PhD course "title"
SYLLABUS

1 Lecturer information

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2 Title of the course

Multinuclear NMR applied to Organic and Biological Chemistry.

3 Course program

NMR is a highly flexible spectroscopic technique, where much information can be extracted about molecules of interest through a plethora of NMR experiments. These include the well-known 1D ^{1}H- and ^{13}C-NMR spectra, used and reported routinely to confirm or identify chemical species, 2D NMR experiments (such as HSQC, COSY and HMBC) used to tease out more structural information from new chemical entities, and exotic 3D NMR experiments used in the advanced study of proteins and genetic materials in physiological-type solutions.
One important and perhaps less studied area of NMR is multinuclear NMR, which is the study of NMR active nuclei of elements other than ^{1}H and ^{13}C. There are dozens of other nuclei that are amenable to study via NMR. One crucially important aspect of multinuclear NMR is that all spin-active nuclei can couple to each other, often producing complex multiplicity patterns. The information obtained from multinuclear NMR can provide great support in working out important chemical and physical properties of the molecules under investigation, including, three-dimensional shape, equilibria, detailed geometry across consecutive bonds.
In this course, we will briefly revise the basics of NMR, expand it to nuclei beyond H and C, and study some applications in organic and biological chemistry of great topical relevance.

4 Course content detailed per lesson of two hours (possibly with dates and room real and virtual)

Tentative Outline:

Lesson 1 – Context, Review of NMR principle, Nuclear Properties, Spin-$^{1}/_{2}$ nuclei, Examples. ^{19}F-NMR, Properties, Couplings. ^{31}P-NMR, Properties, Couplings. Structure Elucidation Worksheet.

Lesson 2 – Nuclei with non-$^{1}/_{2}$ Spin, ^{11}B-NMR and ^{10}B-NMR, Properties, Couplings, Isotope Effect. ^{119}Sn-NMR, ^{117}Sn-NMR and ^{115}Sn-NMR, Properties, Couplings. Other Organic and Biologically Relevant Nuclei. Structure Elucidation Worksheet.

Lesson 3 – Other Organic and Biologically Relevant Nuclei. Structure Elucidation Worksheet.

Lesson 4 – Applications in Solid State NMR, Heteronuclear NMR for Protein and RNA Structure Elucidation. Structure Elucidation Worksheet.

Student input is encouraged through questions and engagement with worksheets.

5 Suggested reading

1. Multinuclear NMR by J. Mason, Springer.
2. Heteronuclear Nuclear Magnetic Resonance, Advances in Pharmacology, 2017.
3. E. Fotopoulou, L. Ronconi, Application of Heteronuclear NMR Spectroscopy to Bioinorganic and Medicinal Chemistry, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, 2018.
4. Other references as course proceeds.

6 Learning Objectives

- Understand how nuclear spins across the periodic table of the elements are affected by a magnetic field, and what happens when radiofrequency radiation is absorbed.
- Be able to unequivocally assign the signals on any NMR spectrum (obtained from any of the compound's NMR-active atoms) in a compound of known structure via their integrations, locations on the chemical shift scale and multiplicities.
- Be able to interpret NMR spectra of NMR-active nuclei, inclusive of number of signals, integrations, location on the chemical shift scale and multiplicity, in order to elucidate the structure of unknown molecular species.
- Be able to strategically plan NMR experiments of NMR-active nuclei, in a research setting, in order to elucidate the structure of complex synthetic and biological molecules.

7 Knowledge and Skills to be acquired

Specific

- Demonstrate an understanding of the fundamental aspects of NMR spectroscopy;
- Extract the wealth of information out of multinuclear NMR spectra, inclusive of the number of signals, integrations, location on the chemical shift scale and multiplicity;
- Interpret and assign multinuclear NMR spectra and use the information to determine the structure of complex synthetic and biological molecules;
- Demonstrate an increased knowledge and understanding in strategically planning NMR experiments to suit research needs;
- Use investigative skills, critical thought and the ability to evaluate information and to analyse experimental NMR data.

General skills in the NMR field relating to improvement of:

- problem-solving and critical thinking skills;
- ability to evaluate the research and professional literature;
- the understanding of the changing knowledge base;
- the capacity to apply concepts developed in one area to a different context;
- the ability to use conceptual models to rationalize experimental observations.

8 Prerequisites

Undergraduate NMR course.

9 Teaching Methods

□ MODE 1 - Pre-recorded lessons uploaded on the moodle platform (a meeting must be organized with PhD students in order to clarify eventual doubts)
X MODE 2 (preferred) - Lessons delivered in-person and in remote with simultaneous recording by the WEBEX platform

(The lessons must be recorded and available to all the students that cannot take part to the lessons in streaming. The Webex platform must be used. All course content should be uploaded to the Moodle platform on the Chemical Sciences PhD page "Courses and Seminars of the PhD in Chemical Sciences 2021-2022")

10 Further information

11 Type of Assessment

The final evaluations will have to be validated maximum 1 month after the end of the course.
Structure Elucidation Assessment with Discussion of Underpinning Principles.

12 Period

Tuesday 2 May-Friday 5 May 2023.