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Reaching metabolomic niches through miniaturization of 1 H-NMR experiments.

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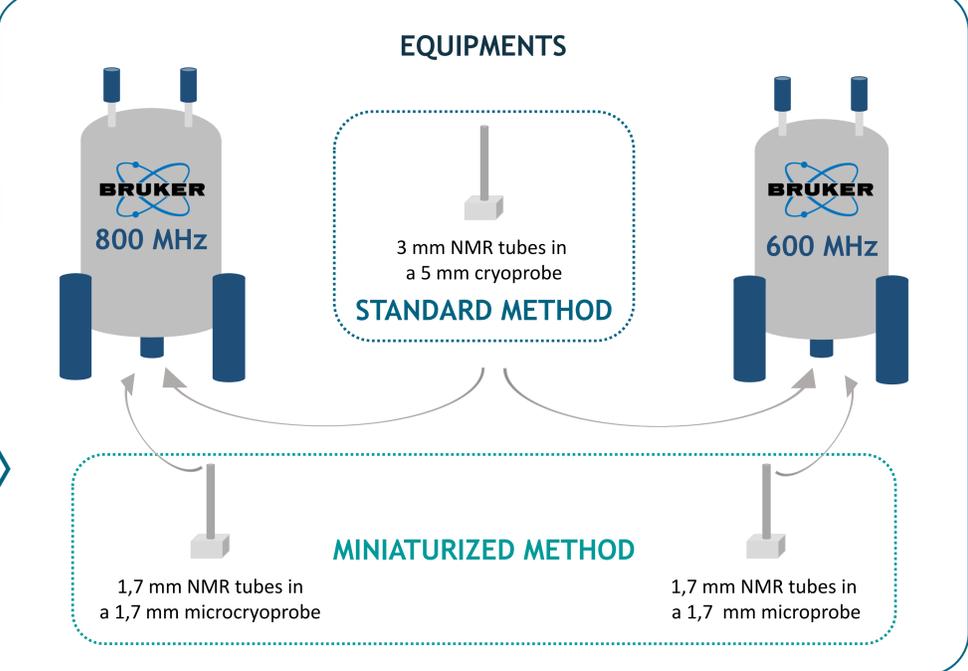
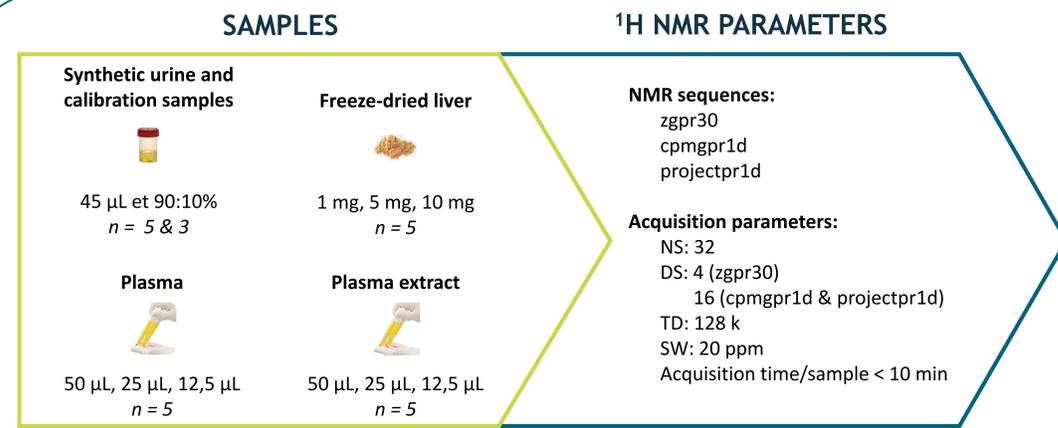
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Introduction

NMR spectroscopy is a great source of information for metabolomics studies. However, one major drawback of NMR is its lack of sensitivity which limits its use for small samples. In such cases, the samples have to be diluted and the experiment time lengthened to accumulate enough signal, which is not optimal. Miniaturization of NMR experiments in the framework of the REACT-EU OCSSIGEN project could be the way to overcome these limitations and reach new metabolomic applications^{1,2}.

Material and methods



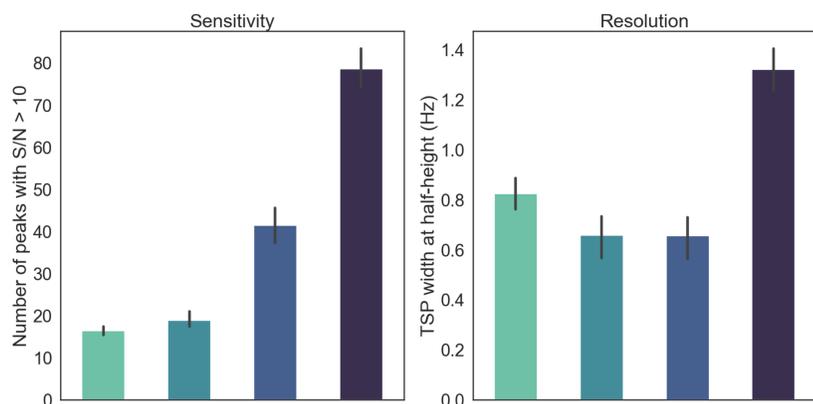
Results and discussion

SYNTHETIC URINE

The normalized LOD for each NMR set-up was determined on 1D ¹H-NMR spectra of 45 µL of synthetic urine³.

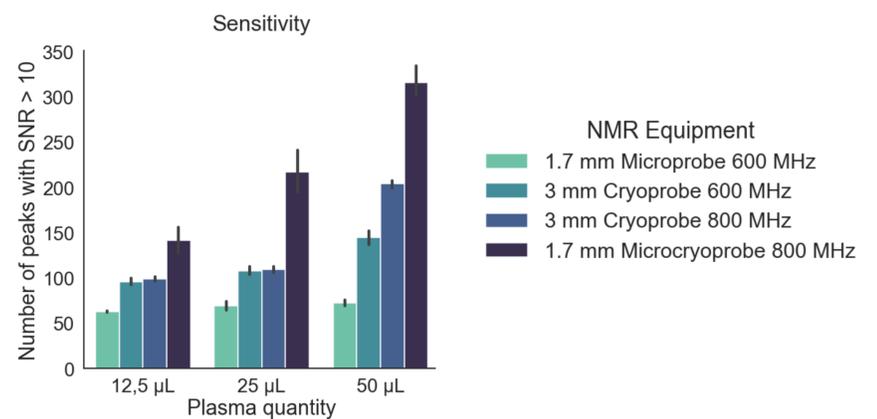
$$LOD^m = \frac{3n_s}{SNR_{exp}} \quad nLOD_f = LOD_f \frac{\sqrt{SW}\sqrt{NS}}{\sqrt{TD}} \quad nLOD_{f,600} = nLOD_f \left(\frac{f_0}{600 \text{ MHz}} \right)^{\frac{7}{4}}$$

	1,7 mm Microprobe 600 MHz	3 mm Cryoprobe 600 MHz	3 mm Cryoprobe 800 MHz	1,7 mm Microcryoprobe 800 MHz
nLOD_{f,600 MHz}^m (nmol.Hz^{1/2})	8,21	6,50	5,11	3,46

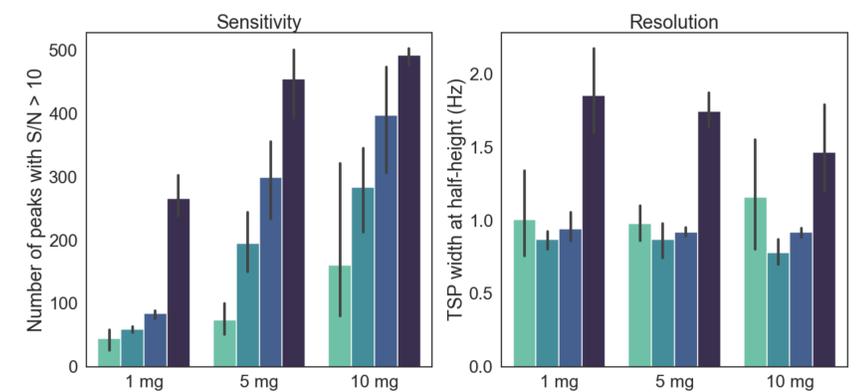


Samples : 45 µL of synthetic urine for 1,7 mm NMR tubes
45 µL of synthetic urine + 135 µL H₂O for 3 mm NMR tubes

PLASMA



LIVER



Conclusions

With the development of the miniaturized NMR method, we can now offer new services when the amount of sample is limited without compromising the high throughput.



APPLICATIONS

- Multi-omics
- Small organisms, spatial analysis of organs
- Multi-omics, kinetics on mice

References

- [1] Mason S, Terburgh K, Louw R. Miniaturized ¹H-NMR method for analyzing limited-quantity samples applied to a mouse model of Leigh disease. *Metabolomics*. 2018 May 21;14(6):74.
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- [3] Lepucki P, Dioguardi AP, Karnausheiko D, Schmidt OG, Grafe HJ. The normalized limit of detection in NMR spectroscopy. *J Magn Reson*. 2021 Nov;332:107077.