

¹²⁹Xe NMR-based biosensing on a benchtop spectrometer

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¹²⁹Xe NMR-based biosensing on a benchtop spectrometer

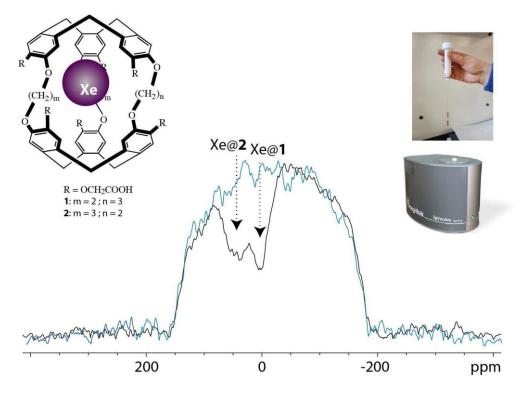
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The nuclear polarization of noble gases, such as xenon, can be enhanced by several orders of magnitude through optical pumping, giving rise to very sensitive NMR probes. Moreover, due to its large and deformable electron cloud, xenon exhibits wide 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 1H-13C 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 13C to 129Xe 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. <u>DOI: 10.1039/c7ano1088e</u>
[2] K. Chighine, E. Léonce, C. Boutin, H. Desvaux & P. Berthault, Magn. Reson., 2021, 2, 409.DOI: 10.5194/mr-2-409-2021