



**HAL**  
open science

## <sup>129</sup>Xe NMR-based biosensing on a benchtop spectrometer

Kévin Chighine, Estelle Léonce, Céline Boutin, Hervé Desvaux, Patrick Berthault

### ► To cite this version:

Kévin Chighine, Estelle Léonce, Céline Boutin, Hervé Desvaux, Patrick Berthault. <sup>129</sup>Xe NMR-based biosensing on a benchtop spectrometer. Compact NMR Conference II, CEISAM research institute, Oct 2021, Nantes (Virtual event), France. cea-03375713

**HAL Id: cea-03375713**

**<https://cea.hal.science/cea-03375713v1>**

Submitted on 13 Oct 2021

**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.

# $^{129}\text{Xe}$ NMR-based biosensing on a benchtop spectrometer

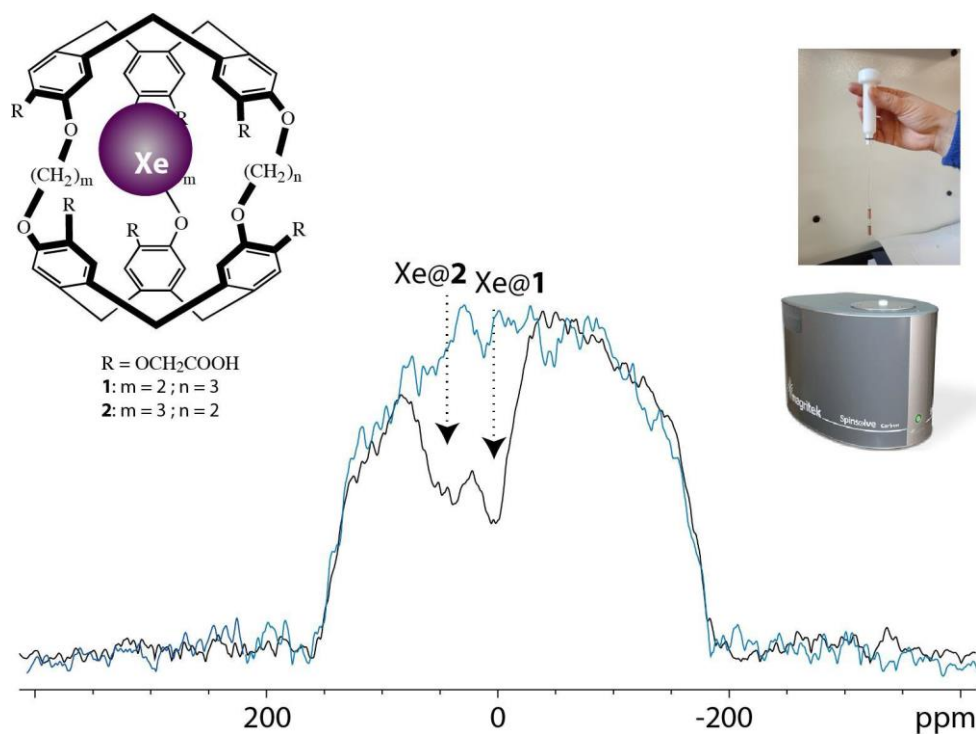
Kévin Chighine, Estelle Léonce, Céline Boutin, Hervé Desvaux & Patrick Berthault

Nanosciences et Innovation pour les Matériaux, la Biomédecine et l'Energie, CEA, CNRS, Université Paris-Saclay, 91191, Gif-sur-Yvette, France

The nuclear polarization of noble gases, such as xenon, can be enhanced by several orders of magnitude through optical pumping, giving rise to very sensitive NMR probes. Moreover, due to its large and deformable electron cloud, xenon exhibits wide chemical shift range (more than 320 ppm for the monoatomic species) and is soluble in most biological fluids. It can be reversibly encapsulated in molecular host systems such as cage-molecules, decorated with ligands in order to target given receptors, and gives rise to sensitive detection of biological events. This two-step procedure, where the xenon host is first introduced and hyperpolarized xenon then delivered, benefits from the difference in resonance frequency between bound xenon and free xenon (in the gas phase or in the dissolved phase) [1].

In a pre-clinical environment, it could be very useful to test the behavior of such bioprobes, using an NMR benchtop spectrometer, less cumbersome and less expensive than a high-field spectrometer. It could be placed very close to the optical pumping setup, working in flow or batch mode. To this aim, we have adapted a method for indirect detection of caged xenon via chemical exchange and spatial encoding on a non-dedicated  $^1\text{H}$ - $^{13}\text{C}$  one-tesla spectrometer. To improve sensitivity and reach the micromolar concentration detection threshold at this intermediate magnetic field, theoretical considerations have been made and instrumental improvements have been proposed, among which shifting the tuning frequency of the probe from  $^{13}\text{C}$  to  $^{129}\text{Xe}$  by wrapping copper foils around the NMR tube on either side of the region to be detected.

This work has recently been published in Magnetic Resonance [2].



[1] E. Mari & P. Berthault, *Analyst*, 2017, 3298. DOI: [10.1039/c7an01088e](https://doi.org/10.1039/c7an01088e)

[2] K. Chighine, E. Léonce, C. Boutin, H. Desvaux & P. Berthault, *Magn. Reson.*, 2021, 2, 409. DOI: [10.5194/mr-2-409-2021](https://doi.org/10.5194/mr-2-409-2021)

