

The logo features a stylized 'V' on the left, composed of a blue arrow pointing upwards and to the right, with a red diagonal bar crossing it. To the right of the 'V' is the word 'Capture' in a large, blue, sans-serif font.

Vx Capture

Vx Capture™

GC/MS and LC/MS File Conversion

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Introduction

Vx Capture is a software utility for converting 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. Use this form if you are interested in customized GC/MS and LC/MS file conversion solutions.

Vx Capture is compatible with these Microsoft operating systems:

- Windows 10
- Windows 8
- Windows 7 SP1
- Windows XP SP3

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

- Adron Systems' Vector/2 and Vx (TKF)
- Adron Systems' Text File (ASC)
- Agilent & HP MSD ChemStation (.D)
- AIA Andi netCDF (CDF)
- Finnigan Incos (MI, MX)
- Finnigan Incos (TI, TX, CT)
- Finnigan ITS40, Magnum and Tracker (MS)
- PerkinElmer TurboMass (RAW)
- 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 MSD 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)

Product Evaluation

Vx Capture is available in “demonstration” mode when acquired from the Adron Systems' website. In this mode, data conversion is limited to $\frac{5}{8}$ ths of data file spectra, with a maximum extracted scan time of ten minutes. All the file formats listed above are supported in “demonstration” mode.

You can submit sample files for conversion to Adron Systems by sending an email to:

support@adronsystems.com

Please submit your data files in a “zipped” format using a utility such as [WinRAR](#), [WinZip](#) or [7-Zip](#). Specify the target format(s) you would like your source files converted to.

Note: For large files, we recommend that you send your “zipped” file to us via [Dropbox](#).

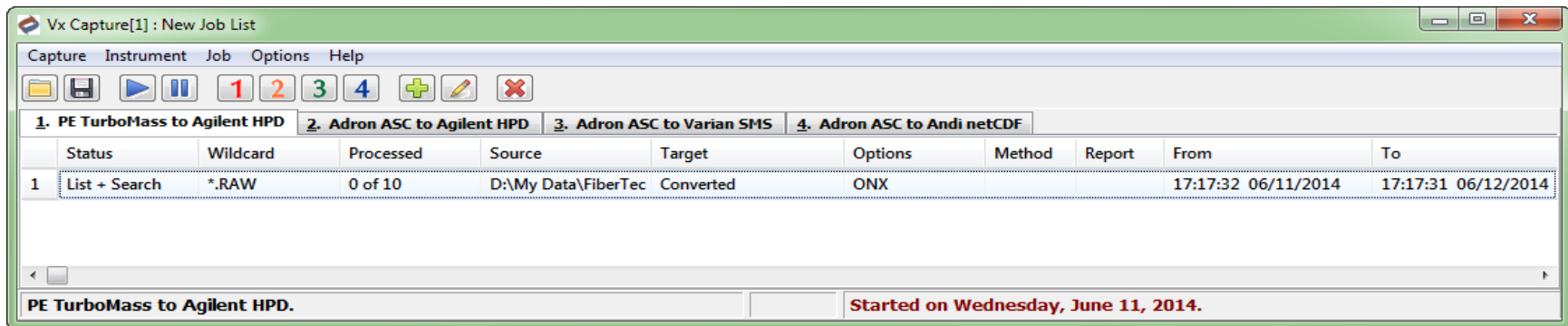
Adron Systems provides *Vx Capture* in an “evaluation” mode on a case-by-case basis. In “evaluation” mode, data conversion is fully functional for a limited number of days. Contact Adron Systems for further details by filling out the [Vx Capture Information Request](#) form.

Vx Capture

Getting Started

To start the *Vx Capture* program, select “Vx Capture” from the “Adron Systems” folder.

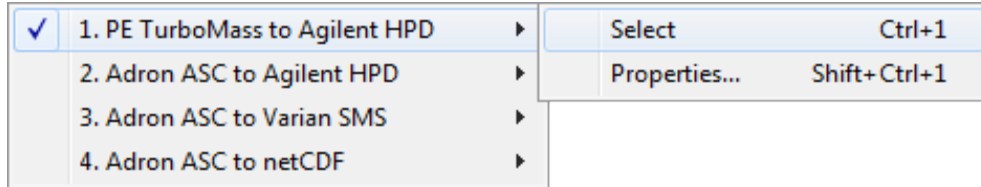
When started, *Vx Capture* appears as:



Instrument Selection

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 different GC/MS or LC/MS systems.

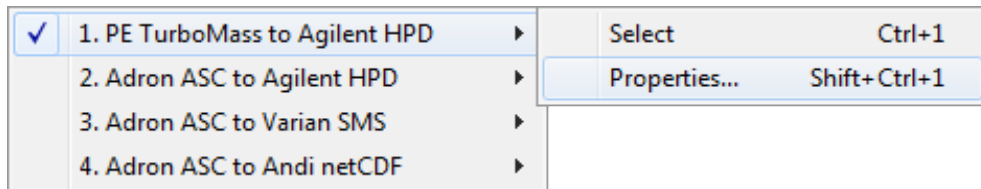
To switch the active instrument, use the toolbar buttons or select the desired tab. Alternatively, from the “Instruments” menu, use the “Select” menuitem as in this example:



The default active instrument is “Instrument #1”. The active instrument's descriptive text (name) is shown in the lower left corner of the status bar. The active instrument number is listed within brackets on the titlebar.

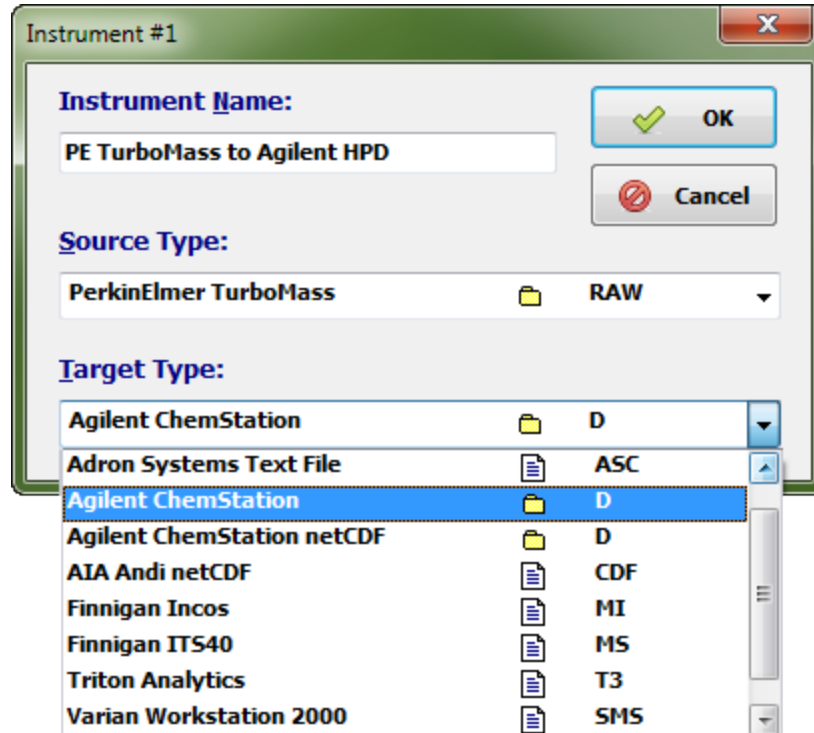
Instrument Configuration

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



Instrument Configuration Continued

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.

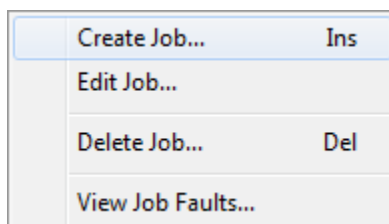
In the example above, the source type is “PerkinElmer TurboMass (RAW)” and the target type is “Agilent ChemStation (.D)”. The “Target Type” is shown with the dropdown list of available target file types.

In the example, the descriptive instrument name is “PE TurboMass to Agilent HPD”.

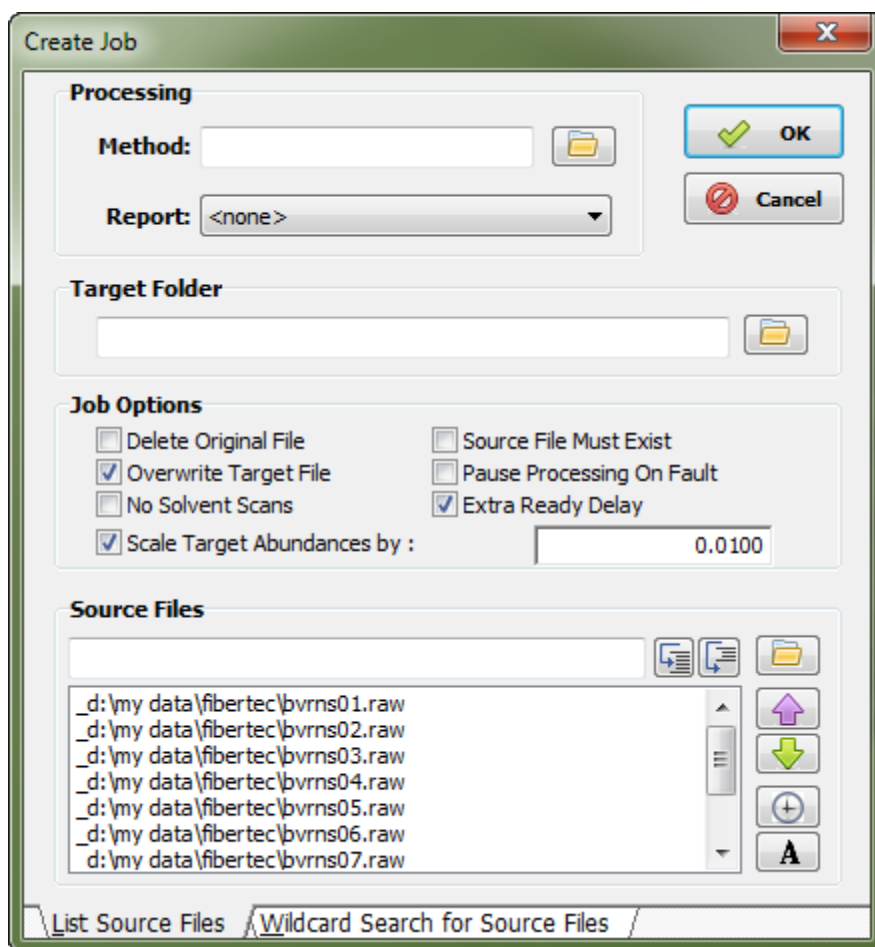
Enter whatever descriptive text you feel is appropriate for the “Instrument Name”.

Job Creation

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. **Note:** 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](#).

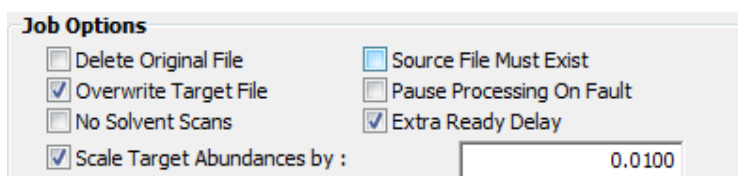
The “Target Folder” group specifies where converted files should be placed. Use the folder icon to select the storage directory.

Leave this field blank to place converted files in the same folder as the source files.

Specify a target sub-folder by entering a name such as “Converted”.

Job Options

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

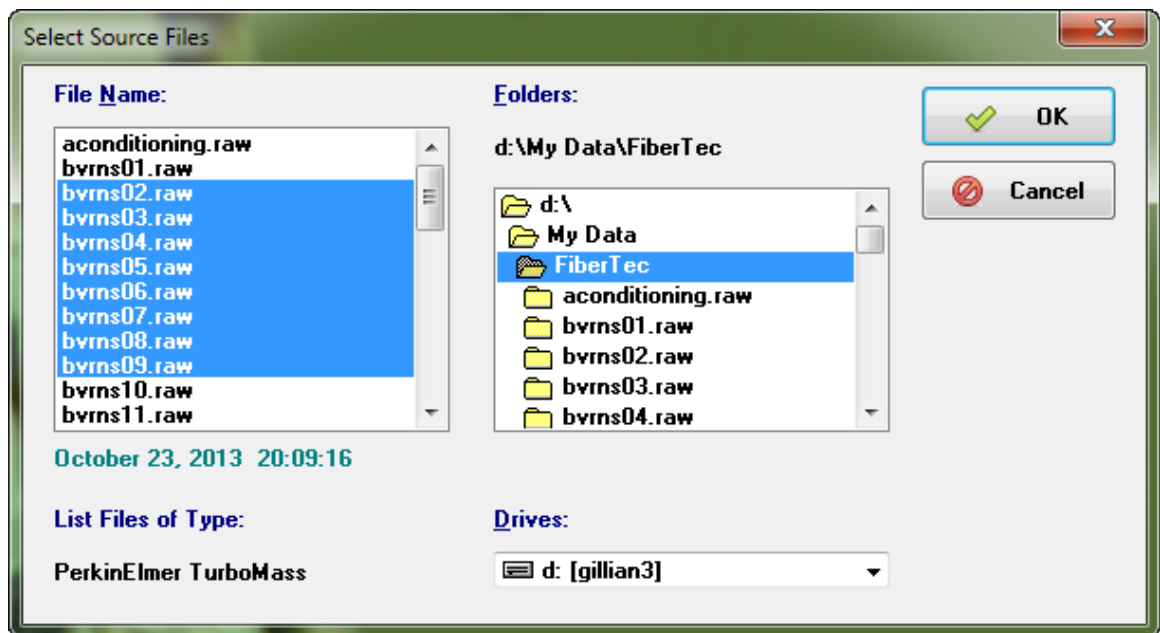


- ✓ *Delete Original File* → After successful conversion, delete the original source file. Use caution when enabling this option!
- ✓ *Source File Must Exist* → Conversion will halt if the listed source doesn't exist. If not enabled (not checked), then conversion will continue with the next file.
- ✓ *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 (checked), 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. Check to enable and specify the scaling factor.

Manual File Selection

The “Source Files” group allows you to specify source files individually. 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.



In this example, with PerkinElmer TurboMass data files, the source files are folder based.

Note: For data files that are file based, the system file selection dialog is utilized.

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.

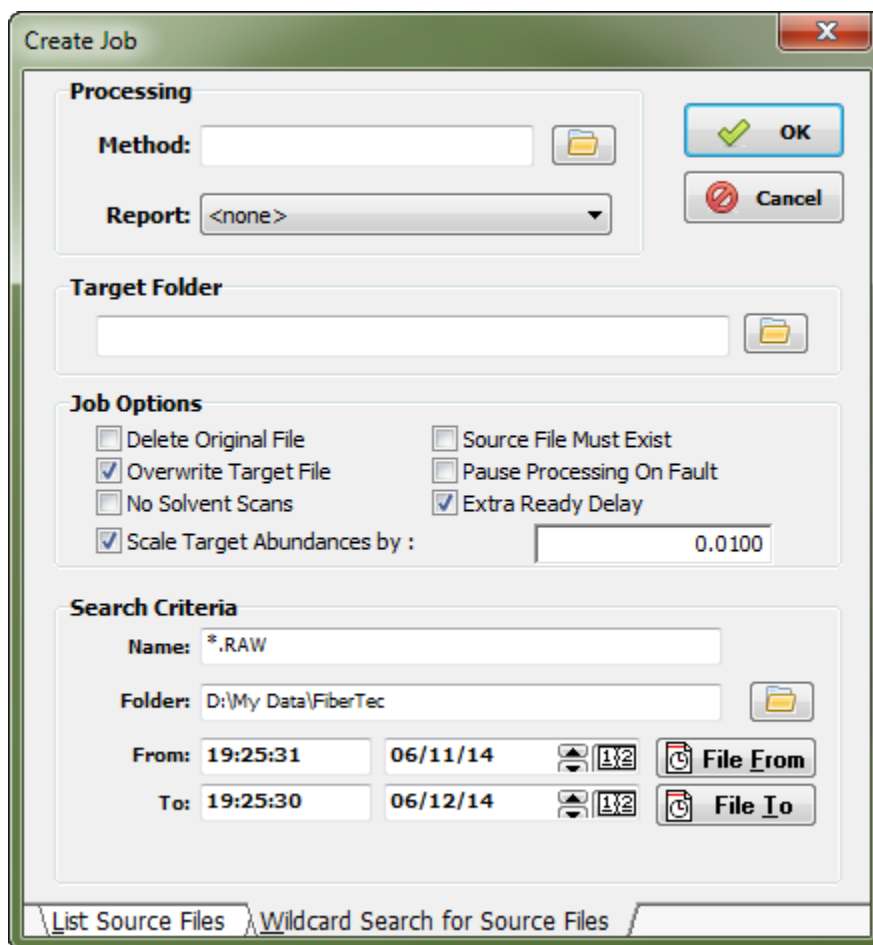
* : An asterisk indicates the file has been processed (converted). This option can be cleared by double-clicking on the line, allowing for re-processing.

~ : A tilde indicates that during file conversion, a problem occurred. Again, the item can be cleared by double-clicking on the line.

Note: Double-click on file entries to reprocess them, i.e., change them back to the “_” prefix.

Wildcard File Selection

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”.



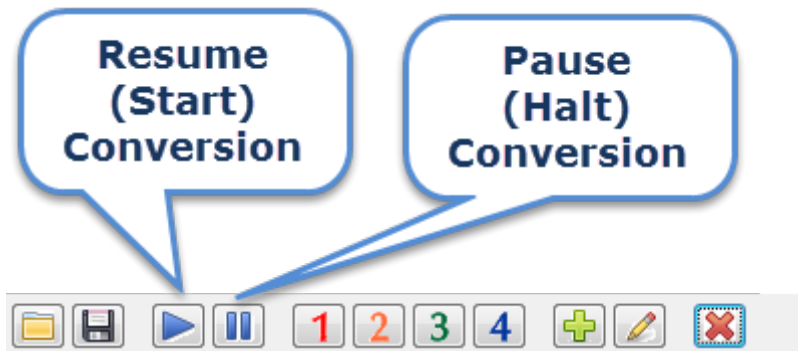
Wildcarding is based on a “From” time to a “To” time, i.e., a time window. This mode is typically used to convert data files as they acquired from the instrument. The default time window is from the present time to plus one day. (Look for files with a creation timestamp starting now through the next 24 hours.)

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.

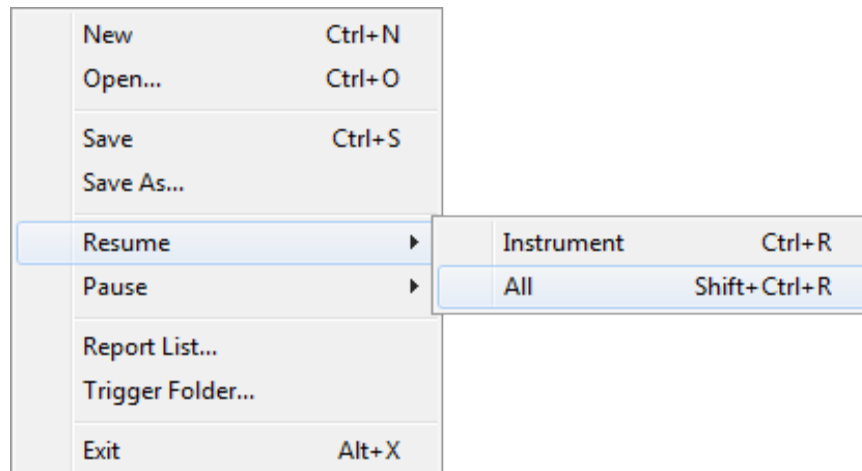
Starting File Conversion

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.

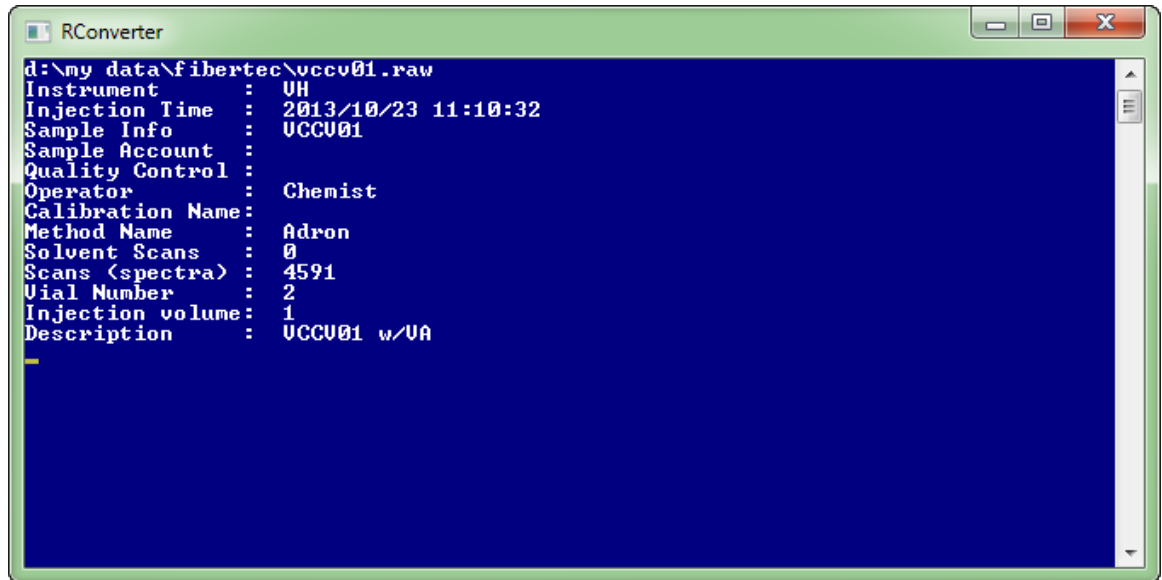
Another method is to select the “Capture” menu and either the “Resume -> All” menuitem or the “Resume -> Instrument” menuitem as shown below:



- “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.

Conversion Window

The *Vx Capture* program launches a window labeled “RConverter” as shown in the example below:

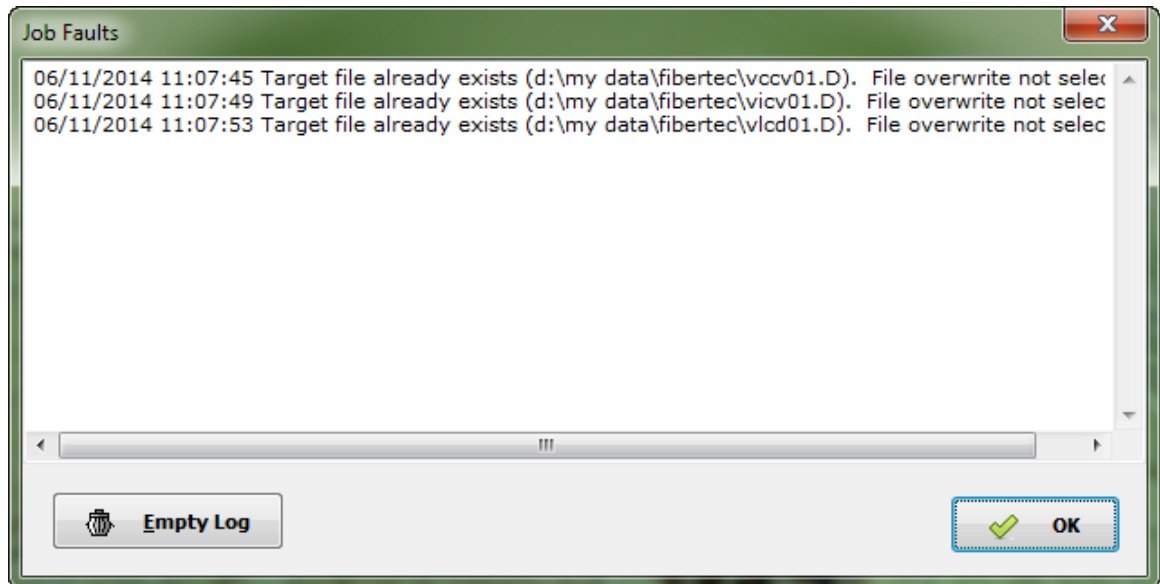


```
d:\my data\fibertec\uccv01.raw
Instrument      : UH
Injection Time : 2013/10/23 11:10:32
Sample Info    : UCCU01
Sample Account :
Quality Control :
Operator       : Chemist
Calibration Name :
Method Name    : Adron
Solvent Scans  : 0
Scans (spectra) : 4591
Vial Number    : 2
Injection volume : 1
Description    : UCCU01 w/UA
```

RConverter is minimized to the Windows taskbar. Click on the window icon 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.

Conversion Faults

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



In this example, three target files already exist, causing a fault when doing the conversion.

In this example, if you wanted to replace the three target files, then, either:

- Manually delete the three target files using Windows Explorer.
- Clear the ~ (tilde) prefix in the “Source Files” section of the “Edit Job” dialog by double-clicking on the file entries.

and

Enable the “Overwrite Target File” option in the “Edit Job” dialog.

and

Restart the Job.

The Adron "ASC" File

Adron Systems designed a simple text based GC/MS file format to facilitate the sharing of GC/MS data between applications. Adron's [Vx.Extract](#) information extraction utility can read and write to this format.

One design goal was to have a human readable format with easy interpretation.

Example "ASC" Syntax

The following is an excerpt from the [Scan_Data.ASC](#) example file:

```
## Source file -- VolData.tkf
## RConverter -- 2.1.00.025
## Scan Count -- 2538
## Generated on -- 2014-06-21T15:54:17-05:00

TimeOfInjection=1991-02-08T12:29:20-06:00
NameOfOperator=Jayne Doe
NameOfInstrument=Jayne's GC/MS
NameOfSample=volstd 100ng
NameOfMethod=D:\VECTOR2\CAL\vol.mth
Description=Volatile Organic standard 100 ng
Description=CyroTrap Analysis
VialNumber=22

IntervalOfScan=1412.07025
157.3009 412
171.1659 360
180.0020 72050
181.0895 5637
182.0411 70126
182.9927 3334
183.9443 16925
185.0319 1671
185.9835 2857

IntervalOfScan=1412.79225
150.0969 573
157.8446 432
170.3503 498
177.8269 1098
180.0020 263568
180.9536 17389
182.0411 276728
182.9927 13482
183.9443 76060
185.0319 5100
185.9835 7020
```

This example starts with four lines of comments, some basic information fields and then two mass spectral scans.

Adron "ASC" Supported Fields

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

TimeOfInjection	<p>For C programmer's, this is a time_t value - 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.</p> <p>Note: Current versions of <i>Vx Capture</i> allow the use of ISO8601 time strings. An example: 2014-06-20T00:02:04-05:00</p>
LocalTimeOfInjection	As above but utilizes local time instead of UTC.
Description	Descriptive text for the run and/or sample. Multiple description lines can be specified as in the example above.
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	<p>Proceed each scan block with this field. Its value is in seconds and specifies when the scan occurred.</p> <p>Blank lines between scans signify the start of a new scan.</p> <p>If the "IntervalOfScan" field isn't used, then each scan time is its ordinal number, in seconds.</p>
StartDataSection	Adron ASC files support parallel data sets. This keyword allows SIM data spectra to follow Scan data spectra. Use of this keyword is optional (implied) for first data section.

Adron "ASC" Comments

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

```
## Source file -- VolData.tkf
## RConverter -- 2.1.00.025
## Scan Count -- 2538
## Generated on -- 2014-06-21T15:54:17-05:00
```

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

These comment lines were generated by *Vx Capture* during its conversion of an Adron Systems' Vx TKF file to Adron's ASC format.

Adron "ASC" Customization

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.

Note: The Thermo Scientific Xcalibur GC/MS and LC/MS data system can generate Adron System ASC files using Thermo's `XcaliburToText` macro. Contact your Thermo representative to obtain this macro.

Vx Capture Configuration

Some behaviors in the *Vx Capture* program can be modified by editing settings in the `ProCaptr.ini` file with a text editor such as Windows' Notepad.

On Windows 7, with the latest version of *Vx Capture* installed, look in the following folder:

```
c:\Programdata\Adron Systems\Vx\Options
```

On Windows XP, with the latest version of *Vx Capture* installed, look in the following folder:

```
c:\Documents and Settings\All Users\application data\Adron Systems\Vx\Options
```

In older versions of *Vx Capture*, the `ProCaptr.ini` file was stored in the "Programs" folder:

```
c:\Adron Systems\Vx\Programs
```

or

```
d:\Adron Systems\Vx\Programs
```

For older Perkin-Elmer *Vx Capture* installations, the `ProCaptr.ini` file was stored in the "Converter" folder:

```
c:\Adron Systems\Converter
```

or

```
d:\Adron Systems\Converter
```

<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 as 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_ASC_Pretty_Columns</code>	When this option is True, make mass and intensity values align to the right. Resulting ASC files are larger when this option is enabled plus extra processing time is required. Extra spaces can make it more difficult to import results into other applications.

Writer_ASC_Use_Commas	When this option is True, use commas to separate mass and intensity values instead of spaces.
Writer_HPD_Military_Time	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.
Writer_CDF_Nominal_Masses	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.
Writer_CDF_Do_Float_Values	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.
Writer_CDF_Use_Local_Time	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.
Writer_SMS_Nominal_Masses	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: Agilent MSD 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: Agilent MSD ChemStation files have a maximum spectral intensity value of 8388096 counts. TIC values can range up to 32 bits or 4294967295 counts. Mass resolution is limited to $\frac{1}{20\text{th}}$ m/z.

PerkinElmer TurboMass Addendum

Conversion Challenge

PerkinElmer TurboMass GC/MS files present a unique challenge for the *Vx Capture* file conversion program.

TurboMass data files can contain up to 32 functions (segments, experiments) within a single acquisition run. The resulting data file is stored as a collection of files within the TurboMass RAW folder.

Spectral index files are stored as `_func001.idx ... _func0xx.idx` files where `xx` represents the last function number.

Spectral data are stored as `_func001.dat ... _func0xx.dat` files where `xx` represents the last function number.

A mix of SIM (selected ion monitoring) and scan functions can comprise an acquisition run within TurboMass.

The challenge is to “re-assemble” TurboMass data into target file formats that are generally not as flexible. *Vx Capture* places some restrictions on the layout of TurboMass acquisition functions.

Vx Capture layout rules for TurboMass are:

- Scan functions must be sequential, in time, with other scan functions.
- SIM functions must be sequential, in time, with other SIM functions.

Scan Function Layouts

Let  represent a TurboMass scan function.

Let  represents a TurboMass SIM function.

These are acceptable layouts for TurboMass functions:

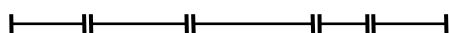
- 1) Mixed SIM and Scan functions:



- 2) Alternating SIM and Scan functions:



- 3) Only Scan functions:

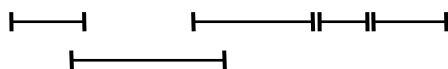


- 4) Only SIM functions:

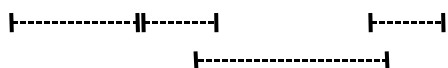


These are unacceptable layouts for TurboMass functions:

1) Non-sequential scan functions:



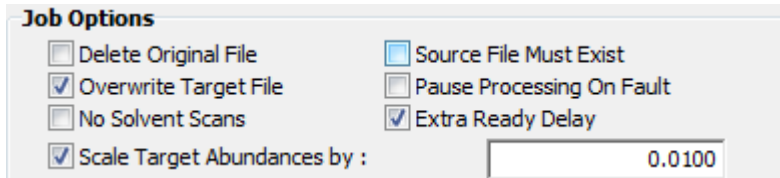
2) Non-sequential SIM functions:



Disclaimer

Using non-sequential layouts will result in the generation of incorrect target files. *Vx Capture* does not generate an error message in these cases.

Data Scaling



When generating Agilent MSD ChemStation files, care must be taken to ensure that the TurboMass file conversion does not exceed the limited range of the ChemStation file. Be sure the "Scale Target Abundances by" option is checked in the Job's dialog and set the scaling factor to 0.01 or another reasonable value.

Other target formats may also have a limited range. Validate your conversions before using results in a production environment!