# Developing an integrated high-throughput spectroscopic strategy for better understanding of food metabolomics

MP 198

**Ruey Leng Loo[1]; Samantha Lodge[1]; Berin Boughton[1]; Melvin Gay[2]; Heino Heyman[3], Christopher Thompson[3], Elaine Holmes[1]; Jeremy Nicholson[1]**
[1]Murdoch University, Perth, Australia;
[2]Bruker Pty. Ltd., Victoria, Australia;
[3]Bruker Daltonics, Billerica, MA, USA

## Introduction

The health value of a specific food is dependent on the growth and storage conditions, as well as the cooking processes. These factors can directly impact various bioactive molecules and affect the food quality and nutritional value.

## Aims

To develop an integrated high throughput spectroscopic strategy involving both the nuclear magnetic resonance spectroscopy (NMR) and mass spectrometer (MS) for phenotyping of fungi (mushrooms).

## Methods

- **Type of foods:** mushroom (truffles, porcini and white button mushroom).
- **Storage conditions:** Mushrooms were extracted and stored in the fridge until analysis.
- **Type of extraction solvents:** water and methanol.
- **NMR analysis:** In 400MHz food screener using both one-dimensional experiment with water pre-saturation and two-dimensional J-resolved experiment.
- **Magnetic resonance mass spectrometry MRMS (Solarix 7T):** Flow injection analysis MRMS in both positive and negative polarities were acquired with 2 mins/sample for each polarity.
- **Data analysis:** NMR data were process using in-house software in R. MRMS data were processed and analyzed with MetaboScape® 5.0.

## Results

**Figure 1:** Different type of mushrooms show different $^1$H NMR metabolite profiles using the same extraction method for regions between **a)** 0.5 – 3.0ppm; and **b)** between 3.0 -4.5ppm.

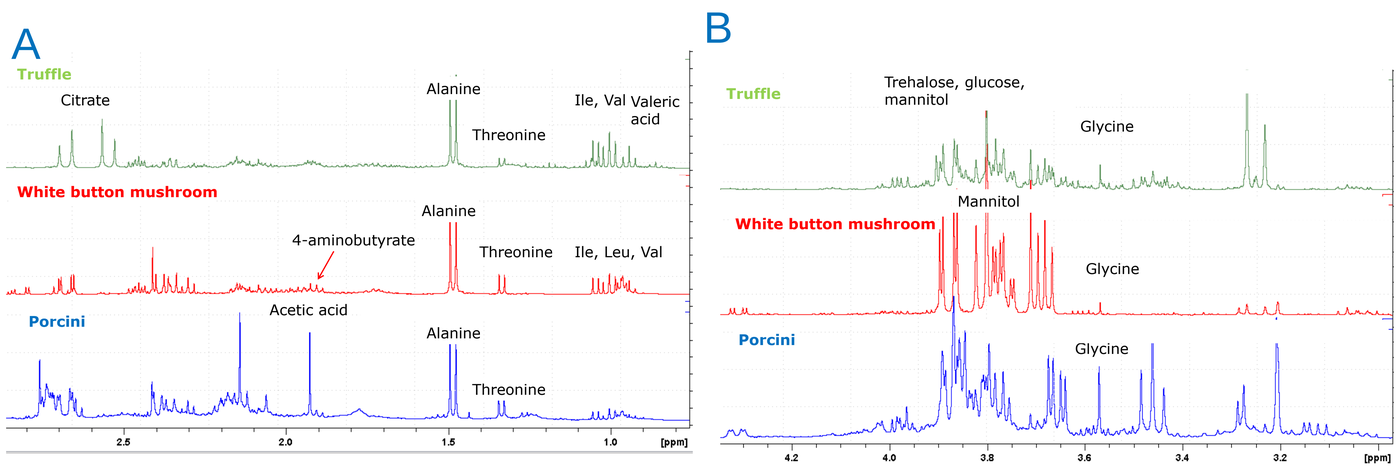



**Figure 2:** Changes in $^1$H NMR metabolic profiles of truffles was observed in principal component analysis (PCA) scores plot.
Color coded to **Green (day 0)**, **blue (day 4), red (day 6)** and **yellow (day 8) .**
M = middle i.e. gleba; C = cap i.e. peridio; S = slice

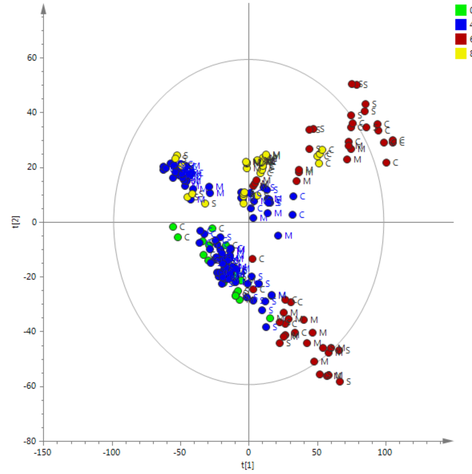
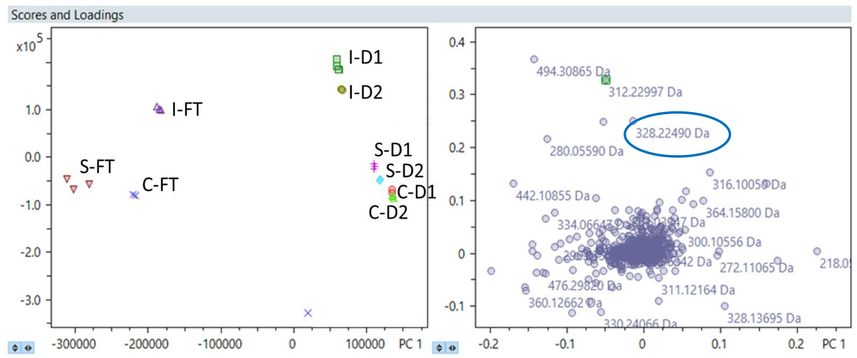
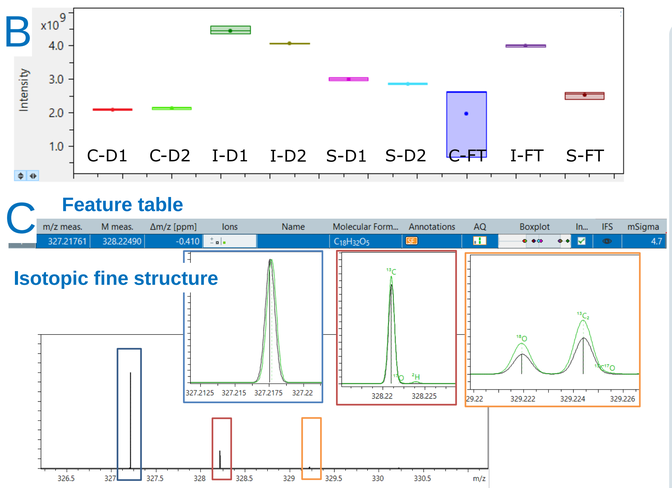



**Figure 3:** Changes in MRMS metabolic profile of truffles and identification of unknown compounds. **A)** PCA scores and loading plots of truffle metabolic profiles based on methanol solvent extraction method over a 2 day period and 1 freeze thaw cycle. **B)** Box plots distribution showing the intensity of metabolite (328.2249 Da) that is double in gleba compared to caps and C) structural elucidation using SmartFomula and isotopic fine structures (IFS) for metabolite 328.2249 Da with a tentative formula of $C_{18}H_{32}O_5$.
Key: D1 = Day 1; D2 = Day 2; FT =1 freeze thaw cycle; I = Inner i.e. gleba; C = cap i.e. peridio; S = slice




## Conclusions

We demonstrate a high-throughput (<10mins/samples) spectroscopic food screening approach using NMR and MRMS for characterizing different type of mushrooms using simple solvent extraction methods.

Our preliminary analysis shows that gleba and peridio of truffle have different chemical compositions. Storage conditions also affects the truffle profiles.

The complementary data by both the NMR and MRMS provide insight into the metabolome profile and could be a valuable tool for quality control monitoring of storage conditions.