University of Groningen

Toward Global Metabolomics Analysis with Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry

Creek, Darren J.; Jankevics, Andris; Breitling, Rainer; Watson, David G.; Barrett, Michael P.; Burgess, Karl E. V.

Published in:
Analytical Chemistry

DOI:
10.1021/ac2021823

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2011

Link to publication in University of Groningen/UMCG research database

Citation for published version (APA):
Creek, D. J., Jankevics, A., Breitling, R., Watson, D. G., Barrett, M. P., & Burgess, K. E. V. (2011). Toward Global Metabolomics Analysis with Hydrophilic Interaction Liquid Chromatography-Mass Spectrometry: Improved Metabolite Identification by Retention Time Prediction. *Analytical Chemistry*, *83*(22), 8703-8710. https://doi.org/10.1021/ac2021823

Copyright
Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

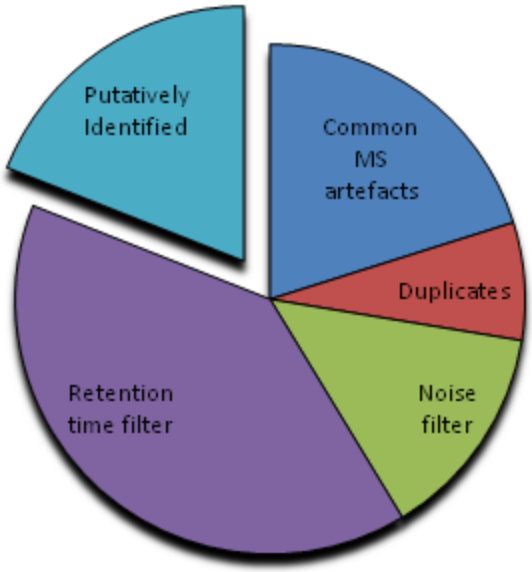
The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment.

Take-down policy
If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): http://www.rug.nl/research/portal. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Supporting information 4: (A) Distribution of 3,133 putatively identified peaks from the mixtures of metabolite standards. 627 peaks were putatively identified; 1,314 peaks rejected based on predicted retention time; 455 were classified as noise if they had very small peaks (< 10,000) or were present in blank samples; 247 were annotated as duplicate or shoulder peaks based on mass and retention time; 667 were common MS artefacts such as isotopes, adducts and fragments (B). (B) Common related peaks observed on HILIC-Orbitrap platform for automated removal in data processing by matching the mass difference (within 3 ppm) and retention time (within 9 seconds) if the peak has a lower intensity than the base peak.

A



B

Related peak	Mass difference
^{13}C isotopes	+1.003355
^{15}N isotopes	+0.997035
^{18}O isotopes	+2.004245
^{34}S isotopes	+1.995796
^{37}Cl isotopes	+1.997050
Double charge	Mass/2
Triple charge	Mass/3
Sodium adduct	+21.98194
Potassium adduct	+37.95588
Sodium–potassium exchange	+15.97394
Sodium–ammonium exchange	–4.95540
Sodium formate adduct	+67.98740
Acetonitrile adduct	+41.02655
Acetonitrile and sodium adduct	+63.00849
Ammonium adduct	+17.02655
Water loss	–18.01057
CO_2 loss	–43.98983
Formic acid loss	–46.00548
Ammonium loss	–17.02655
Centroid/ apodisation artefact	+/– <0.9 [a]

a) Only if peak intensity >50-fold lower than the base peak