

Instruction for Converting the Raw LC-MS Data Obtained by Waters QTOF-MS to an ASCII 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 Waters QTOF-MS needs to be first converted into a CSV file format that is readable by the IsoMS script.
- The Waters LC-MS data processing software package (MassLynx) does not contain a program that would allow a user to directly export the raw data to a CSV file readable by IsoMS. However, a user can use one or two programs (see below) in MassLynx to convert the raw data to its CSV format which can then be processed using the WAFORMATConverter script downloaded from MyCompoundID to a file format readable by IsoMS.
- If a user has acquired the LC-MS data in the centroid mode or dual-mode (centroid and profile), the Dbridge (also called DataBridge) program in MassLynx can be used to convert the raw data to the peak list file in ASCII. If only the profile mode is used for LC-MS data acquisition, MassLynx can be used to convert the profile spectrum data into the centroid spectrum data, followed by using Dbridge to convert it to the peak list file in ASCII.
- The Dbridge program is located in the default installation directory of MassLynx.
- An example of converting the raw LC-MS data into an ASCII file readable by IsoMS is shown below. Waters MassLynx V4.1 was used for this example.

Instruction

1. Steps 1 to 3 can be skipped if the LC-MS data was acquired in the centroid mode. If the data was acquired in the profile mode, to convert the profile spectrum to the centroid spectrum, first assign the folder containing the raw data as the working folder in MassLynx by clicking: Chromatogram → File → Open... (Figure 1).

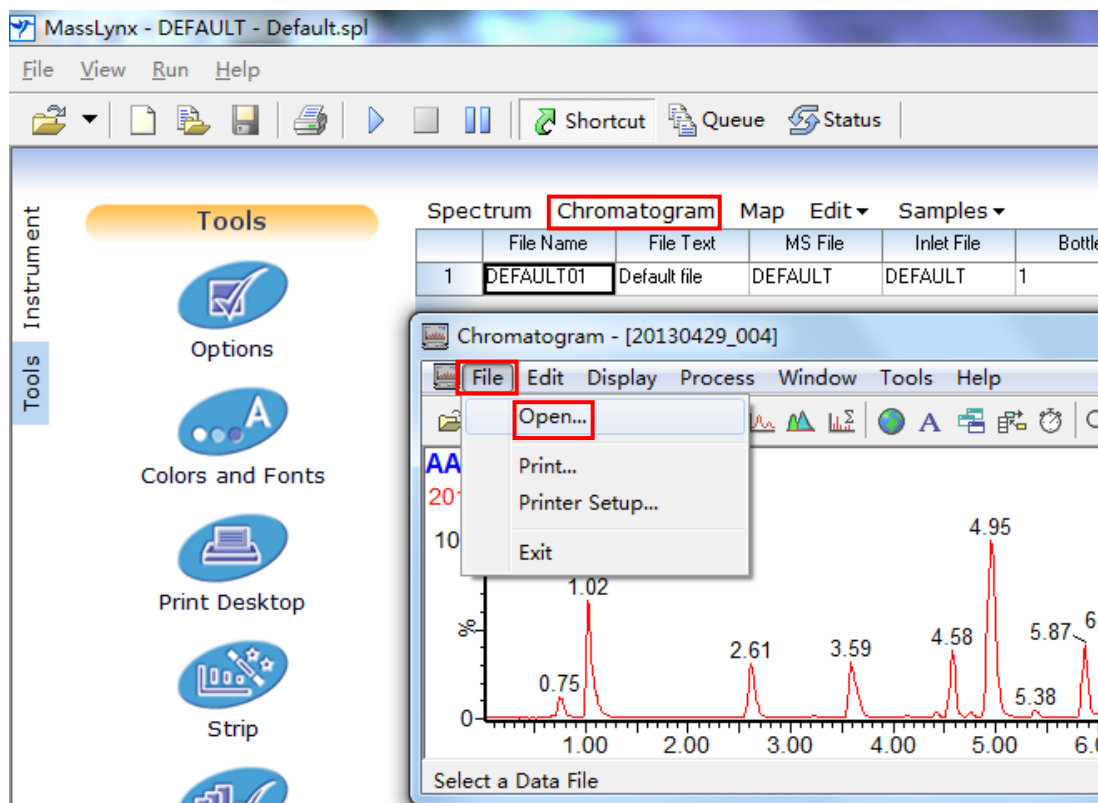


Figure 1. Assign the working folder in MassLynx.

2. To convert the profile spectrum data into the centroid spectrum data in MassLynx, Click: Tools → Accurate Mass Measure (Figure 2).

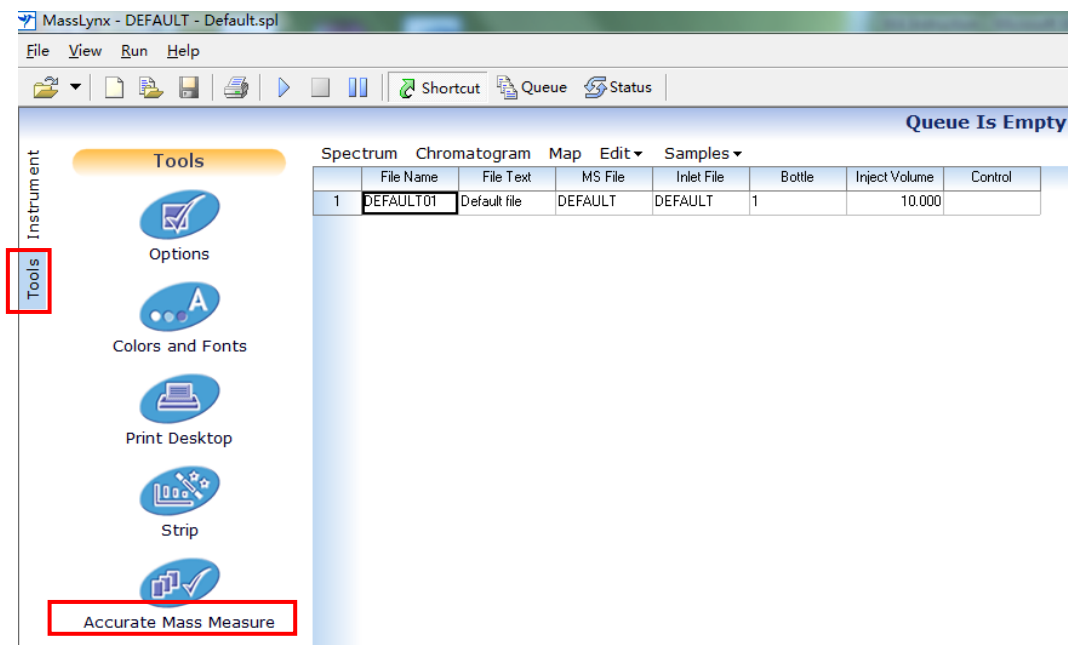


Figure 2. Convert the profile spectrum file into the centroid spectrum file in MassLynx.

3. In the Accurate Mass Measure window, select the raw data to be converted by double clicking the file name (the sign is a green tick) (Figure 3). Choose “Automatic Peak Detection” in the drop-down menu “Process Type”. Finally click “Process”.

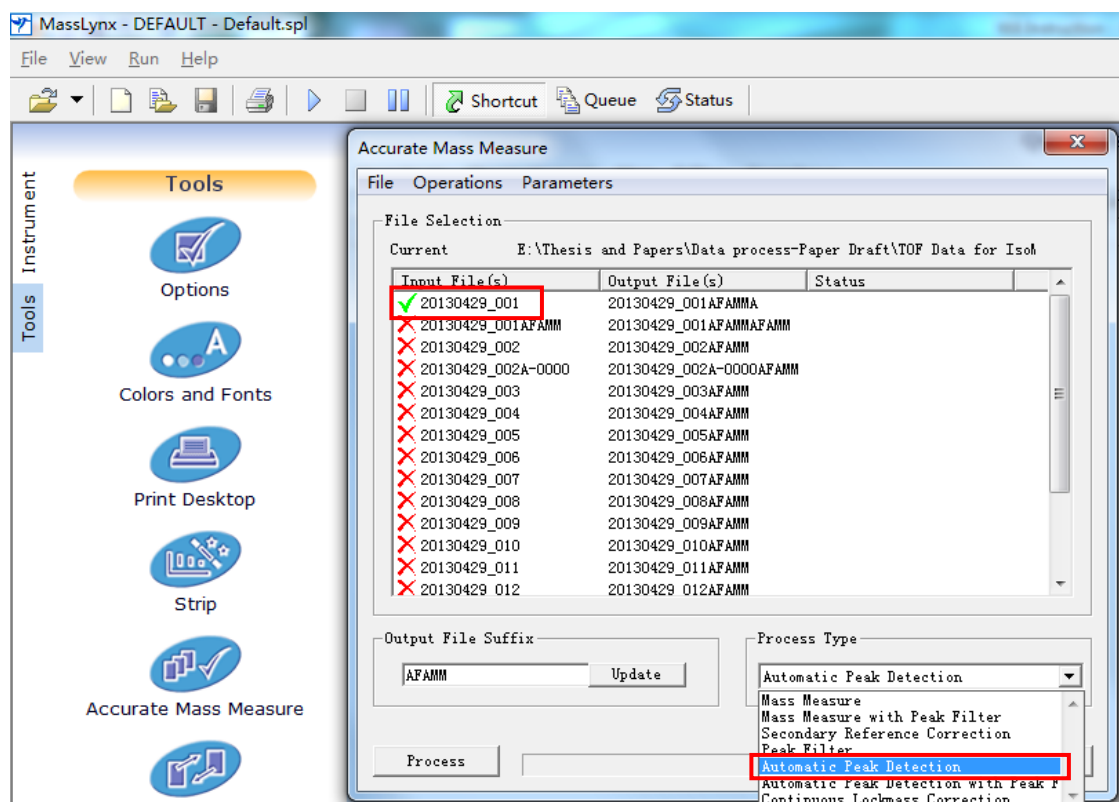


Figure 3. Convert the profile spectrum data into the centroid spectrum data in MassLynx.

4. Peak lists of the centroid spectrum data can be exported in ASCII format by Dbridge (or DataBridge) in MassLynx (Default directory: C:\MassLynx) (Figure 4).

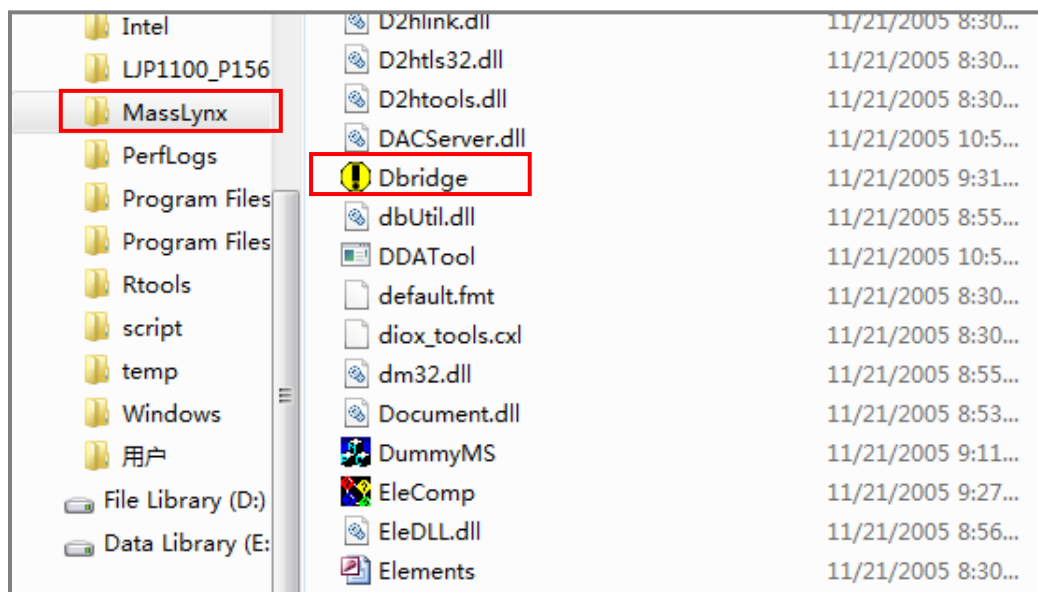


Figure 4. Dbridge is located in the MassLynex folder.

5. In Dbridge, input the centroid raw data by clicking “Select”, and assign a target folder by clicking “Directory” (Figure 5).

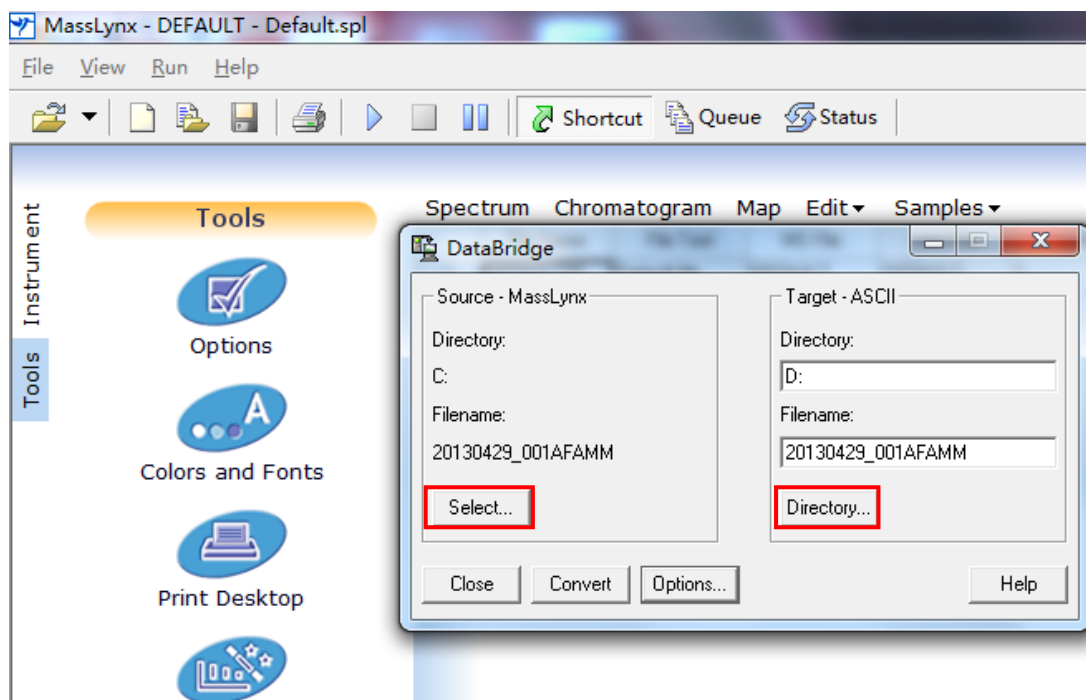


Figure 5. Select the source files and assign the target folder in DBridge.

6. Select the data format of the source file and the target file by clicking "Options..." → MassLynx in Source and ASCII in Target → OK (Figure 6). Finally, start the conversion by clicking “Convert”.

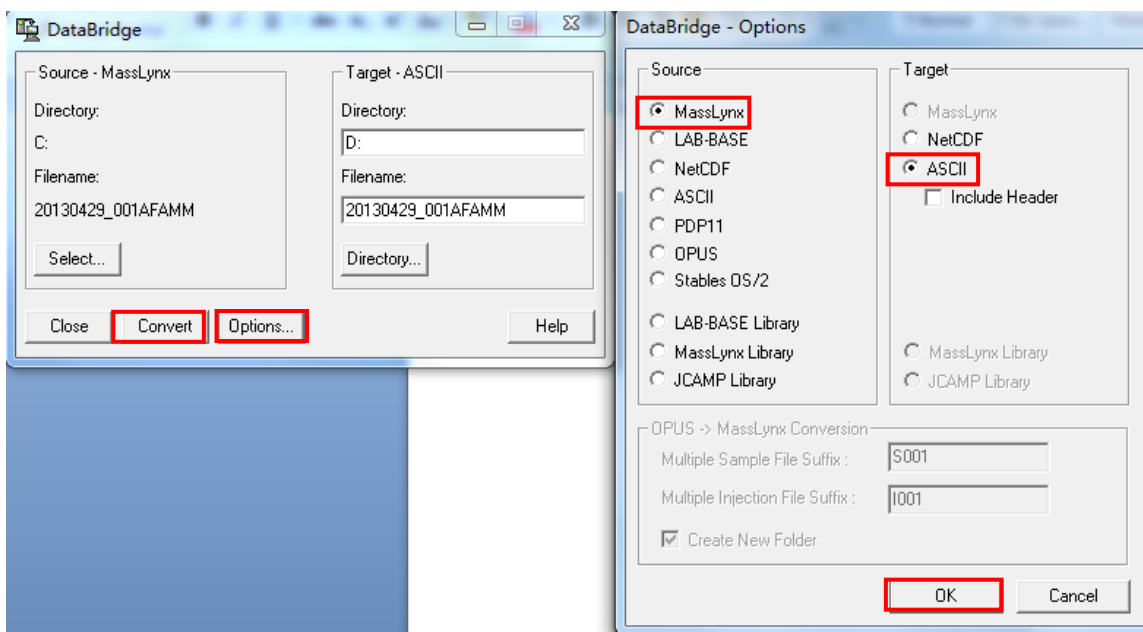


Figure 6. Assign the data formats and run the conversion in Dbridge.