

Getting Started
with the
Vx Acquisition System

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Adron Systems LLC

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Computer Requirements:

Operating System:

- Windows 2000 or Windows XP

PC Specification:

- 400MHz CPU minimum for users with ProLab or Teknivent acquisition units.
- 1.2 GHz CPU minimum; 2.0 GHz or greater Pentium 4 recommended for Finnigan Magnum/ITS40/Tracker and Varian Saturn I users.
- 256 MB RAM minimum for Windows 2000
- 512 MB RAM minimum for Windows XP
- 40 GB or greater recommended
- CD-ROM or CD-RW
- one serial port for chromatograph, if needed
- one serial port for autosampler, if needed
- USB port for dongle; not required in demonstration mode
- 1 full-height PCI port for National Instruments' PCI-GPIB card
or
- 1 PC Card slot for National Instruments' PCMCIA-GPIB card

Display:

- 17" or larger recommended
- 1280x1024 minimum resolution

Installation Considerations for Finnigan ITS40, Magnum and Varian Saturn I Users:

- Communication between the Magnum and the computer (PC) utilizes the National Instruments PCI-GPIB controller. This is part number 778032-01 from National Instruments.
- Notebook users can use the National Instruments PCMCIA-GPIB card. This is National Instruments' part number 778034-02.
- The National Instruments' GPIB driver is currently at revision 2.4. This driver can be obtained from the National Instruments' website at:
<http://www.ni.com/support/gpib/versions.htm>
- Disconnect the GPIB cable from the original Magnum data system. It may interfere with GPIB communications between Vx and the Magnum ion trap. This GPIB cable should be connected to the Vx data system.
- The Magnum ion trap needs a dedicated GPIB controller for its operation. This means other instruments cannot use the GPIB card at the same time.
- **Note:** The original Finnigan data system GPIB card is not usable by the Vx Acquisition System.

The Vx Acquisition System CD

There are three installation programs on the Vx CD. These are:

1. `Setup.exe` is the Vx installer.
2. `Aladdin\HaspUserSetup.exe` is the installer for the Aladdin dongle device driver.
3. `National\NI488224.exe` is the installer for the National Instruments' Windows 2000/XP GPIB driver.

Run each of these programs; order isn't important. For the National Instruments' installer, simply go with the defaults. At the end of the National Instruments' install, select PCI-GPIB or PCMCIA-GPIB as the GPIB type, depending on your card type.

After installing these software items, install the PCI-GPIB or PCMCIA-GPIB card plus the USB software key.

Vx Configure

Once you've installed the above, launch the *Vx Configure* program to configure your instrument setup.

Vx Acquisition - Tune - Getting Started

Start with the *Tune* system. Double-click on Tune or right-click and select Open in the Explorer pane..

The four scan windows have popup menus. Right click to activate and you'll see important items such as setting the scan range. The top three scan windows are normally configured to display peak profile spectra. The bottom scan window is usually configured to display a peak detected spectrum.

The popup menuitems are:

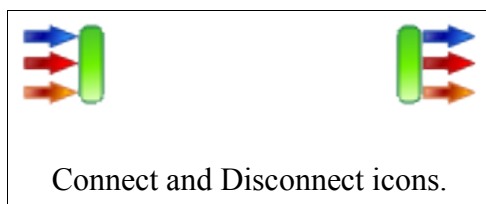
- 100% Peak
Pick one of the top three windows to contain the 100% peak.
- Enable Scanning
Check to enable scanning for this window.
- Freeze Scan
Check to freeze the current scan for this window. Scanning still continues for this window but the window's content is left unchanged.

- **Merged Scan**
Normally, the spectra shown in each scan window is acquired separately. Scan windows that have the “Merged Scan” option checked share the same scan.
- **Normalize**
Normalize the content of the window, with zero as the intensity origin.
- **Auto Normalize**
Automatically normalize the contents of the window, with zero as the intensity origin. It is convenient to check this option!
- **Extremes**
Normalize the content of the window, using the low and high intensity values.
- **Auto Extremes**
Automatically normalize the contents of the window, using the low and high intensity values.
- **Scanning Mode...**
Select between types Scan and SIM with modes of Detected or Profile.
- **Scanning Range...**
The mass scanning range for the window.
- **Diagnostics...**
Allows alternate signals to be swept or monitored by the mass spectrometer.

Vx Acquisition - Tune - Control Panel

In the Tune window, the panel on the right is the Control panel.

To establish communications with the mass spectrometer, press the Connect button. To sever communications with the instrument, press the Disconnect button. **Note:** Disconnect is also used to clear instrument faults.



Note: To view instrument status information, open the Feedback window and the Instrument Status window.

Note: Press the F12 key to show and hide the Explorer pane on the left. Hiding the Explorer reduces “window” clutter when using the Tune section.

The Tune section provides these “Actions”:

- **Tune**
The Tune action allows the user to set voltages, temperatures and other parameters for optimal ion trap performance. These parameters are available in the setpoint list.
- **Calibrate**
The Calibrate action allows the user to calibrate the mass axis values.

The Tune section provides these “Modes”:

- **Scan**
Allows the mass spectrometer to scan. Scans typically sweep the mass axis and monitor ion intensity values.
- **Gain**
In this mode, scanning is disabled. Vx enters a “gain check” mode that determines an optimal voltage (gain) for the electron multiplier (EM). Suggested EM voltages are displayed in the Messenger window, i.e., the lower window of Vx.
- **Off**
Disables the scanning and gain check modes.
- **Channels**
If enabled (checked), then diagnostic voltages, temperatures and other values are pulled in from the ion trap. These values are displayed in the Feedback section of Vx.

Note: These actions and modes only occur if the computer has established communications with the ion trap, i.e., the instrument is “Connected.”

The Tune section provides the “Show” option for hiding and showing the four scan windows.

Note: All of the control panel options are also available through various Vx menus.

Vx Acquisition - Tune - Diagnostics

RF Linearity Check Diagnostic:

- Reset the Tune system by selecting the Tune -> New menuitem. This resets the Magnum back to its default state.
- Disable scanning for scan windows #2, #3, and #4.
- Hide scan windows #2 and #3.
- Right-click on scan window #1 and select the Diagnostics menuitem.
- For the Monitor signal, select the “ModulatorSignal.” Close the dialog by pressing “OK”.
- Right-click on scan window #1 and select the Scanning Range menuitem.
- Select a scan range from 50 to 650. Close the dialog by pressing “OK”.
- Right-click on scan window #1 and enable Auto Normalize.
- In the control panel, select the Tune action, and the Scan mode.
- In the Setpoints list, open the Init_Calibration list. Enable the following items:
 - RF_Enable
 - OneScan_Enable
- Connect to the ion trap using the control panel button.

Scan window #1 should display a roughly linear line starting at the lower left and rising to the upper right of the scan window.

Save the above settings by using the Tune -> Save As menuitem. Save the file as “Linearity” or another appropriate name. The next time you need to run this diagnostic, use this calibration file.

Note: Linearity is adjusted via the large tuning screw on top of the ion trap (cover removed). The resulting line should be fairly linear although there may be some minor "steps" in the display. Non-linearity problems usually are present at the high mass end of the display.

Zero Check Adjustment:

- Reset the Tune system by selecting the Tune -> New menuitem. This resets the Magnum back to its default state.
- Disable scanning for scan windows #2, #3, and #4.
- Hide scan windows #2 and #3.
- Right-click on scan window #1 and select the Scanning Range menuitem.
- Select a scan range from 340 to 400. Close the dialog by pressing "OK".
- Right-click on scan window #1 and enable Auto Normalize.
- In the control panel, select the Tune action, and the Scan mode.
- In the Setpoints list, open the Init_Calibration list. Enable the following items:
 - OneScan_Enable
- Connect to the ion trap using the control panel button.

Using the R11 potentiometer on the Electrometer section of the Analog Input board (front side on Magnum), adjust value to a nearly steady count of 1.

Note: If the "gain check" procedure described above fails, the usual reason is an incorrect zero adjustment.

Save the above settings by using the Tune -> Save As menuitem. Save the file as "Zero Check" or another appropriate name. The next time you need to perform this adjustment, use this calibration file.

Emission Current Adjustment:

This adjustment tries to maximize the sensitivity of the ion trap by balancing emission current and the EM voltage value. Run the “gain” procedure described above to obtain a suggested EM voltage.

- Reset the Tune system by selecting the Tune -> New menuitem. This resets the Magnum back to its default state.
- Connect to the ion trap using the control panel button.
- Disable scanning for scan windows #2, #3, and #4.
- Right-click on scan window #1 and select the Scanning Range menuitem.
- Select a scan range from 50 to 90. Close the dialog by pressing “OK”.
- In the control panel, select the Tune action, and the Scan mode.
- In the Setpoints list, open the Init_Calibration list. Enable the following items:
 - EM_Enable
 - Filament_Enable
 - RF_Enable
- In the Setpoints list, open the Init_Iontrap list. Set the following item:
 - EM_Voltage to value from running “gain check” mode.
- Open the Feedback window, Instrument Status, and Magnum window. Observe the value of “ScanIonTime.”

In the Init_Iontrap list, adjust the values of EM_Voltage and Emission_Current. EM_Voltage can be increased 50 to 100V above that suggested by the “gain check” routine. Setting of Emission_Current is up to the operator's experience.

Ideally, the observed ScanIonTime should be adjusted to roughly 24000 μ S. (The upper limit for ScanIonTime is 24999 μ S.) Note, this adjustment isn't critical and doesn't always succeed as described.

Save the above settings by using the Tune -> Save As menuitem. Save the file as “Emission” or another appropriate name. The next time you need to perform this adjustment, use this calibration file.

Air and Water Check

- Reset the Tune system by selecting the Tune -> New menuitem. This resets the Magnum back to its default state.
- Set the scanning range for window #1 from 15 to 25.
- Set the scanning range for window #2 from 25 to 35.
- Set the scanning range for window #3 from 35 to 45.
- Set the scanning range for window #4 from 10 to 50.
- Enable auto normalize for windows #1, #2, #3, and #4.
- In the control panel, select the Tune action, and the Scan mode.
- Connect to the ion trap using the control panel button.
- In the Setpoints list, open the Init_Calibration list. Enable the following items:
 - EM_Enable
 - Filament_Enable
 - RF_Enable
- In the Setpoints list, open the Init_Iontrap list. Set the following item:
 - EM_Voltage to operating value.
 - Emission_Current to operating value.
- In the Setpoints list, open the Init_CalScan list. Set the following item:
 - EI_Mode to AGC Off. If AGC (Automatic Gain Control) is not turned off, then the mass spectra will be distorted.
- Ionization time can be varied using the AGC_Off_Ion_Time in the Init_EI list. The default value of 100 μ S is usually adequate. Increasing the ionization time will cause more ions to be formed. If spectral peaks look distorted, reduce the ionization time.

If there are no air leaks, then the following should be true:

- 18 m/z > 19 m/z by a factor of at least 5
- 18 m/z > 28 m/z
- 28 m/z > 32 m/z by a factor of at least 2

If the system was recently restarted, it may take a while for water vapor to pump out. (This could vary from a few hours to several days.)

Save the above settings by using the Tune -> Save As menuitem. Save the file as "AirWater" or another appropriate name. The next time you need to perform this check, use this calibration file.

Tuning Procedure

- Reset the Tune system by selecting the Tune -> New menuitem. This resets the Magnum back to its default state.
- Set the scanning range for window #1 from 125 to 135.
- Enable auto normalize for windows #1, #2, #3, and #4.
- Enable scanning for windows #1, #2, #3, and #4.
- In the control panel, select the Tune action, and the Scan mode.
- Connect to the ion trap using the control panel button.
- In the Setpoints list, open the Init_Calibration list. Open the following valve:
 - CalGas_OpenWait a few seconds before continuing on.
- In the Setpoints list, open the Init_Calibration list. Enable the following items:
 - EM_Enable
 - Filament_Enable
 - RF_Enable
- In the Setpoints list, open the Init_Iontrap list. Set the following item:
 - EM_Voltage to operating value.
 - Emission_Current to operating value.

Hint: In the Feedback section for the ion trap, you'll notice the ScanIonTime value. Adjust the calibration gas valve so the ScanIonTime value is between 6000 and 10000 μ S.

If 131/132 m/z is under-resolved, increase EM_Voltage value.

If 131/132 m/z is over-resolved, increase AGC_ON_TIC value in the Init_EI list.

The EM_Voltage and AGC_ON_TIC are the only setpoints used to tune the ion trap.

Save the above settings by using the Tune -> Save As menuitem. This calibration file is utilized when defining an acquisition method. To calibrate the mass axis, continue on with the next section.

Mass Calibration Procedure

Calibration of the mass axis continues from the tuning procedure above.

- In the control panel, select the Tune action, and the Calibrate mode. You'll notice the following list of masses in the left panel:
 - 28
 - 69
 - 131
 - 219
 - 414
 - 502
 - 614
- Double-click on a mass entry. Scan window #1 mass axis changes to reflect the selected mass. A mass “cursor” is also displayed. Use the controls below the mass list to adjust mass position.
- Go through the mass list and adjust mass position.
- When finished, press the Calibrate button.
- Go through the list again, reviewing your calibration.

Save the above settings by using the Tune -> Save As or Tune -> Save menuitem. This calibration file is utilized when defining an acquisition method.

Hint: To calibrate mass 28, you'll probably need to turn AGC off. You may also delete this entry if it isn't important.

EI mass scans are broken in up to 4 segments. Users wishing to meet BFB or DFTPP tuning criteria, may wish to adjust scan boundaries in the Init_EI_Segments list. Be careful that boundaries remain sorted!

Default scan boundaries for the Magnum are:

- 10
- 99
- 249
- 399
- 650

Note: The first and last entries are not editable.

Suggested boundaries for BFB are:

- 10
- 59
- 79
- 119
- 650

Suggested boundaries for DFTPP are:

- 10
- 59
- 129
- 219
- 650

The ionization time for each mass segment can be varied to meet tuning criteria. These parameters are in the Init_EI_Segments list. Parameters are:

- AGC_ON_SF0
- AGC_ON_SF1
- AGC_ON_SF2
- AGC_ON_SF3

Values (scale factors) should be adjusted so that their average is still roughly 100%. For example:

- AGC_ON_SF0 = 100%
- AGC_ON_SF1 = 50%
- AGC_ON_SF2 = 150%
- AGC_ON_SF3 = 100%