

## **OW1 Metabolite profiling of biological extracts**

Damien L. Callahan<sup>1</sup>, Joseph Pesek<sup>2</sup>, Maria Pesek<sup>2</sup>, David DeSouza<sup>3</sup>, Antony Bacic<sup>1,3</sup> Ute Roessner<sup>1</sup>

1. Metabolomics Australia, School of Botany, The University of Melbourne, Victoria 3010, Australia

2. Department of chemistry, San Jose State University, San Jose, California, U.S.A.

3. Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Victoria 3010, Australia

Metabolite profiling, HPLC, LC-QTOF-MS, GC-MS

A workflow will be presented for comprehensive metabolomics using LC- and GC-MS.

Metabolomics is an emerging field in the suite of 'omic' approaches for Systems Biology. The goal of metabolomics is to detect the presence of all small-molecules in a biological sample. This presents a significant challenge due to the chemical diversity and large concentration range of metabolites.

Currently, there is no single method which enables the entire metabolome to be analysed, therefore a suite of analytical approaches are required to increase the coverage of detected metabolites. The routinely used techniques for metabolite profiling are LC- and GC-MS and NMR.

Here we present complementary approaches using MS hyphenated to different chromatographic techniques. GC-MS represent the most robust standardised technique for high throughput metabolite profiling however there are still no standard LC-based methods for profiling. Polar compounds represent the most challenging aspect of LC-based metabolomics. A robust chromatographic technique for profiling polar compounds using HILIC chromatography and QTOF-MS will be presented as well as the complimentary reverse phase LC-MS method. The polar separation was carried out using a diamond hydride column. This unique stationary phase provides stable retention times and fast re-equilibration which contrasts to other forms of HILIC stationary phases.

These LC-based methods will be compared to the well established GC-MS method as well as NMR-based profiling.