Special Issue

Artificial Intelligence in Spectroscopic Techniques: From Data Processing to Discovery

Message from the Guest Editors

Spectroscopic techniques such as Raman, IR, UV-Vis, NMR, XPS, and mass spectrometry generate high-dimensional, information-rich data that are essential for chemical, biological, environmental, and material sciences. However, extracting meaningful patterns, reducing noise, interpreting complex spectra, and correlating spectral signatures with structural or functional properties remain challenging tasks. In recent years, artificial intelligence (AI) has emerged as a transformative tool for spectroscopic analysis. Techniques are reshaping how spectra are processed, interpreted, and applied—from enhanced preprocessing and feature extraction to classification, quantification, inverse design, and autonomous experimentation. This Special Issue aims to showcase cutting-edge research at the intersection of AI and spectroscopy, highlighting both foundational methods and real-world applications. We welcome contributions that focus on AI-enhanced spectral data processing, spectral interpretation, compound identification, predictive modeling, the simulation of spectral data, and autonomous sensing systems across chemical, biomedical, environmental, and industrial domains.

Guest Editors

Prof. Dr. Yiping Zhao

Department of Physics and Astronomy, The University of Georgia, Athens, GA 30602, USA

Prof. Dr. Bo Hu

School of Life Science and Technology, Xidian University, Xi'an 710126, China

Deadline for manuscript submissions

28 February 2026

AI Chemistry

an Open Access Journal by MDPI

mdpi.com/si/250883

AI Chemistry
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
aichem@mdpi.com

mdpi.com/journal/aichem

AI Chemistry

an Open Access Journal by MDPI

mdpi.com/journal/aichem

MDPI

About the Journal

Message from the Editor-in-Chief

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

Rapid Publication:

first decisions in 19 days; acceptance to publication in 4 days (median values for MDPI journals in the first half of 2025).

Recognition of Reviewers:

reviewers who provide timely, thorough peer-review reports receive vouchers entitling them to a discount on the APC of their next publication in any MDPI journal, in appreciation of the work done.