





Agilent Technologies

Converting NIST user library to Agilent Chemstation User Library

The document below describes how to convert NIST libraries to Chemstation format.

In short, the procedure to convert a NIST library to Chemstation format is to export the NIST library as JCAMP file from the NIST search engine application. Subsequently, this JCAMP file can be imported by the Chemstation software to generate the equivalent .L Chemstation library.

How to convert NIST user libraries into Chemstation format:

- Within the NIST Search Program go to Librarian and if there are any spectra listed in the large box on the left hand side, highlight them all (using shift and clicking) and press delete.
- Select the  button which pulls open another box with a drop down menu in it. Look for the user menu you want to export, then click search. A load of files should then be listed in the box you cleared.
- Highlight all the files in the box on the left hand side and click the  button. Choose a name for the file and select the file extension as NIST Text (.msp).

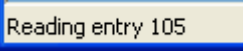
You then need to convert the .MSP file into a format that Chemstation can read. This is done using the lib2NIST converter program in the NIST Mass Spectral Database subdirectory (under start/programs).

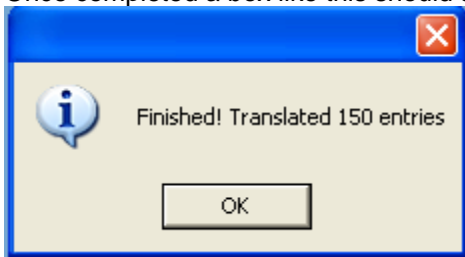
- Open the lib2NIST converter and locate the file you created (normally under C:NIST05(or NIST98)\MSSEARCH).
- Click on the Add Input Libraries/Files button and select the library name you created. The file should appear in the left hand box (labeled Input Libraries or Text Files).
- Once in the left hand box highlight the file and select the output format to be HP JCAMP file (.HPJ). and then click convert.
- Locate the .HPJ file and, if not already there, move it to C:database.

You then need to import the file into Chemstation by:

- Open Chemstation data analysis program.
- Go to view/parametric retrieval
- A dialog box pops open, click cancel.
- Then go to library and select read JCAMP file.
- Locate the file in C:database and click open.
- Another dialog box opens called "enter new library filename". Type in the name you want to give the new library and click okay.

This document is believed to be accurate and up-to-date. However, Agilent Technologies, Inc. cannot assume responsibility for the use of this material. The information contained herein is intended for use by informed individuals who can and must determine its fitness for their purpose.

- You should see something like this  in the bottom left hand corner of the screen.
- Once completed a box like this should appear:



- Click okay and then you can select the library you created in library/ select library.

To return to normal data analysis go to View/ Return to data analysis.