



## ***BANK OF MOLECULES: AN INITIATIVE TO LEVERAGE COLLABORATIVE NATURAL PRODUCT-BASED DRUG DISCOVERY IN BRAZIL***

***Rafael de Felício<sup>1\*</sup>, Joyce B. Guedes<sup>1</sup>, Andreza L. do Nascimento<sup>1</sup>, Beatriz P. Bosque<sup>1</sup>,  
Marcos G. Cunha<sup>1</sup>, Danieli C. Gonçalves<sup>1</sup>, Daniela B. B. Trivella<sup>1</sup>***

rafael.felicio@lnbio.cnpem.br

*<sup>1</sup>Drug Discovery Division, Brazilian Bioscience National Laboratory (LNBio), Brazilian Center for  
Research in Energy and Materials (CNPEM), Campinas/SP, Brazil*

Molecules from Nature (NPs) remain a main source of new drugs. Brazil, a biodiversity hotspot, harbors many molecules yet to be discovered and developed. The Brazilian scientific community is solid and needs to be connected to foster pharmaceutical innovation in Brazil. With this goal, we have established the Bank of Molecules, a multicollaborative initiative that aligns state of the art scientific infrastructure and expertise aimed to avoid early-stage drug discovery bottlenecks and to promote collaborative pharmaceutical innovation in Brazil. How it works: researchers interested in depositing their samples (extracts, fractions, pure compounds) to the Bank of Molecules (depositor) send their samples (2-10 mg) to LNBio/CNPEM, along with basic information that guarantees sample traceability. The samples are received by LNBio/CNPEM, where they are registered at a trackable certified database, processed and stored at low temperature under inert atmosphere, following automated processes under GLP practices. At this first stage, it will be performed two main analyses at LNBio/CNPEM: i) untargeted metabolomic analysis - quality control ( $t_0$ ) and chemical space covered by the samples; and ii) biological evaluation in cellular assays (HCT-116, colon cancer, and HaCat, reference keratinocyte) – aiming to point natural samples with anticancer potential. The first results are expected within 90 days, which are delivered through standard reports on biological and chemical analyses, highlighting the main findings. From there, parties involved can discuss the next steps of the collaboration, including the publication in scientific literature or further developments from the obtained data, according to the interest of the depositor. Remaining samples are stored at LNBio/CNPEM for further analysis, remain property of the depositor, and require consent for use. At the same time, researchers interested in accessing the Bank of Molecules (users) can express their intents and will be connected to the depositor through our system. Once approved, the samples will be sent to the users in “assay ready plates”, containing typically 2.5 nL of the approved chemical samples (384-well format preferred). The “assay ready plates” can be promptly tested by the users, by dispensing their biological samples (bacteria, cells, target proteins, and so on) upon plate arrival at their laboratories. This enables the execution of medium to high throughput screenings at different institutions in Brazil, by avoiding bottlenecks of chemical sample pipetting and trackability, thus speeding up bioprospection in the country. The Bank of Molecules was just launched, attending researchers spanning all regions of Brazil. We invite all researchers to contribute to the Bank of Molecules by depositing their chemical samples, or by accessing them in their drug discovery projects in a collaborative fashion. For more information please consult: <https://lnbio.cnpem.br/>, [Banco.Moleculas@lnbio.cnpem.br](mailto:Banco.Moleculas@lnbio.cnpem.br)

**Keywords:** Drug discovery, Brazilian Biodiversity, Compound Management, Metabolomics, Bioassays

