# Bioanalytical NMR on compact spectrometers

## Summary

*Laboratory of Chemical Physics, National Institute of Chemical Physics and Biophysics is advertising a PhD position in the development of applications for nuclear hyperpolarization in bioanalytical NMR. To date, NMR has been considered as an immensely useful tool in biochemical research. At the same time, NMR is also regarded insensitive and very expensive. These properties hinder development of new applications for NMR. We have demonstrated how parahydrogen sourced nuclear hyperpolarization can be used to increase NMR signals by orders of magnitude, resolving the sensitivity issue. During this PhD project the successful candidate will develop our hyperpolarization technology further towards lower field and more affordable NMR instruments, aiming to solve the cost issue.*

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| Research field: | Physical Sciences |
| Supervisors: | Indrek Reile<br>Kerti Ausmees |
| Availability: | This position is available. |
| Offered by: | National Institute Of Chemical Physics And Biophysics |
| Application deadline: | Applications are accepted between June 01, 2020 00:00 and July 03, 2020 23:59 (Europe/Zurich) |

## Description

Nuclear magnetic resonance (NMR) spectroscopy is a robust chemical analytical technique that is nondestructive, quantitative and not discriminative. It has found widespread use in a wide array of applications ranging from biochemistry to materials science. There are, however, two drawbacks that hinder NMR from being used in several potential applications: insensitivity and instrument cost.

In biochemical applications, this means that a large part of biomolecules cannot be detected since they occur at well below NMR limit of detection. Highest sensitivity instruments also require superconducting magnets that are expensive enough to exclude NMR from several applications where sensitivity would otherwise be sufficient.

Recent advances suggest that parahydrogen (pH2) NMR hyperpolarization (HP) techniques can address both bottlenecks. The pH2 HP-NMR technique generates orders of magnitude signal enhancements in NMR, allowing detection of real-life amounts of a doping drugs and cancer related metabolites in urine – both of which would be impossible by regular NMR. We are finalizing a paper where we demonstrate diagnostic applications of this methodology. This work, however, is still based on high-field NMR spectrometers.

The PhD project will develop these findings towards lower field and more affordable NMR instrumentation. Since in pH2 HP-NMR, sensitivity is no more directly derived from the magnetic field, we can detect our analytes on lower field or even benchtop instruments without sacrificing signal. The project will aim to find the lowest field limits of our pH2 HP-NMR technology, where useful bioanalytical data can still be recorded. The far-reaching goal is to arrive at a method for NMR based diagnostics and analysis that can detect minute amounts of valuable analytes on affordable instruments which do not require liquid helium and specialized personnel to operate them.

**Responsibilities and tasks:**

- The successful applicant will lead the development of the parahydrogen hyperpolarization technique on lower field NMR instruments.
- He/she will develop appropriate sample preparation techniques and optimize experimental parameters.
- The student will also be responsible for day to day maintenance of our hyperpolarization setup and will make hardware improvements to our setup if necessary.

**Qualifications**:

- The applicant should have a masters degree in physics or chemistry.
- We expect the applicant to have some prior exposure to NMR spectroscopy and, at the minimum, be able to interpret basic spectra.

**The applicants should fulfill the following requirements:**

- We expect the successful candidate to have a background either in (metallo)organic chemistry or spectroscopy.
- Skills and prior experience should include one or more of the following:
  - experience with NMR measurements; experience with NMR data analysis;
  - basic understanding of MR physics, experience in biofluid sample preparation (SPE, lyophilization, etc);
  - basic knowledge and experience in analytical chemistry.
- Experience in NMR pulse programming or nuclear hyperpolarization will be considered a plus.

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