

Procedure for creating ASCII text file of mass spectral data using Agilent Chemstation software (tested using v. D.00.00.38)

1. In Enhanced Data Analysis window, with mass spectrum of interest displayed, select Spectrum/Change Spectral Display
2. Select "Choose largest ion of each mass", OK
3. In command line, type "x=y", enter
4. Select Spectrum/Tabulate
5. In Tabulate window, click "Copy", then paste into text editor (NoteTab Light recommended)
6. Save the file

Notes:

- Steps 1-2 convert non-integral masses in the spectral data to their nominal masses, e.g. 57.10 to 57.00.
- Step 3 places the modified spectrum in the active register, from which the data will be tabulated in Step 4. If the command line is not visible, select Tools/Options and click the Command Line box.