# Exploiting and sharing ***existing*** and ***new knowledge*** in the frame of the **Digital Botanical Gardens Initiative**

UNI FR Pierre-Marie Allard
COMMONS Lab
University of Fribourg

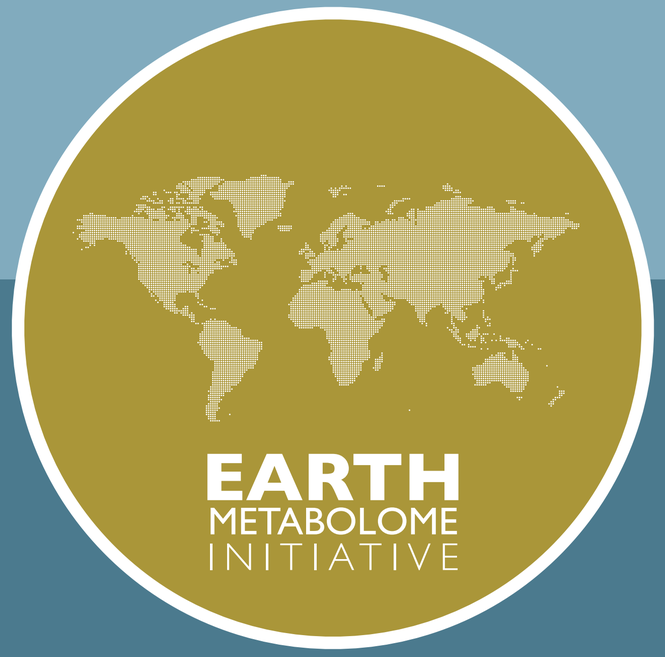
ETH zürich Adriano Rutz
Institute of Molecular Systems Biology
ETHZ

https://doi.org/10.5281/zenodo.10654974

Swiss
Digital Botanical
Gardens Initiative

# EARTH
## METABOLOME
## INITIATIVE

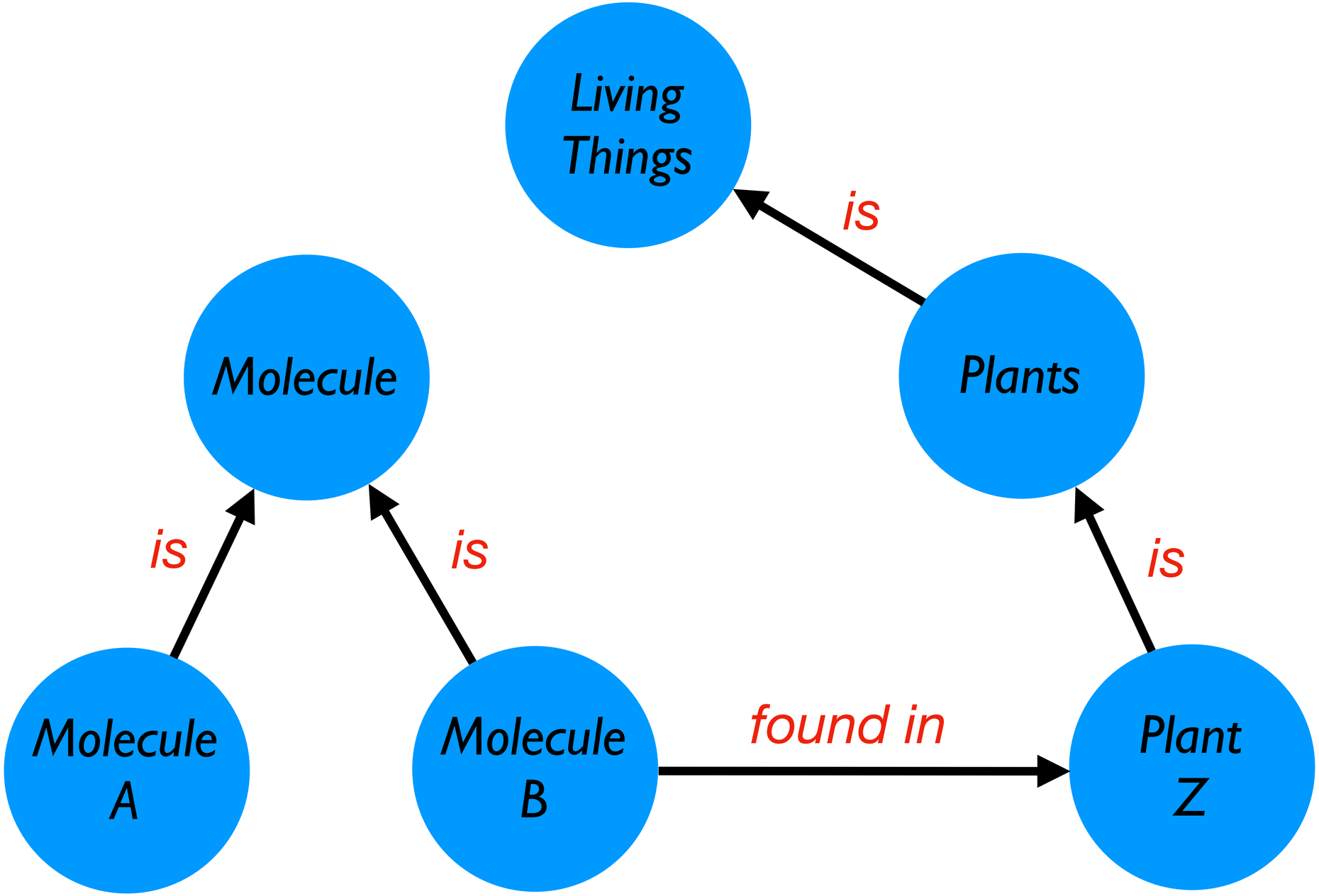
# A massive undertaking ...

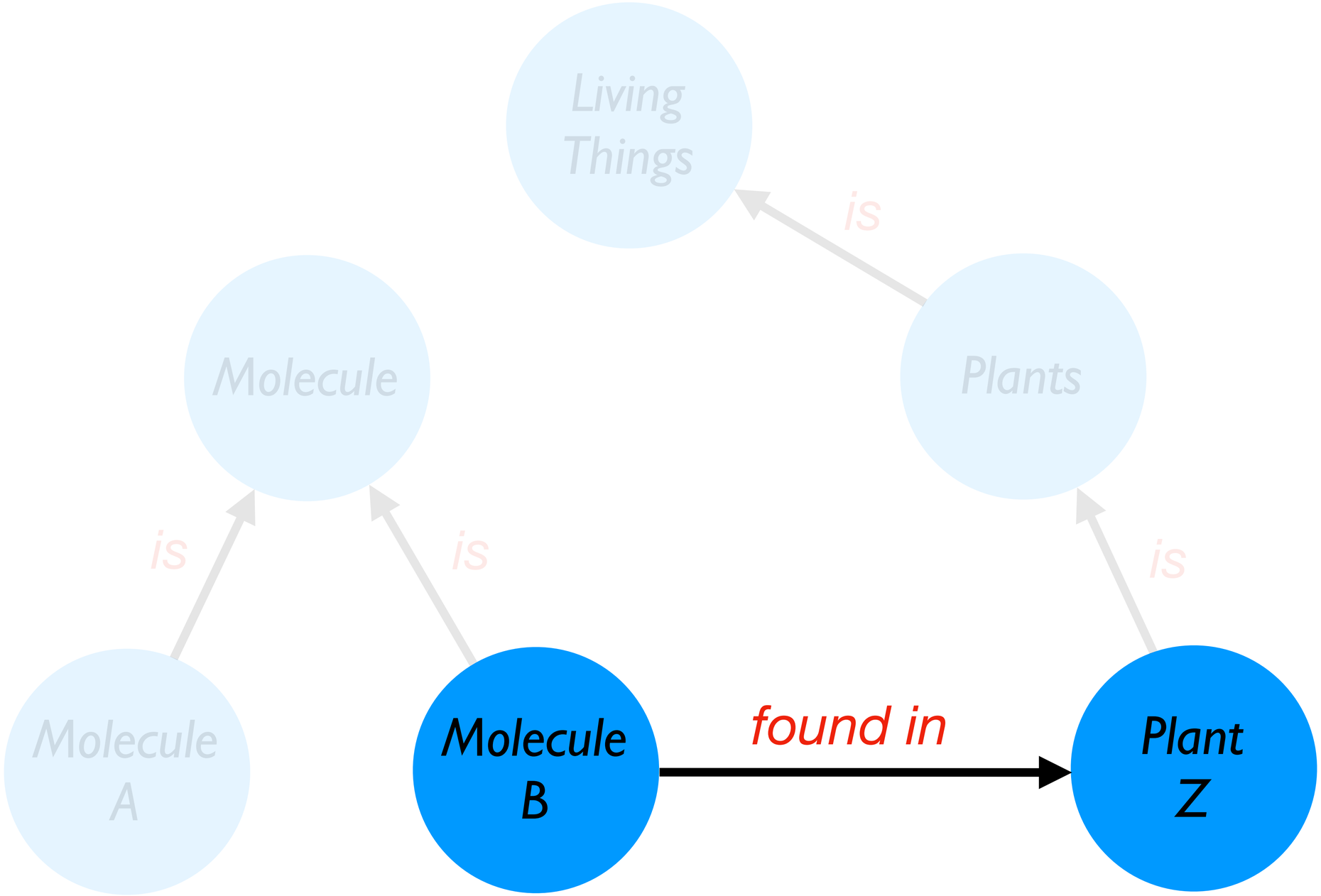



*Profile the metabolic content of all currently known species on Earth.*

## ... with three objectives

- *Explore and understand the chemical foundations of the biosphere*
- *Benefit human society*
- *Protect biodiversity*


Living Things
is
Molecule
Plants
is
is
is
Molecule A
Molecule B
found in
Plant Z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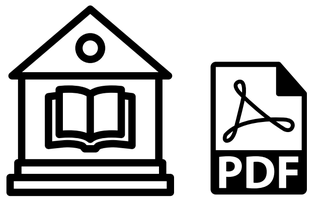


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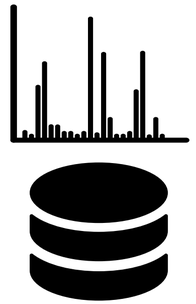
Past knowledge

EARTH METABOLOME INITIATIVE

Future knowledge



Molecule *found in* Organism

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knowledge pixels

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**How do we improve *past* knowledge exploitation ?**

**How do we improve *future* knowledge dissemination ?**

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**How do we improve *past* knowledge exploitation ?**

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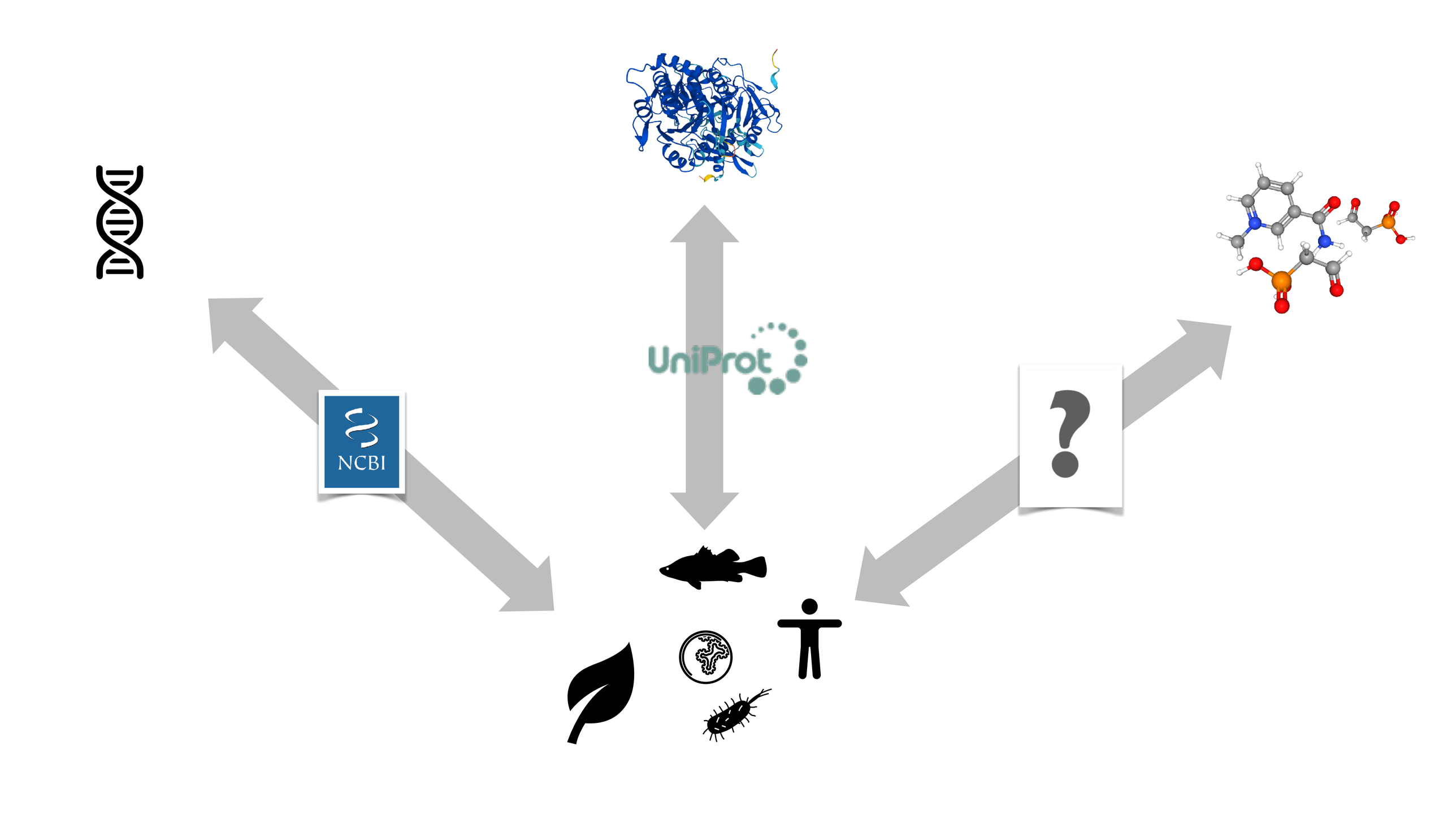
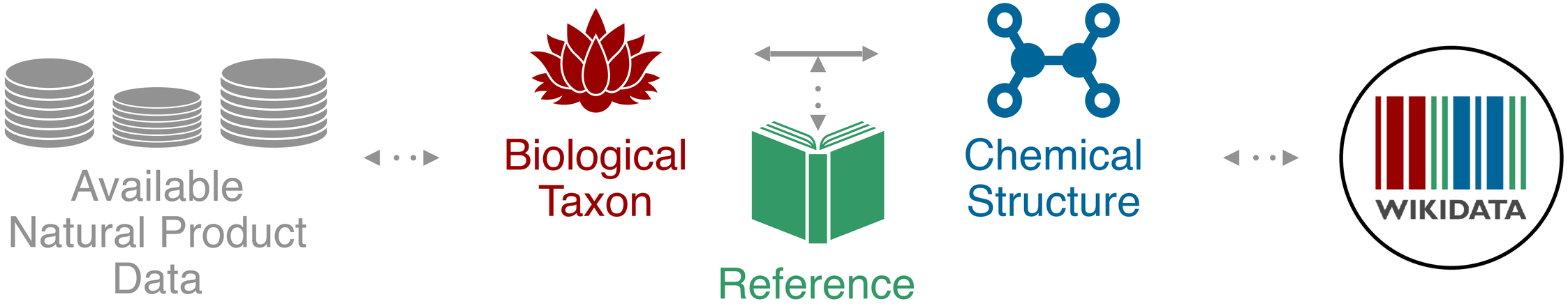

NCBI
UniProt
?

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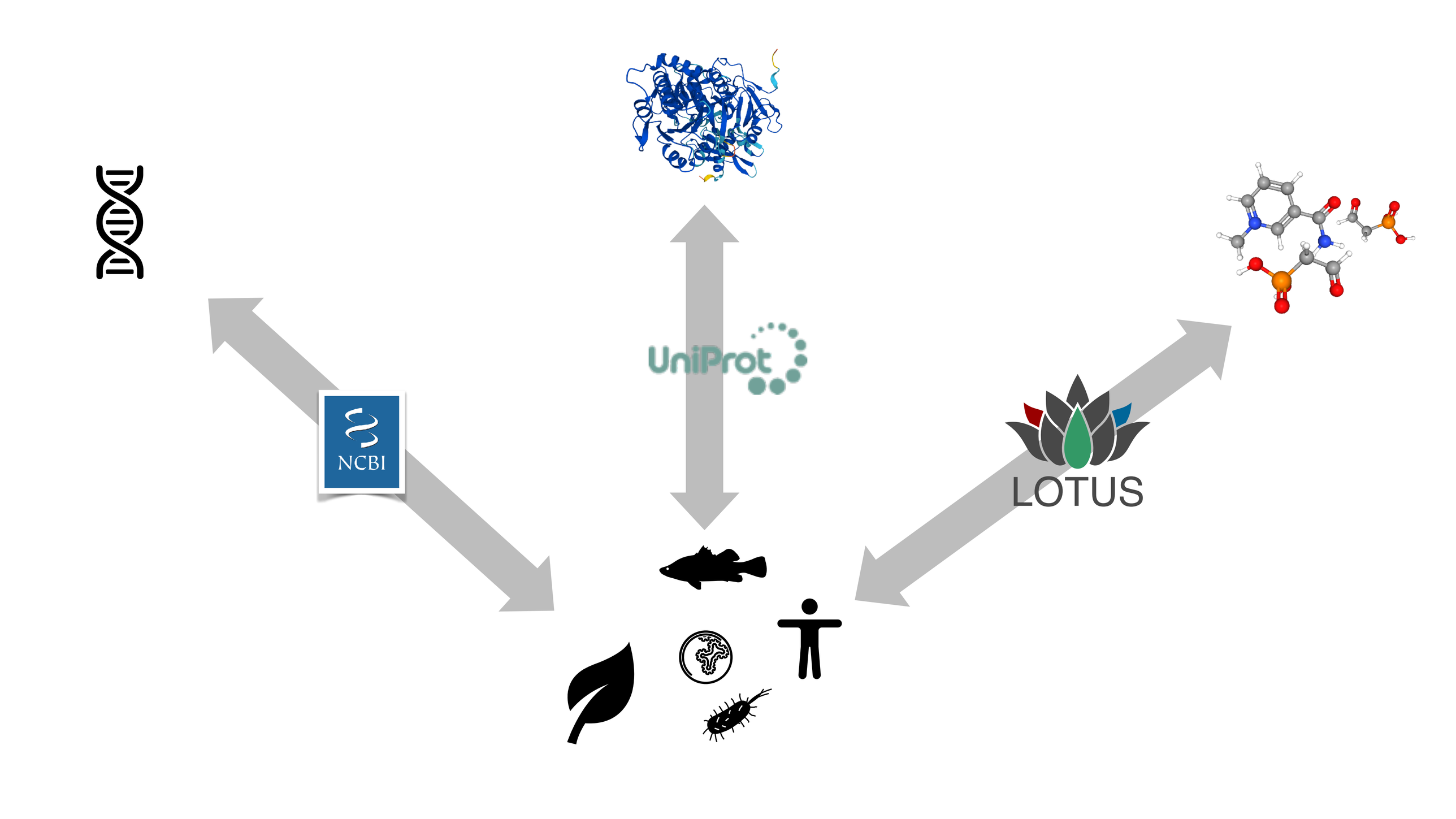
https://doi.org/10.7554/eLife.70780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PLANTES DE NOUVELLE CALÉDONIE. LV.*
ISOBORRÉVÉRINE ET BORRÉVÉRINE, ALCALOÏDES
BIS-INDOLIQUES DE *FLINDERSIA FOURNIERI*


François Tillequin et Michel Koch

*Laboratoire de Matière Médicale, Faculté des Sciences Pharmaceutiques et Biologiques, 4, Ae de l'Observatoire, F-75006-Paris*

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*Laboratoire de Matière Médicale, U.E.R. des Sciences Pharmaceutiques, 1, rue Vaubénard, F-14060-Caen*

Thierry Sevenet

*Laboratoire des Plantes Médicinales du C.N.R.S., Montravel, Noumea, Nouvelle Calédonie*

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JOURNAL OF NATURAL PRODUCTS

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## Cyclic Peptides from the Opportunistic Pathogen *Basidiobolus meristosporus*


Cheng Zhao, Jiaojiao Qu, Fan Peng, Ruili Lu,* Guan-Hu Bao, Bo Huang,* and Fenglin Hu*



Cite This: *J. Nat. Prod.* 2023, 86, 1885−1890 Read Online

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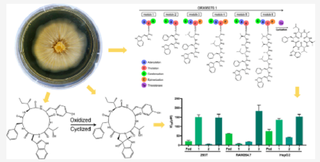
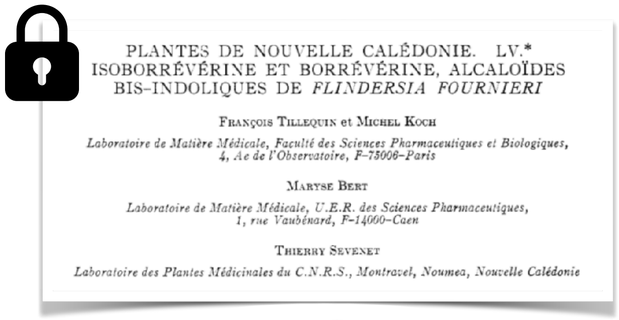
**ABSTRACT:** Three new cyclic peptides, meristosporins A, B, and C (**1**−**3**), one of which features an unusual amino acid, were isolated from the opportunistic pathogen *Basidiobolus meristosporus* and identified by 1D, 2D NMR, MS/MS, and Marfey's analysis. The biosynthetic pathway of the hexapeptide meristosporin A (**1**) was deduced based on nonribosomal peptide synthetase gene clusters analysis. Compounds **1** and **2** showed cytotoxicity to RAW264.7 and 293T cells, respectively. These compounds may be involved in the fungal injury caused to human cells.

Molecule **found in** Organism



PLANTES DE NOUVELLE CALÉDONIE. LV.*
ISOBORRÉVÉRINE ET BORRÉVÉRINE, ALCALOÏDES
BIS-INDOLIQUES DE *FLINDERSIA FOURNIERI*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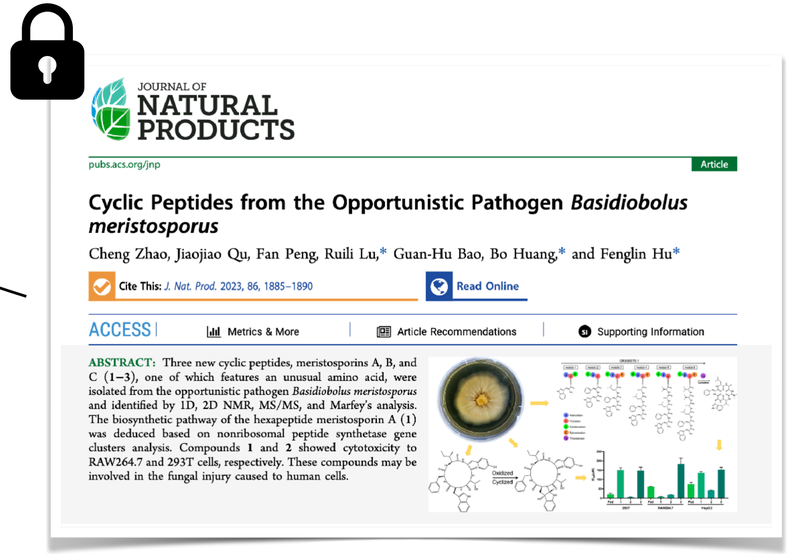

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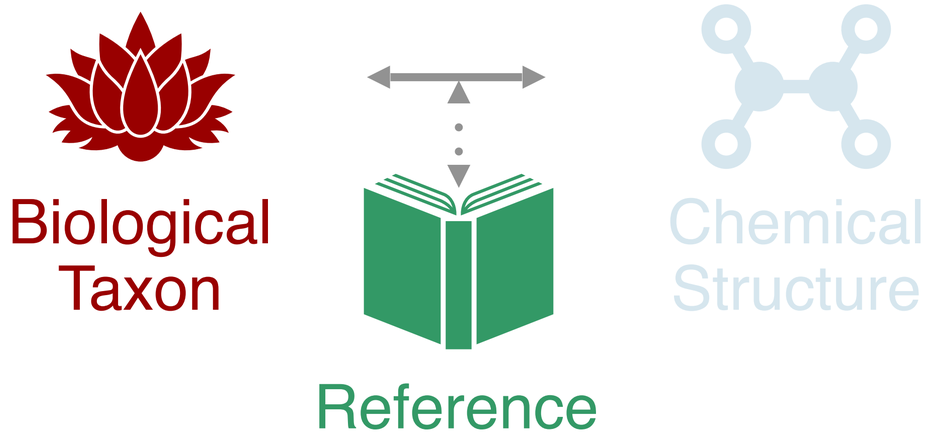
Molecule **found in** Organism

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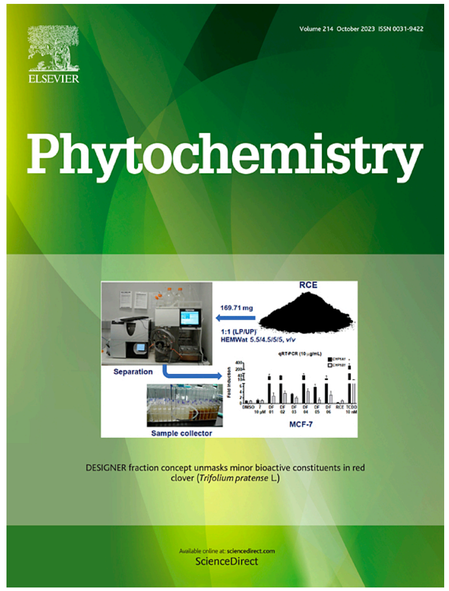


https://www.sciencedirect.com/journal/phytochemistry

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| 233 | 2022 | Phytochemistry |
| 104 | 2023 | Phytochemistry |

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## Graphical abstract

Eight undescribed natural guanidines and one known compound were isolated from the leaves of *Alchornea rugosa*. Rugonines D-G showed strong autophagy inhibitory activity in HEK293 cells stably expressing GFP-LC3.

https://www.sciencedirect.com/science/article/abs/pii/S003194222200437X

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### Alchornea rugosa (Lour.) Muell. Arg.

Doan, Thi-Phuong, Park, Eun-Jin, Ryu, Byeol, Cho, Hyo-Moon, Yoon, Sang-Jun, Jung, Gwan-Young, Thuong, Phuong-Thien & Oh, Won-Keun, 2023, Unique guanidine-conjugated catechins from the leaves of Alchornea rugosa and their autophagy modulating activity, Phytochemistry (113521) 206, pp. 113521-113521 : 2-8

| | |
|---|---|
| publication ID | https://doi.org/ 10.1016/j.phytochem.2022.113521 |
| DOI | https://doi.org/10.5281/zenodo.8169230 |
| persistent identifier | https://treatment.plazi.org/id/9E75879A-FFF7-FF8F-6952-B0FFFF7AF9B6 |
| treatment provided by | Felipe (2023-07-18 16:54:28, last updated 2023-08-17 16:09:01) |
| scientific name | Alchornea rugosa |
| status | |

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Treatment

References

Figures

Tables

Copyright notice

Taxonomy

| | |
|---|---|
| Kingdom | Plantae |
| Phylum | Tracheophyta |
| Class | Magnoliopsida |
| Order | Malpighiales |
| Family | Euphorbiaceae |
| Genus | Alchornea |

Distribution Map

Specimens

Downloads & Links

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Version History

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# Alchornea rugosa (Lour.) Muell. Arg.

Doan, Thi-Phuong, Park, Eun-Jin, Ryu, Byeol, Cho, Hyo-Moon, Yoon, Sang-Jun, Jung, Gwan-Young, Thuong, Phuong-Thien & Oh, Won-Keun, 2023, Unique guanidine-conjugated catechins from the leaves of Alchornea rugosa and their autophagy modulating activity, Phytochemistry (113521) 206, pp. 113521-113521 : 2-8

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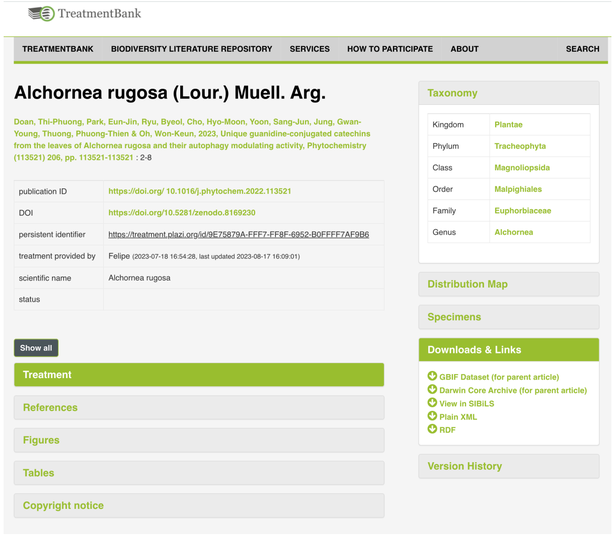


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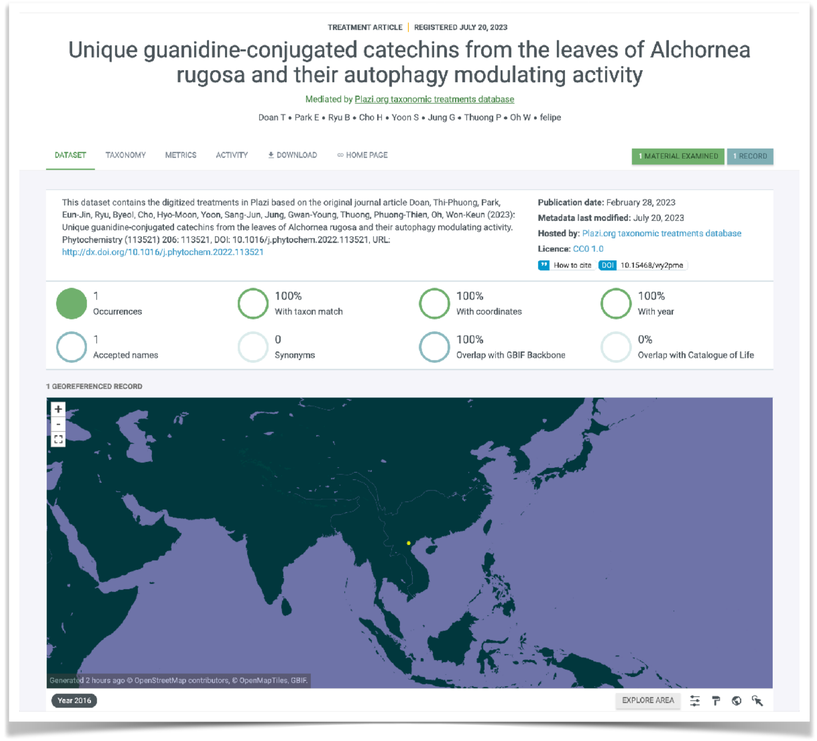

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# Phytochemistry

Year: 2011 – 2023

| | | |
|---|---|---|
| **1742** Articles | **17084** Processed Pages | **554** Taxonomic Treatments |
| **532** Tables | **8868** Figures | **8613** Figures on Zenodo |
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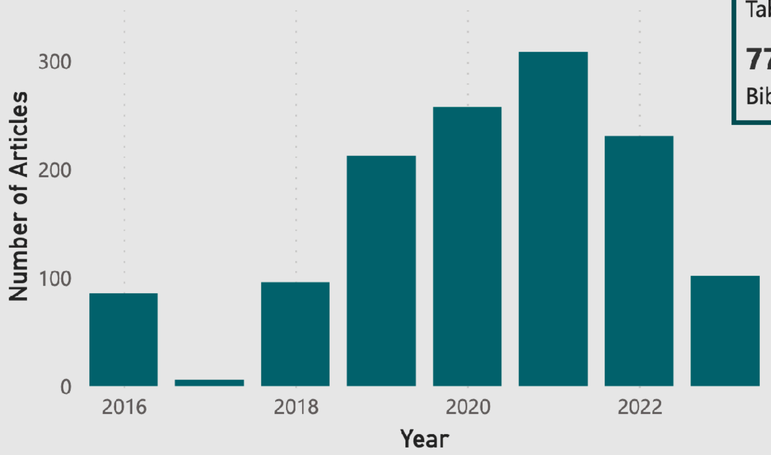
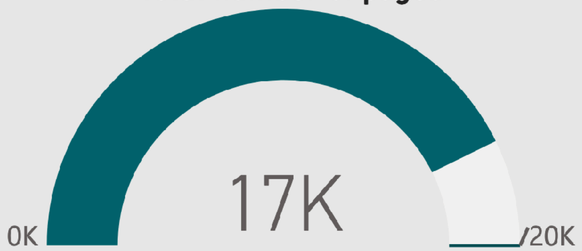
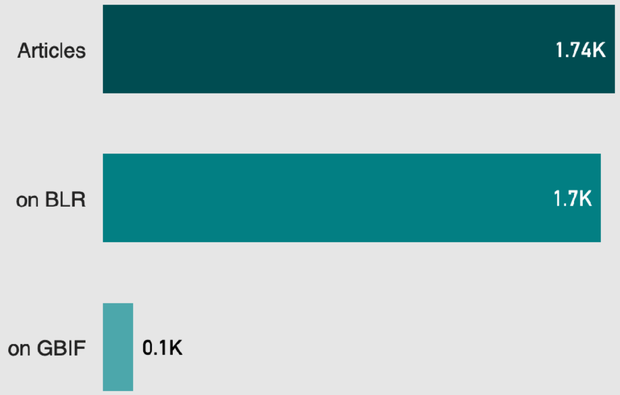
## Number of Articles by Year




## Total number of pages




## Articles, on BLR and on GBIF

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# Phytochemistry

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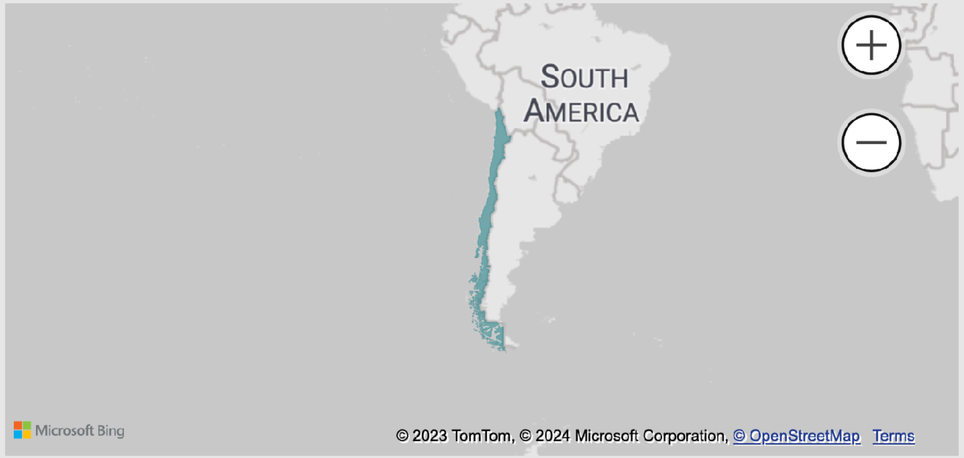
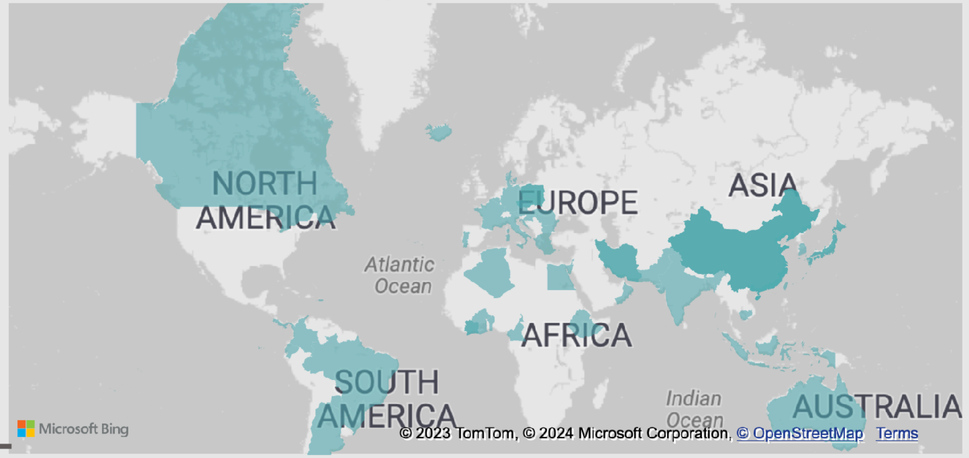



## Author Affiliation by Country




| Authors | Articles |
|---|---|
| Zhang, Yonghui | 30 |
| Zhu, Hucheng | 23 |
| Lin, Bin | 21 |
| Song, Shao-jiang | 21 |
| Chen, Chunmei | 20 |
| Huang, Xiao-Xiao | 19 |
| Li, Xiao-Nian | 18 |
| Wang, Jianping | 16 |
| Chen, Gang | 15 |
| Yao, Guo-Dong | 13 |
| **Total** | **11819** |

| MatCitCountry | Materials Citation |
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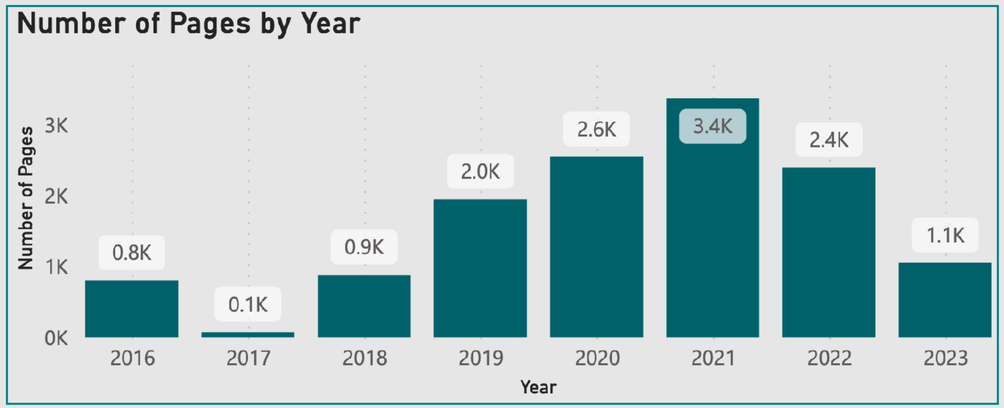
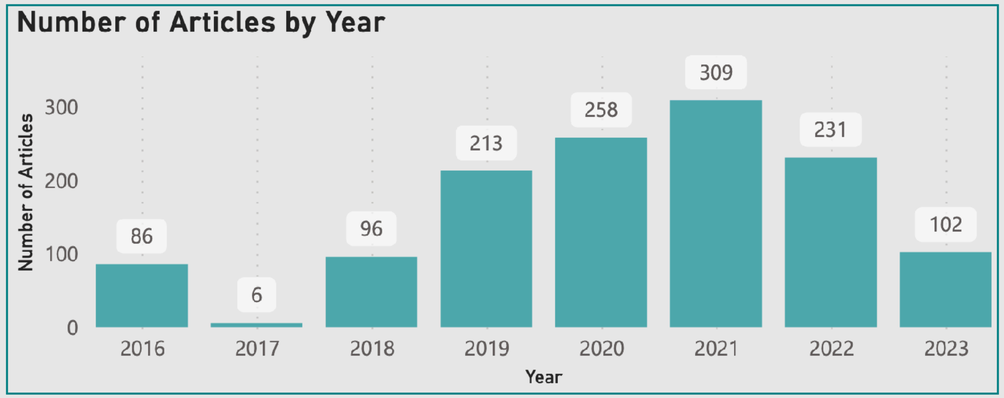
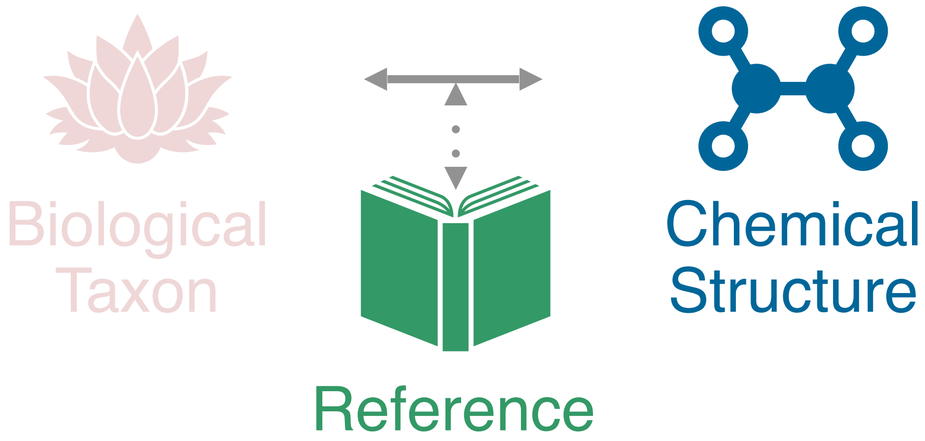
# Phytochemistry



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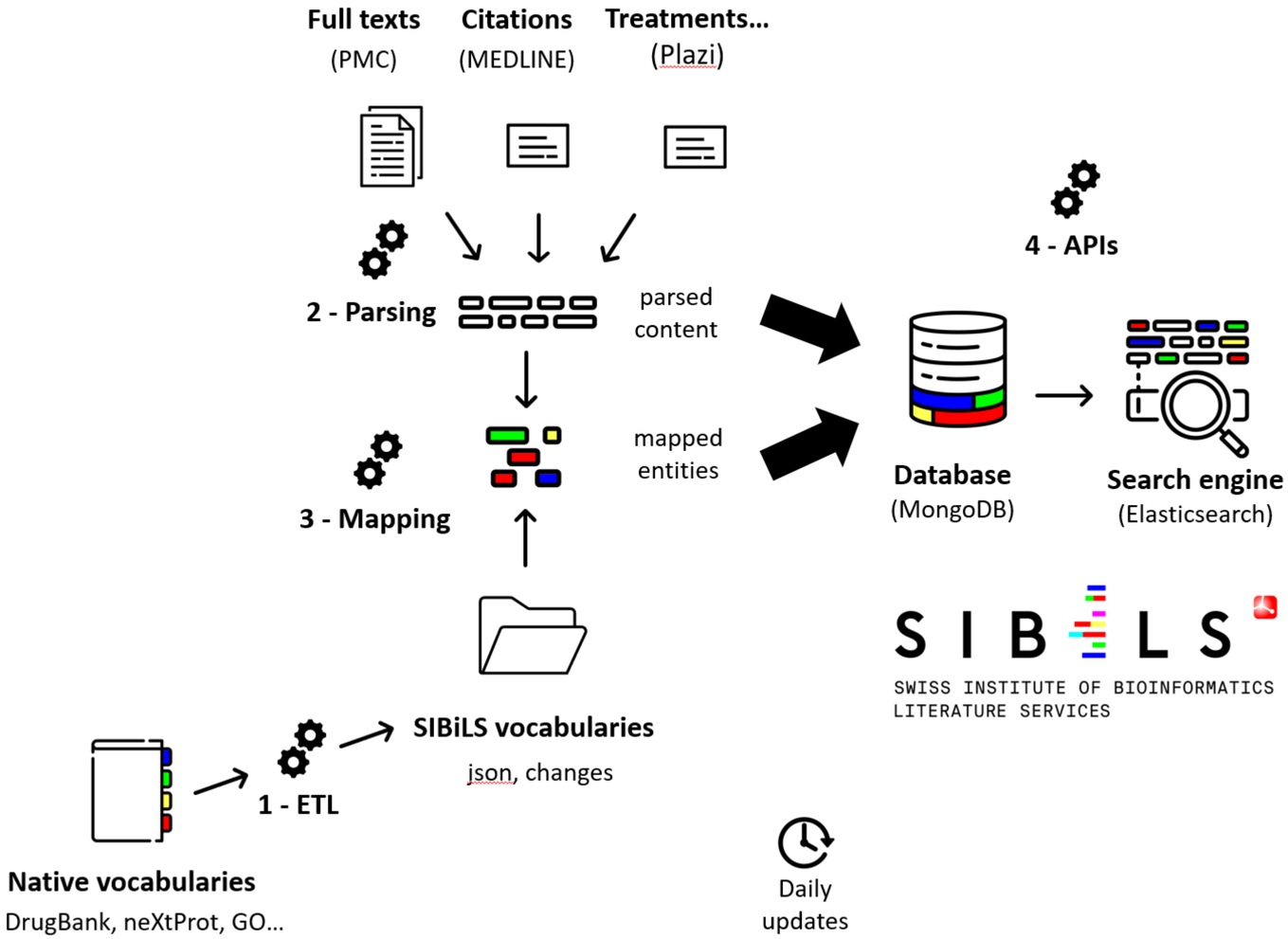

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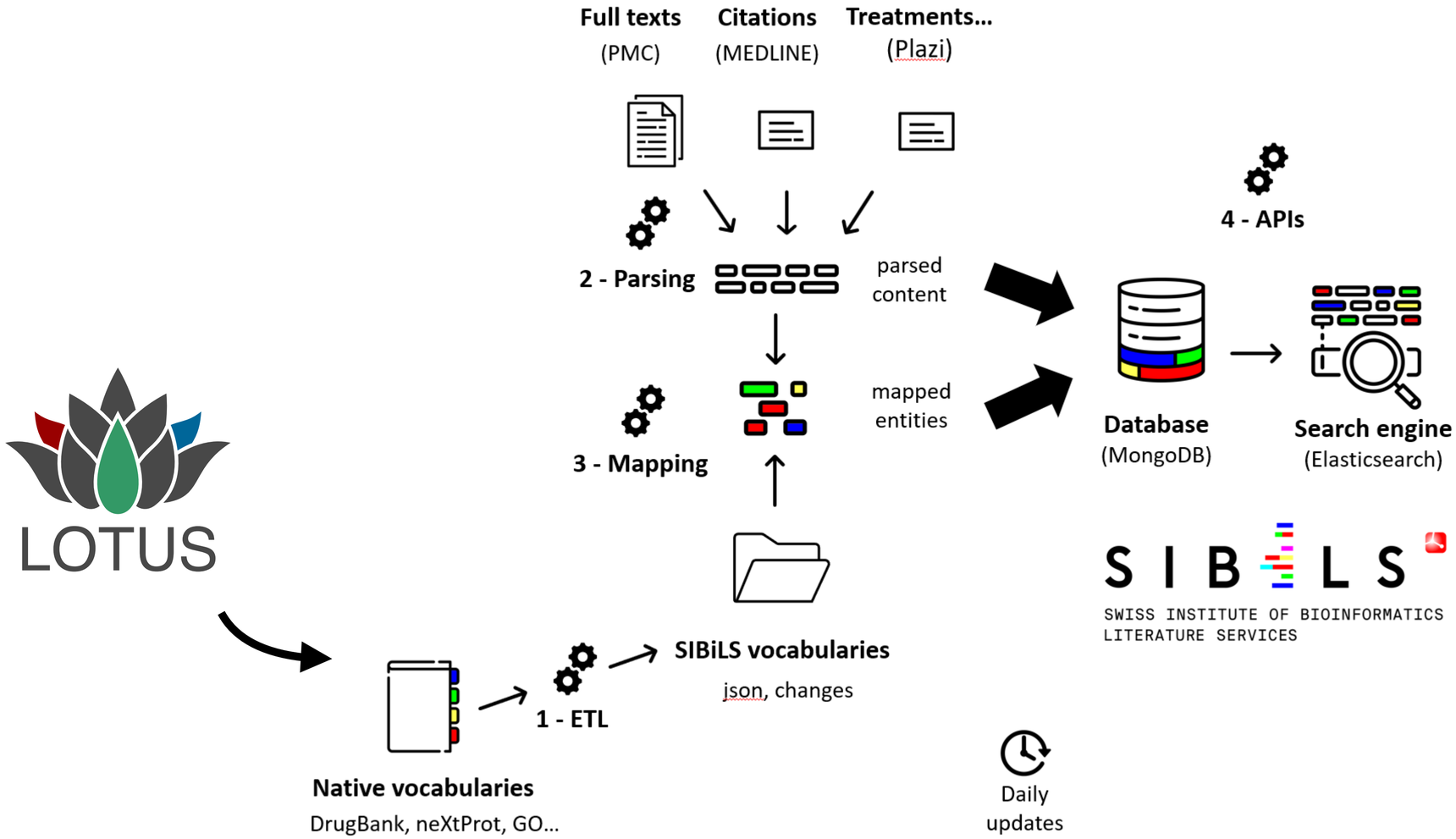

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| *September 2023* | | Medline | PMC | PMC (Author manuscripts) | PMC (Supplementary data) | Plazi | Pensoft |
|---|---|---|---|---|---|---|---|
| Nb documents (files for suppdata) | | 36,142,609 | 5,546,055 | 839,396 | 6,507,981 | 629,807 | 5,524 |
| Nb annotations | **Lotus** | **31,056,431** | **53,110,654** | **10,458,980** | **2,978,799** | **47,551** | **5,507** |
| | **PubChem (subset)** | **338,414,792** | **993,787,345** | **189,916,224** | **76,175,901** | **7,836,483** | **749,143** |
| **Avg biodiv chemicals anns/doc (anns/fils for suppD)** | | **10** | **189** | **12** | **239** | **13** | **137** |

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# Extraction of chemical structures information

1

Trigocherrin A, the first natural chlorinated daphnane diterpene orthoester from Trigonostemon cherrieri.

22182207. Allard Pierre-Marie, Martin Marie-Thérèse, Dau Marie-Elise Tran Huu, Leyssen Pieter, Guéritte Françoise, Litaudon Marc. 2011-12-21. Organic letters. Journal Article, Research Support, Non-U.S. Gov't.
Links

score 70.13

One Tab View

Show concept links

PMCA viewer v1.2

Org Lett - - ():. - PMID: 22182207 - DOI: 10.1021/ol2030907

Author(s): Allard Pierre-Marie , Martin Marie-Thérèse , Dau Marie-Elise Tran Huu , Leyssen Pieter , Guéritte Françoise , Litaudon Marc .

Affiliations

Centre de Recherche de Gif, Institut de Chimie des Substances Naturelles, CNRS, 1, Avenue de la Terrasse, 91198 Gif-sur-Yvette Cedex, France.

## Trigocherrin A lotus, the first natural chlorinated daphnane diterpene orthoester from Trigonostemon ncbitaxon_full ncbitaxon_full cherrieri ncbitaxon_full.

### Abstract

Trigocherrin A lotus, a chlorinated and highly oxygenated daphnane diterpenoid orthoester (DDO), was isolated from the bark of Trigonostemon ncbitaxon_full ncbitaxon_full cherrieri ncbitaxon_full. Trigocherrin A lotus is the first example of a naturally occurring halogenated DDO. Its structure was elucidated by comprehensive analysis of NMR spectroscopic data, and its absolute configuration was determined by comparison of experimental and theoretically calculated ECD spectra. Trigocherrin A lotus exhibited a potent and selective effect against Chikungunya virus ncbitaxon_full in Vero cells.

### MeSH terms

- D000818:Animals
- D000998:Antiviral Agents
- D001688:Biological Products
- D002646: Chikungunya virus ncbitaxon_full

Affiliations (1)
ATC (2)
ChEBI (10)
ICTV International Committee on Taxonomy of Viruses (2)
LOTUS Natural Products (5)
MeSH (17)
NCBI Taxonomy Clinic (1)
NCBI Taxonomy Full (6)
NCI Thesaurus (2)
neXtProt (4)
OTT - Open Tree of Life (4)
psimi (2)

Search: Clear

Trigocherrin A: lotus:Q105674316
Trigonostemon cherrieri: ncbitaxon_full:2606815
Trigonostemon cherrieri: Query terms:
Trigonostemon: Query terms:
cherrieri: Query terms:
Trigocherrin A: lotus:Q105674316
Trigonostemon cherrieri: ncbitaxon_full:2606815
Trigonostemon cherrieri: Query terms:
Trigonostemon: Query terms:
cherrieri: Query terms:
Trigocherrin A: lotus:Q105674316
Trigocherrin A: lotus:Q105674316

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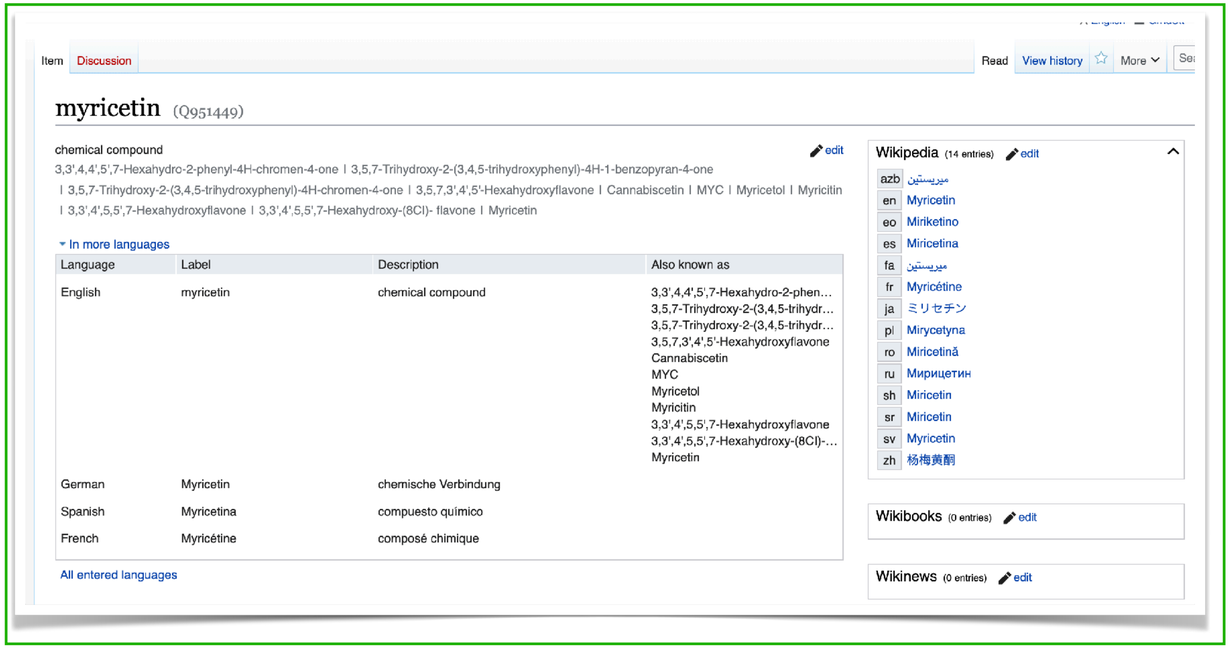
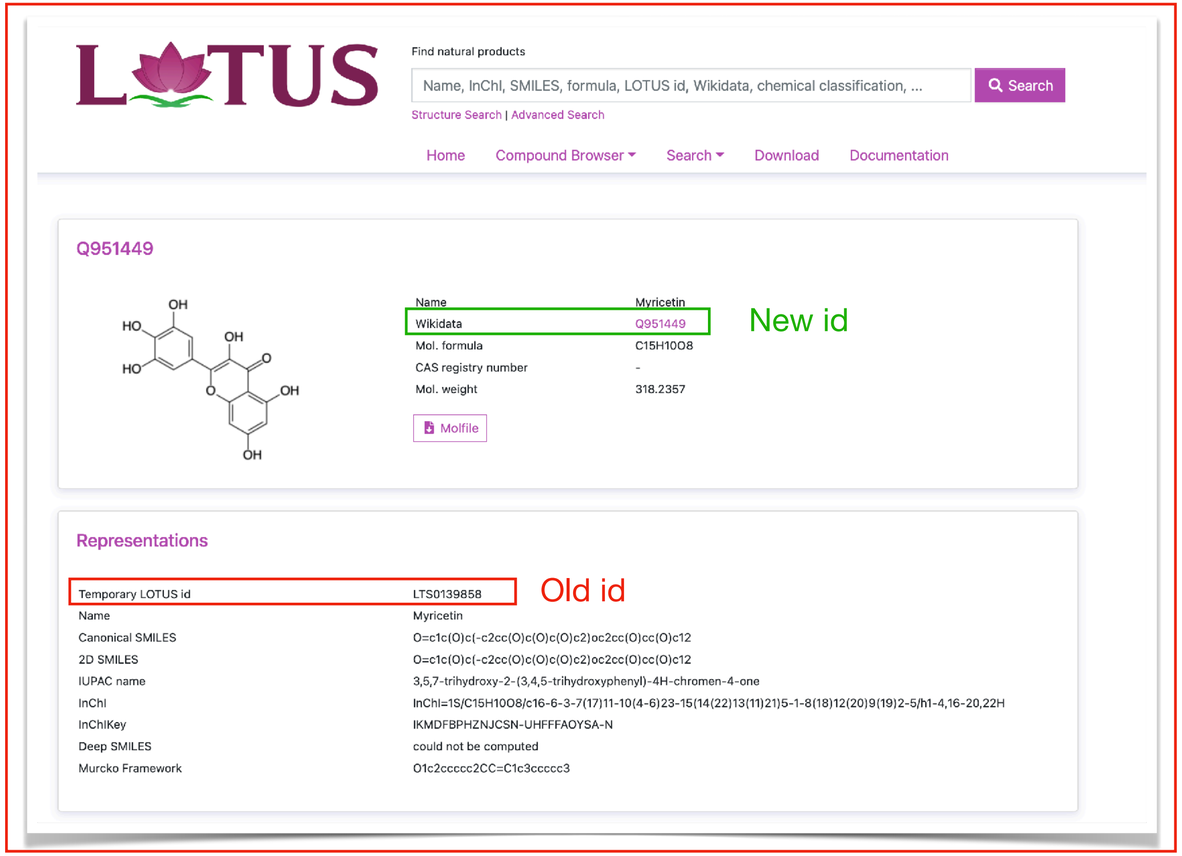
# Extraction of chemical structures information

prefered source

WIKIDATA




Old source

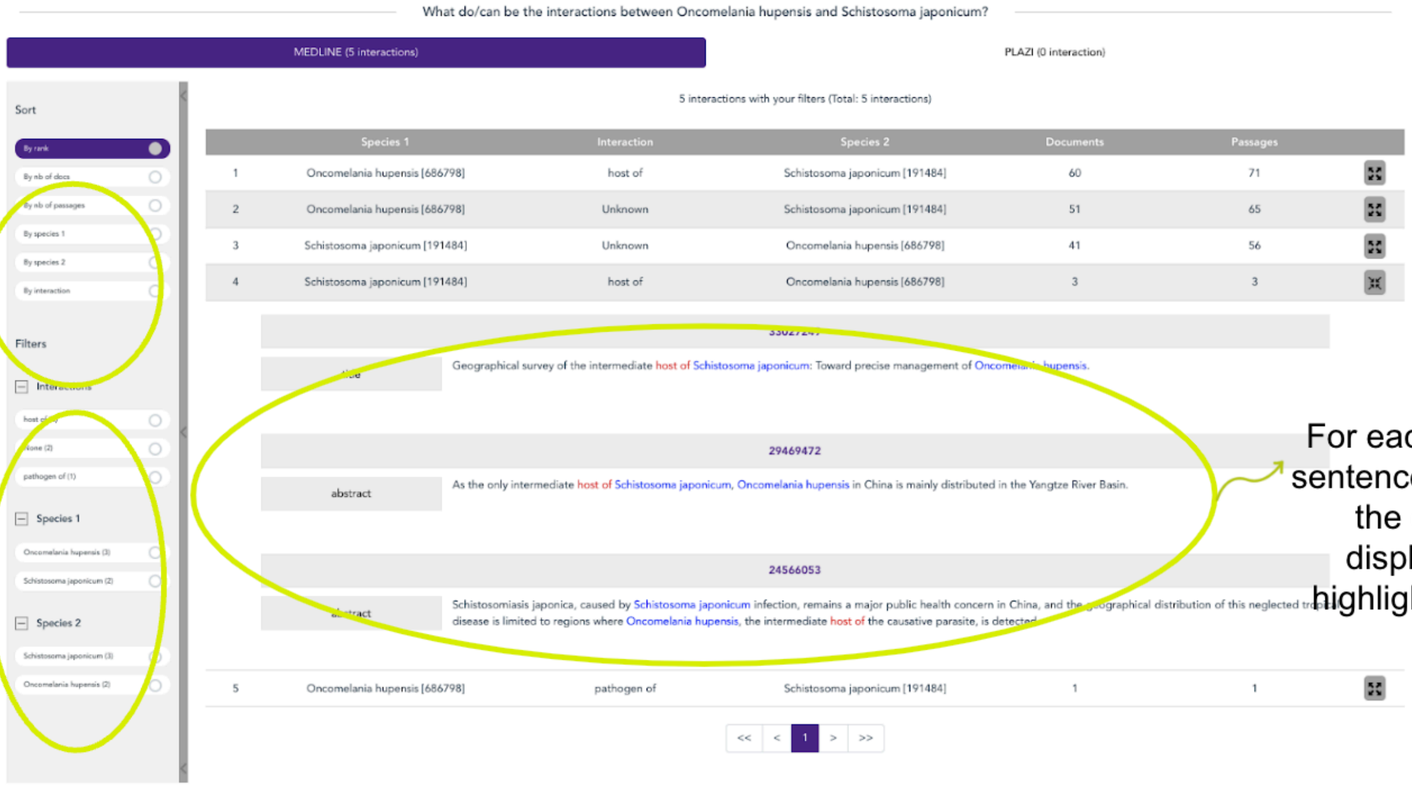


Finding molecules and organisms is not enough !

## *Biotic interaction triplets - User Interface*

Documents can be sorted by relevance, species, etc

Results can be filtered (e.g. species, interactions)




For each triplet, the sentences supporting the claim are displayed with highlighted entities

**Chemical structures / Biological organism relation explorer**

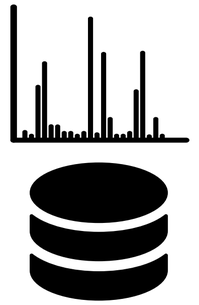
molecule X ***is produced by*** organism Z
molecule X ***is found in*** organism Z
molecule X ***is toxic for*** organism Z
molecule X ***attracts*** organism Z

# OBO Relation Ontology

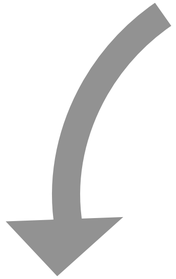
Website for RO

Documentation and User Guide

View Repository on GitHub



Future knowledge



BiC IKL

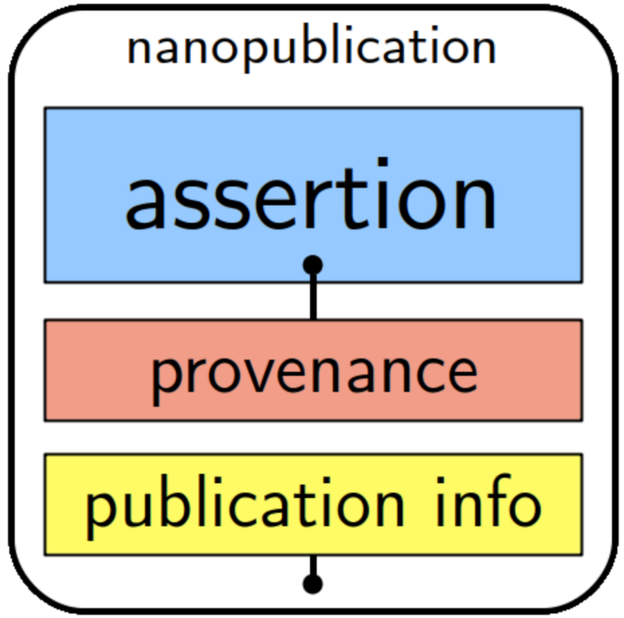
knowledge
pixels

**How do we improve *future* knowledge dissemination ?**

## Nanowhat?

A nanopublication is a tiny snippet of information encoded in a knowledge graph format that computers can understand. This information can be about anything, for example, a relation between a gene and a disease, an opinion, or an assessment of another nanopublication. For more, see nanopub.net.

knowledge pixels




As can be seen in this image, a nanopublication has three basic elements:

1. **Assertion**: The assertion is the main content of a nanopublication in the form of an small atomic unit of information
2. **Provenance**: This part describes how the assertion above came to be. This can include the scientific methods that were used to generate the assertion, for example a reference to the kind of study that was performed and its parameters.
3. **Publication Info**: This part contains metadata about the nanopublication as a whole, such as when and by whom it was created and the license terms for its reuse.

Nanopublications are implemented in the language RDF and come with an evolving ecosystem of tools and systems. They can be published to a decentralized server network, for example, and then queried, accessed, reused, and linked. To find out more, see the guidelines, the examples, or the published articles about nanopublications.

https://nanodash.petapico.org/publish?11&template=http:**Apurl.org*np*RA1ekjkshpkdtjNKNnCbdHlGRfT65IkN6sttki16dzvvw

# Publish a new Nanopublication

**Assertion:** Expressing a sample metabolite annotation ^

An extract has as lab process a sample .

The extract has the taxon the taxon (e.g. species) .

The sample has the label " the label of the sample " .

The sample has the analysis an LCMS analysis .

The LCMS analysis has as feature list a feature list .

The feature list has as LCMS feature a feature .
The feature has the annotation a sirius annotation .
The sirius annotation is identified by the InChIkey2D InChIKey2D .
The sirius annotation has the sirius score " the sirius score value " .
The sirius annotation has the sirius adduct " the sirius adduct value " .

**Provenance:** Attributed to myself ^

The assertion above is attributed to me (Pierre-Marie Allard) .

**Publication info** add element...

Creator: ^

This nanopublication is created by me (Pierre-Marie Allard) .

With license: ^

This nanopublication is published under the license Attribution 4.0 International (CC BY 4.0) .

I understand that publishing cannot be fully undone and that the provided information will be publicly visible and openly connected to my ORCID identifier (but nanopublications can be retracted, which makes them invisible in most situations).

Publish

https://nanodash.petapico.org/explore?3&id=http://purl.org/np/RAtD9MFh9nso72l76ntW7V7_i5FhFE19Ze9M5OArIyxGI
http://purl.org/np/RAtD9MFh9nso72l76ntW7V7_i5FhFE19Ze9M5OArIyxGI

## Nanopublication: RAtD9MFh9n

RAtD9MFh9n

```
extract   has as lab process   sample   .
extract   has the taxon   Tabernaemontana coffeoides (species)   .
feature   has the annotation   sirius-annotation   .
feature-list   has as LCMS feature   feature   .
lcms-analysis   has as feature list   feature-list   .
sample   has the label   "V114006GP-01"   .
sample   has the analysis   lcms-analysis   .
sirius-annotation   is identified by   RWRDIJCXMDTYOZ   .
sirius-annotation   has the sirius score   "35.89209590424093"   .
sirius-annotation   has the sirius adduct   "[M+H]+"   .
```

```
this assertion   is attributed to   sirius_mzspec:MSV000087728:VGF152_B02_features_ms2_pos.mgf:scan:673   .
```

```
this   created   "2023-07-09T07:10:43.610Z"   .
this   is created by   me (Pierre-Marie Allard)   .
this   is published under the license   Attribution 4.0 International (CC BY 4.0)   .
this   introduces   extract   .
this   is an   example nanopublication   .
this   wasCreatedFromProvenanceTemplate   RANUBzTXWg   .
this   wasCreatedFromPubinfoTemplate   RA5gNHxO43   .
this   wasCreatedFromPubinfoTemplate   RAA2MfqdBC   .
this   wasCreatedFromPubinfoTemplate   RAh1gm83Ji   .
this   wasCreatedFromTemplate   RA1ekjkshp   .
sig   hasAlgorithm   "RSA"   .
sig   hasPublicKey
"MIGfMA0GCSqGSIb3DQEBAQUAA4GNADCBiQKBgQCt5+6whGAxG+GntPXngTIho+nH+5j7QoAP98ha0lDVe9+gG2gBASbTY5CD3+6pEh52+JXqPhG+gA78lJWhE6C4YshcPh6wuzRmwmgclvXc5/dTKsVQQX7Ch2i3EavuRHPqJrXyynow5PEWQml
2ojknU5wfpUt5150UdvLbz4bGCwIDAQAB"   .
sig   hasSignature
"CNZ+2K/0hBETcLXMqpQPsE6fimiQV3et5UXnFZeGenzLSVAPuCCBDcil/Q7rDR0DqnJOcCCwASD53UhvT5i6YhltIDTpzU7BtRmVjSqw47TzzfN0pVzXBUPayAsB/Caq/RGyJJ8PumtCxaizu1ssIaAnrYVsdcQcvKqUDB+SSNo="   .
sig   hasSignatureTarget   this   .
Tabernaemontana coffeoides (species)   hasLabelFromApi   "Tabernaemontana coffeoides (species)"   .
```

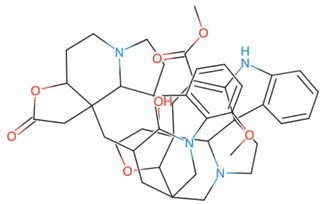
Pierre-Marie Allard 9 Jul 2023, 07:10:43 UTC

## References

| Nanopublication | Part | Subject | Predicate | Object | Published By | Published On |
|---|---|---|---|---|---|---|

No Records Found

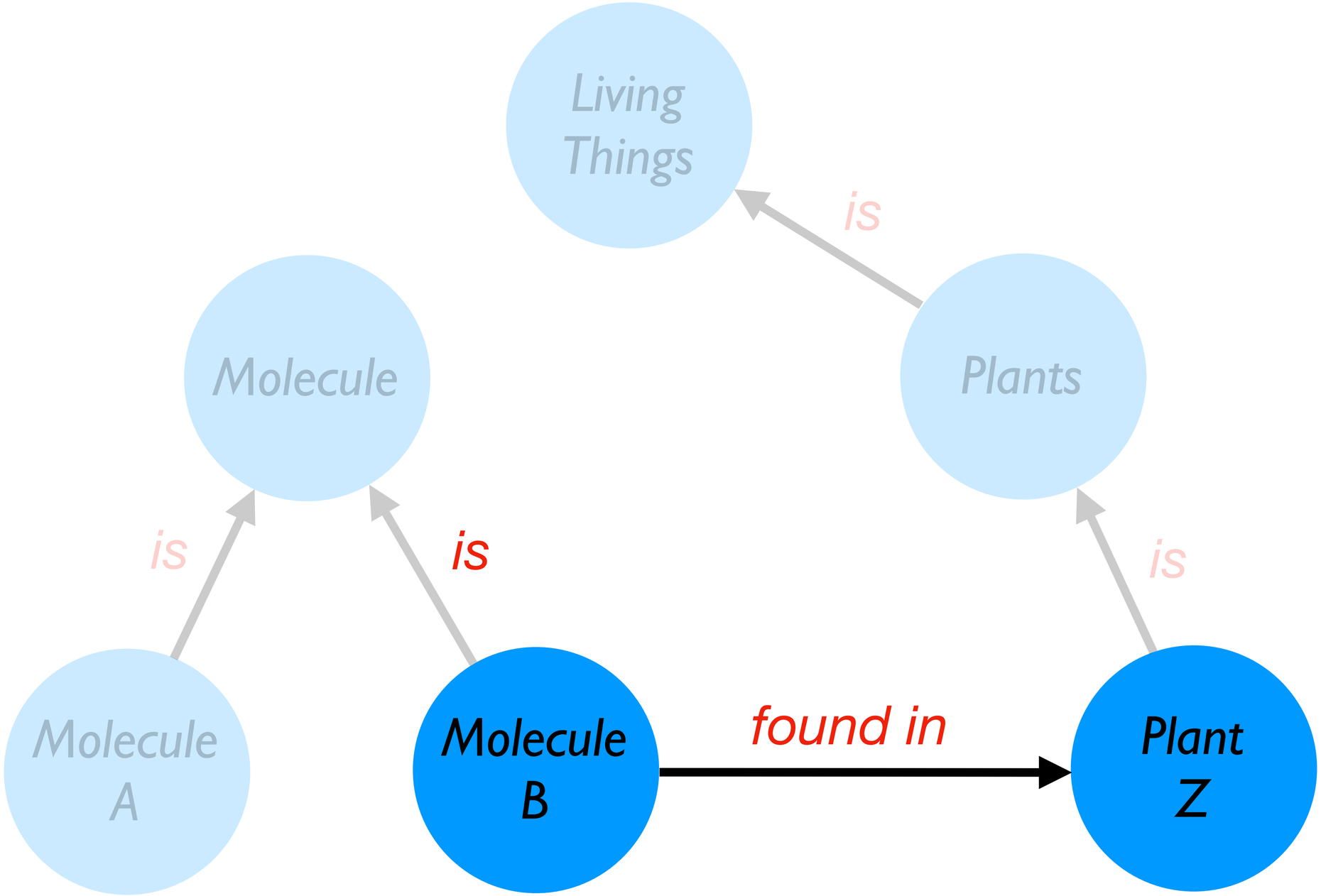
https://www.wikidata.org/wiki/Q82054121

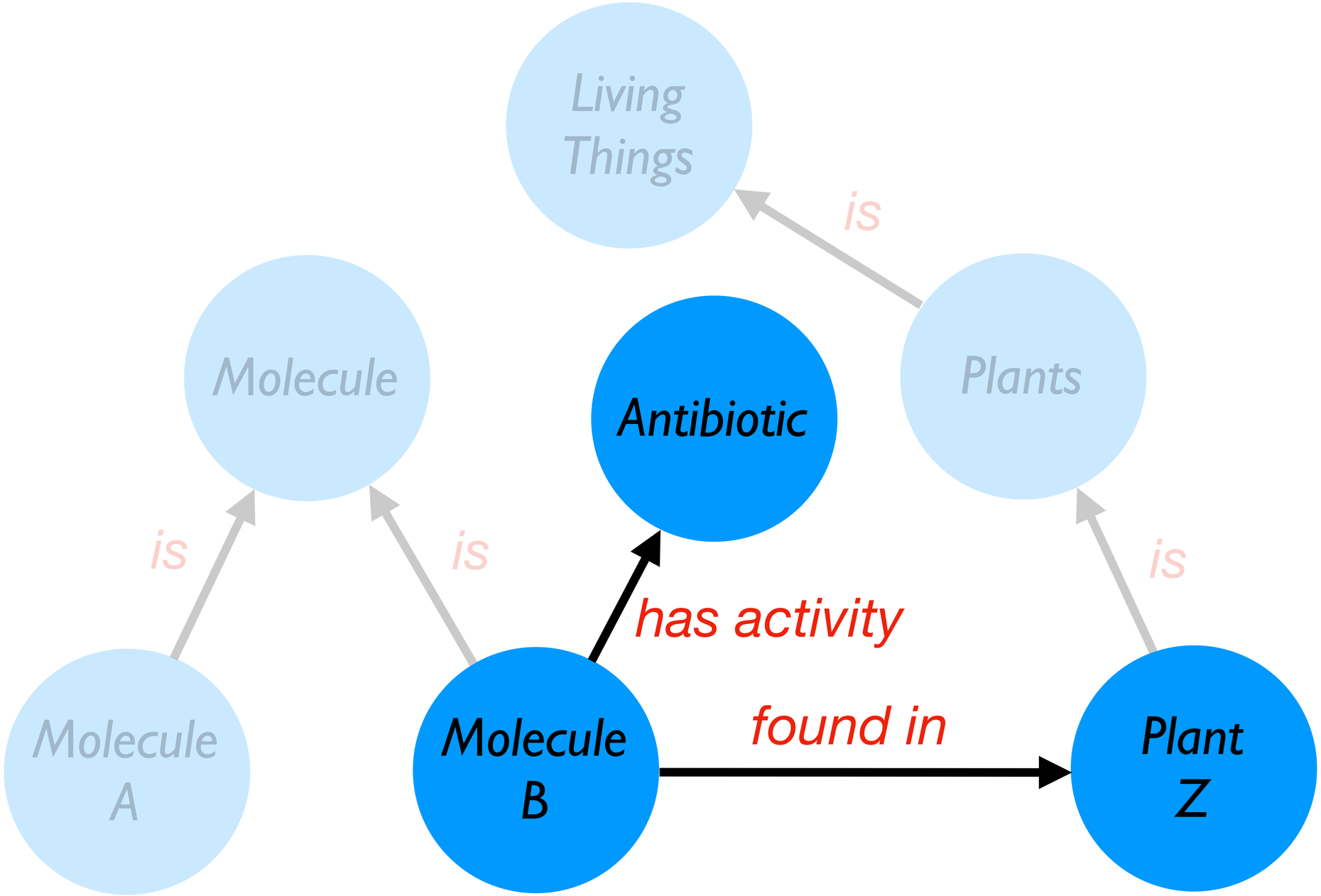
| | | |
|---|---|---|
| canonical SMILES | O=C(OC)C1=C2NC=3C=CC=CC3C24CCN5CC6(CN7C=8C(OC)=CC=CC8C9%10CCN%11CCC%12OC(=O)CC%12(CC(C6)C79O)C%11%10)C%13OCCC%13(C1)C54 | edit |
| | 0 references | |
| | | + add reference |
| |  | |
| | | + add value |

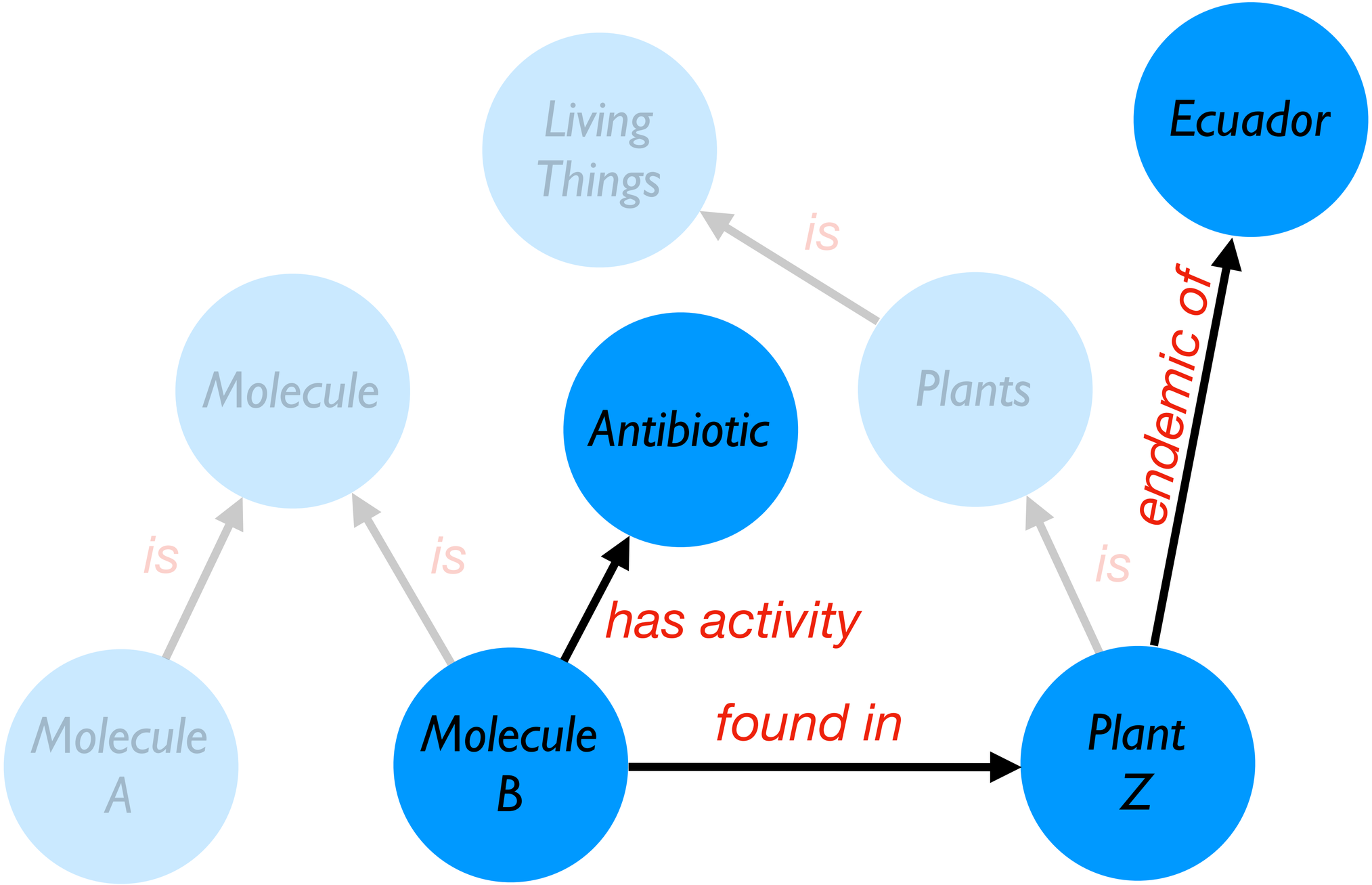
| | | |
|---|---|---|
| found in taxon | Tabernaemontana sphaerocarpa | edit |
| | 1 reference | |
| | stated in: Biscarpamontamines A and B, an aspidosperma-iboga bisindole alkaloid and an aspidosperma-aspidosperma bisindole alkaloid, from Tabernaemontana sphaerocarpa | |
| | | + add reference |
| | Tabernaemontana coffeoides | edit |
| | 1 reference | |
| | reference URL: http://purl.org/np/RAtD9MFh9nso72l76ntW7V7_i5FhFE19Ze9M5OArlyxGI | |
| | | + add reference |
| | | + add value |

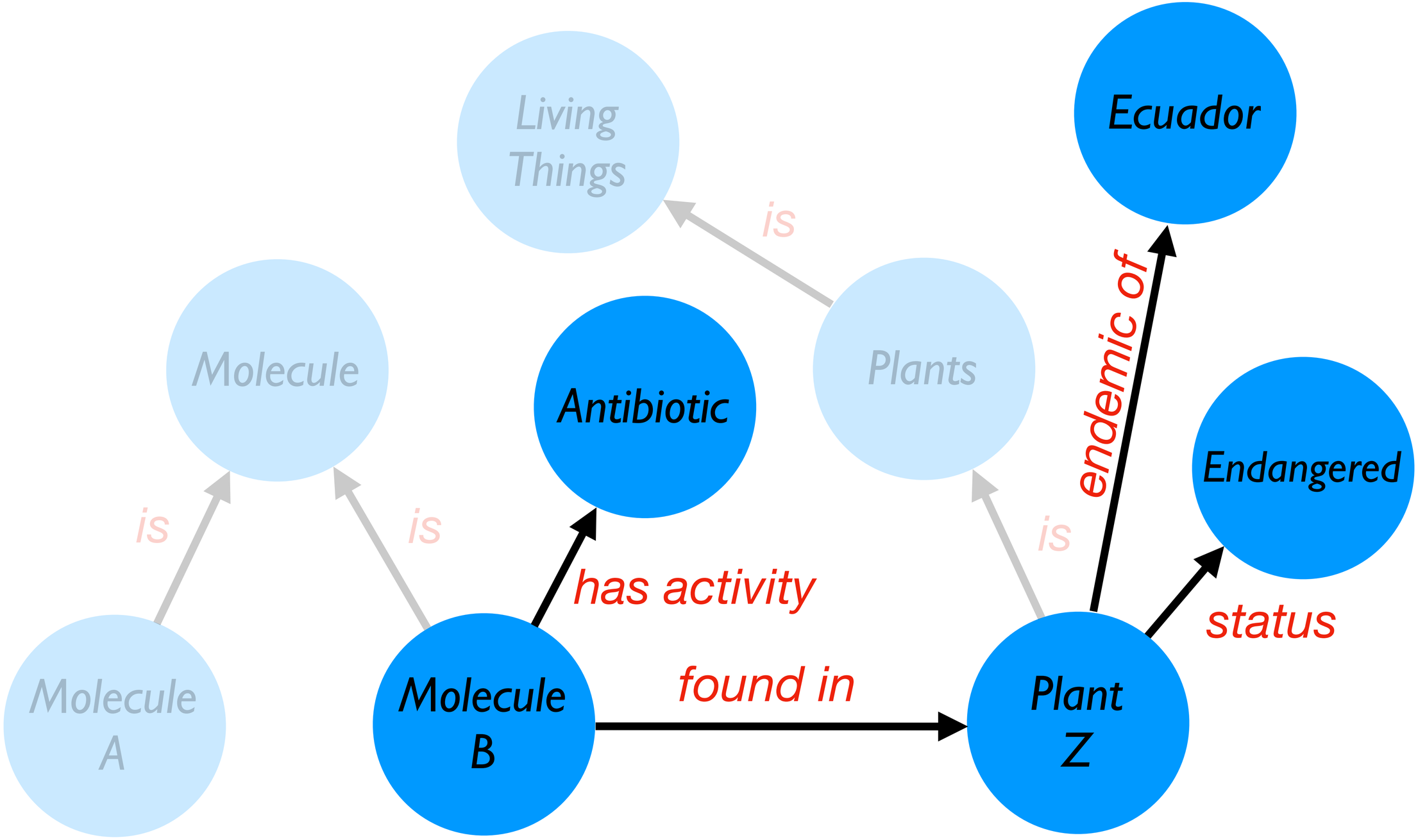
**Classical publication**

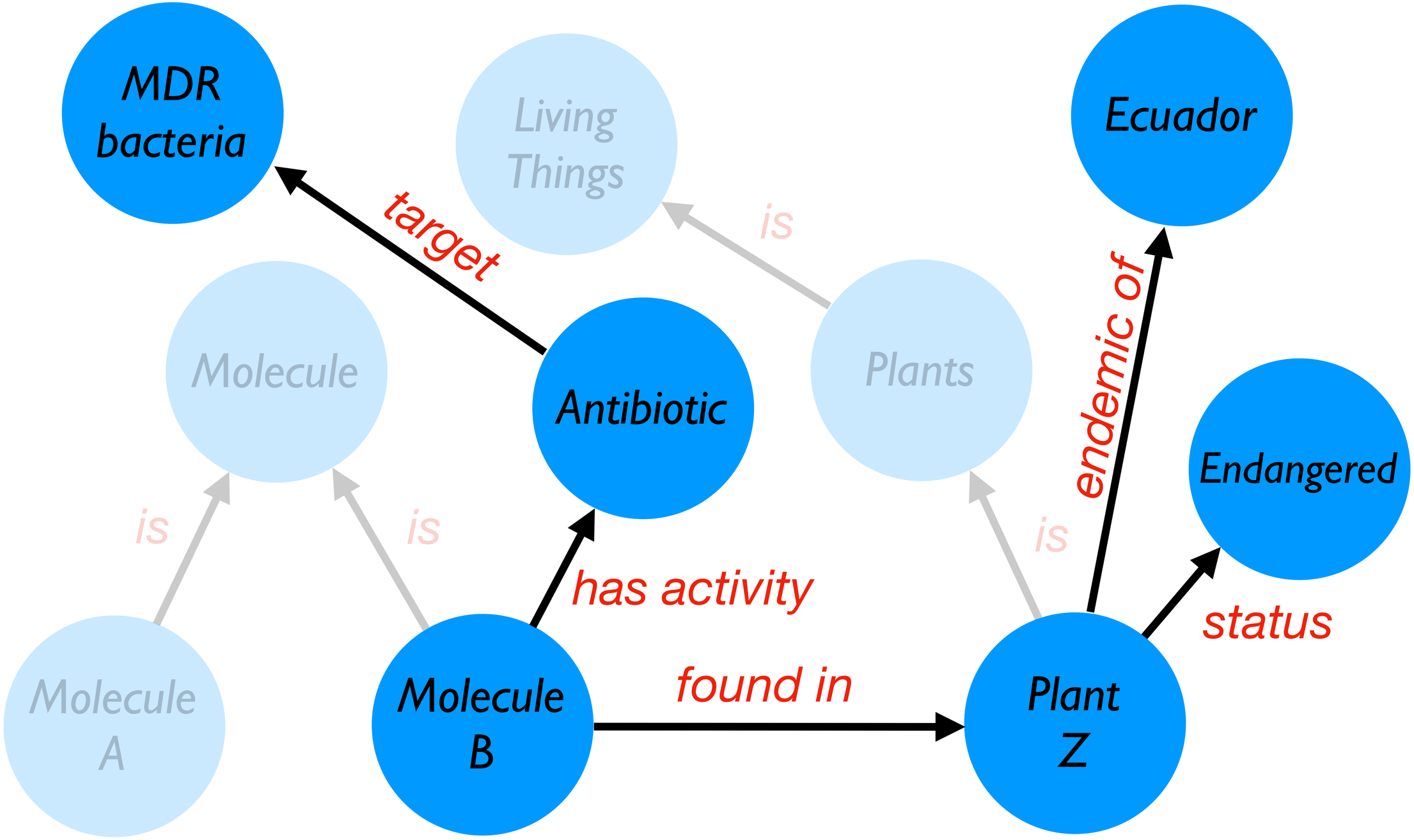
**Nanopublication**

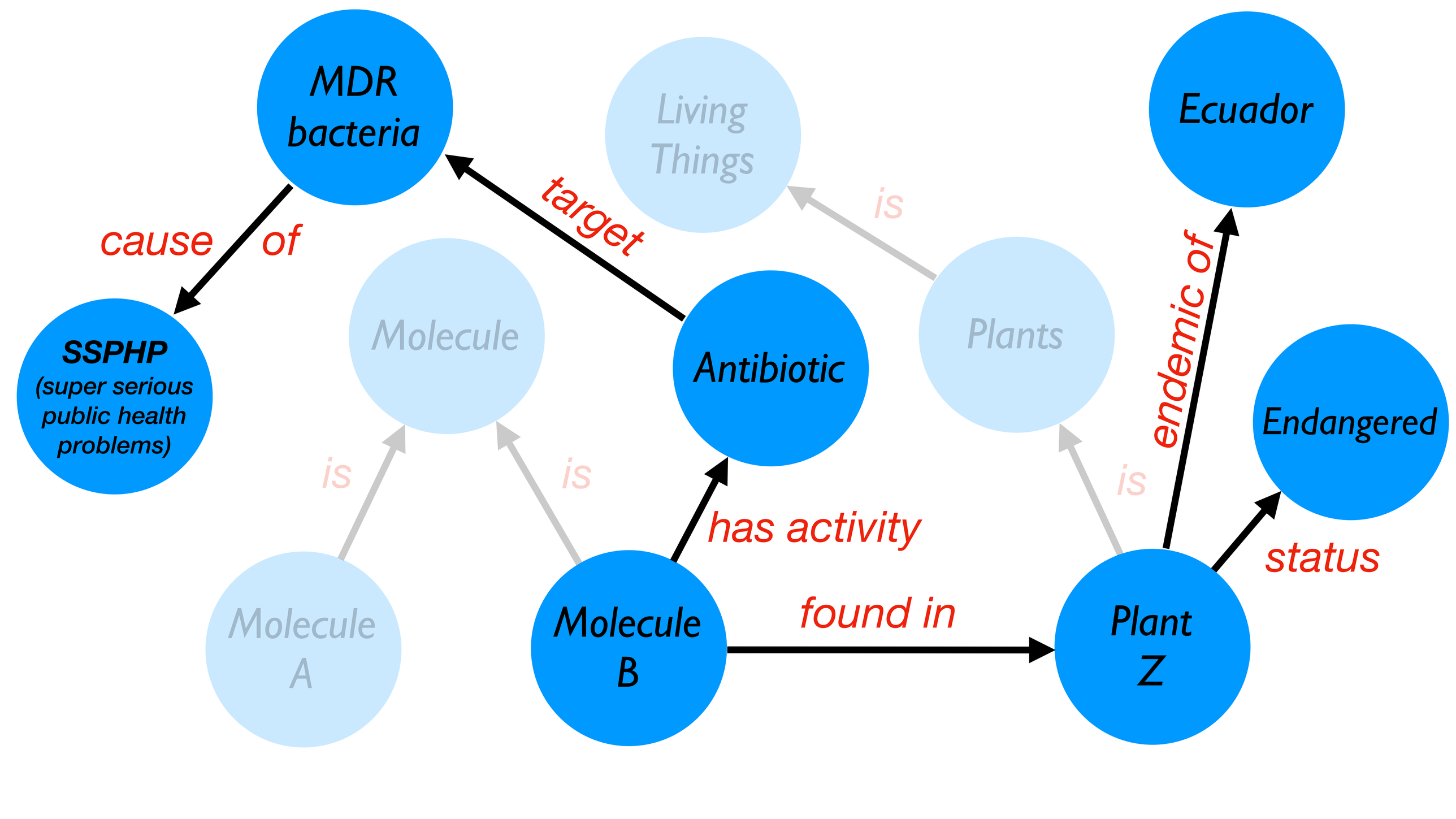

Living Things
is
Molecule
Plants
is
is
is
Molecule A
Molecule B
found in
Plant Z


Living Things
is
Molecule
Antibiotic
Plants
is
is
is
has activity
Molecule A
Molecule B
found in
Plant Z


Living Things
is
Ecuador
Molecule
Antibiotic
Plants
endemic of
is
is
has activity
is
Molecule A
Molecule B
found in
Plant Z


Living Things
is
Ecuador
Molecule
Antibiotic
Plants
endemic of
is
is
is
Endangered
has activity
status
Molecule A
Molecule B
found in
Plant Z


MDR bacteria
Living Things
Ecuador
target
is
endemic of
Molecule
Antibiotic
Plants
Endangered
is
is
is
has activity
status
Molecule A
Molecule B
found in
Plant Z


MDR bacteria
Living Things
Ecuador
cause of
target
is
endemic of
SSPHP
(super serious public health problems)
Molecule
Antibiotic
Plants
Endangered
is
is
is
has activity
status
Molecule A
Molecule B
found in
Plant Z

Donat Agosti

BiCIKL

EARTH METABOLOME INITIATIVE

LOTUS

DBGI
The Digital Botanical Gardens Initiative
www.dbgi.org

PLAZI
TAKING CARE OF FREEDOM

Guido Sauter

Felipe Simões

Tobias Kühn

knowledge pixels

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