**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 | | | Mass Spectrometry | | | | | | |
| 2.2 Teacher responsible for lectures | | | | | Prof. Dr. Anca Silvestru | | | | |
| 2.3 Teacher responsible for seminars | | | | | Prof. Dr. Anca Silvestru | | | | |
| 2.4 Year of study | I | 2.5 Semester | | II | | 2.6. Type of evaluation | E | 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 |  Access to internet and data bases, as well as experimental  spectra are used. |
| 5.2 Conducting seminars / laboratory classes |  Access to internet and data bases, as well as experimental  spectra are used. |

**6. Specific competences acquired**

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|  |  Definition of notions, concepts, theories and models in the field of Mass  Spectrometry and their proper use in professional communication.   Using in-depth knowledge in the field of chemistry to explain and interpret  specific notions of Mass Spectrometry.   Identification and application of advanced concepts, methods and theories to  solve problems specific to Mass Spectrometry.   Critical analysis and use of advanced methods and techniques for the  quantitative and qualitative evaluation in Mass Spectrometry.   Application of advanced concepts and theories in the field of Mass Spectrometry  for project development and problems solving. |
|  |  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 predetermined work plan.   Solving the required tasks in accordance with the general objectives set by the  integration within a working group.   Permanent information and documentation in the field of activity   Concern for the improvement of the results of the professional activity by  getting involved in the tasks carried out.   Ability to draw up 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 |  Acquiring notions regarding the structural  characterization of materials and precursors using mass spectrometry. |
| 7.2 Specific objectives |  Acquiring basic theoretical knowledge in Mass  Spectrometry   Developing the capacity to interpret spectra,  establish mechanisms for reacting and assigning the structure of compounds by using data from mass spectra. |

**8. Content**

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| 8.1 Lectures | Teaching methods | Comments |
| 8.1.1. General notions, specific to mass spectrometry. Ionization methods, sample preparation. | Presentation, discussion, case studies, exercises |  |
| 8.1.2. General principles for recording and interpreting mass spectra. |  |
| 8.1.3. Mass spectra obtained by the EI ionization method. The principle of the method, the characteristics of the spectra, the interpretation of the data. |  |
| 8.1.4. Mass spectra obtained by the CI ionization method. The principle of the method, the characteristics of the spectra, the interpretation of the data. | Presentation, discussion, case studies, exercises |  |
| 8.1.5. Mass spectra obtained by the FAB ionization method. The principle of the method, the | Presentation, discussion, case studies, exercises |  |

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| characteristics of the spectra, the interpretation of the data. |  |  |
| 8.1.6 Mass spectra obtained by the ESI ionization method. The principle of the method, the characteristics of the spectra, the interpretation of the data. |  |  |
| 8.1.7. Mass spectra obtained by the MALDI ionization method. The principle of the method, the characteristics of the spectra, the interpretation of the data. |  |  |
| 8.1.8. Tandem mass spectrometry. The principle of the method, the characteristics of the spectra, the interpretation of the data. |  |  |
| 8.1.9. Equipments used in mass spectrometry. Constructive variants and technical performance. |  |  |
| 8.1.10. Applications of mass spectrometry in the investigation of reaction mechanisms. |  |  |
| 8.1.11. Applications of mass spectrometry in biology. |  |  |
| 8.1.12. Use of mass spectrometry in the qualitative and quantitative analysis of mixtures. |  |  |
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| 8.2 Seminars / laboratory classes | Teaching methods | Comments |
| Case studies prepared with the doctoral students, based on their individual doctoral research topics | Presentation, discussion, exercises |  |
| 8.2.1. Interpretation of EI mass spectra. | Presentation, discussion, exercises, case studies |  |
| 8.2.2. Interpretation of CI mass spectra. |  |
| 8.2.3. Interpretation of FAB mass spectra. |  |
| 8.2.4. Interpretation of ESI+ mass spectra. |  |
| 8.2.5. Interpretation of ESI- mass spectra. |  |
| 8.2.6. Interpretation of MALDI+ mass spectra. |  |
| 8.2.7. Interpretation of MALDI- mass spectra. |  |
| 8.2.8. Matrices and solvents used in mass spectrometry. Preparation of samples. | Presentation, discussion, exercises, case studies |  |
| 8.2.9. Applications of mass spectrometry in establishing the mechanisms of catalytic reactions. Interpretation of experimental data. Tandem mass spectrometry. |  |
| 8.2.10. Applications of mass spectrometry in the determination of protein structure. Interpretation of experimental data. |  |
| 8.2.11. Applications of mass spectrometry in the qualitative analysis of mixtures. Interpretation of experimental data. |  |
| 8.2.12. Applications of mass spectrometry in the identification of compounds. Establishing the structure and chemical composition. Correlation of MS data with those provided by other structural methods (NMR, IR, etc.). |  |

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Bibliography:

1. W. Henderson, J. S. McIndoe, *Mass spectrometry of Inrganic and Organometallic Compounds*, Wiley, Chichester, 2005.

2. J. R. Chapman, *Practical Organic Mass Spectrometry*, Wiley, Chichester, 1997.

3. Original papers in the field, published in journals e.g. Angew. Chem. Int. Ed.; Chem. Eur. J.; Eur. J. Inorg. Chem; Chem. Commun.; Chem. Sci.; Dalton Trans.; Org. Lett.; Organometallics; Inorg. Chem., J. Org. Chem. și Mass Spectrometry.

**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**

 By acquiring the theoretical and methodological concepts and approaching the

practical aspects included in the discipline Mass Spectrometry, the PhD students acquire a consistent baggage of knowledge, in accordance with the partial competences required for the possible occupations provided in Grid 1 – RNCIS.

**10. Examination**

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| Activity type | 10.1 Evaluation criteria | 10.2 Evaluation methods | 10.3 Weight in the final grade |
| 10.4 Lectures | Assessment of knowledge | Oral exam | 60% |
| 10.5 Seminars / laboratory classes | Activity during seminars | Discussions, answers to questions at seminars | promoted |
| Assessment of knowledge | Ongoing tests | 40% |
| 10.6 Minimum performance standard | | | |
|  Grade 5 (five) / promoted | | | |

Date of issue

10.04.2021

Signature of the teacher responsible for lectures

Signature of the teacher responsible for seminars

Date of approval by the doctoral school council

Signature of the doctoral

school director

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