

# **MSFileReader**

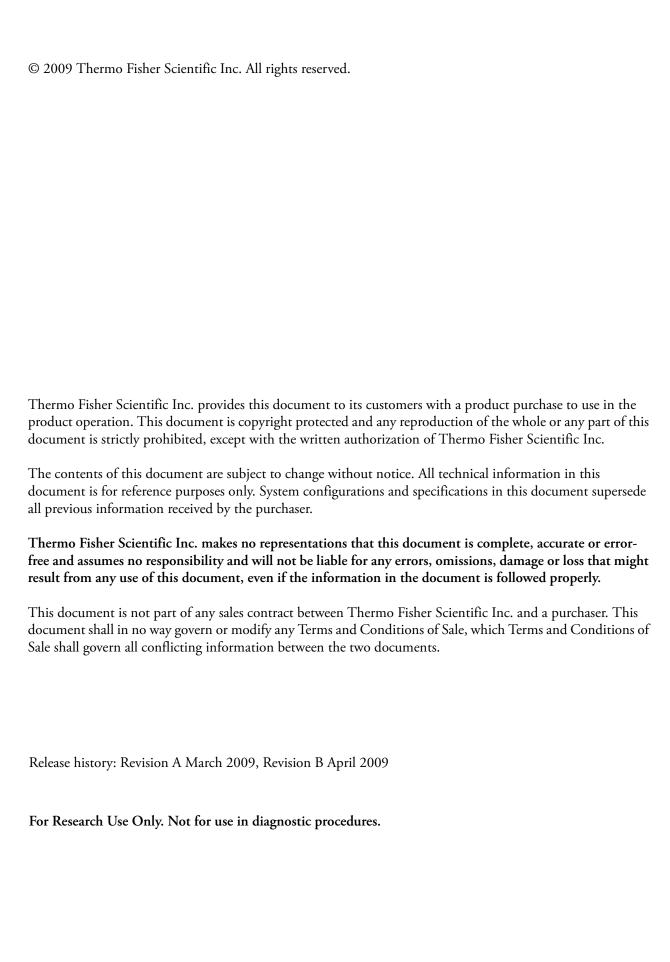
Version 1.0

**Reference Guide** 

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IsCentroidScanForScanNum	
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# **Library Definitions**

MSFileReader is designed to support read access to Xcalibur .raw files in a simple-to-use standard COM object without requiring installation of the Xcalibur data system. It is designed to be used with C++-based applications, but since it is a COM object, you can use any language that supports the COM interface.

Most of the functions described in this document are simple data access functions, but the manual also includes a number of higher-level functions that extract and manipulate the data in commonly used ways.

The description of each function includes the following information:

- The function calling sequence
- Return values
- · Definition of both input and output parameters
- An example using the function

The enumeration types described in this chapter standardize the handling of the following components: the variables set by the instrument (or instruments) during acquisition, and algorithms in the post-acquisition processing of data. Using these variables, you can determine the instrument type (mass spectrometer, analog signal, and so on), and you can select the number of the instrument (with a multiple instrument configuration) used to generate data to the raw file. The described enumerators also handle access to selected channels from multiple-channel data.

All of the described methods provide for systematic error checking and handling. This chapter also provides descriptions related to the error codes returned as a result of trapped errors.

#### **Contents**

- Enumerated Types
- Error Codes

## **Enumerated Types**

Several functions expect or return a parameter of type "long" that defines, typically, a type parameter.

#### 1 Library Definitions

**Enumerated Types** 

- Sample Type
- Controller Type
- Cutoff Type
- Chromatogram Type
- Chromatogram Operator
- Smoothing Type

## **Sample Type**

Sample type is returned in the GetSeqRowSampleType(...) function. The returned value has the following meaning.

Value	Sample type
0	Unknown
1	Blank
2	QC
3	Standard Clear (None)
4	Standard Update (None)
5	Standard Bracket (Open)
6	Standard Bracket Start (multiple brackets)
7	Standard Bracket End (multiple brackets)

## **Controller Type**

Controller type determines the type of data being accessed. This type is set or returned in the calls to Get or Set controller information. This value has the following meaning.

Value	Controller type
-1	No device
0	MS
1	Analog
2	A/D card
3	PDA
4	UV

## **Cutoff Type**

Cutoff type is specified in calls to GetMassListXYZ(...). The purpose of this cutoff type is to determine how the cutoff value is interpreted. This value has the following meaning.

Value	Cutoff type
0	None (all values returned)
1	Absolute (in intensity units)
2	Relative (to base peak)

## **Chromatogram Type**

Chromatogram type is specified in the GetChroData(...) function. The value of this field depends on the current controller and whether or not this is the first chromatogram type parameter or the second chromatogram type parameter to this function. This value has the following meaning:

For MS devices (chromatogram trace type values are in parentheses).

Chro type 1	Chro operator	Chro type 2
Mass Range (0)	+ or -	Mass Range (0)
TIC (1)	-	Mass Range (0)
TIC (1)	-	Base Peak (1)
Base Peak (2)	+ or -	Mass Range (0)

For PDA devices (chromatogram trace type values are in parentheses).

Chro Type 1	Chro Operator	Chro Type 2
Wavelength Range (0)	+ or -	Wavelength Range (0)
Total Scan (1)	-	Wavelength Range (0)
Total Scan (1)	-	Spectrum Maximum (1)
Spectrum Maximum (2)	+ Or -	Wavelength Range (0)

# 1 Library Definitions Enumerated Types

For UV devices (chromatogram trace type values are in parentheses).

Chro Type 1	Chro Operator	Chro Type 2
Channel A (0)	+ or -	Channel B (0)
Channel A (0)	+ or -	Channel C (1)
Channel A (0)	+ or -	Channel D (2)
Channel B (1)	+ or -	Channel A (0)
Channel B (1)	+ or -	Channel C (1)
Channel B (1)	+ or -	Channel D (2)
Channel C (2)	+ or -	Channel A (0)
Channel C (2)	+ or -	Channel B (1)
Channel C (2)	+ or -	Channel D (2)
Channel D (3)	+ or -	Channel A (0)
Channel D (3)	+ or -	Channel B (1)
Channel D (3)	+ or -	Channel C (2)

For Analog devices (chromatogram trace type values are in parentheses).

Chro Type 1	Chro Operator	Chro Type 2
Analog 1 (0)	+ or -	Analog 2 (0)
Analog 1 (0)	+ or -	Analog 3 (1)
Analog 1 (0)	+ or -	Analog 4 (2)
Analog 2 (1)	+ or -	Analog 1 (0)
Analog 2 (1)	+ or -	Analog 3 (1)
Analog 2 (1)	+ or -	Analog 4 (2)
Analog 3 (2)	+ or -	Analog 1 (0)
Analog 3 (2)	+ or -	Analog 2 (1)
Analog 3 (2)	+ or -	Analog 4 (2)
Analog 4 (3)	+ or -	Analog 1 (0)
Analog 4 (3)	+ or -	Analog 2 (1)
Analog 4 (3)	+ or -	Analog 3 (2)

For A/D card devices (chromatogram trace type values are in parentheses).

Chro Type 1	Chro Operator	Chro Type 2
A/D Card Ch. 1 (0)	+ or -	A/D Card Ch. 2 (0)
A/D Card Ch. 1 (0)	+ or -	A/D Card Ch. 3 (1)
A/D Card Ch. 1 (0)	+ or -	A/D Card Ch. 4 (2)
A/D Card Ch. 2 (1)	+ or -	A/D Card Ch. 1 (0)
A/D Card Ch. 2 (1)	+ or -	A/D Card Ch. 3 (1)
A/D Card Ch. 2 (1)	+ or -	A/D Card Ch. 4 (2)
A/D Card Ch. 3 (2)	+ or -	A/D Card Ch. 1 (0)
A/D Card Ch. 3 (2)	+ or -	A/D Card Ch. 2 (1)
A/D Card Ch. 3 (2)	+ or -	A/D Card Ch. 4 (2)
A/D Card Ch. 4 (3)	+ or -	A/D Card Ch. 1 (0)
A/D Card Ch. 4 (3)	+ or -	A/D Card Ch. 2 (1)
A/D Card Ch. 4 (3)	+ or -	A/D Card Ch. 3 (2)

## **Chromatogram Operator**

The chromatogram operator type is specified in the GetChroData(...) function. This value has the following meaning.

Value	Chro operator
0	None (single chro only)
1	Minus (subtract chro 2 from chro 1)
2	Plus (add chro 1 and chro 2)

## **Smoothing Type**

The smoothing type is specified in the GetChroData(...) function. This value has the following meaning.

Value	Smoothing type
0	None (no smoothing)
1	Boxcar
2	Gaussian

## 1 Library Definitions

Error Codes

## **Error Codes**

List of error codes	
cINO_DATA_PRESENT	= 0x80002101;
Does not typically indicate an error. This code may be returned if optional data is not contained in the current raw file.	
cISUCCESS	= 0;
Indicates that the function call to the dll was processed without error.	
cIFAILED	= 0x80004005;
Indicates that a general error has occurred. This code may be returned whenever an error of indeterminate origin occurs.	
clCOL_INDEX_OUT_OF_RANGE	= 0x80002206;
Returns if the column index is out of the range.	
cluser_index_out_of_range	= 0x80002205;
Returns if the user index is out of the range.	
clSEQ_ROW_INVALID	= 0x80002204;
Returns if the sequence row is invalid.	
clSEQ_FILE_READONLY	= 0x80002203;
Returns if the sequence file is read only.	
cINEW_FILE_READONLY	= 0x80002202;
Returns if the file to be created is read only.	,
clSEQ_FILE_INVALID	= 0x80002201;
Returns if the sequence file is invalid.	0.00002201,

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clincomplete\_parameter\_set = 0x80002117;

Returns if the parameter set is wrong.

clFILE\_CRC\_CHECK\_FAILED = 0x80002116;

Returns if the CRC check fails.

cIFILE\_ALREADY\_EXISTS = 0x80002115;

Returns if creating a file that already exists.

 $cifile_NOT_FOUND = 0x80002114;$ 

Returns if the file specified is not found.

 $cifile_INVALID = 0x80002113;$ 

Returns if no valid raw file is currently open.

cIMETHOD\_SCAN\_EVENTS\_NOT\_INITIALIZED = 0x80002112;

Returns if the scan event in the method file is not initialized.

cITUNE\_DATA\_HEADER\_NOT\_INITIALIZED = 0x80002111;

Returns if the tune data header is not initialized.

cISTATUS\_LOG\_HEADER\_NOT\_INITIALIZED = 0x80002110;

Returns if the status log header is not initialized.

cITRAILER\_HEADER\_NOT\_INITIALIZED = 0x8000210f;

Returns if the trailer header is not initialized.

 $cIVIRUV\_CREATION\_FAILED$  = 0x8000210e;

Returns if the UV file creation fails.

### 1 Library Definitions

**Error Codes** 

List of error codes	
cIVIRUV_INVALID	= 0x8000210d;
Returns if the UV data is invalid.	
cIVIRMS_CREATION_FAILED	= 0x8000210c;
Returns if the MS data creation fails.	
cIVIRMS_INVALID	= 0x8000210b;
Returns if the MS data is invalid.	
AIDANN EILE SANE FAILED	= 0x8000210a;
cIRAW_FILE_SAVE_FAILED	- 0x0000210a,
Returns if the raw file saving fails.	
clRAW_FILE_CREATION_FAILED	= 0x80002109;
Returns if the raw file creation fails.	
clMASS_RANGE_FORMAT_INCORRECT	= 0x80002108;
Returns if an incorrectly formatted mass range is passed in a function	
call. Mass ranges should have the same format as entered in Xcalibur applications.	
applications.	
cIFILTER_FORMAT_INCORRECT	= 0x80002107;
Returns if an incorrectly formatted scan filter is passed in a function	
call. See the topic <b>scan filters – format, definition</b> in Xcalibur Help	
for scan filter format specifications.	
clOPERATION_NOT_SUPPORTED_ON_CURRENT_CONTROLLER	= 0x80002105;
Returns if the requested action is inappropriate for the currently	
defined controller. Some functions only apply to specific controllers.	
This code might also be returned if a parameter is passed in a call that	
is not supported by the current controller. For example, scan filters	

may only be passed in calls when the current controller is of mass

spectrometer type (MS\_DEVICE).

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cICURRENT\_CONTROLLER\_INVALID = 0x80002104;

Returns if no current controller has been specified.

 $cIRAW_FILE_INVALID$  = 0x80002103;

Returns if the raw file is invalid.

 $cINO_DATA_PRESENT$  = 0x80002101;

Returns if there is no data in the specified file.

 $cIRAW_FILE_OPEN_FAIL$  = 0x80002100;

Returns if the raw file cannot be opened.

 $clinstmethod_not_embedded$  = 0x80002099;

Returns if there is no emebedded instrument method in the raw file.

 $cIRAW_FILE_TOOOLDVER$  = 0x80002098;

Returns if the raw file version is too old that is not supported by Xcalibur.

clinstmethod\_create\_fall = 0x80002097;

Returns if the instrument method file creation fails.

const long cIMPE\_SCANFILTER = 0x80002117;

Empty scan filters.

const long cIMPE\_EMPTY\_SCANHEADER = 0x80002118;

Scan header is empty.

const long cIMPE\_FILTER = 0x80002119;

The filter format is not supported.

const long clRAW\_FILE\_OPEN\_FAIL = 0x80002100;

Failed to open raw file.

#### 1 Library Definitions

**Error Codes** 

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const long cIMPE\_RESOLUTIONERROR = 0x80002101;

The resolution value is wrong with the raw file.

const long cliNSTMETHOD\_NOT\_EMBEDDED = 0x80002099;

In the raw file, the instrument method is not embedded.

const long clRAW\_FILE\_TOOOLDVER = 0x80002098;

The version of the raw file is too old or is not supported.

const long cliNSTMETHOD\_CREATE\_FAIL = 0x80002097;

Failed to create instrument method extracted from the raw file.

const long cIMPE\_INVALID\_SCANHEADER = 0x8000211a;

Returns when the scan header is invalid.

const long clMPE\_INVALID\_SCANTRAIL = 0x8000211b;

Returns when the scan trail data is invalid.

const long cIMPE\_INVALID\_RAWDATA = 0x8000211c;

Returns when the raw data is invalid.

const long cIMPE\_INVALID\_LABELDATA = 0x8000211d;

Returns when the label data is invalid.

## **Function Reference**

This chapter provides extensive descriptions on the function or methods available to programmers using MSFileReader.dll. The examples contained are written using the C programming language but should also serve experienced programmers of other common programming languages well.

## **Open**

## long Open(LPCTSTR szFileName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

szFileName

A NULL terminated string containing the fully qualified path name of the raw file to open.

#### **Remarks**

Opens a raw file for reading only. This function must be called before attempting to read any data from the raw file.

#### **Example**

```
// example for Open
TCHAR* szPathName[] = _T("c:\\xcalibur\\examples\\data\\steroids15.raw");
long nRet = XRawfileCtrl.Open( szPathName );
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error opening file"), _T("Error"), MB_OK );
     ...
}
```

## Close

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## long Close()

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

This function has no parameters.

#### **Remarks**

Closes a raw file and frees the associated memory.

### **Example**

```
// example for Close
long nRet = XRawfileCtrl.Close();
if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error closing file"), _T("Error"), MB_OK );
          ...
}
```

## **GetFileName**

### long GetFileName(BSTR FAR\* pbstrFileName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrFileName A valid pointer to a BSTR variable. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the fully qualified path name of an open raw file.

## **Example**

## **GetCreatorID**

### long GetCreatorID(BSTR FAR\* pbstrCreatorID)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrCreatorlD A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the creator ID. The creator ID is the logon name of the user when the raw file was acquired.

### **Example**

## **GetVersionNumber**

### long GetVersionNumber(long FAR\* pnVersion)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnVersion A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the file format version number.

## **Example**

```
// example for GetVersionNumber
long nVersionNumber;
long nRet = XRawfileCtrl.GetVersionNumber ( &nVersionNumber );
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting version number"), _T("Error"), MB_OK );
     ...
}
```

## **GetCreationDate**

## long GetCreationDate(DATE FAR\* pCreationDate)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pCreationDate A valid pointer to a DATE variable. This variable must exist.

#### **Remarks**

Returns the file creation date in DATE format.

### **Example**

```
// example for GetCreationDate
DATE CreationDate;
long nRet = XRawfileCtrl.GetCreationDate ( &CreationDate );
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting creation date"), _T("Error"), MB_OK );
     ...
}
```

## **IsError**

## long lsError(BOOL FAR\* pblsError)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pblsError A

A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

Returns the error state flag of the raw file. A return value of TRUE indicates that an error has occurred. For information about the error, call the GetErrorCode or GetErrorMessage functions.

#### **Example**

```
// example for IsError
BOOL bError;
long nRet = XRawfileCtrl.IsError ( &bError );
if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error getting error flag"), _T("Error"), MB_OK );
          ...
}
```

## **IsNewFile**

### long IsNewFile(BOOL FAR\* pblsNewFile)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pblsNewFile A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

Returns the creation state flag of the raw file. A return value of TRUE indicates that the file has not previously been saved.

### **Example**

```
// example for IsNewFile
BOOL bNewFile;
long nRet = XRawfileCtrl.IsNewFile ( &bNewFile );
if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error getting new file flag"), _T("Error"), MB_OK );
          ...
}
```

## **GetErrorCode**

## long GetErrorCode(long FAR\* pnErrorCode)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnErrorCode A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the error code of the raw file. A return value of 0 indicates that there is no error.

### **Example**

```
// example for GetErrorCode
long nErrorCode;
long nRet = XRawfileCtrl.GetErrorCode ( &nErrorCode );
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting error code"), _T("Error"), MB_OK );
     ...
}
```

## **GetErrorMessage**

### long GetErrorMessage(BSTR FAR\* pbstrErrorMessage)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrErrorMessage A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns error information for the raw file as a descriptive string. If there is no error, the returned string is empty.

#### **Example**

## **GetWarningMessage**

### long GetWarningMessage(BSTR FAR\* pbstrWarningMessage)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrWarningMessage A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns warning information for the raw file as a descriptive string. If there is no warning, the returned string is empty.

#### **Example**

## **GetSeqRowNumber**

## long GetSeqRowNumber(long FAR\* pnSeqRowNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnSeqRowNumber A valid pointer to a variable of type long. This variable must exist.

#### Remarks

Returns the sequence row number for this sample in an acquired sequence. The numbering starts at 1.

## **Example**

## **GetSeqRowSampleType**

## long GetSeqRowSampleType(long FAR\* pnSampleType)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnSampleType A valid pointer to a variable of type long. This variable must exist.

#### Remarks

Returns the sequence row sample type for this sample. See Sample Type in the Enumerated Types section for the possible sample type values.

### **Example**

## GetSeqRowDataPath

## long GetSeqRowDataPath(BSTR FAR\* pbstrDataPath)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrDataPath A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the path of the directory where this raw file was acquired.

## **Example**

## **GetSeqRowRawFileName**

#### long GetSeqRowRawFileName(BSTR FAR\* pbstrRawFileName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrRawFileName A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the file name of the raw file when the raw file was acquired. This value is typically used in conjunction with GetSeqRowDataPath to obtain the fully qualified path name of the raw file when it was acquired.

### **Example**

## **GetSeqRowSampleName**

### long GetSeqRowSampleName(BSTR FAR\* pbstrSampleName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrSampleName A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the sample name value from the sequence row of the raw file.

### **Example**

## **GetSeqRowSampleID**

### long GetSeqRowSampleID(BSTR FAR\* pbstrSampleID)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrSamplelD A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the sample ID value from the sequence row of the raw file.

### **Example**

## **GetSeqRowComment**

### long GetSeqRowComment(BSTR FAR\* pbstrComment)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrComment A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the comment field from the sequence row of the raw file.

### **Example**

## **GetSeqRowLevelName**

#### long GetSeqRowLevelName(BSTR FAR\* pbstrLevelName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrLevelName A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the level name from the sequence row of the raw file. This field is empty except for standard and QC sample types, which may contain a value if a processing method was specified in the sequence at the time of acquisition.

### **Example**

## GetSeqRowUserText

### long GetSeqRowUserText(long nIndex, BSTR FAR\* pbstrUserText)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nlndex* The index value of the user text field to return.

pbstrUserText A valid pointer to a BSTR. This variable must exist and be initialized to

NULL.

#### **Remarks**

Returns a user text field from the sequence row of the raw file. There are five user text fields in the sequence row that are indexed 0 through 4.

#### **Example**

# **GetSeqRowInstrumentMethod**

### long GetSeqRowInstrumentMethod(BSTR FAR\* pbstrInstrumentMethod)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstrumentMethod A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the fully qualified path name of the instrument method used to acquire the raw file. If the raw file is created by file format conversion or acquired from a tuning program, this field is empty.

#### **Example**

# **GetSeqRowProcessingMethod**

### long GetSeqRowProcessingMethod(BSTR FAR\* pbstrProcessingMethod)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrProcessingMethod A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the fully qualified path name of the processing method specified in the sequence used to acquire the raw file. If no processing method is specified at the time of acquisition, this field is empty.

## **Example**

# **GetSetRowCalibrationFile**

### long GetSetRowCalibrationFile(BSTR FAR\* pbstrCalibrationFile)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrCalibrationFile A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the fully qualified path name of the calibration file specified in the sequence used to acquire the raw file. If no calibration file is specified at the time of acquisition, this field is empty.

#### **Example**

# **GetSeqRowVial**

# long GetSeqRowVial(BSTR FAR\* pbstrVial)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrVial

A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the vial or well number of the sample when it was acquired. If the raw file is not acquired using an autosampler, this value should be ignored.

### **Example**

# **GetSeqRowInjectionVolume**

### long GetSeqRowInjectionVolume(double FAR\* pdInjVol)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdlnjVol A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Returns the autosampler injection volume from the sequence row for this sample.

### **Example**

# **GetSeqRowSampleWeight**

# long GetSeqRowSampleWeight(double FAR\* pdSampleWt)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdSampleWt A valid pointer to a variable of type double. This variable must exist.

### **Remarks**

Returns the sample weight from the sequence row for this sample.

#### **Example**

# **GetSeqRowSampleVolume**

# long GetSeqRowSampleVolume(double FAR\* pdSampleVolume)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdSampleVolume A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Returns the sample volume from the sequence row for this sample.

### **Example**

# **GetSeqRowISTDAmount**

### long GetSeqRowISTDAmount(double FAR\* pdISTDAmount)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdlSTDAmount A valid pointer to a variable of type double. This variable must exist.

#### Remarks

Returns the bulk ISTD correction amount from the sequence row for this sample.

#### **Example**

# GetSeqRowDilutionFactor

### long GetSeqRowDilutionFactor(double FAR\* pdDilutionFactor)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdDilutionFactor A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Returns the bulk dilution factor (volume correction) from the sequence row for this sample.

### **Example**

# **GetSeqRowUserLabel**

### long GetSeqRowUserLabel(long nIndex, BSTR FAR\* pbstrUserLabel)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

```
nlndex The index value of the user text field to return.pbstrUserLabel A valid pointer to a BSTR. This variable must exist and be initialized to NULL.
```

#### **Remarks**

Returns a user label field from the sequence row of the raw file. There are five user label fields in the sequence row that are indexed 0 through 4. The user label fields correspond one-to-one with the user text fields.

#### Example

# **InAcquisition**

# long InAcquisition(BOOL FAR\* pbInAcquisition)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pblnAcquisition A valid pointer to a variable of type BOOL. This variable must exist.

#### Remarks

Returns the acquisition state flag of the raw file. A return value of TRUE indicates that the raw file is being acquired or that all open handles to the file during acquisition have not been closed.

### **Example**

42

# **GetNumberOfControllers**

## long GetNumberOfControllers(long FAR\* pnNumControllers)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumControllers A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the number of registered device controllers in the raw file. A device controller represents an acquisition stream such as MS data, UV data, etc. Devices that do not acquire data, such as autosamplers, are not registered with the raw file during acquisition.

### **Example**

# **GetNumberOfControllersOfType**

# long GetNumberOfControllersOfType(long nControllerType, long FAR\* pnNumControllersOfType)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nControllerType The controller type that are requested for the number of registered

controllers of that type.

pnNumControllers A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the number of registered device controllers of a particular type in the raw file. See Controller Type in the Enumerated Types section for a list of the available controller types and their respective values.

## **Example**

# **GetControllerType**

## long GetControllerType(long nIndex, long FAR\* pnControllerType)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nlndex* The index value of the controller type that is returned.

pnControllerType A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the type of the device controller registered at the specified index position in the raw file. Index values start at 0. See Controller Type in the Enumerated Types section for a list of the available controller types and their respective values.

#### **Example**

# **SetCurrentController**

#### SetCurrentController(long nControllerType, long nControllerNumber) long

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nControllerNumber

nControllerType The type of controller for which information is subsequently requested. The number of the controller of the specified type.

#### **Remarks**

Sets the current controller in the raw file. This function must be called before subsequent calls to access data specific to a device controller (for example, MS or UV data) may be made. All requests for data specific to a device controller are forwarded to the current controller until the current controller is changed. The controller number is used to indicate which device controller to use if there is more than one registered device controller of the same type (for example, multiple UV detectors). Controller numbers for each type are numbered starting at 1. See Controller Type in the Enumerated Types section for a list of the available controller types and their respective values.

#### **Example**

```
// example for SetCurrentController
long nControllerType = 0;
                          // 0 == mass spec device
long nContorllerNumber = 1; // first MS device
long nRet = XRawfileCtrl.SetCurrentController ( nControllerType, nControllerNumber );
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error setting current controller"), _T("Error"), MB_OK );
}
```

// Calls to access the current controller data may now be made.

# **GetCurrentController**

# long GetCurrentController(long FAR\* pnControllerType, long FAR\* pnControllerNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnControllerType A valid pointer to a variable of type long. This variable must exist.

pnControllerNumber A valid pointer to a variable of type long. This variable must exist.

#### Remarks

Gets the current controller type and number for the raw file. The controller number is used to indicate which device controller to use if there is more than one registered device controller of the same type (for example, multiple UV detectors). Controller numbers for each type are numbered starting at 1. See Controller Type in the Enumerated Types section for a list of the available controller types and their respective values.

### **Example**

```
// example for GetCurrentController
long nControllerType;
long nContorllerNumber;
long nRet = XRawfileCtrl.GetCurrentController ( &nControllerType, &nControllerNumber );
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting current controller"), _T("Error"), MB_OK );
     ...
}
```

# **GetNumSpectra**

# long GetNumSpectra(long FAR\* pnNumberOfSpectra)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumberOfSpectra A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the number of spectra acquired by the current controller. For non-scanning devices like UV detectors, the number of readings per channel is returned.

# **Example**

48

# **GetNumStatusLog**

# long GetNumStatusLog(long FAR\* pnNumberOfStatusLogEntries)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumberOfStatusLogEntries A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the number of status log entries recorded for the current controller.

# **Example**

# **GetNumErrorLog**

# long GetNumErrorLog(long FAR\* pnNumberOfErrorLogEntries)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumberOfErrorLogEntries A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the number of error log entries recorded for the current controller.

# **Example**

50

# **GetNumTuneData**

# long GetNumTuneData(long FAR\* pnNumTuneData)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumTuneData A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the number of tune data entries recorded for the current controller. Tune Data is only supported by MS controllers. Typically, if there is more than one tune data entry, each tune data entry corresponds to a particular acquisition segment.

### **Example**

# **GetMassResolution**

# long GetMassResolution(double FAR\* pdMassResolution)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdMassResolution A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the mass resolution value recorded for the current controller. The value is returned as one half of the mass resolution. For example, a unit resolution controller returns a value of 0.5. This value is only relevant to scanning controllers such as MS.

### **Example**

```
// example for GetMassResolution
double dHalfMassRes;
long nRet = XRawfileCtrl.GetMassResolution (&dHalfMassRes);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting mass resolution"), _T("Error"), MB_OK );
     ...
}
```

# GetExpectedRunTime

# long GetExpectedRunTime(double FAR\* pdExpectedRunTime)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdExpectedRunTime A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the expected acquisition run time for the current controller. The actual acquisition may be longer or shorter than this value. This value is intended to allow displays to show the expected run time on chromatograms. To obtain an accurate run time value during or after acquisition, use the GetEndTime function.

#### **Example**

# **GetNumTrailerExtra**

# long GetNumTrailerExtra(long FAR\* pnNumberOfTrailerExtraEntries)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumberOfTrailerExtraEntries A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the trailer extra entries recorded for the current controller. Trailer extra entries are only supported for MS device controllers and are used to store instrument specific information for each scan if used.

#### **Example**

# **GetLowMass**

# long GetLowMass(double FAR\* pdLowMass)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdLowMass A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the lowest mass or wavelength recorded for the current controller. This value is only relevant to scanning devices such as MS or PDA.

### **Example**

# **GetHighMass**

# long GetHighMass(double FAR\* pdHighMass)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdHighMass A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the highest mass or wavelength recorded for the current controller. This value is only relevant to scanning devices such as MS or PDA.

### **Example**

```
// example for GetHighMass
double dHighMass;
long nRet = XRawfileCtrl.GetHighMass (&dHighMass);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting high mass"), _T("Error"), MB_OK );
     ...
}
```

# **GetStartTime**

56

# long GetStartTime(double FAR\* pdStartTime)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdStartTime A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the start time of the first scan or reading for the current controller. This value is typically close to zero unless the device method contains a start delay.

# **Example**

```
// example for GetStartTime
double dStartTime;
long nRet = XRawfileCtrl.GetStartTime (&dStartTime);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting start time"), _T("Error"), MB_OK );
     ...
}
```

# **GetEndTime**

# long GetEndTime(double FAR\* pdEndTime)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdEndTime A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the start time of the last scan or reading for the current controller.

# **Example**

58

# **GetMaxIntegratedIntensity**

# long GetMaxIntegratedIntensity(double FAR\* pdMaxIntegIntensity)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdMaxIntegIntensity A valid pointer to a variable of type double. This variable must exist.

#### Remarks

Gets the highest integrated intensity of all the scans for the current controller. This value is only relevant to MS device controllers.

#### **Example**

# **GetMaxIntensity**

# long GetMaxIntensity(long FAR\* pnMaxIntensity)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdMaxIntensity A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the highest base peak of all the scans for the current controller. This value is only relevant to MS device controllers.

### **Example**

```
// example for GetMaxIntensity
double dMaxInt;
long nRet = XRawfileCtrl.GetMaxIntensity (&dMaxInt);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting max intensity"), _T("Error"), MB_OK );
     ...
}
```

60

# **GetFirstSpectrumNumber**

## long GetFirstSpectrumNumber(long FAR\* pnFirstSpectrum)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnFirstSpectrum A valid pointer to a variable of type long. This variable must exist.

#### Remarks

Gets the first scan or reading number for the current controller. If data has been acquired, this value is always one.

## Example

# **GetLastSpectrumNumber**

### long GetLastSpectrumNumber(long FAR\* pnLastSpectrum)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnLastSpectrum A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the last scan or reading number for the current controller.

### **Example**

```
// example for GetLastSpectrumNumber
long nLastScan;
long nRet = XRawfileCtrl.GetLastSpectrumNumber (&nLastScan);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting last scan number"), _T("Error"), MB_OK );
     ...
}
```

# **GetInstrumentID**

# long GetInstrumentID(long FAR\* pnInstrumentID)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnInstrumentID A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the instrument ID number for the current controller. This value is typically only set for raw files converted from other file formats.

# **Example**

```
// example for GetInstrumentID
long nInstID;
long nRet = XRawfileCtrl.GetInstrumentID (&nInstID);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting inst ID number"), _T("Error"), MB_OK );
     ...
}
```

# **GetInletID**

# long GetInletID(long FAR\* pnInletID)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnlnletlD A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the inlet ID number for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

```
// example for GetInletID
long nInletID;
long nRet = XRawfileCtrl.GetInletID (&nInletID);
if( nRet != 0 )
{
         ::MessageBox( NULL, _T("Error getting inlet ID number"), _T("Error"), MB_OK );
         ...
}
```

# **GetErrorFlag**

# long GetErrorFlag(long FAR\* pnErrorFlag)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnErrorFlag A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the error flag value for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

```
// example for GetErrorFlag
long nErrorFlag;
long nRet = XRawfileCtrl.GetErrorFlag (&nErrorFlag);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting error flag value"), _T("Error"), MB_OK );
     ...
}
```

# **GetSampleVolume**

# long GetSampleVolume(double FAR\* pdSampleVolume)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdSampleVolume A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the sample volume value for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

66

# **GetSampleWeight**

# long GetSampleWeight(double FAR\* pdSampleWeight)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdSampleWeight A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the sample weight value for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetVialNumber**

## long GetVialNumber(long FAR\* pnVialNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnVialNumber A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Gets the vial number for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

68

## **GetInjectionVolume**

## long GetInjectionVolume(double FAR\* pdInjectionVolume)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdlnjectionVolume A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Gets the injection volume for the current controller. This value is typically only set for raw files converted from other file formats.

## **Example**

```
// example for GetInjectionVolume
double dInjVol;
long nRet = XRawfileCtrl.GetInjectionVolume (&dInjVol);
if( nRet != 0 )
{
     ::MessageBox( NULL, _T("Error getting injection volume"), _T("Error"), MB_OK );
     ...
}
```

## **GetFlags**

## long GetFlags(BSTR FAR\* pbstrFlags)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrFlags A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the acquisition flags field for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

# **GetAcquisitionFileName**

## long GetAcquisitionFileName(BSTR FAR\* pbstrFileName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrFileName A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the acquisition file name for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetInstrumentDescription**

### long GetInstrumentDescription(BSTR FAR\* pbstrInstrumentDescription)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstrumentDescription A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the instrument description field for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetAcquisitionDate**

## long GetAcquisitionDate(BSTR FAR\* pbstrAcquisitionDate)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrAcquisitionDate A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the acquisition date for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetOperator**

## long GetOperator(BSTR FAR\* pbstrOperator)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrOperator A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the operator name for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetComment1**

## long GetComment1(BSTR FAR\* pbstrComment1)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrComment1 A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the first comment for the current controller. This value is typically only set for raw files converted from other file formats.

## **Example**

## **GetComment2**

## long GetComment2(BSTR FAR\* pbstrComment2)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrComment2 A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the first comment for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

# **GetSampleAmountUnits**

## long GetSampleAmountUnits(BSTR FAR\* pbstrSampleAmountUnits)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrSampleAmountUnits A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the sample amount units for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetInjectionAmountUnits**

### long GetInjectionAmountUnits(BSTR FAR\* pbstrInjectionAmountUnits)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnjectionAmountUnits A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the injection amount units for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

# ${\bf Get Sample Volume Units}$

## long GetSampleVolumeUnits(BSTR FAR\* pbstrSampleVolumeUnits)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrSampleVolumeUnits A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the sample volume units for the current controller. This value is typically only set for raw files converted from other file formats.

### **Example**

## **GetInstName**

## long GetInstName(BSTR FAR\* pbstrInstName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstName A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the instrument name, if available, for the current controller.

## **Example**

```
// example for GetInstName
BSTR bstrInstName = NULL;
long nRet = XRawfileCtrl.GetInstName ( &bstrInstName );
if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error getting instrument name"), _T("Error"), MB_OK );
          ...
}
...
SysFreeString(bstrInstName);
```

## **GetInstModel**

## long GetInstModel(BSTR FAR\* pbstrInstModel)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstModel A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the instrument model, if available, for the current controller.

## **Example**

## **GetInstSerialNumber**

## long GetInstSerialNumber(BSTR FAR\* pbstrInstSerialNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstSerialNumber A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the serial number, if available, for the current controller.

### **Example**

## **GetInstSoftwareVersion**

### long GetInstSoftwareVersion(BSTR FAR\* pbstrInstSoftwareVersion)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstSoftwareVersion A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns revision information for the current controller software, if available.

## **Example**

## **GetInstHardwareVersion**

### long GetInstHardwareVersion(BSTR FAR\* pbstrInstHardwareVersion)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstHardwareVersion A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns revision information for the current controller hardware or firmware, if available.

## **Example**

## **GetInstFlags**

## long GetInstFlags(BSTR FAR\* pbstrInstFlags)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrlnstFlags A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

Returns the experiment flags, if available, for the current controller. The returned string may contain one or more fields denoting information about the type of experiment performed.

These are the currently defined experiment fields:

```
TIM - total ion map

NLM - neutral loss map

PIM - parent ion map

DDZMap - data-dependent ZoomScan map
```

### **Example**

## **GetInstNumChannelLabels**

### long GetInstNumChannelLabels(long FAR\* pnInstNumChannelLabels)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnlnstNumChannelLabels A valid pointer to a variable of type long. This variable must

#### **Remarks**

Returns the number of channel labels specified for the current controller. This field is only relevant to channel devices such as UV detectors, A/D cards, and Analog inputs. Typically, the number of channel labels, if labels are available, is the same as the number of configured channels for the current controller.

## **Example**

## **GetInstChannelLabel**

# long GetInstChannelLabel(long nChannelLabelNumber, BSTR FAR\* pbstrInstChannelLabel)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nChannelLabelNumber The index value of the channel number field to return.

pbstrFlags A valid pointer to a BSTR. This variable must exist and be

initialized to NULL.

#### **Remarks**

Returns the channel label, if available, at the specified index for the current controller. This field is only relevant to channel devices such as UV detectors, A/D cards, and Analog inputs. Channel label indices are numbered starting at 0.

## **Example**

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## **GetFilters**

### long GetFilters(VARIANT FAR\* pvarFilterArray, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pvarFilterArray A valid pointer to a variable of type VARIANT. This variable must exist and be initialized to VT\_EMPTY.pnArraySize A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the list of unique scan filters for the raw file. This function is only supported for MS device controllers. If the function succeeds, *pvarFilterArray* points to an array of BSTR fields, each containing a unique scan filter, and *pnArraySize* contains the number of scan filters in the *pvarFilterArray*.

## **Example**

```
// example for GetFilters
VARIANT varFilters;
VariantInit(&varFilters);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetFilters ( & varFilters, &nArraySize );
if( nRet != 0 )
{
        ::MessageBox( NULL, _T("Error getting array of scan filters"), _T("Error"), MB_OK
);
        return
}
if(!nArraySize|| varFilters.vt!= (VT_ARRAY | VT_BSTR))
        ::MessageBox( NULL, _T("No valid filters returned"), _T("Error"), MB_OK );
        return:
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psa = varFilters.parray;
varFilters.parray = NULL;
BSTR* pbstrFilters = NULL;
if( FAILED(SafeArrayAccessData( psa, (void**)(&pbstrFilters) ) ) )
        SafeArrayUnaccessData( psa );
```

#### **2** Function Reference

GetFilters

```
SafeArrayDestroy( psa );
::MessageBox( NULL, _T("Failed to access scan filter array"), _T("Error"), MB_OK
);
return;
}

// display filters one at a time
TCHAR szTitle[16];
for( long i=0; i<nArraySize; i++ )
{
    __stprintf( szTitle, _T("Scan Filter %d"), i );
    ::MessageBox( NULL, pbstrFilters[i], szTitle, MB_OK );
}

// Delete the SafeArray
SafeArrayUnaccessData( psa );
SafeArrayDestroy( psa );
```

## **ScanNumFromRT**

### long ScanNumFromRT(double dRT, long FAR\* pnScanNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

dRT The run time or retention time, in minutes, that is returned for the closest scan number.

pnScanNumber A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

Returns the closest matching scan number that corresponds to *dRT* for the current controller. For non-scanning devices, such as UV, the closest reading number is returned. The value of *dRT* must be within the acquisition run time for the current controller. The acquisition run time for the current controller may be obtained by calling GetStartTime and GetEndTime.

## **Example**

## **RTFromScanNum**

## long RTFromScanNum(long nScanNumber, double FAR\* pdRT)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the closest run time or retention time.

pdRT A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

Returns the closest matching run time or retention time that corresponds to *nScanNumber* for the current controller. For non-scanning devices, such as UV, the *nScanNumber* is the reading number. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

## **Example**

## **GetFilterForScanNum**

## long GetFilterForScanNum(long nScanNumber, BSTR FAR\* pbstrFilter)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the corresponding scan filter.

pbstrFilter A valid pointer to a BSTR. This variable must exist and be initialized to

NULL.

#### **Remarks**

Returns the closest matching run time that corresponds to *nScanNumber* for the current controller. This function is only supported for MS device controllers. The value of *nScanNumber* must be within the range of scans for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

### **Example**

## **GetFilterForScanRT**

## long GetFilterForScanRT(double dRT, BSTR FAR\* pbstrFtiler)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

dRT The run time that is returned for the corresponding scan filter.

pbstrFilter A valid pointer to a BSTR. This variable must exist and be initialized to

NULL.

#### **Remarks**

Returns the scan filter for the closest matching scan that corresponds to *dRT* for the current controller. This function is only supported for MS device controllers. The value of *dRT* must be within the acquisition run time for the current controller. The acquisition run time for the current controller may be obtained by calling GetStartTime and GetEndTime.

## **Example**

## **GetMassListFromScanNum**

long GetMassListFromScanNum(long FAR\* pnScanNumber, LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult, VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding mass list data.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan corresponding to *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan to *pnScanNumber* that matches the scan filter is returned. The requested scan number must be valid for the current controller. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### Example

```
// example for GetMassListFromScanNum
typedef struct _datapeak
       double dMass:
       double dintensity;
} DataPeak;
long nScanNumber = 12;
                              // read the contents of scan 12
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetMassListFromScanNum (
                                                     &nScanNumber,
                                                     NULL.
                                                                            // no
                                             filter
```

```
0,
                                                                                // no
                                                cutoff
                                                        0,
                                                                                // no
                                                cutoff
                                                                                // all
                                                        0,
                                                peaks returned
                                                        FALSE,
                                                                                // do not
                                                centroid
                                                                                // mass
                                                        &varMassList,
                                                list data
                                                        &varPeakFlags,
                                                                                // peak
                                                flags data
                                                        &nArraySize);
                                                                                // size
                                                of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
                // Do something with mass intensity values
        }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varMassList.parray;
        varMassList.parray = NULL;
        // Delete the SafeArray
        SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY)
```

## **2** Function Reference

 ${\sf GetMassListFromScanNum}$ 

```
{
    SAFEARRAY FAR* psa = varPeakFlags.parray;
    varPeakFlags.parray = NULL;

// Delete the SafeArray
    SafeArrayDestroy( psa );
}
```

## **GetMassListFromRT**

long GetMassListFromRT(double FAR\* pdRT, LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult,

VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a double precision variable containing the

retention time, in minutes, that is returned for the corresponding

mass list data.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the closest scan to *pdRT* is returned. If a scan filter is provided, the closest matching scan to *pdRT* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pdRT* contains the actual retention time of the returned scan. Valid retention time limits may be obtained by calling GetStartTime and GetEndTime.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### Example

```
// example for GetMassListFromRT
typedef struct _datapeak
       double dMass:
       double dintensity;
} DataPeak;
double dRT = 3.8;
                       // read the contents of the scan at RT = 3.8 minutes
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetMassListFromRT ( &dRT,
                                                                       // no filter
                                               NULL.
                                                                       // no cutoff
                                               0,
                                               0.
                                                                       // no cutoff
```

```
0,
                                                                       // all peaks
returned
                                               FALSE.
                                                                       // do not
centroid
                                               &varMassList,
                                                                       // mass list data
                                               &varPeakFlags,
                                                                       // peak flags
data
                                               &nArraySize);
                                                                       // size of mass
list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
{
        SAFEARRAY FAR* psa = varMassList.parray;
        varMassList.parray = NULL;
        // Delete the SafeArray
        SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varPeakFlags.parray;
        varPeakFlags.parray = NULL;
        // Delete the SafeArray
```

## **2** Function Reference

 ${\sf GetMassListFromRT}$ 

```
SafeArrayDestroy( psa ); }
```

## **GetNextMassListFromScanNum**

long GetNextMassListFromScanNum(long FAR\* pnScanNumber,

LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult, VARIANT FAR\* pyarMassList

VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags,

long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number after

which the corresponding mass list data is returned.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan after *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan after *pnScanNumber* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pnScanNumber* contains the actual scan number of the returned scan. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### Example

```
// example for GetNextMassListFromScanNum
typedef struct _datapeak
       double dMass:
       double dintensity;
} DataPeak;
long nScanNumber = 12;
                              // read the contents of the scan after scan 12
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetNextMassListFromScanNum (
                                                             &nScanNumber,
                                                             NULL.
                                                                            // no
filter
```

```
0,
                                                                                // no
cutoff
                                                                0,
                                                                                // no
cutoff
                                                                                // all
                                                                0,
                                                        peaks returned
                                                                FALSE,
                                                                                // do not
                                                        centroid
                                                                &varMassList, // mass
                                                        list data
                                                                &varPeakFlags, // peak
                                                        flags data
                                                                &nArraySize ); // size
                                                        of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for next scan after 12."),
_T("Error"), MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
                // Do something with mass intensity values
        }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varMassList.parray;
        varMassList.parray = NULL;
        // Delete the SafeArray
        SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY)
```

### **2** Function Reference

 ${\sf GetNextMassListFromScanNum}$ 

```
{
    SAFEARRAY FAR* psa = varPeakFlags.parray;
    varPeakFlags.parray = NULL;

// Delete the SafeArray
    SafeArrayDestroy( psa );
}
```

### **GetPrevMassListFromScanNum**

long GetPrevMassListFromScanNum(long FAR\* pnScanNumber,

LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult,

VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags,

long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number before

which the corresponding mass list data is returned.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan before *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan before *pnScanNumber* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pnScanNumber* contains the actual scan number of the returned scan. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### Example

```
// example for GetPrevMassListFromScanNum
typedef struct _datapeak
       double dMass:
       double dintensity;
} DataPeak;
long nScanNumber = 12;
                              // read the contents of the scan before scan 12
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetPrevMassListFromScanNum (
                                                             &nScanNumber,
                                                             NULL.
                                                                            // no
filter
```

```
0,
                                                                                // no
cutoff
                                                                0,
                                                                                // no
cutoff
                                                                                // all
                                                                0,
                                                        peaks returned
                                                                FALSE,
                                                                                // do not
                                                        centroid
                                                                &varMassList, // mass
                                                        list data
                                                                &varPeakFlags, // peak
                                                        flags data
                                                                &nArraySize ); // size
                                                        of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for next scan after 12."),
_T("Error"), MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
                // Do something with mass intensity values
        }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varMassList.parray;
        varMassList.parray = NULL;
        // Delete the SafeArray
        SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY)
```

### **2** Function Reference

 ${\sf GetPrevMassListFromScanNum}$ 

```
{
    SAFEARRAY FAR* psa = varPeakFlags.parray;
    varPeakFlags.parray = NULL;

// Delete the SafeArray
    SafeArrayDestroy( psa );
}
```

# **GetMassListRangeFromScanNum**

long GetMassListRangeFromScanNum(long FAR\* pnScanNumber,

LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult,

VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, LPCTSTR csMassRange1, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding mass list data.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

csMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan corresponding to *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan to *pnScanNumber* that matches the scan filter is returned. The requested scan number must be valid for the current controller. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// read the contents of scan 12
long nScanNumber = 12;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nRet = XRawfileCtrl.GetMassListFromScanNum (
                                                       &nScanNumber,
                                                       NULL,
                                                                               // no
filter
                                                       0,
                                                                               // no
cutoff
                                                       0,
                                                                               // no
cutoff
                                                                               // all
                                                       0.
                                               peaks returned
                                                       FALSE,
                                                                               // do not
                                               centroid
                                                       &varMassList,
                                                                               // mass
                                               list data
                                                       &varPeakFlags,
                                                                               // peak
                                               flags data
                                                       szMassRange1,
                                                                               // mass
                                               range
                                                       &nArraySize);
                                                                               // size
                                               of mass list array
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
}
if( nArraySize )
       // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
       {
               double dMass = pDataPeaks[i].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
       // Release the data handle
        SafeArrayUnaccessData( psa );
```

#### **2** Function Reference

Get Mass List Range From Scan Num

# **GetMassListRangeFromRT**

long GetMassListRangeFromRT(double FAR\* pdRT, LPCTSTR szFilter,

long nIntensityCutoffType, long

nIntensityCutoffValue,

long nMaxNumberOfPeaks, BOOL

bCentroidResult, VARIANT FAR\* pvarMassList,

VARIANT FAR\* pvarPeakFlags,

LPCTSTR szMassRange1, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a double precision variable containing the

retention time, in minutes, that is returned for the corresponding

mass list data.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

szMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### Remarks

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the closest scan to *pdRT* is returned. If a scan filter is provided, the closest matching scan to *pdRT* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pdRT* contains the actual retention time of the returned scan. Valid retention time limits may be obtained by calling GetStartTime and GetEndTime.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// read the contents of the scan at RT = 3.8 minutes
double dRT = 3.8;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nArraySize = 0;
long nRet = XRawfileCtrl.GetMassListRangeFromRT ( &dRT,
                                                                       // no filter
                                               NULL.
                                               0,
                                                                       // no cutoff
                                               0,
                                                                       // no cutoff
                                               0,
                                                                       // all peaks
returned
                                               FALSE,
                                                                       // do not
centroid
                                               &varMassList,
                                                                       // mass list data
                                               &varPeakFlags,
                                                                       // peak flags
data
                                               czMassRange1,
                                                                       // mass range
                                                                       // size of mass
                                               &nArraySize );
list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varMassList.parray;
```

#### **2** Function Reference

GetMassListRangeFromRT

# **GetNextMassListRangeFromScanNum**

long GetNextMassListFromScanNum(long FAR\* pnScanNumber,

LPCTSTR szFilter.

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, **BOOL** bCentroidResult,

**VARIANT FAR\* pvarMassList,** VARIANT FAR\* pvarPeakFlags, LPCTSTR szMassRange1, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number after

which the corresponding mass list data is returned.

szFilter A string containing the optional scan filter.

nIntensityCutoffType The type of intensity cutoff to apply.

nIntensityCutoffValue The intensity cutoff value.

nMaxNumberOfPeaks The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

szMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan after *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan after *pnScanNumber* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pnScanNumber* contains the actual scan number of the returned scan. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// read the contents of the scan after scan 12
long nScanNumber = 12;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nArraySize = 0;
long nRet = XRawfileCtrl.GetNextMassListFromScanNum (
                                                                &nScanNumber.
                                                                NULL.
                                                                               // no
filter
                                                               0.
                                                                               // no
cutoff
                                                               0.
                                                                               // no
cutoff
                                                               0.
                                                                               // all
                                                       peaks returned
                                                                               // do not
                                                               FALSE,
                                                       centroid
                                                                &varMassList, // mass
                                                       list data
                                                                &varPeakFlags, // peak
                                                       flags data
                                                                szMassRange1,// mass
                                                       range
                                                                &nArraySize); // size
                                                       of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for next scan after 12."),
_T("Error"), MB_OK );
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
        {
               double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
       // Release the data handle
```

### **GetPrecursorInfoFromScanNum**

# long GetPrecursorInfoFromScanNum(long nScanNumber, LPVARIANT pvarPrecursorInfos, LPLONG pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the corresponding precursor info.

pvarPrecursorInfos A valid pointer to a VARIANT variable to receive the precursor info.

pnArraySize A valid pointer to a long variable to receive the number of precursor info

packets returned in the precursor info array.

#### **Remarks**

This function is used to retrieve information about the parent scans of a data dependent MSn scan.

You retrieve the scan number of the parent scan, the isolation mass used, the charge state, and the monoisotopic mass as determined by the instrument firmware. You will get access to the scan data of the parent scan in the form of a XSpectrumRead object.

Further refine the charge state and the monoisotopic mass values from the actual parent scan data.

#### **Example**

```
struct PrecursorInfo
{
    double dIsolationMass;
    double dMonoIsoMass;
    long nChargeState;
    long nScanNumber;
};

void CTestOCXDIg::OnOpenParentScansOcx()
{
    try
    {
        VARIANT vPrecursorInfos;
        VariantInit(&vPrecursorInfos);
        long nPrecursorInfos = 0;
```

#### ${\sf GetPrecursorInfoFromScanNum}$

```
// Get the precursor scan information
  m_Rawfile.GetPrecursorInfoFromScanNum(m_nScanNumber,
                                                     &vPrecursorInfos,
                                                     &nPrecursorInfos);
  // Access the safearray buffer
  BYTE* pData;
  SafeArrayAccessData(vPrecursorInfos.parray, (void**)&pData);
  for (int i=0; i < nPrecursorInfos; ++i)
    // Copy the scan information from the safearray buffer
    PrecursorInfo info;
     memcpy(&info,
                     pData + i * sizeof(MS_PrecursorInfo),
                     sizeof(PrecursorInfo));
     // Process the paraent scan information ...
  }
  SafeArrayUnaccessData(vPrecursorInfos.parray);
}
catch (...)
  AfxMessageBox(_T("There was a problem while getting the parent scan
                             information."));
```

# **GetPrevMassListRangeFromScanNum**

long GetPrevMassListFromScanNum(long FAR\* pnScanNumber,

LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult,

BUOL bCentroidKesult, VARIANT FAR\* pvarMassList,

VARIANT FAR\* pvarPeakFlags, LPCTSTR szMassRange1, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number before

which the corresponding mass list data is returned.

szFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

szMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan before *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan before *pnScanNumber* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pnScanNumber* contains the actual scan number of the returned scan. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// example for GetPrevMassListFromScanNum typedef struct _datapeak {
```

```
double dMass;
       double dintensity;
} DataPeak;
long nScanNumber = 12;
                               // read the contents of the scan before scan 12
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nArraySize = 0;
long nRet = XRawfileCtrl.GetPrevMassListFromScanNum (
                                                               &nScanNumber,
                                                               NULL.
                                                                               // no
filter
                                                               0,
                                                                               // no
cutoff
                                                               0,
                                                                               // no
cutoff
                                                                               // all
                                                               0.
                                                       peaks returned
                                                               FALSE,
                                                                               // do not
                                                       centroid
                                                               &varMassList, // mass
                                                       list data
                                                               &varPeakFlags, // peak
                                                       flags data
                                                               szMassRange1,// mass
                                                       range
                                                               &nArraySize ); // size
                                                       of mass list array
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting mass list data for next scan after 12."),
_T("Error"), MB_OK );
}
if( nArraySize )
       // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
       {
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
```

### GetPrevMassListRangeFromScanNum

```
}
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
{
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

# GetAverageMassList

long GetAverageMassList(long FAR\* pnFirstAvgScanNumber,

long FAR\* pnLastAvgScanNumber, long FAR\* pnFirstBkg1ScanNumber, long FAR\* pnLastBkg1ScanNumber, long FAR\* pnFirstBkg2ScanNumber, long FAR\* pnLastBkg2ScanNumber,

LPCTSTR szFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnFirstAvgScanNumber A valid pointer to a long variable containing the first scan number of

the scan number range that is returned for the corresponding

averaged mass list data.

pnLastAvgScanNumber A valid pointer to a long variable containing the last scan number of

the scan number range that is returned for the corresponding

averaged mass list data.

pnFirstBkg1ScanNumber A valid pointer to a long variable containing the first scan number of

the first scan number range to be subtracted from the averaged mass

list data.

pnLastBkg1ScanNumber A valid pointer to a long variable containing the last scan number of

the first scan number range to be subtracted from the averaged mass

list data.

pnFirstBkg2ScanNumber A valid pointer to a long variable containing the first scan number of

the second scan number range to be subtracted from the averaged

mass list data.

pnLastBkg2ScanNumber A valid pointer to a long variable containing the last scan number of

the second scan number range to be subtracted from the averaged

mass list data.

szFilter A string containing the optional scan filter.

# **2 Function Reference** GetAverageMassList

*nlntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### Remarks

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scans between pnFirstAvgScanNumber and pnLastAvgScanNumber, inclusive, are returned. Likewise, all the scans between pnFirstBkg1ScanNumber and pnLastBkg1ScanNumber and pnFirstBkg2ScanNumber and pnLastBkg2ScanNumber, inclusive, are averaged and subtracted from the pnFirstAvgScanNumber to pnLastAvgScanNumber averaged scans. If a scan filter is provided, the scans in the preceding scan number ranges that match the scan filter are utilized in obtaining the background subtracted mass list. The specified scan numbers must be valid for the current controller. If no background subtraction is performed, the background scan numbers should be set to zero. On return, the scan number variables contain the actual first and last scan numbers, respectively, for the scans used. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set nMaxNumberOfPeaks to a value greater than zero. To have all data peaks returned, set nMaxNumberOfPeaks to zero.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// example for GetAverageMassList
typedef struct datapeak
       double dMass:
       double dIntensity;
} DataPeak;
long nFirstAvgScanNumber = 12;
                                      // average scans 12 through 18
long nLastAvgScanNumber = 18;
long nFirstBkg1ScanNumber = 5;
                                      // subtract scans 5 through 8
long nLastBkg1ScanNumber = 8;
long nFirstBkg2ScanNumber = 0;
                                      // do not use second background scan number
range
long nLastBkg2ScanNumber = 0;
VARIANT varMassList:
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet = XRawfileCtrl.GetAverageMassList ( &nFirstAvgScanNumber,
                                              &nLastAvgScanNumber,
                                              &nFirstBkg1ScanNumber,
                                              &nLastBkg1ScanNumber,
                                              &nFirstBkg2ScanNumber,
                                              &nLastBkg2ScanNumber,
                                              NULL,
                                                             // no filter
                                              0,
                                                             // no cutoff
                                              0,
                                                             // no cutoff
                                              0,
                                                             // all peaks returned
                                              &varMassList, // mass list data
                                              &varPeakFlags, // peak flags data
                                              &nArraySize ); // size of mass list array
if( nRet != 0 )
       ::MessageBox( NULL, T("Error getting average mass list data."), T("Error"),
MB OK);
}
if( nArraySize )
       // Get a pointer to the SafeArray
       SAFEARRAY FAR* psa = varMassList.parray;
```

```
DataPeak* pDataPeaks = NULL;
       SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
       {
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

# **GetAveragedMassSpectrum**

long GetAveragedMassSpectrum(long FAR\* pnScanNumbers,

Iong nScansToAverage, BOOL bCentroidResult, VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, Iong FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumbers A valid pointer to an array of scan numbers that this routine will average.

*nScansToAverage* The number of scans that are averaged.

bCentroidData A flag indicating if the mass spectral data is centroided before it is

returned by this function.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks

returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS.

GetAveragedMassSpectrum returns the average spectrum for the list of scans that are supplied to the function in *pnScanNumbers*. If no scans are provided in *pnScanNumbers*, or if *nScansToAverage* is zero, then the function returns an error code.

If the bCentroidData value is true, then profile data is centroided before it is returned by this routine.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// example for GetAveragedMassSpectrum
typedef struct _datapeak
        double dMass;
        double dIntensity;
} DataPeak;
long nScans[3];
long nScans[0] = 12;
long nScans[1] = 18;
long nScans[2] = 25;
long nScansToAverage =3;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet;
nRet = XRawfileCtrl.GetAveragedMassSpectrum ( nScans,
                                                nScansToAverage, // the number of
scans
                                                bCentroidData, // centroid the data
                                                &varMassList, // mass list data
                                                &varPeakFlags, // peak flags data
                                                &nArraySize ); // size of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting average mass spectrum data."),
_T("Error"),
                       MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
                double dMass = pDataPeaks[j].dMass;
```

```
double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

#### **2 Function Reference** GetSummedMassSpectrum

# **GetSummedMassSpectrum**

long GetSummedMassSpectrum(long FAR\* pnScanNumbers,

long nScansToSum, BOOL bCentroidResult, VARIANT FAR\* pvarMassList, VARIANT FAR\* pvarPeakFlags, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumbers A valid pointer to an array of scan numbers that this routine will sum.

*nScansToSum* The number of scans that is summed.

bCentroidData A flag indicating if the mass spectral data is centroided before it is returned

by this function.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks

returned in the mass list array.

#### Remarks

This function is only applicable to scanning devices such as MS.

GetSummedMassSpectrum returns the summed spectrum for the list of scans that are supplied to the function in *pnScanNumbers*. If no scans are provided in *pnScanNumbers*, or if *nScansToSum* is zero, then the function returns an error code.

If the bCentroidData value is true, then profile data is centroided before it is returned by this routine.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// example for GetSummedMassSpectrum
typedef struct _datapeak
        double dMass;
        double dIntensity;
} DataPeak;
long nScans[3];
long nScans[0] = 12;
long nScans[1] = 18;
long nScans[2] = 25;
long nScansToSum =3;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
long nRet;
nRet = XRawfileCtrl.GetSummedMassSpectrum ( nScans,
                                               nScansToSum, // the number of scans
                                               bCentroidData, // centroid the data
                                               &varMassList, // mass list data
                                               &varPeakFlags, // peak flags data
                                               &nArraySize ); // size of mass list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting summed mass spectrum data."),
_T("Error"),
                       MB_OK);
}
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
```

#### **2** Function Reference

GetSummedMassSpectrum

```
// Do something with mass intensity values
       }
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

### **GetLabelData**

### long GetLabelData(VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarFlags, long FAR\* pnScanNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pvarLabels A valid pointer to a VARIANT variable to receive the label data.

pvarFlags A valid pointer to a VARIANT variable to receive the flags.

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding label data.

#### **Remarks**

This method enables you to read the FT-PROFILE labels of a scan represented by the scanNumber.

pvarFlags can be NULL if you are not interested in receiving the flags.

The label data contains values of mass (double), intensity (double), resolution (float), baseline (float), noise (float) and charge (int).

The flags are returned as unsigned char values. The flags are saturated, fragmented, merged, exception, reference, and modified.

#### **Example**

// example for GetLabelData

long nRet;

long nScanNumber = 1; // get the label data of the first scan.

int dim, inx, charge;

double \*pdval; unsigned char \*pcval;

SAFEARRAY \*parray, \*parray2;
\_variant\_t vSpecData, vFlags;
VARIANT varLabels, \*pvarLabels;
VARIANT varFlags, \*pvarFlags;

double dMass, dInt;

unsigned char cMerged, cFragmented, cReference, cException, cModified, cSaturated;

TCHAR flags[7];

float fRes, fBase, fNoise;

```
= &varLabels;
pvarLabels
pvarFlags
               = &varFlags;
nRet = XRawfileCtrl.GetLabelData(pvarLabels, pvarFlags, &nScanNumber);
if( nRet != 0 )
{
        ::MessageBox( NULL, _T("Error getting label data."), _T("Error"), MB_OK );
}
               = pvarLabels;
vSpecData
               = vSpecData.parray;
parray
               = parray->rgsabound[0].cElements;
dim
pdval
               = (double *) parray->pvData;
if(pvarFlags)
        vFlags = pvarFlags;
        parray2 = vFlags.parray;
        pcval = (unsigned char *) parray2->pvData;
}
for (inx = 0; inx < dim; inx++)
                       = (double)
        dMass
                                       pdval[((inx)*6)+0];
        dInt
                       = (double)
                                       pdval[((inx)*6)+1];
       fRes
                       = (float)
                                        pdval[((inx)*6)+2];
       fBase
                       = (float)
                                       pdval[((inx)*6)+3];
       fNoise
                       = (float)
                                       pdval[((inx)*6)+4];
        charge
                       = (int)
                                       pdval[((inx)*6)+5];
        if(pVarFlags)
        {
               cSaturated
                               = (unsigned char) pcval[((inx)*6)+0];
               cFragmented = (unsigned char) pcval[((inx)*6)+1];
                               = (unsigned char) pcval[((inx)*6)+2];
               cMerged
                               = (unsigned char) pcval[((inx)*6)+3];
               cException
                cReference
                               = (unsigned char) pcval[((inx)*6)+4];
                cModified
                               = (unsigned char) pcval[((inx)*6)+5];
               // write the flags into a String
               flags[0] = T('\0');
               if(cSaturated)
                        _tcscat(flags, _T("S"));
               if(cFragmented)
                        _tcscat(flags, _T("F"));
                if(cMerged)
                        _tcscat(flags, _T("M"));
               if(cException)
                        tcscat(flags, _T("E"));
                if(cReference)
```

# GetAveragedLabelData

long GetAveragedLabelData(long FAR\* pnArraySize, long nScansToAverage, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarFlags, long FAR\* pnScanNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnArraySize A valid pointer to a long variable that returns the number of data points.

*nScansToAverage* The number of scans that is averaged.

pvarLabels A valid pointer to a VARIANT variable to receive the label data.

pvarFlags A valid pointer to a VARIANT variable to receive the flags.

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding label data.

#### **Remarks**

This method enables you to read the averaged FT-PROFILE labels for the list of scans represented by the *pnArraySize*. If no scans are provided in *pnArraySize*, or if *nScansToAverage* is zero, then the function returns an error code.

pvarFlags can be NULL if you are not interested in receiving the flags.

The label data contains values of mass (double), intensity (double), resolution (float), baseline (float), noise (float) and charge (int).

The flags are returned as unsigned char values. These flags are saturated, fragmented, merged, exception, reference, and modified.

#### Example

// example for GetLabelData

long nScans[3]; long nScans[0] = 12; long nScans[1] = 18; long nScans[2] = 25; long nScansToAverage =3; long nRet;

```
dim, inx, charge;
int
double
                *pdval;
unsigned char
               *pcval;
SAFEARRAY
               *parray, *parray2;
_variant_t
               vSpecData, vFlags;
VARIANT
               varLabels, *pvarLabels;
VARIANT
               varFlags, *pvarFlags;
double
               dMass, dInt;
unsigned char cMerged, cFragmented, cReference, cException, cModified, cSaturated;
TCHAR
               flags[7];
float
               fRes, fBase, fNoise;
pvarLabels
               = &varLabels;
pvarFlags
               = &varFlags;
nRet = XRawfileCtrl.GetAverageLabelData(nScans, nScansToAverage, pvarLabels,
pvarFlags,
                                          &nScanNumber);
if( nRet != 0 )
{
        ::MessageBox( NULL, _T("Error getting label data."), _T("Error"), MB_OK );
}
vSpecData
               = pvarLabels;
               = vSpecData.parray;
parray
               = parray->rgsabound[0].cElements;
dim
               = (double *) parray->pvData;
pdval
if(pvarFlags)
        vFlags = pvarFlags;
        parray2 = vFlags.parray;
        pcval = (unsigned char *) parray2->pvData;
}
for (inx = 0; inx < dim; inx++)
        dMass
                       = (double)
                                       pdval[((inx)*6)+0];
        dInt
                       = (double)
                                       pdval[((inx)*6)+1];
        fRes
                       = (float)
                                       pdval[((inx)*6)+2];
       fBase
                       = (float)
                                       pdval[((inx)*6)+3];
        fNoise
                       = (float)
                                       pdval[((inx)*6)+4];
        charge
                       = (int)
                                       pdval[((inx)*6)+5];
        if(pVarFlags)
        {
               cSaturated
                               = (unsigned char) pcval[((inx)*6)+0];
               cFragmented
                               = (unsigned char) pcval[((inx)*6)+1];
               cMerged
                               = (unsigned char) pcval[((inx)*6)+2];
                               = (unsigned char) pcval[((inx)*6)+3];
               cException
```

#### **2** Function Reference

 ${\sf GetAveragedLabelData}$ 

```
cReference
                                 = (unsigned char) pcval[((inx)*6)+4];
                cModified
                                 = (unsigned char) pcval[((inx)*6)+5];
                // write the flags into a String
                flags[0] = _T('\0');
                if(cSaturated)
                        _tcscat(flags, _T("S"));
                if(cFragmented)
                         _tcscat(flags, _T("F"));
                if(cMerged)
                         _tcscat(flags, _T("M"));
                if(cException)
                         _tcscat(flags, _T("E"));
                if(cReference)
                         _tcscat(flags, _T("R"));
                if(cModified)
                         _tcscat(flags, _T("O"));
        // Do something with the data.
}
```

## **GetNoiseData**

# long GetNoiseData( VARIANT FAR\* pvarNoisePacket, long FAR\* pnScanNumber )

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pvarNoisePacket A valid pointer to a VARIANT variable to receive the noise packets.

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding noise packets.

#### **Remarks**

This method enables you to read the FT-PROFILE noise packets of a scan represented by the scanNumber.

The noise packets contain values of mass (double), noise (float) and baseline (float).

#### **Example**

```
// example for GetNoiseData
```

```
long
               nScanNumber = 1; // get the noise packets of the first scan.
long
int
               dim, inx;
               *pdval;
double
SAFEARRAY
               *parray;
_variant_t
               vSpecData;
VARIANT
               varNoisePackets, *pvarNoisePackets;
double
               dMass:
               fBase, fNoise;
float
pvarNoisePackets = &varNoisePackets;
nRet = XRawfileCtrl.GetNoiseData(pvarNoisePackets, &nScanNumber);
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting noise packets."), _T("Error"), MB_OK );
}
vSpecData
               = pvarNoisePackets;
parray
               = vSpecData.parray;
               = parray->rgsabound[0].cElements;
dim
```

#### **2** Function Reference

 ${\sf GetNoiseData}$ 

### **IsProfileScanForScanNum**

#### long IsProfileScanForScanNum(long nScanNumber, long pblsProfileScan)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the profile data type information. *pblsProfileScan* A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

Returns TRUE if the scan specified by *nScanNumber* is a profile scan, FALSE if the scan is a centroid scan. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

#### Example

### **IsCentroidScanForScanNum**

#### long IsCentroidScanForScanNum(long nScanNumber, long pblsCentroidScan)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nScanNumber The scan number that is returned for the profile data type information.

pblsCentroidScan A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

Returns TRUE if the scan specified by *nScanNumber* is a centroid scan, FALSE if the scan is a profile scan. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

#### **Example**

### **GetScanHeaderInfoForScanNum**

long GetScanHeaderInfoForScanNum(long nScanNumber, long FAR\*

pnNumPackets, double FAR\*

pdStartTime,

double FAR\* pdLowMass,

double FAR\* pdHighMass, double FAR\* pdTIC, double FAR\* pdBasePeakMass, double FAR\* pdBasePeakIntensity,

long FAR\* pnNumChannels,

long pbUniformTime,

double FAR\* pdFrequency)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nScanNumber The scan number that is returned for the scan header information.

pnNumPackets A valid pointer to a variable of type long to receive the number of mass

intensity value pairs in the specified scan. This variable must exist.

pdStartTime A valid pointer to a variable of type double to receive the retention

time of the specified scan. This variable must exist.

pdLowMass A valid pointer to a variable of type double to receive the low mass

value of the specified scan. This variable must exist.

pdHighMass A valid pointer to a variable of type double to receive the high mass

value of the specified scan. This variable must exist.

pdTIC A valid pointer to a variable of type double to receive the integrated

total ion current value for the specified scan. This variable must exist.

pdBasePeakMass A valid pointer to a variable of type double to receive the base peak

mass of the specified scan. This variable must exist.

pdBasePeakIntensity A valid pointer to a variable of type double to receive the intensity of

the base peak mass for the specified scan. This variable must exist.

pnNumChannels A valid pointer to a variable of type long to receive the number of

channels acquired at the specified scan number index. This variable

must exist.

pbUniformTime A valid pointer to a variable of type BOOL to receive the flag

indicating whether or not the sampling time increment for the current

controller is uniform. This variable must exist.

pdFrequency A valid pointer to a variable of type double to receive the sampling

frequency for the current controller if *pbUniformTime* is TRUE. This

variable must exist.

#### **Remarks**

For a given scan number, this function returns information from the scan header for the current controller. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The validity of these parameters depends on the current controller. For example, *pdLowMass*, *pdHighMass*, *pdTIC*, *pdBasePeakMass*, and *pdBasePeakIntensity* are only likely to be set on return for MS or PDA controllers. *PnNumChannels* is only likely to be set on return for Analog, UV, and A/D Card controllers. *PdUniformTime*, and *pdFrequency* are only likely to be set on return for UV, and A/D Card controllers and may be valid for Analog controllers. In cases where the value is not set, a value of zero is returned.

#### **Example**

```
// example for GetScanHeaderInfoForScanNum
long nScanNum = 12; // get info for the twelfth scan
long nPackets = 0;
double dStartTime = 0.0;
double dLowMass = 0.0;
double dHighMass = 0.0;
double dTIC = 0.0;
double dBasePeakMass = 0.0;
double dBasePeakIntensity = 0.0;
long nChannels = 0;
long bUniformTime = FALSE;
double dFrequency = 0.0;
long nRet = XRawfileCtrl. GetScanHeaderInfoForScanNum (
                                                             nScanNum,
                                                             &nPackets.
                                                             &dStartTime.
                                                             &dLowMass,
                                                             &dHighMass,
                                                             &dTIC,
                                                             &dBasePeakMass,
                                                             &dBasePeakIntensity,
                                                             &nChannels.
                                                             &bUniformTime,
                                                             &dFrequency);
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting scan header info"), _T("Error"), MB_OK );
```

} ...

# **GetStatusLogForScanNum**

# long GetStatusLogForScanNum(long nScanNumber, double\* pdStatusLogRT, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarValues, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for status log information.

pdStatusLogRT A valid pointer to a variable of type double to receive the retention time

when the status log entry was recorded. This variable must exist.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested status log information. This variable must exist

and be initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text

string values for the requested status log information. This variable must

exist and be initialized to VT EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* and *pvarValues* arrays. This variable must exist.

#### **Remarks**

Returns the recorded status log entry labels and values for the current controller. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

On return, *pdStatusLogRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time corresponding to the specified scan number but is the closest status log entry to the scan time.

The variables *pvarLabels* and *pvarValues* must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* and *pvarValues* arrays.

#### Example

// example for GetStatusLogForScanNum long nScan = 12; // use twelth scan double dStatusLogRT = 0.0;

```
VARIANT varLabels;
VariantInit(&varLabels);
VARIANT varValues;
VariantInit(&varValues);
long nArraySize = 0;
long nRet = XRawfileCtrl. GetStatusLogForScanNum (
                                                      nScan,
                                                       &dStatusLogRT,
                                                       &varLabels,
                                                       &varValues,
                                                       &nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting status log information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
SAFEARRAY FAR* psaValues = varValues.parray;
varValues.parray = NULL;
BSTR* pbstrLabels = NULL;
BSTR* pbstrValues = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
if( FAILED(SafeArrayAccessData( psaValues, (void**)(&pbstrValues) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        SafeArrayUnaccessData( psaValues );
        SafeArrayDestroy( psaValues );
        ::MessageBox( NULL, _T("Failed to access values array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
       sLabel = pbstrLabels[i];
       sData = pbstrValues[i];
       // do something with label and value
}
```

# **2 Function Reference**GetStatusLogForScanNum

// Delete the SafeArray SafeArrayUnaccessData( psaLabels ); SafeArrayDestroy( psaLabels ); SafeArrayUnaccessData( psaValues ); SafeArrayDestroy( psaValues );

# **GetStatusLogForRT**

# long GetStatusLogForRT(double FAR\* pdRT, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarValues, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the retention time

that is returned for the closest status log entry.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested status log information. This variable must exist

and be initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text

string values for the requested status log information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* and *pvarValues* arrays. This variable must exist.

#### **Remarks**

Returns the recorded status log entry labels and values for the current controller. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

On return, *pdRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time specified but is the closest status log entry to the specified time.

The variables *pvarLabels* and *pvarValues* must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* and *pvarValues* arrays.

#### Example

```
&varLabels,
                                               &varValues,
                                               &nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting status log information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
SAFEARRAY FAR* psaValues = varValues.parray;
varValues.parray = NULL;
BSTR* pbstrLabels = NULL;
BSTR* pbstrValues = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
if( FAILED(SafeArrayAccessData( psaValues, (void**)(&pbstrValues) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        SafeArrayUnaccessData( psaValues );
        SafeArrayDestroy( psaValues );
        ::MessageBox( NULL, _T("Failed to access values array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
        sLabel = pbstrLabels[i];
       sData = pbstrValues[i];
       // do something with label and value
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
SafeArrayUnaccessData( psaValues );
SafeArrayDestroy( psaValues );
```

## **GetStatusLogLabeIsForScanNum**

long GetStatusLogLabelsForScanNum(long nScanNumber, double\*
pdStatusLogRT, VARIANT FAR\*
pvarLabels,
long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nScanNumber The scan number that is returned for status log information.

pdStatusLogRT A valid pointer to a variable of type double to receive the retention time

when the status log entry was recorded. This variable must exist.

pvarlabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested status log information. This variable must exist

and be initialized to VT EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* arrays. This variable must exist.

#### **Remarks**

Returns the recorded status log entry labels for the current controller. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

On return, *pdStatusLogRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time corresponding to the specified scan number but is the closest status log entry to the scan time.

The variable *pvarLabels* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* array.

#### Example

## GetStatusLogLabelsForScanNum

```
long nRet = XRawfileCtrl. GetStatusLogLabelsForScanNum (
                                                               nScan,
                                                               &dStatusLogRT,
                                                               &varLabels,
                                                               &nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting status log information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
BSTR* pbstrLabels = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
       sLabel = pbstrLabels[i];
       // do something with label
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
```

# **GetStatusLogLabeIsForRT**

# long GetStatusLogLabelsForRT(double FAR\* pdRT, VARIANT FAR\* pvarLabels, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the retention time

that is returned for the closest status log entry.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested status log information. This variable must exist

and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the pvarLabels arrays. This variable must exist.

#### Remarks

Returns the recorded status log entry labels for the current controller. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

On return, *pdRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time specified but is the closest status log entry to the specified time.

The variable *pvarLabels* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* array.

#### Example

#### **2** Function Reference

GetStatusLogLabelsForRT

```
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
BSTR* pbstrLabels = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++ )</pre>
       sLabel = pbstrLabels[i];
       // do something with label
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
```

# **GetStatusLogValueForScanNum**

# long GetStatusLogValueForScanNum(long nScanNumber, LPCTSTR szLabel, double\* pdStatusLogRT, VARIANT FAR\* pvarValue)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for status log information.

A string containing the label that is returned for the status log parameter

value.

pdStatusLogRT A valid pointer to a variable of type double to receive the retention time

when the status log entry was recorded. This variable must exist.

pvarValue A valid pointer to a variable of type VARIANT to receive the status log

parameter value. This variable must exist and be initialized to VT\_EMPTY.

#### Remarks

Returns the recorded status log parameter value for the specified status log parameter label for the current controller. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

To obtain a list of the status log parameter labels, call GetStatusLogLabelsForScanNum.

On return, *pdStatusLogRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time corresponding to the specified scan number but is the closest status log entry to the scan time.

The variable *pvarValue* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of the paramter type stored in the data file.

#### **Example**

```
// example for GetStatusLogValueForScanNum
long nScan= 1; // status log record for first scan
double dRT = 0.0;
VARIANT varValue;
VariantInit(&varValue);
TCHAR szLabel;
_tcscpy(szLabel, _T("Multiplier (V):")); // call GetStatusLogLabels for correct labels
```

#### Function Reference

GetStatusLogValueForScanNum

# **GetStatusLogValueForRT**

# long GetStatusLogValueForRT(double FAR\* pdRT, LPCTSTR szLabel, VARIANT FAR\* pvarValue)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the retention time

that is returned for the closest status log entry.

SZLabel A string containing the label that is returned for the status log parameter

value.

pvarValue A valid pointer to a variable of type VARIANT to receive the status log

parameter value. This variable must exist and be initialized to VT\_EMPTY.

#### **Remarks**

Returns the recorded status log parameter value for the specified status log parameter label for the current controller. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

To obtain a list of the status log parameter labels, call GetStatusLogLabelsForRT.

On return, *pdRT* contains the retention time when the status log entry was recorded. This time may not be the same as the retention time specified but is the closest status log entry to the specified time.

The variable *pvarValue* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of the paramter type stored in the data file.

#### **Example**

#### **2 Function Reference** GetStatusLogValueForRT

} ...

 $\ensuremath{/\!/}$  determine type and do something with value

• • •

### **GetTrailerExtraForScanNum**

# long GetTrailerExtraForScanNum(long nScanNumber, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarValues, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for trailer extra information.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested trailer extra information. This variable must

exist and be initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text

string values for the requested trailer extra information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* and *pvarValues* arrays. This variable must exist.

#### **Remarks**

Returns the recorded trailer extra entry labels and values for the current controller. This function is only valid for MS controllers. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The variables *pvarLabels* and *pvarValues* must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* and *pvarValues* arrays.

#### Example

// example for GetTrailerExtraForScanNum
long nScan = 12; // use twelth scan
VARIANT varLabels;
VariantInit(&varLabels);
VARIANT varValues;
VariantInit(&varValues);

long nArraySize = 0;

 $long\ nRet = XRawfileCtrl.\ GetTrailerExtraForScanNum\ (\ nScan,$ 

&varLabels, &varValues,

```
&nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting trailer extra information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
SAFEARRAY FAR* psaValues = varValues.parray;
varValues.parray = NULL;
BSTR* pbstrLabels = NULL;
BSTR* pbstrValues = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
if( FAILED(SafeArrayAccessData( psaValues, (void**)(&pbstrValues) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        SafeArrayUnaccessData( psaValues );
        SafeArrayDestroy( psaValues );
        ::MessageBox( NULL, _T("Failed to access values array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
        sLabel = pbstrLabels[i];
       sData = pbstrValues[i];
       // do something with label and value
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
SafeArrayUnaccessData( psaValues );
SafeArrayDestroy( psaValues );
```

### **GetTrailerExtraForRT**

# long GetTrailerExtraForRT(double FAR\* pdRT, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarValues, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the retention time

that is returned for the trailer extra entry.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested trailer extra information. This variable must

exist and be initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text

string values for the requested trailer extra information. This variable must

exist and be initialized to VT EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* and *pvarValues* arrays. This variable must exist.

#### **Remarks**

Returns the recorded trailer extra entry labels and values for the current controller. This function is only valid for MS controllers. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

On return, *pdRT* contains the retention time when the trailer extra entry was recorded. This time may not be the same as the retention time specified but is the scan retention time of the scan closest to the specified time.

The variables *pvarLabels* and *pvarValues* must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* and *pvarValues* arrays.

#### **Example**

// example for GetTrailerExtraForRT double dRT = 3.8; // 3.8 minutes VARIANT varLabels; VariantInit(&varLabels); VARIANT varValues; VariantInit(&varValues); long nArraySize = 0;

```
long nRet = XRawfileCtrl. GetTrailerExtraForRT (&dRT,
                                               &varLabels,
                                               &varValues,
                                               &nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting trailer extra information"), _T("Error"),
MB OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
SAFEARRAY FAR* psaValues = varValues.parray;
varValues.parray = NULL;
BSTR* pbstrLabels = NULL;
BSTR* pbstrValues = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
if( FAILED(SafeArrayAccessData( psaValues, (void**)(&pbstrValues) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        SafeArrayUnaccessData( psaValues );
        SafeArrayDestroy( psaValues );
        ::MessageBox( NULL, _T("Failed to access values array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
{
        sLabel = pbstrLabels[i];
       sData = pbstrValues[i];
       // do something with label and value
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
SafeArrayUnaccessData( psaValues );
SafeArrayDestroy( psaValues );
```

# **GetTrailerExtraLabelsForScanNum**

# long GetTrailerExtraLabelsForScanNum(long nScanNumber, VARIANT FAR\* pvarLabels, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for trailer extra information.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested trailer extra information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the *pvarLabels* arrays. This variable must exist.

#### **Remarks**

Returns the recorded trailer extra entry labels for the current controller. This function is only valid for MS controllers. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The variable *pvarLabels* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* array.

#### Example

#### Get Trailer Extra Labels For Scan Num

```
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
BSTR* pbstrLabels = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
       sLabel = pbstrLabels[i];
       // do something with label
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
```

### **GetTrailerExtraLabelsForRT**

# long GetTrailerExtraLabelsForRT(double FAR\* pdRT, VARIANT FAR\* pvarLabels, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the scan retention

time that is returned for the trailer extra labels.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of text

string labels for the requested trailer extra information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records

returned in the pvarLabels arrays. This variable must exist.

#### **Remarks**

Returns the recorded trailer extra entry labels for the current controller. This function is only valid for MS controllers. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

On return, *pdRT* contains the retention time when the trailer extra entry was recorded. This time may not be the same as the retention time specified but is the retention time of the scan closest to the specified time.

The variable *pvarLabels* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* array.

#### Example

#### Get Trailer Extra Labels For RT

```
::MessageBox( NULL, _T("Error getting trailer extra information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
BSTR* pbstrLabels = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
       sLabel = pbstrLabels[i];
       // do something with label
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
```

### **GetTrailerExtraValueForScanNum**

# long GetTrailerExtraValueForScanNum(long nScanNumber, LPCTSTR szLabel, VARIANT FAR\* pvarValue)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for trailer extra information.

SzLabel A string containing the label that is returned for the trailer extra parameter

value.

pvarValue A valid pointer to a variable of type VARIANT to receive the trailer extra

parameter value. This variable must exist and be initialized to VT\_EMPTY.

#### **Remarks**

Returns the recorded trailer extra parameter value for the specified trailer extra parameter label for the current controller. This function is only valid for MS controllers. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

To obtain a list of the status log parameter labels, call GetTrailerExtraLabelsForScanNum.

The variable *pvarValue* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of the type of the parameter stored in the data file.

#### Example

## **2** Function Reference

Get Trailer Extra Value For Scan Num

 $\ensuremath{/\!/}$  determine type and do something with value

...

### **GetTrailerExtraValueForRT**

# long GetTrailerExtraValueForRT(double FAR\* pdRT, LPCTSTR szLabel, VARIANT FAR\* pvarValue)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a variable of type double containing the retention time

that is returned for the closest trailer extra entry.

SZLabel A string containing the label that is returned for the trailer extra parameter

value.

pvarValue A valid pointer to a variable of type VARIANT to receive the trailer extra

parameter value. This variable must exist and be initialized to VT\_EMPTY.

#### **Remarks**

Returns the recorded trailer extra parameter value for the specified trailer extra parameter label for the current controller. This function is only valid for MS controllers. The value of *pdRT* must be within the retention time range for the current controller. The retention time range for the current controller may be obtained by calling GetStartTime and GetEndTime.

To obtain a list of the trailer extra parameter labels, call GetTrailerExtraLabelsForRT.

On return, *pdRT* contains the retention time when the trailer extra entry was recorded. This time may not be the same as the retention time specified but is the retention time of the scan closest to the specified time.

The variable *pvarValue* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of the type of the parameter stored in the data file.

#### **Example**

```
// example for GetTrailerExtraValueForRT
double dRT = 3.8 minutes;
VARIANT varValue;
VariantInit(&varValue);
TCHAR szLabel;
_tcscpy(szLabel, _T("Charge State:")); // call GetTrailerExtraLabelsForRT for correct labels
long nRet = XRawfileCtrl. GetTrailerExtraValueForRT (&dRT, szLabel, &varValue);
if( nRet != 0 )
{
```

### **2** Function Reference

Get Trailer Extra Value For RT

```
::MessageBox( NULL, _T("Error getting trailer extra information"), _T("Error"), MB_OK ); ... }

// determine type and do something with value ...
```

## **GetErrorLogItem**

## long GetErrorLogItem(long nItemNumber, double FAR\* pdRT, BSTR FAR\* pbstrErrorMessage)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nltemNumber* The error log item number that is returned for information.

pdRT A valid pointer to a variable of type double to receive the retention time

when the error occurred. This variable must exist.

pbstrErrorMessage A valid pointer to a variable of type BSTR to receive the text string

describing the error. This variable must exist and be initialized to

NULL.

#### **Remarks**

Returns the specified error log item information and the retention time when the error occurred. The value of *nItemNumber* must be within the range of one to the number of error log items recorded for the current controller. The number of error log items for the current controller may be obtained by calling GetNumErrorLog.

#### **Example**

### **GetTuneData**

## long GetTuneData(long nSegmentNumber, VARIANT FAR\* pvarLabels, VARIANT FAR\* pvarValues, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nSegmentNumber* The acquisition segment that is returned for tune information.

pdRT A valid pointer to a variable of type double to receive the retention time

when the error occurred. This variable must exist.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of

text string labels for the requested tune information. This variable must

exist and be initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of

text string values for the requested tune information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of

records returned in the *pvarLabels* and *pvarValues* arrays. This variable

must exist.

#### **Remarks**

Returns the recorded tune parameter labels and values for the current controller. This function is only valid for MS controllers. The value of *nSegmentNumber* must be within the range of one to the number of tune data items recorded for the current controller. The number of tune data items for the current controller may be obtained by calling GetNumTuneData.

The variables *pvarLabels* and *pvarValues* must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* and *pvarValues* arrays.

#### **Example**

```
long nRet = XRawfileCtrl. GetTuneData (nSegment, &varLabels, &varValues,
&nArraySize);
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting tune record information"), _T("Error"),
MB_OK);
}
// Get a pointer to the SafeArray
SAFEARRAY FAR* psaLabels = varLabels.parray;
varLabels.parray = NULL;
SAFEARRAY FAR* psaValues = varValues.parray;
varValues.parray = NULL;
BSTR* pbstrLabels = NULL;
BSTR* pbstrValues = NULL;
if( FAILED(SafeArrayAccessData( psaLabels, (void**)(&pbstrLabels) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        ::MessageBox( NULL, _T("Failed to access labels array"), _T("Error"), MB_OK );
}
if( FAILED(SafeArrayAccessData( psaValues, (void**)(&pbstrValues) ) ) )
        SafeArrayUnaccessData( psaLabels );
        SafeArrayDestroy( psaLabels );
        SafeArrayUnaccessData( psaValues );
        SafeArrayDestroy( psaValues );
        ::MessageBox( NULL, _T("Failed to access values array"), _T("Error"), MB_OK );
}
for( long i=0; i<nArraySize; i++)
       sLabel = pbstrLabels[i];
       sData = pbstrValues[i];
       // do something with label and value
}
// Delete the SafeArray
SafeArrayUnaccessData( psaLabels );
SafeArrayDestroy( psaLabels );
SafeArrayUnaccessData( psaValues );
SafeArrayDestroy( psaValues );
```

## **GetTuneDataValue**

## long GetTuneDataValue(long nSegmentNumber, LPCTSTR szLabel, VARIANT FAR\* pvarValue)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nSegmentNumber* The acquisition segment that is returned for tune information.

SZLabel A string containing the label that is returned for the tune parameter

value.

pvarValue A valid pointer to a variable of type VARIANT to receive the tune

parameter value. This variable must exist and be initialized to

VT\_EMPTY.

#### **Remarks**

Returns the recorded tune parameter value for the specified tune parameter label for the current controller. This function is only valid for MS controllers. The value of *nSegmentNumber* must be within the range of one to the number of tune data items recorded for the current controller. The number of tune data items for the current controller may be obtained by calling GetNumTuneData.

To obtain a list of the tune parameter labels, call GetTuneDataLabels.

The variable *pvarValue* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of the type of the parameter stored in the data file.

#### Example

// determine type and do something with value

## **GetTuneDataLabels**

# long GetTuneDataLabels(long nSegmentNumber, VARIANT FAR\* pvarLabels, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nSegmentNumber* The acquisition segment that is returned for tune information.

pvarLabels A valid pointer to a variable of type VARIANT to receive the array of

text string labels for the requested tune information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of

records returned in the pvarLabels array. This variable must exist.

#### **Remarks**

Returns the recorded tune parameter labels for the current controller. This function is only valid for MS controllers. The value of *nSegmentNumber* must be within the range of one to the number of tune data items recorded for the current controller. The number of tune data items for the current controller may be obtained by calling GetNumTuneData.

The variable *pvarLabels* must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY | VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarLabels* array.

#### Example

## **GetNumInstMethods**

#### long GetNumInstMethods(long FAR\* pnNumInstMethods)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnNumInstMethods A valid pointer to a long variable to receive the number of instrument methods contained in the raw file.

#### **Remarks**

Returns the number of instrument methods contained in the raw file. Each instrument used in the acquisition with a method that was created in Instrument Setup (for example, autosampler, LC, MS, PDA) has its instrument method contained in the raw file.

#### **Example**

## **GetInstMethod**

#### long GetInstMethod(long nInstMethodItem, BSTR FAR\* pbstrInstMethod)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nlnstMethodItem A long variable containing the index value of the instrument method to

be returned.

pbstrFilter A valid pointer to a BSTR. This variable must exist and be initialized to

NULL.

#### **Remarks**

Returns the channel label, if available, at the specified index for the current controller. This field is only relevant to channel devices such as UV detectors, A/D cards, and Analog inputs. Channel labels indices are numbered starting at 0.

Returns the instrument method, if available, at the index specified in *nInstMethodItem*. The instrument method indices are numbered starting at 0. The number of instrument methods are obtained by calling GetNumInstMethods.

#### **Example**

## **2 Function Reference** GetChroData

### **GetChroData**

long GetChroData(long nChroType1, long nChroOperator, long nChroType2,

LPCTSTR szFilter, LPCTSTR szMassRanges1,

LPCTSTR szMassRanges2, double dDelay, double FAR\*

pdStartTime,

double FAR\* pdEndTime, long nSmoothingType, long nSmoothingValue, VARIANT FAR\* pvarChroData, VARIANT FAR\* pvarPeakFlags, long FAR\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nChroType1 A long variable containing the first chromatogram trace type of interest.

*nChroOperator* A long variable containing the chromatogram trace operator.

nChroType2 A long variable containing the second chromatogram trace type of

interest.

szFilter A string containing the formatted scan filter.

szMassRanges1 A string containing the formatted mass ranges for the first

chromatogram trace type.

szMassRanges2 A string containing the formatted mass ranges for the second

chromatogram trace type.

dDelay A double precision variable containing the chromatogram delay in

minutes.

pdStartTime A pointer to a double precision variable containing the start time of the

chromatogram time range to return.

pdEndTime A pointer to a double precision variable containing the end time of the

chromatogram time range to return.

*nSmoothingType* A long variable containing the type of chromatogram smoothing to be

performed.

*nSmoothingValue* A long variable containing the chromatogram smoothing value.

pvarChroData A valid pointer to a VARIANT variable to receive the chromatogram

data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks

returned in the chromatogram array.

pnArraySize A pointer to a long variable to receive the size of the returned

chromatogram array.

#### **Remarks**

Returns the requested chromatogram data as an array of double precision time intensity pairs in *pvarChroData*. The number of time intensity pairs is returned in *pnArraySize*.

The chromatogram trace types and operator values of *nChroType1*, *nChroOperator*, and *nChroType2* depend on the current controller. See Chromatogram Type and Chromatogram Operator in the Enumerated Types section for a list of the valid values for the different controller types.

The scan filter field is only valid for MS controllers. If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

The *dDelay* value contains the retention time offset to add to the returned chromatogram times. The value may be set to 0.0 if no offset is desired. This value must be 0.0 for MS controllers. It must be greater than or equal to 0.0 for all other controller types.

The mass ranges are only valid for MS or PDA controllers. For all other controller types, these fields must be NULL or empty strings. For MS controllers, the mass ranges must be correctly formatted mass ranges and are only valid for Mass Range and Base Peak chromatogram trace types. For PDA controllers, the mass ranges must be correctly formatted wavelength ranges and are only valid for Wavelength Range and Spectrum Maximum chromatogram trace types. These values may be left empty for Base Peak or Spectrum Maximum trace types but must be specified for Mass Range or Wavelength Range trace types. See the topic Mass1 (m/z) text box in Xcalibur Help for information on how to format mass ranges.

The start and end times, *pdStartTime* and *pdEndTime*, may be used to return a portion of the chromatogram. The start time and end time must be within the acquisition time range of the current controller which may be obtained by calling GetStartTime and GetEndTime, respectively. Or, if the entire chromatogram is returned, *pdStartTime* and *pdEndTime* may be set to zero. On return, *pdStartTime* and *pdEndTime* contain the actual time range of the returned chromatographic data.

The *nSmoothingType* variable contains the type of smoothing to perform on the returned chromatographic data. See *SmoothingType* in the Enumerated Types section for a list of the valid values for *nSmoothingType*. The value of nSmoothingValue must be an odd number in the range of 3-15 if smoothing is desired.

The chromatogram list contents are returned in a SafeArray attached to the *pvarChroData* VARIANT variable. When passed in, the *pvarChroData* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarChroData* is set to type VT\_ARRAY | VT\_R8. The format of the chromatogram list returned is an array of double precision values in time intensity pairs in ascending time order (for example, time 1, intensity 1, time 2, intensity 2, time 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each time intensity pair.

On successful return, *pnArraySize* contains the number of time intensity pairs stored in the *pvarChroData* array.

#### **Example**

```
// example for GetChroData to return the MS TIC trace
typedef struct _datapeak
       double dTime;
       double dIntensity;
} ChroDataPeak;
XRawfileCtrl.SetCurrentController (0, 1);
                                               // first MS controller
VARIANT varChroData;
VariantInit(&varChroData);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
double dStartTime = 0.0;
double dEndTime = 0.0:
long nRet = XRawfileCtrl.GetChroData (1,
                                                       // TIC trace
                                       0.
                                       0,
                                       NULL,
                                       NULL,
                                       NULL,
                                       0.0.
                                       &dStartTime,
                                       &dEndTime,
                                       &varChroData,
                                       &varPeakFlags,
                                       &nArraySize );
if (nRet! = 0)
       ::MessageBox( NULL, _T("Error getting chro data."), _T("Error"), MB_OK );
```

```
}
if( nArraySize )
       // Get a pointer to the SafeArray
       SAFEARRAY FAR* psa = varChroData.parray;
       ChroDataPeak* pDataPeaks = NULL;
       SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dTime = pDataPeaks[j].dTime;
               double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with time intensity values
       }
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if(varChroData.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varChroData.parray;
       varChroData.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

## **GetMassListRangeFromScanNum**

**HRESULT** GetMassListRangeFromScanNum(long\* pnScanNumber, BSTR

bstrFilter.

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, **BOOL** bCentroidResult,

double\* pdCentroidPeakWidth, VARIANT\* pvarMassList,

VARIANT\* pvarPeakFlags, LPCTSTR csMassRange1,

long\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number that is

returned for the corresponding mass list data.

szFilter A string containing the optional scan filter.

nIntensityCutoffType The type of intensity cutoff to apply.

nIntensityCutoffValue The intensity cutoff value.

nMaxNumberOfPeaks The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pdCentroidPeakWidth The peak width to use when centroiding the peaks.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

csMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the scan corresponding to *pnScanNumber* is returned. If a scan filter is provided, the closest matching scan to *pnScanNumber* that matches the scan filter is returned. The requested scan number must be valid for the current controller. Valid scan number limits may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// read the contents of scan 12
long nScanNumber = 12;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
long nArraySize = 0;
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nRet = XRawfileCtrl.GetMassListFromScanNum ( &nScanNumber,
                                               NULL.
                                                                       // no filter
                                               0,
                                                                       // no cutoff
                                               0,
                                                                       // no cutoff
                                                                       // all peaks
                                               0,
returned
                                               FALSE.
                                                                       // do not
centroid
                                               &varMassList.
                                                                       // mass list data
                                               &varPeakFlags,
                                                                       // peak flags
data
                                               szMassRange1,
                                                                       // mass range
                                               &nArraySize );
                                                                       // size of mass
list array
if( nRet != 0 )
        ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
if( nArraySize )
        // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
        for( long j=0; j<nArraySize; j++ )</pre>
        {
                double dMass = pDataPeaks[j].dMass;
                double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
        // Release the data handle
        SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
```

```
SAFEARRAY FAR* psa = varMassList.parray;
varMassList.parray = NULL;

// Delete the SafeArray
SafeArrayDestroy( psa );
}

if(varPeakFlags.vt != VT_EMPTY )
{
    SAFEARRAY FAR* psa = varPeakFlags.parray;
    varPeakFlags.parray = NULL;

// Delete the SafeArray
SafeArrayDestroy( psa );
```

## **GetMassListRangeFromRT**

HRESULT GetMassListRangeFromRT(double\* pdRT, BSTR bstrFilter,

long nIntensityCutoffType, long nIntensityCutoffValue, long nMaxNumberOfPeaks, BOOL bCentroidResult, double\* pdCentroidPeakWidth,

VARIANT\* pvarMassList, VARIANT\* pvarPeakFlags, LPCTSTR szMassRange1, long\*

pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a double precision variable containing the

retention time, in minutes, that is returned for the corresponding

mass list data.

szFilter A string containing the optional scan filter.

*nIntensityCutoffType* The type of intensity cutoff to apply.

*nIntensityCutoffValue* The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pdCentroidPeakWidth The peak width to use when centroiding the peaks.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

szMassRange1 A string containing the mass range.

pnArraySize A valid pointer to a long variable to receive the number of data

peaks returned in the mass list array.

#### **Remarks**

This function is only applicable to scanning devices such as MS and PDA.

If no scan filter is supplied, the closest scan to *pdRT* is returned. If a scan filter is provided, the closest matching scan to *pdRT* that matches the scan filter is returned. The requested scan must be valid for the current controller. On return, *pdRT* contains the actual retention time of the returned scan. Valid retention time limits may be obtained by calling GetStartTime and GetEndTime.

If no scan filter is provided, the value of *szFilter* may be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the topic **scan filters format, definition** in Xcalibur Help for information on how to construct a scan filter.

To reduce the number of low intensity data peaks returned, an intensity cutoff, *nIntensityCutoffType*, may be applied. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted based on the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that are returned in the mass list, set *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a SafeArray attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* is set to type VT\_ARRAY | VT\_R8. The format of the mass list returned is an array of double precision values in mass intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, etc.).

The pvarPeakFlags variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

To get a range of masses between two points that are returned in the mass list, set the string of szMassRange1 to a valid range.

On successful return, *pnArraySize* contains the number of mass intensity pairs stored in the *pvarMassList* array.

#### **Example**

```
// read the contents of the scan at RT = 3.8 minutes
double dRT = 3.8;
VARIANT varMassList;
VariantInit(&varMassList);
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
TCHAR* szMassRange1[] = _T("450.00-640.00");
long nArraySize = 0;
long nRet = XRawfileCtrl.GetMassListRangeFromRT ( &dRT,
                                                                       // no filter
                                               NULL,
                                               0,
                                                                       // no cutoff
                                               0,
                                                                       // no cutoff
                                               0,
                                                                       // all peaks
returned
                                               FALSE,
                                                                       // do not
centroid
                                               &varMassList,
                                                                       // mass list data
                                               &varPeakFlags,
                                                                       // peak flags
data
                                               czMassRange1,
                                                                       // mass range
                                                                       // size of mass
                                               &nArraySize );
list array
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting mass list data for scan 12."), _T("Error"),
MB_OK);
}
if( nArraySize )
       // Get a pointer to the SafeArray
        SAFEARRAY FAR* psa = varMassList.parray;
        DataPeak* pDataPeaks = NULL;
        SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
               // Do something with mass intensity values
       }
       // Release the data handle
       SafeArrayUnaccessData( psa );
if( varMassList.vt != VT_EMPTY )
        SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
```

## **GetPrecursorInfoFromScanNum**

# HRESULT GetPrecursorInfoFromScanNum(long nScanNumber, VARIANT\* pvarPrecursorInfos, LONG\* pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the corresponding precursor info.

pvarPrecursorInfos A valid pointer to a VARIANT variable to receive the precursor info.

pnArraySize A valid pointer to a long variable to receive the number of precursor info

packets returned in the precursor info array.

#### **Remarks**

This function is used to retrieve information about the parent scans of a data-dependent MSn scan.

You retrieve the scan number of the parent scan, the isolation mass used, the charge state, and the monoisotopic mass as determined by the instrument firmware. You also get access to the scan data of the parent scan in the form of an XSpectrumRead object.

Further refine the charge state and the monoisotopic mass values from the actual parent scan data.

#### **Example**

```
struct PrecursorInfo
{
    double dIsolationMass;
    double dMonoIsoMass;
    long nChargeState;
    long nScanNumber;
};

void CTestOCXDIg::OnOpenParentScansOcx()
{
    try
    {
        VARIANT vPrecursorInfos;
        VariantInit(&vPrecursorInfos);
}
```

```
long nPrecursorInfos = 0;
  // Get the precursor scan information
  m_Rawfile.GetPrecursorInfoFromScanNum(m_nScanNumber,
                                                     &vPrecursorInfos,
                                                     &nPrecursorInfos);
  // Access the safearray buffer
  BYTE* pData;
  SafeArrayAccessData(vPrecursorInfos.parray, (void**)&pData);
  for (int i=0; i < nPrecursorInfos; ++i)
  {
    // Copy the scan information from the safearray buffer
    PrecursorInfo info;
    memcpy(&info,
                     pData + i * sizeof(MS_PrecursorInfo),
                     sizeof(PrecursorInfo));
    // Process the paraent scan information ...
  }
  SafeArrayUnaccessData(vPrecursorInfos.parray);
catch (...)
  AfxMessageBox(_T("There was a problem while getting the parent scan
                             information."));
```

## **RefreshViewOfFile**

#### long RefreshViewOfFile()

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

This function has no parameters.

#### Remarks

Refreshes the view of a file currently being acquired. This function provides a more efficient mechanism for gaining access to new data in a raw file during acquisition without closing and reopening the raw file. This function has no effect with files that are not being acquired.

#### **Example**

```
// example for RefreshViewOfFile
long nRet = XRawfileCtrl.RefreshViewOfFile();
if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error file refreshing view of file"), _T("Error"), MB_OK );
          ...
}
```

## **ExtractInstMethodFromRaw**

#### HRESULT ExtractInstMethodFromRaw(BSTR szInstMethodFileName)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

szlnstMethodFileName The file name of the instrument method.

#### Remarks

This method enables you to save the embedded instrument method in the raw file to a separated .meth file.

### **Example**

## **GetActivationTypeForScanNum**

# long GetActivationTypeForScanNum(long nScanNumber, long nMSOrder, long FAR \*pnActivationType)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the activation type information.

*nMSOrder* The MSn order for the scan.

pnActivationType A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

This function returns the activation type for the scan specified by *nScanNumber* and the transition specified by *nMSorder* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The value returned in the *pnActivationType* variable is one of the following:

CID	0
MPD	1
ECD	2
PQD	3
ETD	4
HCD	5
Any activation type	6
SA	7
PTR	8
NETD	9
NPTR	10

### **Example**

// example for GetActivationTypeForScanNum

```
long nScanNum = 12;  // Is the twelfth scan from the file
long nMSOrder = 2;  // The MS2 transition
long nType;
```

```
long nRet = XRawfileCtrl. GetActivationTypeForScanNum(nScanNum, nMSOrder,
&nType);

if( nRet != 0 )
{
          ::MessageBox( NULL, _T("Error getting the activation type for scan number 12"),
          _T("Error"), MB_OK );
          ...
}
```

## **GetMassAnalyzerTypeForScanNum**

## long GetMassAnalyzerForScanNum(long nScanNumber, long FAR \*pnMassAnalyzerType)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nScanNumber The scan number that is returned for the mass analyzer type

information.

pnMassAnalyzerType A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

This function returns the mass analyzer type for the scan specified by *nScanNumber* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The value returned in the *pnMassAnalyzerType* variable is one of the following:

```
      ITMS
      0

      TQMS
      1

      SQMS
      2

      TOFMS
      3

      FTMS
      4

      Sector
      5
```

#### Example

}

## 2 Function Reference

 ${\sf GetMassAnalyzerTypeForScanNum}$ 

## **GetDetectorTypeForScanNum**

#### 

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the detector type information.

pnDetectorType A valid pointer to a variable of type long. This variable must exist.

#### Remarks

This function returns the detector type for the scan specified by *nScanNumber* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The value returned in the *pnDetectorType* variable is one of the following:

```
CID 0
PQD 1
ETD 2
HCD 3
```

#### **Example**

```
long nScanNum = 12;  // Is the twelfth scan from the file
long nType;
long nRet = XRawfileCtrl. GetDetectorTypeForScanNum(nScanNum, & nType);
```

// example for GetDetectorTypeForScanNum

## **GetScanTypeForScanNum**

#### 

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the scan type information.

pnScanType A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

This function returns the scan type for the scan specified by *nScanNumber* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The value returned in the *pnScanType* variable is one of the following:

```
ScanTypeFull0ScanTypeSIM1ScanTypeZoom2ScanTypeSRM3
```

#### **Example**

## **GetMSOrderForScanNum**

## long GetMSOrderForScanNum(long nScanNumber, long FAR \*pnMassOrder)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nScanNumber The scan number that is returned for the scan type information.pnMassOrder A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

This function returns the MS order for the scan specified by *nScanNumber* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The value returned in the *pnScanType* variable is one of the following:

Neutral gain	-3
Neutral loss	-2
Parent scan	-1
Any scan order	0
MS	1
MS2	2
MS3	3
MS4	4
MS5	5
MS6	6
MS7	7
MS8	8
MS9	9
MS10	10

#### Example

// example for GetMSOrderForScanNum

long nScanNum = 12; // Is the twelfth scan from the file long nOrder;

long nRet = XRawfileCtrl. GetMSOrderForScanNum(nScanNum, & nOrder);

## **GetPrecursorMassForScanNum**

# long GetPrecursorMassForScanNum(long nScanNumber, long nMSOrder, double FAR \*pdPrecursorMass)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nScanNumber* The scan number that is returned for the scan type information.

*nMSOrder* The MSn order for the scan.

pdPrecursorMass A valid pointer to a variable of type double. This variable must exist.

#### **Remarks**

This function returns the precursor mass for the scan specified by *nScanNumber* and the transition specified by *nMSorder* from the scan event structure in the RAW file. The value of *nScanNumber* must be within the range of scans or readings for the current controller. The range of scans or readings for the current controller may be obtained by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

#### Example

```
// example for GetPrecursorMassForScanNum
```

## **Version**

# long Version(long \*pnMajorVersion, long \*pnMinorVersion, long \*pnSubMinorVersion, long \*pnBuildNumber)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnMajorVersion	The major version number for the DLL. This variable must exist.
pnMinorVersion	The minor version number for the DLL. This variable must exist.
pnsubMinorVersion	The sub-minor version number for the dll. This variable must exist.
pnsubBuildNumber	The build number for the dll. This variable must exist.

#### **Remarks**

This function returns the version number for the DLL.

#### **Example**

// example for Version

long nMajorVersion, nMinorVersion, nSubMinorVersion, nBuildNumber;

long nRet = XRawfileCtrl.Version(&nMajorVersion, &nMinorVersion, &nSubMinorVersion, &nBuildNumber);

## **IsThereMSData**

#### long IsThereMSData(BOOL FAR\* pbMSData)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbMSData

A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

This function checks to see if there is MS data in the raw file. A return value of TRUE means that the raw file contains MS data. You must open the raw file before performing this check.

#### **Example**

## **HasExpMethod**

## long HasExpMethod(BOOL FAR\* pbHasMethod)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbHasMethod A valid pointer to a variable of type BOOL. This variable must exist.

#### **Remarks**

This function checks to see if the raw file contains an experimental method. A return value of TRUE indicates that the raw file contains the method. You must open the raw file before performing this check.

### **Example**

## **GetFilterMassPrecision**

## long GetFilterMassPrecision(long\* pnFilterMassPrecision)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnFilterMassPrecision A valid pointer to a variable of type long. This variable must exist.

#### **Remarks**

This function gets the mass precision for the filter associated with an MS scan.

#### **Example**

## **GetStatusLogForPos**

#### 

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

*nPos* The position that the status log information is to be returned for.

pvarRT A valid pointer to a variable of type VARIANT to receive the retention time

when the status log entry was recorded. This variable must exist and be

initialized to VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text

string values for the requested status log information. This variable must

exist and be initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type LONG to receive the number of records

returned in the *pvarRT* and *pvarValues* arrays. This variable must exist.

#### **Remarks**

This function returns the recorded status log entry labels and values for the current controller.

The *pvarRT* and *pvarValues* variables must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY|VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarRT* and *pvarValues* arrays.

#### **Example**

// example for GetStatusLogForPos

VARIANT varRT; VariantInit(&varRT);

VARIANT varValues; VariantInit(&varValues);

long nPosition = 0; long nArraySize = 0;

long nRet = XRawfileCtrl. GetStatusLogForPos ( nPosition, &varRT, & varValues, &nArraySize);

if( nRet != 0 )

```
{
    ::MessageBox( NULL, _T("Error while getting the status log information"),
    __T("Error"), MB_OK );
    ...
}
```

## **GetStatusLogAtIndex**

# long GetStatusLogAtIndex(VARIANT \*pvarIndex, VARIANT \*pvarValues, long \*pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pvarIndex A valid pointer to a variable of type VARIANT to receive the retention time when the

status log entry was recorded. This variable must exist and be initialized to

VT\_EMPTY.

pvarValues A valid pointer to a variable of type VARIANT to receive the array of text string

values for the requested status log information. This variable must exist and be

initialized to VT\_EMPTY.

pnArraySize A valid pointer to a variable of type long to receive the number of records returned in

the pvarIndex and pvarValues arrays. This variable must exist.

#### **Remarks**

This function returns the recorded status log entry labels and values for the current controller.

The *pvarIndex* and *pvarValues* variables must be initialized to VARIANT type VT\_EMPTY. On return, these variables are of type VT\_ARRAY|VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarIndex* and *pvarValues* arrays.

### Example

```
// example for GetStatusLogAtIndex
```

## **2** Function Reference

GetStatusLogAtIndex

}

## **GetInstMethodNames**

### long GetInstMethodNames(long \*pnSize, VARIANT \*pvarNames)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnArraySize A valid pointer to a variable of type long to receive the number of records returned in

the pvarNames array. This variable must exist.

pvarNames A valid pointer to a variable of type VARIANT to receive the array of text string

values for the requested status log information. This variable must exist and be

initialized to VT\_EMPTY.

#### Remarks

This function returns the recorded names of the instrument methods for the current controller.

The *pvarNames* variable must be initialized to VARIANT type VT\_EMPTY. On return, this variable is of type VT\_ARRAY|VT\_BSTR. On return, *pnArraySize* contains the number of entries in the *pvarNames* array.

## **Example**

```
// example for GetInstMethodNames
```

#### **2** Function Reference

GetInstMethodNames

```
SafeArrayUnaccessData( psa );
SafeArrayDestroy( psa );
:::MessageBox( NULL, _T("Failed to access scan filter array"), _T("Error"), MB_OK );
return;
}

// display names one at a time
TCHAR szTitle[24];

for( long i=0; i<nArraySize; i++ )
{
    __stprintf( szTitle, _T("Method name %d"), i );
    :::MessageBox( NULL, pbstrNames[i], szTitle, MB_OK );
}

// Delete the SafeArray
SafeArrayUnaccessData( psa );
SafeArrayDestroy( psa );
```

## **SetMassTolerance**

### long SetMassTolerance(BOOL bUserDefined, double dMassTolerance, long nUnits)

#### **Return Value**

0 if successful;

#### **Parameters**

bUserDefined A flag indicating whether the mass tolerance is user-defined (TRUE) or based on

the values in the raw file (FALSE).

dMassTolerance The mass tolerance value.

*nUnits* The type of tolerance value (amu, mmu, ppm).

#### Remarks

This function sets the mass tolerance that will be used with the raw file.

### **Example**

# **2 Function Reference** GetChros

## **GetChros**

long GetChros(long nChros, double \*pdStartTime, double \*pdEndTime,
VARIANT \*pvarChroParamsArray, VARIANT \*pvarSizeArray,
VARIANT \*pvarChroDataArray, VARIANT \*pvarPeakFlagsArray)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

nChros A long variable containing the number of chromatograms to get from the

raw file.

pdStartTime A pointer to a double-precision variable containing the start time of the

chromatogram time range to return.

pdEndTime A pointer to a double-precision variable containing the end time of the

chromatogram time range to return.

pvarChroParamsArray A valid pointer to a VARIANT variable to parameters that will be used to

generate each chromatogram.

pvarSizeArray A valid pointer to a VARIANT variable to the size of each chromatogram.

pvarChroDataArray A valid pointer to a VARIANT variable to receive the chromatogram data.

pvarPeakFlagsArray A valid pointer to a VARIANT variable to receive the peak flag data.

#### Remarks

This function returns the requested chromatogram data as an array of double-precision time-intensity pairs in *pvarChroDataArray*. The number of time intensity pairs is returned in *pvarSizeArray*.

You can use the start and end times, *pdStartTime* and *pdEndTime*, to return a portion of the chromatogram. The start time and end time must be within the acquisition time range of the current controller, which you can obtain by calling *GetStartTime* and *GetEndTime*, respectively. Alternatively, if the entire chromatogram is to be returned, you can set *pdStartTime* and *pdEndTime* to zero. On return, *pdStartTime* and *pdEndTime* contain the actual time range of the returned chromatographic data.

The parameters that are used to generate the chromatograms are contained in *pvarChroParamsArray*. They include the trace type 1 (int), trace operator (int), trace type 2 (int), filter string (bstr), mass range 1 (bstr), mass range 2 (bstr), delay (double), start RT (double), end RT (double), start scan number (int), end scan number (int), smoothing type (int), and number of smoothing points (int), in this order. The description of the GetChroData function contains additional information on these values.

The chromatogram list contents are returned in a *SafeArray* attached to the *pvarChroDataArray* VARIANT variable. When passed in, the *pvarChroData* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarChroDataArray* will be set to type VT\_ARRAY|VT\_R8. The format of the chromatogram list returned is an array of double-precision values in time-intensity pairs in ascending time order (for example, time 1, intensity 1, time 2, intensity 2, time 3, intensity 3, and so forth).

The *pvarPeakFlags* variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each time-intensity pair.

On successful return, *pvarSizeArray* contains the number of time-intensity pairs stored in *pvarChroDataArray*. When passed in, the *pvarSizeArray* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarSizeArray* will be set to type VT\_ARRAY|VT\_I4.

## **GetSegmentedMassListFromRT**

long GetSegmentMassListFromRT(double \*pdRT, BSTR bstrFilter,

long nIntensityCutoffType, long nIntensityCutoffValue,

long nMaxNumberOfPeaks, BOOL bCentroidResult,

double \*pdCentroidPeakWidth,

VARIANT \* pvarMassList, VARIANT \* pvarPeakFlags,

long \*pnArraySize, VARIANT \*pvarSegments,

long \*pnNumSegments,

**VARIANT \*pvarLowHighMassRange)** 

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pdRT A valid pointer to a double-precision variable containing the retention time,

in minutes, that the corresponding mass list data is to be returned for.

bstrFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

nIntensityCutoffValue The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks

returned in the mass list array.

pvarSegments A valid pointer to a VARIANT variable to receive the segment data.

pnNumSegments A valid pointer to a long variable to receive the number of segments returned

in the segments array.

pvarMassRange A valid pointer to a VARIANT variable to receive the mass range data.

#### Remarks

This function applies only to scanning devices such as MS.

If no scan filter is supplied, the closest scan to *pdRT* will be returned. If a scan filter is provided, the closest matching scan to *pdRT* that matches the scan filter will be returned. The requested scan must be valid for the current controller. On return, *pdRT* contains the actual retention time of the returned scan. You can obtain valid retention time limits by calling GetStartTime and GetEndTime.

If no scan filter is to be provided, the value of *szFilter* can be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the "scan filters format definition" topic in the Xcalibur online help for information on how to construct a scan filter.

To reduce the number of low-intensity data peaks returned, you can apply an intensity cutoff, *nIntensityCutoffType*. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted on the basis of the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that will be returned in the mass list, set the value of *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set *bCentroidResult* to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a *SafeArray* attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* will be set to type VT\_ARRAY|VT\_R8. The format of the mass list returned is an array of double-precision values in mass-intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, and so forth.)

The *pvarPeakFlags* variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass-intensity pair.

On successful return, *pnArraySize* contains the number of mass-intensity pairs stored in the *pvarMassList* array.

The *varSegments* array contains information about the segments, and the *varMassRange* array contains the mass range for each segment. The *nSegments* variable contains the number of segments.

## Example

```
// example for GetSegmentedMassListFromRT
typedef struct _datapeak
{
          double dMass;
          double dIntensity;
} DataPeak;

VARIANT varMassList;
VariantInit(&varMassList);
```

```
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
VARIANT varSegments;
VariantInit(&varSegments);
VARIANT varMassRange;
VariantInit(&varMassRange);
double dRT = 3.8;// read the contents of the scan at RT = 3.8 minutes
long nArraySize = 0;
long nSegments = 0;
long nRet = XRawfileCtrl.GetSegmentedMassListFromRT ( &dRT,
  NULL, 0, 0, 0, FALSE,
  &varMassList,
  &varPeakFlags,
  &nArraySize,
          &varSegments,
  &nSegments,
  &varMassRange);
if( nRet != 0 )
{
       ::MessageBox( NULL, _T("Error getting mass list data for scan at 3.8 minutes."),
      _T("Error"), MB_OK );
}
if( nArraySize )
       // Get a pointer to the SafeArray
       SAFEARRAY FAR* psa = varMassList.parray;
       DataPeak* pDataPeaks = NULL;
       SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
       // Do something with mass intensity values
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
```

```
{
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varSegments.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varSegments.parray;
       varSegments.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varMassRange.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varMassRange.parray;
       varMassRange.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

## **GetSegmentedMassListFromScanNum**

long GetSegmentMassListFromScanNum(long \*pnScanNumber, BSTR bstrFilter,

long nIntensityCutoffType, long nIntensityCutoffValue,

long nMaxNumberOfPeaks, BOOL bCentroidResult,

double \*pdCentroidPeakWidth,

VARIANT \* pvarMassList, VARIANT \* pvarPeakFlags,

long \*pnArraySize, VARIANT \*pvarSegments,

long \*pnNumSegments, VARIANT \*pvarMassRange)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number that the

corresponding mass list data is to be returned for.

bstrFilter A string containing the optional scan filter.

*nlntensityCutoffType* The type of intensity cutoff to apply.

nIntensityCutoffValue The intensity cutoff value.

*nMaxNumberOfPeaks* The maximum number of data peaks to return in the mass list.

bCentroidResult Boolean flag indicating that returned mass list contents should be

centroided.

pvarMassList A valid pointer to a VARIANT variable to receive the mass list data.

pvarPeakFlags A valid pointer to a VARIANT variable to receive the peak flag data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks

returned in the mass list array.

pvarSegments A valid pointer to a VARIANT variable to receive the segment data.

pnNumSegments A valid pointer to a long variable to receive the number of segments returned

in the segments array.

pvarMassRange A valid pointer to a VARIANT variable to receive the mass range data.

#### Remarks

This function is only applicable to scanning devices such as MS.

If no scan filter is supplied, the scan corresponding to *pnScanNumber* will be returned. If a scan filter is provided, the closest matching scan to *pnScanNumber* that matches the scan filter will be returned. The requested scan number must be valid for the current controller. You can obtain valid scan number limits by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

If no scan filter is to be provided, the value of *szFilter* can be NULL or an empty string. Scan filters must match the Xcalibur scan filter format. See the "scan filters format definition" topic in the Xcalibur online help for information on how to construct a scan filter.

To reduce the number of low-intensity data peaks returned, you can apply an intensity cutoff, *nIntensityCutoffType*. The available types of cutoff are None, Absolute (intensity), and Relative (relative intensity). The value of *nIntensityCutoffValue* is interpreted on the basis of the value of *nIntensityCutoffType*. See Cutoff Type in the Enumerated Types section for the possible cutoff type values.

To limit the total number of data peaks that will be returned in the mass list, set the value of *nMaxNumberOfPeaks* to a value greater than zero. To have all data peaks returned, set *nMaxNumberOfPeaks* to zero.

To have profile scans centroided, set bCentroidResult to TRUE. This parameter is ignored for centroid scans.

The mass list contents are returned in a *SafeArray* attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* will be set to type VT\_ARRAY|VT\_R8. The format of the mass list returned is an array of double-precision values in mass-intensity pairs in ascending mass order (for example, mass 1, intensity 1, mass 2, intensity 2, mass 3, intensity 3, and so forth.)

The *pvarPeakFlags* variable is currently not used. This variable is reserved for future use to return flag information, such as saturation, about each mass intensity pair.

On successful return, *pnArraySize* contains the number of mass-intensity pairs stored in the *pvarMassList* array.

The *varSegments* array contains information about the segments, and the *varMassRange* array contains the mass range for each segment. The *nSegments* variable contains the number of segments.

#### **Example**

```
// example for GetSegmentedMassListFromScanNum
typedef struct _datapeak
{
          double dMass;
          double dIntensity;
} DataPeak;

VARIANT varMassList;
VariantInit(&varMassList);
```

```
VARIANT varPeakFlags;
VariantInit(&varPeakFlags);
VARIANT varSegments;
VariantInit(&varSegments);
VARIANT varMassRange;
VariantInit(&varMassRange);
long nScanNumber = 12;// read the contents of scan 12
long nArraySize = 0;
long nSegments = 0;
long nRet = XRawfileCtrl.GetSegmentedMassListFromScanNum ( &nScanNumber,
 NULL, 0, 0, 0, FALSE,
 &varMassList,
&varPeakFlags,
&nArraySize,
&varSegments,
&nSegments,
&varMassRange);
if( nRet != 0 )
{
       ::MessageBox( NULL, _T("Error getting mass list data for scan 12."),
      _T("Error"), MB_OK );
}
if( nArraySize )
       // Get a pointer to the SafeArray
       SAFEARRAY FAR* psa = varMassList.parray;
       DataPeak* pDataPeaks = NULL;
       SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
       // Do something with mass intensity values
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
if( varMassList.vt != VT_EMPTY )
```

```
{
       SAFEARRAY FAR* psa = varMassList.parray;
       varMassList.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varPeakFlags.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varPeakFlags.parray;
       varPeakFlags.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varSegments.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varSegments.parray;
       varSegments.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
if(varMassRange.vt != VT_EMPTY )
       SAFEARRAY FAR* psa = varMassRange.parray;
       varMassRange.parray = NULL;
       // Delete the SafeArray
       SafeArrayDestroy( psa );
}
```

## **GetScanEventForScanNum**

### long GetScanEventForScanNumberTextEx(long nScan, BSTR FAR\* pbstrScanEvent)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

```
nScanThe scan number that the scan event is being requested for.pbstrScanEventA valid pointer to a BSTR. This variable must exist and be initialized to NULL.
```

#### **Remarks**

This function returns a scan event information as a string for the specified scan number.

### **Example**

## **GetSeqRowUserTextEx**

## long GetSeqRowUserTextEx(long nIndex, BSTR FAR\* pbstrUserText)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

### **Parameters**

nlndex The index value of the user text field to return.pbstrUserText A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

This function returns a user text field from the sequence row of the raw file. There are five user text fields in the sequence row that are indexed 0 through 4.

### **Example**

## **GetSeqRowBarcode**

## long GetSeqRowBarcode(BSTR FAR\* pbstrBarcode)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pbstrBarcode A valid pointer to a BSTR. This variable must exist and be initialized to NULL.

#### **Remarks**

This function returns the barcode used to acquire the raw file. This field is empty if the raw file was created by file format conversion or acquired from a tuning program.

### **Example**

## **GetSeqRowBarcodeStatus**

### long GetSeqRowBarcodeStatus(long\* pnStatus)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnStatus

A valid pointer to a long. This variable must exist and be initialized to 0.

#### **Remarks**

This function returns the barcode status from the raw file. This field is empty if the raw file was created by file format conversion or acquired from a tuning program.

## **Example**

## **GetSeqmentAndScanEventForScanNum**

# long GetSeqmentAndScanEventForScanNum(long nScanNumber, long \*pnSegment, long\* pnScanEvent)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

```
pnSegment A valid pointer to a long. This variable must exist and be initialized to 0.pnScanEvent A valid pointer to a long. This variable must exist and be initialized to 0.
```

#### Remarks

Returns the segment and scan event indexes for the specified scan..

## **Example**

## **GetMassPrecisionEstimate**

## long GetMassPrecisionEstimate(long nScanNumber, VARIANT \*pvarMassList, long \*pnArraySize)

#### **Return Value**

0 if successful; otherwise, see Error Codes.

#### **Parameters**

pnScanNumber A valid pointer to a long variable containing the scan number for which the

corresponding mass list data is to be returned.

pvarMassList A valid pointer to a VARIANT variable to receive the mass precision data.

pnArraySize A valid pointer to a long variable to receive the number of data peaks returned in the

mass list array.

#### Remarks

This function is only applicable to scanning devices such as MS. It gets the mass precision information for an accurate mass spectrum (that is, acquired on an FTMS- or Orbitrap-class instrument).

If no scan filter is supplied, the scan corresponding to *pnScanNumber* will be returned. If a scan filter is provided, the closest matching scan to *pnScanNumber* that matches the scan filter will be returned. The requested scan number must be valid for the current controller. You can obtain valid scan number limits by calling GetFirstSpectrumNumber and GetLastSpectrumNumber.

The mass list contents are returned in a *SafeArray* attached to the *pvarMassList* VARIANT variable. When passed in, the *pvarMassList* variable must exist and be initialized to VARIANT type VT\_EMPTY. If the function returns successfully, *pvarMassList* will be set to type VT\_ARRAY|VT\_R8. The format of the mass list returned is an array of double-precision values in the order of intensity, mass, accuracy in MMU, accuracy in PPM, and resolution.

#### Example

```
VariantInit(&varMassList);
long nScanNumber = 12;// read the contents of scan 12
long nArraySize = 0;
long nSegments = 0;
long nRet = XRawfileCtrl. GetMassPrecisionEstimate ( nScanNumber, &varMassList,
                                                    &nArraySize);
if( nRet != 0 )
       ::MessageBox( NULL, _T("Error getting mass precision data for scan 12."),
      _T("Error"), MB_OK );
}
if( nArraySize )
       // Get a pointer to the SafeArray
       SAFEARRAY FAR* psa = varMassList.parray;
       DataPeak* pDataPeaks = NULL;
       SafeArrayAccessData( psa, (void**)(&pDataPeaks) );
       for( long j=0; j<nArraySize; j++ )</pre>
               double dMass = pDataPeaks[j].dMass;
               double dIntensity = pDataPeaks[j].dIntensity;
double dAccuracyMMU = pDataPeaks[j].dAccuracyMMU;
double dAccuracyMMU = pDataPeaks[j].dAccuracyPPM;
double dResolution = pDataPeaks[i]. dResolution;
       // Do something with mass precision values
       // Release the data handle
       SafeArrayUnaccessData( psa );
}
```

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