Freely Available

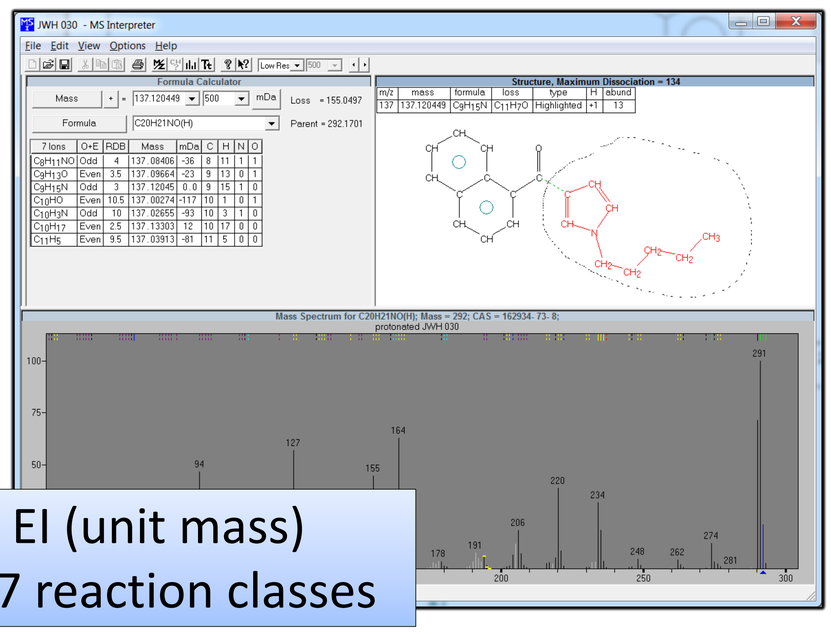
NIST MS Analysis Tools For EI and Tandem Spectra

Recently Updated

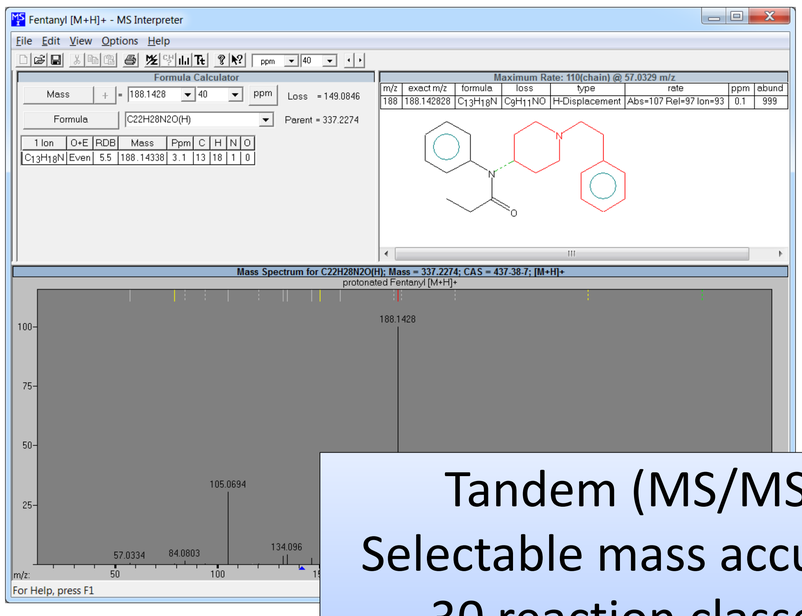
MS Interpreter – 2020 Version – Major Update

Fragmentation Analysis for GC/MS and LC/MS

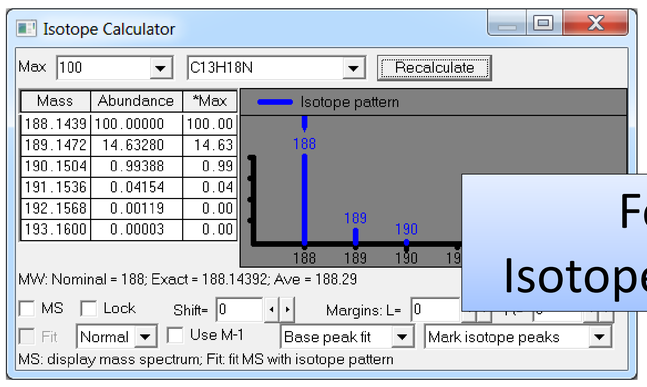
Click on a peak, See its Origin or Isotopic Envelope



EI (unit mass)
107 reaction classes



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

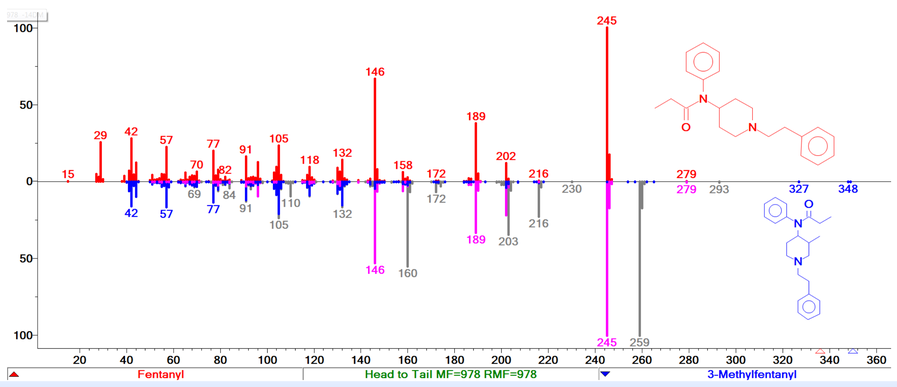


Formula
Isotope calculation

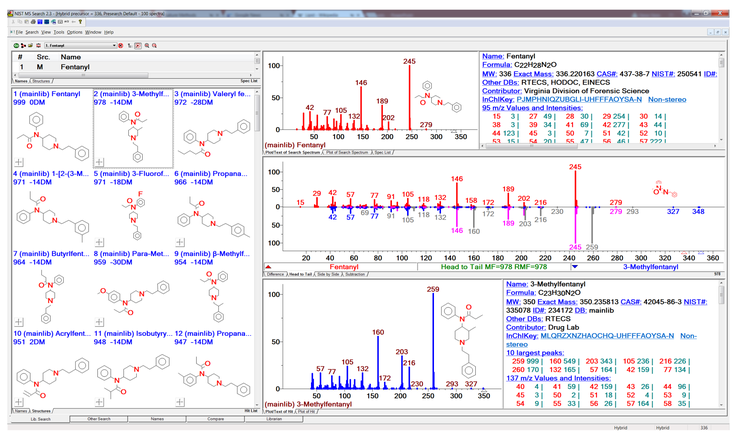
Direct link to NIST MS Libraries
Shows chemical origins of peaks
Rates based on thermochemistry
Many display options

The Hybrid Spectrum Search – Huge Expansion of Chemical Space

EI – Major Advance in 'Mature' Area



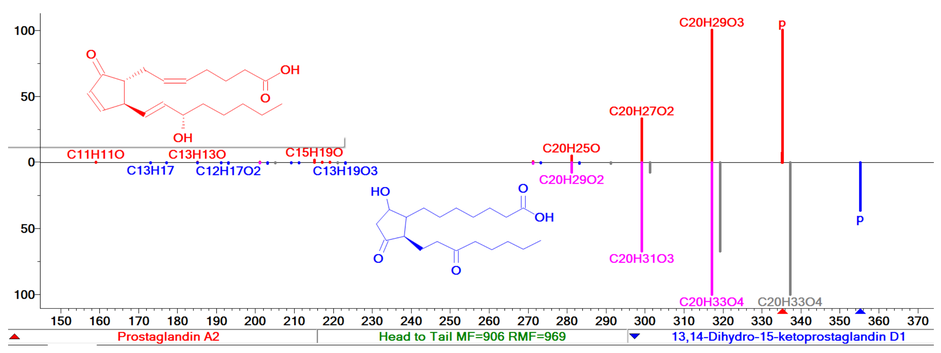
Shift peaks to match spectra for compounds that differ by an 'inert' chemical group. Both original and shifted peaks shown to aid structure analysis.



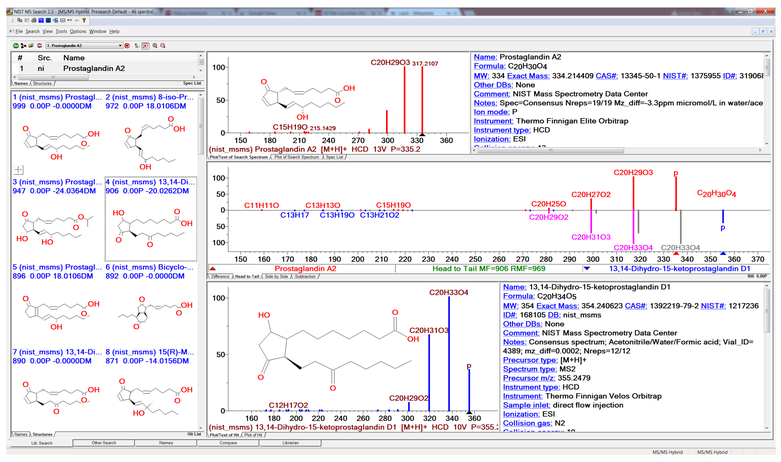
Can greatly increase the number of matching compounds, aiding ID and fragmentation interpretation

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 of ESI generated ions

http://chemdata.nist.gov

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

Hybrid Search Applications

Tandem MS

analytical chemistry

Article

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pubs.acs.org/ac

Hybrid Search: A Method for Identifying Metabolites Absent from Tandem Mass Spectrometry Libraries

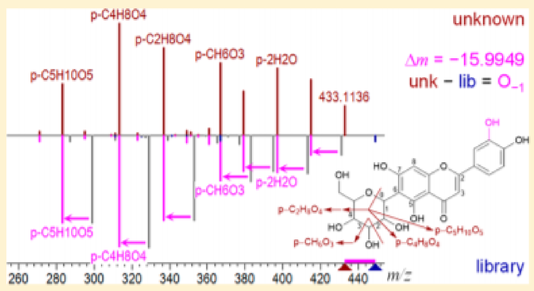
Brian T. Cooper,*[†,‡] Xinjian Yan,[‡] Yamil Simón-Manso,[‡] Dmitrii V. Tchekhovskoi,[‡] Yuri A. Mirokhin,[‡] and Stephen E. Stein[‡]

[†]Department of Chemistry, University of North Carolina at Charlotte, Charlotte, North Carolina 28223, United States

[‡]Mass Spectrometry Data Center, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, United States

Supporting Information

ABSTRACT: Metabolomics has a critical need for better tools for mass spectral identification. Common metabolites may be identified by searching libraries of tandem mass spectra, which offers important advantages over other approaches to identification. But tandem libraries are not nearly complete enough to represent the full molecular diversity present in complex biological samples. We present a novel hybrid search method that can help identify metabolites not in the library by similarity to compounds that are. We call it "hybrid" searching because it combines conventional, direct peak matching with the logical equivalent of neutral-loss matching. A successful hybrid search requires the library to contain "cognates" of the unknown: similar compounds with a structural difference confined to a single region of the molecule, that does not substantially alter its fragmentation behavior. We demonstrate that the hybrid search is highly likely to find similar compounds under such circumstances.



Proteomics

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

Meghan C. Burke*[†], Yuri A. Mirokhin[†], Dmitrii V. Tchekhovskoi[†], Sanford P. Markey[†], Jenny Heidbrink Thompson[‡], Christopher Larkin[‡], and Stephen E. Stein[†]

[†] Mass Spectrometry Data Center, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, Maryland 20899, United States

[‡] Analytical Sciences, MedImmune LLC, One MedImmune Way, Gaithersburg, Maryland 20878, United States

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DOI: 10.1021/acs.jproteome.6b00988

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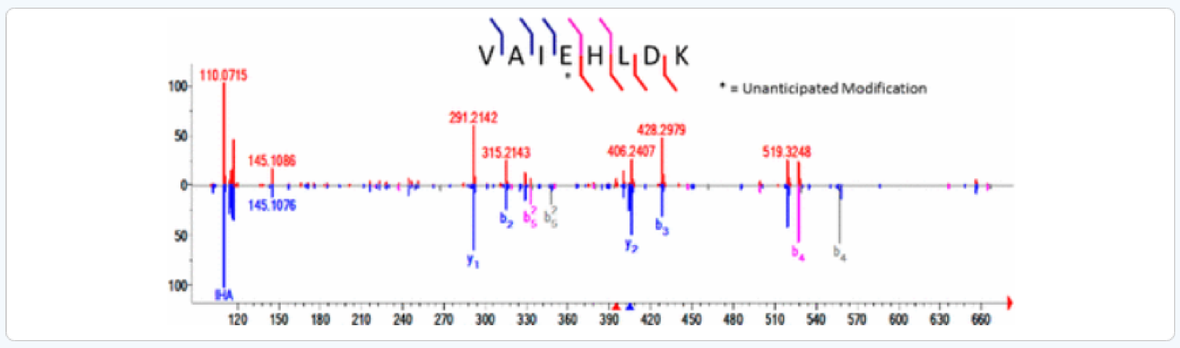
*E-mail: meghan.burke@nist.gov.

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

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*[†]

[†] West Coast Metabolomics Center, University of California, Davis, Davis, California 95616, United States

[‡] School of Food Science, State Key Laboratory of Food Science and Technology, Jiangnan University, Wuxi, Jiangsu 330047, China

[§] Inovatus Ltd., Zagreb 10000, Croatia

[∥] Department of Urology, Inha University College of Medicine, Incheon 22212, South Korea

[⊥] Institute of Microbiology, Technische Universität Braunschweig, Braunschweig 38106, Germany

[#] Braunschweig Integrated Centre of Systems Biology (BRICS), Technische Universität Braunschweig, Braunschweig 38106, Germany

[▽] Departments of Surgery and Biomedical Sciences, Cedars-Sinai Medical Center, Los Angeles, California 90048, United States

[○] Department of Medicine, University of California Los Angeles, Los Angeles, California 90095, United States

[•] Samuel Oschin Comprehensive Cancer Institute, Cedars-Sinai Medical Center, Los Angeles, California 90048, United States

[¶] Department of Urology, Ga Cheon University College of Medicine, Incheon 22212, South Korea

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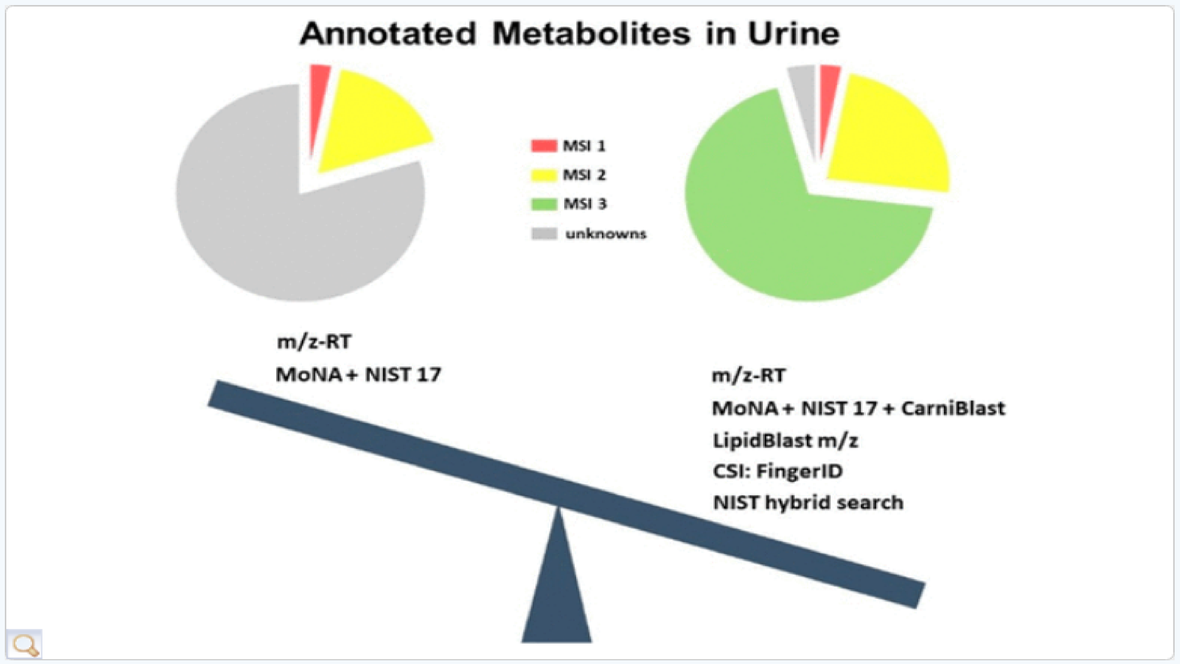
DOI: 10.1021/acs.analchem.8b04698

Publication Date (Web): January 4, 2019

*Phone +1-530-754-8258 (office), +1-530-752-9922 (lab), +1-530-723-4450 (cell). Corresponding author address: NIH West Coast Metabolomics Center, UC Davis Genome Center, Room 1313, 451 Health Sci Drive, Davis, CA 95616.

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

Arun S. Moorthy*[†], William E. Wallace[†], Anthony J. Kearsley[‡], Dmitrii V. Tchekhovskoi[†], and Stephen E. Stein[†]

[†] Mass Spectrometry Data Center, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, United States

[‡] Applied and Computational Mathematics Division, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, United States

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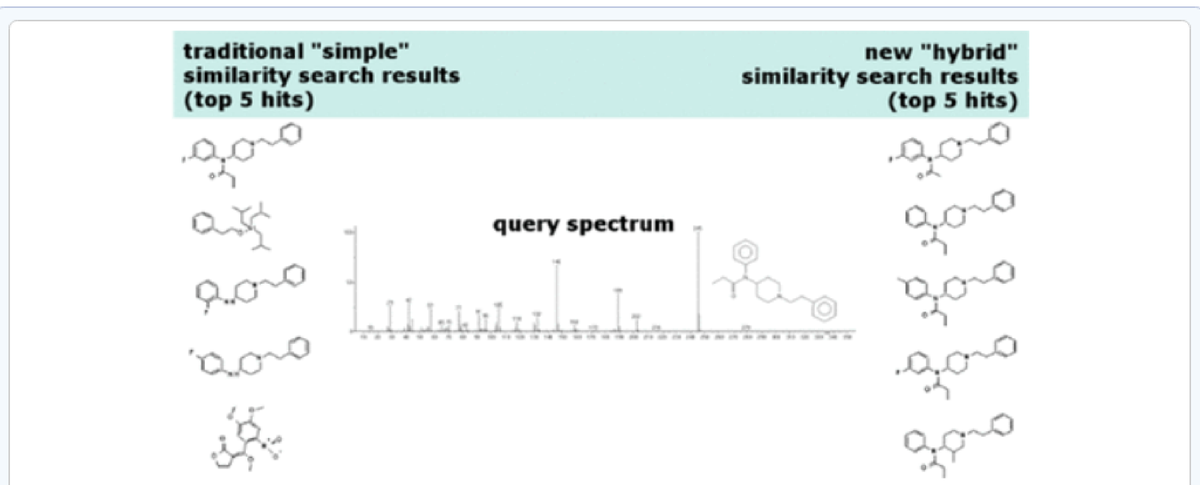
DOI: 10.1021/acs.analchem.7b03320

Publication Date (Web): November 20, 2017

*E-mail: arun.moorthy@nist.gov.

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