

# NIST Tandem Mass Spectral Library

## 2020 Release

**31K Compounds, 2X More than 2017**  
**186K Precursor Ions - 1.3M Spectra**

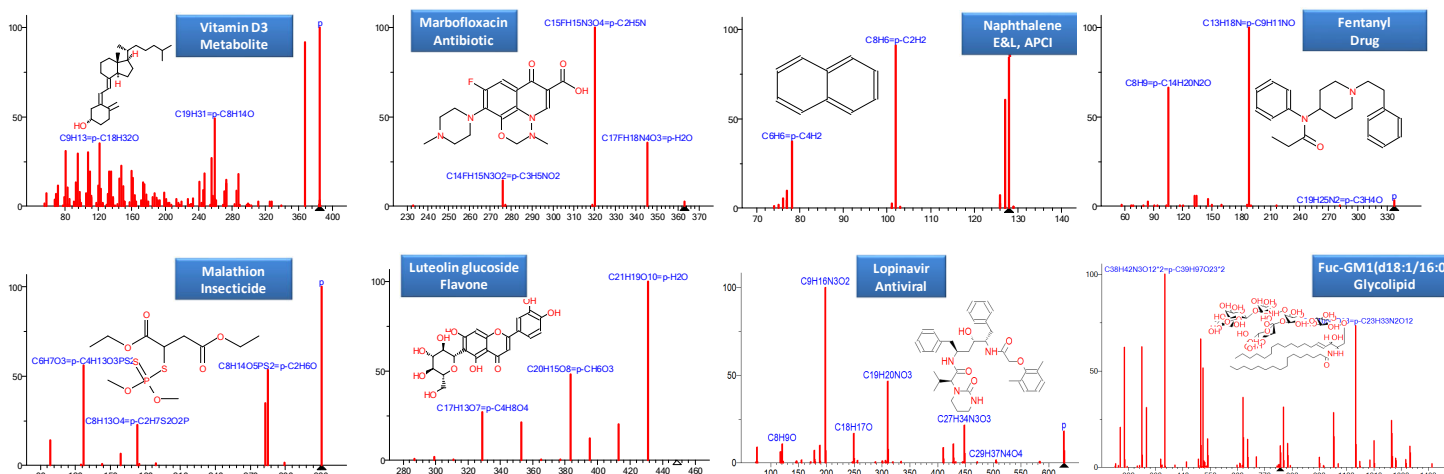
### Fragmentation Methods

27,840 HRAM (High Res Accurate Mass) Compounds  
29,890 QTOF, HCD, IT-HRAM, QqQ Compounds  
29,444 Ion Trap Compounds (Low Res., up to MS<sup>4</sup>)  
246 APCI HRAM 'Extractables and Leachables'

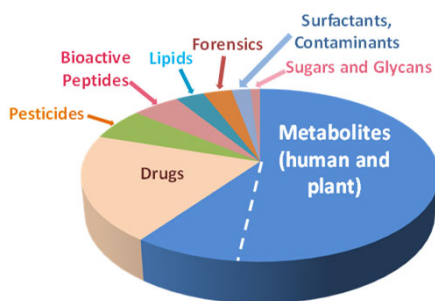
### Precursor Ion Types

26,575 Protonated  
12,589 Deprotonated  
10,032 Water/Ammonia Loss  
24,167 Other In-Source Generated

### Wide Variety of Compounds



### Types of Compounds and Spectra

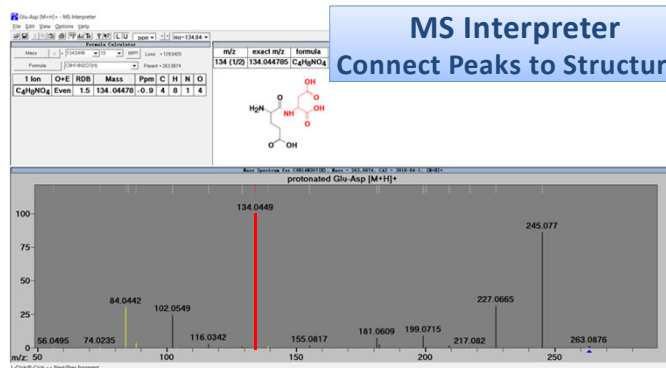


75%(+) 25%(-)  
32% MS<sup>2</sup> in-source  
8% MS<sup>3</sup> and MS<sup>4</sup>  
Over wide energy range

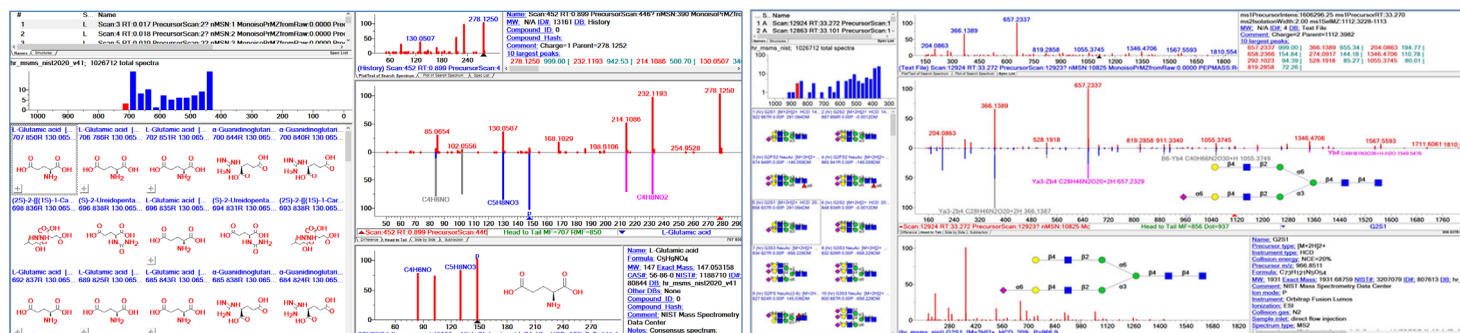
6,000 human metabolites

### MS Interpreter

Connect Peaks to Structures



### Hybrid Search - Identify Compounds Not in the Library



<http://chemdata.nist.gov>

# NIST/EPA/NIH EI-MS LIBRARY

## 2020 Release

### THE LARGEST INCREASE IN COVERAGE **EVER**

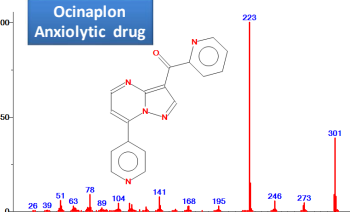
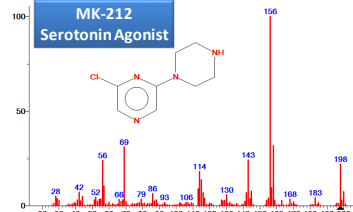
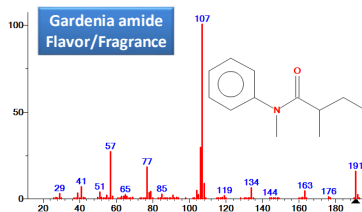
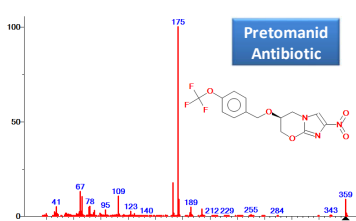
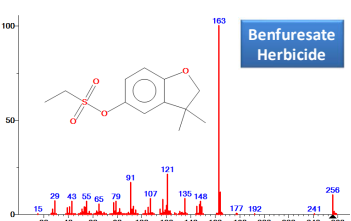
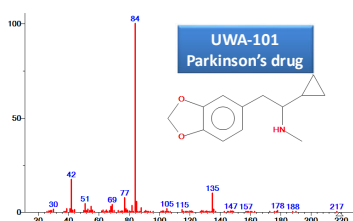
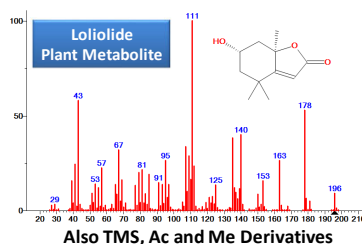
**350,643 Electron Ionization (EI) Spectra**

- 306,869 Compounds, 43,774 Replicate Spectra
- 40 K More Compounds than NIST 17

**447,285 Retention Index (RI) Values**

- 139,963 RI Compounds – 40 K increase
- 112,253 Compounds with both RI & MS

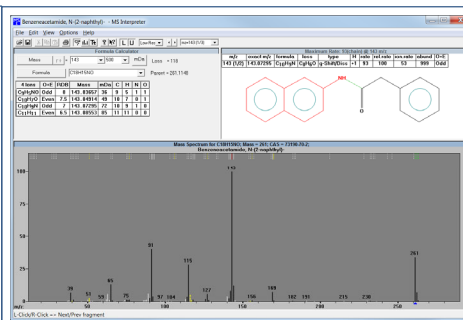
**NEW COMPOUNDS SELECTED FOR IMPORTANCE  
MEASURED AT NIST, THOROUGHLY EVALUATED**



**1,000s of New Compounds of Analytical Interest**  
Human & Plant Metabolites  
Flavor/Fragrance – Food  
Drugs & their Metabolites  
Forensics, Toxins  
Pesticides – Contaminants  
Industrial Chemicals  
Petrochemicals,  
Surfactants, Lipids, ...

**NISTMS.EXE**  
USER INTERFACE  
HYBRID SEARCH  
FOR COMPOUNDS NOT  
IN LIBRARY

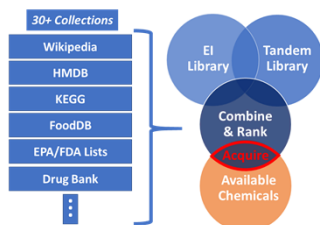
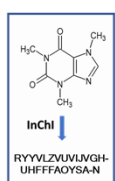
NEW AI RETENTION  
INDEX ESTIMATES



**MS  
INTERPRETER**

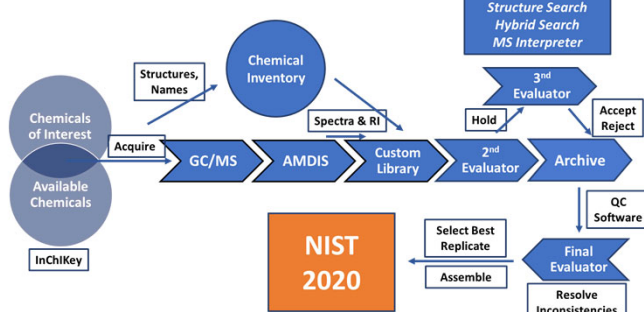
CONNECT PEAKS  
TO STRUCTURES  
MAJOR UPDATE

New Compound Selection Process



**NEW LIBRARY  
BUILDING METHOD**  
SELECT COMPOUNDS,  
MEASURE SPECTRA  
ORGANIZE BY STRUCTURE  
MULTIPLE EVALUATIONS  
MS INTERPRETER  
HYBRID SEARCH

New Evaluation Process



<http://chemdata.nist.gov>