

DEVELOPING ANALYTICAL APPLICATIONS FOR PARAHYDROGEN HYPERPOLARIZATION: URINARY ELIMINATION PHARMACOKINETICS OF NICOTINE

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Nuclear magnetic resonance spectroscopy (NMR) is a valuable analytical tool with applications in a vast array of research fields from chemistry and biology to medicine and beyond. It is used to analyse matter by measuring the interactions of nuclear spins with the magnetic field in a non-destructive and noninvasive manner. NMR is renowned for its straightforward data interpretation and quantitative properties, making it attractive for pharmacokinetic applications, where drug metabolism pathways, concentrations, and kinetics need to be evaluated. However, pharmacologically active compounds and their metabolites in biofluids often appear in minute concentrations, well below the detection limit of NMR. Herein, we demonstrate how parahydrogen hyperpolarization (pH₂ HP) overcomes this sensitivity barrier, allowing us to detect mid-nanomolar concentrations of a drug and a drug metabolite in a biofluid matrix. Performance of the method is demonstrated by monitoring nicotine and cotinine urinary elimination, reflected by their concentrations in urine during the onset and withdrawal from nicotine consumption. An NMR limit of detection of 0.1 μM and a limit of quantitation of 0.7 μM is demonstrated, opening up new prospects in applying NMR in quantitative and qualitative analysis of biofluids.

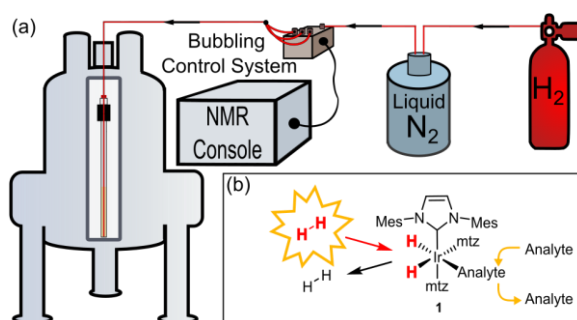


Fig.1 (a) Experimental setup – 50% enriched pH₂ was produced in flow and bubbled through the sample under spectrometer control via a bubbling control system. Sample was loaded to an NMR tube, pressurized, and inserted into the spectrometer; (b) The active iridium catalyst complex **1** responsible for HP chemosensing [1].

References

1. N. K. J. Hermkens, N. Eshuis, B. J. A. van Weerdenburg, M. C. Feiters, F. P. J. T. Rutjes, S. S. Wijmenga, M. Tessari, 2016, *Anal. Chem.* 88, 3406–3412.



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