

Vx Capture[™] – A GC/MS and LC/MS File Conversion Utility from [Adron Systems LLC](#)
September 21, 2009

Vx Capture is a software program to convert between file formats of various GC/MS and LC/MS manufacturers. *Vx Capture* provides:

- Batch conversion of existing GC/MS and LC/MS files.
- Automated conversion of GC/MS and LC/MS files as they are acquired from your instrumentation.

The latest version of *Vx Capture* is available by filling out the [Vx Capture Information Request](#) form on the Adron Systems' website. Also, use this form if you are interested in customized GC/MS file conversions.

Vx Capture is compatible with the following Microsoft operating systems:

- Windows Vista / Windows XP / Windows 2000

Vx Capture converts **from** the following GC/MS source formats:

- Adron Systems' Vector/2 and Vx (TKF)
- Adron Systems' Text File (ASC)
- Agilent & HP ChemStation (.D)
- AIA Andi netCDF (CDF)
- Finnigan Incos (MI,MX)
- Finnigan Incos (TI,TX,CT)
- Finnigan ITS40, Magnum and Tracker (MS)
- Varian Workstation 2000/2100/2200/4000 (SMS)
- Varian Workstation 1200 (XMS)
- Varian Saturn 1, 2, and 3 (MS)

Vx Capture converts **to** the following GC/MS target formats:

- Adron Systems' Text File (ASC)
- Agilent ChemStation (.D\Data.MS)
- Agilent ChemStation netCDF (.D\Data.CDF)
- AIA Andi netCDF (CDF)
- Finnigan Incos (MI,MX)
- Finnigan ITS40, Magnum, and Tracker (MS)
- Triton Analytics CSV File (T3)
- Varian Workstation 2000 (SMS)
- Varian Saturn 1, 2 and 3 (MS)

The *Vx Capture* program is available in "demonstration" mode. In this mode, data conversion is limited to five-eighths of data file spectra, with a maximum scan time of ten minutes. All the file formats listed above are supported in "demonstration" mode.

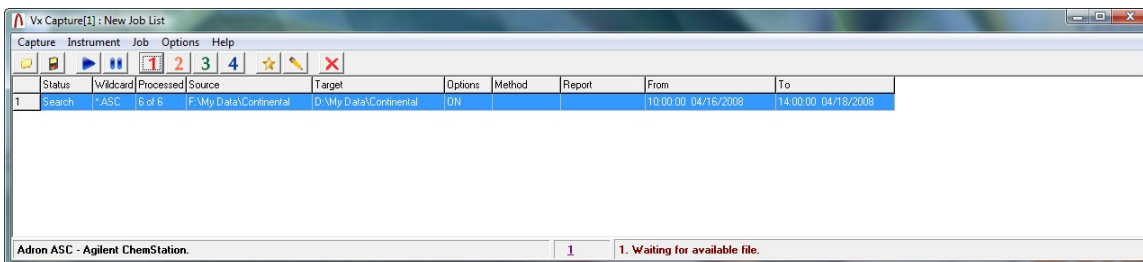
You can also submit sample files for conversion to Adron Systems by sending an e-mail to:

support@adronsystems.com

Please submit your data files in "zipped" format using a utility such as [WinRAR](#) or [WinZip](#). Specify the target format(s) you would like your source files converted to.

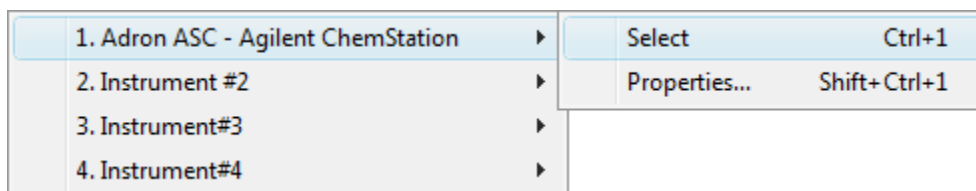
To install *Vx Capture*, run the `Setup.exe` program off of the CD. Alternatively, if you obtained the *Vx Capture* program from the Adron Systems' website, run the `Vx.exe` self-extracting installer.

To start the *Vx Capture* program, select "Vx Capture" from the "Adron Systems" folder. When started, *Vx Capture* appears as:



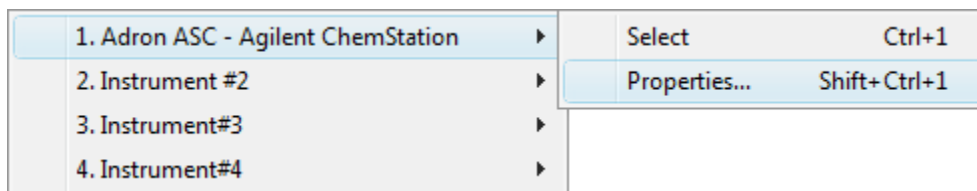
With *Vx Capture*, you can configure up to four separate conversions. In *Vx Capture* these conversions are called "Instruments" because the source files are generated off of GC/MS or LC/MS systems.

To switch the active instrument, use the toolbar buttons "1", "2", "3", or "4". Alternatively, from the "Instruments" menu, use the "Select" menuitem as in this example:

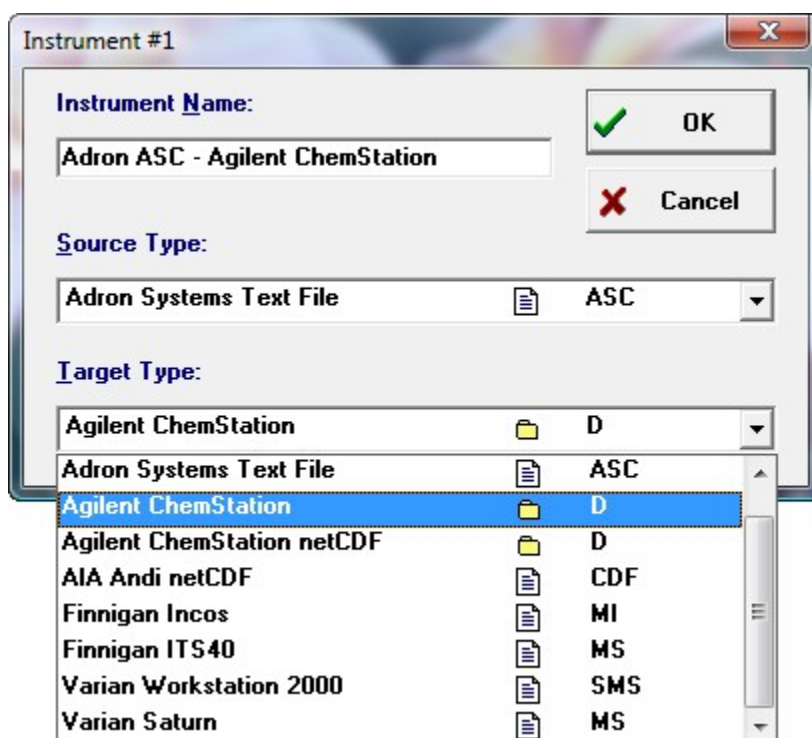


The default active instrument is "Instrument #1". The active instrument is listed in the lower left corner of the status bar. The active instrument number is listed within brackets on the titlebar.

To configure a specific conversion, use the "Instruments" menu, and select the "Properties..." menuitem as in this example:



This will bring up the Instrument properties dialog as shown below:

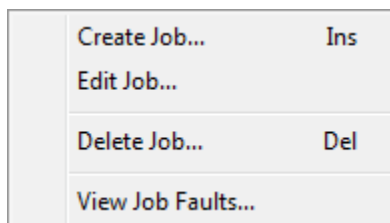


Select the source and target file types from the dropdown lists. Specify a descriptive name for the instrument conversion.

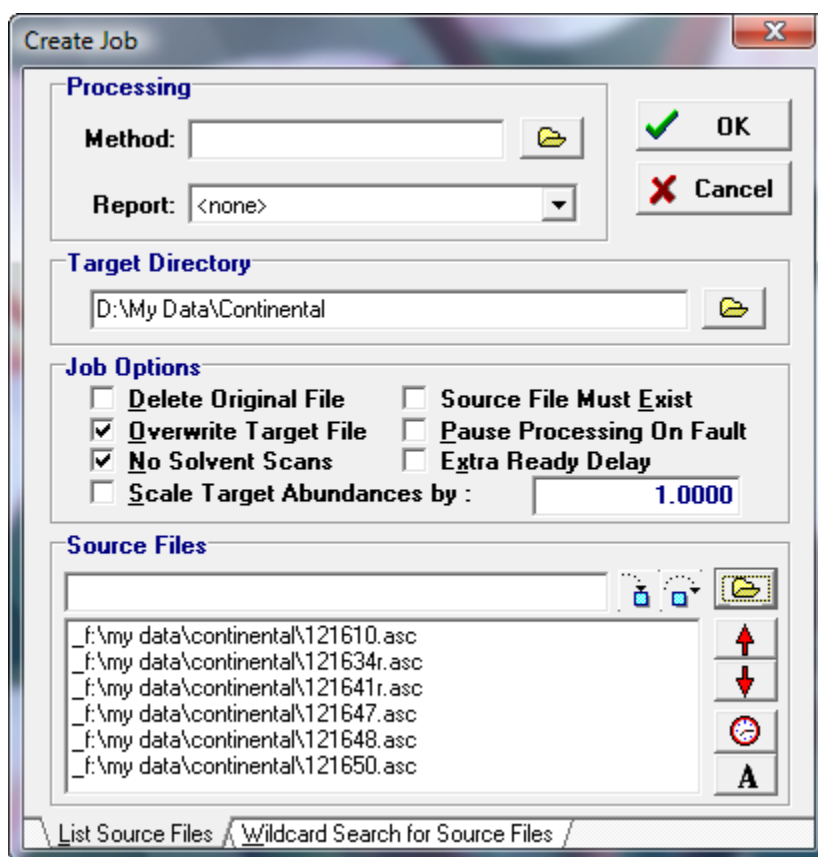
In the example above, the source type is "Adron Systems Text File (ASC)" and the target type is listed as "Agilent ChemStation (.D)". The "Target Type" is shown with the dropdown list of available target file types.

The descriptive instrument name is "Adron ASC - Agilent ChemStation".

The next step is to create a "Job", i.e., a list of files to convert. Go to the "Job" menu and select the "Create Job" menu item as shown in this example:



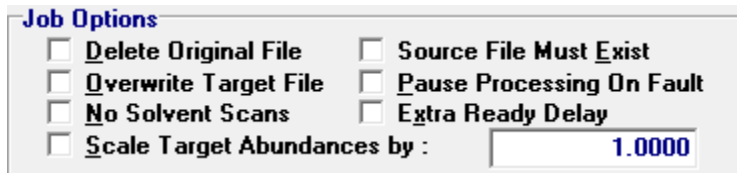
This brings up the "Create Job" dialog as shown below. By-the-way, the "Edit Job" dialog is identical but is used to edit an existing "Job".



Ignore the "Processing" group. This is for customers using the [Extend MS](#) product from [ProLab Resources](#).

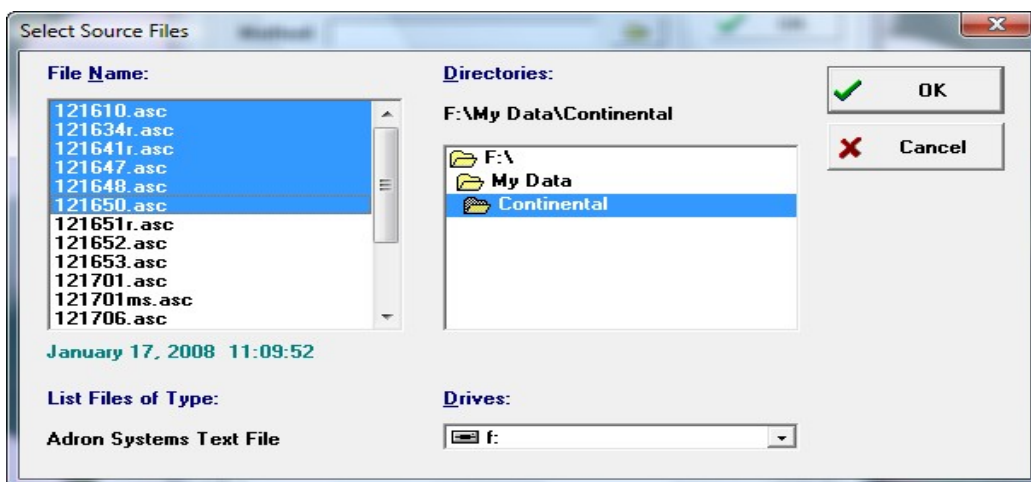
The "Target Directory" specifies where converted files should be placed. Use the folder icon to select the directory.

The "Job Options" group allows you to configure the behavior of the conversion process.



- ✓ *Delete Original File* -- After successful conversion, delete the original source file. Use caution when enabling this option!
- ✓ *Source File Must Exist* -- Conversion will halt if the listed source doesn't exist. If not enabled (not checked), then conversion will continue with the next file.
- ✓ *Overwrite Target File* -- If the target file already exists, the file will be overwritten when option is enabled (checked).
- ✓ *Pause Processing On Fault* -- If the conversion process fails for a given file, then, when this option is enabled, conversion of subsequent files is halted.
- ✓ *No Solvent Scans* -- This doesn't allow "solvent scans" to be placed in the target file. Solvent scans are blank (empty) scans at the beginning the GC/MS or LC/MS file.
- ✓ *Extra Ready Delay* -- Some acquisition systems need extra time to "finish" writing the source data file. Enabling this option provides an extra 60 seconds to complete writing the data file. This option is often used for files acquired from the Varian WorkStation (SMS and XMS) data system.
- ✓ *Scale Target Abundances by* -- This scales data by the specified multiplier. This option is used if the target file format has less dynamic range than the source file, i.e., data is scaled down.

The "Source Files" group allows you to specify source files individually. Typically, the "Select Source Files" dialog is used by invoking the folder button.

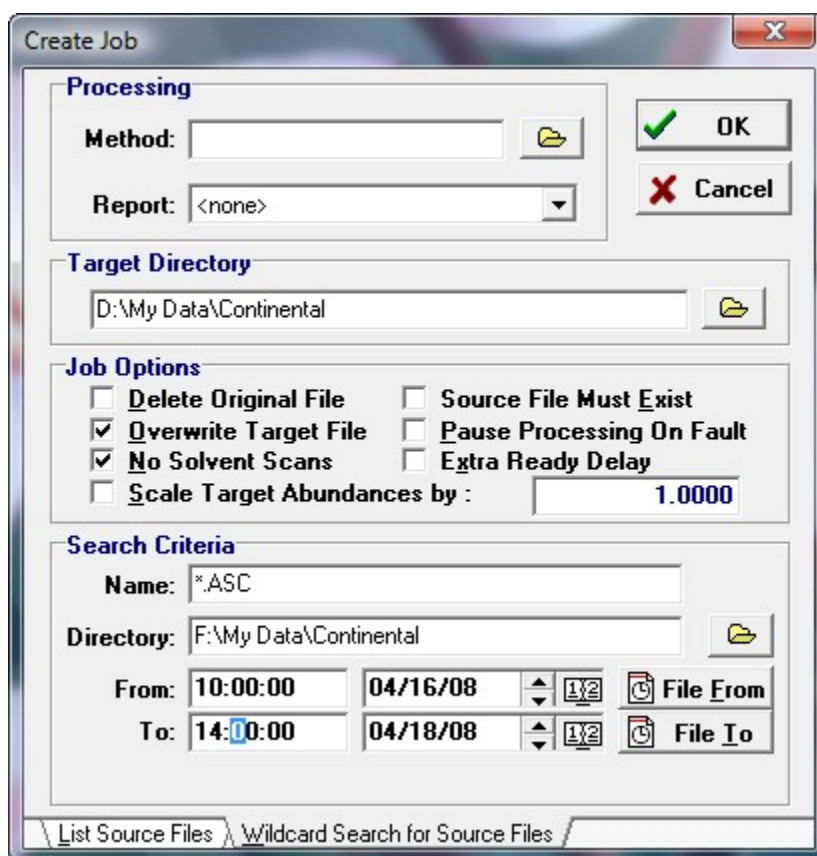


When selecting files with this dialog, you can use the Ctrl and Shift keys to select multiple files.

Note: The files listed in the "Source Files" group have three possible prefixes in front of the file name. These prefixes are:

- _ : An underscore indicates the file has not been processed.
- * : An asterisk indicates the file has been processed (converted). This option can be cleared by double-clicking on the line, allowing for re-processing.
- ~ : A tilde indicates that during file conversion, a problem occurred. Again, the item can be cleared by double-clicking on the line.

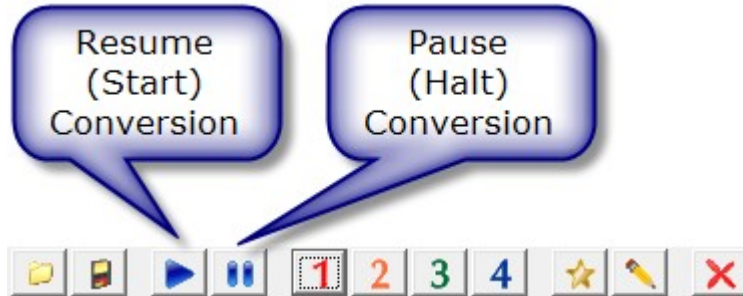
The "Create Job" (or "Edit Job") dialog box also allows for "wildcard" searching of source data files. See the tab at the bottom of the dialog label "Wildcard Search for Source Files".



Wildcarding is based on a "From" time to a "To" time, i.e., a time window. This mode is typically used to convert data files as they acquired from the instrument. This option could also be used to convert a group of files in a specified time window. In this case, the "File From" and "File To" buttons are generally used to select the first and last files in the group.

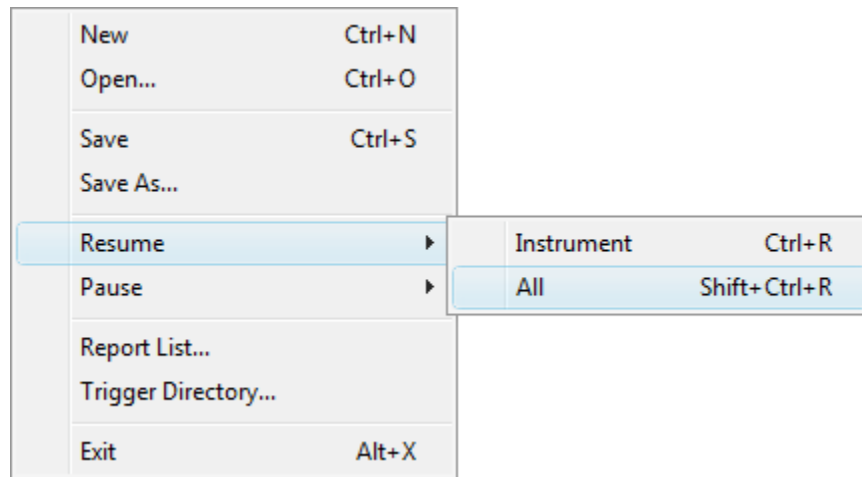
Note: File times must differ by at least one second for "wildcarding" to work!

After creating a "Job" to list the source files, either through the "List Source Files" tab or the "Wildcard Search for Source Files" tab, the next step is to start the conversion process.



The easiest way to start the conversion process for the active instrument is to press the "Resume" button on the *Vx Capture* toolbar.

Another method is to select the "Capture" menu and either the "Resume -> All" menuitem or the "Resume -> Instrument" menuitem as shown below:



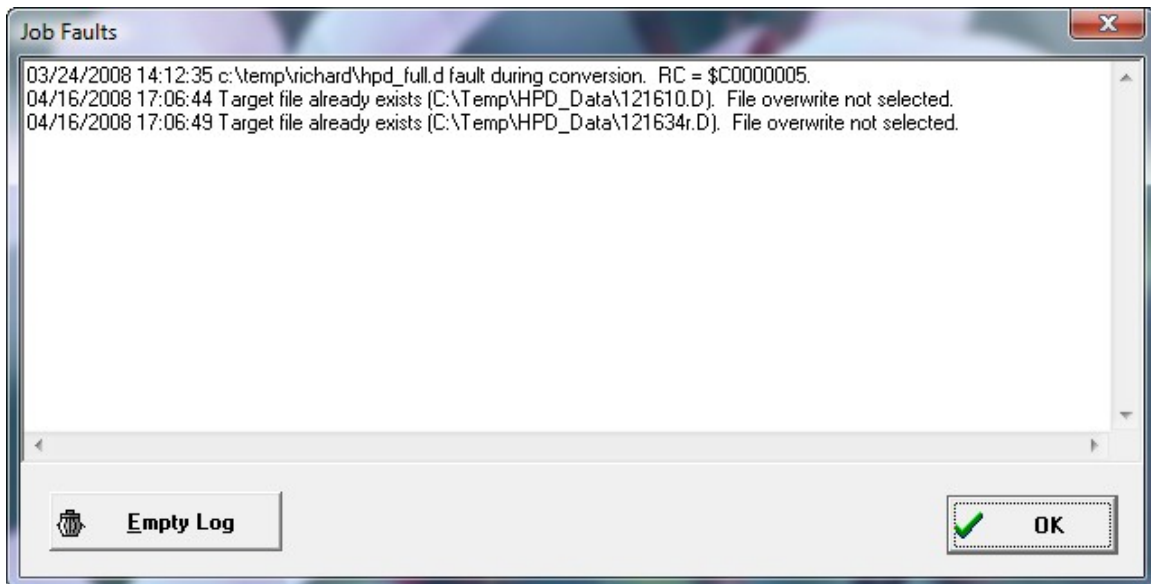
- "Resume -> All" starts conversions for all Jobs on all instruments.
- "Resume -> Instrument" starts conversions only for the active instrument. This is the same behavior as the toolbar "Resume" option shown at the start of this page.

The *Vx Capture* program launches a window labeled "PlaConverter" as shown in the example below:



PlaConverter is minimized to the Windows taskbar. Click on the button to open the window. If the conversion is fast, then this window will be short lived. The speed of the conversion depends on your PC, its capabilities and the type of conversion involved. Basic file information is listed for the source file being converted.

Problems during the conversion process (faults) can be viewed with the "Job Faults" dialog. This dialog is accessed through the "Job" menu.



Adron Systems supports a simple text based GC/MS format with the file extension "ASC". The following is an excerpt from the [Adron_Text.ASC](#) example file:

```
## Generated on   Fri Apr 18 13:32:05 2008 UTC ##  
## Injection time Thr Jan 03 02:56:18 2008 UTC ##
```

```
TimeOfInjection=1199328978  
NameOfOperator=Jayne Doe  
NameOfInstrument=Jayne's GC/MS  
NameOfSample=07121610-5,D1,partial  
Description=Example Adron Systems' ASC file  
VialNumber=22
```

```
IntervalOfScan=63.109
```

35.943	673
38.720	745
39.599	2592
40.106	6744
41.002	1464
41.807	1259
43.008	1168
43.906	177573
44.934	910
45.864	419
50.006	370
54.705	473
82.001	281

```
IntervalOfScan=63.484
```

38.050	351
38.994	1275
39.956	9087
41.180	1404
41.960	252
43.014	2919
43.914	138976
45.028	1064
46.085	985
53.072	389
79.188	263

This above example starts with some basic information fields and then shows the format of two mass spectral scans.

The fields supported by the Adron ASC file format are as follows:

TimeOfInjection	For C programmer's, this is a time_t value, i.e., the number of seconds since midnight, January 1, 1970. If not specified, then the timestamp for the ASC file is used as the acquisition time. The TimeOfInjection value is based on UTC (Universal Coordinated Time); not local time.
LocalTimeOfInjection	As above but utilizes local time instead of UTC.
Description	Descriptive text for the run and/or sample.
NameOfInstrument	Specifies which instrument generated the data.
NameOfMethod	Name of acquisition method used to acquire the data.
NameOfOperator	Name of operator that ran the sample.
NameOfSample	Descriptive name of sample.
VialNumber	Auto-sampler or injection number.
IntervalOfScan	Proceed each scan block with this field. Its value is in seconds and specifies when the scan occurred. <i>If not specified, then each scan time is its scan number.</i> Blank lines between scans signify the start of a new scan. If the "IntervalOfScan" field isn't used, then each scan time is its ordinal number, in seconds.

To comment lines, use the "#" symbol as shown in this example:

```
## Generated on   Fri Apr 18 13:32:05 2008 UTC ##  
## Injection time Thr Jan 03 02:56:18 2008 UTC ##
```

The "#" should be the first non-whitespace character on the line.

If you are interested in customization of the Adron ASC format or have questions, contact us through the [Vx Capture Information Request](#) form on the Adron Systems' website. The Thermo-Fisher Excalibur GC/MS and LC/MS data system can generate Adron System ASC files.

Note: Some behaviors in the *Vx Capture* program can be modified by editing settings in the `ProCaptr.Ini` file. For details, see the [ReadMe.Txt](#) file included in the distribution.

<code>Reader_CDF_Use_Local_Time</code>	NetCDF files have times stored in Coordinated Universal Time (UTC). However, some vendors mistakenly use local time instead of UTC. When this option is True, NetCDF files are processed (read) using local time.
<code>Reader_SMS_Merged_Scans</code>	Varian ion traps can produce MS(n) data files. When this option is True, then such scans are merged together. This is basically the 'All' option found in Varian Workstation. This option is for reading Varian SMS files.
<code>Reader_XMS_Merged_Scans</code>	Varian ion traps can produce MS(n) data files. When this option is True, then such scans are merged together. This is basically the 'All' option found in Varian Workstation. This option is for reading Varian XMS files.
<code>Writer_HPDMilitary_Time</code>	When writing Agilent ChemStation .D data files, store time in military format when this option is set True (default). When False, a civilian format (am, pm) is used.
<code>Writer_CDF_Nominal_Masses</code>	When this option is True, masses are stored with nominal, integer resolution. When False (default), masses are stored with 0.0001 m/z resolution. Use nominal masses for TagFinder and other software packages. Option applies to Vx Capture version 2.12.120 and greater.
<code>Writer_CDF_Do_Float_Values</code>	When this option is True, masses and intensities are stored as floating point numbers. This option is provided for capability with programs that incompletely support the AIA NetCDF standard. Option applies to Vx Capture version 2.17.126 and greater.
<code>Writer_CDF_Use_Local_Time</code>	NetCDF files have times stored in Coordinated Universal Time (UTC). However, some vendors mistakenly use local time instead of UTC. When this option is True, NetCDF files are stored with local time. Option applies to Vx Capture version 2.18.127 and greater
<code>Writer_SMS_Nominal_Masses</code>	When this option is True, SMS data files are stored with integer mass resolution. This option supports Varian Workstation versions 5.x and older. Otherwise, mass resolution is 0.1 m/z.

Writer_T3_Do_Comments	When this option is True, write out data file comments at start of Triton T3 data file.
Writer_T3_Do_Header	When this option is True, write out data file header information. These are the same information fields used in the Adron ASC file described above.
Writer_T3_Do_Scan_Interval	When this option is True, the initial column of the Triton T3 data file is the scan interval (retention time) in seconds.
Writer_T3_Do_Scan_Summation	When this option is True, then the next column of the Triton T3 data file is the ion summation value (TIC, RIC).
Writer_T3_Clip_Trailing_Zeros	When this option is True, then redundant trailing zeros are clipped from output rows in Triton CSV T3 data files.
Writer_T3_Scan_Range	For Triton T3 data files, this specifies the mass scan range.
Writer_T3_Use_Commas	For Triton T3 data files, when True, commas are used to separate items. Otherwise tabs are used as separators.

Note: Hewlett-Packard and Agilent ChemStation files with a small number of scans (<4) are not recognized as valid files. A work-around is to add empty scans until there are at least four scans defined. You can use the "IntervalOfScan" field without scan data to accomplish this. You can add these empty scans at the beginning or end of the text file.

Note: Please read the [License.Txt](#) file for the current *Vx Capture* grant-of-license information.