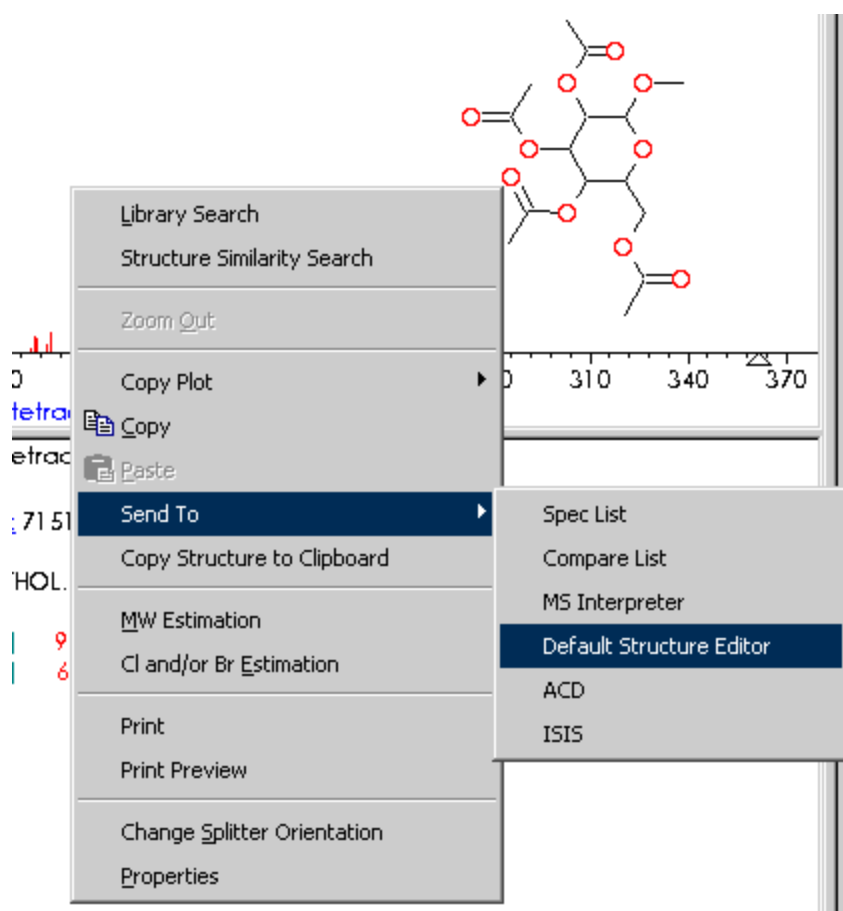


Using Drawing Packages with NIST Version 2

The NIST Version 2 interfaces directly with several drawing packages such as ChemSketch (free download on Web), ISIS Draw (MDL, cost money), and Chemsite Pro. You can also interface indirectly with other programs using mol files.

Direct Approach: I like the direct approach much better than the indirect one. I've personally used ISIS Draw and ChemSketch, the latter is freeware. This approach only works with chemical drawing programs that support command line reading of mol files. A menu will appear by "right-clicking" on a spectrum that has a structure associated with it. A standard option, "Default Structure Editor," will appear which links the user to whichever program automatically processes mol files under windows.



If you want to send the structure to more than one program, you must create a text file named autoimp.str and place it in the same folder as the NISTMS search program. Make sure you display files with extension and the file is truly named autoimp.str and NOT autoimp.str.txt! The file must contain the following general type command line:

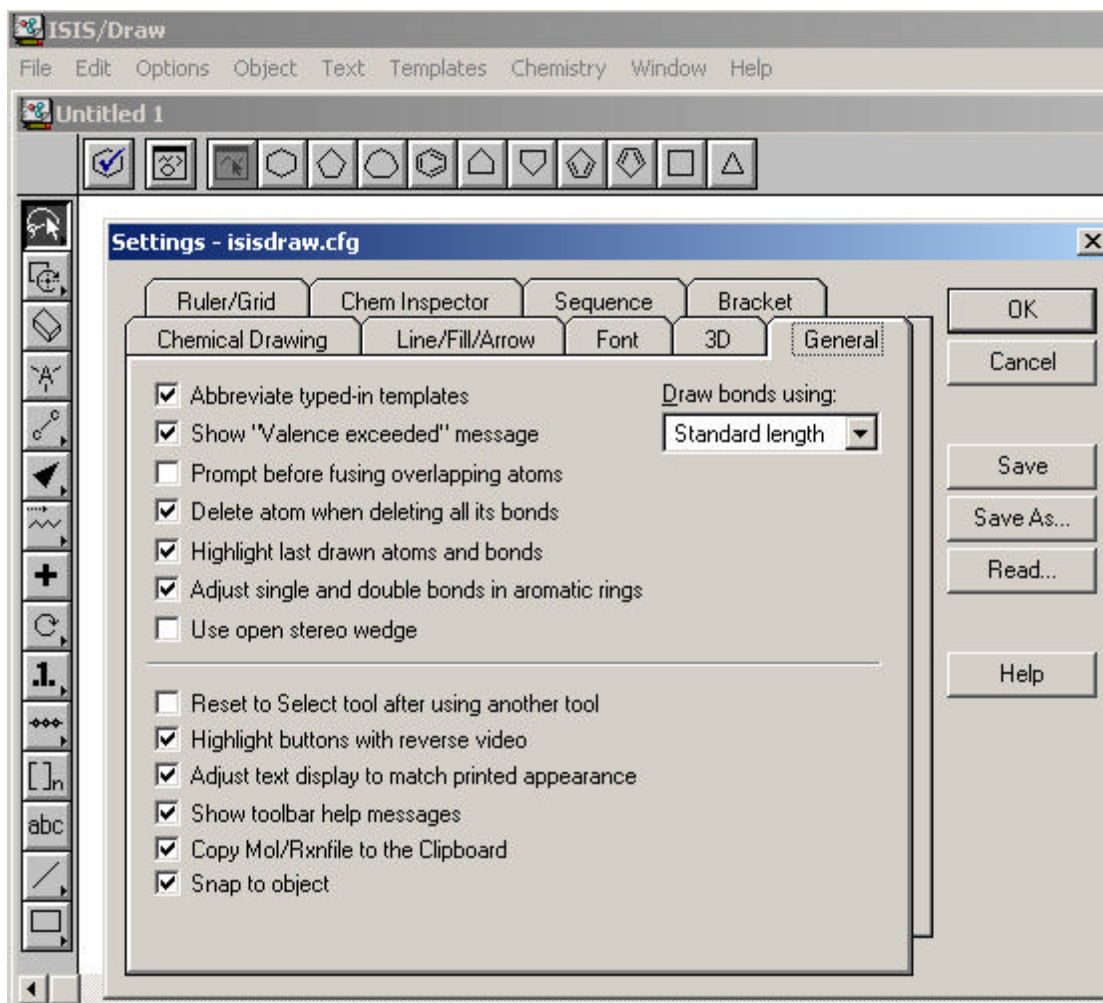
```
"Name" "Fully extended file name" "%1"
```

In my particular case, I created the following autoimp.str file:

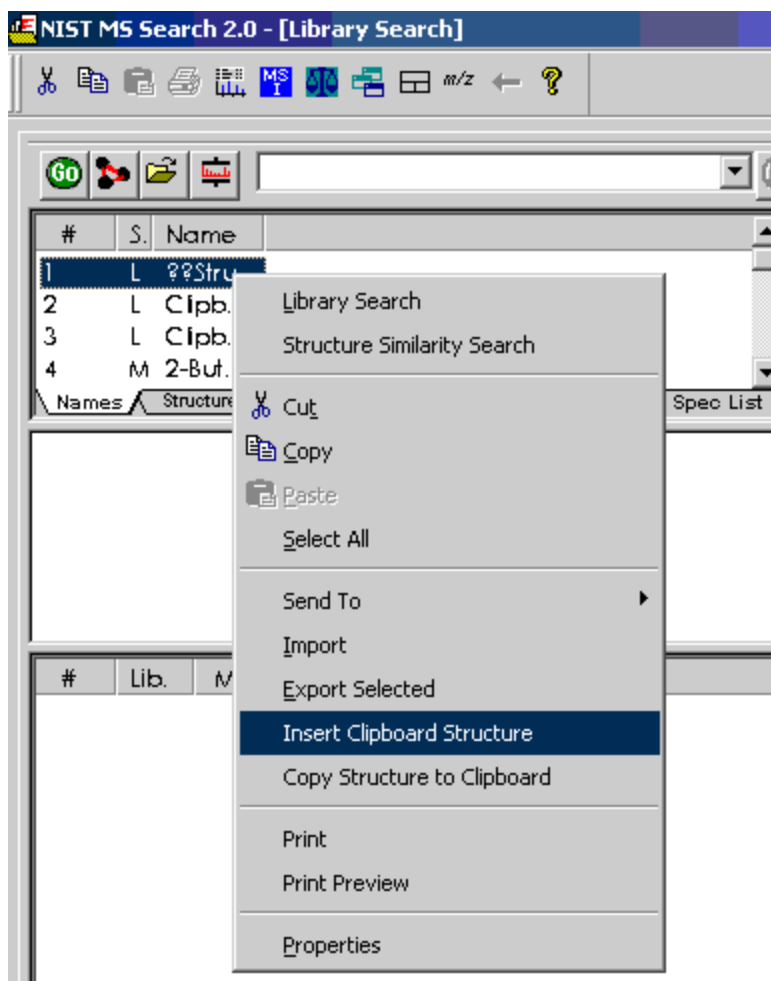
```
"ACD" "C:\ACD50\CHEMSK.EXE" "%1"  
"ISIS" "C:\Program Files\ISIS214\IDraw32.exe" "%1"
```

since I was using two different programs.

To import structures from ChemSketch and ISIS Draw, just select (“lasso”, “box”, etc.) the desired structure (can have many in the drawing program window, but in most cases select you only want to import one structure). Select the copy option in the drawing program. In ICIS Draw, you must make sure that the files are exported in the clipboard in mol format. Go to the options/setting menu and check and save the “Copy Mol/Rxnfile to the Clipboard” option.



In the NIST program, the structure is then stored in the clipboard.mol file. To insert it into NIST, just “right click” on the window you wanted to paste it into and select “Insert Clipboard Structure”.



If you are importing it in the librarian to add to the library, just select the clipboard and then usually select "Clipboard" in the library editor window and then normally one would "From structure" button to automatically calculate and enter the MW and MF.

edi **Spectrum Information** [X]

Name: ??Structure Only

Formula: C8H18OSi

Other Names (Synonyms):

Comments: Chemical Concepts spectrum, possibly the

Mol. Weight: 158 ID Number: 1

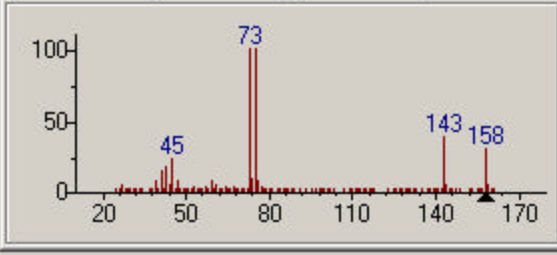
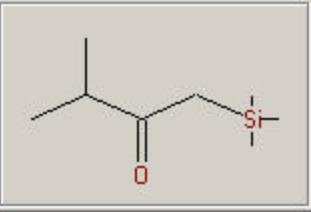
CAS Number: 69561995 Peaks: 115

Library: Spec. List

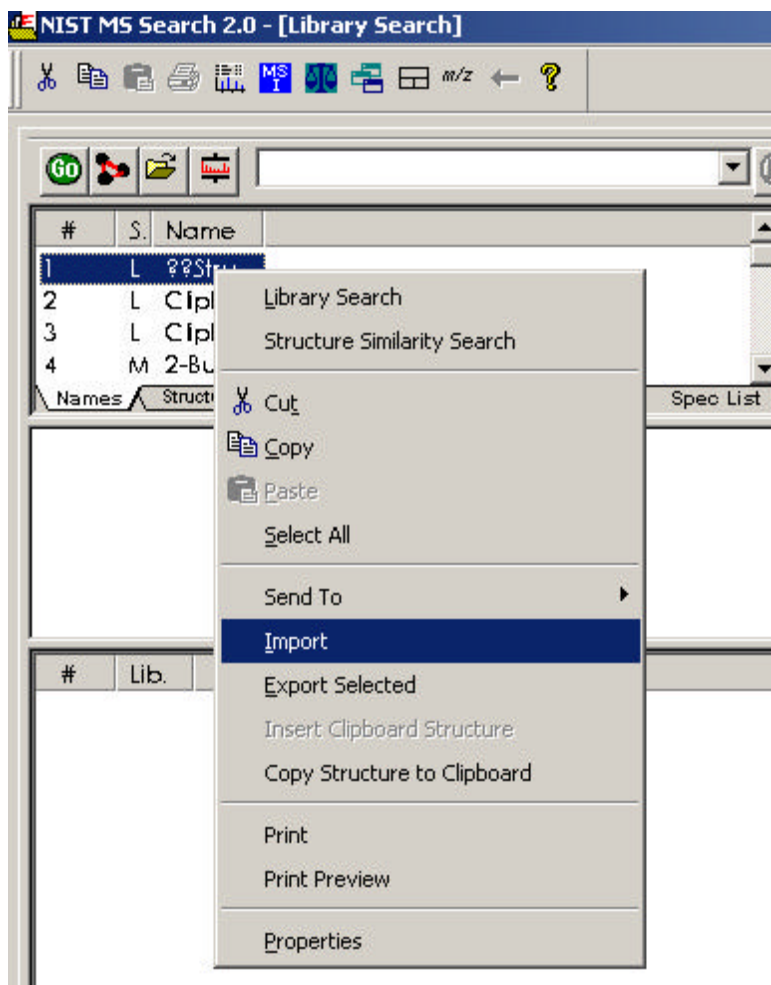
Peak information:

m/z	Abund.
25	0
26	3
27	44
28	12
29	27
30	2
31	15
32	2
33	0
34	0
37	3

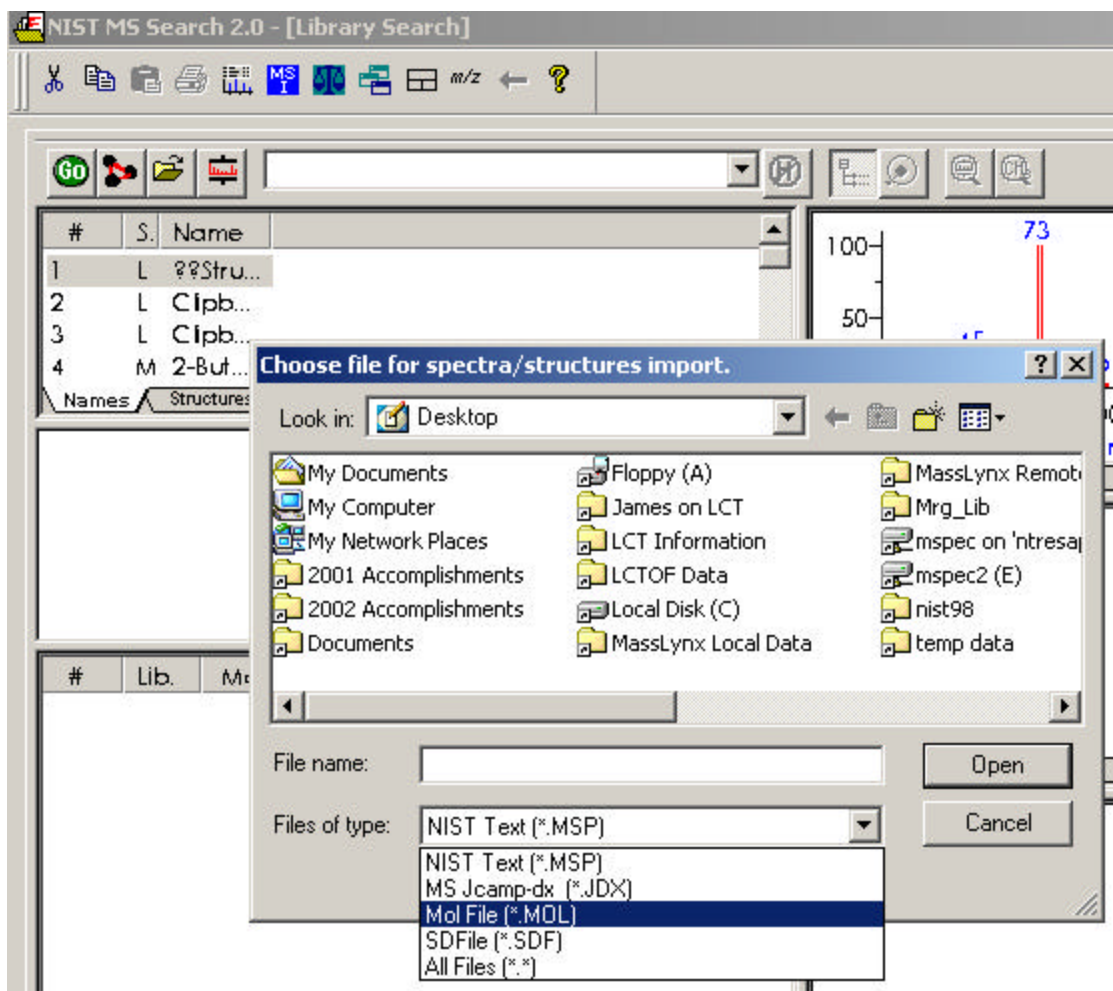
Structure: Clipboard #1

Indirect Approach: The indirect approach involves saving the desired structure as a mol file. Most drawing programs export in mol format in addition to their native format. To do this in most programs, select the desired structure by “lassoing” or “boxing” it, go to the File option on the menu bar, and select Export in Mol format, etc. This is normally different than saving the file, which saves the file in the programs native format. To import into the NIST search, right click in the window in which you want to import the structure and select the “Import” option.



Then select the mol file format and hope you remember where you saved from the drawing program!



The files can also be imported in a similar manner in the Library Editor window in mol format by selecting “Attach Structure” button and then “Another” button.

Spectrum Information

Name:

Formula:

Other Names (Synonyms):

Comments:

Mol. Weight:

CAS Number:

Library:

Peak information

m/z	Abund.
25	0
26	3
27	44
28	12
29	27
30	2
31	15
32	2

NIST MS Search 2.0

? Structure for CAS=69561995 is in the Main Library. Use this structure or attach another one ?

Structure:

CC(C)C(=O)CSi

Now you see why I prefer the direct approach!!