

Organized diversity

Center creates a database of chemical compounds that have potential use in the development of pharmaceuticals

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Detailed information on 640 chemical compounds extracted during studies of Brazilian biodiversity is available on the Internet at www.nubbe.iq.unesp.br/nubbeDB.html. This database contains knowledge generated over 15 years of research by the Center for Natural Products Bioassays, Biosynthesis and Ecophysiology (NuBBE) at São Paulo State University (UNESP) in Araraquara. “We realized that our research results, which have been published in more than 170 articles, could be more useful if they were organized into a database than if they remained dispersed. We have valuable information on the chemical diversity of the species studied, and we decided to make this information available so that other researchers could use it in further studies,” says Vanderlan Bolzani, professor at the Institute of Chemistry (IQ) of UNESP in Araraquara and member of the group coordinating the Biota-FAPESP program. The database was designed in collaboration with Professor Adriano D. Andricopulo of the Medicinal and Computational Chemistry Laboratory (LQMC) of the Physics Institute (USP - São Carlos) and his doctoral student, Ricardo N. Santos, a FAPESP scholarship recipient.

PROPERTIES IDENTIFIED

This resource assembles a variety of types of information, such as the origin of the compound, the species from



Studies on research to develop medicine from *Rubiaceae* species, such as the coffee tree, are part of this online tool

which it was isolated, its chemical properties and its identified biological activities. The results of online research enable users to view the chemical structure and a table with information on the compound, and also to download the three-dimensional structure. The NuBBE database is composed of isolated plant compounds (80%), fungi or microorganisms (6%), synthetic compounds inspired by natural products (7%), semi-synthetic compounds (5%) and biotransformation products (modified by enzymes) (2%). A set of properties helps to define whether a given compound has the potential to be used in the development of new medicines. “The database is chemically diversified and rich. It is an interesting source for identifying bioactive compounds for testing in other, more sophisticated assays,” says Bolzani. His study on the search for cancer-fighting substances in the medicinal shrub *Rubiaceae brasiliensis*, conducted during the 1990s, is one of the oldest accessions in the database.

The data were compiled over a period of two years by a six-person team that included technicians and researchers. The database web site was designed by Leandro Figueira, who holds a Master’s

degree in computer science. “An undergraduate research internship student helped us to analyze all the NuBBE papers and to obtain information on the compounds,” says Marília Valli, a doctoral student at the UNESP Chemistry Institute and FAPESP scholarship recipient who is working on a project that studies the potential of NuBBE natural products as a resource for the rational planning of new anti-tumor agents. Valli’s dissertation, under the guidance of her advisor Bolzani, should be concluded in 2013.

One of the ambitions of the project participants is to cross the NuBBE database with information in the Environmental Information System (SINBIOTA), which links information generated by projects in the Biota-FAPESP program with a cartographic database. “This is not yet available, but we want to show the species to which the compounds are related and the habitats in which these species live. We hope this database will be the starting point for a national database on all the substances that have already been isolated from Brazilian biomes. We need to make our colleagues more aware of the value that such work would represent,” says Bolzani. ■ **Fabício Marques**