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LDA 2 – graphical software package for flexible automatic lipid identification for LC-MS^n data

Highly specific and sensitive detection and quantitation of metabolites due to flexible MS^n structure identification and 3D peak detection.

Ref.no.: E_576

KEYWORDS:
LC-MS^n
Identification
Quantitation
Lipidomics
Metabolomics
Algorithm
Software
Specificity
Sensitivity

INVENTORS:
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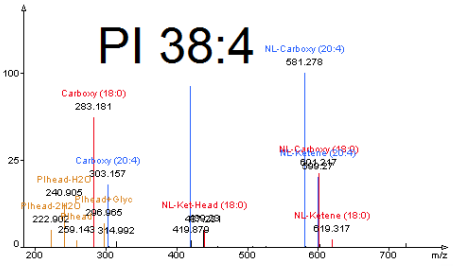
COOPERATION OPTIONS:
- Licensing
- Technical co-operation
- Consulting

DEVELOPMENT STATUS:
Fully operational software package for lipids, including basic statistical tools. Tested on various lipid classes and MS machines

STATUS OF PATENTS:
- EP application
- US-application

BACKGROUND

LC-MS is the most sensitive and specific technique for the analysis of metabolites in general and lipids in particular. However, due to the complex metabolite fragmentation behavior and peak overlaps in MS^1 data, a reliable and generally applicable solution is missing. Existing solutions rely on databases containing fragments which hardly allow the definition of fragments by users or exploit the intensity information of spectra.



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The software package is superior to conventional approaches due to three major innovations: (i) a reliable 3D peak detection algorithm that confines the peak borders in m/z and time direction; (ii) a flexible language for defining of expected MS^n fragments and the relative intensities thereof, and an algorithm that returns structural information about the metabolites (in the case of lipids: head group, fatty acid composition, regio-isomeric position of the fatty acids); (iii) an algorithm for the prediction of the retention time of metabolites from the same class to remove isobaric hits.

ADVANTAGES

We provide an application (algorithms and graphical software package) for the automated identification of structural information and quantitation of lipids based on MS^n data. The expected MS^n fragments and their intensity relationships can be easily defined/changed due to an intuitive mechanism supported by visual feedback. As such the software can flexibly accommodate for changes in the fragmentation behavior (collision energy, adduct ions, MS level, charge state). These changes can be applied by the end users themselves without specific IT knowledge. A sophisticated quantitation algorithm reliably separates overlapping peak intensities and guarantees for accurate and highly specific quantitation. Both methods in concert with an optional retention time prediction algorithm allow for automated identification and quantitation of even very low abundant lipid species where no fragmentation spectra are available.

POTENTIAL FIELDS OF APPLICATION

- General: identification and quantitation of any kind of molecules detected by LC MS^n, including various metabolites, particularly lipids.
- Biological, pharmaceutical and medical research: identification and quantitation of metabolite composition of cells, tissue, and body fluids, and detection of potential drug targets.
- Clinical application: diagnostic purposes, risk prediction of future life threatening events, monitoring progress or treatment of a disease, and determination of effectiveness of treatment
- Food: food quality, identification of food origin, and detection of adulterations
- Chemical industry: identification and quantitation of chemical composition of various analytes, e.g. oils.

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