

## **CHMR430 – Advanced Spectroscopic Elucidation for Organic Chemists (15 credits, optional module, year one-PhD)**

Module leader: Dr. Konstantin Luzyanin

Module teaching staff: Dr. Konstantin Luzyanin

### **Module description and aims**

This module is intended for post-graduate (PhD) students from chemistry and related sciences. The main aims are to provide the students with an in-depth knowledge of modern spectroscopic and spectrometric techniques in the context of the structural elucidation of small organic/organometallic compounds. Both theoretical (knowledge and understanding of techniques) and practical (application of techniques and hands-on operation of equipment as a part of self-learning activities) skills are developed.

### **Learning outcomes and skills**

Having successfully completed this module students will be able to:

- 1) Apply the principles of structural elucidation for identification and characterization of organic/organometallic compounds;
- 2) Demonstrate awareness of the theoretical concepts and applications of NMR spectroscopy, mass-spectrometry (MS), chromatography (GC/HPLC), and hyphenated techniques GC/HPLC-MS in the context of structural elucidation of small organic/organometallic molecules;
- 3) Interpret 1D and 2D NMR spectra, MS and IR spectra;
- 4) To confirm structural assignments by combining various analytical techniques in the structure elucidation routine.

Having successfully completed this module students will acquire the following skills:

- 1) Interpretation of different types of spectra;
- 2) Improved confidence in scientific communication and presentation of data.

### **Syllabus**

1. Principles of structural elucidation. Methods for determination of elemental composition and identification of structure.
2. Solution NMR spectroscopy for structural elucidation. Fundamentals of NMR spectroscopy; principles of 1D and 2D NMR methods and techniques. Recognition of structural fragments by 1D and 2D NMR; determination of relative and absolute configuration and conformation by NMR.
3. Mass-spectrometry for structural elucidation. Fundamentals of mass-spectrometry and instrumentation. Mass-spectrometry and determination of elemental composition
4. Separation sciences and hyphenated techniques as an aid for structural elucidation. Fundamentals of chromatography: liquid chromatography, gas chromatography. Introduction to hyphenation (GC/MS, HPLC/MS, MS/MS). Chromatographic method development.
5. Additional techniques and tools in structural elucidation: UV/vis and IR spectroscopy. Alternative techniques for assignment of relative and absolute configuration of organic compounds. Deuteration and studies of kinetic isotopic effect.
6. Combined approaches for structural elucidation and their application: principles of multi-technique approaches for structural elucidation.

### **Recommended texts**

S. A. Richards and J. C. Hollerton, Essential practical NMR for organic chemistry, Wiley, 2011. Print ISBN: 9780470710920, Online ISBN: 9780470976401

T. Claridge, High-resolution NMR techniques in organic chemistry, 3rd edition, Elsevier, 2016. Print ISBN: 9780080999869, Online ISBN: 9780080999937

**Additional texts**

R. M. Granger, H. M. Yochum, J. N. Granger, and K. D. Sienerth, Instrumental analysis, Oxford University Press, USA, 2018. ISBN: 9780190865337

E. Breitmaier, Structure elucidation by NMR in organic chemistry: a practical guide, 3rd revised edition, Wiley, 2002. Print ISBN: 9780470850060, Online ISBN: 9780470853061

R. G. Linington, P. G. Williams, J. B. MacMillan, Problems in organic structure determination: a practical approach to NMR spectroscopy, CRC Press, Taylor & Francis Group, 2015. ISBN: 9781498719629

J. A. Iggo and K. V. Luzyanin, NMR spectroscopy in inorganic chemistry, 2nd edition, Oxford University Press, 2019. ISBN: 9780198794851

M.-M. Cid (Editor) and J. Bravo (Editor), Structure elucidation in organic chemistry: the search for the right tools, Wiley, 2015. Print ISBN: 9783527333363, Online ISBN: 9783527664610

**Format of delivery and assessment**

Delivery: 32 h lectures, 4x2h classwork seminars, 6x1 h hands-on training sessions, 4 VLE-based workshops on problem solving, and 104 h of self-directed learning.

Assessment: 1 written examination (60% mark), 4 problem(case)-based learning workshops with summary presentation in small groups (4 x 10% each; two of them is peer-assessed by students and staff/using feedback forms; two are assessed by staff only).