07-02: An overview of NMR applications in metabolite profiling of small molecules for plant metabolism studies

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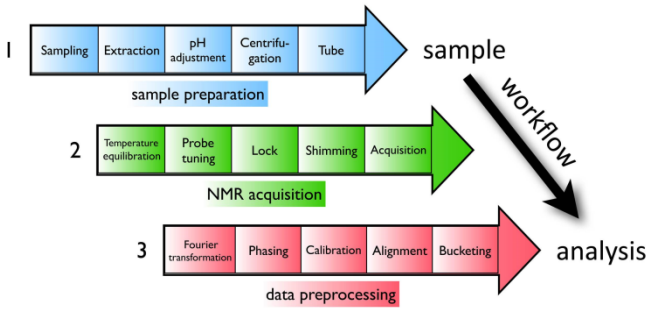
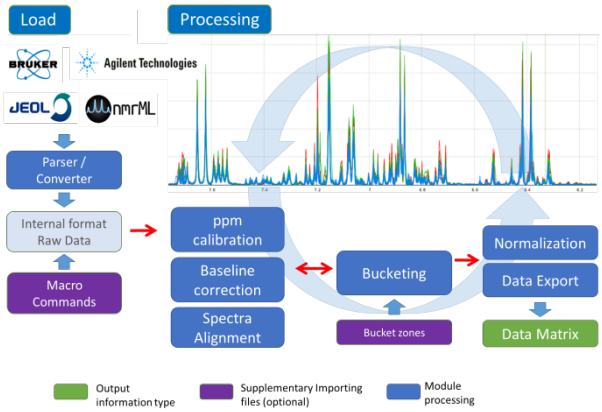
Bordeaux Metabolome Facility (https://metabolome.cgfb.u-bordeaux.fr) is supported by a multidisciplinary team of scientists and engineers from the French National Institute for Agricultural Research (INRA), the French National Centre for Scientific Research (CNRS) and the University of Bordeaux. The Facility contributes to topics of academic and agro-industrial significance in the fields of agronomy, plant science, pharmacology, oenology and aquaculture. It currently houses a 500 MHz magnet dedicated to liquid state NMR-based metabolomics, and also a 600 MHz magnet dedicated to polyphenol structural analysis and wine analysis. A selection of several developments and applications in NMR-based metabolite profiling of small molecules for plant metabolism studies [1] performed with the 500 MHz spectrometer is presented:

- Optimizing 1D ^{1}H-NMR profiling of plant samples: minimizing uncontrolled variability in plant sample preparation before and during NMR profiling, taking into account sample composition, pH and paramagnetic ion concentrations, and NMR spectrometer performances [2].



- Optimizing 1D NMR-based metabolomics processing with an open-source graphical and interactive tool, NMRProcFlow [3] (on-line or downloadable https://www.nmrprocflow.org/): from pre-processing steps including baseline correction, chemical shift calibration and alignment, to processing steps for metabolomics including variable sized and intelligent bucketing and normalization. One of its major strengths is to allow users visually exploring the overlaid or stacked spectra, zooming in on intensity scale, grouping sets of spectra by colouring them based on their factor levels, and thus making the tool valuable to create links between the experimental design and subsequent statistical analyses, and facilitating interactions between plant biologists and NMR spectroscopists.



- Deciphering fleshy fruit biology: 1D and 2D NMR were used to visualize the global composition difference between several fruit species, and to identify major and minor polar metabolites (sugars, organic and amino acids, polyols, alkaloids), in the edible part of the fruit. ^{1}H NMR-based metabolic profiling contributed to get a deeper insight into the regulation of primary metabolism, which provides energy and biosynthetic precursors for fruit growth and ripening, essential for fruit quality and biomass.

These short stories will highlight the work done at Bordeaux Metabolome Facility and illustrate how NMR-based metabolomics remains useful for plant metabolism studies.

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