

NIST / EPA / NIH Mass Spectral Library 2020

A trusted broad and accessible mass spectral library

The NIST/EPA/NIH Mass Spectral Library 2020, the successor to the NIST 2017, is a fully evaluated collection of electron ionization (EI) and MS/MS mass spectra, with chemical and GC data, plus search software to identify your own unknown spectra. NIST 20 contains over a million mass spectra including 350,000 EI spectra for 306,000 compounds and 1,320,000 tandem MS/MS spectra.

It is a product of a more than three-decade, comprehensive evaluation and expansion of the world's most widely used mass spectral reference library by a team of experienced mass spectrometrists at the National Institute of Standards and Technology (NIST) in which each spectrum was examined for correctness.



The collection is comprised of the following three libraries:

- **Electron Ionization (EI) mass spectral library**
- **4 MS/MS libraries**
- **GC Retention Index library**

Library Specifications

- EI Library Spectra: **350,643**
- EI Chemical Structures: **350,643**
- EI Unique Compounds: **306,869**
- EI Retention Index Values: **174,659**
- MS/MS Library Spectra: **1,320,389**
- MS/MS Ions: **185,608**
- MS/MS Unique Compounds: **30,999**
- GC RI Library Unique Compounds: **139,692**
- GC RI Retention Index Values: **447,285**

<https://sciencesolutions.wiley.com>

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Compatibility

- Agilent ChemStation, MassHunter, OpenLab*
- Bruker MS Workstation*
- Chromatec Analytic*
- JEOL msFineAnalysis*
- LECO ChromaTOF*
- NIST MS Search
- PerkinElmer TurboMass
- Scion MS Workstation*
- Shimadzu GCMSsolution
- Thermo Chromeleon*, TraceFinder,* Xcalibur*
- Waters MassLynx

Other versions available:

- ACD/Labs ACD/Spectrus Processor**
- KnowItAll**

*Compatible with the NIST format

**Subscription required

Compound Coverage

Compound coverage can be searched at www.compoundsearch.com. Compound coverage includes:

- Drugs
- Human Metabolites
- Peptides
- Plant Metabolites

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