

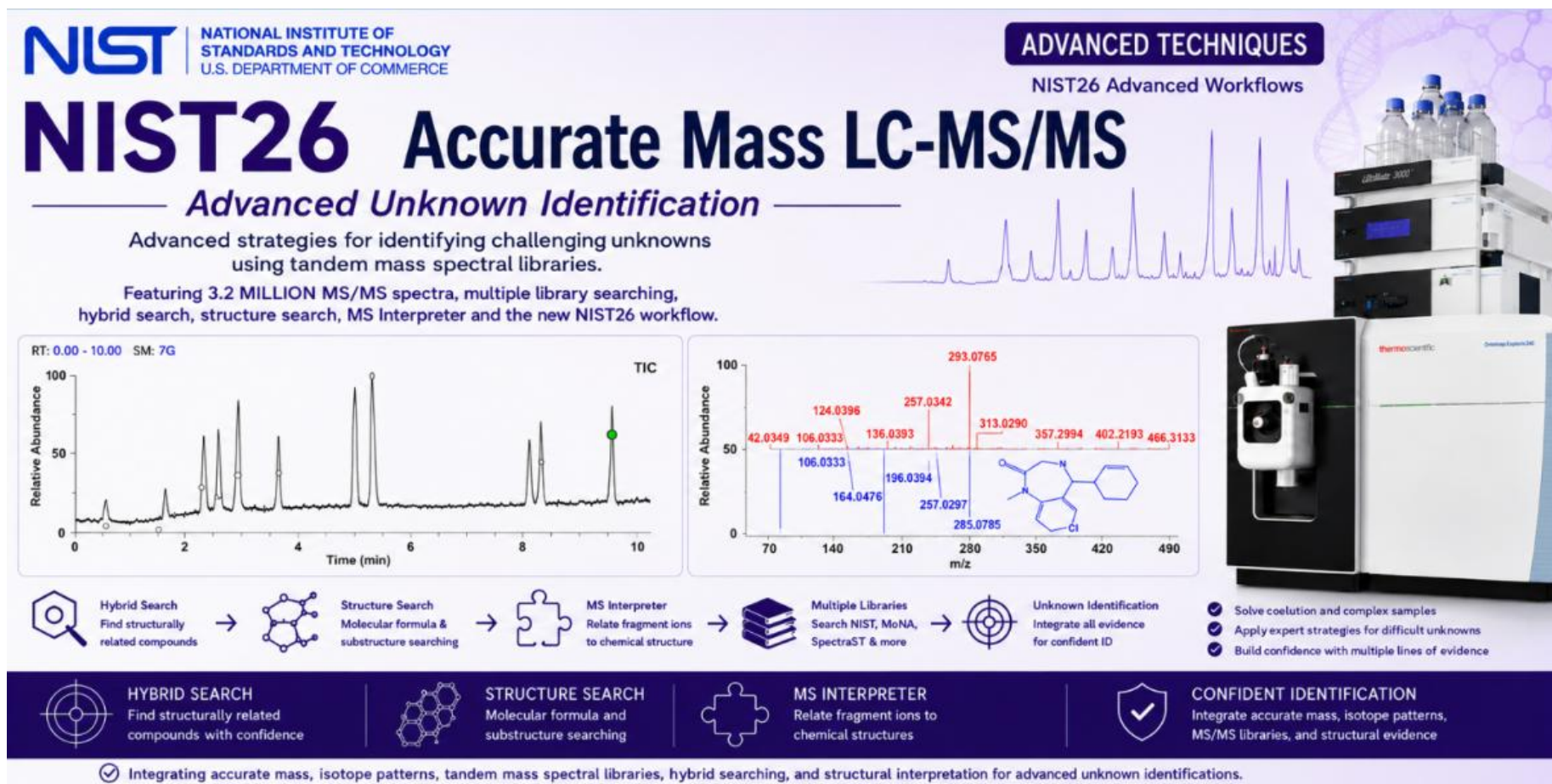
Sending MS/MS (Tandem) Spectra to NIST26 Search

Video and Associated Handout

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Mass Spec Interpretation Services

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Sending MS/MS (Tandem) Spectra to NIST26 Search

Introduction:

- NIST26 Software includes integrated data processing software in Chromatogram tab
- However, in some cases useful to send spectra from Vendor Software for processing

Examples for Not Processing in Chromatogram :

1. Data processing requires conversion (Proteowizard/Msconvert) to mzML format. If deconvolution is not needed and only a few peaks to analyze, more efficient to send from vendor software directly
2. File format of vendor's file not compatible when converted to mzML format.
3. Nominal mass data is not supported in Chromatogram tab. Thus, no choice in this case. See separate [video link](#) and [handout link](#) for details for this type of data.

Process for Vendor Incorporating Sending MS/MS Spectra to NIST Library Search

- Instructions for Vendor incorporating “Send NIST Lib option” found on my website, [see link](#).
- Waters, Agilent ([MassHunter](#) and [Open Lab](#)), and [Thermo](#) (names to left linked to my site info) incorporate NIST “Send NIST Lib option”
- Wiley KnowItAll software imports spectra to NIST search. They have a good manual software package supporting many vendor data file formats.
- Don’t think Sciex or Bruker employ, might have to export from them as txt or msp ASCII format and import into Spec List in Lib Search

Integrate. Interpret. Identify.

Using NIST Search Program with Data Processing and Drawing Programs

Powerful Tools. Seamless Workflow. Confident Results.

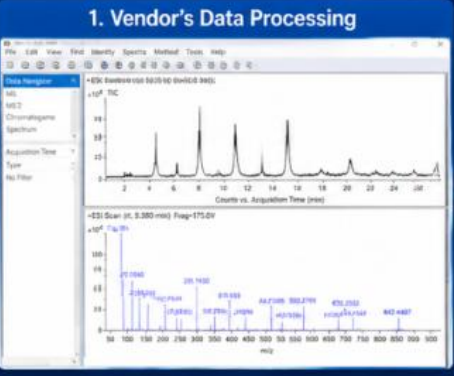
✓ **Process Your Data**
Prepare and examine spectra with your favorite software.

✓ **Search with Confidence**
Submit spectra to the NIST Search Program for high quality library matches.

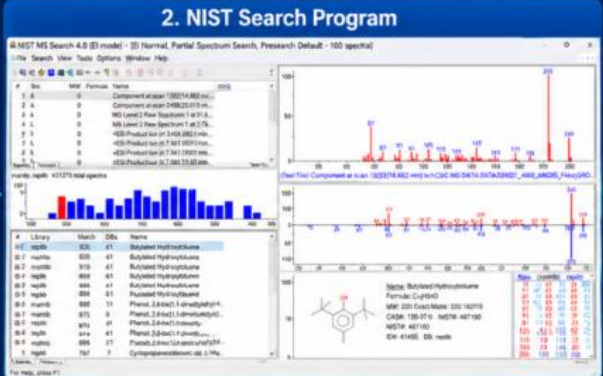
✓ **Interpret with Structure**
Transfer results to drawing programs for visualization and reporting.



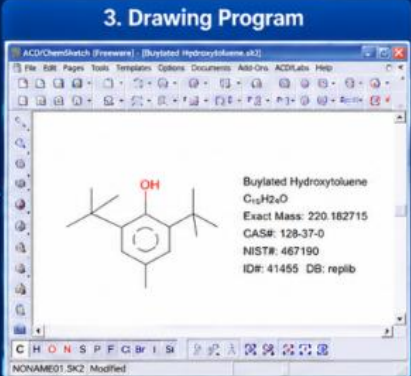
1. Vendor's Data Processing



2. NIST Search Program



3. Drawing Program



Butylated Hydroxytoluene
 $C_{10}H_{12}O$
Exact Mass: 220.162715
CAS#: 128-37-0
NIST#: 467190
ID#: 41455 DB: replib

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From raw data to confident identification.

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Leverage the world's most comprehensive libraries.

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Software Intensity Threshold Bug in Spectrum Import Options Window

- When any Intensity Threshold is used, the imported spectra from Vendor's Software are nominal
- Should be top spectrum with 4 digits to right of decimal
- Instead, nominal as shown on bottom spectrum

Spectrum Import Options

EI Spectrum m/z Rounding
Multiply m/z in imported spectra by and round to the nearest integer
Example: (CH₂)_n correction is 0.99888
Optional: Add this term to all m/z before rounding

Tandem Spectrum Accuracy
Precursor ion m/z decimal places
Product ion m/z decimal places
HiRes No Precursor ion m/z decimal places

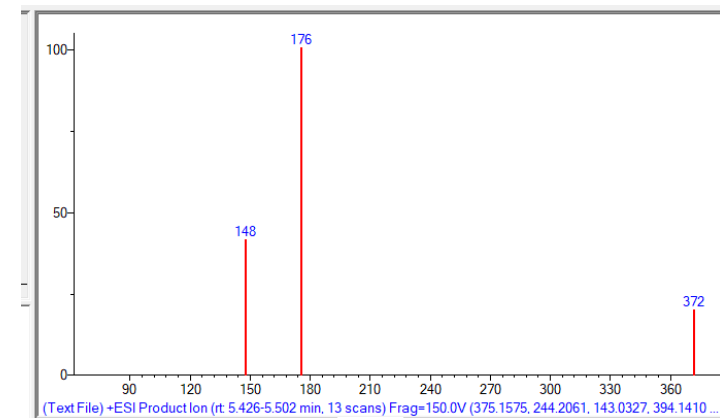
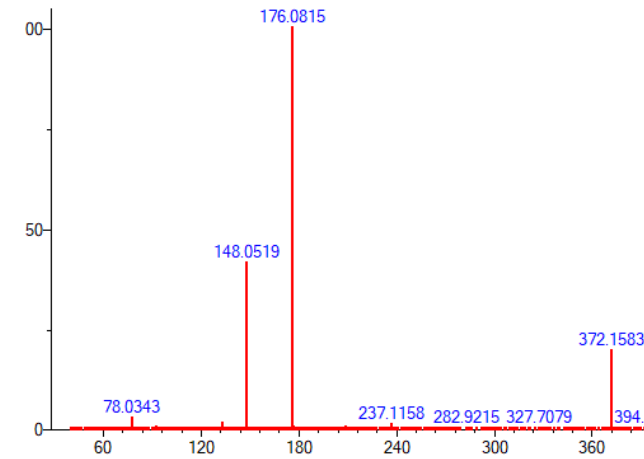
Adding spectra to Spec List
☒ Prepend (add to the top)
☐ Overwrite (replace)
☐ Ask

Intensity threshold
☒ % of max.
☐ absolute

Spectra without precursor ion m/z value are
☒ EI (nominal m/z) ☐ In-source ☐ Accurate m/z

RI type if unspecified:

☒ Include Synonyms



Software Bug in Chromatogram Window Software

- The values used in the Spectrum Import Options “echoed” in the Chromatogram Tab
- Normally these values are shown to 4 significant figures to right of decimal
- When set as zero to import low-resolution spectra, truncated to values selected
- DOES NOT affect the results in accurate mass deconvolution/library searching table!
- Just the “head-to-head” display at top of Chromatogram Tab

