

NIST/EPA/NIH EI-MS LIBRARY

2020 Release

THE LARGEST INCREASE IN COVERAGE *EVER*

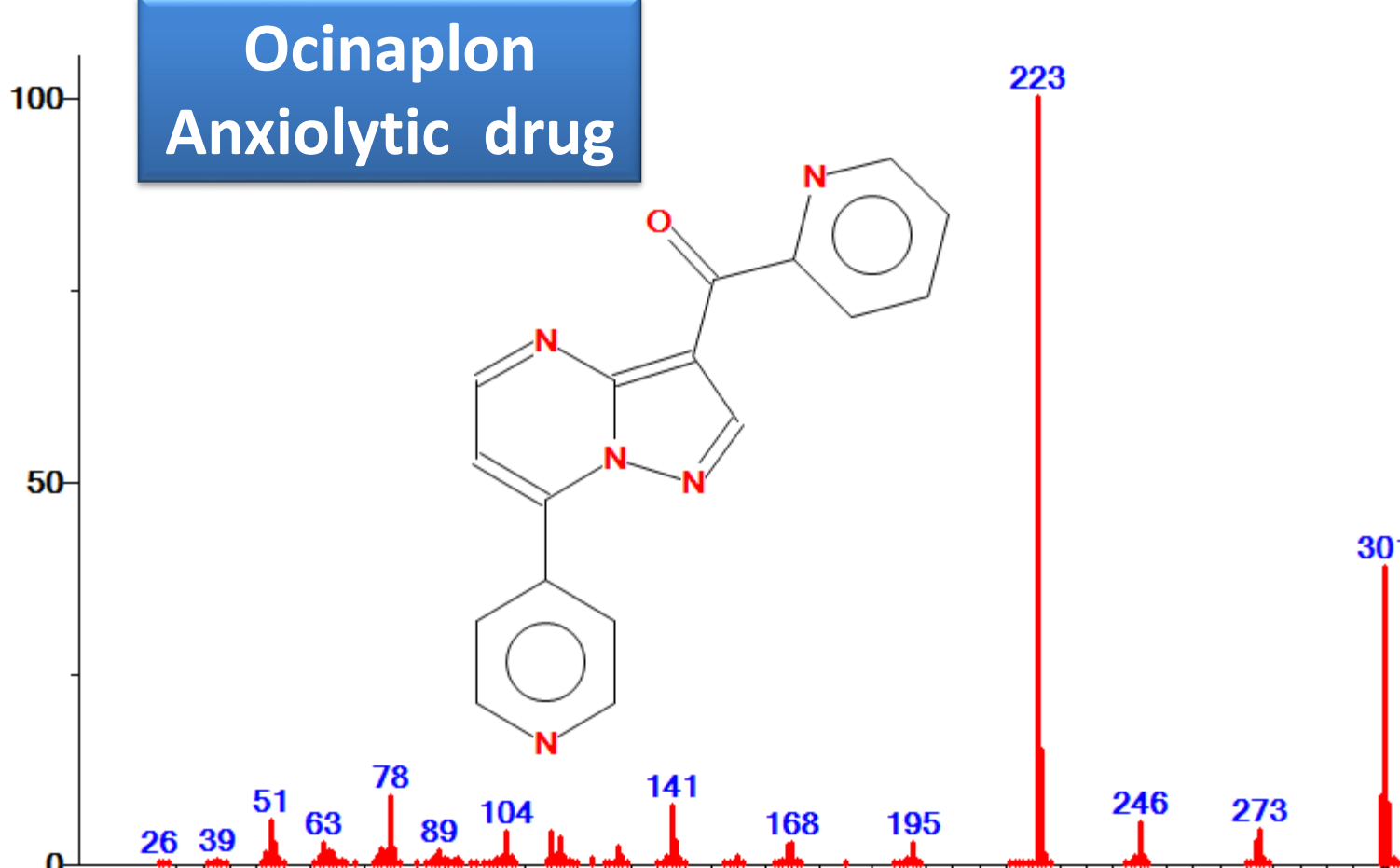
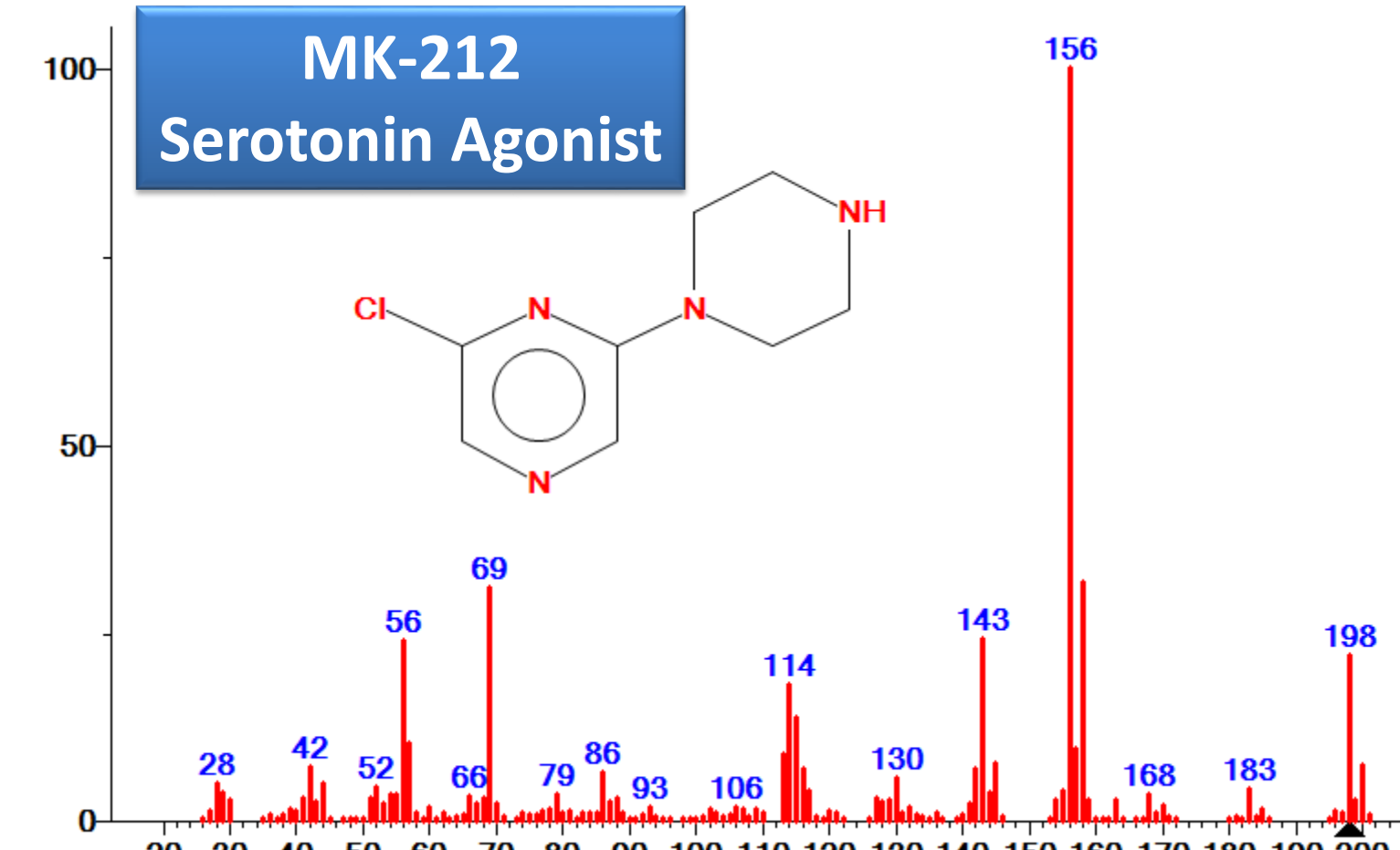
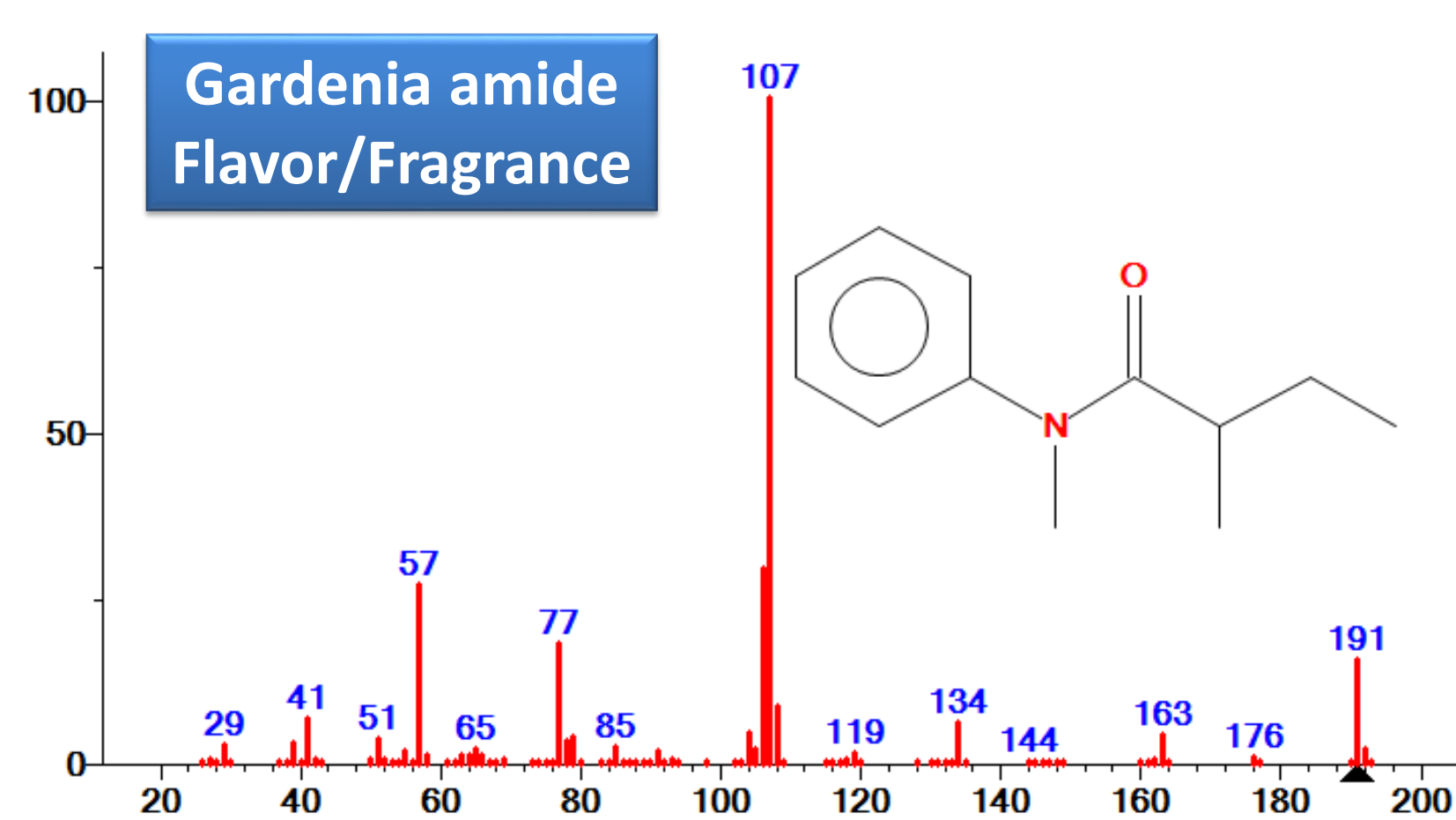
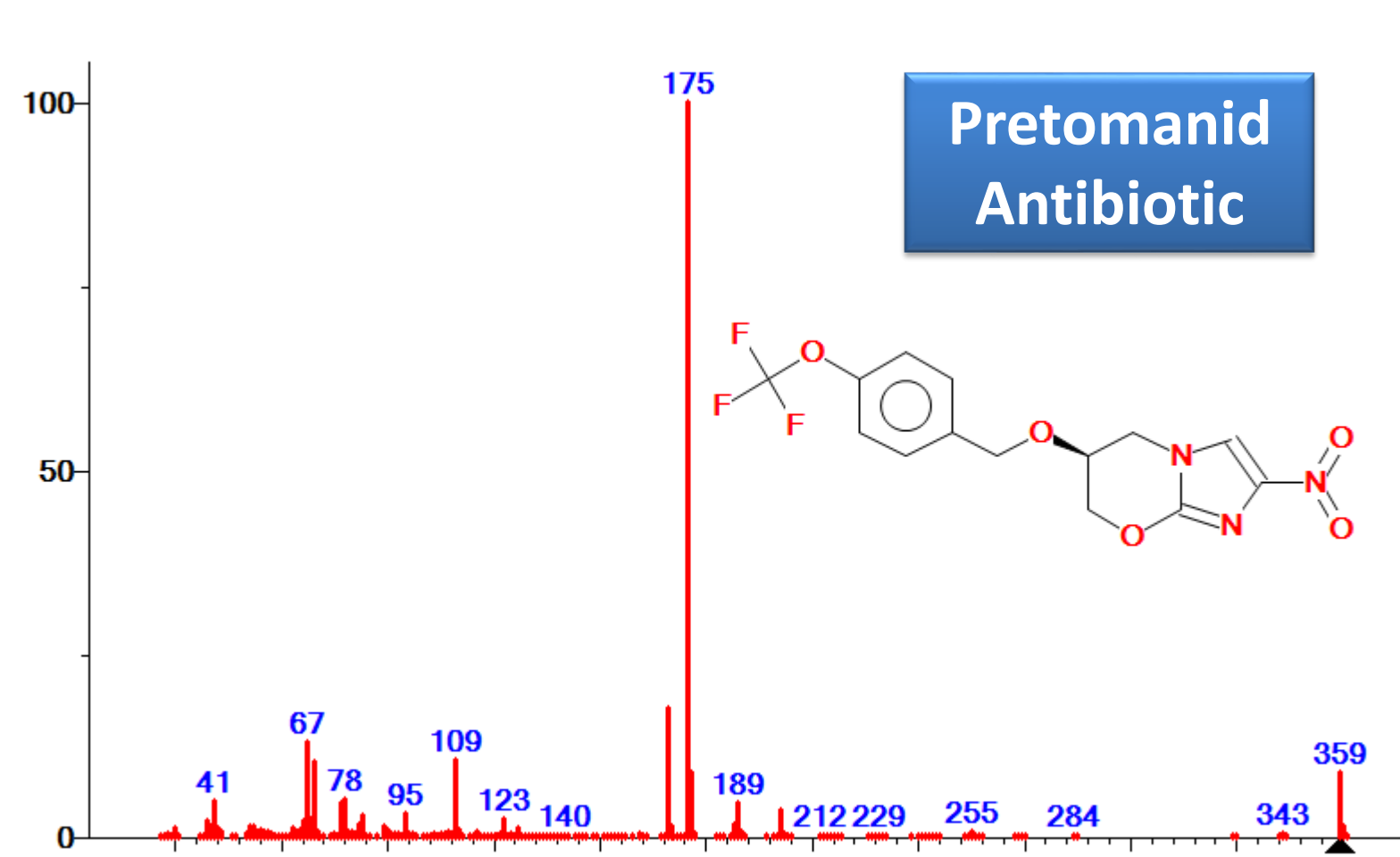
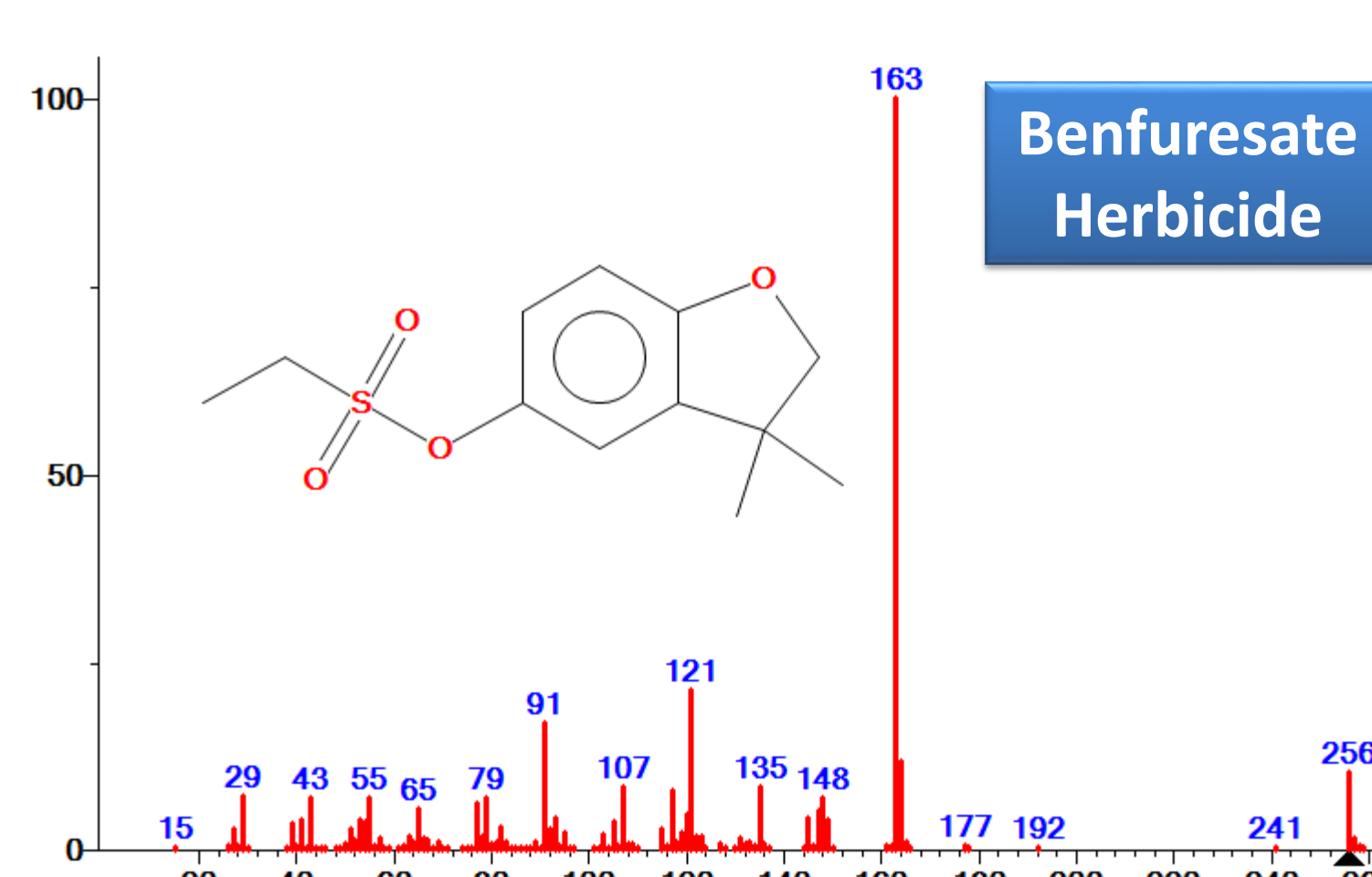
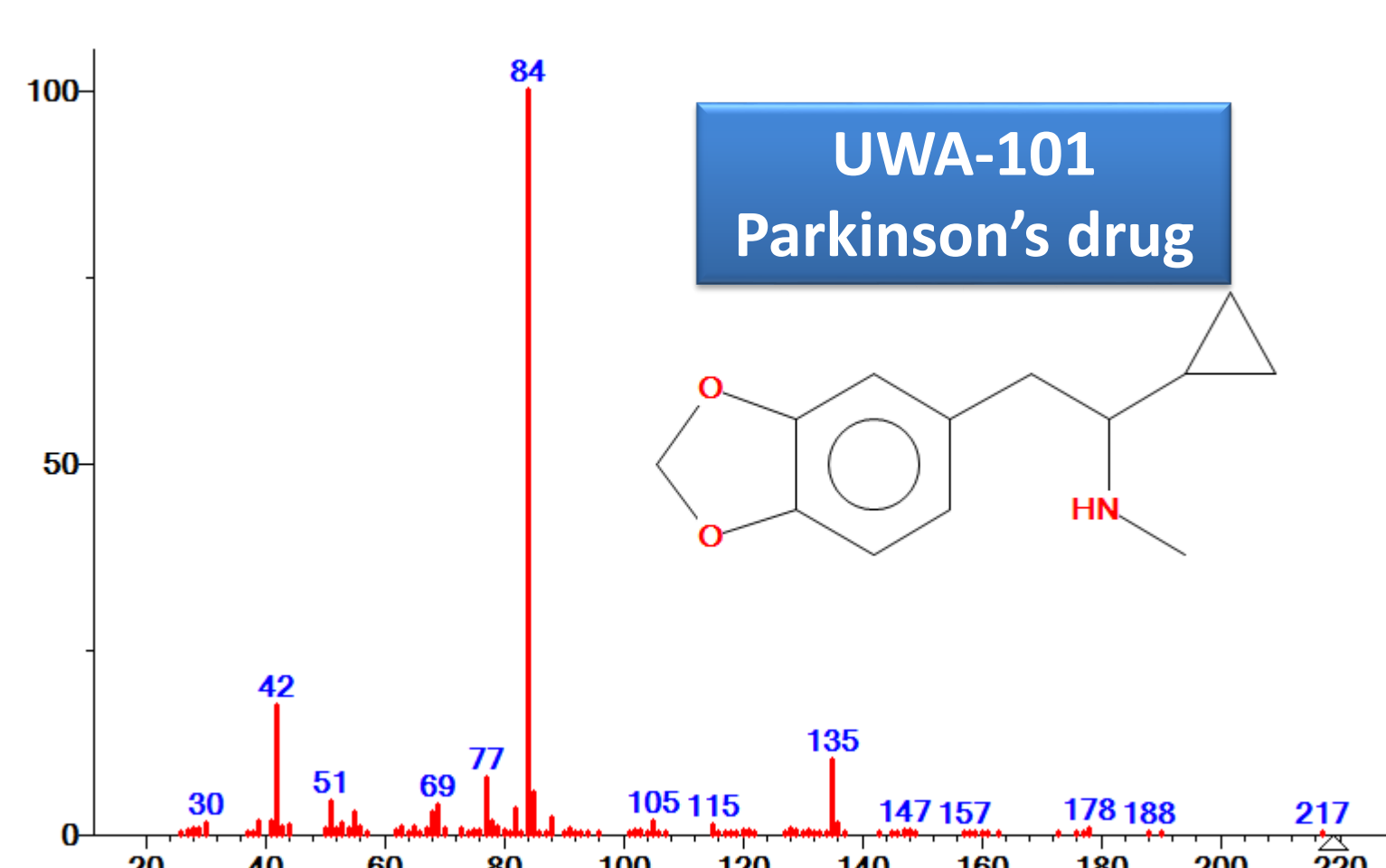
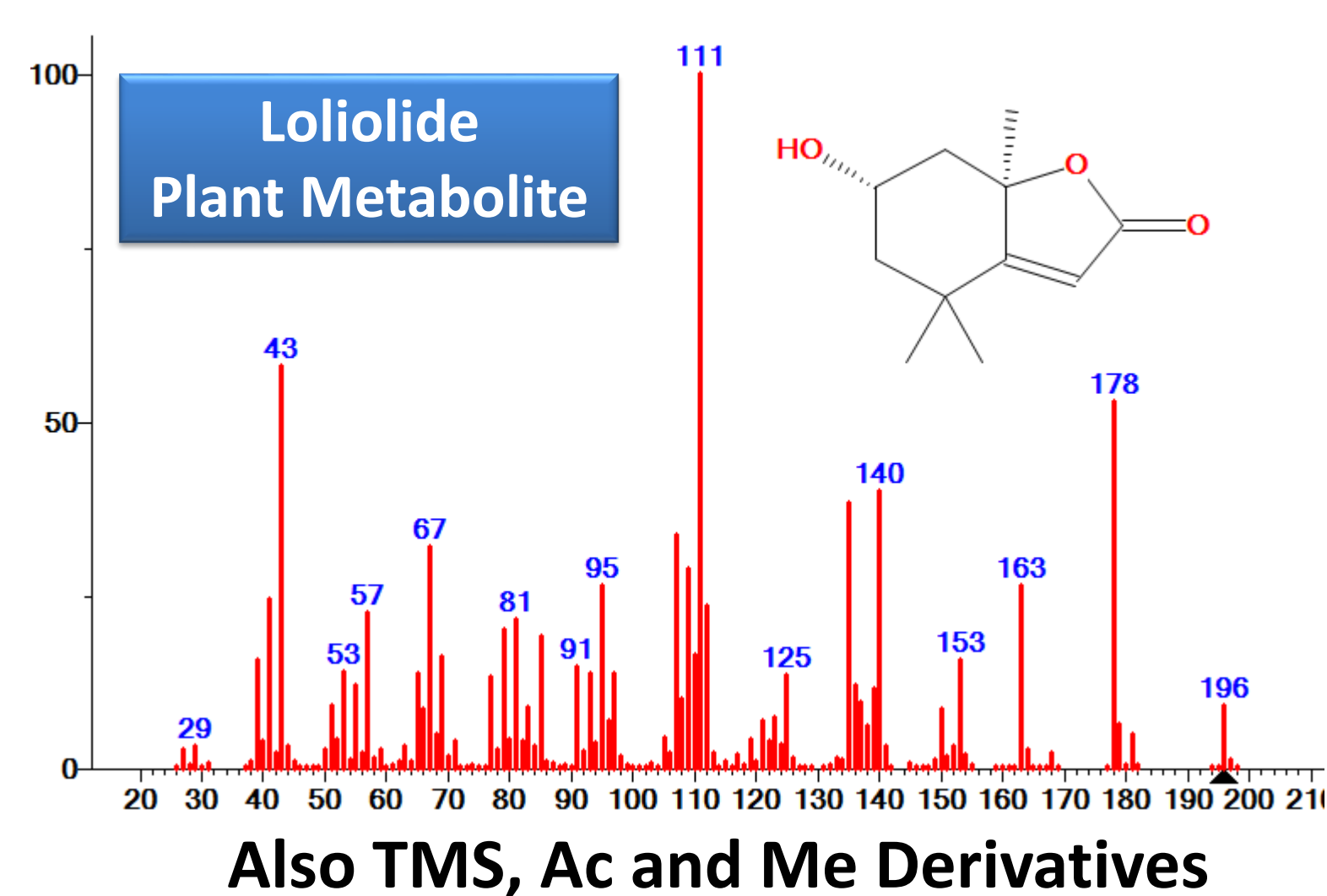
350,643 Electron Ionization (EI) Spectra

- 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



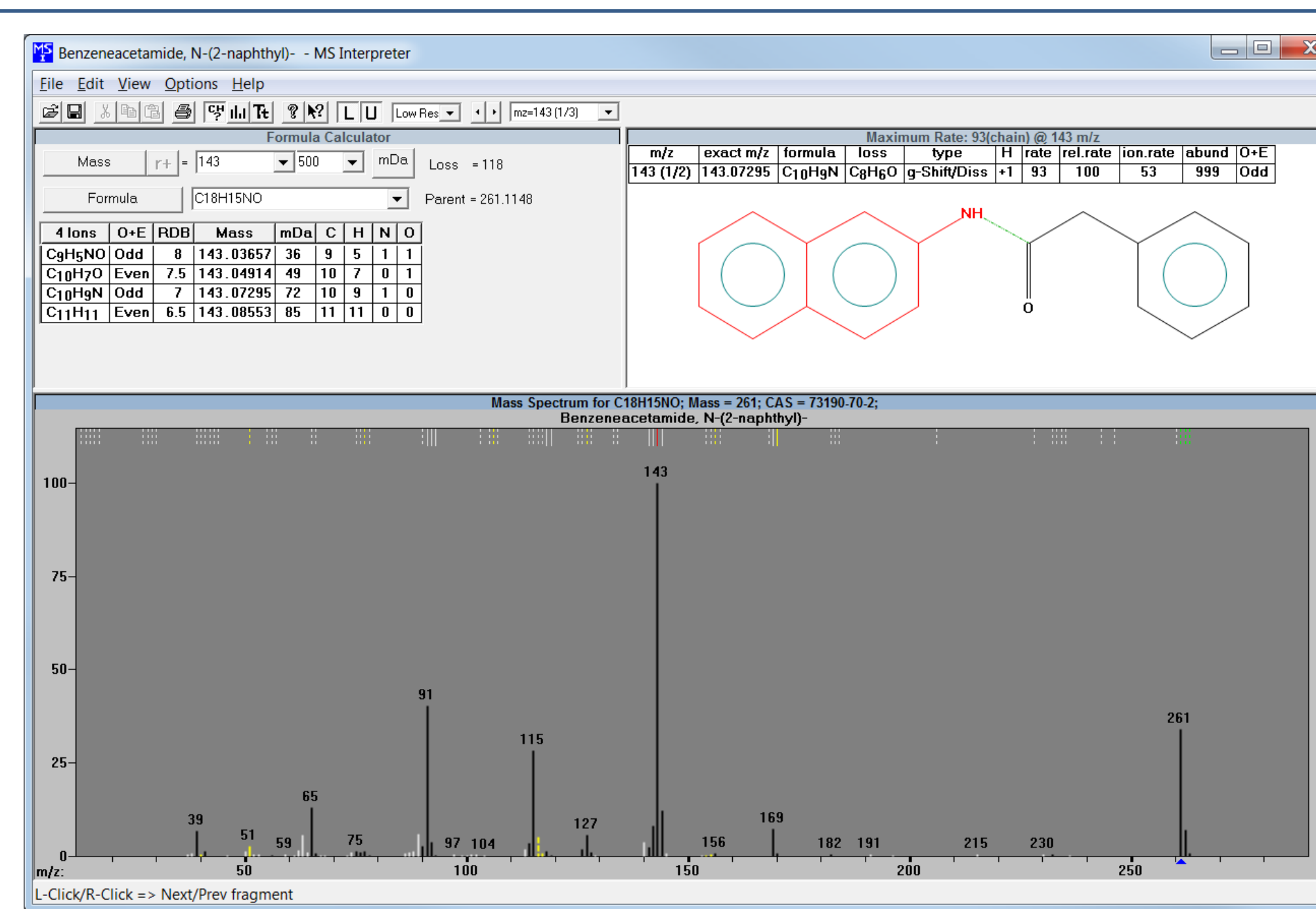
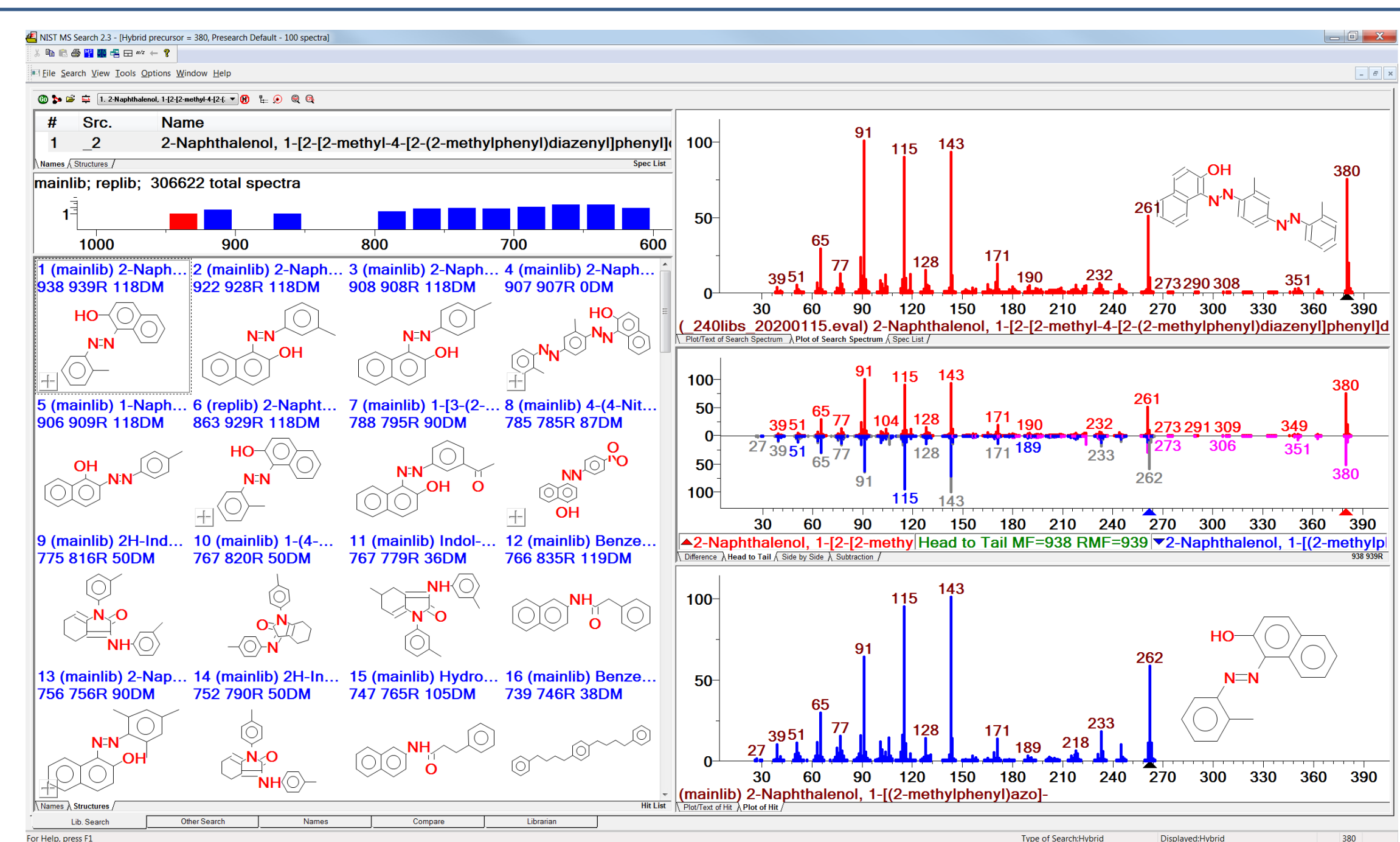
1,000s of New Compounds of Analytical Interest

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

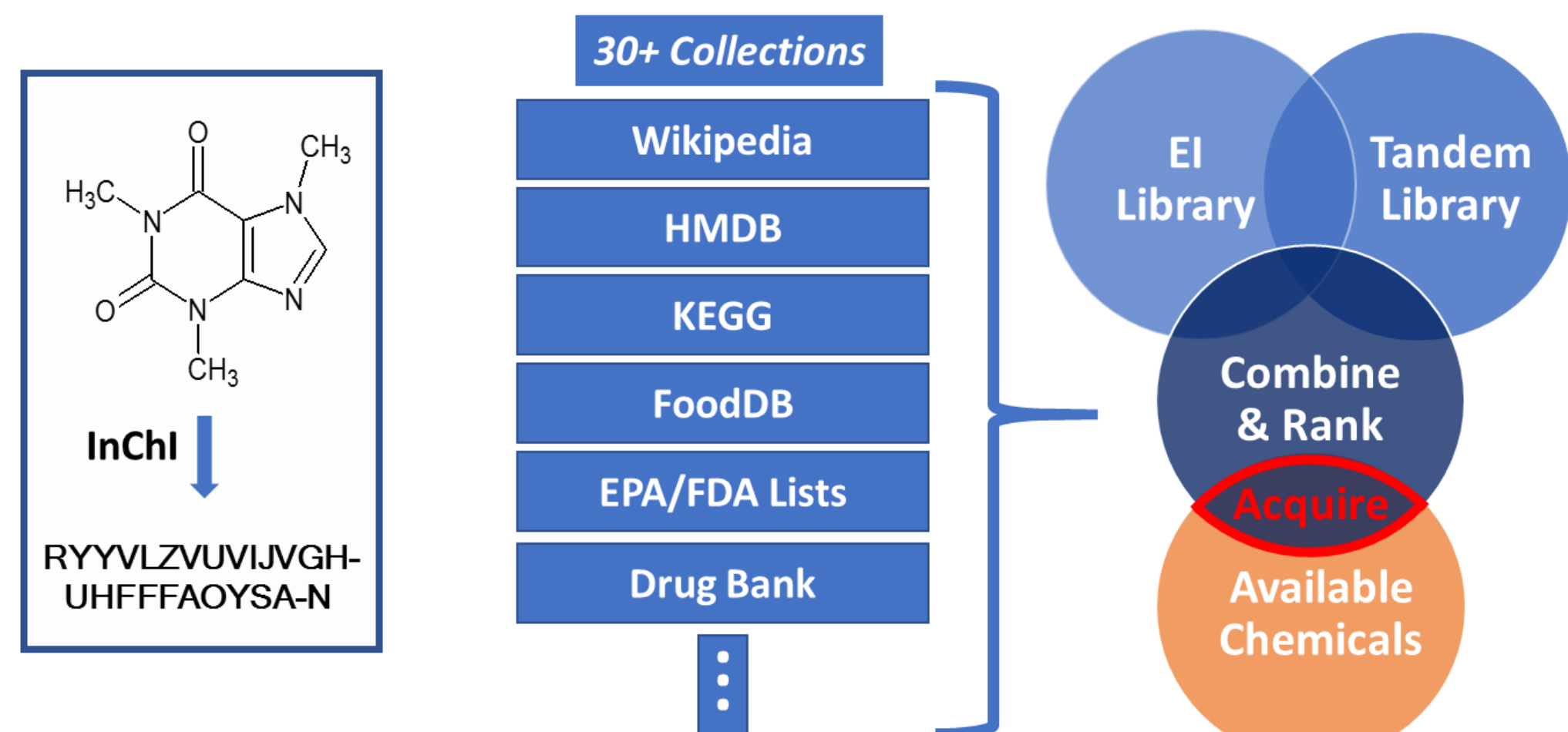


MS INTERPRETER

CONNECT PEAKS
TO STRUCTURES

MAJOR UPDATE

New Compound Selection Process

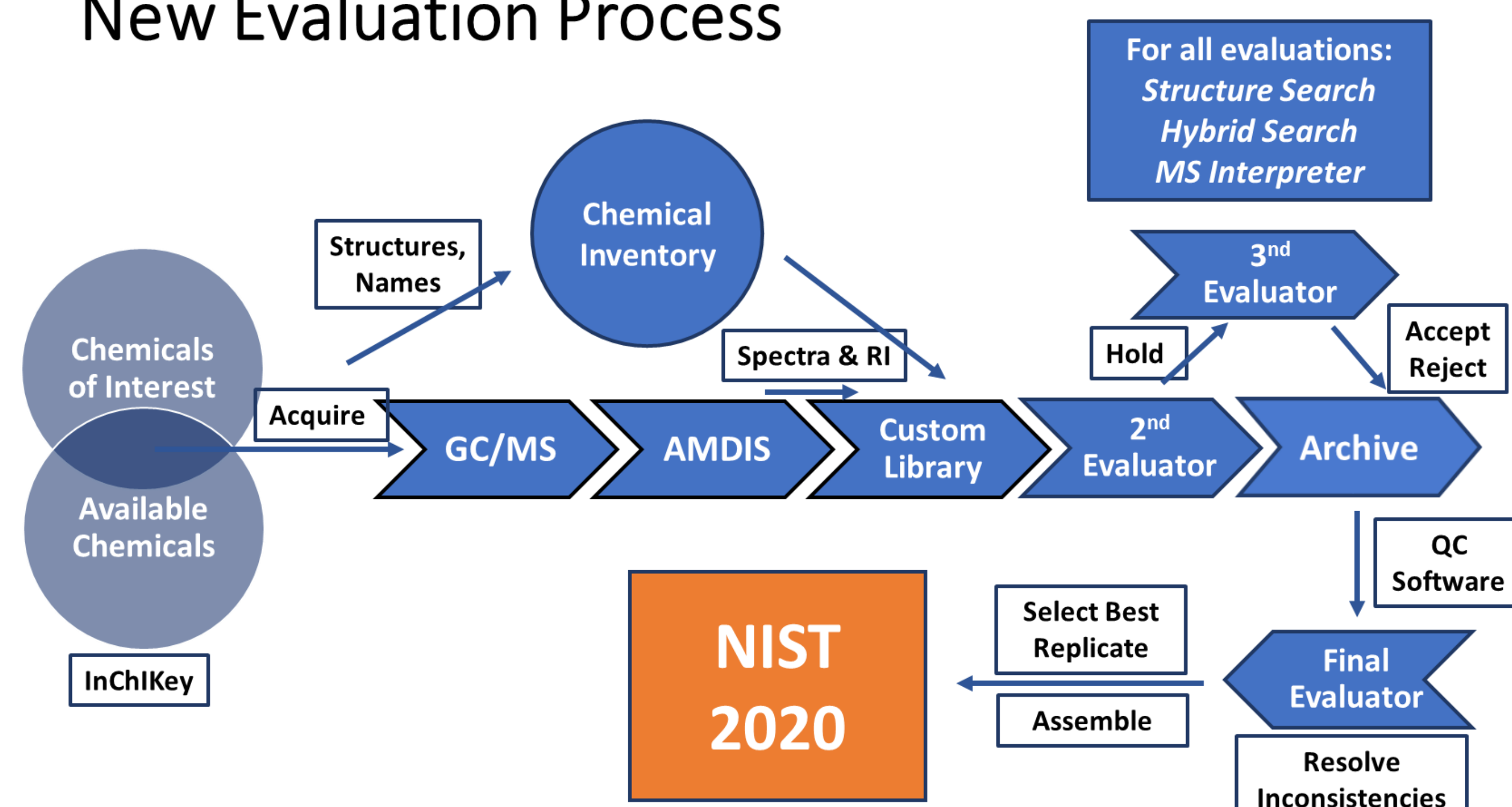


NEW LIBRARY
BUILDING METHOD

SELECT COMPOUNDS,
MEASURE SPECTRA
ORGANIZE BY STRUCTURE
MULTIPLE EVALUATIONS

MS INTERPRETER
HYBRID SEARCH

New Evaluation Process



<http://chemdata.nist.gov>

NIST Tandem Mass Spectral Library

2020 Release

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

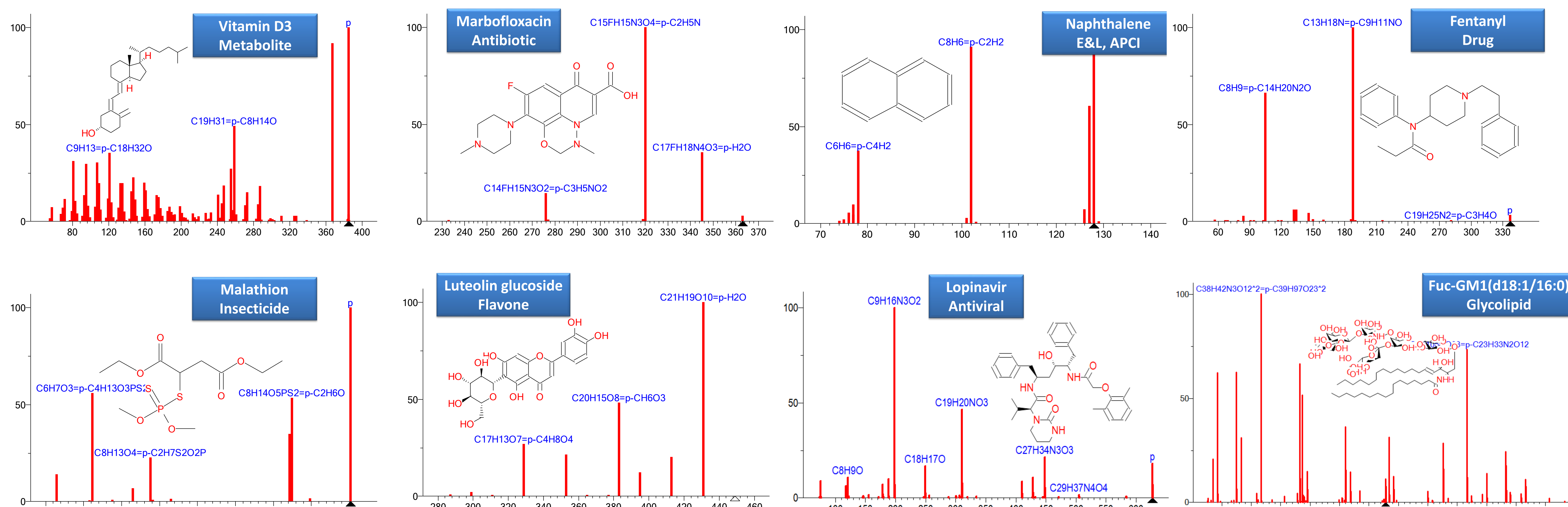
Fragmentation Methods

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'

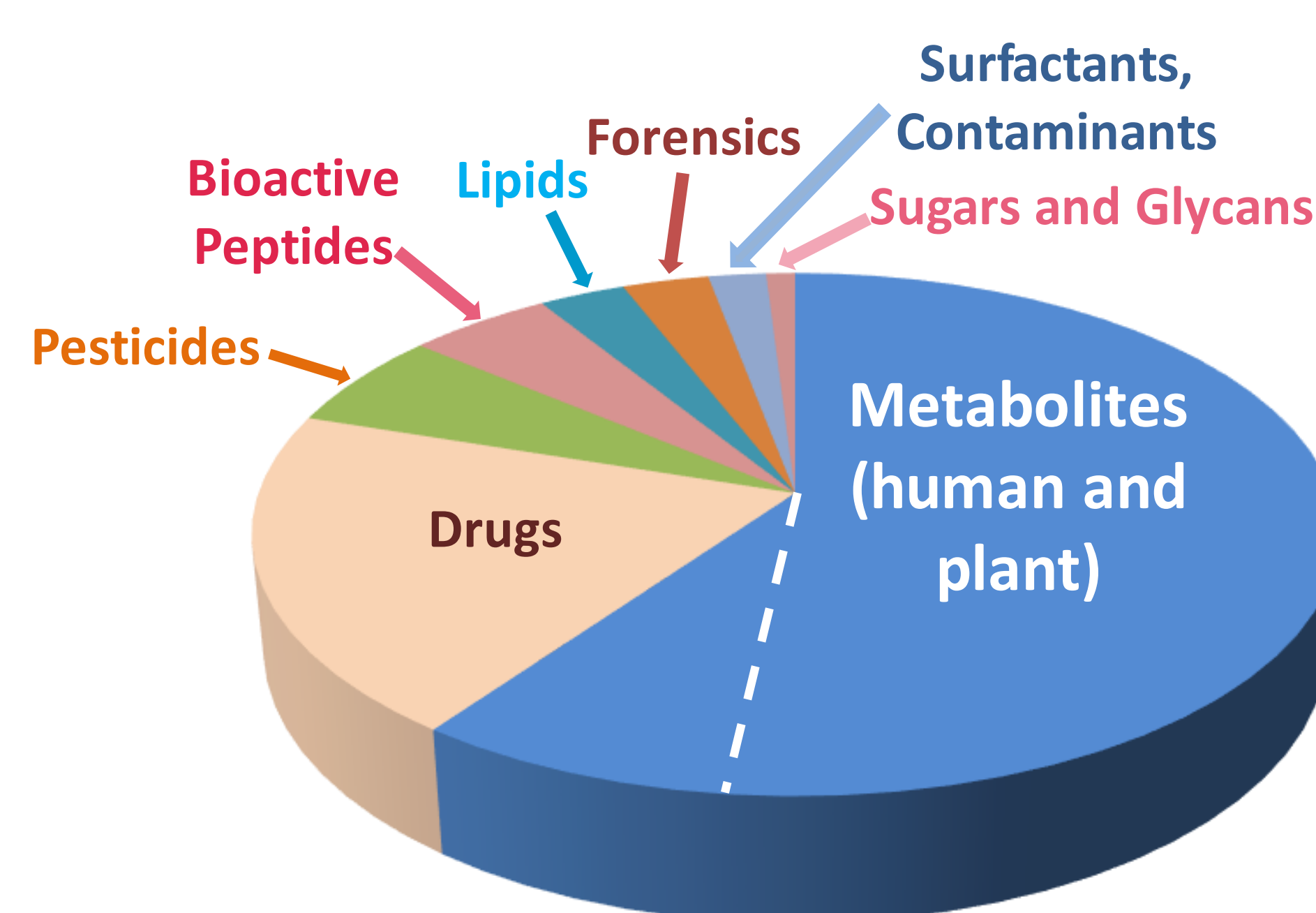
Precursor Ion Types

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

Wide Variety of Compounds



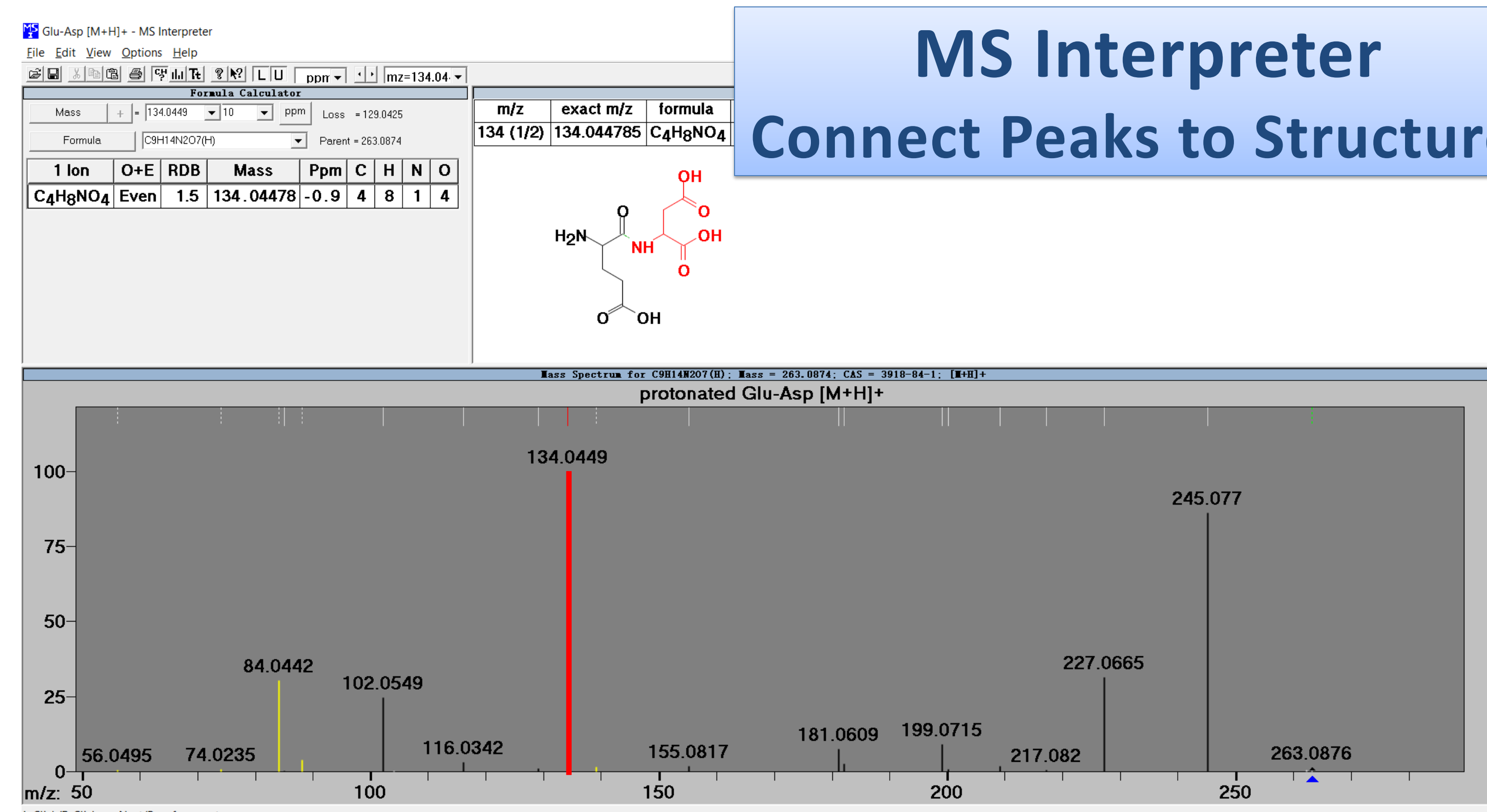
Types of Compounds and Spectra



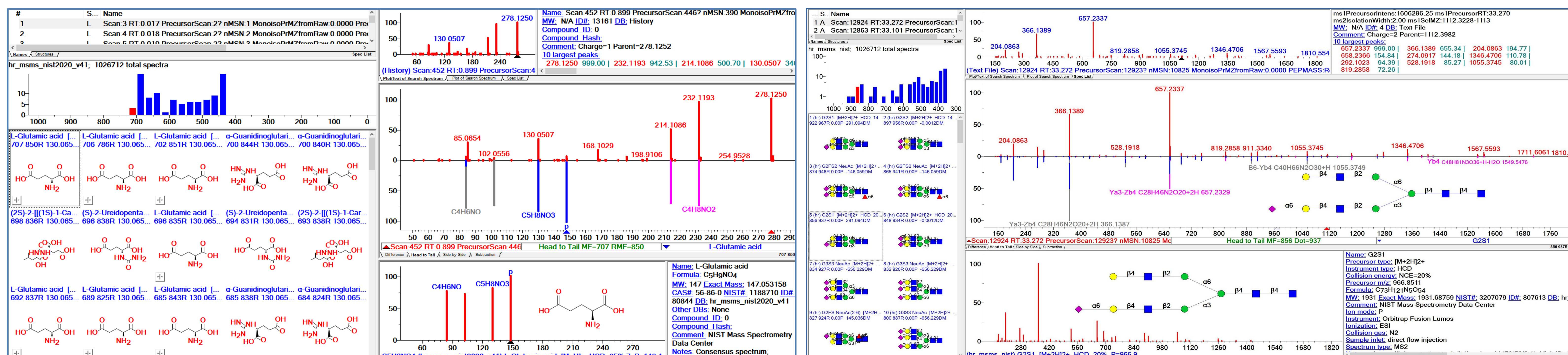
75%(+) 25%(-)
32% MS² in-source
8% MS³ and MS⁴
Over wide energy range

6,000 human
metabolites

MS Interpreter Connect Peaks to Structures



Hybrid Search - Identify Compounds Not in the Library



<http://chemdata.nist.gov>