



**HAL**  
open science

## HR- $\mu$ MAS NMR localized metabolic profiling of $\mu$ g samples: a model study

Covadonga Lucas-Torres, Yusuke Nishiyama, Alan Wong

### ► To cite this version:

Covadonga Lucas-Torres, Yusuke Nishiyama, Alan Wong. HR- $\mu$ MAS NMR localized metabolic profiling of  $\mu$ g samples: a model study. VIII Ibero-American NMR meeting # 6th Iberian NMR Meeting # 9th GERMN # 4th Portuguese RNRMN Meeting, Jun 2018, Lisbon, Portugal. cea-02327970

**HAL Id: cea-02327970**

**<https://cea.hal.science/cea-02327970>**

Submitted on 23 Oct 2019

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# HR- $\mu$ MAS NMR localized metabolic profiling of $\mu$ g samples: a model study

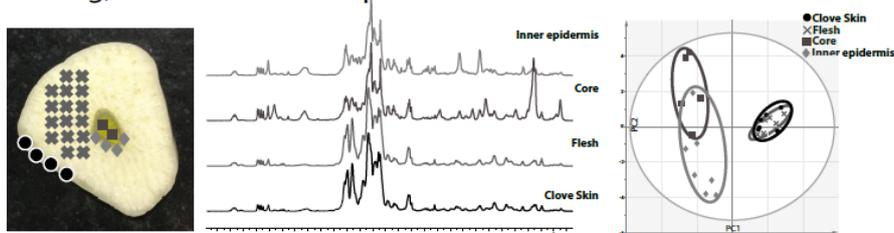
Covadonga Lucas-Torres<sup>a</sup>, Yusuke Nishiyama<sup>b</sup>, Alan Wong<sup>a</sup>

<sup>a</sup> NIMBE, CEA, CNRS, Université Paris-Saclay, CEA Saclay 91191 Gif-sur-Yvette, France  
Covadonga.lucas-torres-perez@cea.fr; <sup>b</sup> JEOL RESONANCE Inc., 3-1-2 Musashino,  
Akishima, Tokyo 196-8558, Japan

NMR has already proven to be a tremendous spectroscopic tool in metabonomics. However, due to its low detection sensitivity, NMR analyses can be challenging especially for mass-limited samples. To overcome this issue, here we introduce a 'new' reliable methodology for profiling  $\mu$ g/nL scale samples based on the Magic Angle Spinning (MAS) technique - High-Resolution  $\mu$ MAS (i.e. 1 mm HR- $\mu$ MAS)<sup>1</sup>.

A model study has been proposed: the localized metabolic profiling (i. e. mapping) of a garlic clove. We have been able to investigate 4 different regions (clove skin, flesh, core and inner epidermis), whereas only 3 regions were distinguished using the standard approach, HR-MAS<sup>2</sup> with larger sample mass (~10 mg). The use of multivariate statistical analysis allowed an initial separation between the different regions by unsupervised PCA. Based on this PCA, a supervised discriminant analysis OPLS was carried out between the previously separated clusters to find the discriminant metabolites. The fact that these micro-detections have been able to offer such precise and accurate results on a model study, opens the way to new applications on heterogeneous biospecimens (such as tissues and cells), on the determination of NMR-based localized metabolic profiles to get the comprehensive fingerprint of their different anatomical regions.

## 0.5 mg, 20 min T2-filter experiments



1. N. T. Duong, Y. Endo, T. Nemoto, H. Kato, A. K. Bouzier-Sore, Y. Nishiyama, and A. Wong. *Analytical Methods*, **2016**, 8(37), 6815–6820.
2. C. Lucas-Torres and A. Wong. *Phytochemical Analysis*, Localized  $^1\text{H}$  HR-MAS NMR metabolic profiling of solid foods: a demonstration on French garlic cloves (*Allium sativum* L.), *submitted manuscript*

This work has been carried out with financial aid of the Agence Nationale de Recherche française (ANR-16-CE11-0023-01 - HRmicroMAS) and JEOL Resonance Inc.