

NIST Tandem Mass Spectral Library

2023 Release

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

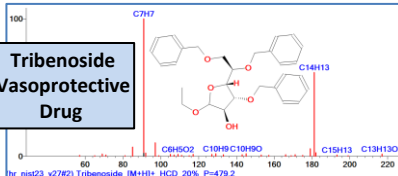
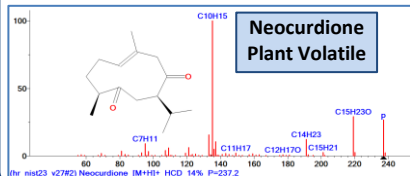
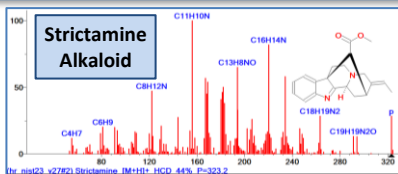
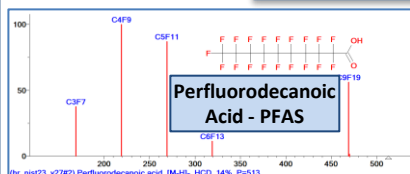
Fragmentation Methods

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 MS⁴)
 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, ...

NIST TANDEM LIBRARY SOFTWARE

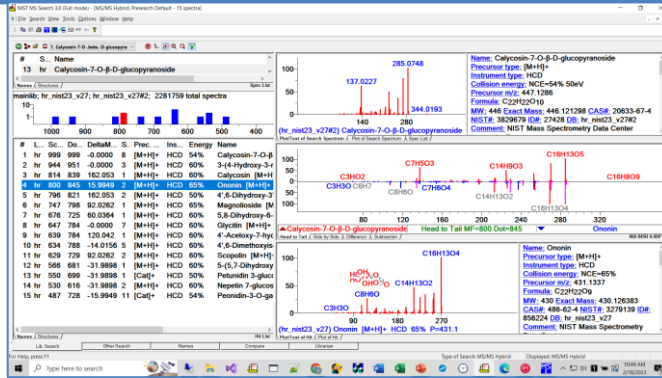
2023 Tandem Release

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

M/SMS Hit List Filter

Enable Filtering (Tandem Only)

Instrument Type: Ion Trap, Ion Trap + FT, Other

Allow Precursors: C16-H, C16-H & C14-HCO2, HCO, H4O, All other (demon/losses), Exclude isotopic precursors

Preferred HCE/Voltage: 20

Priority: Any

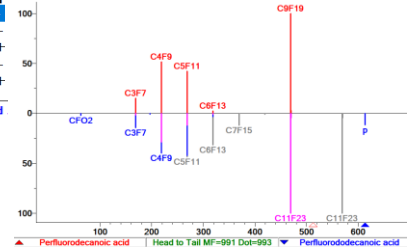
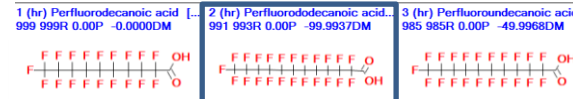
Buttons: OK, Cancel, Help

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%	Perfluoro-octanoic acid [M-H] ⁻
3	hr	866	938	-99.9936	24 WC...	[M-H] ⁻	HCD	14%	Perfluoro-nonoic acid [M-H] ⁻
4	hr	511	796	-249.984	18 CE...	[M-H] ⁻	HCD	27%	Perfluoro-dodecanoic acid [M-H] ⁻
5	hr	466	714	-149.990	22 WC...	[M-H] ⁻	HCD	9%	Perfluoro-decanoic acid [M-H] ⁻
6	hr	460	828	-199.987	18 CE...	[M-H] ⁻	HCD	44%	Perfluoro-undecanoic acid [M-H] ⁻



PFAS ILLUSTRATION: APPLICABLE TO MANY CLASSES

MS Interpreter

DIRECT ACCESS FROM NISTMS

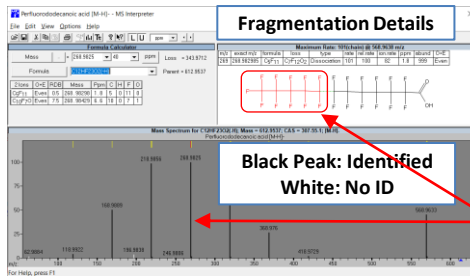
CONNECT PEAKS TO STRUCTURE

Chemical Formula Calculator

Isotope Calculator

Any resolution +/- Charge

Multiple Display Options



Find Formula from Delta Mass

Select Peak Show Structure Fragment

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>