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## MOLECULAR MODELING IN BLUE BIOTECHNOLOGY: A COST-EFFECTIVE AND SUSTAINABLE APPROACH TO EXPLOIT MEDITERRANEAN CHEMICAL DIVERSITY

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### Abstract

Within this study, metabolites isolated from marine organisms living in the Mediterranean Sea have been investigated by both a chemo-ecological and a computational approach to decode the "information content" of marine natural products in terms of possible biotechnological applications. This led us to predict, from 3D chemical structures, the interaction of selected metabolites with macromolecular targets underlying crucial ecological and pharmacological actions.

*Keywords: Biotechnologies, Alien species*

Natural products possess an extraordinary pharmacological effectiveness and specificity compared to artificially designed molecules because evolutionary selection has been the "nature's own high-throughput screening" process for the optimization of biologically active compounds [1, 2]. As a result, a broad range of bioactivities has been found within the increasing number of novel secondary metabolites isolated from the under-explored marine sources [3]. However, similarly to their terrestrial counterparts, marine natural products often interact with more than one specific target, also producing toxicity and other side effects which often prevent their use as drugs. By combining a chemo-ecological approach in the study of the natural function of small molecules isolated from Mediterranean flora and fauna with modern "in silico" target fishing techniques, we propose an efficient method for "a priori" predictions of possible exploitation of marine natural products, or their analogues, in biotechnological fields. Selected cases will be presented, with emphasis on possible uses in biotechnology of undesired biomaterials from invasive alien species, which are altering the Mediterranean community structure [4]. This research has led us to select promising candidates in drug discovery, and to design structural analogues for lead optimization. We believe that our approach to blue biotechnology should prevent the negative impacts of dispersive pharmacological evaluations and randomly-guided sampling activities on the Mediterranean ecosystem, also providing sustainable opportunities for the sea-based economy of coastal communities.

### References

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