NIST Tandem Mass Spectral Library

2026 Release

68,635 Compounds, 33% More than 2023
567 K Precursor Ions – 3.2 M Spectra

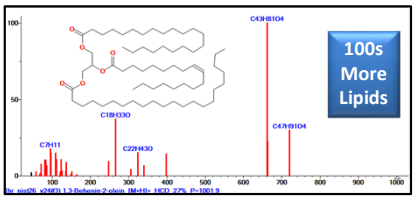
Fragmentation Methods

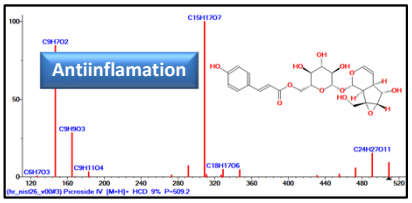
66,782 HRAM (High Res Accurate Mass) Compounds
67,146 QTOF, HCD, IT-HRAM, QqQ Compounds
66,430 Ion Trap Compounds (Low Res., up to MS^4)
623 APCI HRAM Compounds

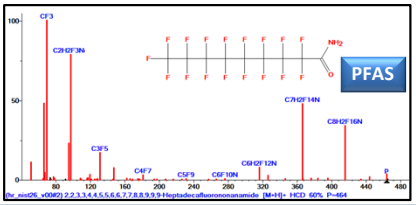
Precursor Ions

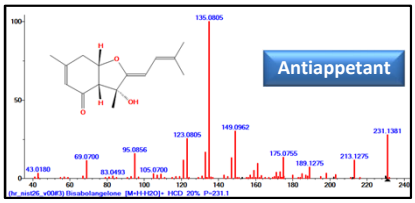
60,178 Protonated
26,100 Deprotonated
18,556 Water/Ammonia Loss
60,962 Other In-Source Ions

All Compounds Selected for Relevance
Measured at NIST, Thoroughly Evaluated







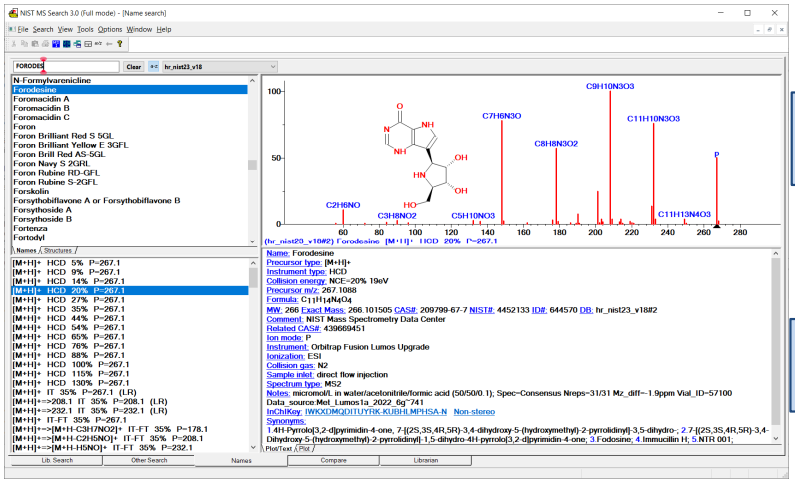


Citation	New	Total
Wikipedia	1271	7510
PubChem Lite	10343	32951
ChEBI	4345	18912
ChEMBL Drugs	866	4449
Protein Data Bank	956	5674
Human Metabolite DB	1387	10197
EPA-PFAS	116	296

View All Spectra for a Compound

Compound Name Structure & Synonyms

All Energies, Polarities, In-Source Entries & Fragmentation Types



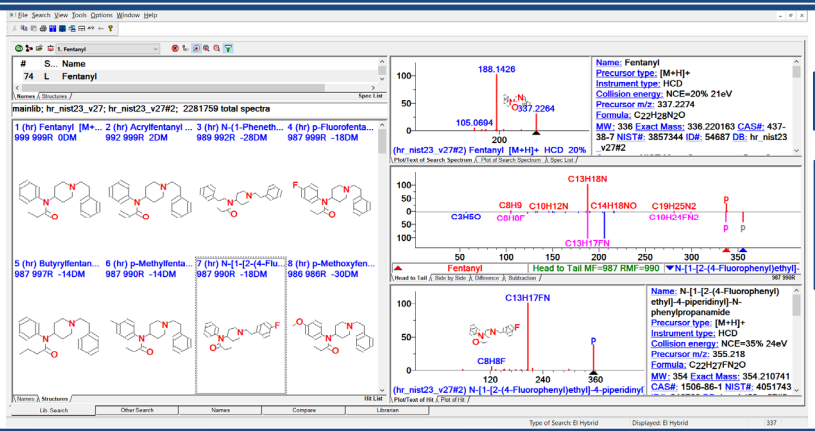
Select Spectrum from List at Lower Left

All Spectrum Text Information

Hybrid Search
For Tandem Spectra

Reports differences in Mass and Formula from Library IDs

Finds Similar Compounds in Library



Query Spectrum

Shifted Library Peaks (gray->red) Contain Modification

Library Spectrum

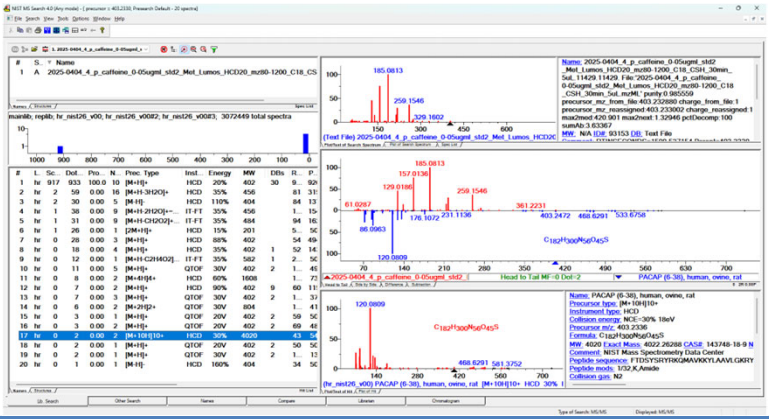
NIST Tandem Library Software

2026 Release

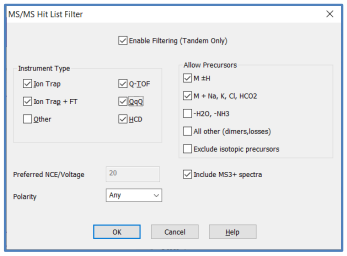
Tandem (MS/MS) Analysis Tools

NISTMS

- All Query Spectra in One List
- Multiple Energies Ion Modes Fragmentation Type In-Source Ions

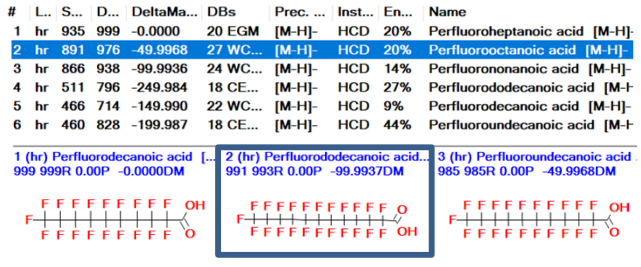


- Filter IDs by Spectrum Type

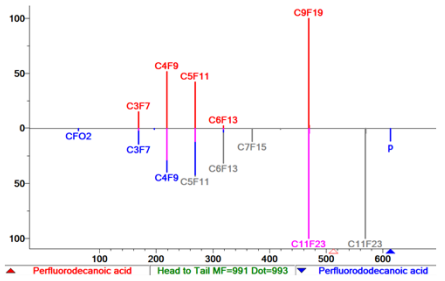


Hybrid Search

- -Finds Compounds Not in Library and Confirms IDs
- -Uses Peaks and Losses
- -Shows Shifted Peaks
- Needs MW Estimate



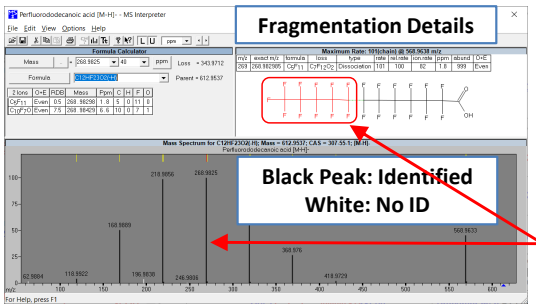
- PFAS Illustration: Applicable to Many Classes

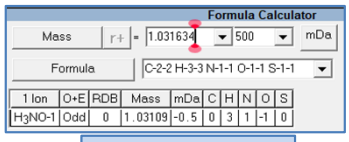


MS Interpreter

- Direct Access From NISTMS
- Connect Peaks to Structure

- Chemical Formula Calculator
- Isotope Calculator
- Any resolution +/- Charge
- Multiple Display Options





- Find Formula from Delta Mass

NIST Website Chemdata.nist.gov

- Freely Available Libraries and Software

Downloadable Libraries

- Annotated Recurrent Unidentified Spectra
  - Urine, Plasma/Serum (ARUS)
- Tryptic Peptides (Human, …)
- Oligosaccharide Libraries (Milk)
- Glycopeptides (mAb, Glycan Distributions)
- Acyl Carnitines

Software

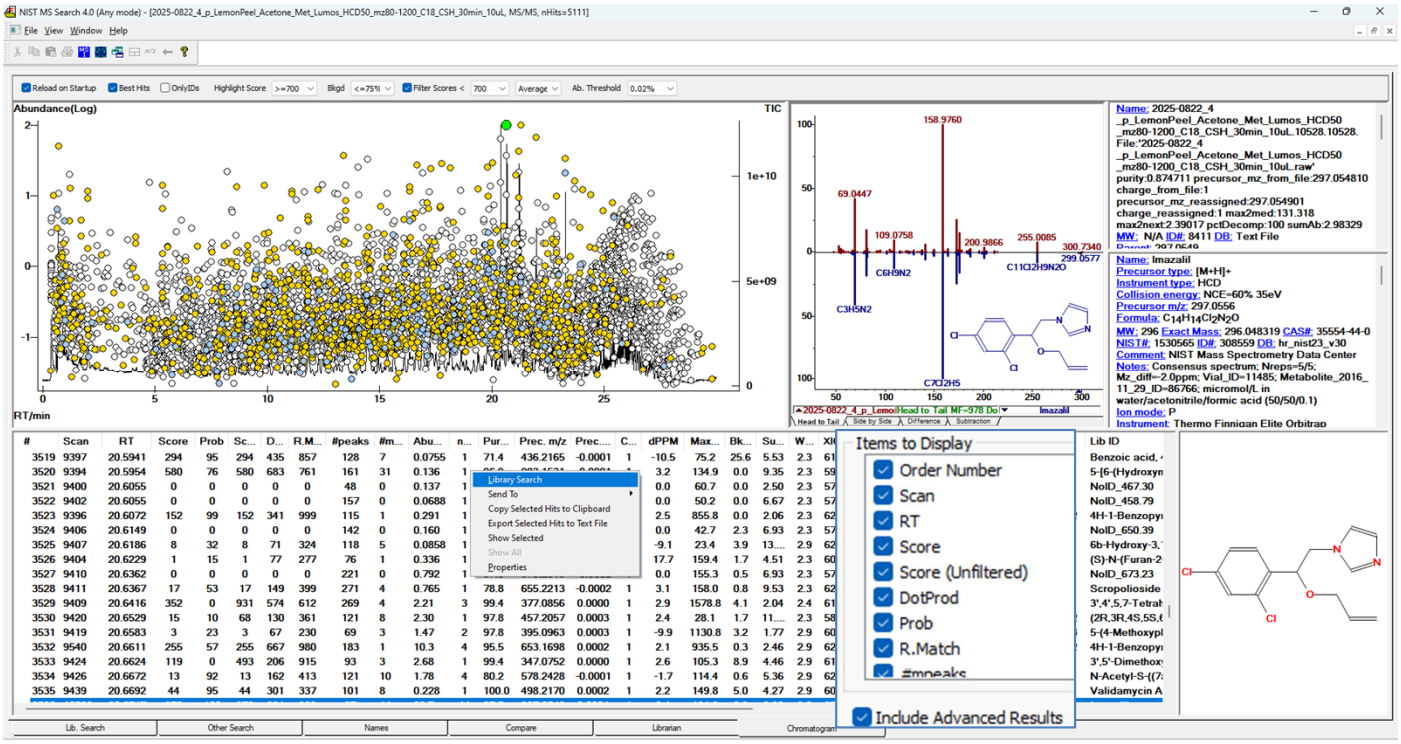
- NISTMS (2026)
- MS Piano (Peptide a\Annotation)
- MS Pepsearch – General Search Utility for NIST Libraries
- MS Interpreter
- Lib2NIST – Library Conversion

http://chemdata.nist.gov

NIST National Institute of Standards and Technology U.S. Department of Commerce

NEW

LC/MS-MS Chromatogram Analysis by NIST Tandem Library

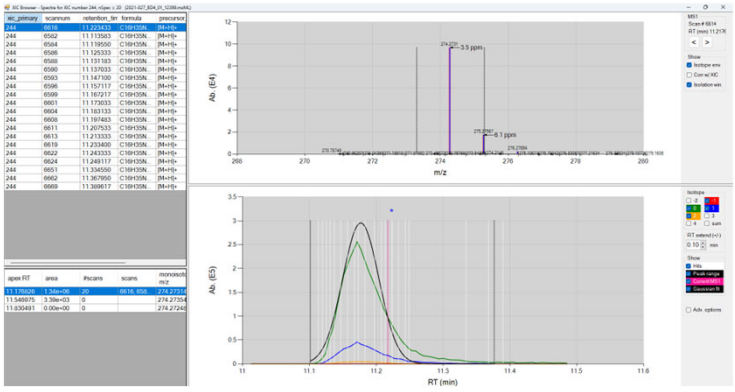


Unique, Extensive, Multilevel Analysis

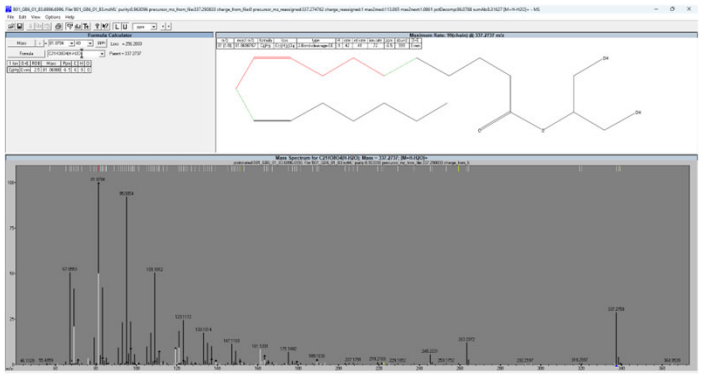
XIC Based Analysis
In-Source RT Alignment
Access External Libraries
Customize/Zoom Display
Eliminate Background MS2

MS1 & MS2 Analysis
Show/Sort 30 Items
Enhanced Hybrid Search
Export to Spreadsheet
Multiple ID Methods

Each Spectrum Can Access All Search/Display Capabilities of NISTMS

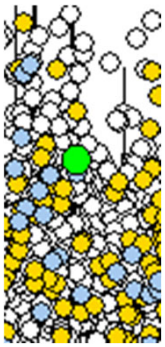


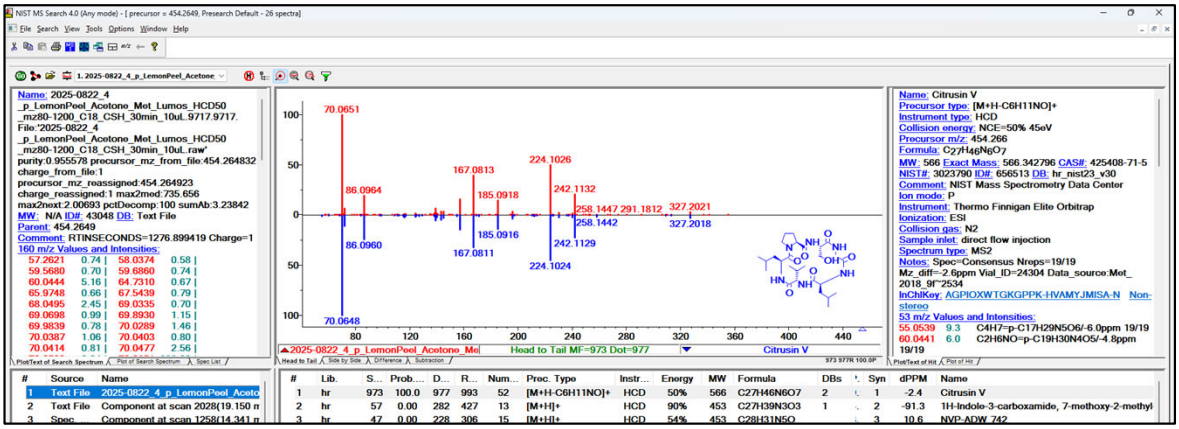
XIC Analyzer (MS1)



MS Interpreter (MS2)

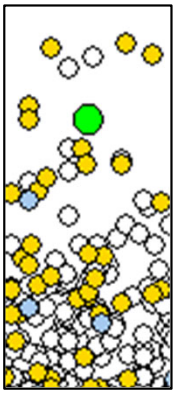
The Power of In-Source Identification

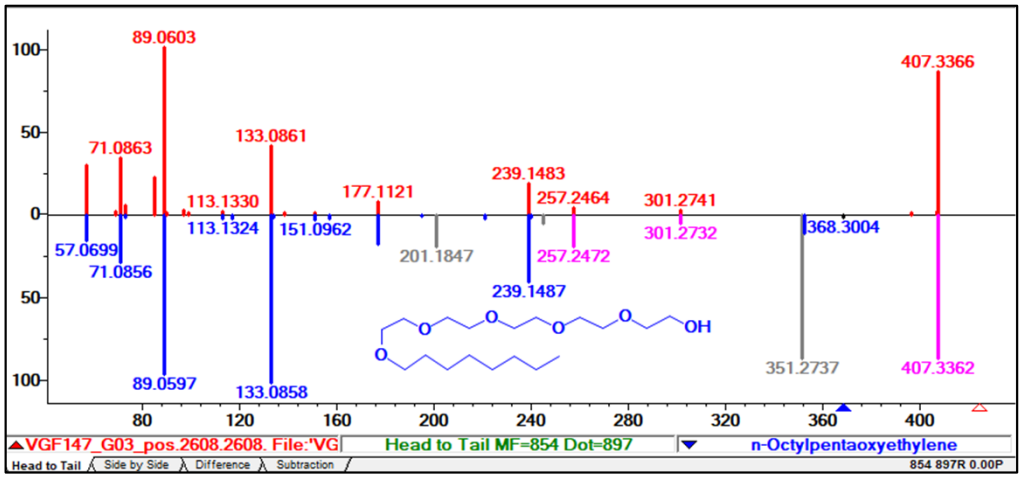




Score 7 -> 973 in-source: Citrusin V (sugar loss)

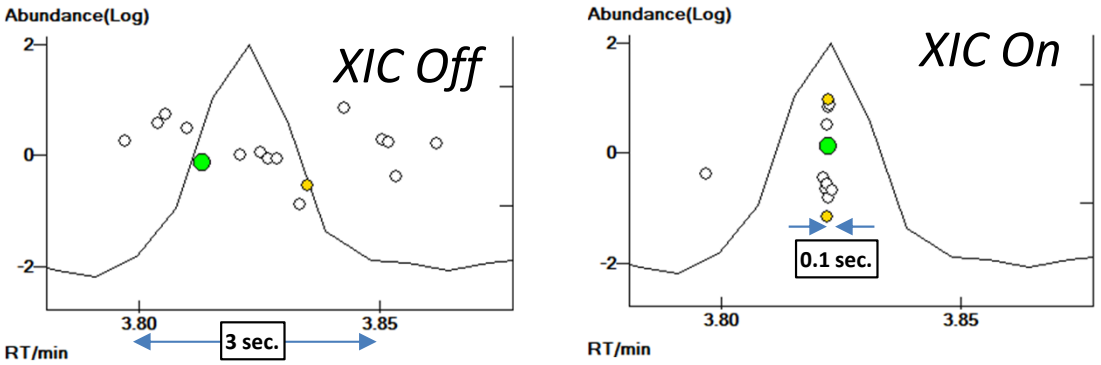
The Power of the Hybrid Search





n-Octylpentaoxyethylene [M+NH4]+ Score 0 -> 854 dMass = 56.0625 (C4H8)

The Power of XIC Analysis



XIC Analysis gives Accurate Retention Times and Abundances