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| <b>Study program:</b> Integrated Academic Studies in Pharmacy  |               |                   |                     |
| <b>Course title:</b> Chemometrics  |               |                   |                     |
| <b>Teacher:</b> Ana S. Pilipović, Mihalj M. Poša   |               |                   |                     |
| <b>Course status:</b> elective   |               |                   |                     |
| <b>ECTS Credits:</b> 3   |               |                   |                     |
| <b>Condition:</b> Mathematics  |               |                   |                     |
| <b>Course aim</b><br>The main aim of this course is to develop logical thinking about information related to binding molecular structure (of the medication) with biological activity, as well as physical and chemical properties of mathematical models.   |               |                   |                     |
| <b>Expected outcome of the course:</b><br>Students should acquire basic knowledge in linear algebra, and mathematical statistics.<br>Students should also gain knowledge in basic mathematical methods which are used in chemometrics realized by using computer software.   |               |                   |                     |
| <b>Course description</b><br><i>Theoretical education</i><br>1. Molecular descriptors.<br>2. Basic principles of QSAR.<br>3. Data scaling: centering, autoscaling, maximum scaling, range scaling, generalized range scaling.<br>4. Molecular grouping in a multidimensional space: clustering, fuzzy grouping.<br>5. Factor analysis, principal component analysis.<br>6. Model setting using multiple regressions.<br>7. Genetic algorithms.<br>8. Artificial neural networks – Cohon's network<br><br><i>Practical education</i><br>Application of computer softwares: SPSS, Statistica, Sybyl, Chem 3D ultra |               |                   |                     |
| <b>Literature</b><br><i>Compulsory</i><br>1. Masart DL, Vandeginste BGM, Buydens LMC, De Yong S, Levi PJ, Smeyers-Verbeke J. Handbook of Chemometrics and Qualimetrics: Part B. Elsevier, Amsterdam, 1998.<br>2. Kowalski BR, Sharaf MA, Illman DL. Chemometrics. Wiley, New York, 1986  |               |                   |                     |
| <b>Number of active classes</b>  |               | <b>Theory:</b> 30 | <b>Practice:</b> 15 |
| <b>Teaching methods:</b> lectures, laboratory practice, colloquia, essays, consultations   |               |                   |                     |
| <b>Student activity assessment</b> (maximally 100 points)  |               |                   |                     |
| <b>Pre-exam activities</b>   | <b>Points</b> | <b>Final exam</b> | <b>points</b>       |
| Lectures   | 10            | Written           | 70                  |
| Practices  |               | Oral              |                     |
| Colloquium   |               | .....             |                     |
| Essay  | 20            |                   |                     |