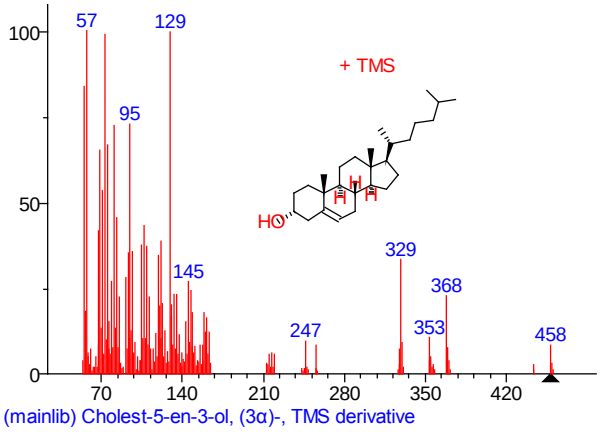
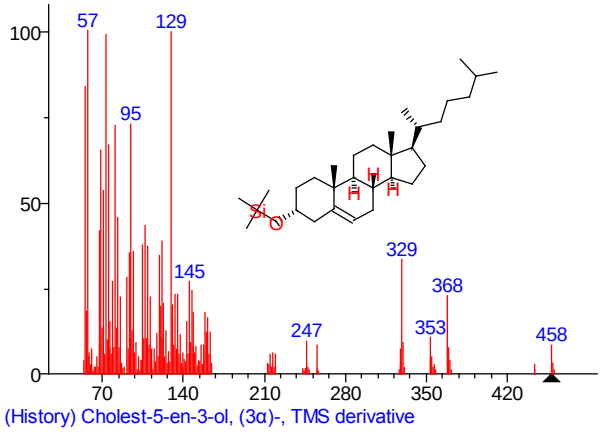
New features in the NIST MS Search Program (version 2.2) for the 2014 Version of the NIST/EPA/NIH Mass Spectral Library (NIST 14)

- Use of NIST GC Method/Retention Index Database data (385,872 records for 82,868 compounds, 56,216 of which there are EI spectra) in user spectrum searches.
- Display of relevant RI values in Hit List.
- Import, export and editing compound RI values for user spectrum searches and user libraries.
- An optional new way for the display of structures of derivatives is provided. Display either the derivatized structure or the structure of the precursor compound with a graphical indication of the derivatizing reagent.





- All small molecule mass spectra in NIST libraries have InChIKeys linked to PubChem. These InChIKeys may also be used for searching compound information on the Web or for exact structure search in libraries.
- Importing and displaying Glycan structures in KCF format; adding them to mass spectra in a user library
- Improve Editing of spectra to include more header information with User spectra in user libraries and accurate *m/z* values, intensities, and peak annotations in the built-in mass spectrum editor.
- In-source/EI with accurate ion m/z spectra - High resolution mass spectra
    - Import of in-source tandem spectra, or EI with accurate ion *m/z* spectra, which do not include a defined m/z of the precursor ion. To import these spectra, select "in-source / EI (accurate m/z)" in Spectrum Import Options.
    - In-source/EI with accurate ion m/z spectra have accurate ion peak m/z and intensities. The accuracy is set in Spectrum Import Options.
    - In-source/EI with accurate ion m/z spectra may be searched in In-source/EI with accurate ion m/z library and/or MS/MS library with the new In-source HiRes search (ion peak m/z tolerance down to 0.015 ppm or 6×10^{-5} m/z units), Similarity Simple, Identity Normal or MS/MS Presearch OFF search options. For this purpose, adding Reverse Search option may useful.

- In-source/EI with accurate ion m/z spectra may be added to a user library. Currently, in-source/EI with accurate ion m/z spectra added with NIST MS Search to a user library may be searched with In-source HiRes search only with Presearch OFF option. Rebuild the library with Lib2NIST to get in-source HiRes presearch benefits.

A number of new features have been added to the version distributed with the 2012 release of NIST Tandem Mass Spectral Libraries as well as to v.2.0g which was distributed with NIST 11. To view those, look at the What's New in the MS Search Program in the v.2.2 Help file available by selecting this link (Help)