Course: Structure Determination of Organic Compounds		
Language: English		
Lecturer: Assoc. Prof. Tatjana Gazivoda Kraljević, Prof. Irena Škorić		
TEACHING	**WEEKLY**	**SEMESTER**
Lectures	2	30
Laboratory	0	0
Seminar	2	30
		Overall: 60
		ECTS: 6.0

PURPOSE:

Expose the basic principles of spectroscopic methods: ultraviolet and visible spectroscopy (UV / Vis), infrared spectroscopy (IR), one- and two-dimensional nuclear magnetic resonance (1D and 2D 1H and 13C NMR) and mass spectrometry and its application in determining the structure of organic compounds.

THE CONTENTS OF THE COURSE:

Week 1

1st week: Introduction to spectroscopic methods.

2nd week: Ultraviolet – visible spectroscopy (UV / VIS): electronic transitions, basic photophysical processes, the absorbance (Lambert-Beer's law), chromophores, examples of UV / Vis spectra.

Seminar – Analysis and interpretation of UV / VIS spectra.

3rd week: Infrared spectroscopy (IR): vibrations of covalent bonds in molecules (stretching and bending), the area of the functional groups and the fingerprint area, examples of the IR spectra.

Seminar – Analysis and interpretation of IR spectra.

4th week: Nuclear magnetic resonance (^{1}H and ^{13}C NMR): physical principles, spectral parameters (chemical shift d, spin-spin coupling constant J, relative intensity of signals, factors affecting the chemical shift, the Nuclear Overhauser Effect (NOE).

Seminar – Analysis and interpretation of ^{1}H and ^{13}C NMR spectra.

5th week: ^{1}H NMR spectroscopy: spin-spin coupling (H-H), multiplets (n + 1), the splitting scheme, the first and second order spin systems.

Seminar – Analysis and interpretation of ^{1}H NMR spectra.

6th week: ^{1}H NMR: two spin systems (AX, AB, AM); three spin systems (AX2, AB2 AMX, ABX ABC); four spin systems (AX3, AB3, a2x2, A2B2, AA'XX 'AA'BB'); five spin systems A2X3, A2B3, ABX3; examples of first and second order spin systems.

Seminar – Analysis and interpretation of 1H NMR spectra by first and second

order spin systems.

7th week: 1st partial exam

8th week: ^{13}C NMR spectroscopy: spin-decoupling in ^{13}C NMR; coupled and decoupled spectra, APT, DEPT

Seminar – Analysis and interpretation of ^{13}C NMR spectra.

9th week: Two-dimensional (2D) NMR spectroscopy: Homonuclear correlation methods ^{1}H-^{1}H (COSY, DQF-COSY, ECOSY) and ^{13}C-^{13}C (inadequate)

Seminar – Analysis and interpretation of 2D NMR spectra

10th week: Two-dimensional (2D) NMR spectroscopy: heteronuclear correlation methods 1H-13C (HETCOR, HSQC, HMQC, HMBC); Correlation methods through space ^{1}H-^{1}H (NOESY) and ^{13}C-^{13}C (ROESY).

Seminar – Analysis and interpretation of 2D NMR spectra

11th week: Mass spectrometry (MS): ionization methods, mass spectrometer of high resolution, the fragmentation of organic compounds

Seminar – Analysis and interpretation of mass spectra

12th week: Mass spectrometry (MS): fragmentation of organic compounds, gas chromatography and mass spectrometry (GC / MS), liquid chromatography and mass spectrometry (LC / MS)

Seminar – Analysis and interpretation of mass spectra

13th week: Chirooptical methods: optical activity and rotation of linearly polarized light; Optical rotatory dispersion (ORD) and circular dichroism (CD).

Seminar – Analysis and interpretation of ORD and CD spectra

14th week: Determination of the structure of organic compounds on the basis of complementary information obtained using various spectroscopic methods.

Seminar – Examples of determining the structure of organic compounds on the basis of complementary information obtained using various spectroscopic methods. Analysis and interpretation of spectra.

15th week: 2nd partial exam

GENERAL AND SPECIFIC COMPETENCE:

General competences:

Apply spectroscopic methods to determine the structure of organic compounds on examples from the literature and own experimental data in solving chemical engineering problems. On the basis of complementary information obtained using various spectroscopic methods to analyse and interpret the spectra and determine the structure of organic compounds.

KNOWLEDGE TESTING AND EVALUATION:

2 partial written tests during the semester (60 % of points on each of the exams brings the release of the oral examination).

Written exam (50% of the points needed for passage).

Oral examination.

MONITORING OF THE COURSE QUALITY AND SUCCESSFULNESS:

Student questionary

LITERATURE:

Compulsory:

1. R. M. Silverstein, F. X. Webster, Spectrometric Identification of Organic Compounds, Wiley, 1997.

2. H. Friebolin: Basic One- and Rwo-Dimensional NMR Spectroscopy (3.izd.), Wiley-VCH, Verlag GmbH, Weinheim, 1998.

3. E. Pretzsch, P. Bühlmann, C. Affolter, Structure Determination of Organic Compounds, Springer, 2000.

4. B. D. Smith, B. Boggess, J. Zajicek: Organic Structure Elucidation, University of Colorado, 1998.

5. T. Gazivoda Kraljević, Određivanje struktura organskih spojeva, internal papers, 2012.