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Synthesis, Biological Evaluation and Molecular Modeling of Enzyme Inhibitors

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Deadline for manuscript submissions: closed (20 June 2023)



Message from the Guest Editors

This Special Issue, devoted to "Synthesis, Biological Evaluation, and Molecular Modeling of Enzyme Inhibitors," invites high-quality research papers focusing on the structural investigation of enzymes in interaction with substrates/inhibitors. Topics of interest include the following:

- Design of enzyme inhibitors and prediction of their activity;
- Structure-activity relationship;
- Molecular docking and modeling;
- Screening for active substances.







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Message from the Editor-in-Chief

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