Triple Quadrupole MS Methods

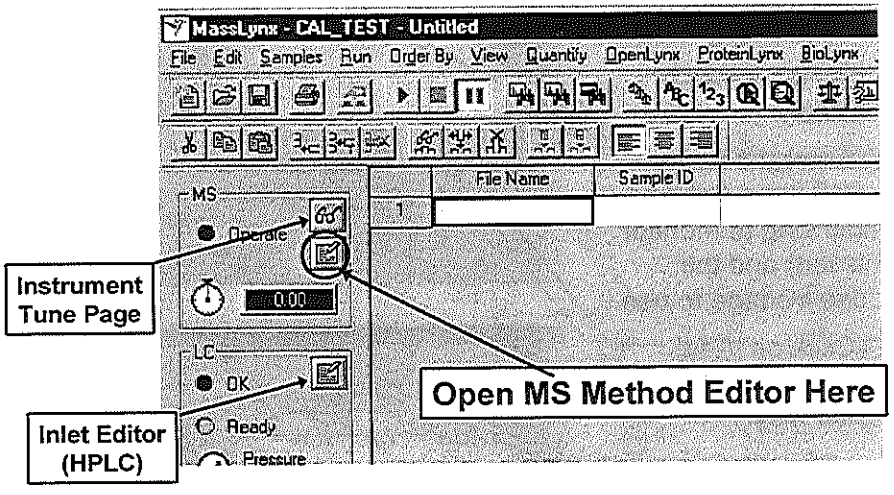
Quattro LC

Quattro Ultima

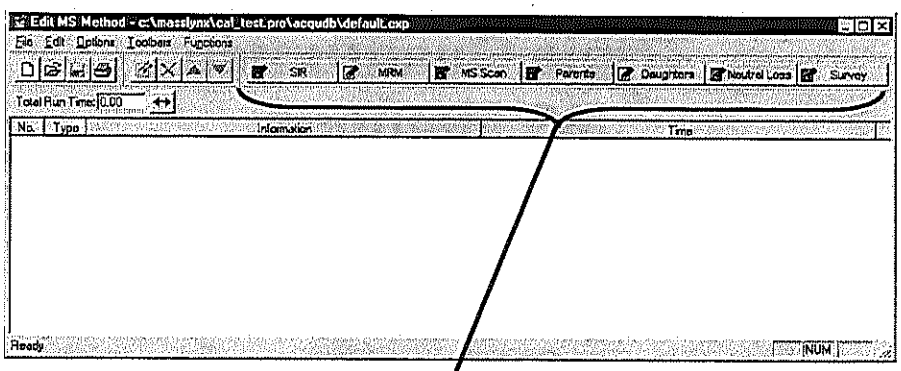
Quattro micro

2A26

Open Up the MS Editor



MS Editor Window



Use these 'Buttons' to Add Functions. There is a different function type for each type of data acquisition (SIR, MRM, etc.)

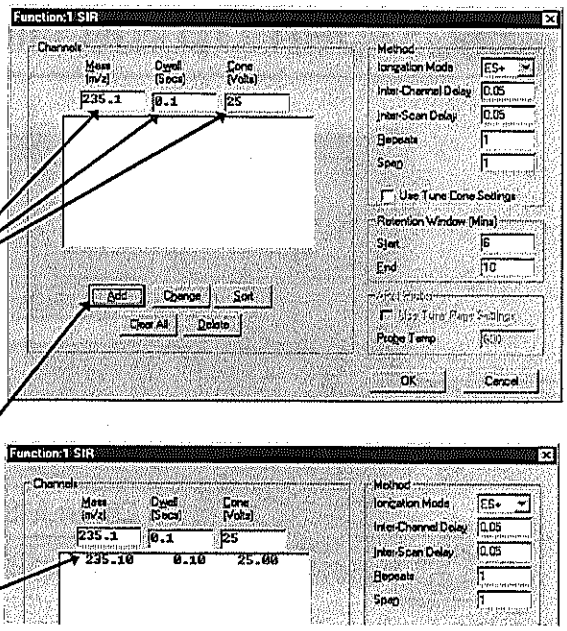
Selected Ion Recording (SIR)

To Add a Ion to Monitor:

1) Enter the Mass (m/z), the dwell time (how long to monitor this ion) and the Cone Voltage to use.

2) Click on 'Add'. Do not press the 'Enter' key.

The desired ion will appear in the table.

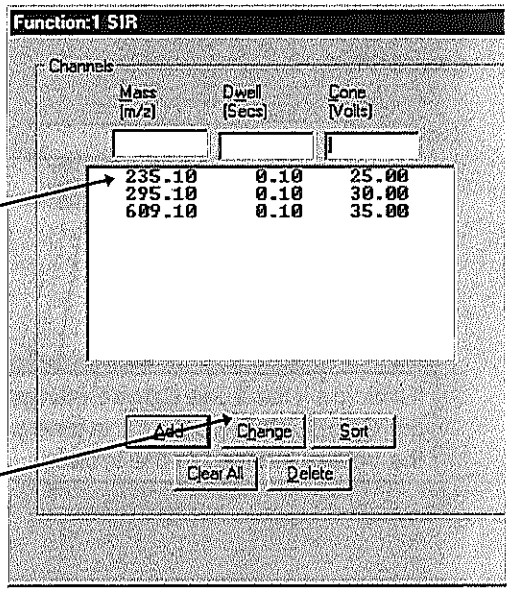


Selected Ion Recording (SIR)

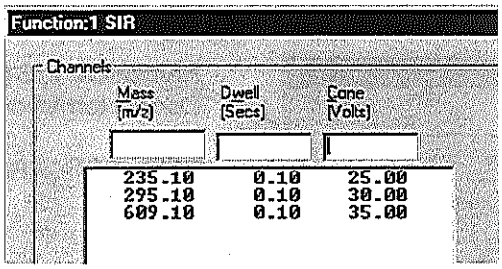
Additional ions that need to me monitored can be added to table.

In this example, this SIR function has 3 channels. A different ion will be monitored in each channel.

To edit a channel, 'double click' on the channel, edit the values and click on 'Change'.



Dwell Times (SIR or MRM)

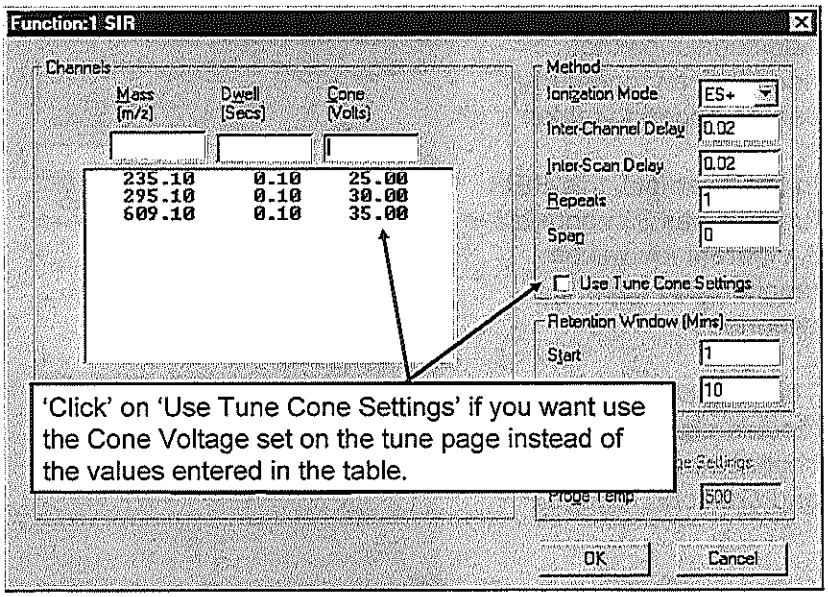


Dwell time is the amount of time the quads "lock" onto the selected mass.

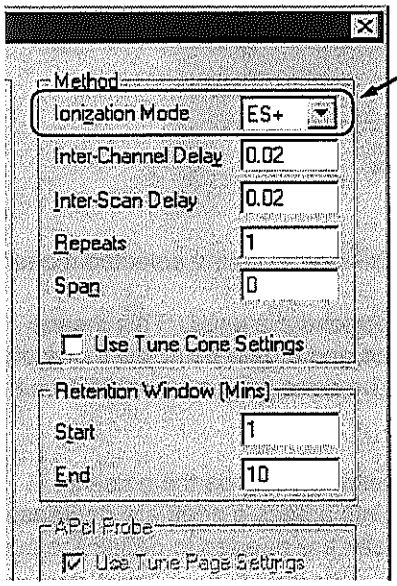
In the above example, dwell times of 0.1 second are used. This means m/z=235.1 will be monitored for 0.1 second and a data point will be recorded for the m/z=235.1 channel. This will then be done for the m/z=295.1 channel, and finally for the m/z=609.1 channel.

Longer dwell times translate to better sensitivity (S/N) as the noise is 'averaged' out, but the number of data points across a peak are decreased. 12-15 points across a chromatographic peak are needed to define the peak.

Selected Ion Recording (SIR)



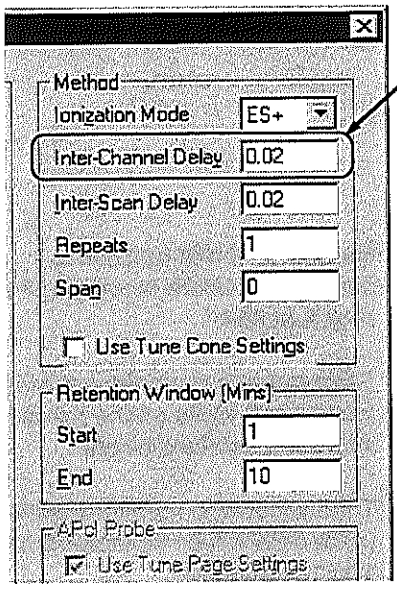
Selected Ion Recording (SIR) Function



Remember to Select the Correct Ion Mode !!!

ESI +, ESI -, APCI + or APCI -

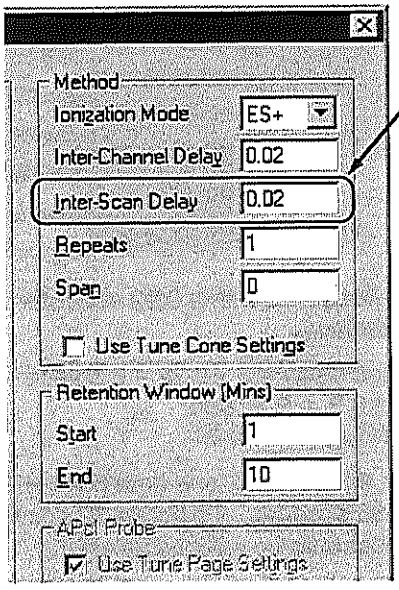
SIR Method: Interchannel Delay



Background: The system monitors one mass (m/z) for a time specified as the dwell time and records a data point for that mass. Before the system can move on and start to monitor the next mass in the list, a short amount of time is needed to reset the electronics and clear the ions from the just measured mass out of the system. This time between the masses listed in a function is called the 'Interchannel Delay'.

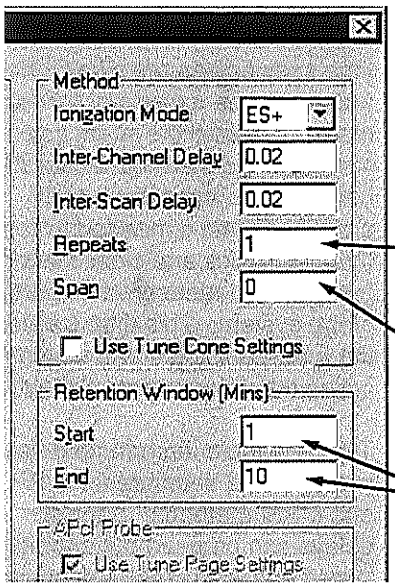
Typically the interchannel delay is set to 0.02 seconds for SIR and MRM methods. Shorter delays can be used but should be tested first (min of 0.01 seconds).

SIR Method: Inter-Scan Delay



Time Between Functions:
In MS Methods were there is more than one function (e.g. a Positive Ion ES SIR function and a Negative Ion ES SIR function), the time when function stops recording data till the next function starts recording data is specified here. If you a method with both positive ion and negative ion functions (switching ion polarity between functions), the interscan delay should be at least 0.3 seconds. Other wise you can use the time specified for the 'interchannel delay' for the 'interscan delay'.

Selected Ion Recording (SIR) Function

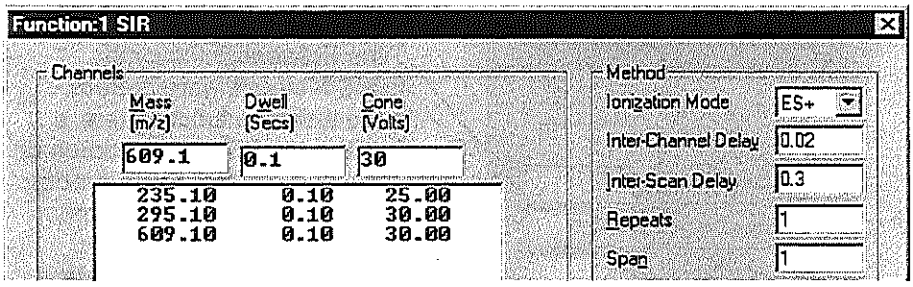


Number of times function is carried out before moving to the next function.

Scan range around the set mass, a span of 0 locks on the mass of interest (best sensitivity).

Time window to monitor function. (here data will be collected from 1 to 10 minutes)

More On Inter-channel delay, & Inter-scan-delay (SIR or MRM)

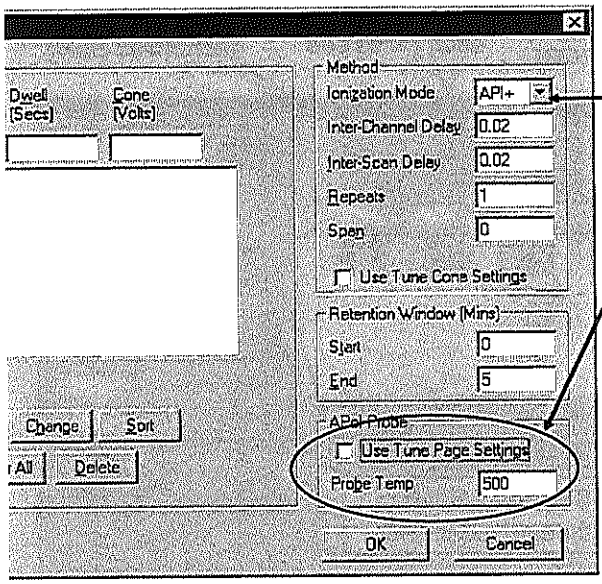


In the above example we have 0.2 sec Dwell times with a 0.02 sec Inter-Channel Delay and a 0.3 sec Inter Scan Delay.

3 compounds with 0.2 sec Dwell + 0.02 sec delay = 3 x 0.22 = 0.66 sec
Inter Scan Delay = 1 x 0.3 = 0.30 sec
Total Function Cycle Time = 0.96 sec

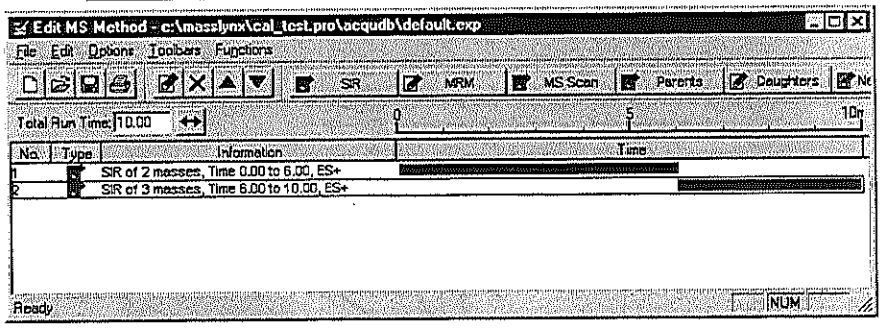
So assuming there is only one function in this method, one data point will be collected for each compound every 0.96 seconds. To obtain 12 points across a peak, the chromatographic peak should be approximately 12 seconds wide.

Selected Ion Recording (SIR) - APCI



For APCI runs specify a probe temperature or check the box to use the tune page settings

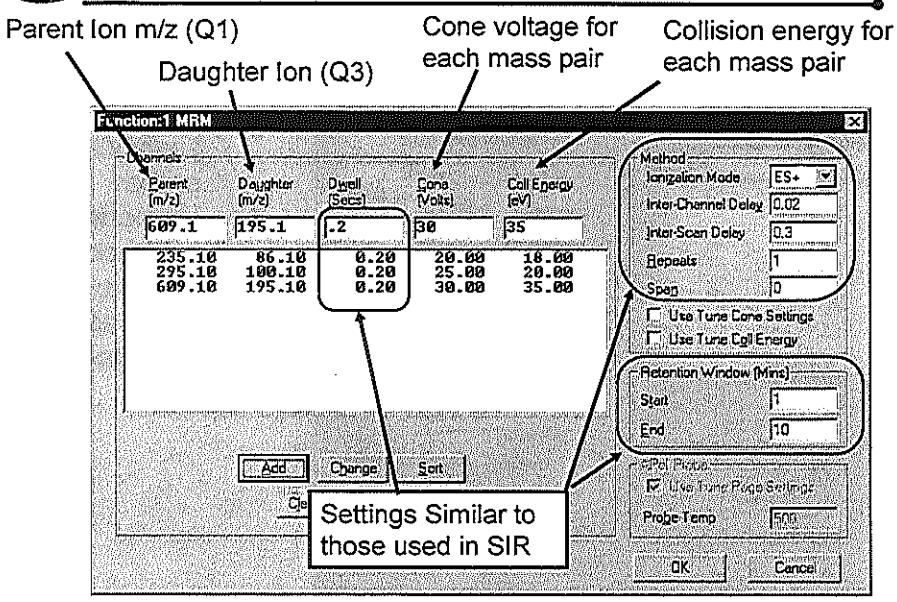
Multiple Functions in One MS Method - SIR Example



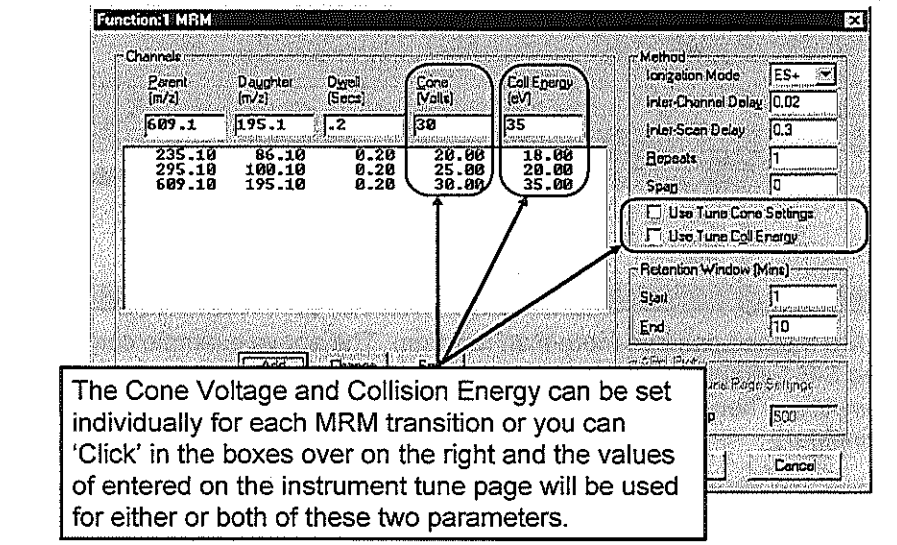
A MS Method can can more than function. The above example contains two SIR functions. Two ions were monitored using Function 1 from 0 to 6 minutes. Then three ions were monitored by Function 2 from 6 to 10 minutes.

This example was set up for an LC run in which two components eluted early in the run and 3 components eluted late in the run. So while Function 1 is monitoring the early components time is not wasted monitoring the late eluting components (and visa versa for Function 2).

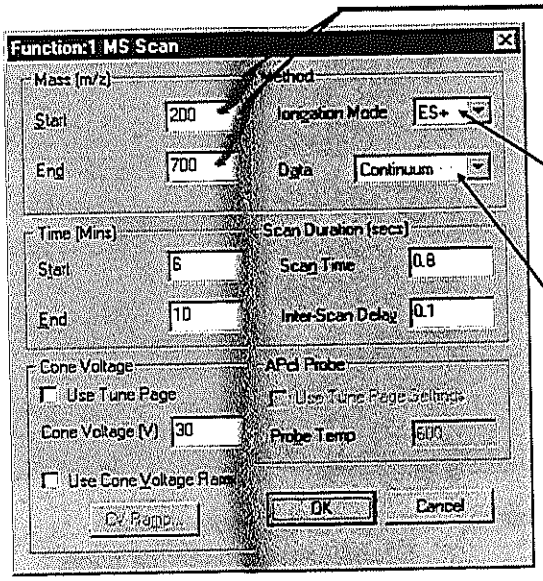
Multiple Reaction Monitoring (MRM)



Multiple Reaction Monitoring (MRM)



MS Scan

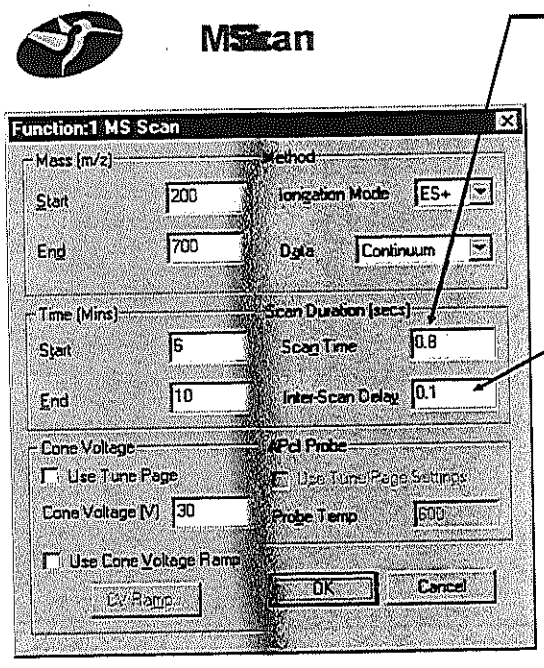


Scan Range
(for this example
m/z=200 to 700 Da)

Choose ES or APCI,
Positive or Negative
Ion

Choose the type of
spectrum desired:
Centroid, Continuum,
or MCA

MS Scan



Scan time: the amount of
time to scan from start
mass to end mass.
Be sure that the scan rate
(amu/sec) is within the
calibrated scan range.
This example is scanning:
500 amu / 0.8 sec =
625 amu/sec.

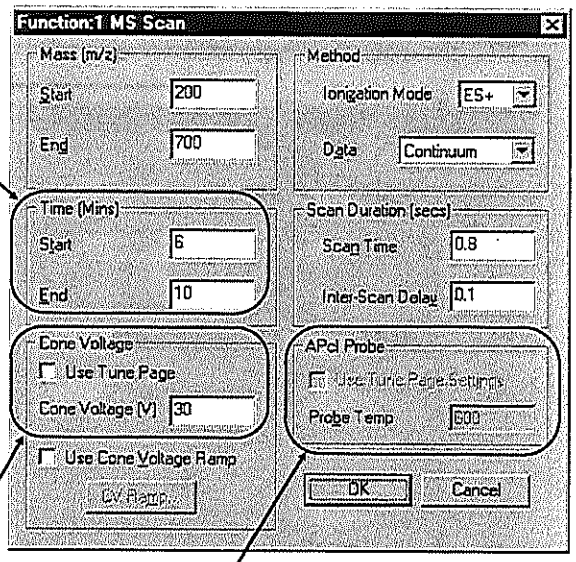
Time Between Scans.

Total cycle time =
Scan Time +
Inter-Scan Delay =0.9 sec

So for this example a
spectrum from 200 to 700
Da will be taken and
stored every 0.9 seconds.

MS Scan

Time window for function -usually +/- 1 min of the retention time of the compound of interest



Specify a cone voltage or use tune setting

For APCI specify a probe temperature or use tune page.

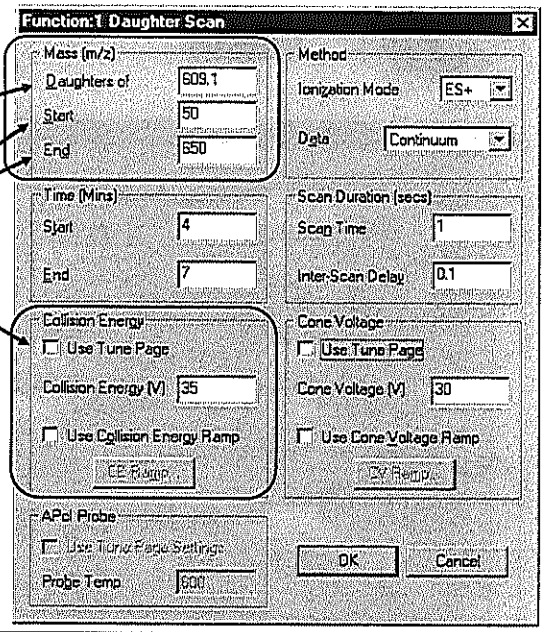
Daughter Scan

Set Mass for MS1 (Parent mass)

Scan range for MS2

Specify a collision energy or use the value entered on the tune page

For this example, a spectrum of the daughter ions of the m/z=609.1 Da parent ion will be obtained using a collision energy of 35 eV.



Other Parameters are the Same as in a MS Scan

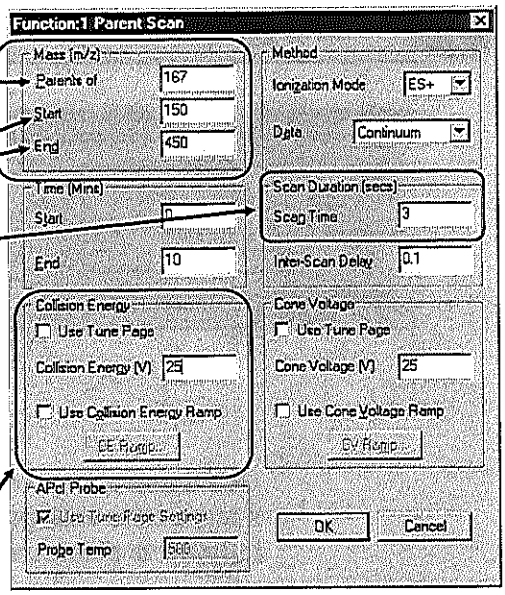
Parent Scan

Set Mass for MS2 (Common product ion)

Scan Range for MS1

Scan time: the amount of time to scan from start mass to end mass. Be sure that the scan rate (amu/sec) is within the calibrated scan range. Parent scans are best done with a slow scan rate ~100 amu/sec

Specify a collision energy or use tune page setting



Other Parameters are the Same as in a MS Scan

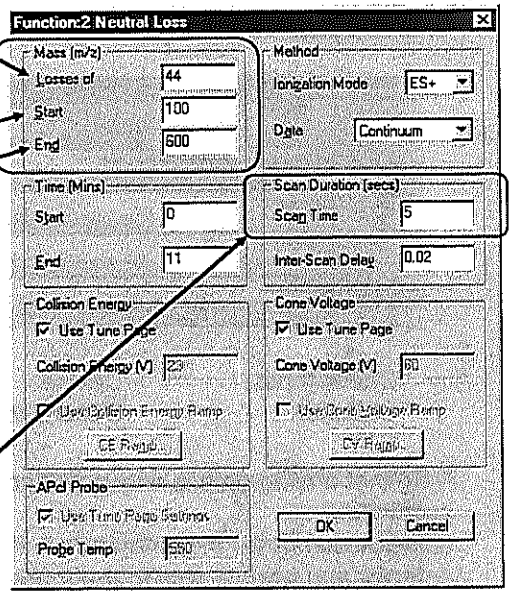
Neutral Loss Scan

Mass offset between scan mass of MS1 and MS2

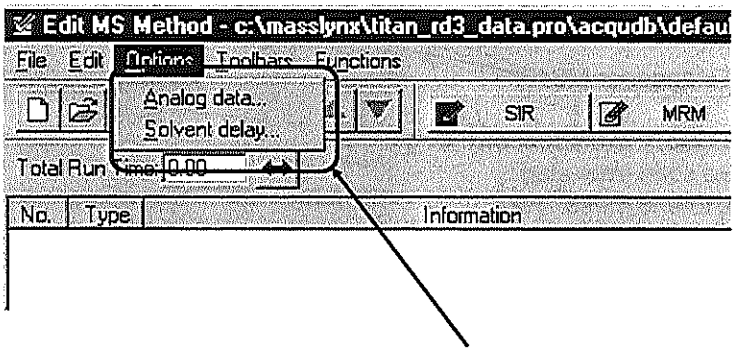
MS1 will be scanned over the specified range:
Start mass of MS1 Range
End mass of MS1 Range

Start mass of MS2 will be the MS1 start mass minus the expected mass loss. End mass of MS2 will be the MS1 end mass minus the expected mass loss (here MS2 will be scanned from 56 to 556)

Other parameters are the same as in daughter and parent scans. As in a parent scan choose a scan time so that the scan rate is around 100 amu/sec.



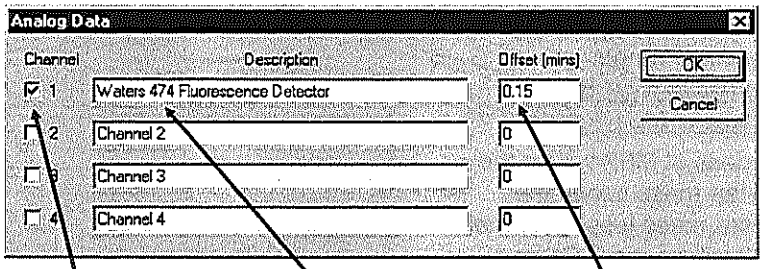
Analog Data (e.g. UV) and Solvent Delay



Use these menu items to collect 'Analog Data' such as the voltage output of a UV detector or to use the divert valve for a 'Solvent Delay'.

Analog Data: -1V to 0V or 0V to 1V

MassLynx can acquire up to 4 channels of analog data



Check Input Channel

Device Description

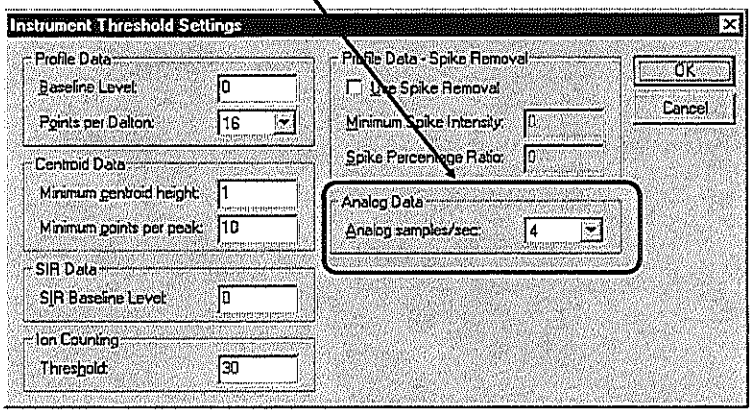
Offset Time Relative to MS

Note that analog data is only acquired while the mass spectrometer is acquiring.
Offset accounts for the difference in time when a peak gets to a analog detector and when it gets to the mass spectrometer.

Analog Data

The rate at which analog data is collected can be set by using the 'Options/Set Instrument Threshold' menu item on the mass spectrometer tune page to display the dialog box shown below.

From this dialog box, you can set the rate at which data from the analog channels is acquired.



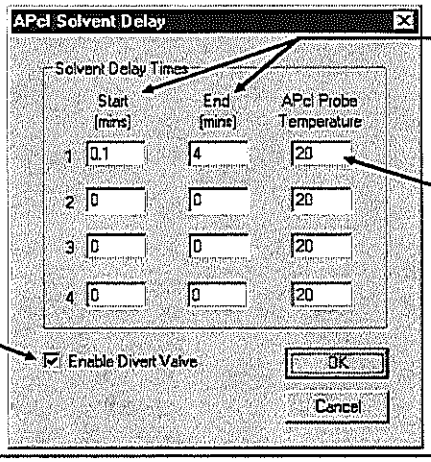
Solvent Delay - Divert Valve

A solvent delay may be set up to divert the LC flow away from the mass spectrometer. For example, the LC effluent early or late in certain analyses may contain matrix materials that might foul the sample cone or RF Lens.

Up to four divert events in one run

This controls the valve on the front of the mass spectrometer.

Make sure to check this box to enable the Divert Valve



Switch valve to MS and divert the flow between these times.

For APCI analyses, the probe temperature can be lowered while diverting to waste or use makeup flow