University of Gdańsk

Subject card

Subject name and code	Computational chemistry tools in forensic analysis, PG_00211811						
Field of study	Forensic Analytics						
Date of commencement of studies	October 2026		Academic year of realisation of subject	2028/2029			
Education level	Bachelor's studies		Subject group	Obligatory subject group in the field of study Optional subject group			
Mode of study	full-time studies		Mode of delivery	at the university			
Year of study	3		Language of instruction	Polish			
Semester of study	5		ECTS credits	3.0			
Learning profile	academic		Assessment form	credit			
Conducting unit	Faculty of Chemistry -> Rector						
Name and surname of lecturer (lecturers)	Subject supervisor		prof. dr hab. Iwona Anusiewicz, prof. UG				
	Teachers						
Lesson types	Lesson type	Lecture	Tutorial	Laboratory	Project	Seminar	SUM
	Number of study hours	0.0	0.0	45.0	0.0	0.0	45
	E-learning hours included: 0.0						
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	45		5.0	25.0	75	
Subject objectives	The aim of the course is to provide students with practical skills in modeling and analyzing the spectroscopic properties of compounds used or identified in forensic science using quantum chemical methods and the Gaussian software package. Students will learn the fundamentals of preparing quantum chemical calculations, molecular geometry optimization, and the interpretation of IR, Raman, UV–Vis, NMR, ECD/VCD, and fluorescence spectra.						

Learning outcomes

Course outcome	Subject outcome	Method of verification
[AKRL3_W08] The graduate knows and understands the application of information technologies in data analysis, interpretation of results, and reporting of forensic research.	The graduate demonstrates knowledge and understanding of the application of information technologies for the analysis of computational data, the interpretation of quantum chemical simulation results, and the reporting of spectroscopic investigations relevant to forensic science, using specialized computational software and data analysis tools.	[SW2] presentation/project/paper/ report
[AKRL3_W02] The graduate knows and understands, at an advanced level, the analytical methods used in forensic laboratories, in particular spectroscopic, chromatographic and electroanalytical methods.	The graduate is able to employ quantum chemical computational methods for the analysis and interpretation of spectroscopic data relevant to forensic science, including IR, Raman, UV–Vis, NMR, ECD, VCD, and fluorescence spectroscopy, thereby supporting the identification of chemical substances.	[SW2] presentation/project/paper/ report
[AKRL3_W03] The graduate knows and understands the structure and chemical properties of compounds relevant in forensic examinations.	The graduate demonstrates knowledge and understanding of the structure and chemical properties of compounds relevant to forensic analyses, as well as the relationship between their molecular characteristics and observed spectroscopic properties within the framework of computational quantum chemistry.	[SW1] oral statement/ conversation/discussion
[AKRL3_K08] The graduate is prepared to think and act in an entrepreneurial manner, seeking innovative solutions, improving analytical processes, and initiating activities that support the modernization of forensic practice	The graduate is prepared to engage in innovative activities by applying computational chemistry methods to spectroscopic analysis, enhancing data interpretation, and contributing to the development of modern tools supporting the identification of chemical compounds in forensic investigations.	[SK8] observation of student's independent or team work
[AKRL3_U06] The graduate is able to use specialised software and advanced ICT techniques to develop and visualise experimental data.	The graduate is able to apply specialized software (e.g., Gaussian, Molden, Avogadro) and computational tools for the processing, analysis, and visualization of quantum chemical simulation results, including the interpretation and visualization of spectroscopic data (IR, Raman, UV–Vis, NMR, ECD, and VCD spectra).	[SU2] presentation/project/paper/ report

Subject contents

The course covers an introduction to computational quantum chemistry methods and their applications in the spectroscopic analysis of compounds of forensic relevance. The topics include the fundamentals of computational software packages (Gaussian, Molden, and Avogadro), preparation of molecular models, and interpretation of quantum chemical calculation results.

In the practical part of the course, students perform quantum chemical calculations and analyze simulated spectroscopic data, including IR, Raman, UV–Vis, NMR, electronic circular dichroism (ECD), vibrational circular dichroism (VCD), and steady-state fluorescence spectra.

The course also addresses molecular geometry optimization, conformational analysis, modeling of intermolecular interactions, and the relationship between molecular structure and spectroscopic properties.

Prerequisites and co-requisites

none

Assessment methods and criteria

Subject passing criteria	Passing threshold	Percentage of the final grade
project	51.0%	100.0%

Recommended reading	Basic literature	Chemia obliczeniowa. J. Harvey, PWN Chemia obliczeniowa w laboratorium organicznym. A. Kaczmarek-Kędziera, M. Ziegler-Borowska, D. Kędziera, Wydawnictwo Naukowe UMK
	Supplementary literature	none
	eResources addresses	
Example issues/ example questions/ tasks being completed	A sample collected during a forensic investigation is suspected to contain an unknown organic compound. Using the Gaussian software package, perform geometry optimization and frequency calculations for the proposed molecular structures at the DFT level of theory (e.g., B3LYP/6-311++G(d,p)). Compare the calculated IR spectra with the experimental spectrum and identify the most likely structure of the unknown compound. Discuss the influence of functional groups and molecular structure on the observed vibrational bands.	
Work placement	Not applicable	

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