**FISA DISCIPLINEI**

**1. Information regarding the program**

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| 1.1 Higher education institution | Babeş-Bolyai University, Cluj-Napoca |
| 1.2 Faculty | Chemistry and Chemical Engineering |
| 1.3 Department | Chemistry |
| 1.4 Field of study | Chemistry |
| 1.5 Study cycle | Doctorate |
| 1.6 Study programme / Qualification | Doctorate |

**2. Information regarding the discipline**

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| 2.1 Name of the discipline | | | Computational Chemistry - **SDC-19-11** | | | | |
| 2.2 Course coordinator | | | Prof. Radu Silaghi-Dumitrescu | | | | |
| 2.3 Seminar coordinator | | | Prof. Radu Silaghi-Dumitrescu | | | | |
| 2.4 Year of study | I | 2.5 Semester | 2 | 2.6. Type of evaluation | E | 2.7 Type of discipline | Op |

**3. Total estimated time** (hours/semester of didactic activities)

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| 3.1 Hours per week | 4 | | Of which: 3.2 course | | 2 | 3.3 seminar/laboratory | 2 |
| 3.4 Total hours in the curriculum | 56 | | Of which: 3.5 course | | 28 | 3.6 seminar/laboratory | 28 |
| Time allotment: | | | | | | | ore |
| Learning using manual, course support, bibliography, course notes | | | | | | | 20 |
| Additional documentation (in libraries, on electronic platforms, field documentation) | | | | | | | 20 |
| Preparation for seminars/labs, homework, papers, portfolios and essays | | | | | | | 20 |
| Tutorship | | | | | | | 6 |
| Evaluations | | | | | | | 3 |
| Other activities: not the case | | | | | | | - |
| 3.7 Total individual study hours | | 69 | |  | | | |
| 3.8 Total hours per semester | | 125 | |
| 3.9 Number of ECTS credits | | 5 | |

**4. Prerequisites** (if necessary)

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| 4.1 curriculum |  Not the case |
| 4.2 competencies |  Not the case |

**5. Conditions** (if necessary)

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| 5.1 for the course |  Students will attend the courses having the materials made available  prior to each course   Students will turn off their mobile phones |
| 5.2 for the seminar /lab activities |  Students will attend the seminar with the course notes referring to the  seminar topic   Students will turn off their mobile phones   A report on practical activities needs to be turned in by each student in  order for them to receive a grade |

**6. Specific competencies acquired**

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|  |  Definition of notions, concepts, theories and advanced models in the field of Computational  Chemistry as well as their proper use within the professional community   Use of in-depth knowledge of chemistry to explain and interpret tools and processes  specific to computational chemistry   Identifying and applying advanced concepts, methods and theories to solve problems  specific to computational chemistry   Critical analysis and use of advanced methods and techniques for the quantitative and  qualitative evaluation of the notions of computational chemistry   Applying concepts and theories in the field of computational chemistry to develop projects  and solve problems   Ability to understand and interpret complementary data for the characterization of  compounds and chemical processes, to express and argue the interpretation of data based on the correlation of results and comparison with data from the literature |
|  |  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   Concern for improving the results of professional activity by getting involved in the  activities carried out   Ability to prepare written reports and to publicly defend/support these reports |

**7. Objectives of the discipline** (outcome of the acquired competencies)

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| 7. General objective of the discipline |  Acquiring notions on the use of computational chemistry to solve  research problems, complementary to other experimental techniques |
| 7.2 Specific objective of the discipline |  Acquisition of basic theoretical knowledge on computational  chemistry   Developing the ability to solve problems . |

**8. Content**

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| 8.1. Course | Teaching methods | Remarks |
| 8.1.1. Introduction to computational chemistry, defining the field, the relationship with the other branches of chemistry | Presentation; Explanation, Conversation; Description; Debate |  |
| 8.1.2. Suprafețe de potențial | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.3. Molecular mechanics | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.4. Molecular orbitals |  |
| 8.1.5. Semiempirical MO methods | Presentation; Explanation, |

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|  | Conversation; Description; Debate |  |
| 8.1.6. Ab initio and post-Hartree-Fock MO methods | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.7. Density functional theory (DFT) | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.8. Hybrid QM/MM methods | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.9. Spectroscopic properties | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.10. Determining charge distributions; molecular electrostatic potentials | Presentation; Explanation, Conversation; Description; Debate |
| 8.1.11-12. Applications in medicinal chemistry | Presentation; Explanation, Conversation; Description; Debate |
| **Bibliography**  1. C.J.Cramer, Essentials of Computational Chemistry, Theories and Models, Wiley, 2004.  2. E.Lewars, Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers, 2003  3. I.Silaghi-Dumitrescu, D. Horvath, Mecanica Moleculara, Presa Universitara Cluj-Napoca, 1996.  4. L. Piela, Ideas of Quantum Chemistry*,* 2nd edition, Elsevier, 2014. | | |
| 8.2 Seminar / Laboratory | Teaching methods | Remarks |
| 8.2.1. Software packages in computational chemistry; basics of file architecture and manipulation | Conversation, Learning by discovery, Problem solving | 2 hours |
| 8.2.2-3. Construction, editing, import, export of models / (bio) molecules; quality criteria | Conversation, Learning by discovery, Problem solving | 4 hours |
| 8.2.4. Types of calculations and methods in the most common software packages; choosing the calculation methodology | Conversation, Learning by discovery, Problem solving | 2 hours |
| 8.2.5-6. Single-point calculations, geometry optimizations, conformation elements; criteria for judging the success of the procedure | Conversation, Learning by discovery, Problem solving | 4 hours |
| 8.2.7-8. Calculations of molecular and supramolecular properties | Conversation, Learning by discovery, Problem solving | 4 hours |
| 8.2.9-10. Calcule ale proprietăților legate de reactivitate; stări de tranziție | Conversation, Learning by discovery, Problem solving | 4 hours |
| 8.2.11-12 Calcule asupra sistemelor biologice; situsuri active. | Conversation, Learning by discovery, Problem solving | 4 hours |
| Bibliography  1. C.J.Cramer, Essentials of Computational Chemistry, Theories and Models, Wiley, 2004.  2. E.Lewars, Computational Chemistry, Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Kluwer Academic Publishers, 2003  3. I.Silaghi-Dumitrescu, D. Horvath, Mecanica Moleculara, Presa Universitara Cluj-Napoca, 1996.  4. F.Jensen, Introduction to Computational Chemistry, Wiley, 1999. | | |

**9. Corroborating the content of the discipline with the expectations of the epistemic community, professional associations and representative employers within the field of the program**

 Acquirement of the theoretical and practical concepts of **Computational Chemistry** course will

provide the students with the competencies requested by ARN.

**10. Evaluation**

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| Type of activity | 10.1 Evaluation criteria | 10.2 Evaluation methods | 10.3 Share in the final grade (%) |
| 10.4 Course | Correctness of answers – proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within new contexts. | Written report with interpretation of practical work | 50% |
| Correct solving of the problems as part of the examination subjects |
| 10.5 Seminar/laboratory | Correctness of answers – proper understanding and learning of notions and concepts discussed during lectures; Correct use of learned concept within  new contexts. | Written report with interpretation of practical work | 50% |
| Quality of reports |
| 10.6 Minimum performance standards | | | |
|  Adequate knowledge of at least one technique for each module. | | | |

Date Signature of course coordinators Signature of seminar coordinators

26.10.2021

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Date of approval Signature of the head of department

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