



NIST 2014 Mass Spectral Reference Libraries

NIST

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The NIST 14 mass spectral database, the successor to the NIST 11, is a set of fully evaluated collections of electron impact (EI) mass spectra, tandem MS (MS/MS) mass spectra and retention index (RI) data. It is the product of a twenty-seven year, comprehensive evaluation and expansion of the world's most widely used mass spectral reference libraries by a team of experienced mass spectrometrists in which each spectrum was examined for correctness.

NIST/EPA/NIH Library of Electron Ionization Spectra

This version contains a total of 242,466 compounds, representing an increase of 29,505 over the prior (2011) version. It also includes 33,782 replicate (alternate) spectra of compounds listed in the main library, an increase of 2,850. New spectra cover a wide range of compound types, with special emphasis given to human and plant metabolites, drugs and compounds of industrial and environmental importance. Thousands of improvements in chemical names, structures and replicate spectra have also been made, including the naming of derivatives.

NIST Tandem MS Library

The number of compounds from the 2012 version has increased by 33% to 9,344 (a 60% increase from 2011 version). With an increased focus on alternate precursor ions, this has led to an increase in the number of precursor ions by a factor of three relative to the 2012 version with a near doubling of the total number of spectra to 234,284. A large fraction of new spectra were acquired at high accuracy and resolving power, over a range of energies, and in both collision cells (beam type) and ion traps (up to MS4) and, when appropriate, in both positive- and negative-ion modes. A substantial proportion of these new compounds are human and plant metabolites, drugs, lipids, sugars, peptides, pesticides, surfactants and glycans (the last with structures in 'cartoon' format). Advanced noise removal processes have improved the quality of a number of spectra that appeared in earlier versions (as described in X. Yang, P. Neta, S. Stein. "Quality Control for Building Libraries from Electrospray Ionization Tandem Mass Spectra". Analytical Chemistry, in press).

NIST GC Methods and Retention Index Library

RI data are provided for 82,868 compounds, an increase of over 12,000 compounds from the 2011 version. Of these, 56,216 compounds are in the EI library. This brings the number of measured retention indices to 387,463.

NIST 14 is available as full version and also as upgrade for owners of a previous edition:

NIST14	NIST 2014 Mass Spectral Libraries, Single User
NIST14U	NIST 2014 Mass Spectral Libraries, Single User, Upgrade

This item includes the library in NIST format. Please note that the library is also available in various other formats, e.g. MassLib, ChemStation, etc. Please contact us for a quote.