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Computer Modeling and Reaction Mechanisms in Chemistry

Guest Editor:

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Deadline for manuscript submissions:
closed (31 December 2023)

Message from the Guest Editor

Computer modeling, machine learning, and artificial intelligence are cutting-edge topics in chemistry today. Application of information technologies in natural sciences can help us to collect big data and understand patterns that are not obvious to humans. In this Special Issue, we plan to collect interdisciplinary works in the fields of computational and quantum chemistry, computational statistics, artificial intelligence, machine learning, neural networks, predictive analytics, data mining, and data science. Both conceptual and applied works in any format (from short communications to comprehensive reviews) are welcome. We look forward to your contributions.

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Editor-in-Chief

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Message from the Editor-in-Chief

As a new international and multidisciplinary peer-reviewed open access journal for multidisciplinary chemistry focused on chemical compounds, Compounds (ISSN 2673-6918) has been founded to publish reviews, original research papers, communications, case reports, letters, and short notes.

Our goal is for Compounds to become a journal where the scientific community can present their results under open access. Our core objective is to provide high-quality research contributions in a wide range of chemistry areas. Manuscripts dealing with chemical compounds; the relationship between structure, properties, and/or functions of all kinds of compounds; as well as chemical theory and applications are welcome.

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