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

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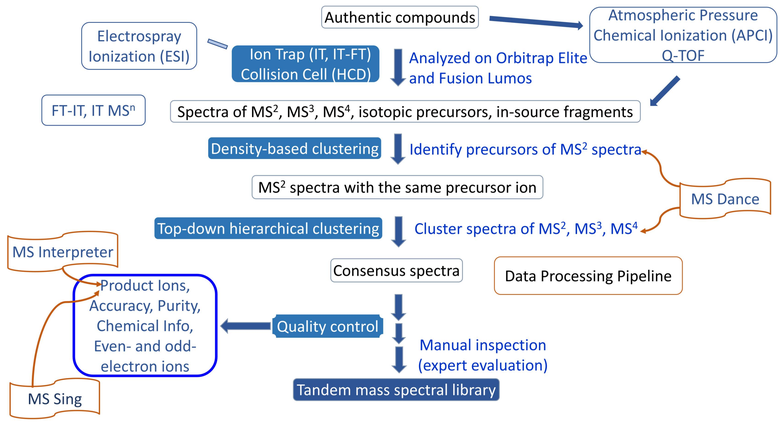
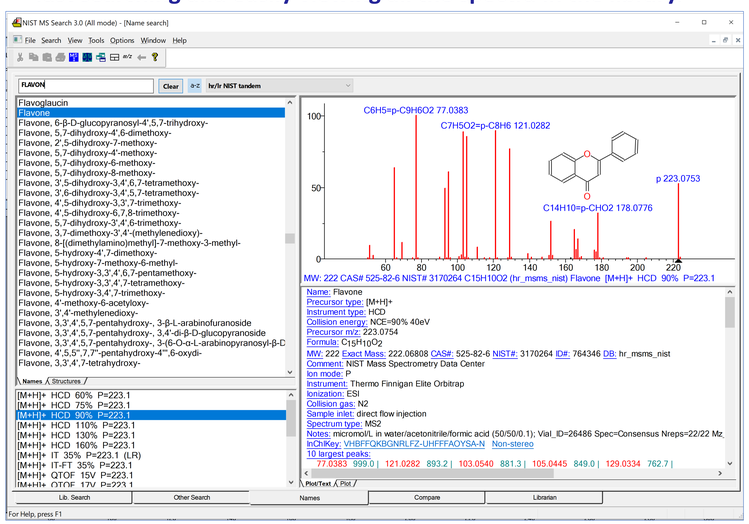
❖ **Overview:** The **NIST23 Tandem Mass Spectral Library** contains **2.4 million high- and low- resolution mass spectra of 51,505 compounds including over 11,000 plant metabolites and natural products** with newly improved quality control and manual inspection procedures. This library will greatly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

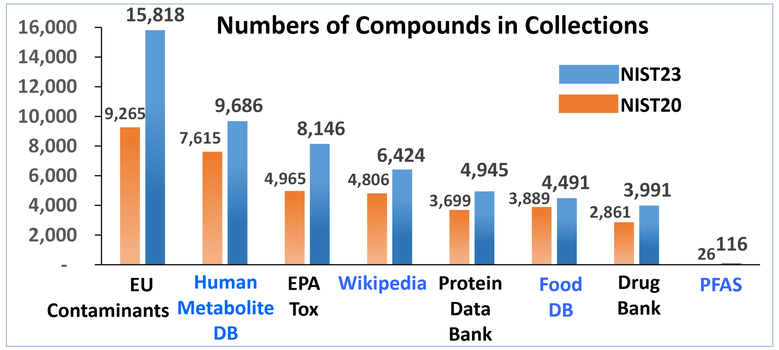
❖ Procedure of Building the NIST Tandem Mass Spectral Libraries



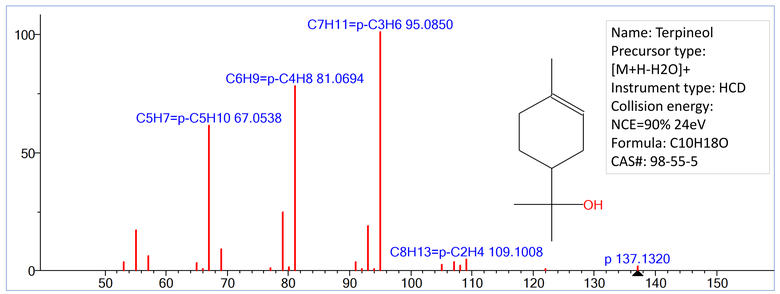
❖ MS Search 3.0: library searching software with new format for fast searching and easily viewing all the spectra in the library.



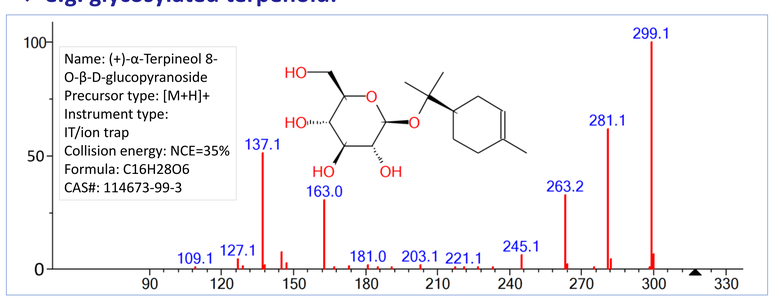
❖ The NIST23 Tandem MS Library contains high quality and comprehensive mass spectra of plant and human metabolites, pesticides, sugars, drugs, bioactive peptides, lipids, and extractable and leachable compounds including in-source fragments and MSⁿ spectra in positive and negative modes.



❖ The NIST23 Tandem Library includes spectra of flavonoids, alkaloids, terpenoids and glycosylated terpenoids, polyketides, shikimates, fatty acid derivatives in plants. e.g. Terpineol

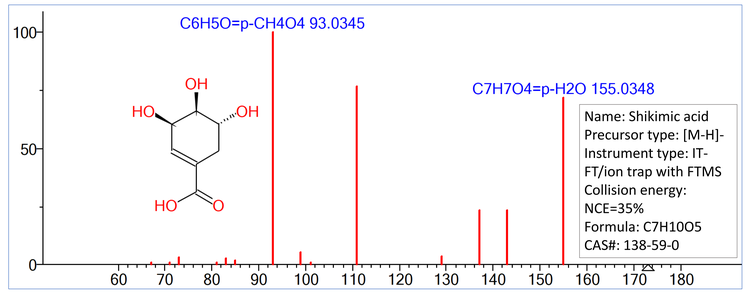


❖ e.g. glycosylated terpenoid:

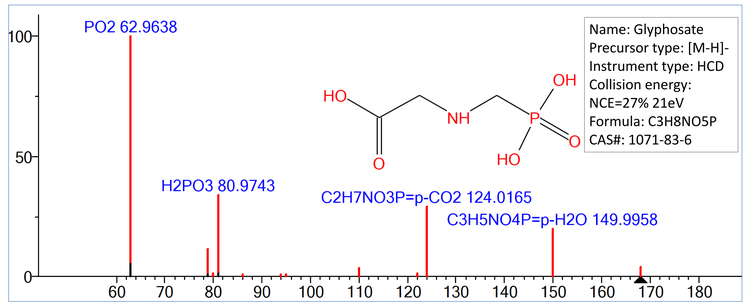


❖ Shikimic acid and its derivatives:

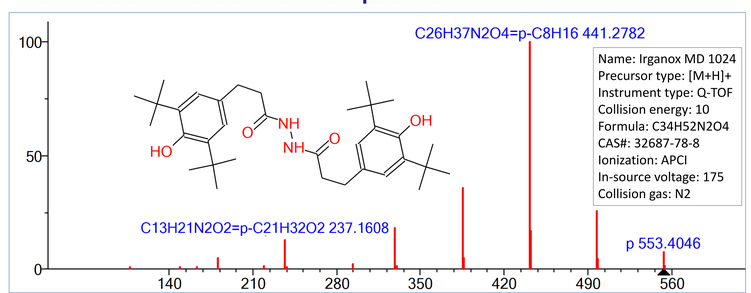
The library has >6,000 spectra of 90 compounds of shikimic acid and its derivatives. The spectra of these metabolites would be greatly helpful to further study the shikimic acid-related pathways and branches in plants and microorganisms as well as herbicide Glyphosate mechanism.



❖ 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