

Some New Features of MS Search in NIST08

NEW Tags in Comments Field

The concept of Tags was added to v.2.0f of MS Search. Tags in the Comments field of a spectrum can be searched. With respect to the spectra in the **mainlib** and/or **replib** databases, when using the Sequential Search, by typing a text string in the dialog box as shown in Figure 1, the **Contributor** field will be searched. All spectra contributed by a single source can be identified in this way.

NEW Tags in User Library and Spec List Spectra

Tag=string (where *Tag* is the name of a Field heading that will be displayed with the Text information of a User Library or Spec List spectrum and can optionally appear in the line below the Plot of the spectrum and string is a contiguous line of characters that contain at least one alpha member) can be entered into the Comments field of a User Library or Spec List spectrum. The *Tag* must be a contiguous string of character (no spaces between characters). The *string* can be entered as "*string*" (open and close quotes) and have spaces. If the following is entered in the **Comments** field of the **Spectrum Information** dialog box of a Spec List or a User Library spectrum:

Structures were provided by O. David Sparkman
Contributor="University of the Pacific Mass Spectrometry Facility"
Instrument="Agilent 5975 Inert XL MSD w/7890 GC"
Tune="Standard Spec w/ PFTBA"
ScanRange=35-400
GC_column="30 m x 250 µm with 0.3 µm film thickness of BD-5"
OvenTemp="50 C 5 min. to 250 C @ 5 C/min"
Synthesized="Matt Cutis", as shown in Figure 2, the information preceding each equal sign (=) will be displayed as a Field title in the Text display of the spectrum and can optional be displayed with the Plot of the spectrum. The information following the equals sign (=) will appear following the Field header. Entry of Field contents (*string*) must conform to the rules above. In order for this display to occur, the Field titles must be registered in the **Display comment field options** dialog box shown in Figure 3 (**View/Comment fields options**). Figure 4 shows a spectrum (Plot and Text) with added Field headers.

When a search is done of a User library that contains *Tags*, it is possible to Constrain that search based on the *Tag* and the partial or whole contents of the *Tag* (Field). Used the Help file for more specific details on the use of *Tags* as Constraints.

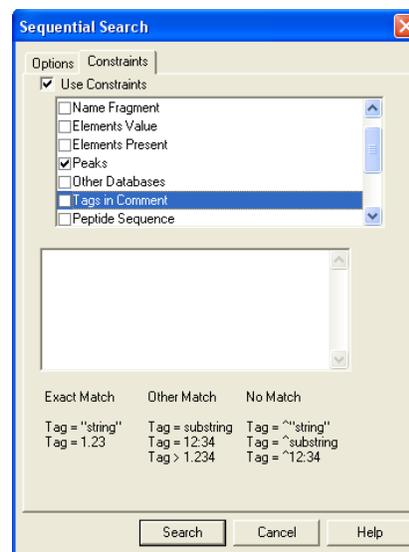


Figure 1

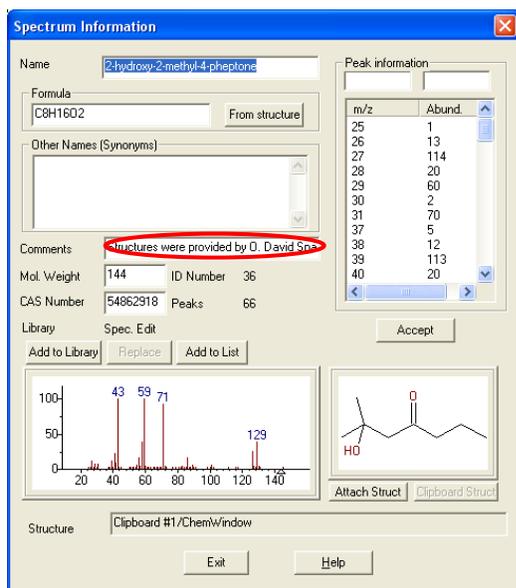


Figure 2

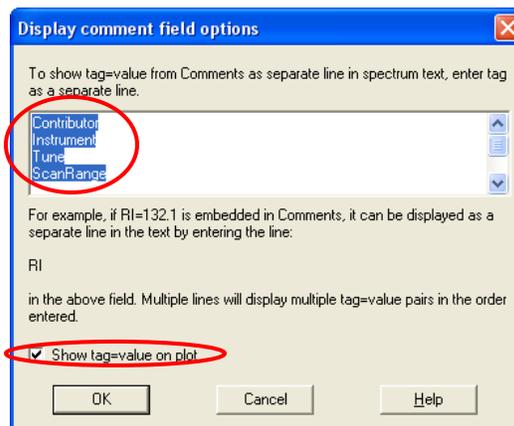


Figure 3

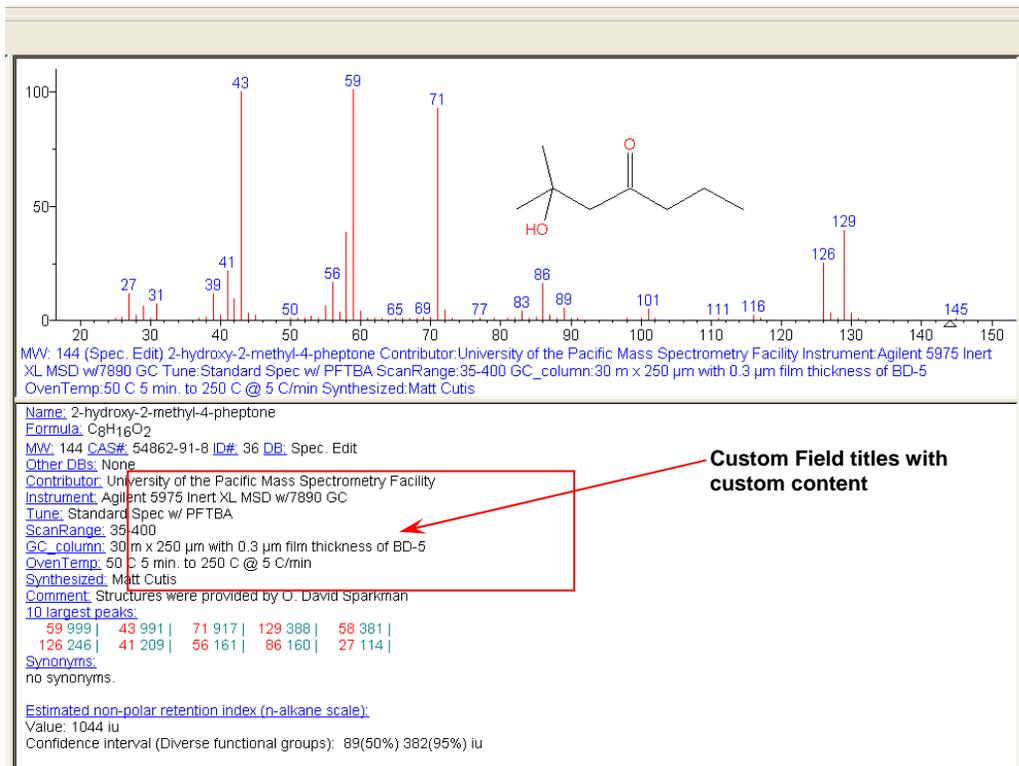


Figure 4

NEW Display of Spectra of Derivatives as Replicate Spectra

One of the major new features with NIST MS Search (v.2.0f) in NIST08 is the ability to display spectra of derivatives as replicate spectra. If a spectrum of 1-octanol is in a Hit List and the **mainlib** or **mainlib** and **replib** databases have spectra of trimethyl silyl, pentamethyldisilyl, and/or acetate derivatives of 1-octanol, these would be listed as replicate spectra. When the replicates are displayed, actual replicates of compounds found in the **replib** database would be designated with an **R**. The spectra of the derivatives would be designated with either an **m** (in the **mainlib** database) or an **r** (in the **replib** database). This display feature is defaulted in MS Search 2.0f. To turn this feature off or modify it, use the **Replicates Display Options** dialog box called by **Options/Replicates**.

NEW Sorting of Hit List

It is now possible to sort a **Lib Search** tab Hit List alphabetically or by Match Factor, Reverse Match Factor and Probability (all high to low or low to high). Hit List in the **Other Search** tab can also be sorted alphabetically. This new feature is especially helpful when doing a Molecular Weight or Formula Search looking for a specific compound and the Hit List has several hundred entries.

NEW Ability to Specify Presence or Absence of Any Part or Parts of a Name

Flexibility has been added to searches using a Name Fragment in constraints. It is now possible to specify the presence or absence of any arbitrary part or parts of a name.

NEW MS/MS Identity Search

This search is designed to work with databases obtained using collisionally activated dissociation (CAD). It will work with User Libraries of MS/MS data or the NIST MS/MS Database provided with NIST08. The Similarity search of the EI database used in conjunction with the Substructure identification feature of MS Search for CAD data (introduced in MS Search 2.0d with NIST05) has been renamed to **MS/MS in EI** and is still an option under Similarity.

NEW Increase Font Flexibility

It is no longer necessary to install NIST Fonts. No longer are fonts limited to *NIST Sans Serif*, *NIST Serif*, *NIST OEM*, *Arial*, and *Terminal*. All the Fonts on a computer are available for the MS Search Program.