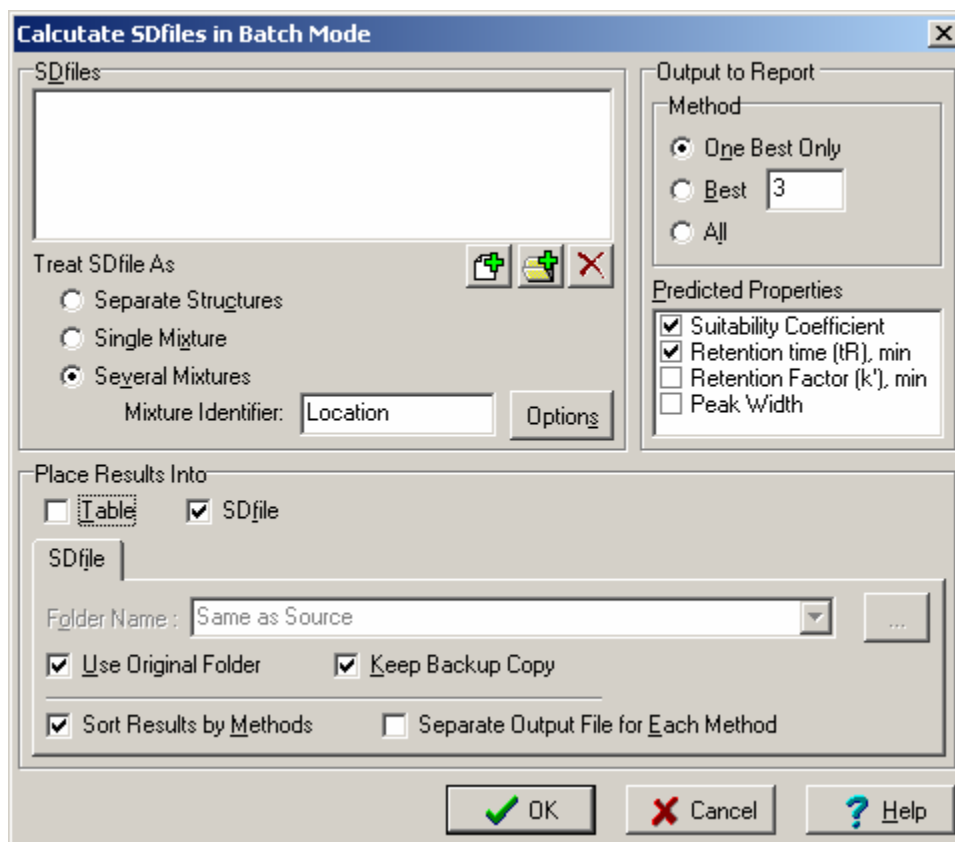
Chemical structure of prednisone is displayed. The structure is a steroid nucleus with a ketone group at C3, a double bond between C4 and C5, a methyl group at C10, and a side chain at C17 containing a ketone group, a methyl group, and a hydroxyl group. Stereochemistry is indicated with wedges and dashes.
- User Data:**


<End of List>
- Bottom Panel:**

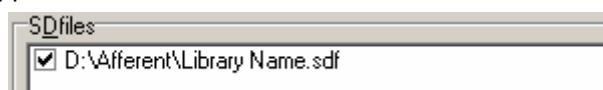
ID: 2 A: 1/876 B: 876 3/25/2004 6:22 PM HPLC
ChemSk Results History Processor CGDatabase

3. The ChromGenius Batch database used for this example was kindly provided by Supelco, Inc. It includes 12 methods.
4. On the **Database** menu, point to **Tools**, and then choose **Calculate SDFFile(s)**.

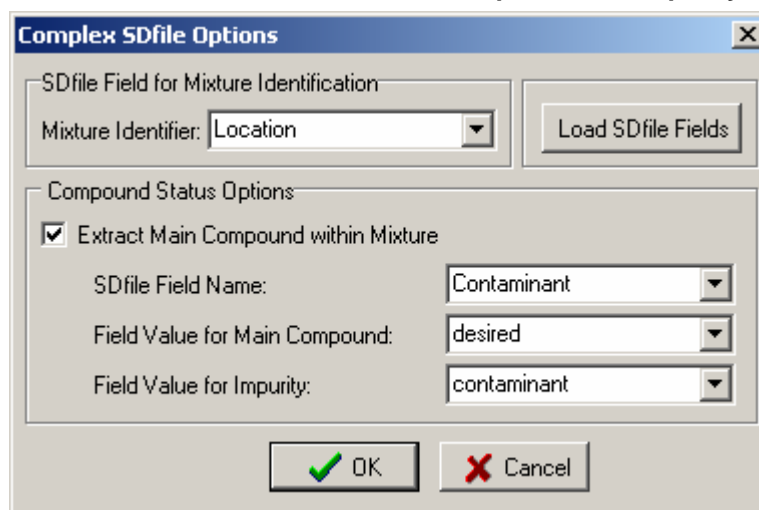
5. A new **Calculate SDFiles in Batch Mode** dialog box appears:



6. Click **Add File**  and specify the location of the SDfile that you exported from MDL Afferent. It will appear in the **SDfiles** area.

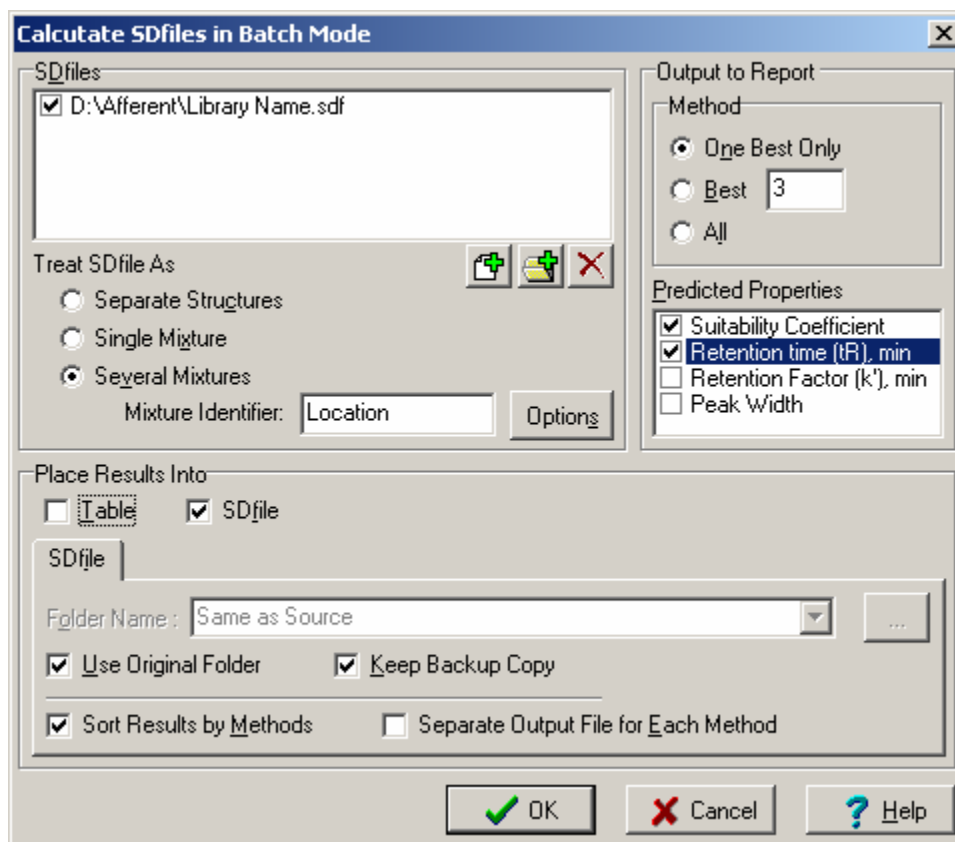


7. Click **Several Mixtures** and then click **Options**. Specify the following options. Type in desired and contaminant in the fields for **Main Compound** and **Impurity**.



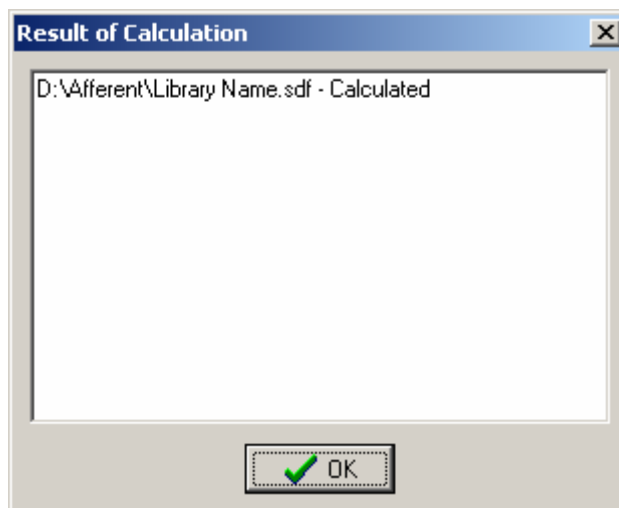
8. Click **OK** to close the **Complex SDfile Options** dialog box.

9. At the end you should have the following:



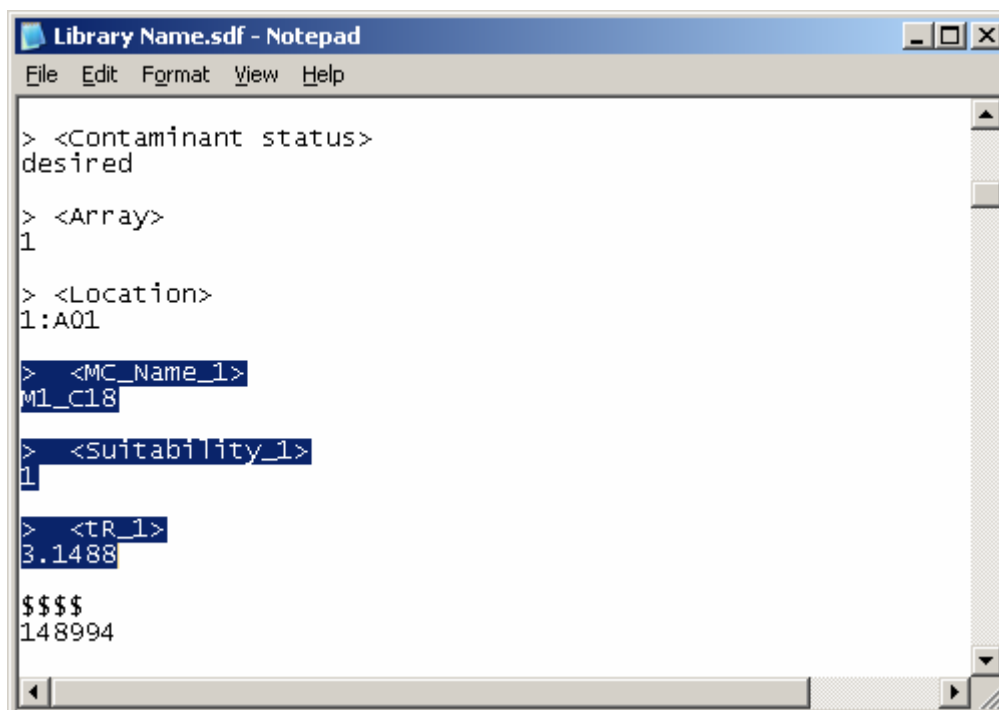
10. Click **OK** to start the calculation.

11. After the calculation is completed, you will get a message:



12. Click **OK**.

13. You can open your SDfile with Notepad to see the additional fields: tR and a name of suggested method (M1_C18 in this case).



```
Library Name.sdf - Notepad
File Edit Format View Help

> <Contaminant status>
desired

> <Array>
1

> <Location>
1:A01

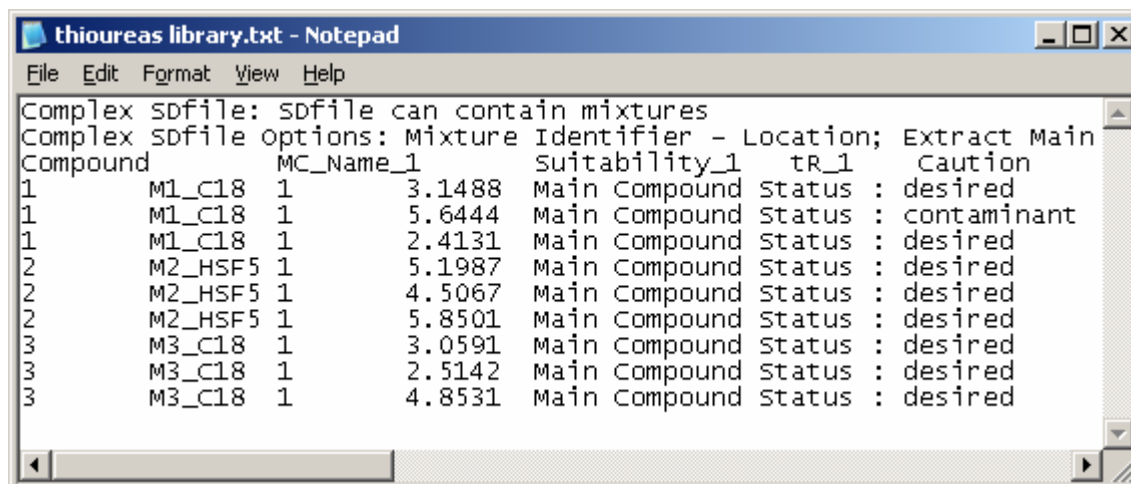
> <MC_Name_1>
M1_C18

> <suitability_1>
1

> <tr_1>
3.1488


$$$$
148994
```

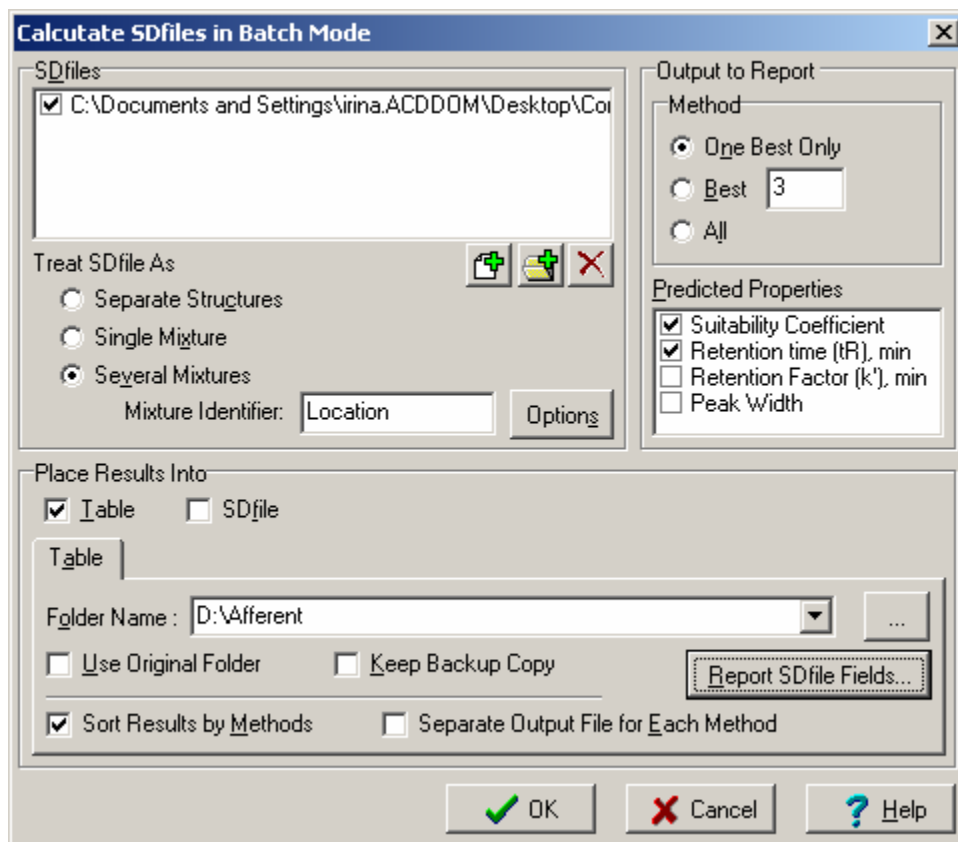
14. Note that you can also export the method choices in text form, omitting the chemical structures. The result will look like this:



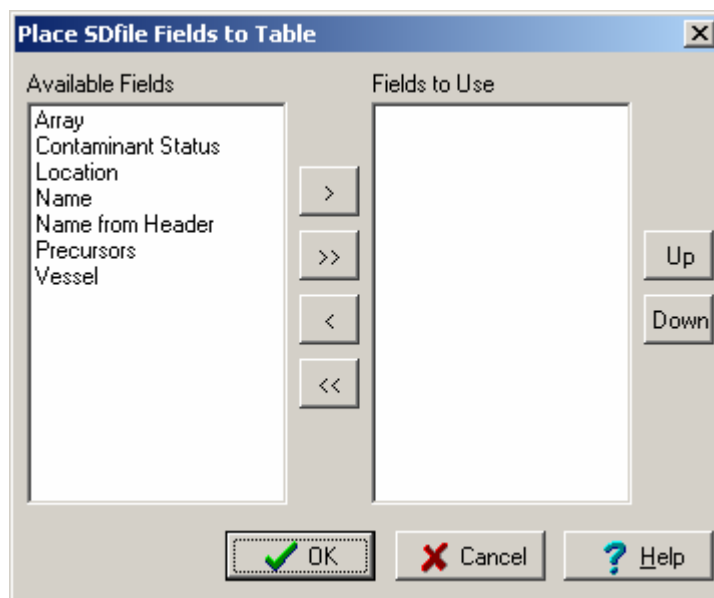
```
thioureas library.txt - Notepad
File Edit Format View Help

Complex SDfile: SDfile can contain mixtures
Complex SDfile Options: Mixture Identifier - Location; Extract Main
Compound      MC_Name_1      Suitability_1  tr_1      Caution
1             M1_C18         1              3.1488    Main Compound Status : desired
1             M1_C18         1              5.6444    Main Compound Status : contaminant
1             M1_C18         1              2.4131    Main Compound Status : desired
2             M2_HSF5        1              5.1987    Main Compound Status : desired
2             M2_HSF5        1              4.5067    Main Compound Status : desired
2             M2_HSF5        1              5.8501    Main Compound Status : desired
3             M3_C18         1              3.0591    Main Compound Status : desired
3             M3_C18         1              2.5142    Main Compound Status : desired
3             M3_C18         1              4.8531    Main Compound Status : desired
```

Note When you place results into a table, all the fields from the SDfile are not automatically transferred into the table. Click **Report SDfile Fields**  in the **Calculate SDfiles in Batch Mode** dialog box shown below:



15. You will see the **Available fields** that need to be used.



16. Click to transfer all the fields at once in the **Fields to Use** section. You can sort them by clicking **Up** and **Down** .

References

1. ACD/ChromGenius Batch. <http://www.chromgeniusbatch.com/>. December 8, 2004.