## *EC oral 1: EC1*

# *ASICS: identification and quantification of metabolites in complex 1H NMR spectra*

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### *Introduction*

Several high-throughput technologies allow to obtain metabolomic profiles in biological fluids: Mass Spectrometry (MS) or Nuclear Magnetic Resonance (NMR) for instance. Among them, NMR has the advantage of being less expensive and is viewed as a promising tool to detect interesting biomarkers easily. However, the interpretation of the obtained spectra is difficult since the identification and the quantification of the metabolites present in a complex mixture is not automatic.

### *Technological and methodological innovation*

To ease and expand the use of NMR, we developed a new R package available on Bioconductor, ASICS (Automatic Statistical Identification in Complex Spectra; [1] and [2]), that proposes a complete pipeline for metabolomic spectra analysis. ASICS contains a statistical method to identify and quantify metabolites in a complex mixture by using a statistical model based on a library of pure metabolite reference spectra.

### *Results and impact*

For some datasets, biochemical dosages of several metabolites were also available. Overall, ASICS exhibited a good sensitivity and specificity to retrieve present metabolites and a quantification that was strongly correlated to most metabolite dosages. In conclusion, ASICS allows a faster and simpler direct biological interpretation than the classical bucket approach and better results than other quantification methods such as Batman [3], Bayesil [4] or Chenomx [5].

### *References*

[1] Tardivel P. et al. 2017. Metabolomics. 13(10) :109
[2] Lefort G. et al. 2019. Bioinformatics. 35(21) :4356-4363.
[3] Hao J. et al. 2012. Bioinformatics. 28(15) :2088-2090
[4] Ravanbakhsh S. et al. 2015. PLOS ONE. 10(5) :e0124219
[5] Weljie A.et al. 2006. Anal. Chem.78: 4430-4442.