هيئة تقويم التعليم والتدريب
Education & Training Evaluation Commission

اعتماد
NCAAA

2024
TPG-153

Course Specification

— (Postgraduate Programs)

Course Title: Applied Analytical Chemistry (Computation by Computers)

Course Code: CHEM 652

Program: Doctor of Philosophy in Chemistry (PhD)

Department: Chemistry

College: College of Science

Institution: King Saud University

Version: TPG-153-2025

Last Revision Date: 19 January 2026

Table of Contents

A. General information about the course:

1. Course Identification:

1. Credit hours:

3 Credit hours

2. Course type

A.	☐University	☐College	☒ Department	☐Track	
B.	☒ Required			☐Elective	

3. Level/year at which this course is offered:

2nd Level / 1st year

4. Course General Description:

Nowadays, computers and artificial intelligence play an essential role across all scientific disciplines, including chemistry. This course introduces advanced computational and AI-driven applications for solving chemical and analytical problems, with particular emphasis on data-intensive research. The course covers three major areas: (i) The use of computers and artificial intelligence in chemical data analysis and statistics, (ii) Computer-assisted chemical structure drawing, molecular modeling, simulation, and AI-based prediction of molecular properties, and (iii) Electronic literature searching, scientific information management, chemical databases, and AI-supported knowledge discovery tools.

The course content is periodically reviewed and updated to reflect recent advances in AI technologies, computational chemistry platforms, and analytical instrumentation, as well as the learning outcomes required by the labor market in academia, industry, and regulatory sectors, thereby ensuring that graduates acquire cutting-edge and state-of-the-art digital, computational, and AI competencies relevant to modern chemical practice.

5. Pre-requirements for this course (if any):

NA

6. Pre-requirements for this course (if any):

NA

7. Course Main Objective(s):

The main objectives of this course are to:

(1) Develop students' ability to employ state-of-the-art computational and AI tools to address chemical and analytical problems.

(2) Equip students with advanced skills in chemical data analysis, chemometrics, statistics, and other techniques relevant to modern research and industrial environments.

(3) Train students to use computer-assisted molecular modeling, simulation, and AI-based property prediction to support analytical method development and chemical investigations.

(4) Enhance students' proficiency in scientific information management, electronic literature searching, chemical databases, and AI-supported knowledge-discovery platforms.

(5) Foster critical evaluation of computational and AI models with respect to accuracy, robustness, interpretability, and uncertainty.

(6) Promote ethical, responsible, and reproducible use of digital and AI technologies in chemical research and professional practice.

(7) Align students' computational competencies with current and emerging labor-market needs in academia, industry, and regulatory sectors.

2. Teaching Mode: (mark all that apply)

No	Mode of Instruction	Contact Hours	Percentage
1	Traditional classroom	45	100
2	E-learning		
3	Hybrid • Traditional classroom • E-learning		
4	Distance learning		

3. Contact Hours: (based on the academic semester)

No	Activity	Contact Hours
1	Lectures	30
2	Laboratory/Studio	
3	Field	
4	Tutorial	15
5	Others (specify)	
	Total	45

B. Course learning outcomes (CLOs), teaching strategies and assessment methods:

Code	Course Learning Outcomes	Aligned PLOs	Teaching Strategies	Assessment Methods
1.0	**Knowledge and understanding**			
1.1	To outline the basic tools of computer and AI in relation with analytical chemistry.	K1	-Lectures -Workshops on software platforms and AI tools	-Mid-term examination -Final examination
1.2	To describe the main applications of computer and AI in terms of statistical data analysis, chemometric, chemical structures drawing, molecular modeling, simulation, AI-based prediction, literature searching, and chemical databases.	K3	-Lectures -Hands-on computational laboratories -Workshops on software platforms and AI tools	-Mid-term examination -Final examination
2.0	**Skills**			
2.1	Select and justify appropriate cutting-edge computational and AI techniques for solving complex chemical problems.	S1	-Lectures -Hands-on computational laboratories -Workshops on software platforms and AI tools	-Mid-term examination -Final examination -Assignments -Reports
2.2	Interpret datasets from spectroscopic, chromatographic, and electrochemical techniques.	S2	-Lectures -Chemical structure drawing software -Statistical data analysis software	-Mid-term examination -Final examination -Assignments -Reports

Code	Course Learning Outcomes	Aligned PLOs	Teaching Strategies	Assessment Methods
			-Literature searching and the chemical databases	-Literature review and critical analysis paper -Exercises
2.3	Implement state-of-the-art software and appropriate environments to perform chemical data analysis and modeling.	S3	-Case-study analysis from literature -Problem-solving sessions	-Mid-term examination -Final examination -Assignments -Reports -Literature review and critical analysis paper -Exercises
2.4	Critically evaluate model performance, uncertainty, robustness, and validation metrics.	S1	-Discussions -Problem-solving sessions	-Mid-term examination -Final examination -Assignments -Reports
3.0	**Values, autonomy, and responsibility**			
3.1	Practice responsible, transparent, and ethical use of digital and AI technologies.	V3	-Research-driven projects -Peer review and group discussions	-Research-based project -Oral presentation -Defense
3.2	Communicate computational results effectively in written reports and oral presentations.	V2	-Research-driven projects -Peer review and group discussions	-Research-based project -Oral presentation -Defense

C. Course Content:

No	List of Topics	Contact Hours
1	An overview of the applications of computer and AI in chemistry and the role of computation in modern analytical chemistry.	3
2	Applications of computers and AI in chemical data analysis and statistics, including statistical foundations and error analysis; calibration models; validation of analytical methods; and spectral and chromatographic data processing, interpretation, and pattern recognition.	4
3	Software for statistical data analysis (e.g., Microsoft excel, OriginLab).	12
4	Applications of computer and AI in chemical structure drawing and molecular modeling.	4
5	Software for molecular modeling and drawing (e.g., ChemOffice, HyperChem, Materials studio).	12
6	Applications of computer and AI in literature searching and the chemical databases.	2
7	Literature searching websites and the chemical databases (e.g., Chemical Abstracts Service).	8
Total		**45**

D. Students Assessment Activities:

No	Assessment Activities*	Assessment timing (in week no)	Percentage of Total Assessment Score
1	Mid-term examination	6–7	20
2	Activities (assignments, discussion, quizzes, homework's, and exercises)	Weekly	20
3	Project, report, and presentation	14–15	20
4	Final examination	16–17	40

*Assessment Activities (i.e., Written test, oral test, oral presentation, group project, essay, etc.)

E. Learning Resources and Facilities:

1. References and Learning Resources:

Essential References	This course does not rely on a single main reference; rather, approved textbooks and peer-reviewed scientific articles relevant to the course objectives and learning outcomes are selected to ensure alignment with recent developments in computational applications and artificial intelligence in analytical chemistry.
Supportive References	-S. Gihar, Computer for Chemists, Neel Kamal Prakashan, 2017. -S. Kulkarni, S. Bhandari, D. Varshney, P. William, Artificial Intelligence for Chemical Sciences, Apple Academic Press, 2025.
Electronic Materials	-Online databases such as SciFinder, PubChem, and ChemSpider. -Scholarly platforms such as Web of Science, Scopus, and Google Scholar. -Open educational resources such as AI for chemistry and computational chemistry. -Publisher journal portals such as Analytical Chemistry, Journal of Chromatography A, Chemometrics and Intelligent Laboratory Systems, Journal of Chemical Information and Modeling, and Trends in Analytical Chemistry.
Other Learning Materials	

2. Educational and Research Facilities and Equipment Required:

Items	Resources
Facilities (Classrooms, laboratories, exhibition rooms, simulation rooms, etc.)	-Dedicated postgraduate computer laboratories designed for advanced computational work. -Seminar rooms equipped for high-level discussions and research presentations. -Secure data-storage facilities compliant with institutional research-data policies. -Access to analytical laboratories for acquiring real experimental datasets from chromatographic, spectroscopic, and electrochemical instruments.
Technology equipment (Projector, smart board, software)	-Smart board and data show. -High-performance desktop computers or workstations capable of running computational, chemometrics, and AI software.

Items	Resources
	-Servers or cloud-computing access for large-scale data analysis and machine-learning applications. -High-speed internet connectivity. -Licensed and open-source software platforms, such as: (1) Statistical data analysis software. (2) Chemical structure drawing and modeling software. (3) Literature searching and the related databases.
Other equipment (Depending on the nature of the specialty)	Access to analytical instrumentation for real data generation, such as HPLC/GC systems, MS instruments, UV-Vis, IR, Raman, and NMR spectrometers, atomic absorption/emission spectrometer, and electrochemical workstations.

F. Assessment of Course Quality:

Assessment Areas/Issues	Assessor	Assessment Methods
Effectiveness of teaching	Students	Direct
Effectiveness of students' assessment	Faculty and program leaders	Direct
Quality of learning resources	Program leaders and peer reviewers	Indirect
The extent to which CLOs have been achieved	Faculty and program leaders	Direct
Other		

Assessor (Students, Faculty, Program Leaders, Peer Reviewer, Others; specify)
Assessment Methods (Direct, Indirect)

G. Specification Approval Data:

COUNCIL /COMMITTEE	
REFERENCE NO.	
DATE	