

Overview:

- High quality and comprehensive reference mass spectral libraries provide a fast and reliable means of assisting the identification of compound identity.
- The most challenging part of building such a library is the need for expert spectrum evaluation.
- Novel evaluation approaches were developed for building a high quality electron ionization mass spectral library.

Methods:

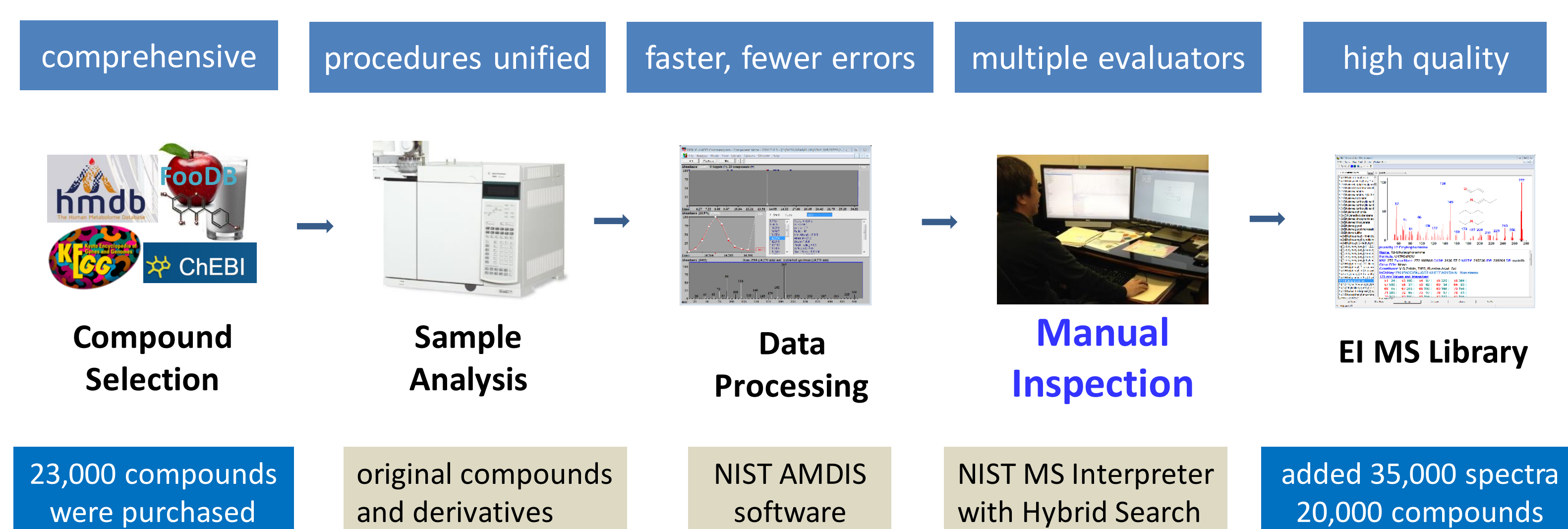
- Each mass spectrum was compared with spectra of similar compounds in the NIST17 and other available mass spectral libraries using the improved hybrid search method.
- The structure similarity search and the MS Interpreter program were used to assess the consistency of chemical structure and spectra.
- Product ions that were not explained or were assigned unreasonable mechanisms were manually examined.
- A new spectral evaluation method was developed in which spectra are passed between evaluators though small libraries in which individual comments are made, leading the eventual incorporation of accepted spectra into the distributed library.
- Software tools used in this study may be freely downloaded from <https://chemdata.nist.gov>.

Results:

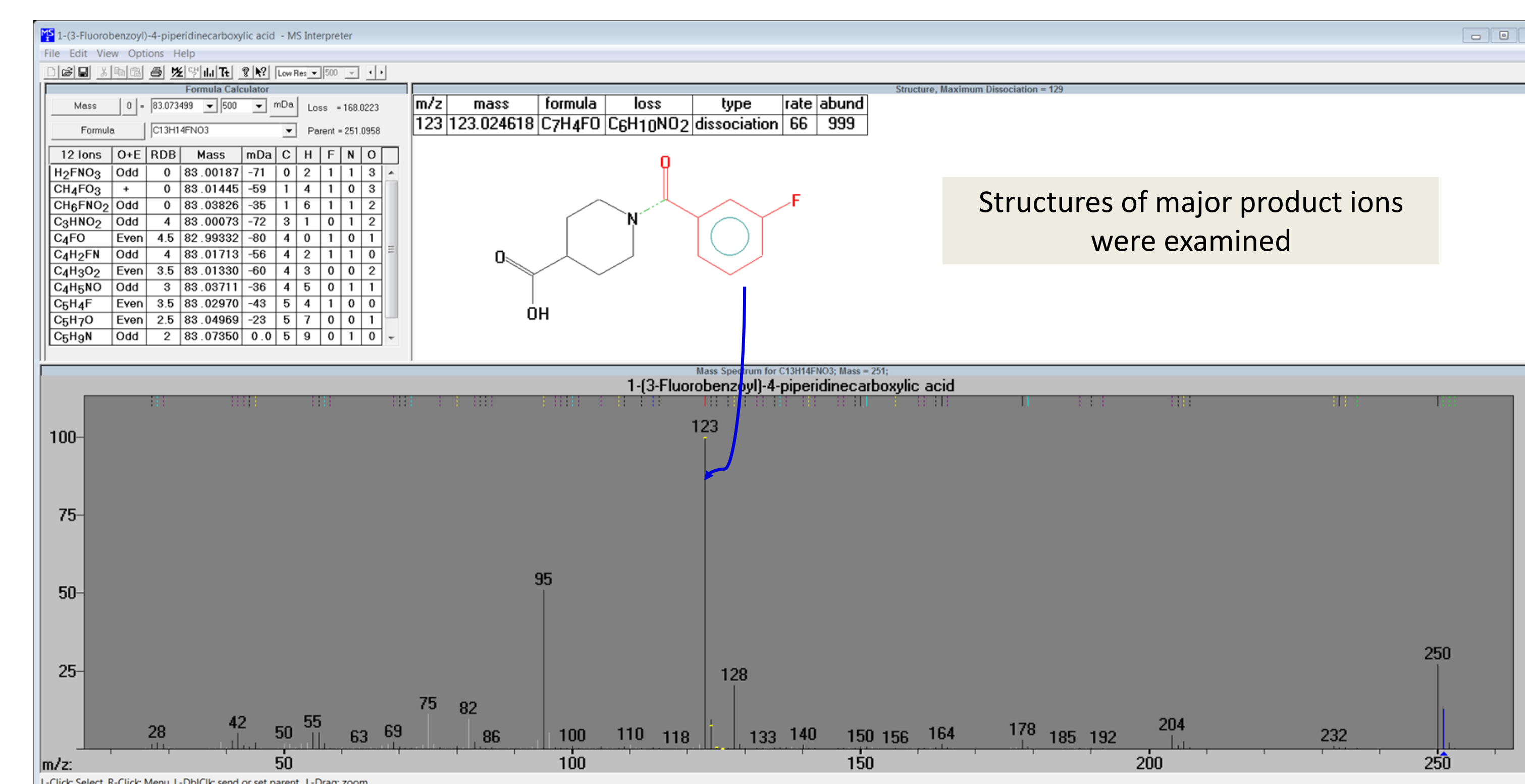
- To date, 36,082 new mass spectra have been evaluated in since NIST17. Low quality spectra, such as those with missing peaks, contaminant peaks or with an uncertain chemical structure were rejected by manual inspection aided by various software.

Please visit booth #616 for more information about NIST Mass Spectral Libraries

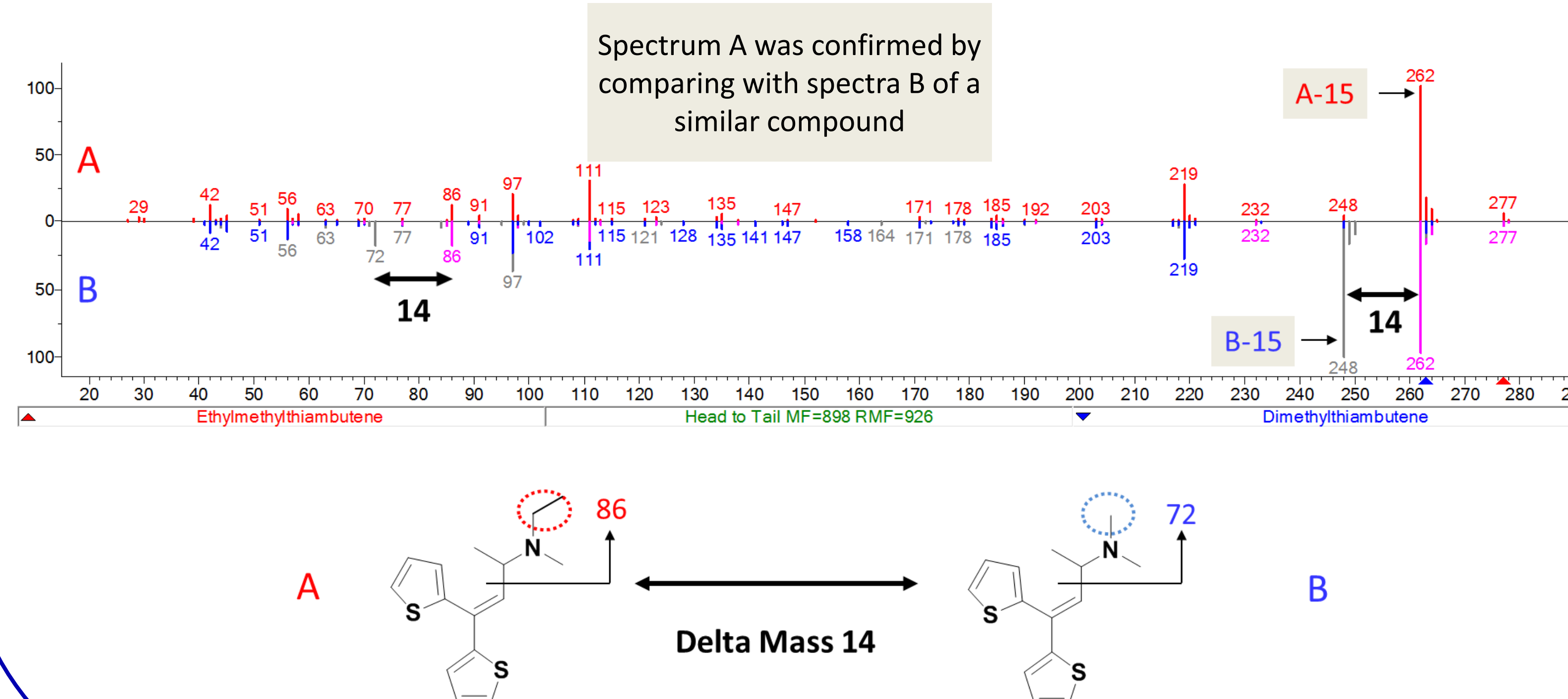
Improved procedure for expanding the EI MS Library



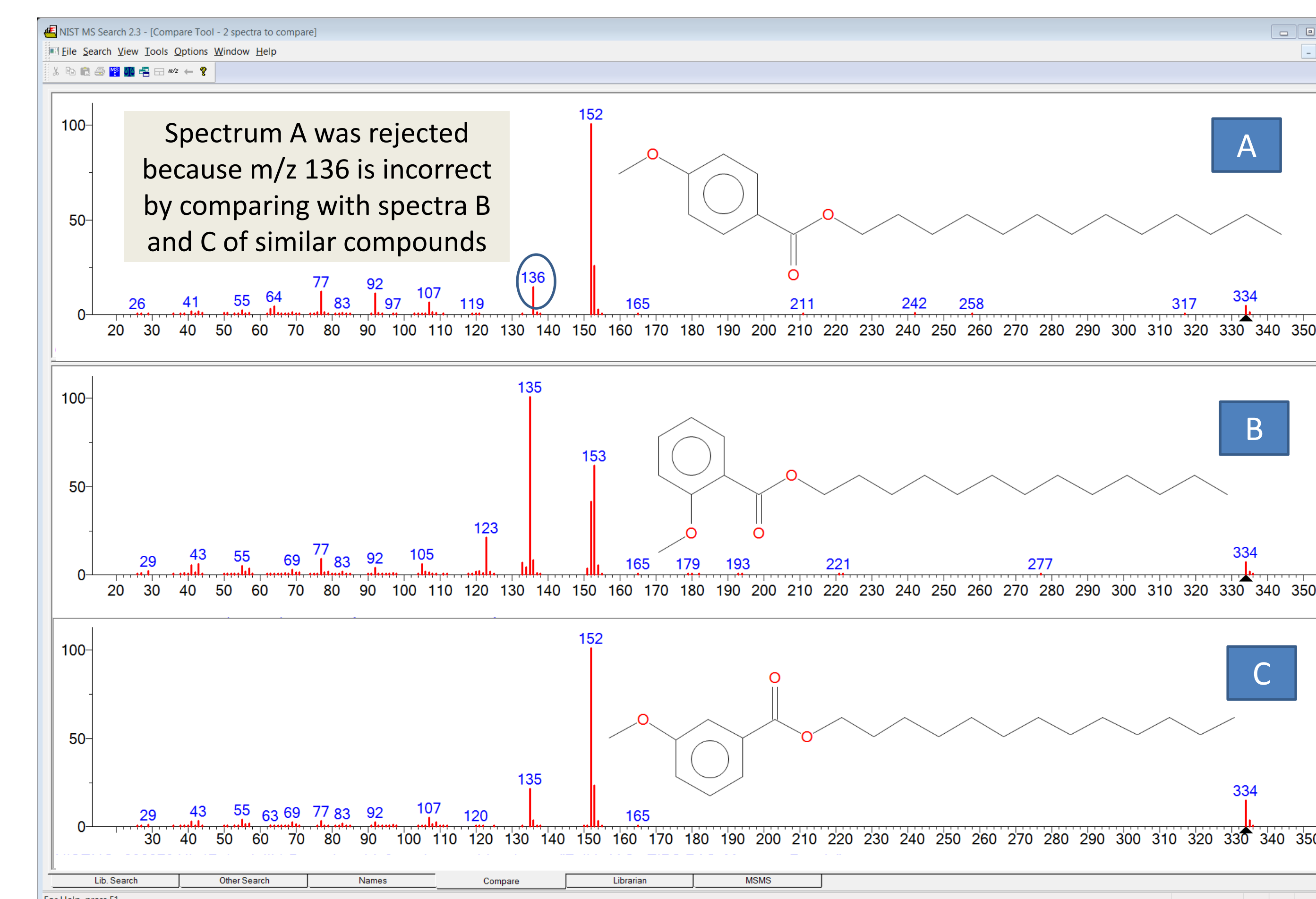
An example of evaluating a spectrum with MS Interpreter



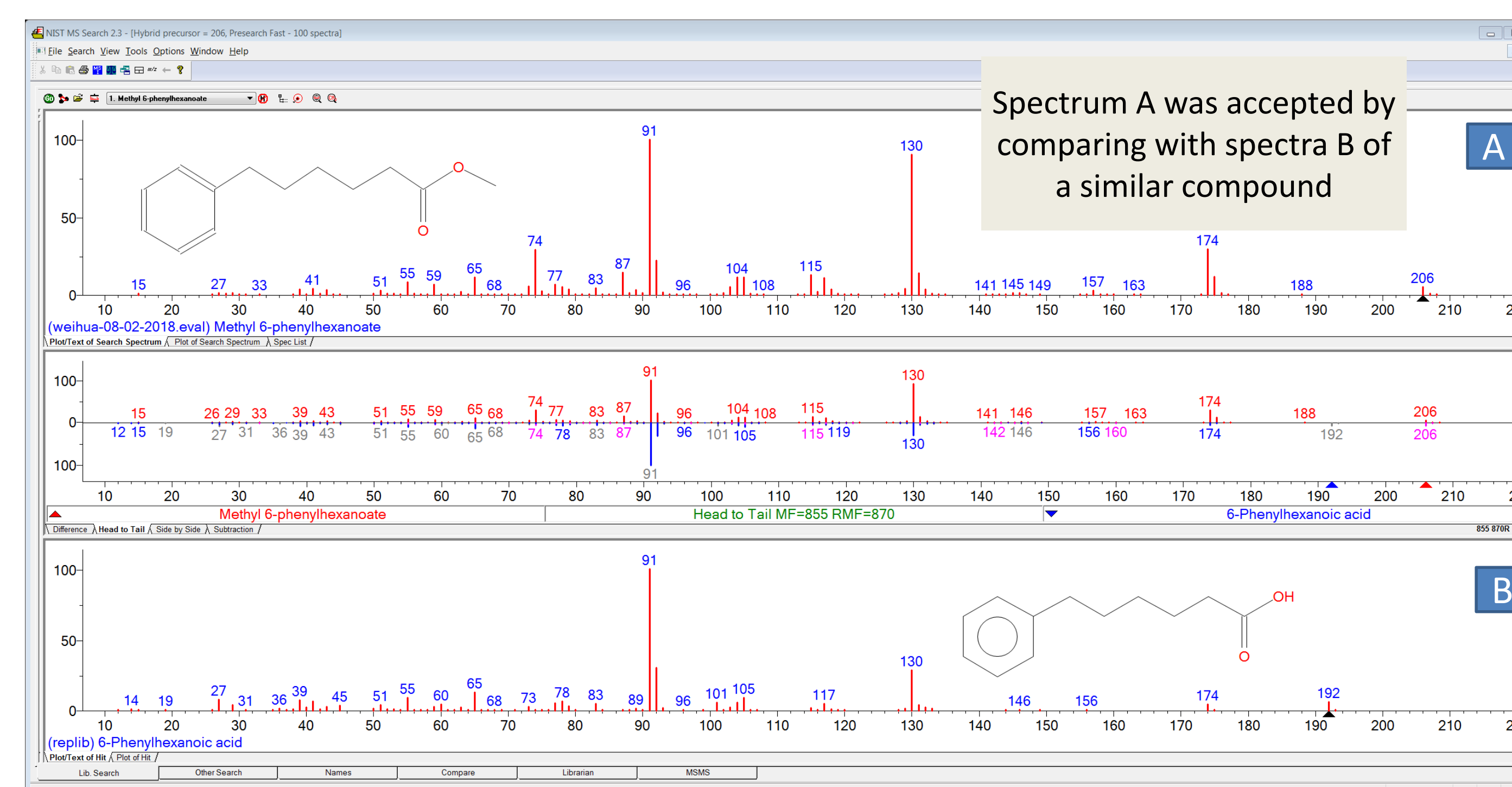
An example of evaluating a spectrum with hybrid search



An example of evaluating a spectrum with structure similarity search



The spectrum of methyl 6-phenylhexanoate was evaluated by using hybrid search



Conclusions:

- The new methods were used in evaluating mass spectra and finding possible errors in the library.
- Approximately 35,000 spectra of 20,000 compounds were critical evaluated and will be added to the library.