marine drugs

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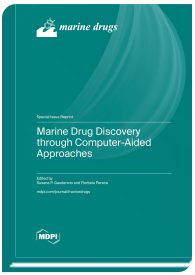
Special Issue Reprint

Marine Drug Discovery through Computer-Aided Approaches



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Computer-Aided Ligand- and Structure-based methodologies are an evolving field in the discovery of Marine Drugs. Computational approaches, chemistry simulation methods using bioinformatics and chemoinformatics tools and databases can be successfully used in the discovery, design and development of new chemical agents for therapeutic purposes by assisting in the structure elucidation of secondary metabolites, repurposing known Marine Natural Products (MNPs) for innovative therapeutic targets, identifying novel hits or leads against selected therapeutic targets and revealing mechanisms of action and supporting medicinal chemistry lead optimization programs.

This Special Issue of Marine Drugs entitled “Marine Drug Discovery through Computer-Aided Approaches” aims to provide a comprehensive overview of the great variety of existing and advanced Computer-Aided Approaches for the discovery and identification of molecular agents with added value and health-promoting properties for the development of biotechnological and medical applications.

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