

Special Issue

Application of Computational Techniques in Analytical Chemistry and Molecular Systems

Message from the Guest Editor

The aim of this Special Issue is to provide a platform for the exchange of knowledge, ideas, and breakthroughs at the intersection of computational science and analytical chemistry. We seek abstract submissions that encompass a wide spectrum of topics, including but not limited to the following:

- Molecular modeling and simulations for drug discovery and development.
- Computational methods for the analysis of complex biomolecular systems.
- Machine learning and artificial intelligence applications in analytical chemistry.
- Quantum chemistry approaches to elucidate molecular behavior.
- Big data analytics for high-throughput chemical analysis.
- Computational advances in spectroscopy and mass spectrometry.
- Chemoinformatics and bioinformatics in chemical analysis.
- Computational methods for material characterization and nanotechnology.
- Predictive modeling and data-driven approaches in analytical instrumentation.
- Innovative software tools and algorithms for analytical chemistry.

Guest Editor

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Deadline for manuscript submissions

closed (30 September 2024)



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