

MassHunter File Reader

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MassHunter File Reader

Welcome to MassHunter File Reader. This free program was developed to enable accessing raw data from Agilent MassHunter binary files, and exporting those data to text files (or an Excel file) for use with other programs. This program is based on inferred data structures that have not been formally defined by Agilent and we cannot be certain that this program will work on your files, nor that the Agilent file structures may not change without notice in the future. However if this program does not work properly with your files then we would appreciate hearing from you since that may enable us to improve the function of this program.

MassHunter File Reader is a read-only application. No MassHunter files are modified in any way during its use. This utility specifically targets Agilent GC/MS and GC/MS/MS files and those are the only files that have been evaluated at this point. Presumably it could work with LC based data also, but that has not been confirmed.

Basic Actions

[Opening a MassHunter .D File](#)

[Reading and Displaying the TIC](#)

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Open a MassHunter File

To open a MassHunter file select File / Open from the menu or simply click the Open File button on the top access bar to display the File_Open window. A few example files are included with this program that represent various types of GC assays by either single or triple quad analysis. If you have any difficulty locating the Demo files please see the topic File Locations.

When you select File / Open the only type of file that can be selected is MSScan.bin. To locate that file, navigate to the .D folder containing the data, open it and then open the folder AcqData. The MSScan.bin file should be visible. You can click on it and then click the Open button, or just double click on MSScan.bin in the usual manner.

The file name will then be displayed with some basic information including the type of data collection (e.g. Scan or MRM), the number of scans collected, collection start time, stop time and the total run time. The time data are preliminary values at this point that may not always accurately represent the true contents. The actual times collected will be available when the data are accessed. When a file has been opened, the Process Scans button is enabled. If this is the file you want to read, then click on Process Scans.

Displaying the TIC

Read and Display Chromatogram

When you click on the Process Scans button, the Total Ion Current chromatogram should be displayed and the data are also listed in the box on the far right of the screen. Each line in the box will consist of the Scan number, the Retention time, and the total abundance collected for that scan. You can zoom in and out of the graphical display to observe selected regions more closely. Note that both the TIC and spectrum displays are meant only to assist in reviewing and selecting data to export. These displays have very limited functionality and are not meant to be used for detailed review or processing of the data.

To view an individual spectrum, either click on a line in the text display box, or click at the desired spot on the TIC. When you access spectra from the TIC scan data, you must click directly on the chromatogram trace. Consequently, for the examination of a specific scan, clicking on the line in the Scan list is usually a simpler and more precise method, but either approach can be used.

Displaying Spectra

Display a Spectrum

When you either click on a line in the Scan list, or at a point on the TIC, the spectrum for that scan will be displayed in the lower part of the plot window by default. The Scan number will display in the title for the spectrum plot, and the number of ions collected for that spectrum and the m/z value for the spectrum's base peak should be displayed on the main form just below the file name. The option to display spectra is only available with scan data. Spectra viewing is not available for SIM or MRM files since they have no meaningful spectra to display. There is no facility provided for further processing such as viewing extracted ion profiles or averaging spectra.

When a spectrum has been displayed, the three buttons to the top right of the plot area are enabled. These let you toggle between displaying the TIC only, the Spectrum only, or the default TIC + Spectrum display. The spectrum display can be zoomed in and out in the same manner as the TIC. You can also click on peaks in the spectrum window which will label the mass for that peak. This is for information only and is not persistent. When you close or switch windows, the mass labels will be lost.

Exporting the data

Export

After you have opened a file and processed the scan data, the Export button will be enabled. The ability to export all or selected data from MassHunter files in plain text format, either individually or in a batch mode, is the main purpose of this program.

Click on either the File / Export menu item or the Export speed button to open the Export Data window. This window provides options to export either the TIC alone including scan number, retention time and total abundance (the data present in the Scan list), or the TIC and each associated spectrum. Note that if you choose the latter option, the file generated can be rather large.

Data can be exported to Condensed Text files, to Formatted Text files, or as Excel Files (.xls). Click on the links for more information on each of those options. By default, the export scan list will be set to all scans from #1 to the last scan in the file, but both of those values can be edited to export a specific scan region of the data.

Also by default, all data with a total abundance greater than 0 will be exported for each selected scan. However, you can optionally set a desired minimum abundance based on the data displayed in the Scan list box to screen out low abundance scans. See the topic Export Options for more information.

After selecting the options that you want to use, click on Export to create the file.

[Export to a condensed text file.](#)

[Export to a formatted text file.](#)

[Export to an Excel file.](#)

{Note: the batch option has not been implemented yet.}

Condensed Text Output

These files are written as a continuous data stream in a defined pattern as described in the [Condensed Format](#) topic. This is the default and most efficient export option. Although these files are in plain text they are not meant to be read directly. Note that depending on the data collected, the file sizes can be quite large. Therefore, unless the exported file is unusually small, you should not attempt to open it using a limited text editor such as Windows Notepad since that would likely cause Notepad to lock up. You should be able to view the files if you want to by using any larger capacity text editor including WordPad.

The numeric data written by MHRReadFile are not truncated or formatted in any way. The output of floating point values is provided at the full precision read from the MassHunter files.

Condensed format text files are meant to be read by other programs and have a consistent structure. All values are written in consecutive order separated by a token. The default token is a comma, but you can also choose to use either a space or a tab as the separation character. Condensed text output files always begin with a single value which defines its content. This is described more fully in the [Condensed Format](#) topic.

Following the initial content code value, the data are written out in consecutive order. The default is to include all scans beginning with scan 1, but both the beginning and ending scan numbers can be revised on the Export screen to output just a portion of the file. Also, no data for a given scan is written if the total abundance is 0. You can enter a higher total abundance cutoff to screen out lower intensity scans. Either scan-only information, or scan plus spectrum information for each scan can be written. For more information on the structure of these files, see the [Condensed Format](#) topic. Text output files can optionally include information for each scan including the Collection Time Segment, the ScanMethod, and/or the Parent Ion for each scan. This is described in the topic [Output Options](#) .

Formatted Text Output

This output is also in plain text, but it is formatted to make it readable. These files are written as scan number, retention time and total abundance separated by spaces, with a blank line between each scan. If spectrum output is selected then each spectrum is written as a mass-intensity table immediately following the spectrum line. Additional values can optionally be included as with the condensed text format. See the topic [Output Options](#) for more information on that.

Remember that these files will often be quite large and the same warning concerning reading them pertains as described for Condensed text. That is, you should never try to open these files with a limited text editor such as Notepad since that may just hang your computer. However, you should be able to open these files with Windows WordPad, or with any high capacity text editor such as gVim or Notepad++.

Excel File Output

This option will create a standard Excel file in the older .xls format (binary, not XML) that can be read by both current and older versions of Microsoft Excel. If the TIC-only option is selected, then the file will consist of the file name on the first line, then a blank line followed by a heading of the three columns of output (Scan number, Retention time and Abundance). All selected scans will then follow in order in the succeeding rows.

If the TIC plus spectrum output is selected, then the same process will be used except that immediately after each scan line the spectrum mass-intensity data will be written in a horizontal format in the next two rows for each ion in the spectrum, with the abundance below each mass. Then the next scan line will be written and so on.

Files in Excel format are convenient for relatively small displays such as scan-only information or for limited scan plus spectrum output. However, a few thousand scans with spectrum data included can quickly grow quite large. For example the MS/MS Q1 scan example file included with this program is only 2,028 scans in length and the scan data alone can be output quickly in Excel format. However, if you export the entire file as scan + spectrum data with no further filtering it can take several seconds to write, and the result will be an Excel file larger than 9 Mb.

Modern Excel worksheets have large capacities. For example, an Excel 2010 worksheet can contain up to 1,048,576 rows and 16,384 columns, so theoretically even huge data files can be output in this format, but it is not recommended since Excel files are more complex than plain text files and are slower to create and to manipulate. The practicality of actually working with an enormous spreadsheet is perhaps another consideration. In general, it is better to reserve Excel output for scan-only data, or for relatively smaller scan plus spectrum files.

Because of the issues outlined above, when you choose to export an Excel file, an estimate of the number of rows and total number of cells that will be output is displayed and you will be asked to confirm that you want to continue before the file is created.

Program Options

The options menu enables you to select a few preferences. The first is to save the current window position when quitting the program. This is the default setting and should be appropriate in most cases, but you can click on the menu item to deselect or select it as you wish.

The second item enables you to change the font used by the program. This normally should also be left at the default, but if you prefer to change the display (e.g. to show larger type) you can use this option. Note that changing fonts, especially increasing the default size, may disrupt the positioning and thus the legibility of some of the objects on screen.

The third option is to set the amount by which the Export abundance cutoff increases or decreases with each click of the up and down arrows in the abundance cutoff value box on the Export window. The choices are to increment by 1, 100 (the default) or 1,000 counts with each click. This is just a minor convenience since you can also simply enter the cutoff value you want directly into the box.

If you change any options, those changes will be saved and used as the defaults in the future.

Open New File

To open a new file, simply click on the Open File button again. There is also an option to Close a currently open file on the File menu that will clear the display, but closing files is not really necessary since this program only opens files to access them and does not leave them open. If a file has already been opened when you click the Open File button then the display data will simply be cleared and you can proceed as described in File Open . For the same reason, you can click the Quit button to close the program at any time that data are not being actively read or written.

Zoom Graphic View

Both the TIC chromatogram and the spectrum plots can be zoomed in and out as needed. To zoom in, click in the display and drag the mouse down and to the right to outline the display area of interest scaled in both the X and Y dimensions.

To restore the unzoomed display, perform the same action in reverse. That is, click in the window and draw a box on screen by dragging the mouse up and to the left.

Condensed Format

The default output file is in Condensed Text format which is intended to be read by another program. To aid in reading the contents, a coded integer value is calculated and written as the first value in the file. This index value will range from 0 to 15 and is constructed when the file is output by combining assigned values for the various options. These options and values are as follows:

Report Option	Value
Scan Only	0
Scan + Spectra	1
Time_Segment	2
Scan_Method	4
Parent_Ion	8

The identity of the data included in the file is then indicated by this number. For example, scan-only data would result in a value of 0, whereas if the spectra are included then it would be 1. Scan-only data with Time_segments included would have a value of 2, Scan+spectra data with Scan_Method and Parent_Ion reported for each scan would be 13, and so on. Note that the basic scan data (the TIC) are always included.

The data in the file after the initial format value is a continuous stream of values in this order:

Scan Number, Retention Time, Total Abundance, Time_Segment (if included), Scan_Method (if included), Parent_Ion (if included), and finally spectral data (if included). When spectra are written, the first value is the number of ions in the spectrum, followed by the paired mass and intensity values, in order by increasing mass.

This sequence then repeats for each subsequent scan included in the file.

Output Options

There are several options included on the Export Data display. The first is the file type with Condensed Text files as the default. The scans selected for output defaults to the entire file, but the initial and final scans to include can be entered into the Scans boxes. Also the minimum total abundance required for reporting data for a scan can be set in the Min Abund box.

The TIC is always included in every export data set. Click on the Tic and Spectra button to include the spectra for each scan. For text files there are a few additional options listed at the bottom of the window including the option to include the Time_Segment for each scan, the Scan_Method for each scan, and/or the scans' Parent_Ion which may be of interest for both product ion and for SIM and MRM data. Finally, the token used to separate each value in the Condensed Data files is a comma by default, but either a space or tab character can be selected instead.

When you click the Export button the File_Save box will open. After choosing the directory and file name, the chosen file will be written. As described in the Writing Excel files topic, if an Excel file is the chosen output then a warning display will appear showing an estimate of the number of rows and total cells that will be written to the file. See the Excel file topic for more information on that.

File Locations

Since it is possible to install MassHunter File Reader as either a standard Windows application or as a portable program, and since different Windows operating systems may have been used, this section describes the expected file locations for MassHunter File Reader after installation and should address any potential difficulty that might arise in locating a file.

Standard Windows Installation

If you used the recommended "No-Questions-Asked" installation then MHFR is registered with Windows and followed the standard conventions. The program itself will be located in "C:\Program Files (x86)\Quadtech Associates, Inc\MassHunter File Reader". In Windows 7 and above, all other files including the Help file, demo files, and any files saved during use will be in subfolders under "C:\Users\<username>\AppData\Roaming\QuadtechAssociates\MassHunter. If you are using Windows XP then the location will be "C:\Documents and Settings\<username>\Application Data\QuadtechAssociates\MassHunter. With a standard installation these locations will be accessed by default by the program during all file read and write operations so you should not have to manually locate them.

The folders present in MassHunter are Documents (contains the Help file), Data (the default location for any files saved), Settings (program support files) and DemoData which contains the example files.

To delete a standard installation, either use the Windows Uninstall feature on the Control panel (Windows XP and 7), or right click on the desktop icon and select Uninstall in Windows 8.0, 8.1 or 10.

Portable Installations

These are simple to use, but you must keep track of where things are since Windows is not tracking the program. When a portable installation is made, all files including the program, help files and the demo data are simply placed in a single folder which is located wherever you choose to place it. That could be on the system hard drive, an attached USB drive, or on other removeable media. The folder name by default is MassHunter File Reader although you can change that if you wish during installation. If you have difficulty locating any files then just look for this folder; all the files should be in the same place. Since portable installations are -- well -- portable, it is not a good idea to create any desktop shortcuts since if the location is not available when you click on the Shortcut it may generate a broken link.

Notice: When you make a portable installation the Show Help option initially will not work correctly because the program will not be able to locate the Help file. Therefore, you should locate the folder in which you placed the program and all its files and open the Documents folder. Either copy or move the Help file in that folder into the main program folder so the program can locate it. This step only pertains to portable installations.

To delete a portable installation, just delete the entire folder and its contents.