



Application of Computational Techniques in Analytical Chemistry and Molecular Systems

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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:

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





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Message from the Editor-in-Chief

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