New Literature regarding MZMine 2, XCMS, and MS-Dial

Krystle Ong, Christian Fay, & Luke Potter
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analytical chemistry

Article

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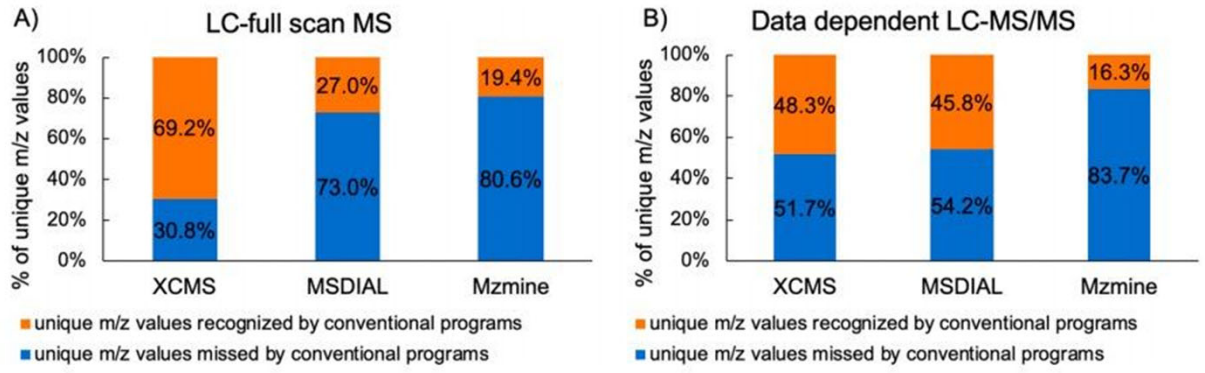
Enhancing Metabolome Coverage in Data-Dependent LC−MS/MS Analysis through an Integrated Feature Extraction Strategy

Yaxi Hu,[†,‡] Betty Cai,[†] and Tao Huan*[,†]

[†]Department of Chemistry, Faculty of Science, University of British Columbia, 2036 Main Mall, Vancouver V6T 1Z1, British Columbia, Canada

[‡]Food, Nutrition and Health Program, Faculty of Land and Food Systems, University of British Columbia, Vancouver V6T 1Z4, British Columbia, Canada

False negative results



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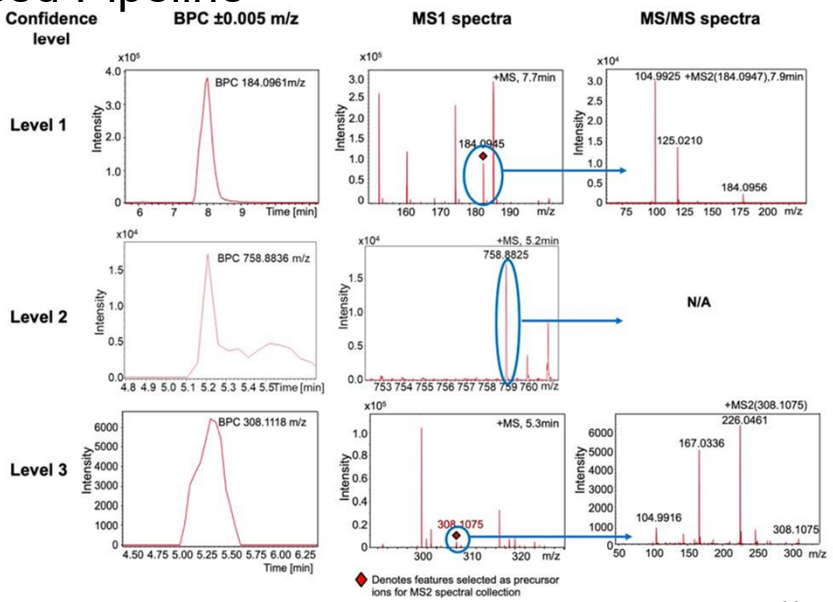
Enhanced Pipeline



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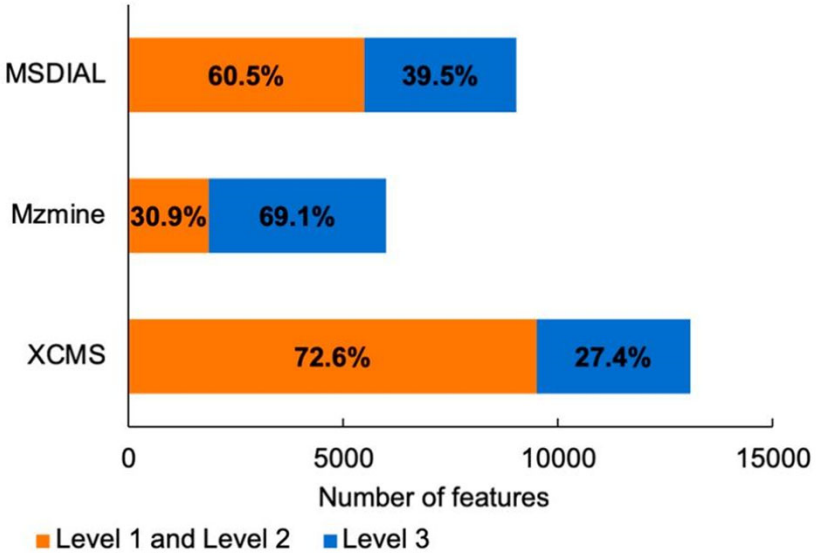
MSDIAL: Missed features



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Proof of Concept: using XCMS

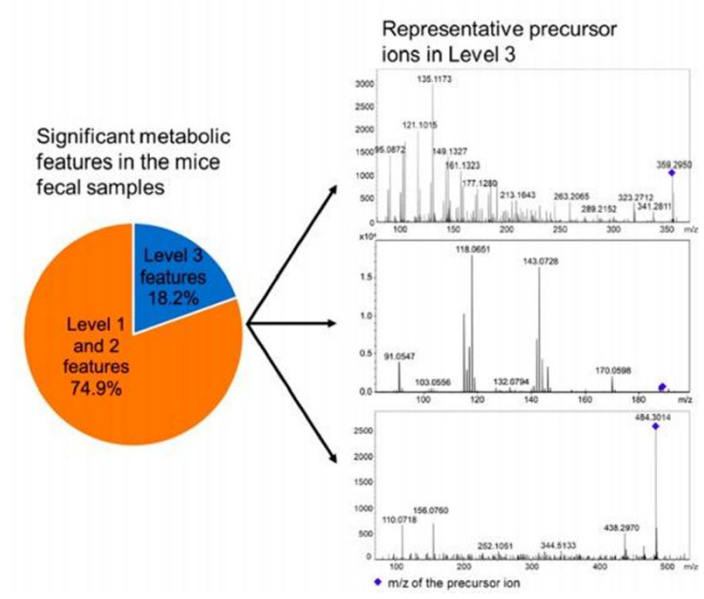

Table S3. Manually annotated level 3 metabolic features.

m/z	Retention time (s)	MS-finder score	Error (ppm)	Manually annotated by MS-Finder	Biological functions (fold change: high fat diet/normal diet)
176.1029	17.71	8.14	3.24	Citrulline	An amino acid made from ornithine and carbamoyl phosphate in one of the central reactions in the urea cycle. Also produced from arginine. (fold change: 0.66, p-value: 0.044)
177.0551	185.20	7.12	-2.72	Ureidosuccinic acid	An intermediary product in pyrimidine biosynthesis. (fold change: 3.21, p-value: 0.012)
357.2783	355.82	7.29	1.42	Tetracosahexaenoic acid	A precursor of docosahexaenoic acid that is formed from dietary linolenic acid. (fold change: 0.42, p-value: 0.004)
362.2690	430.34	6.67	-0.08	N-Arachidonoyl glycine	An endogenous lipid acts as an efficacious agonist at GRP18 to trigger anti-nociceptive and anti-inflammatory activities. (fold change: 0.38, p-value: 0.004)
377.1458	166.21	8.93	0.69	Riboflavin	Supports energy production by aiding the metabolism of fats, carbohydrates and proteins. (fold change: 2.06, p-value: 0.031)

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XCMS

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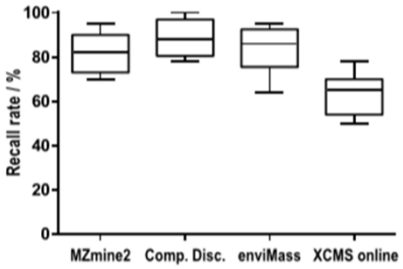
Comparison of Software Tools for Liquid Chromatography−High-Resolution Mass Spectrometry Data Processing in Nontarget Screening of Environmental Samples

Lotta L. Hohrenk,[†,§] Fabian Itzel,[‡,§] Nicolai Baetz,[†,‡] Jochen Tuerk,[‡,§] Maryam Vosough,[∥] and Torsten C. Schmidt*[,†,§,⊥]

[†]Instrumental Analytical Chemistry, University of Duisburg-Essen, Universitätsstrasse 5, D-45141 Essen, Germany
[‡]Institut für Energie- und Umwelttechnik e. V., Bliersheimer Strasse 58-60, 47229 Duisburg, Germany
[§]Centre for Water and Environmental Research, University of Duisburg-Essen, Universitätsstrasse 2, 45141 Essen, Germany
[∥]Department of Clean Technologies, Chemistry and Chemical Engineering, Research Center of Iran, P.O. Box 14335-186, Tehran 1496813151, Iran
[⊥]IWW Water Center, Moritzstrasse 26, 45476 Mülheim an der Ruhr, Germany

XCMS

- XCMS has a lot more “false” peaks that are from noise compared to other software
- XCMS has a higher chance of finding the compound of interest when comparing it to other softwares such as enviMass and MZmine2
- Hohrenk et al. used FOR-IDENT to see if different softwares would lead to altered final interpretation of the results but showed that all gave similar interpretations regardless of feature detection lists



$$\text{recall rate} = \frac{\text{true positives}}{\text{total number of true positives}} \times 100\%$$

Hohrenk et al. 2020. Analytical Chemistry

XCMS

metabolites

MDPI

Article

A Case Report of Switching from Specific Vendor-Based to R-Based Pipelines for Untargeted LC-MS Metabolomics

Álvaro Fernández-Ochoa [1,2,*], Rosa Quirantes-Piné [2], Isabel Borrás-Linares [2], María de la Luz Cádiz-Gurrea [1,2,*], PRECISESADS Clinical Consortium [†], Marta E. Alarcón Riquelme [3], Carl Brunius [4,*,‡] and Antonio Segura-Carretero [1,2,‡]

1 Department of Analytical Chemistry, Faculty of Sciences, University of Granada, Av Fuentenueva s/n, 18071 Granada, Spain; ansegura@ugr.es
2 Research and Development of Functional Food Centre (CIDAF), Health Science Technological Park, Av del Conocimiento, No. 37, s/n, 18016 Granada, Spain; rquirantes@cidaf.es (R.Q.-P.); iborras@cidaf.es (I.B.-L.)
3 Centre for Genomics and Oncological Research (GENYO), Pfizer-University of Granada-Andalusian Government, Health Science Technological Park, Av de la Ilustración 114, 18016 Granada, Spain; marta.alarcon@genyo.es
4 Department of Biology and Biological Engineering, Chalmers University of Technology, SE-412 96 Gothenburg, Sweden
* Correspondence: alvaroferochoa@ugr.es (Á.F.-O.); mluzcadiz@ugr.es (M.d.l.L.C.-G.); carl.brunius@chalmers.se (C.B.); Tel.: +34-958-637-206 (Á.F.-O.)
† Membership of the PRECISESADS Clinical Consortium is provided in the Acknowledgment section.
‡ These authors share co-senior authorship.

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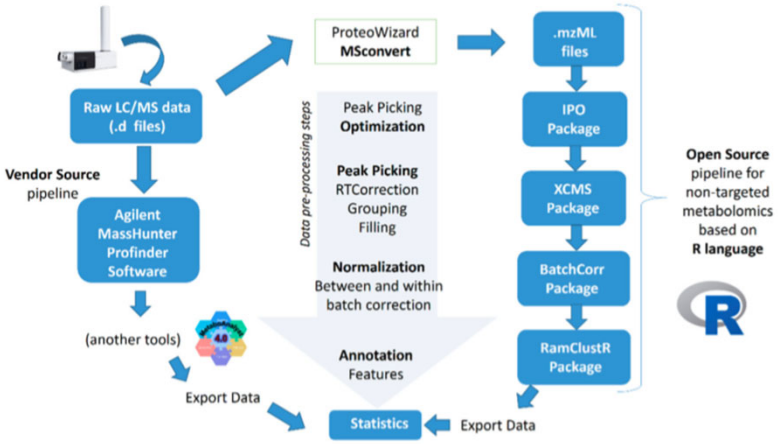
check for updates

XCMS

Profinder Software Methodology		R-Based Methodology	
✓	✗	✓	✗
Easy to use, user-friendly interface	License fee	Open source	Steep learning curve
High quality of the plots	Limited capacity to process a high number of samples	Greater number of packages, functions, and methods (e.g., normalization)	Low plot quality (plots obtained with the specific R packages used)
No need to transform the format of the data	Few normalization techniques. Difficulties to normalize large between-batch effects	High capacity for faster processing of a high number of samples	Data format transformation
Easy to inspect features, integration results, and MS spectra. Easy to predict molecular formula	Errors in peak integration	Possibility of carrying out all the steps of pre-processing and statistical analysis in the same environment	More cumbersome to show integration results, MS spectra, and to predict molecular formula
Easy to manually correct areas	Low control of the processing (only some parameters can be modified)	Flexibility and versatility	Some level of coding skills is required

Modified from: Fernández-Ochoa et al. 2020. Metabolites

XCMS



MS-Dial

Analytical and Bioanalytical Chemistry
pp 1–12 | Cite as

Lipidomic profiling of non-mineralized dental plaque and biofilm by untargeted UHPLC-QTOF-MS/MS and SWATH acquisition

Authors | Authors and affiliations

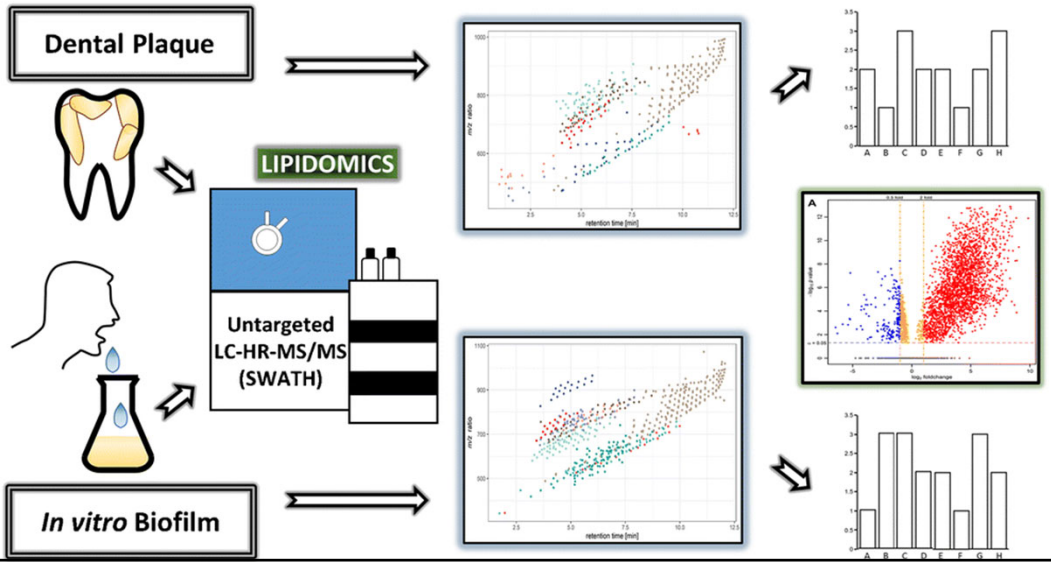
Bernhard Drotleff, Simon R. Roth, Kerstin Henkel, Carlos Calderón, Jörg Schlotterbeck, Merja A. Neukamm, Michael Lämmerhofer

Open Access | Research Paper
First Online: 15 January 2020

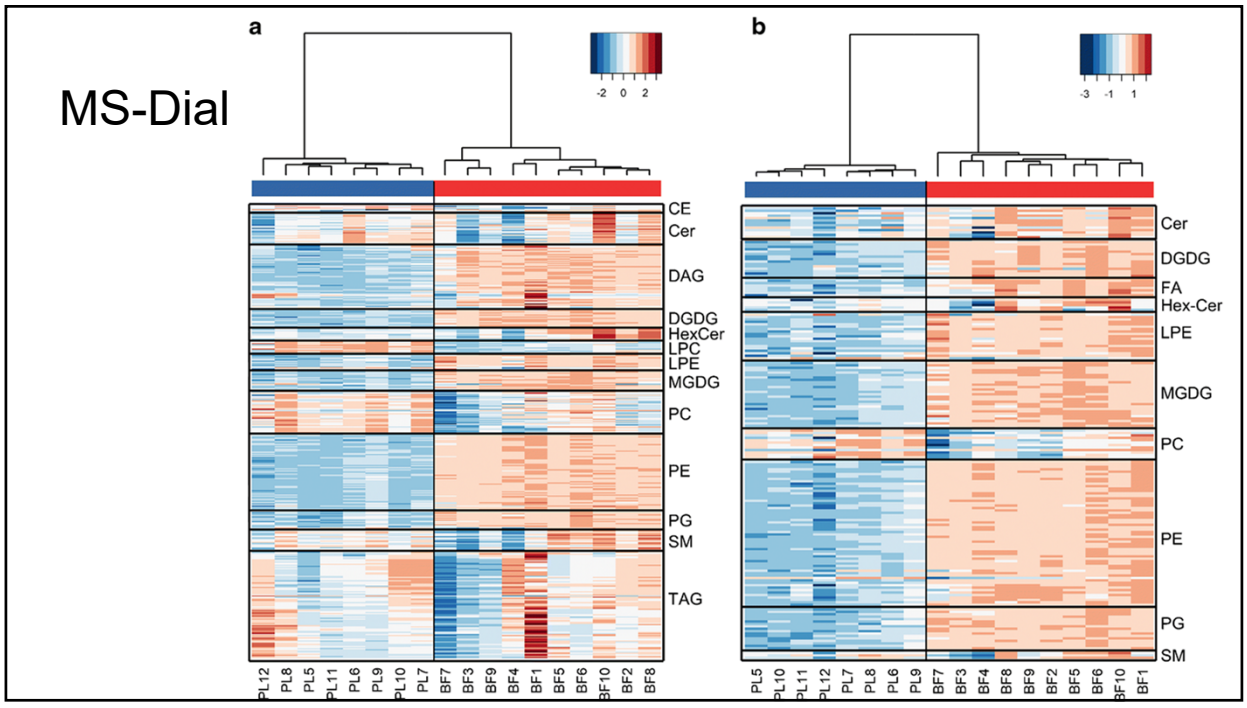
MS-Dial

- Purpose of the study: “a comprehensive lipidomic profiling for determination of lipid compositions of in vivo dental plaque samples and of in vitro cultivated biofilm”

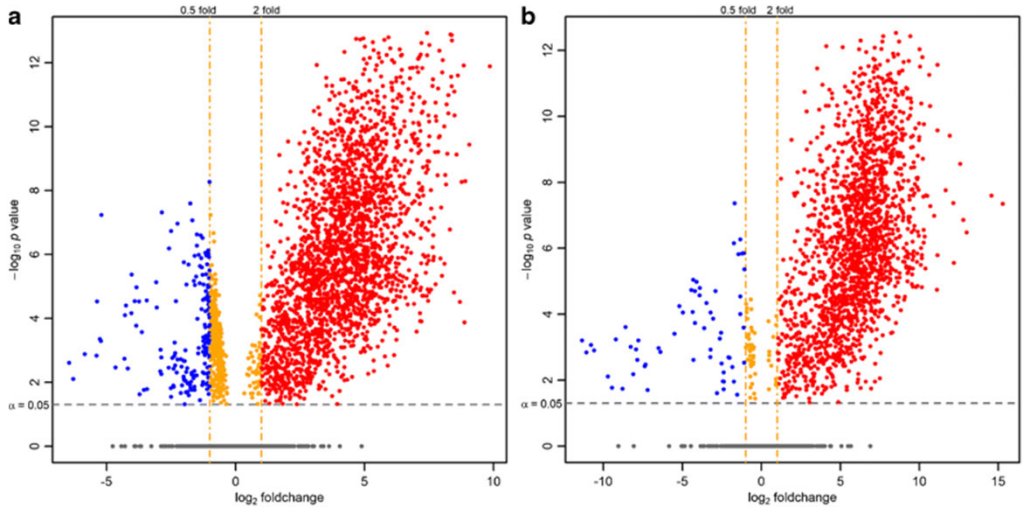
MS-Dial



MS-Dial



MS-Dial



MS-Dial