

Instruction for Converting the Raw LC-MS Data Obtained by Bruker FT-ICR-MS or QTOF-MS to a CSV File Compatible with IsoMS

(Version 1.0; Feb 12, 2014)

- In Step 1 of the data processing process by IsoMS, the raw LC-MS data obtained by Bruker FT-MS or QTOF-MS needs to be first converted into a CSV file format that is readable by the IsoMS script.
- The Bruker LC-MS data processing software package (DataAnalysis) does not contain a program that would allow a user to directly export the raw data to a CSV file readable by IsoMS. However, Bruker allows a user to develop VB scripts to be integrated with the DataAnalysis software to process the raw data into a format compatible with other program.
- We have developed a VB script, BDFormatConverter, that can be used for the data conversion. Before converting any files, the BDFormatConverter code must be cut and pasted to DataAnalysis to create a DataAnalysis Method. The instruction for creating and using the method for converting the raw LC-MS data into a CSV file readable by IsoMS is given below.

Instruction

1. To create a DataAnalysis method, open a LC-MS data file in DataAnalysis (any data file works here).
2. In DataAnalysis, click: Method → Script as shown in Figure 1.

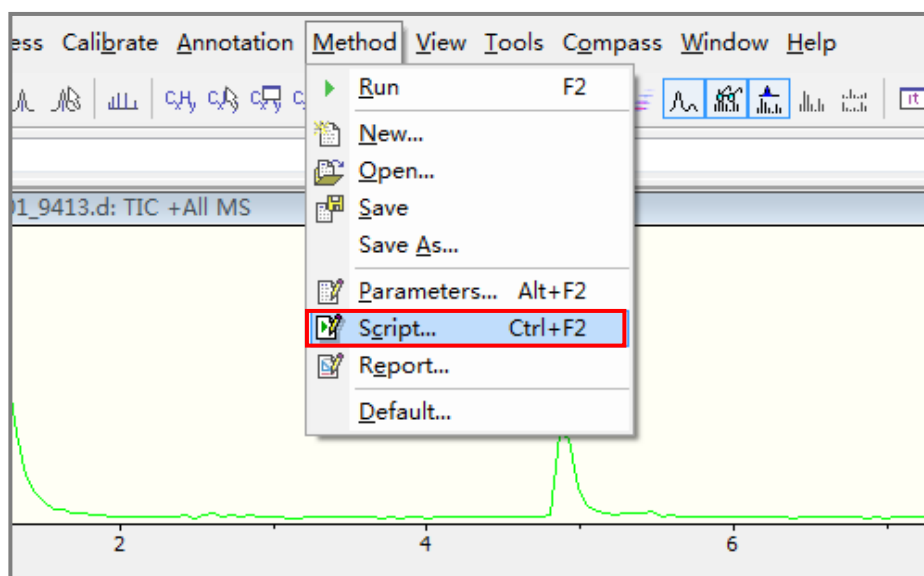


Figure 1. Open the VB script window in Bruker DataAnalysis.

3. Paste the BDFormatConverter code to the pop-up DataAnalysis Script window (Figure 2). Change the parameters in the red box (see Table 1 for the explanation of the parameters that need to be changed).

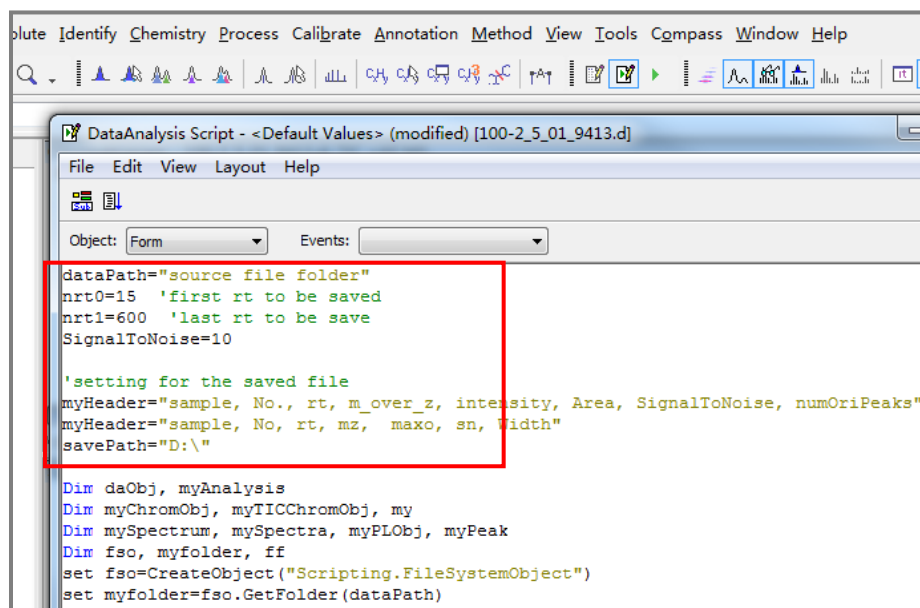


Figure 2. Paste the BDFormatConverter code to the DataAnalysis script window and then change the parameters in the red box.

Table 1. Parameters need to be changed according to the LC-MS data obtained.

Parameter	Function
datapath	The directory of the folder containing the raw LC-MS data.
nrt0	Chromatogram cutoff window: Spectra before this retention time are not formatted.
nrt1	Chromatogram cutoff window: Spectra after this retention time are not formatted.
SignalToNoise	S/N cut off: Spectral peaks with a lower S/N than the cutoff value are not formatted.
savepath	The directory of the folder containing the resultant peak list files.

4. To save the DataAnalysis method, click: Method → Save As... (Figure 3).

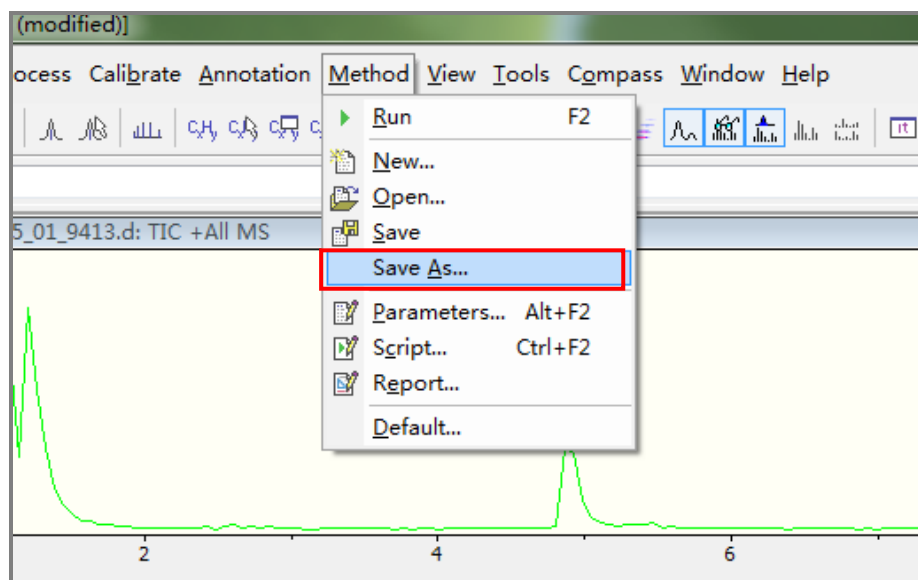


Figure 3. Save the DataAnalysis method.

5. To use an existing method for converting the LC-MS data, load the method in DataAnalysis (Figure 4). If needed, the parameters of the method can be modified.

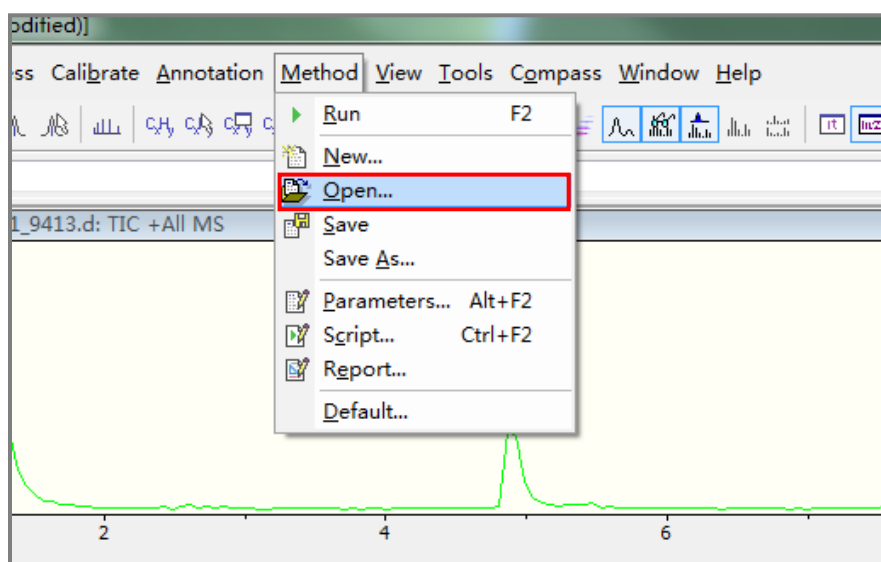


Figure 4. Load the peak list export method.

6. To run the method, click: Method → Run (Figure 5).

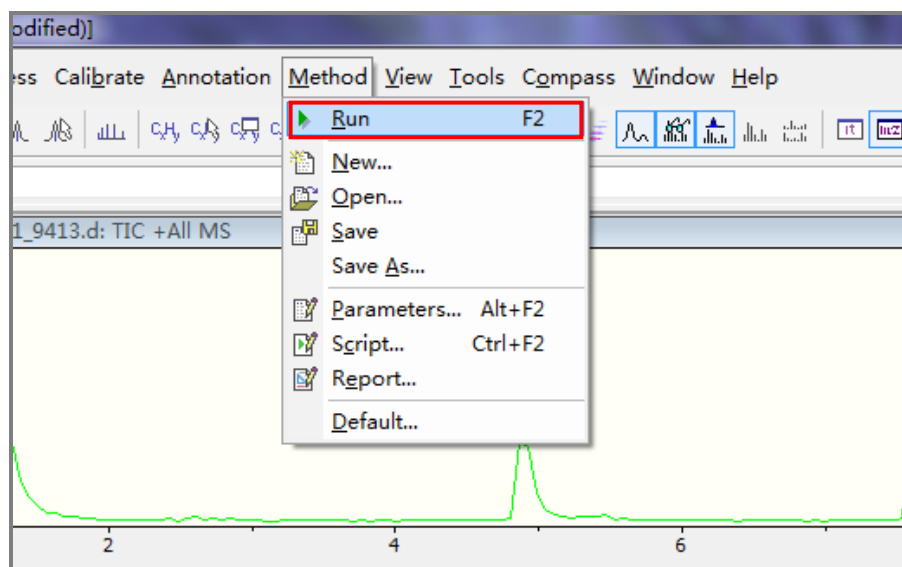


Figure 5. Start the method to convert the raw LC-MS data into a file format readable by IsoMS.