NATURAL PRODUCTS DATABASES AS VALUABLE SOURCES OF BIOACTIVE STRUCTURES FOR VIRTUAL SCREENING

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Lattes

http://buscatextual.cnpq.br/buscatextual/visualizacv.do?metodo=apresentar&id=K4751704U

Research Gate:

https://www.researchgate.net/profile/Marcus_Scotti

Google Scholar:

https://scholar.google.com.br/citations?user=jdVKCTgAAAAJ&hl=es

João Pessoa -PB

Cheminformatics Lab

Conducts studies in:

Computer-assisted drug design: QSAR, Structure-Base Virtual Screening and Ligand-based VS

Environmental Chemoinformatics

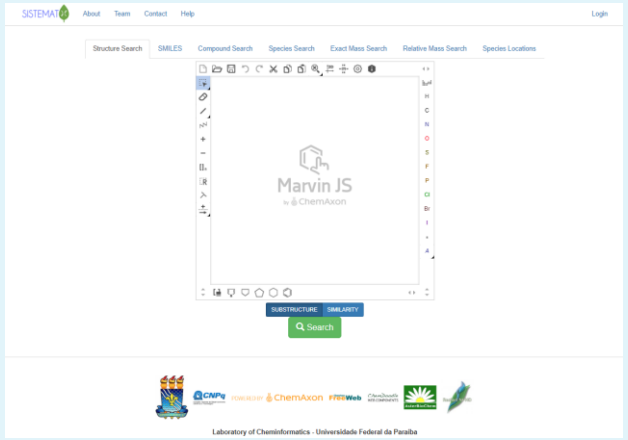
Natural Products Databases:

https://sistematx.ufpb.br

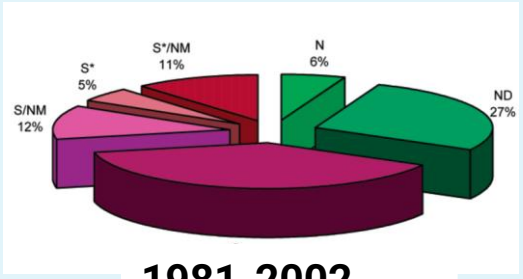
Molecules **2018**, *23*(1), 103; https://doi.org/10.3390/molecules23010103 Open Access Technical Note

SistematX, an Online Web-Based Cheminformatics Tool for Data Management of Secondary Metabolites

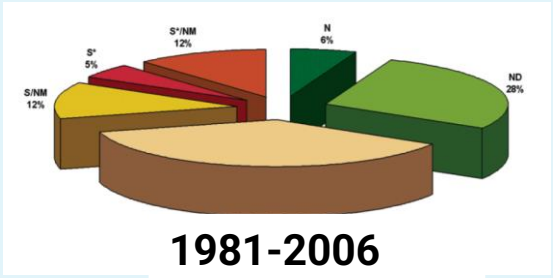
Marcus Tullius Scotti [1,*], Chonny Herrera-Acevedo [1], Tiago Branquinho Oliveira [2,3], Renan Paiva Oliveira Costa [1], Silas Yudi Konno de Oliveira Santos [1], Ricardo Pereira Rodrigues [1], Luciana Scotti [1] and Fernando Batista Da-Costa [3]



Natural products (NP) and their secondary metabolites are promising starting points for the development of prototypes and new drugs, being a large part of the new treatments against countless diseases, directly or indirectly related to them.



1981-2002



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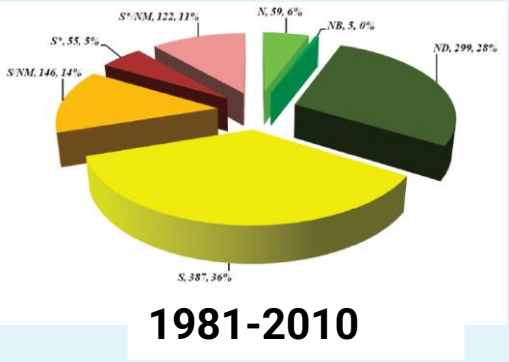
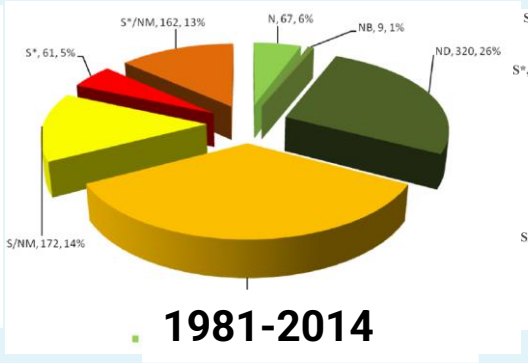
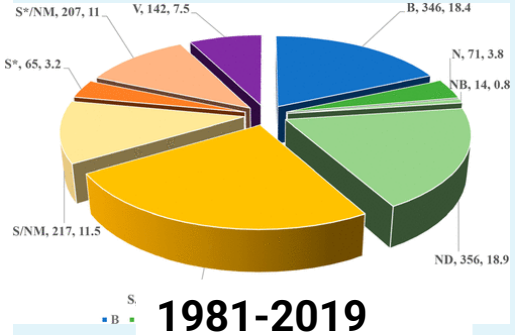


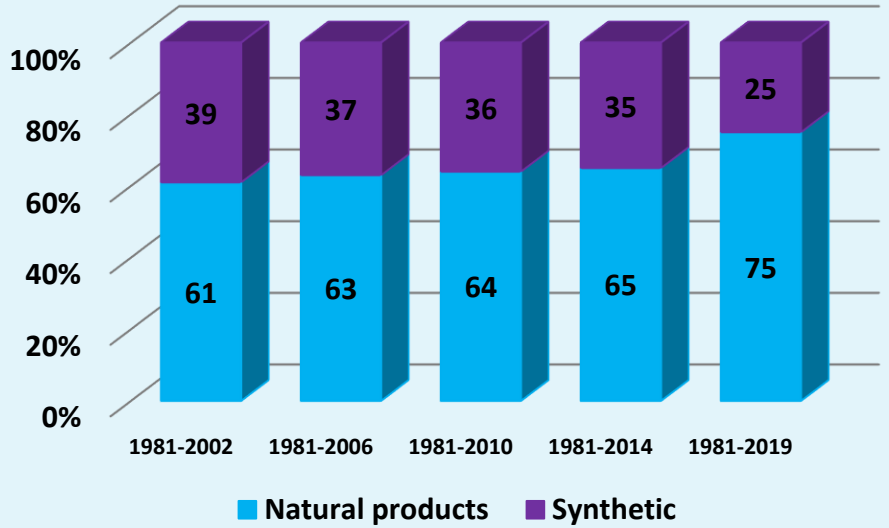
1981-2010



1981-2014



1981-2019



Natural Products as Sources of New Drugs over the Nearly Four Decades from 01/1981 to 09/2019. David J. Newman and Gordon M. Cragg

Newman, David J.; Cragg, Gordon M.; Snader, Kenneth M. *J. Nat. Prod.*, 75, 1022-1037 (2003).

Newman, David J.; Cragg, Gordon M. *J. Nat. Prod.,* 70, 461-477 (2007).

Newman, David J.; Cragg, Gordon M. *J. Nat. Prod.,* 75, 311-335 (2012).

Newman, David J.; Cragg, Gordon M. *J. Nat. Prod.,* 79, 629-661 (2016).

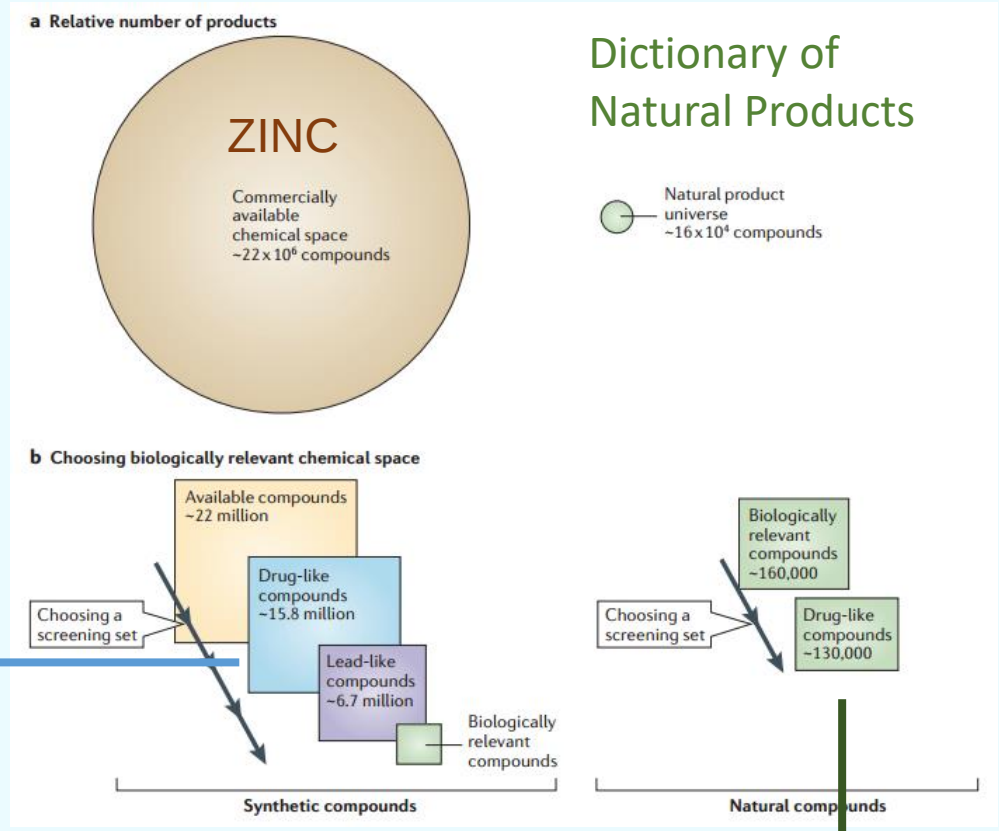
Natural Products

The re-emergence of natural products for drug discovery in the genomics era

Alan L. Harvey, RuAngelie Edrada-Ebel, Ronald J. Quinn

Nature Reviews Drug Discovery 14, 111–129 (2015)

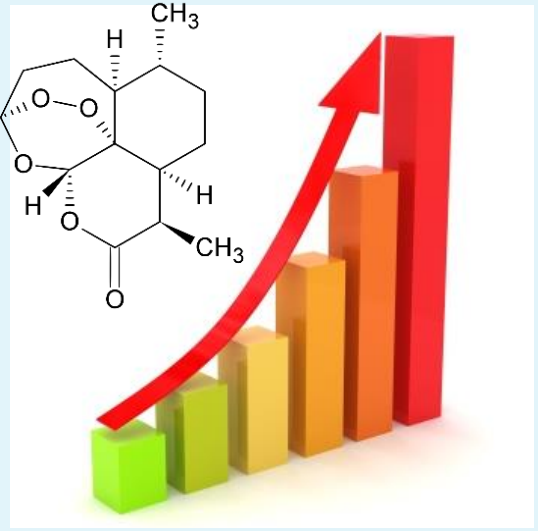
Database	Number of entries	Additional information
Super Natural II	355,000	2D structures; vendor information for over 215,000 compounds
Universal Natural Product Database	197,201	3D structures assembled from other available Chinese databases
Chinese Natural Product Database	53,000	Has been used in a virtual screen for PPAR-γ agonists
Drug Discovery Portal	40,000	Not all natural products, but all based on available samples
iSMART	20,000	Based on components from traditional Chinese medicines
Database from historical medicinal plants, DIOS	6,702	Successfully used in several virtual screening campaigns
AfroDb	1,000	Compounds from African medicinal plants
NuBBE	640	Compounds from Brazilian sources



71.8%

81.2%

Natural Products Databases



The increase in the number of new structures and studies related to biological activity reinforced the development of databases allowing significant support for drug discovery

The classification and organization of information is essential

The databases have provided a collection systematic information on natural products and their derivatives

Natural Products Databases

Computational approaches have played an increasingly prominent role in natural product (NP)-based drug discovery.

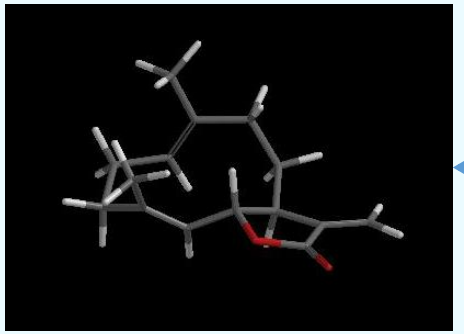
For example, the development and use of NP databases allow access to numerous chemical, biological, pharmacological, toxicological, and structural NP data.

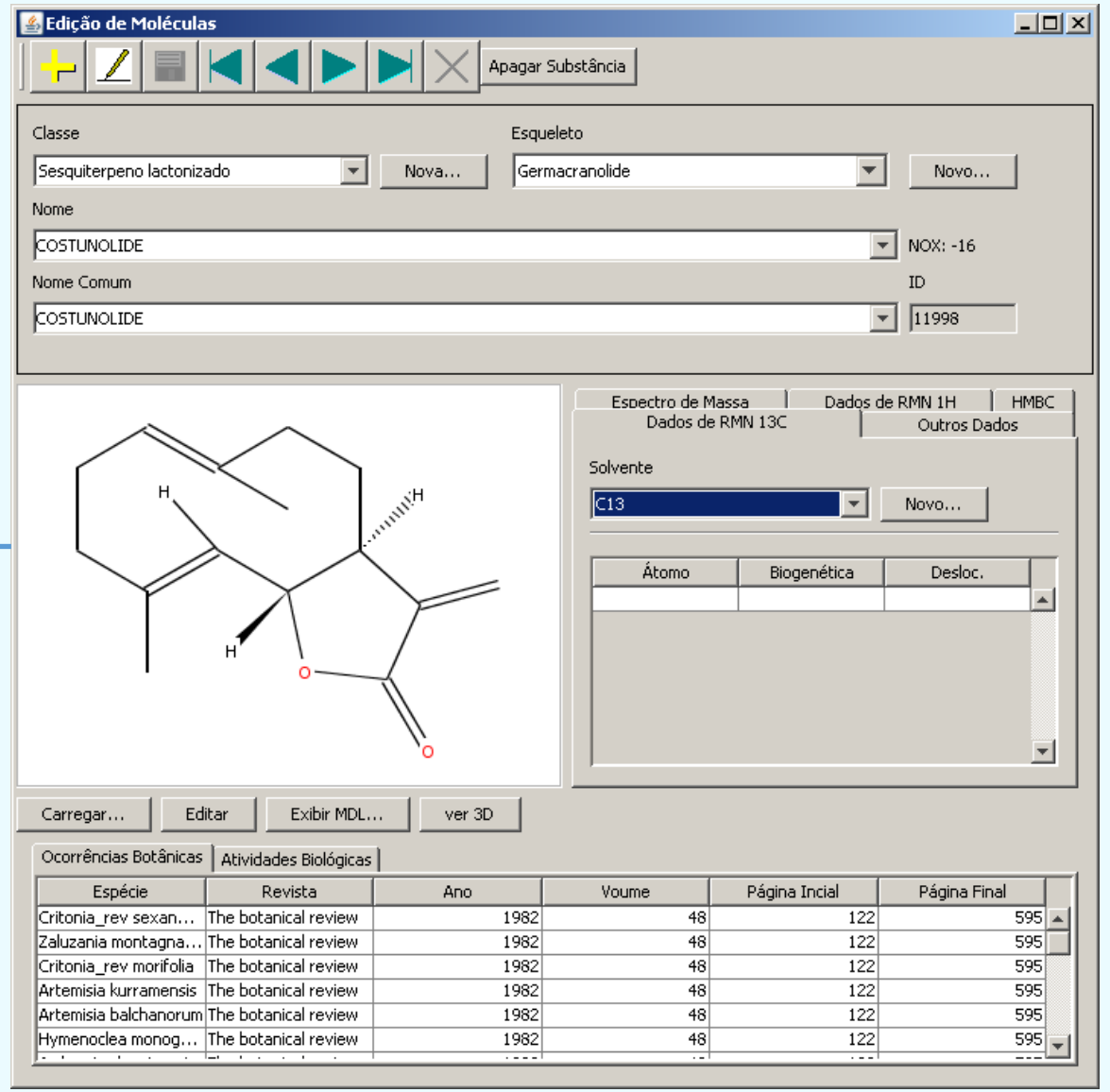
Sorokina and Steinbeck recently reviewed currently available NP databases, citing more than 120 examples, and noted that access to information was limited, and only a few of the databases were sustainably managed and continually developed.

Sorokina, M.; Steinbeck, C. Review on natural products databases: where to find data in 2020. *J. Cheminf.* 2020, 12, 20.

- **JAVA**
- **MySQL database**

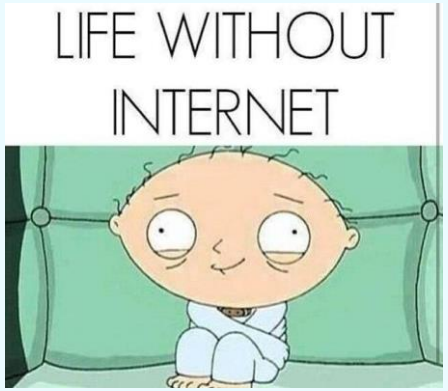
LAN

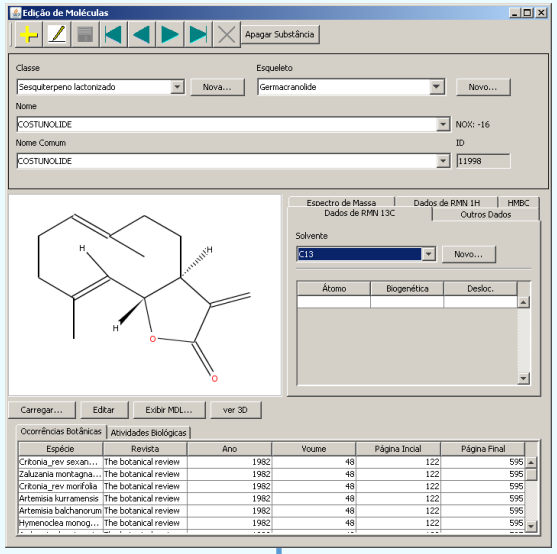




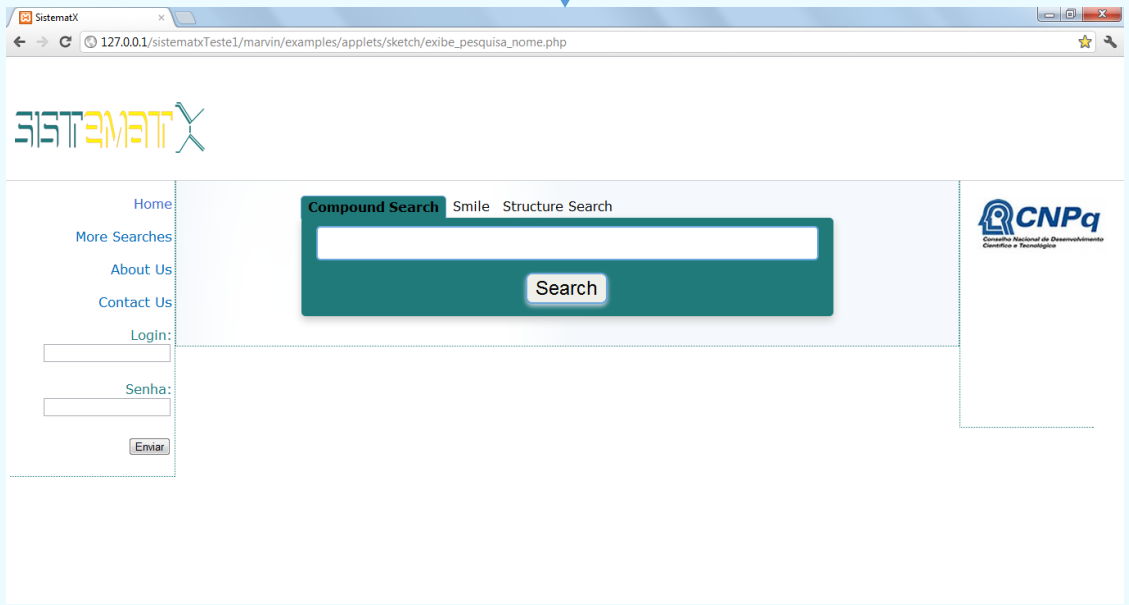
Web tools/applications

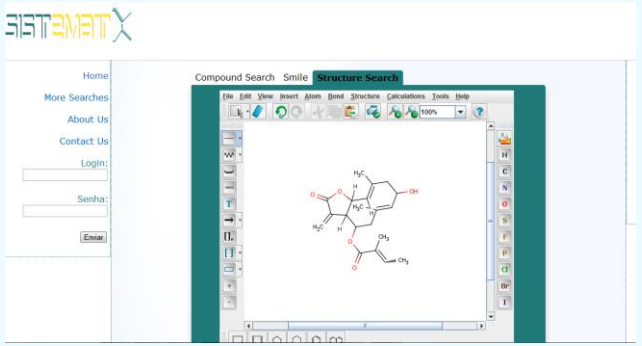
- Don’t need to install
- Don’t need a powerful computer (use a server)
- You can use in different devices
- Browser
- Internet (sometimes you don’t have it)





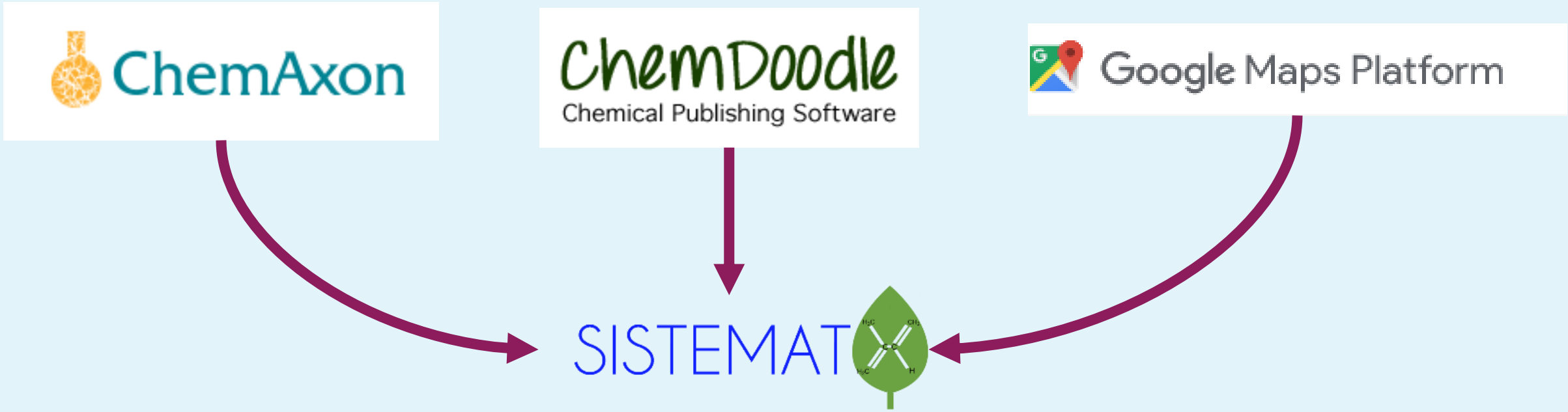
HTML
CSS
Java
JavaScript

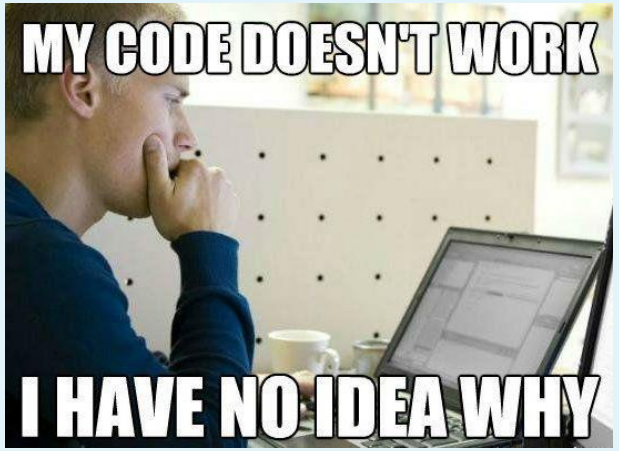


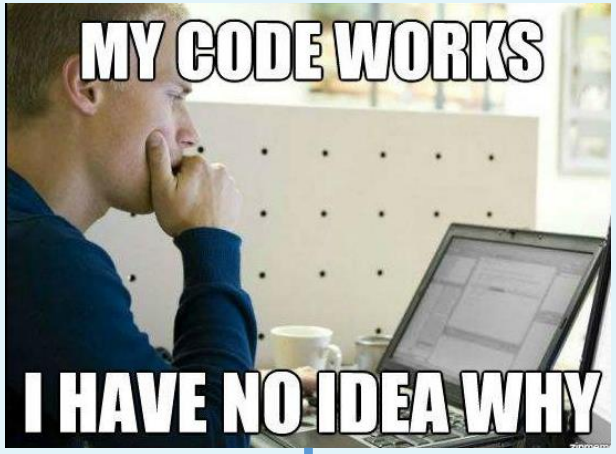


APIs

Several Application Programming Interface (APIs) are used in the SistematX implementation.
API is code that allows two software programs to communicate with each other.

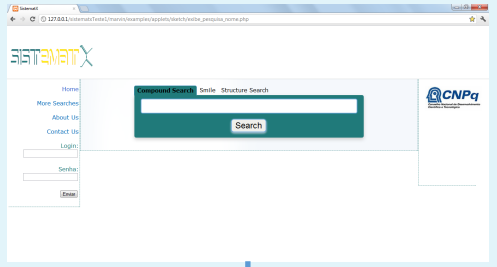


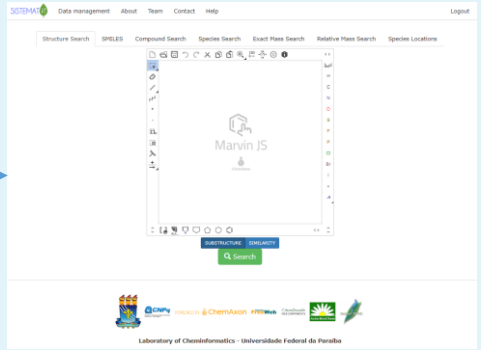

MY CODE DOESN'T WORK
I HAVE NO IDEA WHY

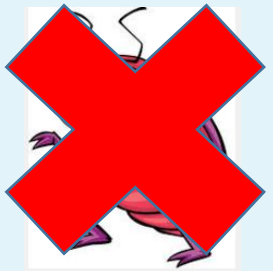

MY CODE WORKS
I HAVE NO IDEA WHY


Ferrari
Ferrari

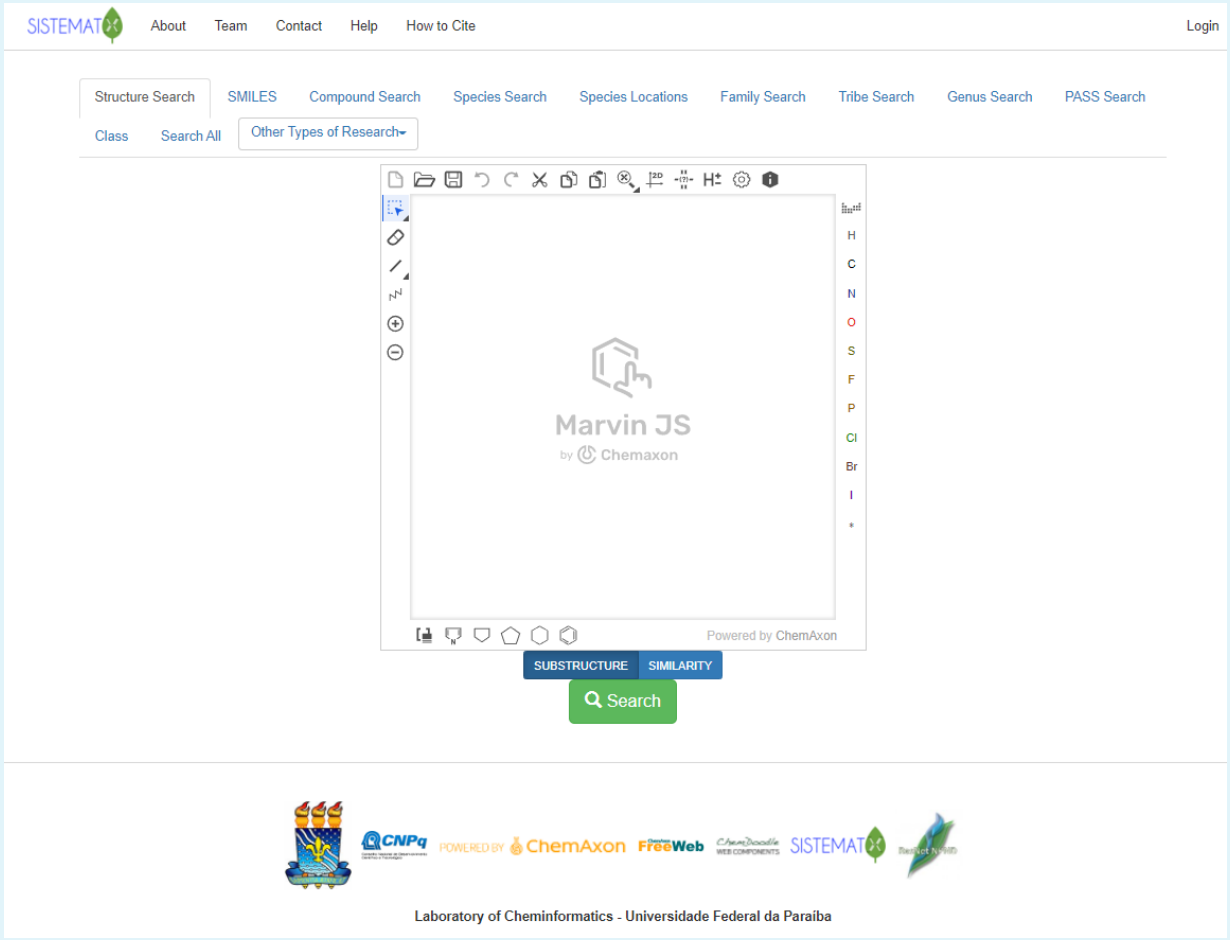
APIs


SISTEMATX
Compound Search
Smile
Structure Search
Search
CNPq


Marvin JS
Search
Laboratory of Cheminformatics - Universidade Federal da Paraíba



SistematX web



sistematx.ufpb.br

register software: Nº: BR 51 2015 000073 0 e BR51 2016 000371 5

INPI - Instituto Nacional da Propriedade Industrial. (National Institute of Industrial Property.)

Some Natural Products Databases

- TIPdb

Lin, Y. C.; Wang, C. C.; Chen, I. S.; Jheng, J. L.; Li, J. H.; Tung, C. W., TIPdb: a database of anticancer, antiplatelet, and antituberculosis phytochemicals from indigenous plants in Taiwan. ScientificWorldJournal 2013, 2013, 736386.
cwtung.kmu.edu.tw/**tipdb**/

- TCM database@Taiwan ,

Chen, C. Y., TCM Database@Taiwan: the world's largest traditional Chinese medicine database for drug screening in silico. PLoS One 2011, 6(1), e15939.
http://tcm.cmu.edu.tw/

- KNApSAcK-3D

Nakamura, K.; Shimura, N.; Otabe, Y.; Hirai-Morita, A.; Nakamura, Y.; Ono, N.; Ul-Amin, M. A.; Kanaya, S., KNApSAcK-3D: a three-dimensional structure database of plant metabolites. Plant Cell Physiol. 2013, 54(2), e4.
knapsack3d.sakura.ne.jp

- 3DMET

Maeda, M. H.; Kondo, K., Three-dimensional structure database of natural metabolites (3DMET): a novel database of curated 3Dstructures. J. Chem. Inf. Model 2013
www.**3dmet**.dna.affrc.go.jp/

- UNPD

Jiangyong Gu, Yuanshen Gui, Lirong Chen, Gu Yuan, Hui-Zhe Lu, Xiaojie Xu. Use of Natural Products as Chemical Library for Drug Discovery and Network Pharmacology.
PLoS ONE. 2013, 8(4): e62839. doi:10.1371/journal.pone.0062839.

- NuBBE database

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 from the biodiversity of Brazil. J. Nat. Prod. 2013, 76(3), 439-44.
nubbe.iq.unesp.br/portal/**nubbedb**.html

Comparison among the queries

2 years

	SistematX	3DMET	$NuBBE_{DB}$	TCM Database @Taiwan	TIPdb	UNPD
Query by structure	YES	YES*	YES	YES*	NO	NO
Name	YES	YES	YES	YES	YES	YES
SMILES	YES	YES	YES	YES	NO	YES
CASRN	YES	YES	NO	NO	NO	YES
InChI	YES	YES	NO	NO	NO	YES
InChIKey	YES	NO	NO	NO	NO	YES
Molecular Formule	YES	YES	YES	YES	NO	YES
Class	YES	NO	YES	NO	YES	NO
Chemical information	YES	YES	YES	YES	YES	YES
Biological Activity	YES	NO	YES	YES	YES	NO
Botanical occurrence	YES	NO	YES	YES	YES	YES
Part of plant	YES	NO	NO	NO	YES	NO
Citação bibliográfica	YES	NO	YES	NO	NO	NO

SistematX database

molecules

MDPI

Technical Note

SistematX, an Online Web-Based Cheminformatics Tool for Data Management of Secondary Metabolites

Marcus Tullius Scotti [1,*], Chonny Herrera-Acevedo [1], Tiago Branquinho Oliveira [2,3], Renan Paiva Oliveira Costa [1], Silas Yudi Konno de Oliveira Santos [1], Ricardo Pereira Rodrigues [1], Luciana Scotti [1] and Fernando Batista Da-Costa [3]

1 Postgraduate Program in Natural Products and Synthetic Bioactive, IPeFarM, Federal University of Paraíba, Campus I, Cidade Universitária, João Pessoa 58051-900, PB, Brazil; chonny622@gmail.com (C.H.-A.); renan0paiva@hotmail.com (R.P.O.C.); syudik12@gmail.com (S.Y.K.d.O.S.); ricardo.p.rodrigues@ufes.br (R.P.R.); luciana.scotti@gmail.com (L.S.)

2 Department of Pharmacy, Federal University of Sergipe (UFS-SE), Av. Marechal Rondon s/n, Jd. Rosa Elze, São Cristóvão 49100-000, SE, Brazil; tiago.branquinho@ufs.br

3 AsterBioChem Research Team, Laboratory of Pharmacognosy, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo (USP), Av. do Café s/n, Ribeirão Preto 14040-903, SP, Brazil; febcosta@fcfrp.usp.br

* Correspondence: mtscotti@gmail.com; Tel.: +55-83-99869-0415

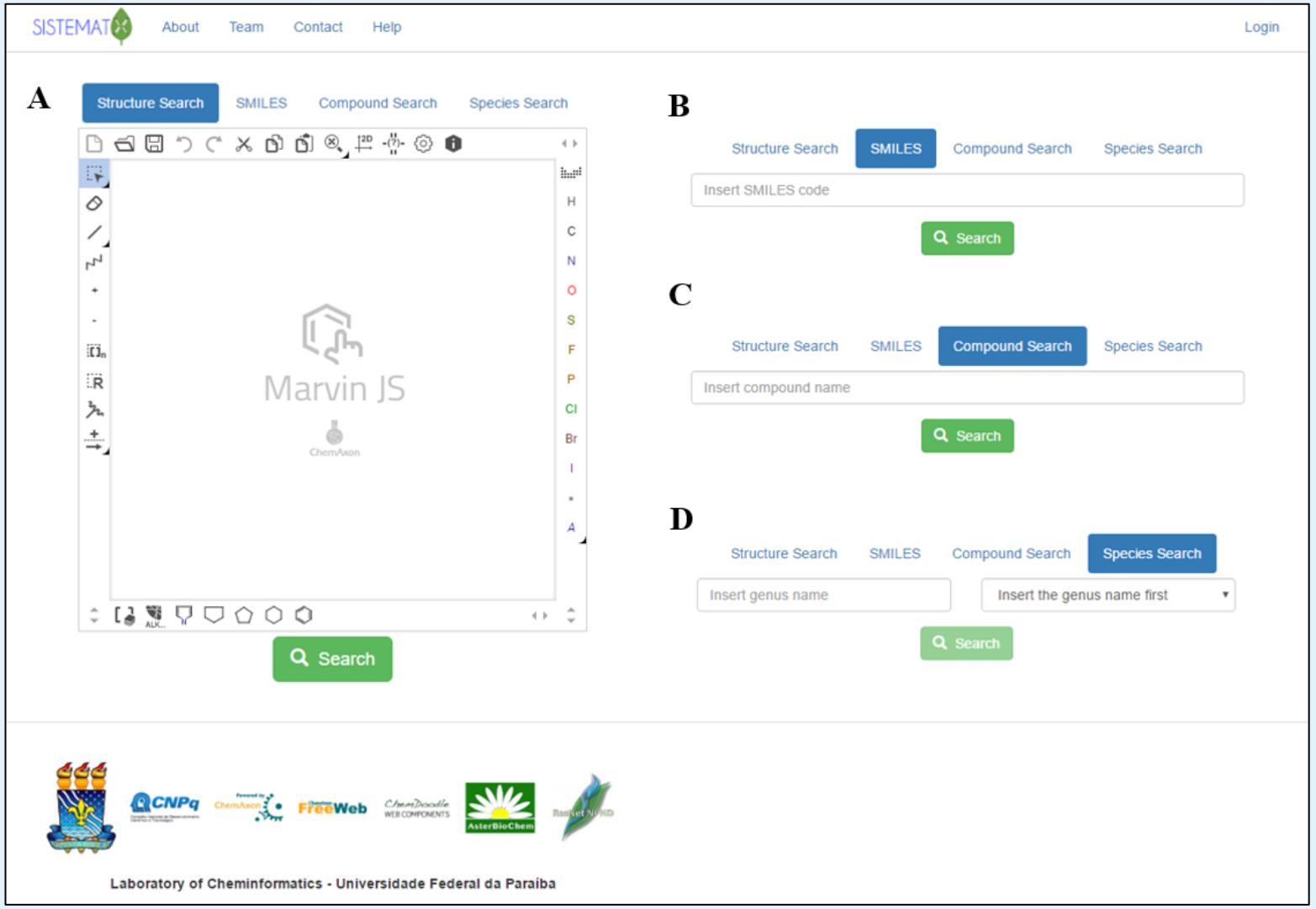
Received: 18 November 2017; Accepted: 28 December 2017; Published: 3 January 2018

SistematX interface

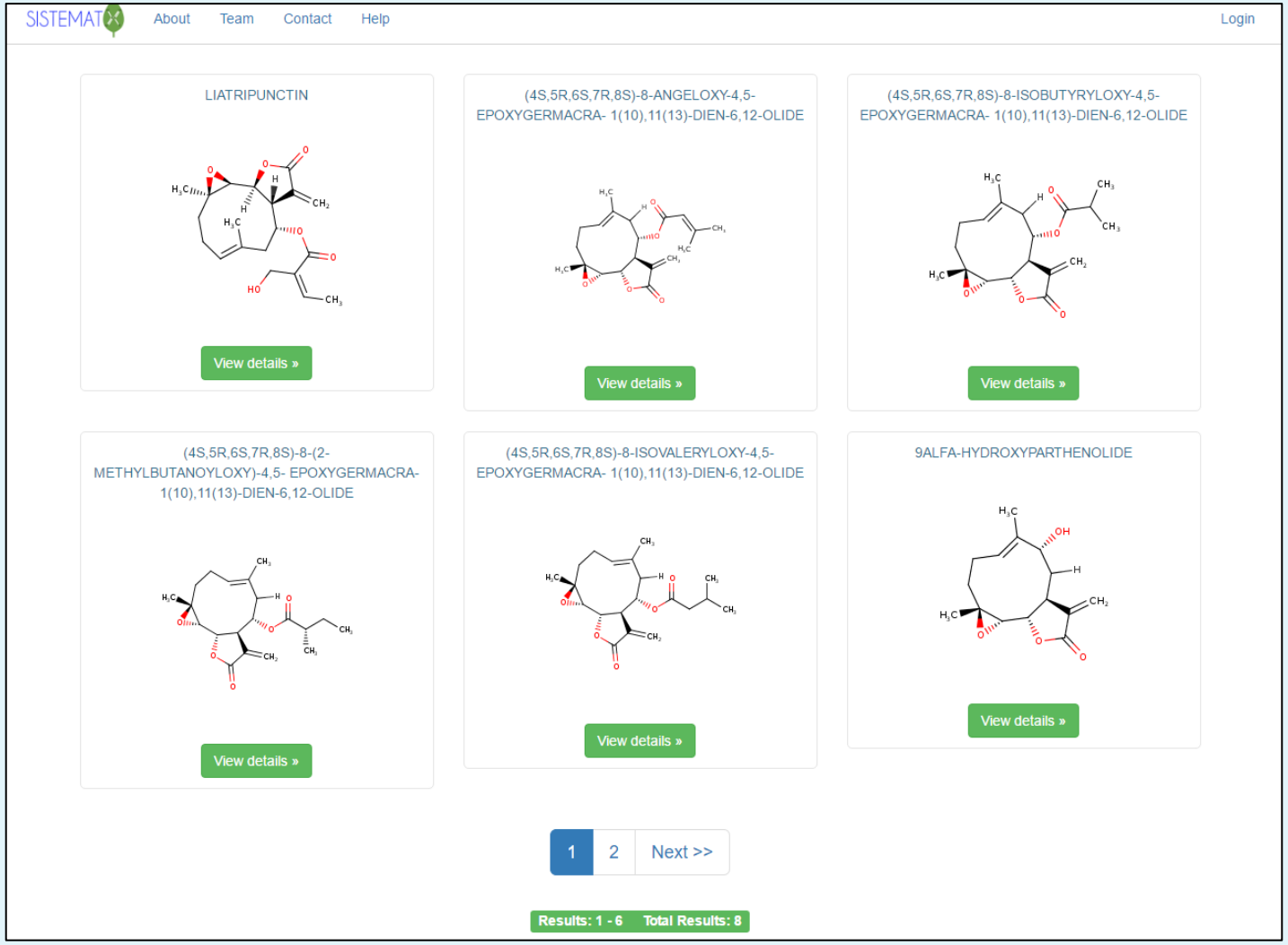
After the user enters the website, the "Structure search" option is seen with the MarvinJS API (Application Programming Interface) at the top of the screen.

Other search options can be exhibited in the interface.

The initial screen of the system also shows the SMILES (Simplified Molecular-Input Line-Entry System) code (B), compound name (C) and plant species search modes (D).



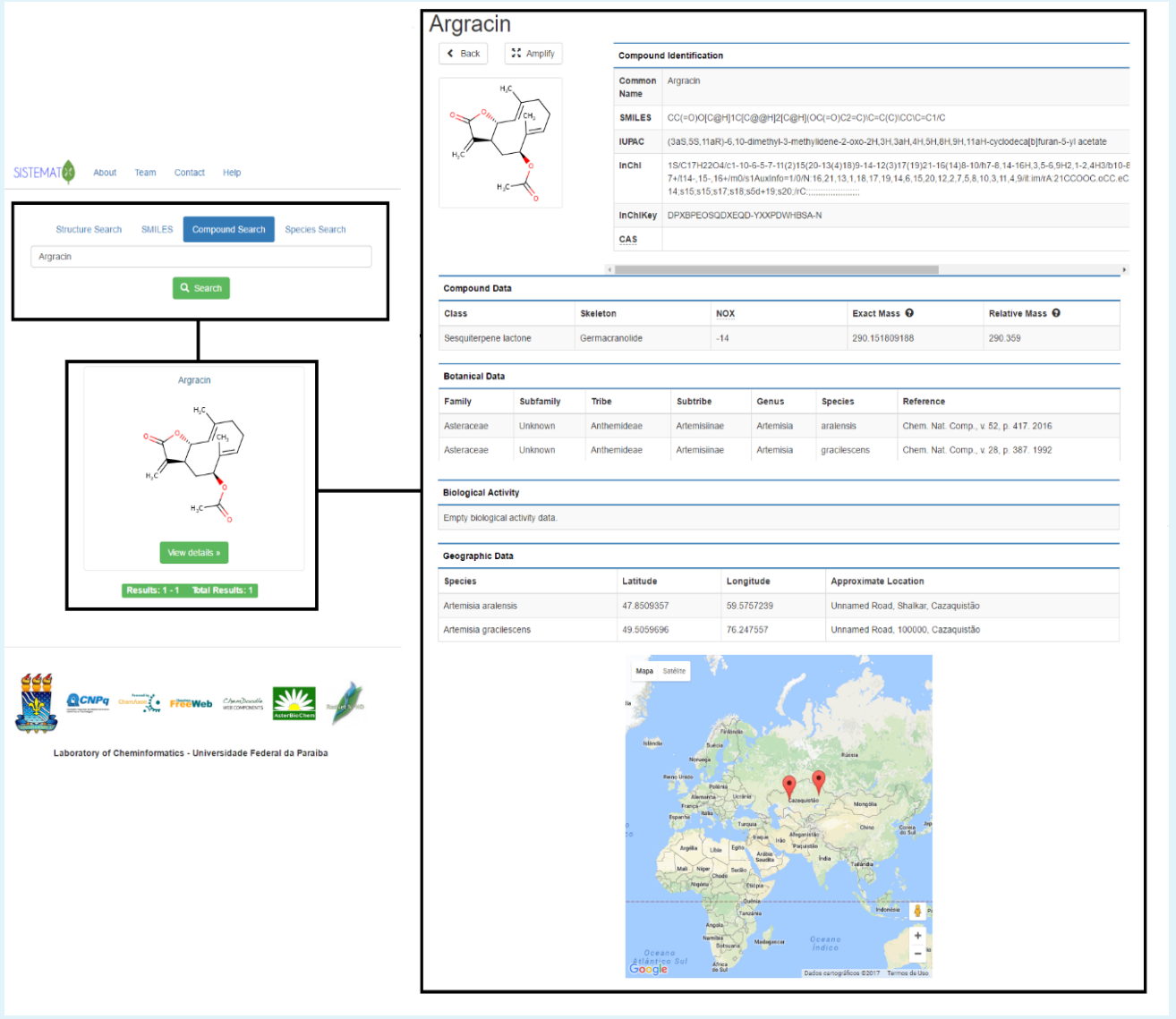
SistematX database



When performing a search, the mechanism generates a results page (six results) using common names; if the compound does not have one, it shows the IUPAC name.

The user can set the number of structure results per page. When a result is selected, the user has access to the data for that compound.

SistematX database

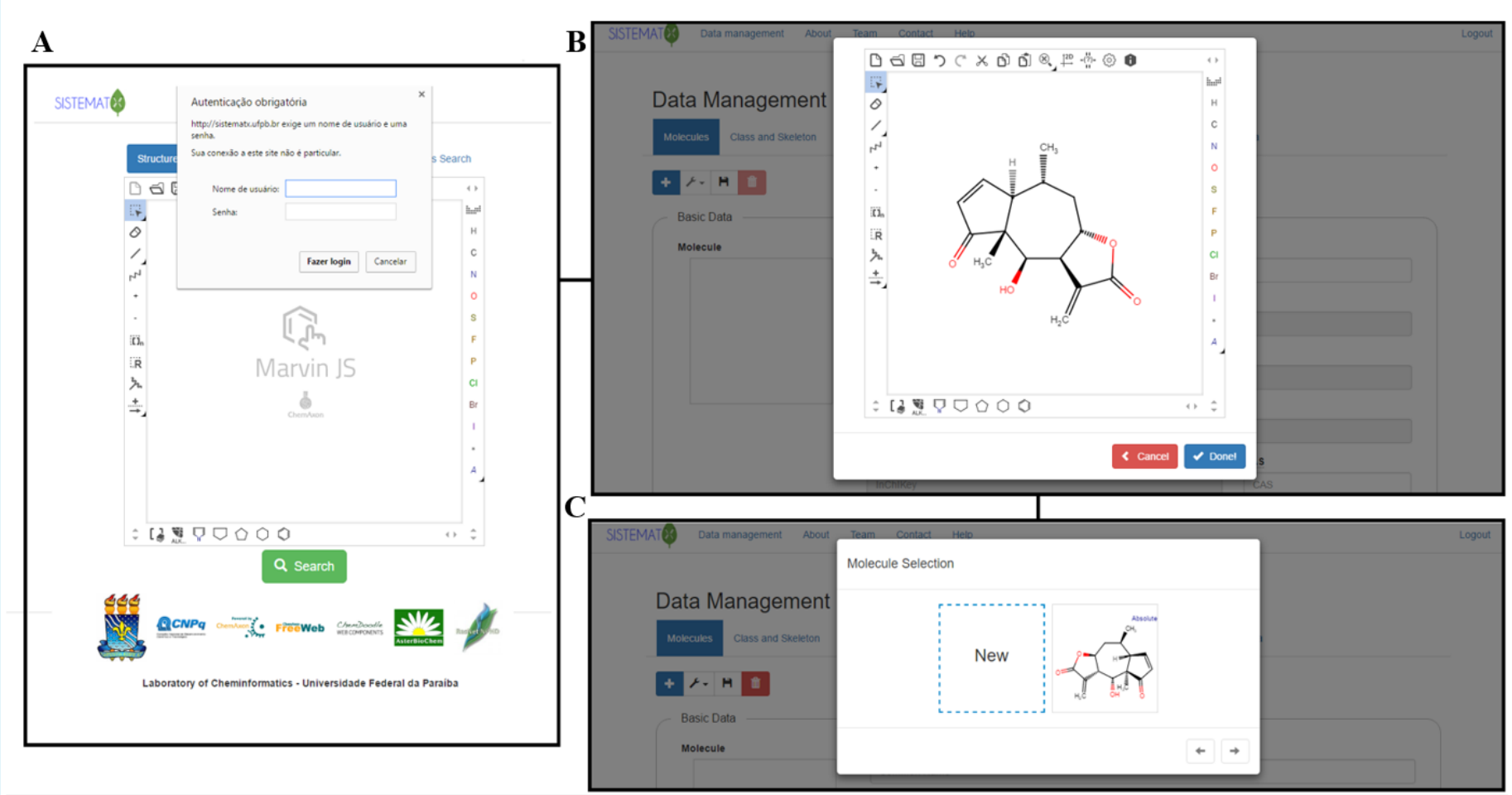


Integrated development environment (IDE)

API	Description	Engine
	1. Structure	
2D drawing	Allows drawing and visualization of chemical structures	ChemAxon
3D generator	Uses 2D drawing to generate a 3D representation of the molecule	ChemAxon
3D	Graphical visualization of 3D molecules with JavaScript	ChemDoodl
	2. Compound Identification	
SMILES	Simplified Molecular Input Line Entry System	ChemAxon
IUPAC	IUPAC Nomenclature	ChemAxon
InChI	IUPAC International Chemical Identifier	ChemAxon
InChIKey	InChIKey is a compact format of the InChI code	ChemAxon
CAS	Chemical Abstracts Service Registry Number	ChemAxon
	3. Compound Data	
NOX	Oxidation number (NOX) of an organic compound	ChemAxon
Exact Mass	Uses the mass of the most abundant isotope of each element	ChemAxon
Relative Mass	Uses the average atomic mass of each element	ChemAxon
	4. Geographic data	
Latitude	Can be inserted by the administrator or appears by clicking in the world map	Google Inc.
Longitude	Can be inserted by the administrator or appears by clicking in the world map	Google Inc.
Approximate	Using the latitude and longitude, appears an an approximate location of the specie	Google Inc.
Visualization	Uses the world map to possible to visualize the localization of the species	Google Inc.

SistematX database

On the SistematX homepage, the user can also log into the data management area using login name and password and from there access the administration pages to edit or register new molecules.
Once the corresponding information has been accepted, the data management interface appears.



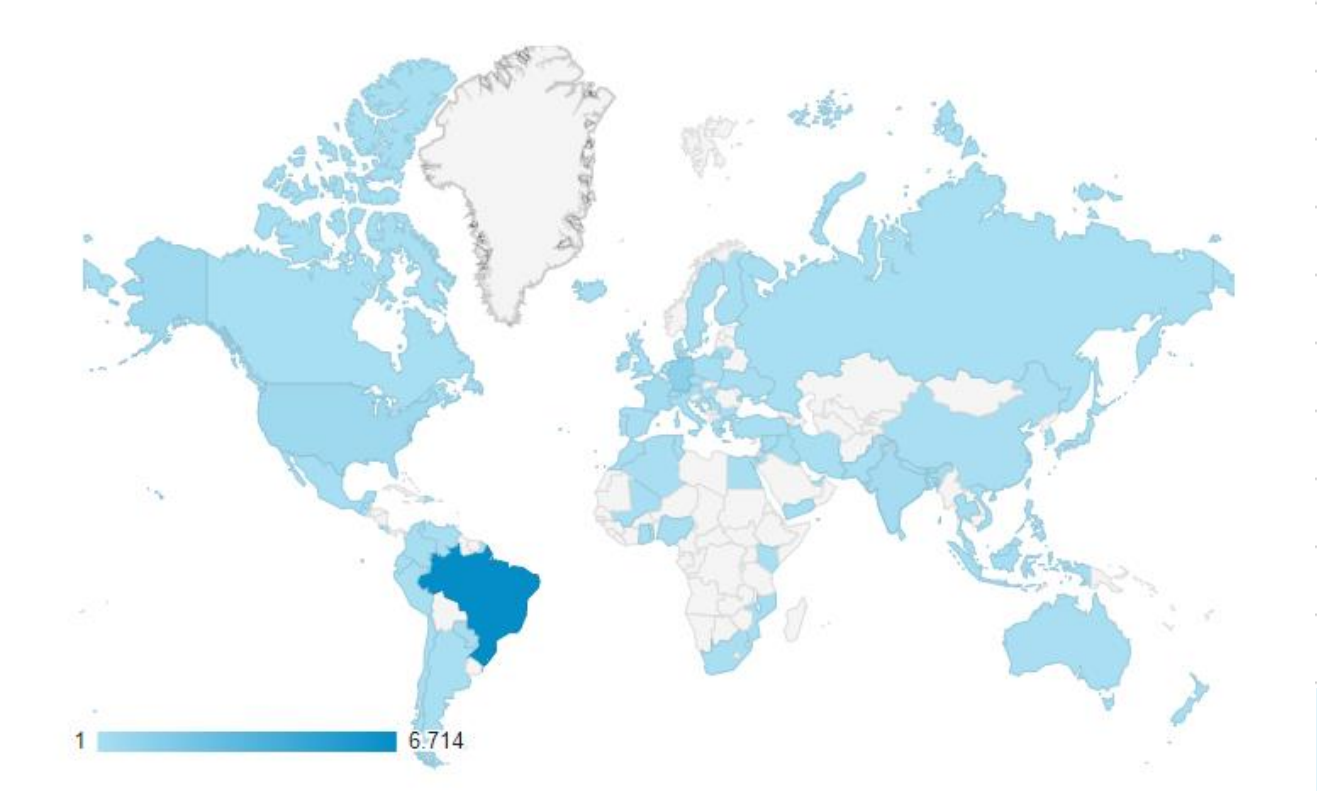
SistematX database

SistematX currently has 9,514 unique secondary metabolites arising from 20,934 botanical occurrences across 5 families:

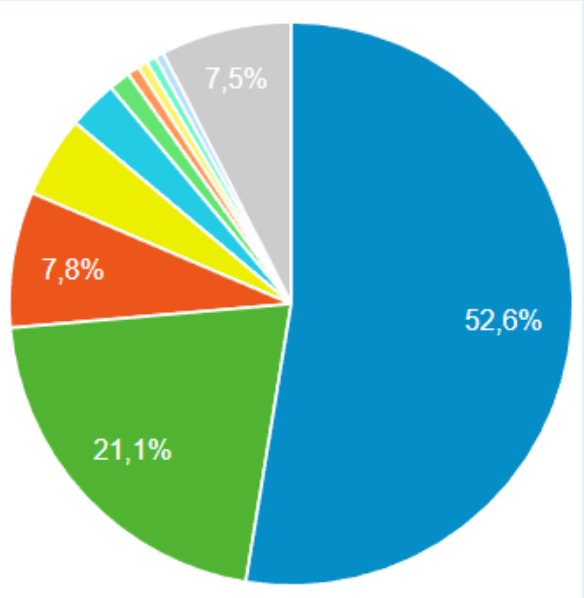
Botanical family	Secondary metabolites	Ocurrences
Asteraceae	2,574	7,879
Apocynaceae	372	620
Annonaceae	1,898	5,335
Lamiaceae	4,097	6,357
Solanaceae	573	743

SistematX database

Since 2018, SistematX has reported 5251 users and more than 9200 sessions (47.4% located outside Brazil)



1.	Brazil
2.	Germany
3.	United States
4.	France
5.	India
6.	Colombia
7.	United Kingdom
8.	Russia
9.	Italy
10.	Mexico



SISTEMAT

Published articles

XXVIII Symposium on Bioinformatics and Computer-Aided Drug Discovery

Molecular Diversity
https://doi.org/10.1007/s11030-021-10245-z

ORIGINAL ARTICLE

Check for updates

Machine learning models to select potential inhibitors of acetylcholinesterase activity from SistematX: a natural products database

Chonny Herrera-Acevedo[1,4] · Camilo Perdomo-Madrigal[2] · Kenyi Herrera-Acevedo[3] · Ericsson Coy-Barrera[4] · Luciana Scotti[1] · Marcus Tullius Scotti[1]

Molecular Diversity
https://doi.org/10.1007/s11030-020-10139-6

ORIGINAL ARTICLE

Check for updates

Selection of antileishmanial sesquiterpene lactones from SistematX database using a combined ligand-/structure-based virtual screening approach

Chonny Herrera-Acevedo[1,2] · Mayara Dos Santos Maia[1] · Élida Batista Vieira Sousa Cavalcanti[1] · Ericsson Coy-Barrera[2] · Luciana Scotti[1] · Marcus Tullius Scotti[1]

ChemPubSoc Europe
DOI: 10.1002/cmdc.201700743
CHEMMEDCHEM Full Papers

SPECIAL ISSUE

In Silico Studies Designed to Select Sesquiterpene Lactones with Potential Antichagasic Activity from an In-House Asteraceae Database

Chonny Herrera Acevedo, Luciana Scotti, and Marcus Tullius Scotti*[a]

Current Topics in Medicinal Chemistry, 2020, *20*, 2126-2145

RESEARCH ARTICLE

BENTHAM SCIENCE

Ligand and Structure-based Virtual Screening of Lamiaceae Diterpenes with Potential Activity against a Novel Coronavirus (2019-nCoV)

Gabriela Cristina Soares Rodrigues[1], Mayara dos Santos Maia[1], Renata Priscila Barros de Menezes[1], Andreza Barbosa Silva Cavalcanti[1], Natália Ferreira de Sousa[1], Érika Paiva de Moura[1], Alex France Messias Monteiro[1], Luciana Scotti[1] and Marcus Tullius Scotti[1,*]

Chagas Diseases, Leishmaniasis, COVID-19, Alzheimer

SistematX

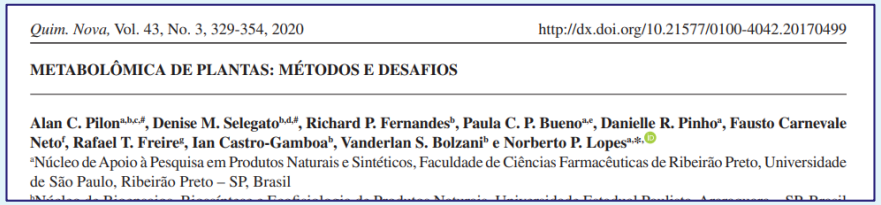
Metabolomics (2019) 15:59
https://doi.org/10.1007/s11306-019-1520-7

ORIGINAL ARTICLE

Untargeted LC–MS metabolomic studies of Asteraceae species to discover inhibitors of *Leishmania major* dihydroorotate dehydrogenase

Lucas A. Chibli[1] · Annylory L. Rosa[1] · Maria Cristina Nonato[2] · Fernando B. Da Costa[1]

Chibli et al. profiled over 2000 metabolites from the Asteraceae family while screening for inhibitors of *Leishmania major* dihydroorotate dehydrogenase



Quim. Nova, Vol. 43, No. 3, 329-354, 2020 http://dx.doi.org/10.21577/0100-4042.20170499

METABOLÔMICA DE PLANTAS: MÉTODOS E DESAFIOS

Alan C. Pilon[a,b,c,#], Denise M. Selegato[b,d,#], Richard P. Fernandes[b], Paula C. P. Bueno[a,e], Danielle R. Pinho[a], Fausto Carnevale Neto[f], Rafael T. Freire[g], Ian Castro-Gamboa[b], Vanderlan S. Bolzani[b] e Norberto P. Lopes[a,*]

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Described the challenges of metabolomics methods in a summary of more than 95 metabolomics tools, software programs, and databases, highlighting SistematX for its use of the Google Maps application program interface (API) as a locational system.

Electrophoresis 2019, *40*, 227–246 227

Review

Tools and resources for metabolomics research community: A 2017–2018 update

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The scale at which MS- and NMR-based platforms generate metabolomics datasets for both research, core, and clinical facilities to address challenges in the various sciences—ranging from biomedical to agricultural—is underappreciated. Thus, metabolomics efforts

Mishra and Mohapatra noted that SistematX was an easy tool for metabolomic studies.

JBC ARTICLE

Author's Choice

A database-driven approach identifies additional diterpene synthase activities in the mint family (Lamiaceae)

Received for publication, September 27, 2018, and in revised form, November 12, 2018 Published, Papers in Press, November 29, 2018, DOI 10.1074/jbc.RA118.006025

Sean R. Johnson[‡1], Wajid Waheed Bhat[§¶1,2], Jacob Bibik[‡], Aiko Turmo[‡], Britta Hamberger[‡], Evolutionary Mint Genomics Consortium[¶], and Björn Hamberger[‡§3]

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Edited by John M. Denu

The authors criticized the inability to perform bulk downloads in the SistematX environment, which limited their ability to assess its completeness and cross-reference it with other data.
They suggested that the development of a tool to download publicly available digital data would be beneficial to the field.

2021: an update

JCIM JOURNAL OF CHEMICAL INFORMATION AND MODELING

pubs.acs.org/jcim Application Note

The SistematX Web Portal of Natural Products: An Update

Renan P. O. Costa, Lucas F. Lucena, Lorena Mara A. Silva, Guilherme Julião Zocolo, Chonny Herrera-Acevedo, Luciana Scotti, Fernando Batista Da-Costa, Nikita Ionov, Vladimir Poroikov, Eugene N. Muratov, and Marcus T. Scotti*

Cite This: https://doi.org/10.1021/acs.jcim.1c00083 Read Online

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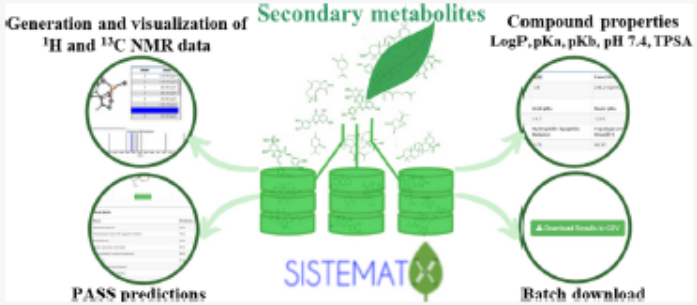
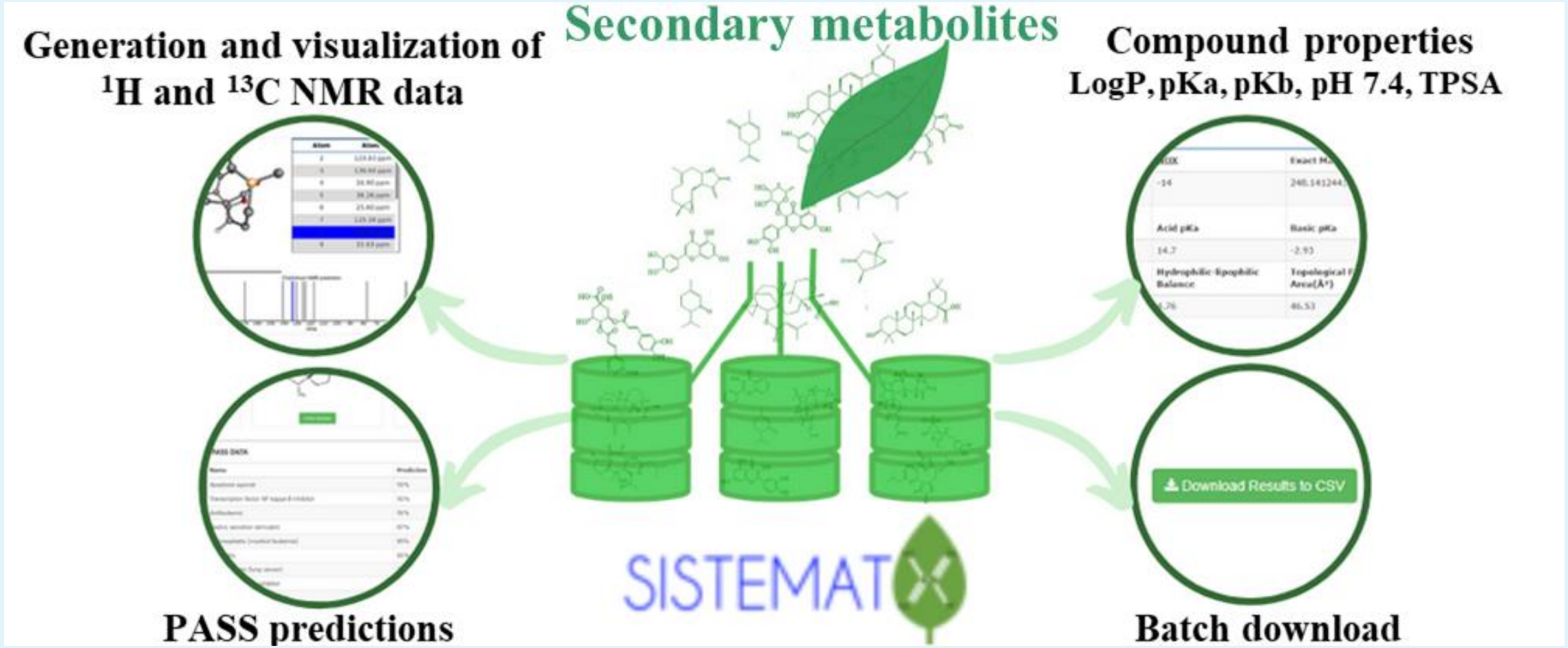
ABSTRACT: Natural products and their secondary metabolites are promising starting points for the development of drug prototypes and new drugs, as many current treatments for numerous diseases are directly or indirectly related to such compounds. State-of-the-art, curated, integrated, and frequently updated databases of secondary metabolites are thus highly relevant to drug discovery. The SistematX Web Portal, introduced in 2018, is undergoing development to address this need and documents crucial information about plant secondary metabolites, including the exact location of the species from which the compounds were isolated. SistematX also allows registered users to log in to the data management area and gain access to administrative pages. This study reports recent updates and modifications to the SistematX Web Portal, including a batch download option, the generation and visualization of ^{1}H and ^{13}C nuclear magnetic resonance spectra, and the calculation of physicochemical (drug-like and lead-like) properties and biological activity profiles. The SistematX Web Portal is freely available at http://sistematx.ufpb.br.



What's the new?



Compound properties

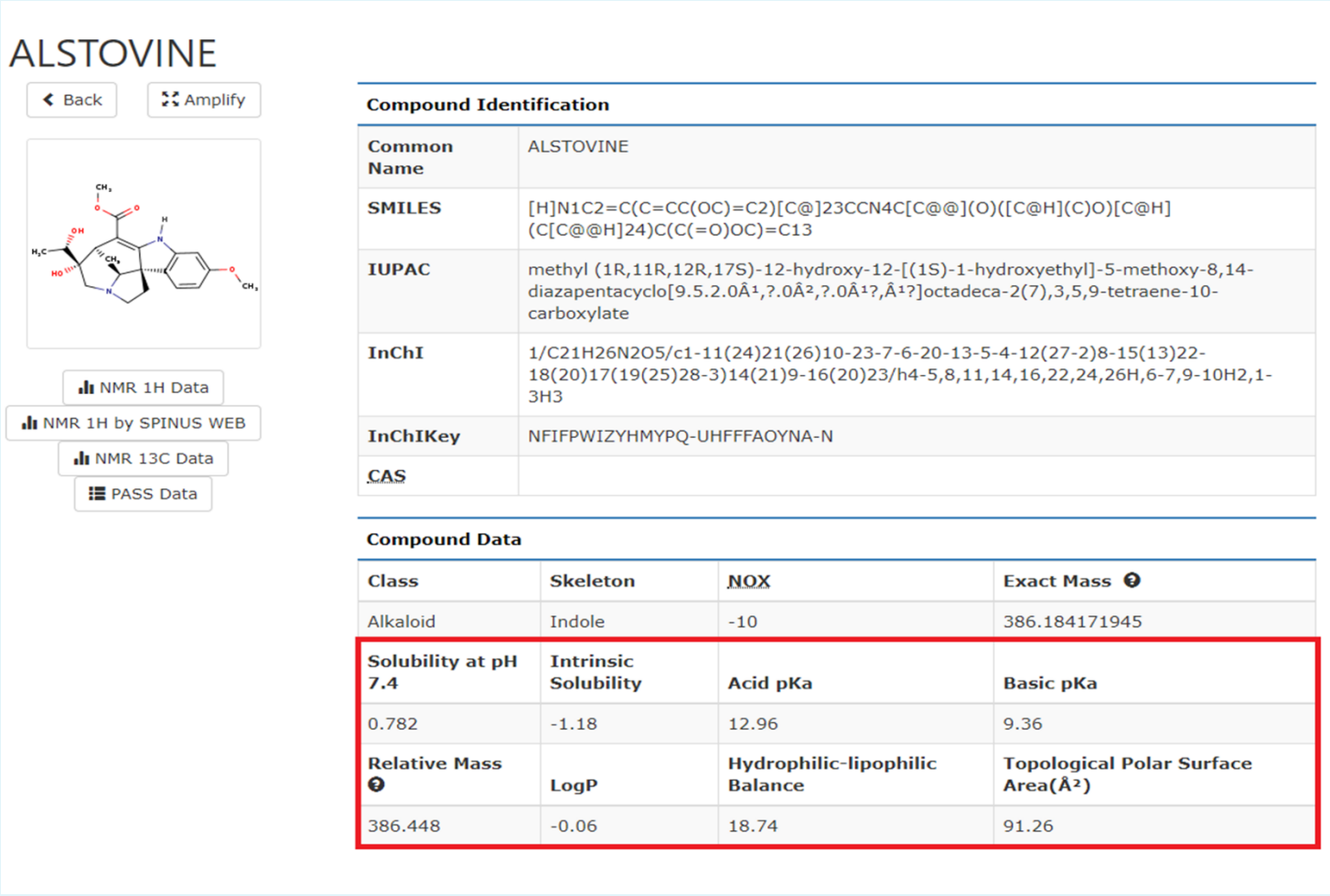
Summary of Application Programming Interface Calculated Physicochemical (Drug-Like and Lead-Like) Properties Recently Implemented in SistematX

API	description
log P	octanol–water partition coefficient
pK_a	decimal cologarithm of the acid dissociation constant
pK_b	decimal cologarithm of the base dissociation constant
solubility (pH 7.4)	maximum quantity of a solute that can be dissolved in a pH 7.4 solution
intrinsic solubility	solubility of a compound in its free acid or free base form
TPSA	sum of the surfaces of polar atoms in a molecule
hydrophilic–lipophilic Balance	measurement determining a compound's hydrophilicity or lipophilicity

Compound properties

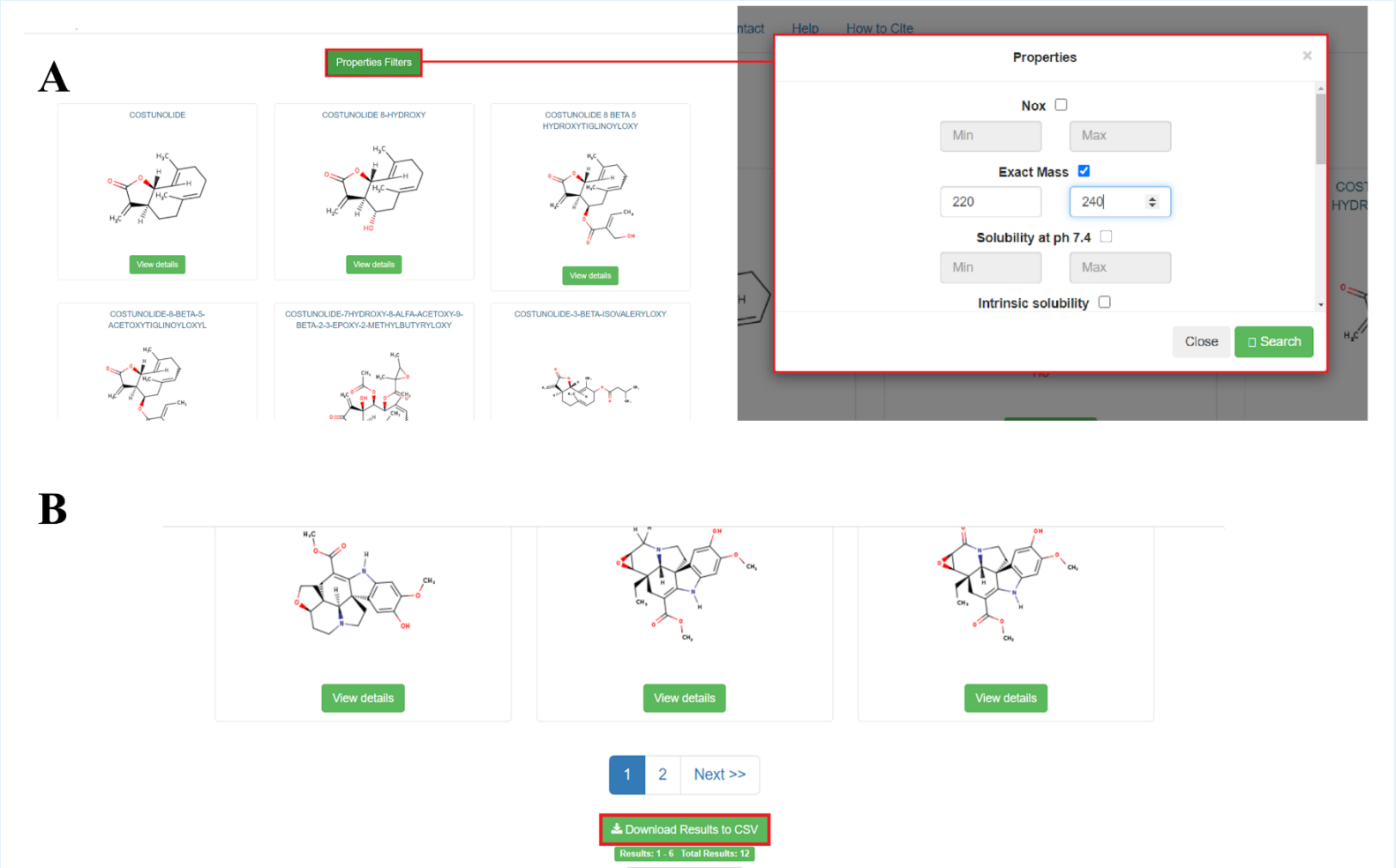
SistematX implemented new features to meet the demands of the scientific community, users, and our partners.

Physicochemical (druglike and lead-like) properties, specifically logP, pKa, pKb, pH 7.4 solubility, intrinsic solubility, TPSA, and hydrophilic– lipophilic balance, are now calculated for compounds in the database



Properties filters

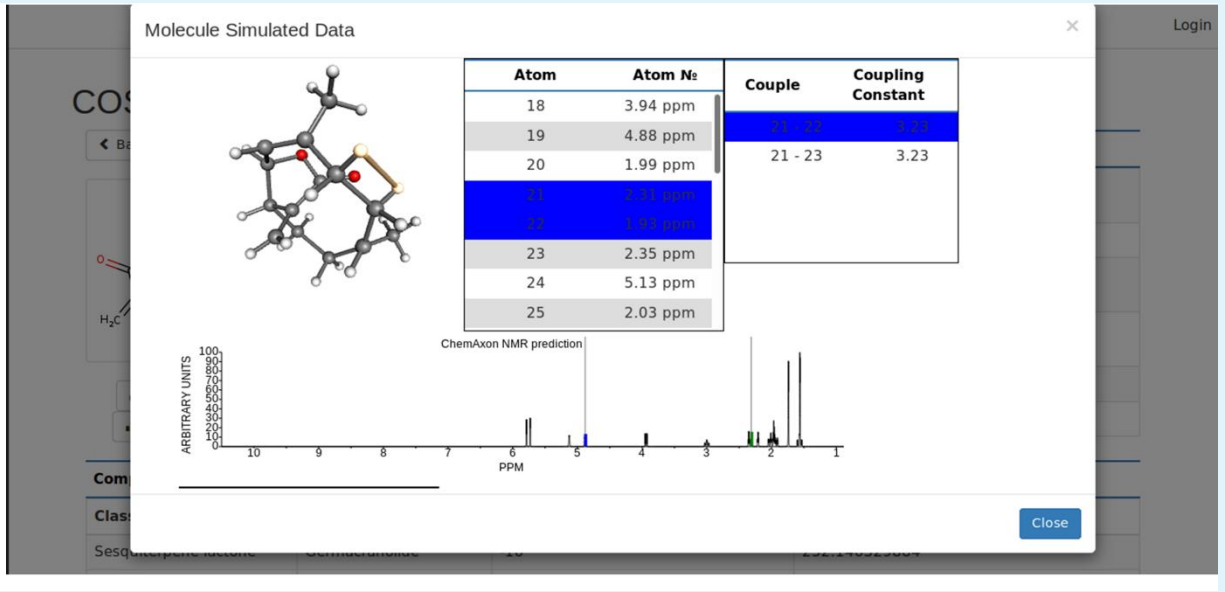
The results page for the molecules of interest now contains new search filters, which are accessible through a new user-responsive button that displays a modal pop-up window

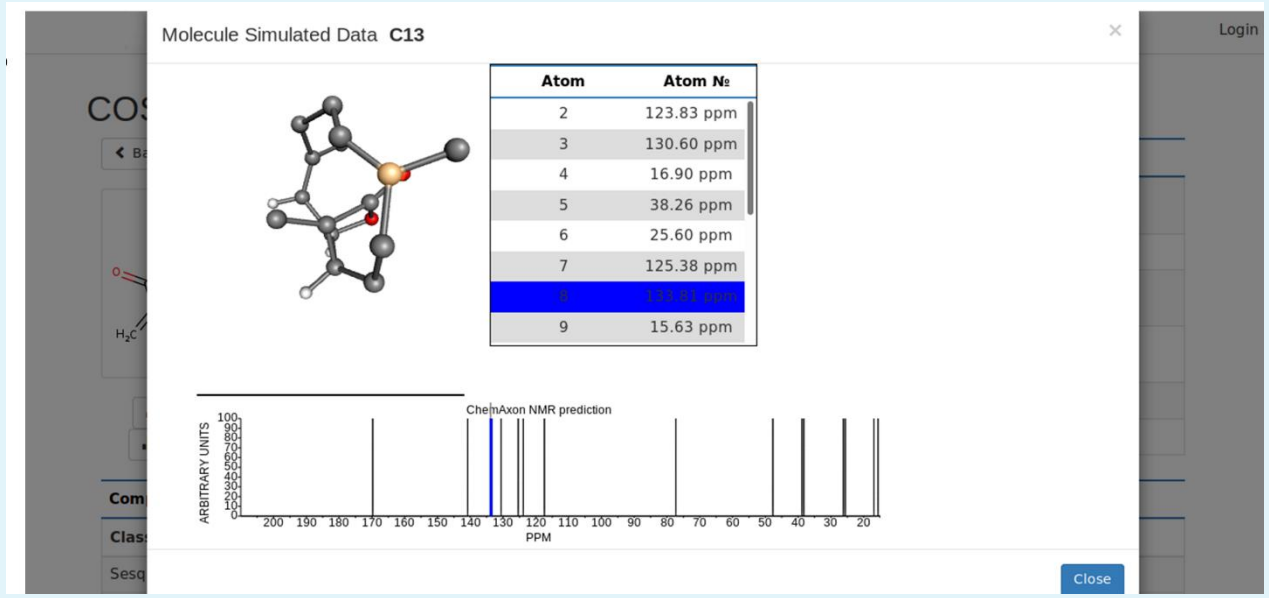


Generation and visualization of ^{1}H and ^{13}C NMR data

SistematX now includes NMR spectra, coupling constants, and chemical shifts, which are relevant to phytochemical studies.

Utilizing the ChemAxon API, predictions are calculated when a new compound is registered in the system.

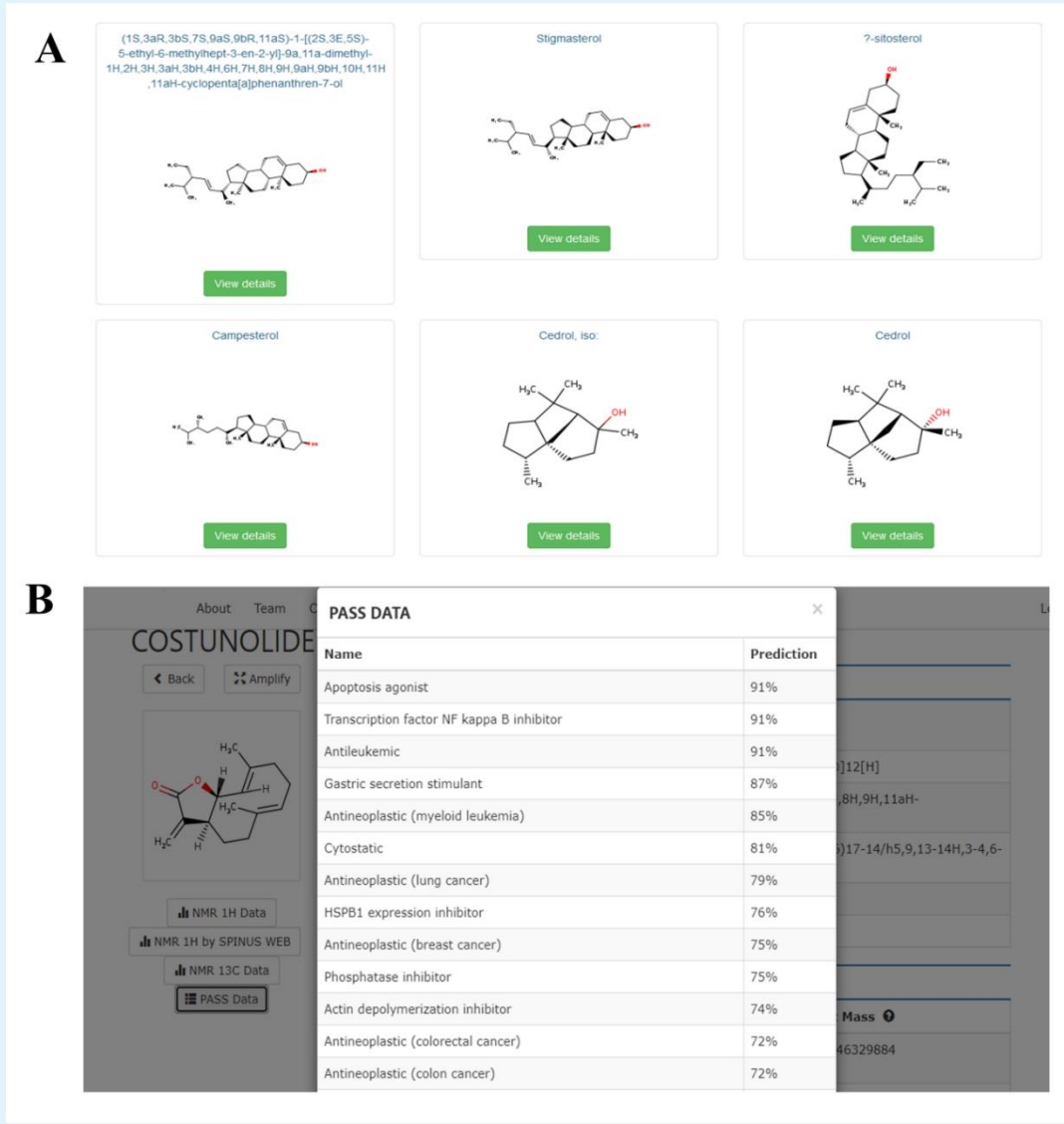




PASS filter

Biological activity profiles of registered structures are estimated using PASS software, which uses NP structural formulas to predict 4686 pharmacological effects and mechanisms of action.

SistematX reports prediction results with a probability of activity cutoff >0.5, resulting in a total of 1571 predicted pharmacological effects and mechanisms of action.



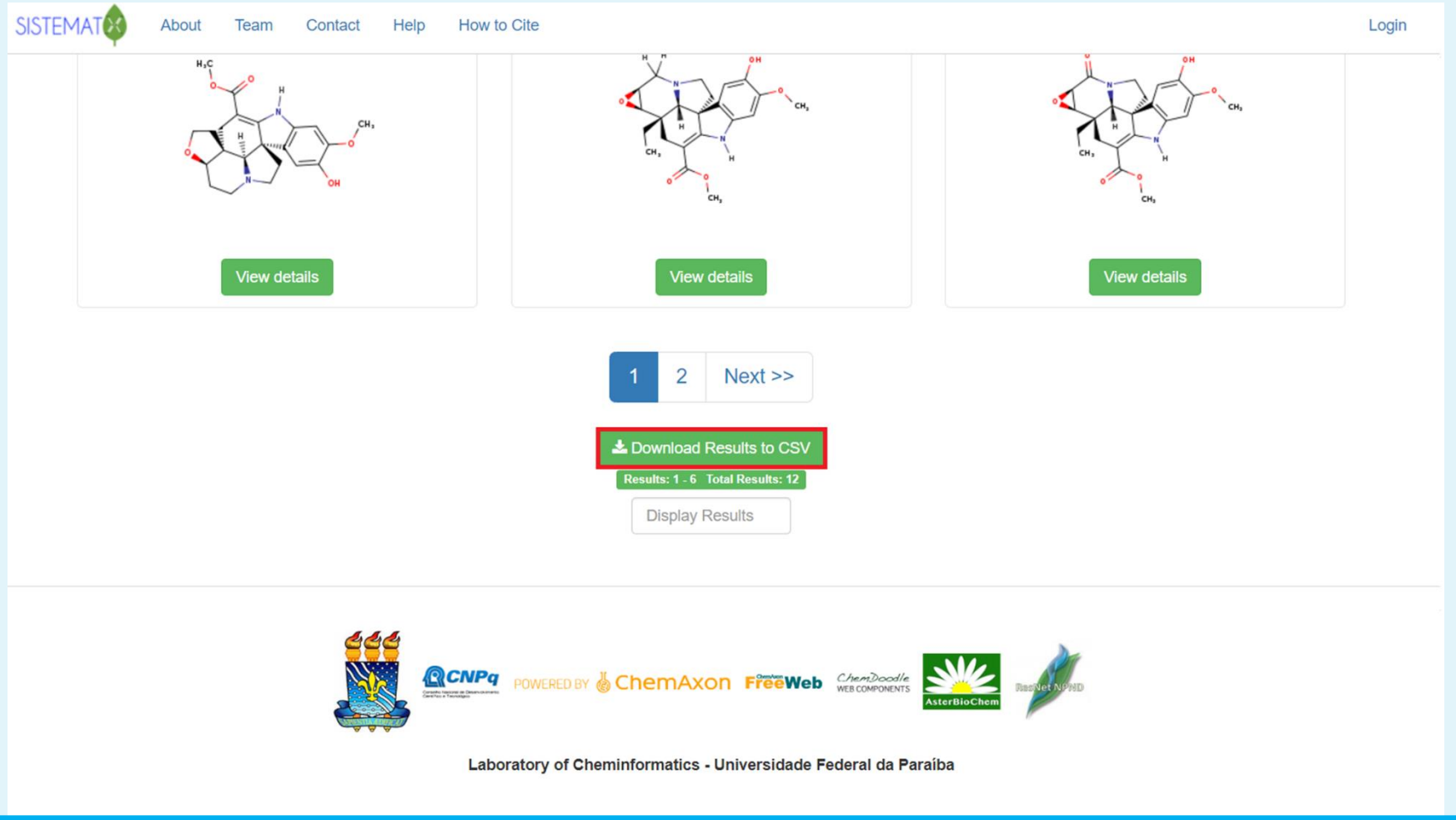
Saldívar-González, F. I.; Aldas-Bulos, V. D.; Medina-Franco, J. L.; Plisson, F., Natural product drug discovery in the artificial intelligence era. *Chemical Science* 2022, 13 (6), 1526-1546.

Lagunin A, Stepanchikova A, Filimonov D, Poroikov V. PASS: prediction of activity spectra for biologically active substances. Bioinformatics. 2000 Aug;16(8):747-8. doi: 10.1093/bioinformatics/16.8.747. PMID: 11099264.

Filimonov D.A., Lagunin A.A., Gloriozova T.A., Rudik A.V., Druzhilovskii D.S., Pogodin P.V., Poroikov V.V. (2014). Prediction of the biological activity spectra of organic compounds using the PASS online web resource. Chemistry of Heterocyclic Compounds, 50 (3), 444-457.

Batch download

The new batch download feature was developed using Java programming language. Downloading the search results creates a *.CSV file containing all botanical occurrences.



New partnership

[Guilherme Juliao Zocolo]

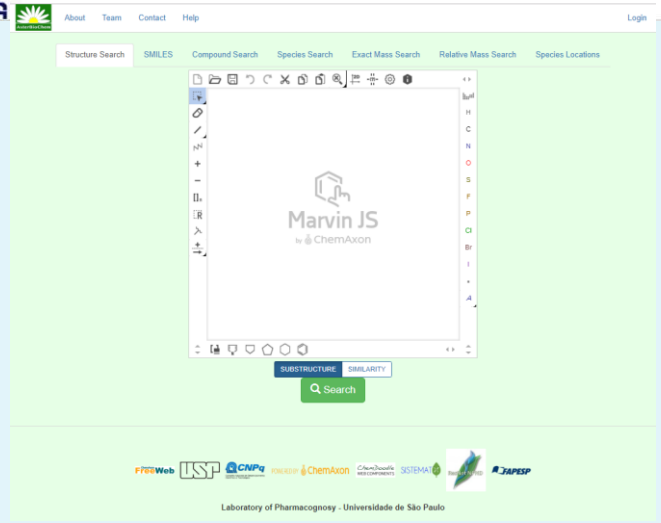
[Lorena Mara Alexandre e Silva]

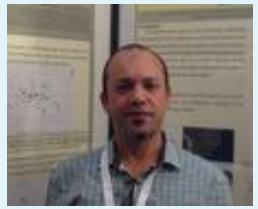
AsterBioChem

2011

Asteraceae database

http://www.asterbiochem.org/asterdb





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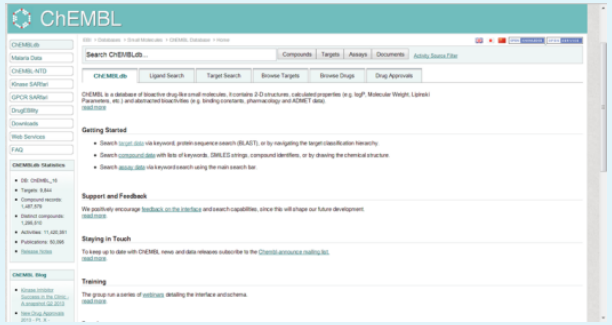
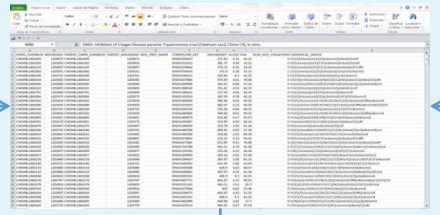
SistematX web

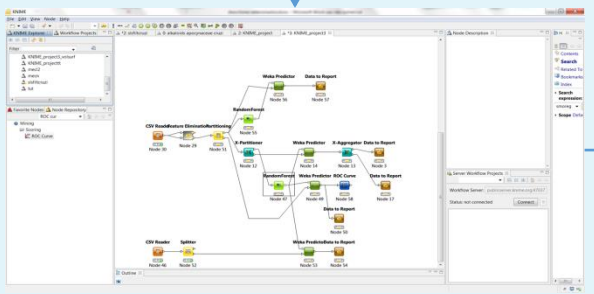


Biological activities
Structures

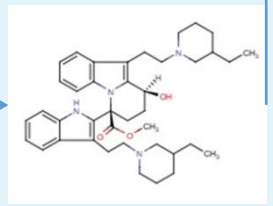
Combine data

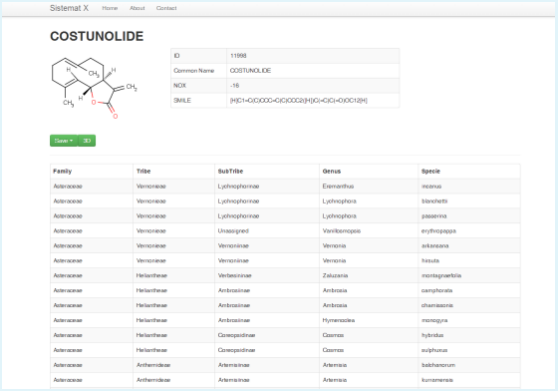


Virtual Screening



Machine Learning





Structures
Biological activities
NMR data
Geographic location
Botanical data

molecules

MDPI

Article

Identification of Kaurane-Type Diterpenes as Inhibitors of Leishmania Pteridine Reductase I

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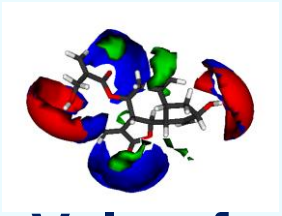
ChEMBL

Structures with IC_{50} values against *L.major*

ChemAxon

JChem
3D structures



Volsurf+
Molecular descriptors

Open for Innovation KNIME

RF classification model

[LB] **Ligand-based VS**

SISTEMAT

360 Kauranes

Combined-approach ***[CA]***

***In vitro* enzymatic activity inhibition against *Lm*PTR1 Leishmania major pteridine reductase I**

RCSB PDB PROTEIN DATA BANK

***L. major* PTR1**

molegro VIRTUAL DOCKER 6.0

Molecular docking

[SB]

Structure-based VS

ChEMBL

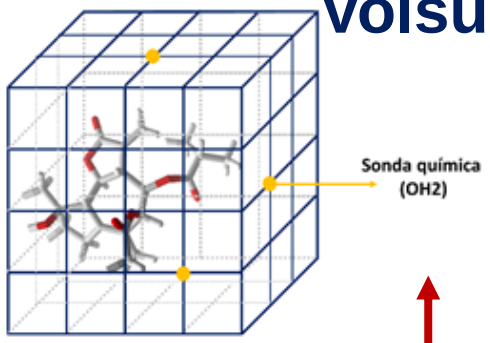
657 Structures with IC_{50} values against *L.major*

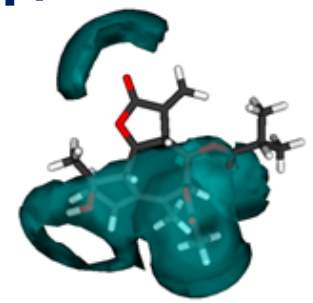
338 structures
Actives (53.1%)

Cutoff value
*$pIC_{50} \geq 5.0$**

298 structures
Inactives (46.9%)

128 Molecular descriptors
Volsurf+

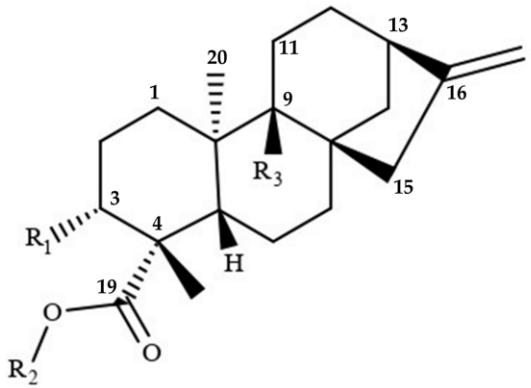


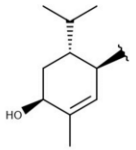
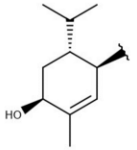
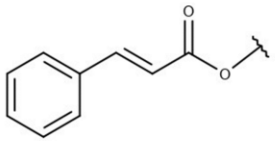
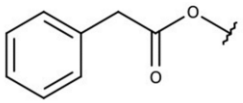


***4.9 < pIC_{50} < 5.0 (21 structures were removed)**

Ligand-based virtual screening

Only 7 of the 360 structures were classified as active (ligand-based probability value [LB] ≥ 0.5)



ID	R_1	R_2	R_3	*LB*
135	H		H	*0.57*
134	H		$\Delta^{9,11}$	*0.55*
302		H	H	*0.54*
298		H	H	*0.53*

Asteraceae

Wedelia chinensis
Asia

Wedelia trilobata
Central America

$$CA = \frac{SB + (1 + \mathrm{TN}) \times LB}{2 + \mathrm{TN}}$$

Specificity (TN) 72.7 %

Kaurane	*SB*	*LB*	CA_{Lm}
135	0.93	0.57	0.70
101	1.00	0.51	0.69
302	0.94	0.54	0.68
134	0.90	0.55	0.68
298	0.93	0.53	0.68

→ ***Ligularia fischeri*** **(Asteraceae)**

Five kauranes from various Asteraceae species were identified as having promising antileishmanial activity against *Lm*PTR1 from a dataset of 360 kauranes

HERRERA-ACEVEDO, C., MAIA, M. D. S., CAVALCANTI, É. B. V. S., COY-BARRERA, E., SCOTTI, L., & SCOTTI, M. T. Molecular Diversity, 1-17, 2020

In vitro enzymatic activity inhibition against *Lm*PTR1

Compound	135	302
IC_{50} (µM)	8.6	9.6
Confidence Interval (95%)	9.4–7.9	10.7–8.6
Ki^{app}	1.88	2.10
	Active	

Machine learning cutoff value

$pIC_{50} \geq 5.0$

$IC_{50} \leq 1 \times 10^{-5} M$ (10 μM)

Natural Products Online is an open-source project for Natural Products (NPs) storage, search and analysis.

https://naturalproducts.net/

This is a portal for the open-source open-data repository for natural products.
The web resources are developed and maintained by the Prof. Dr. Steinbeck group.

Laboratory of Cheminformatics UFPB

Main researchers

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Visiting professor

Prof. Dr. Eugene N. Muratov

Master students

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Ávilla Ítalo de Souza Silva

Lucas Ferreira Calado

Thanks

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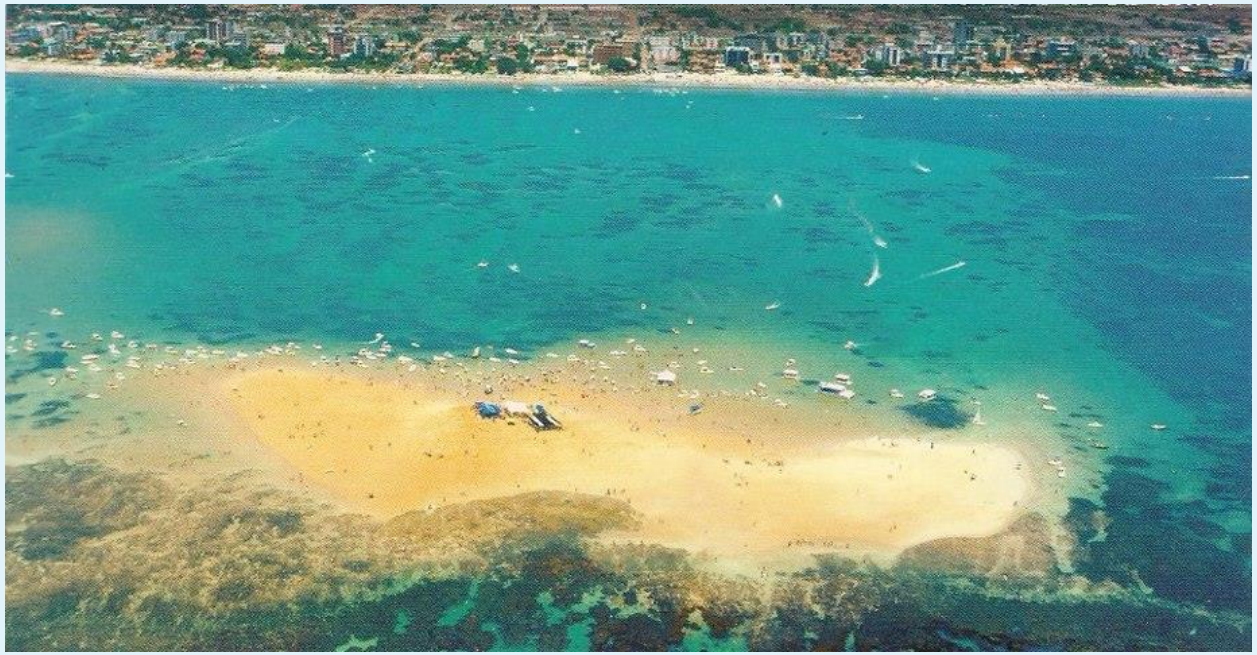

Areia Vermelha