



Singapore Phenome Centre

# Metabolomics Workshop

**4th March 2pm @ Seminar Room Level 1 EMB**

Organised by Singapore Phenome Center

The workshop is designed to introduce the recent technological advancements in state-of-the-art metabolic profiling techniques and share the experts' perspective on the applications of metabolomics as an important method for studying modern biological sciences. The workshop will also be an opportunity to participants to explore and learn the relevant data extraction methods. We hope to provide a better understanding of the science of metabolic profiling and their potential applications. Highly recommended to attend!

**Target Group:** Research scientists, postdoctoral fellows, and students and those who are interested in metabolomics and their applications should attend.

**Zoom link:** Zoom details will be provided after registration closes.

## Agenda:

2:00-2:35pm	Prof Yulan Wang	Introduction of NMR-based metabolomics
2:35-3:10pm	A/Prof. Mingliang Fang	The surging development of global metabolomics/metabonomics in the last decade: instrumentation, databases, and processing platforms
3:10-3:45pm	A/Prof. Guan Xueli	Introduction of LCMS-based lipidomics
3:45-4:20pm	Dr. Wilson Goh	Introduction of data analysis in metabolomics
4:20-5:00pm	Discussion	

At Singapore Phenome Centre (SPC), metabolomics is used to study metabolic profile and discover both diagnostic and prognostic disease biomarkers in clinical and biological samples with high quality data.

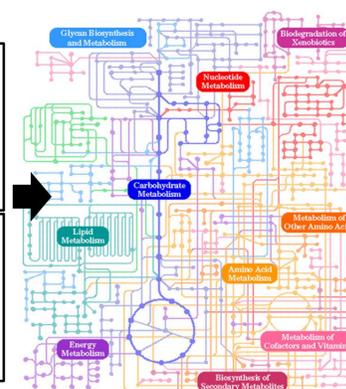
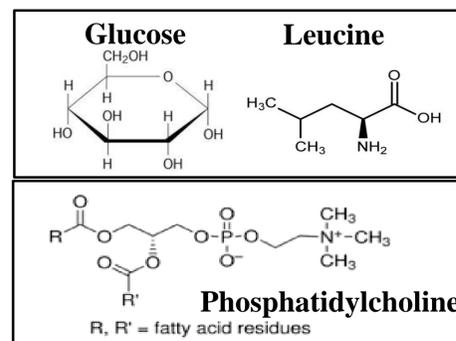
Our facilities include :-

- 1) High-resolution quadrupole/time-of-flight (QToF) mass spectrometers for untargeted profiling and biomarker discovery.
- 2) Tandem quadrupoles (TQ) for quantitative targeted analysis of biomolecules.
- 3) Matrix-assisted laser desorption ionization (MALDI) and desorption electrospray ionization (DESI) for imaging.
- 4) In Vitro Diagnostics Research (IVDr) NMR system.

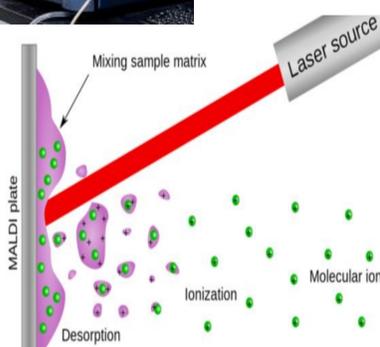
## Liquid Chromatography-Mass Spectrometry (LC-MS)



Small molecule  
100 - 2000 Da



MS Imaging allows molecular imaging on biological tissues and shows the spatial distribution of metabolites, lipids, peptides, neurotransmitter etc. SPC provides both MALDI and DESI imaging method for detailed insight on the distribution of metabolites.



Compound	m/z	Lipid
A	888.63	C24:1 Sulfatide
B	797.53	PI(34:0)
C	788.54	PS(36:1)

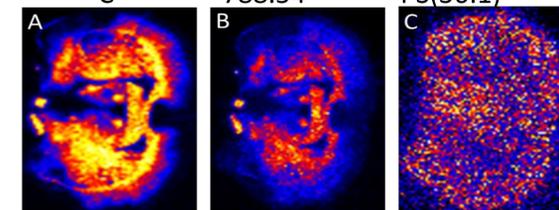
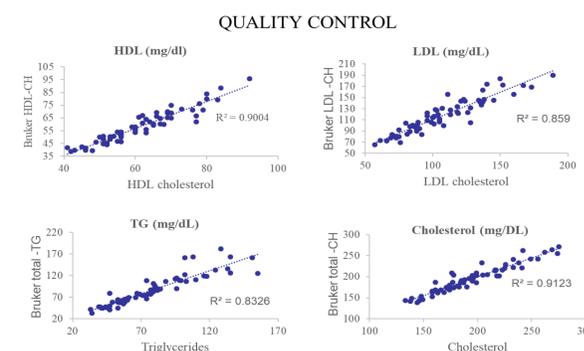


Fig. 1. Illustration of MALDI MS

## Nuclear Magnetic Resonance (NMR)

The reproducibility of high-quality data for metabolites quantification made it the favorite platform for long-term or large-scale clinical metabolomic studies. NMR in SPC is the first to equipped with the In Vitro Diagnostics Research (IVDr) system in Singapore and even South East Asia.



The comparison of lipoproteins derived from 1H NMR of plasma samples shows good linearity with clinical measured lipoproteins.

**Singapore Phenome Centre offers a wide range of services including (but not limited to):**

➤ Untargeted UPLC-MS metabolite profiling	➤ Quantification of about 150 metabolites in urine
➤ Untargeted NMR metabolic profiling	➤ Quantification of 10 classes of phospholipids
➤ Identification and quantitation of over 100 lipoprotein sub-fractions from plasma	➤ Quantification of amino acids
➤ Stable isotope flux analysis	➤ Quantification of a range of neurotransmitters
➤ Quantification of TCA cycle intermediates	➤ Quantification of tryptophan metabolism
➤ Quantification of choline metabolism	➤ Quantification of bile acids
➤ Quantification of arachidonic acid metabolism	➤ Customer tailored targeted analysis
➤ Quantification of short-chain fatty acids and organic acids	➤ Quantification of ceramide
➤ Quantification of vitamins	➤ De-Novo Structural Elucidation from NMR Spectra

## Selected Publications

- [1] Yang Q *et al* (2020) A high-throughput method to characterize the gut bacteria growth upon engineered nanomaterial treatment. *Environmental Science* 7(10), 3155-3166.
- [2] Chen L *et al* (2020) Comparative Blood and Urine Metabolomics Analysis of Healthy Elderly and Young Male Singaporeans. *Journal of Proteome Research* 19(8), 3264-3275.
- [3] Wu *et al* (2020) Gender differences in the bile acid profiles of APP/PS1 transgenic AD mice. *Brain Research Bulletin*. 161, 116-126.
- [4] An Y *et al* (2020) Development and validation of an improved probabilistic quotient normalization method for LC/MS- and NMR-based metabolomic analysis. *Chinese Chemical Letters* 31(7), 1827-1830.
- [5] Hu Q *et al* (2020) Challenges in Analysis of Hydrophilic Metabolites Using Chromatography Coupled with Mass Spectrometry. *Journal of Analysis and Testing* 4(3), 140-162.

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