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Computational Aspects of Organocatalysis

Guest Editor:

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Message from the Guest Editor

The focus of this Special Issue lies on the application of state-of-the-art computational investigations to better understand organocatalytic reactions. This includes, among others, the elucidation of the underlying reaction mechanisms, the rationalization of selectivities observed in these transformations, the prediction of new or more efficient catalysts, benchmarking studies on the performance of computational methods for organocatalystic reactions, or similar studies. Full papers, communications, perspectives, and mini-reviews are most welcome.

Keywords

- Aminocatalysis
- Asymmetric Synthesis
- Computational Chemistry
- Density Functional Theory
- Reaction Mechanisms
- Regioselectivty
- Stereoselectivty