EUROPEAN UNIVERSITY OF THE SEAS

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SEA-EU micro credential course sheet

Course offers for the SEA-EU micro-credential Programmes on Future Skills or Sustainability Studies

General Information

Course Title	**Code**
Hands-on Computer Aided Drug Design	SEAEU-01-2026
Course teacher	
Samanta Romanowska (main teacher), *Lidia Chomicz-Mańka (associated teacher)*	
Organiser/Contact person	
samanta.makurat@ug.edu.pl	
Credits (ECTS)	**Workload**
3	1 ECTS = 25 to 30 h Workload, including _45_ contact hours and _30_ self instructed learning For getting the courses ECTS recognized, please contact your university authorities for more information.
Language of instruction	
English/Polish	
Mode of provision	
☐ Physical attendance of students: 100% ☐ Physical attendance of students: partly required	☐ remote attendance possible X online 100%
Percentage of e-learning (0-100%)	
100% *hybrid, with partial physical attendance of students is also possible on demand (see enrolment requirements).*	
Short course description (for dissemination to students)	
This practical laboratory course provides a comprehensive introduction to computational chemistry and is specifically designed for chemistry-related or closely associated students with no prior experience in computations. Participants will gain a broad understanding of the fundamental methodologies and applications of computational chemistry, beginning with essential technical skills in a Unix/Linux environment and progressing to the management of scientific simulations on High-Performance Computing (HPC) clusters.	

The curriculum is structured around two major pillars of modern computational chemistry, with particular emphasis on applications in computer-aided drug design (CADD) and biomedical research. A central focus is placed on Quantum Mechanics (QM) methods, using the Gaussian software package to investigate and predict the properties and behavior of small molecules, and Molecular Dynamics (MD) simulations, employing the AMBER suite to model and analyze protein–ligand complexes, a key component of modern drug discovery.

As a part of the course, analysis of experimental structures from the Protein Data Bank (PDB) will allow to explore how substrates and inhibitors interact with biological targets while developing a solid conceptual understanding of the theoretical foundations underlying major computational chemistry techniques. Through hands-on work with molecular visualization and analysis tools such as VMD, Molden, and PyMOL, participants will learn to interpret structural data, molecular properties, and simulation trajectories.

Integrated within the SEA-EU "Future Skills" framework, the course fosters the development of essential competencies in digital literacy, data analysis, critical thinking, scientific problem-solving, and collaborative research practices. Upon completion, students will possess both the theoretical background and practical skills necessary to perform and critically evaluate computational studies in chemistry, biochemistry, and drug discovery.

Organisational Information

Course format/teaching and learning method (see SEA-EU list of teaching and learning methods at the end of this document)
Lecture, Seminar and Practical Study Unit
Max. number of participants
Up to 12 students for the lecture, *Up to 12 students for the seminar group,* *Up to 6 students on one practical unit.*
Course enrolment
MS Forms: https://forms.office.com/e/DMWUcBWtdR Please register with your university e-mail. Only selected students will receive feedback information. Enrollment is possible until 15.10.2026 The course will start in the first week of 11.2026, will last 10 weeks, up to an end of 02.2027
Course fees
No fees

Enrolment requirements
Study level X Bachelor (level 6) ☐ Master (level 7) ☐ PhD/Doctorate (level 8) *Master and PhD students can also participate* Entry level of language proficiency: English B2 or Polish B2 Other requirements: *Basic knowledge of physical chemistry and access to a computer with Internet. Students should ideally install several freeware tools prior to the course (e.g., PuTTY, Xming, WinSCP, VMD Molden and Pymol). Alternatively, physical attendance is possible in the faculty's computer lab, where pre-configured Linux workstations are provided.*
Course dates, period and time / Link to the University's website for the course
5 x 2 hours lecture *5 x 2 hours seminar* *5 x 5 hours practice* The course will start in the first week of 11.2026, will last 10 weeks, up to an end of 02.2027 Link to the University's website for the course: under preparation
Other remarks
Enrollment is subject to the first come, first served rule or equal distribution among Partner Universities. In case of any ambiguities or disputes, the final decision rests with the instructor.

Learning Conditions

Course content
• *Tools of computational chemistry: Linux terminal, text editors, HPC environments, crystal structure databases, and visualization programs,* • *Quantum Mechanics (QM) calculations: Geometry optimization, energy analysis, UV spectra, HOMO-LUMO orbitals using Gaussian* • *Molecular Dynamics (MD) simulations: Force fields, system preparation, alanine dipeptide and protein-ligand complex simulations using AMBER* • *Introduction to QM/MM and other computational methods* • *Small molecules and protein systems visualization programs (pyMOL, VMD, Gaussian).* • *Data analysis and interpretation*
Learning outcomes (knowledge, skills, attitudes)
• *Digital/Data Literacy (list and use programming languages and data visualization tools, configure connections in the digital space): Students are able to apply specialized command-line tools and text editors in a Unix-like environment to manage and configure scientific data workflows on High-Performance Computing (HPC) clusters,* • *Critical/Systems Thinking (recognize facts, concepts, theories and principles, student can to carry out an informed, critical analysis): Students are able to recognize and evaluate*

the core concepts and principles of QM, MM, and QM/MM methodologies to carry out an informed, critical analysis of their applicability to complex chemical systems,

- *Data Literacy/Critical Thinking (collect, classify and evaluate data, analyze information to reach factually sound conclusions): Students are able to collect, classify, and evaluate computational data from Quantum Mechanics (QM) calculations to analyze complex information and reach factually sound conclusions regarding molecular electronic properties and spectra,*
- *Problem Solving (evaluate information objectively and form well-reasoned conclusions): Students are able to conduct Molecular Dynamics simulations and interpret molecular trajectories by objectively evaluating structural parameters (RMSD, distances) to form well-reasoned conclusions about biomolecular stability,*
- *Digital Collaboration (exchange information in the digital space and collaborate with the help of digital tools): Students are able to collaborate effectively in the digital space by exchanging simulation data and leveraging digital tools to achieve a common research goal in a hybrid learning environment.*

Student activities

- *Use command-line tools and editors in a Unix-like environment.*
- *Working on HPC clusters*
- *Differentiate between QM, MM, and QM/MM methodologies and apply them correctly.*
- *Run QM calculations, geometry optimizations and interpret electronic properties (dipole moment, frequencies, spectra),*
- *Conduct MD simulations, measure structural parameters (RMSD, distances), and visualize trajectories,*
- *Preparing and delivering group presentations, discussing and giving feedback*
- *Performing data interpretation*

Attendance policy

Attendance to all classes is required; however, in case of unforeseen circumstances, the instructor will make the final decision.

Assessment Methods (see SEA-EU list of assignments in this document)

- *Oral Examination - 3 group presentations: 3x25% = 75% of the grade*
- *Examination - Quiz: 25% of the grade*

Grading

X graded ☐ non-graded (pass/fail)

Study materials/Course literature

F. Jensen, "Introduction to Computational Chemistry";
J. B. Foresman and Æ Frisch, „Exploring Chemistry with Electronic Structure Methods“;
D. Frenkel, B. Smit, „Understanding Molecular Simulation“;
A. R, Leach, „Molecular Modeling: Principles and Applications“
Online manuals for Gaussian, AMBER, VMD, Pymol.

Linkage to SEA-EU micro-credential Programmes

Linked to micro-credential programme and category (choose only one category) (see Future Skills Framework or Sustainability Studies Framework)	
X Future Skills ☐ Higher order thinking competences ☐ Self competences ☐ Social and communication competences ☐ Transformative competences X Digital and media competences	☐ Sustainability Studies ☐ Sustainability as a concept ☐ Sustainable economy ☐ Peace, justice and inclusion ☐ Life on land and in water ☐ Climate change ☐ Sustainable cities and local communities ☐ Industry and Innovation for Sustainability

Linked Competence(s)/Issue(s) in your chosen category you will provide with your teaching

Digital and media competences,

- *Data literacy competences (Students learn to collect, classify, evaluate, and interpret complex computational data using specialized programming tools and databases)*
- *Digital collaboration competences (some tasks are planned for students to be prepared in groups, especially, A significant portion of the assessment is based on group presentations preparing these presentations requires students to create a constructive working atmosphere for virtual collaboration and practice transparency while combining their individual findings into a single digital product)*

Higher order thinking competences,

- *Problem solving competences (Students are tasked with recognizing **complex** problems from the domain of physical chemistry and identifying their key components)*
- *Critical and Systems Thinking Competences (Students must recognize concepts, theories, and principles, such as Quantum Mechanics and Molecular Dynamics, relevant to carrying out an informed, critical analysis of their results)*

Self competences,

- *Complexity and ambiguity competences (This course requires students to manage high-level scientific complexity where there is often no single "correct" answer, but rather a balance of approximations)*

Social and Communication

- *Collaboration and Networking Competences (The laboratory is structured around collaborative problem-solving, for some project students work in groups, jointly plan a common setting for cooperative work and organize roles within their team, A*

significant portion of the course (75% of the final grade) is based on group presentations)

- *Communication Competences (The course emphasizes the ability to translate complex, raw computational data into clear and precise scientific communication)*

Sustainable economy

- *Responsible and sustainable production and consumption (course aligns with the principles of Green Chemistry by replacing physical, resource-heavy experiments with in silico simulations. By using computational methods (QM/MD) instead of traditional laboratory trials, researchers can drastically minimize the consumption of chemical reagents and eliminate the production of hazardous chemical waste, leading to more sustainable research and development processes)*

Life on land and water

- *Public health, poverty and well-being (a special emphasis on technical methods used in drug design and biomedical research, such as analyzing protein-ligand complexes, ools are essential for the advancement of modern medicine, enabling the discovery of new treatments and a better understanding of molecular disease mechanisms, which is vital for enhancing global public health and societal well-being)*

Future Skills Framework

Meta category	Competences
Higher order thinking competences	☐ Adaptability competences ☐ Problem solving competences ☐Critical and Systems thinking competences
Self competences	☐ Active Learning competences ☐ Self-awareness competences ☐ Complexity and ambiguity competences
Social and communication competences	☐ Collaboration and networking competences ☐ Communication competences ☐ Leadership competences
Transformative competences	☐ Entrepreneurship competences ☐ Citizenship competences ☐ Global awareness competences
Digital and media competences	X Data Literacy competences ☐ Media literacy competences X Digital collaboration competences

Sustainability Studies Framework

Meta-category	Issues
Sustainability as a concept	☐ Key concepts and principles of sustainability ☐ Evolution of the concept of sustainable development ☐ Introduction to corporate sustainability ☐ Implementing sustainability
Sustainable economy	☐ Responsible and sustainable production and consumption ☐ Corporate Social Responsibility and decent work ☐ Green, Circular and Blue Economy
Peace, justice and inclusion	☐ Resilience, Preparedness and Emergency Management ☐ Building equitable, inclusive societies ☐ Democracy and citizenship ☐ International and Environmental Law
Life on land and in water	☐ Sustainable food production ☐ Public health, poverty and well-being ☐ Biodiversity in ecosystems ☐ Hydrosphere, Oceans and Water Management
Climate change	☐ Consequences of climate change on the ocean ☐ Greenhouse effect ☐ Social, cultural and economic consequences of climate change
Sustainable cities and local communities	☐ Sustainable city planning ☐ People, Resources and Environment ☐ Sustainable tourism, travel and mobility

	☐ Waste and recycling
Industry and Innovation for Sustainability	☐ Inclusive and sustainable innovation and industrialization ☐ Sustainable, innovative and resilient infrastructure development ☐ Clean Energy and Bioeconomy ☐ The sustainability of information and communication technology (ICT) including supply chains

For details and learning outcomes see SEA-EU micro-credentials Sustainability Studies Framework document

Teaching and learning methods:

Teaching method	Definition
Fieldwork	Educational activities conducted outside the classroom, typically in real-world settings. It involves hands-on experience, data collection, or research in a specific field related to the course.
Lecture	A method of teaching where an instructor presents information to a large group of students. It is a one-way communication where the lecturer imparts knowledge and concepts.
Performance	A teaching method that involves students showcasing their skills or understanding through practical demonstrations, presentations, or performances, often related to the subject matter.
Practical Study-Unit	A study unit focused on hands-on application of theoretical knowledge, often involving practical exercises, experiments, or projects related to the course.
Practicum	Similar to an internship, a practicum is a hands-on learning experience in a professional setting, typically associated with teacher training or counselling programs.
Project	A collaborative or individual task requiring students to plan, execute, and present the results of an in-depth investigation or creative work related to the course.
Seminar	A small-group discussion or workshop led by a facilitator, where students actively engage with the material, discuss concepts, and share ideas. It encourages participation and critical thinking.
Tutorials	Small-group or one-on-one sessions where students receive personalised instruction, clarification of concepts, and guidance from a tutor or instructor. Tutorials supplement larger lectures and allow for individualised learning.

Methods of Assessment:

Teaching method	Definition
Analysis Task	A task which requires students to identify the primary elements of a problem or task at hand, and then outline the steps and skills required to ensure that the task is performed optimally.
Assignment	Normally an essay (or a set of written exercises) to be done away from the classroom and submitted by a set date.
Case Study (Exam conditions)	A research approach that is used to generate in-depth, multi-faceted understanding of a complex issue within a real-life context, which includes the application of discipline specific models, constructs and research literature..
Case Study (take home)	Students are required to work through a case study to identify the problem(s) and to offer potential solutions; useful for assessing students' understanding and for encouraging students to see links between theory and practice. Case studies could be provided in advance of a time-constrained assessment.
Classwork	Written or oral exercises carried out by students whilst in the classroom. Examples include: discussions, debates, translation exercises, etc.
Competencies	Refers to a continuous process which aims at building the student's capabilities (knowledge, skills and abilities), and assessing them against stated (professional) standards.
Essay	An analytical, interpretative, or critical piece of writing that expresses the writer's opinion in response to a set question, problem or issue.
Examination	A written assessment (using traditional pen and paper or a digital platform for the administration of the examination) which is carried out in a predetermined, restricted time span under invigilated conditions. This type of assessment is normally summative in nature.
Fieldwork	Work which is done on site to enable students to gain practical experience and knowledge through first hand observation.
Internship	An internship can be defined as any arrangement in which students are given opportunities to apply their learning and demonstrate their professional capabilities in the workplace, community context or other relevant settings. Assessment will be conducted by academic supervisors, industry supervisors or workplace mentors, or a combination of both.
Logbook	A systematic record of every phase of a project or placement activity.
Long Essay	An analytical, interpretative, or critical piece of writing that enables students to explore a specific subject area in some depth, explain theories and concepts; evaluate arguments, and express and support their own views and opinions.
Oral Examination	An examination during which students are required to verbally reply to questions posed to them in the spoken form.
	Students are asked to give an oral presentation on a particular topic for a specified length of time and could also be asked to prepare

	associated handout(s). Can usefully be combined with self- and peer-assessment.
Portfolio	A systematic and organised collection of a student's work that exhibits to others the direct evidence of a student's efforts, achievements, and progress over a period of time. It should include representative work, providing a documentation of the learner's performance and a basis for evaluation of the student's progress. Portfolios may include a variety of demonstrations of learning that have been gathered in the form of a physical collection of materials, videos, CD-ROMs, reflective journals, etc.
Poster	The production of a large print that can be displayed in a public space. It can include graphical images, text or a mixture of both and is usually designed with the intention of promoting an idea, event, product etc.
Report	A written document in which information is presented in an organised format. A report would normally include a descriptive statement, an account of the conditions that are observed, findings resulting from investigation and inquiry, and a conclusive summary in which the student puts forward any recommendations.
Research Paper	A research paper is an extended essay which is intended to assess the students' written, analytical, interpretative and argumentative skills, based on independent research.
Research Projects	Potential for sampling a wide range of practical, analytical and interpretative skills. Can assess wide application of knowledge, understanding and skills.
Research/Review Paper	A thorough and systematic analysis of published research findings, from which students are expected to provide new insights or interpretations about a topic or field of interest.
Role Play	Students write or give a presentation taking on a particular role, e.g. a journal reviewer/ editor, consultant, art critic etc. This type of assignment could be paired up with a grant application exercise.
Seminar Paper	A seminar paper is an advanced piece of writing which is intended to present an original piece of research to a group of peers.