

Special Issue

Synthesis and Theoretical Study of Bioactive Molecules

Message from the Guest Editor

Not all synthesized compounds exhibit biological activity. Therefore, biological evaluation of synthesized compounds is required, which is unfortunately expensive and time-consuming. To avoid such problems, theoretical studies exploring molecular mechanics, docking, and molecular dynamics can provide info on the physicochemical properties of a compound and its binding interaction with the expected target receptor. Therefore, this Special Issue focuses on the synthesis of bioactive molecules and theoretically studying their binding with target receptor by using different computational tools.

Guest Editor

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Message from the Editor-in-Chief

Editor-in-Chief

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