COCONUT 2.0 DATABASE AND AUTOMATED LITERATURE MINING USING DECIMER.AI

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ChemBioSys

What are Natural Products (NPs)?

- Natural Products (NPs) are organic compounds produced by living organisms such as plants, fungi, bacteria, and marine organisms.
- NPs exhibit a wide range of structures and bioactivities, making them crucial in drug discovery and development.
- Many well-known drugs, such as antibiotics, anticancer agents, and immunosuppressants, are derived from NPs.
- NPs are key sources of new therapeutic agents due to their complex structures and biological activities.

Status of Natural Products Databases as of Early 2024

- Total Databases: Over 63 published databases related to natural products.
- Offline Databases: 14 of these are completely offline.
- Access Challenges:
  - Many databases are difficult to access.
  - Data often fails to meet FAIR (Findable, Accessible, Interoperable, Reusable) standards.
- Data Gaps:
  - Crucial information is frequently missing, including:
    - Organism source
    - Geolocation
    - Compound names
    - Literature references

COCONUT - COlleCtion of Open Natural ProdUcTs

- To create an aggregated dataset of elucidated and predicted NPs.
- Provides a web interface for easy browsing, searching, and downloading.
- Should be freely accessible as a website.
- A complete open-source resource for Natural Product research

COCONUT – 1.0

- Version 1.0 published on Journal of Cheminformatics
- Data sourced from 53 chemical databases and literature.
- Quality control and standardization process.
- Over 406,076 unique "flat" NPs and 730,441 with stereochemistry.
- Search Capabilities
- Data Download

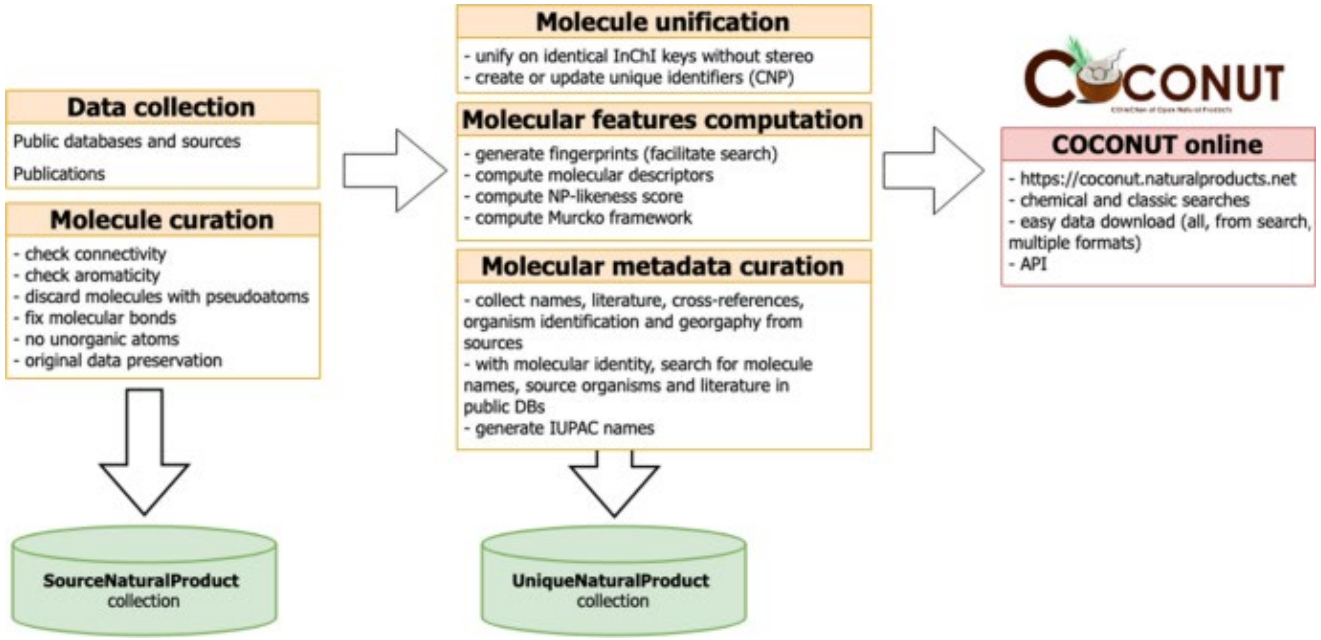
Database | Open access | Published: 10 January 2021

COCONUT online: Collection of Open Natural Products database

Maria Sorokina, Peter Merseburger, Kohulan Rajan, Mehmet Aziz Yirik & Christoph Steinbeck

Journal of Cheminformatics **13**, Article number: 2 (2021) | Cite this article

29k Accesses | **236** Citations | **33** Altmetric | Metrics



Sorokina, M.*et al.* J Cheminform 13, 2 (2021)

COCONUT - Applications

- Natural Product Discovery and Analysis
- Drug Discovery and Development
- Computational Screening and In Silico Applications
- Chemical Informatics and Data Mining
- Educational and Research Resource
- Citation count : **354** and Growing (since 2021)

Issues with COCONUT - 1.0

- Valence Issues and duplicate records.
- Presence of Synthetic Molecules.
- Fluorinated Compounds: Unintended inclusion of fluorinated molecules that aren't typically classified as natural products.
- Unlinked or Non-Normalized Citations
- Missing Organism Information associated with the natural products.
- Difficulty in Local Execution
- Lack of Code Documentation: Insufficient or unclear documentation for code and tools provided.

The DECIMER Project

Deep Learning for scraping, curating and registering compounds from the primary literature

Information in printed literature is not readily available in databases

Biol. Activity

Chemical Class

Organism Name

Chemical Name

Abstract: Agar-based disc diffusion antimicrobial assay has shown that the ethyl acetate extract of the fermented broth of *Aspergillus giganteus* NTU967 isolated from *Ulva lactuca* exhibited significant antimicrobial activity in our preliminary screening of bioactive fungal strains. Therefore, column chromatography of the active principles from liquid- and solid–state fermented products of the fungal strain was carried out, and which had led to isolation of eleven compounds. Their structures were determined by spectral analysis to be seven new highly oxygenated polyketides, namely aspergilsmins A–G (**1**–**7**), along with previously reported patulin, deoxytryptoquivaline, tryptoquivaline and quinadoline B. Among these, aspergilsmin C (**3**) and patulin displayed promising anticancer activities against human hepatocellular carcinoma SK-Hep-1 cells and prostate cancer PC-3 cells with IC_{50} values between 2.7–7.3 μM. Furthermore, aspergilsmin C (**3**) and patulin exhibited significant anti-angiogenic functions by impeding cell growth and tube formation of human endothelial progenitor cells without any cytotoxicity.

Keywords: *Aspergillus giganteus*; Trichocomaceae; bioactive natural products; Polyketides; aspergilsmin

Chemical Structures

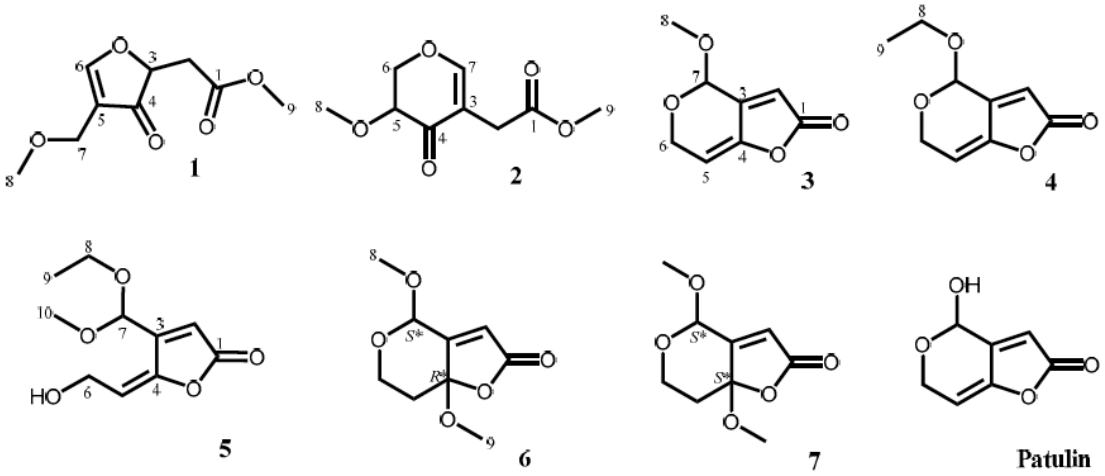


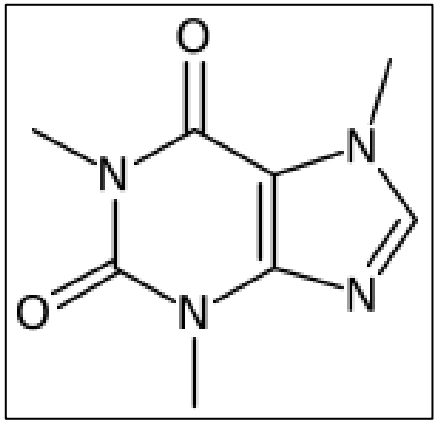
Figure 1. Chemical structures of compounds **1**–**7** and patulin.

Image Source: Chen et al. 2020, J.Nat Prod

Optical Chemical Structure Recognition (OCSR) Tools

Rule based methods

1. Scanning
2. Vectorization
3. Searching for dashed lines and dashed wedges
4. Character recognition
5. Graph compilation
6. Post processing
7. Display and editing

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   -0.9781    0.2079    0.0000 N   0  0  0  0  0  0
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  4  5  1  0     0  0
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Mol file

Review | Open Access | Published: 07 October 2020

A review of optical chemical structure recognition tools

Kohulan Rajan, Henning Otto Brinkhaus, Achim Zielesny & Christoph Steinbeck

Journal of Cheminformatics **12**, Article number: 60 (2020) | Cite this article

7667 Accesses | **2** Citations | **22** Altmetric | Metrics

Image Source: Chen et al. 2020, J.Nat Prod

DECIMER: Deep LEarning for Chemical IMagE Recognition

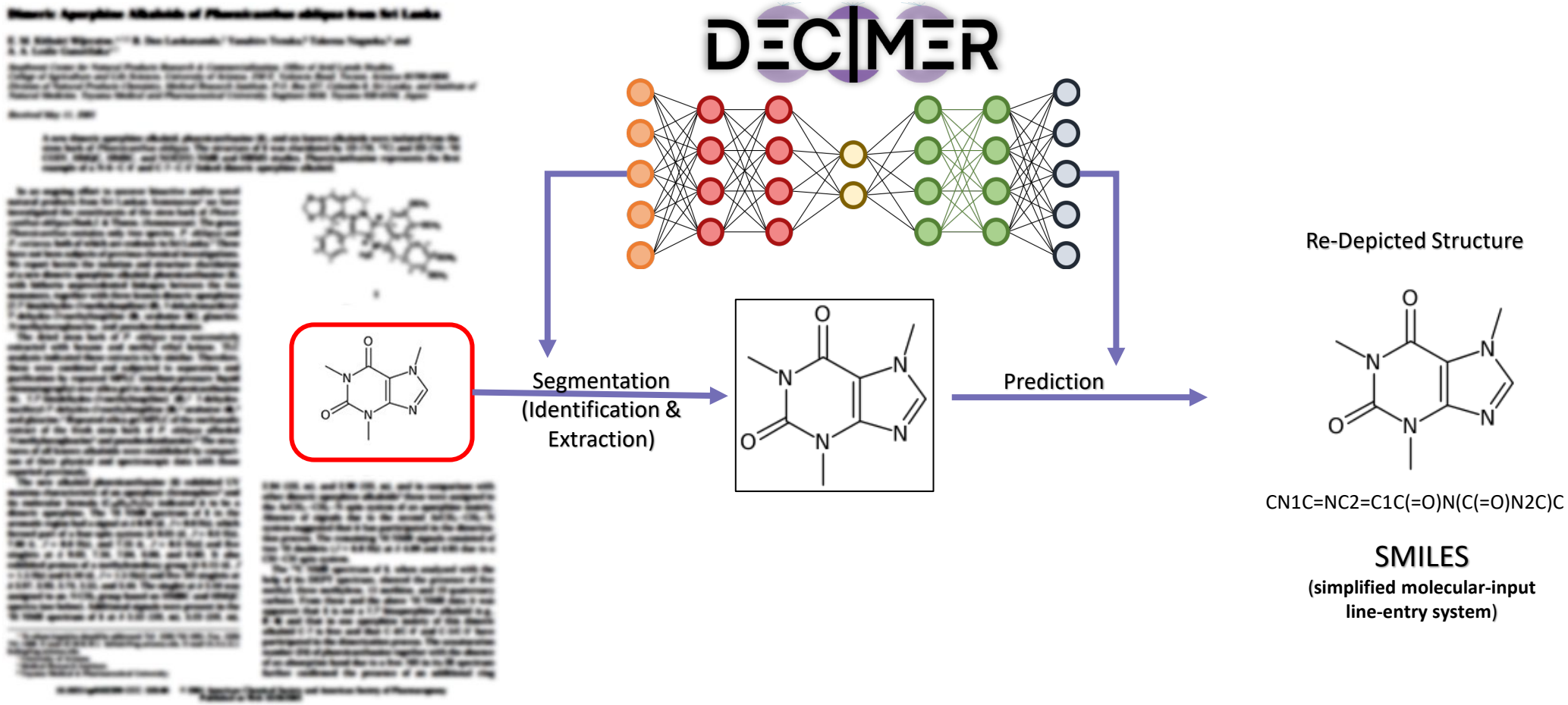


Image Source: Wijeratne et al. 2001, J.Nat Prod

Deep LEarning for Chemical IMagE Recognition

DEC|MER

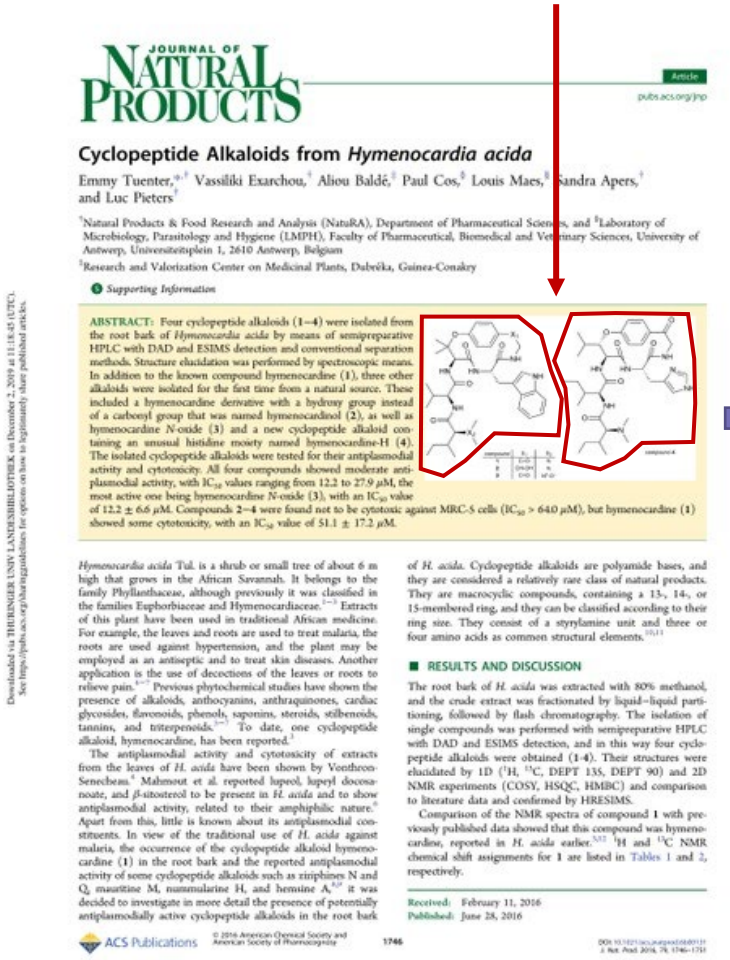
SEGMENTATION

IMAGE CLASSIFIER

IMAGE
TRANSFORMER

DECIMER – Segmentation (Tool)

Detected Chemical Structures



JOURNAL OF NATURAL PRODUCTS

Article

pubs.acs.org/jnp

Cyclopeptide Alkaloids from *Hymenocardia acida*

Emmy Tuenter,[†,‡] Vassiliki Exarchou,[†] Aliou Baldé,[†] Paul Cos,[§] Louis Maes,[§] Sandra Apers,[†] and Luc Pieters[†]

[†]Natural Products & Food Research and Analysis (NatuRA), Department of Pharmaceutical Sciences, and [§]Laboratory of Microbiology, Parasitology and Hygiene (LMPH), Faculty of Pharmaceutical, Biomedical and Veterinary Sciences, University of Antwerp, Universiteitsplein 1, 2610 Antwerp, Belgium

[‡]Research and Valorization Center on Medicinal Plants, Dubréka, Guinea-Conakry

Supporting Information

ABSTRACT: Four cyclopeptide alkaloids (**1**–**4**) were isolated from the root bark of *Hymenocardia acida* by means of semipreparative HPLC with DAD and ESIMS detection and conventional separation methods. Structure elucidation was performed by spectroscopic means. In addition to the known compound hymenocardine (**1**), three other alkaloids were isolated for the first time from a natural source. These included a hymenocardine derivative with a hydroxy group instead of a carbonyl group that was named hymenocardinol (**2**), as well as hymenocardine *N*-oxide (**3**) and a new cyclopeptide alkaloid containing an unusual histidine moiety named hymenocardine-H (**4**). The isolated cyclopeptide alkaloids were tested for their antiplasmodial activity and cytotoxicity. All four compounds showed moderate antiplasmodial activity, with IC_{50} values ranging from 12.2 to 27.9 μM, the most active one being hymenocardine *N*-oxide (**3**), with an IC_{50} value of 12.2 ± 6.6 μM. Compounds **2**–**4** were found not to be cytotoxic against MRC-5 cells (IC_{50} > 640 μM), but hymenocardine (**1**) showed some cytotoxicity, with an IC_{50} value of 51.1 ± 17.2 μM.

Hymenocardia acida Tul. is a shrub or small tree of about 6 m high that grows in the African Savannah. It belongs to the family Phyllanthaceae, although previously it was classified in the families Euphorbiaceae and Hymenocardiaceae.[1−3] Extracts of this plant have been used in traditional African medicine. For example, the leaves and roots are used to treat malaria, the roots are used against hypertension, and the plant may be employed as an antiseptic and to treat skin diseases. Another application is the use of decoctions of the leaves or roots to relieve pain.[4−7] Previous phytochemical studies have shown the presence of alkaloids, anthocyanins, anthraquinones, cardiac glycosides, flavonoids, phenols, saponins, steroids, stilbenoids, tannins, and triterpenoids.[5−7] To date, one cyclopeptide alkaloid, hymenocardine, has been reported.[3]

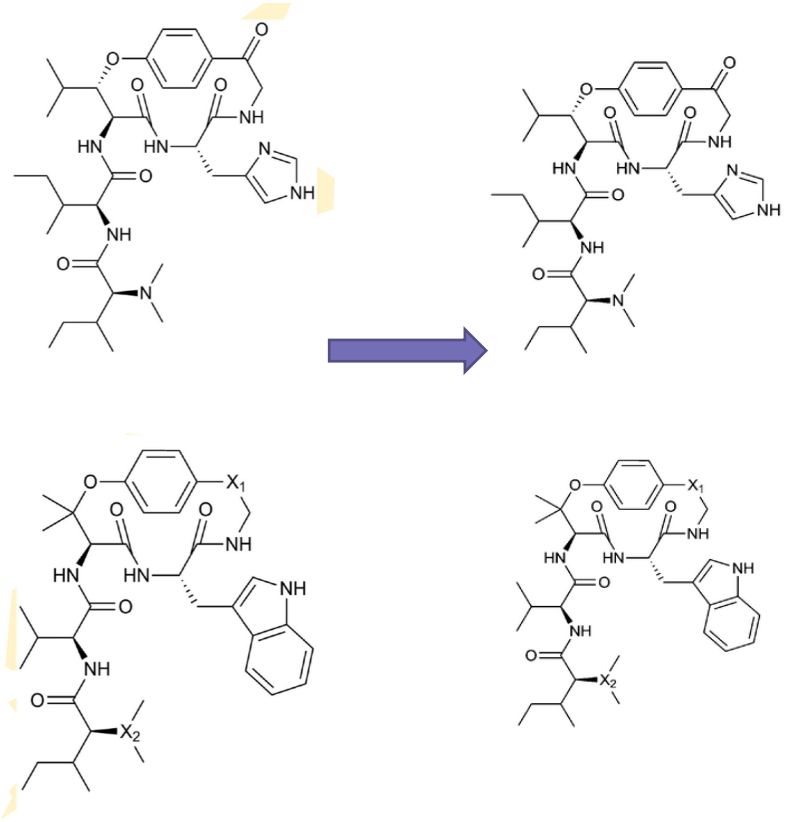
The antiplasmodial activity and cytotoxicity of extracts from the leaves of *H. acida* have been shown by Venthroo-Senechem.[4] Mahmout et al. reported lupeol, lupeyl docosanoate, and β-sitosterol to be present in *H. acida* and to show antiplasmodial activity, related to their amphiphilic nature.[6] Apart from this, little is known about its antiplasmodial constituents. In view of the traditional use of *H. acida* against malaria, the occurrence of the cyclopeptide alkaloid hymenocardine (**1**) in the root bark and the reported antiplasmodial activity of some cyclopeptide alkaloids such as ziziphines N and Q, mauritine M, nummularine H, and hemsine A,[8,9] it was decided to investigate in more detail the presence of potentially antiplasmodially active cyclopeptide alkaloids in the root bark of *H. acida*. Cyclopeptide alkaloids are polyamide bases, and they are considered a relatively rare class of natural products. They are macrocyclic compounds, containing a 13-, 14-, or 15-membered ring, and they can be classified according to their ring size. They consist of a styrylamine unit and three or four amino acids as common structural elements.[10,11]

RESULTS AND DISCUSSION

The root bark of *H. acida* was extracted with 80% methanol, and the crude extract was fractionated by liquid−liquid partitioning, followed by flash chromatography. The isolation of single compounds was performed with semipreparative HPLC with DAD and ESIMS detection, and in this way four cyclopeptide alkaloids were obtained (**1**-**4**). Their structures were elucidated by 1D (^{1}H, ^{13}C, DEPT 135, DEPT 90) and 2D NMR experiments (COSY, HSQC, HMBC) and comparison to literature data and confirmed by HRESIMS.

Comparison of the NMR spectra of compound **1** with previously published data showed that this compound was hymenocardine, reported in *H. acida* earlier.[3,12] ^{1}H and ^{13}C NMR chemical shift assignments for **1** are listed in Tables 1 and 2, respectively.

Received: February 11, 2016
Published: June 28, 2016



Segmented Chemical Structures

Final Cleaned Images

Software | Open Access | Published: 08 March 2021

DECIMER-Segmentation: Automated extraction of chemical structure depictions from scientific literature

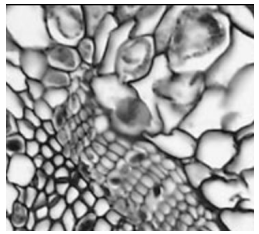
Kohulan Rajan, Henning Otto Brinkhaus, Maria Sorokina, Achim Zielesny & Christoph Steinbeck

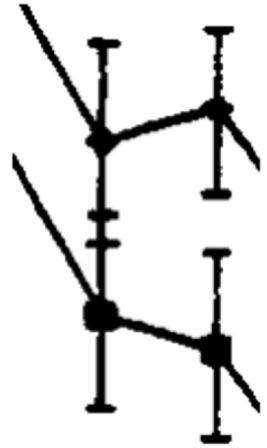
Journal of Cheminformatics **13**, Article number: 20 (2021) | Cite this article

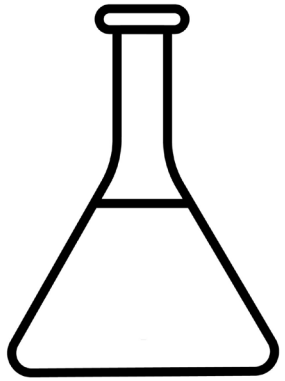
2444 Accesses | **31** Altmetric | Metrics

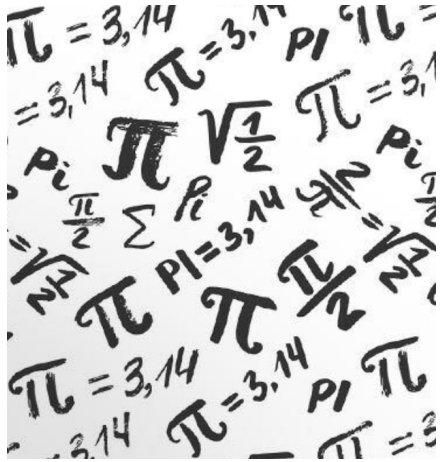
Image source: Rajan et al. 2021, J Cheminform
Tuenter et al. 2016, J.Nat Prod

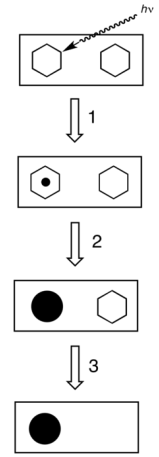
Wrong segments?











DECIMER – Image Classifier

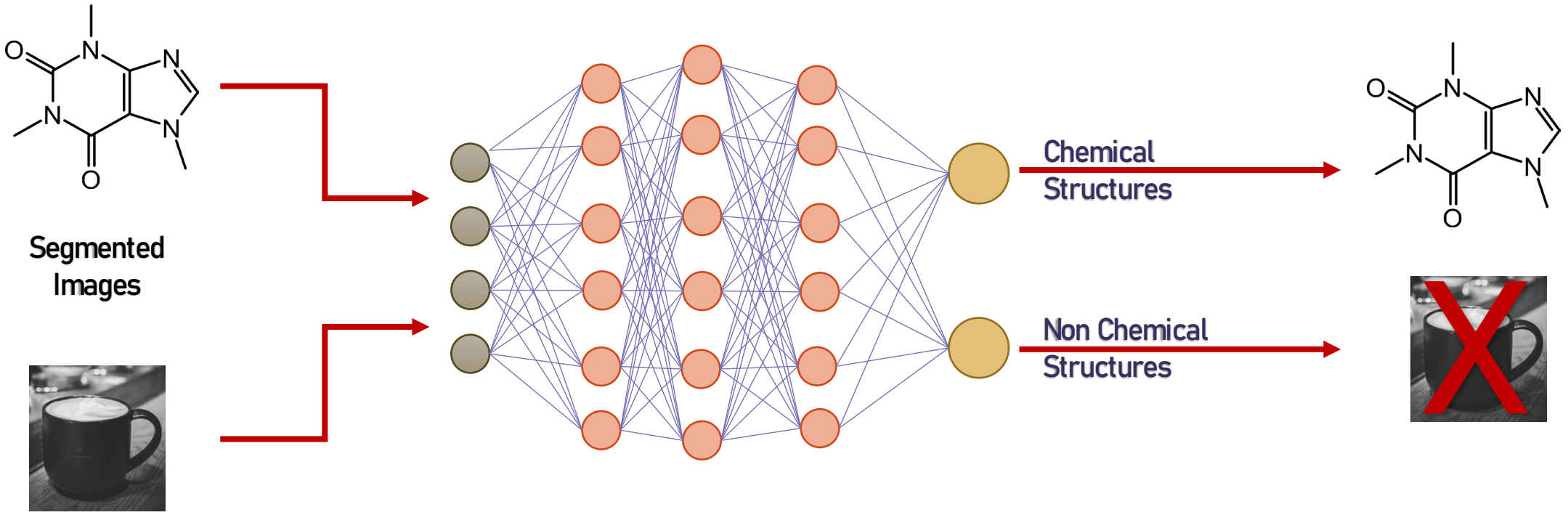
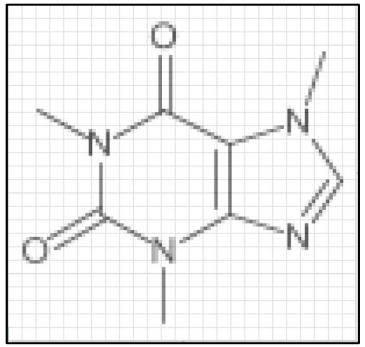


Image classifier based on EfficientNetV1-B0

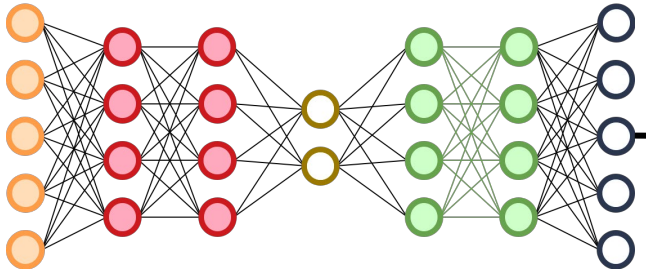
References : Tan and Le 2019, arXiv [cs.LG]

OCSR Engine

DECIMER – Image Transformer V 2.0



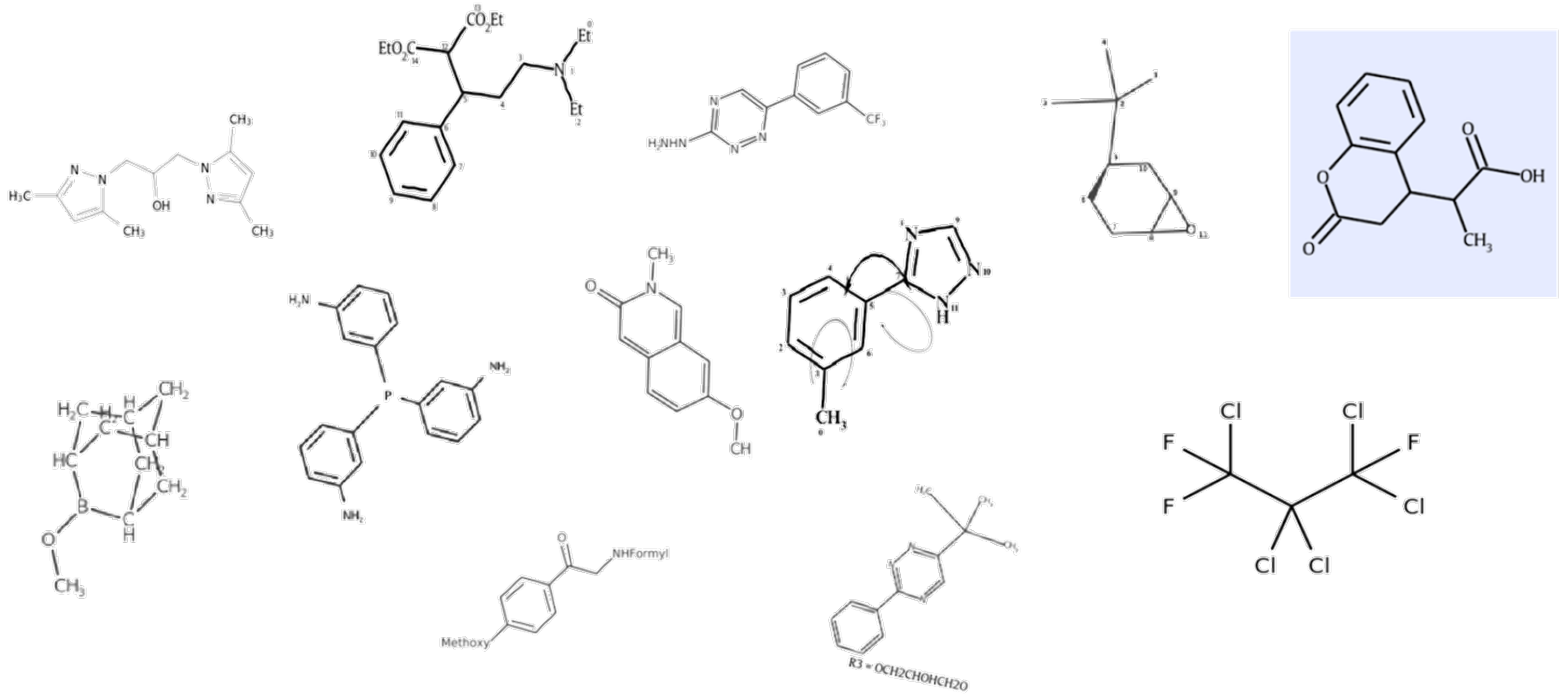
”Caffeine” Depicted using CDK



EfficientNet-V2 Encoder CNN
+
Transformer - Decoder DNN

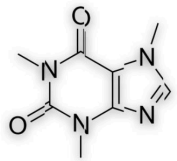
CN1C=NC2=C1C(=O)N(C(=O)N2C)C

SMILES



Training Data

RanDepict, an easy-to-use utility to generate a big variety of chemical structure depictions

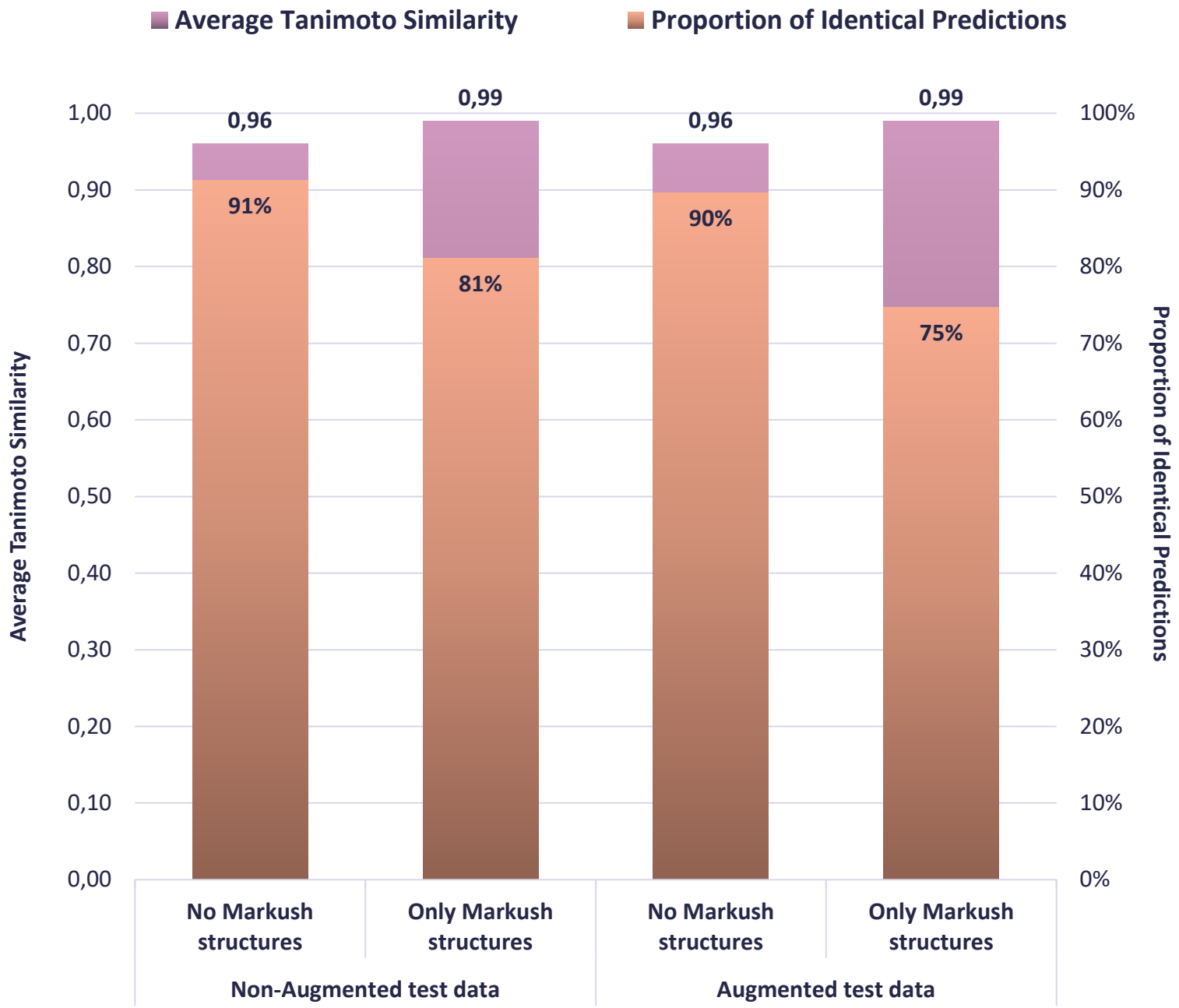


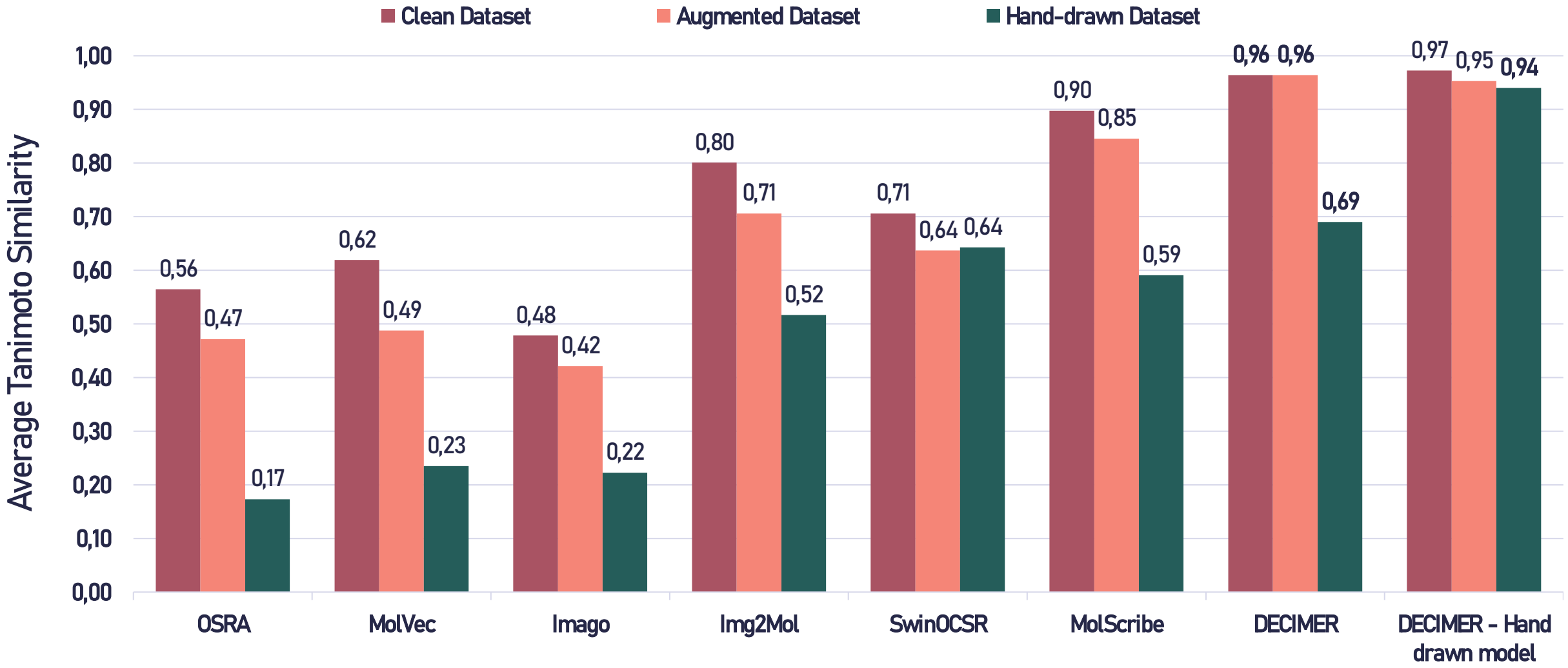
RANDEPICT

Random Chemical Structure Depiction Generator

Poster Board #: 937

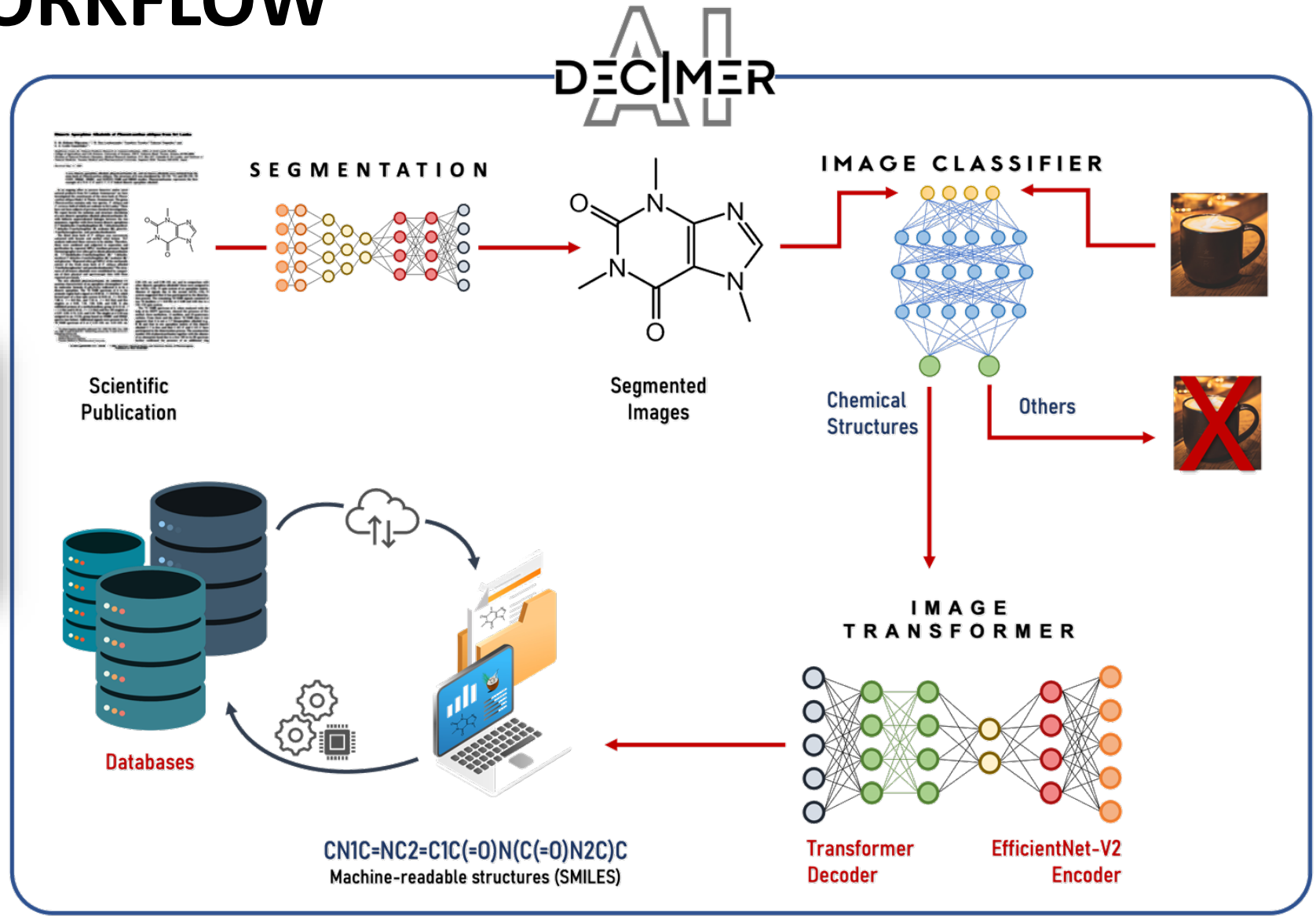
DECIMER Image Transformer Testing





DECIMER Image Transformer - 2024

DECIMER WORKFLOW



nature > nature communications > articles > article

Article | Open access | Published: 19 August 2023

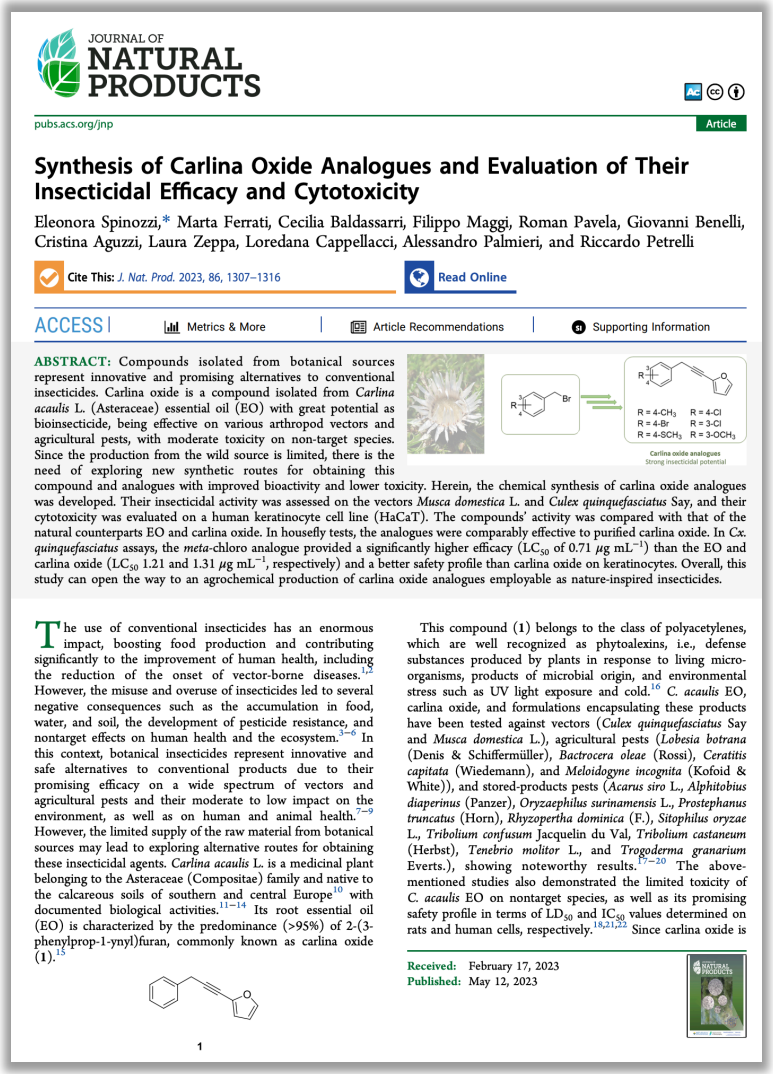
DECIMER.ai: an open platform for automated optical chemical structure identification, segmentation and recognition in scientific publications

Kohulan Rajan, Henning Otto Brinkhaus, M. Isabel Agea, Achim Zielesny & Christoph Steinbeck

Nature Communications **14**, Article number: 5045 (2023) | Cite this article

11k Accesses | **16** Citations | **122** Altmetric | Metrics

Text extraction using LLM



JOURNAL OF NATURAL PRODUCTS

pubs.acs.org/jnp

Article

Synthesis of Carlina Oxide Analogues and Evaluation of Their Insecticidal Efficacy and Cytotoxicity

Eleonora Spinozzi,* Marta Ferrati, Cecilia Baldassarri, Filippo Maggi, Roman Pavela, Giovanni Benelli, Cristina Aguzzi, Laura Zeppa, Loredana Cappellacci, Alessandro Palmieri, and Riccardo Petrelli

Cite This: *J. Nat. Prod.* 2023, 86, 1307−1316 Read Online

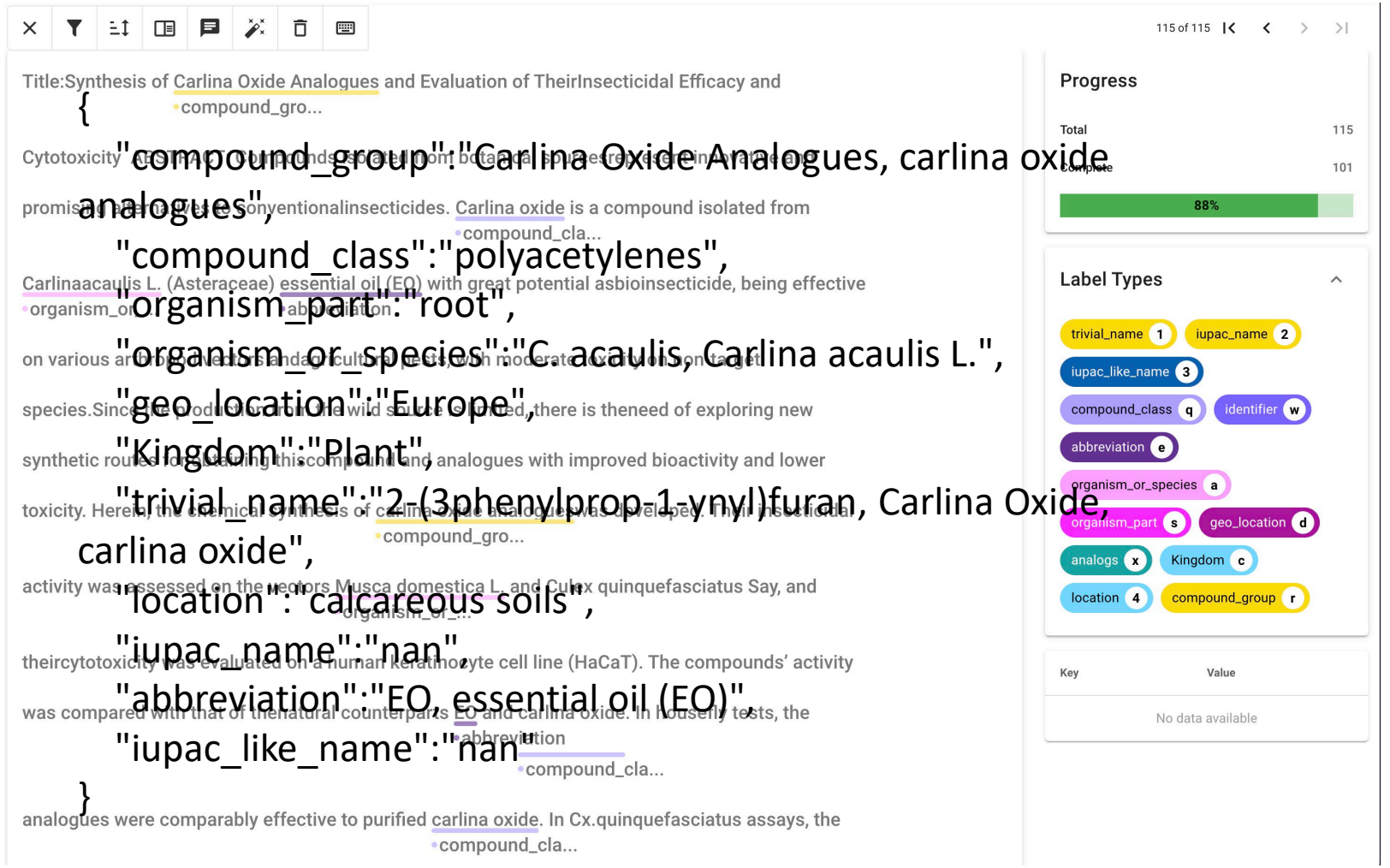
ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: Compounds isolated from botanical sources represent innovative and promising alternatives to conventional insecticides. Carlina oxide is a compound isolated from *Carlina acaulis* L. (Asteraceae) essential oil (EO) with great potential as bioinsecticide, being effective on various arthropod vectors and agricultural pests, with moderate toxicity on non-target species. Since the production from the wild source is limited, there is the need of exploring new synthetic routes for obtaining this compound and analogues with improved bioactivity and lower toxicity. Herein, the chemical synthesis of carlina oxide analogues was developed. Their insecticidal activity was assessed on the vectors *Musca domestica* L. and *Culex quinquefasciatus* Say, and their cytotoxicity was evaluated on a human keratinocyte cell line (HaCaT). The compounds' activity was compared with that of the natural counterparts EO and carlina oxide. In housefly tests, the analogues were comparably effective to purified carlina oxide. In *Cx. quinquefasciatus* assays, the *meta*-chloro analogue provided a significantly higher efficacy (LC_{50} of 0.71 $\mu g\ mL^{-1}$) than the EO and carlina oxide (LC_{50} 1.21 and 1.31 $\mu g\ mL^{-1}$, respectively) and a better safety profile than carlina oxide on keratinocytes. Overall, this study can open the way to an agrochemical production of carlina oxide analogues employable as nature-inspired insecticides.

The use of conventional insecticides has an enormous impact, boosting food production and contributing significantly to the improvement of human health, including the reduction of the onset of vector-borne diseases.[1,2] However, the misuse and overuse of insecticides led to several negative consequences such as the accumulation in food, water, and soil, the development of pesticide resistance, and nontarget effects on human health and the ecosystem.[3−6] In this context, botanical insecticides represent innovative and safe alternatives to conventional products due to their promising efficacy on a wide spectrum of vectors and agricultural pests and their moderate to low impact on the environment, as well as on human and animal health.[7−9] However, the limited supply of the raw material from botanical sources may lead to exploring alternative routes for obtaining these insecticidal agents. *Carlina acaulis* L. is a medicinal plant belonging to the Asteraceae (Compositae) family and native to the calcareous soils of southern and central Europe[10] with documented biological activities.[11−14] Its root essential oil (EO) is characterized by the predominance (>95%) of 2-(3-phenylprop-1-ynyl)furan, commonly known as carlina oxide (**1**).[15]

This compound (**1**) belongs to the class of polyacetylenes, which are well recognized as phytoalexins, i.e., defense substances produced by plants in response to living microorganisms, products of microbial origin, and environmental stress such as UV light exposure and cold.[16] *C. acaulis* EO, carlina oxide, and formulations encapsulating these products have been tested against vectors (*Culex quinquefasciatus* Say and *Musca domestica* L.), agricultural pests (*Lobesia botrana* (Denis & Schiffermüller), *Bactrocera oleae* (Rossi), *Ceratitis capitata* (Wiedemann), and *Meloidogyne incognita* (Kofoid & White)), and stored-products pests (*Acarus siro* L., *Alphitobius diaperinus* (Panzer), *Oryzaephilus surinamensis* L., *Prostephanus truncatus* (Horn), *Rhyzopertha dominica* (F.), *Sitophilus oryzae* L., *Tribolium confusum* Jacquelin du Val, *Tribolium castaneum* (Herbst), *Tenebrio molitor* L., and *Trogoderma granarium* Everts.), showing noteworthy results.[17−20] The above-mentioned studies also demonstrated the limited toxicity of *C. acaulis* EO on nontarget species, as well as its promising safety profile in terms of LD_{50} and IC_{50} values determined on rats and human cells, respectively.[18,21,22] Since carlina oxide is

Received: February 17, 2023
Published: May 12, 2023



COllecTion of Open Natural prodUcTs

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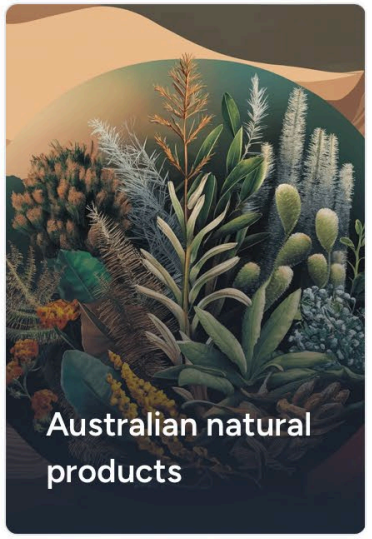

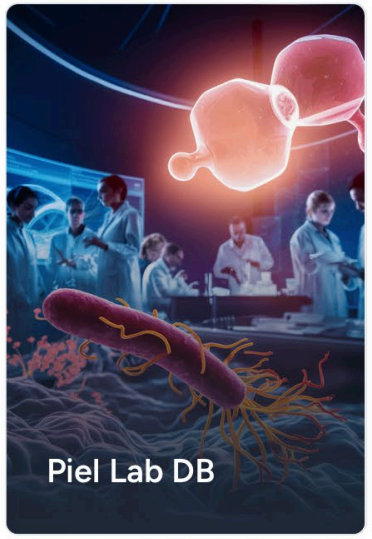

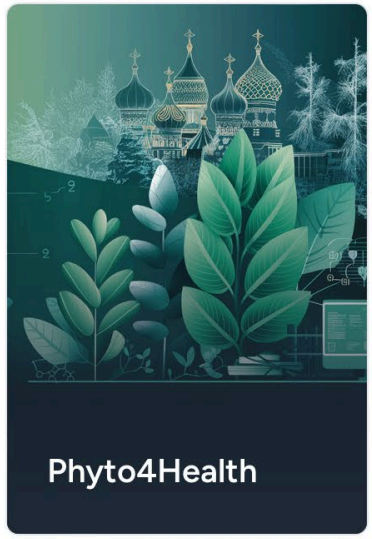

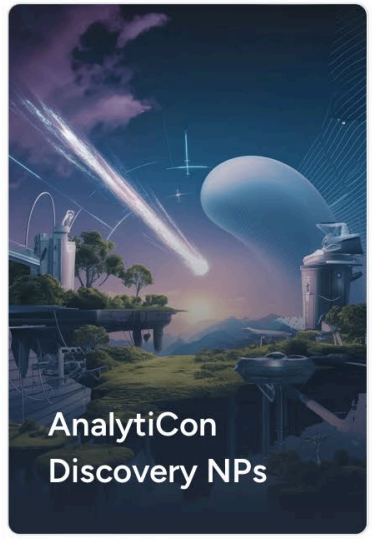

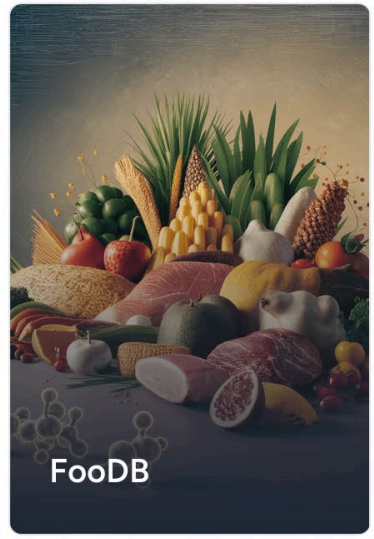

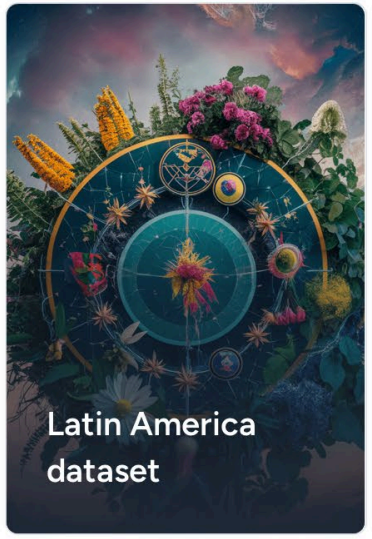

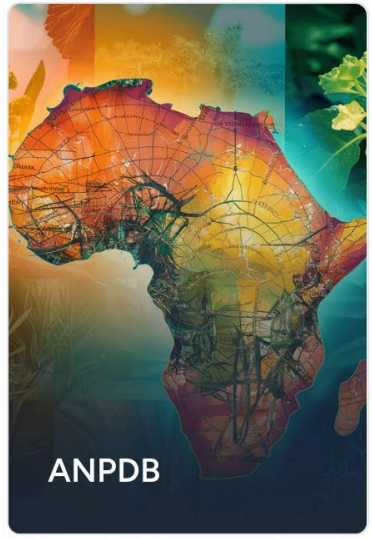

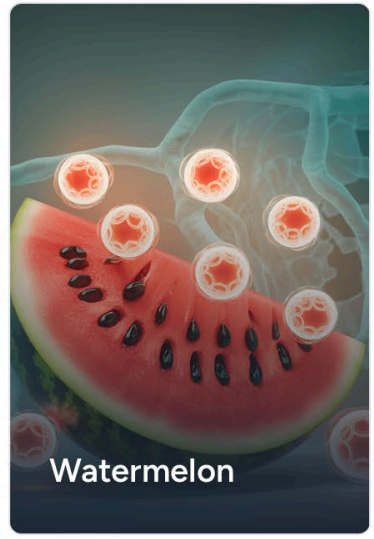

Issue Tracker

Data Sources

JOURNAL ARTICLE

Open Access Article

BIOFACQUIM: A Mexican Compo

JOURNAL ARTICLE

KNApSAcK-3D: A Three-Dimer
Database of Plant Metabolites

Kensuke Nakamura ✉, Naoki Shimura, Yuuki Otabe,
Naoaki Ono, Md Altaf Ul-Amin, Shigehiko Kanaya ✉

Plant and Cell Physiology, Volume 54, Issue 2, February 2013, Page e4,

[Special Issue: Fact Databases and Freewares] RIKEN Natural Products Encyclopedia (RIKEN NPEdia),a Chemical Database of RIKEN Natural Products Depository (RIKEN NPDepo)

Takeshi Tomiki, Tamio Saito, Masashi Ueki, Hideaki Konno, Takeo Asaoka, Ryuichiro Suzuki, Masakazu Uramoto, Hideaki Kakeya, Hiroyuki Osada

⊞ Author information

Keywords: Natural Products Database, Molecular Library, Metabolites, Chemical Biology

JOURNAL FREE ACCESS

2006 Volume 7 Pages 157-162

DOI https://doi.org/10.2751/jcac.7.157

Network of Anti-Inflammatory Natural

ACS Central Science > Vol 5/Issue 11 > Article

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RESEARCH ARTICLE | November 14, 2019

The Natural Products Atlas: An Open Access Knowledge Base for Microbial Natural Products Discovery

Jeffrey A. van Santen, Grégoire Jacob, Amrit Leen Singh, Victor Aniebok, Marcy J. Balunas, Derek Bunsko, Fausto Carnevale Neto, Laia Castaño-Espriu, Chen Chang, Trevor N. Clark, Jessica L. Cleary Little, David A. Delgadillo, Pieter C. Dorrestein, Katherine R. Duncan, Joseph M. Egan, Melissa M. Galey, F.P. Jake Haeckl, Alex Hua, Alison H. Hughes, Dasha Iskakova, Aswad Khadilkar, Jung-Ho Lee, Sanghoon Lee, Nicole LeGrow, Dennis Y. Liu, Jocelyn M. Macho, Catherine S. McCaughey, Marnix H. Medema, Ram P. Neupane, Timothy J. O'Donnell, Jasmine S. Paula, Laura M. Sanchez, Anam F. Shaikh, Sylvia Soldatou, Barbara R. Terlouw, Tuan Anh Tran, Mercia Valentine, Justin J. J. van der Hooft, Duy A. Vo, Mingxun Wang, Darryl Wilson, Katherine E. Zink, and Roger G. Linington*

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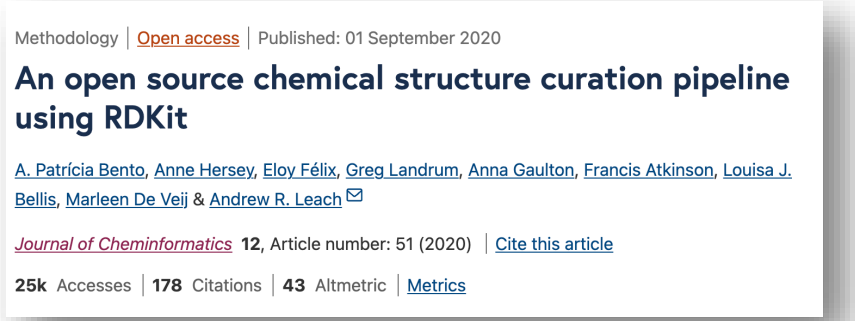
ducts from Northern African Sources

V. Simoben†, Aurélien F. A. Moumbock‡, Yvette I. Malange‡, Leonel E. Njume‖,

Data Curation Process



Data Normalisation

Structure Curation ChEMBL Pipeline with RDKit

Apart from structure depictions

structural and chemical information is processed using RDKit through Cheminformatics Microservice

Standardising data for consistency

Correcting molecular structure errors

Duplicate entries identified and removed

RDKit

Cheminformatics Microservice

Effortlessly integrate cheminformatics tools into your web application or workflows.

Documentation API

Software | Open access | Published: 16 October 2023

Cheminformatics Microservice: unifying access to open cheminformatics toolkits

Venkata Chandrasekhar, Nisha Sharma, Jonas Schaub, Christoph Steinbeck & Kohulan Rajan

Journal of Cheminformatics **15**, Article number: 98 (2023) | Cite this article

1835 Accesses | **5** Altmetric | Metrics

Multi-Tool Kit Support (Portability)

Seamlessly incorporate and utilize various toolkits, such as RDKit, CDK, and OpenBabel, to improve your cheminformatics and computational chemistry tasks without the need for complex setup. Maximize the benefits of different frameworks available.

Consistent and Reproducible Environments (Reproducibility)

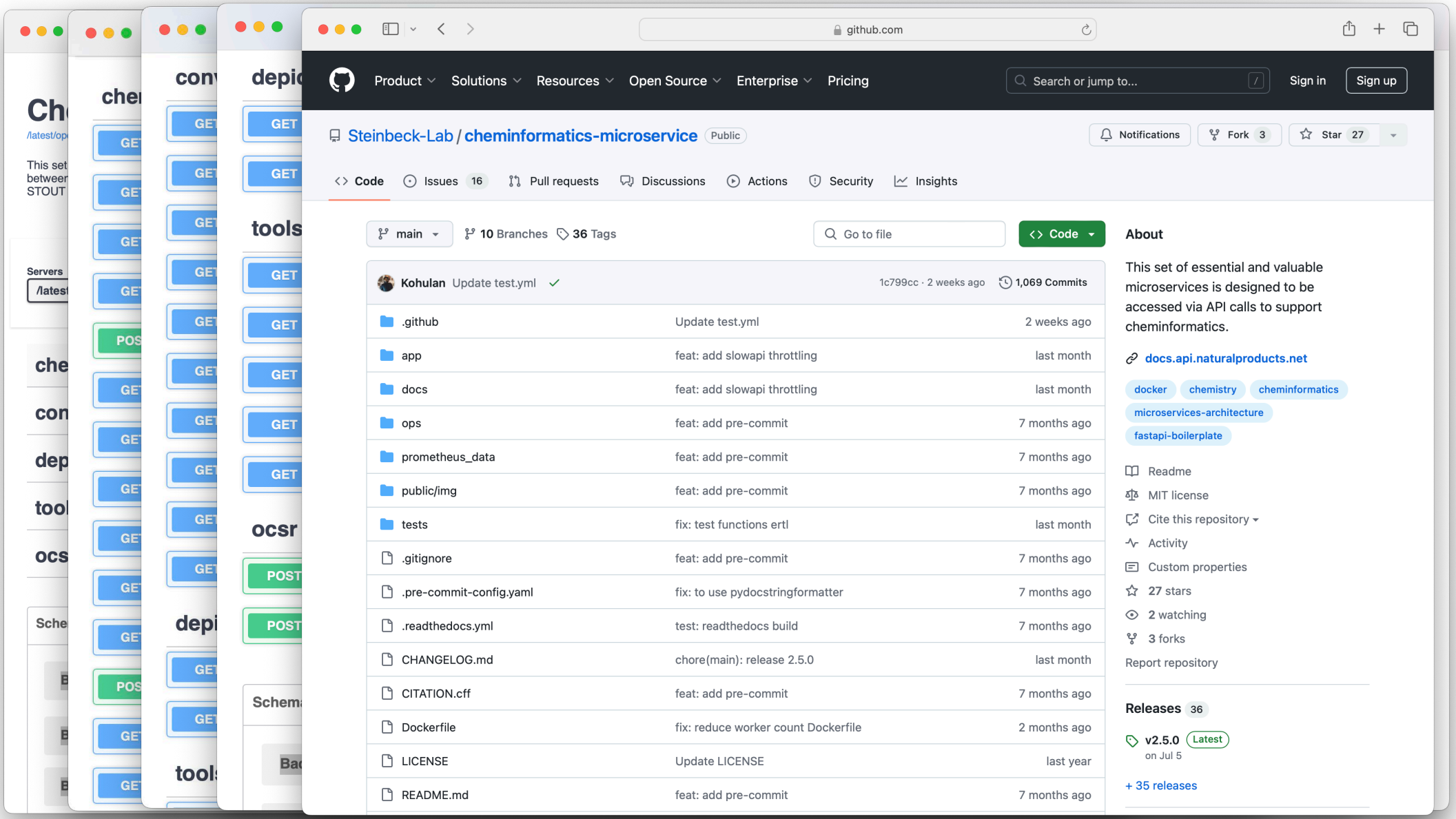
Cheminformatics Microservice packages toolkits and all their dependencies, libraries, and system tools, into a single container (including the entire runtime ensuring consistency across different deployments).

Advanced logging (Metrics)

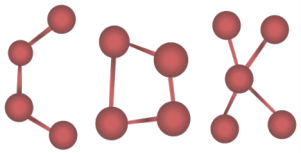
Prometheus and Grafana provide a powerful monitoring solution for Cheminformatics Microservice that collects and visualizes metrics in real time, enabling efficient tracking of system health, performance, and behaviour.

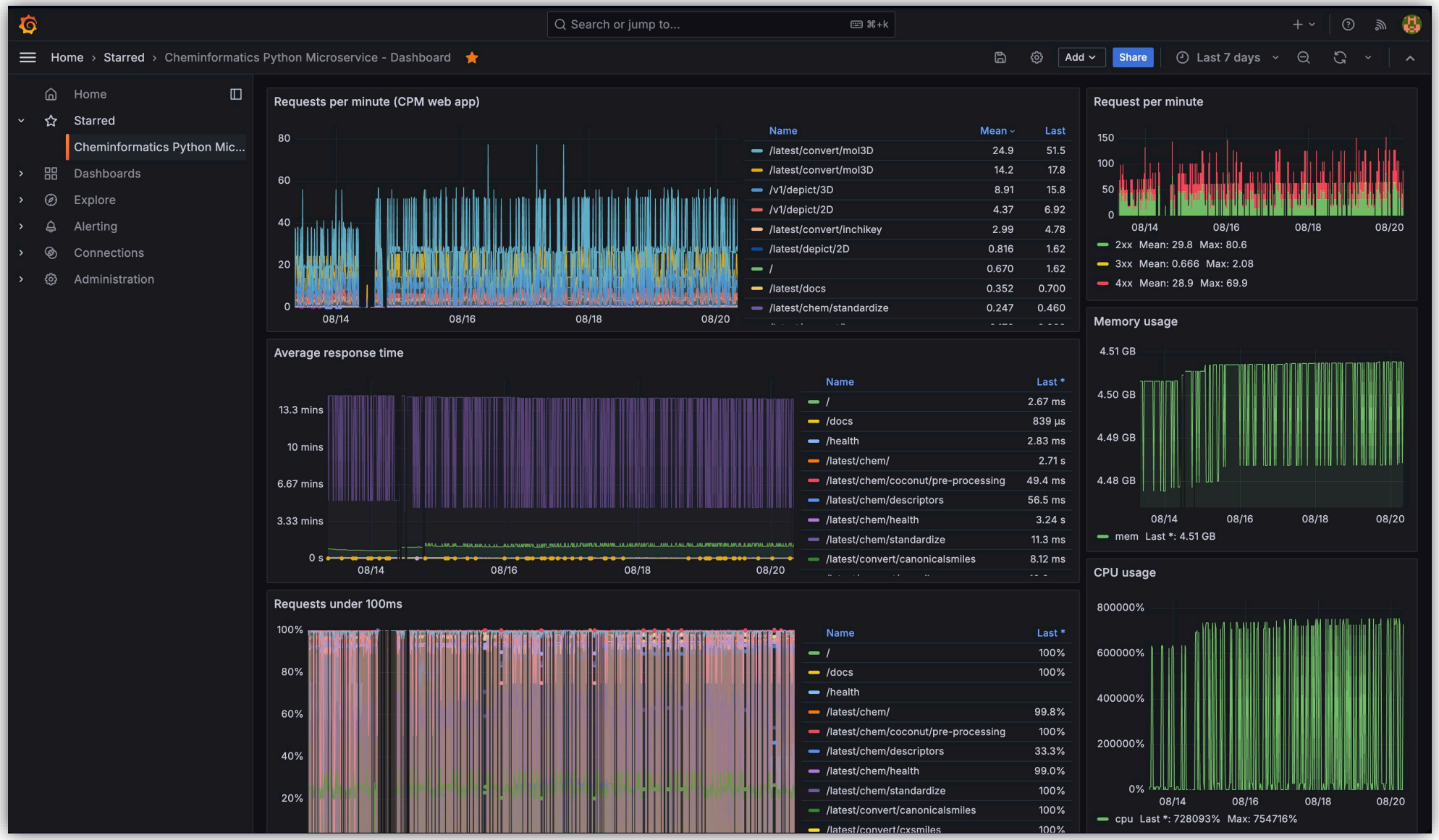
https://api.naturalproducts.net/latest/docs

Cheminformatics Microservice



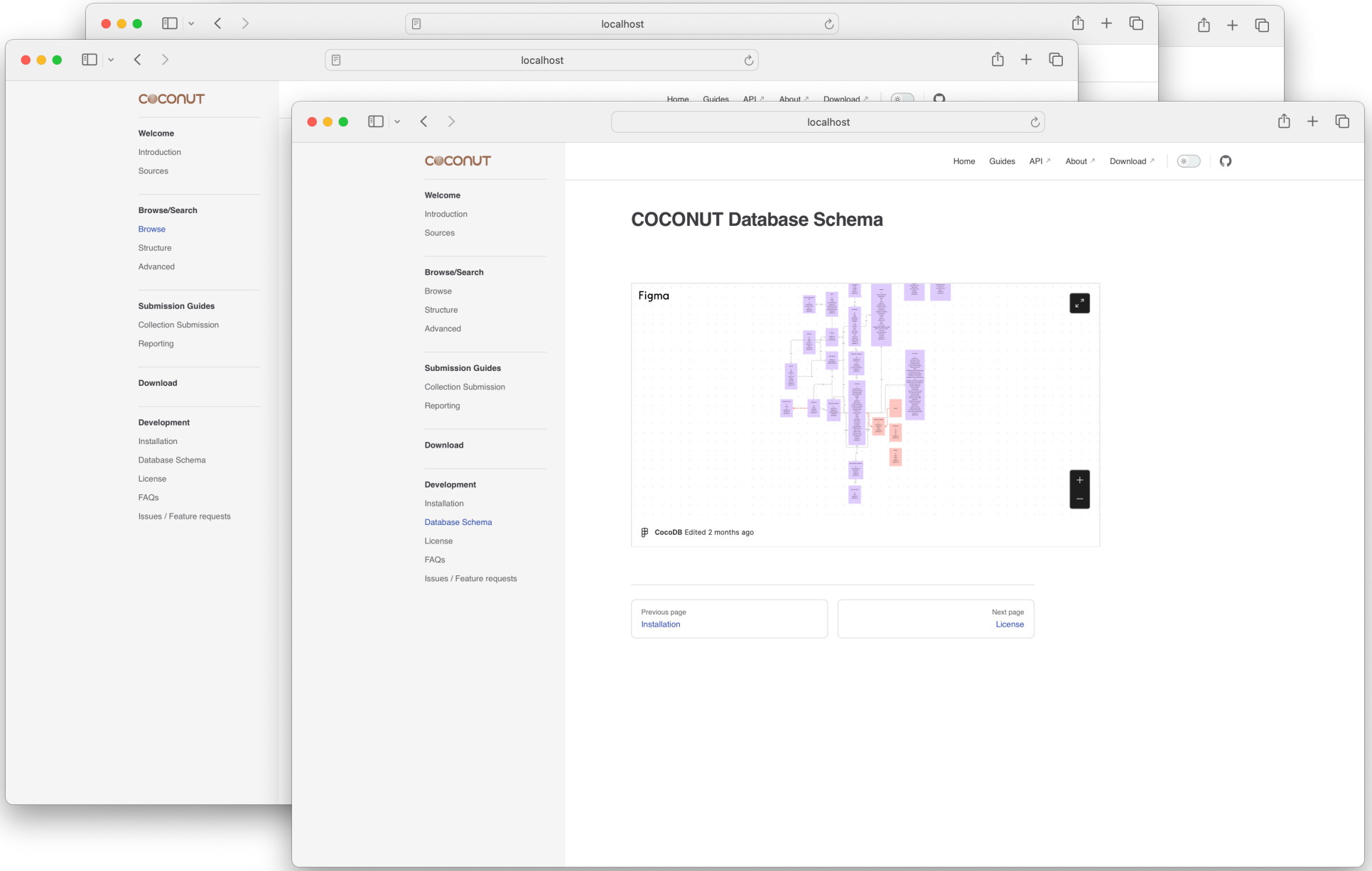
Cheminformatics Microservice





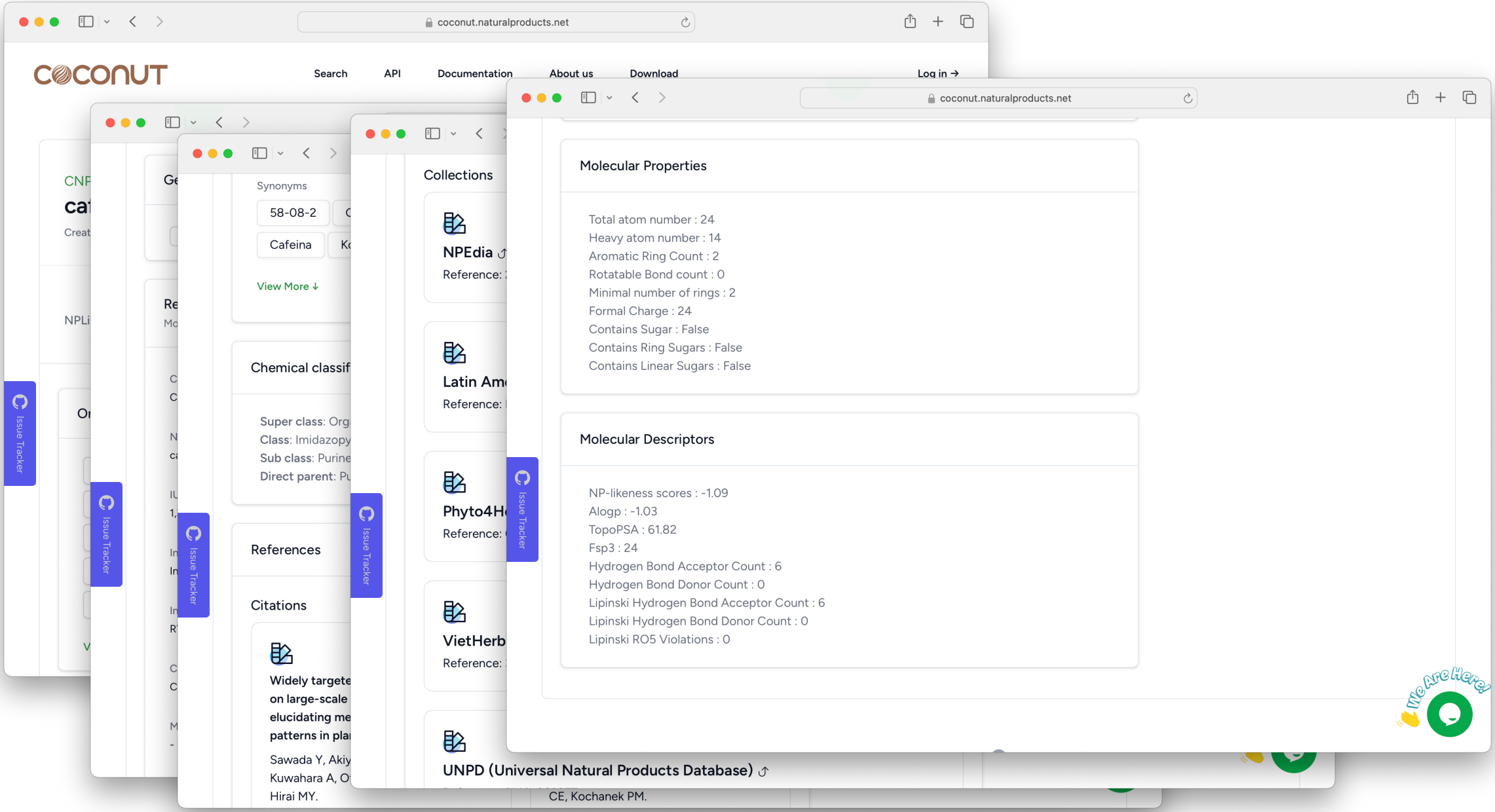
COCONUT 2.0 Architecture

COCONUT Documentation



VitePress Documentation

COCONUT Entries



Collections

- Currently there are 63 collections present

ChEBI

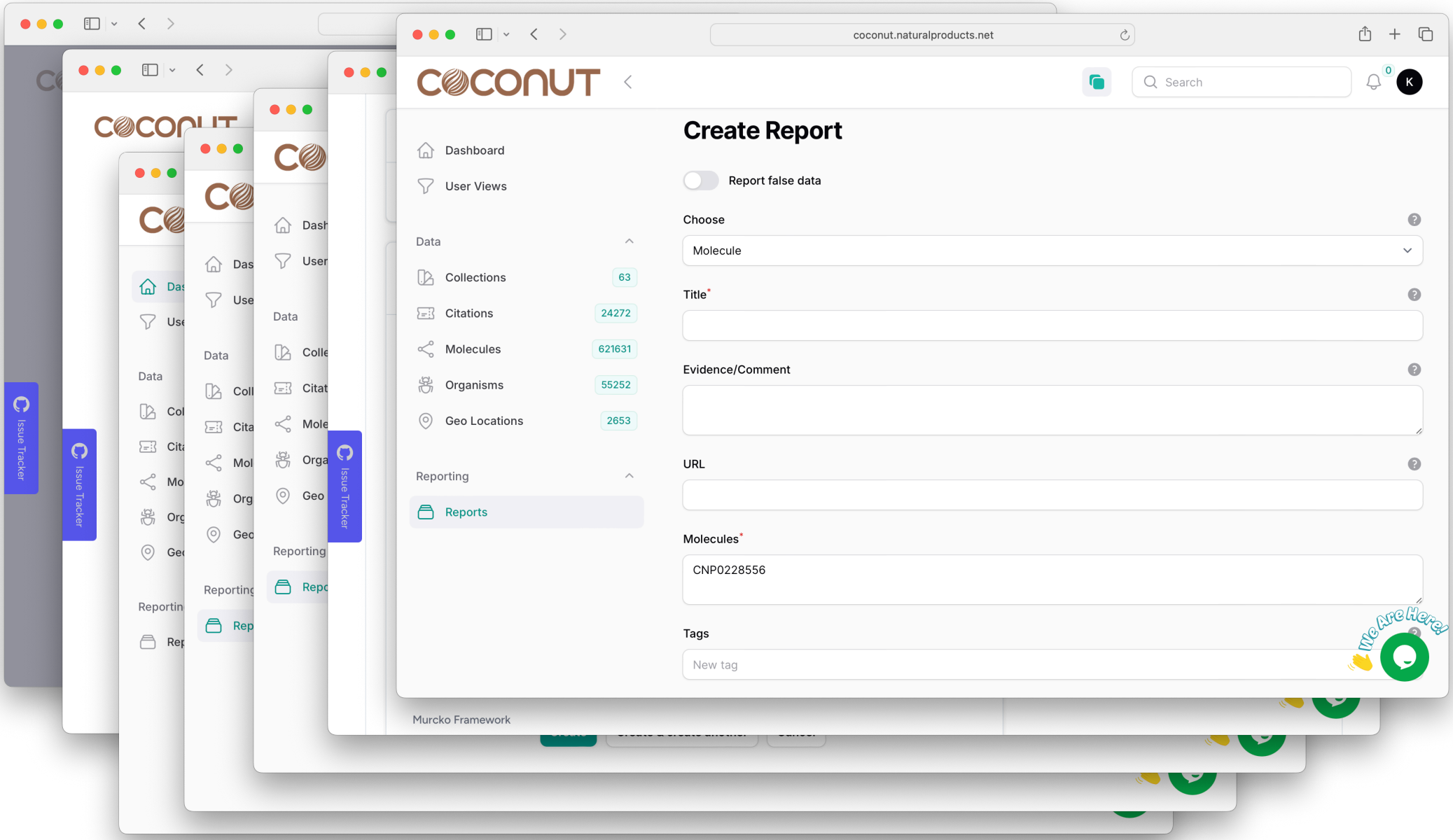
Phyto4Health

ChemSpider
Search and share chemistry

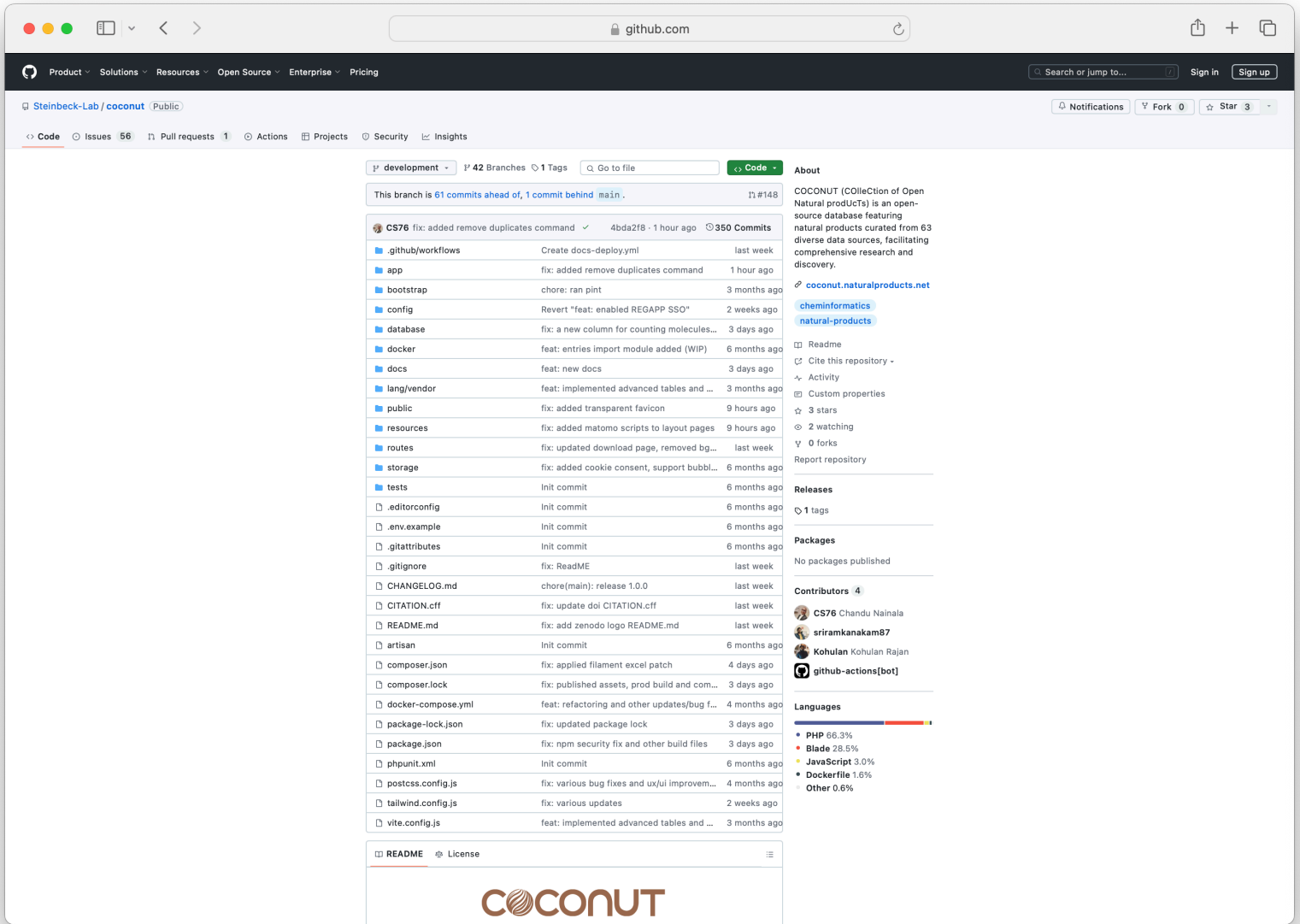
npatlas

bi mx DB

Login and Reports



Sourcecode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Notifications Fork 0 Star 3
Code Issues 56 Pull requests 1 Actions Projects Security Insights
development 42 Branches 1 Tags Go to file Code
This branch is 61 commits ahead of, 1 commit behind main. #148
CS76 fix: added remove duplicates command 4bda2f8 · 1 hour ago 350 Commits
.github/workflows Create docs-deploy.yml last week
app fix: added remove duplicates command 1 hour ago
bootstrap chore: ran pint 3 months ago
config Revert "feat: enabled REGAPP SSO" 2 weeks ago
database fix: a new column for counting molecules... 3 days ago
docker feat: entries import module added (WIP) 6 months ago
docs feat: new docs 3 days ago
lang/vendor feat: implemented advanced tables and ... 3 months ago
public fix: added transparent favicon 9 hours ago
resources fix: added matomo scripts to layout pages 9 hours ago
routes fix: updated download page, removed bg... last week
storage fix: added cookie consent, support bubbl... 6 months ago
tests Init commit 6 months ago
.editorconfig Init commit 6 months ago
.env.example Init commit 6 months ago
.gitattributes Init commit 6 months ago
.gitignore fix: ReadME last week
CHANGELOG.md chore(main): release 1.0.0 last week
CITATION.cff fix: update doi CITATION.cff last week
README.md fix: add zenodo logo README.md last week
artisan Init commit 6 months ago
composer.json fix: applied filament excel patch 4 days ago
composer.lock fix: published assets, prod build and com... 3 days ago
docker-compose.yml feat: refactoring and other updates/bug f... 4 months ago
package-lock.json fix: updated package lock 3 days ago
package.json fix: npm security fix and other build files 3 days ago
phpunit.xml Init commit 6 months ago
postcss.config.js fix: various bug fixes and ux/ui improvem... 4 months ago
tailwind.config.js fix: various updates 2 weeks ago
vite.config.js feat: implemented advanced tables and ... 3 months ago
About
COCONUT (COlleCtion of Open Natural prodUcTs) is an open-source database featuring natural products curated from 63 diverse data sources, facilitating comprehensive research and discovery.
coconut.naturalproducts.net
cheminformatics
natural-products
Readme
Cite this repository
Activity
Custom properties
3 stars
2 watching
0 forks
Report repository
Releases
1 tags
Packages
No packages published
Contributors 4
CS76 Chandu Nainala
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Kohulan Kohulan Rajan
github-actions[bot]
Languages
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Blade 28.5%
JavaScript 3.0%
Dockerfile 1.6%
Other 0.6%
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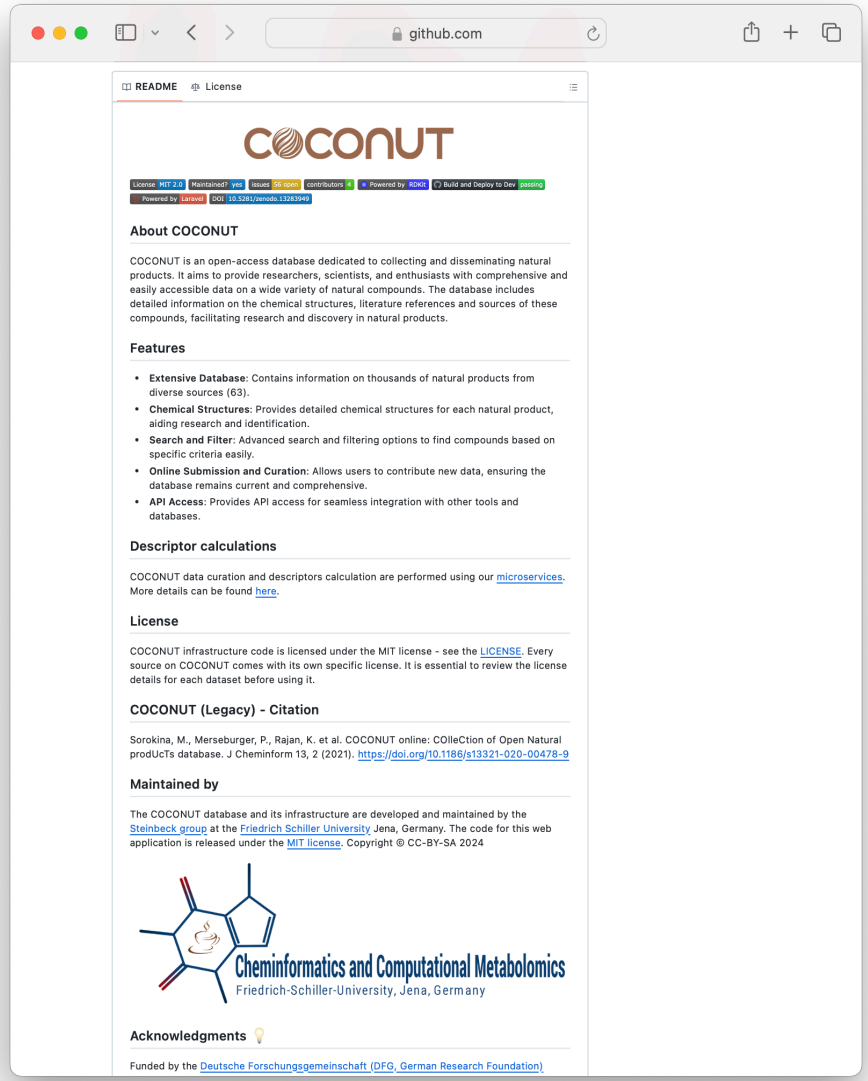
github.com
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COCONUT
About COCONUT
COCONUT is an open-access database dedicated to collecting and disseminating natural products. It aims to provide researchers, scientists, and enthusiasts with comprehensive and easily accessible data on a wide variety of natural compounds. The database includes detailed information on the chemical structures, literature references and sources of these compounds, facilitating research and discovery in natural products.
Features
Extensive Database: Contains information on thousands of natural products from diverse sources (63).
Chemical Structures: Provides detailed chemical structures for each natural product, aiding research and identification.
Search and Filter: Advanced search and filtering options to find compounds based on specific criteria easily.
Online Submission and Curation: Allows users to contribute new data, ensuring the database remains current and comprehensive.
API Access: Provides API access for seamless integration with other tools and databases.
Descriptor calculations
COCONUT data curation and descriptors calculation are performed using our microservices. More details can be found here.
License
COCONUT infrastructure code is licensed under the MIT license - see the LICENSE. Every source on COCONUT comes with its own specific license. It is essential to review the license details for each dataset before using it.
COCONUT (Legacy) - Citation
Sorokina, M., Merseburger, P., Rajan, K. et al. COCONUT online: COlleCtion of Open Natural prodUcTs database. J Cheminform 13, 2 (2021). https://doi.org/10.1186/s13321-020-00478-9
Maintained by
The COCONUT database and its infrastructure are developed and maintained by the Steinbeck group at the Friedrich Schiller University Jena, Germany. The code for this web application is released under the MIT license. Copyright © CC-BY-SA 2024
Cheminformatics and Computational Metabolomics
Friedrich-Schiller-University, Jena, Germany
Acknowledgments
Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)

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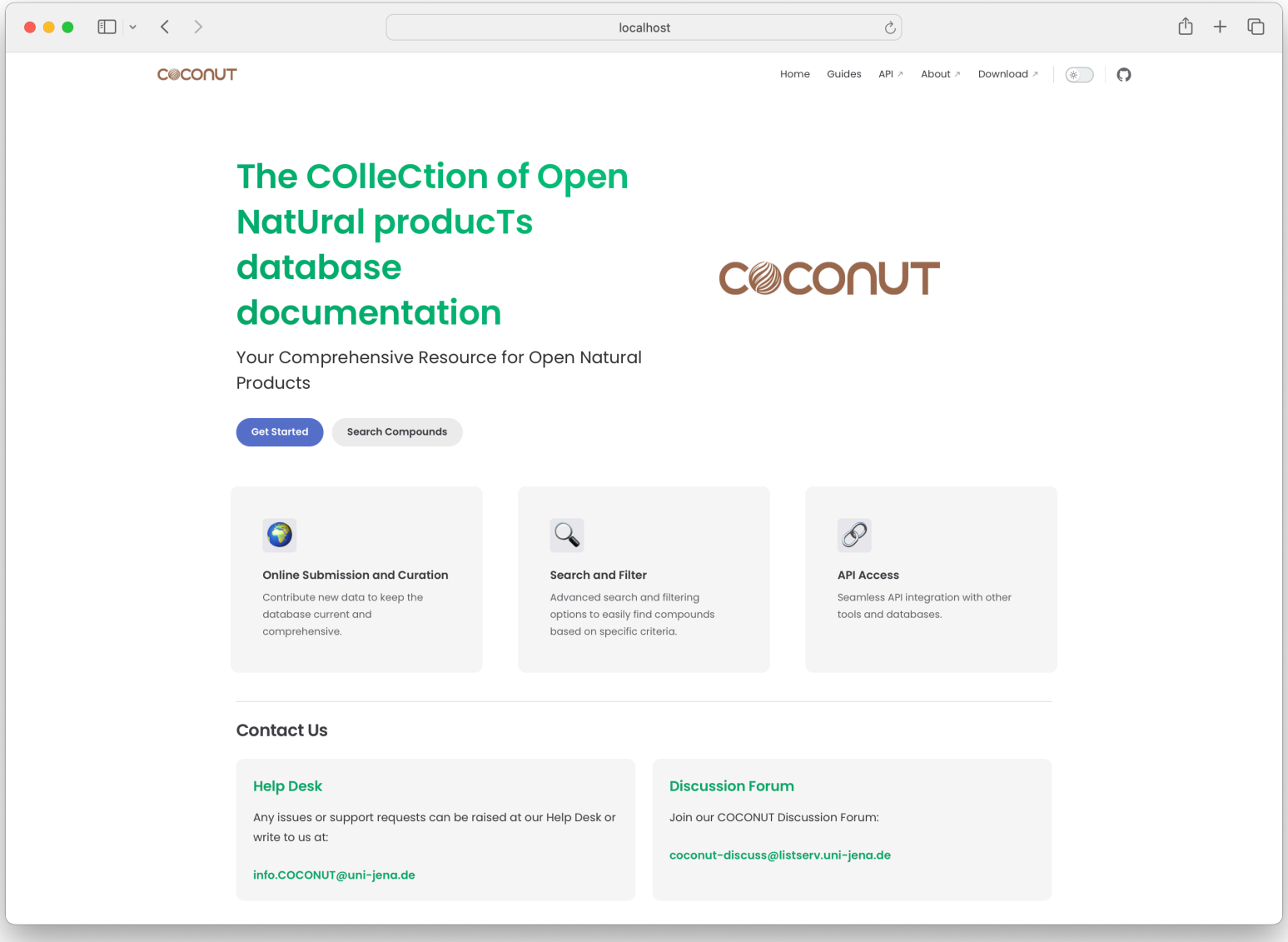
localhost
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API
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Your Comprehensive Resource for Open Natural Products
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Advanced search and filtering options to easily find compounds based on specific criteria.
API Access
Seamless API integration with other tools and databases.
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Acknowledgments

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for your attention.

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