**Course Syllabus**

**1. Data about the program**

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| 1.1 Higher education institution | Babeș-Bolyai University |
| 1.2 Faculty | Faculty of chemistry and chemical engineering |
| 1.3 Doctoral school | Chemistry |
| 1.4 Field of study | Chemistry |
| 1.5 Study cycle | Doctorate |
| 1.6 Study program / Qualification | Doctoral training / PhD in CHEMISTRY |

**2. Course data**

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| 2.1 Name of discipline | | | Supramolecular chemistry and stereochemistry **– SDC-19-3** | | | | | | |
| 2.2 Teacher responsible for lectures | | | | | Prof.. dr. Ion Grosu | | | | |
| 2.3 Teacher responsible for seminars | | | | | Prof.. dr. Ion Grosu | | | | |
| 2.4 Year of study | I | 2.5 Semester | | II | | 2.6. Type of evaluation | - | 2.7 Course framework | OP |

**3. Estimated total time of teaching activities** (hours per semester)

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| --- | --- | --- | --- | --- | --- | --- | --- |
| 3.1 Hours per week | 2 | | Out of which: 3.2 Lectures | | 1 | 3.3 Seminars / Laboratory classes | 1 |
| 3.4 Total hours in the curriculum | 24 | | Out of which: 3.5 Lectures | | 12 | 3.6 Seminars / Laboratory classes | 12 |
| Allocation of study time: | | | | | | |  |
| Study supported by textbooks, other course materials, recommended bibliography and personal student notes | | | | | | | 100 |
| Additional learning activities in the library, on specialized online platforms and in the field | | | | | | | 100 |
| Preparation of seminars / laboratory classes, topics, papers, portfolios and essays | | | | | | | 18 |
| Tutoring | | | | | | | 8 |
| Examinations | | | | | | | - |
| Other activities: - | | | | | | | - |
| 3.7 Individual study (total hours) | | 226 | |
| 3.8 Total hours per semester | | 250 | |
| 3.9 Number of credits | | 10 | |

**4. Preconditions** (where applicable)

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| 4.1 Curriculum |  |
| 4.2 Competences |  |

**5. Conditions** (where applicable)

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| 5.1 Conducting lectures | - |
| 5.2 Conducting seminars / laboratory classes | - |

**6. Specific competences acquired**

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| **Professional competences** | Defining the notions, concepts, theories and models in the field of Stereochemistry and Supramolecular Chemistry and their appropriate use in professional communication  • Use of in-depth knowledge in the field of chemistry to explain and interpret the specific processes of Stereochemistry and Supramolecular Chemistry  • Identification and application of advanced concepts, methods and theories for solving problems specific to Stereochemistry and Supramolecular Chemistry  • Critical analysis and use of advanced methods and techniques for the quantitative and qualitative evaluation of the notions of Stereochemistry and Supramolecular Chemistry  • Application of advanced concepts and theories in the field of Stereochemistry and Supramolecular Chemistry for the elaboration of projects and problem solving  • Ability to understand and interpret complementary data for the characterization of organic compounds and processes, to express and argue the interpretation of data based on the correlation of results and comparison with data from the literature |
| **Transversal competences** | Execution of the requested tasks according to the specified requirements and within the imposed deadlines, in compliance with the norms of professional ethics and moral conduct, following a pre-established work plan  • Solving the requested tasks in accordance with the general objectives established by integration within a working group  • Permanent information and documentation in its field of activity  • Ability to prepare written reports and to publicly support these reports |

**7. Course objectives** (based on the acquired competencies grid)

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| 7.1 The general objective of the course | Acquisition of notions regarding the structural characterization of materials and precursors using specific techniques |
| 7.2 Specific objectives | Acquisition of basic theoretical knowledge on Stereochemistry and Supramolecular Chemistry  • Developing the ability to solve problems |

**8. Content**

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| 8.1 Lectures | Teaching methods | Comments |
| 8.1.1. General notions of stereochemistry | Presentation, discussion, case studies, exercises |  |
| 8.1.2. Symmetry operations, point groups of symmetry |
| 8.1.3. Enantiomerism: optical activity, configuration descriptors |
| 8.1.4. Chirality: central, axial, planar, helical and supramolecular. Prochirality |  |  |
| 8.1.5. Diastereoisomerism. Generalities. Configurational diastereoisomerism; experimental methods for determining configurations. |  |  |
| 8.1.6. Conformational analysis. Types of torsions in acyclic and cyclic compounds |  |  |
| 8.1.7. General notions related to supramolecular chemistry |  |  |
| 8.1.8. Non-covalent interactions |  |  |
| 8.1.9. General methods for the synthesis of macrocyclic compounds and mechanically interconnected compounds |  |  |
| 8.1.10. Physical and chemical properties of macrocyclic compounds and mechanically interconnected compounds |  |  |
| 8.1.11. Supramolecular architectures obtained by self-assembly |  |  |
| 8.1.12. . Adaptive chemistry (covalent dynamics) |  |  |
| Bibliography:  1. S. Mager, I. Grosu, L. David, Stereochemistry of Organic Compounds, Dacia Publishing House, 2006  2. E. L. Eliel, S. Wilen, Sterochemistry of Organic Compounds, WILEY, 1994.  3. P. Y. Bruice, Organic Chemistry, Prentice Hall, 1998.  4. J. March, B. Smith, Advanced Organic Chemistry, Wiley, 2006.  5. Steed J. W., Atwood J. L. Supramolecular Chemistry, Wiley, New York, (2000).  6. Vögtle, F .; Stoddart, J. F. and Shibasaki, M (editors), Stimulating Concepts in Chemistry, Wiley-VCH, Weinheim, Germany (2000).  7 Diederich, F .; Stang, P. G. and Tykwinski, R. R. (editors), Modern Supramolecular Chemistry-Strategies for Macrocycle Synthesis, Wiley-VCH, Weinheim, Germany (2008) | | |
| 8.2 Seminars / laboratory classes | Teaching methods | observations |
| 8.2.1. Symmetry operations, point groups of symmetry. Enantiomerism: optical activity, configuration descriptors | Presentation, discussion, exercises |
| 8.2.2-3. Chirality: central, axial, planar, helical and supramolecular. Prochirality |
| 8.2.4. Applications of NMR in conformational analysis of acyclic compounds, cycloalkanes, and heterocyclic compounds |
| 8.2.5-6. Geometric diastereoisomerism; determination of the stereochemistry of some compounds with geometric isomerism or which have several elements of chirality |
| 8.2.7-8 Problems related to macrocyclic compounds, cryptans and cyclophanes |
| 8.2.9-10 Problems related to host-guest supramolecular systems |
| 8.2.11-12 Problems related to self-assembled supramolecular architectures |
| **Last issues of Angew. Chem. Int. Ed.; Chem. Eur. J.; Eur. J. Org. Chem; Chem. Commun.; Chem. Sci.; Dalton Trans.; Org. Lett.; Organometallics; Inorg. Chem. and J. Org. Chem** |
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**9. Aligning the contents of the discipline with the expectations of the epistemic community representatives, professional associations and standard employers operating in the program field**

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| By acquiring the theoretical-methodological concepts and approaching the practical aspects included in the discipline Stereochemistry and supramolecular chemistry, doctoral students acquire a consistent knowledge, in accordance with the partial competencies required for possible occupations provided in Grid 1 - RNCIS |

**10. Examination**

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| Activity type | 10.1 Evaluation criteria | 10.2 Evaluation methods |  |
| Lectures and seminars | Assessment of knowledge | Oral presentation of a topic |  |
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| Date of issue | Signature of the teacher responsible for lectures | Signature of the teacher responsible for seminars |

10.10.2021

Date of approval by the doctoral school council Signature of the doctoral school director