Way2Drug
PREDICTIVE SERVICES
Understanding Chemical-Biological Interactions

IRACEMA: A Database Management System for Bioactive Compounds Characterized by Brazilian Researchers

XXXI Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD-2025)

Thais A. Lourenço, Renan P. O. Costa, Luis Felipe M. Melo, Uilames A. Ferreira, Eduardo Henrique P. Alves, Luciano P. Oliveira-Filho, Luciana Scotti, Marcus Tullius Scotti, and Gustavo Henrique G. Trossini

October 22nd, 2025

CHEMINFORMATICS LAB

Litec

Bioactive Compounds

Definition and Importance

Bioactive compounds are a vast class of chemical substances found in nature or synthesized in a laboratory that can cause biological (pharmacological or toxicological) responses in cells, tissues, or organisms

National Landscape

The research and development of bioactive compounds, both in Brazil and worldwide, has driven a substantial increase in the amount of available chemical and biological data,

Cheminformatics

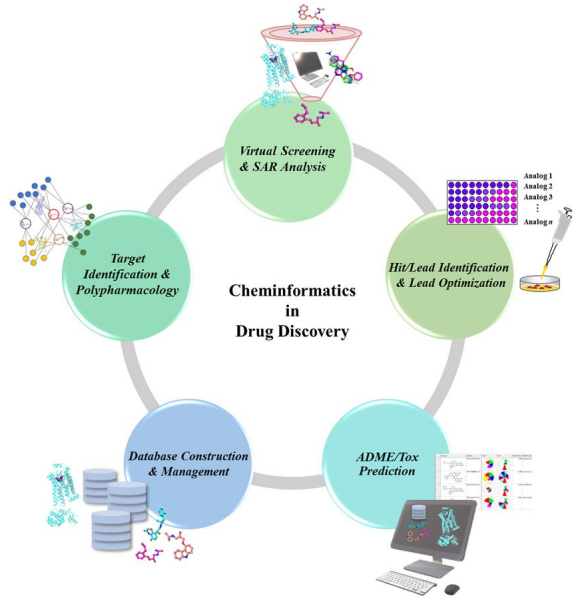


Figure 1. Role of Cheminformatics in the drug discovery process. Cheminformatics is involved in almost every step of the drug discovery pipeline due to the employment and analysis of available data to translate into valuable knowledge, which can in turn be used as a data for further studies. DOI:10.3389/fphar.2018.00128

"A Cheminformatics is the mixing of those information resources to transform data into information and information into knowledge for the intended purpose of making better decisions faster in the area of drug lead identification and optimization."

— Frank Brown, 1998

Databases

Definition

A database is a system optimized for efficient data search, query, and management, enabling the analysis of structured data and the relationship between information.

BrNPDB

Brazilian Biodiversity Natural Products Database

SISTEMATX

PubChem

ChEMBL

DRUGBANK

IRACEMA (Innovative Research, Analysis and Computational Exploration of Molecules Assembled in Brazil)

- The first database of its kind to focus on synthetic compounds in the country
- Provides an intuitive, user-friendly platform for molecular visualization and analysis by integrating cheminformatics tools
- Give national and international visibility to Brazilian laboratories and facilitate collaboration within research groups

Methodology - Data Curation

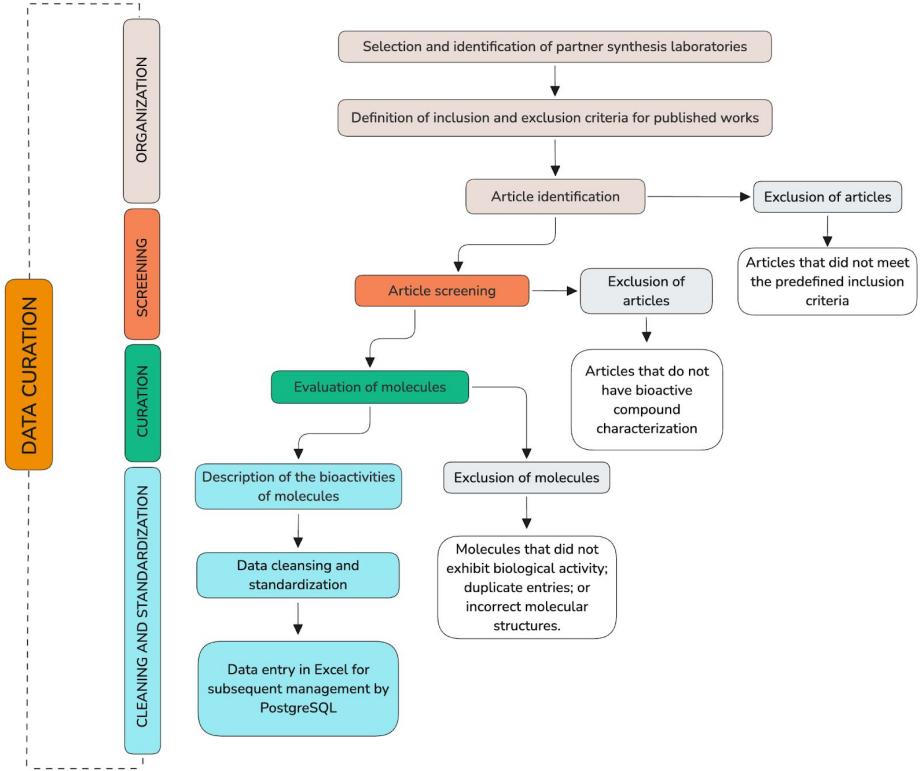


Figure 2. Flowchart of the Data Curation Methodology.

Methodology - System Architecture

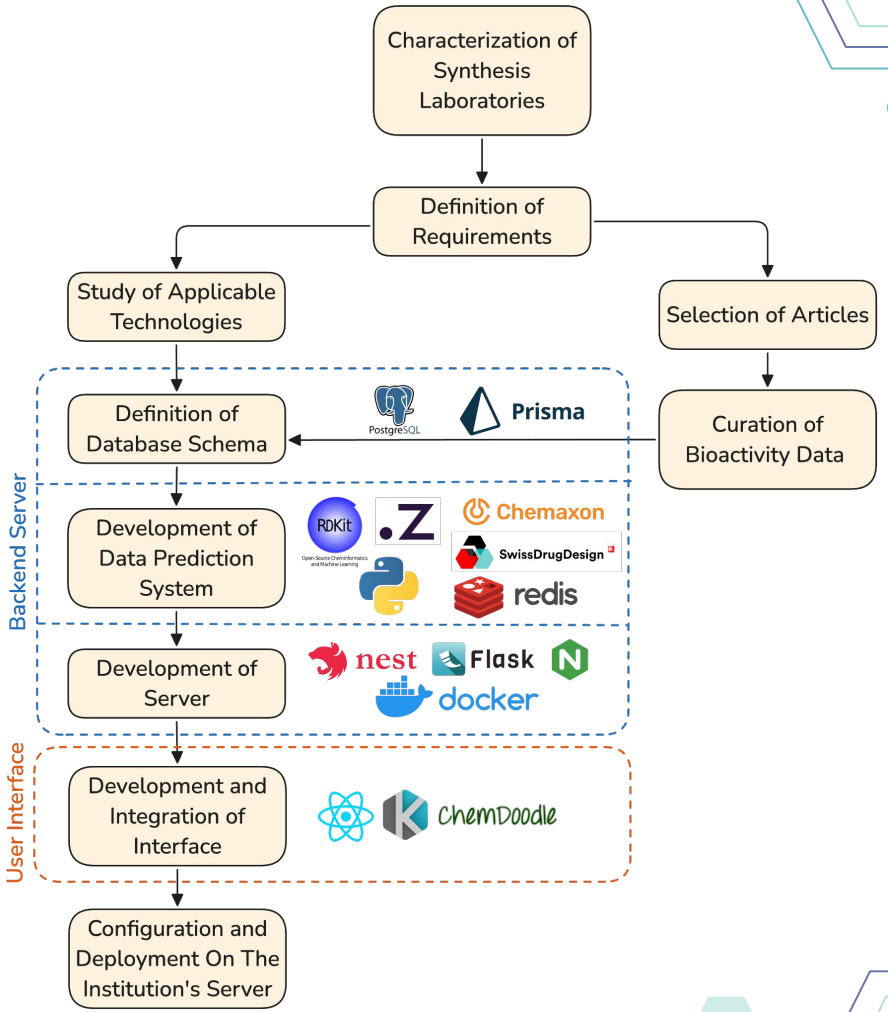


Figure 3. Workflow for compound and bioactivity data curation, alongside the architectural scheme of the IRACEMA system integrating frontend, backend, database, and cheminformatics microservices.

Visual Identity

Figure 4. Moodboard and elements that served as inspiration for visual identity

IRACEMA platform

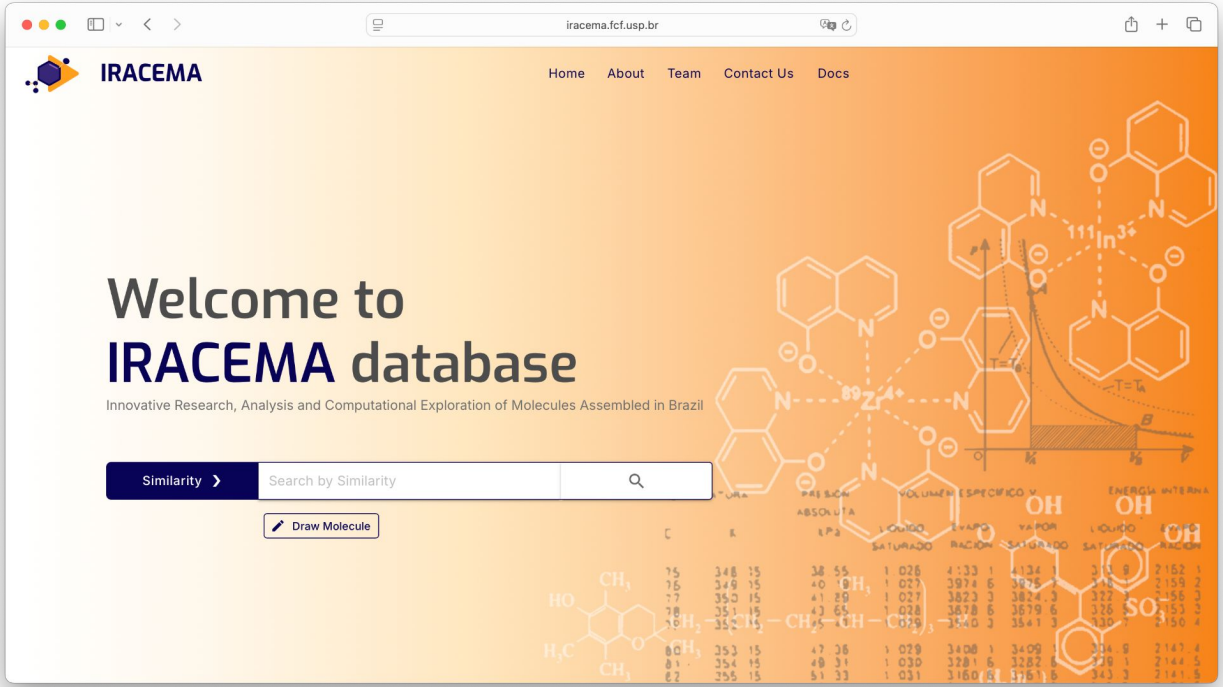
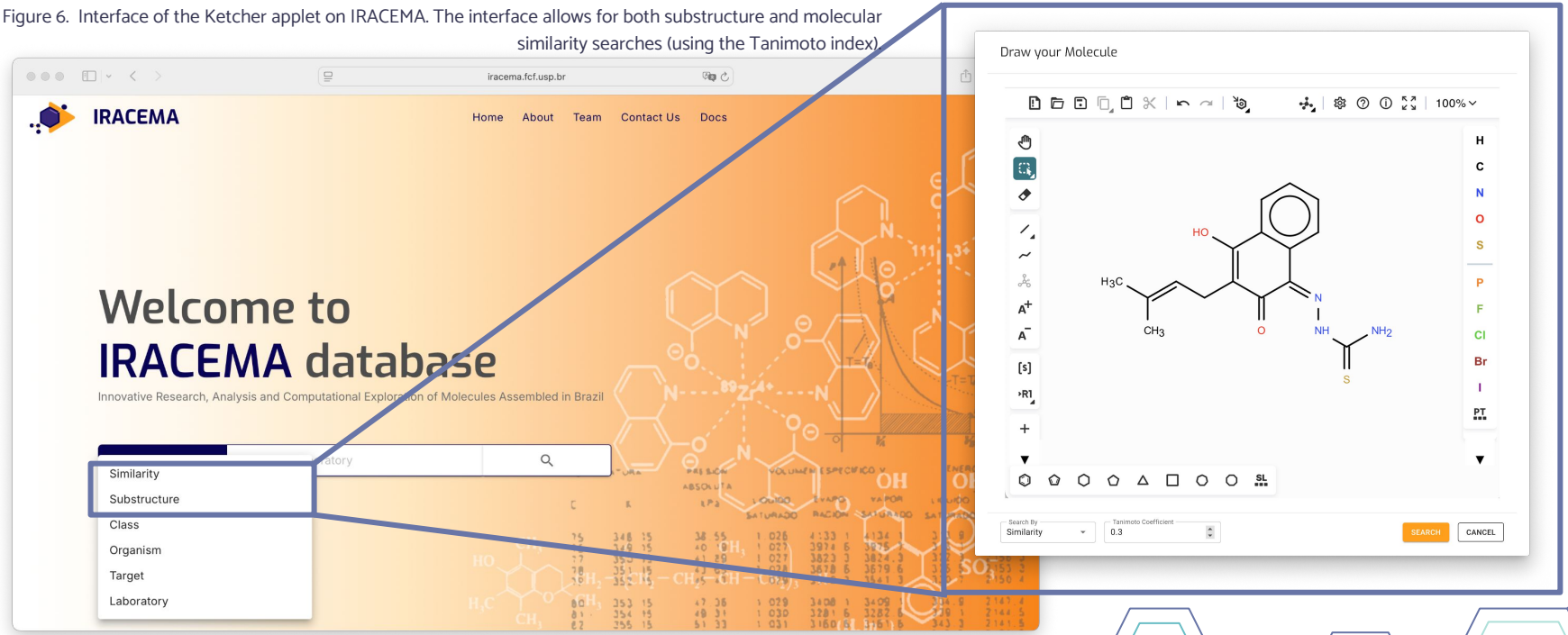


Figure 5. The IRACEMA homepage, with a navigation menu at the top and a search bar in the center.

IRACEMA Search

Figure 6. Interface of the Ketcher applet on IRACEMA. The interface allows for both substructure and molecular similarity searches (using the Tanimoto index).



IRACEMA Results Page

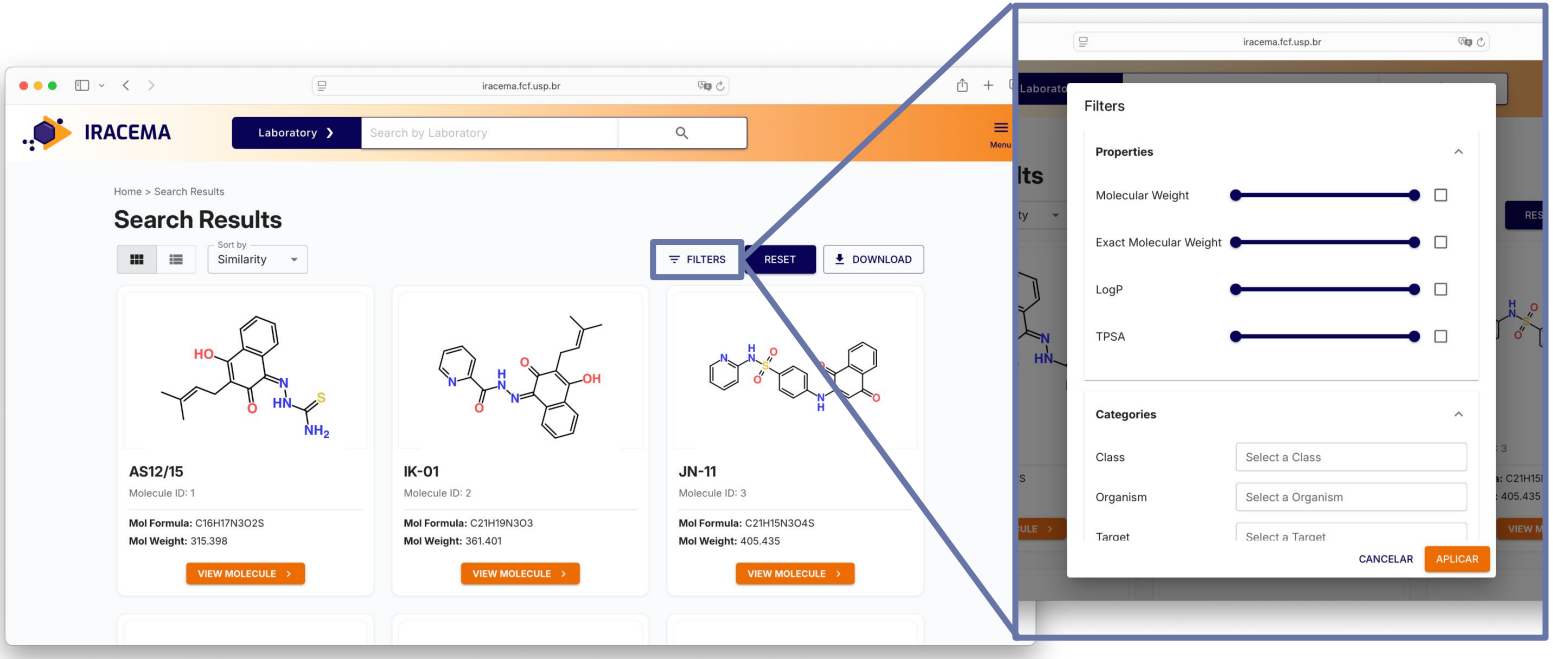


Figure 7. The results page displays the compounds in either gallery or list format, providing a brief description of each molecule.

IRACEMA Molecule Page

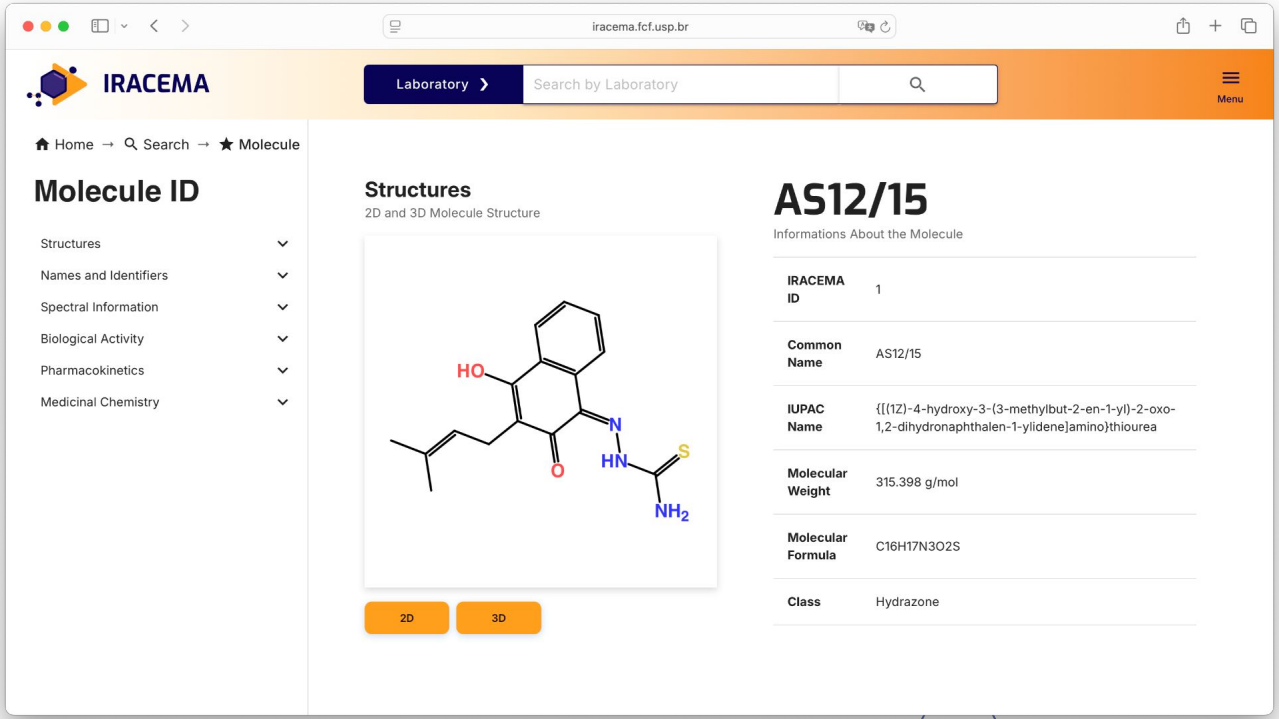


Figure 8. A detailed view of a selected molecule. The molecule page features 2D and 3D structural visualizations, manually curated biological activities, and predicted molecular properties.

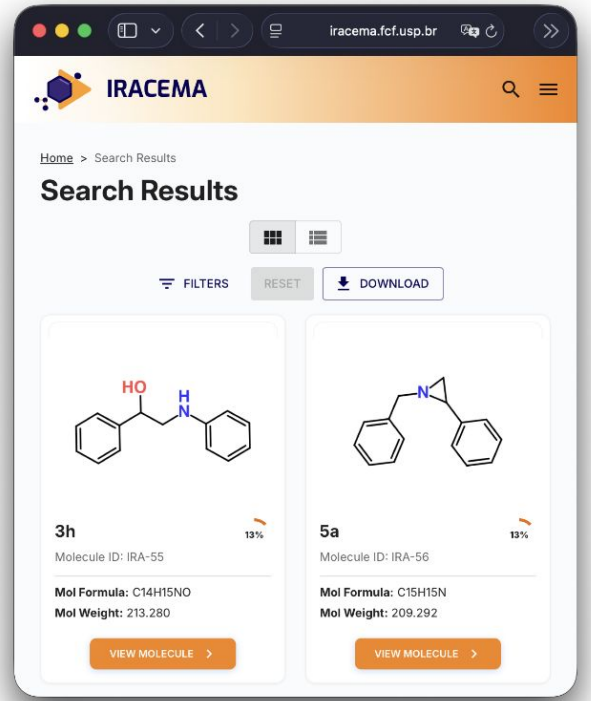
BIOACTIVE MOLECULES

CURATION

PROCESSING

VISUALIZATION


```
{
  "data": {
    "mol": "<rdkit.Chem.rdchem.Mol object at 0x7f44fd2d57b0>",
    "canon_smiles": "O=C(O)c1ccccc1",
    "inchi_str": "InChI=1S/C7H6O2/c8-7(9)6-4-2-1-3-5-6/h1-5H,(H
    "inchikey": "WPYMKLBDIGXBTP-UHFFFAOYSA-N",
    "logp": 1.3848,
    "tpsa": 37.3,
    "mol_formula": "C7H6O2",
    "exact_mol_wt": 122.036779432,
    "mol_wt": 122.12299999999996,
    "coordinates_2d": "string",
    "coordinates_3d": "string"
  }
}
{
  "results": [
    {
      "smiles": "OC(=O)C1=CC=CC=C1",
      "Physicochemical Properties": {
      },
      "Lipophilicity": {
      },
      "Water Solubility": {
      },
      "Pharmacokinetics": {
      },
      "Druglikeness": {
      }
    }
  ]
}
```

Freely available at https://iracema.fcf.usp.br/

IRACEMA Database

Thank You!

References

- GUAÂDAOUI, A. et al. What is a bioactive compound? A combined definition for a preliminary consensus. International Journal of Nutrition and Food Sciences, v. 3, n. 3, p. 174–179, 2014.
- SHRINET, K. et al. Bioactive compounds and their future therapeutic applications. In: Bioactive Compounds: Health Benefits and Potential Applications. p. 337-362, 2021.
- DE MENEZES, R. P. B.; SCOTTI, L.; SCOTTI, M. T. MACHINE LEARNING APLLIED TO QSAR. Quimica Nova, v. 47, n. 7, 2024.
- DING, Y.; XUE, X. Medicinal Chemistry Strategies for the Modification of Bioactive Natural Products. Molecules, v. 29, 2024.
- LEACH, A. R.; GILLET, V. J. An Introduction to Chemoinformatics. Revised ed. Dordrecht: Springer, 2007.
- ARAÚJO, V. R. et al. O crescimento do Brasil na pesquisa e desenvolvimento de novas moléculas sintéticas com propriedades terapêuticas desejadas: uma revisão. Revista Brasileira de Ciências Farmacêuticas, v. 58, n. 1, p. 1-15, jan./mar. 2023.
- SCOTTI, M. T. et al. SistematX, an Online Web-Based Cheminformatics Tool for Data Management of Secondary Metabolites. Molecules 2018, Vol. 23, Page 103, v. 23, n. 1, p. 103, 3 jan. 2018.
- COSTA, R. P. O. et al. The SistematX Web Portal of Natural Products: An Update. Journal of Chemical Information and Modeling, v. 61, n. 6, p. 2516–2522, 28 jun. 2021.

Way2Drug
PREDICTIVE SERVICES
Understanding Chemical-Biological Interactions

IRACEMA: A Database Management System for Bioactive Compounds Characterized by Brazilian Researchers

XXXI Symposium on Bioinformatics and Computer-Aided Drug Discovery (BCADD-2025)

Thais A. Lourenço, Renan P. O. Costa, Luis Felipe M. Melo, Uilames A. Ferreira, Eduardo Henrique P. Alves, Luciano P. Oliveira-Filho, Luciana Scotti, Marcus Tullius Scotti, and Gustavo Henrique G. Trossini

October 22nd, 2025

CHEMINFORMATICS LAB

Litec