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Abstract

NP Navigator: A New Online Tool for the Exploration of 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 the navigation and analysis of the chemical space of NPs and NP-like compounds [1,2]. The basis of this tool is a hierarchical ensemble of 241 Generative Topographic Maps (GTM) [3,4], visualizing chemical space of NPs from the COlleCtion of Open Natural ProductTs (COCONUT) [5], molecules with some biological activity from ChEMBL [6], and purchasable compounds from ZINC [7]. 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"—to trace regions of the NP chemical space containing compounds with desired structural features. In such a manner, the NP Navigator allows searching for NP and NP-like analogues of user-provided compounds. This study was previously published in *Molecular Informatics* (10.1002/minf.202100068) [1].

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

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

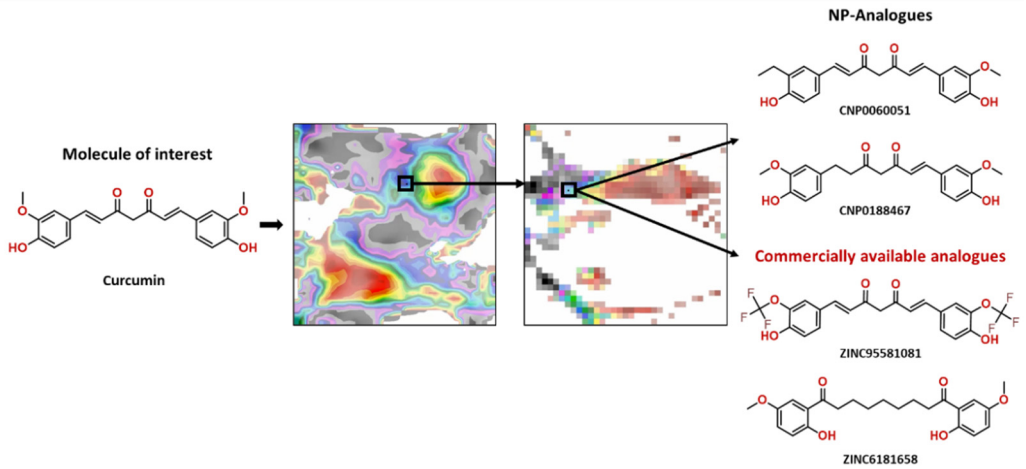

Figure 1. Search of the NPs and commercially available NP-like analogs of provided compound (curcumin) with the help of NP Navigator.

Supplementary Materials: The video demonstration of NP Navigator usage is available at https://sciforum.net/paper/view/10829 (accessed on 20 December 2021).

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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 (accessed on 20 December 2021).

Conflicts of Interest: The authors declare no conflict of interest.

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