NIST/EPA/NIH EI-MS LIBRARY

2017 Release

More Spectra and Compounds

306,622 Electron Ionization (EI) Spectra

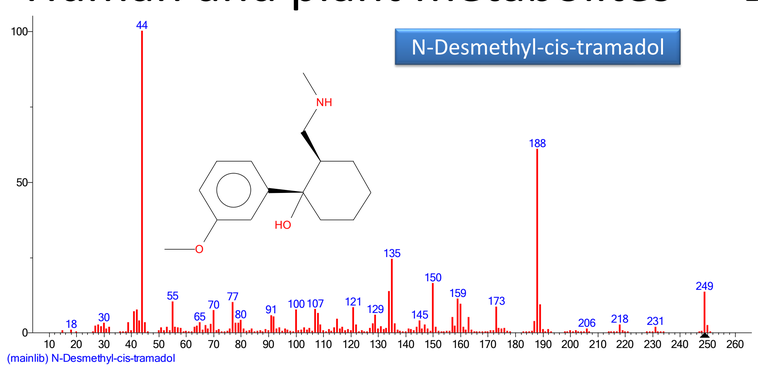
- 267,376 Compounds
- Over 25,000 More Compounds than NIST 14

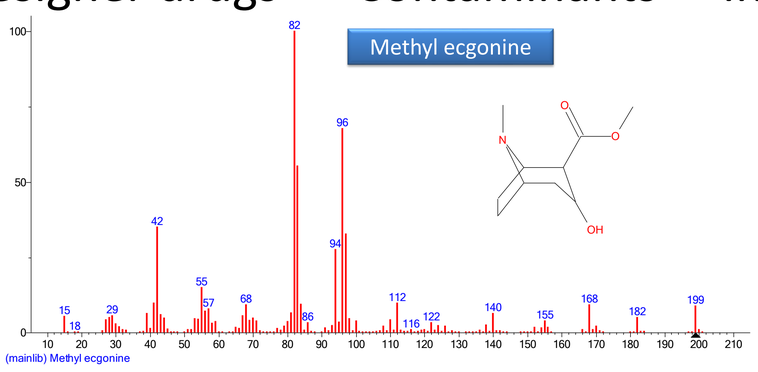
404,045 Retention Index (RI) Values

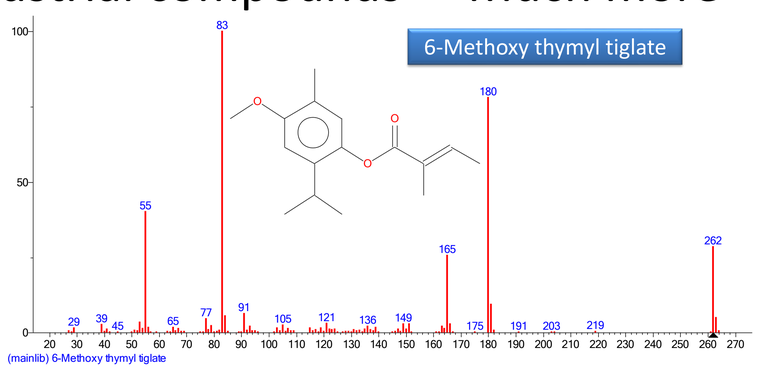
- 99,400 RI Compounds
- 76,361 Compounds with both RI & MS

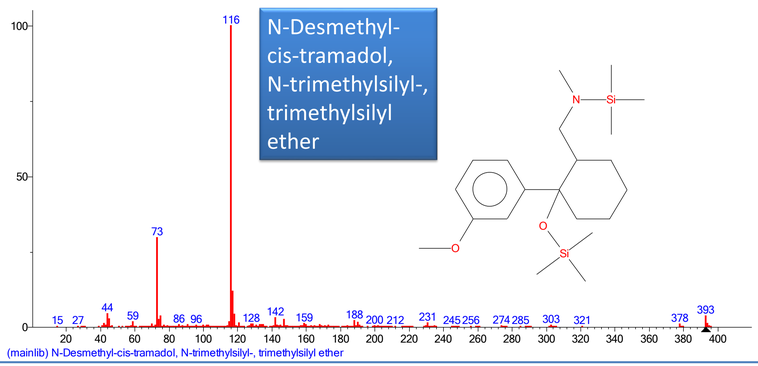
New Compounds (Native and Derivatized)

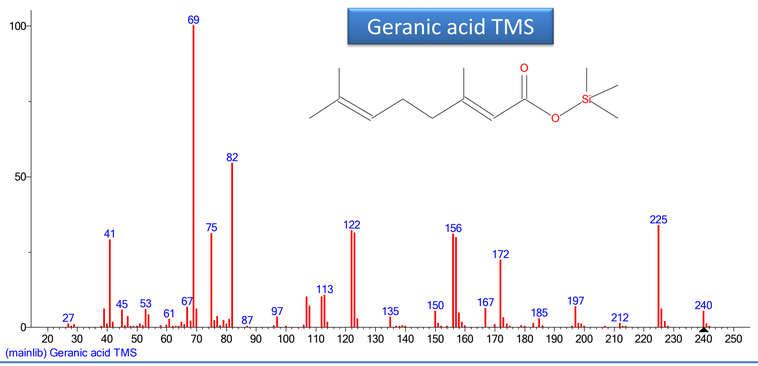
- Human and plant metabolites
- Designer drugs
- Contaminants
- Industrial compounds
- Much more

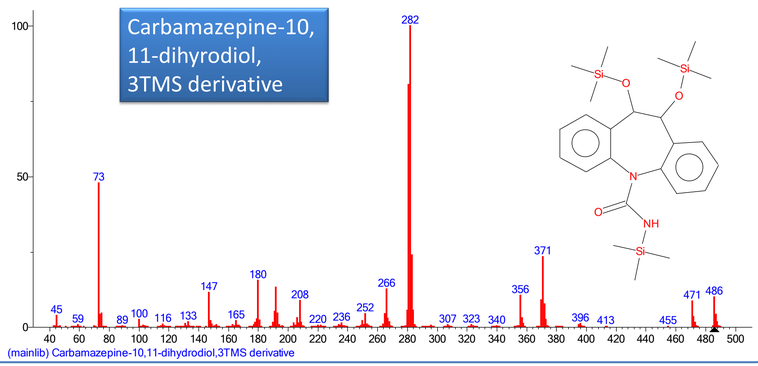






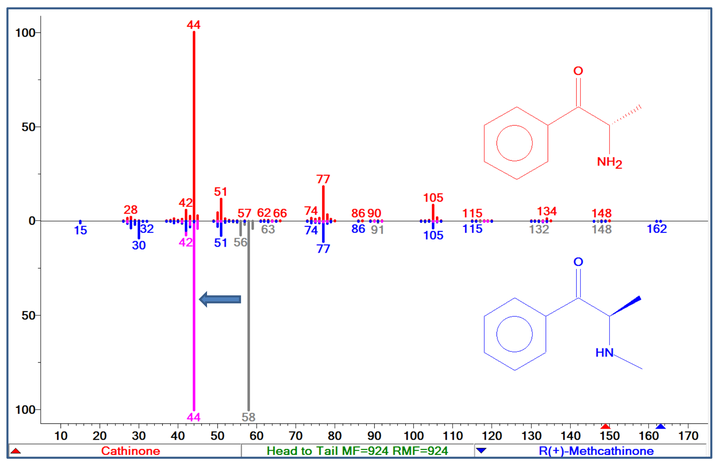


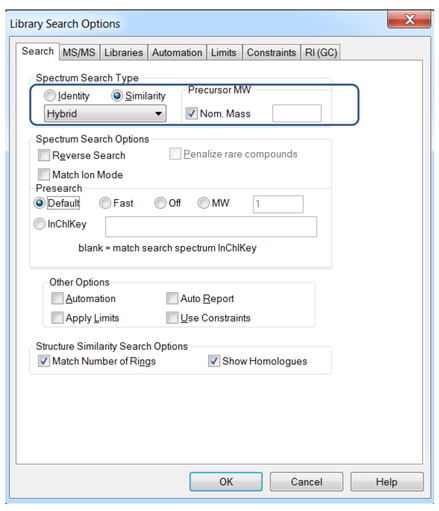




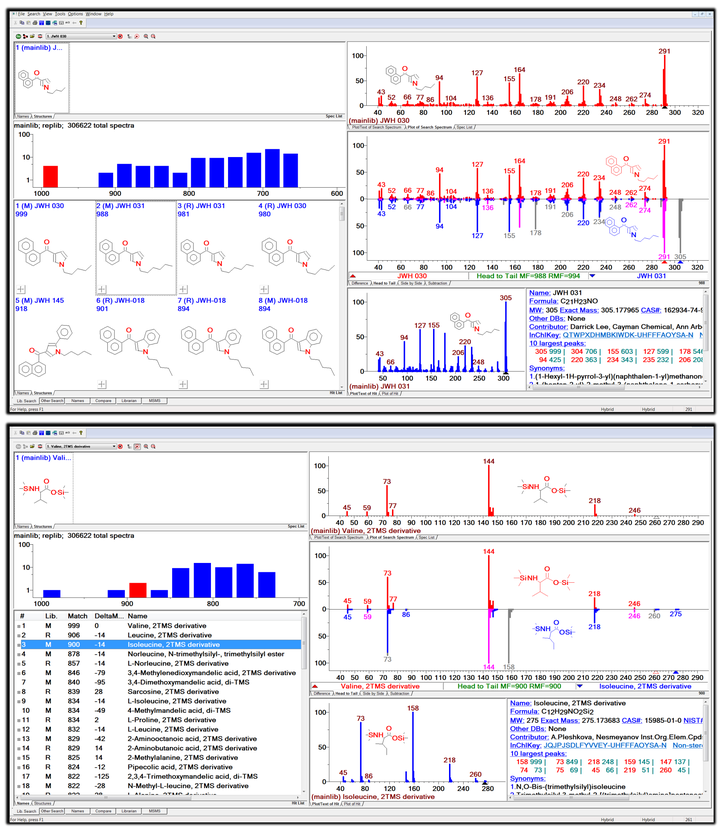
The Hybrid Spectrum Search

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

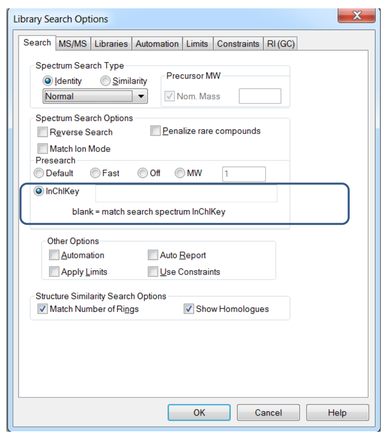


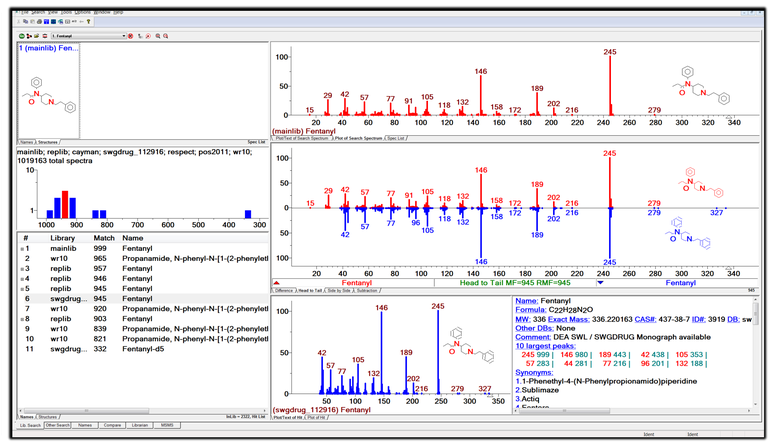


Can greatly increase the number of matching compounds, aiding ID and fragmentation mechanism



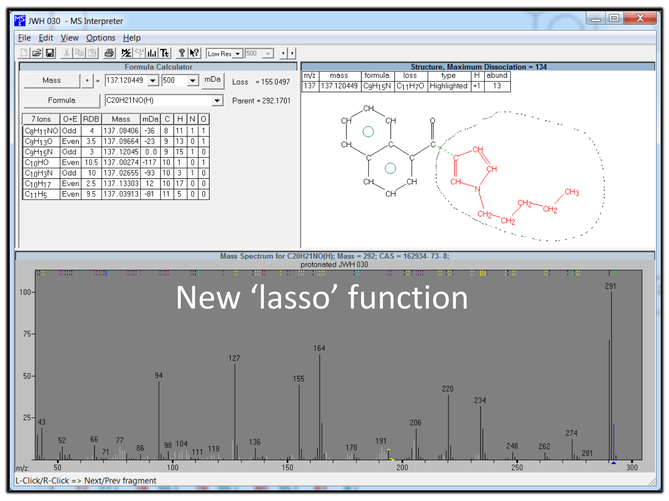
InChI Structure Search





Compare replicates within and between libraries

MS Interpreter Enhancement



Specify structure for mass calculation

http://chemdata.nist.gov

NIST National Institute of Standards and Technology
U.S. Department of Commerce