

## Subject card

| Subject name and code  | Information technology, PG_00053223   |  |  |               |  |                |         |     |
|--|---|--|--|---------------|--|----------------|---------|-----|
| Field of study   | Chemistry   |  |  |               |  |                |         |     |
| Date of commencement of studies  | October 2023  |  | Academic year of realisation of subject  |               | 2023/2024  |                |         |     |
| Education level  | first-cycle studies   |  | Subject group  |               | Obligatory subject group in the field of study   |                |         |     |
| Mode of study  | Full-time studies   |  | Mode of delivery   |               | at the university  |                |         |     |
| Year of study  | 1   |  | Language of instruction  |               | Polish   |                |         |     |
| Semester of study  | 1   |  | ECTS credits   |               | 5.0  |                |         |     |
| Learning profile   | general academic profile  |  | Assessment form  |               |  | assessment     |         |     |
| Conducting unit  | Department of Analytical Chemistry -> Faculty of Chemistry  |  |  |               |  |                |         |     |
| Name and surname   | Subject supervisor  |  | dr hab. inż. Dorota Warmińska  |               |  |                |         |     |
| of lecturer (lecturers)  | Teachers  |  | dr hab. inż. D   | orota Warmińs | ka   |                |         |     |
|  |   |  | dr inż. Mateusz Kogut  |               |  |                |         |     |
| Lesson types and methods   | Lesson type   | Lecture  | Tutorial   | Laboratory    | Projec   | :t             | Seminar | SUM |
| of instruction   | Number of study hours   | 15.0   | 15.0   | 45.0          | 0.0  |                | 0.0     | 75  |
|  | E-learning hours inclu  | uded: 0.0  |  |               |  |                |         |     |
| Learning activity and number of study hours  | Learning activity   | earning activity Participation in classes include plan   |  |               |  | Self-study SUM |         |     |
|  | Number of study hours   | 75   |  | 5.0           |  | 45.0           |         | 125 |
| Subject objectives   | The aim of the course is to familiarize students with the possibilities offered by modern personal computer software in the field of calculation and text editing. In addition, the aim of the course is to develop the student's ability to use the computer for statistical and numerical analysis of a set of a chemical experiment results. |  |  |               |  |                |         |     |
| Learning outcomes  | Course outcome  |  | Subject outcome  |               | Method of verification   |                |         |     |
|  | [K6_U05] can, on the basis of the collected experimental or source material, prepare an oral communication with a multimedia presentation   |  | The student is able to prepare and present a speech along with the presentation of the results using appropriately selected computer programs  |               | [SU1] Assessment of task<br>fulfilment<br>[SU5] Assessment of ability to<br>present the results of task              |                |         |     |
|  | prepare a report describing these   |  | After completing the course, the student should be able to prepare the elaboration of the obtained results, fluently using the advanced functions of MS Office programs (Word, Excel). |               | [SU1] Assessment of task<br>fulfilment<br>[SU3] Assessment of ability to<br>use knowledge gained from the<br>subject |                |         |     |
| [K6_W05] knows and understands the chemical processes and algorithms of mathematical models which are necessary for the design of technological processes, knows chemical structure of contemporary materials and its relation to their properties, enabling the selection of the materials for sustainable development technology and material-efficient and energy-efficient methods |   | The student knows and is able to use mathematical models necessary to design technological processes |  |               | [SW1] Assessment of factual knowledge [SW3] Assessment of knowledge contained in written work and projects           |                |         |     |

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| Subject contents                | Laboratory:   |   |                               |  |  |  |  |
|---------------------------------|---|---|-------------------------------|--|--|--|--|
| ·                               |   |   |                               |  |  |  |  |
|                                 | Working principles in the Windows operating system: local area network, information organization, transfer data between applications. Web browser support, principles of searching for information on the web, search engines, databases, chemical data resources on the Internet. Using the Word editor to prepar chemistry texts: using the equation editor, preparing tabular summaries in a text editor, combining text with graphic elements. Application of Excel spreadsheet for presentation and solving chemical problems. Basic calculations in the spreadsheet, priorities of activities, use of functions embedded, formatting calculation results. Ways of addressing cells and their consequences. Rules for using cell names, areas and formulas. Drawing up graphs: presentation dependencies described by the formula and tabular data, trend lines, scale change on the chart axes. Preparation of an example presentation using the Power Point program. Solving nonlinear equations. Linear regression, linearization of nonlinear dependencies, multiple regression. Numerical integration.  |   |                               |  |  |  |  |
|                                 | Exercises:  |   |                               |  |  |  |  |
|                                 | Evaluation of the correctness of experimental data. Estimating the size of errors. Analysis of results of one-dimensional random variable. Calculation of the mean, median, variance. Determination of the confidence interval. Conducting statistical tests. Analysis of a two-dimensional random variable. Regression and correlation study. Determination of linear and nonlinear regression parameters. Solving nonlinear equations by numerical methods. Interpolation. Numerical calculation of the definite integral.  |   |                               |  |  |  |  |
|                                 | Lectures:   |   |                               |  |  |  |  |
|                                 | Basic concepts of error theory, sources of errors. The difference between concepts: uncertainty and error. Systematic and random errors. Maximum error, probability and error propagation and rounding rules. One-dimensional random variable. Measures of location and dispersion. Normal distribution and t Student (mean and its confidence interval, median and fashion, gross error and its elimination, precision and accuracy, Q-Dixon, F-Snedecor and Student t-tests) Two-dimensional random variable. Regression and correlation. Linear, nonlinear and multiple regression. Residual distribution, residual variance. Regression coefficient confidence interval. Tolerance range for values deviating from the regression lineStages of IT development. Algorithm, algorithm features, construction principles, typical structures of activity networks. Algorithm stability. Examples of numerical instability.  Solving nonlinear and leap equations using bisection, tangent, secant and straight iteration methods. Interpolation and differentiation of a tabular function (Newton's formulas based on finite differences and differential quotients of a function, Lagrange's formula). Numerical integration (Newton-Cotes formulas, generalized trapezoidal formulas, parabolas, Richardson extrapolation). |   |                               |  |  |  |  |
| Prerequisites and co-requisites |   |   |                               |  |  |  |  |
| Assessment methods              | Subject passing criteria  | Passing threshold   | Percentage of the final grade |  |  |  |  |
| and criteria                    | Laboratory-Colloquia during the semester  | 50.0%   | 40.0%                         |  |  |  |  |
|                                 | Classes-Colloquia during the semester   | 50.0%   | 30.0%                         |  |  |  |  |
|                                 | Lecter - Colloquia during the semester  | 50.0%   | 30.0%                         |  |  |  |  |
| Recommended reading             | Basic literature  | J.B. Czermiński i inni, Metody statystyczne dla chemików PWN 1986                   |                               |  |  |  |  |
|                                 | K. Doerffel, Statystyka dla che   |   | emików analityków, WNT 1989   |  |  |  |  |
|                                 |   | J. Arendarski, Niepewność pomiarów, Politechnika Warszawska, 2003                   |                               |  |  |  |  |
|                                 |   | T. Ratajczak, Metody numeryczne przykłady i zadania, Wydawnictwo<br>PG, Gdańsk 2007 |                               |  |  |  |  |
|                                 |   | E. Slavicek, Technika obliczeniowa dla chemików WNT 1991                            |                               |  |  |  |  |

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|  | eResources addresses  | P. Konieczka, J. Namieśnik i inni, Ocena i kontrola jakości wyników pomiarów analitycznych, WNT Warszawa 2007  E. Bulska i inni, Ocena i kontrola jakości wyników pomiarów analitycznych, WNT 2007  Z. Fortuna, B. Macukow, J. Wąsowski, Metody numeryczne, WNT wznawiane każdego roku.  A. Bjork, G. Dahlquist, Metody numeryczne PWN 1987  Adresy na platformie eNauczanie: |  |  |
|--|---|---|--|--|
|  |   | Technologie Informatyczne dla studentów I-ego roku kierunku Chemia, 2023/2024 - Moodle ID: 32881 https://enauczanie.pg.edu.pl/moodle/course/view.php?id=32881   |  |  |
| Example issues/<br>example questions/<br>tasks being completed | Creating a network of simple algorithms for computational methods.  Determining the confidence interval for the arithmetic mean of the experimental data set. |   |  |  |
|  | Performing conformity assessment of the accuracy and precision of the measurement method  Calculation of the optimal regression line.                         |   |  |  |
|  | Preparation of an example presentation using the Power Point program.   |   |  |  |
| Work placement   | Not applicable  |   |  |  |

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