Instruction for Use of NIST MS Search and AMDIS with Third Party Data Systems

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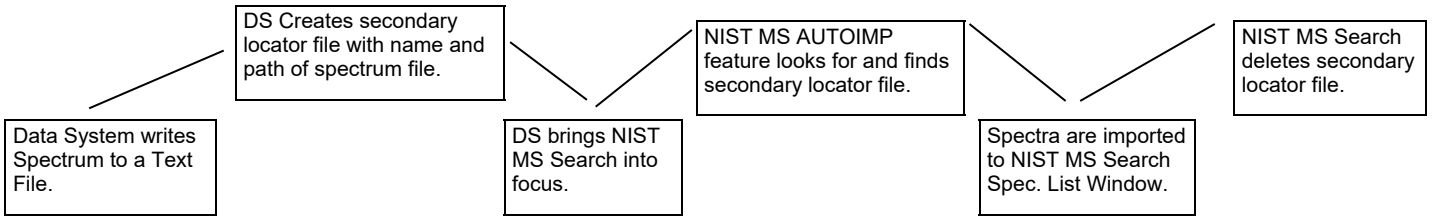
INTRODUCTION

This document describes how to start the NIST MS (Mass Spectral) Search Program Version 2.0 and higher or the AMDIS (Automated Mass spectral Deconvolution and Identification System) program from another application. The document also includes information regarding the text output of the NIST MS Search Program and the use of various command line switches that can be used with the NIST MS Search Program and AMDIS.

> **NOTE: These instructions are different from those for previous versions of the NIST MS Search Program.** The **NAMES** of the Search Program and its calling program **HAVE CHANGED FROM** those used with various releases of **Version 1.X**. Instructions for interfacing the NIST MS Search Program are on page 1. Instructions for interfacing AMDIS are on page 11.

USE OF NIST MS SEARCH PROGRAM WITH INSTRUMENT DATA SYSTEMS

The use of the automation features were implemented to enhance the performance of the NIST MS Search Program when used with proprietary mass spectral data systems (DS).



If your data system is capable of exporting spectra in the NIST format (described in **USER LIBRARIES** below) or in JCAMP format and you can call a Windows program from within your data system, these features are available to you. Implementation of these features has been provided on some manufacturers' data systems.

The command string used to start or bring into focus the NIST MS Search Program for Windows is:

C:\NISTXX\MSSEARCH\NISTMS$.EXE <*space*> *possibility of several switches described below*

assuming the program is in the **C:\NISTXX\MSSEARCH** folder (the default installation directory; if it is in some other folder, make the appropriate substitution (see **Location of the NIST MS Search Program** below).

Two locator files are required to use the automatic spectral import features, a primary locator file AUTOIMP.MSD in the NIST MS Search Program's folder and secondary locator file which can be located in any desired folder and have any selected name and extension.

It is best if you write your linking routine so that it first looks to see if there is a file with name AUTOIMP.MSD in the NIST MS Search Program's folder. This primary locator file contains the name and location of the secondary locator file. If an AUTOIMP.MSD file is present, **YOUR PROGRAM SHOULD** examine its contents and use the contained name and location for writing your secondary locator file. It is **NOT NECESSAY to rewrite** the AUTOIMP.MSD file each time your program calls the NIST Program. Once put in place, the AUTOIMP.MSD file should not be modified.

WARNING: If your routine automatically creates the primary locator file AUTOIMP.MSD, it will overwrite an existing AUTOIMP.MSD file and can cause other programs to No Long Function properly with the spectral import feature of the NIST MS Search Program. It is best that your routine look at the contents of **NIST MS Search Program's** folder to determine if an **AUTOIMP.MSD** file is present. If one is present, then the name of the second locator file and it is location, specified in the **AUTOIMP.MSD** file, should be used in the writing of the second locator file to avoid interferences with other programs. This is the way that **AMDIS** functions.

1. The first locator file MUST be in the SAME Folder as the NIST MS Search Program and have the name **AUTOIMP.MSD**. The AUTOIMP.MSD file should be written only **ONCE** and **ONLY** in the case where there is **NO** AUTOIMP.MSD file present in the NIST MS Search Program's folder. If an AUTOIMP.MSD file already exists, the secondary locator file name and location listed in it should be used in the writing of the secondary locator file.

   The AUTOIMP.MSD contains the text string describing the location and name of the second locator file, i.e.:

   C:\MYMSDS\DATA\FILESPEC.FIL
   Where: **C:\MYMSDS\DATA** is the folder where the file, **FILSPEC.FIL (example name)**, resides. In the case of the Agilent ChemStation the contents of the AUTOIMP.MSD file is C:\MSDchem\HPNIST.txt

The **AUTOIMP.MSD** file can be created with any ASCII text editor.

> **NOTE:** If you use Microsoft NotePad, the default extension is .TXT even though you type AUTOIMP.MSD. The default settings for Windows Explorer will not show this .TXT extension. The file will not work unless the .TXT extension is removed.

> **NOTE:** If your routine creates the AUTOIMP.MSD file, it must put both a CR and line-feed at the end of the line containing the secondary locator file name and location.

2. The second locator file is written each time you save spectra to a separate file (.MSP). This file contains the text string that describes the location and name of the text file (the *.MSP file) containing the spectrum (or spectra) in the NIST text format described below. You can specify whether the spectra in the NIST MS Search Program's **Spec. List** Window (called MS Search Clipboard Window in ver 1.x) are added to or replaced by the automatic import. An example of the contents of the second locator file is:

   C:\MYMSDS\DATA\DATAFILE.MSP <*space*> **Overwrite** *or* **Append**
   23 62789
   Where: **C:\MYMSDS\DATA** is the directory location of the spectra file, **DATAFILE.MSP** is name of the file containing the spectra, and **Overwrite** or **Append**[1] is the instruction as to how the spectra are added to the **Spec List**. If the Overwrite/Append argument is NOT part of the string, the user will be prompted as to whether or not to overwrite or prepend the contents of the NIST MS Search Program's **Spec. List** when the MS Search Program is brought into focus.

[1] More recent versions of MS Search (v.2.2 or higher) allow the **Append/Import** function to be set in the **Spectrum Import Options** dialog box. By selecting Prepend or Overwrite in the **Adding spectra to Spec List** part of this dialog box will override the above command line statement. If Ask is selected, the command line statement will be use. If there is no command line statement the operator will be ASKED at the time of the import as to Prepend or Overwrite.

23 62789 are separated by a space decimal positive values of high-order and low-order words of your application's main window handle; they are necessary to enable **Switchback** Desktop Button feature (see below). Obtain your program's main window handle. In 32 Windows, this is a 32 bit unsigned integer. Divide this number by 65,536. The result of the division (quotient) is the first number and the remainder is the second number. The first number must cannot be greater than or equal to 65,535. The second number is the remainder and cannot be equal to or greater than 65,535.

This secondary locator file is automatically deleted by the NIST MS Search Program each time the MS Search Program is brought into focus and/or spectra are imported.

The **DATAFILE.MSP** is described below under **NIST Text Format of Individual Spectra** (page 8). This file can contain a single spectrum or multiple spectra.

Special Switches

Version 2.0 and higher of the NIST MS Search Program allows **NISTMS$.EXE** to be called using five different command-line switches (explained later in this document on page 5):

/Instrument
/PAR=2
/PAR=4
/PAR=8
/MOL="<full pathname>"

Introduction

More than one switch can be used when **NISTMS$.EXE** is started:

Example: **C:\NISTXX\MSSEARCH\NISTMS$.EXE /instrument /par=4***

This command string starts the NIST MS Search Program, activate the **Switchback** Desktop Button and **par=4** creates a file (**NISTLOG.TXT**, located in the \MSSearch folder) that contains the results of every search done. Upper- or lower-case characters can be used for these switches. Case is not an issue.

Passed Spectrum: Previous versions of the NIST MS Search Program would only handle integer *m/z* values. If a decimal value was passed, it was truncated. This meant that if the value 123.14 and 123.89 were in the passed spectrum, the NIST Program would read this as two values of 123. Version 2 of the NIST MS Search Program has user settable mass defect correction. Your linking software should pass the raw *m/z* value including any decimal place values.

Prior to Version 1.7 of the NIST MS Search Program, a **/V1.5** switch was required for Versions 1.5 and later. This requirement has been eliminated since V1.7. **NOTE**: The command line to start Version 2 or later of the NIST MS Search Program is: **C:\NISTXX\MSSEARCH\NISTMS$.EXE**

Location of the NIST MS Search Program

Rather than hard coding a location for the NIST MS Search Program, it is better to have your program to determine the location each time the NIST Program is called from another application or, at least, the first time the Program is called. This is accomplished by looking in the WIN.INI section labeled NISTMS. Depending on what NIST/AMDIS Programs you have installed, this section will appear as follows:

[NISTMS]
Path16=C:\NISTXX\MSSEARCH\ *only used with Version numbers <2.0*
WorkDir16=C:\NISTXX\MSSEARCH\ *only used with Version numbers <2.0*
Amdis32Path=C:\NISTXX\AMDIS32\ ***THIS IS NEW in V.2.0 and higher***
Path32=C:\NISTXX\MSSEARCH\ ***only used with Version 2.0 and higher***
WorkDir32=C:\NISTXX\MSSEARCH\

Use Path16= for all versions before 2.0 and Path32= for Version 2 and higher.

* NISTXX is used in this document to indicate the root directory for the NIST software (MSSearch and AMDIS) and the NIST Libraries (EI and Tandem) as well as other libraries used by NIST MS Search. In some cases it may be NIST, NISTMS, NIST02, NIST05, NIST08, NIST11, or a later release, such as NIST14, NIST17, or NIST20.

Support of Structure Programs in the NIST MS Search Program, V2

Version 2 of the NIST MS Search Program provides more support of structures than previous versions. There is a Structure Search Command. If a structure rather than a spectrum is in the Spec. List pane of the Lib Search Tab, this structure can be searched to retrieve spectra of all compounds with similar structures by clicking on the Structure Search button (second button from the left) with the structure highlighted in the Spec. List pane.

When Version 2 saves a structure to the Windows Clipboard using the Right Mouse button (RMB) menu's command "Copy Structure to Clipboard", a file in MOL File format with the name Clipboard.MOL is written to the NIST MS Search Program's directory (by default, \NIST08\MSSearch). Other programs can either use the file as it appears on the Windows Clipboard or this file for structure importation.

If a spectrum containing a chemical structure is selected, the right mouse button menu's command "Send to" will result in a "Send to" menu that can have up to three additional items. These "Send to" menu items are a function of the first three lines in a text file in the NIST MS Search Program's directory (the WorkDir32 in [NISTMS] in the WIN.INI file) with the name AUTOIMP.STR. Each line contains three double-quoted strings:

1) A program name as it appears in the "Send to" menu
2) Program executable and path
3) Program startup parameters. %1 will be replaced by the mol file name.

The following is an example of the contents of an AUTOIMP.STR file:

"ChemSite" "C:\MolSuite\ChemSite\ChemSite.exe" "%1"
"ISIS Draw" "D:\ISIS Draw 2.2.1\IDraw32.exe" "%1"
"ACD/ChemSketch" "C:\acd40tl\chemsk.exe" "%1"

The last line of the above example results in ACD lab's ChemSketch starting with the contents of clipboard.mol being imported when ChemSketch opens.

When a program that is to be interactive with the NIST MS Search Program is installed, it must UPDATE or CREATE the AUTOIMP.STR file, or the AUTOIMP.STR file must be edited by the user before the third-party program will appear on and function from the "Send to" menu.

A third-party program can call the NIST MS Search Program by issuing the command:

C:\NISTXX\MSSEARCH\NISTMS$.EXE /MOL=<molfile>

assuming the NIST MS Search Program is in the **C:\NIST08\MSSEARCH** directory; if it is in some other directory, make the appropriate substitution (see **Location of the NIST MS Search Program** above).

where <molfile> is a full pathname of the MOL file. If there is a space in the name, e.g., example c:\program files\a.mol, the name should be double quoted:

C:\NISTXX\MSSEARCH\NISTMS$.EXE /MOL="c:\program files\a.mol"

Third-party program can obtain the path to NISTMS$ from Path32 in [NISTMS] in WIN.INI (see **Location of the NIST MS Search Program** above).

Explanation of Command Line Switches

/Instrument

The **/instrument** switch is used to make the **sWitchBack** Desktop Button active. If this switch is not used, the **sWitchBack** button is grayed. The **/instrument** also causes the program from which the NIST MS Search Program was called to automatically come back into focus after an automated search if the **Return Focus to Caller upon Completion** check box in the **Automation** tab of the **Library Search Options** dialog box has been selected.

/PAR=2

The **/PAR=2** switch is used when the NIST MS Search Program is called from within another application. This allows spectra to be passed from the other application and searched with the MS Search without bringing MS Search into focus. The text results (spectrum header, match factor, reverse match factor, and probability) for a specified number of hits is stored in a text file, which can be accessed by the calling application for reporting purposes.

The **/PAR=2** switch causes spectra to be searched in background (if the **Automation** check box has been selected in the **Automations** tab of the **Library Search Options** dialog box or if the **Automation** check box is selected **Search** tab view if the **Library Search Options** dialog box) and produces the files **SRCRESLT.TXT** and **SRCREADY.TXT** in the NIST MS Search Program's folder (\MSSearch) each time the NIST MS Search Program is called using this switch in the command string. The NIST MS Search Program never comes into focus. If the NIST MS Search Program is not running, it starts Minimized and does not display the **User Spectrum Search** progress dialog box. The Program's main window is disabled while the search is in progress. If neither the Append nor Overwrite switch is used in the command line, then the NIST MS Search Program will search in background as if **Append** were added and the new spectra are added to the **Spec List**.

The results of a specified number of hits from the search are written into **SRCRESLT.TXT**. If more than one spectrum is imported, the search results for each spectrum will be in the file. The number of hits for each search that are stored is determined by the value in the "Number of First Hits to Print" entry box in the **Automation** tab view of the **Library Search Options** dialog box, displayed by selecting the **Automation**/**No Automation** button in the **Library Search Options** dialog box.

If either or both **SCRESLT.TXT** and **SRCREADY.TXT** exist, they will be deleted each time the NIST MS Search Program is called with **NISTMS$.EXE** and the **/PAR=2** switch before the search starts. **SCREADY.TXT** is created immediately after the search is completed and **SRCRESLT.TXT** is closed.

The format for the **SRCRESLT.TXT** file is in this example containing the first two hits for each of two imported spectra:

Unknown: Scan 493 (8.216 min): 50P0830C.D Compound in Library Factor = 197
Hit 1 : <<Methane, dibromo->>;<<CH2Br2>>; MF: 824; RMF: 856; Prob: 98.10; CAS: 74-95-3; Mw: 172; Lib: <<replib>>; Id: 10054; RI: 0.[2]
Hit 2 : <<Methane, dibromo->>;<<CH2Br2>>; MF: 820; RMF: 853; Prob: 98.10; CAS: 74-95-3; Mw: 172; Lib: <<replib>>; Id: 10055; RI 654.
Hit 3 : <<Methane, dibromo->>;<<CH2Br2>>; MF: 810; RMF: 865; Prob: 98.10; CAS: 74-95-3; Mw: 172; Lib: <<replib>>; Id: 17162; RI 0.
Hit 4 : <<Methane, dibromo->>;<<CH2Br2>>; MF: 809; RMF: 839; Prob: 98.10; CAS: 74-95-3; Mw: 172; Lib: <<replib>>; Id: 17161; RI 816.
Unknown: Scan 385 (6.416 min): 50P0830C.D Compound in Library Factor = -1187
Hit 1 : <<6-Chloromethyl-5-methylidene>>;<<C9H11ClO>>; MF: 613; RMF: 803; Prob: 23.43; CAS:66728-04-9; Mw: 170; Lib: <<mainlib>>; Id: 52538; RI.
Hit 2 : <<Trichloronitromethane>>;<<CCl3NO2>>; MF: 612; RMF: 842; Prob: 22.52; CAS: 76-06-2; Mw: 163; Lib: <<replib>>; Id: 12645; RI: 891.
Hit 3 : <<Acetic acid, trichloro-, ethyl ester>>;<<C4H5Cl3O2>>; MF: 604; RMF: 624; Prob: 16.80; CAS: 515-84-4; Mw: 190; Lib: <<replib>>; Id: 242; RI.
Hit 4 : <<Acetic acid, trichloro-, anhydride>>;<<C4Cl6O3>>; MF: 581; RMF: 590; Prob: 6.13; CAS: 4124-31-6; Mw: 306; Lib: <<mainlib>>; Id: 52533.

[2] Prior to NIST 14 (V.2.2) the RI, which appears at the end of the line was not included. The Included RI values are only the experimental values for the type of column selected in the G/MS tab of the **Library Search Option** dialog box's **RI(GC)** tab view.

Extended character codes in chemical names in the file **SRCRESLT.TXT** should be interpreted as follows (codes are decimal numbers):

.alpha.	.beta.	.gamma.	.delta.	.epsilon.	.pi.	.sigma.	.mu.	.omega.	.+/-.	.eta.
224	225	231	235	238	227	229	230	234	241	252

The **SRCREADY.TXT** file contains the number of spectra searched. This file can be used as an indicator for other programs that the NIST User Spectrum Search of the imported spectrum or spectra has completed. The contents of the **SRCRESLT.TXT** file can be used in the preparation of reports that contain the results of library searches by other programs.

/PAR=4

The **/PAR=4** switch will cause **User Spectrum Search** results to be written to a user spectrum search log file, **NISTLOG.TXT**, which will be created in the NIST MS Search Program's directory, e.g., **C:\NISTXX\MSSearch**. The **NISTLOG.TXT** file has the same format as the **SRCRESLT.TXT** file, and its contents are determined in the same way as the **SRCRESLT.TXT** file. Once NIST$.EXE has been called using the **/PAR=4** switch, User Spectrum Search results will be recorded in **NISTLOG.TXT** even if the NIST MS Search Program is brought back into focus without the switch, i.e., C:\NISTXX\MSSEARCH\NISTMS$.EXE.

There is no facility within the NIST MS Search Program to remove the **NISTLOG.TXT** file. It must be removed with Windows Explorer. Once the NIST MS Search Program is exited and then restarted, the **/PAR=4** switch must be used to have the User Spectrum Search result recording resume in this subsequent session.

The **NISTLOG.TXT** file is always appended. It is the user's responsibility to delete it if necessary. This process of logging each search can be done concurrently with the background search (use of the **/PAR=2** switch).

/PAR=8

To stop recording User Spectrum Search results in **NISTLOG.TXT**, the NIST MS Search Program has to be brought into focus with **C:\NIST08\NIST$.EXE /PAR=8**. Stopping the recording of User Spectrum Search results can be done without exiting the Program.

USER LIBRARIES

One of the primary features of the NIST MS Search Program is the ability to do comparisons of user-generated mass spectra and create **User libraries** to search against. The Program will allow up to fourteen **User libraries**. These may be searched in conjunction with the NIST/EPA/NIH Mass Spectral Main and/or Replicates Libraries, or they may be searched by themselves. A maximum of 127 libraries can be included for search at one time. The order of the Libraries selected for search of an unknown spectrum is not relevant. The sample spectrum is searched against ALL the selected libraries. The HIT LIST is ordered by best Match Factor to poorest Match Factor regardless of which library the spectrum is in. For **Other Searches**, the Program allows for the searching of combinations of libraries in any order. The inclusion of libraries and their order of search can be set from the **Options** tab view of the various Search's dialog box. The search order is determined by the position in the list. Highlight the library name to be repositioned in the **Include Libs** section of the **Options** tab view of the **Search** dialog box and use the arrows on the upper left to change the position.

User libraries exist as folders under the Program's root directory: **C:\NSTXX\MSSearch**. The name given to the **User library** is the name of the folder. This folder will contain a number of files that are used by the **User library**. These files exist in a proprietary format. The spectrum, structure, and compound information are put in these files through the **Spectrum Information** dialog box in the **Librarian** tab view of the Program. This dialog box if displayed for an existing spectrum in by highlighting the spectrum in the **Spec List** (vertical window on the left side of the display) and then selecting the **Edit spectrum** button in the button bar just above the **Spec List**. The **Spectrum Information** dialog box is also displayed by selecting this the **New spectrum** button in this same button bar.

The spectrum and compound information can originate in a Text file in the NIST MS Text file format described in the **NIST Text Format of Individual Mass Spectra** at the end of this section. The NIST Search Program, will read a number of different formats. Select **Open** from the **File** menu on the main menu. On the **Choose file for spectra/structures import** dialog box (lower right) there is drop-down list box that shows the various format that can be imported by MS Search. Currently there are ten formats.

The NIST MS Search Program's **User libraries** support **chemical structures**. Starting with V1.6 of the NIST MS Search Program, users may import their own chemical structures for use with selected user spectra. This is done in the **Librarian** pane by connecting a user-drawn structure in standard MOL-file format with a user spectrum. Such structure-drawing programs are widely available:

ISIS/Draw may be freely downloaded from http://www.mdli.com/downloads/isisdraw.html
Advanced Chemistry Development's ChemSketch 4.0 from http://www.acdlabs.com/download/

As has always been the case, if a user spectrum is given its CAS registry number and the Main Library has a structure for that CAS#, this structure will automatically be displayed with the associated spectrum unless an imported structure has been attached to the spectrum.

Beginning with Version 2.0 of the NIST MS Search Program, chiral structures are supported for User Library chemical structures. Chiral Structures began to appear in NIST 14.

User libraries are very easy to create and maintain. You may want to create them using specific sets of spectra from the NIST/EPA/NIH Main or Replicates Library. Any spectrum in the **Spec. List** Window can be added to a **User library**. Any spectrum in the **Hit List** Window can be copied to the **Spec. List** Window. Structures in the MOL file format can be copied from MS Search to the Windows Clipboard by putting the Mouse pointer on the spectrum with structure, clicking the Right Mouse button, and selecting **Copy Structure to Clipboard** from the RMB menu.

MS Search can read user-submitted spectra in the JCAMP, U.S. EPA, or the NIST Text formats as well as formats of files submitted by various instrument manufacturers' mass spectrometer data systems. You should check with the manufacturer of your mass spectrometer's data system to see if there is file compatibility.

Instructions on building **User libraries** are included in the Librarian Help Screens. These also include the information necessary to add structures to **User library** spectra.

Utilities are provided that allow for the association of structures with spectra in the **User libraries**. There is also a utility that allows ChemStation user libraries with associated structures to be copied to the NIST **User library** format.

NIST Text Format of Individual Mass Spectra

The NIST Text file format is very simple. A file can contain as many spectra as you want. Each spectrum must start with the field title "Name:". There must be something in this field in order for the spectrum to be imported, i.e., the data file name and the scan number of the spectrum's fetus. The last required field title is "Num Peaks:". The contents of this field must be the number of *m/z*–intensity pairs that make up the spectrum. Optional fields with the titles of "Comments:", "Formula:", "MW:", and "CAS#:" can be between the "Name:" and "Num Peaks:" fields.

When a spectrum is saved to a Text file from the NIST/EPA/NIH Main or Replicates Library, it will also contain fields with the names "NIST#:" and "DB#:". The field with the name "NIST#:" is on the same line as the "CAS#:" field and separated by a semicolon (;). The mass/intensity list begins on the line following the line with the field title "Num Peaks:". Lines of the *m/z*–intensity pairs list have no field title.

When you create a file with all the allowable fields, each field title should be on a separate line. Use the following format. The format for each spectrum in a Text file usable by the Program should be as follows:

Line 1: NAME: Molecule (Required, up to 511 characters)
Line 2: COMMENT: Run 23, 8/8/88 (Optional, up to 511 characters)
Line 3: FORMULA: C6H6 (Optional)
Line 4: MW: 78 (Optional)

If the user spectrum contains a CAS registry number with its appropriate prefix (**CAS:**), the display of the spectrum in the **Plot**, **Compare**, and **Structure** Windows will have the structure of the compound with that CAS registry number in the NIST/EPA/NIH Main Library.

Line 5: CAS#: 71-43-2 (Optional) **Note that** CAS# and CASNO are synonymous.

The actual mass spectral data (number of peaks in the spectrum) must begin on the next line. It does not actually matter what line this is, as long as it precedes the line that starts the mass/intensity pair data. The VERY NEXT line and subsequent lines MUST contain the paired mass/intensity values.

Line 6: Num Peaks: 18 (This prefix and the number of mass/intensity pairs are Required.)

Line 7: 26 430; 27 340; 28 40; 37 480; 38 611; 39 1411; 49 300; 50 1792; 51 2052; 52 1962; 63 340; 73 160; 74 480; 75 180;

Line n: 76 721; 77 1401; 78 9806; 79 651;

The peaks need not be normalized, and the masses need not be ordered. The exact spacing and delimiters used for the mass/intensity pairs are unimportant. For example, the peaks above could equally be presented as:

(26,430),(27,340),(28,40),(37,480),(38,611),(39,1411),
(49,300), (75,180),(50,1792),(51,2052),(52,1962),(63,340),
(73,160),(74,480),(75,180),(76,721),(77,1401),(78,9806),(79,651)

or each mass intensity pair could be on an individual line.

You can give the file any valid name. However, it is best to use the extension “MSP”. This is the recognized default extension in the Program when you want to import user spectra.

NOTE: The above examples show that the *m/z* values are integers. Version 1.7 and higher of the NIST MS Search Program has user settable mass defect correction and the passed *m/z* value can be a fraction, when available.

NOTE: The NIST MS Search Program can also import spectra in the JCAMP format.

Synonym Codes for MS Search Field Headers:

v.2.0g (May xx, 2011 and Feb 2, 2012 builds) Prepare February 10, 2013

Spectra in the NIST Tandem Library have a number of fields displayed in the Text Information pane. These fields provide important information about how the spectrum was acquired. These fields can be added to user generated spectra. The field headers and their contents can be exported in MSP files and stored in user libraries. When the codes are present in MSP files and imported into MS Search, the field headers and their contents will be display in the Text Information pane.

Currently there are two versions of v.2.0g in use: the one that is being distributed with NIST 11 (May xx, 2011) and the version that will was released with the next version of the NIST Tandem Library (June 2012). This document relates to both versions and distinctions are clearly pointed out.

The following are field codes, displays in MSP files, and displays in the Text Info. window:

Syn. Tag	MSP File Tag	MS Search Display
$:00	Spectrum_type	Spectrum type
$:01	Compound_type	Compound type
$:02	Ion_name	Ion name
$:03	Precursor_type	Precursor type
$:04	PrecursorMZ	Precursor m/z
$:05	Collision_energy	Collision energy
$:06	Instrument_type	Instrument type
$:07	Instrument	Instrument
$:08	Special_fragmentation	Special fragmentation
$:09	Sample_inlet	Sample inlet
$:10	Ionization	Ionization
$:11	Ion_mode	Ion mode
$:12	Collision_gas	Collision gas
$:13	Pressure	Pressure
$:14	Mass_range	Mass range
$:15	Maximum_intensity	Maximum intensity
$:16	In-source_voltage	In-source voltage “Cone voltage” is translated to In-source voltage
$:17	AUX	AUX
$:18	Link	Link <= never displayed
$:19	Ion_Formula	Ion Formula
$:20	Ion_MW	Ion MW
$:21	Charge	Charge
$:22	Salt	Salt
$:23	Known_impurity	Known impurity
$:24	Related_CAS#	Related CAS#
$:25	Salt/mix_CAS#	Salt/Mix CAS#
$:26*	Peptide_sequence	Peptide sequence
$:27*	Peptide_mods	Peptide mods
$:28	InChIKey	InChIKey

* Neither of these codes are recognized by either version of the MS Search Program discussed in this document.

For example, msp file line

SYNON: $:04123.45

(the colon after SYNON and the space between the *synon* colon and $xx is important) There should be no space between the last digit of $:xx and the first character of the field content.

Is displayed by MS Search as

Precursor m/z: 123.45

Example, msp file line

PrecursorMZ: 123.45

When MS Search exports these special field headers and their contents, it inserts the space between the colon at the end of the field header name and the first character of the contents.

Is also displayed by MS Search as

Precursor m/z: 123.45

When a spectrum is opened in the **Spectrum Information** dialog box (Spectrum Editor), the $:xx codes followed by the field contents appear in the **Other Names (Synonyms)** pane. Any normal synonyms not preceded by a SYNON: $:xx(field content) will be displayed under the normal **Synonyms** field title in the spectrum **Text Information** pane.

To import these special synonyms into NIST 11 MS Search, it is necessary to select the **Include Synonyms** check box in **Spectral Import Options** dialog box. Without this, all synonyms are ignored by the currently distributed version of MS Search.

When an MSP file is being created or appended, be sure that the **Include Synonyms** check box in the **Choose file for spectra/structure export** dialog box has been selected. If it is not selected the *Synonyms Field Codes* will not be in the resulting file.

The next version of MS Search to be distributed (in test), reads these SYNON: $xx(field contents) synonyms always, no matter whether **Include Synonyms** in the **Spectral Import Options** dialog box has been selected or not. The same is true for the **Choose file for spectra/structure export** dialog box.

The currently distributed version of the software writes both **$:04123.45** *AND* **PrecursorMZ:** 123.45 into the MSP file. All other field headers appear as $:xx in the MSP file when formed from the currently distributed version of the software, The next version (in test) will replace the $:xx with the above **MSP File Tags**. The next version will import either **MSP File Tags** or the SYNON: $:xx tags.

If an input MSP file contains both **Synon: $:04** and **PrecursorMZ:** lines, the latter is used; the former is ignored.

Calling AMDIS from Within A Third-Party Program

AMDIS can be called from within a third-party program by starting AMDIS32$.exe. This ensures the communications happen with only one copy of AMDIS. AMDIS_32.EXE should be in the same folder as AMDIS32$.EXE. The format of the AMDIS call from a third-party program is:

C:\NIST08\AMDIS32\AMDIS32$.EXE <*space*><datafile><space><switches>

Where:
<datafile> is the full pathname of the data file to be loaded into AMDIS and <switches> is described below.

This example assumes that AMDIS is in the C:\NISTXX**AMDIS32** folder; if it is in some other folder, make the appropriate substitution (see **Location of the NIST MS Search Program** above).

You can specify the type of analysis and the analysis mode for AMDIS with the switches.

For example, the command *C:\NISTXX\AMDIS32\AMDIS32$.exe c:\data\grob.d\data.ms /x* will call AMDIS and use the RI Calibration data in the analysis.

The following switches work with **AMDIS32$.exe**

Switch	Type of Analysis
/S	Simple
/X	Use RI Calibration Data
/I	Use Internal Standards
/N	Use RI Calibration data + Internal Standards.
/C	RI Calibration/Performance
/K	Performance Check
/M	Manual (Loads in data file, does not perform analysis, leaves AMDIS in the forefront)
/Range=X:Y or /R=X:Y	This will cause the range bound by spectrum no. X to spectrum no. Y to be displayed in AMDIS

Only /M will bring AMDIS to the foreground. Using AMDIS32$ without /M will load the data file and run AMDIS in the background.

For example, the command Run c:\NIST08\AMDIS32\amdis32$.exe /s d:\data\cal.d\data.ms will open AMDIS, load in cal.d, and do a simple analysis. AMDIS will stay in the background.

The command Run c:\amdis\amdis32$.exe /m d:\data\cal.d\data.ms will open AMDIS and load cal.d. AMDIS will not do any analysis.

Additionally there are three switches that work with AMDIS_32.exe but do not function with AMDIS32$.exe. The format of the call for AMDIS_32.exe is the same as for AMDIS32$.exe. Note that running AMDIS_32.exe creates a new copy of AMDIS.

The following switches work with **AMDIS_32.exe**

Switch	Analysis Mode	Action
/A	Results	Loads in data file, analyzes the data file within the Results Window.
/D	Direct Confirm	Loads in data file in the Confirm Window., and analyzes the data file.
/E	Auto Exit	Loads data file, analyzes data file and shuts down.

For example, the command *c:\NISTXX\AMDIS32\AMDIS_32.exe c:\data\grob.d\data.ms /e /x* will call AMDIS, use the RI Calibration data in the analysis, and close out of AMDIS.

Sending Spectra from AMDIS to a Third-Party Program

AMDIS can send deconvoluted spectra to the NIST MS Search Program; however, currently, there is no straightforward way to send AMDIS deconvoluted spectra to a third-party program.

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