

NIST/EPA/NIH EI-MS LIBRARY

2017 Release

MORE SPECTRA AND COMPOUNDS

306,622 Electron Ionization (EI) Spectra

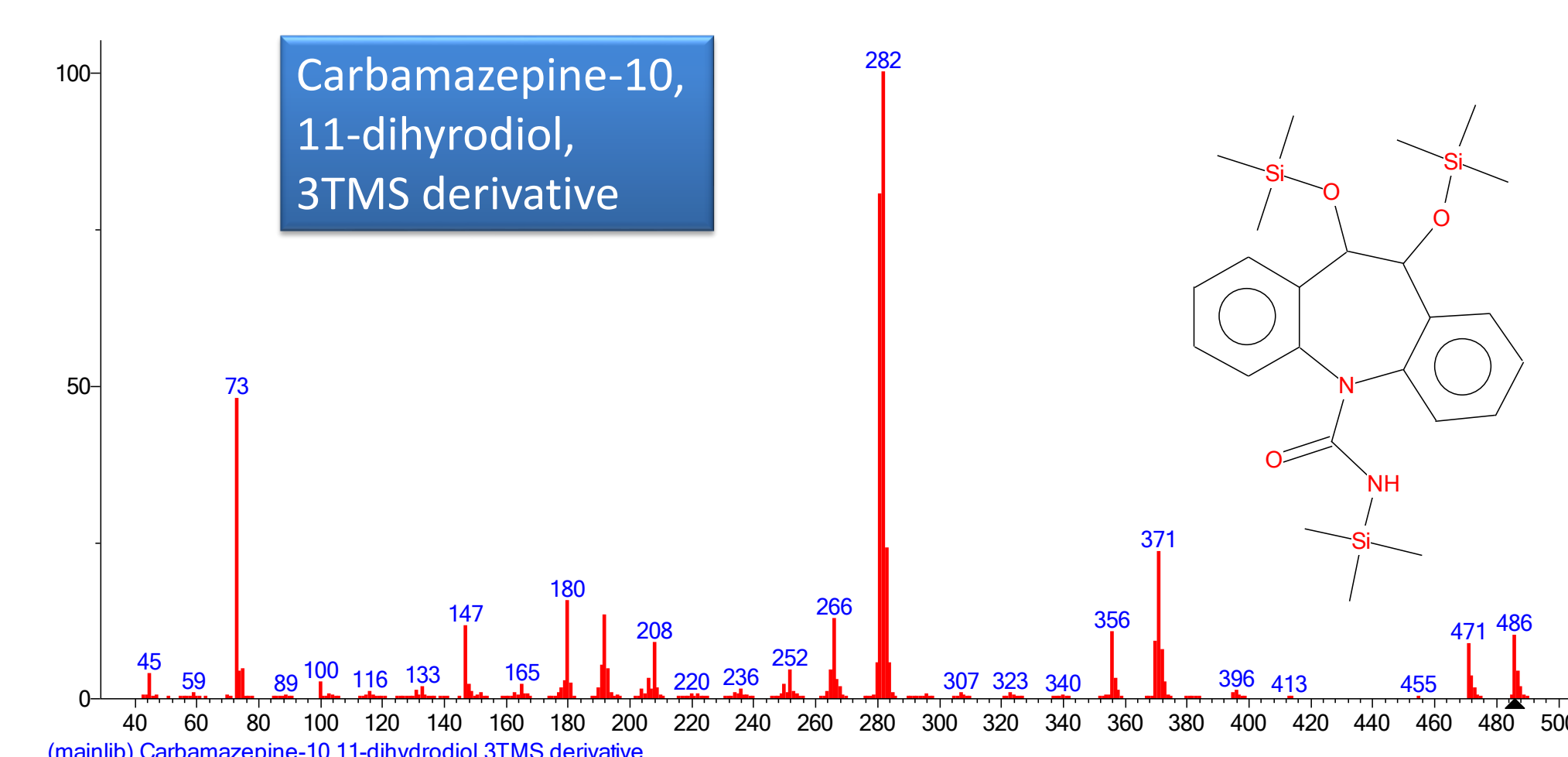
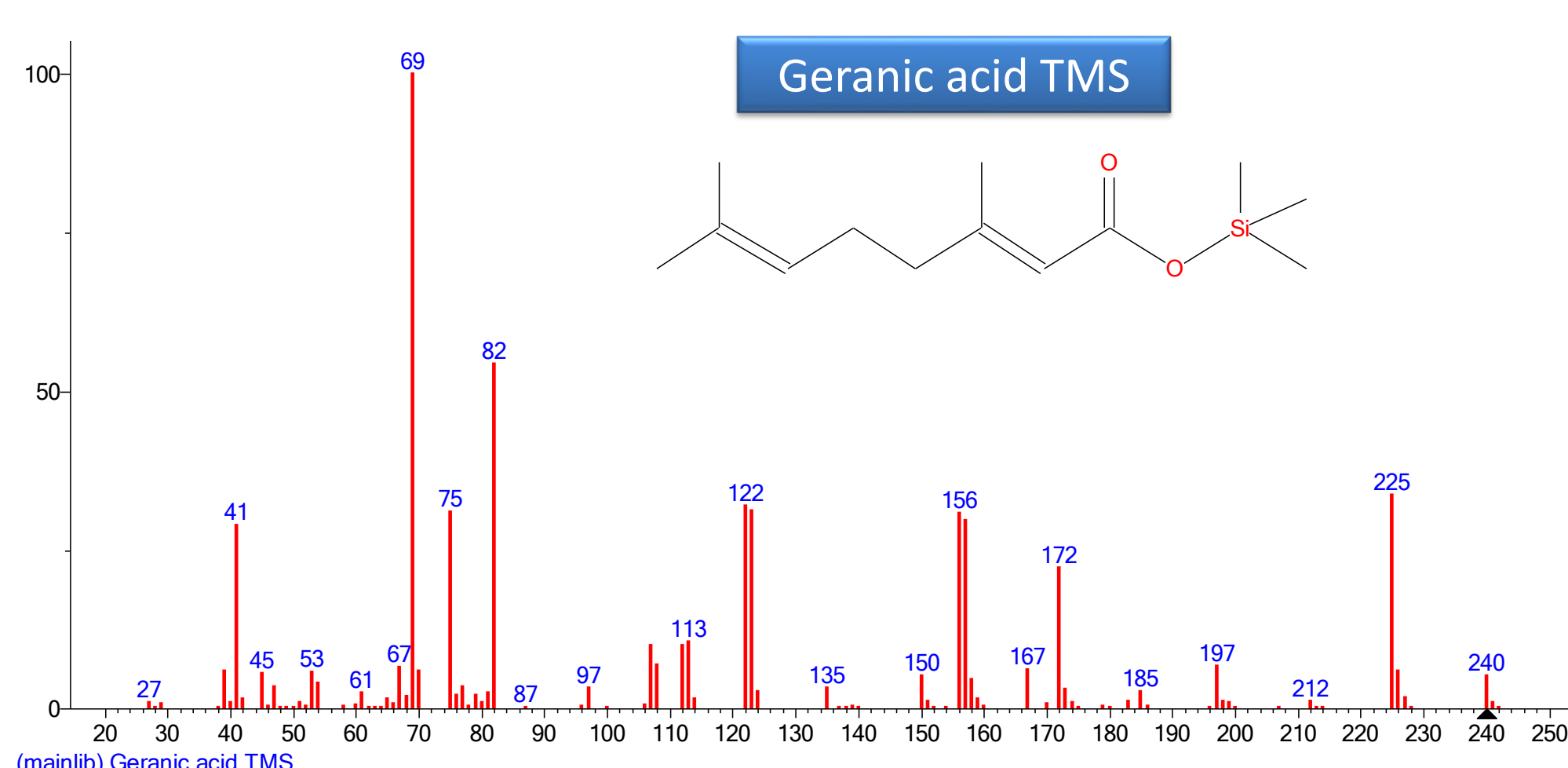
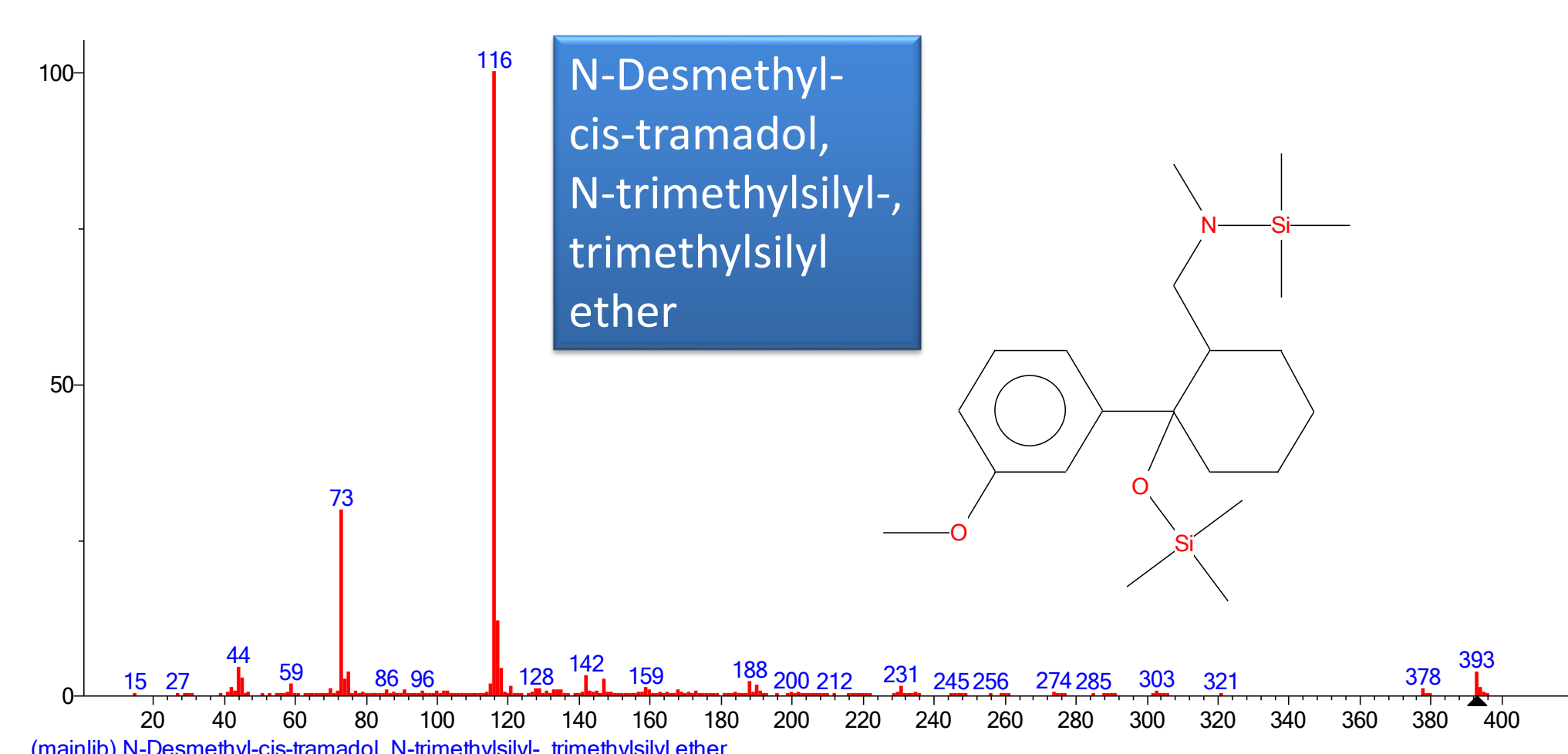
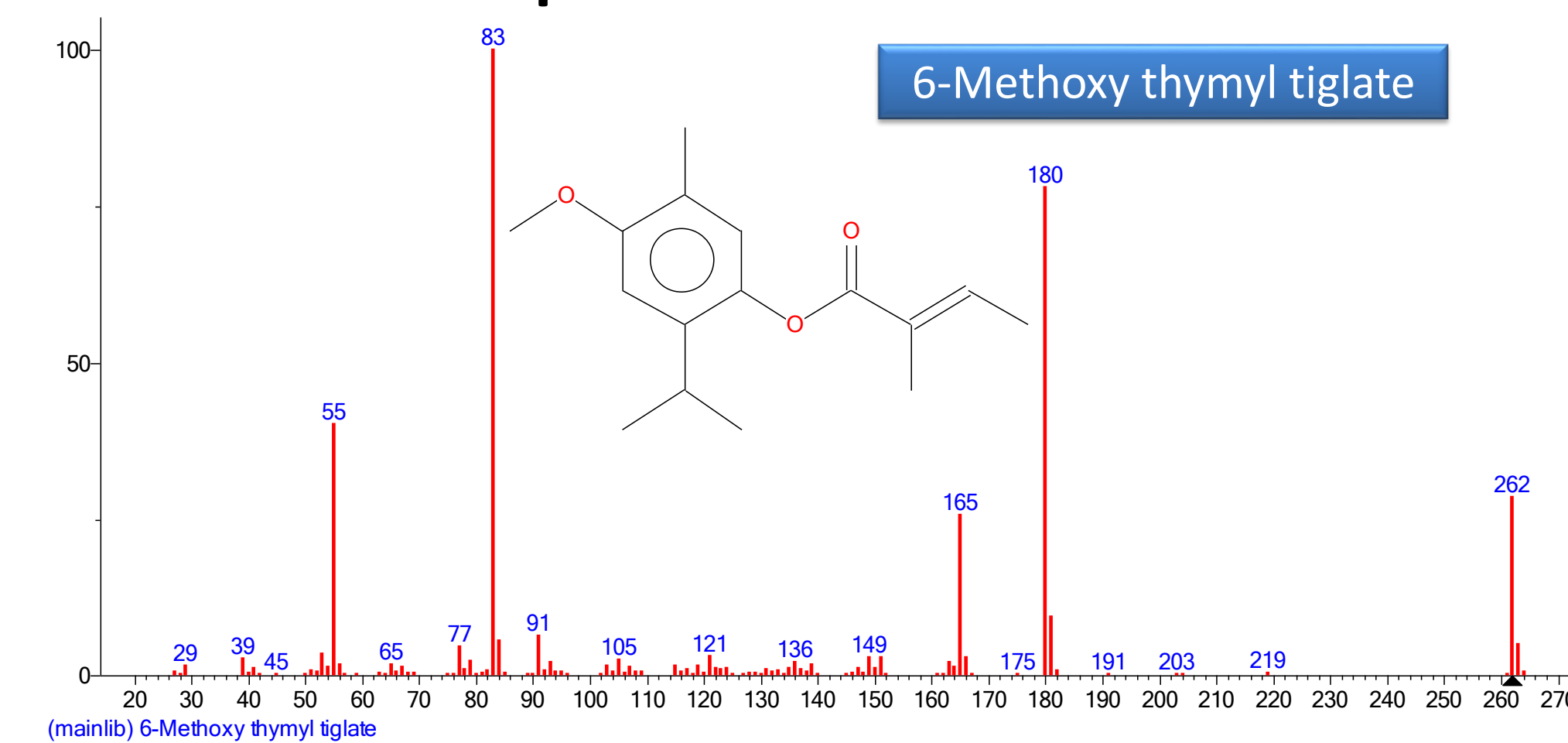
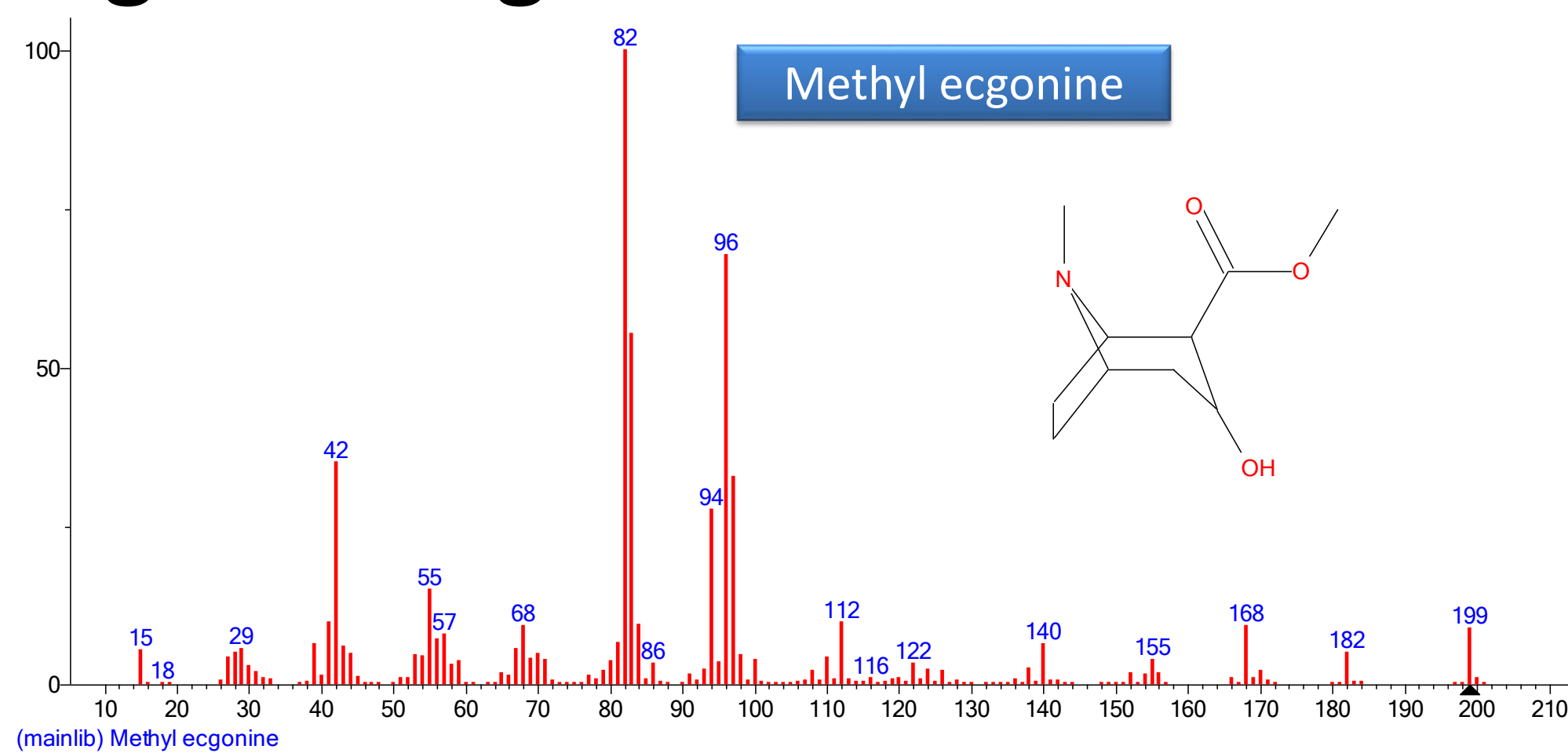
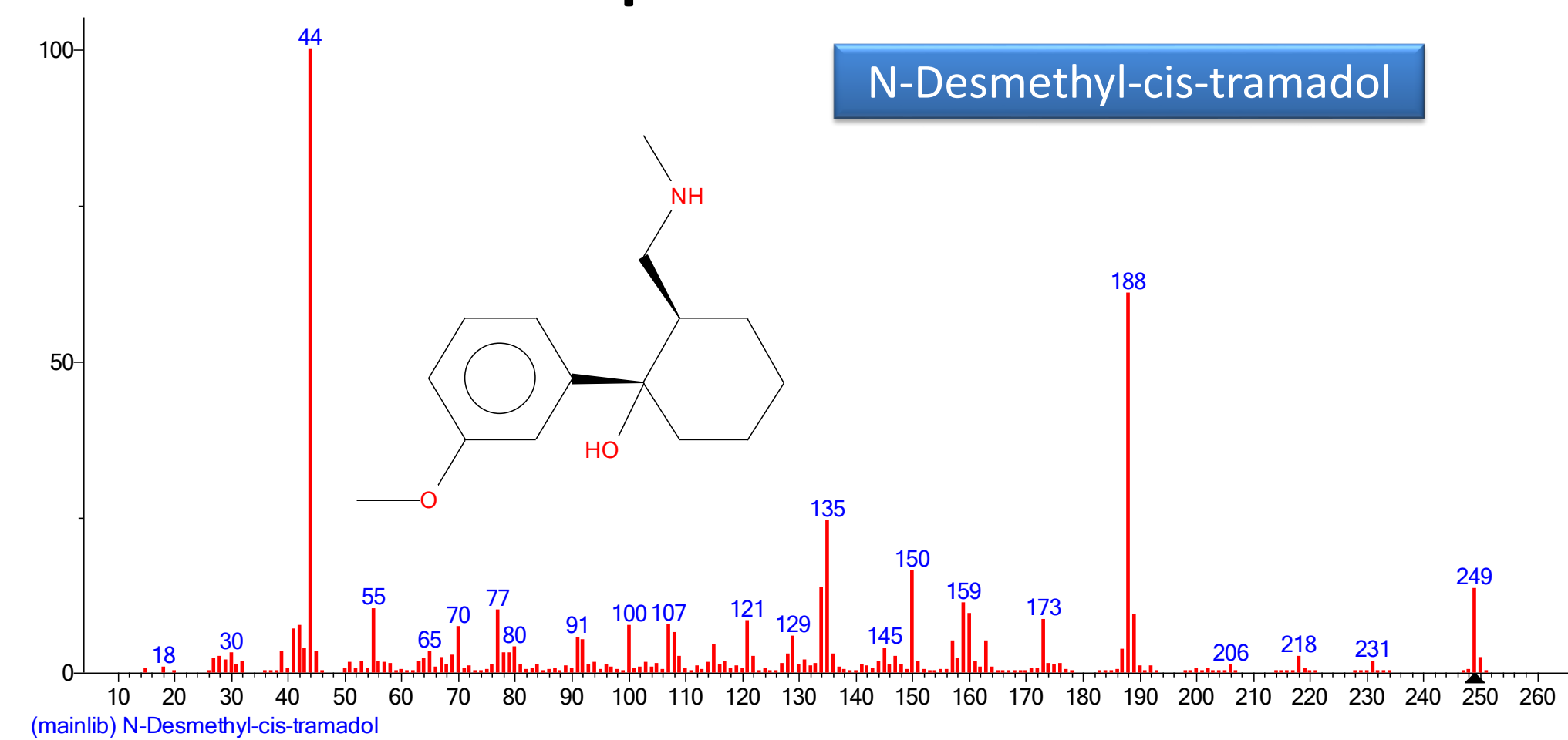
- 267,376 Compounds
- Over 25,000 More Compounds than NIST 14

404,045 Retention Index (RI) Values

- 99,400 RI Compounds
- 76,361 Compounds with both RI & MS

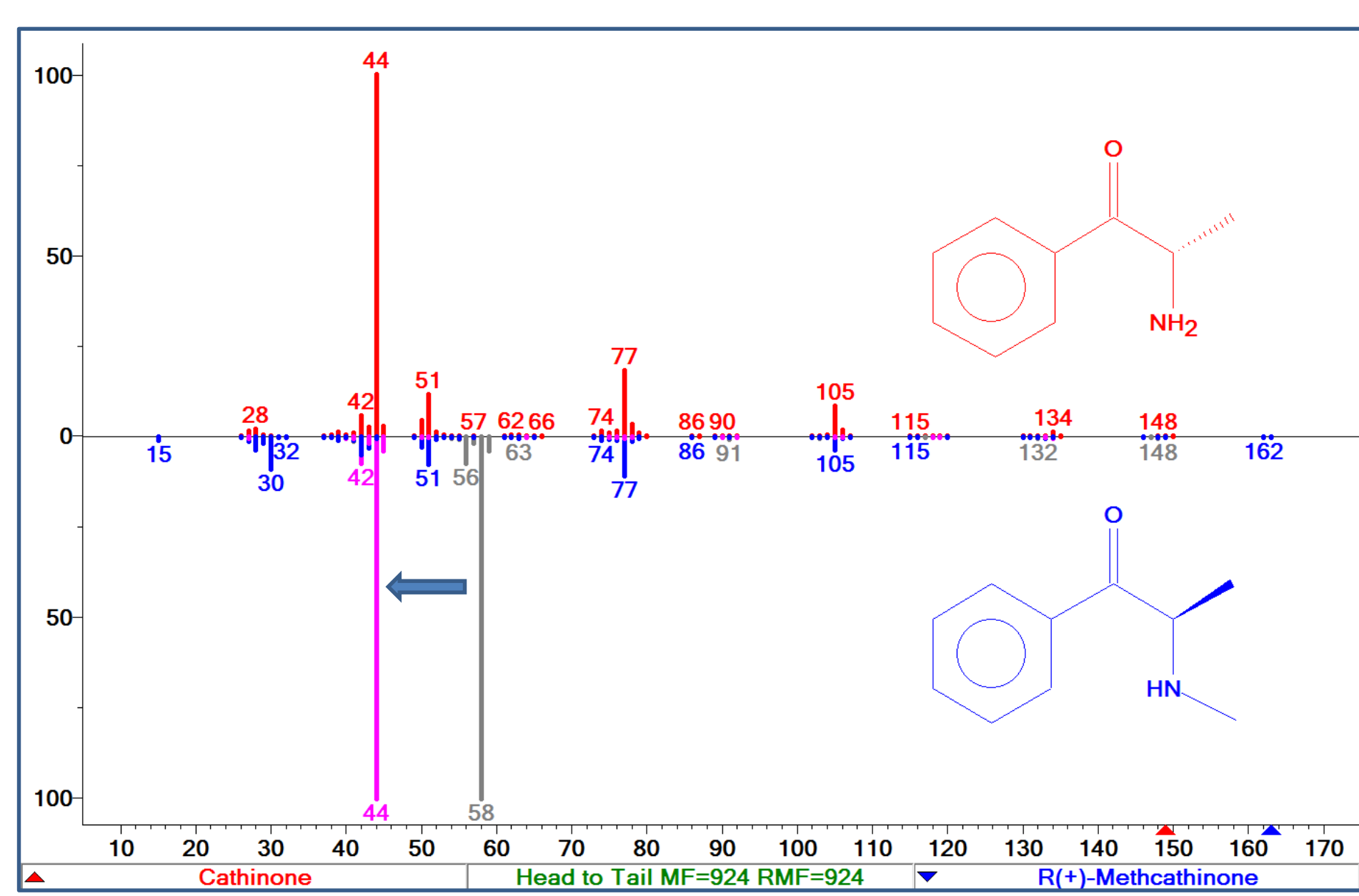
NEW COMPOUNDS (NATIVE AND DERIVATIZED)

- Human and plant metabolites
- Designer drugs
- Contaminants
- Industrial compounds
- Much more



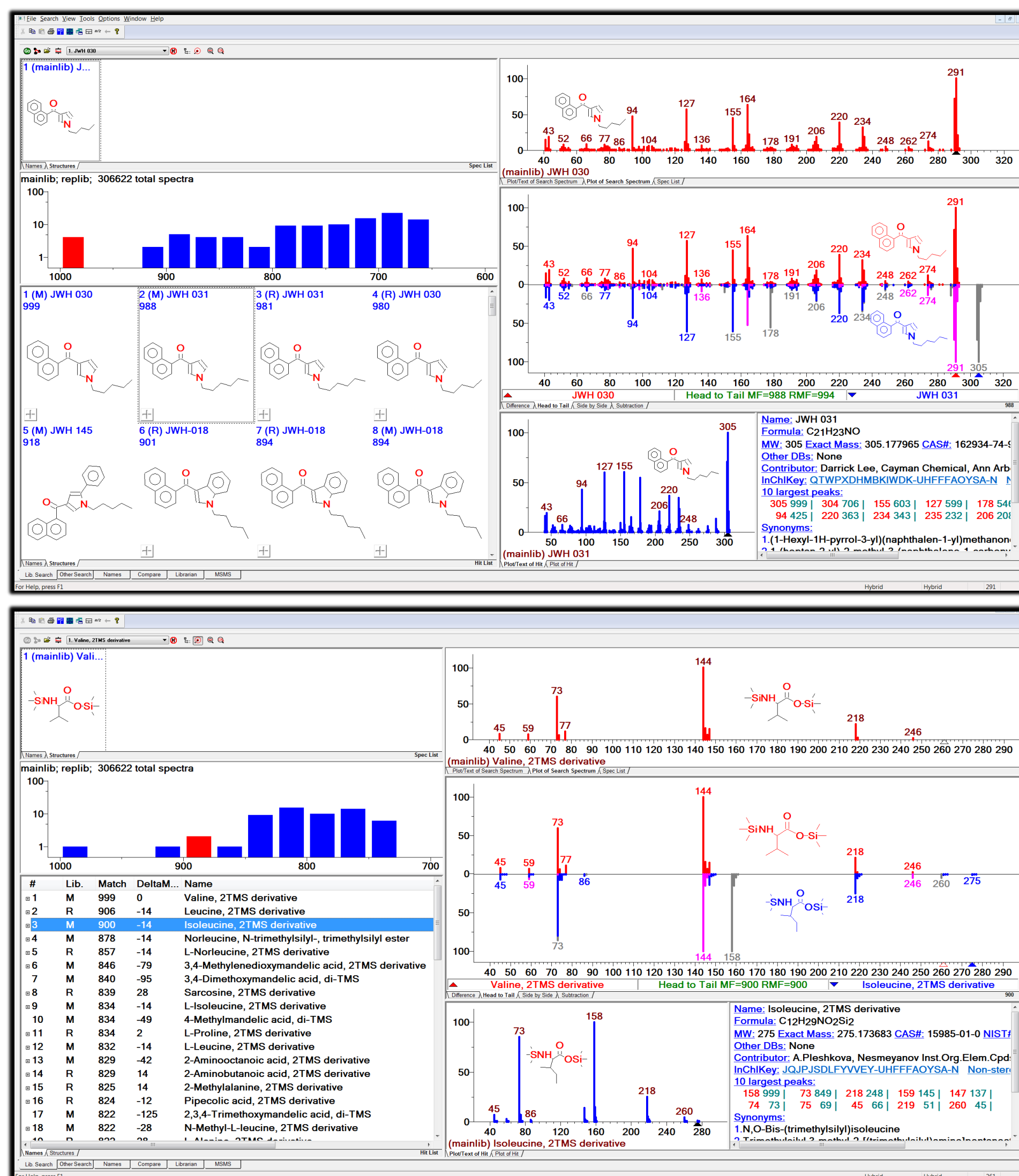
THE HYBRID SPECTRUM SEARCH

Shift peaks to match spectra for compounds that differ by an 'inert' chemical group. Both original and shifted peaks shown to aid structure analysis.



Library Search Options dialog box. The 'Spectrum Search Type' is set to 'Hybrid'. The 'Spectrum Search Options' include 'Reverse Search', 'Match Ion Mode', and 'Presearch' (Default, Fast, Off, MW). The 'Structure Similarity Search Options' include 'Match Number of Rings' and 'Show Homologues'. The 'Other Options' include 'Automation', 'Auto Report', 'Apply Limits', and 'Use Constraints'.

Can greatly increase the number of matching compounds, aiding ID and fragmentation mechanism



INCHI STRUCTURE SEARCH

InChI Structure Search interface. The 'Library Search Options' dialog box is shown on the left. The main window displays a search results table with columns for 'Library', 'Match', 'Name', and 'Formula'. The results include various compounds such as Fenpropyl, Fenpropyl, and Fenpropyl. The chemical structures of the top results are shown.

Compare replicates within and between libraries

MS INTERPRETER ENHANCEMENT

MS Interpreter interface. The 'Mass' field is set to 137.12048. The 'Formula' field is set to C12H12O9. The 'Parent' field is set to 155.8497. The 'Structure, Maximum Observation = 134' field is set to 137.12048. The 'New 'lasso' function' is highlighted. The chemical structure of the compound is shown.

Specify structure for mass calculation



<http://chemdata.nist.gov>

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