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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