Freely Available

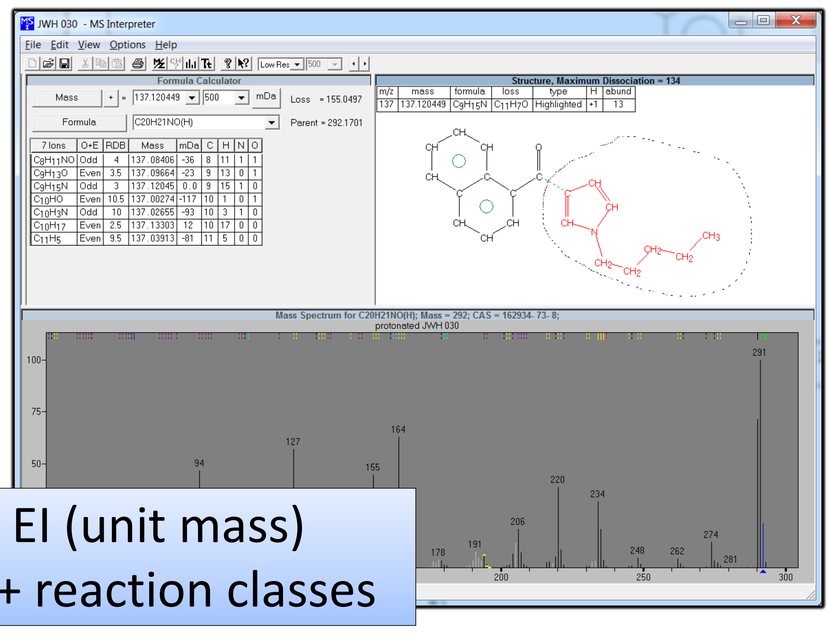
NIST MS Analysis Tools For EI and Tandem Spectra

Recently Updated

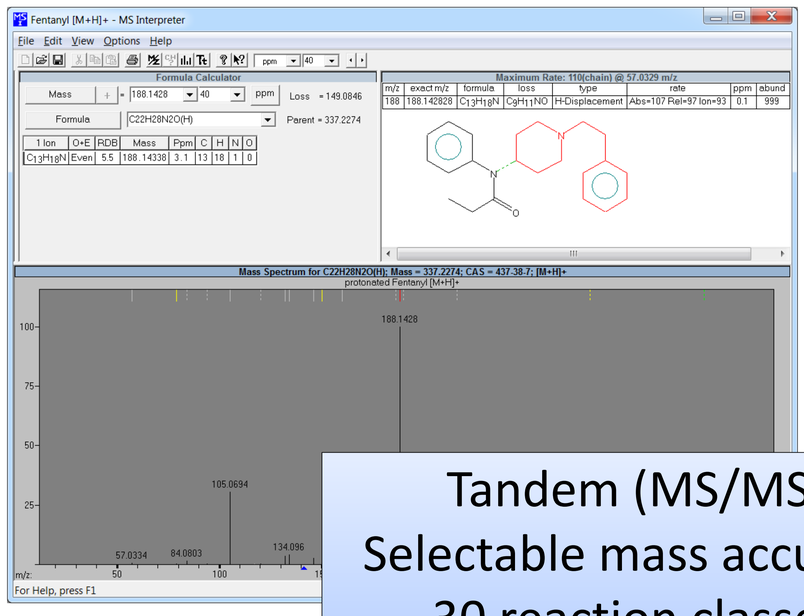
MS Interpreter – 2019 Version – Major Update

Fragmentation Analysis for GC/MS and LC/MS

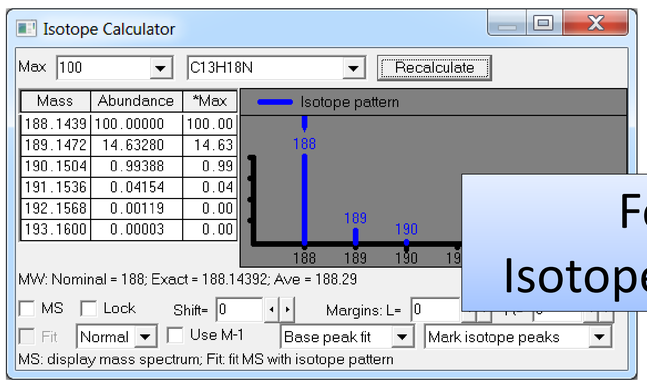
Click on a peak, See its Origin or Isotopic Envelope



EI (unit mass)
90+ reaction classes



Tandem (MS/MS)
Selectable mass accuracy
30 reaction classes
Uncertain peaks highlighted

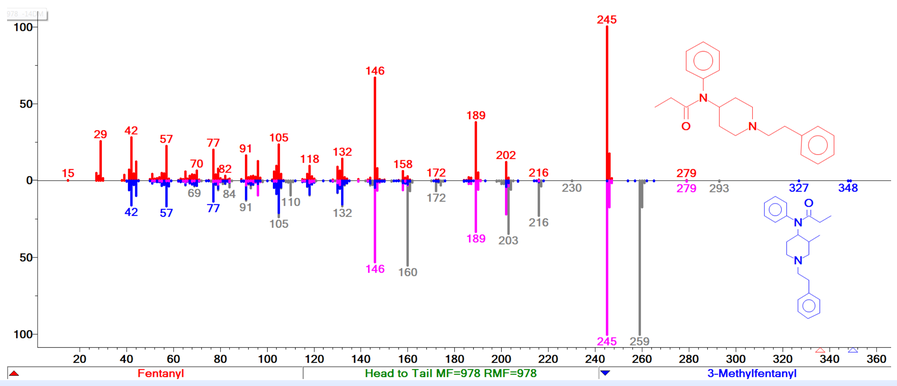


Formula
Isotope calculation

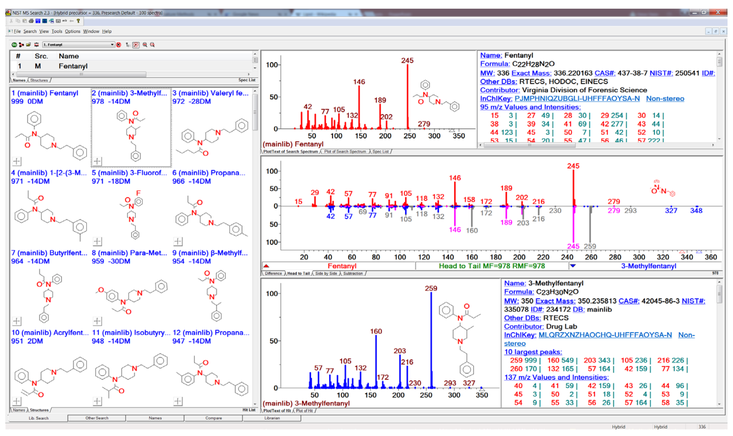
Direct link to NIST MS Libraries
Shows chemical origins of peaks
Rates based on thermochemical estimates
Many options

The Hybrid Spectrum Search – Huge Expansion of Chemical Space

EI – Major Advance in 'Mature' Area



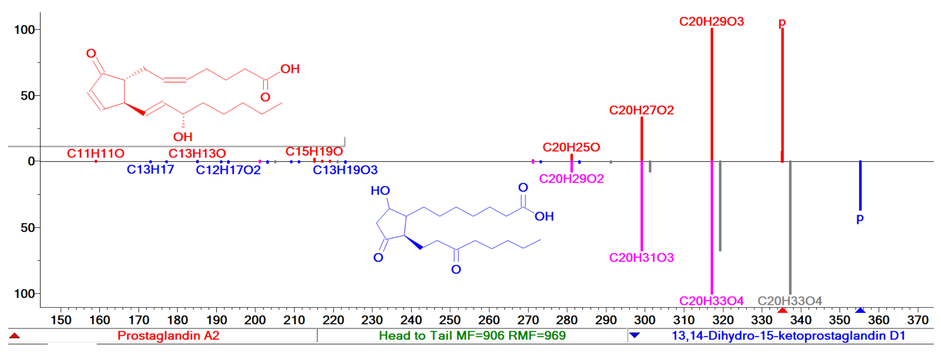
Shift peaks to match spectra for compounds that differ by an 'inert' chemical group. Both original and shifted peaks shown to aid structure analysis.



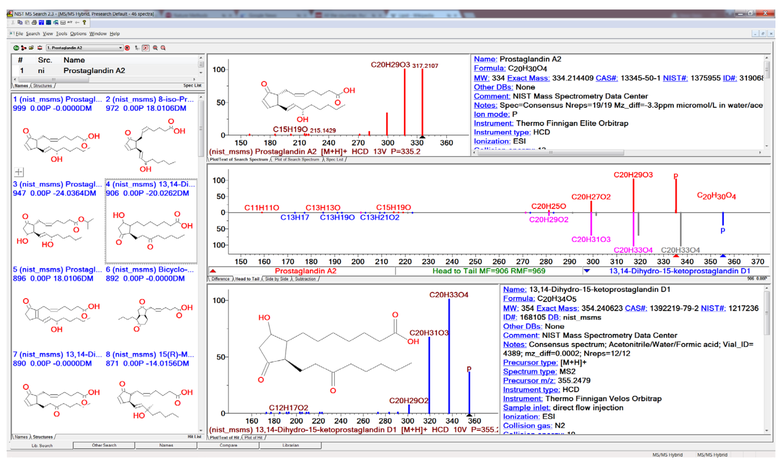
Can greatly increase the number of matching compounds, aiding ID and fragmentation interpretation

Derivatives, designer drugs, pesticides, botanicals, among many more classes. MW estimate required

Identifies 'Dark Matter' in LC/MS



Shown to increase identification rates from 12% to >90 % in Urine and Plasma



A large fraction of compounds in biological fluids are members of a small number of classes: ideal for the hybrid search

Lipids, amino acids, carnitines, nucleic acids, drugs, …
Compensates for larger search space and smaller library size of ESI generated ions

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Proteomics

The Hybrid Search: A Mass Spectral Library Search Method for Discovery of Modifications in Proteomics

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DOI: 10.1021/acs.jproteome.6b00988

Publication Date (Web): April 3, 2017

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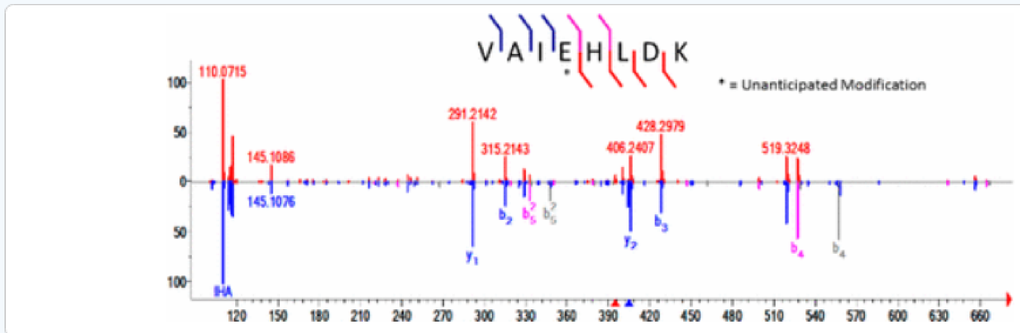
Abstract



We present a mass spectral library-based method to identify tandem mass spectra of peptides that contain unanticipated modifications and amino acid variants. We describe this as a “hybrid” method because it combines matching both ion *m*/*z* and mass losses. The mass loss is the difference between the mass of an ion peak and the mass of its precursor. This difference, termed DeltaMass, is used to shift the product ions in the library spectrum that contain the modification, thereby allowing library product ions that contain the unexpected modification to match the query spectrum. Clustered unidentified spectra from the Clinical Proteomic Tumor Analysis Consortium

Metabolomics/Tandem

Structure Annotation of All Mass Spectra in Untargeted Metabolomics

Ivana Blaženović†, Tobias Kind†, Michael R. Sa†, Jian Ji‡, Arpana Vaniya†, Benjamin Wancewicz†, Bryan S. Roberts†, Hrvoje Torbašinović§, Tack Lee∥, Sajjan S. Mehta†, Megan R. Showalter†, Hosook Song∥, Jessica Kwok†, Dieter Jahn⊥#, Jayoung Kim∇○•¶, and Oliver Fiehn*†

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Anal. Chem., **2019**, *91* (3), pp 2155–2162

DOI: 10.1021/acs.analchem.8b04698

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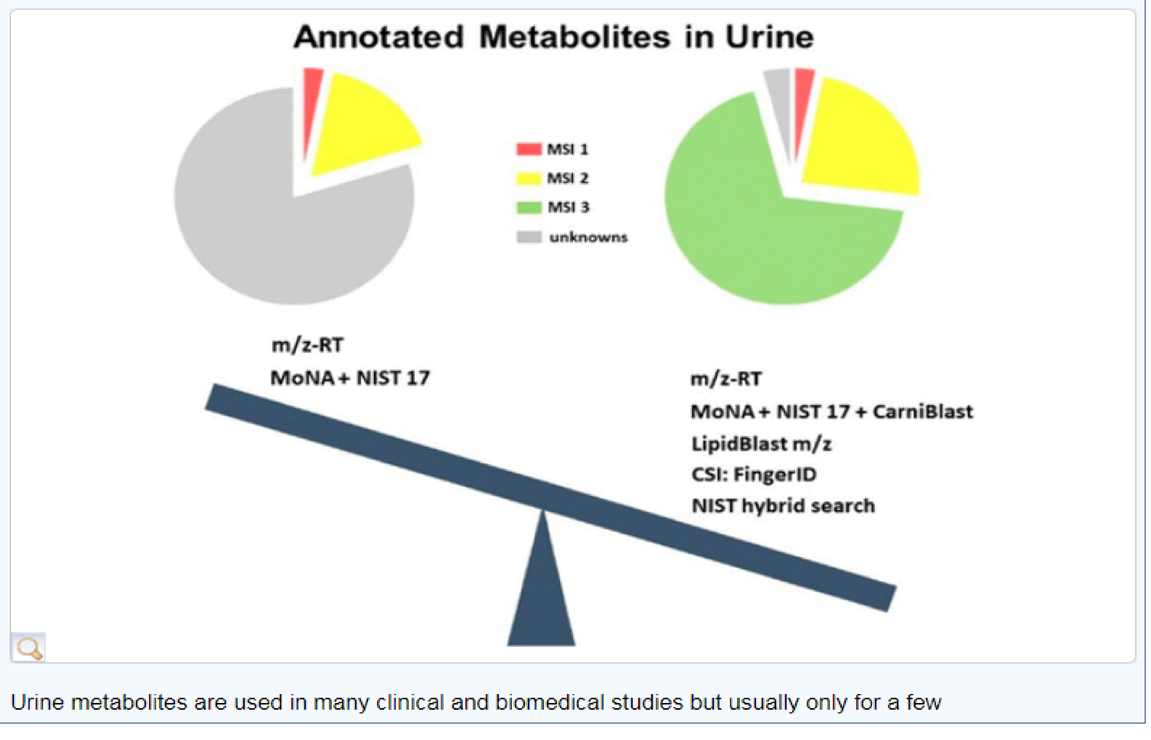
Abstract

Jump to a section



Urine metabolites are used in many clinical and biomedical studies but usually only for a few

GC/MS

Combining Fragment-Ion and Neutral-Loss Matching during Mass Spectral Library Searching: A New General Purpose Algorithm Applicable to Illicit Drug Identification

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Anal. Chem., **2017**, *89* (24), pp 13261–13268

DOI: 10.1021/acs.analchem.7b03320

Publication Date (Web): November 20, 2017

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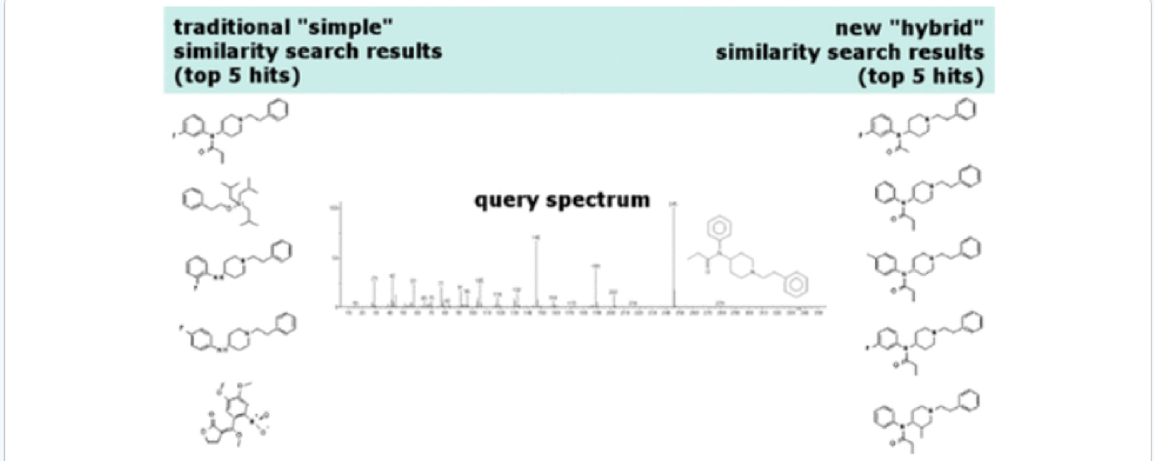
Abstract



A mass spectral library search algorithm that identifies compounds that differ from library compounds by a single “inert” structural component is described. This algorithm, the *Hybrid Similarity Search*, generates a similarity score based on matching both fragment ions and neutral losses. It employs the parameter DeltaMass, defined as the mass difference between query and library compounds, to shift neutral loss peaks in the library spectrum to match corresponding neutral loss peaks in the query spectrum. When the spectra being compared differ by a single

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