

## Contact-free MRI and MRS on self-standing droplets

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### Introduction:

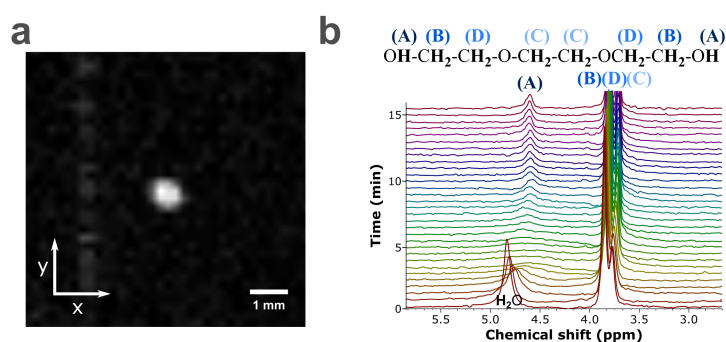
Magnetic resonance spectroscopy and imaging are versatile techniques that provide key information about the structure, dynamics and interactions of molecules. Yet, experimental magnetic resonance studies are often limited to the use of sample holders. Addressing this constraint would allow the implementation of real-time, dynamic studies on the molecular level of liquid samples undergoing for example evaporation, or phase transitions. Previous efforts to study self-standing droplets under a magnetic field have primarily focused on molten aluminum beads *via* aerodynamic levitation<sup>1</sup> or buoyancy forces of immiscible liquids<sup>2</sup>. However, these methods are constrained to non-volatile samples and lack direct access to the interface. Recent advancements have explored magnetic resonance studies on surface-resting sessile droplets, providing real-time dynamic insights<sup>3</sup>, yet without endowing a fully contact-free environment.

### Methodology and results:

In this study, we utilize a demagnetized acoustic levitator to investigate liquid samples in a contact-free manner. Initially, the performance of the levitator (Fig. 1a) inside a 300 MHz magnetic field was assessed. Then, magnetic resonance images of the levitator and the levitated samples were collected (Fig 1b), which acted as a direct proof-of-concept. Following, resolved NMR spectra of the levitated droplets were collected by applying localized and non-localized pulses. Finally, we examined the impact of the droplet shape on the chemical shift and conducted time-resolved experiments using pure solvents and mixtures, yielding valuable insights into physical and chemical interactions.

### Conclusions:

This approach allows the implementation of contact-free, time-resolved studies at the molecular level, advancing the capabilities of magnetic resonance research.



**Figure 1.** a) MRI of acoustically levitated droplet of hexadecane, recorded with True Fast Imaging with Steady State Precession, with 20x20 mm<sup>2</sup> field of view, 64x64 mm<sup>2</sup> resolution, 1 mm slices, 5 averages, echo time of 1.143 ms, repetition time of 2.287 ms, 21 segments, segment mode sequential, scan repetition time of 35 ms, and flip angle of 90°, and b) Series of NMR spectra of a 50 wt% triethylene glycol aqueous solution during evaporation, recorded with Image-Selected In vivo Spectroscopy by applying a 3000 ms repetition time, 8 scans, on a 5x5x5 mm<sup>3</sup> voxel, and 5 Hz exponential line broadening.

### References

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