



# amaZon Series

## Getting Started



**Bruker Daltonics**

# Legal and Regulatory Notices

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## Document History

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## Safety Class

The instrument is a Safety Class I instrument and has been designed and tested in accordance with IEC Publication 1010: Safety Requirements for Electrical Equipment for Measurement, Control, and Laboratory Use.

Class 1 LED Product

# Warnings

## WARNING

Connecting an instrument to a power source which has not equipped with a protective earth contact creates a shock hazard for the operator and can damage the instrument. Likewise, interrupting the protective conductor inside or outside the instrument or disconnecting the protective earth terminal creates a shock hazard for the operator and can damage the instrument.

## WARNING

The instrument has to be disconnected from its power source before the inner cover is removed or the instrument is otherwise opened

All connections of the instrument have to be used in correct way.

It is only permitted to use wires and cables provided by the manufacturer.

## Noise Declaration

Deutsch

LpA<< 70 dB am Arbeitsplatz normaler Betrieb nach EN 27779: 1991

English

LpA<< 70 dB operator position normal operation per ISO 7779: 1988

## Limitations on Use

**For Research Use Only (RUO). Not for use in diagnostic procedures.**

## Hyperlink Disclaimer

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## Safety Symbols

### GENERAL WARNING



This symbol is placed on the product where it is necessary for you to refer to the manual in order to understand a hazard.

### ELECTRICITY, ELECTRIC SHOCK



This symbol is placed on the product within the area where hazardous voltage is present or shock hazard can occur. Only trained service personnel should perform work in this area.

### HOT SURFACE



This symbol is placed on the product within the area where hot parts and surfaces are present. Allow the product to cool before performing work in this area.

### BIOLOGICAL HAZARD



This symbol is placed on the product within the area where biohazards are present. Handle these areas with the appropriate care.

### SHARP HAZARD



This symbol is placed on the product where sharp components (e.g. thin needles) may present a hazard.

**CORROSIVE SUBSTANCES**

This symbol indicates corrosive chemicals (e.g. acids). Wear appropriate safety clothing when handling such substances.

**WARNING**

The source chamber may not be opened until the sample flow has stopped.  
Health Risk!  
Fire danger!  
Contamination of the Environment and Air!

**Additional Safety Symbols for ETD****FIRE HAZARD**

This symbol is placed on the product where extremely flammable substances (e.g. methane – CH<sub>4</sub>) may present a fire hazard. Handle these substances with the respective care. Ignition sources have to be kept away. Take precautionary measures against static discharges.  
Methane can form explosive mixtures with air.

**IRRITANT SUBSTANCE**

This symbol is placed on the product within the area where substances are present, which are harmful or irritant (e.g. fluoranthene - C<sub>16</sub>H<sub>10</sub> - or other ETD reagents). Handle these areas with the respective care. Wear appropriate safety clothing when handling such substances.

## Table of Changes

Revision	Date	Changes	Remarks
1	July 2009	First edition	-
1.1	November 2009	Minor corrections to all chapters	-

### Instrument Identification

Each instrument is identified by two unique serial numbers. These serial numbers are located on a label on the lower left side near the rear of the instrument.

When corresponding with Bruker Daltonik GmbH about your instrument, be sure to include the model number and the full serial number.

Write the serial number of your instrument here for reference:

**Serial #:**

### Manual Conventions

### Cautions

Cautions call attention to procedures which, if not correctly performed or adhered to, could result in damage to the instrument.

### Warnings

Warnings call attention to procedures which, if not correctly performed or adhered to, could result in personal injury.

### Part Numbers

In this manual, Bruker Daltonik GmbH part numbers are generally listed in parentheses after the name of the part or in tables in the parts chapter.

A few tools and supplies listed have no part numbers and are not available from Bruker Daltonik GmbH. Most of these can be obtained from laboratory supply companies.

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# 1 Starting Up the Instrument

This document provides a quick start up procedure for the amaZon instrument. This takes a system in Shutdown state through acquiring data to postprocessing and getting results. More detailed information is given in the instrument user manual.

## 1.1 Requirements

The following requirements must be met:

- The instrument has been properly installed by Bruker Service and is operational.
- The base calibration of the instrument is correct.
- The vacuum and helium conditions are within the specified range.
- The ESI-source is mounted on the instrument.
- trapControl software has been properly installed on the computer.

## 1.2 Starting the Computer

### 1) Switch on the computer.

Windows XP starts up.

### 2) Login with your user name and password, press Return.

If several users are installed, login with the correct username and password.

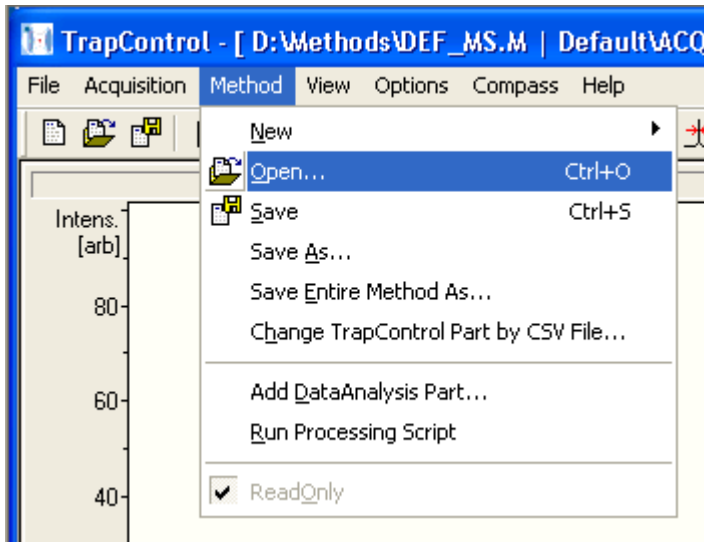
### 3) The desktop with its icons is then displayed.



## 1.3 Starting the Software

- 1) Start the trapControl software by clicking on the desktop icon or via the start button in the task bar Start > Programs > Bruker Daltonics > trapControl.
- 2) Load the default method (DEFAULT.ms).

This is done via the menu using **Method > Open** or by using the **Ctrl +O** shortcut.



## 2 Introducing a Sample

### 1) Prepare a sample.

**Material:** TuneMix (# 18220)  
HPLC grade acetonitrile e.g. #208543  
HPLC grade water e.g. #49145

Prepare a 1:100 dilution of TuneMix in a solvent mixture of 95% acetonitrile and 5% water. For a 50 mL stock solution mix:

TuneMix	0.5 mL
Water	2.5 mL
Acetonitrile	47.0 mL

### WARNING

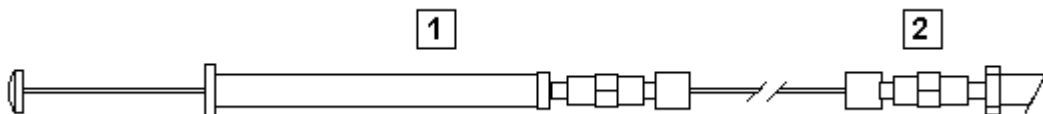


The amaZon series ion traps are very sensitive instruments. To avoid memory effects do not use TuneMix concentrations above 1:100.

### 2) Prepare sample infusion.

Fill the sample syringe with the TuneMix stock solution. Ensure that no air bubbles are present in the syringe.

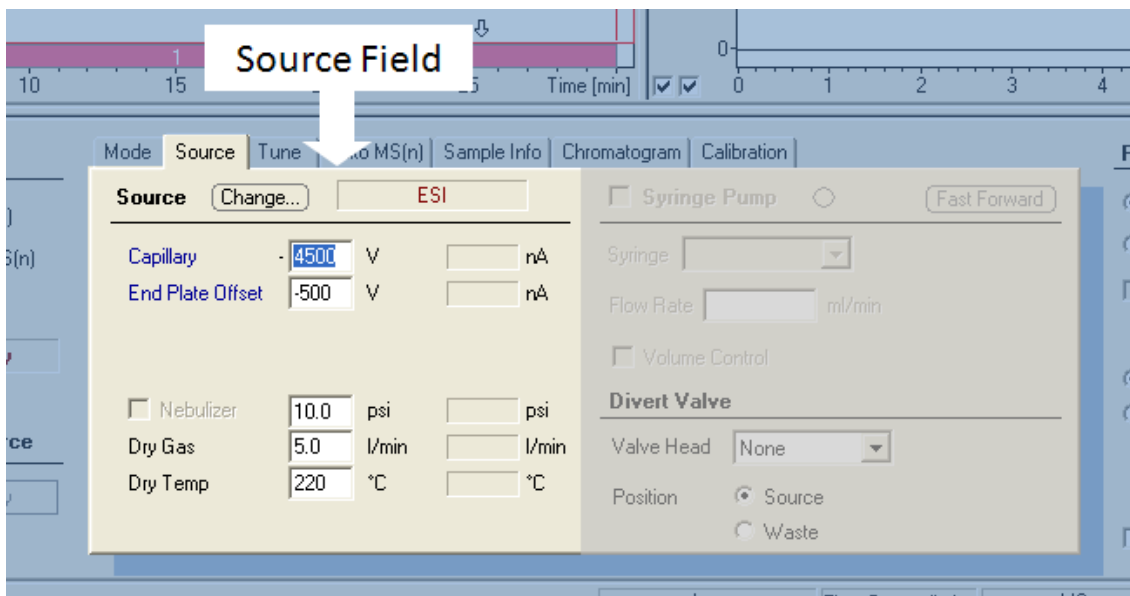
Insert the syringe into the syringe pump and connect it to the nebulizer (2). Ensure that all connections are leak-tight.



## 3 Obtaining a Spectrum

### 3.1 Setting the Ion Source Conditions

1) Set the parameter values in the Source field on the Source page.



The following parameter set is recommended for sample infusion with a syringe pump and typical flow rates between 120  $\mu\text{L/h}$  – 240  $\mu\text{L/h}$ :

- ⇒ Nebulizer      5 psi – 15 psi
- ⇒ Dry Gas        5 L/min
- ⇒ Dry Temp      200 °C

For LC-infusion at flow rates between 100  $\mu\text{L/min}$  – 500  $\mu\text{L/min}$ , the following parameter set is recommended.

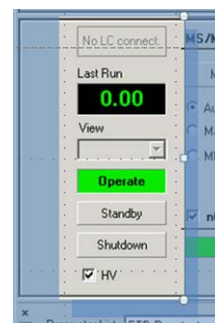
- ⇒ Nebulizer      20 psi – 35 psi
- ⇒ Dry Gas         $\approx$  10 L/min
- ⇒ Dry Temp      250 °C

In general, source conditions depend on the specific application and should always be optimized for best results.

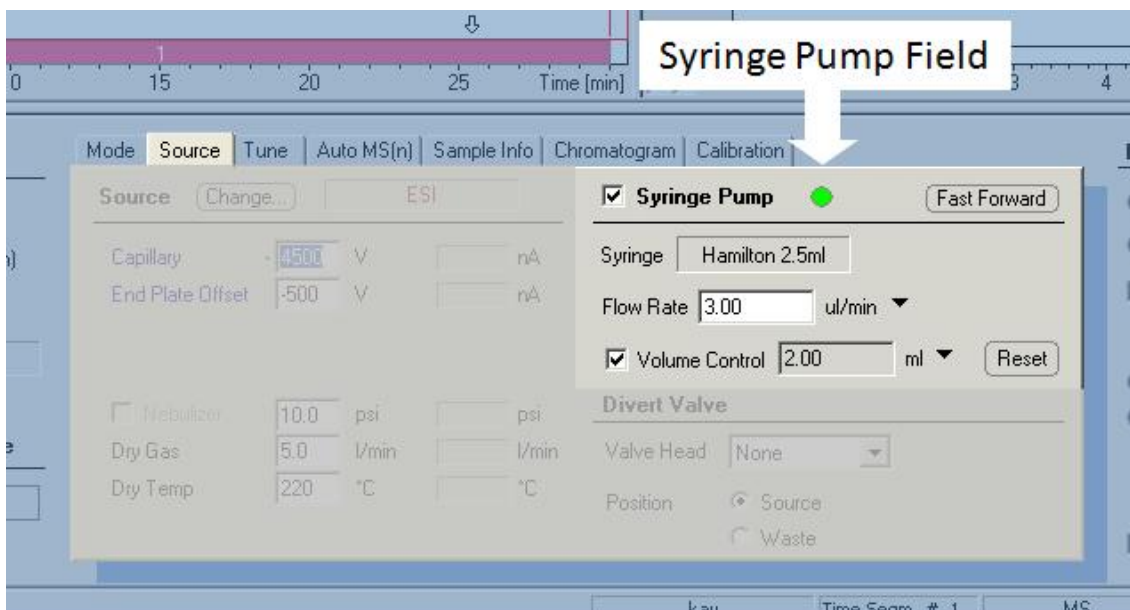
## 3.2 Switching to Operate Mode

### 1) Go to the Main panel.

Click on the **Operate** button. The button will turn green and the instrument is fully powered up.



### 2) Set the parameter values in the Syringe Pump field on the Source page.



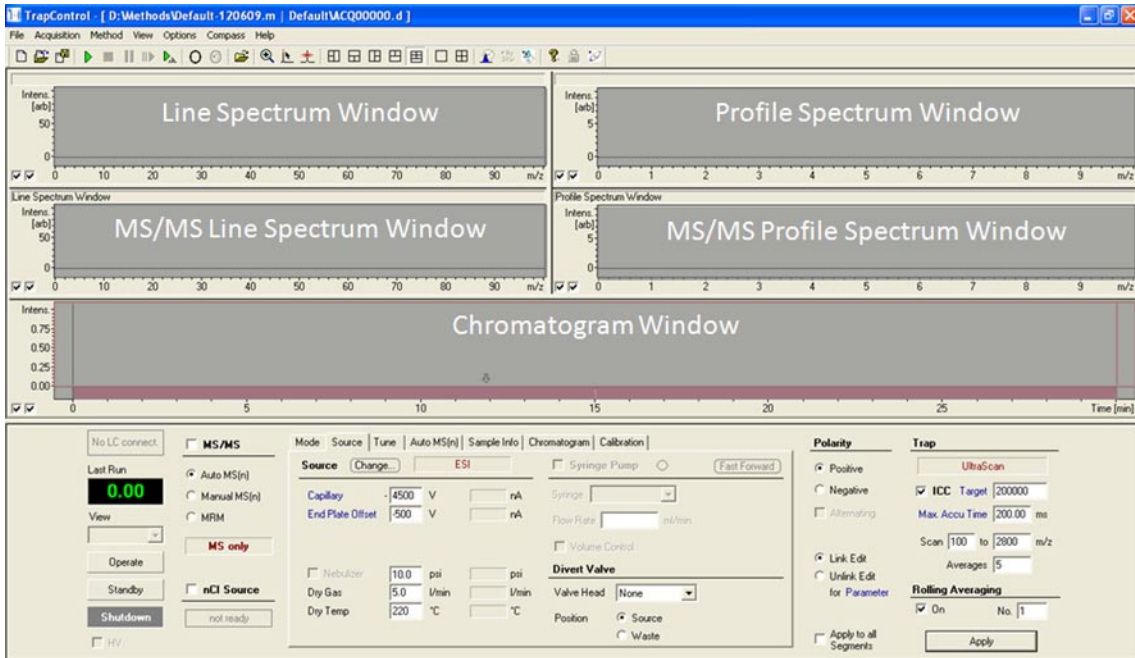
- Select the syringe size from the drop-down menu or select User Define to utilize a non-standard syringe.
- Set the flow rate to 3  $\mu\text{L}/\text{min}$ .
- If the syringe pump is to be left unattended, check the checkbox and set the volume control to an appropriate figure below the maximum capacity of the syringe.

### 3) Switch on the flow of the syringe pump.

Click the **Syringe Pump** check box (the indicator will turn green).



Allow the Nebulizer Gas, the Dry Gas and the Dry Temp to reach stable values.



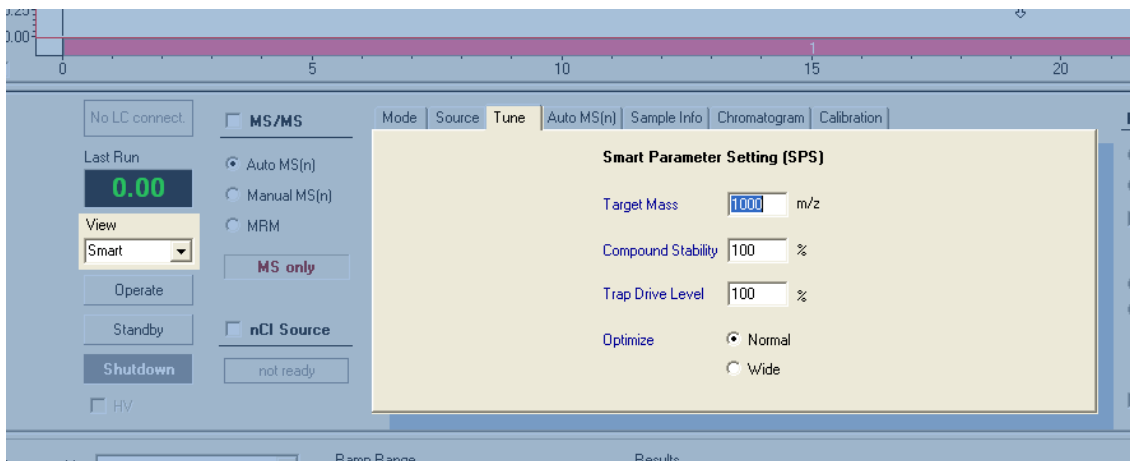
## Windows

- Top left** The Line Spectrum Window shows the identified peaks in the mass spectrum
- Top right** The Profile Spectrum Window displays the original mass spectrum as measured
- Middle left** Displays the MS/MS Line Spectrum
- Middle right** Displays the MS/MS Profile Spectrum
- Bottom** The Chromatogram Window displays the ion trace(s) over time and segments


## 3.3 Setting the Target Mass

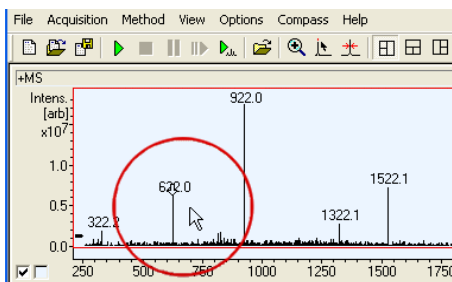
### 1) Set the transfer parameters of the ion optics via the **Smart Parameter Setting**.

In the **Smart Parameters Setting (SPS)** field on the **Tune** page, enter the desired target mass.

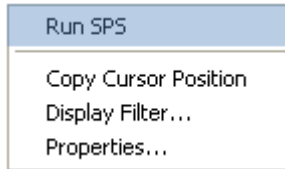


This can be done in any of the following ways:

- ⇒ Manually by using the keyboard to enter a value in the **Target Mass** numeric entry field
- ⇒ Using the mouse wheel to increment the value up or down (the incremental steps can be increased by holding down the **Shift** or **Ctrl** key)
- ⇒ Using peaks in the line spectrum window. To do this:
  - a) Activate the maximum cursor in the toolbar  or F10 or **View > Maximum Cursor**
  - b) Left mouse click next to the selected peak in the line spectrum window



- c) Right mouse click next to the peak in the line spectrum window and select Run SPS in the context menu.



- d) **Run SPS** (Smart parameter Settings) copies the cursor position into the Smart target field.

## 3.4 Save Method as...

### 1) General method handling.

The toolbar has three buttons for handling a method.

The **New Method** icon generates a new method. The default settings are loaded as start parameters.

The **Open Method** icon displays the Open Method dialog;

The **Method Save** icon is for saving a method. The **Ctrl + S** shortcut also saves the method.

### 2) Save the created method under a new name.

The method can be saved under a new name, such as `NEWMETHOD.MS`, by using **Method > Save Method as....**

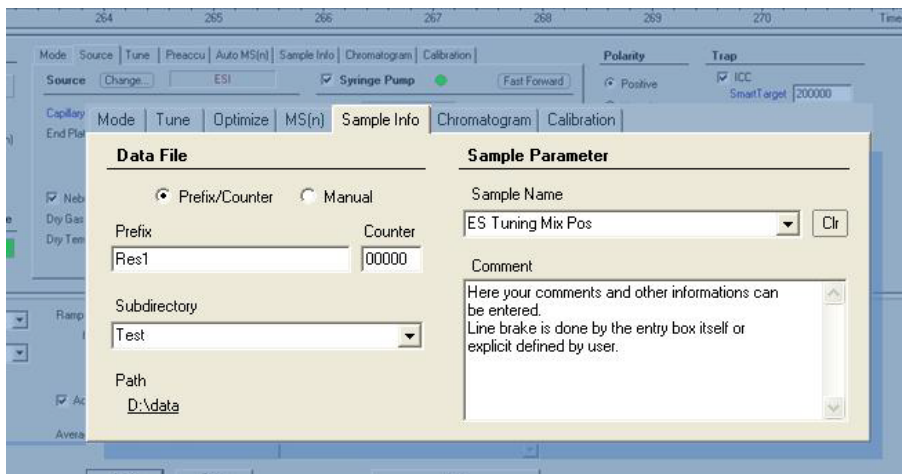
The default method is read-only and can not be changed. Therefore, all changes must be saved under a new method name.

## 4 Acquiring Data

### 4.1 Entering Sample Info

1) Enter information about the sample on the Sample Info page.

This information will be saved with the spectrum data for later review. Open the Sample Info page.




2) Enter the Filename information.

In the **Data File** field click on the **Prefix / Counter** radio button, enter a prefix and counter for the file name, and type in the name of a new subdirectory. Enter a description of the sample in the **Comment** field and enter a **Sample Name** in the **Sample Parameter** field if desired. The **Comment** and the **Sample Name** entered here will be displayed in the **Analysis Info** window in Bruker Daltonics DataAnalysis program (see section 5).

3) To accept the information, press “Enter” on the keyboard.

### 4.2 Acquiring a Single Spectrum

1) Save single mass spectrum.

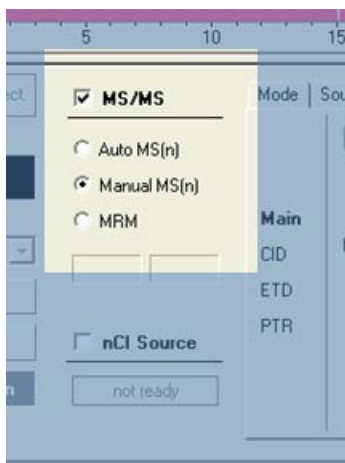
Save the desired mass spectra by using the toolbar button .

2) The saved file will be named Res10000 .d.

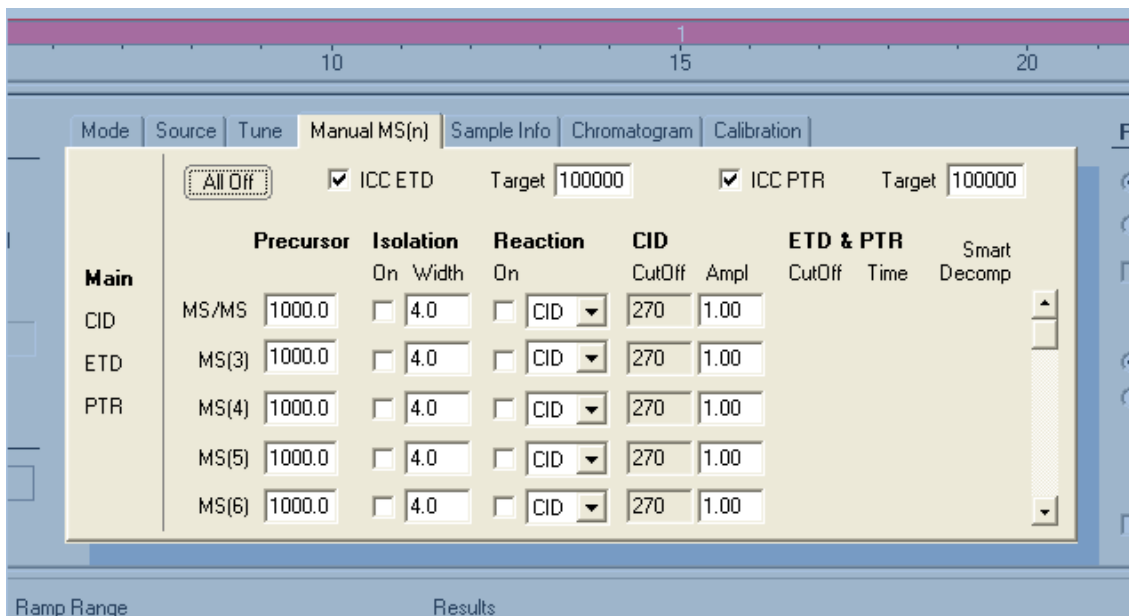


## 4.3 Acquiring an MS/MS Spectrum


- 1) Click on the Manual MS(n) radio button.



- 2) Click on the Manual MS(n) tab to open the page.



- 3) Select an ion in the line spectrum window to fragment.

This can be done with the maximum cursor from the toolbar  or **F10** or **View > Maximum Cursor**.

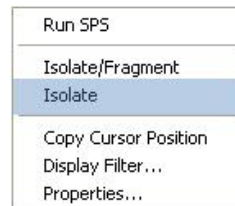
**4) Double click in the line spectrum window to the right of the relevant peak.**

The mass will be centered in the profile spectrum window.

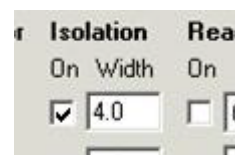
**5) Enter the isolation mass, with an isolation width of 4 mass units.**

**6) Right click on the line spectrum window to open the context menu and select Isolate.**

The previously selected mass will be set as the isolation mass.



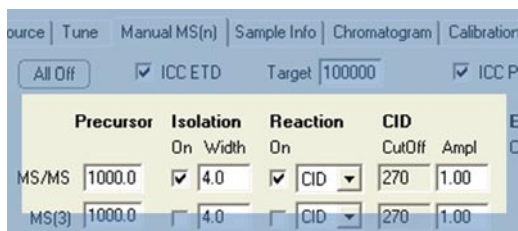
The check box for stage 1 isolation will be automatically checked.



**7) Check that the ion is isolated and all other ions in the line spectrum window disappear.**

**8) Switch on fragmentation.**

Ensure that the Reaction drop-down menu is set to CID fragmentation and switch on fragmentation by clicking on the checkbox.



**9) Optimize the spectrum by adjusting the Fragmentation Amplitude.**


Increase or decrease the amplitude in increments of 0.1 until the isolated ion is reduced to ~ 10 % of its initial intensity, and the fragment ions can be easily seen.

Enter a new amplitude using one of these alternatives:

- ⇒ the keyboard,
- ⇒ the scroll-bar buttons or
- ⇒ the mouse wheel.

**10) Save single mass spectrum.**

Save the desired mass spectra with one of these alternatives:

- ⇒ toolbar button ,
- ⇒ shortcut **F7**,
- ⇒ or **Acquisition > Save Profile Now**.

**11) The saved file will be named Res100001.d.****12) Enter another mass for isolation (e.g. 922) and fragmentation and save the mass spectrum again. The saved file will be named Res100002.d.****13) Turn off the isolation / fragmentation.**


Click **All Off** on the **Manual MS(n)** page.



## 4.4 Chromatogram Data


**1) Save chromatogram data.**

To obtain the chromatogram data, start the acquisition via one of these alternatives:

- ⇒ toolbar button ,
- ⇒ shortcut **F5**,
- ⇒ or **Acquisition > Run Method**.

**2) The default runtime stop is 30 min.**

The method can be stopped manually via one of these alternatives:

- ⇒ toolbar button ,
- ⇒ shortcut **F8**,
- ⇒ or **Acquisition > Stop Run**.

## 5 Postprocessing

### 5.1 Opening an Analysis File

Switch to the DataAnalysis program via the task bar or using the toolbar button .

#### Load the acquired data file

The data file is loaded into the DataAnalysis program via the **File > Open...** dialog or the shortcut **Ctrl + O**. A display window is opened by the program.

In the **File > Open** dialog, go to the directory `d:\data\test` and open the files `Res100000.d`, `Res100001.d`, and `Res100002.d` by double-clicking on them. To open all files simultaneously, hold down the **Shift** key and highlight them all before pressing **Enter**.

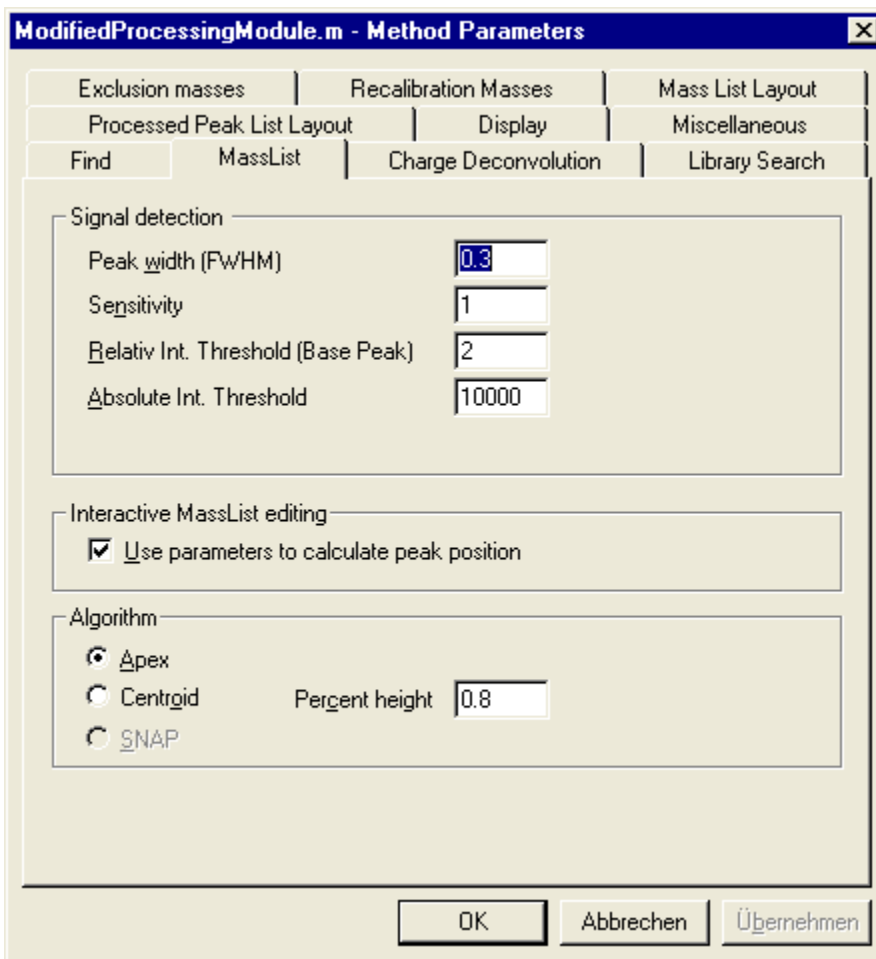
Mass spectra and chromatogram spectra are loaded by name and shown in the **File** menu.

When the desired trace is selected in the **Analysis List** window, the spectrum is activated in the appropriate spectrum window.

### 5.2 Mass Spectra

Changing the detection of mass peaks is performed using the **MassList > Parameter** dialog:

The following dialog is used to set the new parameters for detecting mass peaks in the spectrum.



For further information about creating and modifying Method parameters, see the *Bruker Daltonics DataAnalysis User Manual*.

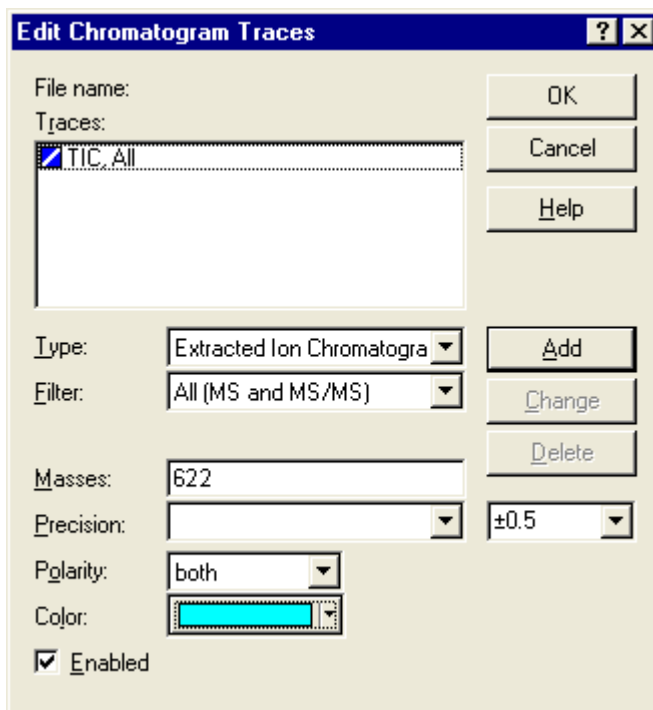
## 5.3 Chromatogram Data

### 1) Full scan chromatogram.

Load the data file (e.g. Res100003.d). The TIC (Total Ion Chromatogram) is displayed.

To extract a single ion chromatogram open the Edit Chromatogram Traces dialog via the menu **Edit** and select the **Chromatograms..** option.

You can use also the **F7** shortcut to open the **Edit Chromatogram Traces** dialog.



For this example extract the trace 622. For other chromatograms type in the desired masses of the desired extract.

Click **Add** to create a new trace and then click **OK**.

To change the properties of an existing trace, select that trace with the cursor, enter the changes, and click **OK** to confirm the changes to the trace.

## 2) Generate a peak list with Find Compounds.

A quick and effective way to generate a peak list is to use the **Find... Compounds** function.

The **Compounds > Chromatogram** function (shortcut: **Ctrl + F2**) generates its own chromatographic trace and generates the peak list on the trace. The Compound Mass Spectra window is opened. A mouse click on this spectra window opens the tree view showing all compounds.

The **Compounds > MS(n)** function generates all traces for the MS(n) steps used and generates the peak list.

The **Compound > AutoMS(n)** function generates the trace for MS- and MS/MS-chromatograms.


## 6 Reporting


To generate informative reports from your data, a variety of report layouts are available.

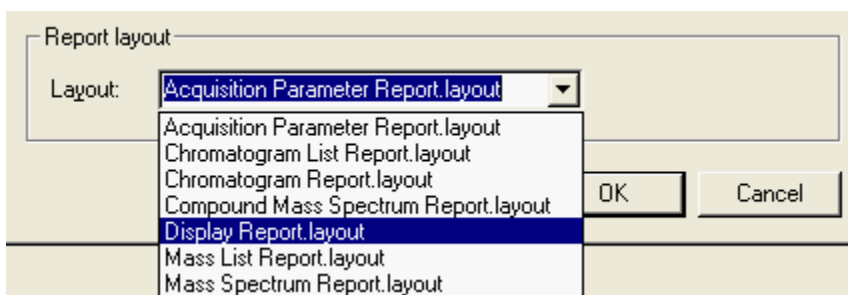
**To print directly, select:**

- ⇒ the Print button 
- ⇒ the menu **File > Print** or
- ⇒ the shortcut **CTRL + P**

**To print via the print preview, select:**

- ⇒ the Print Preview button  or
- ⇒ the menu **File > Print Preview**.

In the **Report Preview** window select the print button  to print the file. The Report layout list shows all available report layouts. The available report layouts depend on your local installation.



### 6.1 Acquisition Parameter Report

Select this layout to print the acquisition parameters of the selected analysis.

### 6.2 Display Report

Select this layout to print the currently displayed windows (Chromatogram window, Mass Spectrum View window, Compound Mass Spectra window, Mass Spectrum window).

## 6.3 Mass Spectra

The following report layouts are available.

### **Mass List Report**

Select this layout to print the Mass List Report of the selected mass spectrum.

### **Mass Spectrum Report**

Select this layout to print the Mass Spectrum Report of the selected mass spectrum.

## 6.4 Chromatogram Data

The following report layouts are available.

### **Chromatogram List Report**

Select this layout to print the Chromatogram List Report of the selected chromatogram.

### **Chromatogram Report**

Select this layout to print the Chromatogram Report of the selected chromatogram.

### **Compound Mass Spectrum Report**

Select this layout to print the Compound Mass Spectrum Report of the selected chromatogram.



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