

## **Combination of experimental and computational approaches: Recent developments in catalytic organic and bioorganic reactions**

In the last few decades, catalyzed organic and bioorganic reactions have attracted much attention in chemical and pharmaceutical researches. Recently, the design of novel catalysts and enzymes are in much demands to circumvent certain intractable synthetic problems.

In this light, the modeling of catalytic procedures seems to be necessary and also important in the synthesis of emerging classes of organic compounds that are becoming the targets of molecular and biomedical researches.

Strictly speaking, combination of computational approaches with experimental methods to model and interpret the mechanistic features of catalytic and enzymatic organic reactions provides more detailed information about the structure, bonding, stereochemistry and spectroscopic properties of compounds through the reaction path and consequently leads to the new opportunities for production of novel chemicals and discovery of useful drugs.

In this context, the main goal of this thematic issue is to present a comprehensive joint experimental and computational researches set in the field of catalytic organic synthesis and their rational mechanistical underpinning and the conjunction of experimental features of catalytic and enzymatic reactions with computational approaches will be covered.

This thematic issue contains 7 reviews, written by highly knowledgeable teams with tremendous amount of experience in the field of computational organic chemistry.

As the result, the thematic issue contains the reviews of emerging and cutting edge researches in the field of computational organic chemistry and hopefully attracts substantial attentions and stirs up the interest of readers in the related research community.

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