Course title in English	Chemoinformatics Seminar
Course title in Polish	Konwersatorium chemoinformatyczne
Course code	
Type of course	Seminar
Level of course	PhD
Year of study	1-4
Semester/trimester	1/3/5/7; 2/4/6/8
Number of hours/ credits allocated	30/2
Name of lecturer	Tomasz Puzyn
Objective of the course (expected learning outcomes and competences to be acquired)	*Knowledge*: After completing the course each PhD student: 1. can list the most important chemoinformatic scientific journals 2. knows the current state of knowledge and the latest scientific achievements in chemoinformatics, with particular emphasis on the new type of chemical structure descriptors and methods of profiling and modeling dependencies 3. can indicate the most important currently implemented scientific projects and research groups active in the subject area 4. can mention the latest software used in chemoinformatics and indicate its application. *Skills*: After completing the course, each PhD student: 1. is able to find the necessary information in the literature and critically evaluate their scientific value 2. critically verifies the quality of scientific publications in the field of chemoinformatics 3. efficiently uses the English and Polish vocabulary of the subject 4. in a concise and correct manner presents the results and conclusions of scientific projects carried out by other researchers

	5. correctly selects individual methods of material modeling accordingly to types of solving research problems.
	Social competence:
	<u>After completing the course each PhD student:</u>
	1. sees the need to follow the latest developments in the field of the subject.
Prerequisites	knowledge of the basics of chemoinformatics
Course contents	**1.** Recent achievements in predicting properties and activity of chemical compounds by means of chemoinformatic methods **2.** Anticipation of properties of selected groups of chemical species of high importance: pharmaceuticals, ionic liquids and nanomaterials **3.** The latest software used in chemoinformatics **4.** The most important scientific projects and research groups in the subject area.
Recommended reading	**List of literature** **A. Literature required for the final passing of the course (passing the exam):** A.1. used during classes • *Nanotoxicology (scientific journal)* • *Journal of Nanotoxicology and Nanomedicine (scientific journal)* • *ACS Nano (scientific journal)* • *Small (scientific journal)* • *Environmental Health Perspectives (scientific journal)* • *Nano Research (scientific journal)* • *Green Chemistry (scientific journal)* • *Nanoscale (scientific journal)* • *Nanomedicine-Nanotechnology Biology and Medicine (scientific journal)* • *Journal of Chemoinformatics (scientific journal)* • *Journal of Materials Chemistry A (scientific journal)* • *American Journal of Materials Science (scientific journal)* • *Journal of Chemical Information and Modeling (scientific journal)* • *Journal of Computational Chemistry (scientific journal)* • *Environmental Modelling & Software (scientific journal)*

	• *SAR and QSAR in Environmental Research (scientific journal)* • *Chemometrics and Intelligent Laboratory Systems (scientific journal)* • *Journal of Chemometrics (scientific journal)* • *Structural Chemistry (scientific journal)* • *International Journal of Quantitative Structure-Property Relationships (scientific journal)* A.2. studied individually by the student **B. Supplementary literature.**
Teaching methods	seminars: presentation of the latest works in the field of applications of chemoinformatic methods, problem solving by PhD students with the participation of the person conducting the classes, analysis of various possibilities of solutions combined with a discussion.
Assessment methods	**A. Way of passing,** according to Regulations of Studies at UG • pass with grade **B. Forms of passing** The final grade from the course will be issued as a weighted average of two partial grades for: • a recapitulation of the issue agreed with the teacher based on the latest scientific publications (weight 50%); • activity during classes (weight 50%). **C. Basic criteria of grade or examination requirements** Recapitulation of a scientific publication: • Preparation and comprehensive reporting of the issue agreed with the lecturer based on the latest scientific publications. • Correct use of the vocabulary of the subject. Activity: • Active participation in seminars' discussions. • Correct use of the subject vocabulary. **A. The way of verification of the planned results of the taught course** • Observation of the skills of class participants during the course • Assessment of tasks completed by students.

Language of instruction	Polish