

## Ultrafast Laplace NMR to monitor molecular exchange

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NMR relaxation and diffusion measurements provide versatile information about dynamics and structures of e.g. porous materials, and reveal interactions of nuclei within their microscopic environment. Since relaxation and diffusion data comprise exponentially decaying components, the processing requires Laplace inversion to extract the diffusion coefficient and relaxation time distributions. Thus, these methods are called as Laplace NMR (LNMR). [1]

Multidimensional approach increases chemical resolution of an NMR experiment. Multidimensional and even some 1D-experiments are time consuming, since the experiments needs to be repeated several times with varying evolution delay or gradient strength to acquire multidimensional data. This restricts the applicability of multidimensional LNMR methods and is considered general problem of multidimensional NMR. Moreover, in many cases it prevents the use of hyperpolarization methods for signal amplification. The problem can be tackled by introducing spatial encoding of two-dimensional data, as was originally done in ultrafast NMR spectroscopy [2] and later in ultrafast LNMR [3-6]. Price to pay is reduced sensitivity. However, single-scan approach enables use of hyperpolarization methods (e.g.PHIP, DNP[4], SEOP[5]), providing higher sensitivity boost than the loss due to spatial encoding.

In this presentation we exploit, multidimensional ultrafast LNMR methods to monitor physical exchange phenomena [6]. We demonstrate the feasibility of the methods with interesting test systems that have important role in biology, chemistry and in industrial applications. These methods are also applicable with mobile NMR instruments, thus widening the application range even further [6].

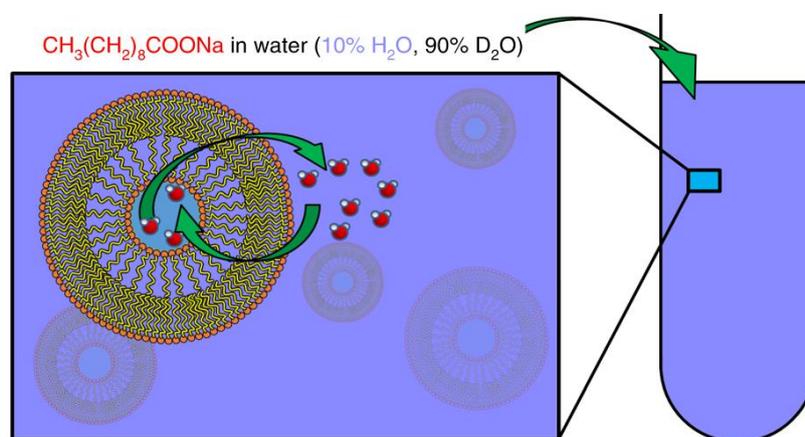


Figure 1: Illustration of diffusion driven exchange between water molecules encapsulated within vesicles formed by decanoate molecules and free water molecules.

### References

- [1] Y.Q. Song: *Magnetic resonance of porous media (mrpm): a perspective*. J. Magn. Reson. **229**, 12-24 (2013).
- [2] A. Tal and L. Frydman: *Single-scan multidimensional magnetic resonance*, Prog. Nucl. Mag. Res. Sp. **57**, 241-92 (2010).
- [3] S. Ahola et.al.: *Ultrafast multidimensional Laplace NMR for a rapid and sensitive chemical analysis* Nat. Commun. **6**, 8363-7 (2015).
- [4] O. Mankinen et.al.: *Ultrafast Laplace NMR with hyperpolarized xenon gas*, Microporous Mesoporous Mater. **269**, 75-78 (2018)
- [5] O. Mankinen et.al.: *Ultrafast diffusion exchange nuclear magnetic resonance*, Nat. Commun. **11**, 3251-8 (2020).
- [6] J.N. King et.al.: *Ultrafast Multidimensional Laplace NMR Using a Single-Sided Magnet*, Angew. Chem. Int. Ed. **55**, 5040-5043 (2016).