Building and Editing RTL Screener/Quant Databases and Libraries

Technical Overview

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Introduction

The techniques of Retention Time Locking (RTL) [1], Target Compound Screening [2], and Deconvolution Reporting [3] all use retention times (RTs) for an additional level of compound confirmation. It is important that for maximum productivity and quality, RTs are constant/reproducible and embedded in mass spectral libraries [4]. However, not all compounds are in a commercially available mass spectral library, and most mass spectral libraries do not have RTs.

This technical overview describes building and editing (for example, adding compounds) the following:

RTL Screener databases, RTL Quant databases, and Mass Spectral Libraries. These tasks are accomplished using the GC/MSD ChemStation software and Microsoft Excel. RTL Quant databases and Mass Spectral Libraries can also be used with Agilent's Deconvolution Reporting Software [3].

Software Requirements

- GC/MSD revision D.01.01 (D.01.00 sp1) or higher
- Microsoft Excel

File Locations (File types: *.d, *.l, *.scd, and *.tab)

- Data files (*.d) in C:\MSDchem\1\data\
- Library files (*.l) in C:\Database\
- Screener database files (*.scd) in C:\Database
- TAB-delimited files (*.tab) in C:\Database

Building an MS Spectral Library

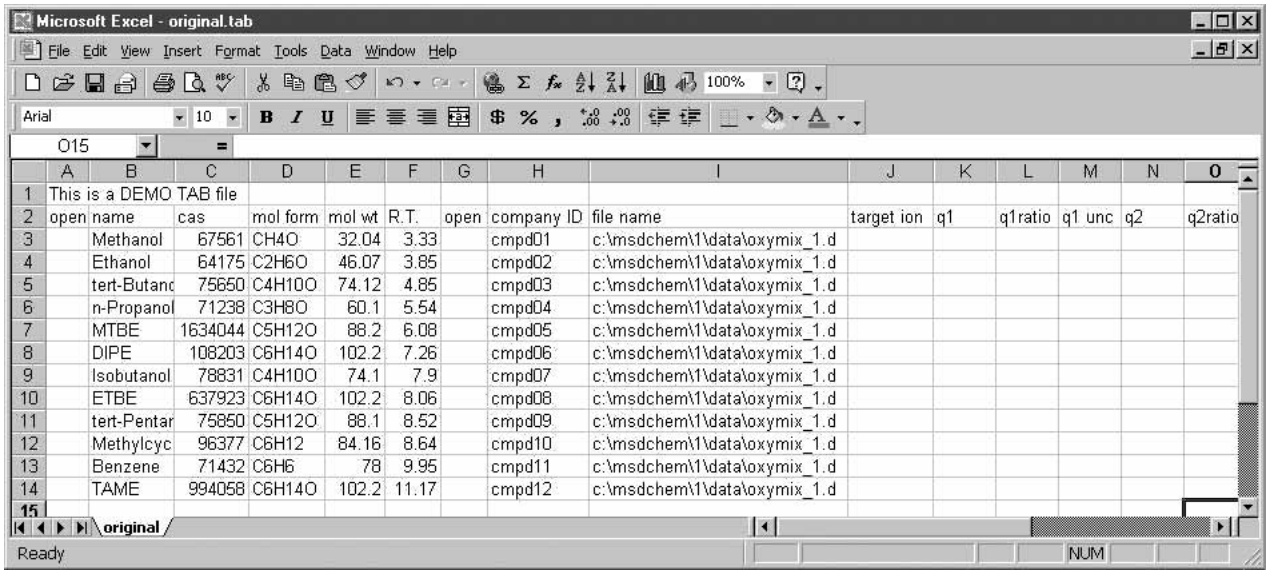
1. Build a (Screener) Library from datafiles (*.d) and a .tab file. See Table 1. The *.d files consist of the peaks/spectra of the library entries.

Table 1. Explanation of Columns in .tab File

Column	Header
A	open (column A is used in GC for retention time (RT), not used in MSD)
B	name (compound name, for example dimethyl...)
C	cas (CAS number without dashes, for example, 12345, not 00012-34-5)
D	molecular formula (for example, C6H14N2O, no commas, dashes, quotes etc)
E	molecular weight (for example, 32.04)
F	RT (GC/MSD, in minutes, for example, 12.34)
G	open (not used)
H	company ID (a unique identifier, for example, cmpd01 - more explanation on this later)
I	file name (complete file path for .d used for library creation such as C:\MSDchem\1\data\oxymix.d)
J	target ion (scd target ion)
K	q1 (qualifier 1)
L	q1ratio (qualifier 1 ratio)
M	q1 unc (qualifier 1 uncertainty)
N	q2 (qualifier 2)
O	q2ratio (qualifier 2 ratio)
P	q2 unc (qualifier 2 uncertainty)
Q	q3 (qualifier 3)
R	q3ratio (qualifier 2 ratio)
S	q3 unc (qualifier 3 uncertainty)
T	unc tp: 0=rel, 1=abs (uncertainty type)
U	Ref Lib Name (library name)*
V	Ref Lib entry num (entry number in the library, such as 15)*

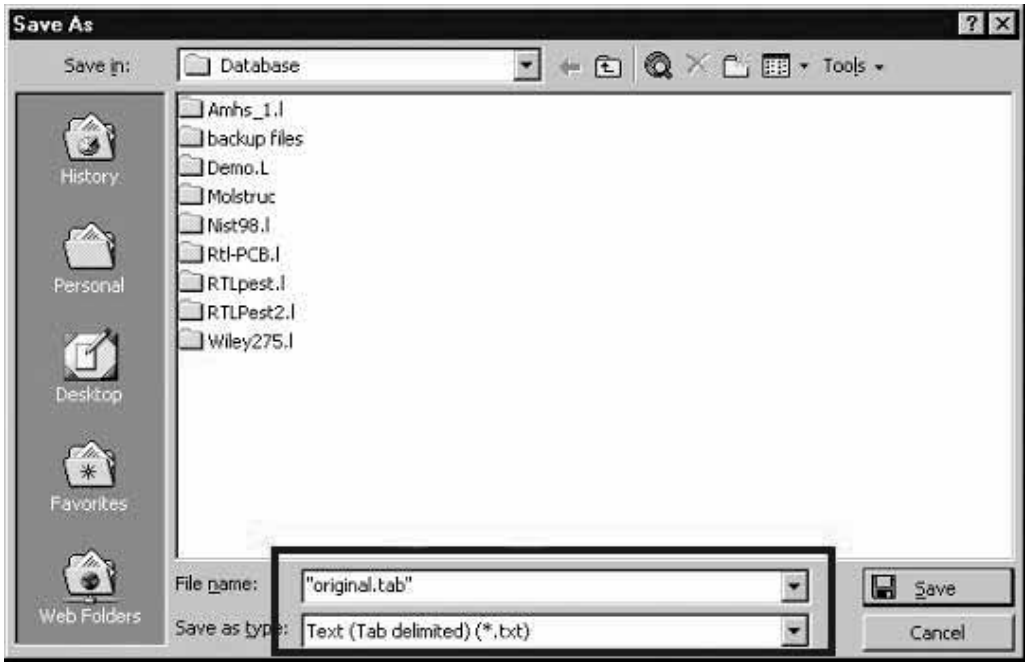
* Not used for original library creation.

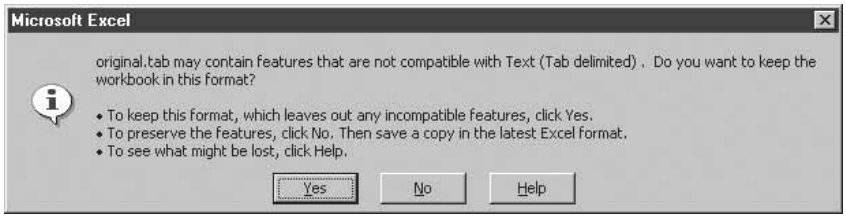
The columns B, C, D, E, F, and I are required. All other columns are left blank. Use one compound per row. See the example below: Note the first two lines (and only two lines) are for comment and header information.



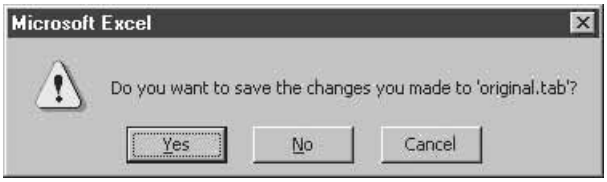
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	This is a DEMO TAB file														
2	open	name	cas	mol form	mol wt	R.T.	open	company ID	file name	target ion	q1	q1ratio	q1 unc	q2	q2ratio
3		Methanol	67561	CH4O	32.04	3.33		cmpd01	c:\msdchem\1\data\oxymix_1.d						
4		Ethanol	64175	C2H6O	46.07	3.85		cmpd02	c:\msdchem\1\data\oxymix_1.d						
5		tert-Butanc	75650	C4H10O	74.12	4.85		cmpd03	c:\msdchem\1\data\oxymix_1.d						
6		n-Propanol	71238	C3H8O	60.1	5.54		cmpd04	c:\msdchem\1\data\oxymix_1.d						
7		MTBE	1634044	C5H12O	88.2	6.08		cmpd05	c:\msdchem\1\data\oxymix_1.d						
8		DIPE	108203	C6H14O	102.2	7.26		cmpd06	c:\msdchem\1\data\oxymix_1.d						
9		Isobutanol	78831	C4H10O	74.1	7.9		cmpd07	c:\msdchem\1\data\oxymix_1.d						
10		ETBE	637923	C6H14O	102.2	8.06		cmpd08	c:\msdchem\1\data\oxymix_1.d						
11		tert-Pentar	75850	C5H12O	88.1	8.52		cmpd09	c:\msdchem\1\data\oxymix_1.d						
12		Methylcyc	96377	C6H12	84.16	8.64		cmpd10	c:\msdchem\1\data\oxymix_1.d						
13		Benzene	71432	C6H6	78	9.95		cmpd11	c:\msdchem\1\data\oxymix_1.d						
14		TAME	994058	C6H14O	102.2	11.17		cmpd12	c:\msdchem\1\data\oxymix_1.d						
15															

2. Make sure you save the spreadsheet file in .tab format in the Database folder. Go to **File|Save as|** and choose Text (Tab delimited)(*.txt). Put the file name in quotes with a .tab extension such as “original.tab”. This will save in a tab-delimited format with a .tab extension.



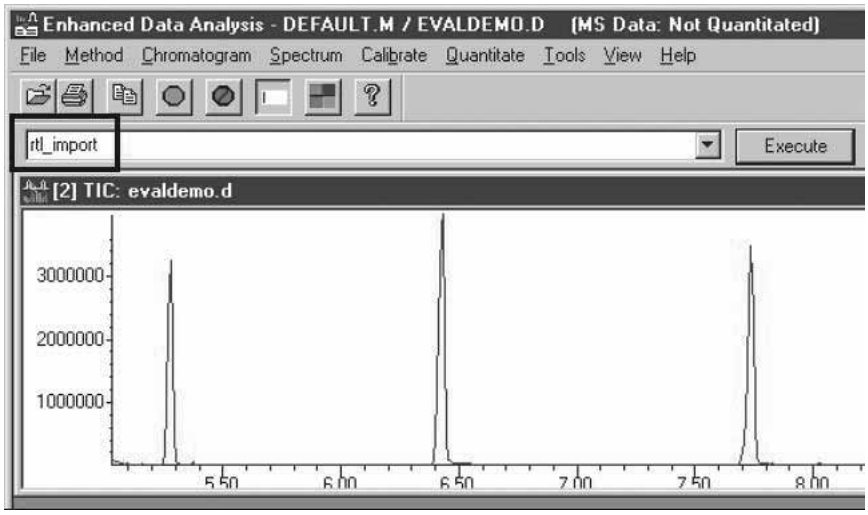


3. Click **Yes** to keep the format.
4. CLOSE the Excel file, otherwise you will get an error message (Could not open file: C:\database\original.tab) from MSD ChemStation.

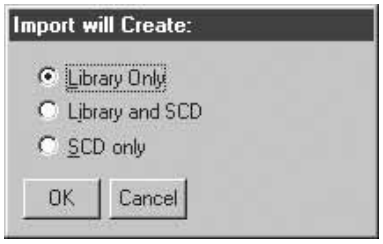


5. Click **No**.

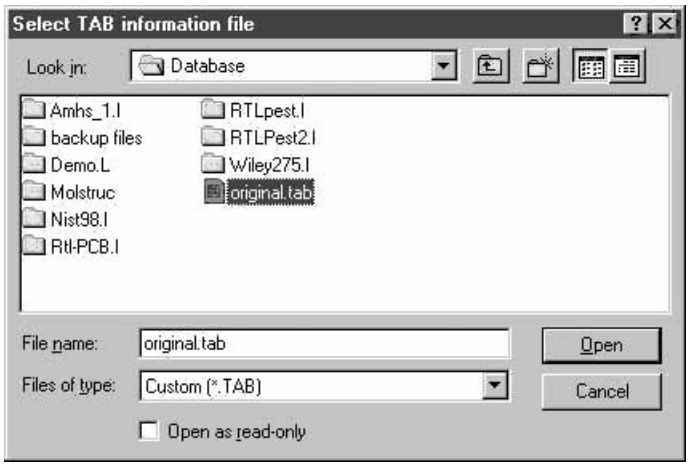
6. Go to Enhanced Data Analysis. On the command line type **rtl_import** and then click **Execute**.



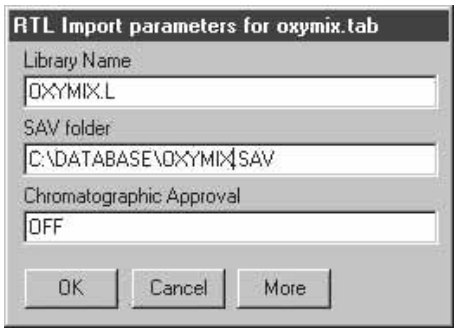
7. Select **Library only**, click **OK**.



(The screener database can also be generated at the same time by selecting the “Library and SCD” option as seen in a later section.)



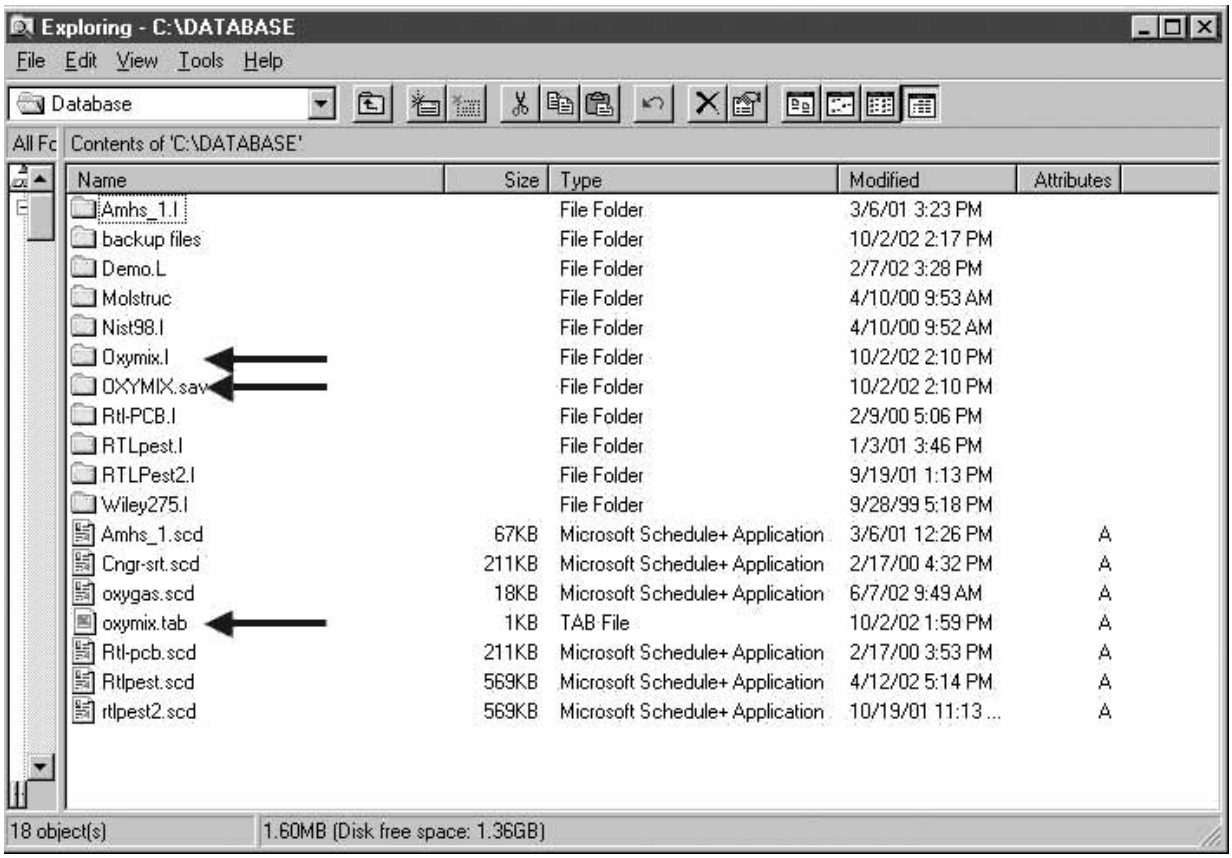
8. You will be prompted for a file to select from the Database folder. Select the .tab you want, click **Open**.



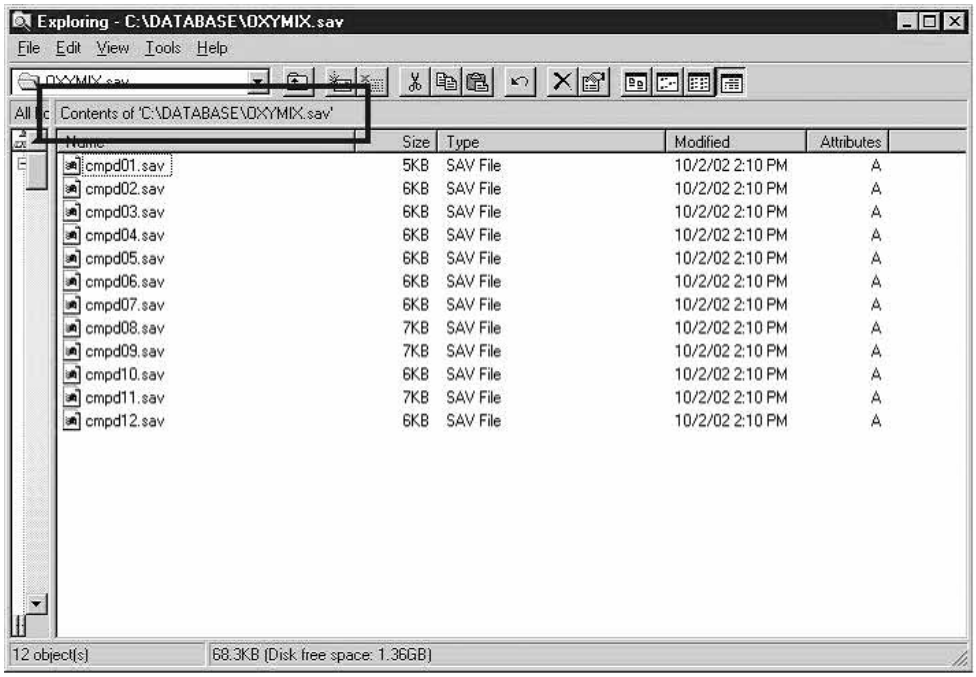
9. Give the library a name (maximum eight characters), such as oxymix.L and click **OK**.

Enhanced DA will call each of the files in Column I of your .tab file. It will then go to the RT you specified in Column F and create a Library entry using that spectrum and the information from Columns B, D, and E. You should see chromatograms flashing before your eyes. If you fill in column H of the *.tab file, you will get a .sav directory when the library is built.

The following screen shows the new library, Oxymix.L, the oxymix.tab file, and the .sav directory.



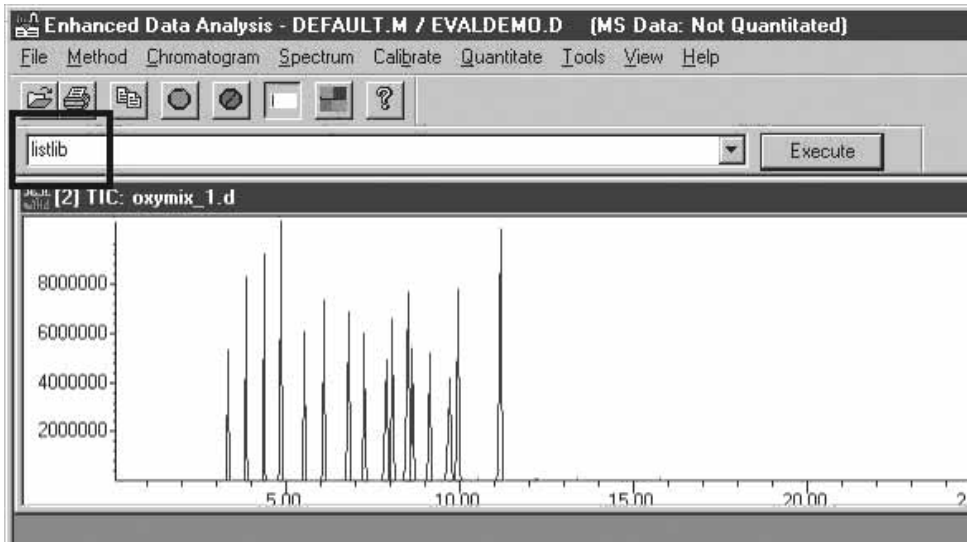
What is the .sav directory? The .sav is a folder created in Database folder when you create a Library from a .tab. The .sav folder contains one .sav file for each entry in the Library you just created.



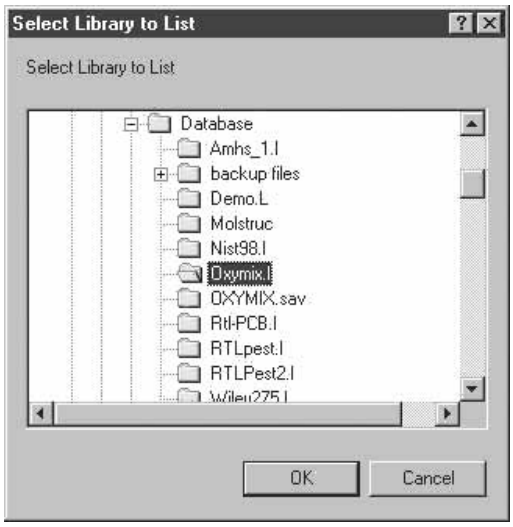
Each .sav file contains the spectrum of the Library entry. The .sav file name is taken from Column H. If Column H is left blank you will get no usable .sav files. You can rebuild the Library using the .sav files if you lost the original data files. In the dialogue box where you entered the Library name when you first created it, there is a “more” button. Clicking “more” gives you a field to specify whether you're using original data or .sav files.

List the Content of a Library (*.l)

1. After the library is built, type **listlib** on the command line and then click **Execute**.

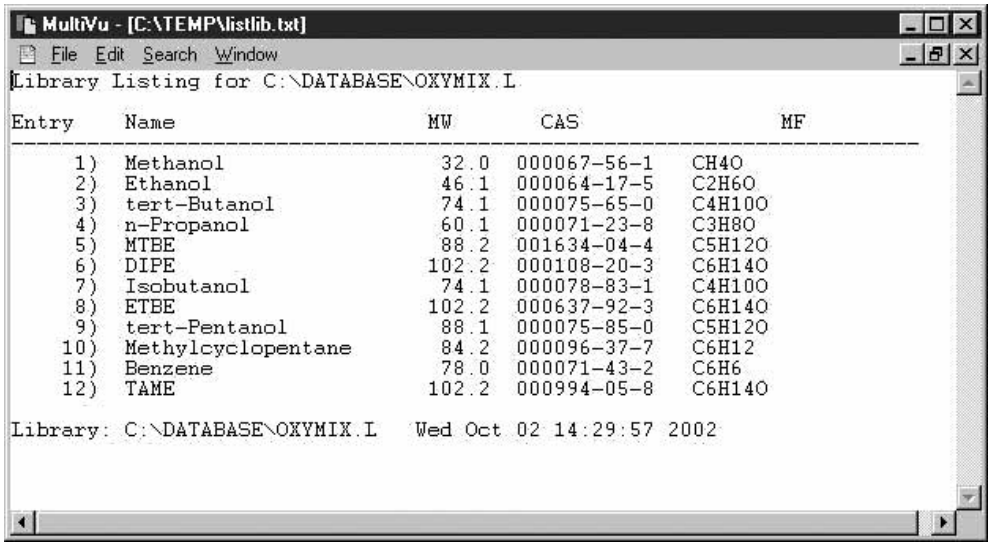


2. Choose the library name you just created then click **OK**.



3. Click **No** to the detailed graphics question.

If all went well you will see a list of your library entries, compound names, MW, CAS, etc.

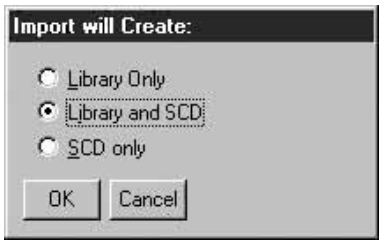


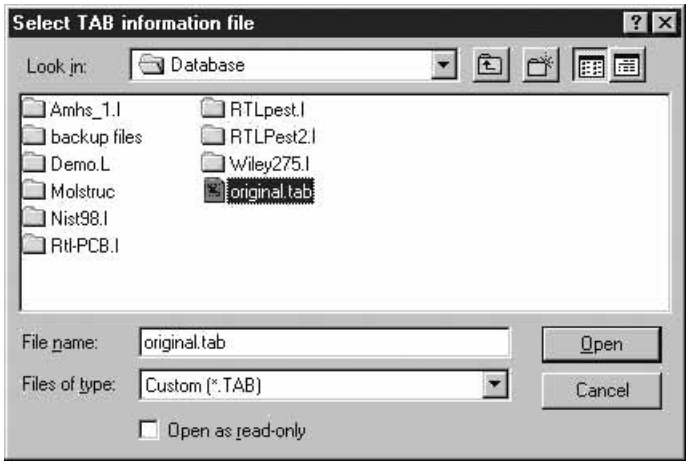
If you see only a few lines of text at the top, the library was not built properly. Go back and follow the build-a-library steps again carefully, especially entering the correct datafile name and the data path in column I of the .tab file.

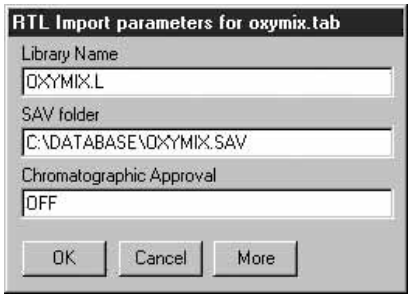
Create an SCD and a Library From a .tab File

The best way to create an .scd is to create it when you create the Library. Do ALMOST exactly what you did to create a Library in the previous section.

1. After you execute the **rtl_import** command, select "**Library and SCD**".



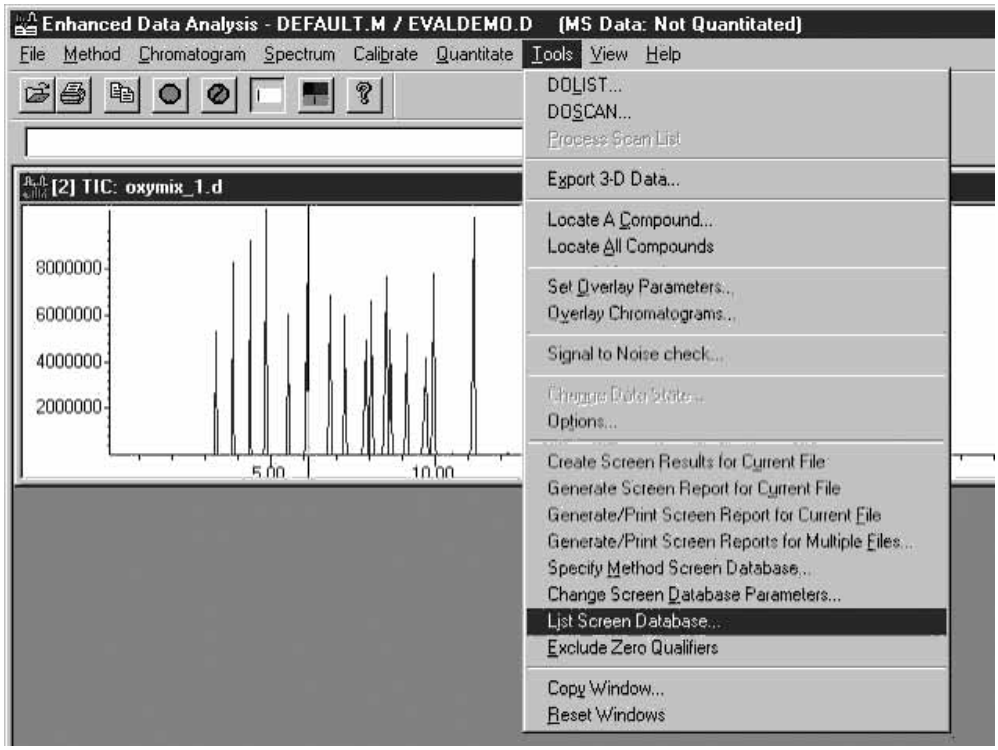


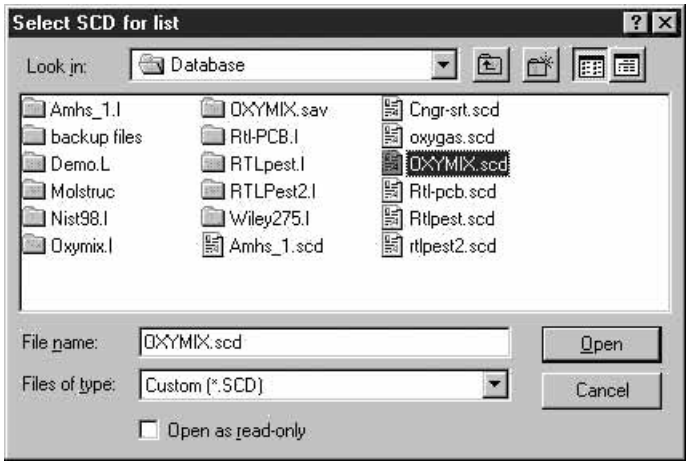


2. Click **Yes**. An .scd will be created with the same name you give the library.

The largest ion will be the target ion, and then the next three largest ions will be the qualifiers. Uncertainty percent will be globally set to 20. Uncertainty type will be globally set to 0=relative.

3. From the Tools menu item, select "**List Screen Database**...".





4. You will see a listing of your .scd. Select the .scd you just created.

MultiVu - [C:\MSDCHEM\2\METHODS\DEFAULT.M\scdlist.txt]

File Edit Search Window

SCD Compound List Report

Screen Database : C:\DATABASE\OXYMIX.scd
Total SCD Cpnds : 12

Cpd#	Compound Name	TIon	Exp_RT	Q1	Q2	Q3
1	Methanol	31	3.33	29	30	33
2	Ethanol	31	3.85	45	29	46
3	tert-Butanol	59	4.85	31	43	41
4	n-Propanol	31	5.54	59	42	27
5	MTBE	73	6.08	43	57	41
6	DIPE	45	7.26	43	87	41
7	Isobutanol	43	7.90	41	42	31
8	ETBE	59	8.06	87	57	29
9	tert-Pentanol	59	8.52	73	55	31
10	Methylcyclopentane	56	8.64	69	41	55
11	Benzene	78	9.95	77	51	50
12	TAME	73	11.17	87	43	55

Cal A = Average L = Linear LO = Linear w/origin Q = Quad QO = Quad w/origin
#Qual = number of qualifiers
A/H = Area or Height
ID R = R.T. B = R.T. & Q Q = Qvalue L = Largest A = All

DEFAULT.M Wed Oct 02 16:14:29 2002

5. Close the window.

The macro that does the .scd listing also creates a .tab file (in the c:\database folder) with the same name as the .scd. In this case, you will have oxymix.scd and oxymix.tab.

6. Go into Excel and open the .tab file (oxymix.tab) of the same name as the .scd you just listed. Click **Finish**.

Now you have a tab file with the proper headers in row 2. This is a .tab of your .scd NOT of your library.

Microsoft Excel - oxymix.tab

File Edit View Insert Format Tools Data Window Help

A1 = SCD tabbed list for oxymix.scd; list created Tue Oct 08 16:50:42 2002

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V
1	SCD tabbed list for oxymix.scd; list created Tue Oct 08 16:50:42 2002																					
2	open	name	cas	mol form	mol wt	R.T.	op	company	file	target	q1	q1ratio	q1 unc	q2	q2ratio	q2 unc	q3	q3ratio	q3 unc	unc tp	Ref Lib Na	Ref Lib entr
3	3.33	Methanol	67561	CH4O	32.04	3.33		cmpd01		31	29	81.6	20	30	9.2	20	33	2.6	20	0	oxymix.L	1
4	3.85	Ethanol	64175	C2H6O	46.07	3.85		cmpd02		31	45	71.3	20	29	31.5	20	46	27.2	20	0	oxymix.L	2
5	4.85	tert-Butar	75650	C4H10O	74.12	4.85		cmpd03		59	31	18.1	20	43	16	20	41	14.8	20	0	oxymix.L	3
6	5.54	n-Propanc	71238	C3H8O	60.1	5.54		cmpd04		31	59	28.8	20	42	19.5	20	27	17.8	20	0	oxymix.L	4
7	6.08	MTBE	1634044	C5H12O	88.2	6.08		cmpd05		73	43	18.8	20	57	18.7	20	41	15.3	20	0	oxymix.L	5
8	7.26	DIPE	108203	C6H14O	102.2	7.26		cmpd06		45	43	50.5	20	87	47.6	20	41	18.9	20	0	oxymix.L	6
9	7.9	Isobutano	78831	C4H10O	74.1	7.9		cmpd07		43	41	79.4	20	42	61.2	20	31	44.2	20	0	oxymix.L	7
10	8.06	ETBE	637923	C6H14O	102.2	8.06		cmpd08		59	87	57.3	20	57	29.7	20	29	8.3	20	0	oxymix.L	8
11	8.52	tert-Penta	75850	C5H12O	88.1	8.52		cmpd09		59	73	74.9	20	55	40.7	20	31	13.8	20	0	oxymix.L	9
12	8.64	Methylcy	96377	C6H12	84.16	8.64		cmpd10		56	69	54.8	20	41	47.1	20	55	26.4	20	0	oxymix.L	10
13	9.95	Benzene	71432	C6H6	78	9.95		cmpd11		78	77	25.2	20	51	15.4	20	50	14.5	20	0	oxymix.L	11
14	11.2	TAME	994058	C6H14O	102.2	11.17		cmpd12		73	87	31.3	20	43	27.6	20	55	21.1	20	0	oxymix.L	12
15																						

oxymix

Ready NUM

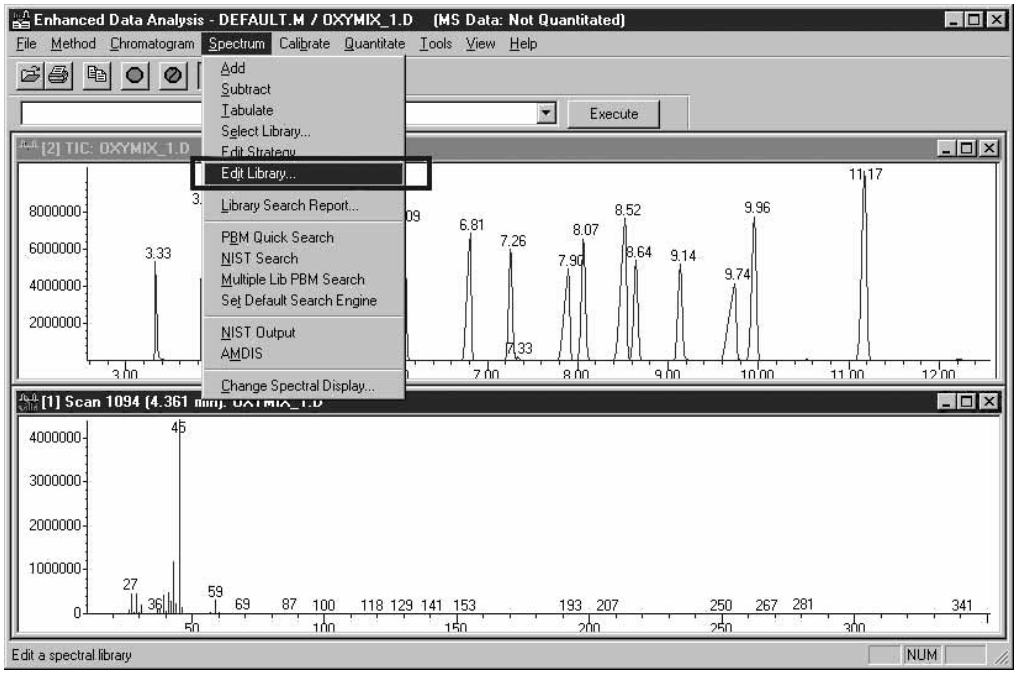
This also is NOT the original .tab from which you created the Library and .scd. You will notice the datafile paths (column I) are gone. Columns J-V are filled in. The software has associated each scd entry with a library name (column U) and library entry number (column V). Information depicted in Columns U and V is used for the XCR (cross correlation) on the screener report [2].

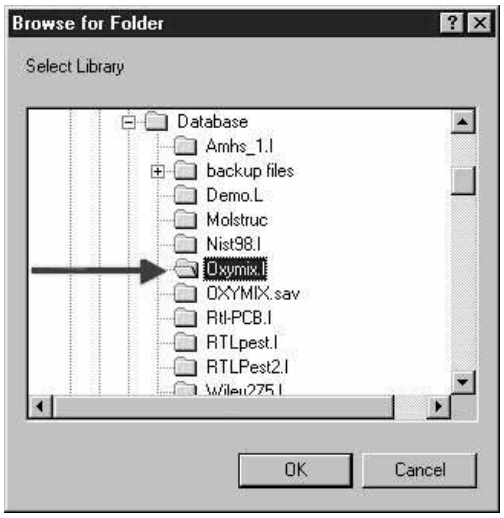
Add Additional Entries to an Existing Library

When you need to add spectra to an existing library and you have not made changes to the corresponding .scd file, you can rebuild your library and .scd using the procedures described above. Just add the new entries to the original.tab file, sort the RT, and save the file. Then use **rtl_import** command to build the library.

If you have made changes to your .scd file, for example, picked different target/qualifier ions or changed ion ratios etc., you should follow these steps.

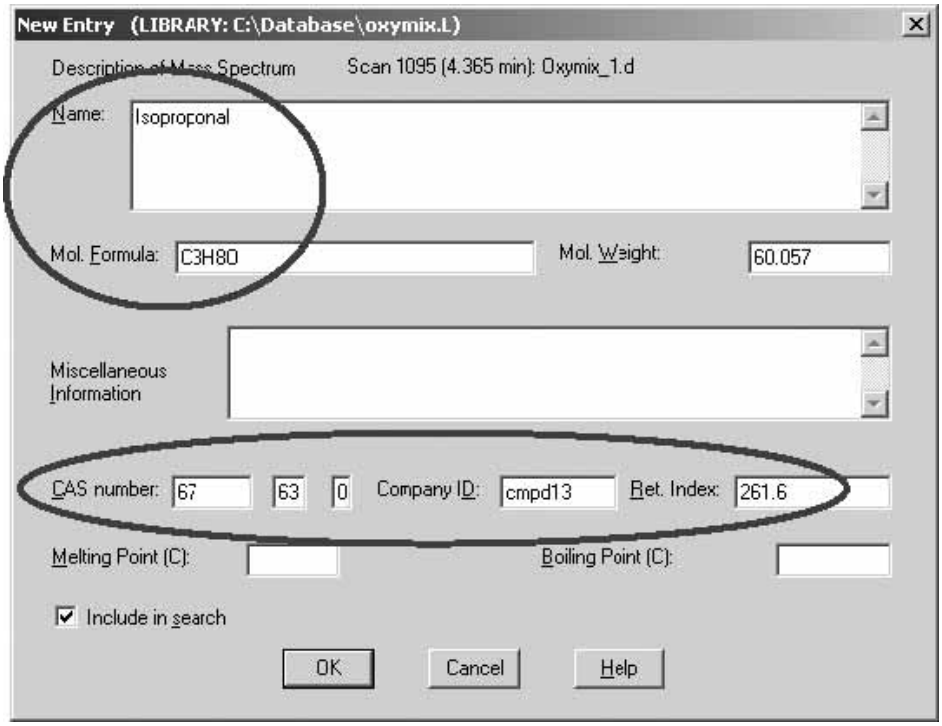
1. Display the spectrum (preferably averaged over the width at the half-height of the peak) to be added to the library. Go to **Spectrum | Edit Library|**, and select the library to add the compound into.



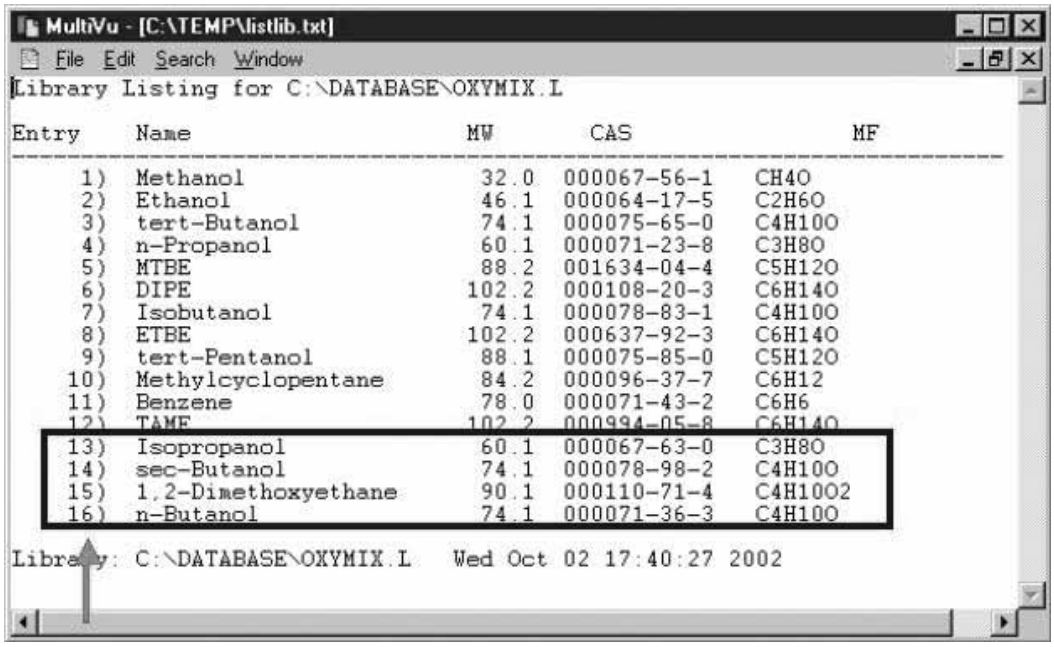


2. After the library is chosen, select the "**Add New Entry**" option.

3. Enter the information associated with each entry. The Retention Index should be filled in with the RT converted to seconds. In this case, it is $4.36 \times 60 = 261.6$



4. Repeat the steps to add all the entries. In this case, we have added a total of four new entries.
5. Go to Enhanced DA and execute a **listlib** command on the command line to list all the library entries.



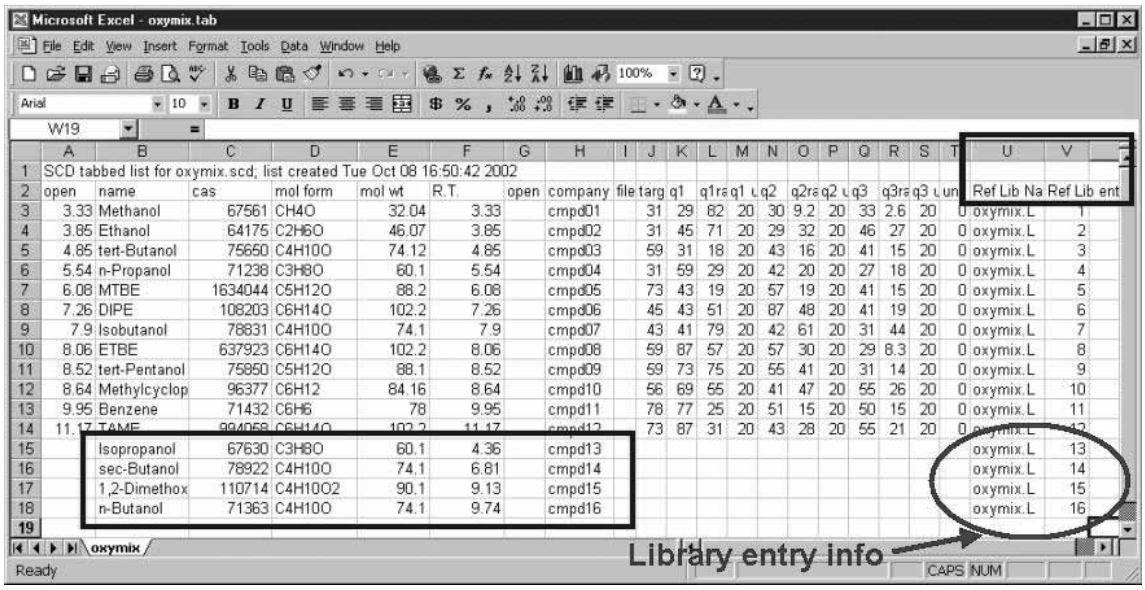
The entry numbers in the above picture (13, 14, 15, and 16) are needed in the .tab file for building the .scd file.

Screener Database

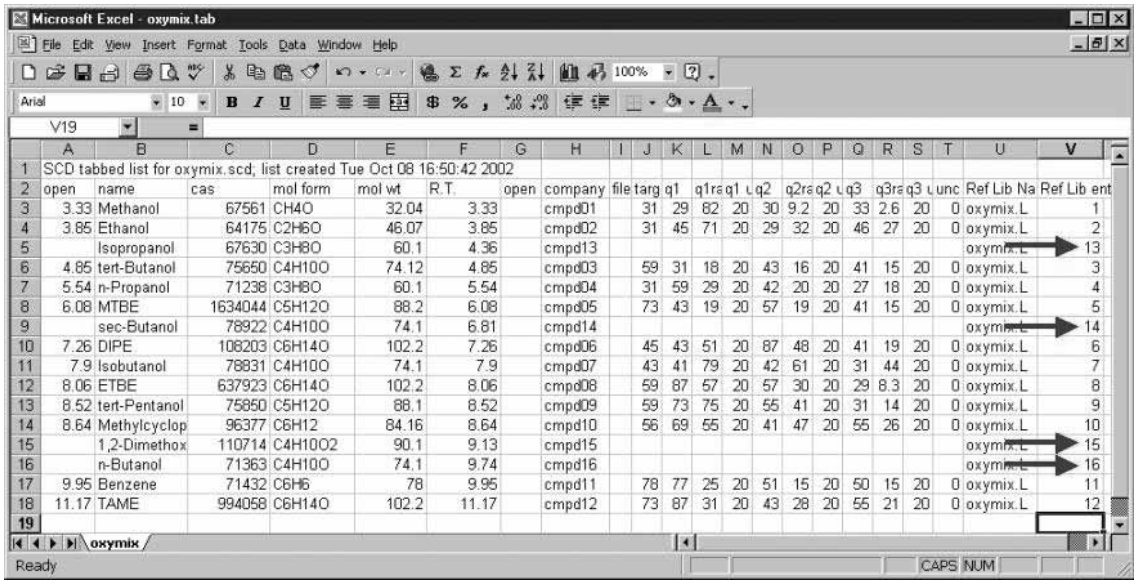
Create Only the SCD From Your .tab

This is used with an existing Library you edited (for example, entries added).

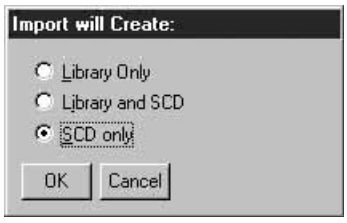
1. In Excel, open your exisiting oxymix.tab (not original.tab) file for editing.
2. Fill in columns B, C, D, E, F, U, and V (column H is optional). You will need to know the existing Library name (enter in column U) and entry number (enter in column V) for each compound.



3. Sort the rows using the RT (column F).

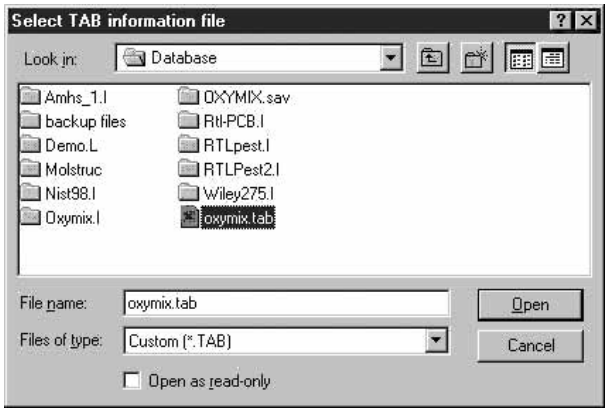


4. Save the **.tab file** and close Excel.
5. Go to **Enhanced DA** and execute an **rtl_import** command on the command line.

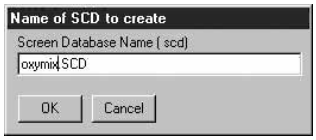


6. Select "**SCD only**" and click **OK**. You will be prompted to select a .tab file from the Database folder.

7. Select the .tab you want and then click **Open**.



8. Give the scd a name (maximum eight characters), such as oxymix.scd, and click **OK**.



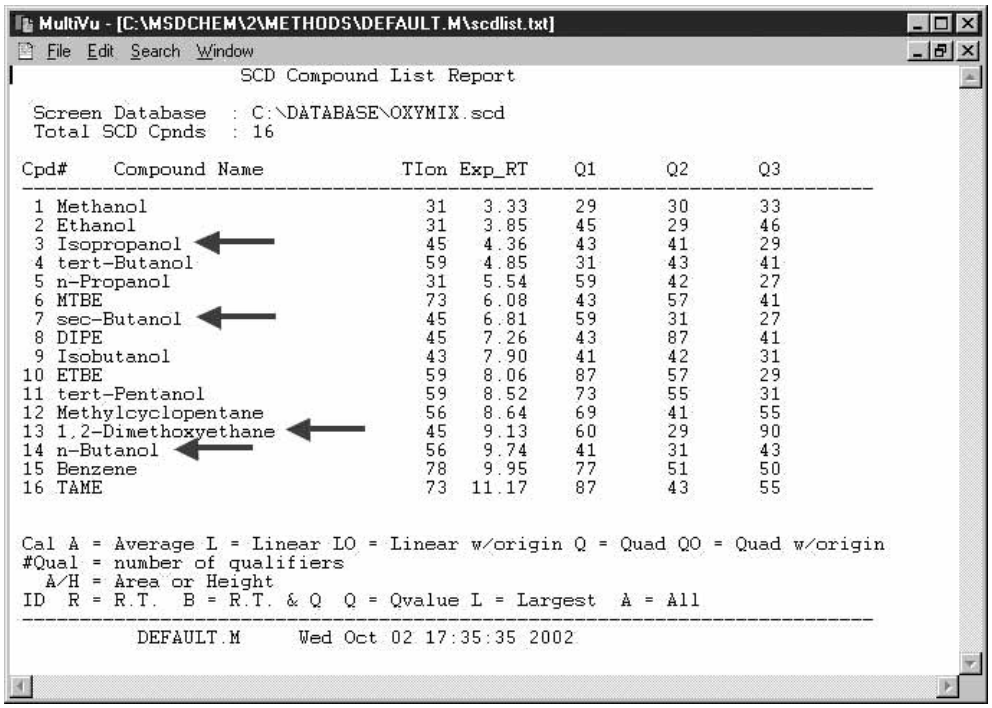
An .scd will be created using the spectra from the library. The largest ion will be the target ion, and then the next three largest ions will be the qualifiers. Uncertainty percent will be globally set to 20. Uncertainty type will be globally set to 0=relative.

Make an ASCII File of the Screener Database

The information in a .scd can be saved in ASCII format (text) for sharing or for future reference.

1. From MSD software, enhanced DA, go to **Tools | List Screen Database...|**. A dialogue box comes up.
2. Choose an existing Screen Database (oxymix.scd) in the Database folder and click **Open**. You will get a text listing in a MultiVu window.

The following graphic shows that the four compounds that were added to the library are successfully added to the screener database in the proper RT order.

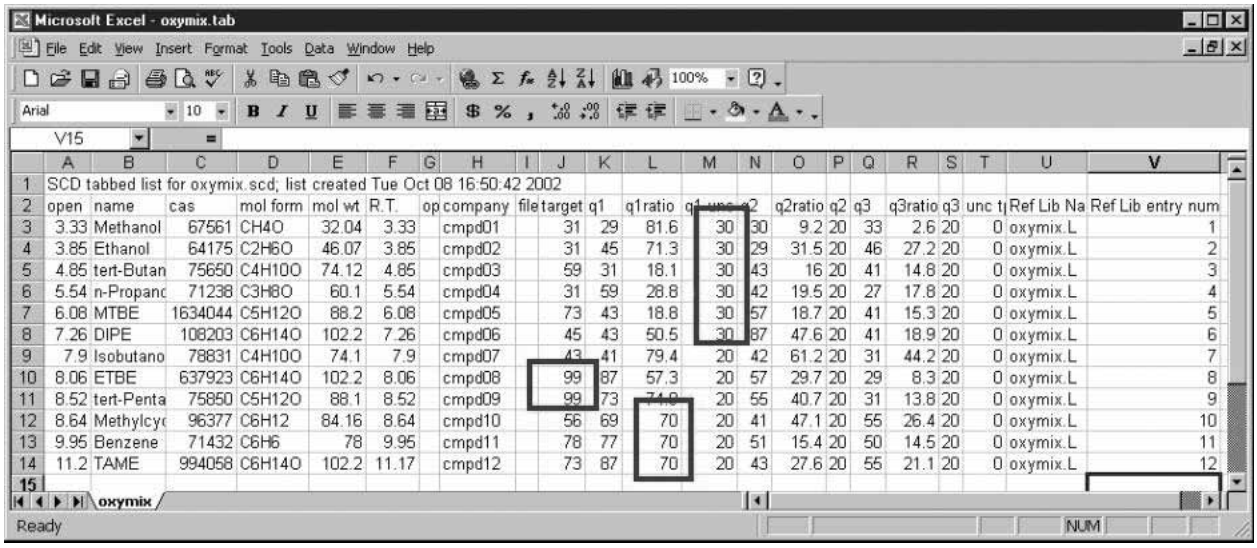


Save the MultiVu window to a file (**File|Save as...|**), for example, oxymix.txt, to be kept as a record.

Edit a *.scd Using a *.tab

If you want to change individual ions, ion ratios, and/or uncertainties etc.

1. Use the "**List Screener Database...**" to generate a .tab file for the .scd to be edited.
2. Open the .tab in Excel. Edit existing entries (select a different target ion, change the qualifier ion ratios etc.). See the example below.



Be very careful in columns U and V. Do not change anything in these two columns.

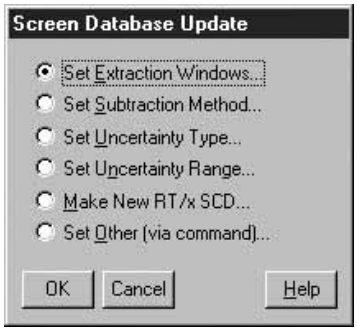
3. Save the **.tab file**, then close Excel.
4. Go to **Enhanced DA**, execute an **rtl_import** command on the command line.
5. Select **SCD only**. The software preserves the edits you have made in the .tab for the .scd.
6. Go to **Tools | List Screen Databases...|** to confirm the changes.

FAQ

When to Use "Set Other (via command)..." Function?

Global changes to the *.scd can be made using the menu item

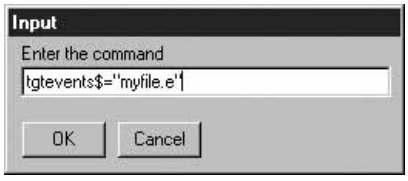
1. **Tools | Change Screen Database Parameters....** The following will appear:



The **Set Other** (via command) is used to make global changes not included in the list.

For instance, if you want to use a specific ChemStation Integrator Parameter file for target ion integration:

2. Choose **Set Other** (via command) and click **OK**.



3. Input the ChemStation Integrator Parameter file you saved, in this case myfile.e, enclosed in quotation marks.
4. Click **OK** and you will see your currently specified method screen database file updated by watching the gray message line at the bottom.

To update qualifier ion intergration parameter files, repeat the above procedure using q1events$, q2events$ and q3events$ for qualifier ion q1, q2 and q3 respectively.

Caution: Global changes made using either one of the preset choices or Set Other will AFFECT ALL COMPOUNDS in the *.scd.

How to Use the Integration Parameters with the Screener?

The screener is always using the "AutoIntegrate Function" when the ChemStation integrator is selected. Because the "AutoIntegrate Function" does not use any of the events files, none of the integration events will be used in the screening process unless an event file was specified for a compound. The screener does not use the autoint.e parameter file. This file is NOT related to the "AutoIntegrate Function".

The screener is integrating extracted ion chromatograms (EICs), not total ion chromatograms (TIC). Therefore, the screener integration parameters should be determined by integrating the EICs. When the optimal parameters are found, save them in an event file (for example, myfile.e).

To associate an event file to all the compounds, refer to the discussion above.

Does RTE Integrator Use any Parameter File?

Yes, the RTE integrator uses rteint.p from your method directory.

1. After selecting the RTE integrator, go to **Chromatogram|MS Signal Integration Parameter...|** to change the integrator parameters.
2. Click **OK**; the parameters are automatically saved to rteint.p.

The screener will always use rteint.p for integration unless you use Set Other (via command) to select another .p file.

Different from the RTE integrator, the ChemStation Integrator always uses the "AutoIntegrate Function" for integration. You have to associate an .e file to the compounds to specify the integration parameters.

How Can I Get the Screener Report to Show Just the Hits and Probable Hits?

1. Go to **|Quantitate|Report Options...|**
2. Check the box next to "**Omit Target Compounds that Are Missed**".

How Can I Get the Screener Report to Show Just the Hits (x)?

1. Go to **|Quantitate|Report Options...|**
2. Check the box next to "**Omit Target Compounds that Are Missed**" and check the box next to "**Have qualifiers Out of Range**".

What Does Tools|Exclude Zero Qualifiers Do?

You get probable hits (designated by a ?) when one or more of the qualifiers do not meet criteria. Many times a qualifier will not meet criteria because its ion abundance is zero. If the ion abundance is zero, the compound probably is not present. Exclude Zero Qualifiers, when checked, eliminates probable hits from the report if any of the qualifiers is zero.

Caution: If a qualifier is small, it could be absent even when the compound is present, so do not use small abundance qualifier ions.

Can I Append Entries to the Library Using Excel?

If you choose to create a Library only or a Library and SCD after executing the rtl_import command, your Library or Library and SCD will be created from scratch, with all counters set to zero. In other words, Excel .tab files can NOT be used to append Library entries to an existing library nor to edit existing Library entries.

How Do I Get Screener Report of a GC Detector on the MS System?

There is no GC mode screener report in the MSD DA, but, here is the work-around. After you load the MS and ECD signal into the ChemStation:

1. Go to **|File|Select Signals...|** and uncheck the **MS signal**.
2. Now, select **|Tools|Create Screen Results for Current File|**.

This will create a screener report for the GC data and save the report to RTLPEST(2).RES. (Depending on the pesticide library revision, you may or may not get the 2 in the file name.)

3. To generate a "pseudo" GC screener report, go back to **|File|Select Signals...|** and check the **MS signal**. Use **|Tools|Generate Screener Report for Current File|** to get a report.

Note: The GC and MS screeners use the same RTLPEST.RES file. They overwrite each other when you screen. If you do not uncheck the MS signal, you will screen and then report the MS signal.

Screen 0,1,"F"

This command, when executed on the command line in Data Analysis View, produces a multipage Screener report for a data file that has already been screened. The first page of the report is a summary report identical to the report from Tools|Generate Screen Report for Current File. Each hit is then reported on a separate page, complete with all the graphics you normally see in Results Screener View. This multipage report is sent to the default printer and is not viewable on the monitor.

What is "Subtraction Method" and Which Method Should I Use ?

The subtraction method that is used is printed near the top of the Screener Report, on the right side. Under Tools | Change Screen Database parameters, one of the choices is Set Subtraction Method. There are four methods from which to choose:

Use Relative Areas - qualifier ion ratios are based on area comparisons to the target ion area. It is NOT recommended to use this method. Small areas may not be integrated or matrix may add significantly to an area. There is NO subtraction done when using this method.

No Subtraction - qualifier ion ratios are based on ion abundances using the spectrum at the apex of the chromatographic peak. This method can be used if there are no interfering ion abundances from matrix. There is NO subtraction done using this method.

Lower of First and Last - qualifier ion ratios are based on ion abundances using the spectrum at the apex of the chromatographic peak MINUS the ion abundances just before the start of the peak or just after the end of the peak. The ion abundances that are subtracted are those that are the lower of either the start or end of the peak. This subtraction method can compensate for ions abundances due to matrix.

Average of First and Last - qualifier ion ratios are based on ion abundances using the spectrum at the apex of the chromatographic peak MINUS the average of the ion abundances just before the start of the peak and just after the end of the peak. This subtraction method can compensate for ion abundances due to matrix, and is the recommended subtraction method to use.

How Do I Build a Quant Database from a Screener Database?

A Quant database is used for quantitating identified compounds and is calibrated. A Screener database is used for identifying compounds, without quantitating them. A Quant database (qdb.mth in the mymethod.m folder) has the same format as a Screener database (such as oxymix.scd in the Database directory). To convert a Screener database to a Quant database, do the following:

1. In the method folder, say mymethod.m, locate the file **qdb.mth.**
2. Rename **qdb.mth** to **qdb.mth.ori** (for original).
3. Copy your Screener database, say **oxymix.scd** from C:\database, and paste it into your method folder, **mymethod.m**.
4. Rename **oxymix.scd** (in the mymethod.m folder) to **qdb.mth**.
5. Reload your method, **mymethod.m**, in Enhanced Data Anaylsis.
6. Select **Calibrate>Edit Compounds** to view the Quant database.
7. Calibrate the Quant database as you normally would.

What Else Can I Do with my Quant Database and Mass Spectral Library?

Agilent introduced Deconvolution Reporting Software (DRS), product # G1716AA. Application Note 5989-1157EN describes the product, its use and performance in detail. DRS uses the results from Quant databases as part of its report. DRS also uses Mass Spectral Libraries in producing its reports. The DRS Help files provide detailed procedures for converting Agilent format Mass Spectral Libraries for use with DRS. So the Quant databases and Libraries you have built using this technical overview have wider application. DRS is a powerful software tool to aid the analyst in finding trace compounds in complex matrices for different industries, for example, forensic toxicology, food safety, flavor and fragrance (that is, allergens), environmental, and homeland security.

Troubleshooting Questions

"When I Execute a Listlib Command, I Only See the Header of the Report, No Entries Listed".

Make sure the file name and the data path is entered correctly

"Could Not Open File: C:\database\oxymix.tab"

Close the file in Excel

"Array Index 6 Out of Bounds"

The TAB file is in Excel (not text tab delimited) format. Re-save the file in tab format.

"Index Out of Range"

There is a mismatch between a library entry number in the *.scd and the library.

The library entry with that number does not exist. To find which *.scd entry has the wrong number, screen a sample with the *scd. Go to **View|Results Screener**. Under the menu item Spectrum, select **|Display Reference Spectra**. The lower left panel should now display the unknown spectrum above the library reference spectrum for that compound. Double click through the compound list until no library reference spectrum is displayed. This compound(s) has an incorrect or missing spectrum in the library.

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3. P. Wylie, M. Szelewski, and C.K. Meng, “Comprehensive Pesticide Screening by GC/MSD using Deconvolution Reporting Software”, Agilent Technologies, publication 5989-1157EN www.agilent.com/chem
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Printed in the USA
June 8, 2004
5989-0916EN

Agilent Technologies