An Updated Review on Marine Anticancer Compounds: The Use of Virtual Screening for the Discovery of Small-Molecule Cancer Drugs

Marine secondary metabolites are a promising source of unexploited drugs that have a wide structural diversity and have shown a variety of biological activities. These compounds are produced in response to the harsh and competitive conditions that occur in the marine environment. Invertebrates are considered to be among the groups with the richest biodiversity. To date, a significant number of marine natural products (MNPs) have been established as antineoplastic drugs. This review gives an overview of MNPs, both in research or clinical stages, from diverse organisms that were reported as being active or potentially active in cancer treatment in the past seventeen years (from January 2000 until April 2017) and describes their putative mechanisms of action. The structural diversity of MNPs is also highlighted and compared with the small-molecule anticancer drugs in clinical use. In addition, this review examines the use of virtual screening for MNP-based drug discovery and reveals that classical approaches for the selection of drug candidates based on ADMET (absorption, distribution, metabolism, excretion, and toxicity) filtering may miss potential anticancer lead compounds. Finally, we introduce a novel and publically accessible chemical library of MNPs for virtual screening purposes.

Fuente de la publicación:

- Ruiz-Torres, V.; Encinar, J.A.; Herranz-López, M.; Pérez-Sánchez, A.; Galiano, V.; Barrajón-Catalán, E.; Micol, V. An Updated Review on Marine Anticancer Compounds: The Use of Virtual Screening for the Discovery of Small-Molecule Cancer Drugs [1]. Molecules 2017, 22, 1037.

Proyectos relacionado:

- Simulaciones moleculares de docking (acoplamiento molecular) para buscar potenciales inhibidores de diferentes virus [2].

Noticias relacionadas:

- CénitS colabora en la búsqueda de anticancerígenos junto a investigadores de la Universidad Miguel Hernández de Elche y el Instituto de Salud Carlos III de Mallorca [3].

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[1] http://www.mdpi.com/1420-3049/22/7/1037 [2] http://www.cenits.es/proyectos/simulaciones-moleculares-docking-acoplamiento-molecular-buscar-potenciales-inhibidores [3] http://www.cenits.es/noticias/20072017-cenits-colabora-busqueda-anticancerigenos-junto-investigadores-universidad-miguel