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ABSTRACT BOOK

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P33. ISOTOPIC PATTERN ANALYSIS APPLIED TO MS-BASED LABELLING EXPERIMENTS IN METABOLOMICS

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MS-based metabolomics has been gaining more and more popularity, also because of recent advances in terms of instrumentation performances. As a consequence, many are the metabolomics applications to medical and biological problems. However, this analytical field has to face some limitations and challenging issues, including the elucidation of metabolic pathways, which would require the direct measurement of metabolic fluxes. To date, most of the commonly used approaches only measure pool sizes of metabolites, from which they infer changes in flux.

Some metabolomics limitations can be overcome by using stable isotopes to label metabolites in living cells, and stable isotope tracer-based metabolomics approaches have already been established for metabolite identification, quantification, and pathway analyses. In the past, radioactive tracers were commonly used, and they were easily detected by scintillation counters. The ever-improving sensitivities in analytical techniques such as Nuclear Magnetic Resonance (NMR) spectroscopy and Mass Spectrometry (MS), however, have made it possible to replace the dangerous radioactive tracers with stable isotopes, mainly ^{2}H and ^{13}C.

MS is particularly suitable for labelling experiments in metabolomics, because if analytes incorporate the label, their natural isotopic pattern will be affected, and therefore it will change its "shape", to a degree that depends on the label incorporation. Although many software packages have been devised to predict natural isotopic patterns, there is limited software as yet available for dealing with "labelled" experimental isotopic patterns.

We will discuss how it is possible to estimate the relative isotopic abundance of the labelling isotope inside target analytes by analyzing their experimental isotopic patterns. We will also present the informatics tool we have recently developed for tackling this important issue in biological labelling experiments, where some of the metabolites could have partly incorporated the "label", thus resulting in its unknown relative abundance within them. Our software tool will soon be made available to the scientific community as an R package.