

Chemical space of food chemicals and natural products from Latin America

José L. Medina-Franco, Alejandro Gómez-García, Juan F. Avellaneda-Tamayo

DIFACQUIM research group, National Autonomous University of Mexico, Avenida Universidad 3000, 04510, Mexico City, Mexico.

Compound databases are significant for several practical applications, including drug discovery, compound design, and the generation of predictive models. Databases of natural products have increased substantially, and there are several compound databases from diverse geographical regions. Latin America is rich in biodiversity, and some databases are being assembled or under development. Collecting, organizing, and systematizing the information available across these compound collections is valuable and significant. In a collective effort from eight Latin American countries, we are assembling and exploring the chemical space of the so-called “Latin American Natural Products Database (LANaPD)” [1]. This public compound collection gathers the chemical information of natural products in diverse databases from this geographical region. The project collects data from compound databases from Argentina, Brazil, Colombia, Costa Rica, El Salvador, Mexico, Panama, and Peru. We anticipate that the chemical space of LANaPD will continue growing and evolving with the update of more compounds from each existing database, plus the addition of databases from other Latin American countries. It is also anticipated that LANaPD can be integrated into other large public databases of natural products such as LOTUS or COCONUT [1]. As part of navigating the chemical space of natural products from Latin America, we are also exploring the structural diversity and coverage in the chemical space of food chemicals that overlap with natural products but also have distinct structural characteristics [2]. As part of the presentation, we will address the concept of the chemical multiverse as an extension of chemical space. Indeed, since chemical space depends on molecular representation, it can be concluded that there is no unique chemical space. In parallel to the continued growth of molecules that are enumerated, there are a plethora of descriptors and sets of properties relevant for different chemical applications, for example, to represent small organic molecules typically used in drug discovery, metallodrugs, natural products, food chemicals, and peptides. Therefore, the Chemical Space of a set of compounds – defined as multidimensional descriptor space – may have alternative versions and representations depending on the descriptors used to determine it, giving rise to the Chemical Multiverse [3]. Finally, in this presentation, we will discuss briefly how the visual representation of the chemical space and the chemical multiverse of natural products and food chemicals can be used as means of artistic representations expected to contribute to the education and dissemination of chemoinformatics [4].

Bibliography :

- [1] Gómez-García, A., Acuña Jimenez, D.A., Zamora, W. et al. *Pharmaceuticals* 16 (2023) 1388.
- [2] Naveja, J.J., Rico-Hidalgo, M.P., Medina-Franco, J. L. *F1000Research*, 7(ChemInf Sci) (2018) 993.
- [3] Medina-Franco, J.L., Chávez-Hernández, A.L., López-López, E., Saldivar-González, F.I. *Mol. Inf.* 41 (2022) 2200116.
- [4] Gaytán-Hernández, D., Chávez-Hernández, A. L., López-López, E., Miranda-Salas, J., Saldivar-González, F., Medina-Franco, J.L. *J. Cheminf.* 15 (2023) 100.