

Instruction for Converting the Raw LC-MS Data Obtained by Agilent TOF-MS to a CSV File Compatible with IsoMS

(Version 1.0; March 9, 2014)

- In Step 1 of the data processing process by IsoMS, the raw LC-MS data obtained by Agilent TOF-MS needs to be first converted into a CSV file format that is readable by the IsoMS script.
- If a user has acquired the LC-MS data in the centroid mode or dual-mode (centroid and profile), the ExportMHDDataFile program in MassHunter can be used to convert the raw data to the peak list file in CSV. If only the profile mode is used for LC-MS data acquisition, the AgtTofReprocessUi program in MassHunter can be used to convert the profile spectrum data into the centroid spectrum data, followed by using ExportMHDDataFile to convert it to the peak list file in CSV.
- The two programs (AgtTofReprocessUi and ExportMHDDataFile) are located in the default installation directory of MassHunter:
C:\Program Files\Agilent\MassHunter\Workstation\Qual\B.06.00\Bin.
- An example of converting the raw LC-MS data into a CSV file readable by IsoMS is shown below.

Instruction

1. This step can be skipped if the LC-MS data was acquired in the centroid mode or dual mode. If the data was acquired in the profile mode, to convert the profile spectrum to the centroid spectrum, click AgtTofReprocessUi and select the LC-MS data to be converted. Check Recentroid (Figure 1). The parameters of Recentroid can be adjusted, if needed.

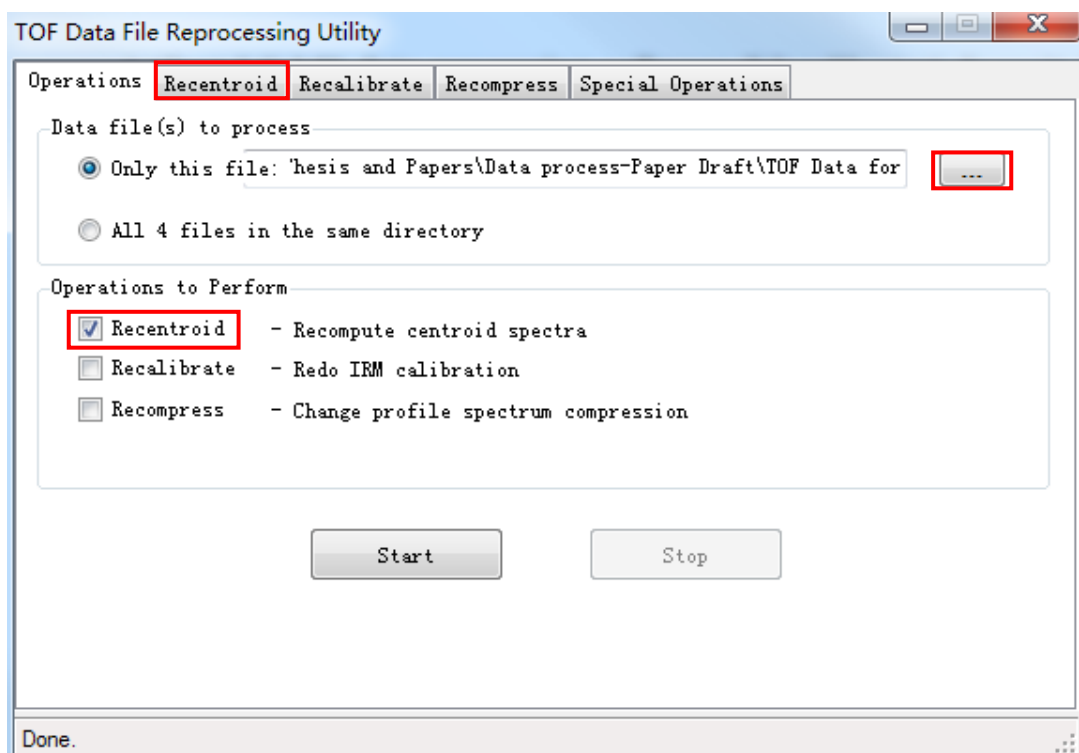


Figure 1. Use AgtTofReprocessUi to convert profile-spectrum to centroid-spectrum.

2. In ExportMHDDataFile, right-click the selected files to add the raw data. The target folder can be selected as shown Figure 2.

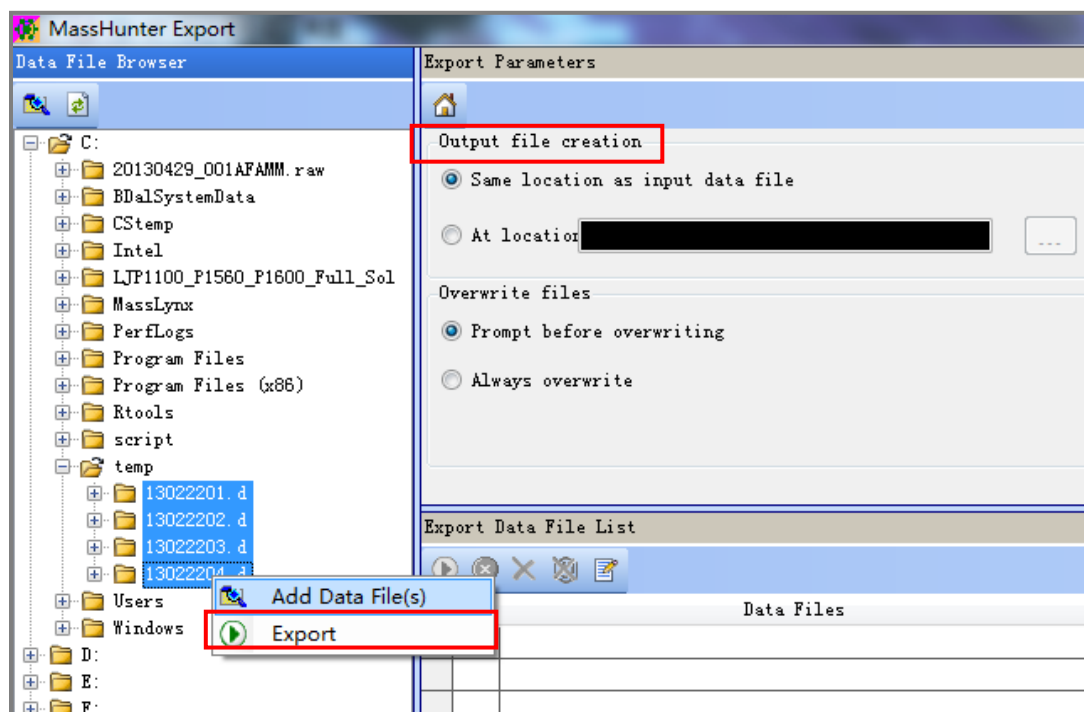


Figure 2. Select the source files and the target folder in ExportMHDDataFile.

3. Select the export file type as CSV in the pull-down menu in ExportMHDDataFile (Figure 3).

Export Parameters

Output file creation

☒ Same location as input data file

☐ At location: ...

Overwrite files

☒ Prompt before overwriting

☐ Always overwrite

Export type

File type: **TOF format text file (*.txt, *.csv)**

With delimiter: (Default: comma)

Data filters

MS Level: MS

☐ Restrict m/z to m/z

☐ Restrict retention time to minutes

Export Data File List

	Data Files	Output Files	Status
▶	C:\temp\13022201.d	13022201.csv	Completed

Figure 3. Select the export file type in ExportMHDDataFile.