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$NuBBE_{DB}$: A BRAZILIAN DATABASE OF SECONDARY METABOLITES

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The NuBBE database ($NuBBE_{DB}$) was designed and developed as a new Web-based database, which incorporates a variety of information about secondary metabolites obtained from Brazilian biodiversity since 1950. Informations available at $NuBBE_{DB}$ include chemical structure, chemical class, source, biological activity, and the DOI of isolated compounds. Chemical structure is represented by SMILES, which generates molecular and physicochemical properties, such as number of rotatable bonds (nRotb), partition coefficients (cLogP), number of hydrogen-bond donors and acceptors, number of Lipinski's "rule of five" violations, topological polar surface area (TPSA), molecular volume, and molecular mass [1]. The main objective of $NuBBE_{DB}$ is to provide specialized information to the worldwide scientific community and serve as a useful tool for studies on the multidisciplinary interfaces related to chemistry and biology, including virtual screening, dereplication, metabolomics, and medicinal chemistry. Nowadays $NuBBE_{DB}$ has approximately 1,300 compounds of which 82% were isolated from plants, 8% from microorganisms, 4% are products of biotransformation using fungi extract, and 6% are semisynthetic. The chemical diversity is rather large, with compounds belonging to several different chemical classes, including 34% of terpenoids, 25% of alkaloids, 13% of flavonoids, 9% of coumarins, 7% of aromatic derivatives, and 12% of other classes. The mainly biological activities of the isolated compounds are antiprotozoal (35%), antifungal (20%), cytotoxic and anticancer (17%), antioxidant (16%), and acetylcholinesterase inhibitors (8%). As a future perspective we will include the geographical location where the studied species were collected (City, Estate) and the predicted ^{1}H and ^{13}C NMR spectra. In conclusion, the information comprised at $NuBBE_{DB}$ could be useful to the scientific community for studies involving virtual screening, dereplication, metabolomics, and the design of new bioactive compounds.

[1] Valli, M; dos Santos, R.N.; Figueira, L.D.; Nakajima, C.H. Castro-Gamboa, I.; Andricopulo, A.D.; Bolzani, V.S. Development of a Natural Products Database form the Biodiversity of Brazil. J. Nat. Prod., 2013, 76 (3): 439-444.