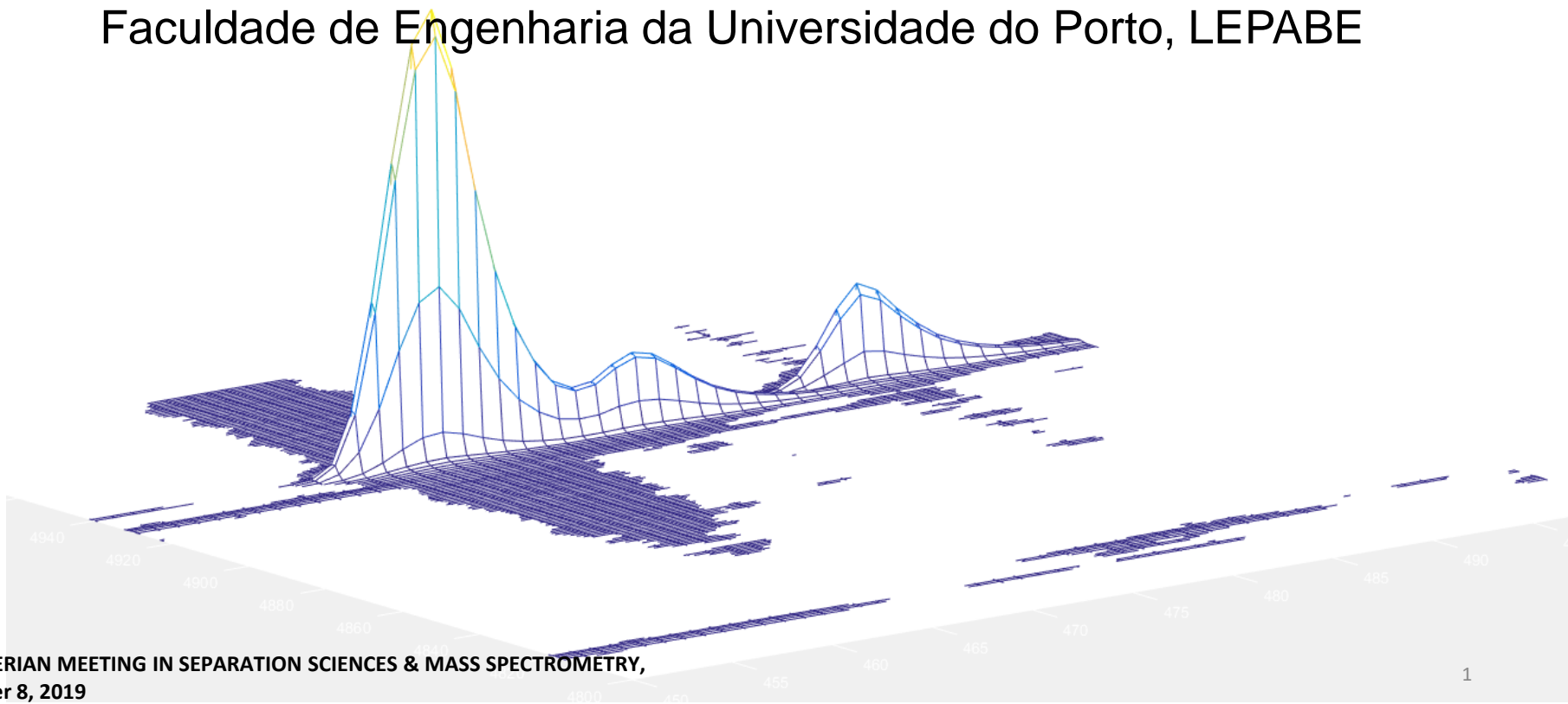


Untargeted metabolomics of full scan MS hyphenated data – mining for minor peaks with Finnee, risks and benefit

Guillaume Erny, Arminda Alves,
Faculdade de Engenharia da Universidade do Porto, LEPABE



THE PROJECT – FINNEE FROM SPECTRA TO FORMULAE



Chronic Diseases Research Center

- Prof. Dr. Nuno Neupart
- Dr. Pedro Martins



Instituto de Biologia Experimental e Tecnológica

- Dr. Patricia Gomes-Alves
- Ricardo Gomes



Laboratory for Process Engineering, Environment, Biotechnology and Energy

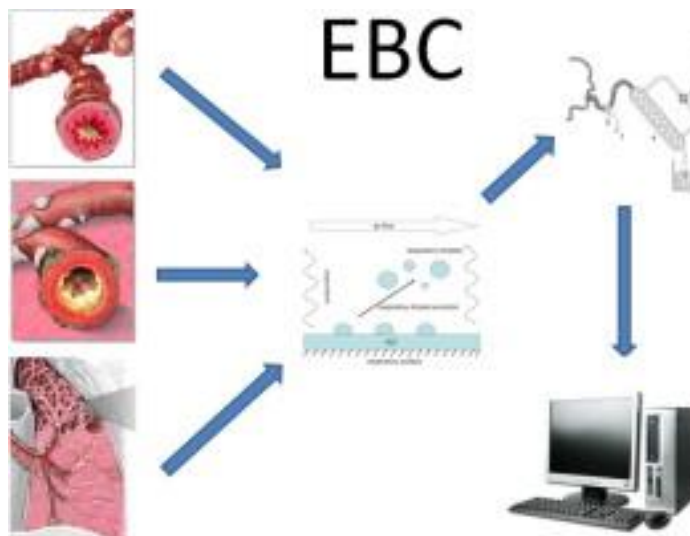
- Dr. Guillaume Erny
- Dr. Monica Santos

ANALYSIS OF EXHALED BREATH CONDENSATES – THE NEW GRAIL?

Exhaled breath condensate (EBC) is the exhalate from breath, that has been condensed, typically via cooling using a collection device (commonly to 4 °C or subzero temperatures using a refrigerating device). EBC reflects changes in the respiratory fluid that lines the [airways](#) and is an inexpensive, non-invasive tool that has potential for scientific research. **Despite its promises, it has not been proven for screening or diagnosing diseases of the lung and other conditions,**



What can I find in my EBC samples?

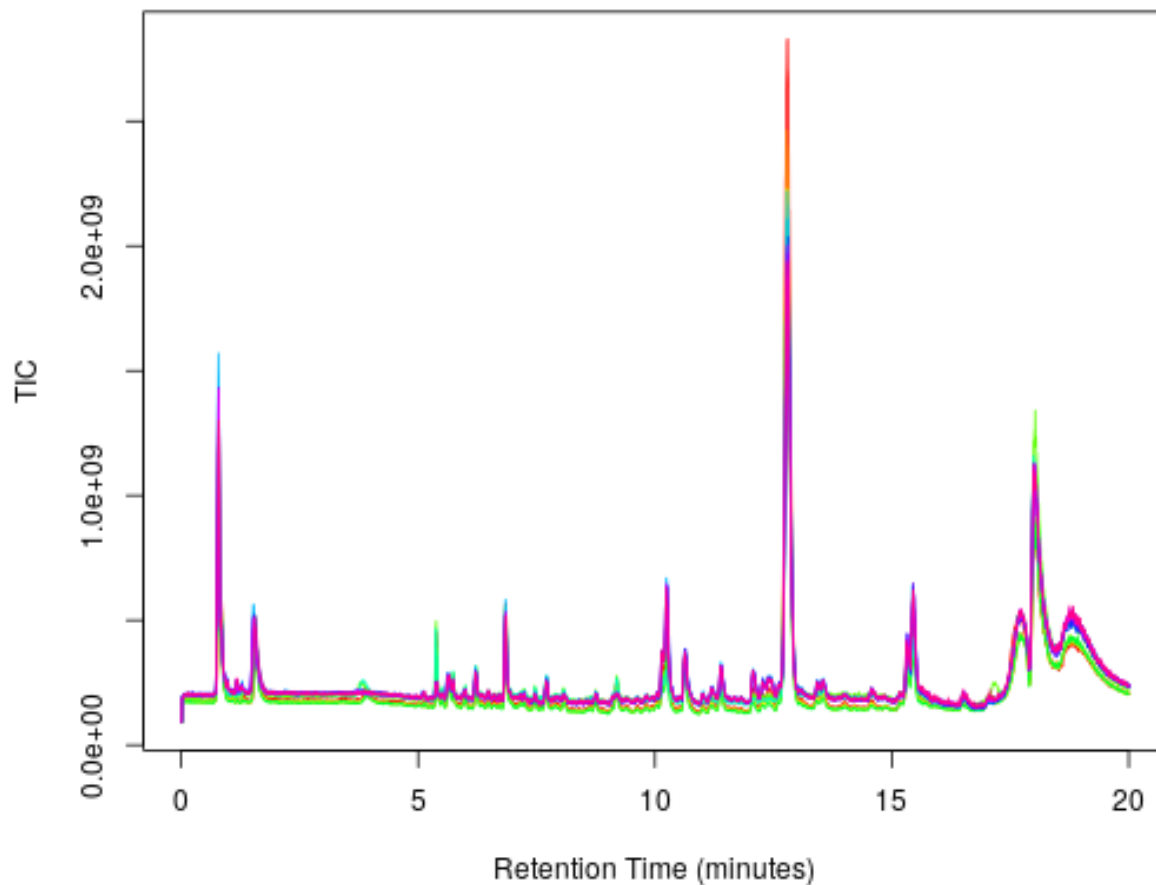


SEPARATION WITH NANO-LC-ESI-MS (ORBITRAP)

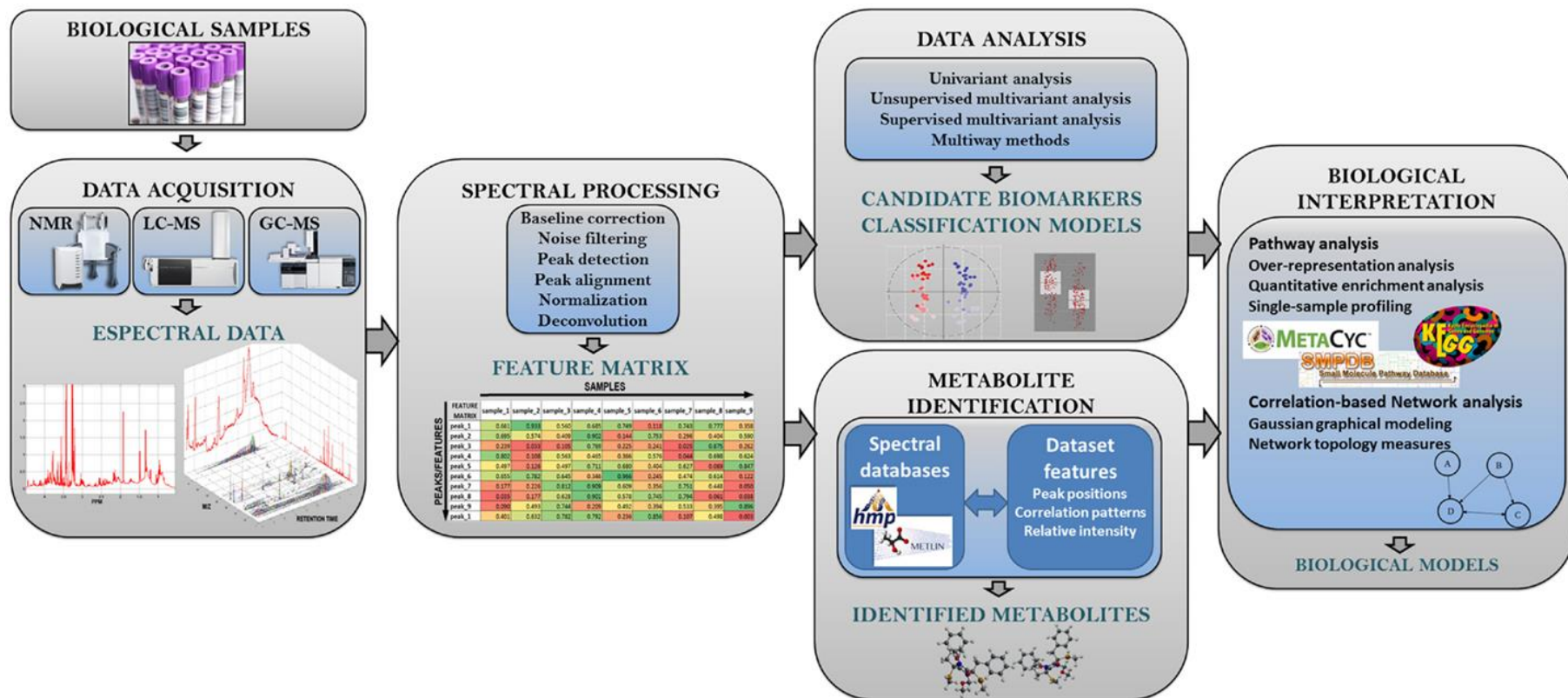


We can have a look!

Total Ion Chromatograms (original)

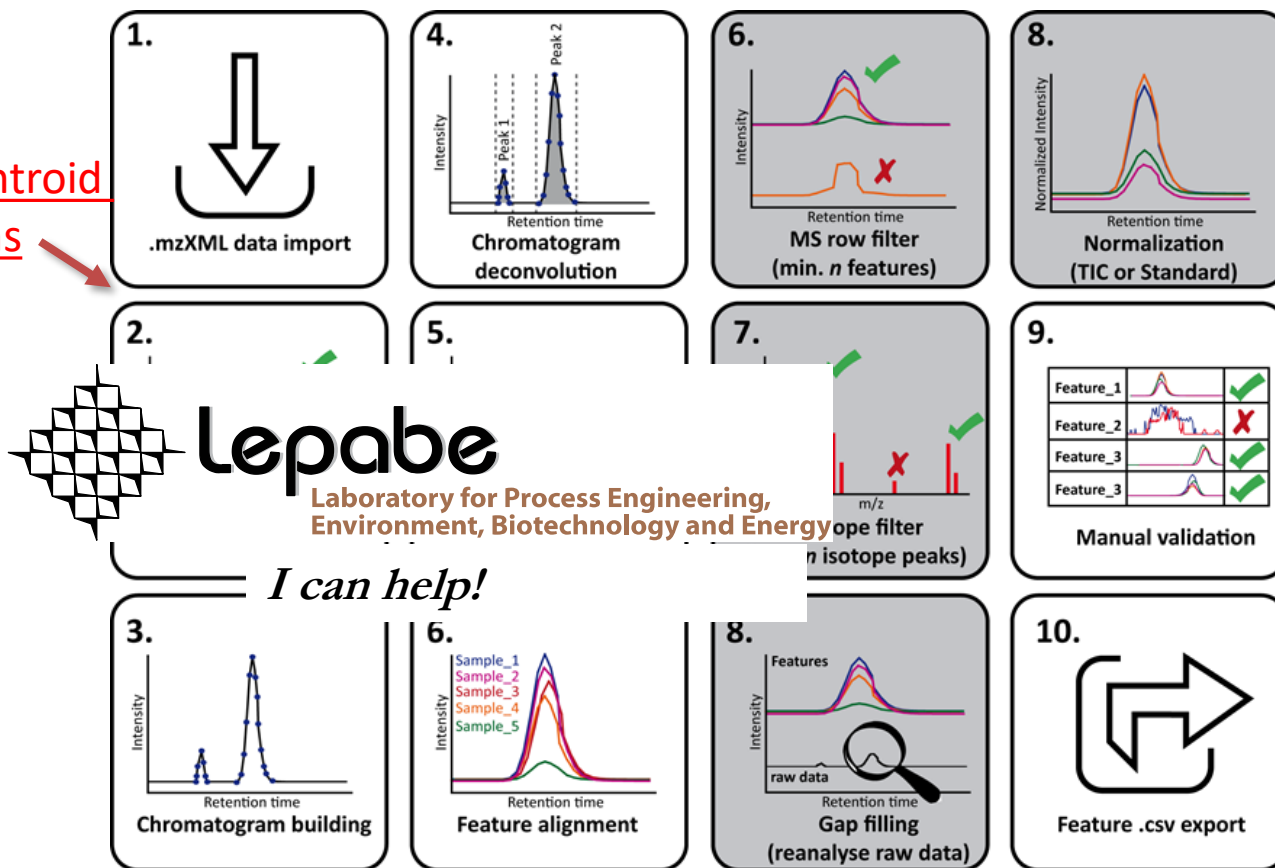


NEED OF AN UNTARGETED ANALYSIS



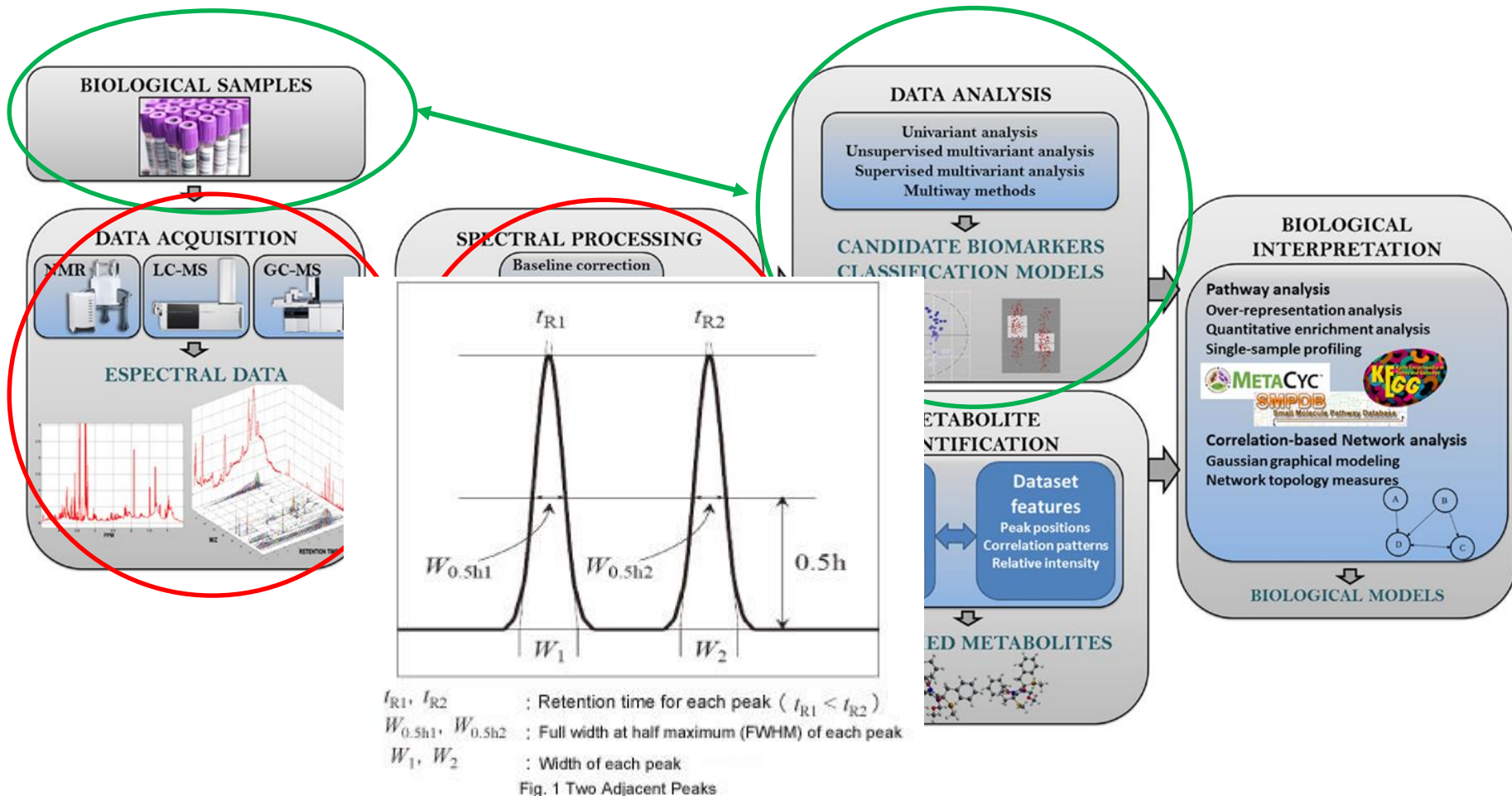
CLASSICAL WORKFLOW FOR SPECTRAL PROCESSING (XCMS & MZMINE)

Profile to centroid
MS scans

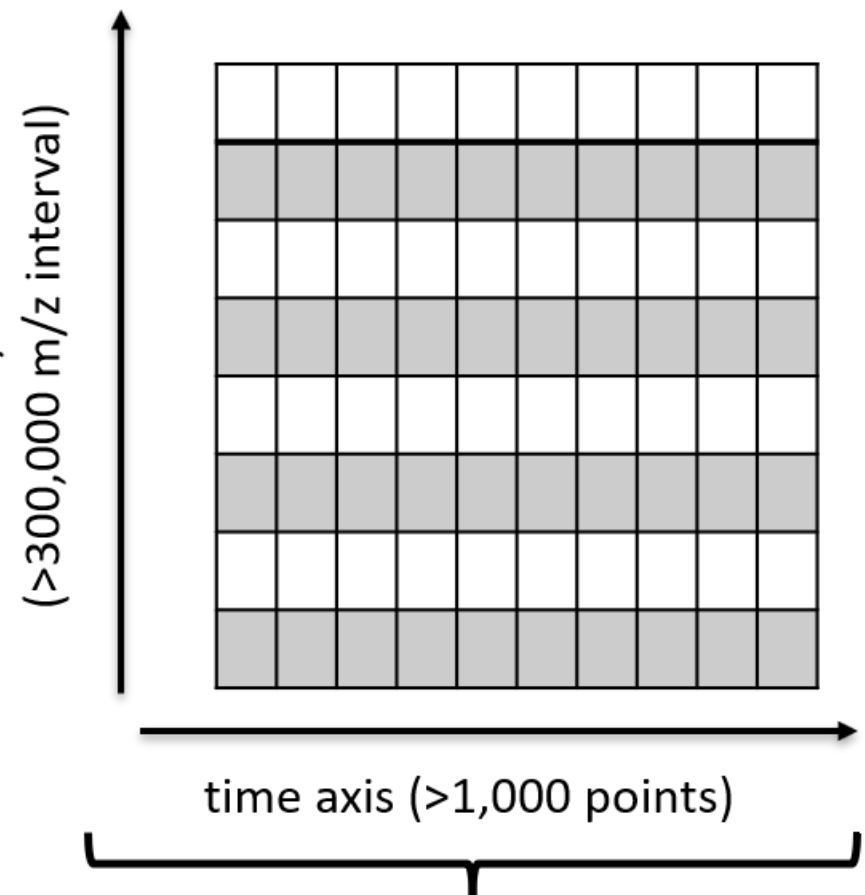
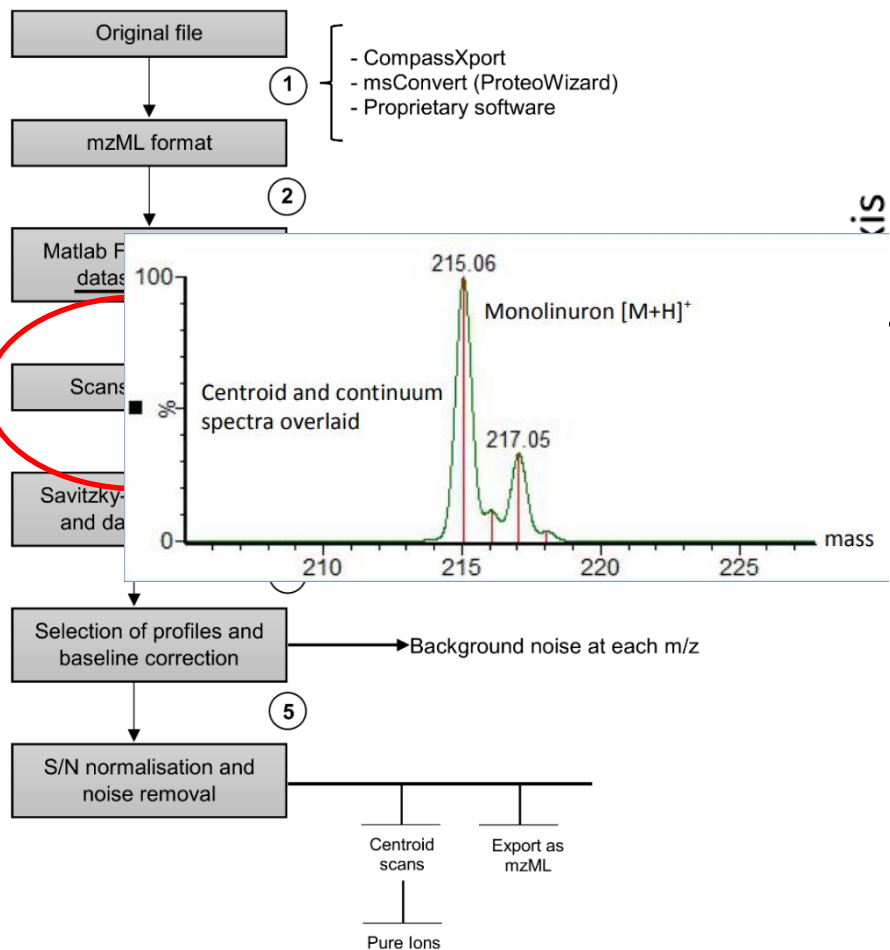


<https://xcmsonline.scripps.edu>

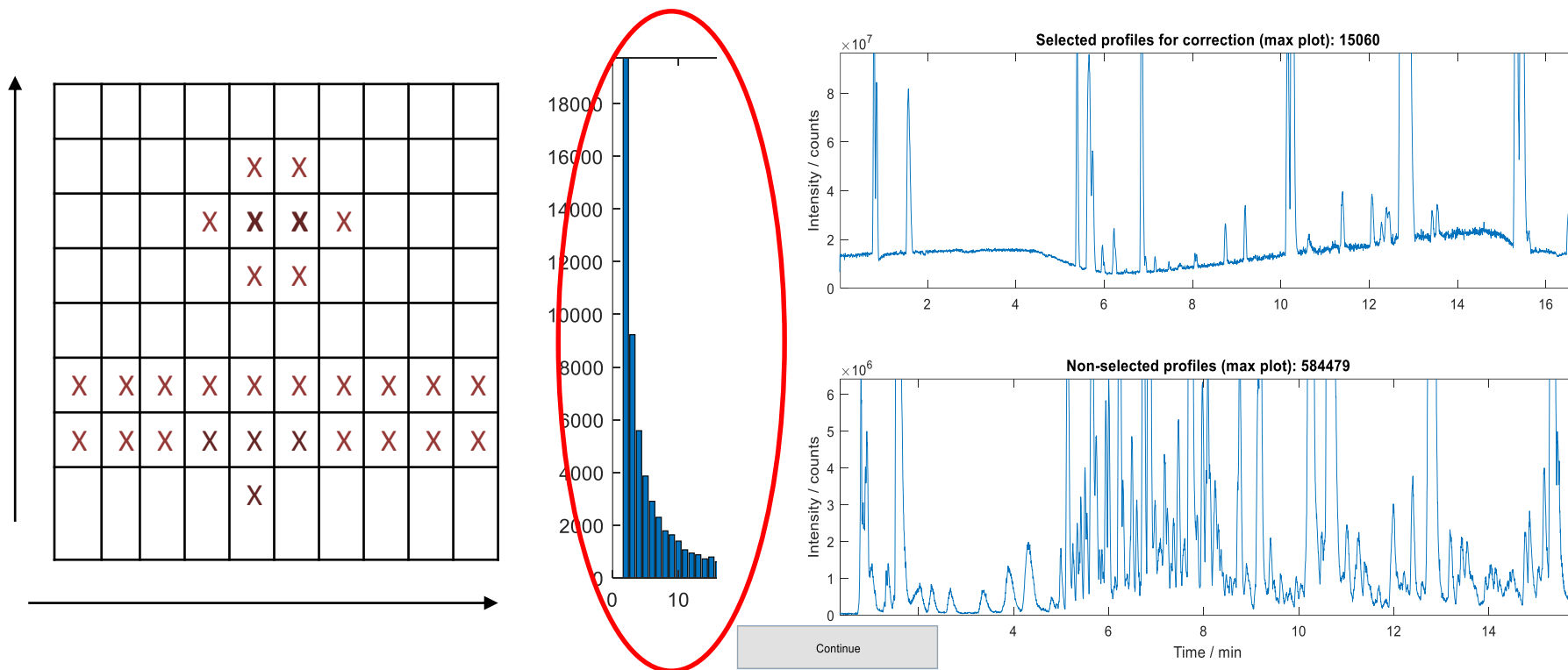
GARBAGE IN, GARBAGE OUT (GIGO)



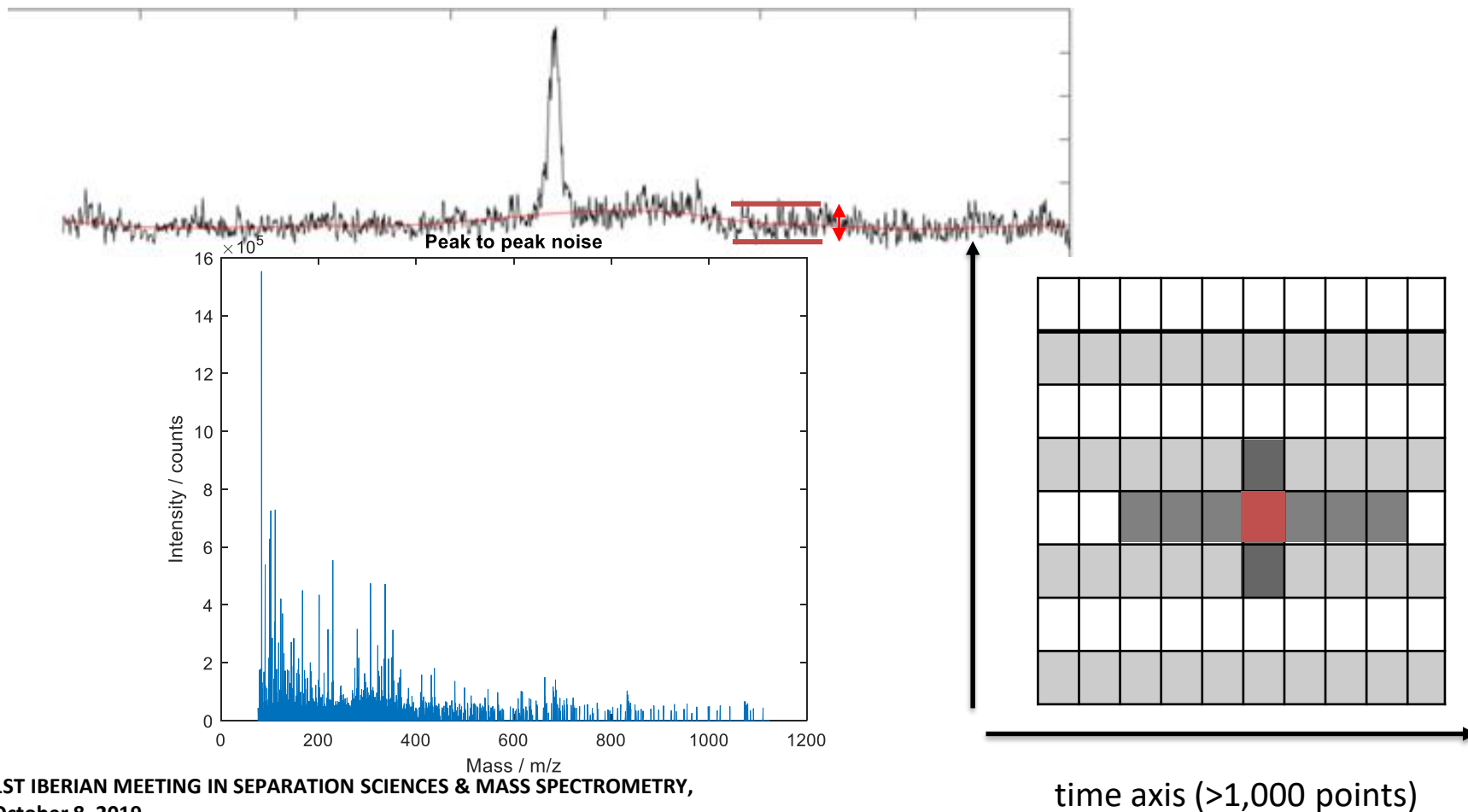
FINNEE WORKFLOW



SELECTION OF INDIVIDUAL MZ INCREMENT TO CORRECT

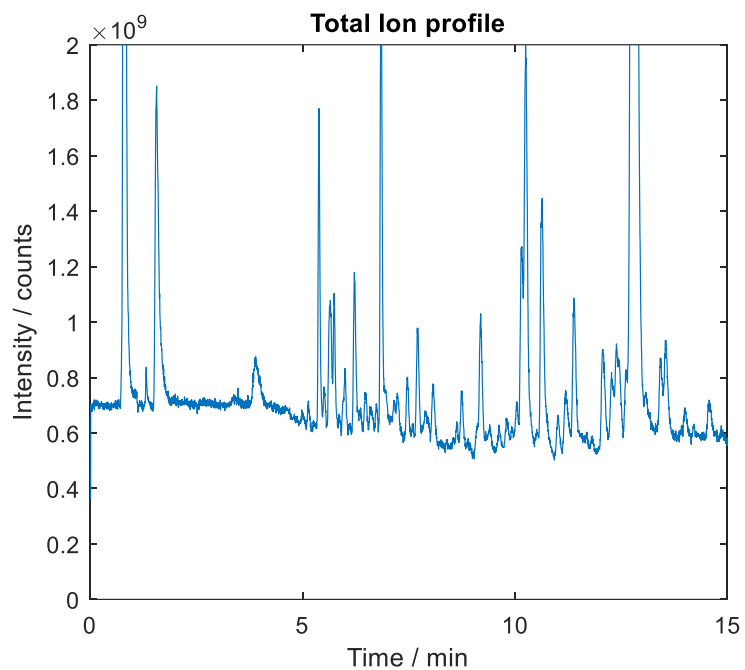


BASELINE DRIFT CORRECTION, NOISE ESTIMATION AND NOISE REMOVAL

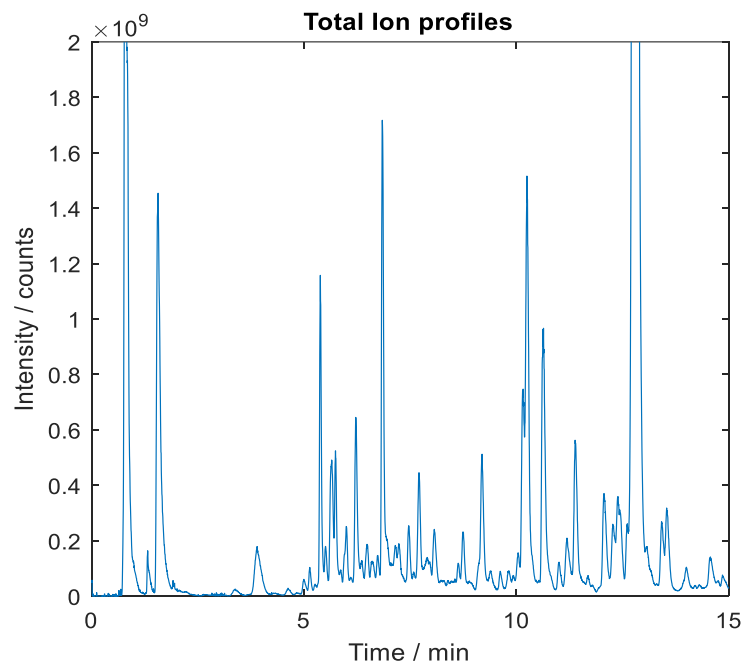


RESULTING TOTAL ION PROFILES

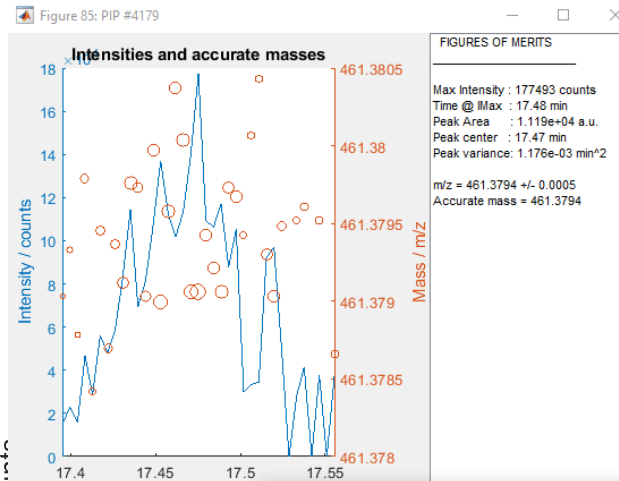
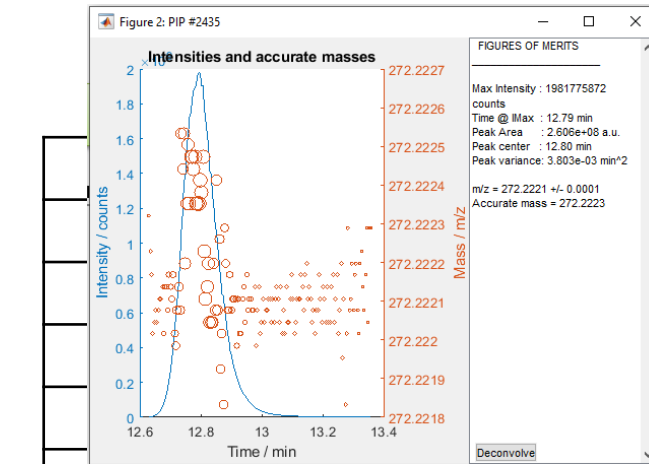
Data file size: ~ 300,00 KB



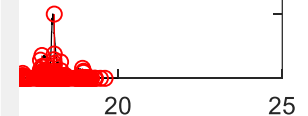
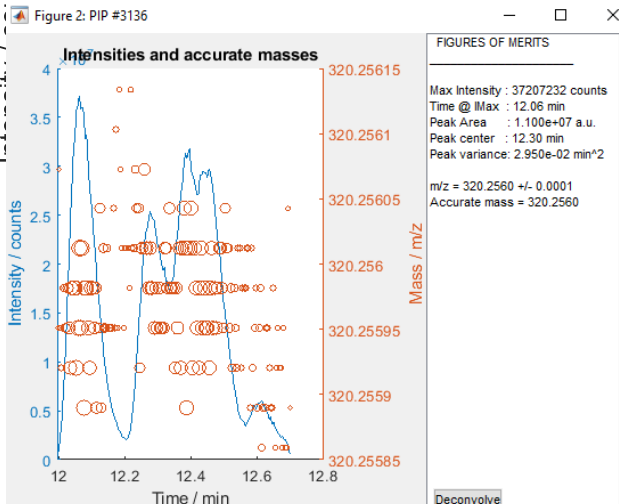
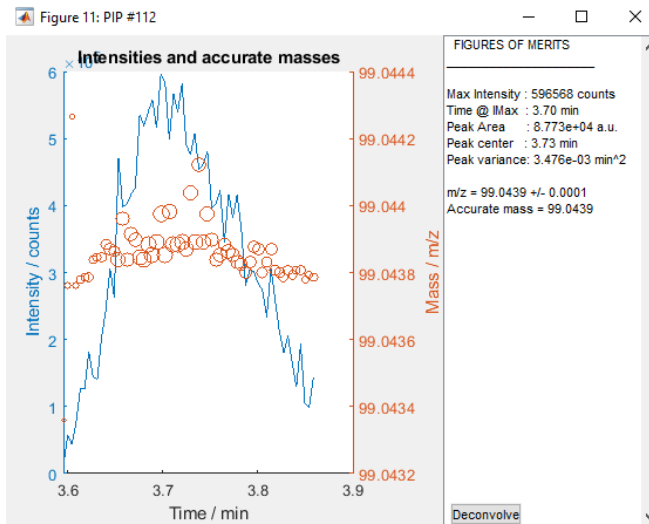
Data file size: ~50,000 KB



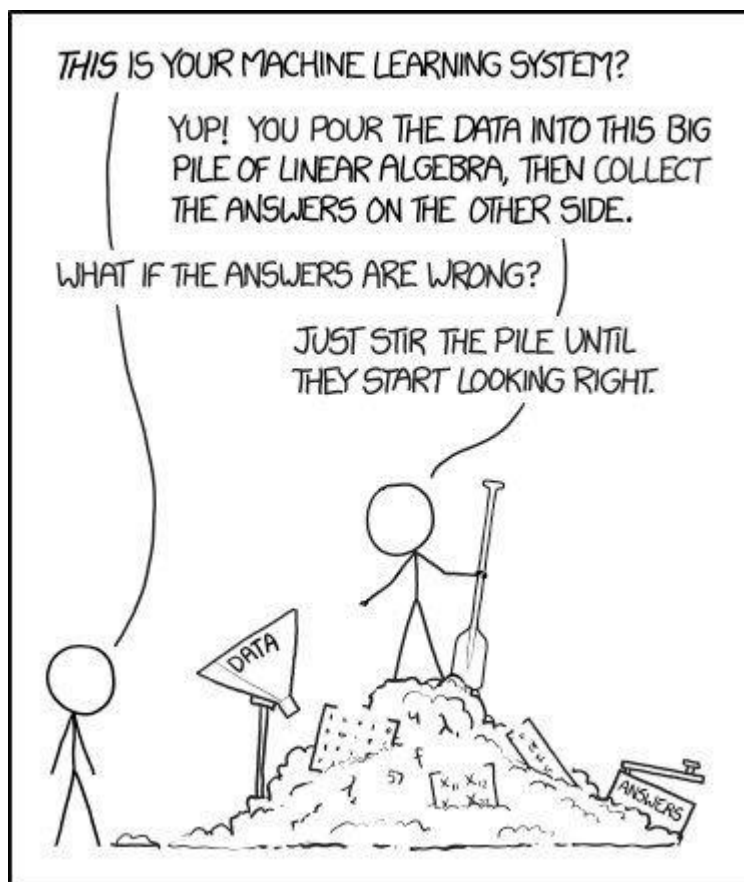
PEAK MINING



popup PIP on



ALIGNMENT AND VALIDATION WITH QC SAMPLES



QC Samples: The quality control (QC) sample should qualitatively and quantitatively representative the entire collection of samples included in the study, providing an average of all of the metabolomes analysed in the study. The QC samples are analysed intermittently for the duration of the analytical study to assess the variance observed in the data throughout the sample preparation, data acquisition and **data processing step**.

=> Assessment of goodness of the peak mining approach

1. Peaks present in all QC samples
2. Peak whose RSD (peak Area) is below 20 %

RESULTS

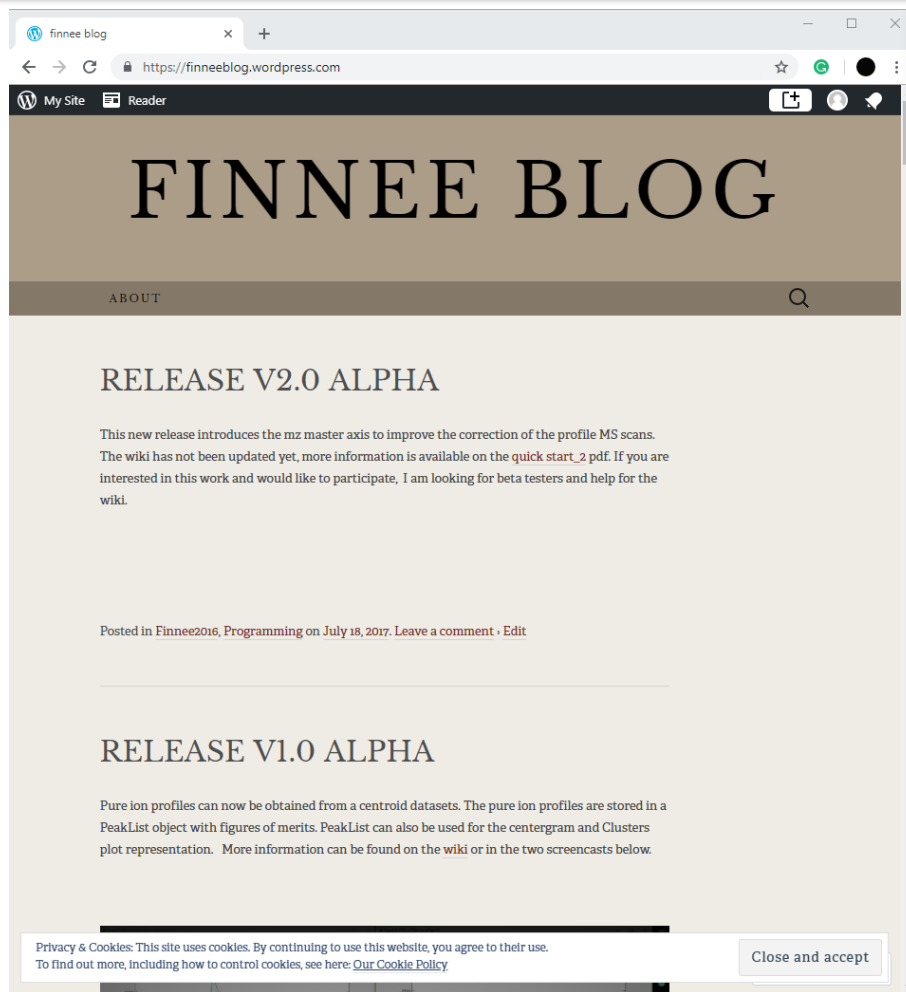
xcms: <https://xcmsonline.scripps.edu/>

msDial: http://prime.psc.riken.jp/Metabolomics_Software/MS-DIAL/

					Finnee	xcms	msDial	
	Peaks	Aligned	Aligned	Aligned	Finnee	438	0	0
	per dts	peaks¹	peaks²	peaks³	xcms	0	273	0
Finnee	5000	4610	3627	1773	msDial	0	0	564
Xcms	8000	4132	4123	1587	Finnee[^]	574	574	
msDial	>20,000	19859	16972	1454	xcms			
					Finnee[^]	150	0	150
					msDial			
					xcms[^]	0	129	129
					msDial			
					all	611	611	611
						1773	1587	1454

1. Peaks with at least 9 match out of 11
2. Peaks with a least 11 match out of 11
3. RSD of the area below 20%

FINNEE: AN OPEN-SOURCE MATLAB® TOOLBOX



finnee blog

https://finneeblog.wordpress.com

FINNEE BLOG

ABOUT

RELEASE V2.0 ALPHA

This new release introduces the mz master axis to improve the correction of the profile MS scans. The wiki has not been updated yet, more information is available on the quick start_2.pdf. If you are interested in this work and would like to participate, I am looking for beta testers and help for the wiki.

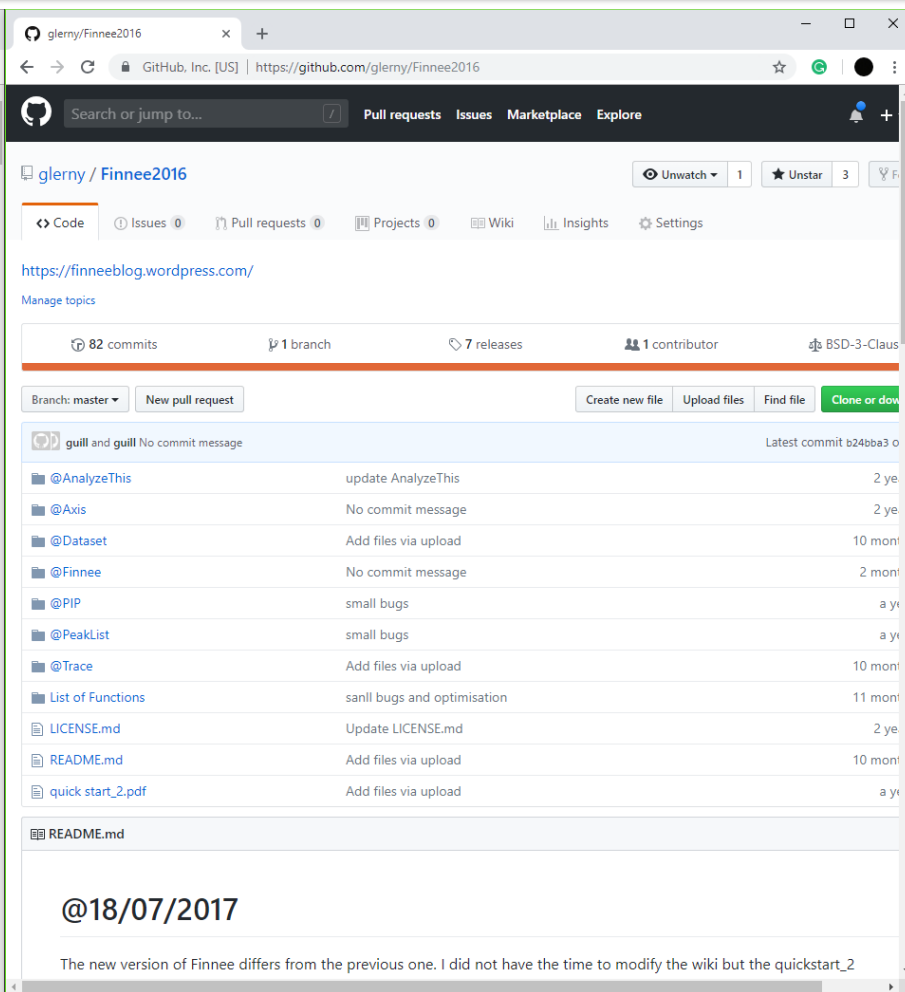
Posted in Finnee2016, Programming on July 18, 2017. Leave a comment · Edit

RELEASE V1.0 ALPHA

Pure ion profiles can now be obtained from a centroid datasets. The pure ion profiles are stored in a PeakList object with figures of merits. PeakList can also be used for the centergram and Clusters plot representation. More information can be found on the wiki or in the two screencasts below.

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File	Commit Message	Latest Commit	Time
@AnalyzeThis	update AnalyzeThis	b24ba30	2 ye
@Axis	No commit message		2 ye
@Dataset	Add files via upload		10 mon
@Finnee	No commit message		2 mon
@PIP	small bugs		a y
@PeakList	small bugs		a y
@Trace	Add files via upload		10 mon
List of Functions	sanll bugs and optimisation		11 mon
LICENSE.md	Update LICENSE.md		2 ye
README.md	Add files via upload		10 mon
quick_start_2.pdf	Add files via upload		a y

README.md

@18/07/2017

The new version of Finnee differs from the previous one. I did not have the time to modify the wiki but the quickstart_2

ACKNOWLEDGEMENTS

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- (i) project UID/EQU/00511/2019 - Laboratory for Process Engineering, Environment, Biotechnology and Energy – LEPABE funded by national funds through FCT/MCTES (PIDDAC);
- (ii) Project POCI-01-0145-FEDER-029702, funded by FEDER funds through COMPETE2020 – Programa Operacional Competitividade e Internacionalização (POCI) and by national funds (PIDDAC) through FCT/MCTES;
- (iii) Project “LEPABE-2-ECO-INNOVATION” – NORTE-01-0145-FEDER-000005, funded by Norte Portugal Regional Operational Programme (NORTE 2020), under PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund (ERDF).