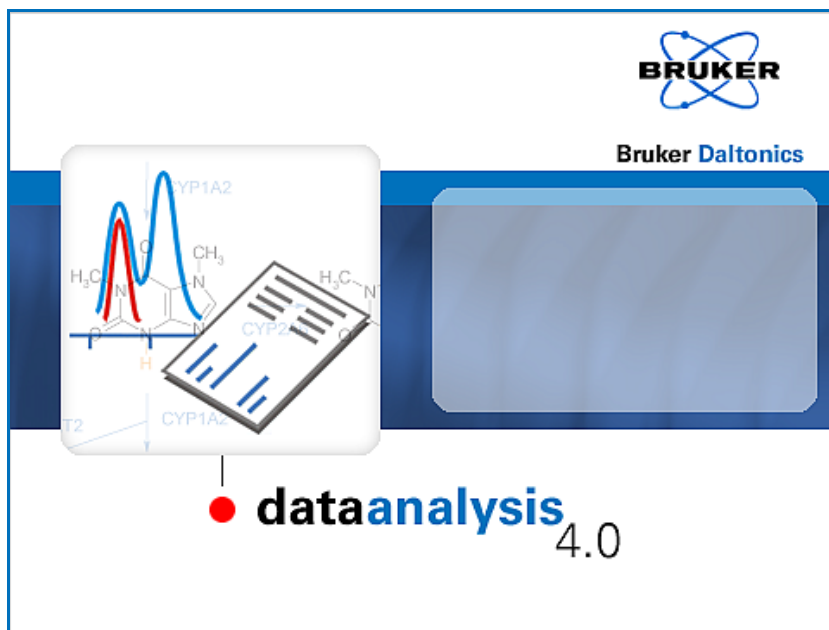

dataanalysis 4.0

Scripting Reference Manual



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1 **PREFACE**

The *Bruker Daltonics DataAnalysis 4.0* application (in the following 'DataAnalysis') can be controlled programmatically by manipulating it through Automation (formerly OLE Automation). For example, in a Visual Basic Script, you can control an open analysis by manipulating its corresponding **Analysis** object.

The DataAnalysis object model enables you to automate analysis processing tasks. This object model consists of the hierarchy of DataAnalysis objects, and their associated properties, methods and events.

The DataAnalysis 4.0 Scripting Reference Manual describes each object, along with its properties, methods and events.

For reference on how to work with DataAnalysis 4.0, please refer to the DataAnalysis 4.0 User Manual, and for reference on DataAnalysis 4.0 menus and commands, please refer to the DataAnalysis 4.0 Reference Manual. The DataAnalysis 4.0 manuals are available as PDF documents on the installation CD.

2 AUTOMATION OBJECTS AND OBJECT HIERARCHY

2.1 Object Hierarchy

Each `DataAnalysis` object implements a dual interface through which you can manipulate the object. Each object implements an **IDispatch** interface for Automation and a Component Object Model (COM) interface for direct access to object members (properties, methods, events).

Overview of each `DataAnalysis` object

Each `DataAnalysis` object is described below.

<u>Object</u>	<u>Represents</u>
Analyses	All open analyses; a collection of Analysis objects.
Analysis	An open analysis.
Annotation	An annotation of a mass spectrum.
Annotations	All annotations of a mass spectrum. A collection of Annotation objects.
Application	The <code>DataAnalysis</code> application.
ChildSpectra	All derived spectra of a mass spectrum.
Chromatogram	A chromatogram of an analysis.
ChromatogramDefinition objects	
TICChromatogramDefinition	ChromatogramDefinition object for Total Ion Chromatograms.
EICChromatogramDefinition	ChromatogramDefinition object for Extracted Ion Chromatograms.
BPCChromatogramDefinition	ChromatogramDefinition object for Base Peak Chromatograms.
CNLChromatogramDefinition	ChromatogramDefinition object for Constant Neutral Loss Chromatograms.
MassPosChromatogramDefinition	ChromatogramDefinition object for Mass Position Chromatograms.
UVChromatogramDefinition	ChromatogramDefinition object for 1D UV Chromatograms.

<u>Object</u>	<u>Represents</u>
UV2DChromatogramDefinition	ChromatogramDefinition object for extracted chromatograms of a 2D UV data file.
LCChromatogramDefinition	ChromatogramDefinition object for LC Chromatograms.
VARChromatogramDefinition	ChromatogramDefinition object for Acquisition Parameter Chromatograms.
ICACHromtogramDefinition	ChromatogramDefinition object for Isotope Cluster Analysis Chromatograms.
ImportedDataChromatogramDefinition	ChromatogramDefinition object for Imported External Data Chromatograms.
ExtDataChromatogramDefinition	ChromatogramDefinition object for imported external comma-separated-value data.
Chromatograms	All chromatograms of an analysis; a collection of Chromatogram objects.
Compound	A compound of a chromatogram analysis; a collection of Spectrum objects.
Compounds	All compounds of a chromatogram analysis; a collection of Compound objects.
Form	The script form in the AutomationEngine and in DataAnalysis.
LibrarySearchResult	The library search result of a compound or mass spectrum for a chromatogram analysis, resp. spectrum analysis.
LibrarySearchResults	All library search results of a compound or spectrum from a chromatogram analysis, resp. spectrum analysis; a collection of LibrarySearchResult objects.
MSFilter	Defines mass spectrum specific information of a ChromatogramDefinition object.
MSPeak	A peak of a mass spectrum.
MSPeakList	All peaks of a mass spectrum (= Mass List); a collection of one or more MSPeak objects.
Properties	Represents an open analysis.

Object

SmartFormulaParameters

SmartFormulaResult

SmartFormulaResultItem

SmartFormulaResults

Spectra

Spectrum

SumFormula

Variable

Variables

Represents

Defines all parameters used for generating sum formulae from a specified region of a mass spectrum.

A single SmartFormula result of a mass spectrum; a collection of one or more **SmartFormulaResultItem** objects.

A single item of a SmartFormula result.

All SmartFormula results of a mass spectrum; a collection of one or more **SmartFormulaResult** objects.

All mass spectra of a mass spectrum analysis; a collection of **Spectrum** objects.

A mass spectrum of a mass spectrum analysis or a compound of a chromatogram analysis.

A sum formula of a chemical compound.

A variable item of the **Variables** collection class.

The variable table of a **Spectrum** object.

DataAnalysis object hierarchy for automation

To manipulate DataAnalysis objects, you must know the relationships between them. The **Application** object is at the top, and the other objects are subordinate to it. This relationship allows you to directly access objects subordinate to the **Application** object by using the properties and methods of the **Application** object. The **Form** object is not related to the other objects. It is used to control the VBScripting form in the Automation-Engine and in DataAnalysis.

The "has-a" tree is shown below. For example, the **Analyses** object has, as one of its properties, an **Analysis** object.

```
Application
```

```
    Application (Application is its own parent)
```

```
        Analyses
```

```
            Analysis
```

```
                Properties
```

```
                Chromatograms (for "Chromatogram" analysis types)
```

```
                    Chromatogram
```

Definition (gets a ChromatogramDefinition object)
Compounds (for "Chromatogram" analysis types)
 Compound
 Spectrum
 ChildSpectrum
 Spectrum
 ...
 MSPeakList
 MSPeak
 Variables
 Variable
 LibrarySearchResults
 LibrarySearchResult
 Annotations
 Annotation
 SmartFormulaResults
 SmartFormulaResult
 SmartFormulaResultItem
 Variables
 Variable
 LibrarySearchResults
 LibrarySearchResult
Spectra (for "MassSpectrum" analysis types and averaged
 spectrum entries in Compound Spectra not relating to
 compounds)
 Spectrum
 ChildSpectrum
 Spectrum
 ...
 MSPeakList
 MSPeak
 Variables
 Variable
 LibrarySearchResults
 LibrarySearchResult
 Annotations
 Annotation
 SmartFormulaResults

```
SmartFormulaResult
    SmartFormulaResultItem
ChromatogramDefinition____
SmartFormulaParameters
MSFilter
SumFormula
Form
```

Implied objects

The **Analysis**, the **Application** and the **Form** objects are the topmost objects for a script running in DataAnalysis. These objects are implicitly available in the VBScript in DataAnalysis. The **Form** object is the topmost object in the AutomationEngine. This object is also implicitly available in the VBScript in the AutomationEngine.

2.2 Analyses Object

The **Analyses** object represents all open analyses. The **Analyses** object is a collection of one or more **Analysis** objects.

The **Analyses** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

Item

Open

The **Analyses** object is a collection object that contains all **Analysis** objects. To find a particular object, iterate through the collection by using the **Analyses** object of the **Application** object. Consider the following code snippet from a DataAnalysis Script.

```
Dim myAnalysis
set Application = GetObject("",
"BDal.DataAnalysis.Application")
For Each myAnalysis in Application.Analyses
    ' Access myAnalysis here.
    ' For example:
```

```
MsgBox myAnalysis.Name
```

Next

See Also

Analysis object

2.3 Analysis Object

The **Analysis** object represents an open analysis.

The **Analysis** object has the following objects, properties and methods:

Objects

Chromatograms

Properties

Compounds

Spectra

Properties

FullName

Path

IsChromatographicAnalysis

ScriptVariable

IsLockMassCalibrationActive

Type

Name

Methods

ApplyLockMassCalibration

PrepareSurveyView

AddChromatogramRangeSelection

Print

ClearChromatogramRangeSelections

PrintToPDF

ClearResults

ProcessAutoMSn

Close

RecalculateLineSpectra

DeleteRecalculatedLineSpectra

RecalibrateAutomatically

DeleteScriptTable

RecalibrateExternal

Deselect

RecalibrateInternal

Export

RunScript

FindAutoMSn

Save

FindDissect

Select

FindMolecularFeatures

SendReport

FindMSn

SetScriptTableCellText

Methods

LoadMethod
MascotSearch
SetScriptTableColumnHeader

Each open analysis in `DataAnalysis` is represented by an **Analysis** object. This object has members (properties, methods, and events) that you can use to process the analysis.

The **Analysis** object is a top-most object in a script running in `DataAnalysis`. You can access the **Analysis** object directly by its name.

All open analyses belong to the analyses collection represented by the **Analyses** object. You can find a particular analysis by iterating through this collection.

2.4 Annotation Object

The **Annotation** object represents an annotation in a **Spectrum** object.

The **Annotation** object has the following objects, properties and methods:

Objects

Properties

ShowLine	Y1
Text	Y2
X1	YText
X2	

Methods

All defined annotations belong to the **Annotations** collection represented by the **Annotations** object. You can find a particular annotation by iterating through this collection.

See Also

Annotations object

2.5 Annotations Object

The **Annotations** object represents all annotations in a **Spectrum** object. The **Annotations** object is a collection of one or more **Annotation** objects.

The **Annotations** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

AddAnnotation

DeleteAnnotation

The **Annotations** object is a collection object that contains all **Annotation** objects. To find a particular object, iterate through the collection by using the **Annotations** object of the **Spectrum** object.

See Also

Annotation object

2.6 Application Object

The **Application** object represents DataAnalysis and is the topmost object in the DataAnalysis object hierarchy. From the **Application** object, you can directly access other DataAnalysis objects by using the **Application** object's properties and methods, or you can indirectly access objects through other objects obtained by these properties and methods.

The **Application** object is also the first object being opened and accessed when using the AutomationEngine. When running the script in DataAnalysis both the **Application** object and the **Analysis** object are implicitly available.

The **Application** object has the following objects, properties and methods:

Objects

Analyses

Properties

Active	Name
ActiveAnalysis	Path
FullName	Version
Logging	Visible

Methods

Activate	SelectNone
Hide	Show

The **Application** object is a top-most object in a script running in DataAnalysis. You can access the **Application** object directly by its name.

2.7 ChildSpectra Object

The **ChildSpectra** object represents all spectra in a spectrum analysis. The **ChildSpectra** object is a collection of one or more **Spectrum** objects.

The **ChildSpectra** object has the following objects, properties and methods:

Objects**Properties**

Count

Methods

Item

The **ChildSpectra** object is a collection object that contains all **Spectrum** objects. To find a particular object, iterate through the collection by using the **ChildSpectra** object of the **Spectrum** object.

Example

```
Option Explicit
Analysis.Spectra.Smooth

Dim Spectrum
```

```
For Each Spectrum in Analysis.Spectra
    MsgBox Spectrum.ChildSpectra(1).Name
Next
```

See Also

Spectrum object

2.8 Chromatogram Object

The **Chromatogram** object represents a chromatogram defined for an analysis.

The **Chromatogram** object has the following objects, properties and methods:

Objects

Properties

Color	MaximumIntensity
Definition	MinimumIntensity
FirstRetentionTime	Name
Intensity(n)	RetentionTime property
LastRetentionTime	Size

Methods

AddRangeSelection	FindCompounds
AverageMassSpectrum	IntegrateOnly
ChromatogramData	Noise
ClearRangeSelections	RelatedCompounds
Deselect	Select
Enable	Smooth
Export	

All defined chromatograms belong to the **Chromatograms** collection represented by the **Chromatograms** object. You can find a particular chromatogram by iterating through this collection.

See Also

Chromatograms object

2.9 ChromatogramDefinition Objects

The **ChromatogramDefinition** objects represent the description of a particular chromatogram trace.

There exist several different **ChromatogramDefinition** objects, each for a specific type of chromatogram trace. These are:

TICChromatogramDefinition	for Total Ion Chromatograms
EICChromatogramDefinition	for Extracted Ion Chromatograms
BPCChromatogramDefinition	for Base Peak Chromatograms
CNLChromatogramDefinition	for Constant Neutral Loss Chromatograms
MassPosChromatogramDefinition	for Mass Position Chromatograms
UVChromatogramDefinition	for 1D UV Chromatograms
UV2DChromatogramDefinition	for extracted chromatograms of a 2D UV data file
LCChromatogramDefinition	for LC Chromatograms
VARChromatogramDefinition	for Acquisition Parameter Chromatograms
ICACHromatogramDefinition	for Isotope Cluster Analysis Chromatograms
ImportedDataChromatogramDefinition	for Imported External Data Chromatograms
ExtDataChromatogramDefinition	for imported external comma-separated-value data (for description of the data format refer to the DataAnalysis Reference Manual, Chromatograms command)

Each of these **ChromatogramDefinition** objects has the following objects, properties and methods:

Objects

Properties	<u>TIC...</u>	<u>EIC...</u>	<u>BPC...</u>	<u>CNL...</u>	<u>Mass...</u>	<u>UV...</u>	<u>UV2...</u>
Type	X	X	X	X	X	X	X
Name	X	X	X	X	X	X	X
Color	X	X	X	X	X	X	X
MSFilter	X	X	X	X			
ScanMode	X	X	X				
Polarity	X	X	X	X			
BackgroundTyp	X	X	X				
Range		X	X	X	X		X
WidthRight, WidthLeft		X	X	X	X		

Properties	<u>TIC...</u>	<u>EIC...</u>	<u>BPC...</u>	<u>CNL...</u>	<u>Mass...</u>	<u>UV...</u>	<u>UV2...</u>
Filename						(X)	(X)
RetentionTimeOffset							
Signal						X	
VariableName							
GroupName							
Delta_m_over_z							
ToleranceDelta_m_over_z							
IntensityRatio							
ToleranceIntensityRatio							
RawValues					X		
ExtractionMode							X

Properties	<u>LC...</u>	<u>VAR...</u>	<u>ICA...</u>	<u>Imp...</u>	<u>Ext...</u>
Type	X	X	X	X	
Name	X	X	X	X	
Color	X	X	X	X	
MSFilter					
ScanMode					
Polarity			X		
BackgroundTyp					
Range					
WidthRight, WidthLeft					
Filename				X	X
RetentionTimeOffset					X
Signal	X				
VariableName		X			
GroupName		X			
Delta_m_over_z			X		
ToleranceDelta_m_over_z			X		
IntensityRatio			X		
ToleranceIntensityRatio			X		
RawValues					
ExtractionMode					

Methods

ChromatogramDefiniton objects are used in two situations: First to define a new chromatogram and to add it to the analysis and second to get information about an existing chromatogram.

Example

The following example first adds a single TIC and then a set of three traces, another TIC, a BPC, and an acquisition variable trace to the list of loaded and displayed traces in DataAnalysis:

```
Dim TIC, BPC, UV, Var
Dim Chroms(3)          ' define an array of four chromatogram
definitions

' define a "TIC, +All MS FullScan" chromatogram trace
Set TIC =
CreateObject("DataAnalysis.TICChromatogramDefinition")
TIC.MSFilter.Type      = daMSFilterMS
TIC.ScanMode           = daScanModeFullScan
TIC.Polarity           = daPositive
' load and display the "TIC, +All MS FullScan " chromatogram
trace
Analysis.Chromatograms.AddChromatogram TIC

' alter the TIC definition to "TIC -MS2(390.4) FullScan" and
add it to the array of chromatogram definitions
TIC.MSFilter.Type      = daMSFilterMSMS
TIC.MSFilter.FragmentationPath = "390.4"
TIC.ScanMode           = daScanModeFullScan
TIC.Polarity           = daNegative
Set Chroms(0)          = TIC

' define a base peak chromatogram definition of "BPC 200-500;
700; 800-1000 +All MSn FullScan" with spectral background
subtracted and add it to the array of chromatogram definitions
Set BPC =
CreateObject("DataAnalysis.BPCChromatogramDefinition")
BPC.MSFilter.Type      = daMSFilterAllMSMS
BPC.ScanMode           = daScanModeFullScan
BPC.Polarity           = daPositive
BPC.BackgroundType     = daBgrdTypeSpectral
BPC.Range              = "200-500; 700; 800-1000"
BPC.WidthLeft          = 0.8
BPC.WidthRight         = 1.0
Set Chroms(1)          = BPC
```

```
' define a constant wavelength UV chromatogram from HyStar
Set UV = CreateObject("DataAnalysis.UVChromatogramDefinition")
UV.Signal = "214 nm"
Set Chroms(2) = UV

' define an acquisition parameter chromatogram definition of
the "Vacuum High (Vacuum System)" variable and add it to the
array of chromatogram definitions
Set Var =
CreateObject("DataAnalysis.VARChromatogramDefinition")
Var.VariableName = "Vacuum High"
Var.GroupName = "Vacuum System"
Set Chroms(3) = Var

' load and display the array of four chromatogram definitions
at once
Analysis.Chromatograms.AddChromatograms(Chroms)

' define an isotope cluster analysis chromatogram definition
dim icachrom
set icachrom =
createObject("DataAnalysis.ICACHromatogramDefinition")

icaChrom.Delta_m_over_z = 1.003
icaChrom.ToleranceDelta_m_over_z = 0.1
icaChrom.IntensityRatio = 3.5
icaChrom.ToleranceIntensityRatio = 0.1
icaChrom.Polarity = daPOSITIVE

' load and display the isotope cluster analysis chromatogram
analysis.chromatograms.addChromatogram icaChrom
```


2.10 Chromatograms Object

The **Chromatograms** object represents all chromatograms defined for an analysis. The **Chromatograms** object is a collection of one or more **Chromatogram** objects.

The **Chromatograms** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

Add FindsCompounds

AddChromatogram IntegrateOnly

AddChromatograms Item

BaselineSubtract Smooth

Clear

The **Chromatograms** object is a collection object that contains all **Chromatogram** objects. To find a particular object, iterate through the collection by using the **Chromatograms** object of the **Analysis** object. Consider the following code snippet from an AutomationEngine Script:

Example

```
Dim DataAnalysis, myAnalysis, Chrom
Set DataAnalysis = GetObject("",
"BDal.DataAnalysis.Application")
Set myAnalysis = DataAnalysis.Analyses.Open "C:\Data
Files\Demo\Sample.d\Analysis.yep"
For Each Chrom in myAnalysis.Chromatograms
    ' Access Chrom here.
    ' For example:
    Chrom.IntegrateOnly
Next
```

See Also

Chromatogram object

2.11 Compound Object

The **Compound** object represents a compound of an analysis. The **Compound** object is a collection of one or more **Spectrum** objects.

The **Compound** object has the following objects, properties and methods:

Objects

LibrarySearchResult Variables

Properties

Area	Name
BaselineEndIntensity	PeakEndIntensity
BaselineStartIntensity	PeakStartIntensity
Chromatogram	RetentionTime
Count	RetentionTimeEnd
HasLibrarySearchResults	RetentionTimeStart
Height	SeparationType
Intensity(n)	SignalToNoise
Molweight	Width
MSFilter	

Methods

Deconvolute	Export
Deselect	Item
Enable	Select

All defined compounds belong to the **Compounds** collection represented by the **Compounds** object. You can find a particular compound by iterating through this collection.

Example

In the following sample `compd` is the first compound and `ms2` is the second spectrum of this compound:

```
dim compd, ms2
set compd = Analysis.Compounds(1)
set ms2 = compd(2)
```

The following sample code exports every second spectrum of all compounds in BSC format:

```
For i = 1 to Analysis.Compounds.Count
    Analysis.Compounds(i)(2).Export CStr(i), daBSC
Next
```

See Also

Compounds object

2.12 Compounds Object

The **Compounds** object represents all compounds of a chromatogram analysis. The **Compounds** object is a collection of one or more **Compound** objects.

The **Compounds** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

Clear	Identify
Deconvolute	Item
DeleteCompound	MassListClear
Export	MassListFind

The **Compounds** object is a collection object that contains all **Compound** objects. To find a particular object, iterate through the collection by using the **Compounds** object of the **Analysis** object. Consider the following code snippet from a DataAnalysis Script:

Example

```
Dim Cmpd
For Each Cmpd in Analysis.Compounds
    ' Access Cmpd here.
    ' For example:
    Cmpd.Deconvolute
Next
```

See Also**Compound** object

2.13 Form Object

The **Form** object represents the VBScripting form in the AutomationEngine and in DataAnalysis.

The **Form** object has the following objects, properties and methods:

Objects**Properties****Methods**

Caption	Maximize
Close	Minimize
DoEvents	Restore
Enable	Show
Hide	ShowMenu
HideMenu	

2.14 LibrarySearchResult Object

The **LibrarySearchResult** object contains the library search result of a compound or mass spectrum for a chromatogram analysis resp. a spectrum analysis.

The **LibrarySearchResult** object has the following objects, properties and methods:

Objects**Properties**

CASRegistryNumber	HasIdentifiedPositivePolarity
CompoundComment	LibraryNames
CompoundName	MolWeight
Fit	Purity

Properties

FitPurity	RetentionTime
Formula	RFit
HasIdentifiedMS	SpectrumComment
HasIdentifiedMSMS	SpectrumInfo
HasIdentifiedNegativePolarity	

Methods**See Also**

LibrarySearchResults object

2.15 LibrarySearchResults Object

The **LibrarySearchResults** object represents all library search results of a compound or spectrum from a chromatogram analysis resp. a spectrum analysis. The **LibrarySearchResults** object is a collection of one or more **LibrarySearchResult** objects.

The **LibrarySearchResults** object has the following objects, properties and methods:

Objects**Properties**

Count

Methods

Item

The **LibrarySearchResults** object is a collection object that contains all **LibrarySearchResult** objects. To find a particular object, iterate through the collection by using the **LibrarySearchResults** object of a **Compound**, resp. **Spectrum** object.

Example

The following example displays a message box with the library search result for the first compound:

```
dim Results
set Results = Analysis.Compounds(1).LibrarySearchResults
```

```
dim i
dim output
for i = 1 to Results.Count
    output = output + vbLf + " " + Results(i).CompoundName +
    ", Purity = " + CStr(Results(i).Purity)
next

if Results.Count > 0 then
    MsgBox "Compound 1 has been identified as:" + output
else
    MsgBox "Compound 1 has not been identified."
end if
```

See Also

LibrarySearchResult object

2.16 MSFilter Object

The **MSFilter** object defines mass spectrum specific information of a **Chromatogram-Definition** object.

The **MSFilter** object has the following objects, properties and methods:

Objects

Properties

FragmentationMode	Type
FragmentationPath	

Methods

Example

The following example creates a total ion chromatogram of the intensity of all MS³ fragment spectra of precursors *m/z* 490.8 followed by *m/z* 300.5.

```
Dim TIC
Set TIC =
CreateObject("DataAnalysis.TICChromatogramDefinition")
```

```
TIC.MSFilter.Type = daMSFilterMSMS
TIC.MSFilter.FragmentationPath = "490.8/300.5"
```

```
Analysis.Chromatograms.AddChromatogram TIC
```

The following example creates an extracted ion chromatogram of the intensity all ETD fragment spectra:

```
Dim EIC
Set EIC = CreateObject("DataAnalysis.EICChromatogramDefinition")
```

```
EIC.MSFilter.Type = daMSFilterAllMSMS
EIC.MSFilter.FragmentationMode = daETD
```

```
Analysis.Chromatograms.AddChromatogram EIC
```

See Also

ChromatogramDefinition objects

2.17 MSPeak Object

The **MSPeak** object represents a peak of a mass spectrum.

Note: The GUI elements to which the **MSPeak** object corresponds are named as 'Mass List' and 'MassList menu'.

The **MSPeak** object has the following objects, properties and methods:

Objects

Properties

Algorithm	PeakEnd
Area	PeakEndIntensity
ChargeState	PeakStart
DeconvolutedMolweight	PeakStartIntensity
DeconvolutionComponent	RawValue
Intensity	SignalToNoise
m_over_z	Width

Methods

See Also

MSPeakList object

2.18 MSPeakList Object

The **MSPeakList** object represents all peaks of a mass spectrum. The **MSPeakList** object is a collection of one or more **MSPeak** objects.

Note: The GUI elements to which the **MSPeakList** object corresponds are named as 'Mass List', and 'MassList menu'.

The **MSPeakList** object has the following objects, properties and methods:

Objects

Properties

Count

IndexOfNMostIntensePeaks

Methods

DeletePeak

The **MSPeakList** object is a collection object that contains all **MSPeak** objects. To find a particular object, iterate through the collection by using the **MSPeakList** object of the **Spectrum** object. Consider the following code snippet from a DataAnalysis Script:

Example

```
Dim Peak
For Each Peak in Spectrum.MSPeakList
    ' Access Peak here.
    ' For example:
    MsgBox Peak.m_over_z
Next
```

See Also

MSPeak object

Spectrum object

2.19 Properties Object

The **Properties** object represents an open analysis.

The **Properties** object has the following objects, properties and methods:

Objects

Properties

Comment	InstrumentSerialNumber
DateCreated	SampleInfo
InstrumentName	

Methods

Example

The following example displays a message box with analysis properties:

```
Dim Properties
Dim CR
CR = chr(13)
Properties = "Analysis name: " + Analysis.Name + CR
Properties = Properties + " Comment: " +
Analysis.Properties.Comment + CR
Properties = Properties + " Date created: " +
Analysis.Properties.DateCreated + CR
Properties = Properties + " Instrument name: " +
Analysis.Properties.InstrumentName + CR
Properties = Properties + " Sample info: " +
Analysis.Properties.SampleInfo + CR
MsgBox Properties
```

2.20 SmartFormulaParameters Object

The **SmartFormulaParameters** object defines all parameters used for generating sum formulae from a specified region of a mass spectrum.

The **SmartFormulaParameters** object has the following objects, properties and methods:

Objects

Properties

ApplyNitrogenRule	HCRatioMaximum
AutoSearchMonoIsotopicPeak	HCRatioMinimum
Charge	LowerBoundaryFormula
DoubleBondEquivalenceMaximum	NumberOfFormula
DoubleBondEquivalenceMinimum	SearchMass
ElectronConfiguration	SearchRange
EstimateCarbonNumber	Tolerance
Evaluate	HCRatioMinimum

Methods

Example

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.Charge      =      +1
SFP.DoubleBondEquivalenceMinimum  =      3
SFP.DoubleBondEquivalenceMaximum  =      8
SFP.LowerBoundaryFormula          =      "C5H5Fe0"
SFP.UpperBoundaryFormula          =      "C30H30Fe3"
SFP.NumberOfFormula               =      50
SFP.Tolerance                     =      0.001
SFP.SearchMass                    =      186
SFP.SearchRange                   =      0.5
```

See Also

SmartFormulaAndExport method

2.21 SmartFormulaResult Object

The **SmartFormulaResult** object represents a single SmartFormula result of a mass spectrum. The **SmartFormulaResult** object is a collection of one or more **SmartFormulaResultItem** objects.

The **SmartFormulaResult** object has the following objects, properties and methods:

Objects

SmartFormulaResultItem

Properties

Intensity Parameters

m_over_z

Methods

DeleteResultItem

The **SmartFormulaResult** object is a collection object that contains all **SmartFormulaResultItem** objects. To find a particular object, iterate through the collection by using the **SmartFormulaResult** object of the **SmartFormulaResults** object.

Example

```
Dim SmartFormulaResults
Set SmartFormulaResults =
    Analysis.spectra(1).SmartFormulaResults

Dim SmartFormulaResult
Dim SmartFormulaResultItem

For each SmartFormulaResult in SmartFormulaResults
    For each SmartFormulaResultItem in SmartFormulaResult

        MsgBox SmartFormulaResultItem.SumFormula

    Next
Next
```

See Also

SmartFormulaResults object

SmartFormulaResultItem object

2.22 SmartFormulaResultItem Object

The **SmartFormulaResultItem** object represents a single item of a SmartFormula result.

The **SmartFormulaResultItem** object has the following objects, properties and methods:

Objects

Properties

CombinedDeviation	Sigma
CombinedDeviationRank	SigmaRank
ElectronConfiguration	StdDevIntensity
Error	StdDevIntensityRank
m_over_z	StdDevIntensityVarNorm
MeanError	StdDevIntensityVarNormRank
NitrogenRule	StdDevMassDiffs
Probability	StdDevMassDiffsRank
RingsAndDoubleBonds	StdDevMeanMass
Score	StdDevMeanMassRank
ScoreRank	SumFormula

Methods

FormulaPattern	MeasuredPattern
----------------	-----------------

See Also

SmartFormulaResults object

SmartFormulaResult object

2.23 SmartFormulaResults Object

The **SmartFormulaResults** object represents all SmartFormula results of a mass spectrum. The **SmartFormulaResults** object is a collection of one or more **SmartFormulaResult** objects.

The **SmartFormulaResults** object has the following objects, properties and methods:

Objects

SmartFormulaResult

Properties

Methods

DeleteResult

The **SmartFormulaResults** object is a collection object that contains all **SmartFormulaResult** objects. To find a particular object, iterate through the collection by using the **SmartFormulaResults** object of the **Spectrum** object.

See Also

SmartFormulaResult object

SmartFormulaResultItem object

Spectrum object

2.24 Spectra Object

The **Spectra** object represents all spectra in a spectrum analysis. The **Spectra** object is a collection of one or more Spectrum objects.

The **Spectra** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

BaselineSubtract	MassListClear
Deconvolute	MassListFind
Export	SmartFormulaAndExport
Identify	Smooth
Item	

The **Spectra** object is a collection object that contains all **Spectrum** objects. To find a particular object, iterate through the collection by using the **Spectra** object of the **Analysis** object.

See Also

Spectrum object

2.25 Spectrum Object

The **Spectrum** object represents a mass spectrum of a spectrum analysis or a compound of a chromatogram analysis.

The **Spectrum** object has the following objects, properties and methods:

Objects

Annotations	MSPeakList
ChildSpectra	SmartFormulaResults
LibrarySearchResults	Variables

Properties

Annotations	MaximumIntensity
BackgroundType	MinimumIntensity
CollisionEnergy	MSFilter
FirstMass	MSPeakList
HasLibrarySearchResults	Name
Intensity(n)	Polarity
LastMass	ScanMode
Mass	Size

Methods

AddRangeSelection	MassListFind
ClearRangeSelection	Noise
Deconvolute	Recalibrate
Deselct	RecalibrateInternal
Enable	Select
Export	SmartFormulaAndExport
ExportMassList	Smooth
Identify	SpectrumData
MassListClear	

For a spectrum analysis all defined spectra belong to the **Spectra** collection represented by the **Spectra** object. For a chromatogram analysis all defined spectra belong to the **Compound** collection represented by the **Compound** object; the **Compound** object is in turn a collection of the **Compounds** object. You can find a particular spectrum by iterating through this collection.

See Also

Spectra object

Compound object

2.26 SumFormula Object

The **SumFormula** object represents a sum formula of a chemical compound.

The **SumFormula** object has the following objects, properties and methods:

Objects**Properties**

AverageMass	MonoisotopicMass
ElementalCounts	NominalMass
Formula	

Methods

Add	Pattern
-----	---------

ElementalComposition Subtract

Example

The following example calculates and displays the average mass of the singly charged ion of Ethanol (C₂H₅OH) and also displays the hill-sorted sum formula of Ethanol:

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C2H5OH"
MsgBox SF.AverageMass(+1)
MsgBox SF.Formula
```

2.27 Variable Object

The **Variable** object represents a variable item of the **Variables** object.

The **Variable** object has the following objects, properties and methods:

Objects

Properties

Group	Unit
Name	Value

Methods

Example

The following example displays the accumulation time of the first spectrum of compound 1 for an esquire analysis:

```
dim i, var, Variables
set Variables = Analysis.Compounds(1)(1).Variables

for i = 1 to Variables.Count
    set var = Variables(i)
    if var.Group = "Trap" and var.Name = "Accumulation Time"
then
    MsgBox "The accumulation time is "+var.Value+"
"+var.Unit
```



```
        exit for
    end if
next
```

See Also

Variables object

2.28 Variables Object

The **Variables** object is a collection class of **Variable** items and represents variables of a **Spectrum** object.

The **Variables** object has the following objects, properties and methods:

Objects

Properties

Count

Methods

Item

Example

The following example displays the number of variables of the first spectrum of compound 1:

```
dim Cmpd, nVars
set Cmpd = Analysis.Compounds(1)
nVars = Cmpd(1).Variables.Count
msgbox "The first spectrum of compound """+Cmpd.Name+""""
contains "+CStr(nVars)+" variables."
```

See Also

Spectrum object

Variable object

3 AUTOMATION PROPERTIES

Properties are characteristics of objects. For example, analysis objects have **Name** and **Path** properties. These properties correspond to the name and path of an analysis. For examples of using properties, see the macro samples provided with DataAnalysis.

The following properties are available:

<u>Property</u>	<u>Description</u>
Active	Gets or sets whether DataAnalysis is active.
ActiveAnalysis	Gets the Application object representing the active analysis.
Algorithm	Gets the algorithm which was used for finding the peak of an MSPeak object.
Annotations	Gets the annotations list of a Spectrum object.
ApplyNitrogenRule	Gets or sets the state of applying nitrogen rule of a SmartFormulaParameters object.
Area	Gets the area of the peak of a Compound or MSPeak object.
AutoSearchMonoisotopicPeak	Gets or sets the “auto-search mono-isotopic peak” option of a SmartFormulaParameters object.
AverageMass	Gets the average mass of the SumFormula object.
BackgroundType	Gets or sets the background subtraction type of an MS type ChromatogramDefinition object or Spectrum object.
BaselineEndIntensity	Gets the intensity of the baseline at the end of a Compound object.
BaselineStartIntensity	Gets the intensity of the baseline at the start of a Compound object.
CASRegistraNumber	Gets the Chemical Abstracts Registry Number of a LibrarySearchResult object.
Charge	Gets or sets the charge of a SmartFormulaParameters object.
ChargeState	Gets the charge state of an MSPeak object.

<u>Property</u>	<u>Description</u>
Chromatogram	Gets the chromatogram from which the chromatographic peak of the Compound object was derived.
CollisionEnergy	Gets the collision energy of a Spectrum object.
Color	Gets or sets the color of a Chromatogram or ChromatogramDefinition object.
CombinedDeviation	Gets the Combined Deviation value of a SmartFormulaResultItem object.
CombinedDeviationRank	Gets the rank according to sorting for Combined Deviation value of a SmartFormulaResultItem object.
Comment	Gets the comment of an analysis for a Properties object.
CompoundComment	Gets the compound comment text of a LibrarySearchResult object.
CompoundName	Gets the compound name of a LibrarySearch-Result object.
Count	Gets the number of items in a collection.
DateCreated	Gets the Date an analysis was created for a Properties object.
DeconvolutedMolweight	Gets the deconvoluted molweight of an MSPeak object.
DeconvolutionComponent	Gets the deconvolution component related to an MSPeak object.
Definition	Gets a ChromatogramDefinition object.
Delta_m_over_z	Gets or sets the $\Delta m/z$ value of an ICACHromatogramDefinition object.
DoubleBondEquivalenceMaximum	Gets or sets the double bond equivalence maximum of a SmartFormulaParameters object.
DoubleBondEquivalenceMinimum	Gets or sets the double bond equivalence minimum of a SmartFormulaParameters object.
ElectronConfiguration	Gets or sets the electron configuration of a SmartFormulaParameters object. Gets the electron configuration of a SmartFormula-ResultItem object.

<u>Property</u>	<u>Description</u>
ElementalCounts	Gets the total number of different elements of a sum formula. It also retrieves the number of occurrences of each element from the formula of a SumFormula object.
Error	Gets the error of measured and theoretical m/z value of a SmartFormulaResultItem object.
EstimateCarbonNumber	Gets or sets whether a SmartFormulaParameters object should estimate the number of carbons.
Evaluate	Gets or sets whether a SmartFormulaParameters object should calculate sigma fit and statistical properties.
ExtractionMode	- not documented yet -
Filename	Gets or sets the filename of a ChromatogramDefinition object.
FirstMass	Gets the first mass of a Spectrum object.
FirstRetentionTime	Gets the first retention time value of a Chromatogram object in seconds.
Fit	Gets the effective Fit score of a LibrarySearchResult object.
FitPurity	Gets the effective Fit/Purity score of a LibrarySearchResult object.
Formula	Gets or sets the chemical formula of a SumFormula object. Gets the chemical formula of a LibrarySearchResult object.
FragmentationMode	Gets or sets the fragmentation mode of an MSFilter object.
FragmentationPath	Gets or sets the fragmentation path of a ChromatogramDefinition object.
FullName	Gets the full path of an Analysis or Application object.
Group	Gets the group string value of a Variable object.
GroupName	Gets or sets the group name of a ChromatogramDefinition object.

<u>Property</u>	<u>Description</u>
HasIdentifiedMS	Gets the condition of a LibrarySearchResult object if the compound has been identified by its precursor spectra.
HasIdentifiedMSMS	Gets the condition of a LibrarySearchResult object if the compound has been identified by its fragment spectra.
HasIdentifiedNegativePolarity	Gets the condition of a LibrarySearchResult object if the compound has been identified by negative polarity spectra.
HasIdentifiedPositivePolarity	Gets the condition of a LibrarySearchResult object if the compound has been identified by positive polarity spectra.
HasLibrarySearchResults	Gets the condition of a Compound or Spectrum object if has been identified.
HCRatioMaximum	Gets or sets the maximum H/C ratio of a SmartFormulaParameters object.
HCRatioMinimum	Gets or sets the minimum H/C ratio of a SmartFormulaParameters object.
Height	Gets the height of a Compound object.
InstrumentName	Gets the name of the instrument the analysis was acquired on (Properties object).
InstrumentSerialNumber	Gets the serial number of the instrument the analysis was acquired on (Properties object).
Intensity	Gets the intensity value of an MSPeak or SmartFormulaResult object.
Intensity(n)	Gets the intensity value at defined index of a Chromatogram , Compound or Spectrum object.
IntensityRatio	Gets or sets the intensity ratio of an ICAChromatogramDefinition object.
IsChromatographicAnalysis	Gets the condition of an Analysis object if the analysis is a chromatogram analysis.
IsLockMassCalibrationActive	Gets whether lock mass calibration is active or not for an Analysis object.
LastMass	Gets the last mass of a Spectrum object.

<u>Property</u>	<u>Description</u>
LastRetentionTime	Gets the last retention time value of a Chromatogram object in seconds.
LibraryNames	Gets the names of the mass-spectral library of a LibrarySearchResult object.
Logging	Turns on/off logging of all incoming automation calls.
LowerBoundaryFormula	Gets or sets the lower boundary formula of sum formulae to be generated of a SmartFormulaParameters object.
m_over_z	Gets the m/z value of an MSPeak , SmartFormulaResult or SmartFormulaResultItem object.
Mass	Gets the m/z value at defined index of a Spectrum object.
MaximumIntensity	Gets the maximum intensity of a Chromatogram or Spectrum object.
MeanError	Gets the mean m/z error of the complete isotopic pattern of a SmartFormulaResultItem object.
MinimumIntensity	Gets the minimum intensity of a Chromatogram or Spectrum object.
MolWeight	Gets the deconvoluted m/z value of the precursor that was used for creating the compound of a Compound object (AutoMSn algorithm). Gets the molecular weight of a LibrarySearchResult object.
MonoisotopicMass	Gets the nominal m/z value of the SumFormula object at a specific charge state.
MSFilter	Gets the MS/MS Info of the spectrum/spectra related to a Compound or Spectrum object.
MSPeakList	Gets the Mass List (MS peak list) of a Spectrum object.
Name	Gets the name of an Analysis , Application , Chromatogram , ChromatogramDefinition , Compound , Spectrum or Variable object.
NitrogenRule	Gets whether the nitrogen rule of a SmartFormulaResultItem object is fulfilled.
NominalMass	Gets the nominal m/z value of the SumFormula object at a specific charge state.

<u>Property</u>	<u>Description</u>
NumberOfFormula	Gets or sets the maximum number of formulae to be generated of a SmartFormulaParameters object.
Parameters	Gets the parameters used for generating molecular formulae for that particular observed MS peak of a SmartFormulaResult object.
Path	Gets the path to an object. This path never ends with a backslash, unless the path has the format "C:\."
PeakEnd	Gets the m/z value at the end of an MSPeak object.
PeakEndIntensity	Gets the intensity at the end of a Compound or MSPeak object.
PeakStart	Gets the m/z value at the start of an MSPeak object.
PeakStartIntensity	Gets the intensity at the start of a Compound or MSPeak object.
Polarity	Gets or sets the polarity of an MS type ChromatogramDefinition object or Spectrum object.
Probability	Gets the probability for that item of a SmartFormulaResultItem object.
Purity	Gets the effective Purity score of a LibrarySearchResult object.
Range	Gets or sets the range of a ChromatogramDefinition object.
RawValue	Gets the raw value of an MSPeak object.
RawValues	- not documented yet -
RetentionTime	Gets the retention time value at defined index of a Chromatogram object. Gets the retention time of a Compound object. Gets the retention time of a LibrarySearchResult object.
RetentionTimeEnd	Gets the retention time at which the Compound object ends.
RetentionTimeOffset	- not documented yet -
RetentionTimeStart	Gets the retention time at which the Compound object starts.

<u>Property</u>	<u>Description</u>
RFit	Gets the effective RFit score of a LibrarySearchResult object.
RingsAndDoubleBonds	Gets the number of rings and double bonds of a SmartFormulaResultItem object.
SampleInfo	Gets the sample info of the analysis (Properties object).
ScanMode	Gets or sets the scan mode of an MS type ChromatogramDefinition object or Spectrum object.
ScriptVariable	Gets and sets a string value to a variable of an Analysis object.
Score	Gets the Score value of a SmartFormulaResultItem object.
ScoreRank	Gets the rank according to sorting for Score value of a SmartFormulaResultItem object.
SearchMass	Gets or sets the search mass of a SmartFormulaParameters object to be looked for in a mass spectrum.
SearchRange	Gets or sets the range of a SmartFormulaParameters object within the search mass should be searched in a mass spectrum.
SeparationType	Gets the type of separation of a Compound object.
SequenceNumbers	Gets the sequence numbers which contributed to a Spectrum object.
ShowLine	Gets or sets the state of visibility of an Annotation object.
Sigma	Gets the Sigma value of a SmartFormula-ResultItem object.
SigmaRank	Gets the rank according to sorting for Sigma value of a SmartFormulaResultItem object.
Signal	Gets the signal of an UVChromatogramDefinition object or LCChromatogramDefinition object.
SignalToNoise	Gets the signal to noise ratio of a Compound or MSPeak object.

<u>Property</u>	<u>Description</u>
Size	Gets the number of data points of a Spectrum object.
SpectrumComment	Gets the spectrum comment text of a Library-SearchResult object.
SpectrumInfo	Gets the spectrum information text of a Library-SearchResult object.
StdDevIntensity	Gets the StdIntensity value of a SmartFormula-ResultItem object.
StdDevIntensityRank	Gets the rank according to sorting for StdIntensity value of a SmartFormulaResultItem object.
StdDevIntensityVarNorm	Gets the StdIntensityVarNorm value of a SmartFormulaResultItem object.
StdDevIntensityVarNormRank	Gets the rank according to sorting for StdIntensityVarNorm value of a SmartFormulaResultItem object.
StdDevMassDiffs	Gets the StdDevMassDiffs value of a SmartFormulaResultItem object.
StdDevMassDiffsRank	Gets the rank according to sorting for StdDevMassDiffs value of a SmartFormulaResultItem object.
StdDevMeanMass	Gets the StdDevMeanMass value of a SmartFormulaResultItem object.
StdDevMeanMassRank	Gets the rank according to sorting for StdDevMeanMass value of a SmartFormulaResultItem object.
SumFormula	Gets the sum formula of a SmartFormula-ResultItem object.
SumIntensity	Gets the sum of all intensity values of a Spectrum object.
Text	Gets the text of an Annotation object.
Tolerance	Gets or sets the tolerance of a SmartFormulaParameters object.
ToleranceDelta_m_over_z	Gets or sets the tolerance of the Δ m/z value of an ICChromatogramDefinition object.
ToleranceIntensityRatio	Gets or sets the tolerance of the intensity ratio of an ICChromatogramDefinition object.

<u>Property</u>	<u>Description</u>
Type	Gets the type of a ChromatogramDefinition object.
Unit	Gets the unit string value of a Variable object.
UpperBoundaryFormula	Gets or sets the upper boundary formula of sum formulae to be generated of a SmartFormulaParameters object.
Value	Gets the string value of a Variable object.
VariableName	Gets or sets the variable name of a ChromatogramDefinition object.
Version	Gets the version of DataAnalysis.
Visible	Gets the condition of an Application object if the application is visible.
Width	Gets the full-width at half-maximum (FWHM) of the peak of a Compound object or the peak width of an MSPeak object.
WidthLeft	Gets or sets the tolerance to the left of a ChromatogramDefinition object.
WidthRight	Gets or sets the tolerance to the right of a ChromatogramDefinition object.
X1	Gets the left x-value of the position of an Annotation object.
X2	Gets the right x-value of the position of an Annotation object.
Y1	Gets the left lower y-value of the position of an Annotation object.
Y2	Gets the right lower y-value of the position of an Annotation object.
YText	Gets the upper y-value of the position of an Annotation object.

3.1 Active Property

Applies to: **Application** object

Gets or sets whether DataAnalysis is active.

Syntax

object.Active = *boolean*

boolean = *object.Active*

Parameters

object An expression that evaluates to an **Application** object. When you access the **Active** property of the **Application** object, you can omit *object* because the name of the **Application** object is implied when you access its properties and methods.

boolean A **Boolean** value that gets or sets the state of the object. Possible values are:

True The object is active resp. activates the object.

False The object is inactive resp. deactivates the object.

Return Values

The **Active** property returns one of the following values:

- **True** The object is active.
- **False** The object is not active.

Remarks

The **Active** property has the **Boolean** type.

Example

```
set Application = GetObject("", "BDal.DataAnalysis.Application")
Application.Active = FALSE
```

3.2 ActiveAnalysis Property

Applies to: **Application** object

Retrieves the active analysis from an **Application** collection.

Syntax

object.ActiveAnalysis

Parameters

object An expression that evaluates to an **Application** object.

Example

The following *AutomationEngine* example displays the analysis name of the active analysis in *DataAnalysis*:

```
Dim DA
' open or connect to DataAnalysis
set DA = GetObject("", "BDal.DataAnalysis.Application")
' display the analysis name of the active analysis
MsgBox DA.ActiveAnalysis.Name
```

3.3 Algorithm Property

Applies to: **MSPeak** object

Gets the algorithm which was used for finding the peak of an **MSPeak** object.

Syntax

object.**Algorithm**

Parameters

object An expression that evaluates to an **MSPeak** object.

3.4 Annotations Property

Applies to: **Spectrum** object

Gets the annotations list of a **Spectrum** object.

Syntax

object.**Annotations**

Parameters

object An expression that evaluates to an **Spectrum** object.

3.5 ApplyNitrogenRule Property

Applies to: **SmartFormulaParameters** object

Gets or sets the state of applying nitrogen rule of a **SmartFormulaParameters** object.

Syntax

object.ApplyNitrogenRule = *boolean*

boolean = *object.ApplyNitrogenRule*

Parameters

object An expression that evaluates to an **SmartFormulaParameters** object.

boolean A **Boolean** value that gets or sets whether the nitrogen rule should be applied. Possible values are:

True Applies the rule.

False Deactivates the rule.

3.6 Area Property

Applies to: **Compound** object, **MSPeak** object

Gets the area of the chromatographic peak of a **Compound** object or the mass peak of an **MSPeak** object.

Syntax

object.Area

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.7 AutoSearchMonoIsotopicPeak Property

Applies to: **SmartFormulaParameters** object

Gets or sets the “auto-search mono-isotopic peak” option of a **SmartFormulaParameters** object.

Syntax

object.AutoSearchMonoIsotopicPeak = *boolean*

boolean = *object*.**AutoSearchMonoIsotopicPeak**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

boolean A **Boolean** value that gets or sets whether the “auto-search mono-isotopic peak” should be applied. Possible values are:

True Applies the option.

False Deactivates the option.

Example

The following example sets/gets the auto-search mono-isotopic peak option of a **SmartFormulaParameters** object and displays it in a message box.

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.AutoSearchMonoIsotopicPeak = true
MsgBox SFP.AutoSearchMonoIsotopicPeak
```

3.8 AverageMass Property

Applies to: **SumFormula** object

Gets the average mass of a **SumFormula** object.

Syntax

mass = *object*.**AverageMass**(*charge*)

Parameters

object An expression that evaluates to a **SumFormula** object.

charge Charge state for which the m/z value should be calculated.

Example

The following example calculates and displays the average mass of Ethanol (C₂H₅OH):

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")
SF.Formula = "C2H5OH"
MsgBox SF.AverageMass(0)
```

3.9 BackgroundType Property

Applies to: MS type **ChromatogramDefinition** objects (**TICChromatogramDefinition** object, **BPCChromatogramDefinition** object, **EICChromatogramDefinition** object), **Spectrum** object

Gets or sets the background subtraction type of an MS type **ChromatogramDefinition** or **Spectrum** object.

Syntax

object.**BackgroundType** = *BackgroundType*

BackgroundType = *object*.**BackgroundType**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

<i>BackgroundType</i> = <i>daBgrdTypeNone</i>	no background subtraction
<i>daBgrdTypeConstant</i>	background subtraction of a constant, previously defined Background Mass Spectrum
<i>daBgrdTypeSpectral</i>	two dimensional, spectral background subtraction

Example

The following example sets the background type of **TICChromatogramDefinition**:

```
TIC.BackgroundType = daBgrdTypeSpectral
```

3.10 BaselineEndIntensity Property

Applies to: **Compound** object

Gets the intensity of the baseline at the end of a **Compound** object.

Syntax

object.**BaselineEndIntensity**

Parameters

object An expression that evaluates to a **Compound** object.

3.11 BaselineStartIntensity Property

Applies to: **Compound** object

Gets the intensity of the baseline at the start of a **Compound** object.

Syntax

object.**BaselineStartIntensity**

Parameters

object An expression that evaluates to a **Compound** object.

3.12 CASRegistryNumber Property

Applies to: **LibrarySearchResult** object

Gets the Chemical Abstracts Registry Number of a **LibrarySearchResult** object.

Syntax

object.**CASRegistryNumber**

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.13 Charge Property

Applies to: **SmartFormulaParameters** object

Gets or sets the charge of a **SmartFormulaParameters** object.

Syntax

object.**Charge** = *charge*

charge = *object*.**Charge**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

charge An integer that gets or sets the charge state.

Example

The following example sets/gets the charge of a **SmartFormulaParameters** object and displays it in a message box.

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.Charge = -5
MsgBox SFP.Charge
```

3.14 ChargeState Property

Applies to: **MSPeak** object

Gets the charge state of an **MSPeak** object.

Syntax

object.ChargeState

Parameters

object An expression that evaluates to an **MSPeak** object.

3.15 Chromatogram Property

Applies to: **Compound** object

Gets the chromatogram from which the chromatographic peak of the **Compound** object was derived.

Syntax

object.Chromatogram

Parameters

object An expression that evaluates to a **Compound** object.

3.16 CollisionEnergy Property

Applies to: **Spectrum** object

Gets the collision energy of a **Spectrum** object.

Syntax

object.CollisionEnergy

Parameters

object An expression that evaluates to a **Spectrum** object.

3.17 Color Property

Applies to: **Chromatogram** object, **ChromatogramDefinition** objects

Gets or sets the color of a **ChromatogramDefinition** or **Chromatogram** object.

Syntax

object.Color = *color*

color = *object*.Color

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

<i>color</i>	=	<i>daBlack</i>	black
<i>color</i>		<i>daWhite</i>	white
		<i>daRed</i>	red
		<i>daBrightGreen</i>	bright green
		<i>daBlue</i>	blue
		<i>daYellow</i>	yellow
		<i>daPink</i>	pink
		<i>daTurquoise</i>	turquoise
		<i>daDarkRed</i>	dark red
		<i>daGreen</i>	green
		<i>daDarkBlue</i>	dark blue
		<i>daDarkYellow</i>	dark yellow
		<i>daViolet</i>	violet
		<i>daTeal</i>	teal
		<i>daGray25</i>	25% gray

<i>daGray50</i>	50% gray
<i>daSkyBlue</i>	sky blue
<i>daLightTurquoise</i>	light turquoise
<i>daLightGreen</i>	light green
<i>daLightYellow</i>	light yellow
<i>daPaleBlue</i>	pale blue
<i>daRose</i>	rose
<i>daLavender</i>	lavender
<i>daTan</i>	tan
<i>daLightBlue</i>	light blue
<i>daAqua</i>	aqua
<i>daLime</i>	lime
<i>daGold</i>	gold
<i>daLightOrange</i>	light orange
<i>daOrange</i>	orange
<i>daBlueGray</i>	blue gray
<i>daGray40</i>	40% gray
<i>daDarkTeal</i>	dark teal
<i>daSeaGreen</i>	sea green
<i>daDarkGreen</i>	dark green
<i>daOliveGreen</i>	olive green
<i>daBrown</i>	brown
<i>daPlum</i>	plum
<i>daIndigo</i>	indigo
<i>daGray80</i>	80% gray

Example

The following example sets the color of the first chromatogram to red:

```
Analysis.Chromatograms(1).Color = daRed
```

3.18 CombinedDeviation Property

Applies to: **SmartFormulaResultItem** object

Gets the Combined Deviation value of a **SmartFormulaResultItem** object.

Syntax

object.**CombinedDeviation**

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.19 CombinedDeviationRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for Combined Deviation value of a **SmartFormula-ResultItem** object.

Syntax

object.**CombinedDeviationRank**

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.20 Comment Property

Applies to: **Properties** object

Gets the analysis comment of a **Properties** object.

Syntax

object.**Comment**

Parameters

object An expression that evaluates to a **Properties** object.

Example

```
MsgBox Analysis.Properties.Comment
```

3.21 CompoundComment Property

Applies to: **LibrarySearchResult** object

Gets the compound comment text of a **LibrarySearchResult** object.

Syntax

object.**CompoundComment**

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.22 CompoundName Property

Applies to: **LibrarySearchResult** object

Gets the compound name of a **LibrarySearchResult** object.

Syntax

object.**CompoundName**

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.23 Count Property

Applies to: **Analyses** object, **ChildSpectra** object, **Chromatograms** object, **Compounds** object, **LibrarySearchResults** object, **MSPeakList** object, **Spectra** object, **Variables** object

Gets the number of items in a collection.

Syntax

object.**Count**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

The **Count** property has the **Long** type.

Use the **Count** property, for example, to get the number of analyses in the **Analyses** collection.

Example

The following example prints each analysis in the **Analyses** collection:

```
For i = 1 to Application.Analyses.Count
```

```
Application.Analyses.Item(i).Print("Chromatogram  
Report.layout")  
Next
```

3.24 DateCreated Property

Applies to: **Properties** object

Gets the date an analysis was created.

Syntax

object.DateCreated

Parameters

object An expression that evaluates to a **Properties** object.

Example

```
MsgBox Analysis.Properties.DateCreated
```

3.25 DeconvolutedMolweight Property

Applies to: **MSPeak** object

Gets the deconvoluted molweight of an **MSPeak** object.

Syntax

object.DeconvolutedMolweight

Parameters

object An expression that evaluates to an **MSPeak** object.

3.26 DeconvolutionComponent Property

Applies to: **MSPeak** object

Gets the deconvolution component related to an **MSPeak** object.

Syntax

object.DeconvolutionComponent

Parameters

object An expression that evaluates to an **MSPeak** object.

3.27 Definition Property

Applies to: **Chromatogram** object

Gets the definition of a **Chromatogram** object.

Syntax

object.Definition

Parameters

object An expression that evaluates to a **Chromatogram** object.

Example

The following example gets the definition and displays the name of each chromatogram:

```
Dim Definition
For each Chromatogram in Analysis.Chromatograms
    MsgBox Chromatogram.Definition.Name
    If Chromatogram.Definition.Type = daTICChromType Then
        MsgBox "This is a TIC"
    End If
next
```

3.28 Delta_m_over_z Property

Applies to: **ICChromatogramDefinition** object

Gets or sets the Δ m/z value of an **ICChromatogramDefinition** object.

Syntax

object.Delta_m_over_z = *mz*

mz = *object*.Delta_m_over_z

Parameters

object An expression that evaluates to an **ICChromatogramDefinition** object.

mz Delta m/z value.

3.29 DoubleBondEquivalenceMaximum Property

Applies to: **SmartFormulaParameters** object

Gets or sets the double bond equivalence maximum of a **SmartFormulaParameters** object.

Syntax

object.**DoubleBondEquivalenceMaximum** = *DoubleBondEquivalence*

DoubleBondEquivalence = *object*.**DoubleBondEquivalenceMaximum**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

DoubleBondEquivalence An integer that gets or sets the maximum of the double bound equivalence.

Example

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.DoubleBondEquivalenceMaximum = 13
MsgBox SFP.DoubleBondEquivalenceMaximum
```

3.30 DoubleBondEquivalenceMinimum Property

Applies to: **SmartFormulaParameters** object

Gets or sets the double bond equivalence minimum of a **SmartFormulaParameters** object.

Syntax

object.**DoubleBondEquivalenceMinimum** = *DoubleBondEquivalence*

DoubleBondEquivalence = *object*.**DoubleBondEquivalenceMinimum**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

DoubleBondEquivalence An integer that gets or sets the minimum of the double bound equivalence.

Example

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.DoubleBondEquivalenceMinimum = 4
MsgBox SFP.DoubleBondEquivalenceMinimum
```

3.31 ElectronConfiguration Property

Applies to: **SmartFormulaParameters** object, **SmartFormulaResultItem** object

Gets or sets the electron configuration of a **SmartFormulaParameters** object.

Gets the electron configuration of a **SmartFormulaResultItem** object.

Syntax

object.**ElectronConfiguration** = *ElectronConfiguration*

ElectronConfiguration = *object*.**ElectronConfiguration**

Parameters

<i>object</i>	An expression that evaluates to one of the objects in the Applies To list above.
<i>ElectronConfiguration</i>	= <i>daEven</i> even number of electrons
	<i>daOdd</i> odd number of electrons
	<i>daEvenOdd</i> either even or odd number of electrons

3.32 ElementalCounts Property

Applies to: **SumFormula** object

Gets the total number of different elements of a sum formula. It also retrieves the number of occurrences of each element from the formula of a **SumFormula** object.

Syntax

number of elements = *object*.**ElementalCounts** (**symbols, counts**)

Parameters

<i>object</i>	An expression that evaluates to a SumFormula object.
<i>symbols</i>	An array storing the symbols of each different element.
<i>counts</i>	An array storing the number of occurrences of each different element.

Example

The following example gets the number of different elements and retrieves the number of occurrences of each element.

Note: Arrays starting with index zero.

```
dim symbols()
dim counts()

dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C10H10Fe"
MsgBox SF.ElementalCounts symbols, counts

'how many different symbols are available
MsgBox UBound(symbols) + 1

for n = 0 to UBound(symbols)
    MsgBox symbols(n) & " " & counts(n)
next
```

3.33 Error Property

Applies to: **SmartFormulaResultItem** object

Gets the error of measured and theoretical m/z value of a **SmartFormulaResultItem** object.

Syntax

object.Error

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.34 EstimateCarbonNumber Property

Applies to: **SmartFormulaParameters** object

Gets or sets whether a **SmartFormulaParameters** object should estimate the number of carbons.

Syntax

object.**EstimateCarbonNumber** = *boolean*

boolean = *object*.**EstimateCarbonNumber**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

boolean A **Boolean** value that gets or sets whether the carbon number should be estimated. Possible values are:

True Carbon number will be estimated.

False Carbon number will not be estimated.

3.35 Evaluate Property

Applies to: **SmartFormulaParameters** object

Gets or sets whether a **SmartFormulaParameters** object should calculate sigma fit and statistical properties.

Syntax

object.**Evaluate** = *boolean*

boolean = *object*.**Evaluate**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

boolean A **Boolean** value that gets or sets whether sigma fit and statistical properties should be calculated. Possible values are:

True Sigma fit and statistical properties will be calculated.

False Sigma fit and statistical properties will not be calculated.

3.36 ExtractionMode Property

Not documented yet.

3.37 Filename Property

Applies to: **ImportedDataChromatogramDefinition** object, **UVChromatogramDefinition** object, **UV2DChromatogramDefinition** object

Gets or sets the filename of an UV data or imported external data file.

Syntax

object.**Filename** = *filename*

filename = *object*.**Filename**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above. For **UVChromatogramDefinition** or **UV2DChromatogramDefinition** object:

filename Filename of UV data file without path information. The UV data file must be located in the same folder as the mass spectral data file, e.g., "analysis.yep". For **ImportedDataChromatogramDefinition** object:

filename Relative filename of an external data file. The external data file <link to format description> may be located in any folder and is not limited to the analysis folder.

Remarks

The **Filename** property for UV and UV2D only applies for ChemStation data. HyStar UV data do not need a **Filename** property being defined.

Examples

The following example adds a chromatogram acquired by ChemStation to the **Chromatograms** collection:

```
dim UV
set UV = CreateObject("DataAnalysis.UVChromatogramDefinition")

' add the first of the UV traces stored by ChemStation
UV.Filename = "vwd1A.ch"

Analysis.Chromatograms.AddChromatogram UV
```

The following example adds an imported external data chromatogram to the **Chromatograms** collection from the parent folder of the analysis folder:

```
dim IC
set IC =
CreateObject("DataAnalysis.ImportedDataChromatogramDefinition")
IC.FileName = "..\Biological Activity.csv"
Analysis.Chromatograms.AddChromatogram IC
```

3.38 FirstMass Property

Applies to: **Spectrum** object

Gets the first mass of a **Spectrum** object.

Syntax

object.FirstMass

Parameters

object An expression that evaluates to a **Spectrum** object.

3.39 FirstRetentionTime Property

Applies to: **Chromatogram** object

Gets the first retention time value of a **Chromatogram** object in seconds.

Syntax

object.FirstRetentionTime

Parameters

object An expression that evaluates to a **Chromatogram** object.

Example

The following example displays the retention time range of the first chromatogram loaded:

```
set chrom = analysis.chromatograms(1)
msgbox "Retention time: " +
CStr(Int(chrom.FirstRetentionTime)) + " - " +
CStr(Int(chrom.LastRetentionTime))
```

See Also

LastRetentionTime property

3.40 Fit Property

Applies to: **LibrarySearchResult** object

Gets the effective Fit score of a **LibrarySearchResult** object.

Syntax

object.Fit

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.41 FitPurity Property

Applies to: **LibrarySearchResult** object

Gets the effective Fit/Purity score of a **LibrarySearchResult** object.

Syntax

object.FitPurity

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

Remarks

The **LibrarySearchResult** object must be part of a **Compound** object. If the **LibrarySearchResult** object of a **Spectrum** object is used this property is empty.

See Also

LibrarySearchResults object

3.42 Formula Property

Applies to: **LibrarySearchResult** object, **SumFormula** object

Gets the chemical formula of a **LibrarySearchResult** object.

Gets or sets the chemical formula of a **SumFormula** object.

Syntax

object.**Formula** = *formula*

formula = *object*.**Formula**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

formula A string that gets or sets the chemical formula.

Example

The following example displays the hill-sorted sum formula of Ethanol (C₂H₅OH):

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C2H5OH"
MsgBox SF.Formula
```

See Also

LibrarySearchResults object

3.43 FragmentationMode Property

Applies to: **MSFilter** object

Gets or sets the fragmentation mode of an **MSFilter** object.

Syntax

object.**FragmentationMode**

Parameters

object An expression that evaluates to an **MS Filter** object.

The following types are defined:

daAny any frgamnetation mode (default)

<i>daCID</i>	Collision Induced Dissociation (CID)
<i>daETD</i>	Electron Detachment Dissociation (ETD)
<i>daCIDETD</i>	CID and ETD
<i>daPTR</i>	Proton Transfer Reaction (PTR)

Example

The following example gets the fragmentation mode of a total ion chromatogram and displays it in a message box:

```
Dim Chrom
' get first chromatogram and check if it is a TIC chromatogram
Set Chrom = Analysis.Chromatograms(1)
If Chrom.Definition.Type = daTICChromType Then
    If Chrom.Definition.MSFilter.FragmentationMode = daAny Then
        MsgBox "This is a TIC of any fragmentation mode"
    Else
        MsgBox "This is a TIC of a specific fragmentation mode"
    End If
End If
```

3.44 FragmentationPath Property

Applies to: **MSFilter** object

Gets or sets the fragmentation path of an **MSFilter** object.

Syntax

object.**FragmentationPath** = *FragmentationPath*

FragmentationPath = *object*.**FragmentationPath**

Parameters

object An expression that evaluates to an **MSFilter** object.

FragmentationPath String of the fragmentation path.

Remarks

The **FragmentationPath** property has the **String** type.

Example

The following example gets the fragmentation path of a chromatogram definition object and displays it in a message box:

```
MsgBox TIC.MSFilter.FragmentationPath
```

3.45 FullName Property

Applies to: **Analysis** object, **Application** object

Gets the full path of an **Analysis** or **Application** object.

Syntax

object.FullName

Parameters

object An expression that evaluates to one of the objects in the Applies To list above. When you access the **FullName** property of the **Application** object, you can omit *object* because the name of the **Application** object is implied when you access its properties and methods.

Remarks

The **FullName** property has the **String** type.

The following table summarizes the results of using the **FullName** property with the objects in the Applies To list:

Object	Results
Application	Gets the full path to the DataAnalysis executable, for example: "C:\Program Files\DataAnalysis\DataAnalysis.exe"
Analysis	Gets the full path to the file containing the analysis, for example: "C:\Data Files\Demo\Sample.d\Analysis.yep"

Example

The following example displays the full path to each analysis in the **Analyses** collection:

```
set Application = GetObject("",  
"BDal.DataAnalysis.Application")  
dim myAnalyses  
set myAnalyses = Application.Analyses  
For i = 1 to myAnalyses.Count  
    MsgBox myAnalyses.Item(i).FullName  
Next
```

See Also

Name property

Path property

3.46 Group Property

Applies to: **Variable** object

Gets the group string value of a **Variable** object.

Syntax

object.Group

Parameters

object An expression that evaluates to a **Variable** object.

See Also

Variable object

Variables object

3.47 GroupName Property

Applies to: **VarChromatogramDefinition** object

Gets or sets the group name of a **VarChromatogramDefinition** object.

Syntax

object.GroupName = *GroupName*

GroupName = *object*.GroupName

Parameters

object An expression that evaluates to a **VarChromatogramDefinition** object.

GroupName Name of group to which an acquisition parameter belongs as shown in Edit Chromatograms dialog.

Example

The following example displays the variable name:

```
MsgBox Var.GroupName
```

See Also

VariableName property

3.48 HasIdentifiedMS Property

Applies to: **LibrarySearchResult** object

Gets the condition of a **LibrarySearchResult** object if the compound has been identified by its precursor spectra.

Syntax

object.HasIdentifiedMS

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.49 HasIdentifiedMSMS Property

Applies to: **LibrarySearchResult** object

Gets the condition of a **LibrarySearchResult** object if the compound has been identified by its fragment spectra.

Syntax

object.HasIdentifiedMSMS

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.50 HasIdentifiedNegativePolarity Property

Applies to: **LibrarySearchResult** object

Gets the condition of a **LibrarySearchResult** object if the compound has been identified by negative polarity spectra.

Syntax

object.HasIdentifiedNegativePolarity

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.51 HasIdentifiedPositivePolarity Property

Applies to: **LibrarySearchResult** object

Gets the condition of a **LibrarySearchResult** object if the compound has been identified by positive polarity spectra.

Syntax

object.HasIdentifiedPositivePolarity

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.52 HasLibrarySearchResults Property

Applies to: **Compound** object, **Spectrum** object

Gets the condition of a **Compound** or **Spectrum** object if has been identified.

Syntax

object.HasLibrarySearchResults

Parameters

object An expression that evaluates to a **Compound** or **Spectrum** object.

See Also

LibrarySearchResults object

3.53 HCRatioMaximum Property

Applies to: **SmartFormulaParameters** object

Gets or sets the maximum H/C ratio of a **SmartFormulaParameters** object.

Syntax

object.HCRatioMaximum

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

3.54 HCRatioMinimum Property

Applies to: **SmartFormulaParameters** object

Gets or sets the minimum H/C ratio of a **SmartFormulaParameters** object.

Syntax

object.HCRatioMinimum

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

3.55 Height Property

Applies to: **Compound** object

Gets the height of a **Compound** object.

Syntax

object.Height

Parameters

object An expression that evaluates to a **Compound** object.

3.56 InstrumentName Property

Applies to: **Properties** object

Gets the name of the instrument the analysis was acquired on.

Syntax

object.InstrumentName

Parameters

object An expression that evaluates to a **Properties** object.

Example

```
MsgBox Analysis.Properties.InstrumentName
```

3.57 InstrumentSerialNumber Property

Applies to: **Properties** object

Gets the serial number of the instrument the analysis was acquired on.

Syntax

object.InstrumentSerialNumber

Parameters

object An expression that evaluates to a **Properties** object.

Example

```
MsgBox Analysis.Properties.InstrumentSerialNumber
```

3.58 Intensity Property

Applies to: **MSPeak** object, **SmartFormulaResult** object

Gets the intensity value of an **MSPeak** or **SmartFormulaResult** object.

Syntax

intensity = *object*.Intensity

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.59 Intensity(n) Property

Applies to: **Chromatogram** object, **Compound** object, **Spectrum** object

Gets the intensity value at defined index of a **Chromatogram**, **Compound** or **Spectrum** object.

Syntax

`intensity = object.Intensity(n)`

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

n An index value for the intensity to retrieve.

Remarks

When accessing numerous intensity values of a chromatogram or spectrum, the **ChromatogramData** method, resp. **SpectrumData** method, will be significantly faster.

Example

The following example finds and displays the maximum intensity of the first chromatogram.

```
dim chrom
set chrom = analysis.chromatograms(1)

dim i, MaxIntensity
MaxIntensity = 0
for i = 1 to chrom.size
    if MaxIntensity < chrom.Intensity(i) then
        MaxIntensity = chrom.Intensity(i)
    end if
next

MsgBox "The maximum intensity in the chromatogram is " +
CStr(MaxIntensity) + "."
```

See Also

ChromatogramData method

SpectrumData method

Mass property

RetentionTime property

3.60 IntensityRatio Property

Applies to: **ICACHromatogramDefinition** object

Gets or sets the intensity ratio of an **ICACHromatogramDefinition** object.

Syntax

object.IntensityRatio = *IntensityRatio*

IntensityRatio = *object.IntensityRatio*

Parameters

object An expression that evaluates to an **ICACHromatogramDefinition** object.

IntensityRatio Intensity ratio value.

See Also

ToleranceIntensityRatio property

3.61 IsChromatographicAnalysis Property

Applies to: **Analysis** object

Gets the condition of an **Analysis** object if the analysis is a chromatogram analysis.

Syntax

object.IsChromatogramAnalysis

Parameters

object An expression that evaluates to an **Analysis** object.

3.62 IsLockMassCalibrationActive

Applies to: **Analysis** object

Gets whether lock mass calibration is active or not for an **Analysis** object.

Syntax

object.IsLockMassCalibrationActive

Parameters

object An expression that evaluates to an **Analysis** object.

3.63 LastMass Property

Applies to: **Spectrum** object

Gets the last mass of a **Spectrum** object.

Syntax

object.LastMass

Parameters

object An expression that evaluates to a **Spectrum** object.

3.64 LastRetentionTime Property

Applies to: **Chromatogram** object

Gets the last retention time value of a **Chromatogram** object in seconds.

Syntax

object.LastRetentionTime

Parameters

object An expression that evaluates to a **Chromatogram** object.

Example

The following example displays the retention time range of the first chromatogram loaded:

```
set chrom = analysis.chromatograms(1)
msgbox "Retention time: " +
CStr(Int(chrom.FirstRetentionTime)) + " - " +
CStr(Int(chrom.LastRetentionTime))
```

See Also

FirstRetentionTime property

3.65 LibraryNames Property

Applies to: **LibrarySearchResult** object

Gets the names of the mass-spectral library of a **LibrarySearchResult** object.

Syntax

object.LibraryNames

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.66 Logging Property

Applies to: **Application** object

Turns on/off logging of all incoming automation calls.

Syntax

object.Logging = *boolean*

boolean = *object*.Logging

Parameters

object An expression that evaluates to an **Application** object.

boolean A **Boolean** value that sets the state of the object. Possible values are:

- | | |
|--------------|-------------------------|
| True | Activates the object. |
| False | Deactivates the object. |

Return Values

The **Logging** property returns one of the following values:

- **True** The object is active.
- **False** The object is not active.

Remarks

The **Logging** property has the **Boolean** type.

Example

The following example first displays a message box with the current logging status and then turns on logging.

```
MsgBox(Application.Logging)
Application.Logging = true
```

3.67 LowerBoundaryFormula Property

Applies to: **SmartFormulaParameters** object

Gets or sets the lower boundary formula of sum formulae to be generated of a **SmartFormulaParameters** object.

Syntax

object.Formula = *formula*

formula = *object*.Formula

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

formula A string that gets or sets the chemical formula.

Example

The following example sets/gets the lower boundary formula of a **SmartFormulaParameters** object and displays it in a message box:

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.LowerBoundaryFormula = "C24H30N0O2S3"
MsgBox SFP.LowerBoundaryFormula
```

3.68 m_over_z Property

Applies to: **MSPeak** object, **SmartFormulaResult** object, **SmartFormulaResultItem** object

Gets the m/z value of an **MSPeak**, **SmartFormulaResult** or **SmartFormulaResultItem** object.

Syntax

object.m_over_z

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

In case of an **MSPeak** or **SmartFormulaResult** object *m_over_z* represents the experimentally observed value, whereas in case of a **SmartFormulaResultsItem** object *m_over_z* represents the theoretically calculated value based on the sum formula of that object.

3.69 Mass Property

Applies to: **Spectrum** object

Gets the *m/z* value at defined index of a **Spectrum** object.

Syntax

object.Mass(*n*)

Parameters

object An expression that evaluates to a **Spectrum** object.

n Index value for the *m/z* value to retrieve.

Remarks

When accessing numerous mass values of a spectrum, the **SpectrumData** method will be significantly faster.

Example

The following example finds and displays the most intense *m/z* value of the first spectrum in the first compound.

```
dim spec
set spec = Analysis.Compounds(1)(1)

dim i, MaxIntensity, MaxMass
MaxIntensity = 0
MaxMass = 0

for i = 1 to spec.size
    if MaxIntensity < spec.Intensity(i) then
        MaxIntensity = spec.Intensity(i)
        MaxMass = spec.Mass(i)
    end if
next
```

```
MsgBox "The most intense is at m/z " + FormatNumber(MaxMass,  
2) + "." + "."
```

See Also

SpectrumData method

Intensity property

3.70 MaximumIntensity Property

Applies to: **Chromatogram** object, **Spectrum** object

Gets the maximum intensity of a **Chromatogram** or **Spectrum** object.

Syntax

object.**MaximumIntensity**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.71 MeanError Property

Applies to: **SmartFormulaResultItem** object

Gets the mean m/z error of the complete isotopic pattern, which is calculated from all individual m/z error values for each isotopomeric peak of a **SmartFormulaResultItem** object.

Syntax

object.**MeanError**

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.72 MinimumIntensity Property

Applies to: **Chromatogram** object, **Spectrum** object

Gets the minimum intensity of a **Chromatogram** or **Spectrum** object.

Syntax

object.MinimumIntensity

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.73 MolWeight Property

Applies to: **Compound** object, **LibrarySearchResult** object

Gets the deconvoluted m/z value of the precursor that was used for creating the compound of a **Compound** object (AutoMSn algorithm).

Gets the molecular weight of a **LibrarySearchResult** object.

Syntax

object.MolWeight

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

See Also

LibrarySearchResults object

3.74 MonoIsotopicMass Property

Applies to: **SumFormula** object

Gets the nominal m/z value of a **SumFormula** object at a specific charge state.

Syntax

mass = *object*.MonoIsotopicMass(charge)

Parameters

object An expression that evaluates to a **SumFormula** object.

charge Charge state for which the m/z value should be calculated.

Example

The following example calculates and displays the monoisotopic mass of the double charged ion of Ethanol (C₂H₅OH):

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C2H5OH"
MsgBox SF.MonoIsotopicMass(+2)
```

3.75 MSFilter Property

Applies to: **Compound** object, **Spectrum** object

Gets the MS/MS Info of the spectrum/spectra related to a **Compound** or **Spectrum** object.

Syntax

object.MSFilter

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example displays a message box with the precursor of the 2nd spectrum of the first compound:

```
Dim Cmpd
Dim Spec
set Cmpd = Analysis.Compounds(1)
set Spec = Cmpd(2)
msgbox "Precursor: " + Spec.MSFilter.FragmentationPath
```


3.76 MSPeakList Property

Applies to: **Spectrum** object

Gets the Mass List (MS peak list) of a **Spectrum** object.

Syntax

object.MSPeakList

Parameters

object An expression that evaluates to a **Spectrum** object.

3.77 Name Property

Applies to: **Analysis** object, **Application** object, **Chromatogram** object, all **ChromatogramDefinition** objects, **Compound** object, **Spectrum** object, **Variable** object

Gets the name of an object.

Syntax

object.Name

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

The **Name** property has the **String** type.

The following table summarizes the results of using the **Name** property with the objects in the Applies To list:

Object	Results
Analysis	Gets the name of the analysis.
Application	Gets the name of the application.
Chromatogram	Gets the description for the chromatogram.
Compound	Gets the description for the processed mass spectrum.
Spectrum	Gets the description for the mass spectrum.
ChromatogramDefinition	Gets the name of chromatogram trace

The **Name** property does not get an analysis' drive and directory. To get the drive and directory use the **Path** or **FullName** property.

Example

The following example gets the name of the analysis and displays it in a message box:

```
MsgBox Analysis.Name
```

See Also

FullName property

Variable object

Variables object

3.78 NitrogenRule Property

Applies to: **SmartFormulaResultItem** object

Gets whether the nitrogen rule of a **SmartFormulaResultItem** object is fulfilled.

Syntax

object.**NitrogenRule**

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.79 NominalMass Property

Applies to: **SumFormula** object

Gets the nominal m/z value of a **SumFormula** object at a specific charge state.

Syntax

mass = *object*.**NominalMass(charge)**

Parameters

object An expression that evaluates to a **SumFormula** object.

charge Charge state for which the m/z value should be calculated.

Example

The following example calculates and displays the nominal mass of Ethanol (C₂H₅OH):

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")
```

```
SF.Formula = "C2H5OH"  
MsgBox SF.NominalMass(0)
```

3.80 NumberOfFormula Property

Applies to: **SmartFormulaParameters** object

Gets or sets the maximum number of formulae to be generated of a **SmartFormulaParameters** object.

Syntax

object.NumberOfFormula = *number*

number = *object*.NumberOfFormula

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

number An integer that gets or sets the maximum number of formulae.

Example

The following example sets/gets the number of formulae of a **SmartFormulaParameters** object and displays it in a message box:

```
GPF.NumberOfFormula = 42  
MsgBox GPF.NumberOfFormula
```

3.81 Parameters Property

Applies to: **SmartFormulaResult** object

Gets the parameters used for generating molecular formulae for that particular observed MS peak of a **SmartFormulaResult** object.

Syntax

object.Parameters

Parameters

object An expression that evaluates to a **SmartFormulaResult** object.

3.82 Path Property

Applies to: **Analysis** object, **Application** object

Gets the path to an object. This path never ends with a backslash, unless the path has the format "C:\."

Syntax

object.**Path**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above. When you access the **Path** property of the **Application** object, you can omit *object* because the name of the **Application** object is implied when you access its properties and methods.

Remarks

The **Path** property has the **String** type.

The **Path** property does not get an object's file name and extension. To get the file name and extension use the **Name** or **FullName** property.

The following table summarizes the results of using the **Path** property with the objects in the Applies To list:

Object	Results
Application	Gets the path to the DataAnalysis executable, for example: "C:\Program Files\DataAnalysis"
Analysis	Gets the path to the file containing the analysis, for example: " "C:\Data Files\Demo\Analysis.d"

The **Path** property does not end the path with a backslash, unless the path has the format "C:\."

Example

The following example gets the path to the analysis and displays it in a message box:

```
MsgBox Analysis.Path
```

3.83 PeakEnd Property

Applies to: **MSPeak** object

Gets the m/z value at the end of an **MSPeak** object.

Syntax

object.PeakEnd

Parameters

object An expression that evaluates to an **MSPeak** object.

3.84 PeakEndIntensity Property

Applies to: **Compound** object, **MSPeak** object

Gets the intensity at the end of a **Compound** or **MSPeak** object.

Syntax

object.PeakEndIntensity

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.85 PeakStart Property

Applies to: **MSPeak** object

Gets the m/z value at the start of an **MSPeak** object.

Syntax

object.PeakStart

Parameters

object An expression that evaluates to an **MSPeak** object.

3.86 PeakStartIntensity Property

Applies to: **Compound** object, **MSPeak** object

Gets the intensity at the start of a **Compound** or **MSPeak** object.

Syntax

object.**PeakStartIntensity**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.87 Polarity Property

Applies to: MS type **ChromatogramDefinition** objects (**TICChromatogramDefinition** object, **BPCChromatogramDefinition** object, **EICChromatogramDefinition** object, **CNLChromatogramDefinition** object), **Spectrum** object

Gets or sets the polarity of an MS type **ChromatogramDefinition** or **Spectrum** object.

Syntax

object.**Polarity** = *polarity*

polarity = *object*.**Polarity**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Polarity = *daPositive* positive polarity
daNegative negative polarity
daBoth positive and negative polarity

Example

The following example sets the polarity of **TICChromatogramDefinition**:

```
TIC.Polarity = daPositive
```

3.88 Probability Property

Applies to: **SmartFormulaResultItem** object

Gets the probability for that item of a **SmartFormulaResultItem** object.

Syntax

object.Probability

Parameters

object An expression that evaluates to an **SmartFormulaResultItem** object.

3.89 Purity Property

Applies to: **LibrarySearchResult** object

Gets the effective Purity score of a **LibrarySearchResult** object.

Syntax

object.Purity

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.90 Range Property

Applies to: **BPCChromatogramDefinition** object, **EICChromatogramDefinition** object, **CNLChromatogramDefinition** object, **MassPosChromatogramDefinition** object, **UV2DChromatogramDefinition** object

Gets or sets the range of a **ChromatogramDefinition** object. The range defines the intensities which has to be summed up (EIC, NL, UV2D) or within the maximum intensity should be retrieved (BPC, MassPos).

Syntax

object.Range = *range*

range = *object*.Range

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Range = {*range*} combined range, e.g., "290 – 350; 400" or single value 400

Example

The following example sets the range of **BPCChromatogramDefinition**:

```
BPC.Range = "300-400"
```

Comment UV2DChromatogramDefinition

In rare cases a single wave length definition can result in a zero-line output. To avoid this change trace definition to wider range, e.g. UV2D.Range = "252-256".

3.91 RawValue Property

Applies to: **MSPeak** object

Gets the raw value of an **MSPeak** object. The raw value depends on the kind of instrument. For a time-of-flight instrument, this is the time of flight. For an FTMS instrument, this is the frequency. All other instruments deliver the non-recalibrated mass here.

Syntax

object.RawValue

Parameters

object An expression that evaluates to an **MSPeak** object.

3.92 RawValues Property

Not documented yet.

3.93 RetentionTime Property

Applies to: **Chromatogram** object, **Compound** object, **LibrarySearchResult** object

Gets the retention time value at defined index of a **Chromatogram** object.

Gets the retention time of a **Compound** object.

Gets the retention time of a **LibrarySearchResult** object.

Syntax

object.RetentionTime

object.RetentionTime(*n*)

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

n An index value for the retention time to retrieve; applies only to the **Chromatogram** object.

Remarks

When accessing numerous retention time values of a chromatogram, the **ChromatogramData** method will be significantly faster.

Example

The following example displays the retention time end value of the first chromatogram.

```
dim chrom
set chrom = analysis.chromatograms(1)

MsgBox "The chromatogram ends at " +
CStr(chrom.RetentionTime(chrom.Size)/60) + " minutes."
```

See Also

ChromatogramData method

Intensity property

LibrarySearchResults object

3.94 RetentionTimeEnd Property

Applies to: **Compound** object

Gets the retention time at which a **Compound** object ends.

Syntax

object.RetentionTimeEnd

Parameters

object An expression that evaluates to a **Compound** object.

3.95 RetentionTimeOffset Property

Not documented yet.

3.96 RetentionTimeStart Property

Applies to: **Compound** object

Gets the retention time at which a **Compound** object starts.

Syntax

object.RetentionTimeStart

Parameters

object An expression that evaluates to a **Compound** object.

3.97 RFit Property

Applies to: **LibrarySearchResult** object

Gets the effective RFit score of a **LibrarySearchResult** object.

Syntax

object.RFit

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.98 RingsAndDoubleBonds Property

Applies to: **SmartFormulaResultItem** object

Gets the number of rings and double bonds of a **SmartFormulaResultItem** object.

Syntax

object.RingsAndDoubleBonds

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.99 SampleInfo Property

Applies to: **Properties** object

Gets the sample info of the analysis.

Syntax

object.**SampleInfo**

Parameters

object An expression that evaluates to a **Properties** object.

Example

```
MsgBox Analysis.Properties.SampleInfo
```

3.100 ScanMode Property

Applies to: MS type **ChromatogramDefinition** objects (**TICChromatogramDefinition** object, **BPCChromatogramDefinition** object, **EICChromatogramDefinition** object, **CNLChromatogramDefinition** object), **Spectrum** object

Gets or sets the scan mode of an MS type **ChromatogramDefinition** object or **Spectrum** object.

Syntax

object.**ScanMode** = *scanMode*

scanMode = *object*.**ScanMode**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

<i>ScanMode</i> = <i>daScanModeFullScan</i>	standard full scan mode
<i>daScanModeMaxRes</i>	high resolution scan mode
<i>daScanModeAll</i>	includes all scan modes
<i>daScanModeISCID</i>	In-Source CID (isCID) scan mode
<i>daScanModeBBCID</i>	Broad-Band CID (bbCID) scan mode

Example

The following example sets the scan mode of **TICChromatogramDefinition**:

```
TIC.ScanMode = daScanModeFullScan
```

3.101 Score Property

Applies to: **SmartFormulaResultItem** object

Gets the Score value of a **SmartFormulaResultItem** object.

Syntax

object.Score

Parameters

object An expression that evaluates to an **SmartFormulaResultItem** object.

3.102 ScoreRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for Score value of a **SmartFormulaResultItem** object.

Syntax

object.ScoreRank

Parameters

object An expression that evaluates to an **SmartFormulaResultItem** object.

3.103 ScriptVariable Property

Applies to: **Analysis** object

Gets and sets a string value to a variable of an **Analysis** object.

Syntax

variable = *object*.ScriptVariable(VariableName)

object.ScriptVariable(VariableName) = variable

Parameters

object An expression that evaluates to an **Analysis** object.

variableName A unique name for the variable. Variable names are not case-sensitive.

Remarks

Variables are stored in the results of an analysis. The content of a variable can be included in a print report using the dedicated report layout component.

Example

The following example creates and sets a variable named 'Test' and assigns the string value '15' to it:

```
ScriptVariable("Test") = "15"
```

The following example displays the content of the variable named 'Test':

```
MsgBox ScriptVariable("Test")
```

3.104 SearchMass Property

Applies to: **SmartFormulaParameters** object

Gets or sets the search mass of a **SmartFormulaParameters** object to be looked for in a mass spectrum.

Syntax

object.**SearchMass** = *mass*

mass = *object*.**SearchMass**

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

mass A float that gets or sets the search mass.

Example

The following example sets/gets the search mass of a **SmartFormulaParameters** object and displays it in a message box:

```
GPF.SearchMass = 243.3
```

```
MsgBox GPF.SearchMass
```

3.105 SearchRange Property

Applies to: **SmartFormulaParameters** object

Gets or sets the range of a **SmartFormulaParameters** object within the search mass should be searched in a mass spectrum.

Syntax

object.SearchRange = *range*

range = *object*.SearchRange

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

range A float that gets or sets the search range.

Example

The following example sets/gets the search range of a **SmartFormulaParameters** object and displays it in a message box:

```
GPF.SearchRange = 0.1  
MsgBox GPF.SearchRange
```

3.106 SeparationType Property

Applies to: **Compound** object

Gets the type of separation of a **Compound** object.

Syntax

object.SeparationType

Parameters

object An expression that evaluates to a **Compound** object.

3.107 SequenceNumbers Property

Applies to: **Spectrum** object

Gets the sequence numbers which contributed to a **Spectrum** object.

Syntax

object.SequenceNumbers

Parameters

object An expression that evaluates to a **Spectrum** object.

3.108 ShowLine Property

Applies to: **Annotation** object

Gets the state of visibility of the line of a single **Annotation** object.

Syntax

boolean = *object*.ShowLine

Parameters

object An expression that evaluates to an **Annotation** object.

boolean A **Boolean** value that gets the state of the object. Possible values are:

True The line is visible.

False The line is not visible.

3.109 Sigma Property

Applies to: **SmartFormulaResultItem** object

Gets the Sigma value of a **SmartFormulaResultItem** object.

Syntax

object.Sigma

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.110 SigmaRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for Sigma value of a **SmartFormulaResultItem** object.

Syntax

object.**SigmaRank**

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.111 Signal Property

Applies to: **UVChromatogramDefinition** object, **LCChromatogramDefinition** object

Gets the signal of an **UVChromatogramDefinition** object or **LCChromatogramDefinition** object.

Syntax

object.**Signal**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example adds an LC chromatogram from HyStar to the chromatograms selection:

```
dim LC
set LC = CreateObject("DataAnalysis.LCChromatogramDefinition")

LC.Signal = "Solvent B"

Analysis.Chromatograms.AddChromatogram LC
```


3.112 SignalToNoise Property

Applies to: **Compound** object, **MSPeak** object

Gets the signal to noise ratio of a **Compound** or **MSPeak** object.

Syntax

object.SignalToNoise

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

The following drawing illustrates the *Signal* and the *Noise* values.

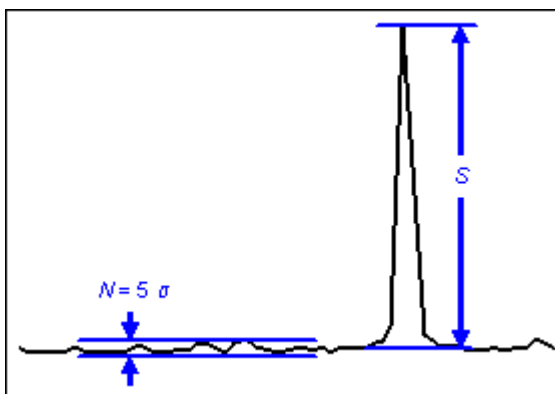


Figure 3-1 Illustration of the *Signal* and the *Noise* values

3.113 Size Property

Applies to: **Chromatogram** object, **Spectrum** object

Gets the number of data points of a **Chromatogram** or **Spectrum** object.

Syntax

object.Size

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.114 SpectrumComment Property

Applies to: **LibrarySearchResult** object

Gets the spectrum comment text of a **LibrarySearchResult** object.

Syntax

object.SpectrumComment

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.115 SpectrumInfo Property

Applies to: **LibrarySearchResult** object

Gets the spectrum information text of a **LibrarySearchResult** object.

Syntax

object.SpectrumInfo

Parameters

object An expression that evaluates to a **LibrarySearchResult** object.

See Also

LibrarySearchResults object

3.116 StdDevIntensity Property

Applies to: **SmartFormulaResultItem** object

Gets the StdDevIntensity value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevIntensity

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.117 StdDevIntensityRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for StdDevIntensity value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevIntensityRank

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.118 StdDevIntensityVarNorm Property

Applies to: **SmartFormulaResultItem** object

Gets the StdDevIntensityVarNorm value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevIntensityVarNorm

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.119 StdDevIntensityVarNormRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for StdDevIntensityVarNorm value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevIntensityVarNormRank

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.120 StdDevMassDiffs Property

Applies to: **SmartFormulaResultItem** object

Gets the StdDevMassDiffs value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevMassDiffs

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.121 StdDevMassDiffsRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for StdDevMassDiffs value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevMassDiffsRank

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.122 StdDevMeanMass Property

Applies to: **SmartFormulaResultItem** object

Gets the StdDevMeanMass value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevMeanMass

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.123 StdDevMeanMassRank Property

Applies to: **SmartFormulaResultItem** object

Gets the rank according to sorting for StdDevMeanMass value of a **SmartFormulaResultItem** object.

Syntax

object.StdDevMeanMass

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.124 SumFormula Property

Applies to: **SmartFormulaResultItem** object

Gets the sum formula of a **SmartFormulaResultItem** object.

Syntax

object.SumFormula

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

3.125 SumIntensity Property

Applies to: **Spectrum** object

Gets the sum of all intensity values of a **Spectrum** object.

Syntax

object.SumIntensity

Parameters

object An expression that evaluates to a **Spectrum** object.

3.126 Text Property

Applies to: **Annotation** object

Gets the text of **Annotation** object.

Syntax

text = *object*.Text

Parameters

object An expression that evaluates to an **Annotation** object.

text A **string** that gets the text.

3.127 Tolerance Property

Applies to: **SmartFormulaParameters** object

Gets or sets the tolerance of a **SmartFormulaParameters** object in ppm.

Syntax

object.Tolerance = *tolerance*

tolerance = *object*.Tolerance

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

tolerance A float the gets or sets the tolerance.

Example

The following example sets the tolerance to 0.01 ppm and then gets it again and displays it in a message box:

```
GPF.Tolerance = 0.01  
MsgBox GPF.Tolerance
```

3.128 ToleranceDelta_m_over_z Property

Applies to: **ICACHromatogramDefinition** object

Gets or sets the tolerance of the delta m/z value of an **ICACHromatogramDefinition** object.

Syntax

object.ToleranceDelta_m_over_z = tolerance

tolerance = object.ToleranceDelta_m_over_z

Parameters

object An expression that evaluates to an **ICACHromatogramDefinition** object.

tolerance Tolerance of the delta m/z value.

3.129 ToleranceIntensityRatio Property

Applies to: **ICACHromatogramDefinition** object

Gets or sets the tolerance of the intensity ratio of an **ICACHromatogramDefinition** object.

Syntax

object.ToleranceIntensityRatio = tolerance

tolerance = object.ToleranceIntensityRatio

Parameters

object An expression that evaluates to an **ICACHromatogramDefinition** object.

tolerance Tolerance of the intensity ratio.

See Also

IntensityRatio property

3.130 Type Property

Applies to: **MSFilter** object, all **ChromatogramDefinition** objects

Gets the type of object.

Syntax

object.Type

Parameters

object An expression that evaluates to one of the objects in the Applies To list above. The following types are defined:

MS Filter object:

<i>daMSFilterNONE</i>	No filter defined.
<i>daMSFilterAll</i>	All mass spectra.
<i>daMSFilterMS</i>	MS ¹ spectra only.
<i>daMSFilterAllMSMS</i>	All MS ⁿ spectra.
<i>daMSFilterMSMS</i>	A specific MS ⁿ spectrum of defined precursor.
<i>daMSFilterMSMSplus</i>	A specific MS ⁿ spectrum of defined precursor and all fragment spectra of it.
<i>daMSFilterAllMSMS_2</i>	All MS ² spectrum of defined precursor.
<i>daMSFilterAllMSMS_3</i>	All MS ³ spectrum of defined precursor.
<i>daMSFilterAllMSMS_4</i>	All MS ⁴ spectrum of defined precursor.
<i>daMSFilterAllMSMS_5plus</i>	All MS ⁿ (n ≥ 5) spectrum of defined precursor.

ChromatogramDefinition objects:

<i>daTICChromType</i>	Total Ion Chromatogram
<i>daEICChromType</i>	Extracted Ion Chromatogram
<i>daBPCCChromType</i>	Base Peak Chromatogram
<i>daCNLChromType</i>	Constant Neutral Loss Chromatogram
<i>daMPChromType</i>	Mass Position Chromatogram
<i>daVARChromType</i>	Acquisition Parameter Chromatogram
<i>daUVChromType</i>	1D UV Chromatogram
<i>daUV2DChromType</i>	extracted chromatogram of a 2D UV data file
<i>daLCChromType</i>	LC Chromatogram
<i>dalImportChromType</i>	Imported External Data Chromatogram
<i>dalCAChromType</i>	Isotope Cluster Analysis Chromatogram

Example

The following example gets the type of an **MSFilter** object and a **TICChromatogram-Definition** object and displays them in a message box:

```
MsgBox TIC.MSFilter.Type
MsgBox TIC.Type
```


3.131 Unit Property

Applies to: **Variable** object

Gets the unit string value of a **Variable** object.

Syntax

object.Unit

Parameters

object An expression that evaluates to a **Variable** object.

See Also

Variable object

Variables object

3.132 UpperBoundaryFormula Property

Applies to: **SmartFormulaParameters** object

Gets or sets the upper boundary formula of sum formulae to be generated of a **SmartFormulaParameters** object.

Syntax

object.UpperBoundaryFormula = *formula*

formula = *object*.UpperBoundaryFormula

Parameters

object An expression that evaluates to a **SmartFormulaParameters** object.

formula A string the gets or sets the upper boundary formula.

Example

The following example sets/gets the upper boundary formula of a **SmartFormulaParameters** object and displays it in a message box:

```
Dim SFP
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")

SFP.UpperBoundaryFormula = "C54H100N3O2S6"
MsgBox SFP.UpperBoundaryFormula
```

3.133 Value Property

Applies to: **Variable** object

Gets the string value of a **Variable** object.

Syntax

object.Value

Parameters

object An expression that evaluates to a **Variable** object.

See Also

Variable object

Variables object

3.134 VariableName Property

Applies to: **VarChromatogramDefinition** object

Gets or sets the variable name of a **VarChromatogramDefinition** object.

Syntax

object.VariableName = variableName

variableName = object.VariableName

Parameters

object An expression that evaluates to a **VarChromatogramDefinition** object.

VariableName Name of a variable as shown in Edit Chromatograms dialog.

Example

The following example sets the variable name:

```
Var.VariableName = "Vacuum High"
```

See Also

GroupName property

3.135 Version Property

Applies to: **Application** object

Gets the version of DataAnalysis.

Syntax

object.Version

Parameters

object An expression that evaluates to an **Application** object.

Remarks

The version is formatted as "*major.minor.build.sub-build*", e.g., "3.2.100.0".

Example

The following example gets the version of DataAnalysis and displays it in a message box:

```
MsgBox Application.Version
```

3.136 Visible Property

Applies to: **Application** object

Gets the condition of an **Application** object if the application is visible.

Syntax

object.Visible

Parameters

object An expression that evaluates to an **Application** object.

See Also

Hide method

Show method

3.137 Width Property

Applies to: **Compound** object, **MSPeak** object

Gets the full-width at half-maximum (FWHM) of the peak of a **Compound** object.

Gets the peak width of an **MSPeak** object.

Syntax

object.Width

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

3.138 WidthLeft, WidthRight Property

Applies to: **BPCChromatogramDefinition** object, **EICChromatogramDefinition** object, **CNLChromatogramDefinition** object, **MassPosChromatogramDefinition** object

Extends the range if it is defined with single values to the left and to the right of a **ChromatogramDefinition** object.

Syntax

object.WidthLeft

object.WidthRight

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

The default values are "0.5".

Example

The following example sets the left and right width of a **BPCChromatogramDefinition** object:

```
BPC.Range      = 400.5
BPC.WidthLeft  = 0.5
BPC.WidhtRight = 0.8
```

3.139 X1 Property

Applies to: **Annotation** object

Gets the x-coordinate of the left border of an **Annotation** object.

Syntax

$x = \text{object.X1}$

Parameters

object An expression that evaluates to an **Annotation** object.

x An **integer** that gets the x-coordinate.

3.140 X2 Property

Applies to: **Annotation** object

Gets the x-coordinate of the right border of an **Annotation** object.

Syntax

$x = \text{object.X2}$

Parameters

object An expression that evaluates to an **Annotation** object.

x An **integer** that gets the x-coordinate.

3.141 Y1 Property

Applies to: **Annotation** object

Gets the lower y-coordinate of the left border of an **Annotation** object.

Syntax

$y = \text{object.Y1}$

Parameters

object An expression that evaluates to an **Annotation** object.

y An **integer** that gets the y-coordinate.

3.142 Y2 Property

Applies to: **Annotation** object

Gets the lower y-coordinate of the right border of an **Annotation** object.

Syntax

$y = \text{object.Y2}$

Parameters

object An expression that evaluates to an **Annotation** object.

y An **integer** that gets the y-coordinate.

3.143 YText Property

Applies to: **Annotation** object

Gets the upper y-coordinate (height where the text appears) of the right border of an **Annotation** object.

Syntax

$y = \text{object.YText}$

Parameters

object An expression that evaluates to an **Annotation** object.

y An **integer** that gets the y-coordinate.

4 AUTOMATION METHODS

Methods are actions you take against objects. For example, to add a document to the collection of open documents, you use the **Add** method of the **Documents** object.

For examples of using methods, see the macro sample provided with DataAnalysis.

The following methods are available:

<u>Method</u>	<u>Description</u>
Activate	Activates DataAnalysis
Add	Adds a simple chromatogram to a Chromatograms object. Adds a partial sum formula string to the formula in a SumFormula object.
AddAnnotation	Adds an Annotation object to Annotations object.
AddChromatogram	Adds a fully defined chromatogram to a Chromatograms object.
AddChromatogramRangeSelection	Adds a selection range to the current set of selected ranges for the chromatograms of an Analysis object.
AddChromatograms	Adds several fully defined chromatograms at once to a Chromatograms object.
AddRangeSelection	Adds a selection range to the current set of selected ranges for a Chromatogram object.
ApplyLockMassCalibration	Turns applying lock mass calibration on or off in an Analysis object.
AverageMassSpectrum	Calculates the average spectrum of the selected range of a Chromatogram object and creates a new Compound Mass Spectra entry with the averaged spectrum.
BaselineSubtract	Performs a baseline subtraction on spectra in a Spectra object.
Caption	Sets the caption in the script form of a Form object.
ChromatogramData	Gets the retention time and intensity vector of a Chromatogram object.
Clear	Deletes all items of a Chromatograms or Compounds object.

<u>Method</u>	<u>Description</u>
ClearChromatogramRangeSelections	Clears the chromatograms selection of an Analysis object.
ClearRangeSelections	Clears all selection ranges of a Chromatogram object. If no selected ranges are defined, the full retention time and intensity range is then applied to other methods of the Chromatogram object.
ClearResults	Deletes the results of an Analysis object.
Close	Closes the analysis of an Analysis object or the script form of a Form object.
Deconvolute	Deconvolutes all spectra in a Compounds or Spectra object.
DeleteAnnotation	Deletes a specific annotation from an Annotations object.
DeleteCompound	Deletes a specific compound from a Compounds object.
DeletePeak	Deletes a specific peak from an MSPeakList object.
DeleteRecalculatedLineSpectra	Deletes recalculated line spectra from an Analysis object.
DeleteResult	Deletes the SmartFormula results from a SmartFormulaResults object.
DeleteResultItem	Deletes a result item from a SmartFormula-Result object.
DeleteScriptTable	Deletes the script table of an Analysis object.
Deselect	Deselects an analysis of an Analysis object, a chromatogram of a Chromatogram object, a compound of a Compound object or a spectrum of a Spectrum object.
DoEvents	Handles pending timer, sizing, or painting events in the script form of a Form object.
ElementalComposition	Calculates the elemental composition from the formula of a SumFormula object.

<u>Method</u>	<u>Description</u>
Enable	Enables/Disables a chromatogram of a Chromatogram object, a compound of a Compound object or a mass spectrum of a Spectrum object. Enables/Disables the script form of a Form object.
Export	Exports a single item or all items of an Analysis, Chromatogram, Compound, Compounds, Spectra or Spectrum object.
ExportMassList	Exports the Mass List of a Spectrum object.
FindAutoMSn	Finds peaks in an Auto-LC-MS/MS Analysis object using the AutoMS(n) algorithm.
FindCompounds	Finds peaks and integrates a chromatogram trace of a Chromatogram object.
FindDissect	Finds peaks and integrates an Analysis object using the Dissect algorithm.
FindMolecularFeatures	Find compounds on the LC/MS data of an Analysis object using the FindMolecular-Features algorithm.
FindMSn	Performs an automatic integration on an MRM Analysis object.
FormulaPattern	Retrieves the simulated pattern for the sum formula value of a SmartFormulaResultItem object.
Hide	Hides the complete DataAnalysis application. Hides the script form of a Form object.
HideMenu	Hides the menu of the script form of a Form object.
Identify	Identifies all spectra in a Compounds or Spectra object.
IndexOfNMostIntensePeaks	Retrieves indices of N most intense peaks from an MSPeakList object.
IntegrateOnly	Performs integration on a Chromatogram object, but creates no average MS spectra.

<u>Method</u>	<u>Description</u>
Item	Gets a specified Analysis , Chromatogram , Compound , or Spectrum object from an Analyses , Chromatograms , Compounds , LibrarySearchResults , Spectra or Variables object.
LoadMethod	Loads a new method for an Analysis object.
MascotSearch	Performs a Mascot Search of a protein or peptide Analysis object using BioTools.
MassListClear	Deletes the Mass List of all spectra in a Compounds , Spectra or Spectrum object.
MassListFind	Performs peak detection within specified m/z range of all spectra in a Compounds , Spectra or Spectrum object.
Maximize	Maximizes the script form of a Form object.
MeasuredPattern	Retrieves the measured isotopomeric pattern for a SmartFormulaResultItem object.
Minimize	Minimizes the script form of a Form object.
Noise	Calculates the noise of the selected range of a Chromatogram object.
Open	Opens an analysis with a specified file name in an Analyses object.
Pattern	Calculates the theoretical pattern from the formula of a SumFormula object.
PrepareSurveyView	Prepares an internal, reduced data set for being displayed in the Survey View for an Analysis object.
Print	Prints a report for an Analysis object.
PrintToPDF	Prints a report to a PDF file for an Analysis object.
ProcessAutoMSn	Performs FindAutoMsn, deconvolution and export of AutoMSn compounds iteratively.
RecalculateLineSpectra	Recalculates line spectra in an Analysis object.
Recalibrate	Recalibrates a spectrum of a Spectrum object.

<u>Method</u>	<u>Description</u>
RecalibrateAutomatically	Automatically recalibrates the spectra of an Analysis object using the calibrant spectra in a predefined retention time range.
RecalibrateExternal	Recalibrates the spectra of an Analysis object externally by applying the recalibration coefficients of another analysis.
RecalibrateInternal	Recalibrates all spectra or a single spectrum of an Analysis object internally as specified in the parameter settings.
RelatedCompounds	Gets the numbers of the compounds related to a Chromatogram object.
Restore	Restores the script form of a Form object.
RunScript	Starts the script of an Analysis object.
Save	Saves the processing state of an Analysis object including changes made to the attached method.
Select	Selects an analysis of an Analysis object, a chromatogram of a Chromatogram object, a compound of a Compound object or a spectrum of a Spectrum object.
SelectNone	Deselects all selected items in the analysis tree of an Application object.
SendReport	Sends a report of an Analysis object as PDF file attachment of an email.
SetScriptTableCellText	Sets the cell content of a script table of an Analysis object.
SetScriptTableColumnHeader	Sets the column names of the script table of an Analysis object.
Show	Shows the DataAnalysis application after it has been hidden completely. Shows a hidden script form of a Form object again.
ShowMenu	Shows a hidden menu of the script form of a Form object again.
SmartFormulaAndExport	Generates a list of sum formulae in a Spectra or Spectrum object and exports it.

<u>Method</u>	<u>Description</u>
Smooth	Smooths the chromatogram or the spectrum of a Chromatogram or Spectrum object respectively all chromatograms or spectra of a Chromatograms or Spectra object.
SpectrumData	Gets the mass and intensity vector of a Spectrum object.
Subtract	Subtracts a partial sum formula string from the formula of a SumFormula object.

4.1 Activate Method

Applies to: **Application** object

Activates DataAnalysis. If DataAnalysis is minimized its size will be restored, too.

Syntax

object.**Activate(reserved)**

Parameters

object An expression that evaluates to an **Application** object.

reserved This parameter is ignored.

Example

The following example activates DataAnalysis without changing its current size, unless it is minimized:

```
Set DA = GetObject("", "BDal.DataAnalysis.Application")
DA.Activate(0)
```

4.2 Add Method

Applies to: **Chromatograms** object, **SumFormula** object

Adds a simple chromatogram to a **Chromatograms** object. Adds a partial sum formula string to the formula in a **SumFormula** object.

Syntax

object.**Add (ChromatogramType, MSType, range, polarity)**

object.**Add formula**

Parameters

<i>object</i>		An expression that evaluates to one of the objects in the Applies To list above.
<i>ChromatogramType</i>	=	<i>daTIC</i> Total ion chromatogram <i>daEIC</i> Extracted ion chromatogram <i>daBPC</i> Base peak chromatogram
<i>MSType</i>	=	<i>daAll</i> , All MS and MS/MS spectra <i>daAllMS</i> All MS spectra <i>daAllMSn</i> All MS(n) spectra <i>{ions}</i> daughter ions, e.g., "289" or "672/289")
<i>range</i>	=	<i>{range}</i> combined range , e.g., "290 – 350; 400"
<i>polarity</i>	=	<i>daPositive</i> positive polarity <i>daNegative</i> negative polarity <i>daBoth</i> positive and negative polarity
<i>formula</i>		A partial formula to add to a SumFormula object.

Example

The following example adds a total ion chromatogram of all positive MS and MSn spectra to the **Chromatograms** collection:

```
Analysis.Chromatograms.Add daTIC, daAll, "", daPositive
```

The following example adds a total ion chromatogram of all MS³ spectra with parent *m/z* 290 in the first generation and *m/z* 150 in the second to the **Chromatograms** collection:

```
Analysis.Chromatograms.Add daTIC, "290/150", "", daBoth
```

The following example adds a Methylen group (C2H) to Ethanol (C2H5OH) making up Propanol and displays the hill-sorted sum formula of it:

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C2H5OH"
SF.Add "CH2"
MsgBox SF.Formula
```

See Also

AddChromatogram method

AddChromatograms method

4.3 AddAnnotation Method

Applies to: **Annotations** object

Adds an annotation to an **Annotations** object.

Syntax

object.AddAnnotation (X1, Y1, X2, Y2, YText, Text, ShowLine)

Parameters

object An expression that evaluates to an **Annotations** object.

X1 Start of the **Annotation** object.

Y1 End of the **Annotation** object.

X2 Height of left starting point.

Y2 Height of right starting point.

YText Height where the upper portion of annotation should be placed.

Text String representing the text of annotation.

ShowLine A **Boolean** value indicating whether to draw lines of annotation. This parameter does not apply to difference annotations; default is *true*.

Example

The following example places a difference annotation on the first spectrum of an analysis:

```
Analysis.Spectra(1).Annotations.AddAnnotation 500, 1500, 556,  
2000, 5000, "Loss of Iron"
```

The following example places a single annotation on the first spectrum of the first compound of an analysis:

```
Analysis.Compounds(1)(1).Annotations.AddAnnotation 100, 0, 100,  
0, 1000, "Oligomycin", false
```

See Also

Annotation object

Spectrum object

4.4 AddChromatogram Method

Applies to: **Chromatograms** object

Adds a fully defined chromatogram to a **Chromatograms** object.

Syntax

object.AddChromatogram ChromatogramDefinition

Parameters

<i>object</i>	An expression that evaluates to a Chromatograms object.
<i>ChromatogramDefinition</i>	An expression that evaluates a ChromatogramDefinition object. This can be one the following objects: TICChromatogramDefinition EICChromatogramDefinition BPCChromatogramDefinition CNLChromatogramDefinition MassPosChromatogramDefinition UVChromatogramDefinition UV2DChromatogramDefinition LCChromatogram VARChromatogramDefinition ICAChromatogramDefinition ImportedDataChromatogramDefinition

Examples

The following example adds a chromatogram to the **Chromatograms** collection:

```
Dim TIC, VAR
Set TIC =
CreateObject("DataAnalysis.TICChromatogramDefinition")
Set Var =
CreateObject("DataAnalysis.VARChromatogramDefinition")
' do some definitions of TIC and Var...
Analysis.Chromatograms.AddChromatogram TIC
Analysis.Chromatograms.AddChromatogram Var
```

The following example adds a chromatogram acquired by HyStar to the **Chromatograms** collection:

```
dim UV
set UV = CreateObject("DataAnalysis.UVChromatogramDefinition")

' add the first of the UV traces stored by HyStar
```

```
UV.FileName = HyStarUNTFileName + ": (1)"
UV.RetentionTimeOffset = 0

Analysis.Chromatograms.AddChromatogram UV

function HyStarUNTFileName
    n = InStrRev(Analysis.Name, ".")
    HyStarUNTFileName = Left(Analysis.Name, n-1) + ".unt"
end function
```

See Also

Add method

AddChromatograms method

ChromatogramDefinition objects

4.5 AddChromatogramRangeSelection Method

Applies to: **Analysis** object

Adds a selection range to the current set of selected ranges for the chromatograms of an **Analysis** object. The selected range is then applied to other methods of the **Analysis** object.

Syntax

object.AddChromatogramRangeSelection (**RetTimeStart**, **RetTimeEnd**, **IntensityStart**, **IntensityEnd**)

Parameters

object An expression that evaluates to an **Analysis** object.

RetTimeStart Start of the retention time range in minutes.

RetTimeEnd End of the retention time range in minutes.

IntensityStart (reserved for future use).

IntensityEnd (reserved for future use).

Example

The following example defines two selected ranges (10-15min and 20-22min) of the **Analysis** object and runs the Find AutoMS(n) algorithm:


```
Analysis.AddChromatogramRangeSelection 10, 15, 0, 0  
Analysis.AddChromatogramRangeSelection 20, 22, 0, 0  
Analysis.FindAutoMSn
```

See Also

FindAutoMSn method

ClearChromatogramRangeSelections method

FindDissect method

4.6 AddChromatograms Method

Applies to: **Chromatograms** object

Adds several fully defined chromatograms at once to a **Chromatograms** object.

Syntax

object.AddChromatograms (**chroms**)

Parameters

object An expression that evaluates to a **Chromatograms** object.

Chroms An array of **ChromatogramDefinition** objects. These can be one the following objects:

- TICChromatogramDefinition
- EICChromatogramDefinition
- BPCChromatogramDefinition
- CNLChromatogramDefinition
- MassPosChromatogramDefinition
- UVChromatogramDefinition
- UV2DChromatogramDefinition
- LCChromatogram
- VARChromatogramDefinition
- ICACHromatogramDefinition
- ImportedDataChromatogramDefinition

Example

The following example adds a three chromatogram traces to **Chromatograms** collection at once:

```
Dim Chroms(3)  
Dim TIC, BPC, EIC  
  
Set TIC =
```

```
CreateObject("DataAnalysis.TICChromatogramDefinition")
Set EIC =
CreateObject("DataAnalysis.EICChromatogramDefinition")
Set BPC =
CreateObject("DataAnalysis.BPCChromatogramDefinition")

' do some definitions with TIC, EIC, and BPC...
Set Chroms(0) = TIC
Set Chroms(1) = BPC
Set Chroms(2) = EIC

Analysis.Chromatograms.AddChromatograms(Chroms)
```

See Also

Add method

AddChromatogram method

ChromatogramDefinition objects

4.7 AddRangeSelection Method

Applies to: **Chromatogram** object

Adds a selection range to the current set of selected ranges for a **Chromatogram** object. The selected range is then applied to other methods of the **Chromatogram** object.

Syntax

object.AddRangeSelection (RetTimeStart, RetTimeEnd, IntensityStart, Intensity-End)

Parameters

object An expression that evaluates to a **Chromatogram** object.

RetTimeStart Start of the retention time range in minutes.

RetTimeEnd End of the retention time range in minutes.

IntensityStart (reserved for future use).

IntensityEnd (reserved for future use).

Example

The following example defines two selected ranges (10-15min and 20-22min) of the **Chromatogram** object of the first chromatogram loaded:

```
Analysis.Chromatograms(1).AddRangeSelection 10, 15, 0, 0  
Analysis.Chromatograms(1).AddRangeSelection 20, 22, 0, 0
```

See Also

AverageMassSpectrum method

ClearRangeSelections method

FindCompounds method

IntegrateOnly method

4.8 ApplyLockMassCalibration Method

Applies to: **Analysis** object

Turns applying lock mass calibration on or off in an **Analysis** object.

Syntax

object.**ApplyLockMassCalibration** **bLockMassCalibration**

Parameters

<i>object</i>	An expression that evaluates to an Analysis object.
<i>bLockMassCalibration</i>	A Boolean value that sets the state of the lock mass calibration. Possible values are: True Turns on applying lock mass calibration. False Turns off applying lock mass calibration.

Remarks

Existing compounds are not removed by this method and will become invalid. They should be deleted before, e.g., using the **Clear** method.

Example

The following example turns on applying lock mass calibration after deleting all previous compounds.

```
Analysis.Compounds.Clear  
Analysis.ApplyLockMassCalibration true
```

See Also

Clear method

4.9 AverageMassSpectrum Method

Applies to: **Chromatogram** object

Calculates the average spectrum of the selected range of a **Chromatogram** object and creates a new Compound Mass Spectra entry with the averaged spectrum. The mass spectra being used for averaging are filtered to match the chromatogram definition of the **Chromatogram** object.

Syntax

object.AverageMassSpectrum (bLine, bProfile)

Parameters

object An expression that evaluates to a **Chromatogram** object.

bLine A **Boolean** value. **True** will create an averaged line spectrum.

bProfile A **Boolean** value. **True** will create an averaged profile spectrum.

Example

The following example defines two selected ranges (10-15min and 20-22min) of the **Chromatogram** object of the first chromatogram loaded and then calculates a profile spectrum placed in the Compound Mass List.

```
Analysis.Chromatograms(1).AddRangeSelection 10, 15, 0, 0  
Analysis.Chromatograms(1).AddRangeSelection 20, 22, 0, 0  
Analysis.Chromatograms(1).AverageMassSpectrum false, true
```

See Also

AddRangeSelection method

ClearRangeSelections method

4.10 BaselineSubtract Method

Applies to: **Spectra** object

Performs a baseline subtraction on spectra in a **Spectra** object. The parameters for this algorithm will be taken from method.

Syntax

object.BaseLineSubtract

Parameters

object An expression that evaluates to a **Spectra** object.

Example

The following example baseline subtracts each spectrum in the **Spectra** collection:

```
Analysis.Spectra.BaseLineSubtract
```

4.11 Caption Method

Applies to: **Form** object

Sets the caption in the script form of a **Form** object.

Syntax

```
object.Caption ( title )
```

Parameters

object An expression that evaluates to a **Form** object.

title A string specifying the new caption.

Example

The following example sets the caption "Demo" in the script form:

```
Form.Caption "Demo"
```

4.12 ChromatogramData Method

Applies to: **Chromatogram** object

Gets the retention time and intensity vector of a **Chromatogram** object.

Syntax

```
object.ChromatogramData retentiontime_vector, intensity_vector
```

Parameters

object An expression that evaluates to a **Chromatogram** object.

retentiontime_vector A vector for the retention time values.

intensity_vector A vector for the intensity values.

Remarks

When accessing numerous retention time/intensity values of a chromatogram, this method will be significantly faster than using the **RetentionTime** or **Intensity** properties. The vectors being filled with retention time and intensity values are zero-based.

Example

The following example calculates the total sum intensity of a chromatogram.

```
dim rt()
dim intensity()

dim chrom
set chrom = Analysis.Chromatograms(1)

chrom.ChromatogramData rt, intensity

dim sum
sum = 0

MsgBox "The first chromatogram contains " +
    CStr(UBound(intensity)) + 1 " values."

dim i
for i = 0 to UBound(intensity)
    sum = sum + intensity(i)
next

MsgBox "The total sum intensity is " + CStr(sum) + "."
```

See Also

SpectrumData method

RetentionTime property

Intensity property

4.13 Clear Method

Applies to: **Chromatograms** object, **Compounds** object

Deletes all items of a **Chromatograms** or **Compounds** object.

Syntax

object.Clear

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example deletes all compounds in the **Compounds** collection:

```
Analysis.Compounds.Clear
```

4.14 ClearChromatogramRangeSelections Method

Applies to: **Analysis** object

Clears the chromatograms selection of an **Analysis** object.

Syntax

object.ClearChromatogramRangeSelections

Parameters

object An expression that evaluates to an **Analysis** object.

See Also

AddChromatogramRangeSelection method

4.15 ClearRangeSelections Method

Applies to: **Chromatogram** object

Clears all selection ranges of a **Chromatogram** object. If no selected ranges are defined, the full retention time and intensity range is then applied to other methods of the **Chromatogram** object.

Syntax

object.ClearRangeSelections

Parameters

object An expression that evaluates to a **Chromatogram** object.

Example

The following example clears all selected of the **Chromatogram** object of the first chromatogram loaded:

```
Analysis.Chromatograms(1).ClearRangeSelections
```

See Also

AddRangeSelection method

AverageMassSpectrum method

FindCompounds method

IntegrateOnly method

4.16 ClearResults Method

Applies to: **Analysis** object

Deletes the results of an **Analysis** object.

Syntax

object.ClearResults

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following example deletes the results in an **Analysis**.

```
Analysis.ClearResults
```

4.17 Close Method

Applies to: **Analysis** object, **Form** object

Closes the analysis of an **Analysis** object or the script form of a **Form** object.

Syntax

object.Close

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

The `Analysis.Close` command cannot be invoked in a script attached to an analysis. This command can only be used from external scripts, e.g., from the Automation-Engine, or applications other than DataAnalysis.

Example

The following example closes the script form.

```
Form.Close
```


4.18 Deconvolute Method

Applies to: **Compounds** object, **Spectra** object, **Spectrum** object

Deconvolutes all spectra of a **Compounds**, **Spectra** or **Spectrum** object.

Syntax

object.Deconvolute

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example deconvolutes each spectrum in the **Compounds** collection:

```
Analysis.Compounds.Deconvolute
```

4.19 DeleteAnnotation Method

Applies to: **Annotations** object

Deletes a specific annotation from an **Annotations** object.

Syntax

object.DeleteAnnotation (*n*)

Parameters

object An expression that evaluates to a **Annotations** object.

n Number of annotation to delete

Example

The following example deletes the first compound in the **Compounds** collection:

```
Analysis.Spectra(1).Annotations.DeleteAnnotation 1
```

4.20 DeleteCompound Method

Applies to: **Compounds** object

Deletes a specific compound from a **Compounds** object.

Syntax

object.DeleteCompound (n)

Parameters

object An expression that evaluates to a **Compounds** object.
n Number of compound to delete

Example

The following example deletes the first compound in the **Compounds** collection:

```
Analysis.Compounds.DeleteCompound 1
```

The following example deletes all compounds in the **Compounds** collection, except for the first:

```
For i = Analysis.Compounds.Count to 2 step -1  
    Analysis.Compounds.DeleteCompound i  
Next
```

See Also

Clear method

4.21 DeletePeak Method

Applies to: **MSPeakList** object

Deletes a specific peak from an **MSPeakList** object.

Syntax

object.DeletePeak (n)

Parameters

object An expression that evaluates to an **MSPeakList** object.
n Number of peak to delete

Example

The following example deletes all peaks of all precursor spectra of the first compound:

```
Dim Spec  
For Each Spec in Analysis.Compounds(1)  
    If Spec.MSFilter.Type = daMSFilterMS Then  
        For i = Spec.MSPeakList.Count to 1 to by -1  
            Spec.MSPeakList.DeletePeak i  
        Next
```

```
End If
Next
```

4.22 DeleteRecalculatedLineSpectra Method

Applies to: **Analysis** object

Deletes the recalculated line spectra from an **Analysis** object. Afterwards the line spectra calculated during acquisition will be used further on.

Syntax

object.DeleteRecalculatedLineSpectra

Parameters

object An expression that evaluates to an **Analysis** object.

4.23 DeleteResult Method

Applies to: **SmartFormulaResults** object

Deletes the SmartFormula results from a **SmartFormulaResults** object.

Syntax

object.DeleteResult

Parameters

object An expression that evaluates to a **SmartFormulaResults** object.

4.24 DeleteResultItem Method

Applies to: **SmartFormulaResult** object

Deletes a result item from a **SmartFormulaResult** object.

Syntax

object.DeleteResultItem

Parameters

object An expression that evaluates to a **SmartFormulaResult** object.

4.25 DeleteScriptTable Method

Applies to: **Analysis** object

Deletes the script table of an **Analysis** object.

Syntax

object.DeleteScriptTable **TableName**

Parameters

object An expression that evaluates to an **Analysis** object.

TableName Name of the table to delete

Remarks

The `Analysis.Close` command cannot be invoked in a script attached to an analysis. This command can only be used from external scripts, e.g., from the Automation-Engine, or applications other than DataAnalysis.

Example

The following example deletes the script table "MyTable" of the analysis.

```
Analysis.DeleteScriptTable "MyTable"
```

See Also

SetScriptTableCellText method

SetScriptTableColumnHeader method

4.26 Deselect Method

Applies to: **Analysis** object, **Chromatogram** object, **Compound** object, **Spectrum** object

Selects an analysis of an **Analysis** object, a chromatogram of a **Chromatogram** object, a compound of a **Compound** object or a spectrum of a **Spectrum** object.

Syntax

object.Deselect

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example deselects the first compound.

```
analysis.compounds(1).Deselect
```

The following example deselects the first mass spectrum in the second compound.
`analysis.compounds(2)(1).Deselect`

See Also

Select method

4.27 DoEvents Method

Applies to: **Form** object

Handles pending timer, sizing or painting events in the script form of a **Form** object.

Syntax

object.DoEvents

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example handles pending events in the script form:

```
Form.DoEvent
```

4.28 ElementalComposition Method

Applies to: **SumFormula** object

Calculates the elemental composition from the formula of a **SumFormula** object.

Syntax

object.ElementalComposition *symbols*, *fractions*

Parameters

object An expression that evaluates to a **SumFormula** object.

symbols An array used to store the symbols of each present element.

fractions An array used to store the relative amount of each element.

Example

The following example calculates the elemental composition for ferrocene and demonstrates how to access the resulting data.

Note: the arrays are start with index zero

```
dim symbols()
dim fractions()

dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C10H10Fe"
SF.ElementalComposition symbols, fractions

'how many different elements are available
MsgBox UBound(symbols) + 1

for n = 0 to UBound(symbols)
    MsgBox symbols(n) & " " & fractions(n)
next
```

4.29 Enable Method

Applies to: **Chromatogram** object, **Compound** object, **Form** object, **Spectrum** object

Enables or disables a chromatogram of a **Chromatogram** object, a compound of a **Compound** object or a mass spectrum of a **Spectrum** object.

Enables or disables the script form of a **Form** object.

Syntax

object.Enable [boolean]

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

boolean A **Boolean** value that enables or disables a chromatogram of a **Chromatogram**, a compound of a **Compound** or a mass spectrum of a **Spectrum** object. Possible values are:

True Enables the object (Default).

False Disables the object.

A **Boolean** value that sets the state of the **Form** object. Possible values are:

True Enables the script form.

False Disables the script form.

Note

A disabled script form cannot be closed or enabled again interactively. This must be accomplished by external control, too.

Example

The following example enables the first mass spectrum of every compound.

```
Dim Cmpd
For Each Cmpd in Analysis.Compounds
    Dim Spec
    set Spec = Cmpd(1)
    Spec.Enable
Next
```

4.30 Export Method

Applies to: **Analysis** object, **Chromatogram** object, **Compound** object, **Compounds** object, **Spectra** object, **Spectrum** object

Exports a single item or all items in an **Analysis**, **Chromatogram**, **Compound**, **Compounds**, **Spectra** or **Spectrum** object.

Syntax

object.**Export filename type**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

filename Destination, to which the export should be saved, if the filename is empty DataAnalysis will generate a filename based on name of the analysis.

type **Analysis** object:
= *daMzXML* Export in mzXML format (*.mzXML)
 daMzData Export in mzData format (*.mzData)

	Compound and Compounds object:	
<i>type</i>	= <i>daMGF</i>	Export in Mascot format (*.mgf)
	<i>daCSV</i>	Export in comma-separated-value ASCII format (*.csv)
	<i>daXML</i>	Export in XML format (*.xml)
	Spectrum and Spectra object:	
<i>type</i>	= <i>daMGF</i>	Export in Mascot format (*.mgf)
	<i>daASCII</i>	Export in ASCII format (*.ascii)
	<i>daXY</i>	Export in a simple ASCII format containing x-y values only (*.xy)
	<i>daCSV</i>	Export in comma-separated-value ASCII format (*.csv)
	<i>daBSC</i>	Export a profile spectrum in BioTools ASCII format (*.bsc)
	<i>daXML</i>	Export in XML format (*.xml)
	Chromatogram object:	
<i>type</i>	= <i>daChemStation</i>	Export spectra in Agilent ChemStation format (*.d)
	<i>daASCII</i>	Export spectra in ASCII format (*.ascii)
	<i>daXY</i>	Export the chromatogram in a simple ASCII format containing x-y values only (*.xy)
	<i>daCDF</i>	Export spectra in andi netCDF format (*.cdf)
	Chromatogram object and <i>daChemStation</i> , <i>daASCII</i> or <i>daCDF</i> type or Analysis object only:	
<i>spectrum</i>	= <i>daLine</i>	Export line spectra; optional parameter, default is <i>daLine</i>
	<i>daProfile</i>	Export profile spectra; optional parameter

Remarks

The export to ASCII format (*.ascii) will export profile spectra if the *spectrum* parameter is set to *daProfile* and if profile spectra are available. Otherwise, line spectra are exported.

Example

The following example deconvolutes each spectrum in the **Compounds** collection object and exports the result as a Mascot file:

```
Analysis.Compounds.Deconvolute
Analysis.Compounds.Export "", daMGF
```

The following example exports the line spectra of the raw data to an mzXML file:

```
Analysis.Export "", daMzXML, daLine
```


4.31 ExportMassList Method

Applies to: **Spectrum** object

Exports the Mass List of a **Spectrum** object.

Syntax

object.ExportMassList filename type

Parameters

object An expression that evaluates to a **Spectrum** object.

filename Destination, to which the export should be saved, if the filename is empty DataAnalysis will generate a filename based on name of the analysis.

type = *daASCII* Export in blank-separated ASCII format (*.ascii)
daCSV Export in comma-separated-value ASCII format (*.csv)

Remarks

The mass list of a line spectrum contains all lines. The mass list of a profile spectrum contains the peaks being found with one of the mass list peak finder algorithms. The items of the Mass List being exported are determined by the Mass List Layout defined in the related method parameters.

Example

The following example exports the first averaged spectrum in the Compound Mass List.

```
Analysis.Spectra(1).ExportMassList "", daASCII
```

See Also

Export method

4.32 FindAutoMSn Method

Applies to: **Analysis** object

Finds peaks in an Auto-LC-MS/MS analysis **Analysis** object using the AutoMS(n) algorithm. This will create a list of compounds, each with a FullScan, a MaxRes and an MSn compound mass spectrum.

Syntax

object.FindAutoMSn

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following finds the compounds of an AutoMS(n) analysis.

```
Analysis.FindAutoMSn
```

See Also

AddChromatogramRangeSelection method

4.33 FindCompounds Method

Applies to: **Chromatogram** object, **Chromatograms** object

Finds peaks and integrates all chromatograms in the **Chromatograms** object or on a single **Chromatogram** object. This will create a list of compounds with averaged compound mass spectra. If ranges have been selected using the **AddRangeSelection** method, only peaks within the selected ranges will be found.

Syntax

object.FindCompounds

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following performs an automatic integration on analyses.

```
Dim MyChromatogram
For each MyChromatogram in Analysis.Chromatograms
    MyChromatogram.FindCompounds
Next
' which is fully equivalent to:
Analysis.Chromatograms.FindCompounds
```

See Also

AddRangeSelection method

ClearRangeSelections method

4.34 FindDissect Method

Applies to: **Analysis** object

Finds peaks and integrates an **Analysis** object using the Dissect algorithm. This will create a list of compounds with averaged compound mass spectra.

Syntax

object.FindDissect

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following performs an automatic integration on MRM analysis.

```
Analysis.FindDissect
```

See Also

AddChromatogramRangeSelection method

4.35 FindMolecularFeatures Method

Applies to: **Analysis** object

Finds compounds on LC/MS data of an **Analysis** object using the FindMolecularFeatures algorithm. This will create a list of compounds, each with a clean compound mass spectrum.

Syntax

object.FindMolecularFeatures

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following performs an automatic integration on MRM analysis.

```
Analysis.FindMolecularFeatures
```

4.36 FindMSn Method

Applies to: **Analysis** object

Performs an automatic integration on an MRM analysis **Analysis** object.

Syntax

object.FindMSn

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following performs an automatic integration on MRM analysis.

```
Analysis.FindMSn
```

4.37 FormulaPattern Method

Applies to: **SmartFormulaResultItem** object

Retrieves the simulated pattern for the sum formula value of a **SmartFormulaResultItem** object.

Syntax

object.FormulaPattern

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

4.38 Hide Method

Applies to: **Application** object, **Form** object

Hides the complete DataAnalysis application. Hides the script form of a **Form** object.

Syntax

object.Hide

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example hides the script form:

```
Form.Hide
```

The following example temporarily hides the DataAnalysis application during some processing:

```
Application.Hide  
' do some processing...  
Application.Show
```

See Also

Show method

4.39 HideMenu Method

Applies to: **Form** object

Hides the script form menu of a **Form** object.

Syntax

```
object.HideMenu
```

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example hides the menu of the script form:

```
Form.HideMenu
```

4.40 Identify Method

Applies to: **Compounds** object, **Spectra** object, **Spectrum** object

Identifies all spectra of a **Compounds** or **Spectra** object.

Syntax

```
object.Identify
```

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example identifies each spectrum in the **Compounds** collection:

```
Analysis.Compounds.Identify
```

4.41 IndexOfNMostIntensePeaks Method

Applies to: **MSPakList** object

Retrieves indices of N most intense peaks in an **MSPeakList** object.

Syntax

```
object.IndexOfNMostIntensePeaks ( n, Indices )
```

Parameters

object An expression that evaluates to an **MSPeakList** object.

n Number of most intensive peaks to retrieve

indices Array for index values

Example

The following retrieves the N most intense peaks of all precursor spectra of the first compound:

```
Dim Spec
For Each Spec in Analysis.Compounds(1)
    If Spec.MSFilter.Type = daMSFilterMS Then
        Dim index()
        Spec.MSPeakList.IndexOfNMostIntensePeaks 10, index
    End If
Next
```

4.42 IntegrateOnly Method

Applies to: **Chromatogram** object, **Chromatograms** object

Performs integration on all chromatograms in the **Chromatograms** object or on a single **Chromatogram** object, but creates no average MS spectra. If ranges have been selected using the **AddRangeSelection** method, only peaks within the selected ranges will be found.

Syntax

```
object.IntegrateOnly
```

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following performs an automatic integration on analyses.

```
Dim MyChromatogram
For each MyChromatogram in a Analysis.Chromatograms
    MyChromatogram.IntegrateOnly
Next
' which is fully equivalent to:
Analysis.Chromatograms.IntegrateOnly
```

See Also

AddRangeSelection method

ClearRangeSelections method

4.43 Item Method

Applies to: **Analyses** object, **ChildSpectra** object, **Chromatograms** object, **Compounds** object, **LibrarySearchResults** object **Spectra** object, **Variables** object

Gets a specified **Analysis**, **Chromatogram**, **Compound** or **Spectrum** object from an **Analyses**, **ChildSpectra**, **Chromatograms**, **Compounds**, **LibrarySearchResults**, **Spectra** or **Variables** object.

Syntax

object.Item [*index*]

-or-

object *index*

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

index A **Variant** that is a **Long** or **String** representing the appropriate analysis, layout, processed spectrum, spectrum, or trace.

- If you specify a **Long**, the **Item** method fetches the object by its one-based index in the collection.

- If you specify a **String**, it must be one of the strings described in the following table:

Object	String
---------------	---------------

Analyses

Remarks

If you specify numbers for *index*, do not store these for later use because the indices might change as objects are added or removed.

The **Item** method is the default. Accordingly, you don't have to reference **Item** explicitly, as shown in the syntax.

Note that the first valid index is '1' – not '0'.

Example

The following example prints all open analyses:

```
for num = 1 to Analyses.Count
    MsgBox Analyses.Item(num).Name
    Analyses(num).Print("Chromatogram Report")
next
```

4.44 LoadMethod Method

Applies to: **Analysis** object

Loads a new method for an **Analysis** object.

Syntax

object.LoadMethod (**MethodName**)

Parameters

object An expression that evaluates to an **Analysis** object.

MethodName A **String** that specifies the method file name. If no drive and path is included the method is loaded from the default method folder.

Example

The following loads a method from the default method folder.

```
Analysis.LoadMethod "Metabolite.m"
```

The following loads a method by specifying the full path name.

```
Analysis.LoadMethod "D:\MyMethods\Test.m"
```


4.45 MascotSearch Method

Applies to: **Analysis** object

Performs a Mascot Search of a protein or peptide **Analysis** object using BioTools.

Syntax

object.MascotSearch

Parameters

object An expression that evaluates to an **Analysis** object.

Remarks

This method requires that the Bruker Daltonics BioTools™ 2.0 application is installed on the system and BioTools being properly setup to search on a Mascot database.

Example

The following performs an automatic integration on analyses.

```
Analysis.FindAutoMSn  
Analysis.Compounds.Deconvolute  
Analysis.MascotSearch
```

4.46 MassListClear Method

Applies to: **Compounds** object, **Spectra** object, **Spectrum** object

Deletes the Mass List of all spectra in a **Compounds**, **Spectra** or **Spectrum** object.

Syntax

object.MassListClear

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following code performs MassListClear on each spectrum in a **Spectra** object:

```
Analysis.Spectra.MassListClear
```

4.47 MassListFind Method

Applies to: **Compounds** object, **Spectra** object, **Spectrum** object

Performs peak detection within specified m/z range of all spectra in a **Compounds**, **Spectra** or **Spectrum** object.

Syntax

object.MassListFind (**start**, **end**)

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Start Start m/z value

End End m/z value

Example

The following code performs MassListFind on each spectrum in a **Spectra** object:

```
val = Analysis.Spectra.MassListFind(250, 400)
```

4.48 Maximize Method

Applies to: **Form** object

Maximizes the script form of a **Form** object.

Syntax

object.Maximize

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example maximizes the script form:

```
Form.Maximize
```

4.49 MeasuredPattern Method

Applies to: **SmartFormulaResultItem** object

Retrieves the measured isotopomeric pattern for a **SmartFormulaResultItem** object.

Syntax

object.MeasuredPattern

Parameters

object An expression that evaluates to a **SmartFormulaResultItem** object.

4.50 Minimize Method

Applies to: **Form** object

Minimizes of the script form of a **Form** object.

Syntax

object.Minimize

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example minimizes the script form:

```
Form.Minimize
```

4.51 Noise Method

Applies to: **Chromatogram** object

Calculates the noise of the selected range of a **Chromatogram** object.

The signal-to-noise ratio determination differs to the one used in the *Find Compounds algorithm* only, that it is using a fixed, small smoothing width. The steps for determination the noise level simplifies to:

1. The third derivative of the chromatogram is calculated using the *Savitsky Golay* algorithm with a smoothing width $m=1$. The simplified formula then is:

$$y'_i = \frac{1}{2} y_{i+1} - \frac{1}{2} y_{i-1}$$

- The standard deviation σ of all values of the third derivative y''' is determined.

$$\sigma = \sqrt{\frac{\sum_{i=1}^N \frac{y'''_i{}^2}{N}}$$

For chromatograms only: The determination of an internal threshold by a histogram approach as in the signal-to-noise determination in *Find Compounds* does not apply, if the region selected does not contain chromatographic peaks.

- The signal-to-noise ratio S/N of each peak is then calculated as:

$$S/N = S/5\sigma, \text{ with } S = \text{peak height above the peak baseline.}$$

The noise N is determined as 5σ ; statistically 99% of the noise values are within this range.

The following drawing illustrates the *Signal* and the *Noise* values.

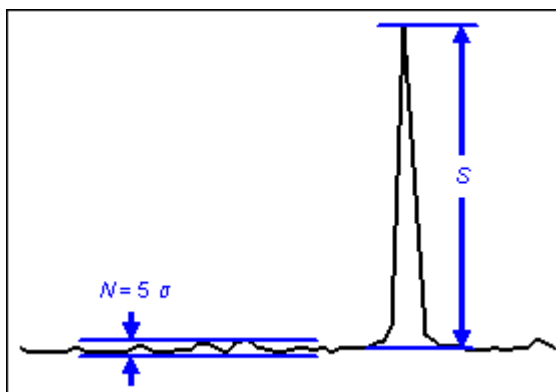


Figure 4-1 Illustration of the *Signal* and the *Noise* values

Syntax

`object.Noise`

Parameters

object An expression that evaluates to a **Chromatogram** object.

Example

The following example defines a selected range (10-15min) of the first chromatogram loaded and then determines and displays the noise.

```
Analysis.Chromatograms(1).AddRangeSelection 10, 15, 0, 0
noise = Analysis.Chromatograms(1).Noise
MsgBox "Noise (10-15min) = " + CStr(noise)
```

See Also**AddRangeSelection** method**ClearRangeSelections** method

4.52 Open Method

Applies to: **Analyses** objectOpens an analysis with a specified file name in an **Analyses** object.**Syntax***object*.Open (**PathName**)**Parameters***object* An expression that evaluates to an **Analyses** object.*PathName* A **String** that specifies the full path to the analysis.**Example**

The following example opens the analysis file C:\Data Files\Demo\Sample.d\Analysis.yep:

```
set myAnalysis = Application.Analyses.Open("C:\Data  
Files\Demo\Sample.d\Analysis.yep")
```

See Also**Close** method

4.53 Pattern Method

Applies to: **SumFormula** objectCalculates the theoretical pattern from the formula of a **SumFormula** object.**Syntax***object*.Pattern **charge**, **bHighResolution**, **m_over_z**, **intensities****Parameters***object* An expression that evaluates to a **SumFormula** object.*charge* The charge state which should be considered for calculation.*bHighResolution* A flag indicating whether to resolve isobaric species or not.

m_over_z An array used to store calculated *m/z* values.
intensities An array used to store relative abundances of each resulting peak.

Example

The following example calculates the pattern for ferrocene and demonstrates how to access the resulting data.

Note: Arrays starting with index zero.

```
dim m_over_z()  
dim intensities()  
  
dim SF  
set SF = CreateObject("DataAnalysis.SumFormula")  
  
SF.Formula = "C10H10Fe"  
SF.Pattern 1, 0, m_over_z, intensities  
  
'how many m/z I pairs are available  
MsgBox UBound(m_over_z) + 1  
  
for n = 0 to UBound(m_over_z)  
    MsgBox m_over_z(n) & " " & I(n)  
next
```

4.54 PrepareSurveyView Method

Applies to: **Analysis** object

Prepares an internal, reduced data set for being displayed in the Survey View for an **Analysis** object.

Syntax

object.**PrepareSurveyView**

Parameters

object An expression that evaluates to an **Analysis** object.

Remarks

The Survey View initially displays a reduced data set calculated from line spectra. Usually, this is done in the background for all acquired polarities and with and without spectral background subtraction. This command makes sure these reduced data are calculated and saved for fast display of density data any time in the future.

Note: Depending on the size and complexity of the data this command can take a considerable time!

4.55 Print Method

Applies to: **Analysis** object

Prints a report for an **Analysis** object.

Syntax

object.Print layout

Parameters

object An expression that evaluates to an **Analysis** object.

layout Report layout name.

Remarks

Layouts for DataAnalysis are currently exclusively being stored below the dedicated folder “C:\BDalSystemData\Report Layouts\DataAnalysis”.

The Report layout name may be specified without the instrument category and without the “.layout“ extension of the report layout filename. Thus, “Display Report”, “Esquire\Display Report”, or “Display Report.layout” are all legal and equivalent settings.

Printing through automation (this command) always uses the non-direct printing mode. The direct printing mode available in the **Print** dialog cannot be applied here.

Example

The following example prints the “Display Report” report.

```
Analysis.Print "Display Report"
```

4.56 PrintToPDF Method

Applies to: **Analysis** object

Prints a report to a PDF file for an **Analysis** object.

Syntax

object.PrintToPDF layout [, filename]

Parameters

object An expression that evaluates to an **Analysis** object.

layout Report layout name.

filename Full path of the PDF file to write. This parameter is optional; if it is not specified, the PDF will be stored in the analysis folder with the filename "Report.pdf".

Remarks

Layouts for DataAnalysis are currently exclusively being stored below the dedicated folder "C:\BDalSystemData\Report Layouts\DataAnalysis".

The Report layout name may be specified without the instrument category and without the ".layout" extension of the report layout filename. Thus "Display Report", "Esquire\Display Report" or "Display Report.layout" are all legal and equivalent settings.

Example

The following example prints the "Generic Display Report" report to "Report.pdf" in the analysis folder.

```
Analysis.PrintToPDF "Generic Display Report"
```

4.57 ProcessAutoMSn Method

Applies to: **Analysis** object

Processes an AutoMSn analysis. It iteratively creates an AutoMSn compound, deconvolutes it, exports it to an mgf file and an XML file, and removes the data immediately.

Syntax

object.**ProcessAutoMSn**

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following example processes an AutoMSn analysis.

```
Analysis.ProcessAutoMSn
```


4.58 RecalculateLineSpectra Method

Applies to: **Analysis** object

Recalculates line spectra in an **Analysis** object using the current mass peak finder with its current settings and stores them side by side to the analysis.baf file. Existing recalculated line spectra will be replaced. All algorithms using line spectra will take the recalculated line spectra instead of retrieving those generate during acquisition.

Syntax

object.RecalculateLineSpectra

Parameters

object An expression that evaluates to an **Analysis** object.

4.59 Recalibrate Method

Applies to: **Spectrum** object

Recalibrates a spectrum of a **Spectrum** object.

Syntax

boolean = *object*.Recalibrate

Parameters

object An expression that evaluates to a Spectrum object.

boolean A **Boolean** value that gets the state of the calibration. Possible values are:
True If the calibration was successful.
False If the calibration failed.

Remarks

This method is equivalent to 'Recalibrate Spectrum Only' in the Calibration dialog.

Example

The following sample code recalibrates the first mass spectrum of every compound.

```
Dim Cmpd
For Each Cmpd in Analysis.Compounds
    Dim Spec
    set Spec = Cmpd(1)
    If not Spec.Recalibrate Then
```

```
        MsgBox "Calibration of spectrum '"+Spec.Name+"'  
failed."  
    End If  
Next
```

4.60 RecalibrateAutomatically Method

Applies to: **Analysis** object

Automatically recalibrates the spectra of an **Analysis** object using calibrant spectra from a preselected retention time range as defined in method parameters.

Syntax

object.RecalibrateAutomatically

Parameters

object An expression that evaluates to an **Analysis** object.

boolean A **Boolean** value that gets the state of the calibration. Possible values are:

True If the calibration was successful.

False If the calibration failed.

Remarks

The details for automatic recalibration are defined in the parameters.

Example

The following sample code recalibrates the analysis and displays an error message if the calibration failed.

```
If not Analysis.RecalibrateAutomatically Then  
    MsgBox "Calibration of the analysis '"+Analysis.Name+"'  
failed."  
End If
```

The following sample code recalibrates the analysis and raises an error if the calibration failed. This can be useful when running scripts externally through the ProcessQueueer, e.g., from the AutomationEngine or in combination with HyStar. In the later case, the HyStar Sample Table flags this analysis as 'Processing failed'.

```
If not Analysis.RecalibrateAutomatically Then  
    err.Raise 51 'raises an "Internal Error" error  
End If
```

Succeeding versions of DataAnalysis will offer a generic solution to provide such feedback into the HyStar Sample Table.)

4.61 RecalibrateExternal Method

Applies to: **Analysis** object

Recalibrates the spectra of an **Analysis** object externally by applying the recalibration coefficients of another analysis.

Syntax

object.RecalibrateExternal (**PathName**)

Parameters

object An expression that evaluates to an **Analysis** object.

PathName A **String** that specifies the full path to the analysis.

Example

The following example recalibrates the analysis with the calibration from another analysis:

```
Analysis.RecalibrateExternal "D:\Data\RefAnalysis.d"
```

4.62 RecalibrateInternal Method

Applies to: **Analysis** object, **Spectrum** object

Recalibrates all spectra or a single spectrum of an **Analysis** or **Spectrum** object internally as specified in the parameter settings.

Syntax

object.RecalibrateInternal

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Remarks

If a complete chromatographic analysis is to be recalibrated internally, the analysis is recalibrated based on the first spectrum in the Compound List (**Analysis.Spectra(0)**) which is not part of a Compound. The internal recalibration is performed on this spectrum and then applied to all other spectra of this analysis. Note, that the method parameter settings for the recalibration must be properly set to contain peaks being found in this first spectrum.

If a specific spectrum of a chromatographic analysis is recalibrated the recalibration is also applied to all other spectra.

If a single-spectrum analysis is to be recalibrated internally, the analysis is also recalibrated based on the first spectrum, too (**Analysis.Spectra(0)**).

Example

The following example recalibrates the analysis internally based on the recalibration of the first spectrum not being part of a compound:

```
Analysis.RecalibrateInternal
```

The following example recalibrates a chromatographic analysis internally based on the recalibration of the second spectrum of the first compound:

```
Analysis.Compounds(1)(2).RecalibrateInternal
```

4.63 RelatedCompounds Method

Applies to: **Chromatogram** object

Gets the numbers of the compounds related to a **Chromatogram** object.

Syntax

object.RelatedCompounds **compound_nr_vector**

Parameters

object An expression that evaluates to a **Chromatogram** object.

compound_nr_vector A vector for the compound number values.

Remarks

The vector being filled with compound numbers is zero-based.

Example

The following example displays the related compounds for the first chromatogram:

```
dim cpmds()  
dim text, i, c  
  
dim Chrom  
set Chrom = Analysis.Chromatograms(1)  
  
Chrom.RelatedCompounds cpmds  
  
if UBound(cpmds) >= 0 then
```

```
text = "Chromatogram 1 has the following related
compounds:" & vbCR
for i = 0 to UBound(cpmds)
    c = cpmds(i)
    text = " " & text & " " & CStr(c) & ": "
    text = text & Analysis.Compounds(c).Name & vbCR
next
else
    text = "Chromatogram 1 has no related compounds."
end if

MsgBox text
```

4.64 Restore Method

Applies to: **Form** object

Restores the script form of a **Form** object.

Syntax

object.Restore

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example restores the script form:

```
Form.Restore
```

4.65 RunScript Method

Applies to: **Analysis** object

Starts the script of an **Analysis** object.

Syntax

object.RunScript

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following example starts the script of an analysis:

```
Analysis.RunScript
```

4.66 Save Method

Applies to: **Analysis** object

Saves the processing state of an Analysis object including changes made to the attached method.

Syntax

object.Save

Parameters

object An expression that evaluates to an **Analysis** object.

Example

The following example saves the analysis:

```
Analysis.Save
```

4.67 Select Method

Applies to: **Analysis** object, **Chromatogram** object, **Compound** object, **Spectrum** object

Selects an analysis of an **Analysis** object, a chromatogram of a **Chromatogram** object, a compound of a **Compound** object or a spectrum of a **Spectrum** object.

Syntax

object.Select

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example selects the first mass spectrum of every compound.

```
Dim Cmpd  
For Each Cmpd in Analysis.Compounds
```

```
Dim Spec
set Spec = Cmpd(1)
Spec.Select true
Next
```

See Also

Deselect method

4.68 SelectNone Method

Applies to: **Application** object

Deselects all currently selected items in the analysis tree of an **Application** object.

Syntax

object.**SelectNone**

Parameters

object An expression that evaluates to an **Application** object.

4.69 SendReport Method

Applies to: **Analysis** object

Sends a report of an **Analysis** object as PDF file attachment of an email.

Syntax

object.**SendReport** *layout*, *email*

Parameters

object An expression that evaluates to an **Analysis** object.

layout Report layout name.

email Email address.

Remarks

Layouts for DataAnalysis are currently exclusively being stored below the dedicated folder "C:\BDalSystemData\Report Layouts\DataAnalysis".

The Report layout name may be specified without the instrument category and without the ".layout" extension of the report layout filename. Thus, "Display Report", "Esquire\Display Report" or "Display Report.layout" are all legal and equivalent settings.

Example

The following sends an email with the “Generic Display Report” report attached to an email recipient defined in the local address book (My Colleague).

```
Analysis.SendReport "Generic Display Report", "My Colleague"
```

4.70 SetScriptTableCellText Method

Applies to: **Analysis** object

Sets the cell content of a script table of an **Analysis** object.

Syntax

object.SetScriptTableCellText **TableName, ColumnNumber, RowNumber, CellText**

Parameters

<i>object</i>	An expression that evaluates to an Analysis object.
<i>TableName</i>	Name of the table
<i>ColumnNumber</i>	Column number of the cell
<i>RowNumber</i>	Row number of the cell
<i>CellText</i>	Text to set into the cell

Remarks

Script tables can only be filled through the automation interface. Its content can only be examined by printing (or print preview).

Example

The following example creates a script table named "MassAccuracyTable" with 4 columns and fills in 2 rows:

```
Dim i
Dim TableName
Dim TargetMass(2)
Dim ActualMass(2)
Dim Accuracy(2)

TableName = "MassAccuracyTable"
TargetMass(1) = "509.20"
TargetMass(2) = "612.40"
ActualMass(1) = "509.25"
ActualMass(2) = "509.42"
Accuracy(1) = "0.05"
```



```
Accuracy(2) = "0.02"

'Delete any previous table
Analysis.DeleteScriptTable TableName

'Fill table header
Analysis.SetScriptTableColumnHeader TableName, 1, "Peak"
Analysis.SetScriptTableColumnHeader TableName, 2, "Mass
target"
Analysis.SetScriptTableColumnHeader TableName, 3, "Mass actual"
Analysis.SetScriptTableColumnHeader TableName, 4, "Mass
accuracy"

'Fill table
for i = 1 to 2
    Analysis.SetScriptTableCellText TableName, 1, i, CStr(i)
    Analysis.SetScriptTableCellText TableName, 2, i,
TargetMass(i)
    Analysis.SetScriptTableCellText TableName, 3, i,
ActualMass(i)
    Analysis.SetScriptTableCellText TableName, 4, i,
Accuracy(i)
Next
```

This Sample can be printed out using a report layout containing a "Scripting Table" component with the "Variable Name" property set to "MassAccuracyTable".

4.71 SetScriptTableColumnHeader Method

Applies to: **Analysis** object

Sets the column names of the script table of an **Analysis** object.

Syntax

object.SetScriptTableColumnHeader **TableName**, **ColumnNumber**, **HeaderText**

Parameters

object An expression that evaluates to an **Analysis** object.

TableName Name of the table

ColumnNumber Column number

HeaderText Text to set as header

Remarks

Script tables can only be filled through the automation interface. Its content can only be examined by printing (or print preview).

See Also

SetScriptTableCellText method

4.72 Show Method

Applies to: **Application** object, **Form** object

Shows the DataAnalysis application after it has been hidden completely. Shows a hidden script form of a **Form** object again.

Syntax

object.**Show**

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following example shows a hidden script form again:

```
Form.Show
```

The following example temporarily hides the DataAnalysis application during some processing:

```
Application.Hide  
' do some processing...  
Application.Show
```

See Also

Hide method

4.73 ShowMenu Method

Applies to: **Form** object

Shows a hidden menu of the script form of a **Form** object again.

Syntax

object.ShowMenu

Parameters

object An expression that evaluates to a **Form** object.

Example

The following example shows a hidden script form again:

```
Form.ShowMenu
```

4.74 SmartFormulaAndExport Method

Applies to: **Spectra** object, **Spectrum** object

Generates a list of sum formulae of a **Spectra** or **Spectrum** object and exports it.

Syntax

object.SmartFormula *parameters*, *filename*

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

parameters An expression that evaluates to a **SmartFormulaParameters** object

filename Destination, to which the results list should be saved. If the file name is empty DataAnalysis will generate a file name based on location and name of the analysis.

Remarks

The results list will be written as a *.csv file.

Example

The following example generates formulae on each spectrum in the **Spectra** collection object and exports the result to the specified file:

```
Dim SFP  
Set SFP = CreateObject("DataAnalysis.SmartFormulaParameters")
```

```
SFP.Charge = +1
SFP.DoubleBondEquivalenceMinimum = 3
SFP.DoubleBondEquivalenceMaximum = 8
SFP.LowerBoundaryFormula = "C5H5Fe0"
SFP.UpperBoundaryFormula = "C30H30Fe3"
SFP.NumberOfFormula = 50
SFP.Tolerance = 0.001
SFP.SearchMass = 186
SFP.SearchRange = 0.5
```

```
Analysis.Spectra.SmartFormulaAndExport SFP ,
    "D:\Data\MyAnalysis.d\FormulaResult0.csv"
```

4.75 Smooth Method

Applies to: **Chromatogram** object, **Chromatograms** object, **Spectra** object, **Spectrum** object

Smooths the chromatogram or the spectrum of a **Chromatogram** or **Spectrum** object respectively all chromatograms or spectra of a **Chromatograms** or **Spectra** object. The parameters for this algorithm are specified in the method.

Syntax

object.Smooth

Parameters

object An expression that evaluates to one of the objects in the Applies To list above.

Example

The following code smooths all spectra of a mass spectrum analysis:

```
Analysis.Spectra.Smooth
```

4.76 SpectrumData Method

Applies to: **Spectrum** object

Gets the mass and intensity vector of a **Spectrum** object.

Syntax

object.SpectrumData **mass_vector**, **intensity_vector**

Parameters

object An expression that evaluates to a **Spectrum** object.

mass_vector A vector for the m/z values.

intensity_vector A vector for the intensity values.

Remarks

When accessing numerous mass/intensity values of a chromatogram, this method will be significantly faster than using the **Mass** or **Intensity** properties.

The vectors being filled with m/z and intensity values are zero-based.

Example

The following example calculates the total sum intensity of a chromatogram.

```
dim mass()
dim intensity()

dim spec
set spec = Analysis.Compounds(1)(1)

spec.SpectrumData mass, intensity

dim sum
sum = 0

MsgBox "The first MS contains " + CStr(UBound(intensity)) + 1 "
      values."

dim i
for i = 0 to UBound(intensity)
    sum = sum + intensity(i)
next

MsgBox "The total sum intensity is " + FormatNumber(sum) + "."
```

See Also**ChromatogramData** method**Mass** property**Intensity** property

4.77 Subtract Method

Applies to: **SumFormula** objectSubtracts a partial sum formula string from the formula of a **SumFormula** object.**Syntax***object*.**Subtract** formula**Parameters***object* An expression that evaluates to a **SumFormula** object.*formula* A partial formula**Example**

The following example subtracts a Methylen group (CH₂) to Ethanol (C₂H₅OH) making up Methanol and displays the hill-sorted sum formula of it:

```
dim SF
set SF = CreateObject("DataAnalysis.SumFormula")

SF.Formula = "C2H5OH"
SF.Subtract "CH2"
MsgBox SF.Formula
```

5 AUTOMATION EVENTS

Events are not supported.

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