

## Subject card

|                                             |                                                                                                                                                                                                                      |                                                          |                                         |                                     |                        |            |     |
|---------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|----------------------------------------------------------|-----------------------------------------|-------------------------------------|------------------------|------------|-----|
| Subject name and code                       | Introduction to molecular modeling, PG_00033260                                                                                                                                                                      |                                                          |                                         |                                     |                        |            |     |
| Field of study                              | Chemistry                                                                                                                                                                                                            |                                                          |                                         |                                     |                        |            |     |
| Date of commencement of studies             | October 2025                                                                                                                                                                                                         |                                                          | Academic year of realisation of subject |                                     | 2026/2027              |            |     |
| Education level                             | Bachelor's studies                                                                                                                                                                                                   |                                                          | Subject group                           |                                     | Optional subject group |            |     |
| Mode of study                               | full-time studies                                                                                                                                                                                                    |                                                          | Mode of delivery                        |                                     | at the university      |            |     |
| Year of study                               | 2                                                                                                                                                                                                                    |                                                          | Language of instruction                 |                                     | Polish                 |            |     |
| Semester of study                           | 3                                                                                                                                                                                                                    |                                                          | ECTS credits                            |                                     | 1.0                    |            |     |
| Learning profile                            | academic                                                                                                                                                                                                             |                                                          | Assessment form                         |                                     | credit                 |            |     |
| Conducting unit                             | Laboratory of Carbohydrate Chemistry -> Department of Organic Chemistry -> Faculty of Chemistry -> Rector                                                                                                            |                                                          |                                         |                                     |                        |            |     |
| Name and surname of lecturer (lecturers)    | Subject supervisor                                                                                                                                                                                                   |                                                          | dr hab. Rafał Ślusarz                   |                                     |                        |            |     |
|                                             | Teachers                                                                                                                                                                                                             |                                                          |                                         |                                     |                        |            |     |
| Lesson types                                | Lesson type                                                                                                                                                                                                          | Lecture                                                  | Tutorial                                | Laboratory                          | Project                | Seminar    | SUM |
|                                             | Number of study hours                                                                                                                                                                                                | 15.0                                                     | 0.0                                     | 0.0                                 | 0.0                    | 0.0        | 15  |
|                                             | E-learning hours included: 0.0                                                                                                                                                                                       |                                                          |                                         |                                     |                        |            |     |
|                                             | Additional information:                                                                                                                                                                                              |                                                          |                                         |                                     |                        |            |     |
|                                             | Methods:<br><br><ul style="list-style-type: none"><li>multimedia presentation</li><li>analysis of critical events (cases)</li><li>discussion on the subject forum</li><li>work with the computer (on-line)</li></ul> |                                                          |                                         |                                     |                        |            |     |
| Learning activity and number of study hours | Learning activity                                                                                                                                                                                                    | Participation in didactic classes included in study plan |                                         | Participation in consultation hours |                        | Self-study | SUM |
|                                             | Number of study hours                                                                                                                                                                                                | 15                                                       |                                         | 2.0                                 |                        | 8.0        | 25  |
| Subject objectives                          | Introduction of the student to the subject of molecular modeling.                                                                                                                                                    |                                                          |                                         |                                     |                        |            |     |

|                                                                |                                                                                                                                                                                                                                                                                                                                            |                                                                                                                                                                                                                             |                                   |
|----------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------|
| Learning outcomes                                              | Course outcome                                                                                                                                                                                                                                                                                                                             | Subject outcome                                                                                                                                                                                                             | Method of verification            |
|                                                                | [CHEML3_U05] Uses basic statistical methods and IT techniques to describe chemical processes and analyse experimental data.                                                                                                                                                                                                                | student names the projection methods and defines the scope of the transmitted information in selected molecular systems                                                                                                     | [SU4] test/exam - oral or written |
|                                                                | [CHEML3_U10] Prepares papers on various fields of chemistry in Polish and English, using acquired knowledge and skills as well as various sources of scientific information.                                                                                                                                                               | student assesses the usefulness of types of representations in the presentation of results, proposes the best methods of visualization of chemical compounds, shows creativity in the preparation of chemical presentations | [SU4] test/exam - oral or written |
|                                                                | [CHEML3_W08] Demonstrates knowledge of basic computational methods to solve problems in chemistry, physics, mathematics.                                                                                                                                                                                                                   | student calculates simple profiles of energy changes, constructs correct queries to bioinformatics databases, indicates the causes of conformation changes                                                                  | [SW4] test/exam - oral or written |
|                                                                | [CHEML3_W09] Describes the practical applications of IT tools (computer programmes) for chemical calculations and data analysis.                                                                                                                                                                                                           | student illustrates changes occurring in systems, selects tools specialized in measurement, construction or analysis of collected data                                                                                      | [SW4] test/exam - oral or written |
| Subject contents                                               | <ul style="list-style-type: none"><li>• learning to visualize chemical structures in various computer programs</li><li>• preparation of two- and three-dimensional representations of structures of chemical compounds</li><li>• simple computer simulations of dynamics and geometry optimization of modeled chemical compounds</li></ul> |                                                                                                                                                                                                                             |                                   |
| Prerequisites and co-requisites                                | A basic knowledge of English and a general understanding of the structure of chemical compounds is required.                                                                                                                                                                                                                               |                                                                                                                                                                                                                             |                                   |
| Assessment methods and criteria                                | Subject passing criteria                                                                                                                                                                                                                                                                                                                   | Passing threshold                                                                                                                                                                                                           | Percentage of the final grade     |
|                                                                | multi-component online test; one test for each of the topics covered; the arithmetic average of all tests is calculated                                                                                                                                                                                                                    | 51.0%                                                                                                                                                                                                                       | 100.0%                            |
| Recommended reading                                            | Basic literature                                                                                                                                                                                                                                                                                                                           | none                                                                                                                                                                                                                        |                                   |
|                                                                | Supplementary literature                                                                                                                                                                                                                                                                                                                   | none                                                                                                                                                                                                                        |                                   |
|                                                                | eResources addresses                                                                                                                                                                                                                                                                                                                       |                                                                                                                                                                                                                             |                                   |
| Example issues/<br>example questions/<br>tasks being completed | <ul style="list-style-type: none"><li>• Assign colors to chemical elements according to IUPAC convention.</li><li>• What kind of coordinates contain information about bond lengths, valence and torsion angles?</li></ul>                                                                                                                 |                                                                                                                                                                                                                             |                                   |
| Work placement                                                 | Not applicable                                                                                                                                                                                                                                                                                                                             |                                                                                                                                                                                                                             |                                   |

Document generated electronically. Does not require a seal or signature.