



# **Analyst**

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# **Software Tutorial**

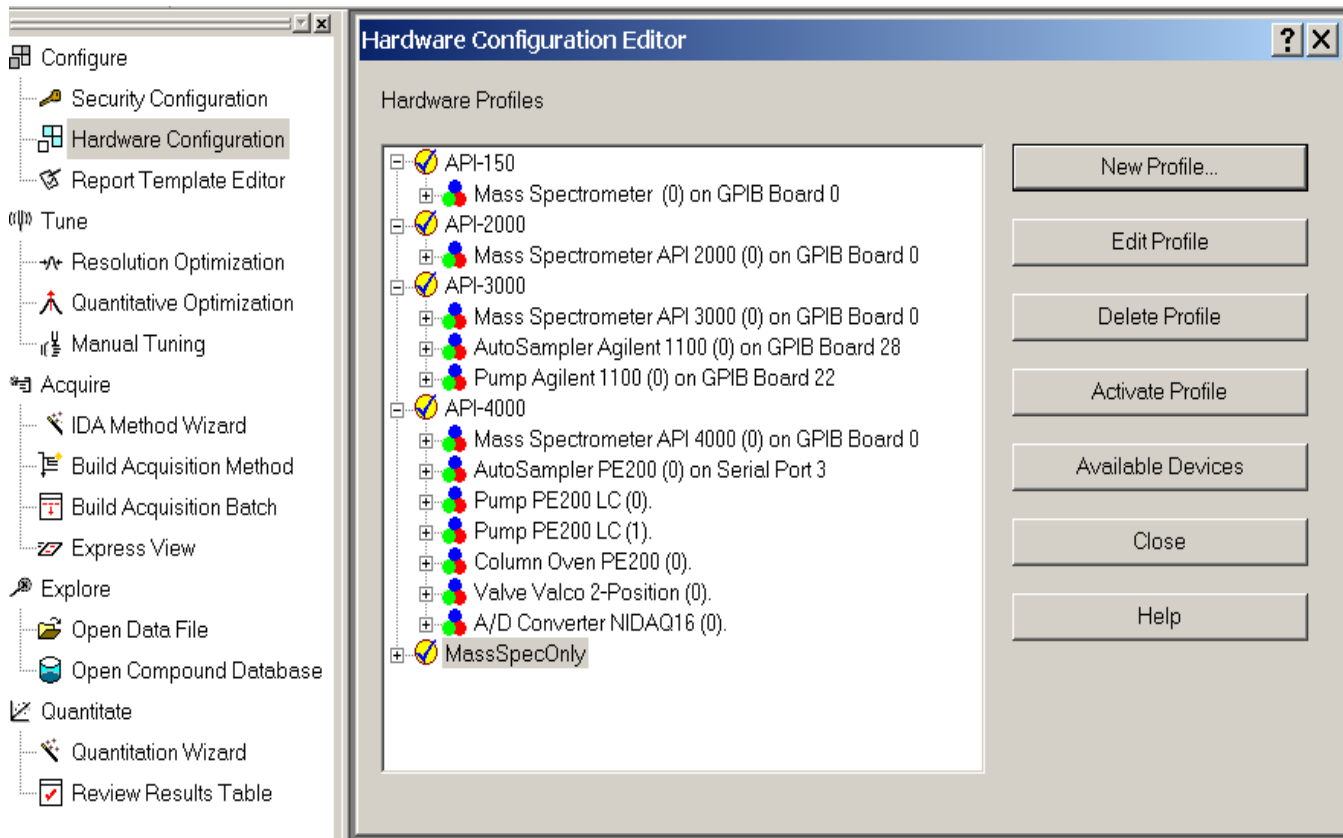
**April 10<sup>th</sup>, 2003**

# Hardware Configuration:

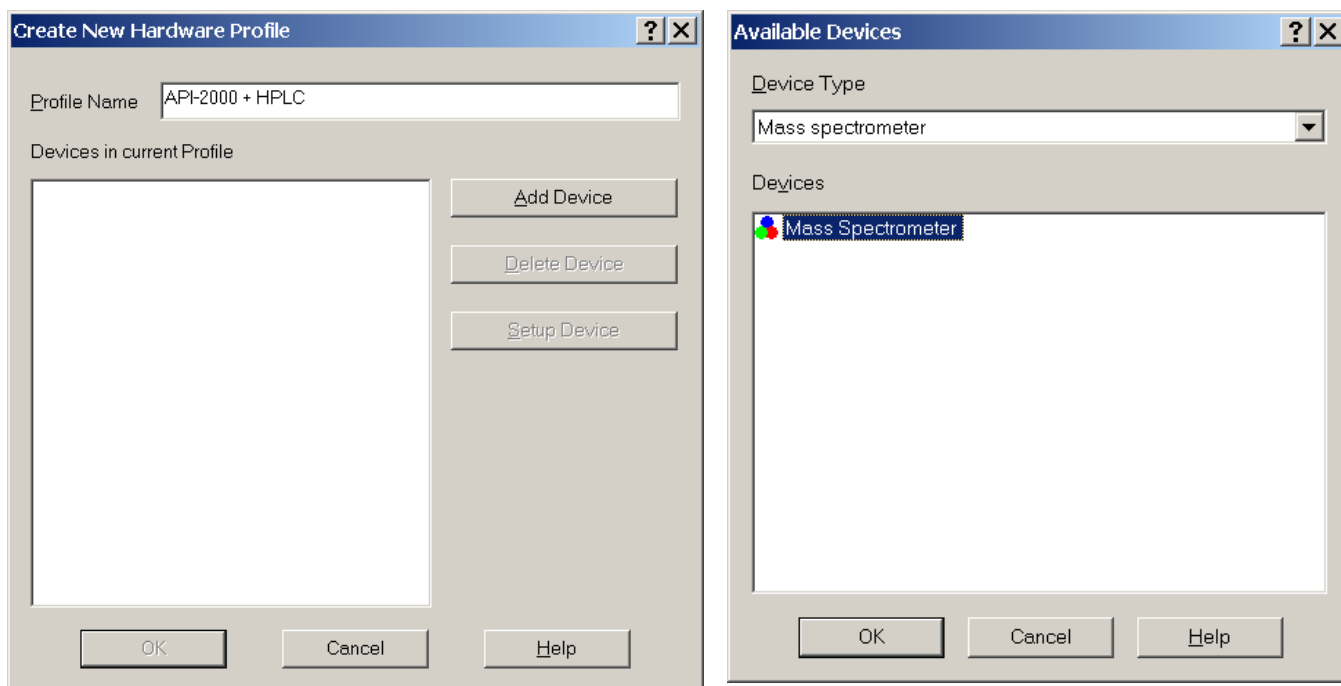
Used to connect the Mass Spec & HPLC to the Analyst computer.

## Hardware Configuration Profile Setup: (API-2000 example)

1. Open analyst
2. Double click on Hardware Configuration.
3. Highlight any running profile click Deactivate Profile. (Green check mark turns yellow).
4. Click New Profile.



5. Type **API-2000 + HPLC** for new profile name.
6. Click Add Device.
7. Choose Mass Spectrometer.
8. OK

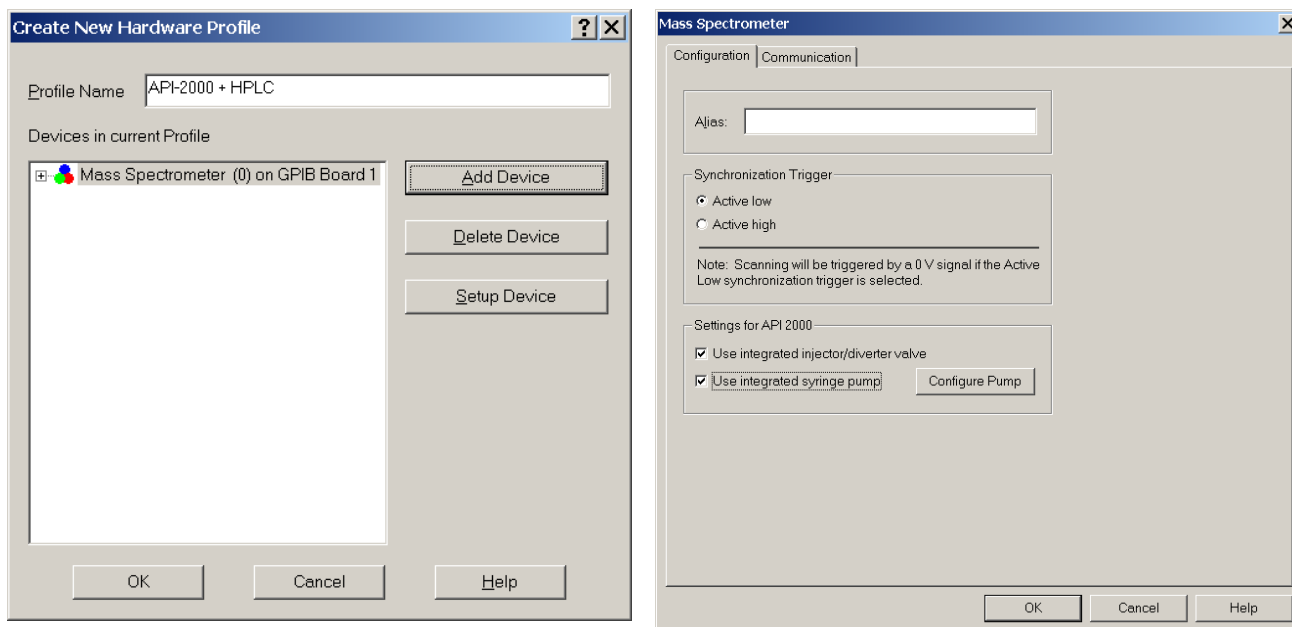


9. Click Setup Device.

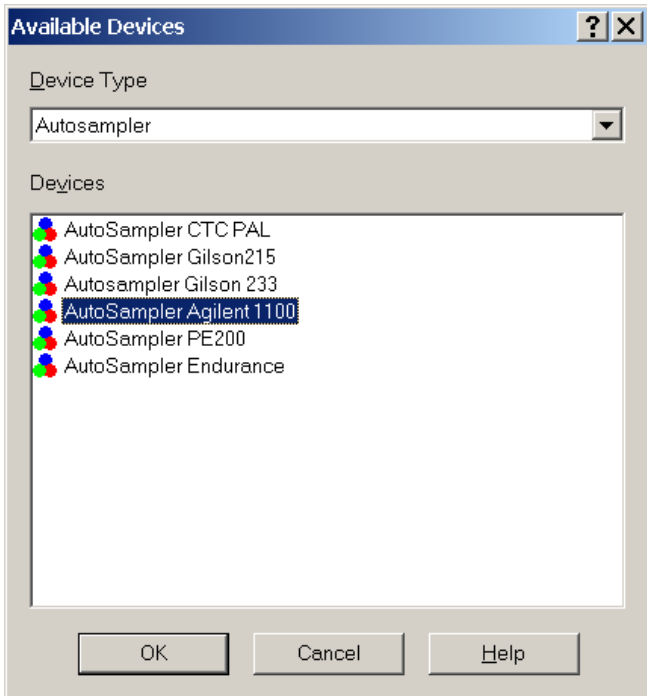
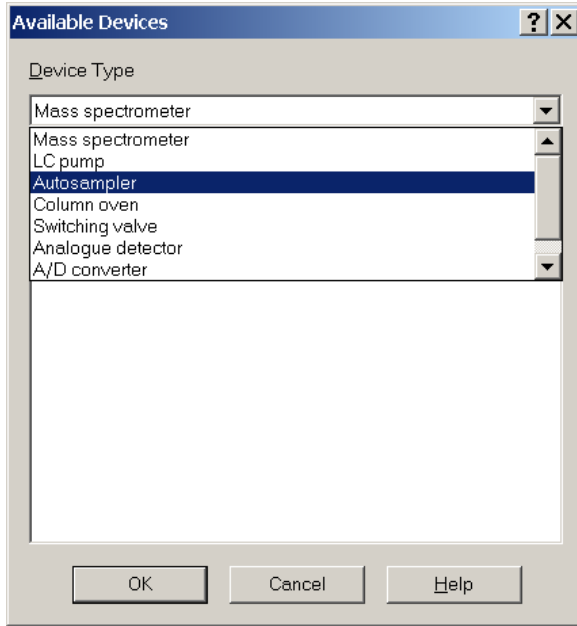
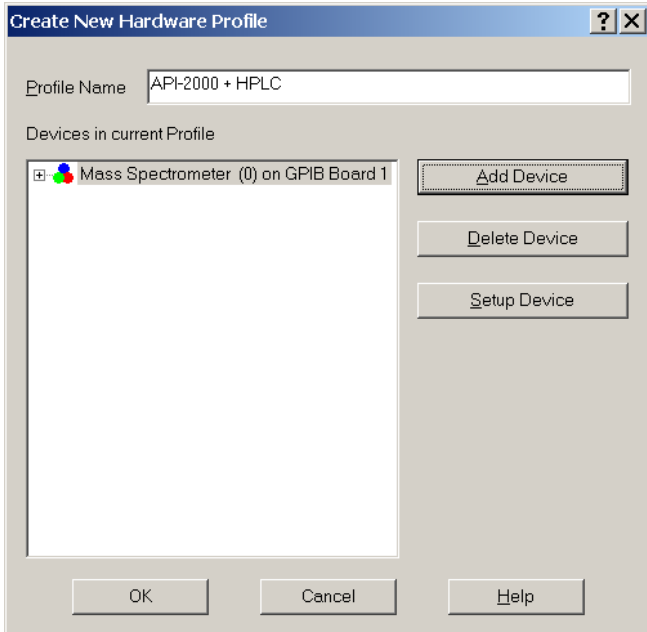
For API-2000 & QTrap

- Use integrated injector / diverter
- Use integrated syringe pump

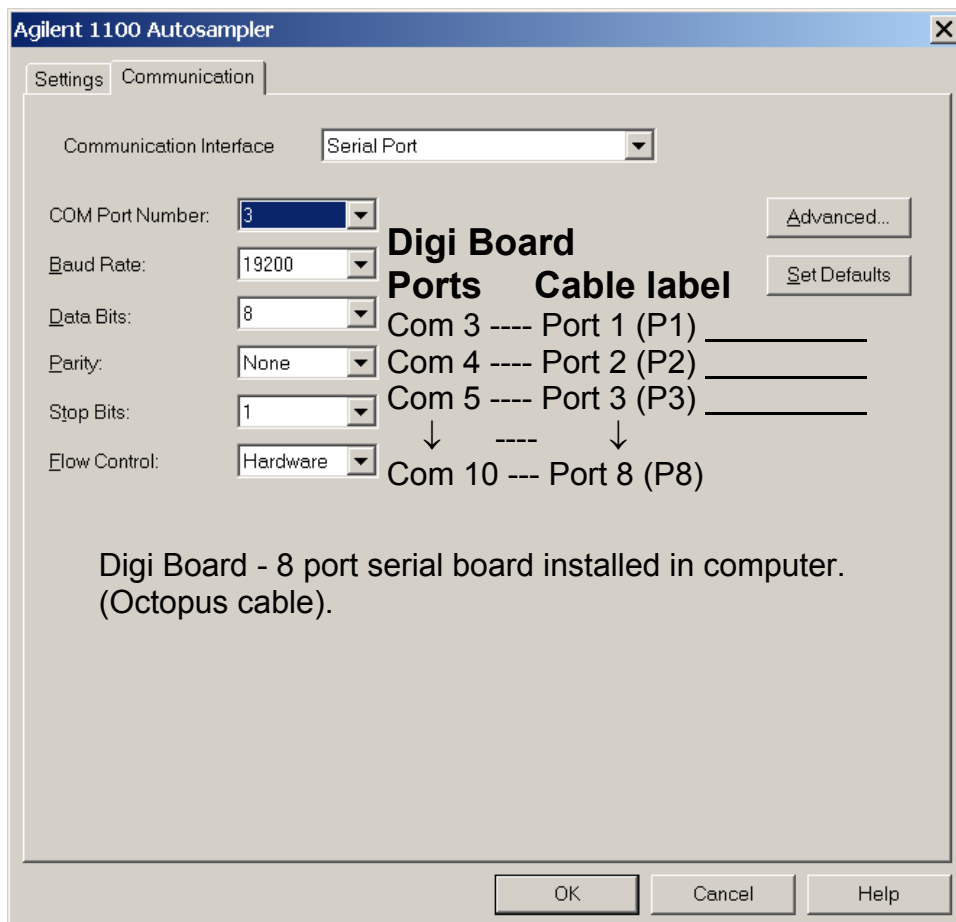
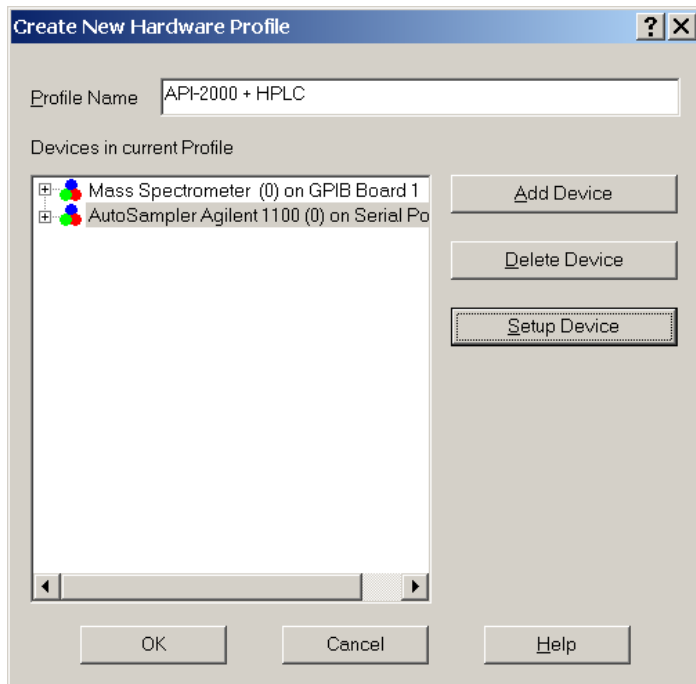
10. OK



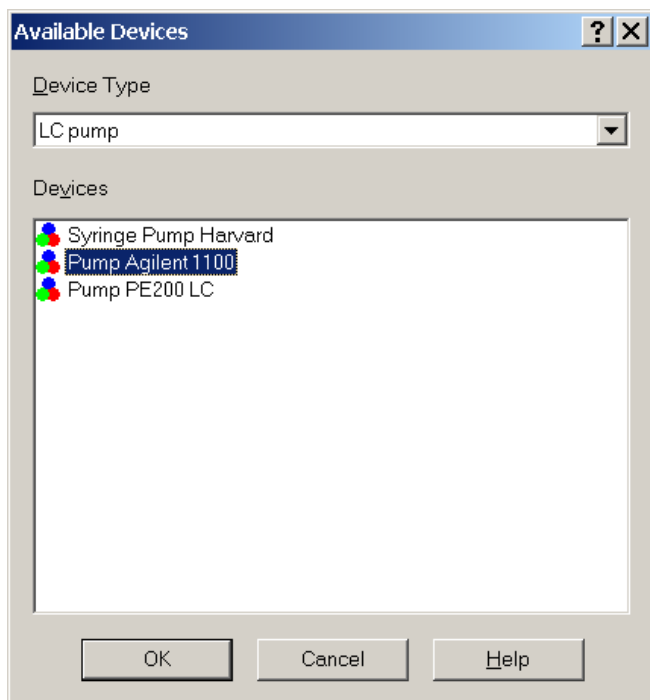
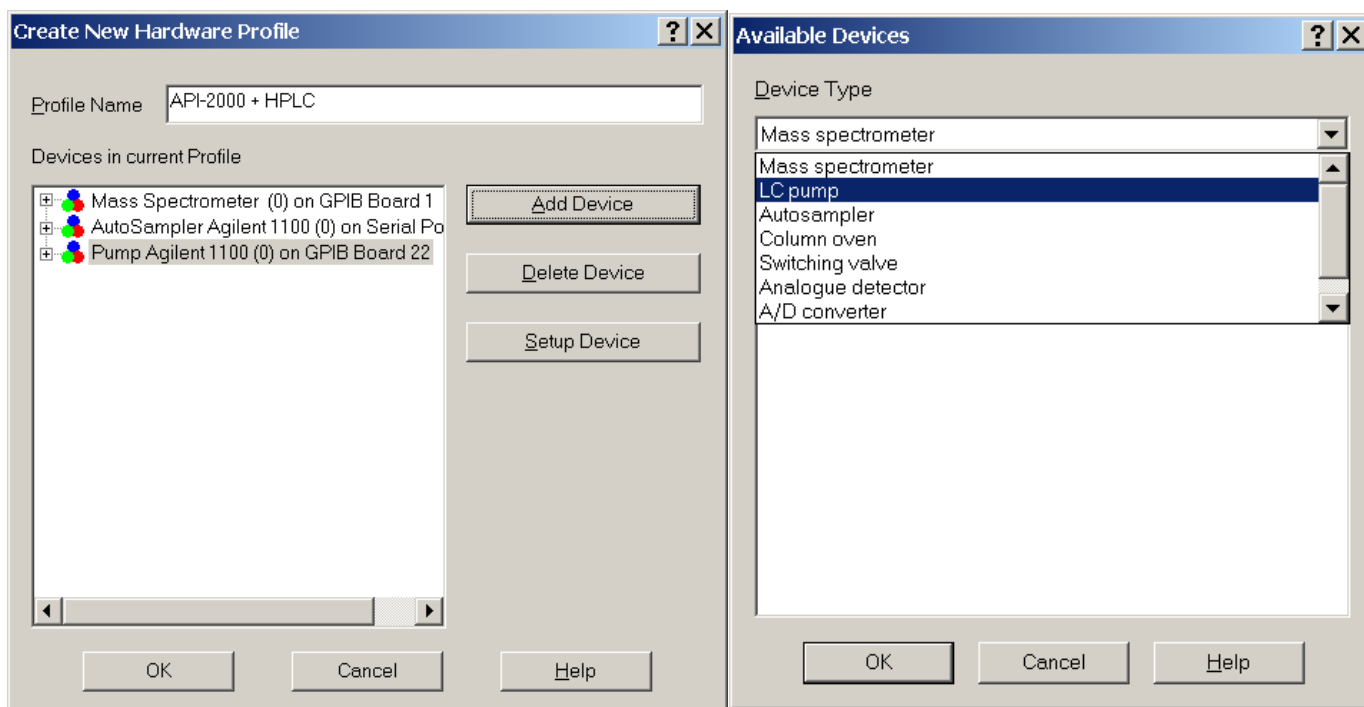
11. Add Device
12. Choose AutoSampler.
13. Highlight AutoSampler specific to your install. *Example: Agilent 1100*
14. OK



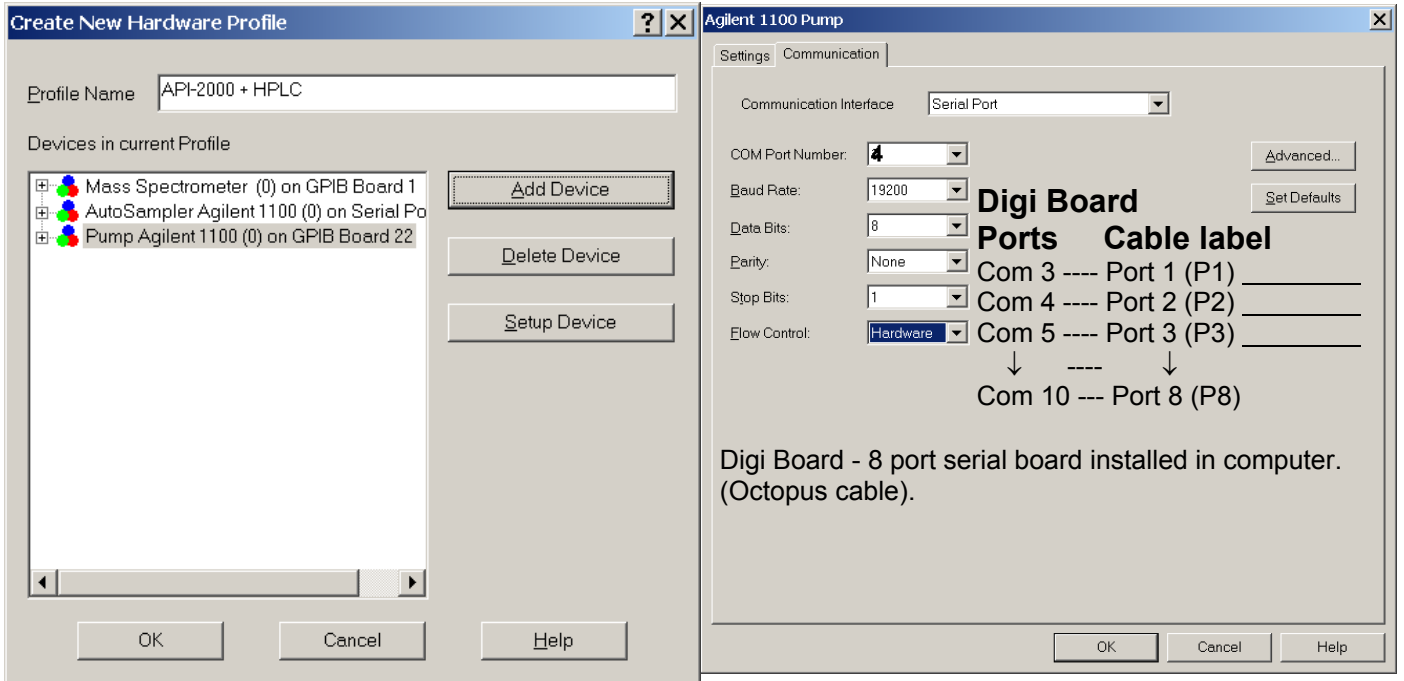
15. Click Setup Device. **See LC Device Manual for detailed instructions.**
16. Choose: Com Port number 3 & Baud Rate (see LC device manual)
17. OK



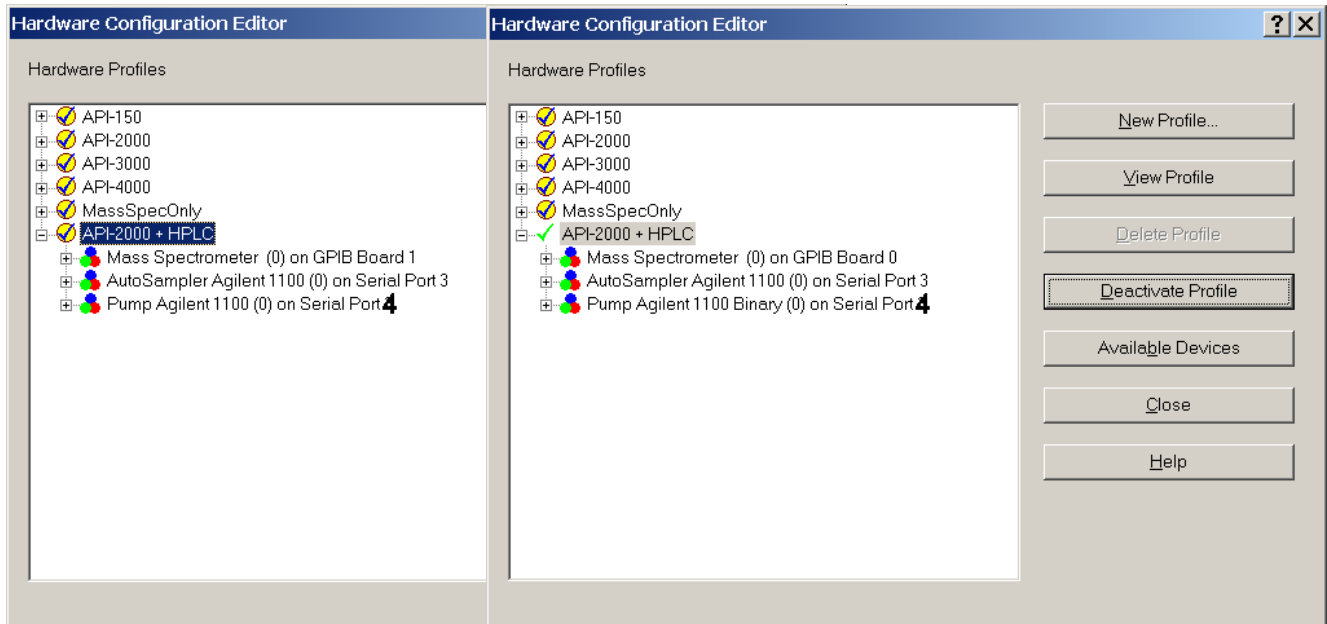
18. Add Device
19. Choose LC Pump.
20. Highlight Pump. *Example: Agilent 1100*
21. OK



22. Click Setup Device. **See LC Device Manual for detailed instructions.**
23. Choose: Com Port number 4 & Baud Rate (see LC device manual)
24. OK



25. Highlight new Profile API-2000 + HPLC.
26. Click Activate Profile.
27. Green check mark means connection was made successfully



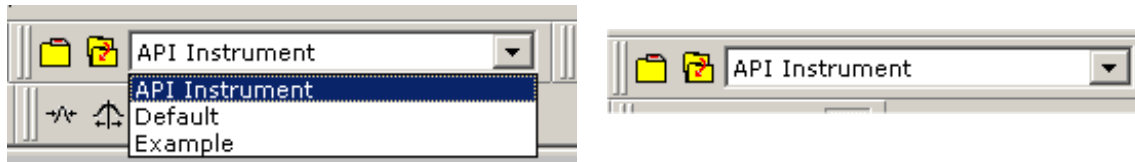
28. Done

# Manual Tuning

This is extremely important.

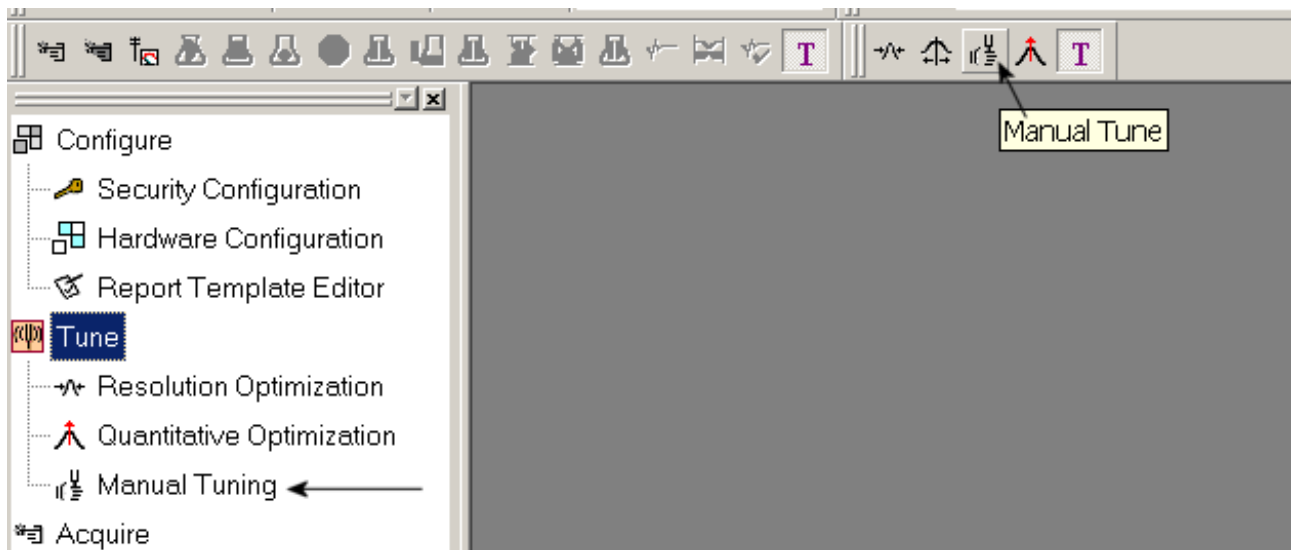
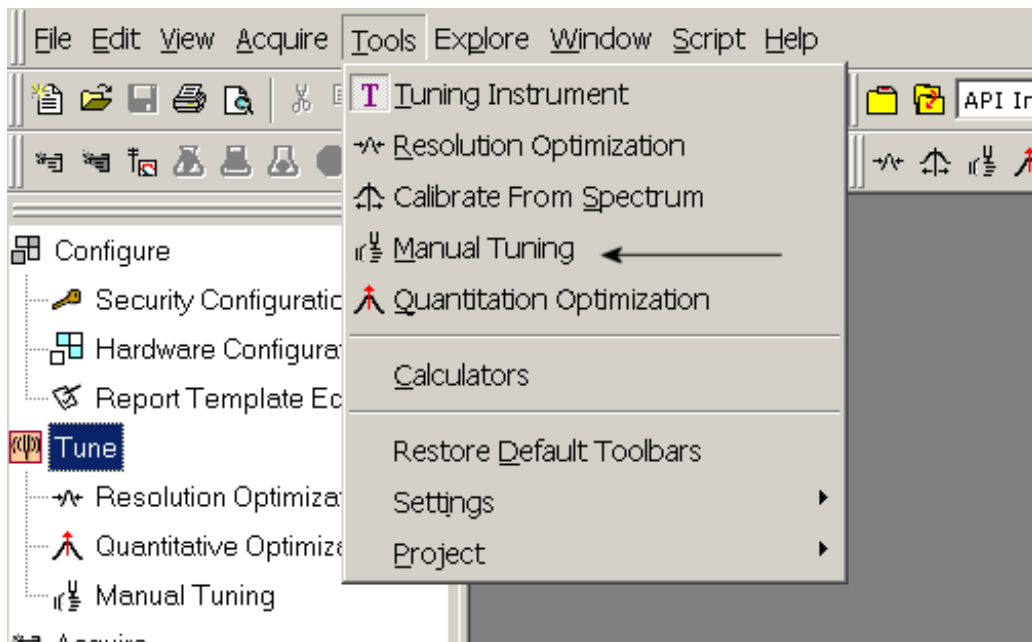
## Select the API Instruments Project

Resolution Optimization may not work properly if PPG are optimized using another project.



## Open “Blank” Manual Tuning File

Use one the options below. This file takes its values from the “Parameter Settings Table”.





## The “Blank” Tune file must be opened first.

### Note:

The reason it must be opened first is so that the PPG file opened next opens in it's proper tuning format. Failing this the PPG file will open in a Sample Acquisition format.

Analyst - [Tune Method Editor]

File Edit View Acquire Tools Explore Window Script Help

Tune Mode API Instrument

Configure

- Security Configuration
- Hardware Configuration
- Report Template Editor
- Tune (1)
- Resolution Optimization
- Quantitative Optimization
- Manual Tuning
- Acquire
  - IDA Method Wizard
  - Build Acquisition Method
  - Build Acquisition Batch
  - Express View
- Explore
  - Open Data File
  - Open Compound Database
- Quantitate
  - Quantitation Wizard
  - Review Results Table

Acquire... Start Ramp Parameter Edit Ramp... MS Method Use

Source/Gas Compound Resolution Detector

Declustering Potential (DP) 20.0

Focusing Potential (FP) 200.0

Entrance Potential (EP) 10.0

MS Advanced MS

Scan type: Q1 MS (O1)

	Start (amu)	Stop (amu)	Time (sec)
1			

Polarity

Positive

Negative

Center / Width

Parameter Range

Total Scan Time (includes Pause): 0.0050 (secs)

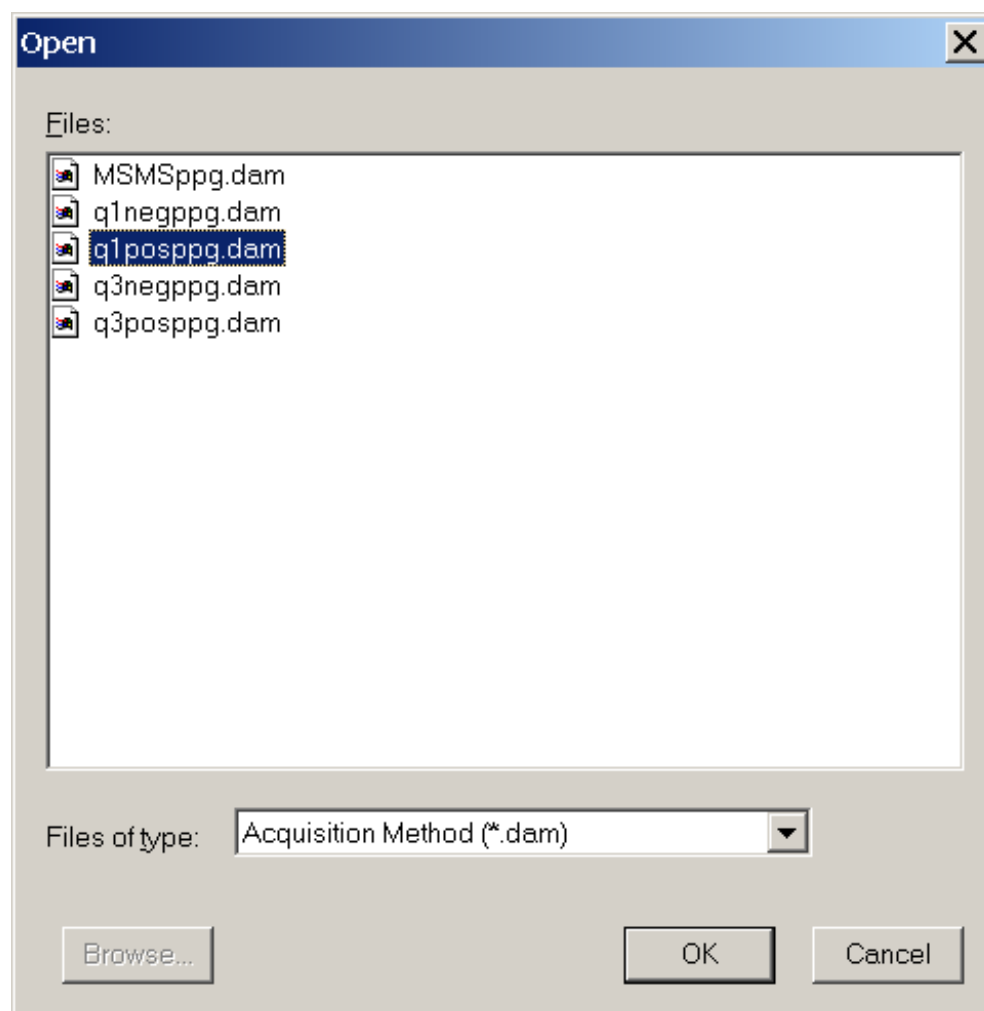
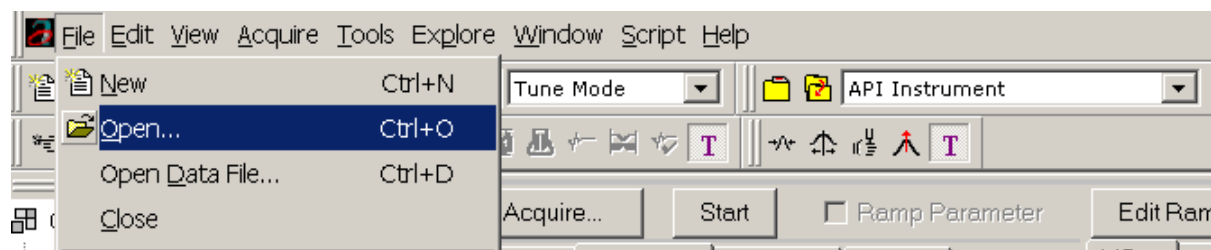
Period

Duration: 0.000 (mins) Cycles: 1 Delay Time: 0 (secs)

For Help, press F1 C:\Analyst Data Idle

Start R... A... A... A... J... M... H... \_Tech Memo's-1 7:04 AM

Choose File / Open / q1posppg.dam.  
This opens the Q1 PPG Acquisition method used for calibration.



# Q1 PPG Acquisition Method used for Calibration

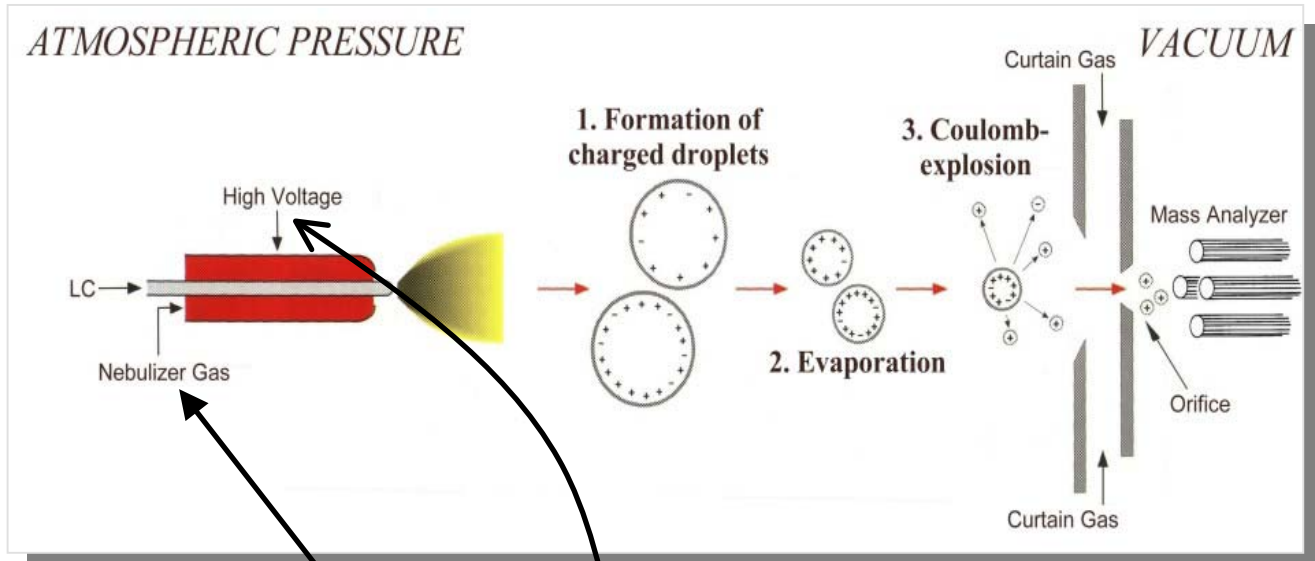
The screenshot displays the Analyst - [Tune Method Editor] software interface. The title bar shows the file path: C:\Analyst Data\Projects\API Instrument\Acquisition Methods\q1posppg.dam. The interface is divided into several sections:

- Left Panel (Navigation):** Includes sections for Configure (Security Configuration, Hardware Configuration, Report Template Editor), Tune (1) (Resolution Optimization, Quantitative Optimization, Manual Tuning), Acquire (IDA Method Wizard, Build Acquisition Method, Build Acquisition Batch, Express View), Explore (Open Data File, Open Compound Database), and Quantitate (Quantitation Wizard, Review Results Table).
- Central Panel (Configuration):** Contains tabs for Source/Gas, Compound, Resolution, and Detector. The Resolution tab is active, showing:
  - Declustering Potential (DP): 90
  - Focusing Potential (FP): 350
  - Entrance Potential (EP): 10.0
- Right Panel (MS Parameters):** Contains tabs for MS and Advanced MS. The MS tab is active, showing:
  - Scan type: Q1 MS (Q1)
  - Polarity: Positive (selected), Negative
  - Center / Width: checked
  - Parameter Range: checked
  - Total Scan Time (includes Pause): 4.8401 (secs)
  - Period: Duration: 80.668 (mins), Cycles: 1000, Delay Time: 0 (secs)
- Table (Scan Data):** A table with 6 rows and 4 columns: Center (amu), Width (amu), Time (sec), and an unlabeled column. The data is as follows:

	Center (amu)	Width (amu)	Time (sec)	
1	59.000	6.000	0.6000	
2	175.116	6.033	0.6032	
3	616.432	6.064	0.6063	
4	906.635	6.070	0.6069	
5	1254.913	6.025	0.6025	
6	1545.117	6.034	0.6033	

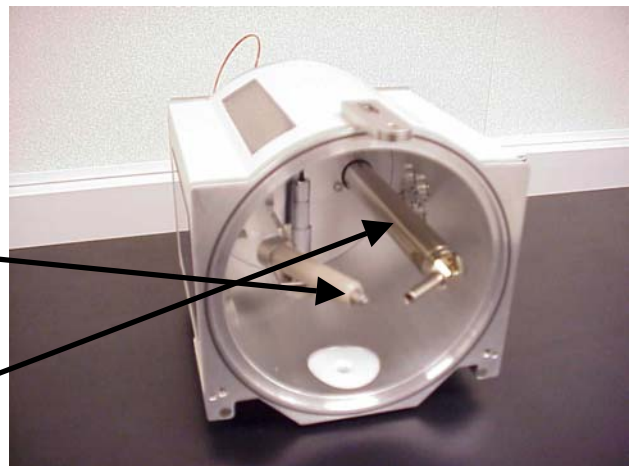
# Method File Evaluation

- Nebulizer Gas, Ion Spray voltage, Heater Temp



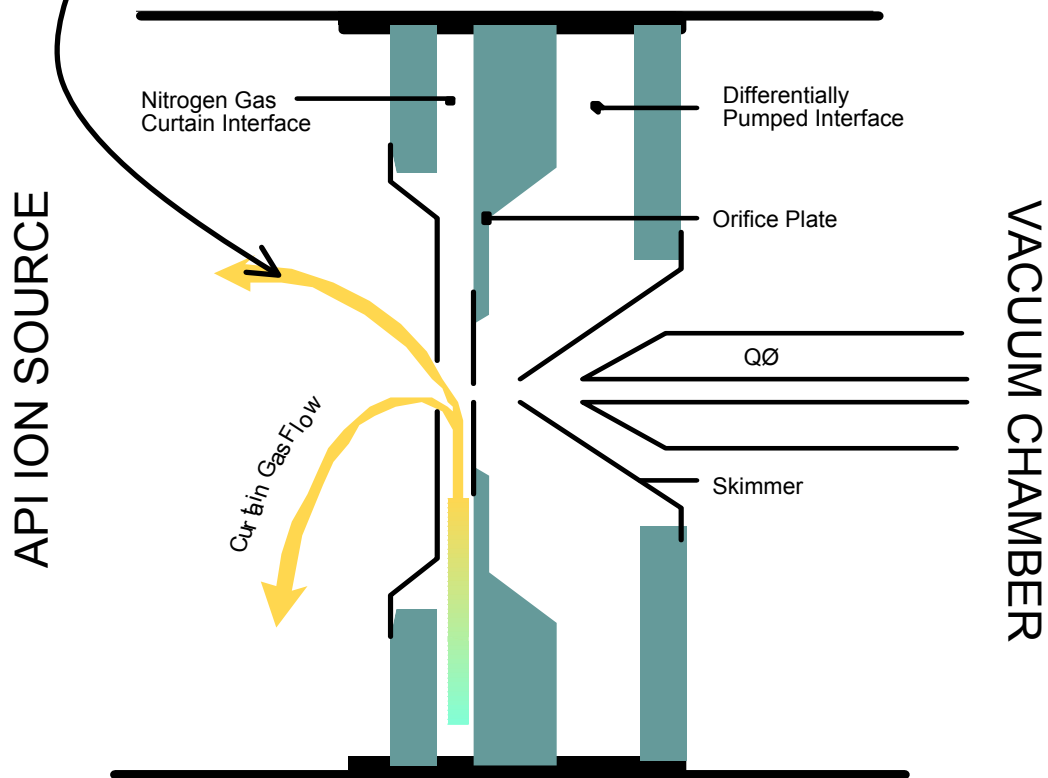
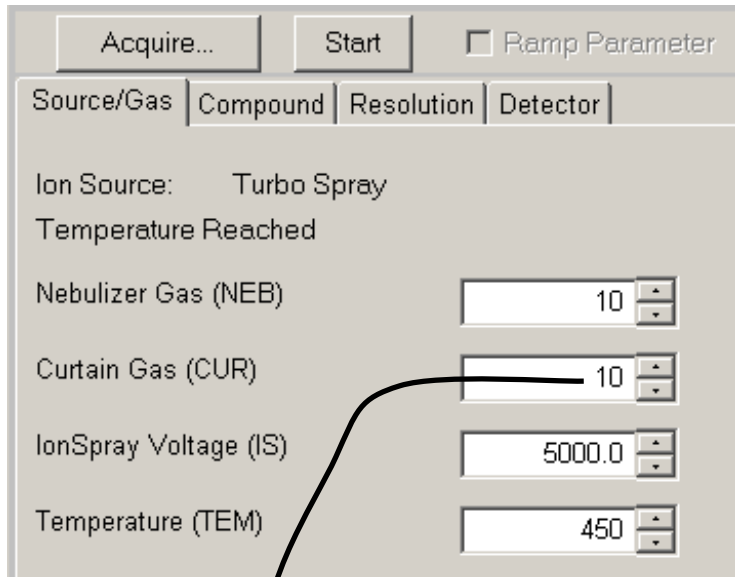
Acquire... Start  Ramp Parameter

Source/Gas	Compound	Resolution	Detector
Ion Source: Turbo Spray			
Temperature Reached			
Nebulizer Gas (NEB)		10	
Curtain Gas (CUR)		10	
IonSpray Voltage (IS)		5000.0	
Temperature (TEM)		450	



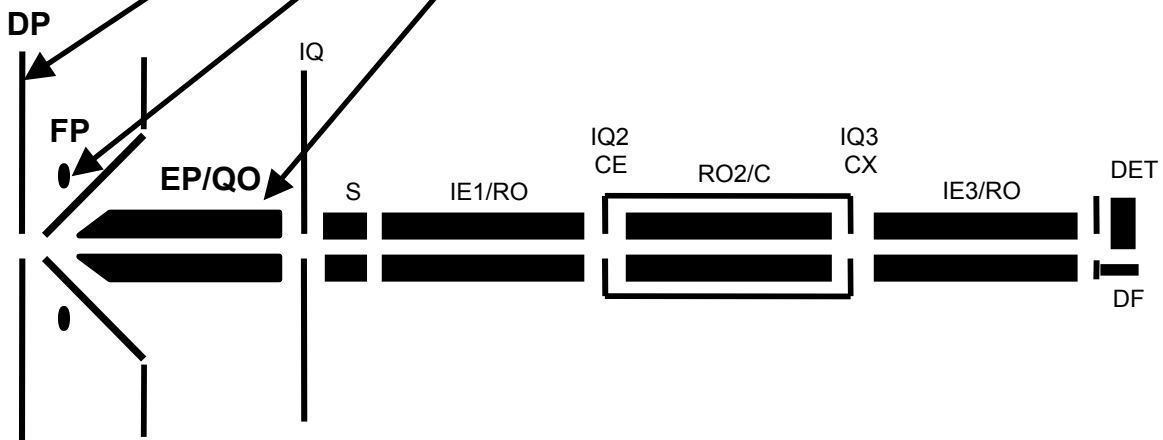
# • Curtain Gas

Curtain Gas keeps the atmosphere out of the Mass Spec.  
The higher the gas the more the sample is blocked.  
Higher Curtain gas settings are desirable for high HPLC flow rates.



- Declustering Potential-DP (Orifice)
- Focusing Potential-FP (Focusing Ring)
- Entrance Potential-EP (Q0)

Source/Gas	Compound	Resolution	Detector
Declustering Potential (DP)		90.0	
Focusing Potential (FP)		350.0	
Entrance Potential (EP)		10.0	



- Ion Energy (IE1) (R01)

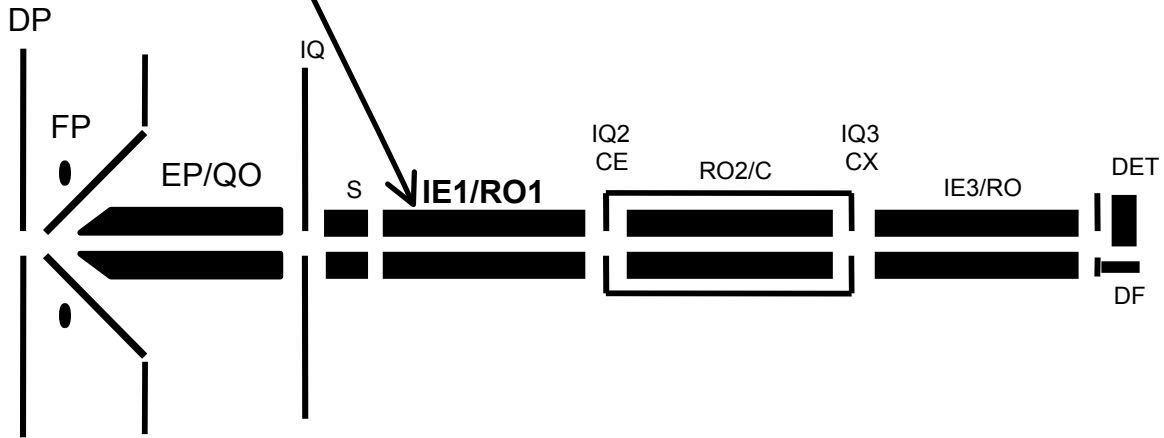
The screenshot shows two windows from a mass spectrometer control software. On the left is the 'Resolution' tab of a main control panel, and on the right is a 'ResolutionTableQ1 +unit' window.

**ResolutionTableQ1 +unit Window:**

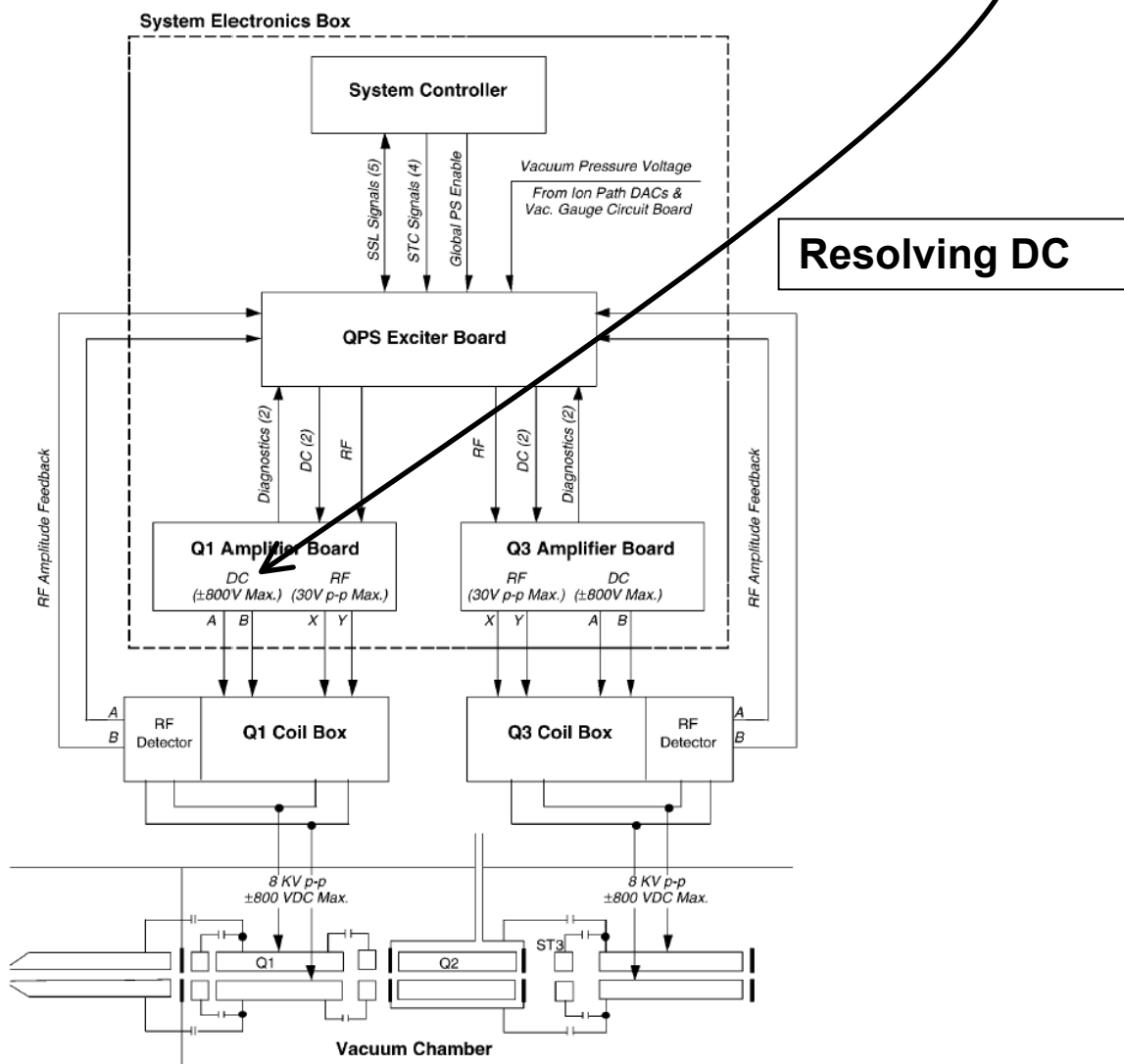
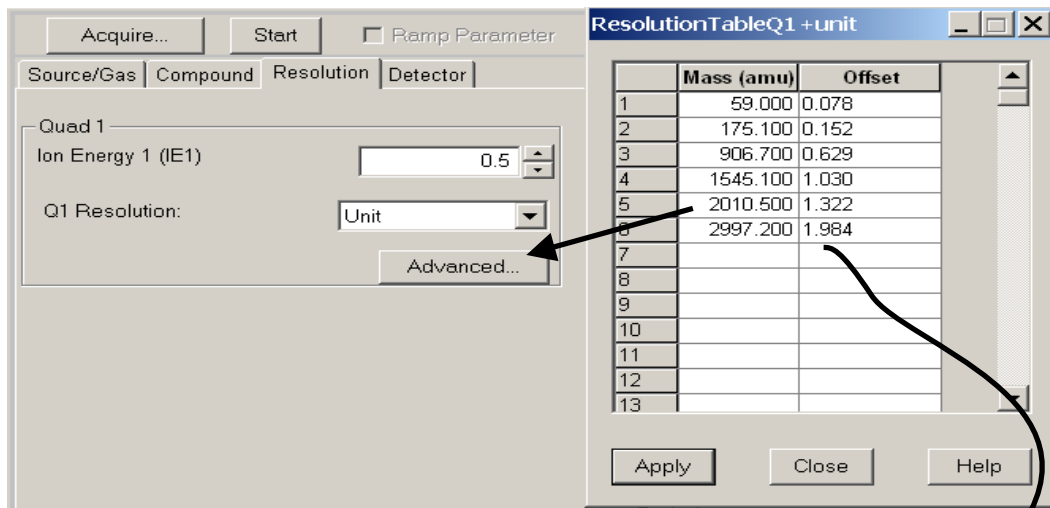
	Mass (amu)	Offset
1	59.000	0.078
2	175.100	0.152
3	906.700	0.629
4	1545.100	1.030
5	2010.500	1.322
6	2997.200	1.984
7		
8		
9		
10		
11		
12		
13		

**Main Control Panel (Resolution Tab):**

- Buttons: Acquire..., Start, Ramp Parameter (checkbox)
- Tabs: Source/Gas, Compound, Resolution, Detector
- Quad 1: Ion Energy 1 (IE1) [0.5]
- Q1 Resolution: [Unit]
- Advanced... button



# Resolution offsets (Resolving DC)





- RF + Resolving DC (Mass selectivity)

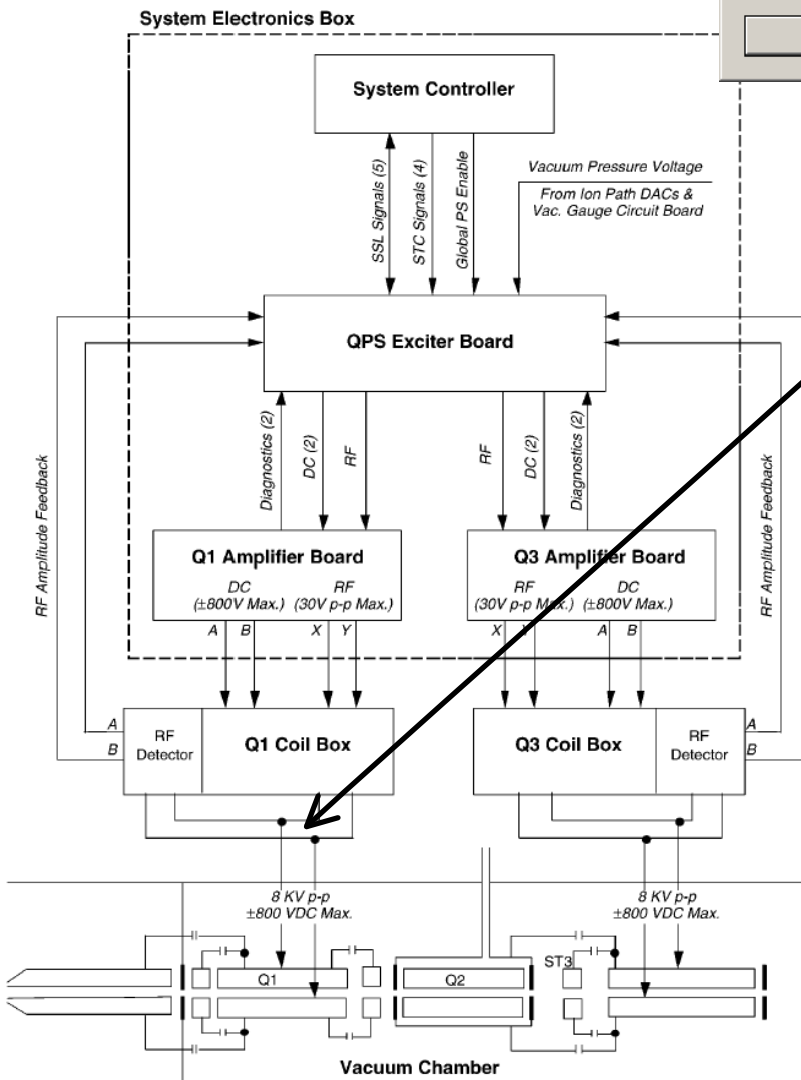
	Center (amu)	Width (amu)	Time (sec)
1	59.000	6.000	0.6000
2	175.116	6.033	0.6032
3	616.382	6.164	0.6161
4	906.635	6.070	0.6069
5	1254.913	6.025	0.6025
6	1545.117	6.034	0.6033

Calibration Table

Calibration Table: CalibrationTableQ1+unit

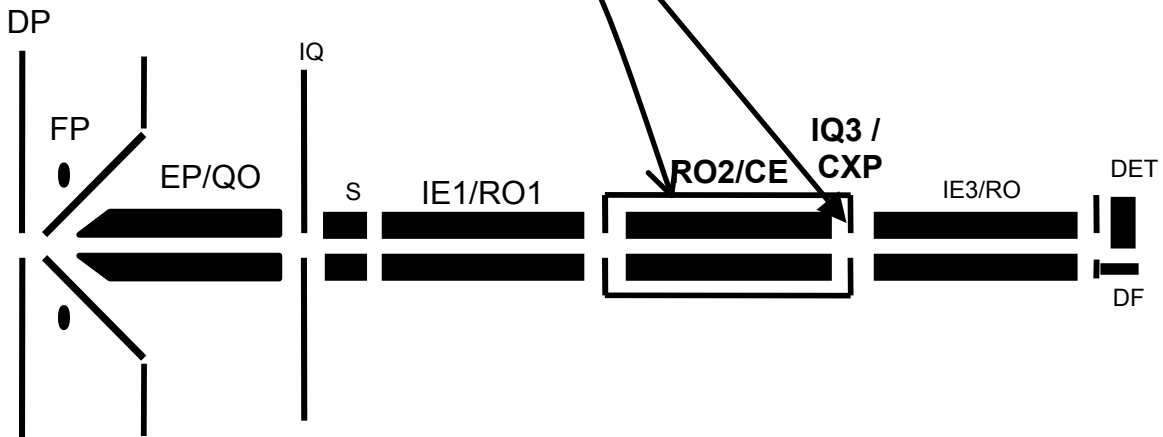
	Mass (amu)	Dac
1	59.000	1093
2	175.133	3295
3	616.464	11667
4	906.670	17175
5	1254.925	23781
6	1545.134	29287
7	2010.469	38120
8	2242.637	42523
9		
10		
11		
12		

OK Cancel Help



- **Collision Cell Rod Offset (R02)**
- **Collision Cell Exit Potential (CXP)**

Acquire...	Start	<input type="checkbox"/> Ramp Parameter	
Source/Gas	Compound	Resolution	Detector
Declustering Potential (DP)	90.0		
Focusing Potential (FP)	350.0		
Entrance Potential (EP)	10.0		
Collision Cell Rod Offset (R02)	-20.0		
Collision Cell Exit Potential (CXP)	15.0		



# Scan Parameters

## • Q3: Collision Cell Exit Potential (CXP)

### Mass dependant parameters:

Some masses have a better transmission efficiency with different parameter settings.

CXP is increased in value as the masses increase.

Example API-3000 CXP: 59=5, 175=10 ... (See table below)

## Selecting and Deselecting CXP Scan Parameter

**Right Click**

Scan type: Q3 MS (Q3)

Polarity:  Positive  Negative

Center / Width

Parameter Range

**CXP is grayed out if checked at experiment**

	Time (sec)	CXPstart (volt)	CXPstop (volt)
1	0.6000	15.000	15.000
2	0.6032	15.000	15.000
3	0.6161	15.000	15.000
4	0.6069	15.000	15.000
5	0.6025	15.000	15.000

1	Declustering Potential DP		
2	Focusing Potential FP		
3	Entrance Potential EP		
4	Collision Cell Exit Potential CXP		
5	Collision Cell Rod Offset RO2		
6	1545.117	6.034	0.6033

Collision Cell Exit Potential (CXP)

If "all" the scan numbers are the same "unchecking" CXP brings back control.

**Note:** Don't be confused with **Edit Ramp**.

That's used in factory for optimizing one lens at a time.

MASS	CXP
59	5
175	10
616	10
907	15
1255	25
1545	30
2010	35
2242	40

Acquire... Start  Ramp Parameter Edit Ramp... MS Method Use

Source/Gas Compound Resolution Detector MS Advanced MS

Declustering Potential (DP)

Focusing Potential (FP)

Entrance Potential (EP)

Collision Cell Rod Offset (RO2)

Collision Cell Exit Potential (CXP)

Scan type: Q3 MS (Q3)

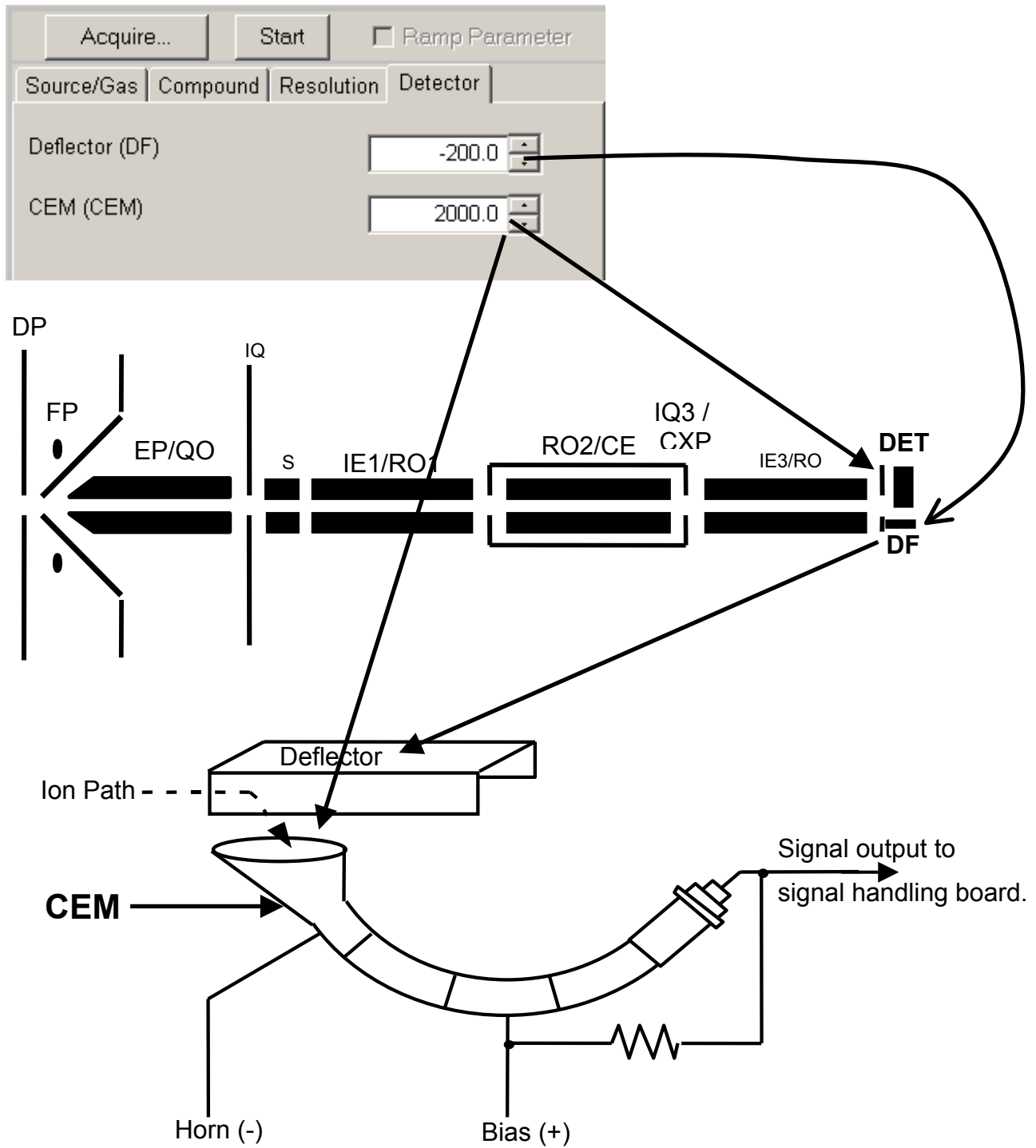
Polarity:  Positive  Negative

Center / Width

Parameter Range

	Time (sec)	CXPstart (volt)	CXPstop (volt)
1	0.6000	5.000	5.000
2	0.6032	10.000	10.000
3	0.6161	10.000	10.000
4	0.6069	15.000	15.000
5	0.6025	25.000	25.000

# • CEM & Deflector (DF)



# Parameters Settings Table Evaluation

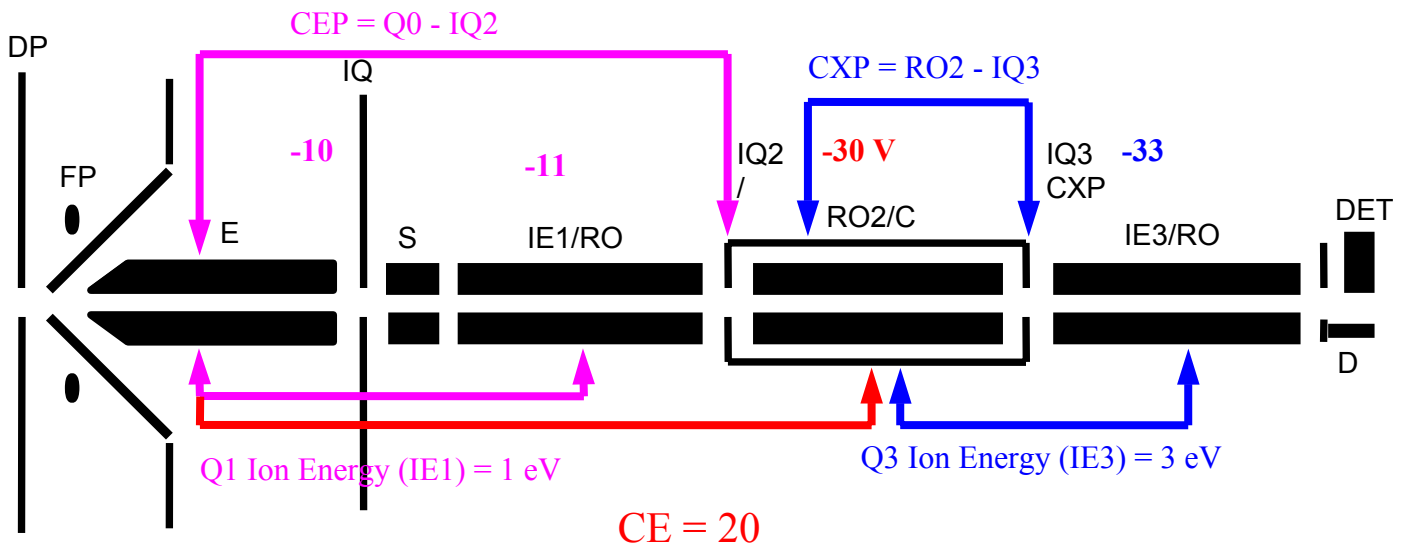
Parameter Settings Editor - ParamSettingsDef.psf

Scan Category: **Q1+ Scan**

Param. ID	Access ID	Access Name	Default	Group	Ion Sources	Access Type												
NEB	NEB	Nebulizer Gas	8	Source/Gas	All	Operator												
CUR	CUR	Curtain Gas	8	Source/Gas	All	Operator												
CAD	CAD	Collision Gas	0	Source/Gas	All	Fixed												
IS	IS	IonSpray Voltage	5000.000	Source/Gas	TIS,IS	Operator												
NC	NC	Nebulizer Current	3.000	Source/Gas	HN	Operator												
TEM	TEM	Temperature	350.000	Source/Gas	TIS,HN	Operator												
OR	DP	Declustering Potential	20.000	Compound	All	Potential Diff.												
RNG	FP	Focusing Potential	200.000	Compound	All	Potential Diff.												
Q0	EP	Entrance Potential	10.000	Compound	All	Potential Diff.												
IQ1	IQ1	Focusing Lens 1	n/a	Compound	All	Param. Dep.												
ST	ST	Prefilter	n/a	Compound	All	Param. Dep.												
RO1	IE1	Ion Energy 1	1.000	Resolution	All	Potential Diff.												
IQ2	IQ2	Focusing Lens 2	n/a	Compound	All	Param. Dep.												
RO2	RO2	Collision Cell Rod Offset	-60.000	Compound	All	Fixed												
ST3	ST3	Prefilter 3	-80.000	Compound	All	Fixed												
RO3	RO3	Q3 Rod Offset	-62.000	Compound </tr <tr> <td>DF</td> <td>DF</td> <td>Deflector</td> <td>0.000</td> <td>Detector</td> <td>All</td> <td>Operator</td> </tr> <tr> <td>CEM</td> <td>CEM</td> <td>CEM</td> <td>1800.000</td> <td>Detector</td> <td>All</td> <td>Operator</td> </tr>	DF	DF	Deflector	0.000	Detector	All	Operator	CEM	CEM	CEM	1800.000	Detector	All	Operator
DF	DF	Deflector	0.000	Detector	All	Operator												
CEM	CEM	CEM	1800.000	Detector	All	Operator												

The parameter Settings Table is where the linking of voltages takes place. See diagram below. Unlinking any of these parameters will cause the "Quantitation Optimization" to malfunction. Do not change or unlink any parameters unless you know the consequences or have consulted a specialist.

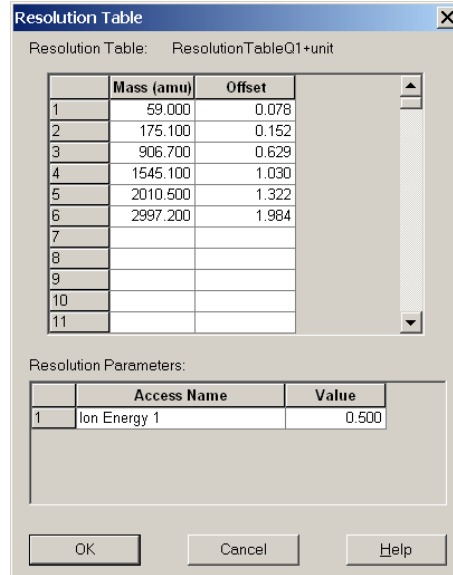
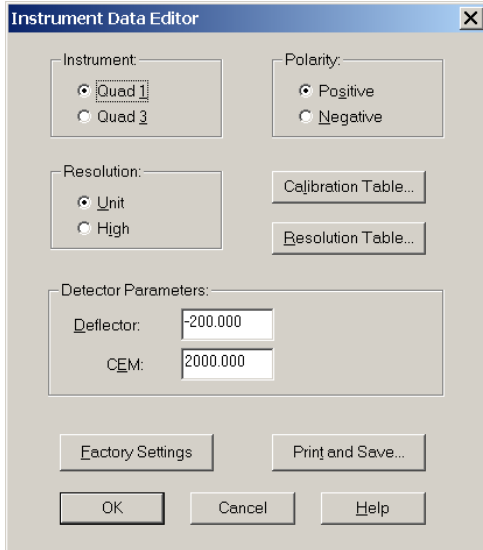
Factory Settings    Print and Save...    OK    Cancel    Help



# Parameter Settings Table: Safe changes

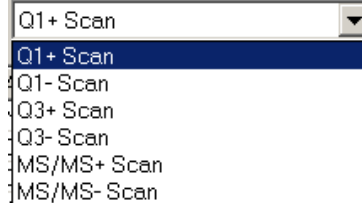
There are valid reasons you may want to check and modify this table. Here are a few examples.

Note: The Ion Energies, Deflector (DF), CEM are “not” set in this table. These are global numbers and are set in the Tools / Settings / Instrument Options.



## 1) TEM: change to 0.

Since the Parameters Settings Table is the default values when you open a Manual tuning file you may want to make the turbo Ion Sprav temperature 0. You can do this in each parameter settings table.



NC	NC	Nebulizer Current	3.000	Source/Gas
TEM	TEM	Temperature	350.000	Source/Gas
OR			0	Compound
RNG			0	Compound
Q0			0	Compound
IQ1			a	Compound
ST			a	Compound
RO1			0	Resolution
IQ2			a	Compound
RO2			0	Compound
ST3			0	Compound
RO3			0	Compound
DF			0	Detector
CEM			0	Detector

**Detail Parameter Setting**

Parameter ID:

Access Name:

Group:

Access Type:  Default...

Access Range:  to

Access Default:   Apply value to all scan categories

Change 350 to 0.

## 2) CAD Gas: collisionally Activated and Dissociation = Collision Gas

Q1+Scan & Q1-Scan CAD = 0.

Parameter Settings Editor - ParamSettingsDef.psf

Scan Category: Q1+ Scan

Param. ID	Access ID	Access Name	
NEB	NEB	Nebulizer Gas	
CUR	CUR	Curtain Gas	
CAD	CAD	Collision Gas	

**Detail Parameter Setting**

Parameter ID: CAD

Access Name: Collision Gas

Group: Source/Gas

Access Type: Fixed Operator...

Value: 0

OK Cancel Help

Q3+Scan & Q3-Scan CAD = 1 or 2.

Parameter Settings Editor - ParamSettingsDef.psf

Scan Category: Q3+ Scan

Param. ID	Access ID	Access Name	
NEB	NEB	Nebulizer Gas	
CUR	CUR	Curtain Gas	
CAD	CAD	Collision Gas	

**Detail Parameter Setting**

Parameter ID: CAD

Access Name: Collision Gas

Group: Source/Gas

Access Type: Fixed Operator...

Value: 2

OK Cancel Help

**The End**