

Importing Spectra into NIST Search Software from Other Programs and Correcting for Mass Sufficiency/Deficiency

Importing Spectra: The spectra (ASCII) must be saved from the data processing program in either JCAMP (.jdx) or NIST (.msp) format. The spectra preferably should include 2 digits to the right of the decimal (see Correcting for Mass Sufficiency/Deficiency below). The NIST program then uses two files to import the saved spectra. The primary file, AUTOIMP.MSP, is found in the C:\NIST directory. In this file is written the following text in the default format:

```
C:\HPCHEM\HPNIST.TXT
```

This is where the NIST program expects the secondary file to be created. This can be changed to whatever you desire, but it is convenient to leave it at its default setting if you want to interchange between the HP (Agilent) and other programs for importing spectra. This is because the HP macro assumes this location in its macro.

The secondary file points to the location of the actual JCAMP or MSP ASCII data file. For example, I used the HP software (NIST Output, Create file in x register) to create an msp file and the HPNIST.TXT file was created containing the following information:

```
C:\HPCHEM\1\DATA\EVALDEMO.D\EVALDEMO.MSP
```

I did this manually in this example. Normally when you double right click the HP Spectrum window, the NIST search software is automatically opened by the HP macro. NIST when open always “watches” for the creation of the HPCHEM\hpnist.txt file, imports the spectrum it points to, and then *deletes* the HPNIST.TXT file.

If another manufacturer were using the export format, they wouldn't have to open the NIST search software. The user would open the NIST search software open, and another manufacturer would only have to write the information in the HPCHEM.TXT file. The NIST search program would then import the spectrum and search it automatically.

Manual Test of Spectrum Import. I tested this approach with a JDX file sent to me by Tony Williams. He had modified the ACD software to include a macro button that exported a JDX file. I wrote a HPNIST.TXT file that pointed to the location of the JDX file using Notepad. I then closed notepad, opened the NIST search, and it automatically imported and searched the file from ACD.

David Sparkman suggested that the line pointing to the file to import should also have APPEND attached to it, e.g.

```
C:\HPCHEM\1\DATA\EVALDEMO.D\EVALDEMO.MSP APPEND
```

But it seemed to work without the APPEND attached. If you write OVERWRITE instead of APPEND, all entries in the spectrum list portion of the NIST search software are overwritten.

Batch File Import of Spectrum. I also wrote a batch file to import spectra and either open the NIST Search or bring it into focus if it was already open:

: J. L. Little, Jan 13, 2001

: Approach to export spectra from ACD to NIST Version 1.7 or 2 Search

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: Assumes that a macro is written within ACD that always creates a JDX file at
: c:\acd\ACD.jdx

: Batch File copies a file, C:\hpnist2.txt to C:\hpnist.txt.

: Hpnist2.txt has only one line, C:\acd\acd.jdx APPEND ,which points to the location
: of the JDX file the ACD software created.

: If OVERWRITE is added to the location instead of APPEND, the spectrum
: is added and all the current spectra in the NIST search program spectrum list
: are deleted.

: The copy command creates a new hpnist.txt file every time the batch file is run.
: Needed because when NIST automatically imports file, it deletes hpnist.txt

copy C:\hpchem\hpnist2.txt c:\hpchem\hpnist.txt

: This will start the NIST search if not already open, or bring it into focus if already
open.

start c:/nist98/nist\$.exe

: This is needed to automatically close the batch file in some Versions of Windows.

echo.

echo off

cls

exit

Correcting for Mass Sufficiency/Deficiency: When exporting larger MW compounds, the nominal mass can be above 0.5 m/z due to the mass sufficiency of hydrogen. The same thing can happen with compounds containing excess numbers of elements such as bromines with mass deficiency. NIST can correct for these by using the File/open command to import a JDX or MSP file. *The imported file **must** have one to two digits to the right of the decimal place to make this approach work.*

After selecting the file, another menu will appear which has an IMPORT button. You can correct for m/z sufficiency/deficiency with this button. These selected parameters will still be used for ALL spectra imported after this point in time until it is changed again. Thus even spectra imported in HP by double-left clicking will be automatically corrected for mass sufficiency/deficiency until these parameters are changed again.