NIST26 Mass Spectral Libraries Breakfast Seminar - Meeting Report.

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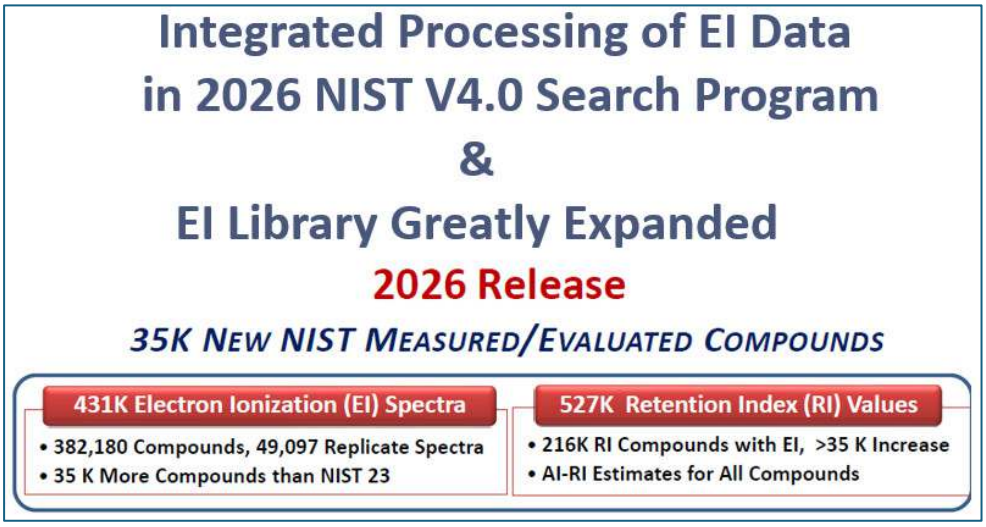
Representing Stanton Scientific, I was pleased to attend the NIST26 Mass Spectral Libraries Breakfast Seminar held Monday, June 1, 2026 from 7.00-8.15am during the 74th ASMS Annual Conference at the San Diego Convention Center.

NIST26 is the latest version of the National Institute of Standards and Technology Mass Spectral Libraries, a full featured MS library search and display program which includes (i) the NIST/EPA/NIH EI-MS Mass Spectral Library, (ii) the NIST GC Retention Index Database, and (iii) the NIST Tandem Mass Spectral Library. This is the most extensive update of the NIST Mass Spectral Library to date.

During the breakfast seminar, following a brief introduction to NIST and the evolution of the NIST Mass Spectral Libraries from Steve Stein, Tytus Mak gave an overview of how (and why) new compounds were selected for NIST26. Weihua Ji then discussed specific details associated with the EI Library Construction and the Quality Control Workflow. Finally, Xiaoyu (Sara) Yang discussed what is new in the NIST26 tandem MS library, including full LC/MS/MS chromatogram analysis.

Significant advances to the **EI-MS Mass Spectral Library** include expanded compound coverage and spectra, which ***now contains 431K spectra from 382,180 compounds, representing an additional 37,200 spectra from 35,000 compounds*** over the previous NIST23 release that were selected from a wide range of sources of analytical relevance and recognised importance to a variety of fields including environmental sciences, space exploration & astrochemistry, and the flavour, fragrance and cosmetics industries.



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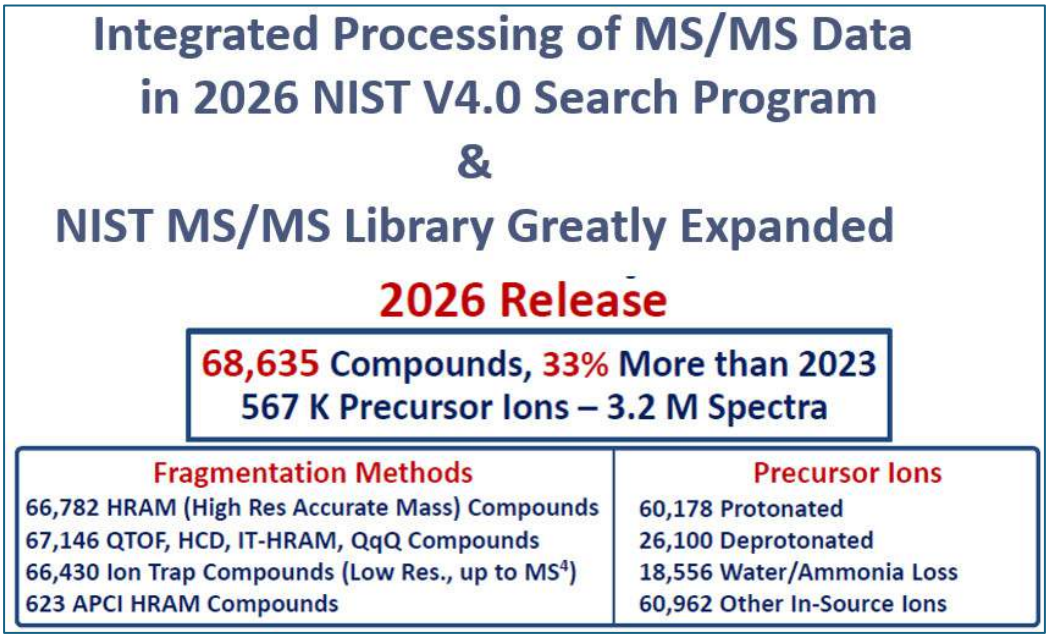
In addition to the ability to evaluate spectra with MS Interpreter, as well as the Hybrid Search function that enables the identification of homologous metabolites not found in the standard library, NIST26 further enhances its EI library search program with a capability for ***(i) integrated GC/MS chromatogram analysis, (ii) integration of deconvolution and subsequent library searching, and (iii) a novel approach for accurate mass EI data deconvolution and library searching***. Together these are a powerful combination for more streamlined and user-friendly compound identification. Further supporting the utility of this library is the **NIST26 GC Retention Index Database**, that now provides 527,993 retention index (RI) values and gas chromatographic conditions for 216,093 compounds measured under a variety of conditions, and covers 188,198 compounds with spectra in the NIST/EPA/NIH Mass Spectral library.

The **NIST26 Tandem Mass Spectral Library** now contains 3.2 M spectra from 567 K precursor ions for 68,635 compounds, which is 33% more than in NIST26.



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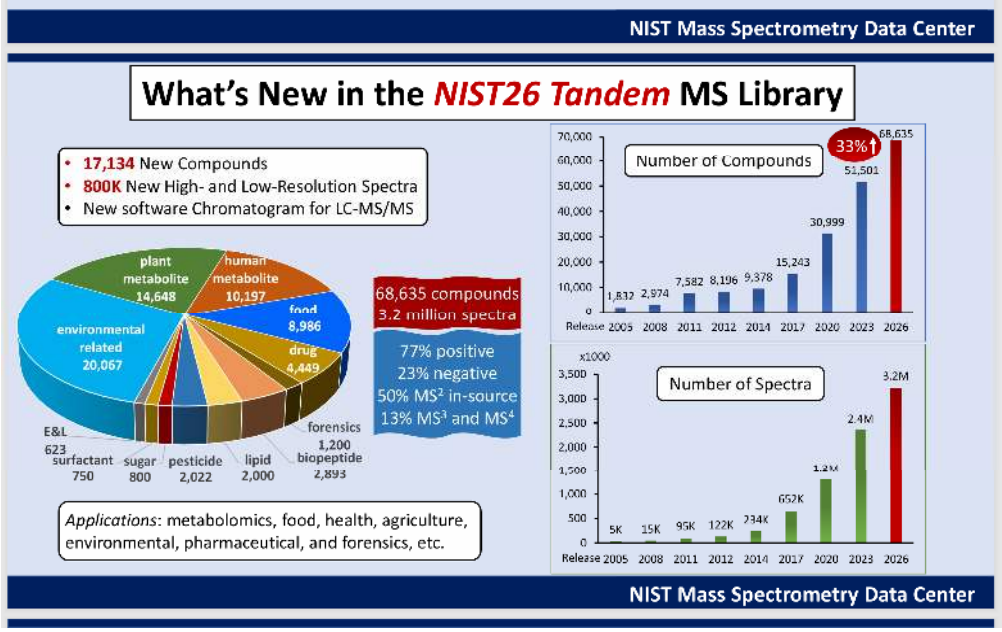
Key application areas include environmental, metabolomics/health, food, forensics, drugs, pharmaceutical, manufacturing, and agriculture.



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Similar to the EI-MS spectral library, a significant advance over the NIST23 release is that ***LC-MS/MS chromatogram-level analysis*** is now enabled within the MS/MS library search program, along with novel data processing approaches such as ***XIC-based analysis, enhanced hybrid searching using accurate mass data, background noise filtering, and combined MS1/MS2 identification / annotation***.

A copy of the slides presented during the Breakfast Seminar can be found in the ***attached nist-2026_nist-presentation.pdf*** document, while additional information can be found in the attached ***NIST26-flyers-EI.pdf*** and ***NIST26-flyers-Tandem.pdf*** documents.

Additional information can be found at https://chemdata.nist.gov/, while a series of resources and tutorials, including a fully functional demo version of the NIST26 LC-MS/MS search, can be found at https://mzinterpretation.com/.

Finally, related to the launch of the NIST26 Mass Spectral Libraries, I also attended the Mass Spectral Libraries Interest Group evening workshop held Tuesday, June 2, 2026 from 5.45-7.00pm on the topic 'The Past, Present, and Future of Mass Spectral Libraries'. Presided by Tytus Mak, Research Scientist at NIST, and including a brief presentation given by Steve Stein from NIST (***see the attached asms26-workshop.pdf document***), the workshop provided an overview of the current 'state of the art' in reference data libraries, and discussed key challenges remaining in the field including curation-at-scale (particularly given the prevalence of increasingly complex, high-resolution datasets), the need to integrate orthogonal data such as retention time and ion mobility, and the future of machine learning and in silico tools in database creation.