

HR- μ MAS NMR localized metabolic profiling of μ g samples: a model study

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HR- μ MAS NMR localized metabolic profiling of μ g samples: a model study

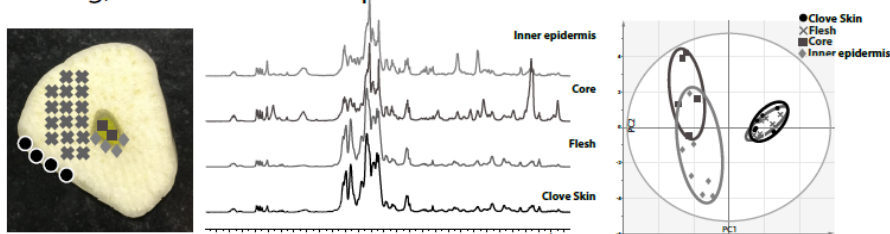
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NMR has already proven to be a tremendous spectroscopic tool in metabonomics. However, due to its low detection sensitivity, NMR analyses can be challenging especially for mass-limited samples. To overcome this issue, here we introduce a 'new' reliable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

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-MAS² 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 ^1H HR-MAS NMR metabolic profiling of solid foods: a demonstration on French garlic cloves (*Allium sativum* L.), *submitted manuscript*

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