

Abstract

NP Navigator: A New Look at the Natural Products Chemical Space [†]

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Abstract: Over the last few billion years, countless organisms populating our planet have produced an extensive reserve of very diverse chemicals called natural products (NPs). Over time, these compounds have evolved to exhibit a wide range of bioactivity and high selectivity in different organisms. That makes them an extremely important source of potential drugs. However, considering the number of reported NPs and their high diversity, it becomes hard to explore the respective chemical space in drug design. In order to simplify this task, we have developed NP Navigator, a free, user-friendly online tool allowing to navigate and analyze the chemical space of NPs and NP-like compounds [1] (https://infochm.chimie.unistra.fr/npnav/chematlas_userspace). The basis of this tool is a hierarchical ensemble of 241 Generative Topographic Maps (GTM) [2, 3], visualizing chemical space of NPs from the COLleCtion of Open Natural ProductTs (COCONUT) [4], molecules with some biological activity from ChEMBL [5], and purchasable compounds from ZINC [6]. NP Navigator can be used for an efficient analysis of various aspects of NPs, including calculated properties, chemotype distribution, biological activity, and commercial availability of NPs. Users can browse through hundreds of thousands of molecules from COCONUT, ZINC, and ChEMBL, selecting a zone of interest based on the color code of the maps, which in turn corresponds to specific values of visualized properties. In addition, it is possible to project several external molecules - “chemical trackers” - that are intentioned to trace regions of the NP chemical space containing compounds with desired structural features. In such a way NP Navigator allows searching for the NP and NP-like analogues of the user-provided compounds.

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Keywords: chemoinformatics; natural products; chemical space; visualization; web tools

Figure 1. Search of the NPs and commercially available NP-like analogs of provided compound with the help of NP Navigator.

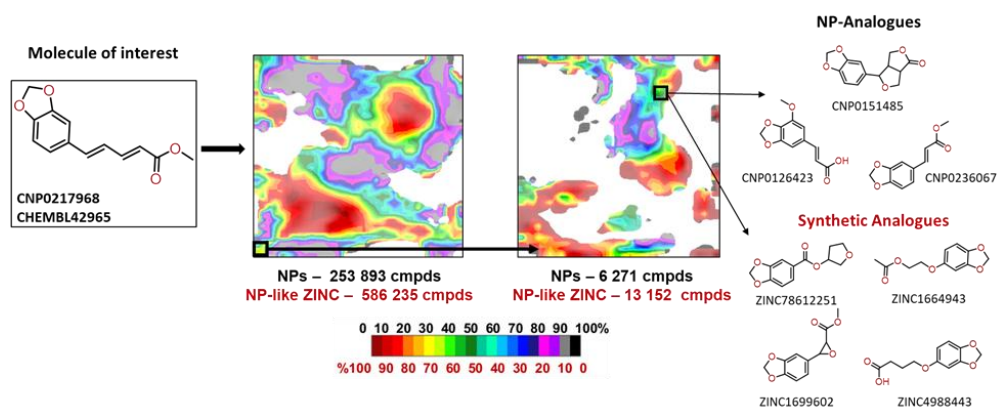


Figure 1. Search of the NPs and commercially available NP-like analogs of provided compound with the help of NP Navigator.

Author Contributions: The research has been performed through the contribution of all authors, and all authors have given approval to the text of this abstract.

Informed Consent Statement: Not applicable.

Data Availability Statement: Publicly available datasets were analyzed in this study. The web implementation of the resulting interactive tool is available here: https://infochm.chimie.unistra.fr/npnav/chematlas_userspace

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