

NIST Tandem Mass Spectral Library

2020 Release

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

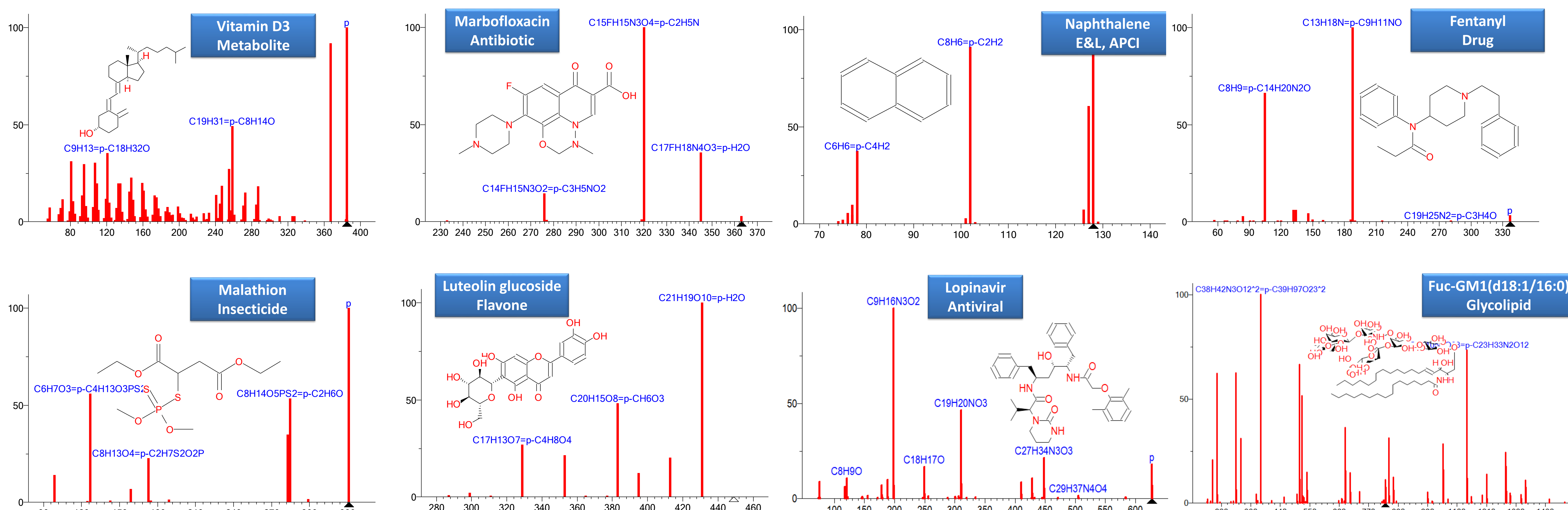
Fragmentation Methods

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 MS⁴)
246 APCI HRAM 'Extractables and Leachables'

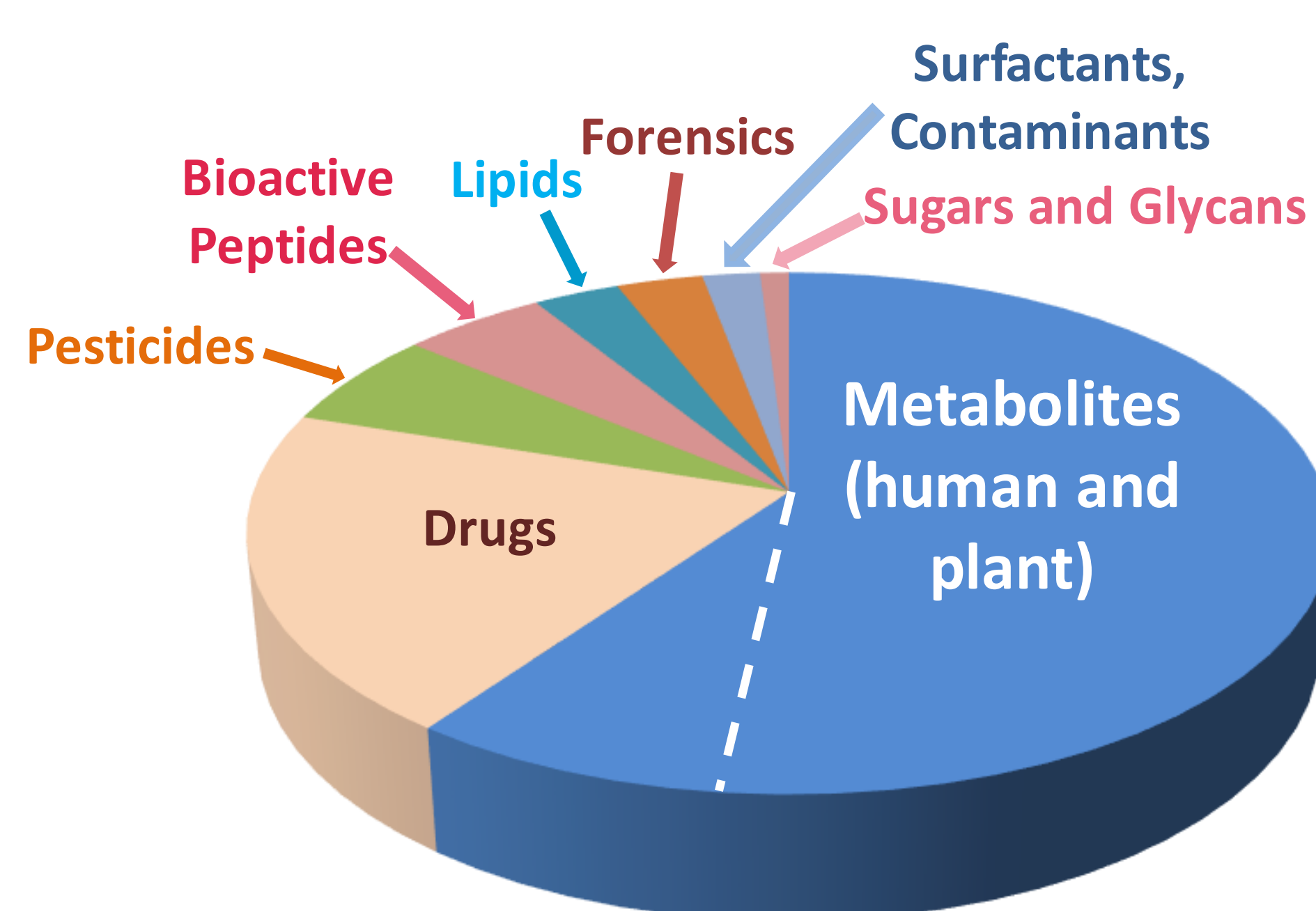
Precursor Ion Types

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

Wide Variety of Compounds



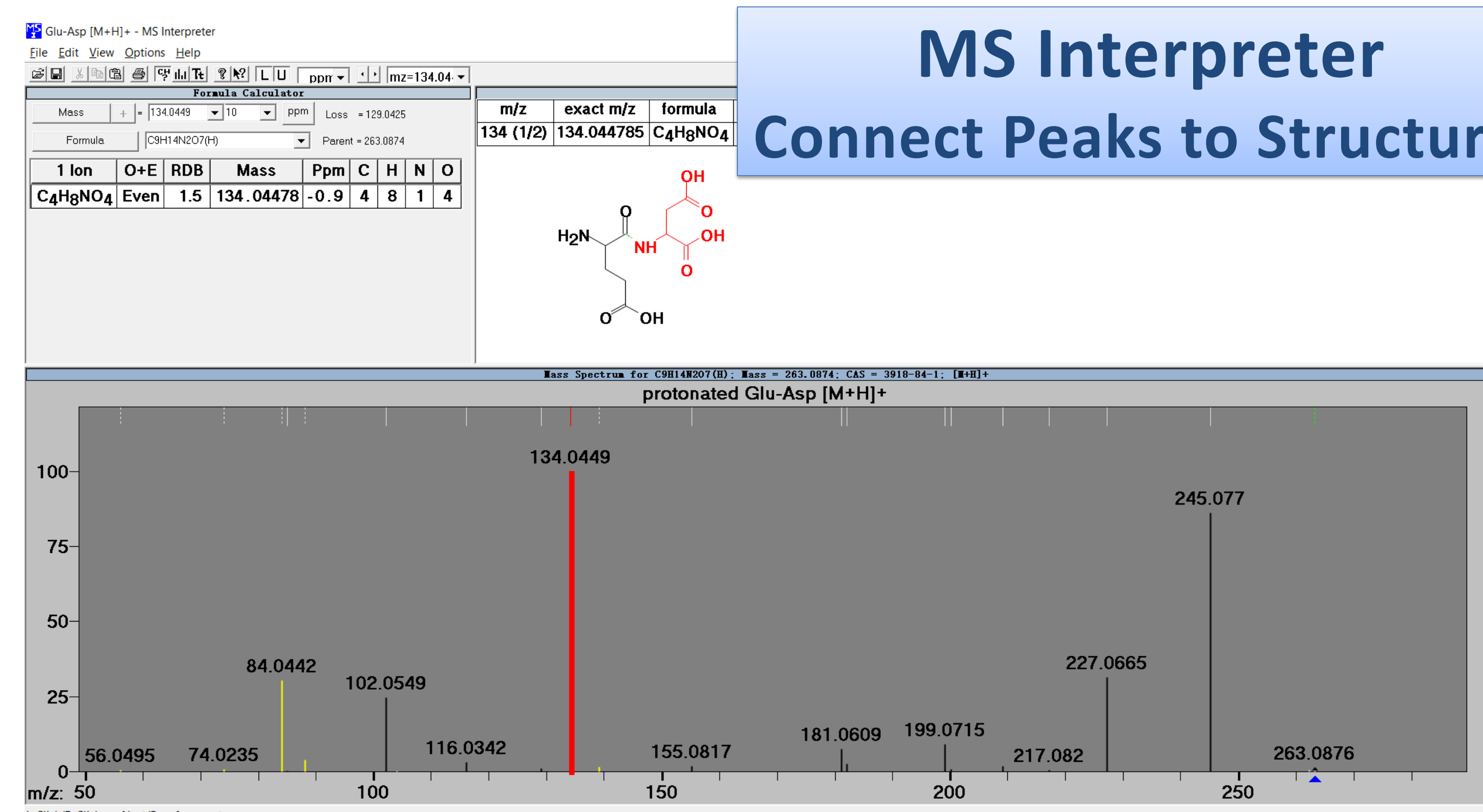
Types of Compounds and Spectra



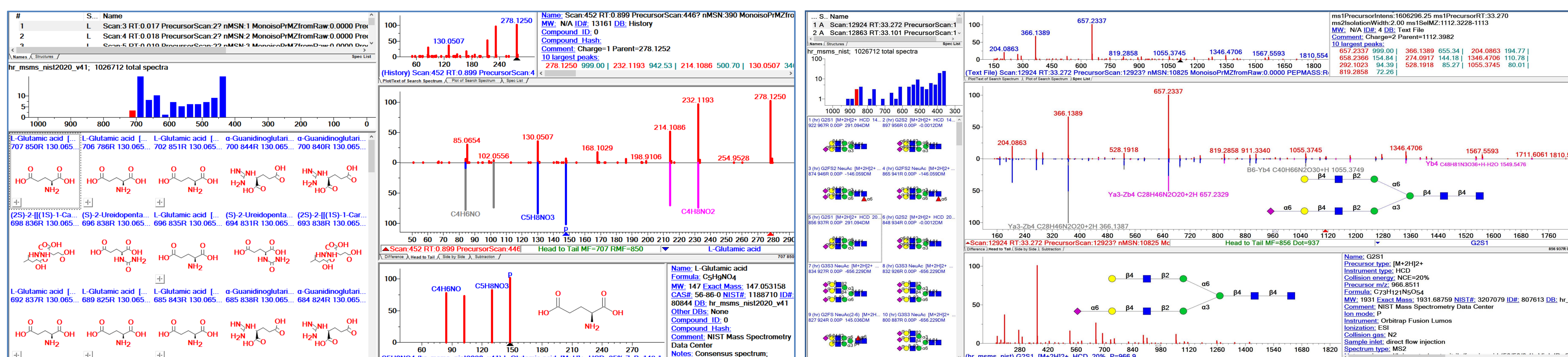
75% (+) 25% (-)
32% MS² in-source
8% MS³ and MS⁴
Over wide energy range

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**

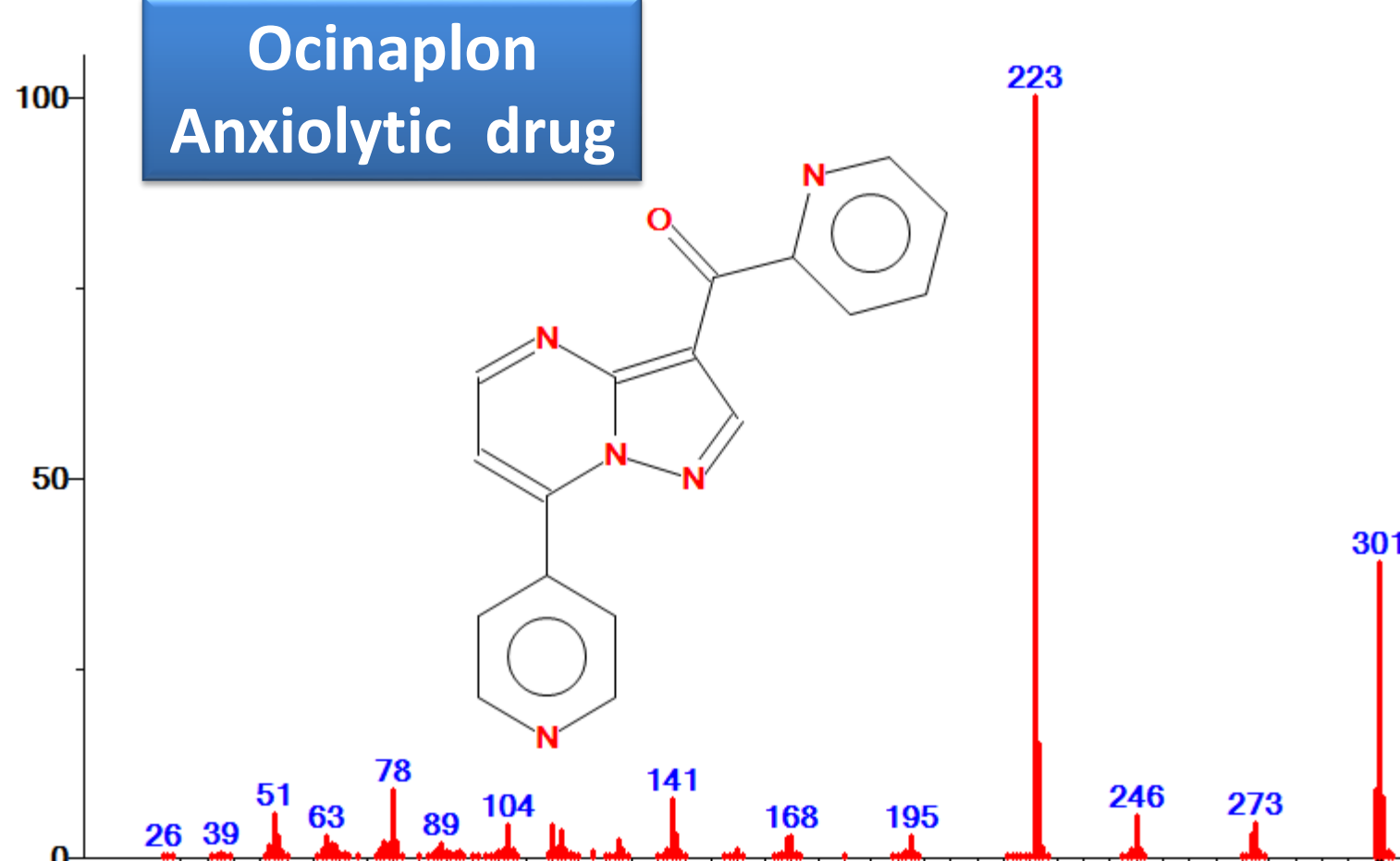
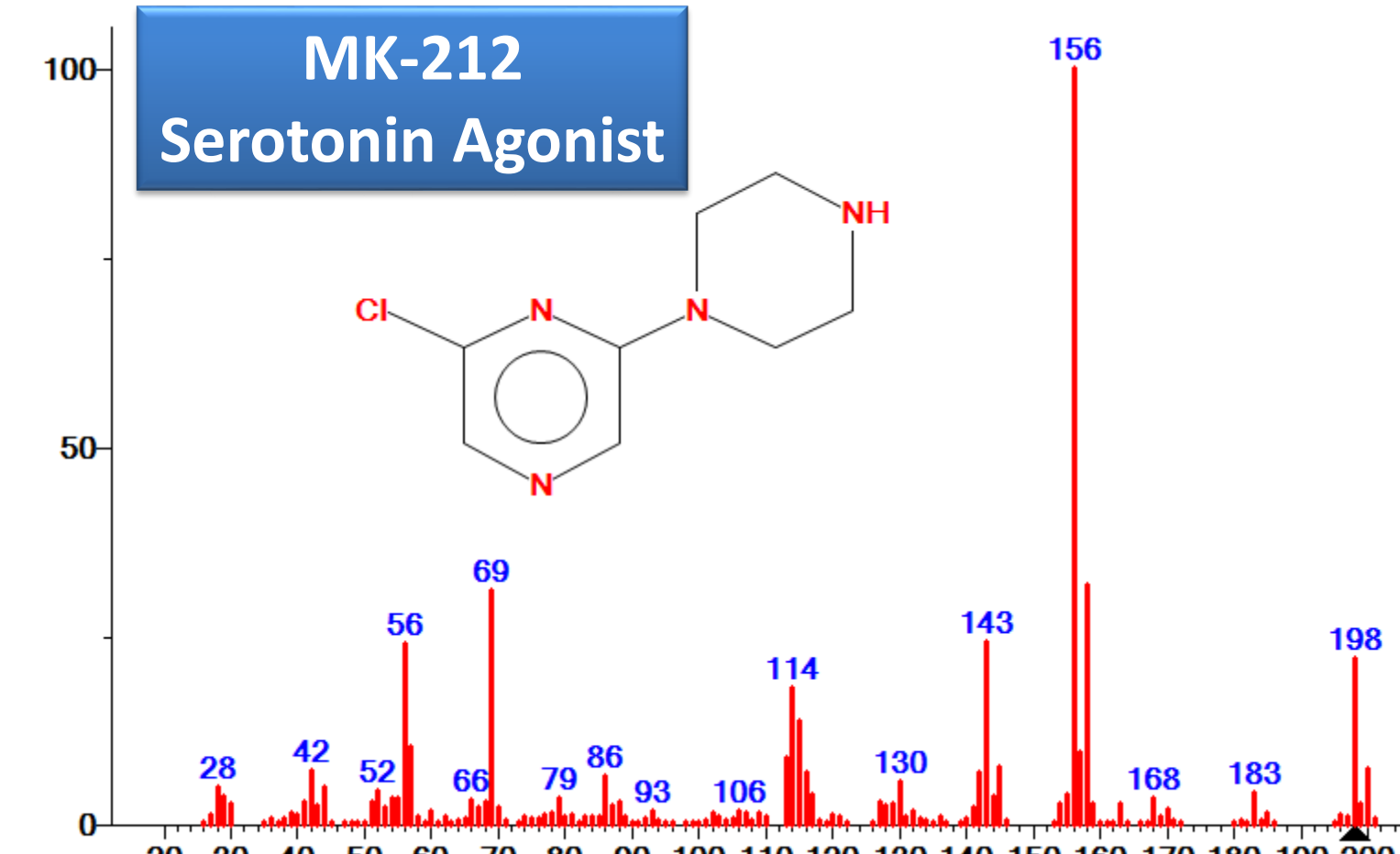
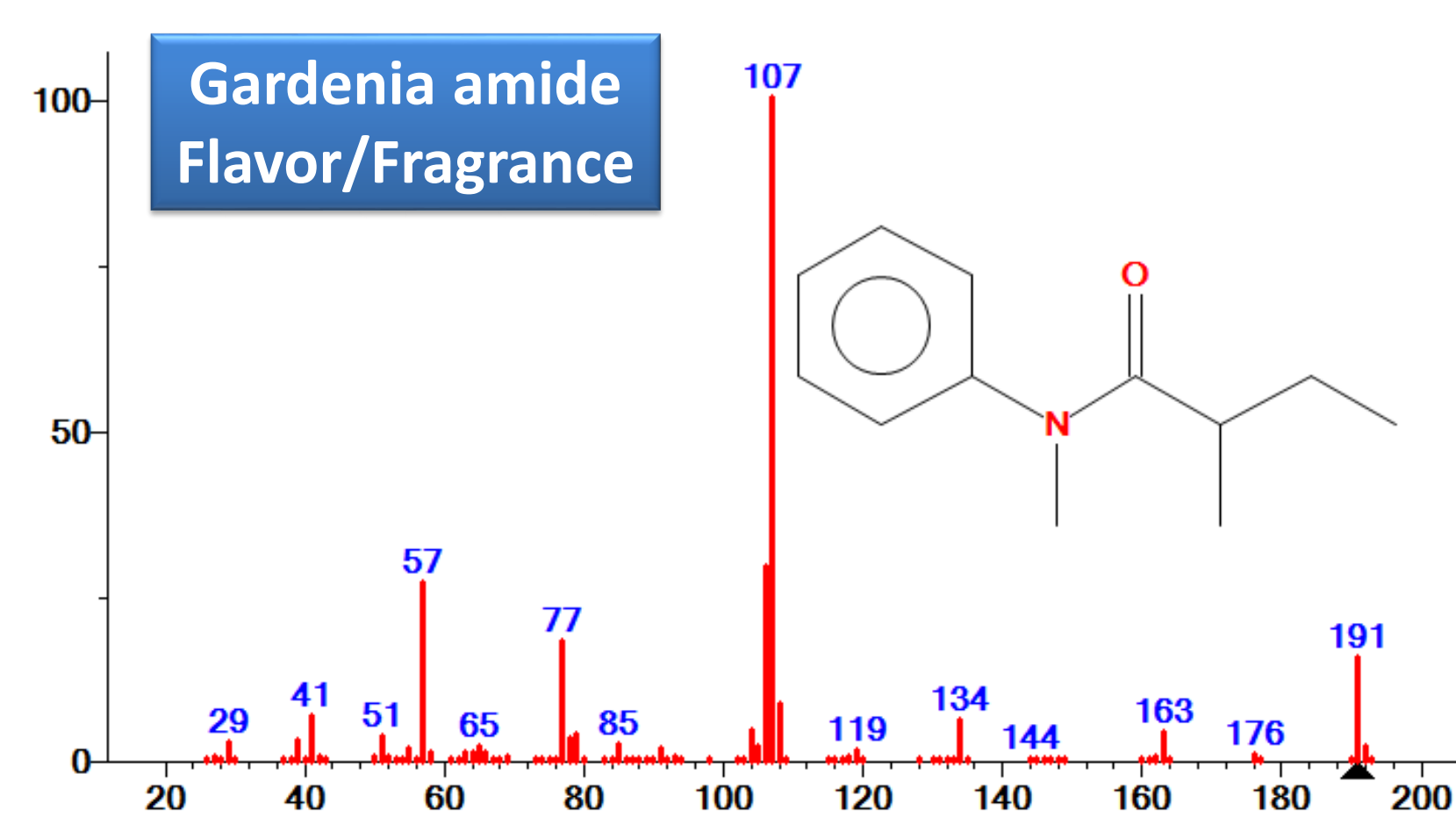
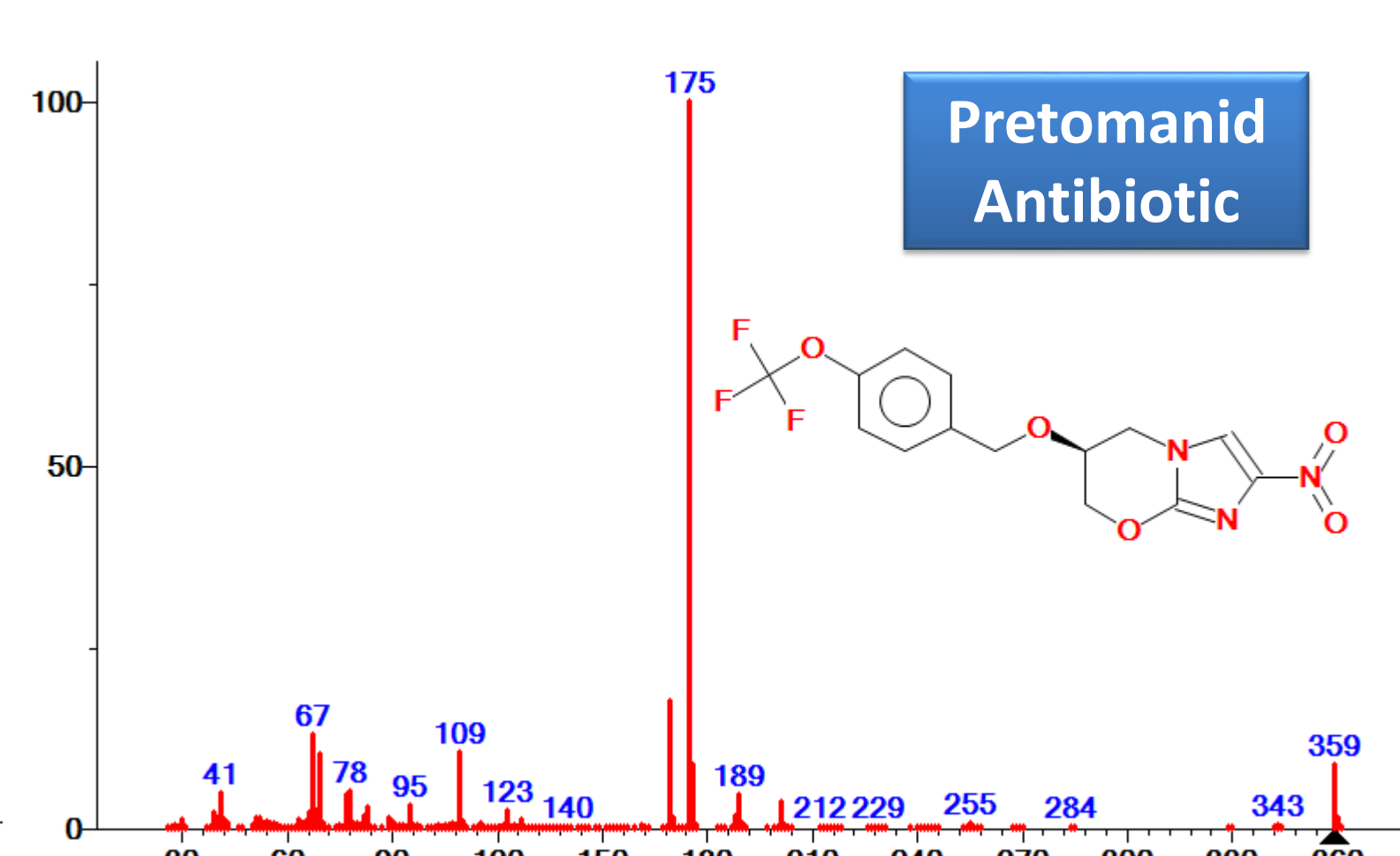
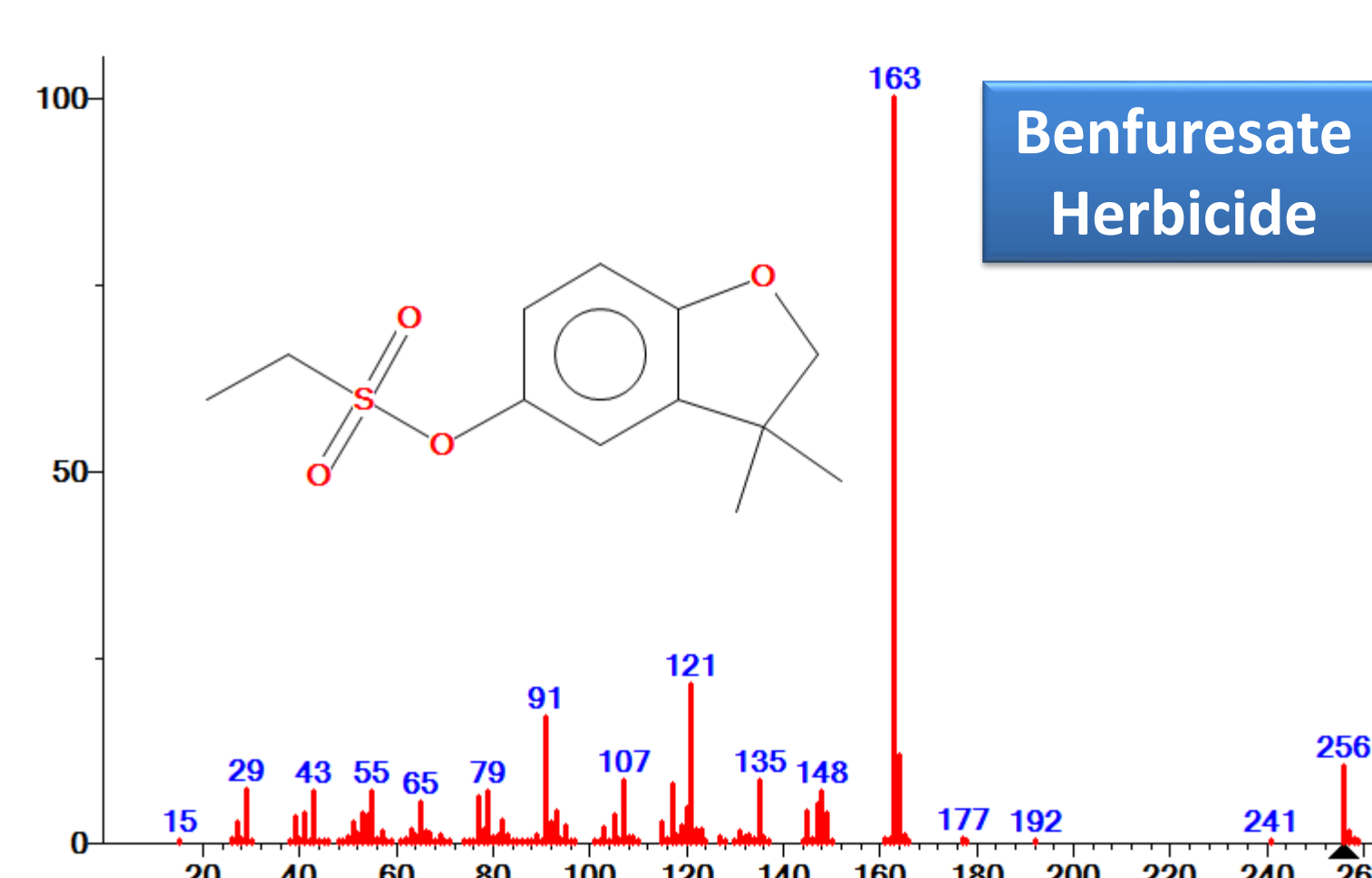
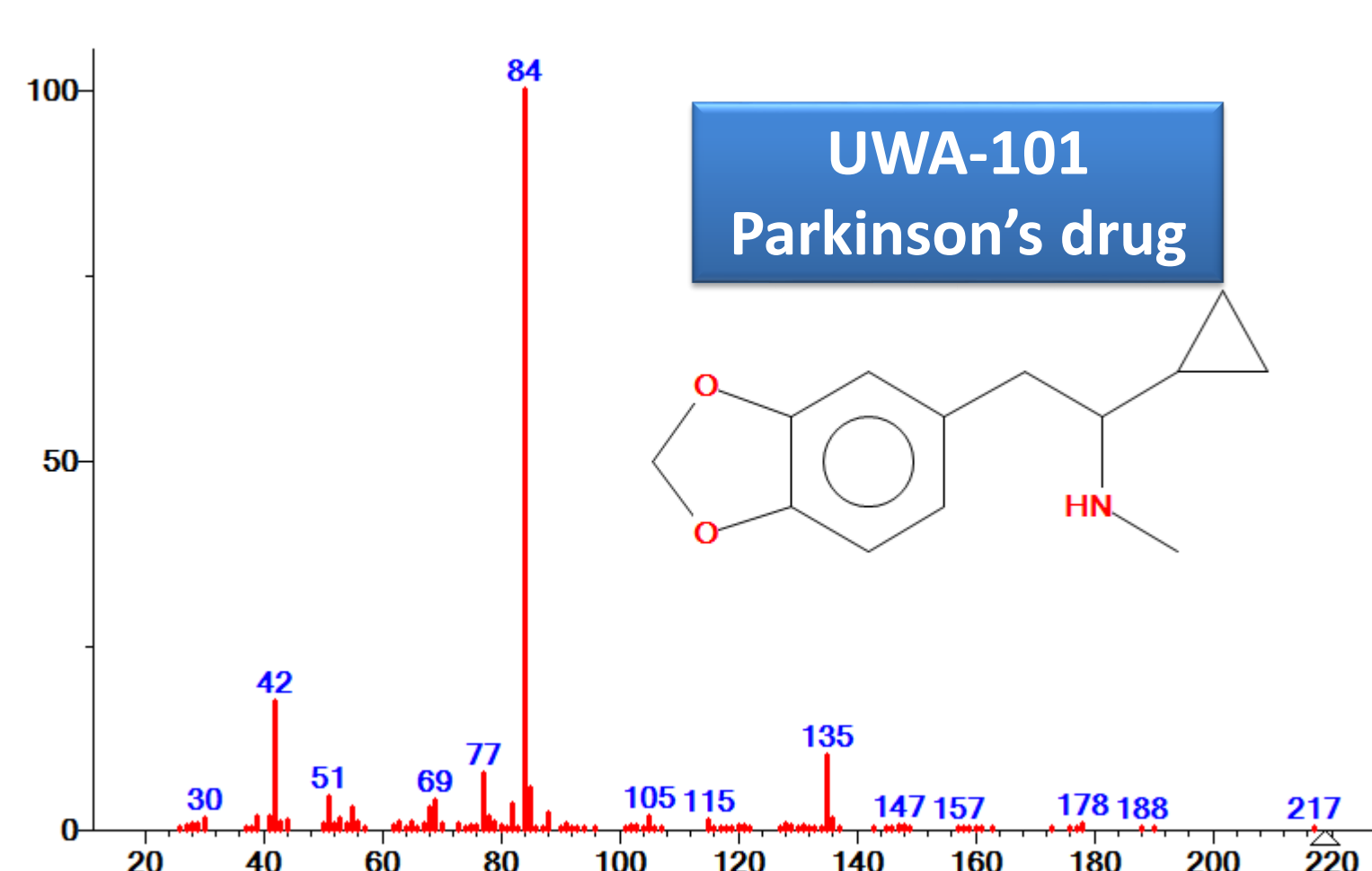
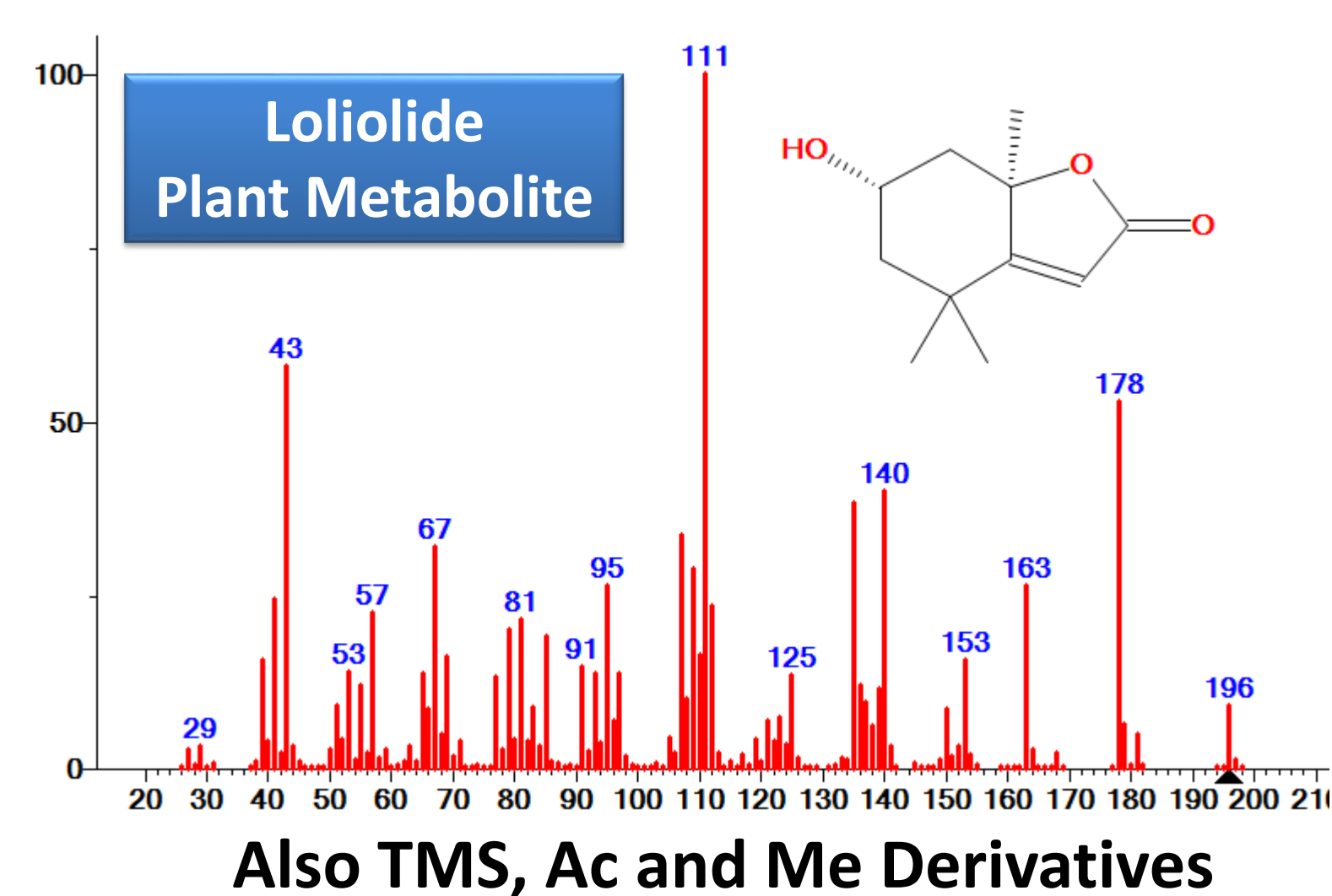
350,643 Electron Ionization (EI) Spectra

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

447,285 Retention Index (RI) Values

- 139,498 RI Compounds – 40 K increase
- 111,788 Compounds with both RI & MS

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

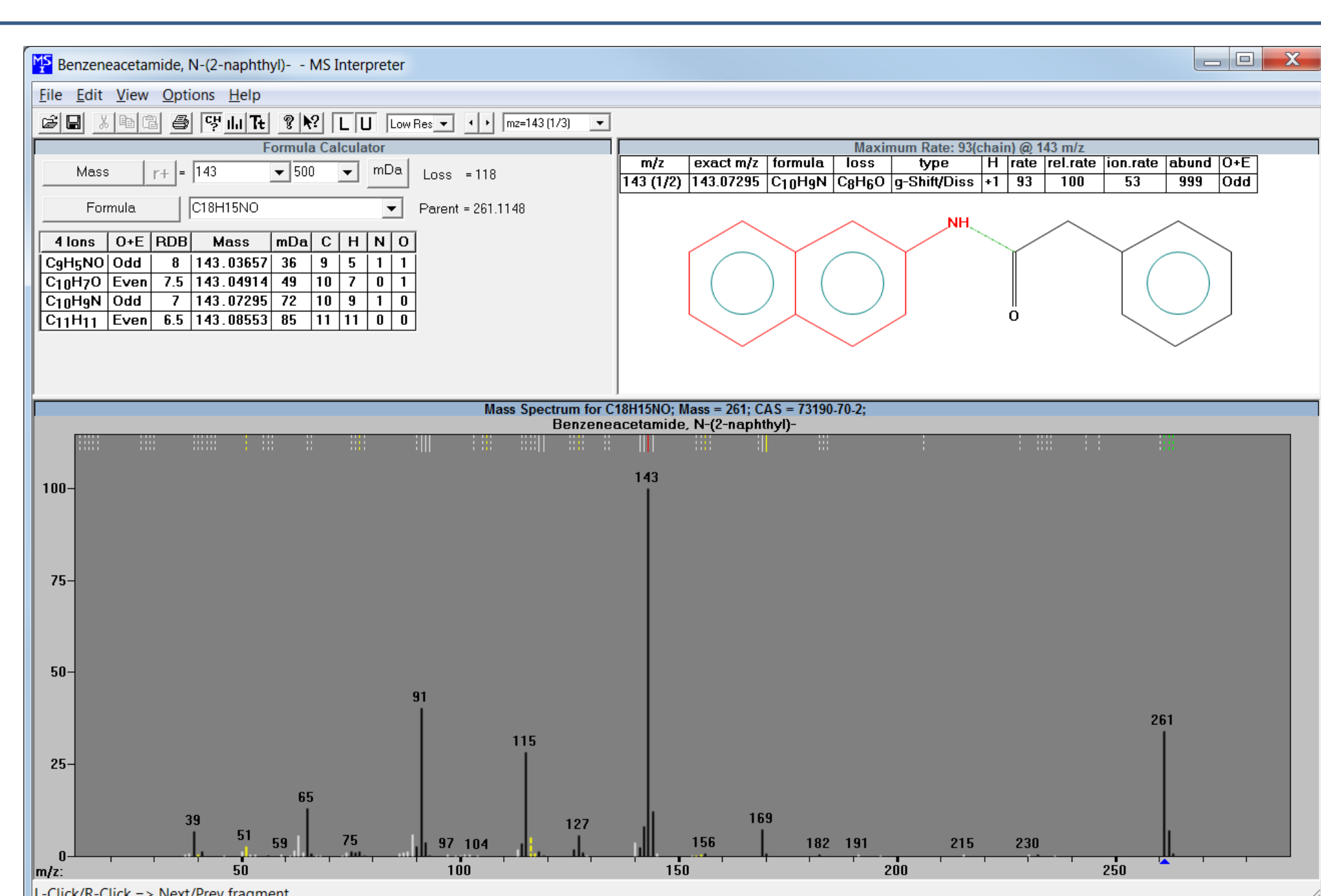
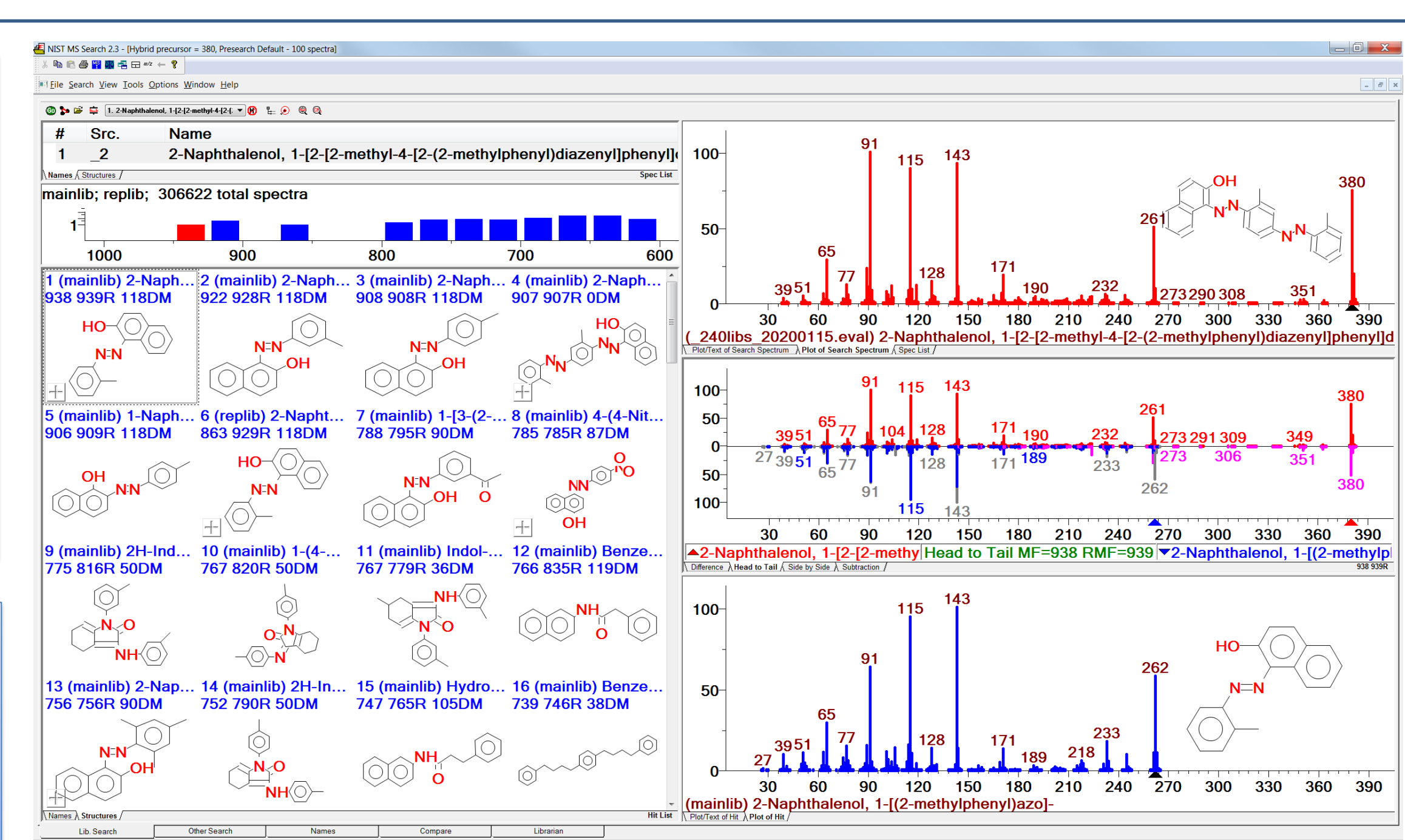


1,000s of New Compounds of Analytical Interest

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**

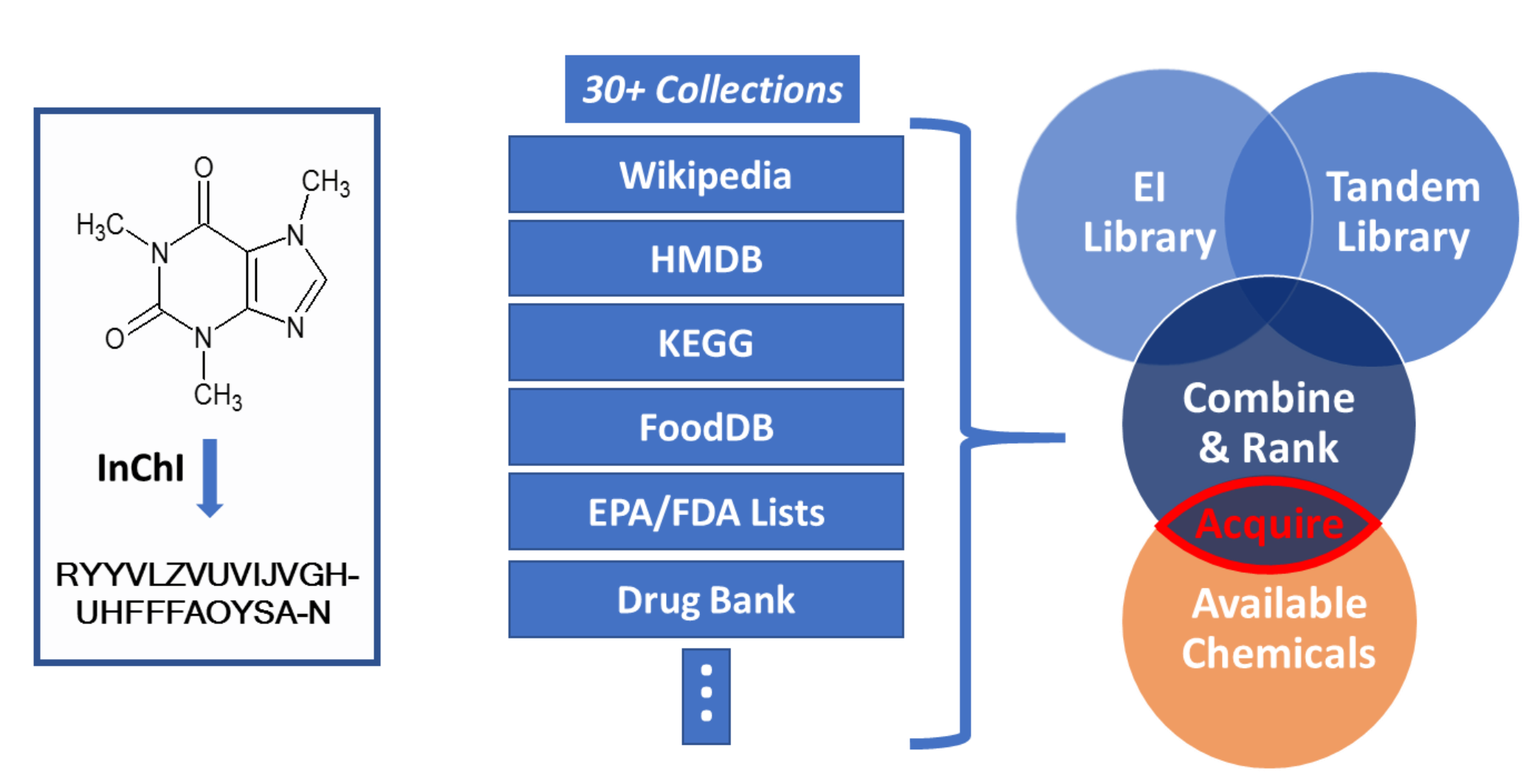


**MS
INTERPRETER**

**CONNECT PEAKS
TO STRUCTURES**

MAJOR UPDATE

New Compound Selection Process

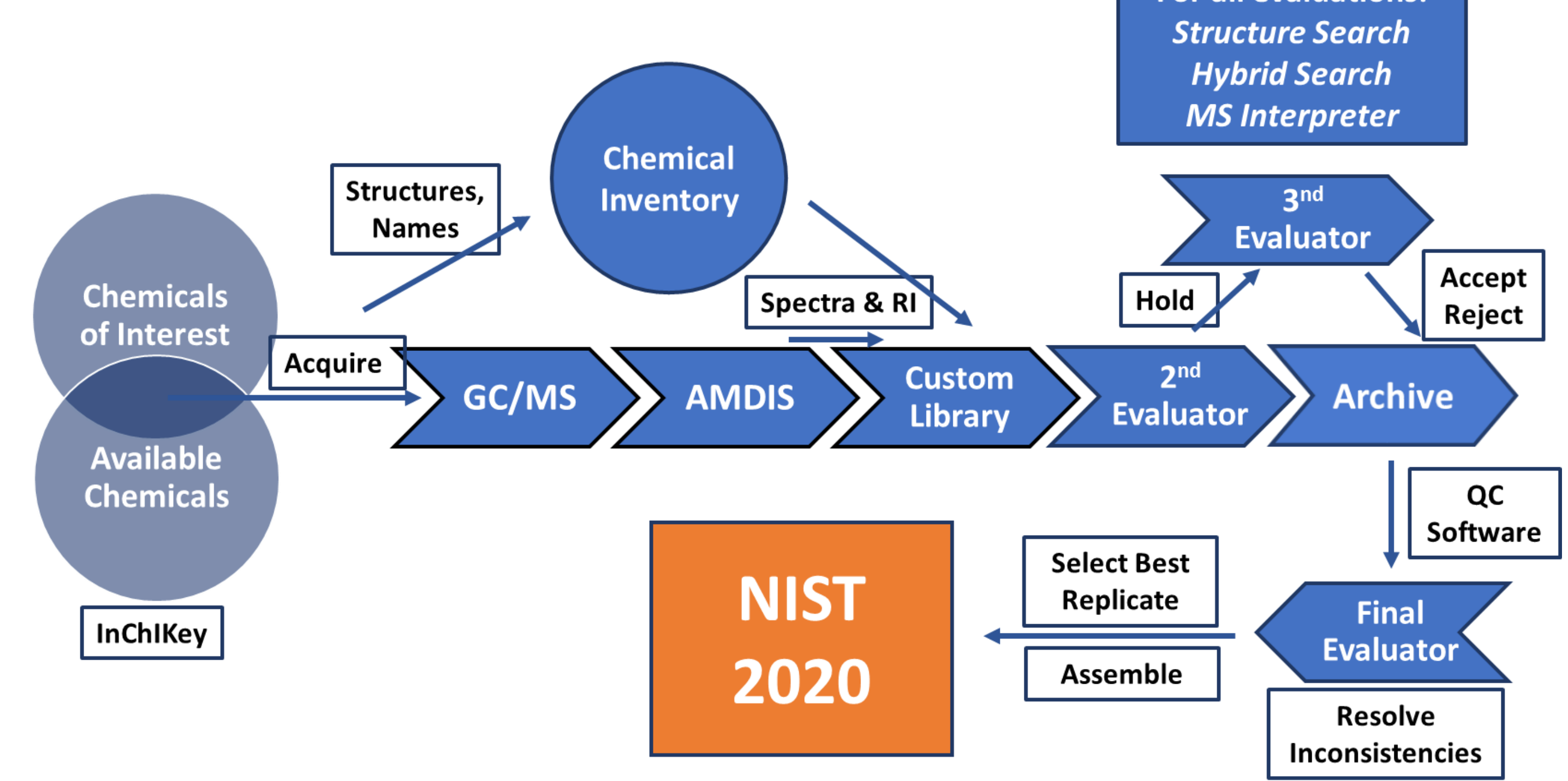


**NEW LIBRARY
BUILDING METHOD**

**SELECT COMPOUNDS,
MEASURE SPECTRA
ORGANIZE BY STRUCTURE
MULTIPLE EVALUATIONS**

**MS INTERPRETER
HYBRID SEARCH**

New Evaluation Process



<http://chemdata.nist.gov>