Special Issue

Theory and Applications of Graphs in Drug Discovery

Message from the Guest Editor

A huge challenge that medical scientists face today is the identification of compounds that are suitable for drug design. In general, selecting the best compounds for drug design is an intricate task because the number of compounds in plants and synthetic libraries is almost infinite. Graph theory, a fast-growing branch of discrete mathematics, offers a natural way of relating compounds with their physical properties or their biological activity. The aim of this Special Issue is to bring together original research and review articles discussing recent developments in the theory and applications of Graphs in Drug Design. The Issue seeks bio-chemically important mathematical results and non-standard applications of mathematical methods to drug discovery problems. Submissions should consider techniques and applications in depth and at a stretch. Additionally, submissions could also include the applications of graphs in biology and chemistry.

Guest Editor

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Deadline for manuscript submissions

closed (28 June 2024)

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About the Journal

Message from the Editor-in-Chief

The journal *Mathematics* publishes high-quality, refereed papers that treat both pure and applied mathematics. The journal highlights articles devoted to the mathematical treatment of questions arising in physics, chemistry, biology, statistics, finance, computer science, engineering and sociology, particularly those that stress analytical/algebraic aspects and novel problems and their solutions. One of the missions of the journal is to serve mathematicians and scientists through the prompt publication of significant advances in any branch of science and technology, and to provide a forum for the discussion of new scientific developments.

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