



NIST 2017 MS/MS Mass Spectral Library

NIST

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NIST Tandem MS Library

This library consists of two sub-libraries:

- Small molecules: Includes 574,826 spectra of 118,082 precursor ions for 13,808 different compounds – a 2/3 increase in numbers of compounds over NIST 14! Spectra of all identifiable precursor ions are included, including fragments, adducts, and isotopic chlorine and bromine peaks. We continue to include spectra for both positive and negative charge states, with fragmentation in both ion trap (at multiple msn levels) and in beam-type collision cells (over a range of energies).
- Biologically relevant peptides: Includes 77,649 spectra of 1,435 biologically relevant peptides. Also included are 12,595 spectra of 469 dipeptides also in small molecules library.

The NIST 2017 MS/MS Library contains all MS/MS data from the full edition of the NIST 2017 Mass Spectral Libraries:

NIST17 MSMS NIST 2017 MS/MS Mass Spectral Library, Single User

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.

Contact: MSP Kofel +41 31 972 31 52 info@msp.ch