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Virtual Screening of Natural Product Databases for Drug Discovery

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Message from the Guest Editors

It is estimated that less than 10% of the world's biodiversity has been evaluated for possible therapeutic applications. Natural products present challenges for drug discovery, which have contributed to a decline in their pursuit by the pharmaceutical industry. Natural products, indeed, are often structurally complex, presenting several hydroxyl and ketone substituents and many chiral centers, and usually have high polarity and molecular weight, which makes them unique and extremely diverse compared to synthetic molecules, but also very difficult to synthetize at a large scale. However, the advent of new technologies has allowed focus on the most promising candidates, thus opening new opportunities for natural products in drug discovery. *In silico* virtual screening is one of the most useful computational methods for filtering large databases of natural compounds. Several virtual screening protocols could be applied to natural product libraries. This Special Issue will cover different aspects of virtual screening methodology and applications, including ligand-, pharmacophore-, and structure-based approaches leading to the identification of hit compounds or to optimized leads.

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Message from the Editor-in-Chief

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