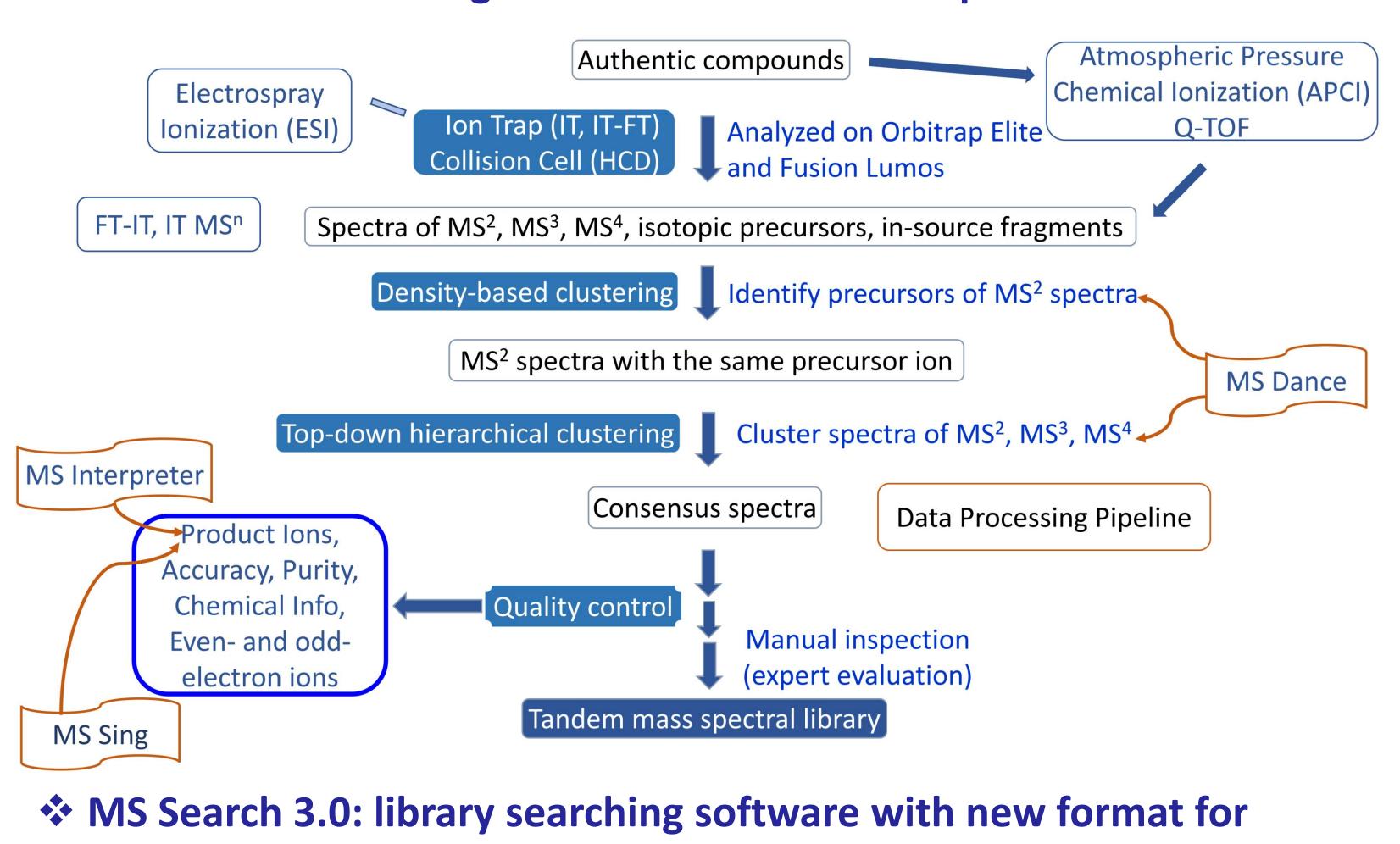


Extending a Tandem Mass Spectral Library with High-Quality Reference Spectra of 11,000 Plant Metabolites

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- ❖ Overview: The NIST23 Tandem Mass Spectral Library contains 2.4 million high- and low- resolution mass spectra of 51,505 compounds including over 11,000 plant metabolites and natural products with newly improved quality control and manual inspection procedures. This library will greatly aid accurate identification of metabolites in plants, food, agriculture, and herbal medicine as well as environmental analysis.
- **Procedure of Building the NIST Tandem Mass Spectral Libraries**



🏅 🖦 👛 🏉 🕎 🌉 📲 🖽 m/z 👉 🦞 Clear a-z hr/lr NIST tandem Flavoglaucin C6H5=p-C9H6O2 77.0383 Flavone, 6-β-D-glucopyranosyl-4',5,7-trihydroxy C7H5O2=p-C8H6 121.0282 lavone, 5.7-dihydroxy-4',6-dimethoxy Flavone, 2',5-dihvdroxy-7-methoxy Flavone, 5.7-dihydroxy-4'-methoxy lavone, 5.7-dihydroxy-6-methoxy Flavone, 5,7-dihydroxy-8-methoxy-Flavone, 3',5-dihydroxy-3,4',6,7-tetramethoxy Flavone, 3',6-dihydroxy-3,4',5,7-tetramethoxy Flavone, 4',5-dihydroxy-3,3',7-trimethoxy C14H10=p-CHO2 178.0776 Flavone, 5.7-dihvdroxy-3',4',6-trimethoxy Flavone, 3,7-dimethoxy-3',4'-(methylenedioxy) Flavone, 8-I(dimethylamino)methyll-7-methoxy-3-methyl-Flavone, 5-hvdroxv-4',7-dimethoxv-Flavone, 5-hydroxy-7-methoxy-6-methyl-140 160 Flavone, 5-hydroxy-3,3',4',6,7-pentamethoxy-MW: 222 CAS# 525-82-6 NIST# 3170264 C15H10O2 (hr_msms_nist) Flavone [M+H]+ HCD 90% P=223.1 Flavone, 5-hydroxy-3,3',4',7-tetramethoxy-Flavone, 5-hydroxy-3,4',7-trimethoxy Precursor type: [M+H]+ Flavone, 4'-methoxy-6-acetyloxy-Instrument type: HCD Flavone, 3',4'-methylenedioxy-Collision energy: NCE=90% 40eV Flavone, 3,3',4',5,7-pentahydroxy-, 3-β-L-arabinofuranosid Flavone, 3,3',4',5,7-pentahydroxy-, 3,4'-di-β-D-glucopyranoside Flavone, 3,3',4',5,7-pentahydroxy-, 3-(6-O-α-L-arabinopyranosyl-β-D MW: 222 Exact Mass: 222.06808 CAS#: 525-82-6 NIST#: 3170264 DB: hr_msms_nist Comment: NIST Mass Spectrometry Data Center Flavone, 4',5,5",7,7"-pentahydroxy-4",6-oxydi-Flavone, 3,3',4',7-tetrahydroxy-Names / Structures / Instrument: Thermo Finnigan Elite Orbitrap [M+H]+ HCD 60% P=223.1 [M+H]+ HCD 75% P=223.1 Sample inlet: direct flow injection [M+H]+ HCD 110% P=223.1 Notes: micromol/L in water/acetonitrile/formic acid (50/50/0.1); Vial_ID=26486 Spec=Consensus Nreps=22/22 M [M+H]+ HCD 130% P=223.1

Plot/Text / Plot

[M+H]+ HCD 160% P=223.1 [M+H]+ IT 35% P=223.1 (LR)

| [M+H]+ | IT-FT 35% P=223.1

[M+H]+ QTOF 15V P=223.1

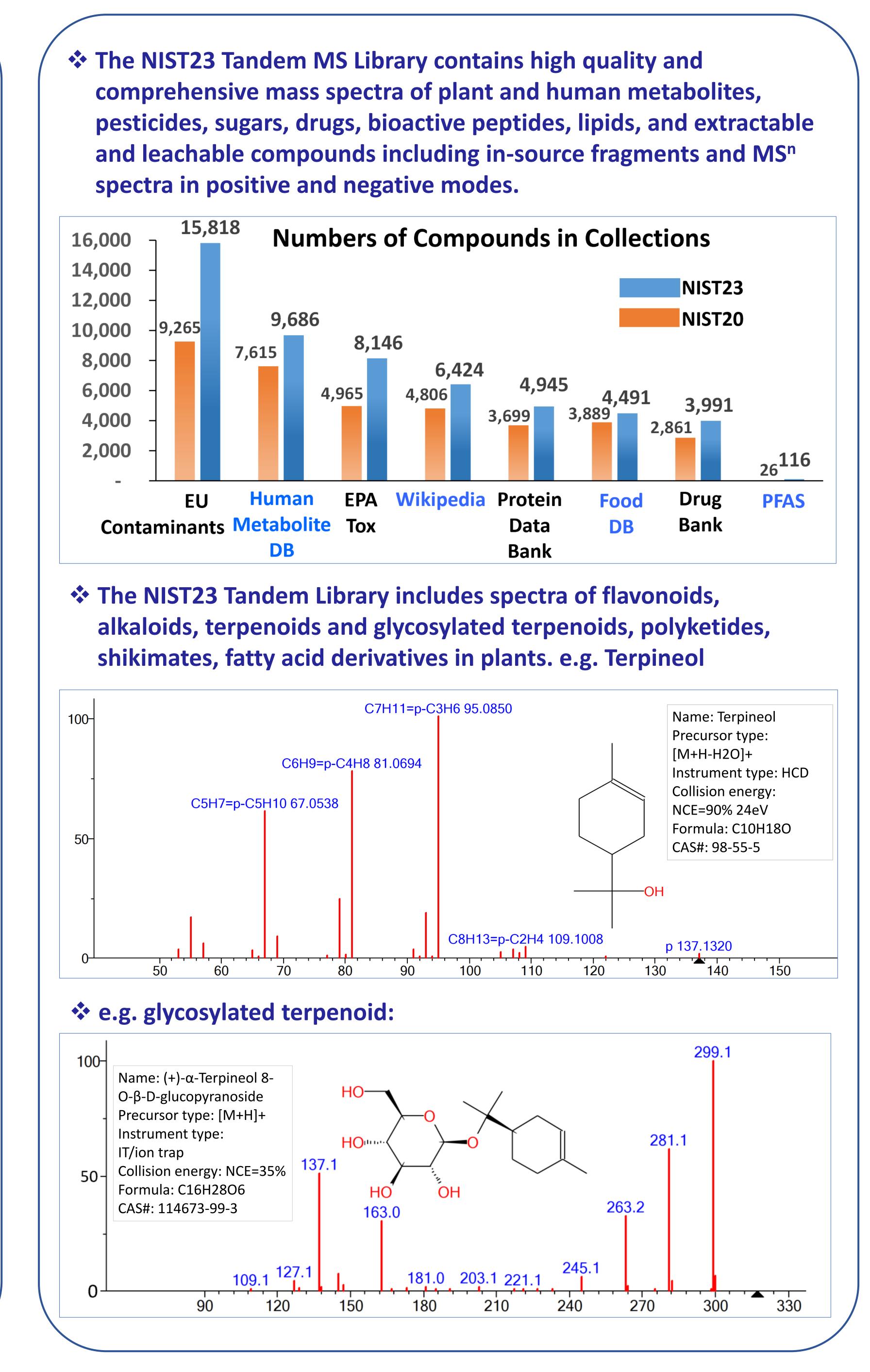
M+H1+ OTOF 17V P=223 1

For Help, press F1

InChikey: VHBFFQKBGNRLFZ-UHFFFAOYSA-N Non-stered

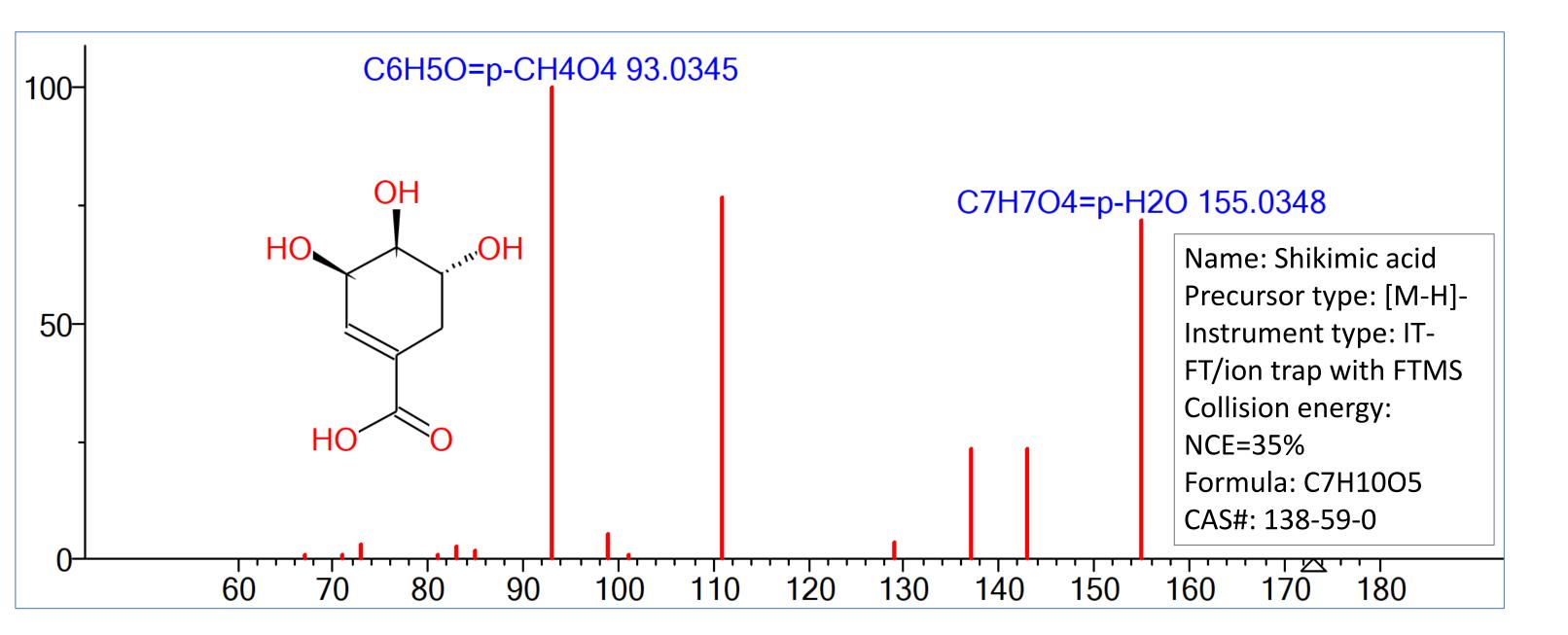
121.0282 893.2 | 103.0540 881.3 | 105.0445 849.0 | 129.0334 762.7 |

fast searching and easily viewing all the spectra in the library.

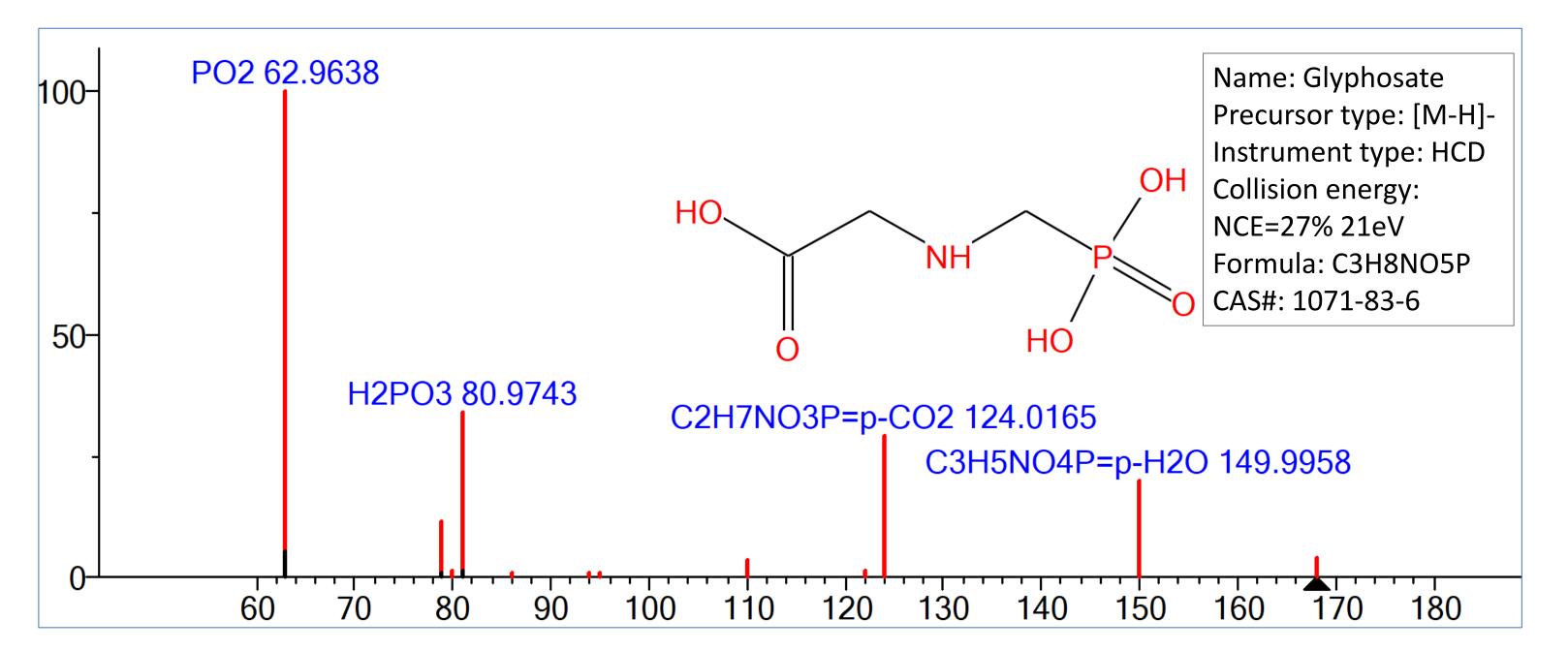


Shikimic acid and its derivatives:

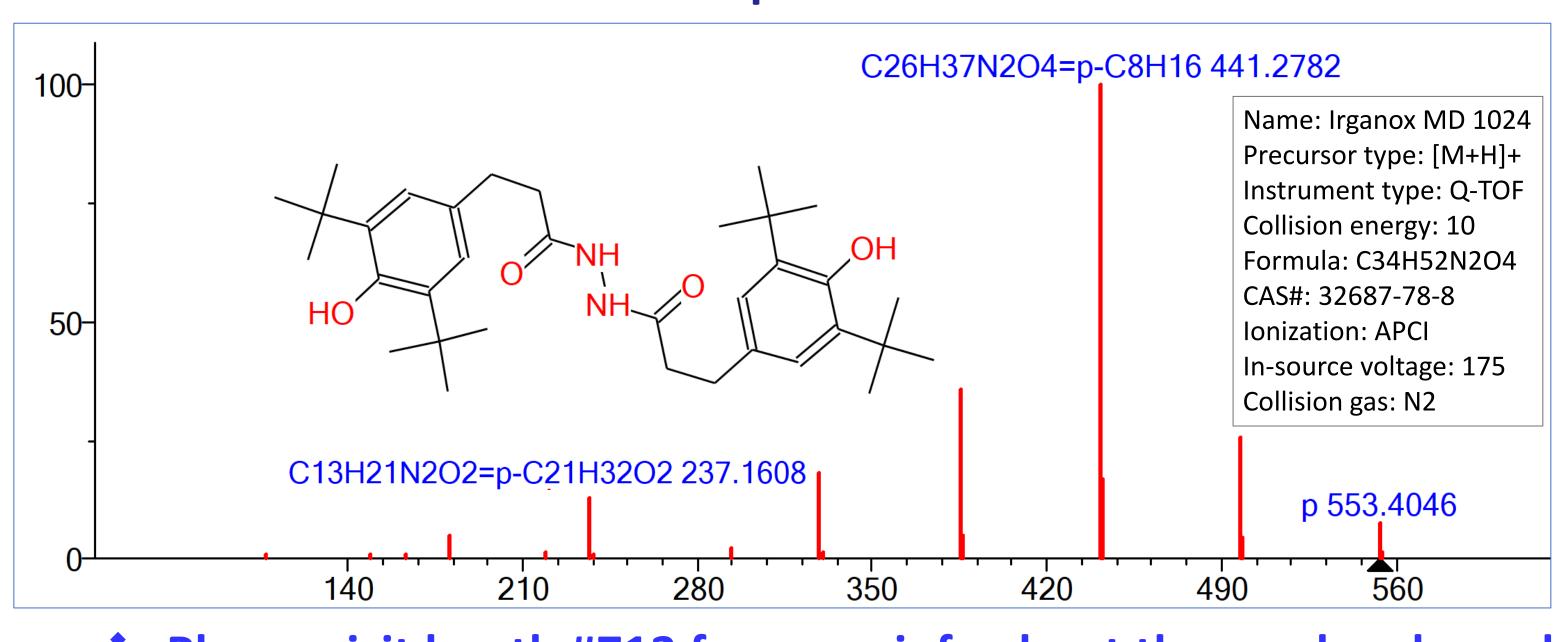
The library has >6,000 spectra of 90 compounds of shikimic acid and its derivatives. The spectra of these metabolites would be greatly helpful to further study the shikimic acid-related pathways and branches in plants and microorganisms as well as herbicide Glyphosate mechanism.



The Library includes >1,200 pesticides. e.g. Glyphosate (Roundup)



❖ The NIST23 APCI Library contains 5,714 Q-TOF spectra of 561 extractable and leachable compounds.



Please visit booth #713 for more info about the newly released NIST23 MS libraries and related software