



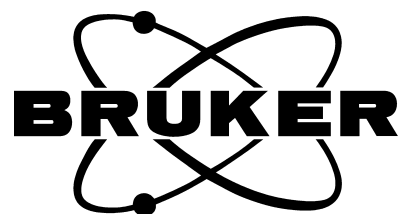
# **OPUS**

Spectroscopy Software

Version 6

## **User Manual**

# **STATISTICS**



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

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# Introduction

OPUS STATISTICS is a software package which consists of three parts. The first part describes the automated evaluation of NIR spectra for qualitative and quantitative analysis in combination with IDENT, QUANT and conformity test methods.

To statistically evaluate spectra series a spectra file list is required. The second part of this manual outlines how to set up such a file list.

Statistical evaluation features, including different evaluation functions, are described in the third part. These functions are used to evaluate single spectrum files, different spectra files which are part of a common file list, or even 3D files.

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# 1 Multi Evaluation

The *Multi Evaluation* function in the OPUS *Evaluate* menu allows the automated evaluation of NIR spectra for qualitative or quantitative analysis. It combines IDENT, QUANT and conformity test methods with the results being displayed in one single report.

If you want to identify an unknown sample, the multi evaluation enables you to first perform an IDENT analysis. Based on the result obtained OPUS continues with a QUANT analysis using the same sample. This procedure can be helpful in many cases to check whether the product to be used for a quantitative analysis has been measured at all. The combination of an IDENT analysis and conformity test may similarly be appropriate.

Multi evaluation parameters are stored in a special method file with the extension *\*.ME*. Before you can start a multi evaluation you have to create a multi evaluation method. If you want to edit the multi evaluation path of this method, make sure that you have the right to change parameters. To verify the user rights select the *User Settings* command in the *Setup* menu, and click on the *21CFR11 Rights* tab. For further details, see chapter 14 in the OPUS Reference Manual.

## 1.1 Setup

To start the multi evaluation analysis you have to set up a method or load a method which has been previously created. Click on the *Multi Evaluation Setup* command in the *Evaluate* menu to open the following dialog:

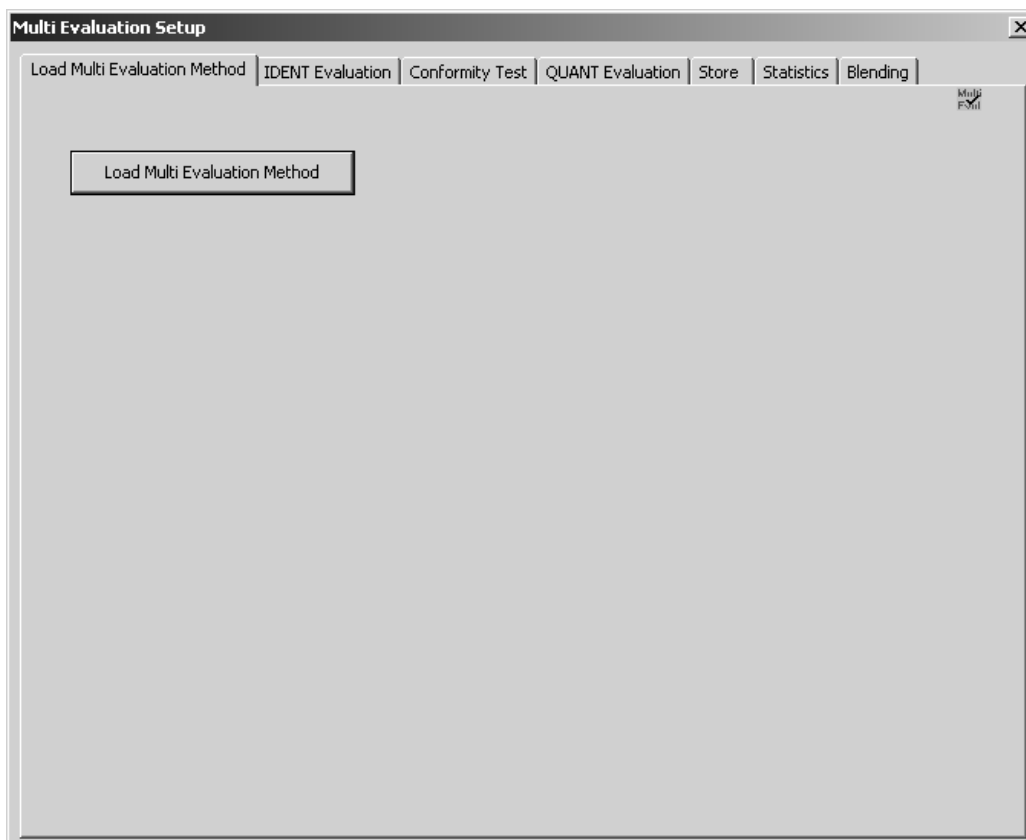


Figure 1: Multi Evaluation Setup - Load Method tab

To load an existing method click on the *Load Multi Evaluation Method* button and select the particular method from the dialog that opens.

Depending on the kind of evaluation you want to perform on the original spectrum or spectra set up a new method by means of the other evaluation option tabs available. The evaluation options correlate with each other, i.e. the sequence of product analysis shall be as follows:

- 1) IDENT (no further test)
- 2) IDENT → Conformity Test
- 3) IDENT → Conformity Test → QUANT
- 4) IDENT → QUANT
- 5) Conformity Test → (no further test)
- 6) Conformity Test → QUANT
- 7) QUANT (no further test)

The sequences 2 and 4 allow to identify the product in a first step by using the *No Reference defined* IDENT test option.

If you use the *IDENT Evaluation* with several substance groups, and the multi evaluation test result shows that several groups may apply to the product to be evaluated, any further test would not be reasonable. This result, however, will only be generated if the basic IDENT library had not been validated properly and overlappings had not been eliminated either.



Otherwise, if only one substance group applies, you can continue by performing the *Conformity Test* and/or *QUANT Evaluation*. This test depends on the substance group selected for the *IDENT Evaluation*.

It is also possible to perform the multi evaluation analysis by the *Conformity Test* only. If one conformity test method turns out to be successful, you can continue with the *QUANT Evaluation*.

Integrating a previous QUANT method, without performing an IDENT or conformity test, can be useful if the original QUANT result has been corrected by, e.g. offset correction, or if warning or alarm limits have to be set.

As soon as you close the *Multi Evaluation Setup* command without saving the changes made the following dialog pops up:

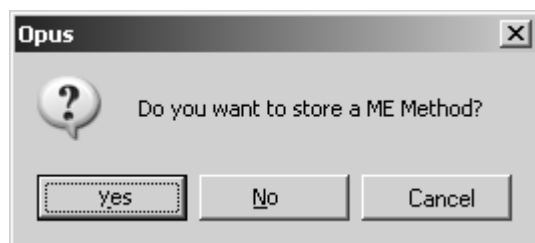


Figure 2: Multi Evaluation Setup - pop-up dialog

This dialog pops up even if you have not made any changes on the method at all, but clicked on one of the *IDENT*, *Conformity Test* or *QUANT* Multi Evaluation tabs.

## 1.1.1 IDENT Evaluation

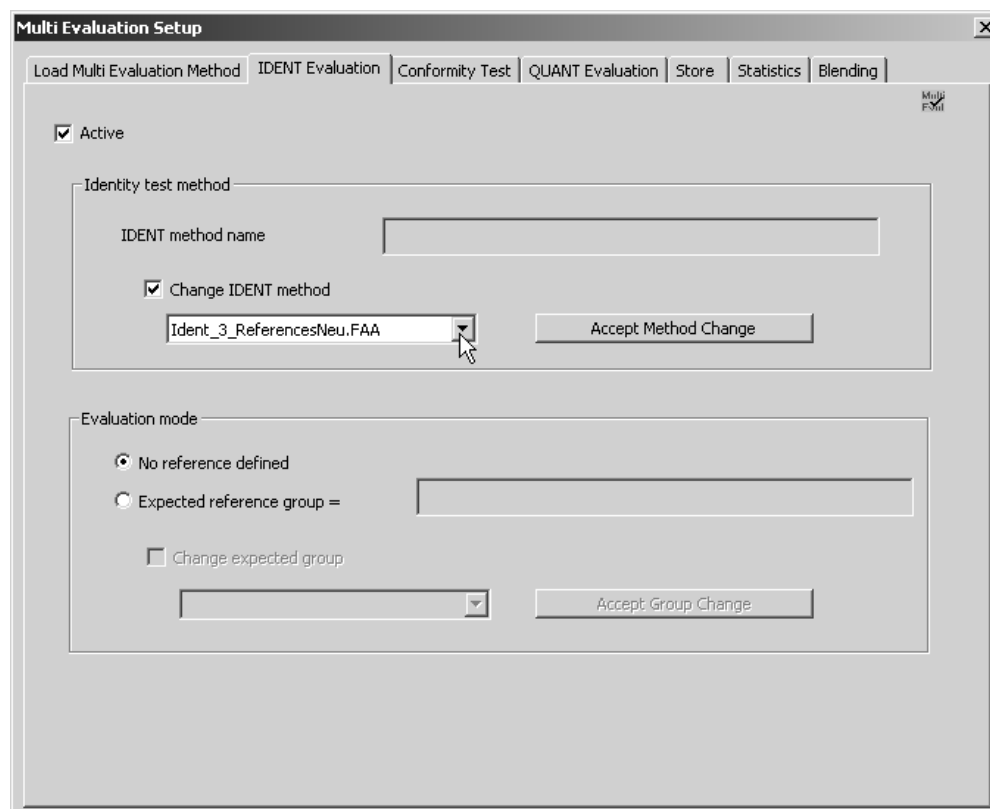


Figure 3: Multi Evaluation Setup - IDENT Evaluation tab

The *Active* check box is deactivated by default and thus all functions and controls are disabled and grayed. Activate the *Active* check box. If you activate the *Change IDENT method* check box, you can select the appropriate IDENT method from the drop-down list.

**Note:** All IDENT, Conformity Test and QUANT methods used for multi evaluation have first to be copied to the sub-directories of the multi evaluation root directory. The following default setting applies:

```

... \OPUS \MultiEvaluation
      \Conformity Test Method
      \IDENT Method
      \QUANT Method
  
```

These paths will be created in OPUS not until the *Multi Evaluation Setup* command has been selected for the very first time. The base path can be changed by means of the *User Settings* command in the *Setup* menu.

Confirm the choice by clicking on the *Accept Method Change* button. The name of the IDENT method file with the extension *\*.FAA* will be displayed in the upper selection field (see A in figure 4).

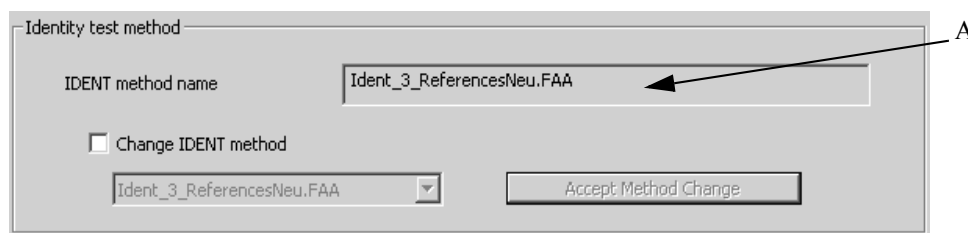


Figure 4: Identity Test Method group field

The *Change IDENT method* check box and the drop-down list will be deactivated again.

For the IDENT analysis two alternative evaluation modes are available. The mode *No reference defined* (see figure 3) works without a pre-defined reference spectrum and allows the complete analysis of all substances available in the IDENT library. This, however, requires the substances to be part of one validated IDENT library, and further evaluation methods, e.g. QUANT, to be assigned properly.

To work with an expected reference group check the *Expected reference group* option button. The reference group selected on this tab will always be set as default on all the other tabs. To change the reference group activate the *Change expected group* check box and select the particular group from the drop-down list. This list includes all groups of the current IDENT library.

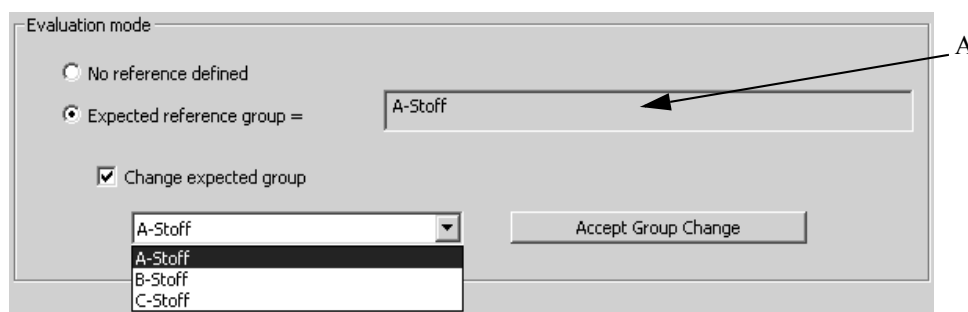


Figure 5: Evaluation Mode group field

Confirm the choice by clicking on the *Accept Group Change* button. The name of the reference group selected will be displayed in the upper selection field (A in figure 5), and the *Change expected group* check box and the drop-down list will be deactivated again.

All the settings made on the *Conformity Test* and *QUANT Evaluation* tab correlate with the expected reference defined.

## 1.1.2 Conformity Test

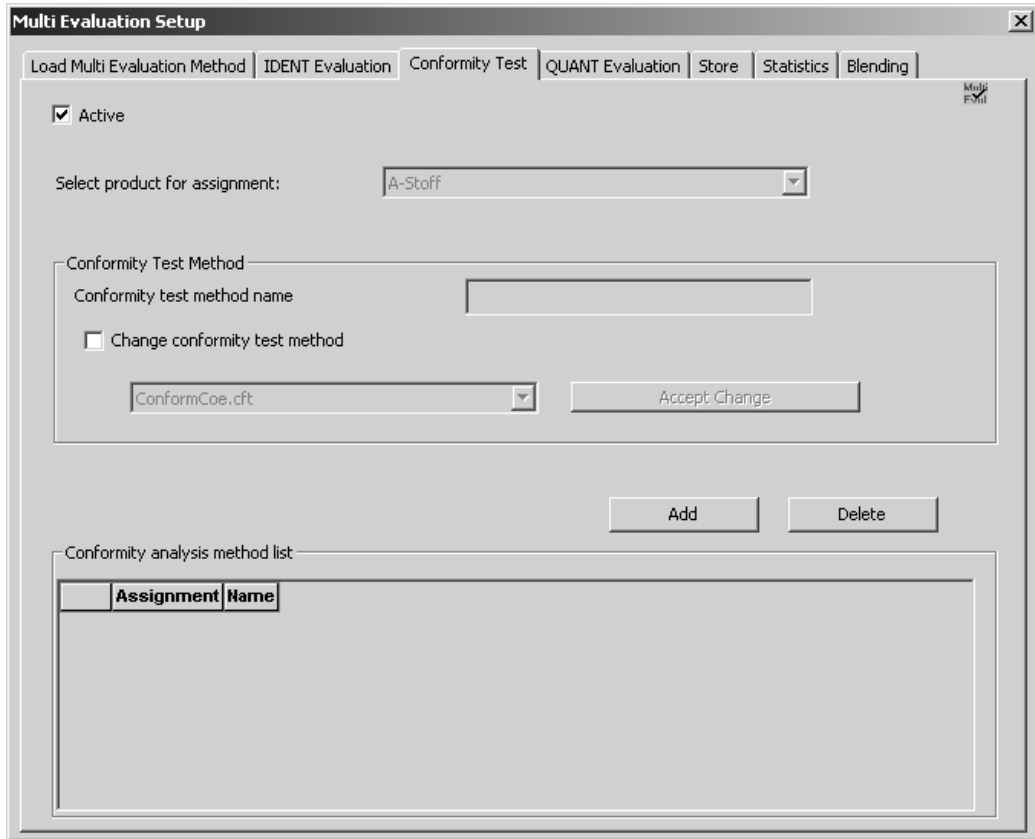


Figure 6: Multi Evaluation Setup - Conformity Test tab

Activate the *Active* check box. If you have defined an expected reference group on the *IDENT Evaluation* tab, the upper drop-down list includes the name of the reference group defined, and will be deactivated. If no reference group has been defined, the drop-down list will be activated and you can select the desired group of the IDENT library (see figure 7).

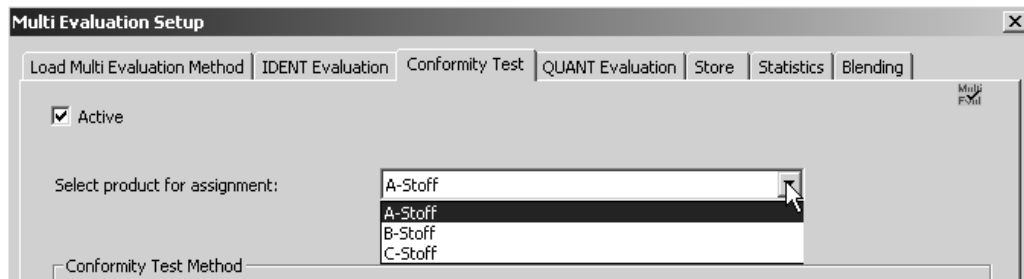


Figure 7: Select Product for Assignment

Assign an individual conformity test method to the selected IDENT library group. Activate the *Change conformity test method* check box and select the appropriate method from the drop-down list. Confirm the choice by clicking on the *Accept Change* button (see figure 8).

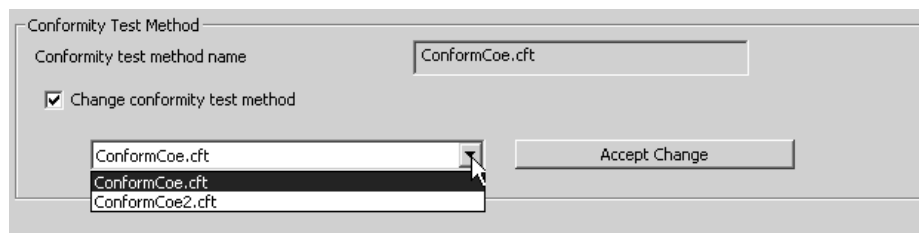


Figure 8: Select Conformity Test Method

If the settings are made, click on the *Add* button (see figure 9). A table will be displayed including the assignments made, and the name of the conformity test method. To remove a particular assignment from the list, select the corresponding line and click on the *Delete* button.

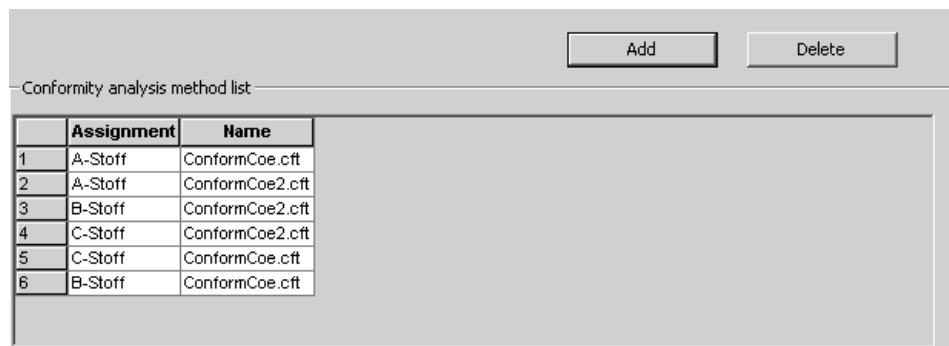


Figure 9: Method List of Conformity Test

### 1.1.3 QUANT Evaluation

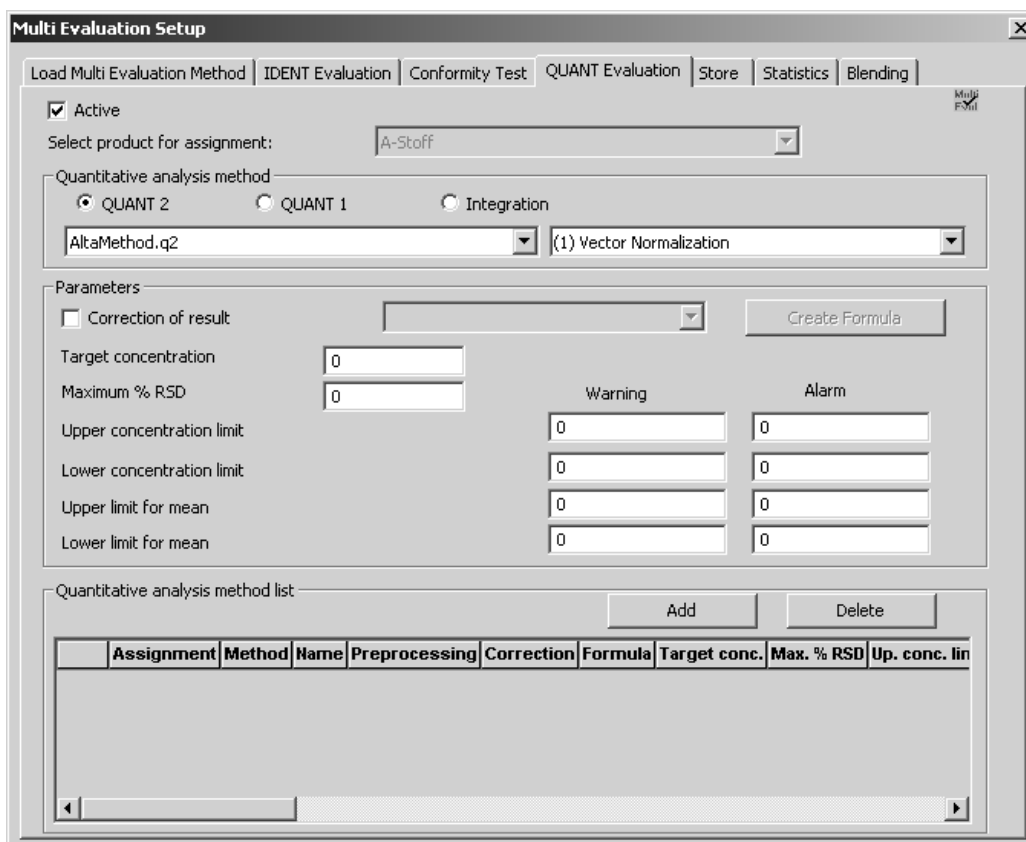


Figure 10: Multi Evaluation Setup - QUANT Evaluation tab

Activate the *Active* check box. If you have defined an expected reference group on the *IDENT Evaluation* tab, the upper drop-down list includes the name of the reference group, and will be deactivated. If no reference group has been defined, the drop-down list will be activated and you can select the desired group of the IDENT library.

Assign an individual QUANT or INTEGRATION method to the selected IDENT library group. Activate one of the *Quantitative analysis method* option buttons and select the appropriate method from the drop-down list.

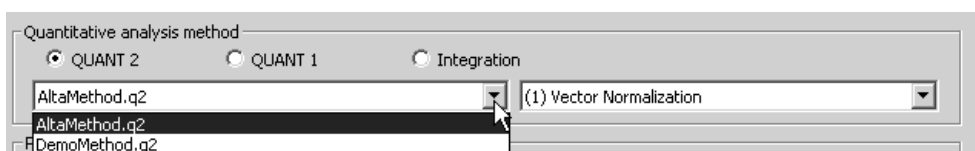


Figure 11: Quantitative Analysis Methods

In case of QUANT 1 and INTEGRATION you can also select between different data preprocessing methods. The methods include *Vector Normalization*, *1st* and *2nd Derivative* and combinations of both methods. Frequently, the *Vector*

*Normalization* method is used to preprocess data. In many cases, however, you even get better results if you select *1st* or *2nd Derivative*. For further details on the preprocessing methods, see chapter 8 in the OPUS Reference Manual.

In the *Parameters* group field you can specify additional values which are set to 0 by default.

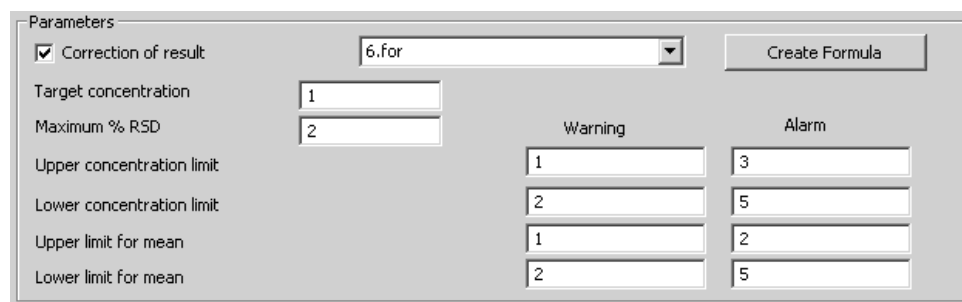


Figure 12: Parameters group field

Activate the *Correction of result* check box and apply a formula from the drop-down list. If you want to create a new formula for the correction of analysis results, click on the *Create Formula* button. The following dialog pops up:

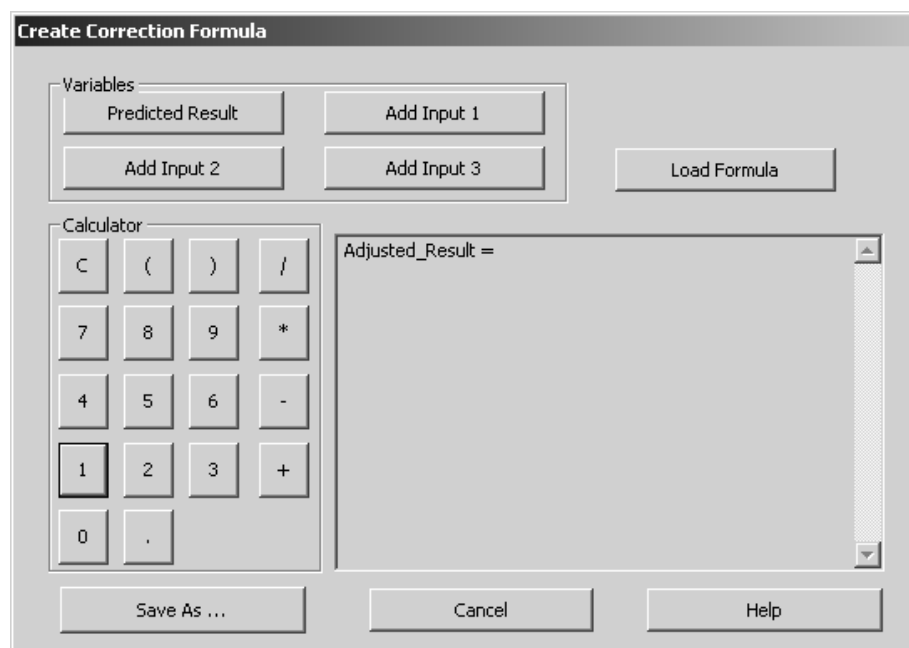


Figure 13: Correction Formula Calculator

By means of the *Load Formula* button you can load an existing formula with the file extension \*.for. The string code begins with the *Adjusted\_Result =* term, and you can add up to 4 different variables:

- 1 variable for the result predicted by the method
- 3 variables for input values which can be set during spectra evaluation

If you click on the *Add Input...* button(s) or *Predicted Result* button or on one of the figure buttons, the string code will be extended according to the entries made.

Example:  $\text{Adjusted\_Result} = \text{Predicted\_Result} * 3.01 / \text{Add\_input } 1 * \text{Add\_input } 2 / 5.2$

Always use the *Calculator* block which includes brackets, decimal point and the four basic arithmetic operations. To save the new formula click on the *Save as...* button. Make sure that you use a valid formula which does not produce any arithmetic error.

No recommendations can be made for the values to be entered for *Target Concentration* or the highest allowable standard deviation in case of several analysis (*Maximum% RSD*). The optimum value has to be determined empirically.

Depending on the test result warning and alarm limits can be set in case of the concentration and average value limit. As soon as the warning limit defined will be exceeded, a warning is given and informs you where the error has occurred. If all parameters have been set, click on the *Add* button to have the method list displayed. The warning and alarm values will be set to 0 again. In this way customized evaluation methods and parameters can be assigned to different components.

	Assignment	Method	Name	Preprocessing	Correction	Formula	Target Conc.	Ma
1	A-Stoff	0	AltalMethod.q2	No Spectral Data Preprocessing	1	6.for	1	2
2	A-Stoff	1	Quant1.q1	No Spectral Data Preprocessing	1	6.for	1	2
3	A-Stoff	2	Co2.int	No Spectral Data Preprocessing	1	6.for	1	2

Figure 14: Quantitative Analysis Method List

The analysis method list includes all the parameters set. The figure displayed in the *Method* column refers to the method selected, i.e.:

- 0 = QUANT 2
- 1 = QUANT 1
- 2 = INTEGRATION

To remove a particular assignment from the list, select the corresponding line and click on the *Delete* button.



## 1.1.4 Store

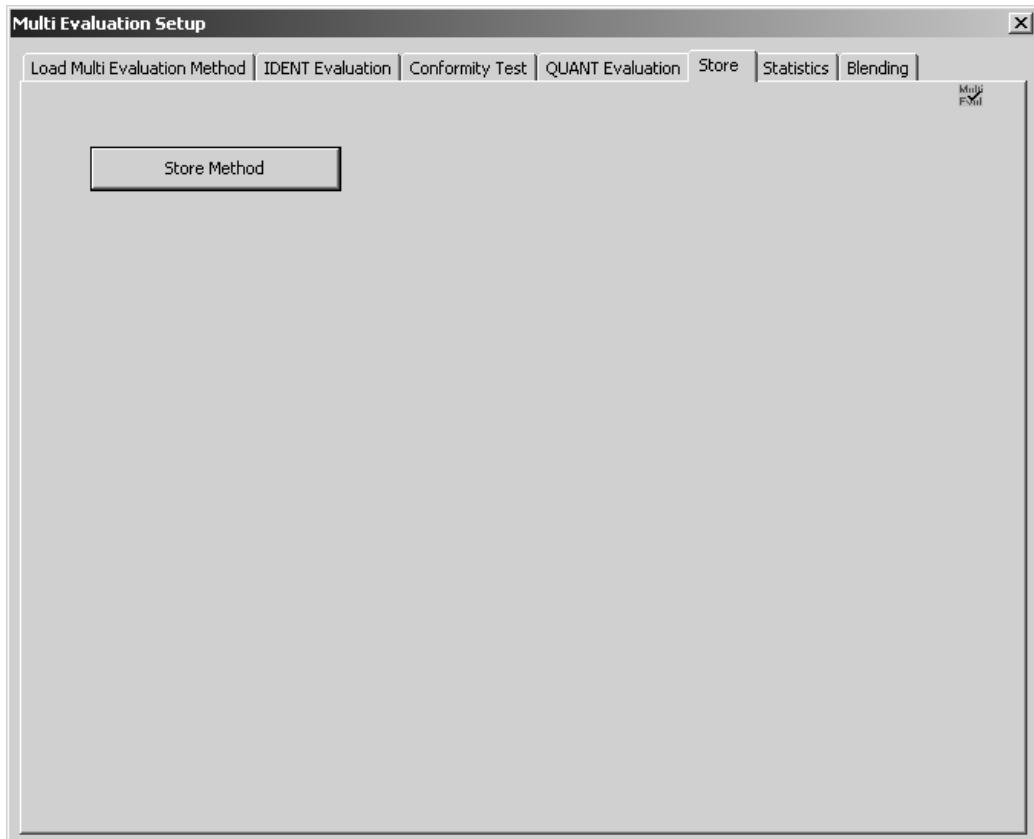


Figure 15: Multi Evaluation Setup - Store tab

To finish the multi evaluation setup procedure click on the *Store Method* button. The method will be stored in the OPUS *MultiEvaluation* directory which root path can be defined in the *Setup* menu by means of the *User Settings* command, provided you have the necessary user rights. For the *MultiEvaluation* directory the default root path will always be the currently used local OPUS directory.

## 1.1.5 Statistics

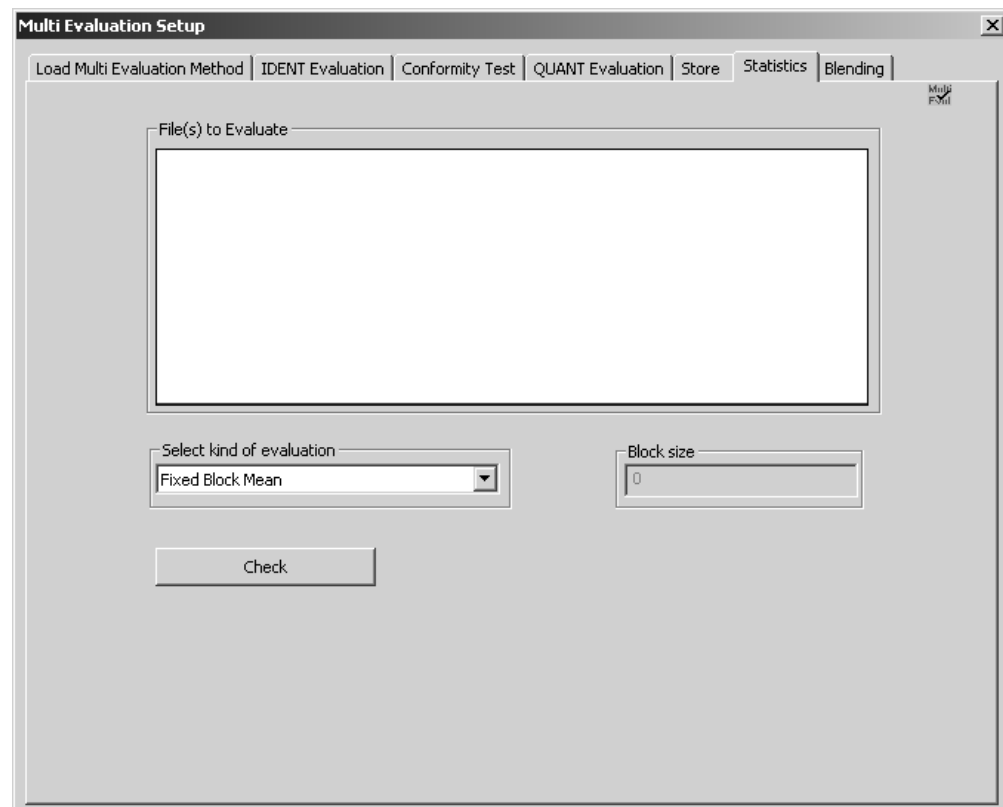



Figure 16: Multi Evaluation Setup - Statistics tab

The settings made on the *Statistics* tab have no effect on the multi evaluation method stored. Drag & drop spectrum files or file lists into the *File(s) to Evaluate* selection field. Select a statistics evaluation function from the drop-down list and define the block size. For further details on the different statistics evaluation functions, refer to chapter 3.

When clicking on the *Check* button a multi evaluation analysis will be performed. The result of this analysis forms the basis for the subsequent statistical evaluation.

### 1.1.5.1 Statistical evaluation of QUANT or INTEGRATION results

The results produced by a QUANT or INTEGRATION evaluation can also be subject to statistical evaluation. The result of this statistical evaluation will be displayed in the OPUS *Online* window.

Click on the *Statistics* tab and *Drag & Drop* a file list, i.e. the LIST data block (  LIST ), from the OPUS browser to the *File(s) to Evaluate* selection field. Make sure that you use the LIST data block only, as OPUS will not accept any other data block in this case.

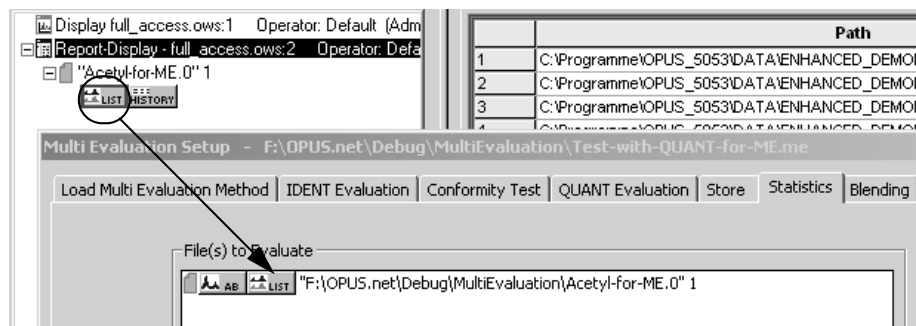


Figure 17: Statistical evaluation with LIST data block

Select the kind of statistical evaluation and click on the *Check* button. Each type of evaluation will be performed (ME, QUANT and STATISTICS), while the different spectra belonging to the file list will be loaded into the OPUS browser.

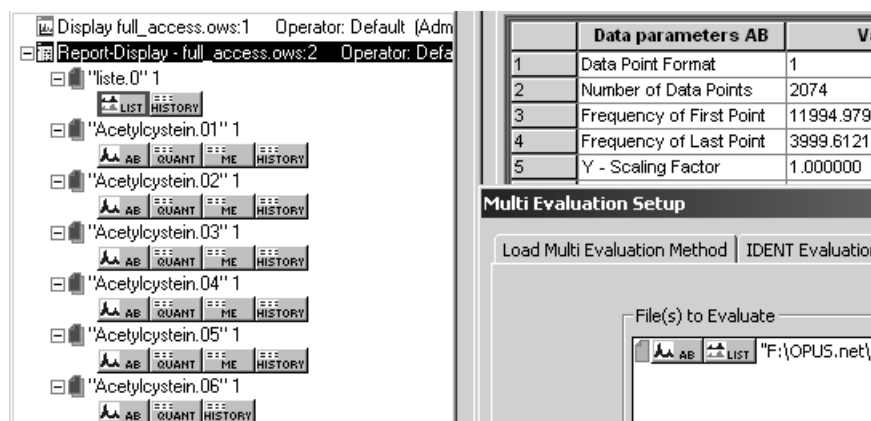


Figure 18: Spectra loaded belonging to the file list

As soon as the evaluation has been finished, the OPUS *Online* window pops up automatically and displays the statistical evaluation results.

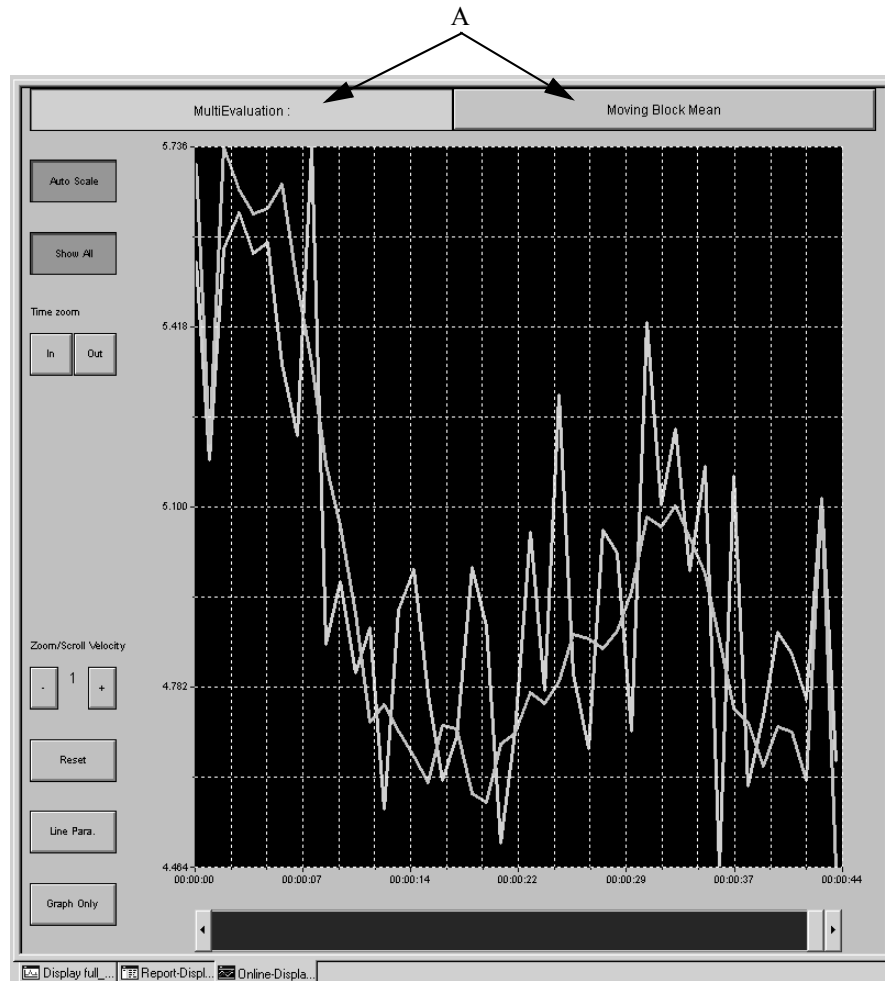



Figure 19: Result view of statistical evaluation

The evaluation result is displayed in the form of bands. These bands show the direct result of the multi evaluation analysis as well as the statistical evaluation result. The button at the top of the display (A in figure 19) has the same color as the corresponding band.

If the evaluation has been finished, the TRC (  ) data block will be attached to the file list in the OPUS browser window. Double clicking on this data block allows to have the result displayed in a report view.

## 1.1.6 Blending

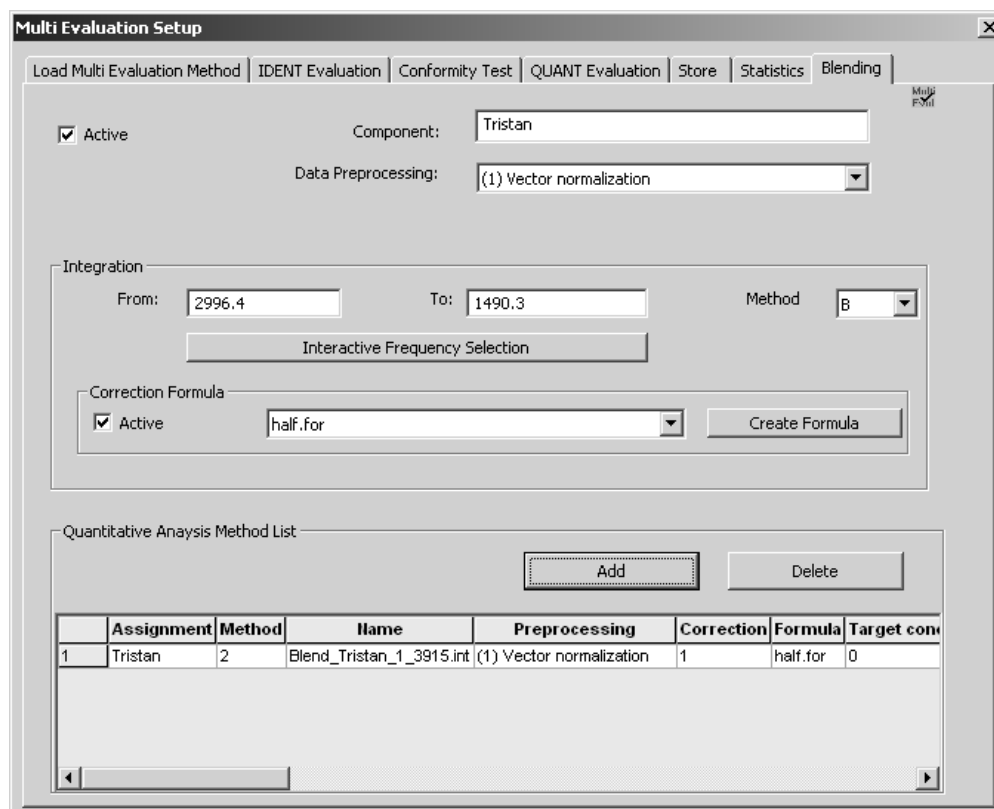


Figure 20: Multi Evaluation Setup - Blending tab

The settings made on the *Blending* tab have no effect on the multi evaluation method stored. This tab can be used to define an integration method and a data preparation method, and to interactively set integration limits.

Activate the *Active* check box and enter the name of the component into the entry field. Select one of the data preprocessing methods from the drop-down list.

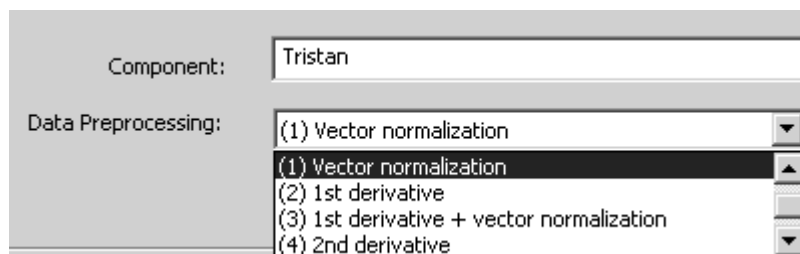


Figure 21: Select Data Preprocessing Method

Define an integration method which specifies the frequencies for one or more areas which are to be integrated.

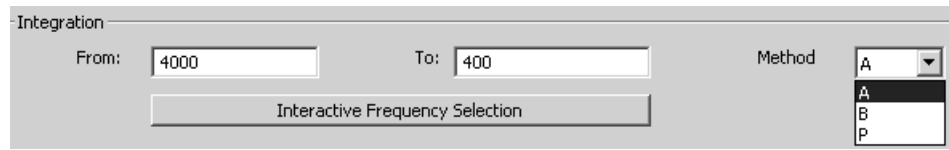


Figure 22: Select Integration Method

The following integration methods are available:

- **Method A:**  
Integration is performed using zero as baseline.
- **Method B:**  
A straight line is drawn between the intensity values of the frequency limits specified. The area above this line is integrated.
- **Method P:**  
The intensity at the frequency specified in the *From* entry field will be applied.

To set the frequency limits either enter the values into the entry fields or click on the *Interactive Frequency Selection* button. The interactive frequency selection is possible both for single spectra and spectra lists.

If you activate the *Active* check box in the *Correction Formula* group field, you can either select a formula from the drop-down list, if available, or create a new formula. For any further details on how to create a formula, refer to chapter 1.1.3.

If you click on the *Add* button, the integration limits and integration method selected (A, B or P) will be grouped into a new method. This method will be registered as new line in the matrix of QUANT methods together with the name of the component and the data preprocessing.

If more than one QUANT method is defined, always the result of the first method indicated in the list will be considered. The name of the method consists of: *Blend\_Name of the component\_Left integration limit\_Right integration limit Random value* (see figure 23).

	Assignment	Method	Name	Preprocessing	Correction	Formula	Target conc
1	Tristan	2	Blend_Tristan_1_3_15.int	(1) Vector normalization	1	half.for	0

Figure 23: Quantitative Analysis Method List

## 1.2 Test

Start the multi evaluation by clicking on the *Multi Evaluation Test* command in the *Evaluate* menu. The following dialog opens:

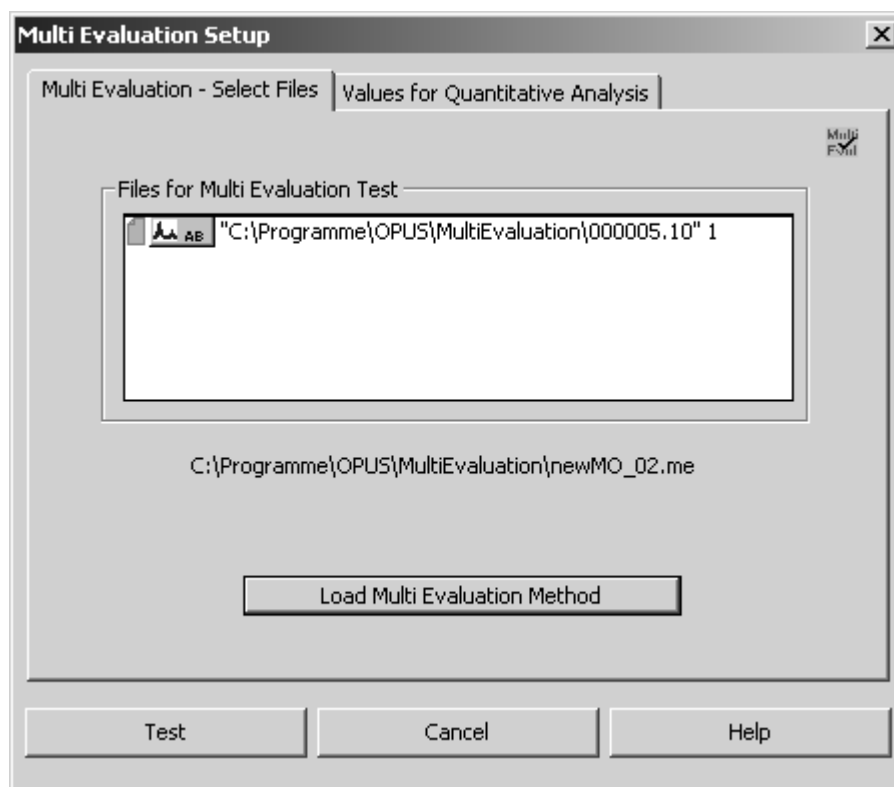


Figure 24: Multi Evaluation Test - Select Files tab

Drag & drop the file(s) to be tested from the OPUS browser window into the *File(s) for Multi Evaluation Test* selection field.

Click on the *Load Multi Evaluation Method* button and load the particular method. Normally, the path of the method previously used is displayed above this button.

The *Values for Quantitative Analysis* tab displays the three input variables defined by means of the formula calculator (see figure 25).

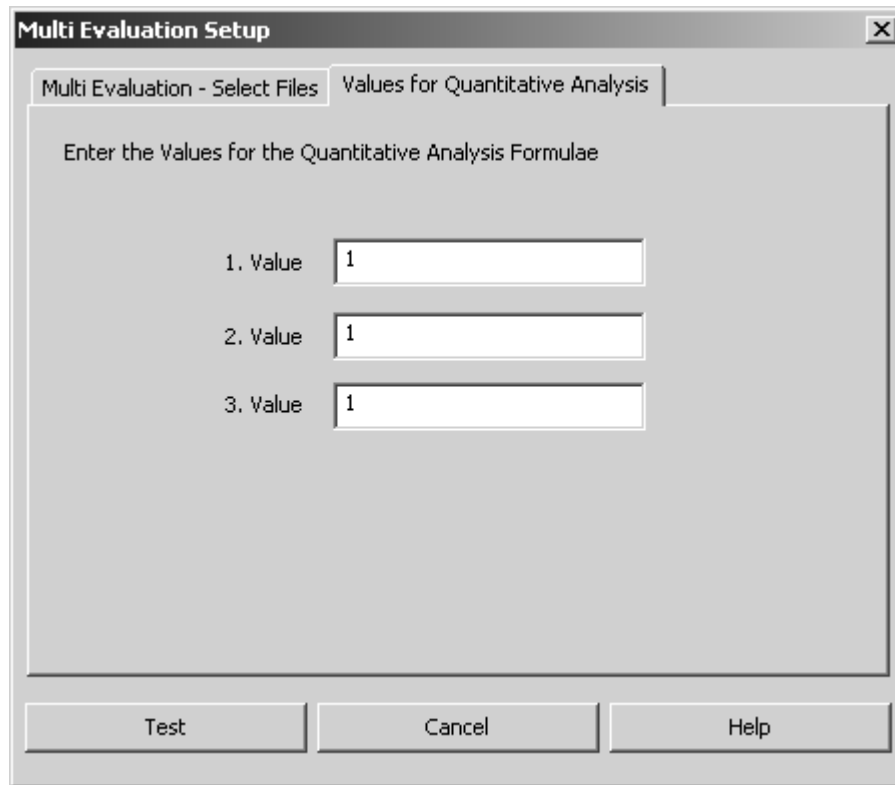



Figure 25: Multi Evaluation Test - Values for Quantitative Analysis tab

Start the multi evaluation analysis and click on the *Test* button. Each step performed during multi evaluation will be indicated by the status bar. The multi evaluation results are stored in an *ME* data block (  ) and displayed in a special report (see figure 26).

Multi Evaluation Test Report		Values					
ME Format Version:	1.1						
Method file	F:\OPUS.net\Release\MultiEvaluation\l1er.me - 2004/11/22 07:30:56 (GMT+1)						
Ident Test active	True						
Ident Test passed	True						
Ident Test Result	L-Alanin						
Confo Tests active	True						
Confo Tests applied	True						
All Confo Tests passed	True						
Confo Test Result	L-Alanin						
Quant Tests active	True						
Methodname	Assignment	Preprocessing	Uncorrected	Use Formula	Formula Name	Final Result	Status
AB_TEST.q2	L-Alanin	(0) No Spectral Data Preprocessing	5.392603e+000	0		5.392603e+000	ALARM
AB_NIR.q1	L-Alanin	(4) 2nd Derivative	7.864650e+000	1	80percent.for	6.29172	UNCHECKED
AB_1.int	L-Alanin	(2) 1st Derivative	-2.915944e-001	1	90prozent.for	-0.26243496	UNCHECKED

Figure 26: Multi Evaluation report

The multi evaluation test report contains the test name and path as well as the results of the different method tests, e.g. QUANT, IDENT or Conformity Test (A in figure 26). The Multi Evaluation final test status is indicated by either ERROR, REGULAR, UNCHECKED, WARNING or ALARM (B in figure 26).



If, e.g., in the QUANT evaluation method the upper and lower concentration limit defined for warning or alarm differs, the final result is checked against these limits.

The concentration limits are not taken into account if all concentration limits are set to 0 (default setting). If they are not evaluated, the status is reported as UNCHECKED unless an ERROR occurs. Any ALARM supersedes a WARNING. An error occurs if, e.g., a data block type does not correspond to a method.



# 2 Setup File List

Several spectra of a particular spectrum type can be combined into one common file list, and edited as one single spectrum. The list which consists of different spectra is stored in the LIST data block (LIST), and displayed when selecting the respective data block.

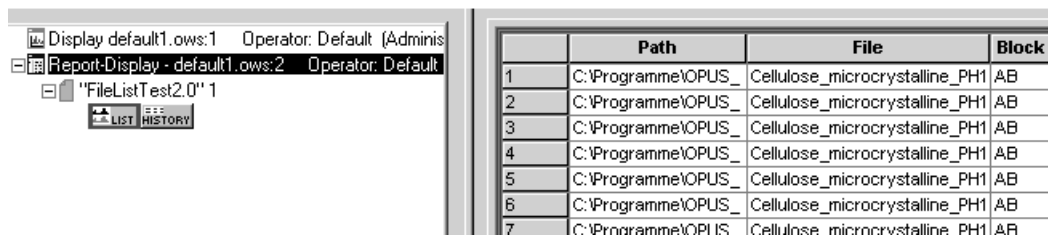


Figure 27: LIST data block

All OPUS commands available for manipulating and evaluating spectra data can be used for the complete spectra file list in the same way as being used for single spectra files.

To create a spectra file list click on the *Setup File List* command in the *Edit* menu, and click on the *Add Spectra* button to load the particular spectra.

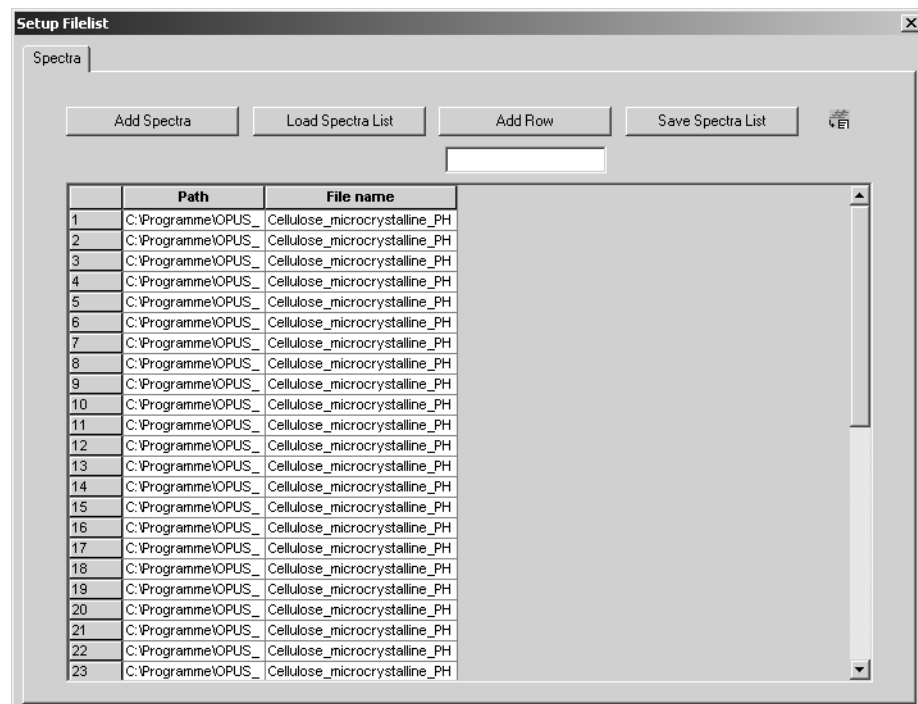


Figure 28: Setup File List - Different spectra

By default, the path and file name of each spectrum is displayed in a table. This table can be customized, i.e. enlarged by as many columns as you like, e.g. to be able to store parameters and input values required for evaluation functions. Enter the name of the column into the entry field below the *Add Row* button. If you click on this button, the new column will be added to the table.

To store the spectra file list click on the *Save Spectra List* button. Define a specific name for the list. Spectra file lists are stored as reports in the OPUS format. The file extension of the list may be incremented, i.e. automatically increased by 1. This is especially helpful if you want to use the same name for different spectra file lists.

In case of evaluating single spectra you can also add specific parameter values to the table in the form of a column. Make sure that you always enter the right parameter code for the specific value into the entry field. The parameter code can be obtained from the Macro Editor, also see the OPUS Programming manual.

If you want to add, e.g. the Mahalanobis distance in case of a QUANT evaluation, or the outlier identification for each single spectrum from the QUANT report to the spectra file list, you first have to create an INFO data block (see also chapter 4 in the OPUS reference manual.)

Select the *Add Information* command in the *Edit* menu. Enter the following data into the *Compound name* line (figure 29): name of the OPUS function (A), result data block (B) as well as the corresponding element from the QUANT report (C), i.e. main report number, sub-report number, line, column.

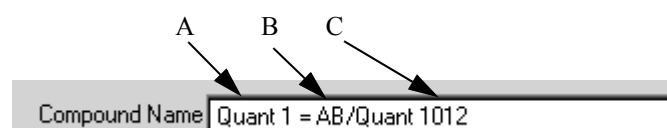


Figure 29: Example of an information input

To perform a statistical evaluation load the file list, which you have created, by means of the *Load File* command from the *File* menu. Select the *Statistics* command from the *Evaluate* menu. For details, see chapter 3. As the list is regarded as one spectrum file, the statistical evaluation result will be displayed as follows.

	Data parameters AB	Values
1	Data Point Format	1
2	Number of Data Points	2074
3	Frequency of First Point	11994.979689
4	Frequency of Last Point	3999.612199
5	Y - Scaling Factor	1.000000
6	Y - Maximum	0.964351
7	Y - Minimum	0.167568
8	Date of Measurement	13/05/2003
9	Time of Measurement	09:33:14.311 (GMT+2)
10	X Units	Wavenumber cm-1

Figure 30: File list parameters

Note that the single spectrum files which make up the file list will all be manipulated after the evaluation statistics has been performed. The manipulation will be indicated by the red symbol in front of the file name.

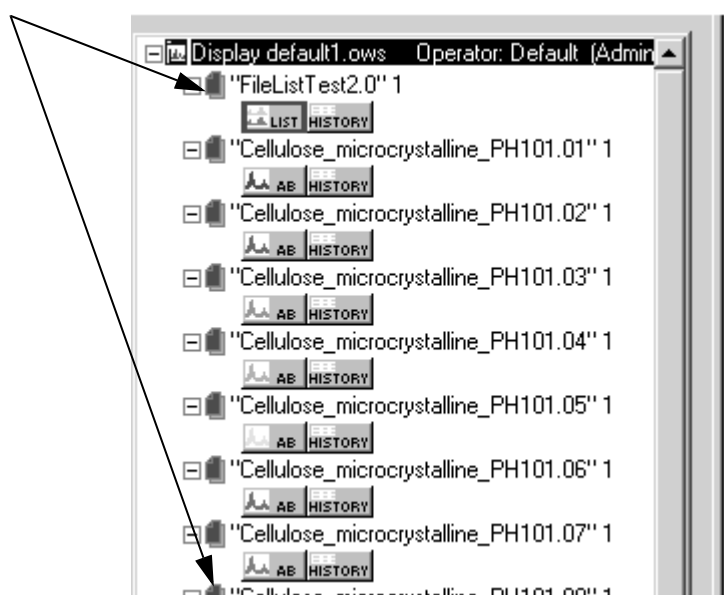


Figure 31: Spectra file list with manipulated files

To restore the original spectrum files, click on the *Undo Changes* command in the *File* menu.



# 3 Statistics

OPUS STATISTICS provides statistical information on single spectra, file lists or 3D spectra files. As even a thorough statistical evaluation cannot rule out all potential analytical problems, the process of method development and validation should address the most common ones.

The OPUS *Statistics* function serves as a basis for the statistical evaluation of quantitative results by means of the *Multi Evaluation* function (see chapter 1.1.5). If you directly use the *Statistics* function, this may only allow a statistical performance on the spectra themselves, which may not be very helpful in case of routine analytics. Therefore, the following chapter has to be seen as reference to the different evaluation methods available in OPUS, and outlines them in more detail by means of a single spectrum.

To start the statistical evaluation select the *Statistics* command in the *Edit* menu. Drag & drop the file(s) to be evaluated into the *File(s) to evaluate* selection field.

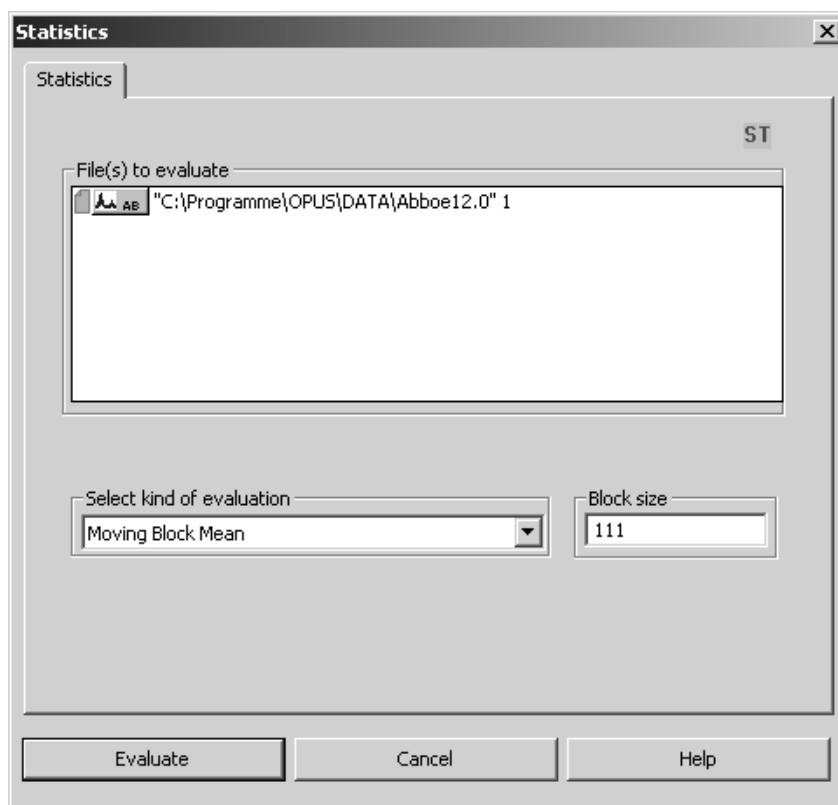


Figure 32: Statistics dialog

Select a statistical evaluation function from the respective drop-down list and enter the number of data points manually into the *Block size* entry field. To get reasonable results always define a meaningful block size. Start the statistical evaluation by clicking on the *Evaluate* button.

The statistical evaluation in OPUS is based on different evaluation functions which are described in the following:

- Maximum/minimum value
- Mean value
- Standard deviation
- Variance

### 3.1 Maximum/Minimum Value

OPUS determines the previous maximum or minimum value of data points. Note that this kind of statistical evaluation function will overwrite the original spectrum.

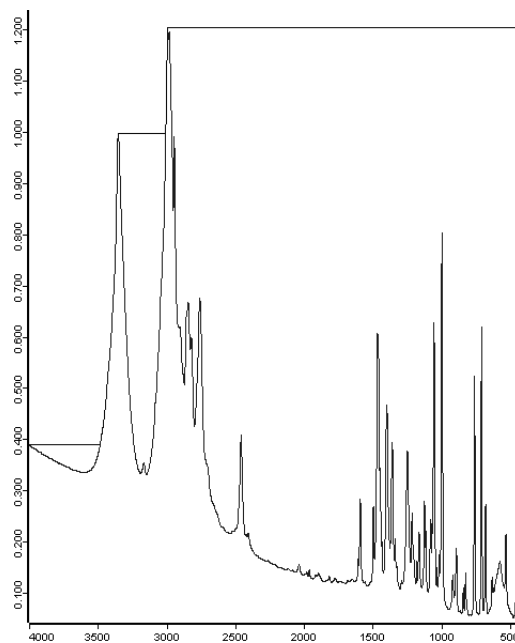
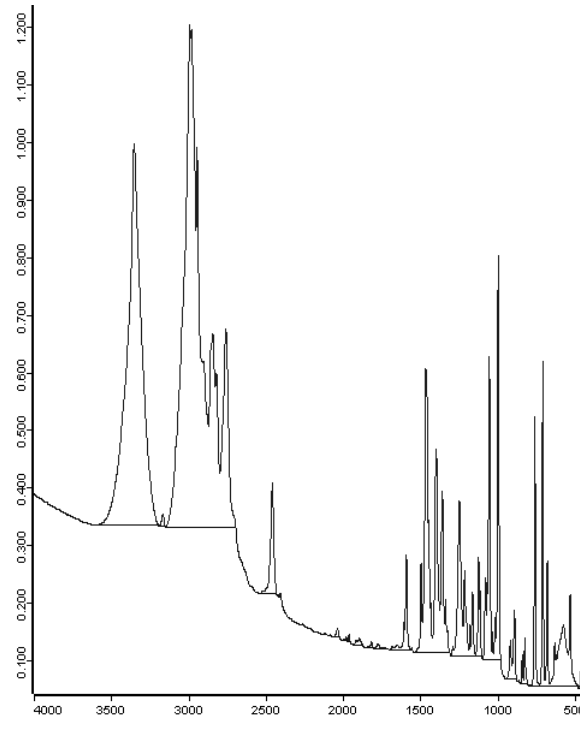


Figure 33: Example of *Maximum Value* function



Figure 34: Example of *Minimum Value* function

## 3.2 Mean Value

The mean value of a spectrum is defined as the sum of all data points divided by the number of data points. *Mean* is another word for the arithmetic average. In case of normal frequency distribution, the mean value is located at the center with most values clustered around the mean and the frequency of occurrence decreasing from this central point.

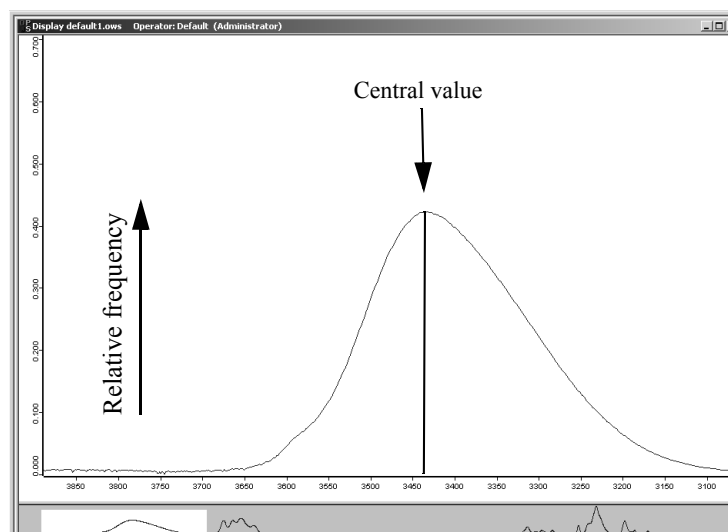


Figure 35: Normal frequency distribution

The total area beneath the curve can be defined as being equal to 1.00 (or as 100% of the data points distributed around the mean).

This kind of statistical evaluation function is used to decrease the noise within a spectrum. In case of the *Mean Value* statistical evaluation function you can either select between

- moving block (average is calculated from all data points)
- fixed block (average is calculated from defined block only)
- overall block (average is calculated from the entire spectrum).

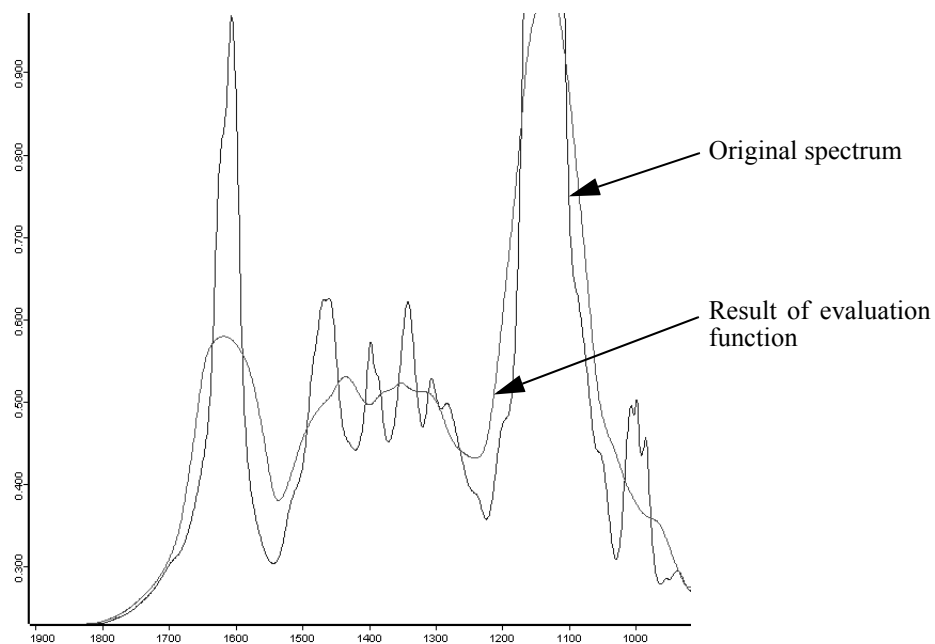


Figure 36: Example of *Moving Block Mean* function

If you use the *Fixed Block Mean* function, the average value is displayed by horizontal sections, see figure 37. This applies to single spectra, file lists and 3D files.

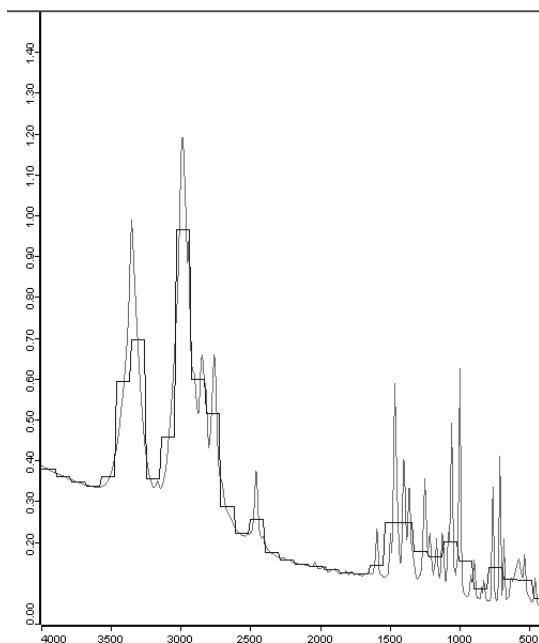


Figure 37: Example of *Fixed Block Mean* function

Using the *Overall Block Mean* function means that the statistical evaluation result is stored in the data block report. To have these parameters displayed in case of single files or file lists, right click on the red file symbol of the spectra file in the OPUS browser window and select the *Show Parameter* command from the pop-up menu. The parameters are displayed as follows:

Data parameters AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4000.146484
Frequency of Last Point	399.243164
Y - Scaling Factor	1.000000
Y - Maximum	1.207416
Y - Minimum	0.044025
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:32:34
Overall Block Mean	0.286445

Figure 38: Data parameters report

If you use 3D files in connection with the *Overall Mean* statistical evaluation function, the result will be stored in a TRC data block (TRC) which is appended to the manipulated file.

### 3.3 Standard Deviation

The standard deviation is defined as the square root of the variance (chapter 3.4). Advantages of using the standard deviation over variance function are:

- The standard deviation is expressed in the measurement units of the data.
- The standard deviation is easily calculated from the variance.
- The areas below the curve of normally distributed data points can be precisely calculated for a given range.

In case of the *Standard Deviation* evaluation function you can either select between

- moving block (useful if no or minor signal changes are expected)
- fixed block
- overall block.

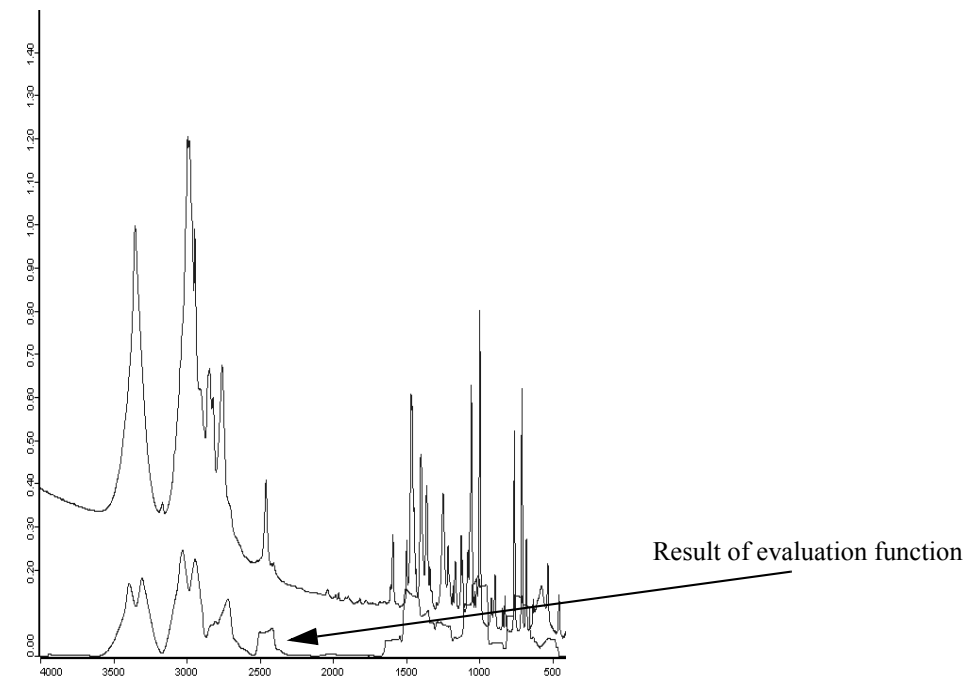


Figure 39: Example of *Moving Block Standard Deviation* function

If you use the *Fixed Block Standard Deviation* function, the standard deviation is displayed by x-axis sections, see figure 40. This applies to single spectra, file lists and 3D files.

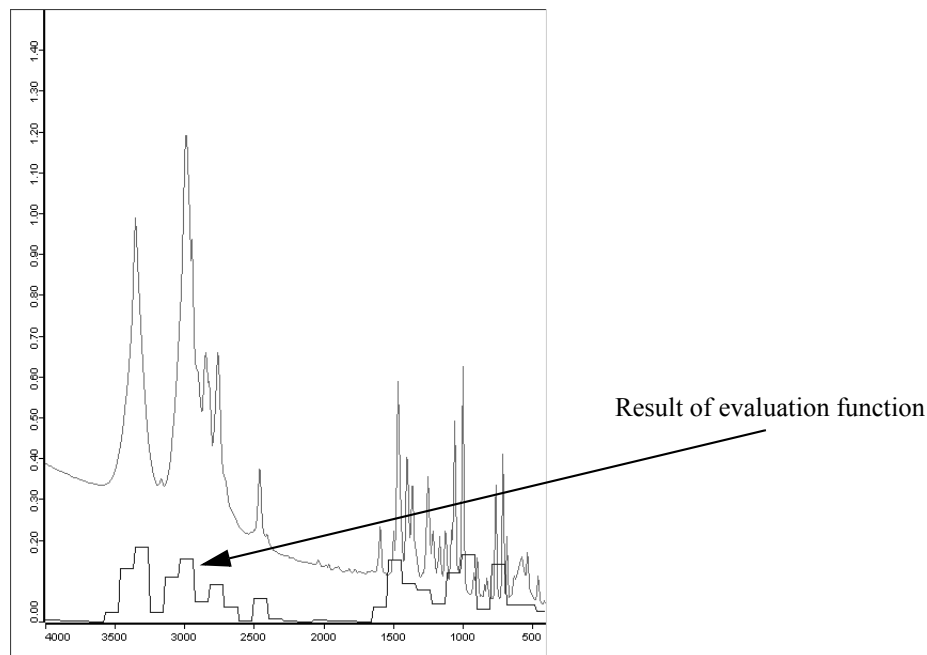



Figure 40: Example of *Fixed Block Standard Deviation* function

Using the *Overall Block Standard Deviation* function means that the evaluation result is stored in the data block report. To have these parameters displayed in case of single files or file lists, right click on the red file symbol of the spectra file in the OPUS browser window and select the *Show Parameter* command. The parameter is displayed as follows:

Data parameters AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4000.146484
Frequency of Last Point	399.243164
Y - Scaling Factor	1.000000
Y - Maximum	1.207416
Y - Minimum	0.044025
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:32:34
Overall Block Standard Deviation	0.213995

Figure 41: Data parameters report

If you use 3D files in connection with the *Overall Block Standard Deviation* evaluation function, a TRC data block (  ) is appended to the manipulated file.

### 3.4 Variance

The variance of a random variable  $x$  is a measure of its statistical dispersion, indicating how far from the expected value its values typically are. The disadvantage of the *Variance* evaluation function is that the variance has a different unit than the data. This is the reason why in many cases one uses the standard deviation which is defined as square root from the mean value.

The variance is based on the following equation:

$$s^2 = \frac{\sum x^2 - (\sum x)^2 / n}{n - 1}$$

with  $n$  being the number of data points per block size,

and  $s^2$  the variance.

In case of the *Overall Block Variance* statistical evaluation function  $n$  is the number of data points of the entire spectrum.

In case of this kind of evaluation function you can either select between

- moving block
- fixed block
- overall block.

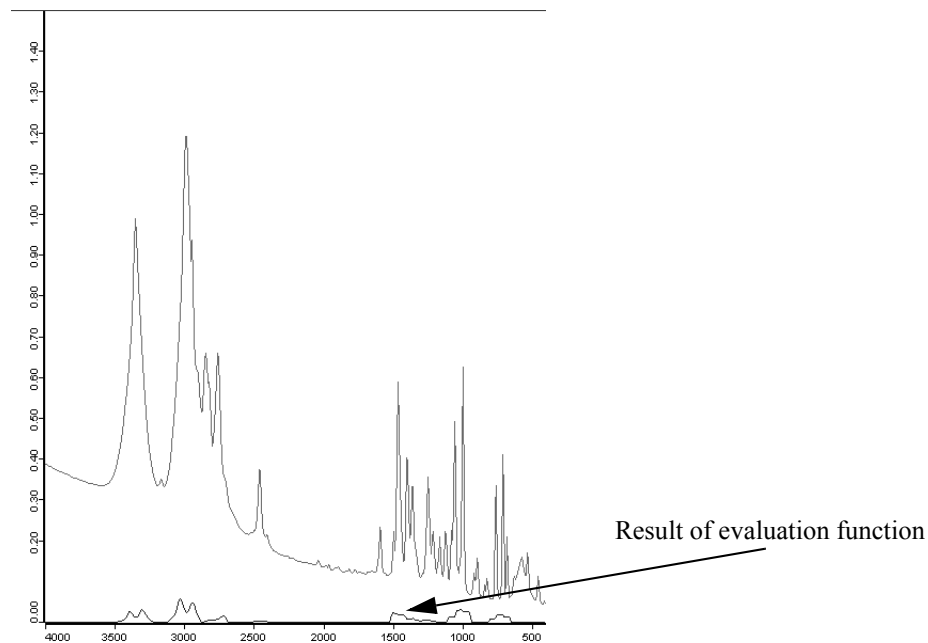


Figure 42: Example of *Moving Block Variance* function

If you use the *Fixed Block Variance* function, the variance is displayed by x-axis sections, see figure 43. This applies to single spectra, file lists and 3D files.

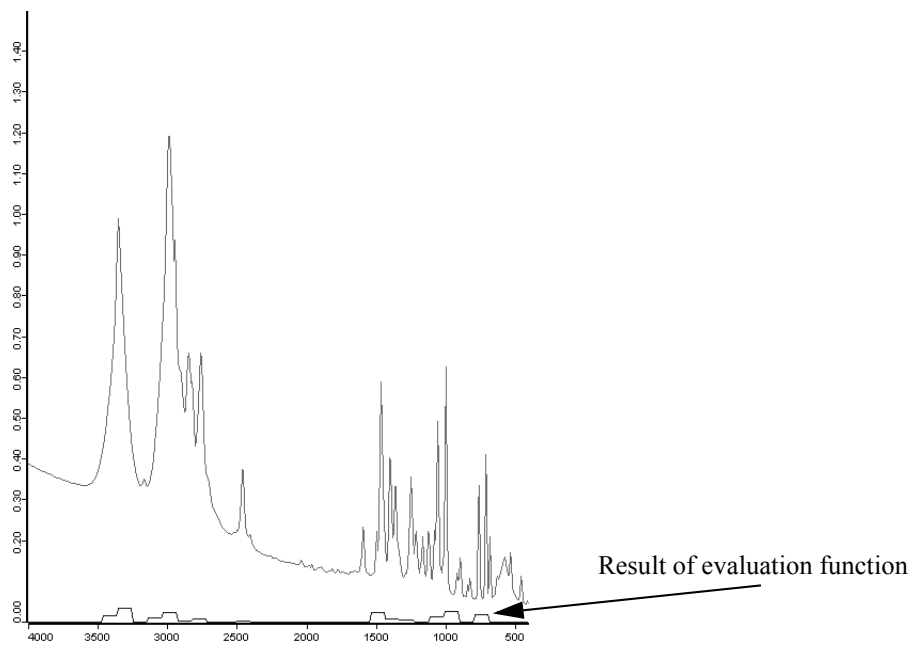



Figure 43: Example of *Fixed Block Variance* function

Using the *Overall Block Variance* function means that the evaluation result is stored in the data block report. To have these parameters displayed in case of single files or file lists, right click on the red file symbol of the spectra file in the OPUS browser window and select the *Show Parameter* command. The parameter is displayed as follows:

Data parameters AB	Values
Data Point Format	1
Number of Data Points	3735
Frequency of First Point	4000.146484
Frequency of Last Point	399.243164
Y - Scaling Factor	1.000000
Y - Maximum	1.207416
Y - Minimum	0.044025
X Units	Wavenumber cm-1
Y Units	Absorbance Units
Derivative	0
Date of Measurement	07/08/84
Time of Measurement	11:32:34
Overall Block Variance	0.045794

Figure 44: Data parameters report

If you use 3D files in connection with the *Overall Block Variance* evaluation function, a TRC data block (  ) is appended to the manipulated file.





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