



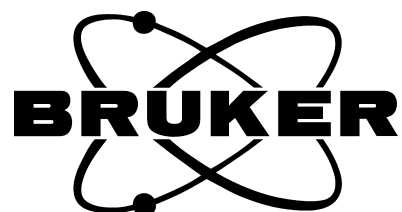
# **OPUS**

Spectroscopy Software

Version 6

## **User Manual**

# **SEARCH**



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This manual is the original documentation for the OPUS spectroscopic software.

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# 1 Introduction

OPUS SEARCH allows to identify unknown spectra by comparing them to spectra libraries. You can use commercially available libraries (e.g. Sadtler), and create your own individual libraries.

OPUS SEARCH can be classified by two functional parts:

- Library Search – to identify unknown substances
- Library Editor – to create individual spectral libraries

The *Library Search* option enables you to search existing libraries. You can select between four different types of search methods:

**a) Spectrum Search**

To identify unknown substances

**b) Peak Search**

To search for one or more specific peaks

**c) Information Search**

To search for names, material characteristics, molecular formulae

**d) Structure Search**

To search for complete or partial substance structures. A structural formula editor helps you to create the respective structural formulae.

The result of such a library search is stored in the form of a report in the SEARCH data block (SEARCH). This report includes links to each spectrum of the substances found. To compare these spectra with the query spectrum it is possible to have them displayed in one window. SEARCH reports can also be used as a basis for further search requests, which also may refine the search method.

The library editor comprises all tools needed to create and maintain your own spectral libraries.


**Note:** OPUS SEARCH utilizes the user name which you have defined for the specific workspace to be able to internally access the database system. Note that this user name will be shortened to 9 characters, and that it only has to include letters and figures. Do not use any special characters (e.g. +\*#) or umlauts (e.g. äöü) as this would cause an error message when trying to access the library system.

## 1.1 Library Structure

A library consists of several files which have the same file name but different file name extensions. This facilitates the providing of backup copies for a library.

FILENAME.D01  
FILENAME.D02  
FILENAME.D03  
FILENAME.D04  
FILENAME.D05  
FILENAME.D06  
FILENAME.D07  
FILENAME.D08  
FILENAME.D09  
FILENAME.D10  
FILENAME.D11  
FILENAME.D12  
FILENAME.D13  
FILENAME.K01  
FILENAME.K02  
FILENAME.K03  
FILENAME.S01  
FILENAME.D02  
FILENAME.TXD

A numbered entry is allocated for each substance within one library. The entry number helps to address the single entries.

Each entry additionally includes an information text which is extracted from the spectrum INFO data block (). The info text mask has to be defined when creating the library and is mandatory for the information input.

The library is restricted to spectra acquired by one single spectroscopic method. Therefore, the library may either include NIR, MIR or Raman spectra, but not a mixture of these types of spectra. Furthermore, you can specify additional OPUS parameters in the method, which will be saved together with the spectrum. The spectrum will then be cut off according to the frequency limits specified and transformed to the digital resolution selected. However, this does not influence the quality of a spectrum search, since the original data files will always be employed for the search.

Optionally, you can define the *Substance Name*, *Molecular Formula*, *Molecular Weight* and *CAS Number* information lines. It is, however, recommended to create these lines at random position in the info mask. If the *Substance Name* line, e.g., cannot be found in the info mask, the content of the first info mask line will automatically be used.

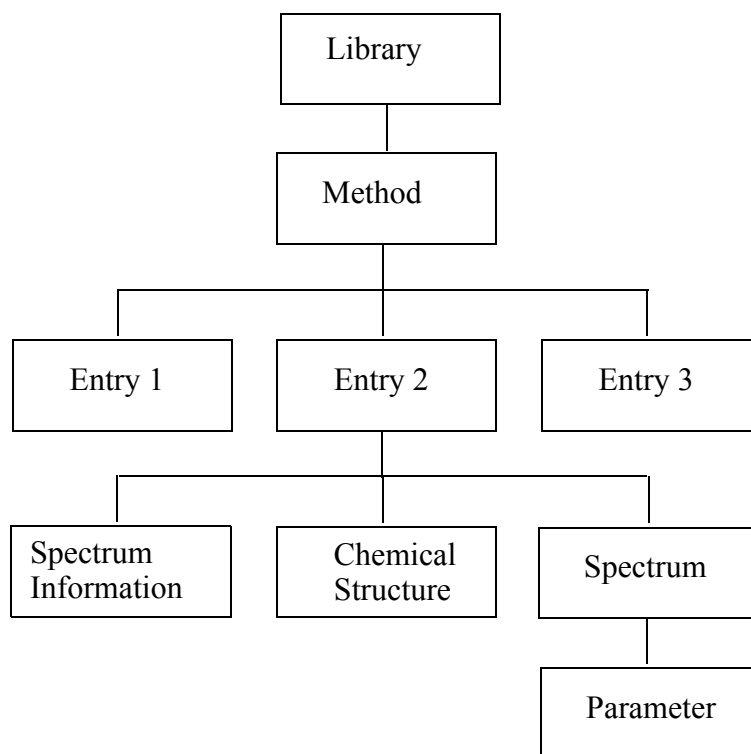


Figure 1: Internal structure of a library entry





# 2 Library Search

The aim of any library search is to identify an unknown substance by its optical spectrum. As already mentioned in chapter 1 four different search methods are available:

**a) Spectrum Search**

An unknown spectrum is compared with the library spectra. Library spectra which show distinct similarities to the unknown spectrum are detected and reported.

**b) Peak Search**

One or several band positions can be entered manually. This allows searching for spectra which are not available in a digital format (i.e. only a hard copy exists).

**c) Information Search**

An information search refers to the kind of information stored together with the spectra. Example: if you search for spectra of substances which have a specific molecular weight, you can narrow down the number of spectra searched for.

**d) Structure Search**

This is the only *reliable* method to find single substances or compound classes in a library. A complete or partial molecular structure is compared with the data stored in the library.

Before starting any search, load the unknown spectrum into the OPUS browser window. OPUS provides a *DEMOLIB* (demo library) which has been used for most of the following examples.

## 2.1 OPUS SEARCH Icons

All OPUS SEARCH commands can easily be accessed by specific OPUS SEARCH icons in the tool bar which you first have to configure. For further details on how to configure the tool bar, refer to the OPUS Reference Manual. OPUS SEARCH commands are listed in the OPUS *Evaluate* menu.

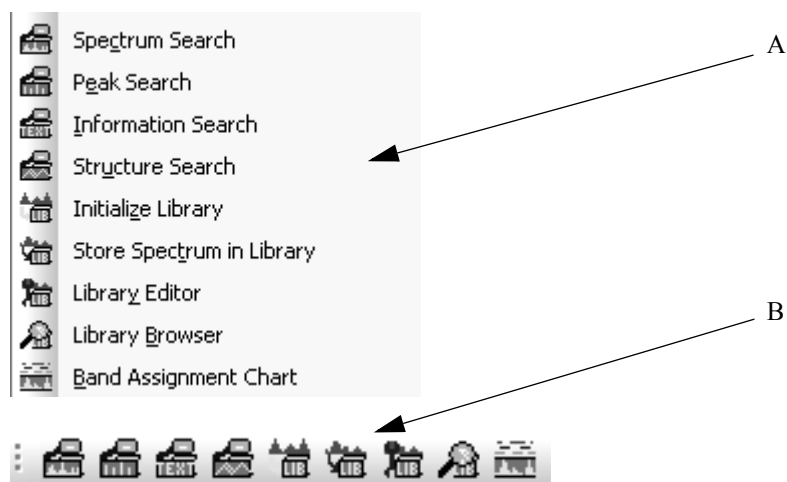


Figure 2: OPUS SEARCH functions

## 2.2 Selecting a Library

You have to define one or more libraries to be used for the search, irrespective of the search method you select. Select any search method described either by defining the respective search command (A) from the *Evaluate* menu or clicking on the respective icon on the tool bar (B). Note that the *Select Libraries* tab will be the same for all search methods.

The following example have been created by using the *Spectrum Search* command. Click on this command and select the *Select Libraries* tab.

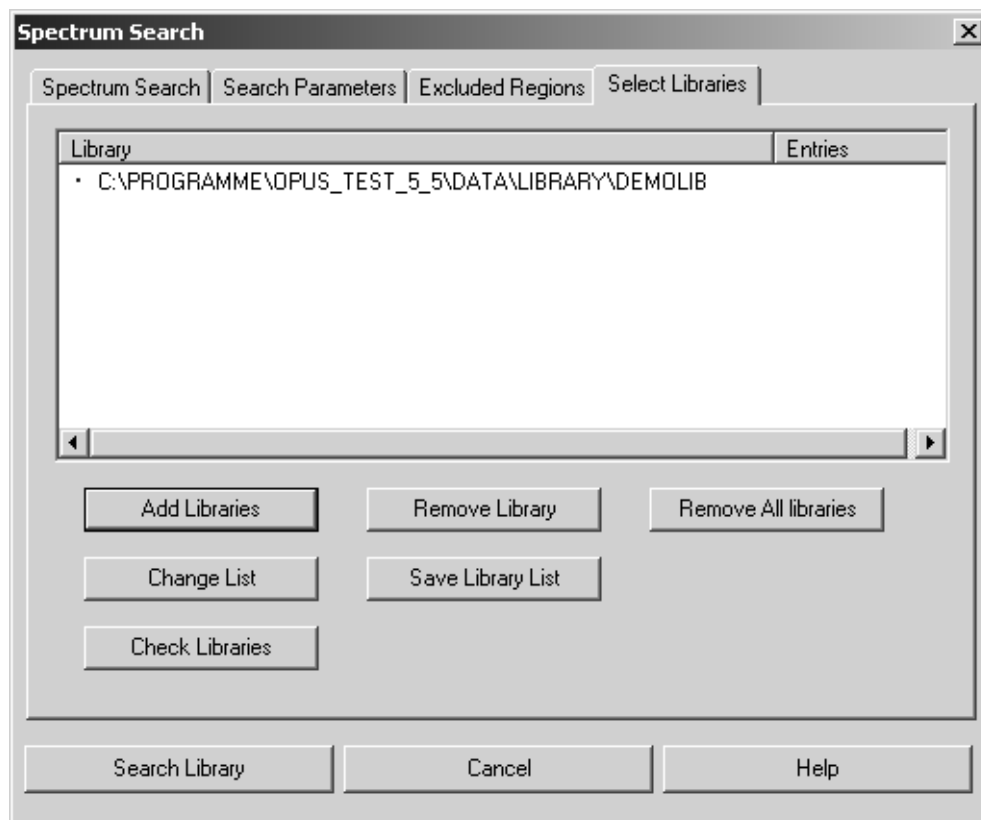


Figure 3: Spectrum Search - Select Libraries tab

As the libraries selected during the last query will automatically be included in the *Library* selection field, the *DEMOLIB* library is displayed in figure 3. You can add libraries to or remove libraries from the library list by clicking on the *Add Libraries* or *Remove Library* buttons.

The libraries displayed in the *Library* selection field will be used for the query. Frequently-used library lists can be saved and re-loaded by clicking on the *Save Library List* and *Change List* buttons.

You can also load Sadtler libraries into the *Library* selection field. Sadtler libraries have the file extension *.IDX*. Any library in OPUS and Sadtler format can be combined for one search.

Sadtler libraries are protected by a dongle. You have to install the dongle drivers which are stored on the OPUS CD (directory: SENTINEL), and copy the *IR.CTL* Sadtler control file to the OPUS directory. This *CTL* file is either stored on the Sadtler libraries CD or on a different disk supplied. To activate the dongle driver you have to reboot the PC.

The library status is indicated in different ways. Library entries checked by a green check mark have been tested and are correct. An exclamation mark indicates an error, whereas a dot means that the library integrity has not been tested.


Therefore, click on the *Check Libraries* button (figure 3). If the library is OK, it will be checked by a green check mark. A red cross indicates the library could not be found. This may occur, if the library has been deleted or the directory changed. If you want to load the library from CD, insert the CD into the CD drive, and keep the CD in the drive during the search run.

If the library has been tested, the number of library entries will be displayed.

Library	Entries	
• Q:\PROGRAMME\OPUS\DATA\LIBRARY\DEMOLIB		
• R:\OPUS LIBS ETC\LIBRARY\SOLVENTS.S01	60	a) not checked
• R:\OPUS LIBS ETC\LIBRARY\LIB-AQ\BAS.F.S01	3929	
• R:\OPUS LIBS ETC\LIBRARY\LIB-IA05\MAGASPH.S01	189	
Library	Entries	
✓ Q:\PROGRAMME\OPUS\DATA\LIBRARY\DEMOLIB		
✓ R:\OPUS LIBS ETC\LIBRARY\SOLVENTS.S01	60	b) test passed
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-AQ\BAS.F.S01	3929	
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-IA05\MAGASPH.S01	189	
Library	Entries	
✗ Q:\PROGRAMME\OPUS\DATA\LIBRARY\DEMOLIB		
✓ R:\OPUS LIBS ETC\LIBRARY\SOLVENTS.S01	60	c) not found
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-AQ\BAS.F.S01	3929	
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-IA05\MAGASPH.S01	189	
Library	Entries	
! Q:\PROGRAMME\OPUS\DATA\LIBRARY\DEMOLIB		
✓ R:\OPUS LIBS ETC\LIBRARY\SOLVENTS.S01	60	d) test failed
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-AQ\BAS.F.S01	3929	
✓ R:\OPUS LIBS ETC\LIBRARY\LIB-IA05\MAGASPH.S01	189	

Figure 4: Different library status

## 2.3 Spectrum Search

Start the *Spectrum Search* command either from the *Evaluate* menu or the tool bar () and load the spectrum by drag & drop from the OPUS browser window into the *Files to Search* selection field (figure 5).

When using the *Spectrum Search* option transmission spectra will automatically be converted into absorption spectra, to get a reasonable result. However, both the query spectrum and the search results will be displayed in transmission.

If you store transmission spectra, they will automatically be converted into absorption spectra. This conversion will be performed internally and will not have any influence on the original spectrum.

**Note:** If you have created a library using transmittance spectra, it is recommended to convert the spectra into absorption spectra.

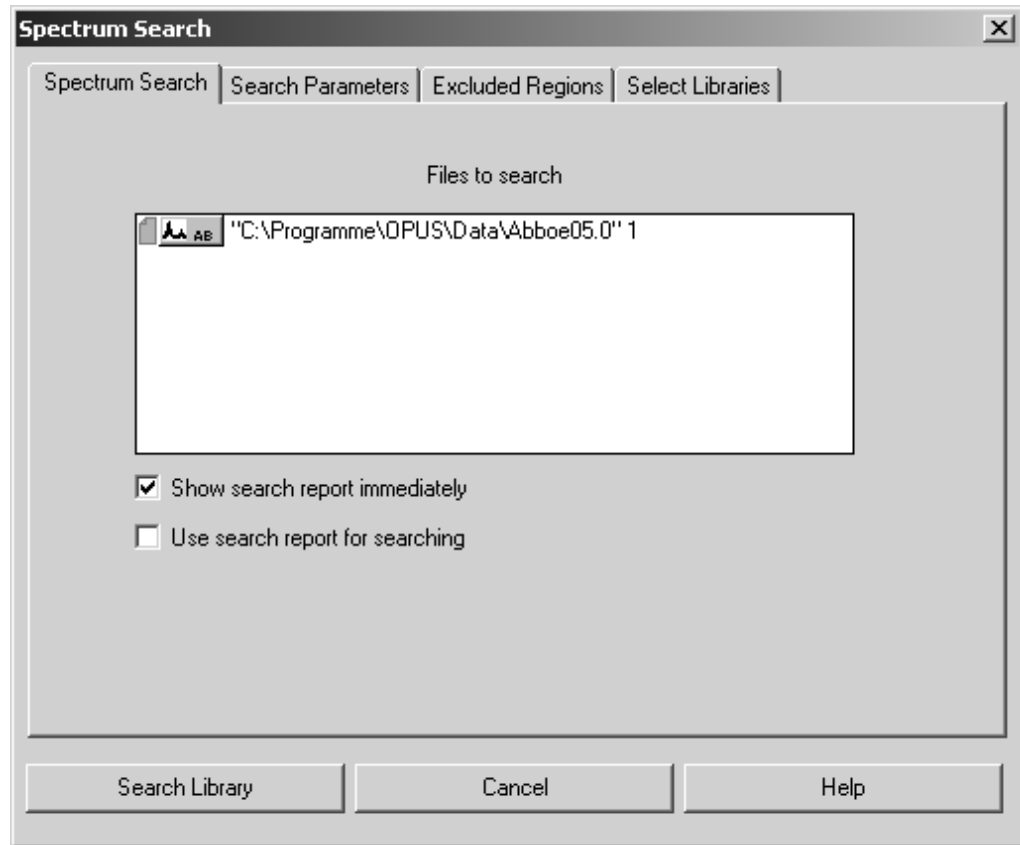


Figure 5: Spectrum Search dialog

If you activate the *Show search report immediately* check box, a library window will automatically be displayed after the search.

If you activate the *Use search report for searching* check box, a dialog pops up from which you can select an already existing search report. In this case the search will not be performed by means of the settings made on the *Select Libraries* tab, but only by those spectra which are included in the search report. This enables to refine a search previously performed.

### 2.3.1 Search Parameters

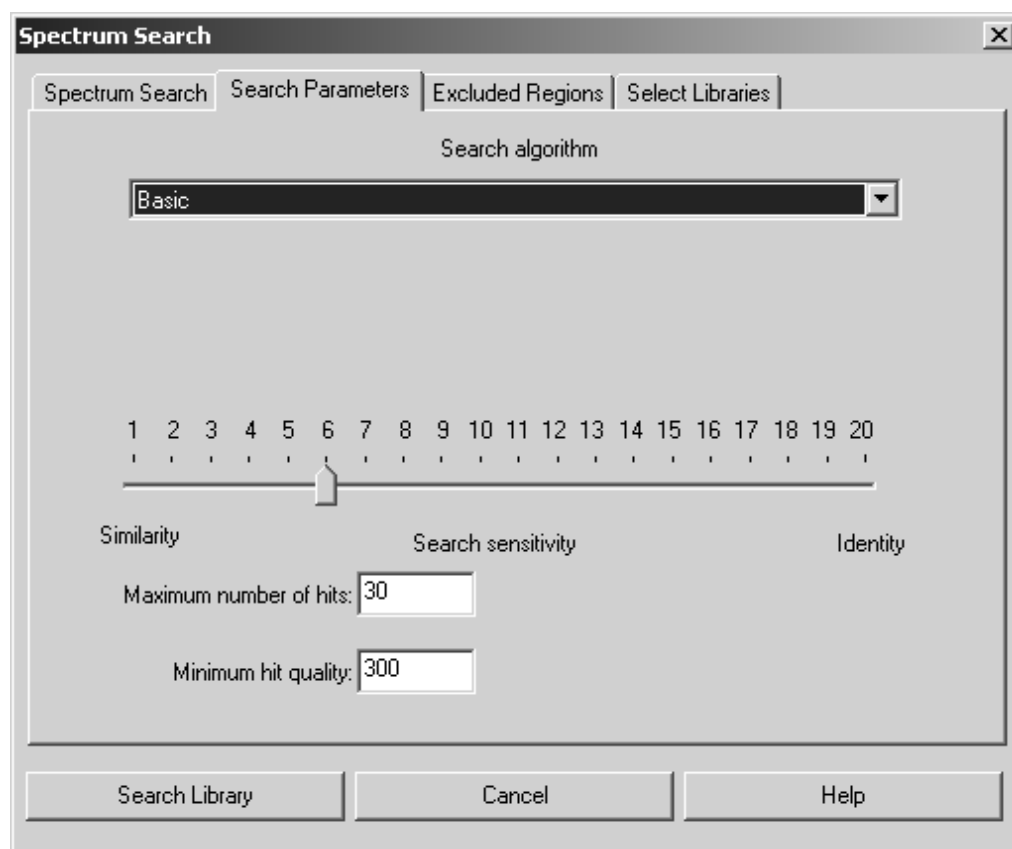


Figure 6: Spectrum Search – Search Parameters tab

Use the drop-down list to select between 4 search algorithms.

**a) Basic**

This algorithm requires a peak table in addition to the search spectrum. This peak table will temporarily be generated during the search.

**b) Standard**

This algorithm is similar to the *Basic* algorithm and additionally takes into account whether the respective peaks in the search or library spectrum have similar intensities. Depending on the substance measured you can also define whether the spectrum to be searched for contains one component (in case of a single substance) or multiple components (in case of compounds). In the first case the hit quality achieved is reduced by a certain factor if the number of bands in the library spectrum is less than the number of bands in the query spectrum.

**c) Weighed Peak Matching**

In case of this algorithm all pieces of band information, which are available from the query and library spectrum, are reflected in the hit quality. The information contains the position, relative intensity and half-width of each band. A library spectrum band is considered to be identified in the query spectrum if this spectrum contains a band

- which position does deviate from the position in the library spectrum by less than the half-width,
- which difference between the half-widths and relative intensities is less than factor 2, respectively.

This algorithm also allows to further specify the search result. Select the appropriate option button to define whether the measurement of the query spectrum has been performed by one main component or by multiple components.

#### d) Use Existing Peak Table

This algorithm uses an already existing peak table, which enables you to suppress the influence of peaks originating from the substrate. If you use this algorithm, the *Search Sensitivity* parameter will not be available. Depending on the measurement you can additionally define whether the spectrum to be searched for contains one component (in case of a single substance) or multiple components (in case of compounds).

#### e) Spectrum Correlation

This algorithm calculates the sum of the squared deviations between the query spectrum and the result spectrum for the data points of the range defined. The summation can be limited to a spectral range selected by the user.

If you use this algorithm, the *Search sensitivity* slider is replaced by two additional drop-down lists, *Normalization Method* and *Derivative*. For details on these methods, see chapter 8 in the OPUS Reference Manual.

The search algorithms described can also be used for Sadtler libraries. However, the *Standard* search algorithm might differ in quality, compared to the search in OPUS libraries, due to the different file formats of Sadtler libraries.

Therefore, it is recommended to test the algorithms first and use a correlation algorithm if you do not get unambiguous results.

### Sensitivity

The *Search sensitivity* allows you to influence the search result. As the search result substantially depends on the type and quality of the spectra acquired, it is not possible to give a general recommendation on how to optimally set the sensitivity value.

In the case of spectra obtained from KBr pellets with a normal signal-to-noise ratio you can start with a sensitivity value between 6 and 10. It is recommended, however, to perform several test runs applied to spectra of known samples to learn about the influence of the *Sensitivity* parameter. As a general rule of thumb, settings greater than 15 rarely produce useful results.

### **Maximum Number of Hits**

Specify the number of hits which will be saved in the search report.

### **Minimum Hit Quality**

A hit quality of 1000 would be a perfect conformity, whereas a value of 0 is obtained if there is no correlation at all. In general, the search algorithm produces a value of  $>0$  even if there are no or negligible similarities between spectra. Therefore, it is reasonable not to include all hits below a certain limit (default setting: 300) into the search report. As the *Minimum hit quality* also depends on the data acquisition method it first should be evaluated by measuring reference samples. Only if such a search yields no hits should you set the *Minimum hit quality* to a lower value.

If you have set all parameters, click on the *Search Library* button to start a search. The search result will be stored in a search report. For further details on the influence of certain search parameters, refer to chapter 2.3.4.



## 2.3.2 Excluded Regions

It is also possible to exclude certain spectral regions from the search. If you click on the *Excluded Regions* tab, the following dialog opens:

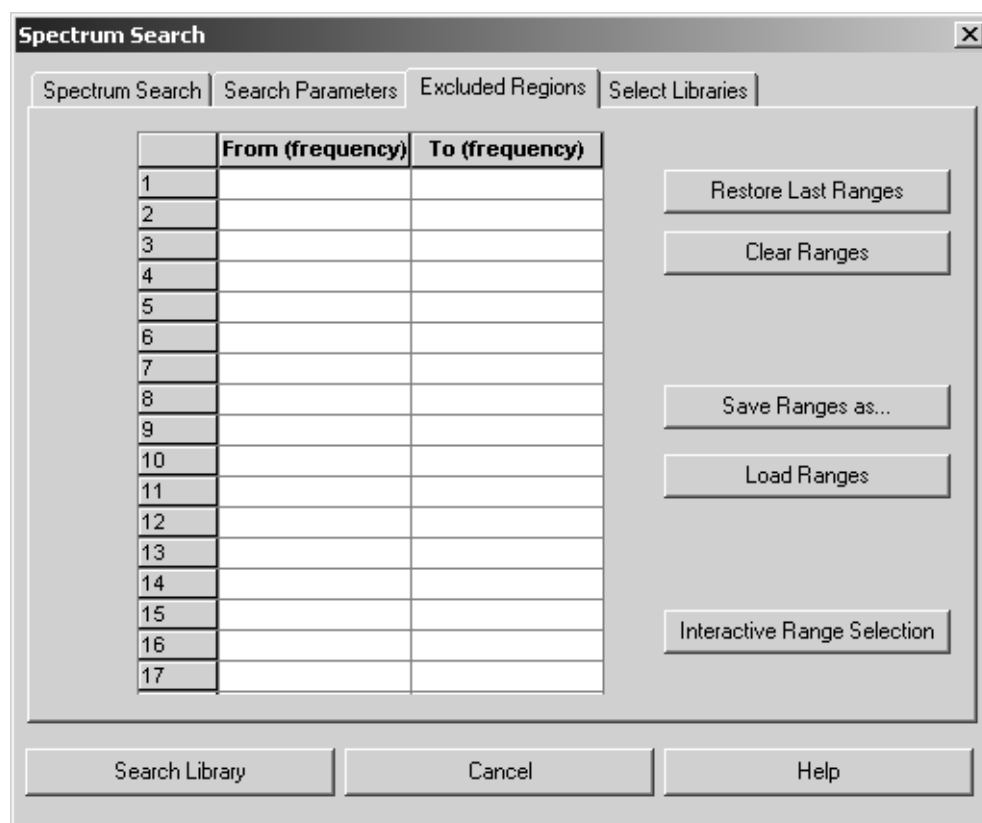


Figure 7: Spectrum Search – Excluded Regions tab

There are several possibilities to define the regions you want to exclude. You can enter the ranges manually into the table. If you want to use the frequency ranges of previous search runs, click on the *Restore Last Ranges* button.

Sometimes it may be advisable to delete CO<sub>2</sub> bands from an MIR spectrum. Click on the *Clear Ranges* button to delete the table entries and enter the new ranges you want to use for the next query.

To delete single lines only, click on the respective line number and press the *DEL* button on the PC keyboard. If you have completed the frequency table, save the settings by clicking on the *Save Ranges as* button. To restore the data sets saved click on the *Load Ranges* button.

If you prefer to interactively select the frequency ranges, click on the *Interactive Range Selection* button. A window opens and displays the query spectrum. Right-click on the spectrum and select the *Add Region* button from the pop-up menu. The spectral ranges to be excluded are displayed on a white background. If you position the cursor on the edges of the spectral ranges and press the left mouse button, you can re-size the ranges.

### 2.3.3 Select Libraries

The *Select Libraries* tab is the same as described for *Spectrum Search* (see section 2.3)

### 2.3.4 Library View and SEARCH Report

The search result is added to the query spectrum in the form of a SEARCH data block (SEARCH), see figure 9. All these SEARCH reports have the same structure, regardless of the search method used. A report will automatically be displayed after a search, provided you have activated the *Show Search Report immediately* check box (see figure 5).

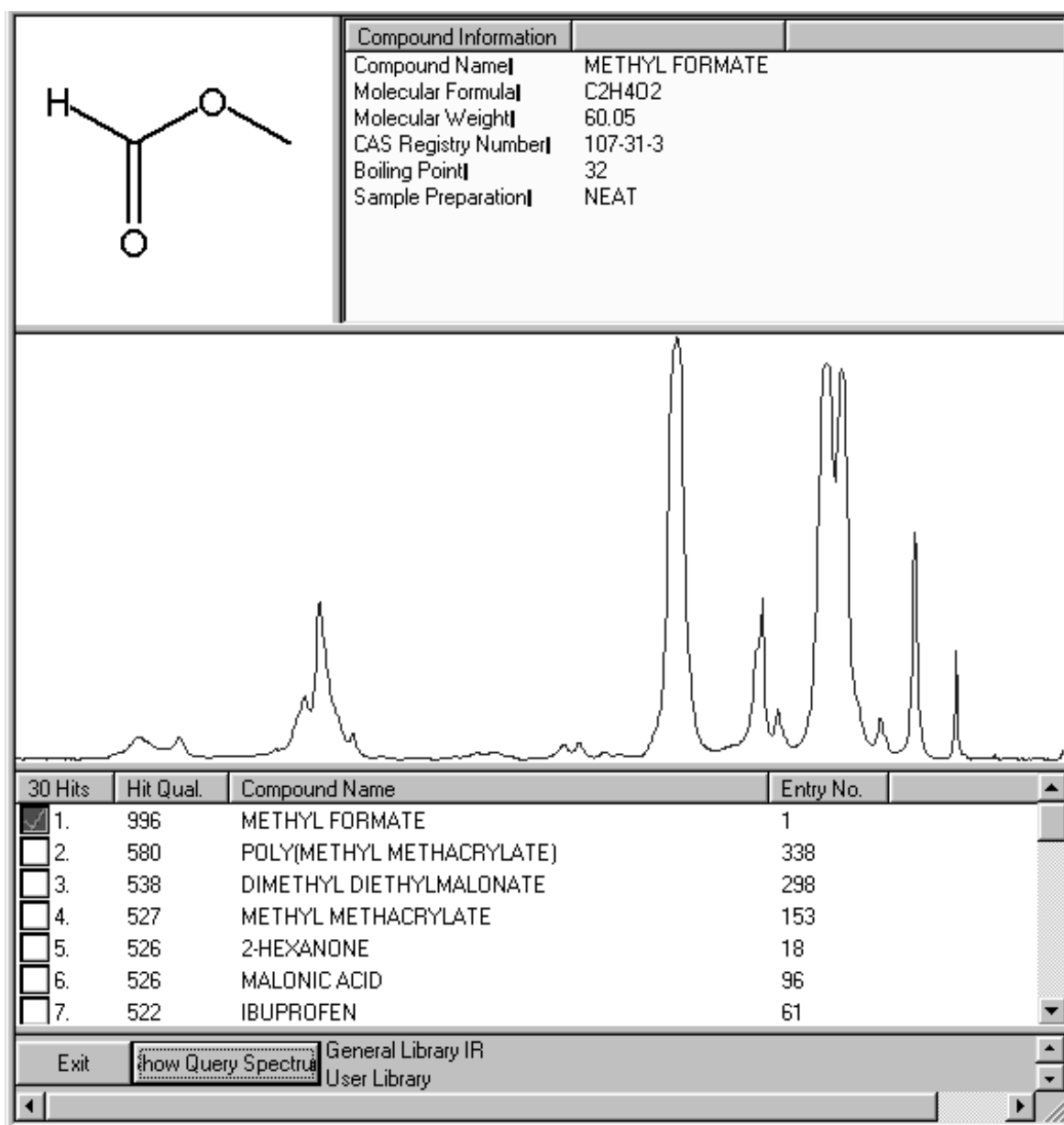


Figure 8: Library windows

The library view consists of four different windows which can be re-sized by moving the window borders (figure 8). The bottom window includes the total number of search hits ranked according to their hit quality. Additional features of the hit list are the compound name, entry number of the substance, molecular formula, molecular weight and the CAS number.

Generally, the first hit is automatically checked and its spectrum is displayed together with the structural formula and compound information. You can deactivate the first hit and activate a different one.

Use the *Show Query Spectrum* button (figure 8) to have the query spectrum displayed. Spectra are automatically displayed in transmittance, if the query spectrum is a transmittance spectrum. If you have clicked on the *Show Query Spectrum* button, the button will change into *Hide Query Spectrum*. Right to this button you can see the library description and copyright.

Closing the library window adds a SEARCH data block (figure 9) to the query spectrum file in the OPUS browser window. If you right click on the data block, the *Show Report* menu pops up. Click on this menu to open the corresponding report window.

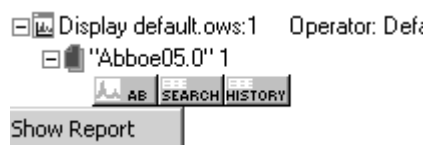


Figure 9: SEARCH data block and Show Report menu

The report window includes its own browser, which helps you to navigate (figure 10). On the right side the number of hits are displayed as well as the library number which is important if several libraries have been used for the search. Additional information on the query are displayed on the lower part of the search report window.

Hit No.	Hit Quality	Compound Name	Entry No.	Lib. Index
1	540	GLYCEROL	106	1
2	540	GLYCEROL	106	2
3	514	ETHYLENE GLYCOL	35	1
4	514	ETHYLENE GLYCOL	35	2
5	502	1,7-DIAMINOHEPTANE	186	1

Figure 10: Search report window

Expand the *Report of Spectrum Search* directory to have the search parameters displayed.

Search Parameters	Values
Report of Spectrum Search	
Algorithm	Standard
Number of Hits	30
Date:	2003/12/05
Time:	11:01:50 (GMT+1)
Searched Method:	
1. Library:	C:\OPUS\DATA\LIBRARY\DEMOLIB
2. Library:	C:\PROGRAMME\OPUS\DATA\LIBRARY\DEMOLIB.S01
Searched Spectrum:	C:\Programme\OPUS\DATA\Abboe05.0
Search Sensitivity:	13

Figure 11: Search parameters

The *Search Parameters* include all relevant details about the search:

- Search algorithm used
- Number of hits
- Date of the search
- Time of the search
- Search method
- List of libraries used for the search (with name and directory)
- Directory and name of the query spectrum
- Sensitivity value used for the search

**Note:** The last two parameters are only valid for the spectrum search. If you use the peak, information or structure search, the parameters will indicate information on:

- Band search: number of bands, band position
- Information search: number of queries, query
- Structure search: name of the structure file

### **Example: Search using the standard algorithm**

Load the *Search 5.0* file from the *OPUS/DATA* directory. This file includes a methyl-propyl-ketone spectrum. Perform several queries using the sensitivity settings listed below:

*Sensitivity: 10*

30 Hits	Hit Qual.	Compound Name	Entry No.	
<input checked="" type="checkbox"/>	1.	911	METHYL PROPYL KETONE	5
<input type="checkbox"/>	2.	701	2-HEXANONE	18
<input type="checkbox"/>	3.	595	DIISOBUTYL KETONE	297
<input type="checkbox"/>	4.	536	3-HEPTANONE	57
<input type="checkbox"/>	5.	477	ISOPROPYL METHYL KETONE	19
<input type="checkbox"/>	6.	464	ISOCTANE	263
<input type="checkbox"/>	7.	451	DIETHYL KETONE	36

Methyl-propyl-ketone has a substantially higher hit quality than all the other substances listed. This kind of setting produces an unambiguous result.

*Sensitivity: 1*

30 Hits	Hit Qual.	Compound Name	Entry No.	
<input checked="" type="checkbox"/>	1.	950	METHYL PROPYL KETONE	5
<input type="checkbox"/>	2.	935	2-HEXANONE	18
<input type="checkbox"/>	3.	675	DIISOBUTYL KETONE	297
<input type="checkbox"/>	4.	638	ISOPROPYL METHYL KETONE	19
<input type="checkbox"/>	5.	623	4-HYDROXY-4-METHYL-2-PENTANONE	33
<input type="checkbox"/>	6.	604	ETHYL BUTYRATE	32
<input type="checkbox"/>	7.	537	4-METHYL-2-PENTANOL	40

Again, methyl-propyl-ketone has been identified as hit no 1. However, the criterion of spectra identity is less stringent. Even hit no. 2 produces a high hit quality.

*Sensitivity: 20*

30 Hits	Hit Qual.	Compound Name	Entry No.	
<input checked="" type="checkbox"/>	1.	828	METHYL PROPYL KETONE	5
<input type="checkbox"/>	2.	706	2-HEXANONE	18
<input type="checkbox"/>	3.	646	ACETONE	93
<input type="checkbox"/>	4.	614	1-PROPANOL	107
<input type="checkbox"/>	5.	599	3-HEPTANONE	57
<input type="checkbox"/>	6.	591	3-PENTANOL	147
<input type="checkbox"/>	7.	569	ISOBUTANOL	131


Even in case of this very extreme setting, which allow only very small deviations from the identity, methyl-propyl-ketone remains hit quality no 1. The absolute hit quality of the spectrum correctly searched is the lowest, compared to the other sensitivity setting as even the smallest deviations are considered.

We know from experience that sometimes too extreme a sensitivity value produces results which could hardly be interpreted. Therefore, it is advisable to test several sensitivity settings, and whether the values found make sense.

## 2.4 Peak Search

A peak search is a very simple but powerful search option. You can perform a search on one or more bands, which will then be compared to the selected libraries using different algorithms. The result of a peak search performed on a Sadtler library substantially depends on the number of bands stored in this library.

According to our experience, sometimes minor peaks may not be recorded in the Sadtler database. The search for strong and medium bands should, however, yield identical results. Different algorithms can be used. To reasonably limit the search results, you can enter a tolerance limit and intensity criteria for each band. This search type is often applied to data obtained from older instruments (where the results are plotted on paper) and digital data is not available. But it can also be used to get an answer to the question *Which spectra show a peak at...?*

To perform a peak search, select the *Peak Search command* from the *Evaluate* menu or click on the  icon.

### 2.4.1 Peak List for Peak Search

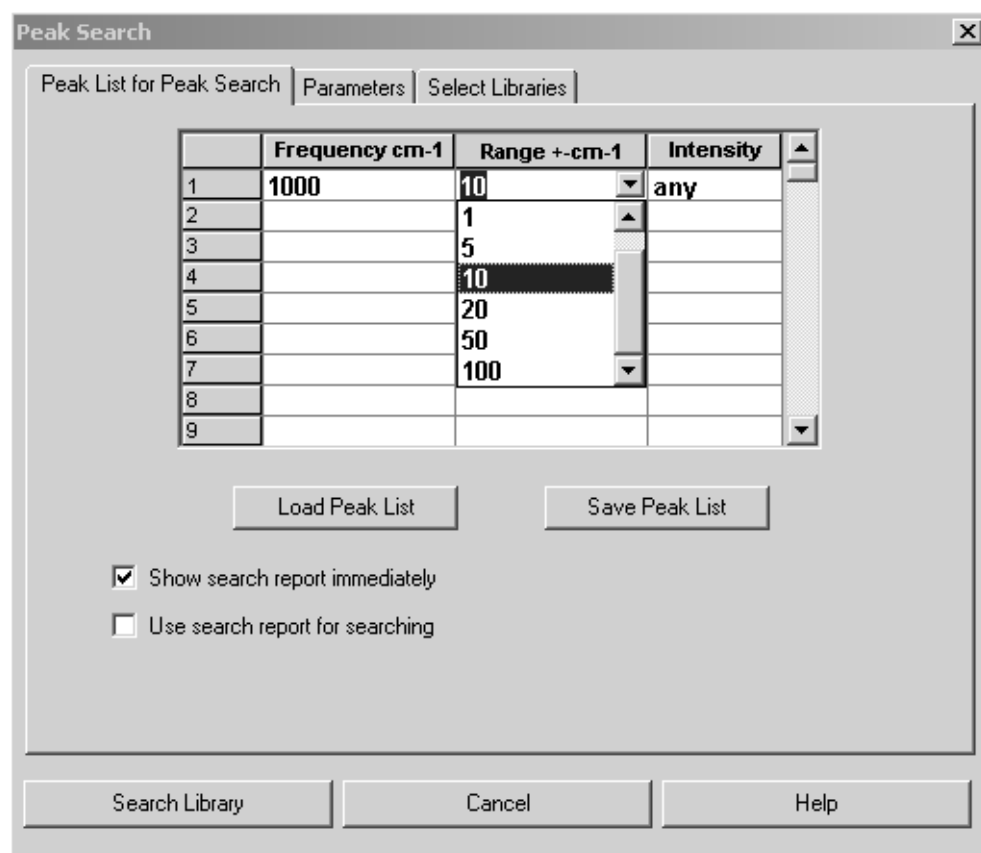


Figure 12: Peak Search – Peak List for Peak Search tab

On the *Peak List for Peak Search* tab a peak table is displayed to be used to enter the peak position, tolerance as well as the intensity of the peaks you want to search for. The *Range* and *Intensity* columns provide drop-down lists for convenient data input. Click on one of the columns to activate this drop-down list.

In the *Range* column you can enter a tolerance value as wavenumbers. This tolerance range will be added to both sides of the peak. If you use a frequency of  $1000\text{cm}^{-1}$  and a tolerance range of  $20\text{cm}^{-1}$ , all peaks between  $980$  and  $1020\text{cm}^{-1}$  will be considered.

In the *Intensity* column you can set the intensity of peaks at 3 different levels, i.e. *strong*, *medium* and *weak*. The range is calculated relatively to the strongest peak (100%) and covers the following areas:

- Weak: 0% - 50%
- Medium: 50% - 75%
- Strong: 50% - 100%

If you do not want to consider the intensity, select the *any* option from the drop-down list in the *Intensity* column.

To save the peak list click on the *Save Peak List* button. To use a peak list previously created click on the *Load Peak List* button. A peak list will always be saved as separate file with the extension *\*.PKL*. When starting a search the current peak list is automatically saved in the *DEFAULT.PKL* file. However, the file content will be updated during the next search run. When using the *Peak Search* algorithm it is also possible to restrict the search to the range of an existing search report, as described in section 2.3.

## 2.4.2 Parameters

On the *Parameters* tab you select the search algorithm, the maximum number of hits as well as the minimum hit quality. The *Minimum Hit Quality* entry field is only available if you have selected the *Calculate Hit Quality* algorithm (see figure 13).

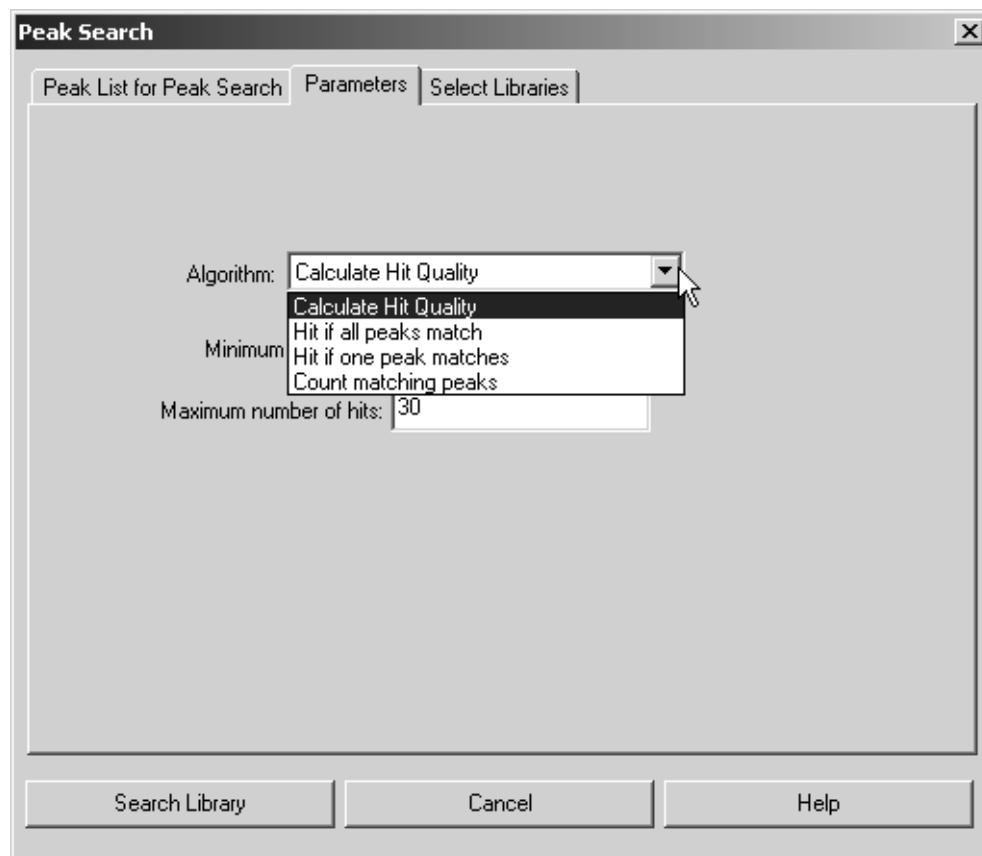


Figure 13: Peak Search – Parameter tab

The following algorithms are available:

**a) Calculate Hit Quality**

The results produced by this algorithm are similar to those produced by using the *Spectrum Search* algorithm. It calculates a hit quality from the difference between the position of the search peak and the peak found in the library. The larger the difference between these two peak positions, the lower will be the resulting hit quality.

**b) Hit if all Peaks match**

A spectrum is only considered to be identical if it includes all peaks specified in the peak list. In this case the hit quality is always “1000”.

**c) Hit if one Peak matches**

A spectrum is considered to be identical if it includes at least one peak specified in the peak list. In this case the hit quality is always “1000”.

**d) Count matching Peaks**

This algorithm indicates the number of peaks found as hit quality. At least one peak has to be congruent with the peak list in order for the spectrum to be included in the hit list.

The result of a peak search will also be stored in a SEARCH data block (see section 2.3.4). The *Select Libraries* tab is the same as described for spectrum search (see section 2.2).



**Example:**

Select the *SEARCH3.0* file as query spectrum and the *DEMOLIB* library as the only library. Enter the following peaks into the peak list on the *Peak List for Peak Search* tab of the *Peak Search* command:

Frequency	Region	Intensity
3434	20	middle
1452	20	middle
1111	20	strong
973	20	middle

Use all 4 algorithms to perform a peak search:

- **Calculate Hit Quality:**  
The correct spectrum is listed as the first hit with a hit quality of “901”.
- **Hit if all Peaks match:**  
The only hit is the correct spectrum.
- **Hit if one Peak matches:**  
Yields 203 hits and each hit has a hit quality of “1000”.
- **Count matching Peaks:**  
A total of 203 hits can be ranked according to the number of matching peaks.

## 2.5 Information Search

The information search allows to search for all data stored, e.g. general compound information or spectral data. You can simultaneously search for several parameters, combining different types of search criteria.

To perform an information search, click on the *Information Search* command in the *Evaluate* menu or click on the  icon.

## 2.5.1 Query for Information Search

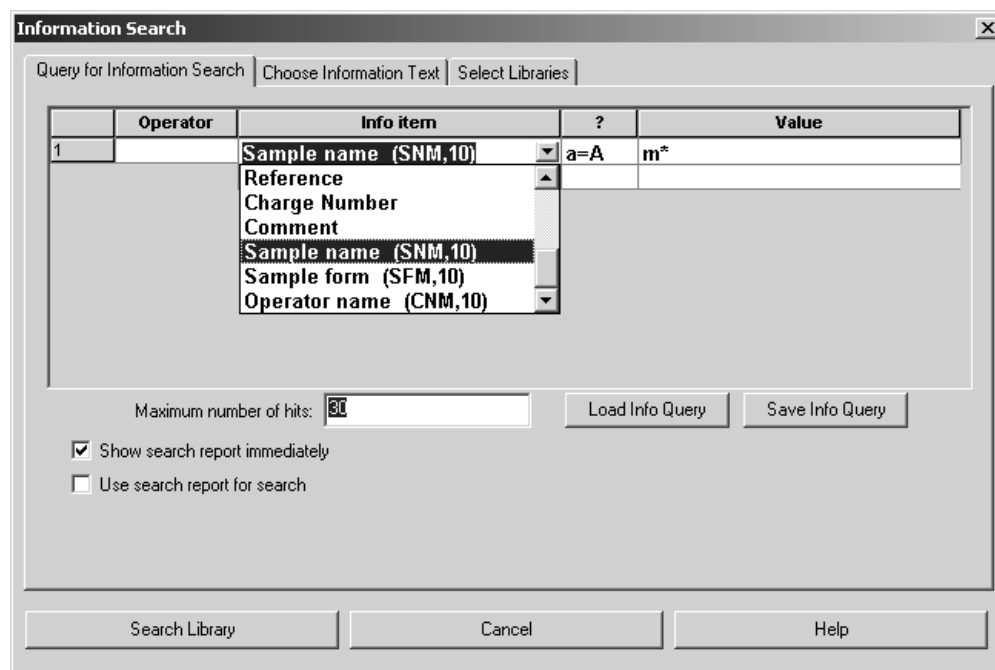


Figure 14: Information Search - Query for Information Search tab

On the *Query for Information Search* tab you set the search criteria. Each row of the table displayed corresponds to a parameter and its corresponding value to be searched. You can either type the entries manually or select them from a drop-down list which will be activated as soon as you click on one of the lines.

You can limit the number of hits, save a search query once created and reload it, and restrict the search to an existing search report.

The search items set cannot be individually configured for each library. There is only a global set of information fields which is the same for all libraries. This may cause empty result lists if there is no information available at all in the specific library file searched. Therefore, it is recommended to check the libraries using the library browser.

The functions of each column will be explained in the following:

### a) Operator

A logical combination of several search criteria in one query can be achieved by using the boolean operators *AND*, *OR*, *OR NOT* and *AND NOT*:

- OR - only one search criterion has to be met to generate a hit.
- AND - all conditions combined with AND have to be met to generate a hit.
- OR/AND NOT - are the negations of the above operators, i.e. these conditions may/must not be met to generate a hit.

**b) Info Item**

In this column you define the parameters to be searched for. The parameters available depend on the libraries selected for the search. Specify the corresponding info item by the drop-down list.

**c) ? – Comparative Operators**

Select the comparative operator for the parameters defined. There are operators for text (a=A, A=A) and numerical comparison (=, <, >, >=, <=):

- a=A: case-insensitive text comparison
- A=A: case-sensitive text comparison
- ==: equality of numbers including the decimals
- >: the number in the library must be greater than the number defined here
- <: the number in the library must be less than the number defined here
- >=: the number in the library must be greater than or equals the number defined here
- <=: the number in the library must be less than, or equals the number defined here

If *Molecular Formula* has been selected as info item, the comparing text operators will not be available.

**d) Value**

Enter the value to be searched for in this column. Depending on the comparison operator the value is treated as text or as a number. In case of text comparison there is an additional set of control characters available to allow a more specific sub-string search:

- \$: the string following the character must be at the beginning of the text
- \*: replaces the rest of a string (wild card)
- ?: replaces exactly one character of a string
- %d: replaces a number
- %l: replaces a character
- %p: replaces either a number or a character
- %w: replaces any sign which is neither a number nor a character
- @: ignores blanks

**Example:**

<i>benzene</i>	returns benzene and methyl benzene
<i>\$benzene</i>	returns benzene but not nitro benzene
<i>benzoi?</i>	returns benzoin and benzoic
<i>benz*</i>	returns benzoin, benzoic, benzopyrene etc.
<i>%d-Methyl*</i>	returns e.g. 1-Methyl..., 2-Methyl... etc.
<i>*%p%d-Methyl*</i>	returns e.g. 3-Methyl... and ...1,3-Methyl...

## 2.5.2 Choose Information Text

The *Choose Information Text* tab is only relevant if you use more than one library for the search. In general, an information search employing several libraries does only make sense if all libraries have an identical information mask. Therefore, the info data sets of all libraries loaded are displayed on the *Choose Information Text* tab.

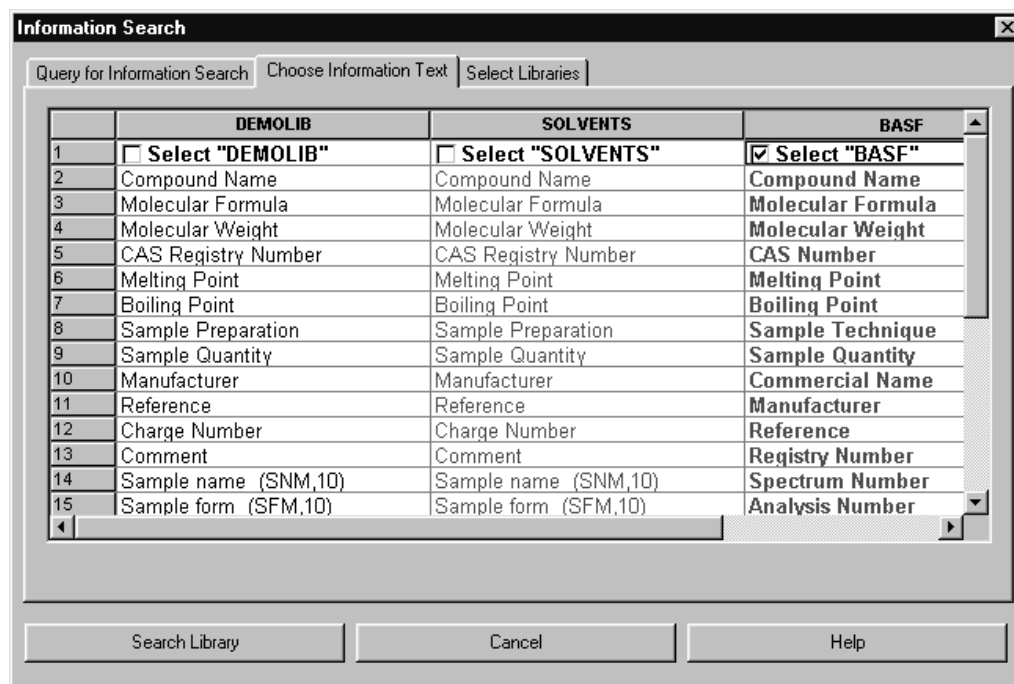
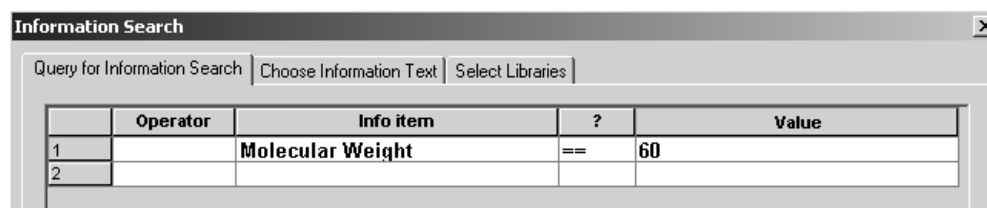


Figure 15: Information Search – Choose Information Text tab

Fig. 15 shows the info data sets of three libraries loaded for an information search. The first two info data sets are identical, whereas the third set differs from the others in some parameters. The deviations are indicated in red.

Click on the *Search Library* button to start the search query. The result will be stored in a SEARCH data block (see chapter 2.3.4). Further information search examples will be described below:

### Example: Numerical Search



This setting generates only one hit if a library entry contains a molecular weight value of 60. A value of 60.05 would not qualify as a hit.

	Operator	Info item	?	Value
1		Molecular Weight	>=	60
2	AND	Molecular Weight	<=	61

This setting retrieves all entries with a molecular weight between 60 and 61.

	Operator	Info item	?	Value
1		Boiling Point	==	60
2	AND	Boiling Point	a=A	Decomposition
3				

Sometimes a numerical field also includes additional text (e.g. *Decomposition* in the second line). The string can either be searched separately or in combination with the numerical value.

The *Compound Name* and *CAS Registry Number* info item options are limited to a text search, the *Molecular Weight* info item option to a numerical search. If the content of a field is recognized as *Molecular Formula*, the *Molecular Formula Search* (see below) will automatically be performed.

The remaining info item options will be treated according to their values. If the first entry in a line is a number, this number will always be stored in numerical form, a following string will be stored as text. The *500 Degrees, Decomposition* entry, e.g., will be stored in a library as a numerical value of *500.0* and as *Degree, Decomposition* text. This allows both a numerical as well as a text search. Even a search query like *Melting Point a=A 500* would generate a hit.

### Example: Molecular Formula Search

	Operator	Info item	?	Value
1		Molecular Formula	a=A	C5,6H5,8
2				

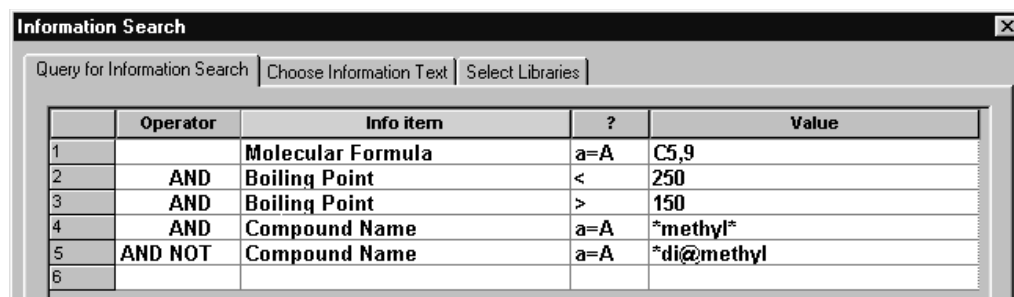
This setting retrieves all entries with 5 or 6 carbon atoms and 5 to 8 hydrogen atoms.

Molecular formula search queries have the following general syntax:

*E1 n,m E2 n,m E3 n,m...*

*E1* and *E2* represent the chemical element. Additionally, you can use *X* as a wild card for halogens and *Ht* for hetero atoms. *N* and *m* specify the range for the number of atoms, *n* being the minimum number and *m* the maximum number in the molecular formula.

**Example: Combined Search**




	Operator	Info item	?	Value
1		Molecular Formula	a=A	C5,9
2	AND	Boiling Point	<	250
3	AND	Boiling Point	>	150
4	AND	Compound Name	a=A	*methyl*
5	AND NOT	Compound Name	a=A	*di@methyl
6				

The following search retrieves substances which have between 5 and 9 carbon atoms, with a boiling point in the range of 150°C to 250°C. In addition, *methyl* should also be part of the name, regardless of whether it is capitalized or not. *Di-methyl* and *di methyl* are excluded from the name.

## 2.6 Structure Search

A structure search is used for the convenient and reliable identification of compounds in libraries. This type of query often yields better results in less time than a spectrum search, as you may not always know the exact spelling of the compound names. In addition, you can also search for a molecular sub-structure, to selectively refine and filter certain compound groups. Searching structures in Sadtler libraries is supported by OPUS/SEARCH 4 and higher.

Prior to performing a search, the molecular structure has to be entered using the structure editor. Details on the structure handling can be obtained from the appendix. Click on the *Structure Search* command in the *Evaluate* pull-down menu or on the  icon.

## 2.6.1 Structure Search

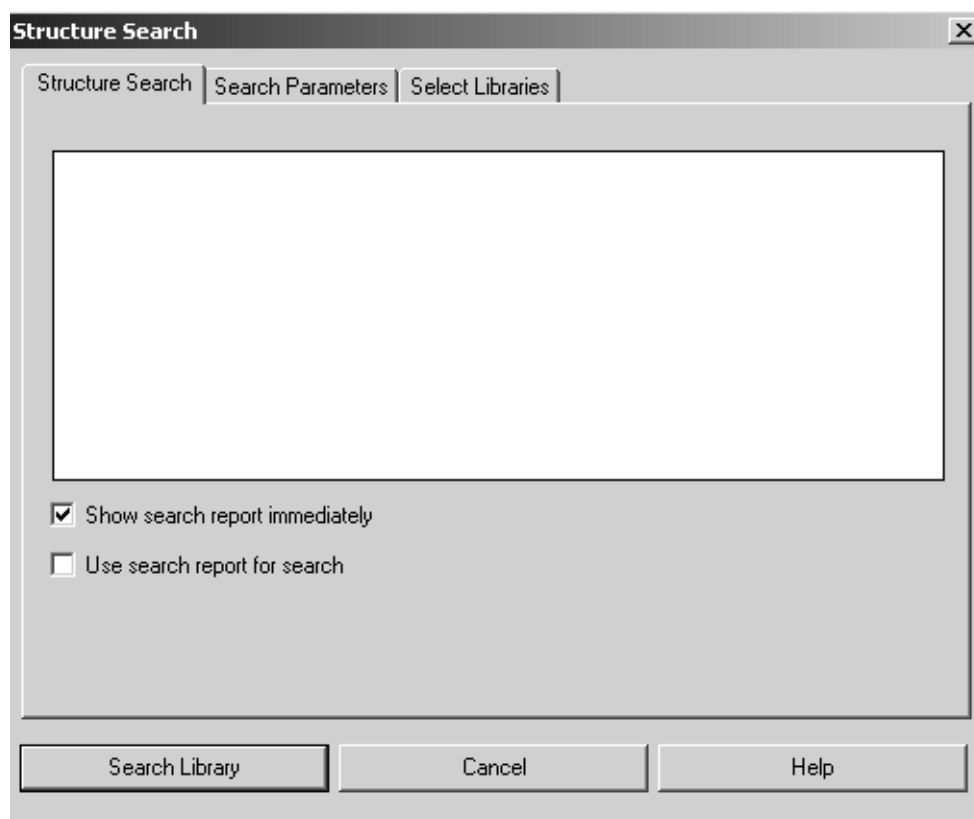


Figure 16: Structure Search - Structure Search tab

Drag & drop the structure blocks created by the editor to the selection field on the *Structure Search* tab. The check boxes are the same as described for the *Spectrum Search*, see section 2.3.

## 2.6.2 Search Parameters

The *Search Parameters* tab provides two different options for the specifications of the search parameters.

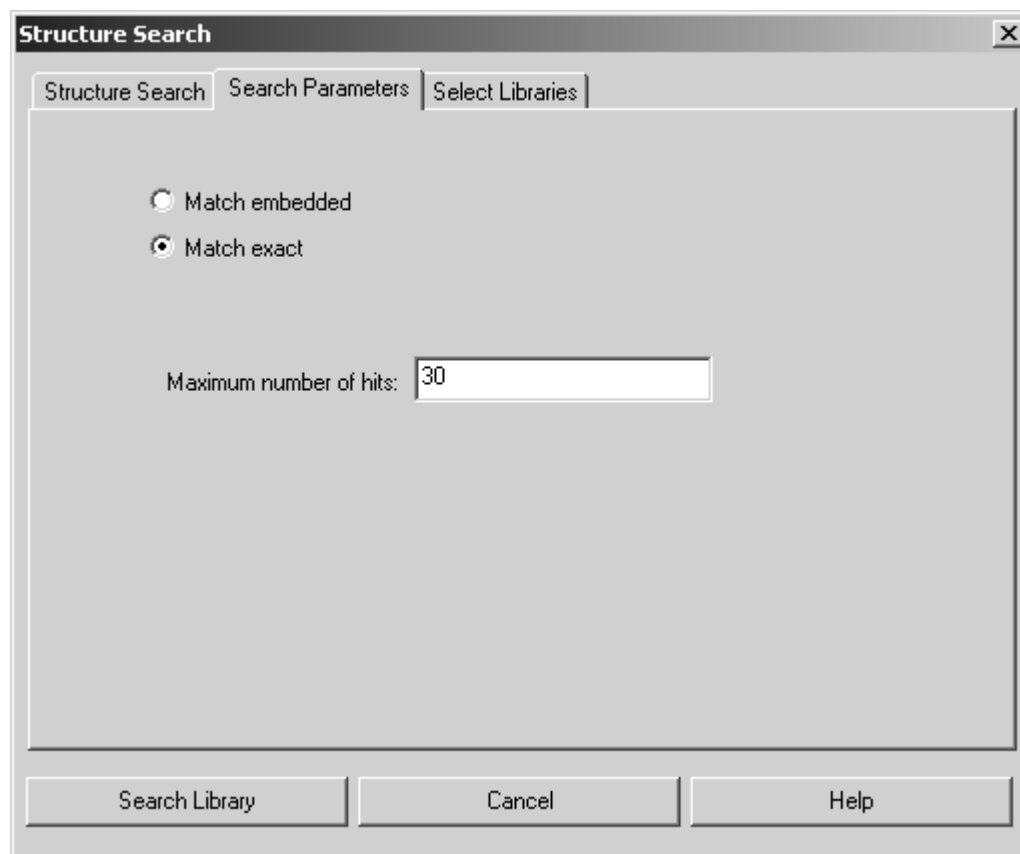


Figure 17: Structure Search – Search Parameters

**a) Match Embedded**

In the query structure this algorithm replaces all hydrogen atoms by free valences which still can have all sorts of remnants. Therefore, molecules even qualify as a hit if the query structure is part of their structure.

**b) Match Exact**

This algorithm only searches for structures (and sub-structures) that exactly match your query.

Define the maximum number of hits in the corresponding entry field.

### 2.6.2.1 Entering Sub-Structures

If you work with an external molecular structure editor, e.g. CHEMWIN or ISISDRAW you can use, apart from element symbols which allow to enter a complete structure, different symbols which allow to define specific sub-structures:

- R** replaces any sub-structure except hydrogen
- Z** replaces any sub-structure including hydrogen
- Y** replaces any single element except hydrogen
- Ht** replaces any single hetero-atom
- X** replaces any single element



### 2.6.2.2 Structure Search Example

Search the following structures in the *DEMOLIB* library:

- Cyclohexane
- Benzene
- Benzene with substitute R
- Benzene with substitute X
- Acetic Acid

Use both search algorithms and compare the results.

### 2.6.3 Select Libraries

On the *Select Libraries* tab you select the libraries for the search. *Structure Search* also generates a SEARCH data block which includes the search result.



# 3

## Generating Library Files

Generating library files can be facilitated by the *Initialize Library* command from the *Evaluate* menu. This command, however, does not provide the possibility to generate or edit library files for Sadtler libraries.

### 3.1 Initializing Library

Use the *Initialize Library* command to integrate several spectra into a new library, or to create an empty library and add different spectra to this library.

Select the *Initialize Library* command or click on the  icon.

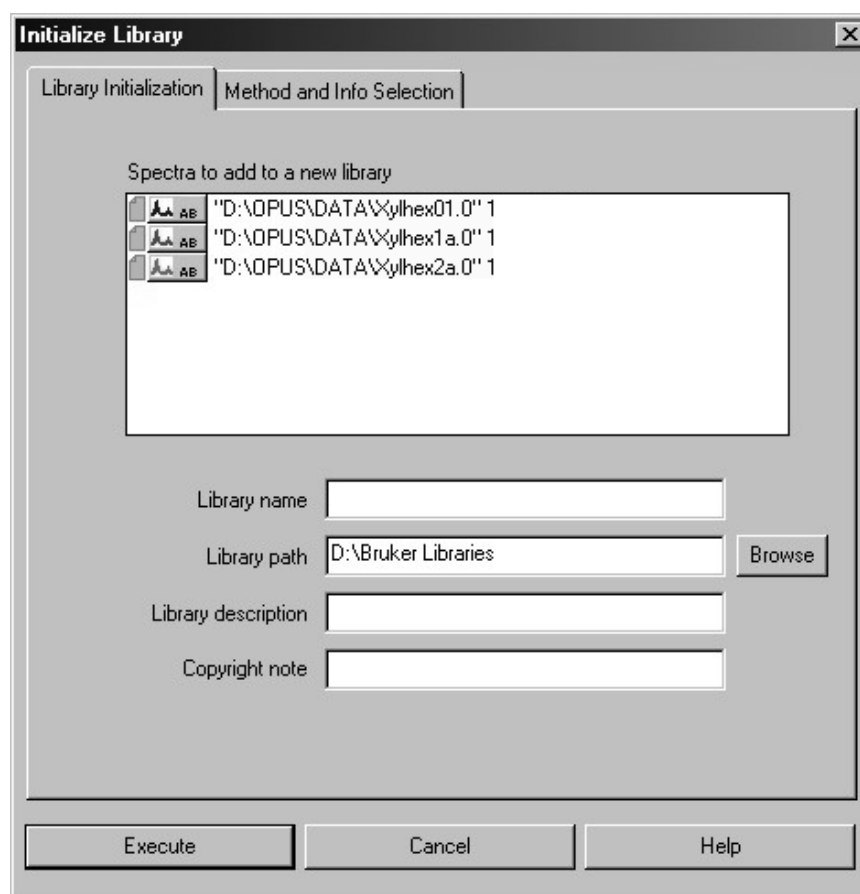


Figure 18: Initialize Library – Library Initialization tab

Define the different entry fields. You can change the default library path by clicking on the *Browse* button. There are two possibilities to proceed:

### 3.1.1 Adding existing spectra to new library

Load the respective spectra by the *Load File* command from the *File* menu to the OPUS browser. Drag & drop the spectra data blocks into the *Spectra to add to a new library* selection field (figure 18). Note that only ratio data blocks, e.g. AB, TR, KM, RAM, Refl or logRefl will be accepted.

If you create the library in this way, the library parameters will be derived from the first spectrum displayed in the selection field. This is the reason why all functions on the *Method and Info Selection* tab are completely deactivated.

### 3.1.2 Creating empty library

If the *Spectra to add to a new library* selection field does not include any spectrum, you have to define certain parameters on the *Method and Info Selection* tab. You can, e.g., define the frequency range of each library spectrum, or specify which kind of spectra information type of each spectrum has to be added to the library.

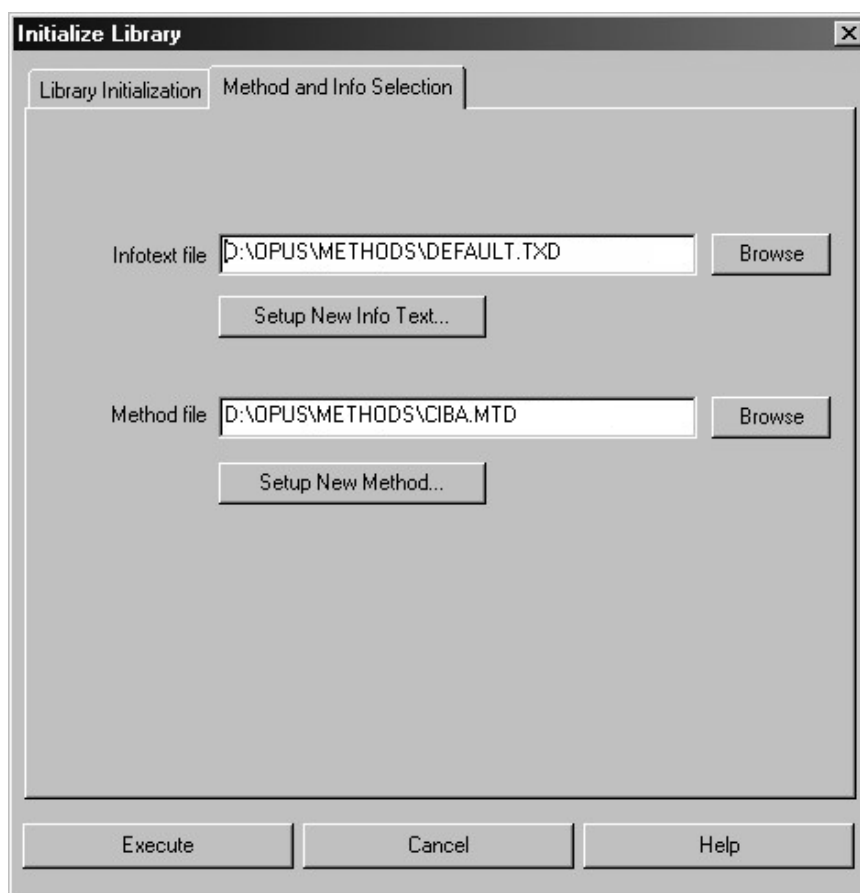



Figure 19: Initialize Library – Method and Info Selection tab

### a) Infotext File

The infotext file determines which kind of information from the INFO data blocks () of OPUS files will be added to the library. For further details on how to create and work with infotext files refer to the OPUS Reference Manual.

If you click on the *Browse* button, you can load an existing infotext file. To create a new infotext file, click on the *Setup New Info Text* button. Infotext files have the file extension \*.TXD.

The infotext file used to create a library has to be identical to the one used for the *Setup Info Mask* command in the *Edit* menu. This applies to all spectra to be added to the library.

### b) Setup New Info Text

To create a new infotext file, click on the *Setup New Info Text* button. The *Setup Information Mask* dialog opens:

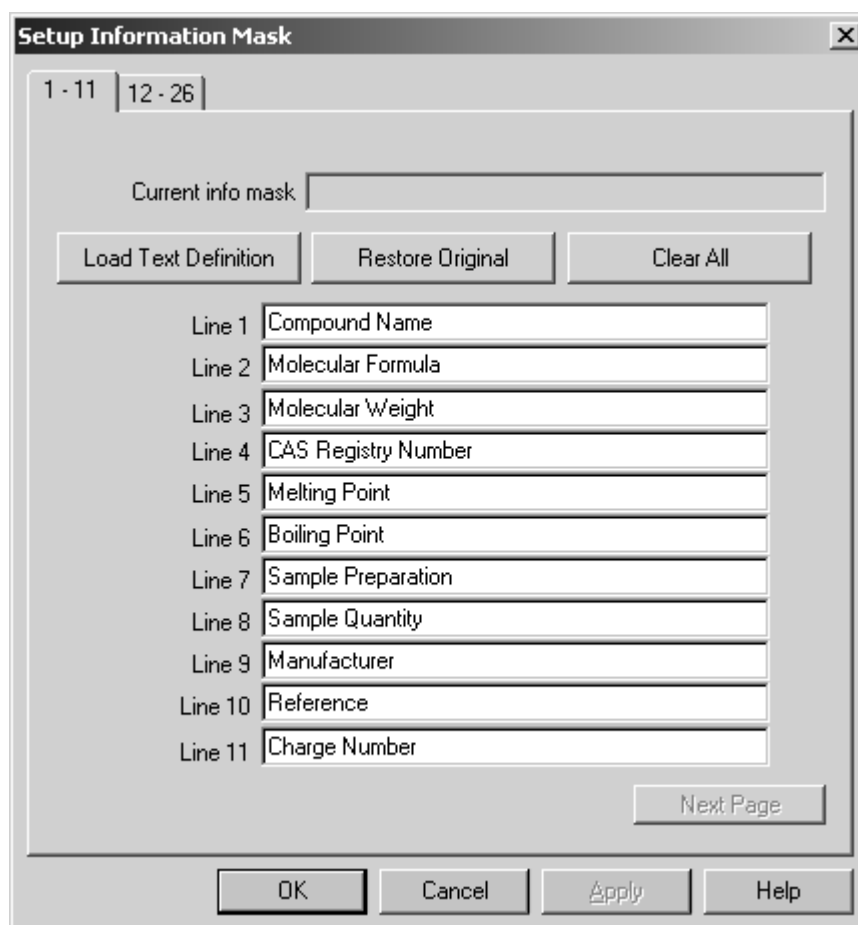


Figure 20: Initialize Library Wizard - Setup Information Mask dialog

If you click on the *Load Text Definition* button, you have access to an existing info mask which you can use as template. The two tabs (1-11 and 12-26) indicate the number of lines displayed. The content of each line will later be available as entry field for the spectrum information input. For the information input use the *Information Input* command from the *Edit* menu.

The *Setup Info Mask* dialog box provides two different possibilities to correct all the changes made. If you click on the *Restore Original* button, the original settings of the template will be restored. To get a template without any entries click on the *Clear All* button. If you click on the *OK* button, the *Save File* dialog opens and allows to store the newly created or modified text mask. The *Method and Info Selection* tab (figure 19) will be displayed again.

### c) Method file

A method file defines the frequency range and digital resolution of spectra used for the library to be created. Besides, you can also select different OPUS parameters which have to be stored for each spectrum in the library. Method files have the extension *\*.MTD*.

Use the *Browse* button to load an existing method file (figure 19). To create a new method click on the *Setup New Method* button. The following dialog opens:

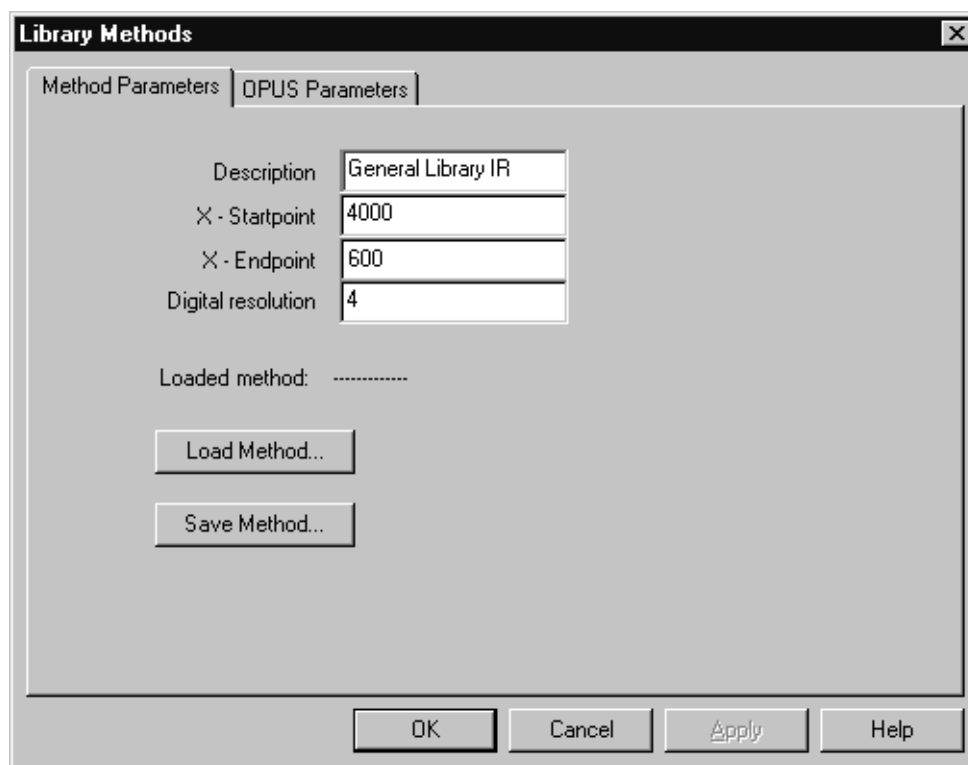


Figure 21: Library Methods - Method Parameters tab

On the *Method Parameters* tab you specify the frequency ranges (x-startpoint, x-endpoint) and digital resolution of the library spectra. Additionally, you have to define a description of the method.

The digital resolution determines the number of data points required to save spectra by using this method. This feature has a direct effect on the space needed by the library on the hard disk. As a rule of thumb, in case of a library using the *DEFAULT* method (4,000 - 400cm<sup>-1</sup>, digital resolution 4cm<sup>-1</sup>) you can anticipate a disk space of about 6 - 7Mbyte per 1,000 spectra.

**Note:** The digital resolution refers to the spectra saved which are used for correlation algorithms, the display, plot and - in case of mixtures - the subtraction. However, the digital resolution does not have any influence on the quality of spectrum searches for the standard algorithm.

If you want to differentiate very identical spectra and if you depend on the correlation algorithm, we recommend a digital resolution of 2 or 1.

You can also load and edit an existing method file. Click on the *Load Method* button. If you do not store a method file created, the *Save File* dialog automatically pops up when clicking on the *OK* button.

On the *OPUS Parameters* tab you define the parameters which are to be stored with each spectrum in the library.

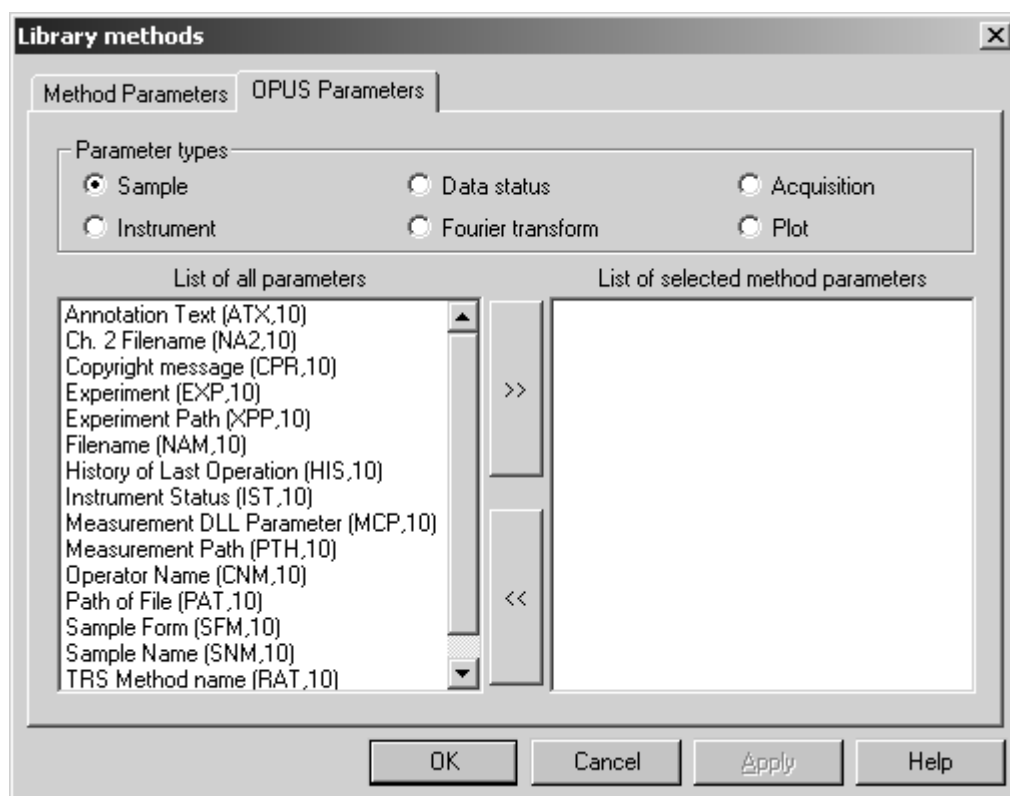


Figure 22: Library Methods - OPUS Parameters tab


The parameters have been grouped into different types. You can switch between these types by clicking on the respective option buttons. The *List of all Parameters* selection field shows all parameters available, and the *List of selected Method Parameters* includes the parameters which have been added to the library. To move a parameter from one selection field to the other, first select the particular parameter and then click on the respective arrow button.

If you click on the *OK* button, the *Save File As* dialog pops up. Save the method file created or modified. The *Method and Info Selection* tab will be displayed again (figure 19). If you click on the *Execute* button, the library will be created. This kind of library can also be used for the searching procedure in libraries, provided the library does include the respective spectra.

To store spectra in a library use the *Store Spectrum in Library* command which will be explained in more detail in the next chapter.

## 3.2 Storing Spectra in a Library

Load all spectra you want to store in the library into the OPUS browser and select the spectral data blocks. Make sure that each file includes an INFO data block which actually contains the information you want to add to the library. To get reasonable search results the spectra to be added should only be absorption or Raman spectra. If you use transmission spectra, they will be converted into absorption spectra and also saved as absorption spectra.

Select the *Store Spectrum in Library* command from the *Evaluate* menu or click on the  icon. The *Store Spectrum in Library* opens.

### 3.2.3 Store Spectrum

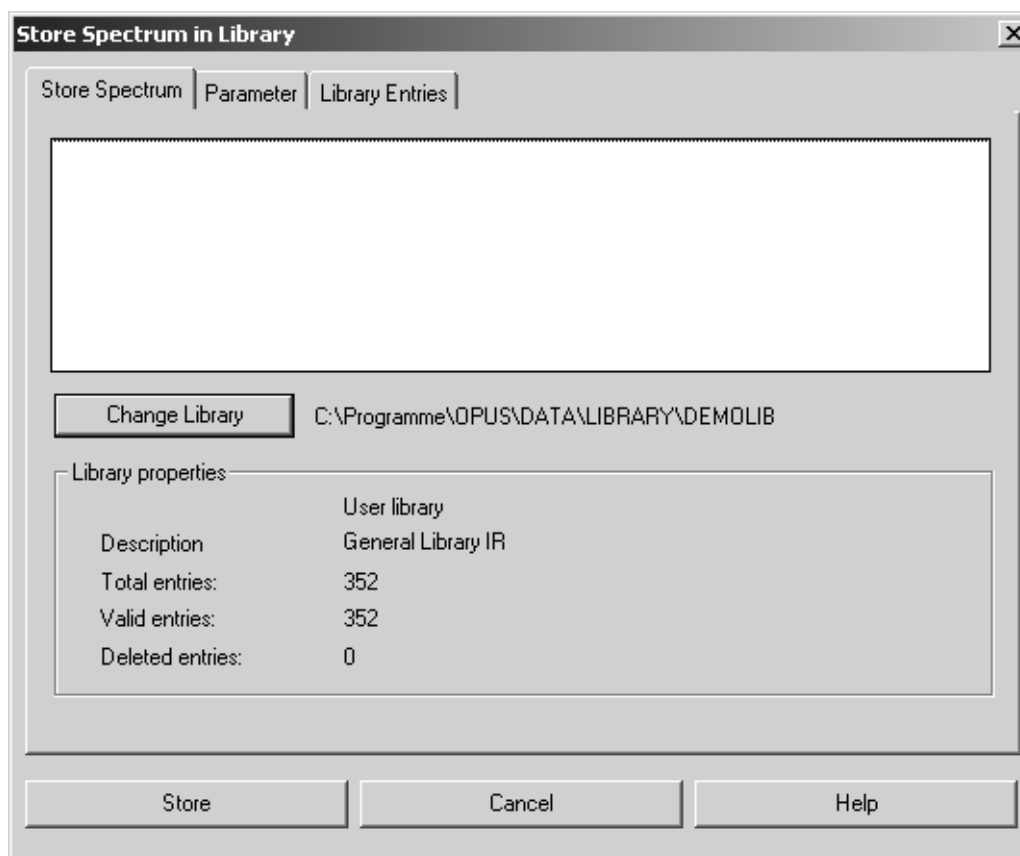


Figure 23: Store Spectrum in Library - Store Spectrum tab

Drag & drop the spectra from the OPUS browser window to the selection field on the *Store Spectrum* tab. If a warning symbol is displayed on the *Store Spectrum* tab, the data block does not match the settings made on the *Parameters* tab. Note that the option buttons checked on the *Parameters* tab for



a previous operation will automatically be selected by default. Data blocks displayed in red will not be added to the library.

The *Library Properties* group field identifies the library as a user library. The library description entered during the setup will also be displayed, together with some library statistics. You also have the possibility to use a different library by clicking on the *Change Library* button.

### 3.2.4 Parameter

On the *Parameter* tab you define how to store data into the library.

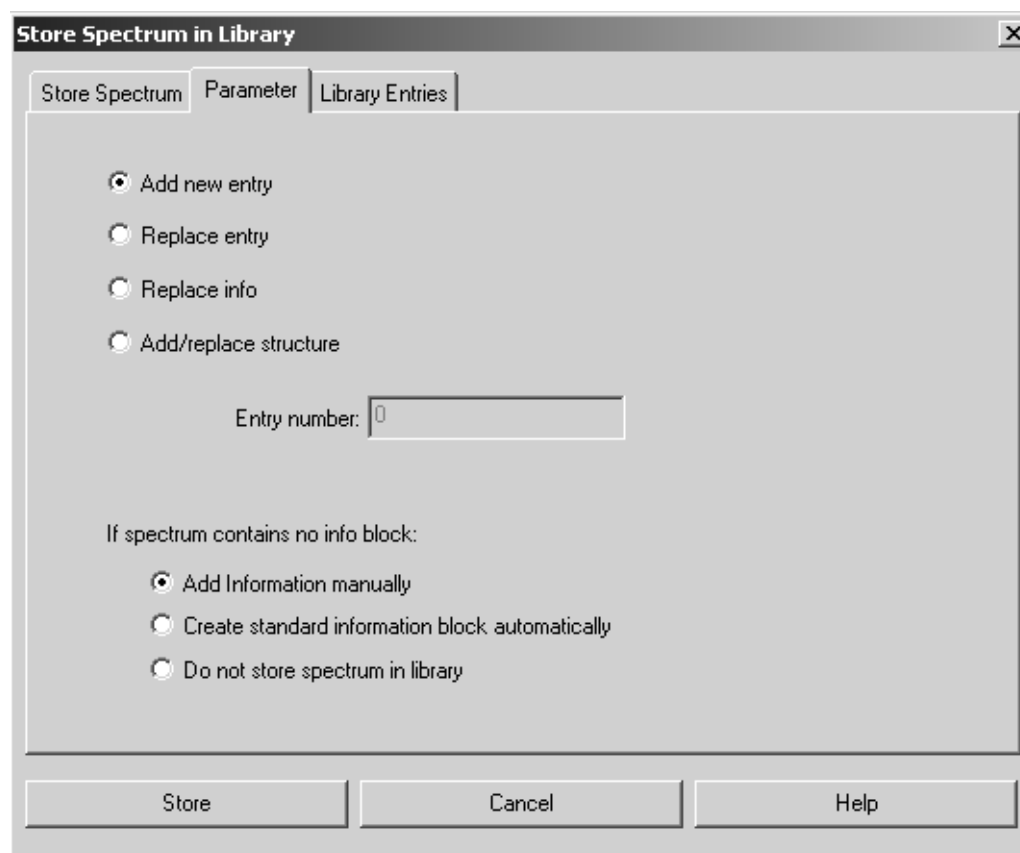


Figure 24: Store Spectrum in Library - Parameter tab

If you select the *Add new entry* option, the spectrum will be stored in the library with an information text added. You can also replace an existing entry by selecting the *Replace entry* option button. Make sure to specify which entry you want to replace by entering the corresponding entry number into the *Entry Number* field.

It is also possible to replace only the info text of an existing library entry. In this case check the *Replace info* option button. Furthermore, you can add and replace a structure by the *Add/replace structure* option button. In both cases, you have to specify which entry you want to replace by entering the corresponding entry number into the *Entry number* field.

Additionally, you can define how to proceed with spectra which do not have an INFO data block. If you check the *Add Information manually* option button and click on the *Store* button, you will be prompted to enter the relevant spectra information.

To automatically create an INFO data block select the *Create standard information block automatically* option button. This kind of INFO data block is based on the sample parameter data available for the sample name, sample type, and operator. Together with the spectrum this data block is stored in the library.

If you check the *Do not store spectrum in library* option button, all spectra which do not have an information block will NOT be stored in the library.

### 3.2.5 Library Entries

Click on the *Library Entries* tab to browse through the different parameters of all entries. The parameters include, e.g. the entry number, compound name, molecular formula, molecular weight and the CAS registry number.

If you click on a particular column header, e.g. *Compound Name*, the entire table entries will be sorted in ascending order according to the column selected. If you click on the particular column header again, the table entries will be sorted in descending order.

A double click on a particular entry would automatically transfer you to the *Parameter* tab. The number of the entry selected will be added to the *Entry Number* field.

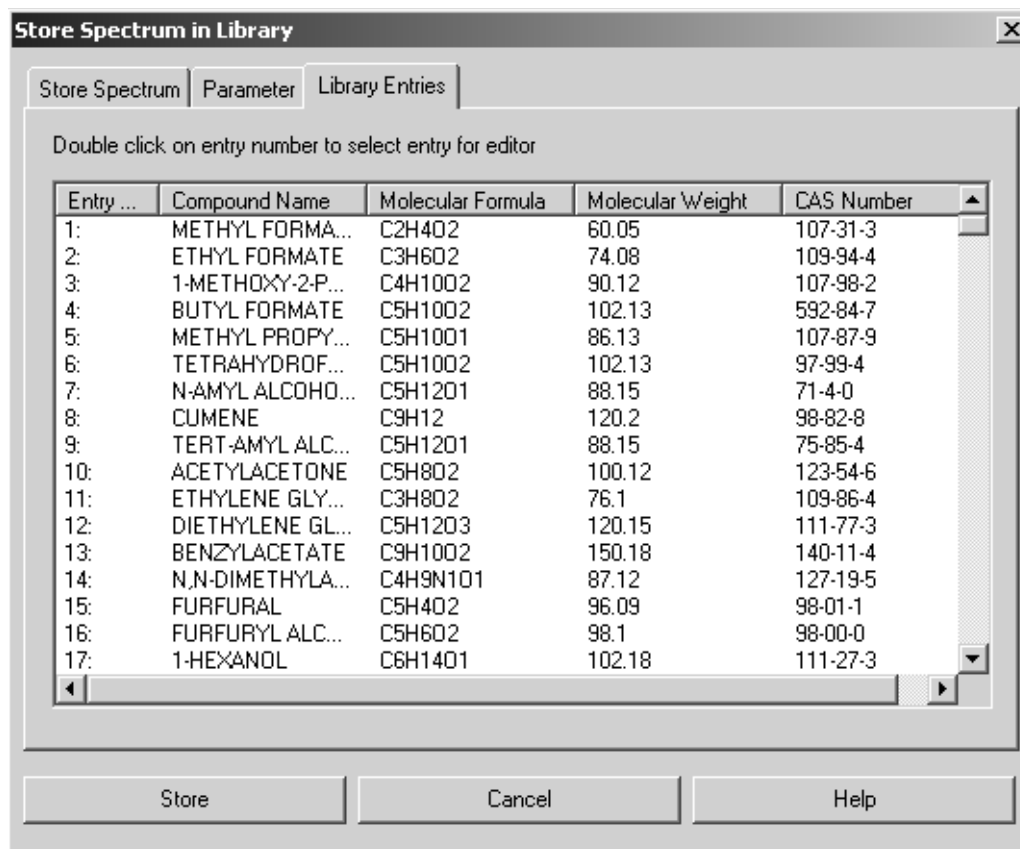


Figure 25: Store Spectrum in Library – Library Entries tab




# 4 Editing Libraries

The library editor allows to maintain self-generated libraries and provides the following options:

- Loading library entries
- Deleting library entries
- Editing library descriptions
- Editing information text

## 4.1 Library Editor

Click on the *Library Editor* command in the *Evaluate* menu or click on the  icon. The following dialog opens:

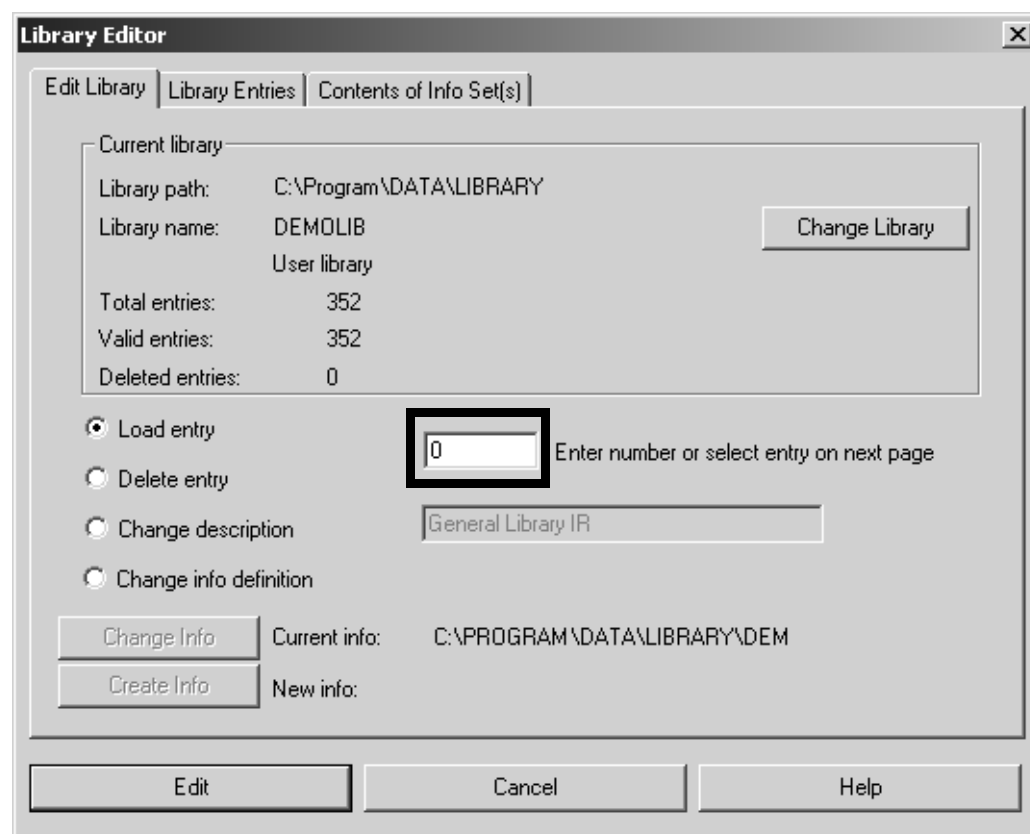


Figure 26: Library Editor - Edit Library tab

### 4.1.1 Edit Library

The *Current Library* group field on the *Edit Library* tab includes information about the currently active library, e.g. library name, path and description, as well as information on the number of entries distinguished between *Valid* and *Deleted*. You can change to a different library by clicking on the *Change Library* button.

You can select between the following editing options:

- **Load Entry**  
Check the *Load entry* option button to extract an entry from the library and save it as a spectral data file by the file name *ENTRYx.0*, with *x* being the entry number in the library. Note that you first have to define an entry number, either manually or by a double-click on the specific entry number on the *Library Entries* tab.
- **Delete Entry**  
Check the *Delete entry* option button to delete an entry from the library. Note that you first have to define an entry number, either manually or by a double-click on the specific entry number on the *Library Entries* tab. The number of entries deleted will be displayed in the *Current Library* group field.
- **Change Description**  
Check the *Change description* option button to change the library description and enter the new description into the entry field on the right.
- **Change Info Definition**  
Check the *Change info definition* option button to change the info mask assigned to a library. Either select an existing mask by clicking on the *Change Info* button or create a new mask by clicking on the *Create Info* button. The *Change Info Definition* option button should only be checked to append lines to an existing mask or to edit typos in an existing mask.

## 4.1.2 Library Entries

If you click on the *Library Entries* tab, the following dialog opens:

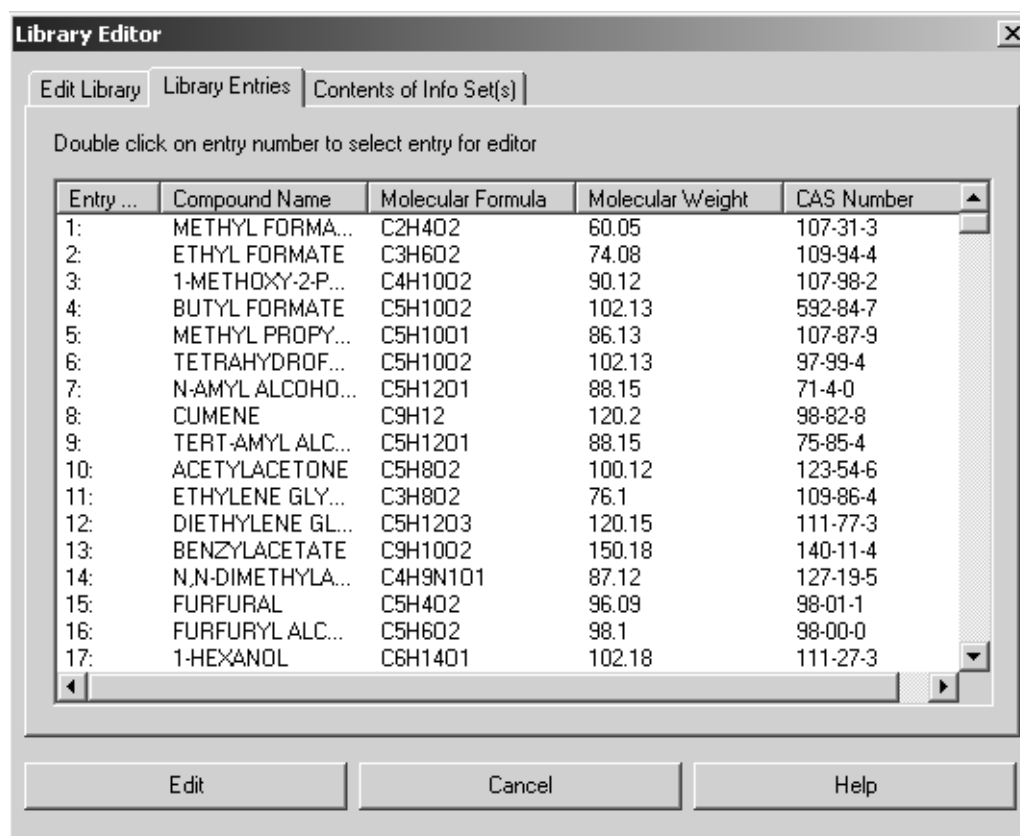


Figure 27: Library Editor - Library Entries tab

The *Library Entries* tab lists all entries of the active library, including the entry number, compound name, molecular formula and weight as well as the CAS number. If you click on a particular column header, e.g. *Compound Name*, the entire table entries will be sorted in ascending order according to the column selected. If you click on the particular column header again, the table entries will be sorted in descending order.

Double-clicking on an entry number automatically copies the entry number into the destined entry field on the *Edit Library* tab (see the mark in figure 26) which will immediately be displayed.

Deleting one or more entries from the library will be noted next to the particular entry number (see figure 28).

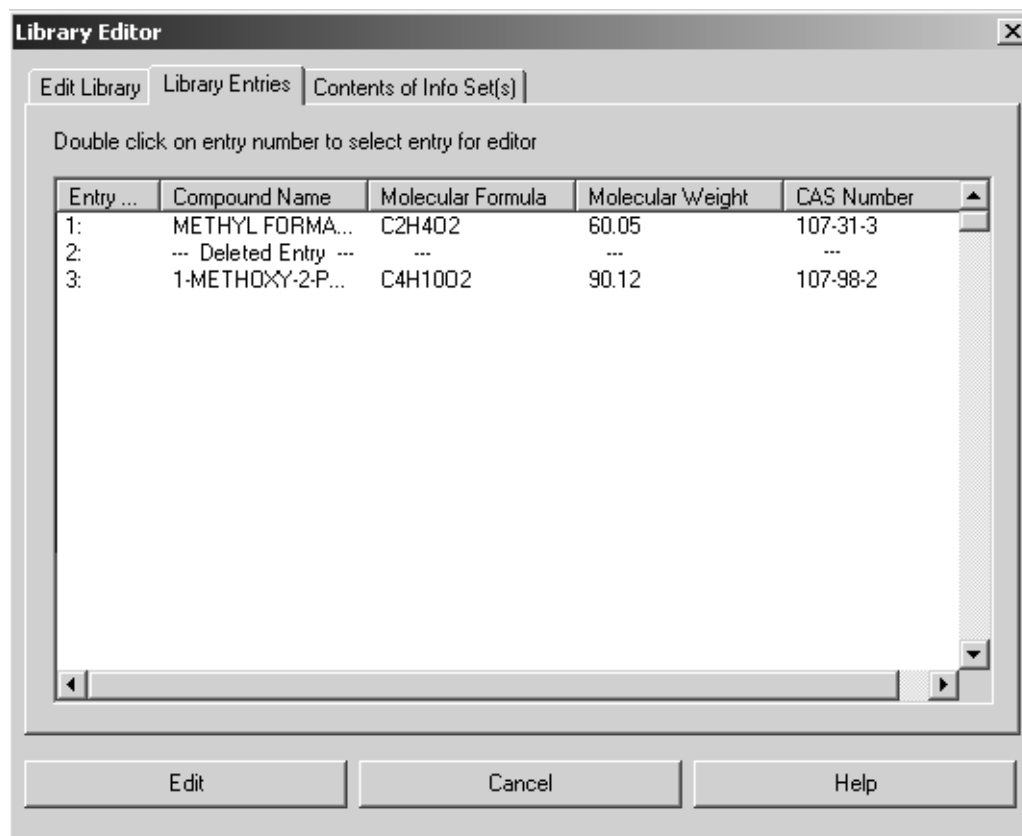


Figure 28: Library Editor - Contents of Info Set(s) tab



### 4.1.3 Contents of the Info Set(s)

If you click on the *Contents of the Info Set(s)* tab, the following dialog opens:

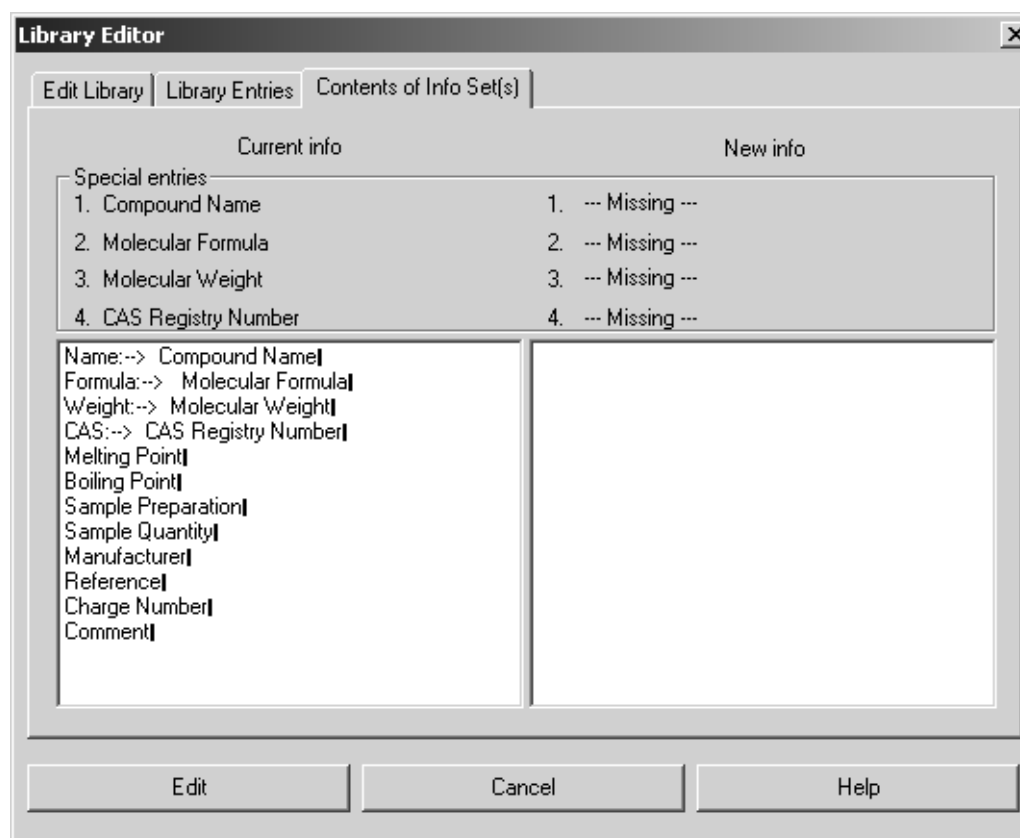


Figure 29: Library Editor - Contents of Info Set(s) tab

The *Contents of Info Set(s)* tab displays the current info text definition of the selected library in the left selection field. If you have checked the *Change info definition* option button on the *Edit Library* tab (see figure 26), the info mask of the file to be newly assigned will be displayed in the right selection field. Thus, it will be easier to see whether the new and the old info mask are compatible. The new info mask must contain all fields included in the old one, and may also list additional fields.

The *Special Entries* group field lists entries that will be automatically assigned to a library (*Compound Name*, *Molecular Formula*, *Molecular Weight* and *CAS Registry Number*). These entries are selected in the respective selection fields.

## 4.2 Library Browser

The *Library Browser* command in the *Evaluate* menu allows to visualize the contents of a library. It is possible to make changes in the library displayed.

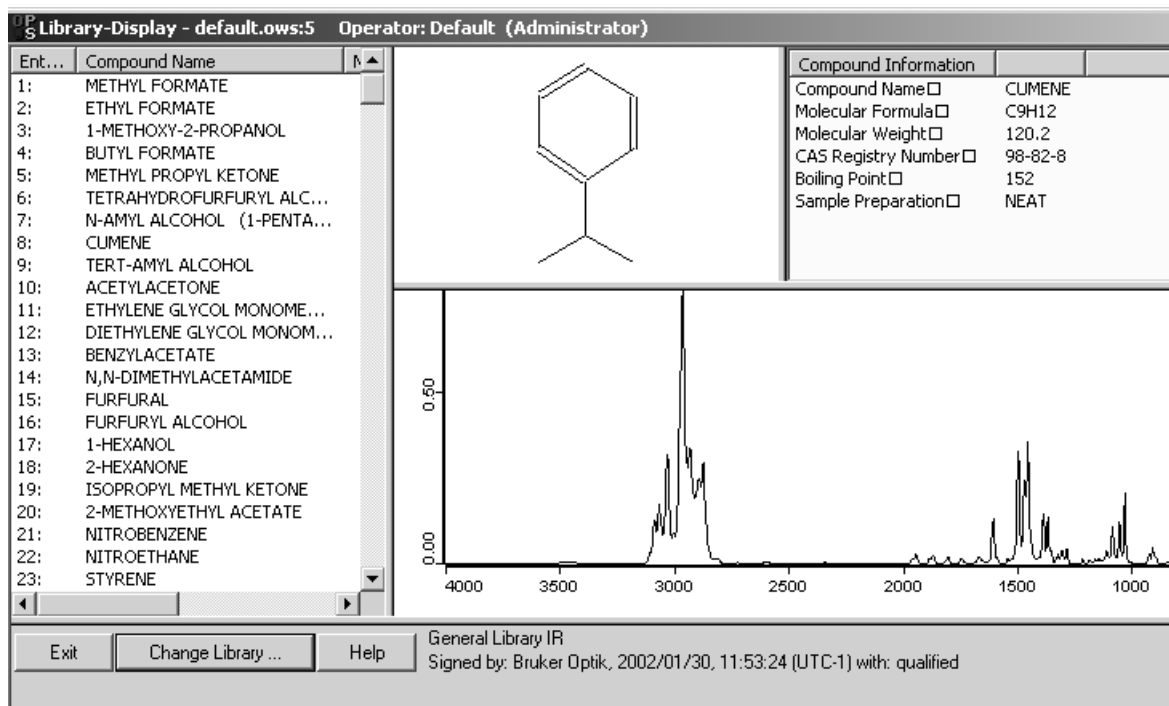


Figure 30: Library browser

The library browser consists of four different windows. All the entries of the library selected are displayed on the left side. It is distinguished between entry number, compound name, molecular formula, molecular weight and CAS number. If you select a particular entry, the information data defined for this entry will be displayed in the respective windows, i.e. the molecular structure (in the middle), compound information (upper window) and the spectrum (lower window). To change the sorting order click on the respective column header, and the table will be sorted in ascending order according to the column selected.

To change to a different library, click on the *Change Library* button. A dialog pops up from which you can select a different library. Click on the *Exit* button to close the library browser. If you open the library browser again by the *Library Browser* command in the *Evaluate* menu, the library previously selected will be displayed.

There are several possibilities to edit the library. However, all the editing options can only be used in connection with unprotected libraries, i.e. libraries which have been created by the user.

**a) Extracting spectra from the library**

Select one entry or several entries in the library list. If you right click on the library list, a window pops up from which you select the *Extract Spectra* command. The entry files are now displayed in the OPUS browser window, and the entry spectra are displayed in the spectrum window.

**b) Deleting spectra from the library**

Select one entry or several entries in the library browser. If you right click on the selection, a window pops up from which you select the *Delete Spectra* command. Before the entries are definitely deleted you will be asked whether you want to continue the deleting operation which is irreversible.

**c) Adding spectra to the library**

If you have loaded a spectrum in a different window, you can add it to the library. Drag & drop the particular data block (AB or TM) into the library list. A dialog pops up and asks whether you want to add this spectrum to the library. Click on the *Yes* button to perform the adding operation. The spectrum is added to the library as a new entry at the end of the library list.

Make sure that the spectra you want to add does include an INFO data block. In case of spectra without any INFO data block a warning pops up, and you will automatically be routed to the *Store Spectrum in Library* dialog described in section 3.2.

**d) Editing compound information**

If you have selected an entry in the library list, you can edit the corresponding compound information. Double click on the *Compound Information* window. The *Add Information* dialog will be displayed and you can make the necessary changes.

The screenshot shows the 'Add Information' dialog box with the following fields and values:

Field	Value
File Path	"C:\Programme\OPUS\Search\Entry007.1" 1
New file	<input type="checkbox"/>
Text definition	From Info Block!
Compound Name	N-AMYL ALCOHOL (1-PENTANOL)
Molecular Formula	C5H12O1
Molecular Weight	88.15
CAS Registry Number	71-4-0
Melting Point	
Boiling Point	138
Sample Preparation	NEAT
Sample Quantity	
Manufacturer	
Reference	
Charge Number	

Figure 31: Add Information

If you click on the *Add* button, a window pops up and asks whether to store the changes into the library. Confirm the procedure by clicking on the *Yes* button.

**e) Adding data blocks from a loaded file to a library entry**

Select the specific library entry to which you want to add an INFO or structure (STR) data block. Drag & drop the respective data block from the OPUS browser to the library list. A dialog pops up, and if you confirm the operation the respective data block will be added to the entry selected. If the entry already includes such a data block type, this data block will automatically be replaced.

## 4.3 Band Assignment Chart

The *Band Assignment Chart* command in the *Evaluate* menu allows to visually assign spectrum bands to functional groups.

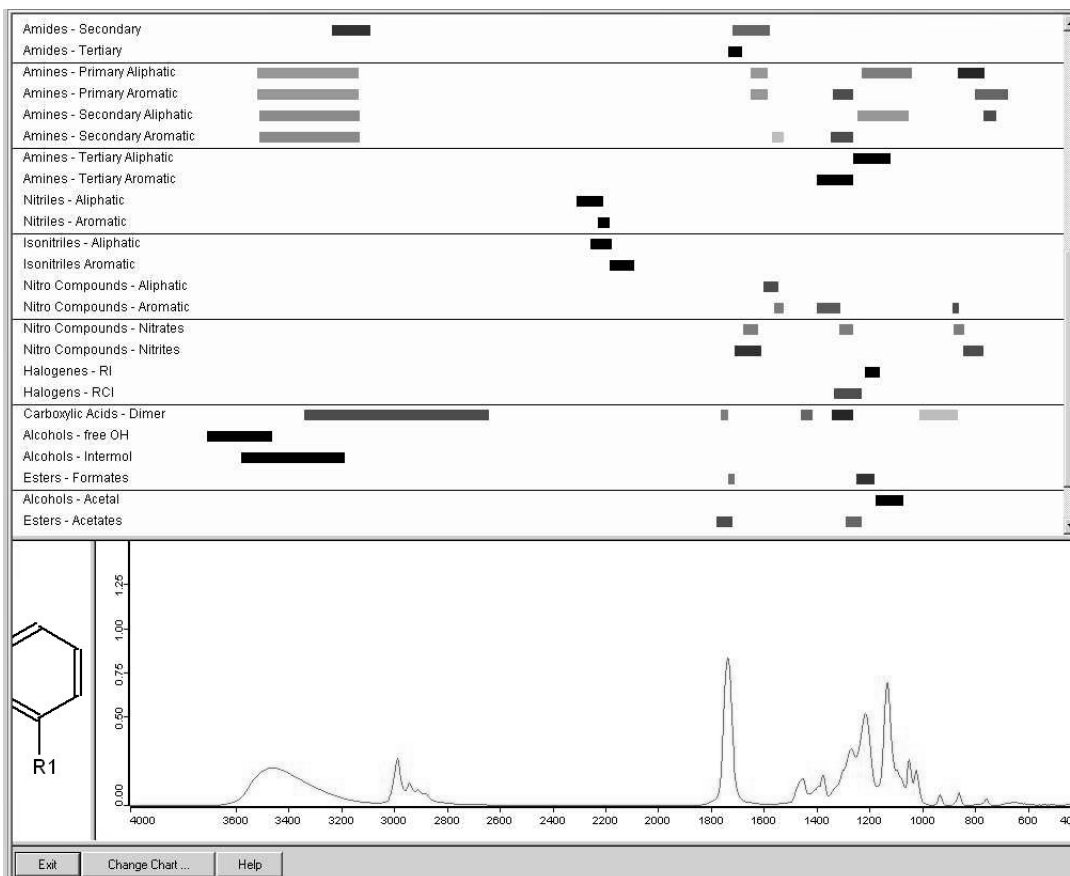


Figure 32: Band Assignment Chart

Three different windows set up the browser of the band assignment chart. The upper window shows a chart which includes the names of the functional groups and their respective band positions in the form of bars. The spectra are displayed in the lower window, which abscissae are always conform with the respective band positions in the upper window. To the left of the spectrum window the molecular structure of the functional group selected is displayed in the so-called structure window.

Apart from the functional group name the band assignment chart also includes information on the position and peaks of the bands created by the functional group. Wavenumber ranges which may include bands are highlighted by a colored bar. The color intensity indicates the band peaks. The less the color intensity of the bar, the less pronounced will be the band expected.

To compare spectra with the band assignment chart, select the *Load File* command from the *File* menu. Load or drag & drop one spectrum from the

OPUS browser window to the spectrum window of the band assignment browser. The latest spectrum only which has been loaded and drawn into the spectrum window will be displayed.

Now, a spectrum search will be performed in the band assignment chart and the entries of the upper window will be sorted according to the result of this particular search. This means that those functional groups which spectra come very close to the spectrum displayed in the spectrum window are shown at the farthest end of the list. Thus, you can quickly get an overview about the functional groups in the substance which forms the basis for the spectrum.

If you right click on the spectrum window, a menu pops up and provides the most important functions required to edit the spectrum display, e.g. *Zoom* and *Scale*. Depending on the spectrum section displayed in the spectrum window the chart in the upper window changes accordingly. This allows to quickly check whether the band positions in the spectrum and the chart are conform with each other.

If you double click on the functional group name, you can have the molecular structure displayed in the structure window. The functional group name will be highlighted in light gray in the upper window. Double click again on the name to undo the selection.

To change to a different band assignment chart, click on the *Change Chart* button. A dialog pops up to be used to select a different band assignment chart. The information provided by the band assignment chart are stored in the OPUS library format. Therefore, it is practically possible to display OPUS libraries in the browser of the band assignment chart, which is, however, not very useful.

Use the *Help* button to open the online help. To close the band assignment chart browser, click on the *Exit* button.

---

# Appendix

## Structure Handling in OPUS


The OPUS base package offers the possibility to import, edit and print structures. There are three functions available in the *Edit* menu:

- Structure Import
- Edit/Create Structure
- Attach Structure

### Structure Import

The *Structure Import* command converts structures, which have been stored in the Molfile format, to the internally used OPUS format. Files stored in this format have the extension *.MOL*.

The Molfile format developed by the company MDL has become a quasi-standard over the last years. Almost all structure programs available can process structures in the Molfile format. The format is published and can be used without any restrictions.

Click on the *Structure Import* command, a dialog opens and shows all files with the extension *.MOL*. Select one or more structure files and click on the *Open* button. All files are converted into the OPUS format, and loaded. The file name is identical to the original file name, and the extension *.0* is automatically added. Double click on the STR data block () in the OPUS browser window to have the structure displayed.

### Edit/Create Structure

The *Edit/Create Structure* command allows to edit a structure or create a new one. OPUS, however, does not include a structure editor but you can load any appropriate structure editor by means of the *Edit/Create Structure* command. The *Edit/Create Structure* command converts an already existing structure from the OPUS format to the Molfile format and writes the structure into a temporary file (*BIRSY.MOL* stored in the OPUS sub-directory SEARCH).

If you now open an appropriate structure editor, the name and path of the temporary file is added to the structure editor using the command line. The temporary file will be loaded and the structure automatically displayed. You can now make as many changes on the structure as you like. Save the changed structure which will be rewritten into the original structure data block. Creating a new structure is similar to editing a structure, except for the fact that an empty temporary file is created before starting the editor.

---

The minimum requirements for a structure editor are:

- The editor has to be compatible with Windows NT/2000/XP.
- The editor has to be able to read and write structures in Molfile format.

Recommended functionality:

- The editor should be able to automatically load and display Molfile format structures.
- If a structure is edited or redrawn, the editor should automatically save this new structure in the Molfile format in the particular file defined.

If you click on the *Edit/Create Structure* command in the *Edit* menu, the following dialog opens:

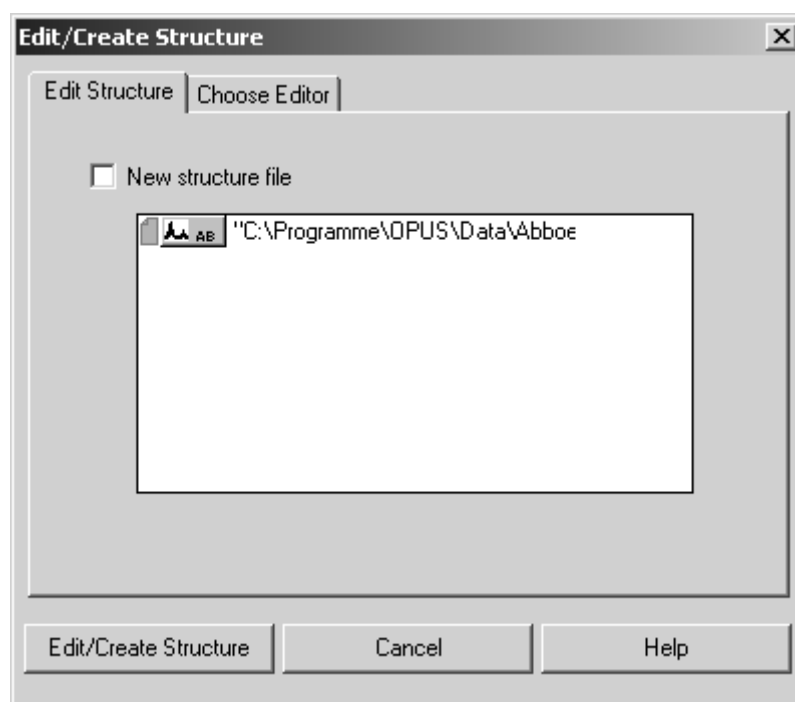


Figure 33: Edit/Create Structure - Edit Structure tab

Select a file and drag & drop it from the OPUS browser into the selection field of the *Edit Structure* tab. If an STR data block already exists, you can edit the structure. If no structure is available, a new structure will be attached.

If you activate the *New structure file* check box, the *Edit/Create Structure* dialog box changes as follows:



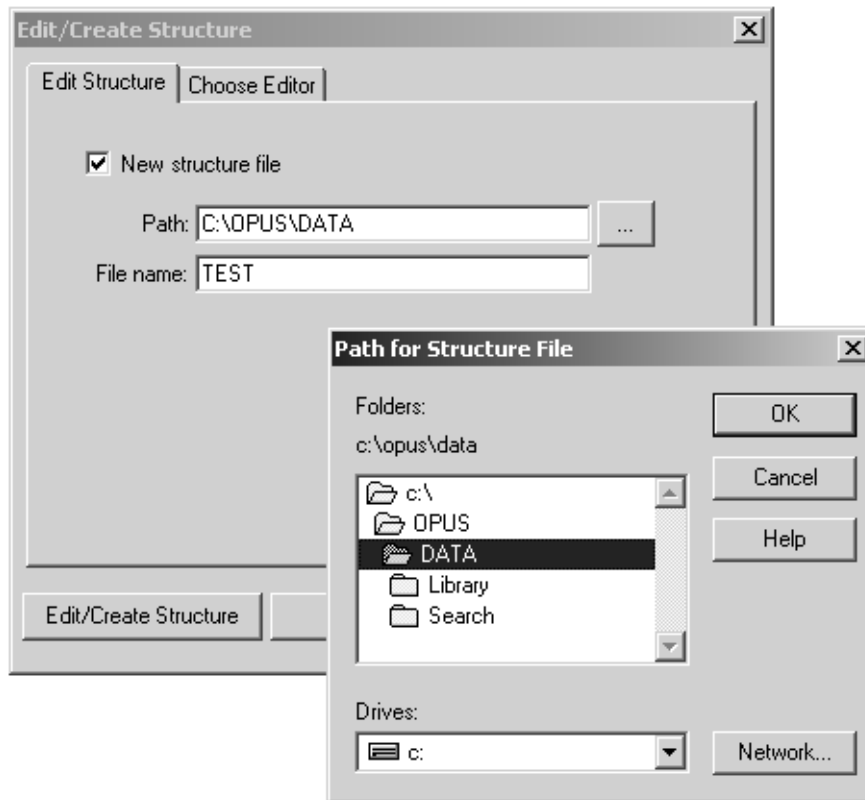



Figure 34: Edit/Create Structure - Edit Structure tab

Enter the path for the new structure file into the *Path* entry field or click on the  button to browse the path. Define the file name (with extension) for the new structure file in the *File Name* entry field.

Click on the *Choose Editor* tab to open the following dialog:

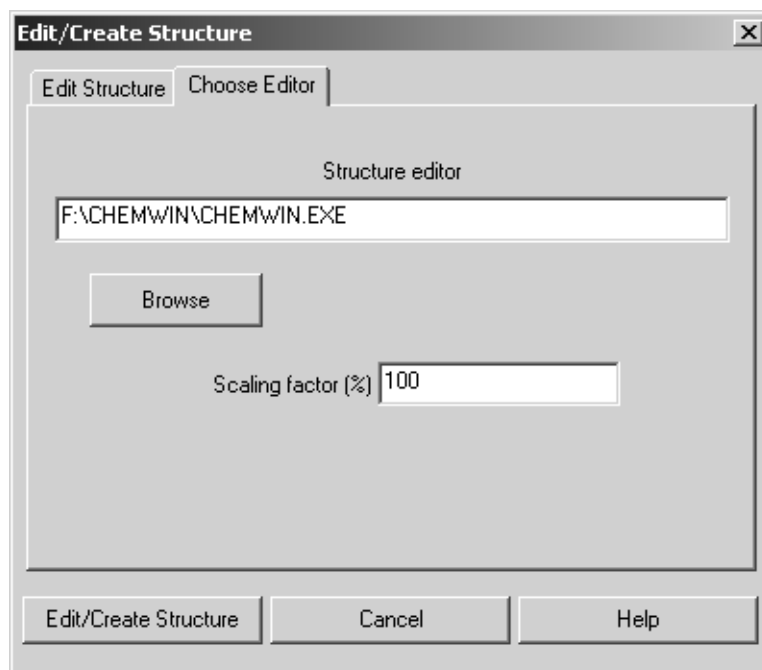


Figure 35: Edit/Create Structure - Choose Editor tab

Enter the path and file name of the structure editor into the *Structure editor* entry field or click on the *Browse* button to select the editor from the dialog that pops up.

Define the *Scaling Factor* for the structure display. The standard setting is 100% which is adequate for most structure editors. Change the scaling factor only if the structure in the editor is displayed in too large or too small a size.

## Attach Structure

The *Attach Structure* command is used to convert a Molfile structure and add the *STR* data block to an existing spectrum file.

Click on the *Attach Structure* command and the following dialog opens:

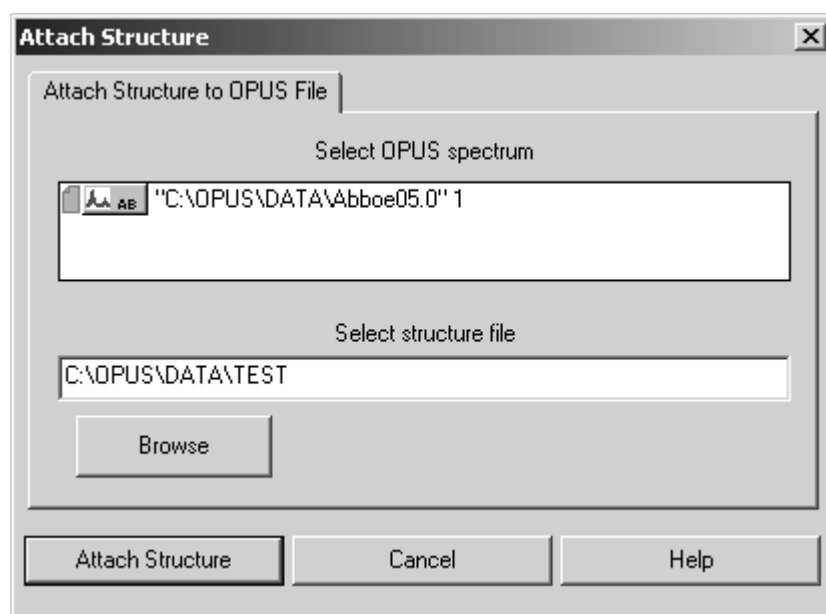


Figure 36: Attach Structure - Attach Structure to OPUS File tab

Select the OPUS file which the structure will be attached to and drag & drop it into the *Select OPUS spectrum* selection field. Define the path and file name of the structure file to be converted or click on the *Browse* button and select the path and file name from the dialog that pops up.

If you click on the *Attach Structure* button, the structure file will be converted and an *STR* data block will be added to the spectrum file.



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