

## COURSE SYLLABUS

### 1. Identification

Code and title: QUP 177 – Nuclear Magnetic Resonance (NMR) I

Professor: Francisco Paulo dos Santos

Level: Master and Doctorate

Credit hours: 3

Revised: August\_2019

### 2. Summary

Fundamentals of the NMR phenomenon, relationship between NMR spectra and molecular structure. Routine spectra ( $^1\text{H}$  and  $^{13}\text{C}$ ): Homo- and heteronuclear correlation (COSY, TOCSY, HSQC, HMBC), Emphasis is on learning the practical and interpretation of NMR spectra of organic compounds.

### 3. Objective

Student has knowledge on the relationship between the substance structure and its  $^1\text{H}$ ,  $^{13}\text{C}$ , COSY, TOCSY, HSQC, HMBC, NMR spectra which can be applied in the determination of the structure of unknown organic compounds.

### 4. Contents

- NMR spectroscopy, basic concepts (chemical shift, spin-spin interaction, the line width).  $^1\text{H}$ -NMR ( $^1\text{H}$ -chemical shift, spin-spin coupling  $^1\text{H}$ - $^1\text{H}$ , interaction with other nuclei),  $^1\text{H}$ -chemical shift and structure relationship. Interpretation of  $^1\text{H}$ -NMR spectra of organic compounds.
- $^{13}\text{C}$ -NMR,  $^{13}\text{C}$ -chemical shifts,  $^1\text{H}$ - $^{13}\text{C}$  interaction,  $^{13}\text{C}$ -chemical shifts and structure of the molecules. Interpretation of  $^{13}\text{C}$ -NMR spectra of organic compounds.
- Analysis of complex NMR spectra of organic compounds, relationship structure-NMR spectrum.

### 5. Assessment

List of exercises, presentation and discussion of scientific articles and final exam. The student, who obtains a final grade of A, B or C, awarded as per the list below, will be considered approved:

A: grade equal to or above 9.0

B: grade equal to or above 7.5 and below 9.0

C: grade equal to or above 5.0 and below 7.5

D: grade below 5

FF: lack of frequency

### 6. Methodology

Lectures, exercises lists, seminars and examinations.

### 7. Bibliography



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- T. D. W. Claridge, High-Resolution NMR Techniques in Organic Chemistry, Tetrahedron Organic Chemistry, 27, Ed. Elsevier, 2009.
- M. Balci, Basic  $^1\text{H}$ - $^{13}\text{C}$ -NMR Spectroscopy, Elsevier, Amsterdam, 2005.
- R. M. Silverstein, G. C. Bassler e T. C. Morrill, Identificação Espectrométrica de Compostos Orgânicos, 7ª Ed. LCT, 2010.
- D. Pavia, G. Lampman, G. Kriz e J. Vyvyan, Introduction to Spectroscopy. 2ª Ed. Cengage Learning, 2015.