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Metabolomics Solutions Workshop

Metabolomics 2017 Brisbane Australia

Date: Wednesday 28th June, 2017
Time: 12:20 - 13:20
Location: Room M 1/2

Quality vs. Quantity - Is Untargeted Metabolomics Fit-For-Purpose?

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Professor of Biostatistics, Machine Learning, & Data Science
Director of the *Centre for Integrative Metabolomics & Computational Biology*
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Unlock the Metabolome - Exploiting the Potential of High Resolution MS for Multiplexed and Standardized Targeted Metabolomics

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Metabolomics is generally defined as the comprehensive study of all metabolites present in a biological system [1]; however, it is clear that with current technologies 'all' is a very distant reality. In fact, the conflict of *concept* vs. *reality* has resulted in a philosophical schism within the metabolomics community. Many believe that hypothesis-driven (semi-) targeted quantification of a select number of well characterised metabolites is the only pragmatic way forward; others doggedly stick to data-driven untargeted workflows, putting their faith in spectral deconvolution, data scrubbing, and the extraordinarily time consuming process of reverse-engineered metabolite identification.

Recently a third way of approaching metabolomics data acquisition has gained momentum. Using on-the-fly LC-MS mass fragmentation (DDA/DIA/AIF) it is possible to concurrently perform both *targeted** (identified but not fully quantified) and full-scan untargeted metabolite screening. By utilizing a combination of in-house and online spectral fragmentation libraries it is now possible, in a single assay, to produce rapid, cheap, high-quality data for a targeted* list of predetermined metabolites (N~400), extended by untargeted identification via spectral fragmentation database matching (N~4,500), whilst keeping the full scan 'peak feature' dataset for deep mining when time permits.

Here I discuss this Semi-Targeted* Rapid Screening (STaRS) from the perspective of data mining, data quality, and data repeatability. Metabolomics is 18-years-old [2], and it is time to move from 'a concept come of age' to a pragmatic systems biology tool.

[1] Fiehn, Metabolomics--the link between genotypes and phenotypes. Plant Mol. Biol., 2002, 48, 155.

[2] Kell & Oliver, *The metabolome 18 years on: a concept comes of age*. Metabolomics (2016) 12:148

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In metabolomics applications, standardized and quantitative assays are of vital importance, particularly in targeted analysis. The Absolute*IDQ*® p400 HR Kit developed for the Q Exactive™ Orbitrap™ HRAM MS platforms delivers a standardized, quality-controlled and reproducible quantitative assay for targeted metabolic profiling.

The kit quantifies up to 408 metabolites, covering 11 different metabolite classes, with high inter-laboratory reproducibility and data comparability. In this presentation we will share how the Biocrates kit and the Q Exactive Orbitrap platform can provide a unique solution for routine quantitative metabolomics applications in your lab.