Advanced NMR Course VT2016 (15Hec)

Course period: 2016-03-01 till 2016-06-03 Main location of the course: Swedish NMR Center, Medicinareg 5C, 41390 Gothenburg	Last day for application: Applications are welcome until 2016-02-15
Course leader/Address for applications: Vladislav Orekhov, vladislav.orekhov@nmr.gu.se Course organizers: Vladislav Orekhov, Mate Erdelyi, Göran Karlsson, and Martin Billeter	
Course description (Advertisement for Ph.D. students): Nuclear Magnetic Response spectroscopy NMR is an invaluable tool broadly used in academia and industry for elucidating structures of small molecules and biopolymers as well as for studies of molecular interactions and dynamics. This course gives an overview, from the perspective of the user, and provides the knowledge one needs to apply NMR methods in an educated way and to avoid common pitfalls. The course starts with five weeks of NMR basic training and then branches into two alternative tracks: Small Molecules and Protein NMR. The laboratory part of the course consists of instrument practice on standard samples in groups of two to three persons using Agilent and/or Bruker spectrometers. In addition, each participant will perform and present a project on defining the full structure of a small molecule or a protein characterization. For these projects, students may use their own suitable samples. Assessment of the students consists of three parts: written lab reports, written exam, and project presentation. All three parts need to be fulfilled for in order to get credit points for the course. A student, who successful accomplishes the course will get a “driving license” for independently performing experiments on the spectrometers at the Swedish NMR Center.	
Responsible department and other participating departments/organisations: Swedish NMR Center & Chemistry and Molecular Biology	
Teachers: Diana Bernin , Martin Billeter , Ulrika Brath, Mate Erdelyi , Göran Karlsson , Daniel Malmodin , Maxim Mayzel, Vladislav Orekhov, Cecilia Persson	
Examiners: Vladislav Orekhov, Mate Erdelyi, Göran Karlsson, and Martin Billeter	

1. Confirmation

Disciplinary domain: Science

Department in charge: Swedish NMR Center & Department of Chemistry and Molecular Biology

Main field of study: chemistry

2. Position in the educational system

Elective course; third-cycle education.

3. Entry requirements

Recommended entry knowledge comprises the courses

- KEM030/031 (Organic Chemistry) or equivalent,
- Familiarity with NMR data processing and analysis with Mestrelab's MestreNova software

4. Course content The course presents experimental NMR spectroscopy with a clear focus on the chemistry user perspective with extensive hands-on exercises. The lectures largely follow the book by Timothy DW Claridge. The course covers the following topics:

1. Nuclear spin and resonance,
2. NMR samples
3. NMR spectrometer, calibrations and experiment starting procedures
4. Data acquisition and processing, sensitivity, and integration
5. Pulses, vector model of NMR
6. Relaxation
7. Polarization transfer, INEPT, DEPT
8. 2D spectroscopy, correlations through the chemical bond, e.g. COSY, TOCSY, HSQC, HMQC, HMBC, and INADEQUATE experiments.
9. The nuclear Overhauser effect
10. Diffusion NMR spectroscopy
11. Spin-systems and dynamic exchange, spectrum prediction
12. Oriented samples in liquids and Residual Dipolar Couplings
13. Experiment automation

5. Outcomes

After completion of the course the Ph.D. student should be able to:

1. Knowledge and understanding

- **Explain** the role of NMR in chemistry and its potential to solve molecular structures
- **Describe** composition of NMR spectrometer and purpose of its main parts
- **Describe** requirements for NMR samples as well as main procedures and parameter settings required for setting up NMR experiment, for obtaining maximum sensitivity and resolution and avoiding spectral artefacts.
- **Explain** meaning of main parameters measured/obtained from in NMR experiment.
- **Explain** concepts of NMR pulse program
- **Explain** concept of NMR relaxation, meaning and origin of T1, T2, and NOE.
- **Explain** concept of NMR spectra processing including use of quadrature detection, FT, weighting functions,

phasing, non-uniform sampling

- **Describe** idea and practical aspects of homo- and hetero-nuclear decoupling.
- **Describe** concepts and practical implementation of correlations through chemical bonds for homo- and hetero-nuclear cases.
- **Describe** concepts and main examples of two-dimensional spectroscopy and its use for molecular characterization. Describe COSY, TOCSY, NOESY, HSQC, HMQC, and HMBC experiments
- **Describe** concepts, main parameters, and practical aspects, of PFG-diffusion experiments.

2. Skills and abilities

- **Independently set up and run** a 1D and 2D for homo- and hetero-nuclear experiments from NMR instrument libraries. Check and adjust important parameters.
- **Process** 1D and 2D spectra and critically assess spectra quality and explain potential problems.
- **Interpret** results of the NMR experiments (signal positions, J-couplings, correlations, relaxation and diffusion measurements) and analysis and **put** them **in context** with the studied molecule.
- **Present** the results of the experiments and analysis in oral and written form.

3. Judgment and approach

Interpret results of the NMR experiments and analysis and **draw conclusions** about the studied system.

Critically assess the reliability of the obtained results and conclusions.

6. Required reading

- Course book: Timothy DW Claridge High-Resolution NMR Techniques in Organic Chemistry (Elsevier)
- Lecture and laboratory notes provided during the course.
- Additional materials, e.g. scientific articles, distributed on the lectures.

7. Assessment Assessment is based on

- Written exam
  The exam questions relate to content of the lectures, the course book, and the additional reading specifically suggested by the lectures. The material presented during the labs only will not be included in the exam.
  The exam may have only two outcomes: pass or not pass. In order to pass, a student need to collects 60% of the maximal number of points.
  If failed or had a valid reason for not attending the exam at the official date, a student will have right to try at least one more time after agreeing the date with the examinors.
- A miniproject
- Compulsory laboratory exercises and corresponding reports.
  In case of a valid reason for not attending a lab student will be given at least one more opportunity to accomplish the lab. The date and time must be agreed with the lab responsible.

8. Grading scale

The grading scale for PhD students comprises Fail (U), Pass (G).

9. Course evaluation

Course evaluation is carried out based on anonymous evaluation survey forms distributed at the end of the course. The results of the evaluation will be used to improve the following courses.

10. Language of instruction

The language of instruction is English.