

## Quick Start for the NISTMS User Interface MS Library Program (2020 Version)

This program is designed to assist in the identification of compounds through their mass spectra with the aid of NIST mass spectral libraries. This document provides a very basic introduction to this program. Both on-line and detailed documentation are also available.

### Overview:

The following five Tabs (shown below) located at the bottom of the display provide different sets of windows for searching and inspecting spectra.



In each Tab you may alter the appearance of the windows, spectra and hit lists by selecting 'Properties' on the RMB (right mouse button) menu or by moving bars between windows of column headers.

Different monitors and Windows versions can affect the appearance of the program. You can customize to your tastes by changing fonts, colors and spectral peak widths. Much of the information shown in columns of hit lists of results can also be changed – many options are available through the 'Properties' associated with each Tab. Choices can depend on specific types of searches and fragmentation (EI vs. tandem, for example).

### Window Positions:

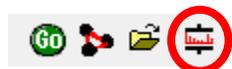


You can reposition windows in most tabs using the above circled button on the button bar (located below the top menu). This button cycles through 3 pre-set configurations. You can also move bars to change the relative sizes of windows.

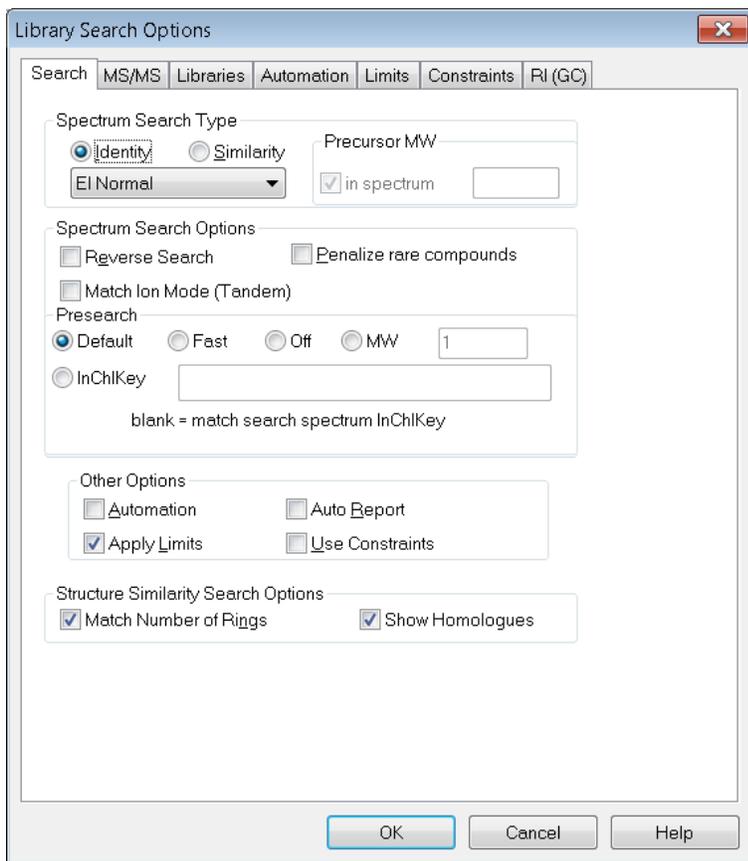
### Saving the Configuration:

After you have configured the program to your taste, you may save it for later restoration using the top menu choice, File/Save Configuration. Restoration is done using File/Restore Configuration. When the program is first started it will use the configuration active when the program was last used. EI and Tandem configuration files (\*.ini) – one for EI and another for Tandem spectra, both in two font sizes.

### Spectrum Library Searching:



The principal function of the program is to find spectra in the library that match yours. Such searching is specified in the Search Options dialog invoked by pressing the circled button above (shown below for a simple EI library search). If the molecular weight (or precursor mass) is known, the 'Hybrid' search will often give more informative results.



### *Searching Spectra:*

Spectra in the upper left window in the Lib. Search Tab (the *Spec. List*) can be searched using current settings by double clicking, pressing the 'Go' button or selecting Library Search on the mouse RMB menu (this will search any NIST library spectrum, regardless of its location).

### *Importing Spectra:*

Adding spectra to the Spec. List for searching depends on the details of your instrument software system. Spectra can be directly added using the File/Open choice (of file Icon in the above button bar) – many formats are supported including the default NIST .msp format. Some instrument data systems send spectra directly to NISTMS which then appear in the Spec. List.

### *MS Interpreter:*

We encourage you to press the F9 button on any NIST spectrum to assist you in understanding of the origin of the peaks.