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► **To cite this version:**

Gaëlle Lefort, Laurence Liaubet, Cécile Canlet, Nathalie Villa, Rémi Servien. ASICS: identification and quantification of metabolites in complex 1H NMR spectra. European RFMF Metabomeeting 2020, Jan 2020, Toulouse, France. hal-02737383

HAL Id: hal-02737383

<https://hal.inrae.fr/hal-02737383v1>

Submitted on 2 Jun 2020

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EC oral 1: EC1

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

Gaëlle LEFORT^{1,2}; Laurence LIAUBET²; Cécile CANLET³; Nathalie VIALANEIX¹; Rémi SERVIEN⁴

¹ MIAT, Université de Toulouse, INRA, Castanet-Tolosan, France

² GenPhySE, Université de Toulouse, INRA, ENVT, Castanet-Tolosan, France

³ Axiom Platform, MetaToul-MetaboHUB, National Infrastructure for Metabolomics and Fluxomics, Toulouse, France ⁴ InTheRes, Université de Toulouse, INRA, ENVT, France

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.