

Área: MED

## IRACEMA: A Database Management System for Bioactive Compounds Isolated and Characterized by Brazilian Researchers.

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### Highlights

First Brazilian bioactive compounds database. Cheminformatic tools for molecular prediction. Modern tech infrastructure. Connects national academic research and advances medicinal chemistry innovation.

### Resumo/Abstract

Bioactive compounds are substances with extra-nutritional properties found in natural sources or synthesized in laboratories. These substances play regulatory roles in metabolic processes, essential for human health. Over time, bioactive compound discovery has become strategically important for scientific advancement, particularly in the pharmaceutical and healthcare industries. Brazil, known for its rich biodiversity and strong expertise in organic chemistry, holds great potential for discovering bioactive molecules, both natural and synthetic. However, the vast amount of data generated in this field is often scattered and difficult to access. This is where cheminformatics becomes essential—helping to organize and analyze chemical data, predict biological activity, and understand mechanisms of action. The IRACEMA project ("Innovative Research, Analysis and Computational Exploration of Molecules Assembled in Brazil") was created to bridge this gap. It aims to build a comprehensive national database dedicated to biologically active compounds identified in Brazil, integrating cheminformatics tools to streamline drug discovery and strengthen collaboration between researchers and the pharmaceutical industry. To achieve this, IRACEMA combines bibliographic review, data collection, predictive modeling, and the development of an interactive web platform for molecular visualization and analysis. The project leverages React and Next.js for the frontend, NestJS and Node.js for backend development, PostgreSQL for data management, and Python/Flask with RDKit and other microservices for cheminformatics applications. Agile methodologies, including tools like Jira and GitHub, support efficient project management and version control. Key challenges include managing chemical data and integrating diverse information sources. By addressing these challenges, IRACEMA not only strengthens Brazil's role in bioactive compound research but also fosters innovation in medicinal chemistry by making this data accessible, bridging the gap between academic discoveries and real-world applications.

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