**Course sheet**

**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 / Doctor |

**2. Course data**

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| 2.1 Name of discipline | | | Molecular Modeling | | | | | | |
| 2.2 Teacher responsible for lectures | | | | | Prof. Lorentz Jäntschi | | | | |
| 2.3 Teacher responsible for seminars | | | | | Prof. Lorentz Jäntschi | | | | |
| 2.4 Year of study | 1 | 2.5 Semester | | 2 | | 2.6. Type of evaluation | col | 2.7 Course framework | DD |

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

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| 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 | | | | | | | 12 |
| Additional learning activities in the library, on specialized online platforms and in the field | | | | | | |  |
| Preparation of seminars / laboratory classes, topics, papers, portfolios and essays | | | | | | | 12 |
| Tutoring | | | | | | |  |
| Examinations | | | | | | | 3 |
| Other activities: - | | | | | | |  |
| 3.7 Individual study (total hours) | | 51 | |
| 3.8 Total hours per semester | | 48 | |
| 3.9 Number of credits | | 10 | |

**4. Preconditions** (where applicable)

|  |  |
| --- | --- |
| 4.1 Curriculum | * MSc in Mathematics, Informatics, Physics, Chemistry, Biology, Geology or Engineering |
| 4.2 Competences |  |

**5. Conditions** (where applicable)

|  |  |
| --- | --- |
| 5.1 Conducting lectures | * Projector: Course in electronic form available |
| 5.2 Conducting seminars / laboratory classes | * Computers |

**6. Specific competences acquired**

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| --- | --- |
| **Professional competences** | * Knowledge and understanding of concepts, models, theories and methods of basic chemistry and their appropriate use in professional communication; * Using basic knowledge of chemistry for explanation and interpretation of concepts and processes specific situations; * Applying the models and modelling basic principles and methods for solving problems; * Use of criteria and evaluation methods to assess the quality, advantages and limitations of processes, concepts, methods and theories. |
| **Transversal competences** | * Responsible execution of laboratory activities in conditions of autonomy and support from the supervisor; * Familiarizing with specific roles and teamwork activities and distribution of tasks within the team conducted experiments in working groups; * Awareness of the need for continuing training; * Efficient use of resources (course support, manual laboratory notebook laboratory list of questions and answers; individual documentation) and learning techniques (reading, writing, communication, exercise, problem solving, building issues) for personal and professional development. |

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

|  |  |
| --- | --- |
| 7.1 The general objective of the course | * Creation and development of abilities to manipulate applications for designing of the molecular structure |
| 7.2 Specific objectives | * Formation of skills and abilities to use the principle of parsimony in the development and use of models of molecular structure and biochemical processes; * Formation of skills and abilities to perform a structure-activity correlation and regression analysis for a class of compounds; * Development of skills for manipulating molecular modeling databases; * Development of skills to use molecular modeling programs. |

**8. Content**

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| --- | --- | --- |
| 8.1 Lectures | Methods | Comments |
| **Molecular structure** |  | C1, C2 |
| Chemical formulas - empirical, raw, molecular and structural | Presentation, discussion, case studies, exercises | 1h |
| Biomolecules - primary, secondary, tertiary, quaternary levels of structure | 1h |
| **Molecular models** | C3, C4 |
| Molecular topology, | 1h |
| Molecular geometry | 1h |
| **Processes models** | C5 |
| Molecular sets, physical interaction | 1h |
| **Molecular properties** | C6 - C8 |
| From and to atomic properties | 1h |
| Intensive vs. extensive | 1h |
| Physical, chemical and biological | 1h |
| **Entropy, energy, and potential** | C9 |
| Hartley, Shannon, Renyi, Lenard-Jones, Mie | 1h |
| **Correlation and regression analysis** | C10 - C12 |
| Pearson, Spearman, Kendall, Goodman-Kruskal | 1h |
| Simple, Multiple, PCA, DCA | 1h |
| Factor analysis, Clustering |  | 1h |
|  | | |
| 8.2 Seminars / laboratory classes | Methods | Comments |
| ChemWindow software | Presentation, discussion, exercises, applications | 1h |
| ChemDraw software |  | 1h |
| ChemOffice software |  | 1h |
| HyperChem software |  | 1h |
| Spartan software |  | 1h |
| Gaussian software |  | 1h |
| PubChem database |  | 1h |
| ChemSpider database |  | 1h |
| NIST database |  | 1h |
| Statistica software |  | 1h |
| <http://l.academicdirect.org> |  | 2h |
| Bibliography:  1. Diudea MV, Gutman I, Jäntschi L. Molecular Topology. Nova Science, Huntington, NY, USA, 2001 (Ed. I), 2002 (Ed. II), 332 p. online: <http://lori.academicdirect.org/books>  2. Ungureşan ML, Jäntschi L, Gligor DM. Aplicaţii educaţionale de chimie pe calculator. MediaMira, Cluj-Napoca, 2004, 250p. online: <http://lori.academicdirect.org/books>  3. Jäntschi L. Microbiologie, toxicology. Studii fitosanitare, Amici, Cluj-Napoca, 2003, 191 p. online: <http://lori.academicdirect.org/books>  4. Jäntschi L, Bolboacă SD. Results from the Use of Molecular Descriptors Family on Structure Property/Activity Relationships. Int J Mol Sci 2007;8:189-203, online: <http://lori.academicdirect.org/articles>  5. Jäntschi L, Prezentarea şi prelucrarea datelor experimentale, U.T.Press: Cluj-Napoca 2013. 70 p. online: <http://lori.academicdirect.org/books>  6. Librăria de soft <http://l.academicdirect.org> | | |

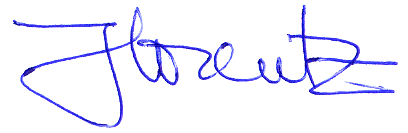
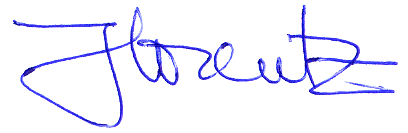
**9. Aligning the contents of the discipline with the expectations of the epistemic community representatives, professional associations and standard employers operating in the program field**

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| * Software programs discussed are in current use and discussion is based on their up-to-date versions. |

**10. Examination**

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| --- | --- | --- | --- |
| Activity type | 10.1 Evaluation criteria | 10.2 Evaluation methods | 10.3 Weight in the final grade |
| Lectures | A short report (1-2 pages) | Conversational | 50% |
| Laboratory | A short presentation (5-8 slides) | Presentation | 50% |
| 10.6 Minimum performance standard | | | |
| * N.A. | | | |

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| --- | --- | --- |
| Date of issue | Signature of the teacher responsible for lectures | Signature of the teacher responsible for seminars |



13.10.21

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

**DIDACTIC LABORATORY FILE**

1. Laboratory Name: Mathematical and computational modelling in biology and chemistry

2. Connected Discipline: Molecular modeling

3. Place (Building block, room): B.-dul Muncii 103-105, C500, C501 & C502 rooms

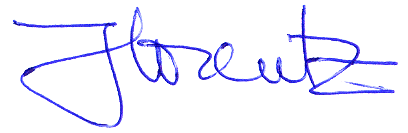
4. Seats (students): 10

5. Surface: 65 m2

6. Infrastructure:

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| Databases | * IP: 193.226.7.200; * Support: MySQL; * Connectivity: * Internet; * IP intranet 172.27.211.4 (mdfv) - cca. 900Gb; * IP intranet 172.27.211.5 (sensors) - cca. 500Gb; |
| Molecular modelling | * IP: 193.226.7.203; * Suport: PHP; * Connectivity: * Internet; * IP intranet 172.27.211.3 (comput) - 8xCPU P4, 32Gb RAM; * IP intranet 172.27.211.4 (mdvf) - 8xCPU P4, 32Gb RAM; |
| Web | * IP: 193.226.7.140; * Support: Apache; * Connectivity: * Internet; * Intranet clients: 172.27.211.2-20; |
| Workstations | * IP intranet 172.27.211.3 (comput); * Support: FreeBSD (Unix); * IP intranet 172.27.211.4 (mdfv); * Support: FreeBSD (Unix); * IP intranet 172.27.211.5 (sensors); * Support: FreeBSD (Unix); |
| Desktops | * Hardware: 10 computers, model ≥P4 * Software: * Software operating: Windows; * Software office: Office; * Software dedicated (see below); * Connectivity: Internet; |
| Dedicated software | Statistica; SPSS; Molecular Modeling Pro; ChemOffice; HyperChem; Dragon; RasMol; deMon2k; GAMESS; MOLDEN; MOPAC; MPQC; NWChem; Octopus; Clustal X; GABRIEL; GAL; GAML; GARLI; GDE; GOAL; LamarckianGA; MacClade; MEGA; Mesquite; metaGA; ModelTest; MrBayes; MS BLAST; NCBI BLAST; PAUP\*; r8s; RAGA; SAGA; S-System; Spartan |

Date: 13.10.2021 Name of discipline titular,

 Prof. Lorentz JÄNTSCHI

Signature

