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Virtual Screening of Marine Natural Products

Guest Editors:

Dr. Florbela Pereira
LAQV, Department of Chemistry, NOVA School of Science and Technology, NOVA University of Lisbon, 2829-516 Caparica, Portugal

Dr. Rachael Mansbach
Theoretical Biology and Biophysics Group, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Deadline for manuscript submissions:
closed (31 December 2020)

Message from the Guest Editors

In recent years, computational methodologies have assisted in the exploration of marine natural products (MNPs) to make the discovery of new leads more efficient, to repurpose known MNPs, to reveal mechanisms of action, and to optimize leads.

Structure-based (SB) and ligand-based (LB) chemoinformatics approaches have become essential tools for the virtual screening of MNPs either in small datasets of isolated compounds or in large-scale databases.

A comprehensive analysis of available MNP databases, biological and chemical space defined by the known MNPs and the most common LB (e.g., quantitative structure–activity relationships (QSAR), estimation of drug likeness, similarity searching, pharmacophore identification), and SB techniques (e.g., molecular dynamics, docking, binding cavity) in the virtual screening of MNPs are the main focus of this Special Issue.

We invite scientists working in this area to submit their original research or review articles for publication in this Special Issue.

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Editor-in-Chief

Prof. Dr. Bill J. Baker
Department of Chemistry, University of South Florida, 4202 E. Fowler Ave., CHE 205, Tampa, FL 33620-5250, USA

Message from the Editor-in-Chief

During the past few decades there has been an ever increasing number of novel compounds discovered in the marine environment. This is exemplified by the robust preclinical and clinical pipeline that currently exists for marine natural products. *Marine Drugs* is inviting contributions on new advances in marine biotechnology, pharmacology, chemical ecology, synthetic biology, and genomics approaches related to the discovery of therapeutically relevant marine natural products. Our goal is to share your contribution in a timely fashion and in a manner that will be valued by the scientific community.

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Contact Us

Marine Drugs Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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