NIST Tandem Mass Spectral Library

2020 Release

31K Compounds, 2X More than 2017
186K Precursor Ions - 1.3M Spectra

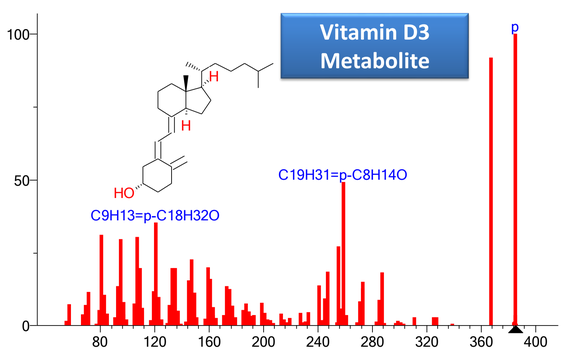
Fragmentation Methods

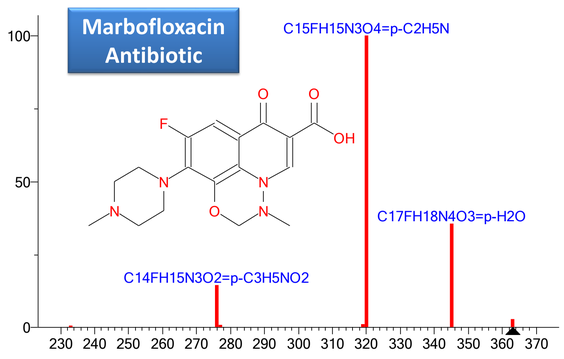
27,840 HRAM (High Res Accurate Mass) Compounds
29,890 QTOF, HCD, IT-HRAM, QqQ Compounds
29,444 Ion Trap Compounds (Low Res., up to MS^4)
246 APCI HRAM 'Extractables and Leachables'

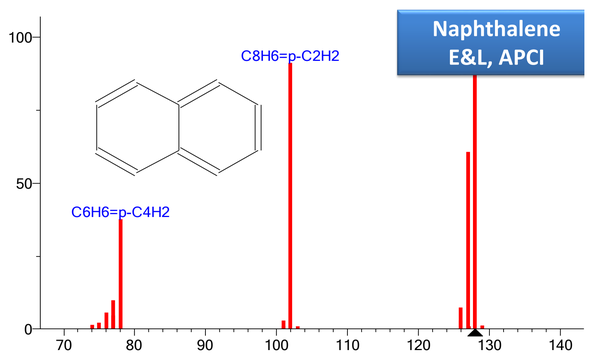
Precursor Ion Types

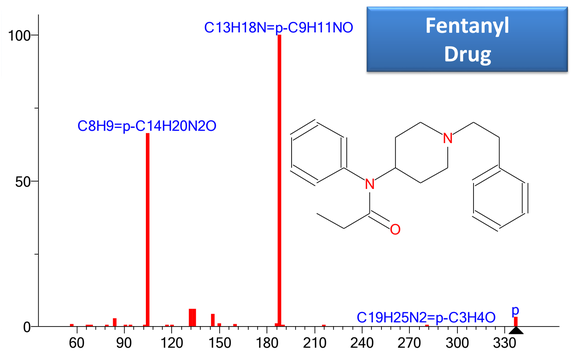
26,575 Protonated
12,589 Deprotonated
10,032 Water/Ammonia Loss
24,167 Other In-Source Generated

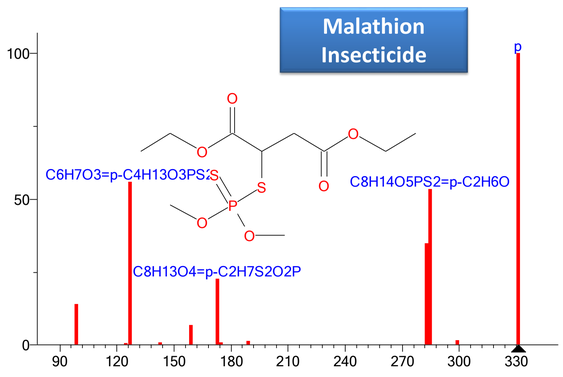
Wide Variety of Compounds

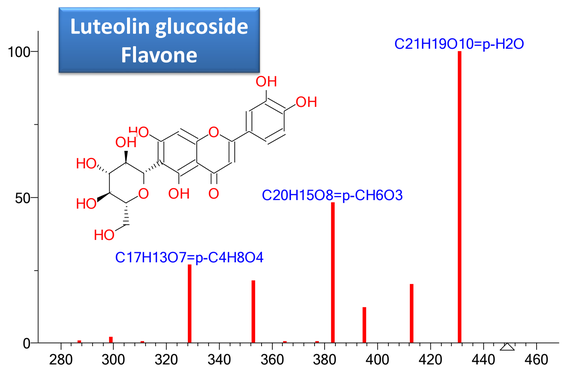


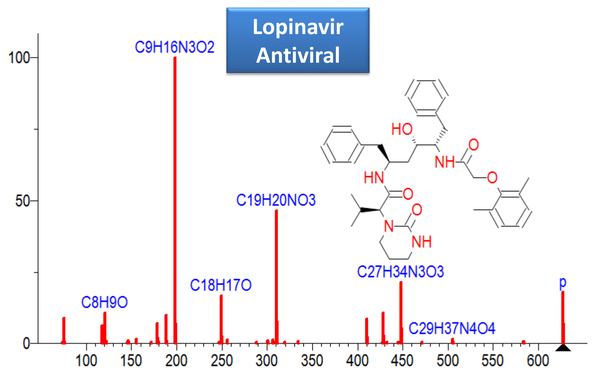


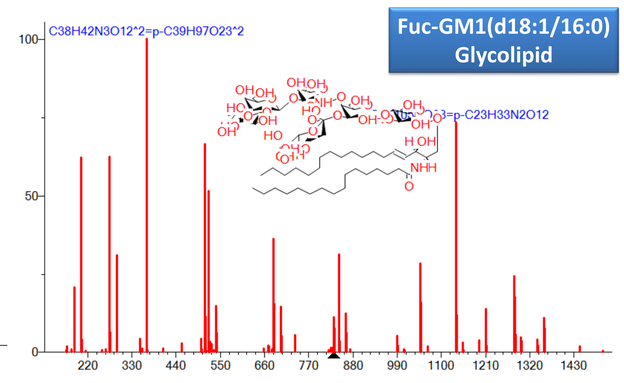




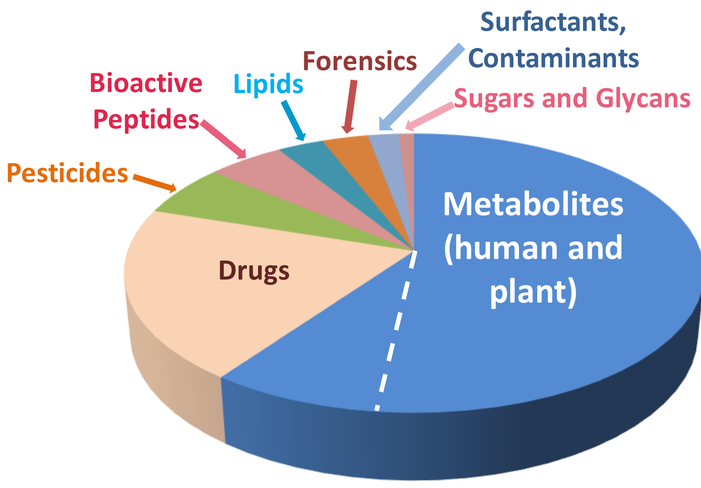








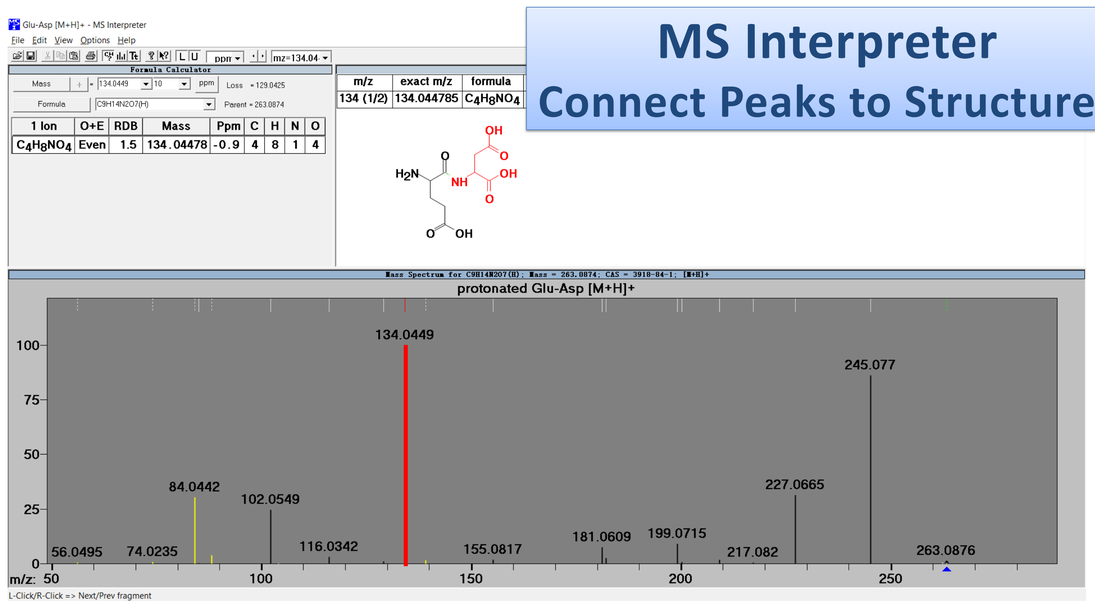
Types of Compounds and Spectra



75%(+) 25%(-)
32% MS^2 in-source
8% MS^3 and MS^4
Over wide energy range

6,000 human metabolites

MS Interpreter
Connect Peaks to Structures



Hybrid Search - Identify Compounds Not in the Library

http://chemdata.nist.gov

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