Procedure for generating MaSC JCAMP-DX mass spectral data:

There are two parts to a JCAMP-DX file – 1.) detailed header information about the sample itself, the instrumental conditions, the submitter, and the data processing, and 2.) the mass spectral data in X, Y format. Currently, the preferred method of submission is the **MaSC Mass Spectrum Template** (a MS Excel file), which is available on the MaSC website: http://www.mascgroup.org/datasubmission.html. You will also need an ASCII text editor in preparing your mass spectral files for submission. Notepad or Wordpad, which come standard with Microsoft Windows, will work but are not recommended. If you don't have a good ASCII text editor, try Notetab Light (http://www.notetab.com) which is freeware.

You will need to have previously saved the mass spectral data you wish to submit as an ASCII text file containing x,y values, where x corresponds to mass, and y corresponds to the intensity at that mass. There are instructions on the MaSC website (http://www.mascgroup.org/datasubmission.html) for several commonly used data collection systems. We apologize if your system is not represented, and if you can supply a procedure for getting x,y data from your system's datafiles we will gladly include it on the MaSC website.

General Notes on JCAMP-DX files:

1. Basic structure:
   A. A JCAMP-DX file consists of a series of linked data records (fields).

   B. Data records are stored in one of three types of field: a *generic labeled data record* (LDR), a *data-type-specific record*, or a *user-defined labeled record*. Only the *user-defined labelnames* are modifiable by MaSC.

   C. General JCAMP: The *generic labeled data records* have the format: ##labelname= dataset
   MS specific: The *data-type-specific records* have the format: ##**.**labelname= dataset
   MaSC specific: The *user-defined labeled records* have the format: ##$labelname= dataset

   D. The first three data records must be ##TITLE=, ##JCAMP-DX=, and ##DATA TYPE= in that order. The file must terminate with ##END=

2. Data records may be no longer than 80 characters per line (including the label), but are allowed to continue on subsequent lines.

3. Comments, which are ignored by data importers and translators, begin with $$ or ##=, and must finish at the end of the line on which they start.

4. Data records can be in any order with the exception of ##TITLE=, ##JCAMP-DX=, ##DATA TYPE=, and ##END= as described above.

INSTRUCTIONS:

1. Open the Excel template and fill in the datafields/metadata tags (rows 2 through 46) as completely as possible. Refer to the notes in the table below and in column C of the Excel template as an aid. You might want to re-save

the Excel template at this point to preserve information that will be used in all your mass spectral submissions.

2. Insert your x,y mass spectral data starting in cell C47, which is marked with a red border. This can be accomplished in at least two ways described below. When finished, the x values should be in column C and the y values should be in column D.
   either:
   a. With the x,y mass spectral data already open in an ASCII text editor, simply highlight the x,y data only, and then select Edit, and then Copy. Click on cell C47 in the Excel template, and then select Edit, and then Paste.
   or:
   b. From within Excel, select File, and then Open, and then navigate to the directory where the x,y mass spectral data files are stored. Make sure to select the appropriate "Files of type:" in the dialog box to enable Excel to see the data files, and double-click on the appropriate data file to open it. You'll be confronted with the text import wizard, which will allow you to select the first x,y data line in the file, and to select the appropriate type of delimiter that separates your x and y values: space, tab, comma, etc. Once you've clicked "Finish," the x,y data will open in an Excel file with the x values in column A and the y values in column B. Highlight these x,y values, select Edit, and then Copy. Click on cell C47 in the MaSC Excel template, and then select Edit, and then Paste.
3. Edit the formula in cell B47 Locate the last y value in column D, and note its corresponding row number. Substitute this row number for "row 1000" in the formula. For instance, if the last y value in column D is in row 193, then change D$1000 to D$193.
4. Next you need to transfer the y values in column D as scaled values into column B as described in a. through c. below.
   a. Copy cell B47, by highlighting it, and then selecting Edit, and then Copy.
   b. Highlight all the cells in column B starting with cell B48 and ending with the cell in column B with the same row number of the last y value in column D. For example, if the last y value in column D is in row 193, then you would highlight all the cells in column B from B48 to B193.
   c. Select Edit, and then Paste. The y values in column D should now be in column B, but scaled appropriately. The base peak will be set to 9999 and all other y values will be scaled to this peak and rounded to the nearest whole number.
5. Transfer the x values in column C to column A as described below:
   a. Highlight all the x values in column C, starting with cell C47, then select Edit, and then Copy.
   b. Highlight cell A47, and then select Edit, and then Paste.
6. You then need to remove extraneous information from the file which is done by selecting only the data in columns A and B as described below:
   a. Highlight the column headings A and B which will select everything in columns A and B.
   b. Select Edit, and then Copy.
   c. Switch to the blank worksheet 3 by clicking on the tab labeled "Sheet3" near the bottom of the screen.

    d. Highlight cell A1, then select Edit, and then Paste Special, and then select Values, and then select OK. The columns might have to be resized to show their full contents.
7. Next save the resulting spreadsheet with the name of the mass spectrum, as a tab-delimited ASCII text file:
    a. Select File, and then Save as …., and then be sure to select *Text (Tab delimited) (*.txt)* in the dialog box labeled "Save as type:"
    b. Enter the name of the mass spectrum as the filename, and select Save.
    c. Answer OK to the dialog box that pops up stating that the selected type does not support multiple worksheets. We no longer care about the other worksheets in this file.
    d. Answer Yes to the dialog box that pops up stating that the file you are about to save has features that are not compatible with tab delimited text. We don't care about losing "special features" that can not be saved as ASCII text.
8. Open the resulting ASCII text file in a text editor (see note in the introduction regarding suitable text editors, Notetab is recommended). It is then necessary to remove the tabs that will have appeared in the metadata/data fields. The quick method for doing this if you are using Notetab is described below:
    a. Within Notetab, highlight all the rows up to, but not including, the actual x,y data.
    b. Select Search, and then Replace.
    c. Enter ^T into the "Find what:" box and simply click in the "Replace with:" box. Now click on "Replace All"
9. Now use the first line of the file, the number line, to determine where lines need to be broken to conform to the 80 characters per line maximum. Once the lines have been corrected (by pressing the Enter key to enter a "carriage-return" to break lines as appropriate), remove the number line, and make the ##TITLE= line the first line in the file.
10. Add ##END= as the final line in the file.
11. Resave the completed file.
12. Check that the file has been formatted properly and contains the correct data by using one of the freely available JCAMP-DX viewers available on the web, such as MSView32 (http://merian.pch.univie.ac.at/pch/download/spectroscopy) or WSearch32 (http://www.wsearch.com.au)
13. Submit both the MS Excel file of the mass spectrum as well as its associated JCAMP-DX file to MaSC. Rename each Excel file and its associated JCAMP-DX file identically – the only difference will be that the Excel file should have the extension .xls and the JCAMP-DX file should have the extension .dx