NIST Tandem Mass Spectral Library

2023 Release

51,501 Compounds, 60% More than 2020
400 K Precursor Ions – 2.4 M Spectra

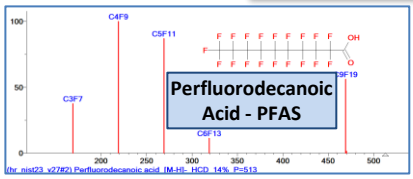
Fragmentation Methods

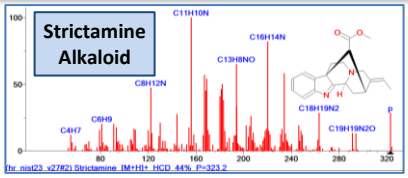
- 49,590 HRAM (High Res Accurate Mass) Compounds
- 50,071 QTOF, HCD, IT-HRAM, QqQ Compounds
- 49,561 Ion Trap Compounds (Low Res., up to MS^4)
- 561 APCI HRAM Compounds

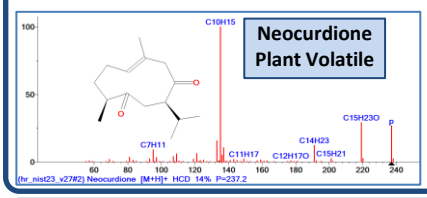
Precursor Ion Types

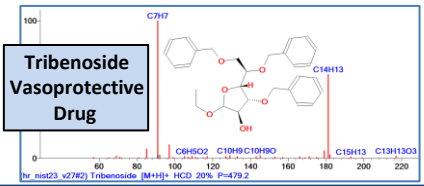
- 44,191 Protonated
- 19,620 Deprotonated
- 14,318 Water/Ammonia Loss
- 44,547 Other In-Source Generated

All Compounds Selected for Relevance
Measured at NIST, Thoroughly Evaluated







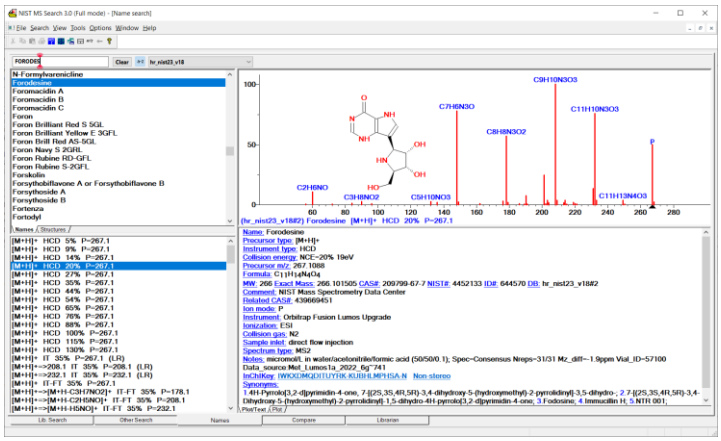


Citation	New	Total
Wikipedia	1618	6424
EPA Tox	3181	8146
Food DB	602	4491
EU Contaminants	6553	15818
Protein Data Bank	1246	4945
Human Metabolite DB	2071	9686
PFAS	90	116

All Spectra Shown for Each Compound

1. Compound Name Many Synonyms

2. All Related Spectra All Energies Fragmentation Types In-Source Ions, …



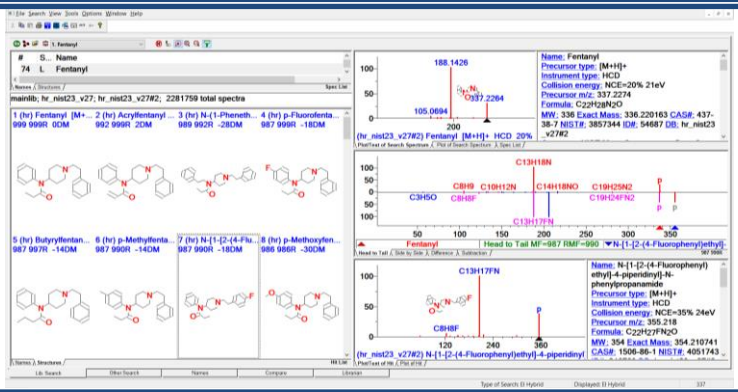
Full Spectrum Selected from List at Lower Left

All Spectrum Text Information

Hybrid Search
Recommended for All Tandem MS Searches

Find Related Compounds Even if Query is not in Library

Differences in masses are 'Modifications'



Query Spectrum

Shifted Library Peaks (gray->red) Contain Modification

Library Spectrum

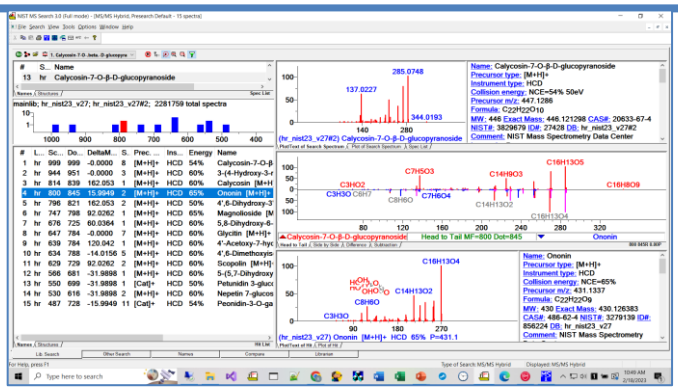
NIST TANDEM LIBRARY SOFTWARE

2023 Tandem Release

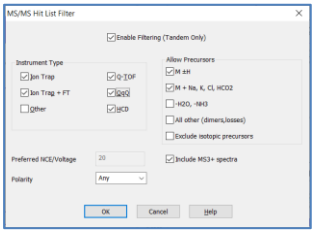
Tandem (MS/MS) Analysis Tools

NISTMS

- All Spectra for Each Compound 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

- Recommended For Routine Use

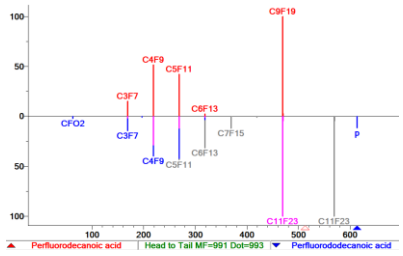
#	L..	S...	D...	DeltaMa...	DBs	Prec. ...	Inst...	En...	Name
1	hr	935	999	-0.0000	20 EGM	[M-H]-	HCD	20%	Perfluoroheptanoic acid [M-H]-
2	hr	891	976	-49.9968	27 WC...	[M-H]-	HCD	20%	Perfluorooctanoic acid [M-H]-
3	hr	866	938	-99.9936	24 WC...	[M-H]-	HCD	14%	Perfluorononanoic acid [M-H]-
4	hr	511	796	-249.984	18 CE...	[M-H]-	HCD	27%	Perfluorododecanoic acid [M-H
5	hr	466	714	-149.990	22 WC...	[M-H]-	HCD	9%	Perfluorodecanoic acid [M-H]-
6	hr	460	828	-199.987	18 CE...	[M-H]-	HCD	44%	Perfluoroundecanoic acid [M-H

1 (hr) Perfluorodecanoic acid [...
999 999R 0.00P -0.0000DM

2 (hr) Perfluorododecanoic acid...
991 993R 0.00P -99.9937DM

3 (hr) Perfluoroundecanoic acid
985 985R 0.00P -49.9968DM

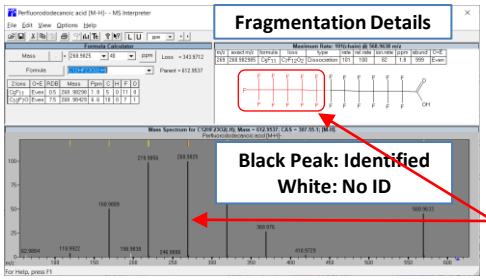
- PFAS Illustration: Applicable to Many Classes

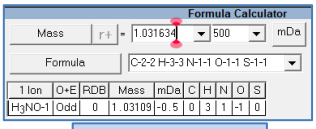


MS Interpreter

- 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 (2019)
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