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| 1. Course title: Structure Elucidation in Organic Chemistry | | | | | |
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| 2. Code: | | 3. Type (lecture, practice etc.): lecture | | | |
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| 4. Contact hours: 3 hoursper week | | 5. Number of credits (ECTS): 4 | | | |
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| 6. Preliminary conditions (max. 3):  Organic Chemistry 1. lecture and lab. completed | | | | | |
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| 7. Announced:fall semester, spring semester, both | | | | | |
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| 8. Limit for participants: | | | | | |
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| 10. Responsible teacher (faculty, institute and department):  Dr. Cecília Sár PhD (Faculty of Medicine, Institute of Organic and Medicinal Chemistry) | | | | | |
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| 11. Teacher(s) and percentage: | | Dr. Cecília Sár | | 75 % | |
| Dr. Tamás Kálai | | 25 % | |
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| 12. Language:English | | | | | |
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| 13. Course objectives and/or learning outcomes:  The aim of this course is to introduce the students how to identify organic compounds from the complementary information afforded by four types of spectra: UV, infrared, mass and NMR. | | | | | |
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| 14. Course outline  week 1: Ultraviolet spectroscopy: transitions of valence electrons; characteristic absorption of chromophore groups; relationship between structure and spectra of biomolecules.  week 2: Infrared Spectroscopy: Introduction, theory, instrumentation, interpretation of spectra.  week 3: Infrared Spectroscopy: Characteristic group absorptions of organic molecules  week 4: Infrared Spectroscopy: Solving problems  week 5: Proton Magnetic Resonance Spectrometry (1H NMR): Introduction, theory, instrumentation.  week 6: 1H NMR: Chemical shift, simple spin coupling  week 7: 1H NMR: Protons on heteroatoms, chemical shift equivalence and magnetic equivalence, effects of a chiral center.  week 8: 13 C NMR Spectroscopy: Interpretation of 13 C spectra. The principles of MRI.  week 9: Mass Spectrometry: Mass spectrometer parts, ionization methods.  week 10: Mass Spectrometry: Appearance of the mass spectrum, mass spectra of various organic compound classes.  week 11: Mass Spectrometry: Interpretation of the mass spectrum through examples.  week 12: Summary of spectroscopic methods: identification of organic molecules from IR, NMR and mass spectra.  week 13: Summary of spectroscopic methods: identification of organic molecules from IR, NMR and mass spectra. | | | | | |
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| 15. Mid-semester works  Attending lectures is highly recommended. | | | | | |
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| 16. Course requirements and grading  Written exam is based on lectures, accessible electronic sources and books. The written evaluation is based on the theory, instrumentation and interpretation of UV, IR, 1H and 13C NMR and mass spectra. | | | | | |
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| 17. List of readings  Silverstein, R.M., Webster, F.X., Kiemle, D.: Spectrometric Identification of Organic Compounds, John Wiley and Sons, 2005.  Reichenbacher, M., Popp, J.: Challenges in Molecular Structure Determination, Springer, Heidelberg, 2012. | | | | | |
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| 18. Recommended texts, further readings  The slides of the lecture are available on Neptun. | | | | | |
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| **Date** | 13 April, 2017 | **Prepared by** |  | | |
| Dr. Cecília Sár  responsible teacher | | |
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| **Endorsed by** | | |  | | |
| program supervisor | | |