

Special Issue

Combining Experimental Reaction Development with Quantum Chemistry and Machine Learning

Message from the Guest Editor

This Special Issue welcomes synergic approaches containing experimental reaction development with quantum chemistry (QM) and/or machine learning (ML). Relevant examples might include studies in which QM mechanistic studies are employed to understand, improve or expand catalyzed reactions and organic synthesis. Furthermore, ML prediction of more efficient reaction components to improve reactivity and selectivity are similarly encouraged.

Guest Editor

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The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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