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

UNI FR
Pierre-Marie Allard
COMMONS Lab
Université de Fribourg

https://doi.org/10.5281/zenodo.8363518

Swiss
Digital Botanical
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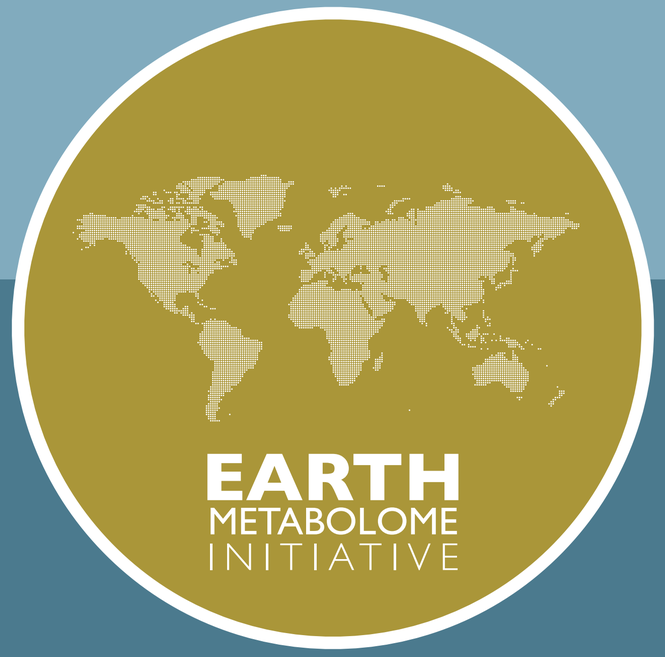
EARTH
METABOLOME
INITIATIVE

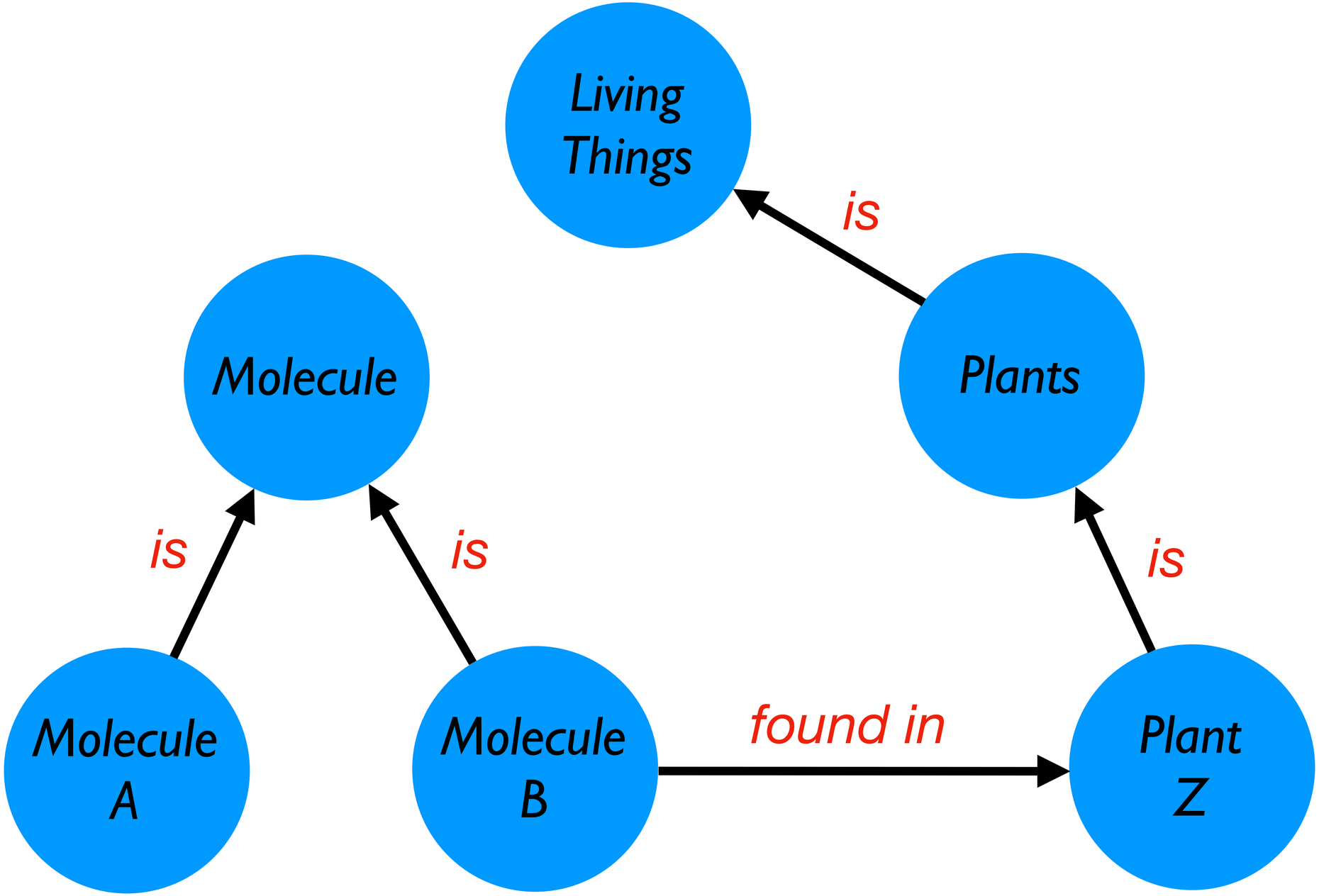
A massive undertaking ...

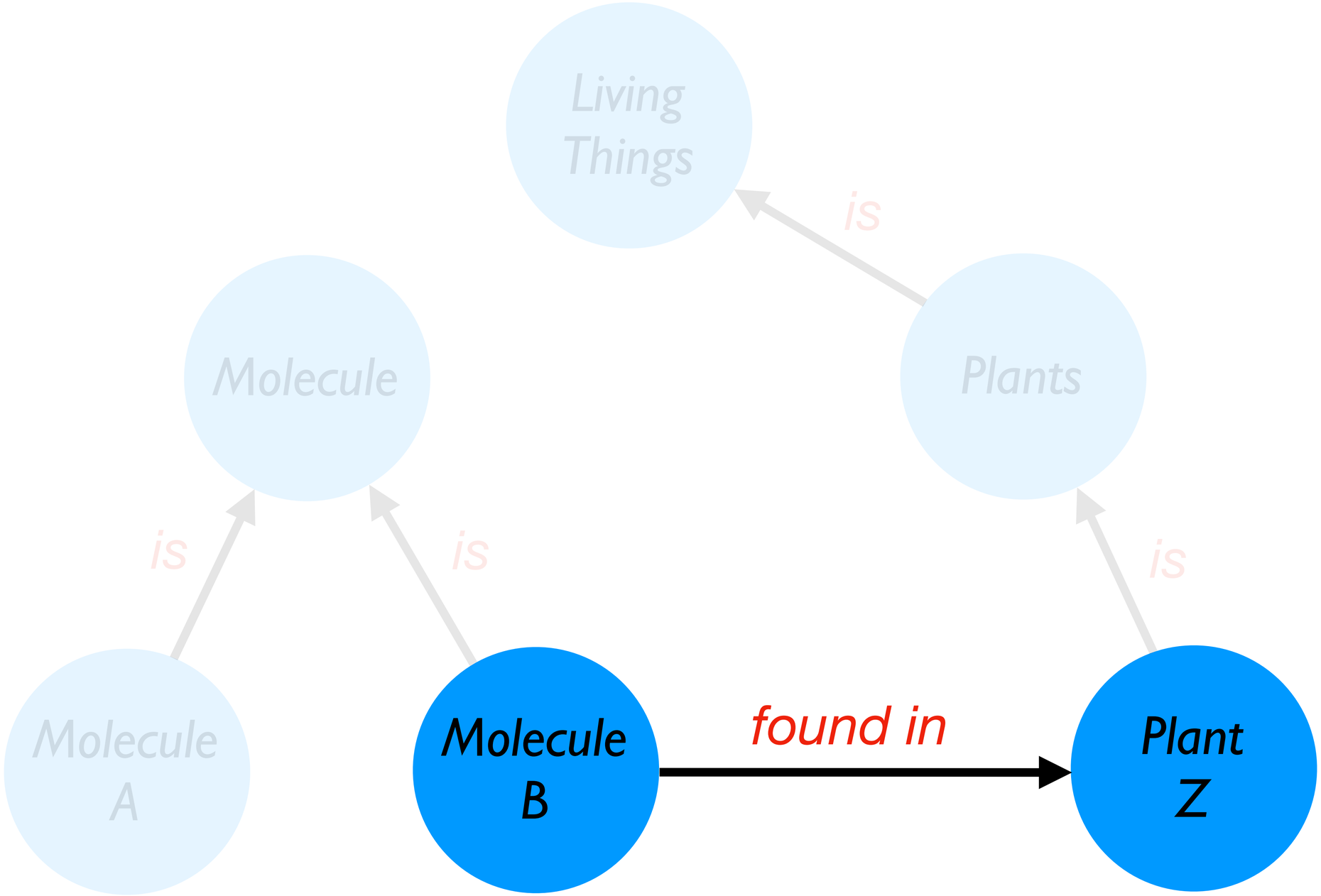


Profile the metabolic content of all currently known species on Earth.

... 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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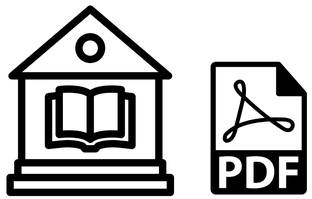

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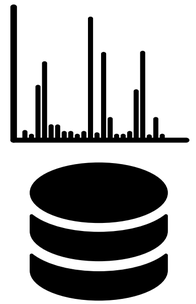
Past knowledge

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 ?

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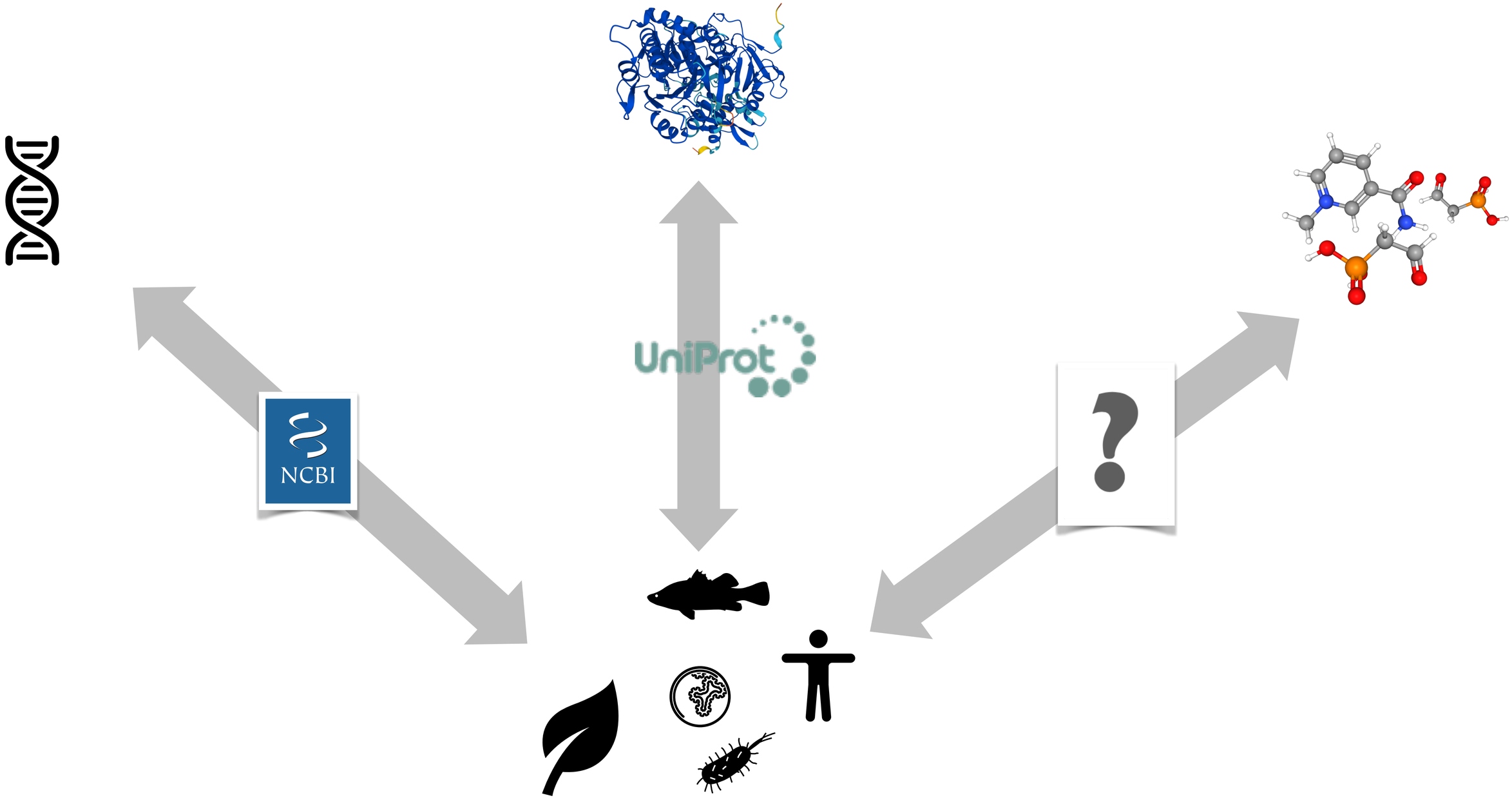
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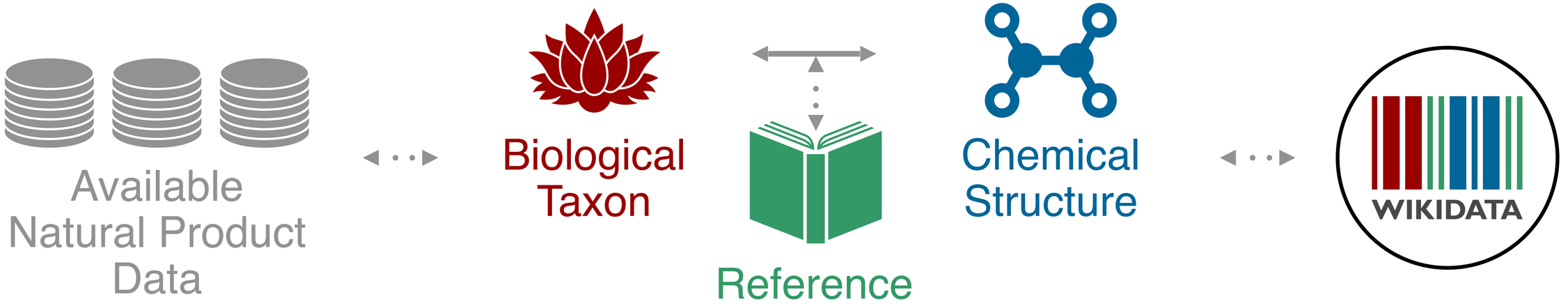

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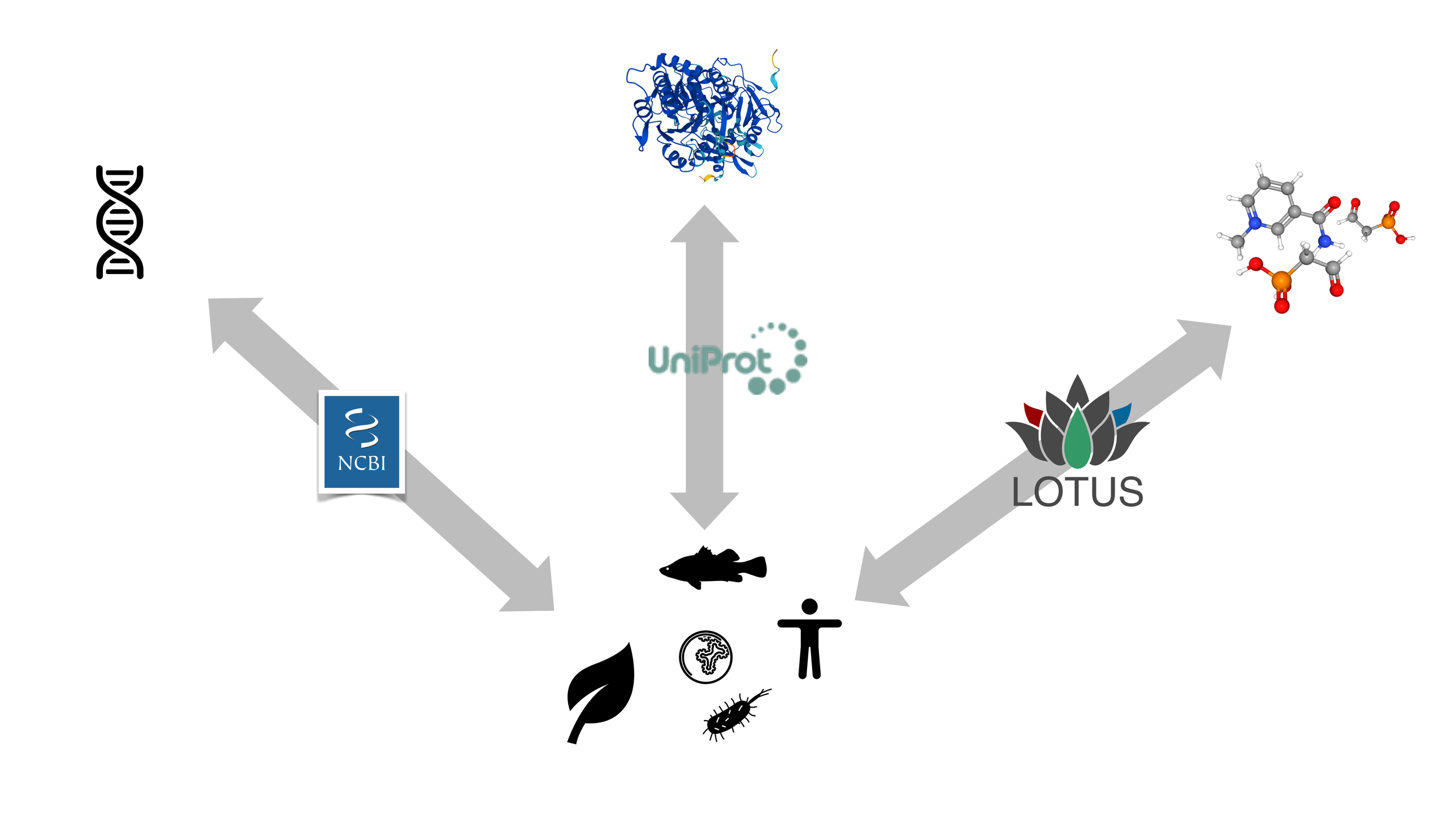
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PLANTES DE NOUVELLE CALÉDONIE. LV.*
ISOBORRÉVÉRINE ET BORRÉVÉRINE, ALCALOÏDES
BIS-INDOLIQUES DE *FLINDERSIA FOURNIERI*

François Tillequin et Michel Koch

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

Maryse Bert

Laboratoire de Matière Médicale, U.E.R. des Sciences Pharmaceutiques, 1, rue Vaubénard, F-14000-Caen

Thierry Sevenet

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

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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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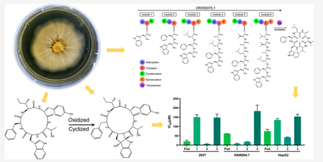
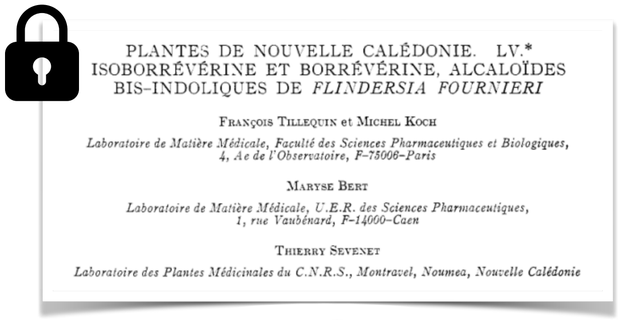
ABSTRACT: Three new cyclic peptides, meristosporins A, B, and C (**1**−**3**), one of which features an unusual amino acid, were isolated from the opportunistic pathogen *Basidiobolus meristosporus* and identified by 1D, 2D NMR, MS/MS, and Marfey's analysis. The biosynthetic pathway of the hexapeptide 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



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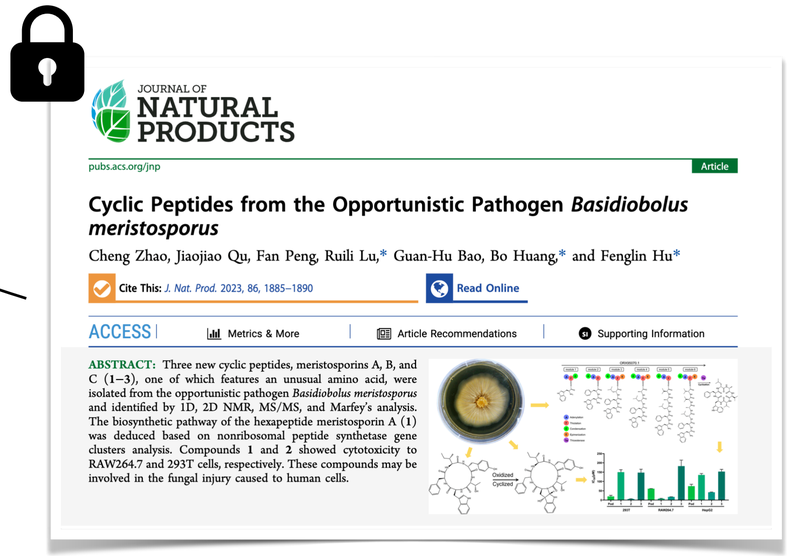

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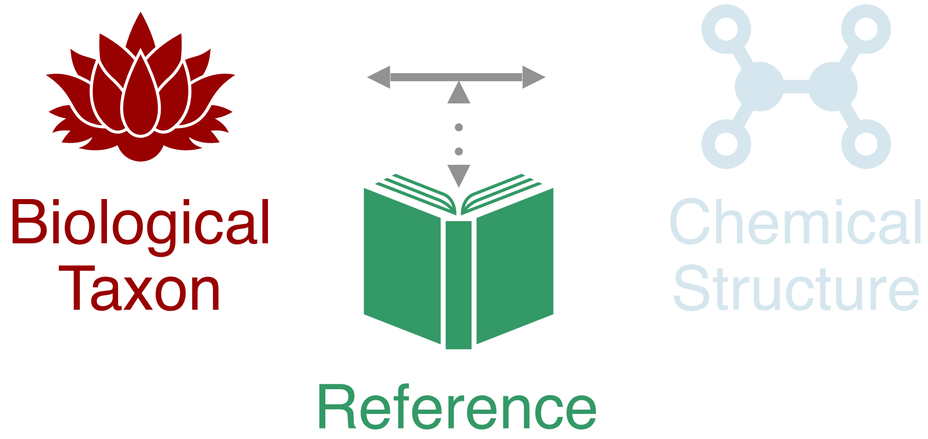
Molecule **found in** Organism



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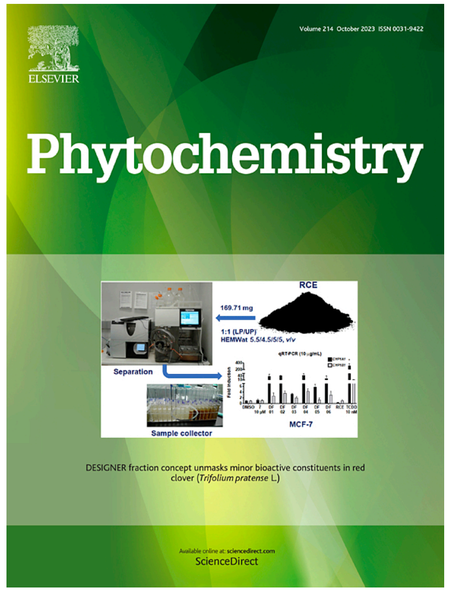

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1	BC47F915FFEB1332DA01FB0A61B1E9CF	407E816DFFED1334D933FF8B6478EF0D	Phytochemistry	In vitro
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Graphical abstract

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 HEK293cells stably expressing GFP-LC3.

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

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Alchornea rugosa (Lour.) Muell. Arg.

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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
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Taxonomy

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

Distribution Map

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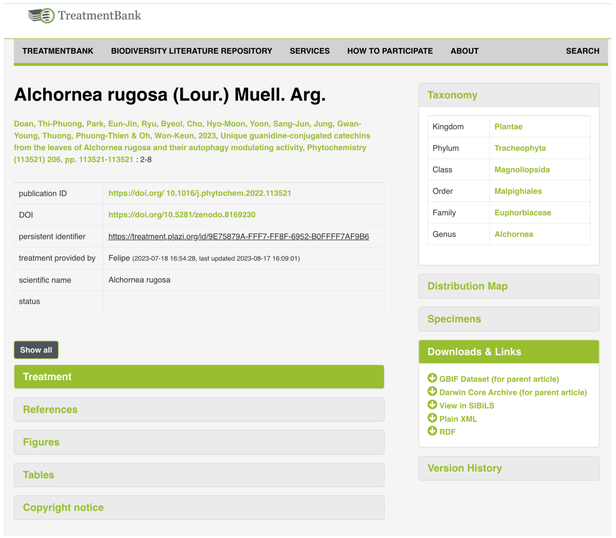

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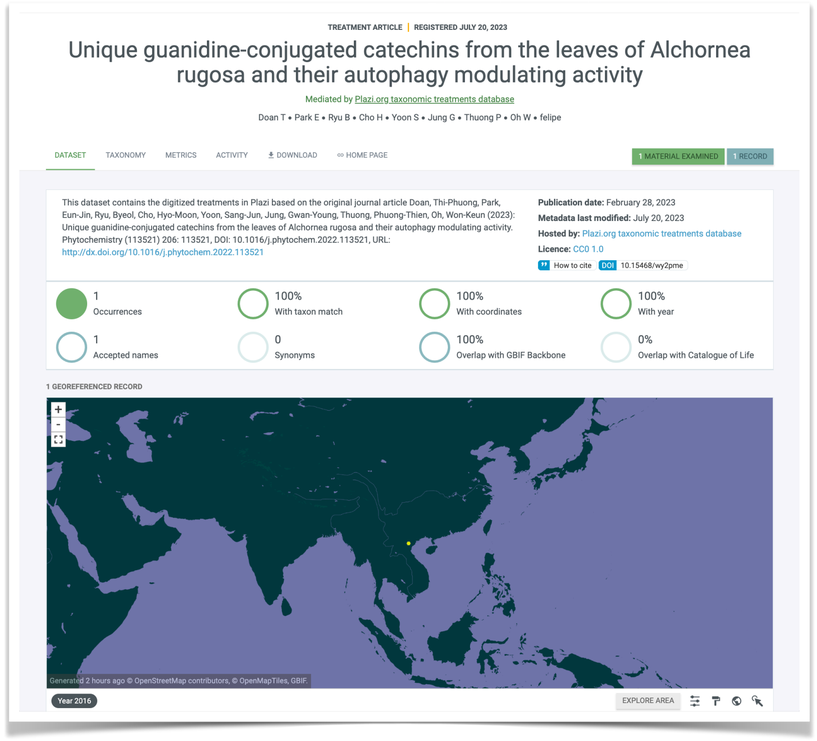

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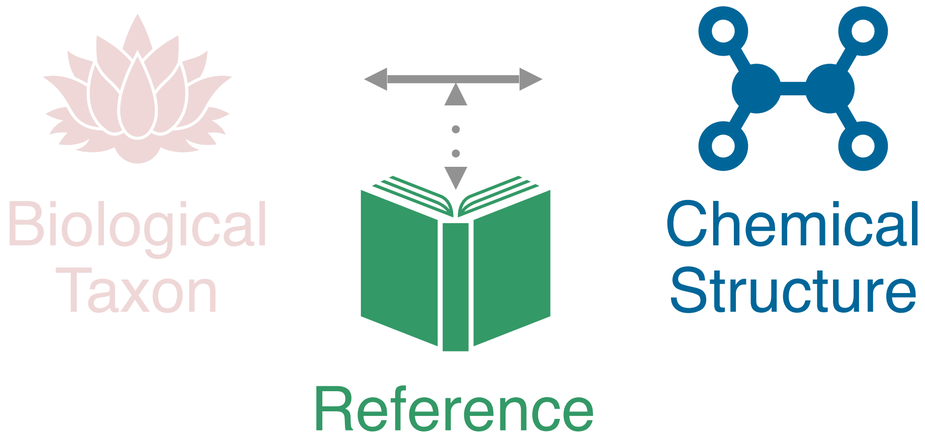

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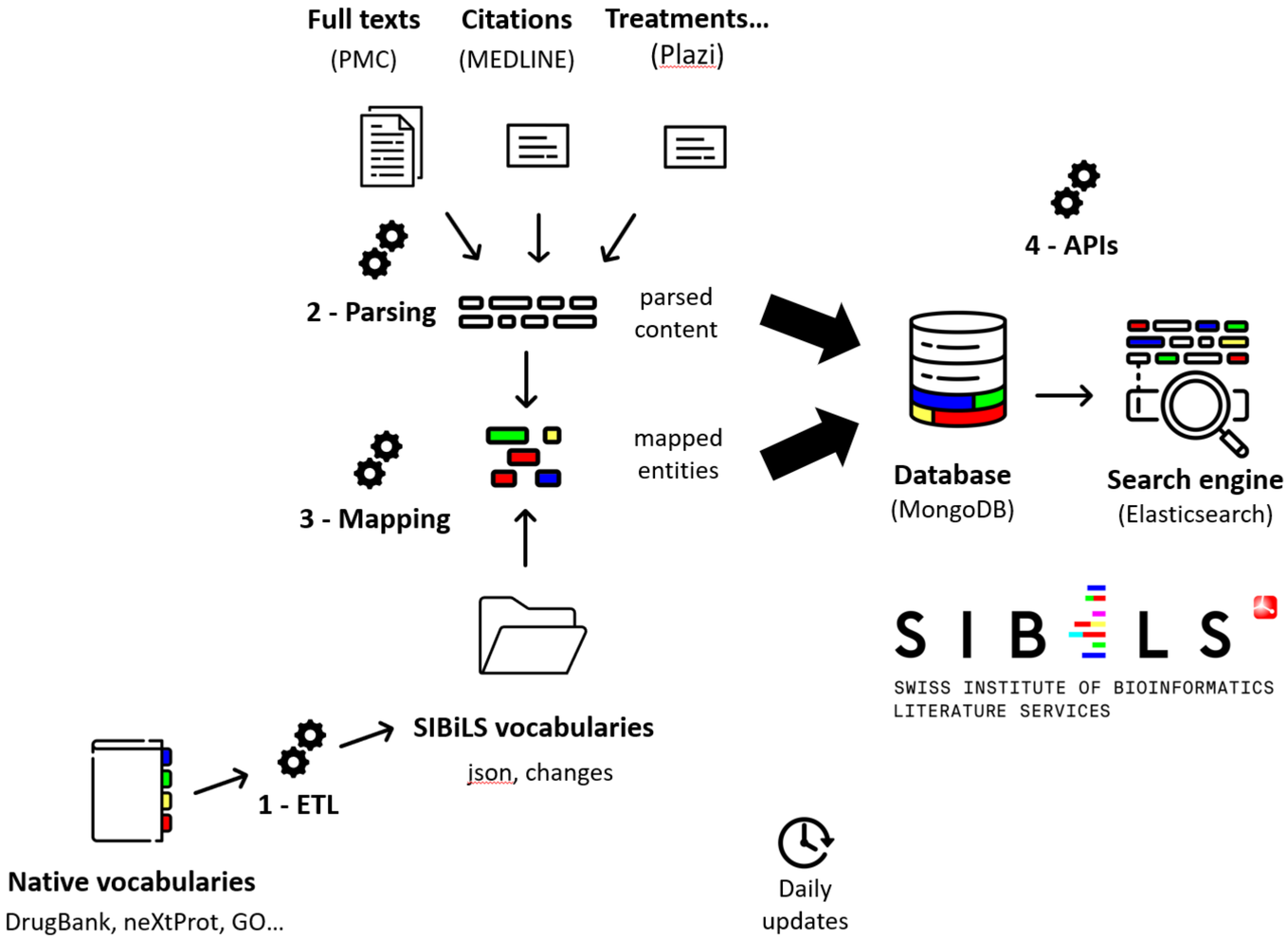

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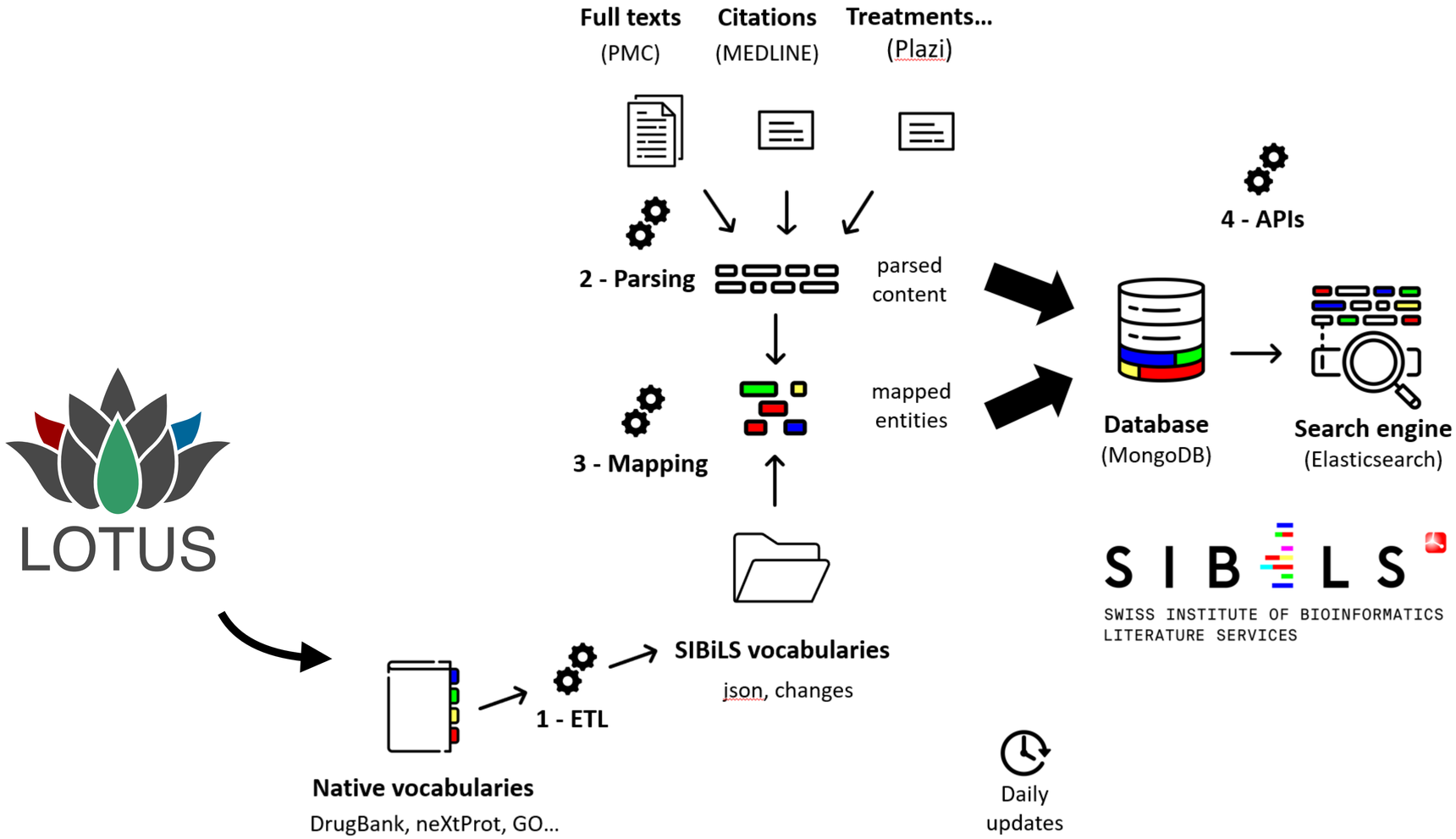

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Nb documents (files for suppdata)		36,142,609	5,546,055	839,396	6,507,981	629,807	5,524
Nb annotations	**Lotus**	**31,056,431**	**53,110,654**	**10,458,980**	**2,978,799**	**47,551**	**5,507**
	PubChem (subset)	**338,414,792**	**993,787,345**	**189,916,224**	**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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Deeper Insights on Alchornea cordifolia (Schumach. & Thonn.) Müll.Arg Extracts: Chemical Profiles, Biological Abilities, Network Analysis and Molecular Docking

PMC7913913. Kouadio Ibrahime Sinan, Gunes Ak, Ouattara Katinan Etienne, József Jekő, Zoltán Cziáky, et al. 2021-02-04. Biomolecules. Licence CC BY. **MEDLINE. PubMedCentral. EuropePMC. PMCViewer. Doi. SIBiLS. BiotXplorer.**

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Abstract

Alchornea cordifolia (Schumach. & Thonn.) Müll. Arg. is a well-known African medicinal plant traditionally used for various healing purposes. In the present study, methanolic, ethyl acetate and infusion extracts of A. cordifolia leaves were studied for their total phenolic and flavonoid contents and screened for their chemical composition. Moreover, the enzyme (acetyl- and butyryl-cholinesterases, α-amylase, α-glucosidase, and tyrosinase) inhibitory and cytotoxicity activities on HepG2: human hepatocellular carcinoma cells, B16 4A5: murine melanoma cells, and S17: murine bone marrow (normal) cells of extracts were evaluated. Finally, components-targets and docking analyzes were conducted with the aim to unravel the putative mechanisms underlying the observed bio-pharmacological effects. Interestingly, the infusion and methanolic extracts showed significantly higher total phenolic and flavonoid contents compared with the ethyl acetate extract (TPC: 120.38–213.12 mg GAE/g and TFC: 9.66–57.18 mg RE/g). Besides, the methanolic extracts followed by the infusion extracts were revealed to contain a higher number of compounds (84 and 74 compounds, respectively), while only 64 compounds were observed for the ethyl acetate extract. Gallic acid, ellagic acid , shikimic acid, rutin , quercetin , myricetin , vitexin , quercitrin , kaempferol , and naringenin were among the compounds that were commonly identified in all the studied extracts. Additionally, the methanolic and infusion extracts displayed higher antioxidant capacity than ethyl acetate extract in all assays performed. In ABTS and DPPH radical scavenging assays, the methanol extract (500.38 mg TE/g for DPPH and 900.64 mg TE/g for ABTS) exhibited the best ability, followed by the water and ethyl acetate extracts. Furthermore, the extracts exhibited differential enzyme inhibitory profiles. In particular, the methanolic and infusion extracts showed better cytotoxic selectivity activity against human hepatocellular carcinoma cells. Overall, this study demonstrated A cordifolia to be a species worthy of further investigations, given its richness in bioactive phytochemicals and wide potentialities for antioxidants and pharmacological agents.

1. Introduction

Alchornea cordifolia (Schumach. & Thonn.) Müll. Arg. belonging to the Euphorbiaceae family is found generally in African regions, and is traditionally used for the treatment of a

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- [ ] NCBI Taxonomy Full (27)
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- [ ] OTT - Open Tree of Life (86)
- [ ] PRI-PTM (41)

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Abstract

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- [ ] GO Biological Process (14)
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- [ ] MeSH (560)
- [ ] NCBI Taxonomy Clinic (5)
- [ ] NCBI Taxonomy Full (27)
- [ ] NCI Thesaurus (99)
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- [ ] OTT - Open Tree of Life (86)

Search: Clear

chemical - ethyl acetate lotus:LTS0196824
chemical - ellagic acid lotus:LTS0037297
chemical - rutin lotus:LTS0042292
chemical - quercetin lotus:LTS0205097
chemical - myricetin lotus:LTS0139858
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chemical - quercitrin lotus:LTS0186298
chemical - kaempferol lotus:LTS0055161
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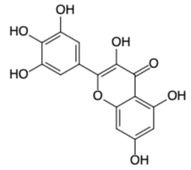

Name	Myricetin
Wikidata	Q951449
Mol. formula	C15H10O8
CAS registry number	-
Mol. weight	318.2357

Molfile

Representations

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2D SMILES	O=c1c(O)c(-c2cc(O)c(O)c(O)c2)oc2cc(O)cc(O)c12
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InChIKey	IKMDFBPHZNJCSN-UHFFFAOYSA-N
Deep SMILES	could not be computed
Murcko Framework	O1c2ccccc2CC=C1c3ccccc3

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Deeper Insights on Alchornea cordifolia (Schumach. & Thonn.) Müll.Arg Extracts: Chemical Profiles, Biological Abilities, Network Analysis and Molecular Docking

PMC7913913. Kouadio Ibrahime Sinan, Gunes Ak, Ouattara Katinan Etienne, József Jekő, Zoltán Cziáky, et al. 2021-02-04. Biomolecules. Licence CC BY. MEDLINE. PubMedCentral. EuropePMC. PMCViewer. Doi. SIBiLS. BiotXplorer.

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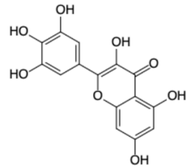

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used source

prefered source WIKIDATA

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myricetin (Q951449)

chemical compound

3,3',4,4',5,7-Hexahydro-2-phenyl-4H-chromen-4-one | 3,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-1-benzopyran-4-one | 3,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-chromen-4-one | 3,5,7,3',4',5'-Hexahydroxyflavone | Cannabiscetin | MYC | Myricetol | Myricitin | 3,3',4',5,5',7-Hexahydroxyflavone | 3,3',4',5,5',7-Hexahydroxy-(8Cl)- flavone | Myricetin

In more languages

Language	Label	Description	Also known as
English	myricetin	chemical compound	3,3',4,4',5,7-Hexahydro-2-phen… 3,5,7-Trihydroxy-2-(3,4,5-trihydr… 3,5,7-Trihydroxy-2-(3,4,5-trihydr… 3,5,7,3',4',5'-Hexahydroxyflavone Cannabiscetin MYC Myricetol Myricitin 3,3',4',5,5',7-Hexahydroxyflavone 3,3',4',5,5',7-Hexahydroxy-(8Cl)-… Myricetin
German	Myricetin	chemische Verbindung	
Spanish	Myricetina	compuesto químico	
French	Myricétine	composé chimique	

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pl Mirycetyna
ro Miricetină
ru Мирицетин
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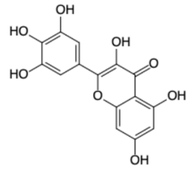

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Murcko Framework	O1c2ccccc2CC=C1c3ccccc3

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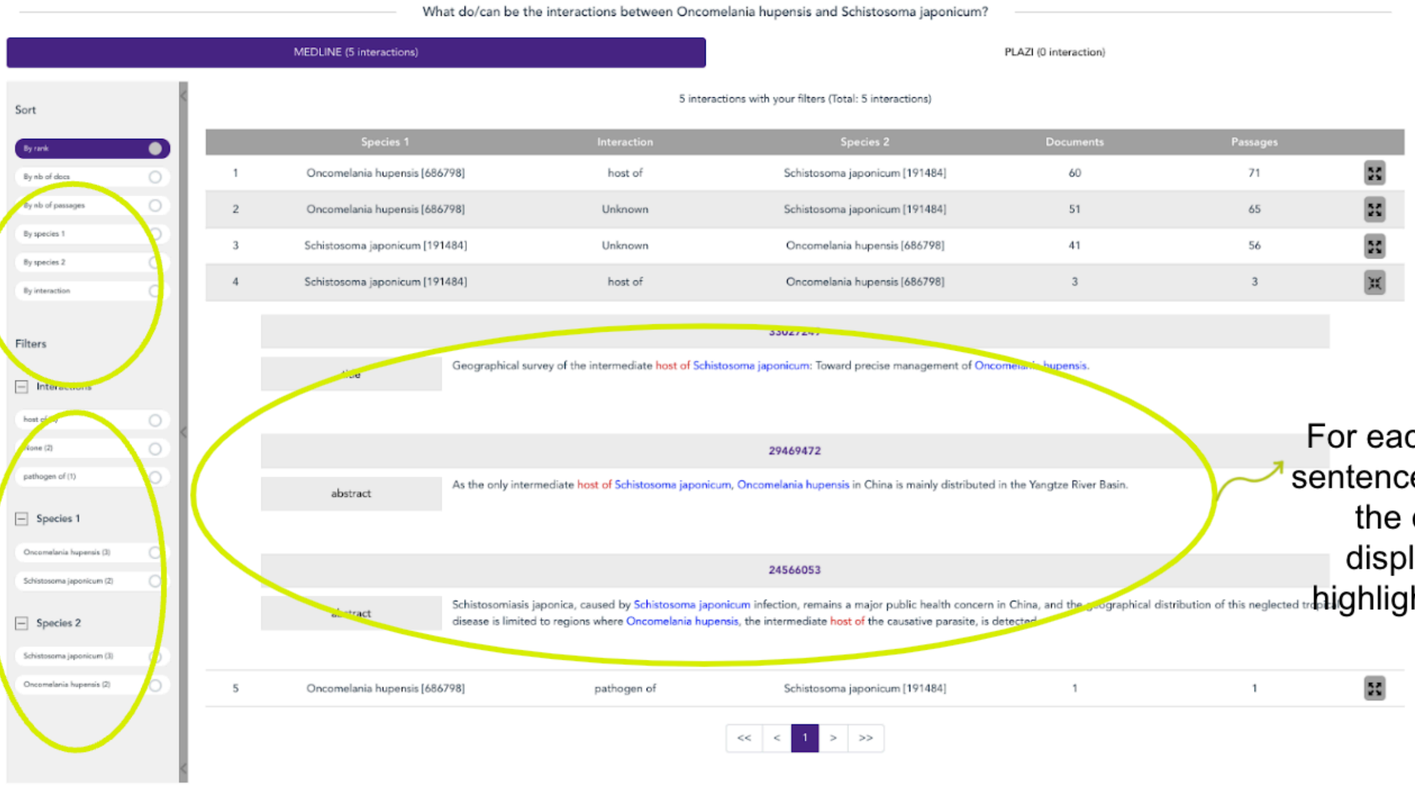
Results can be filtered (e.g. species, interactions)



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OBO Relation Ontology

Website for RO

Documentation and User Guide

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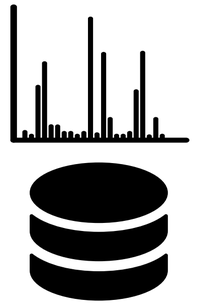
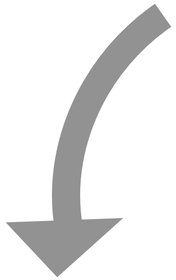
Chemical structures / Biological organism relation explorer

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



Future knowledge



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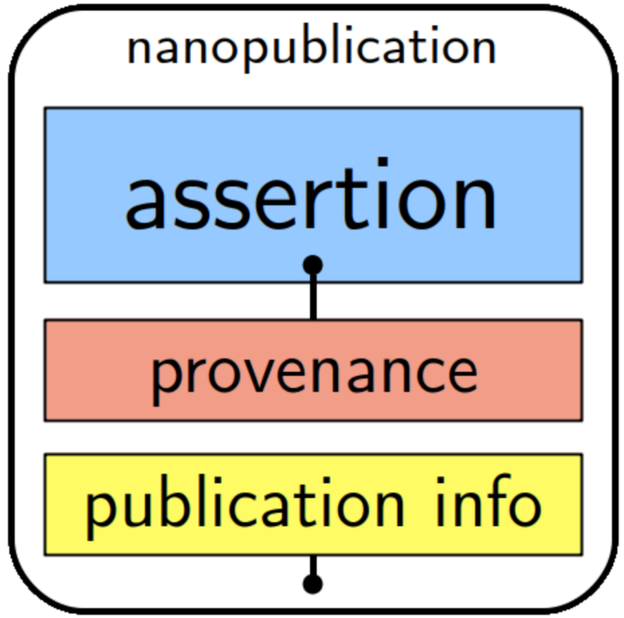

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Assertion: Expressing a sample metabolite annotation ^

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 ^

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

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Nanopublication: RAtD9MFh9n

RAtD9MFh9n

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lcms-analysis   has as feature list   feature-list   .
sample   has the label   "V114006GP-01"   .
sample   has the analysis   lcms-analysis   .
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sirius-annotation   has the sirius score   "35.89209590424093"   .
sirius-annotation   has the sirius adduct   "[M+H]+"   .
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this assertion   is attributed to   sirius_mzspec:MSV000087728:VGF152_B02_features_ms2_pos.mgf:scan:673   .
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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   .
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Pierre-Marie Allard 9 Jul 2023, 07:10:43 UTC

References

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	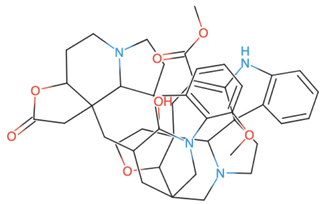	
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	Tabernaemontana coffeoides	edit
	1 reference	
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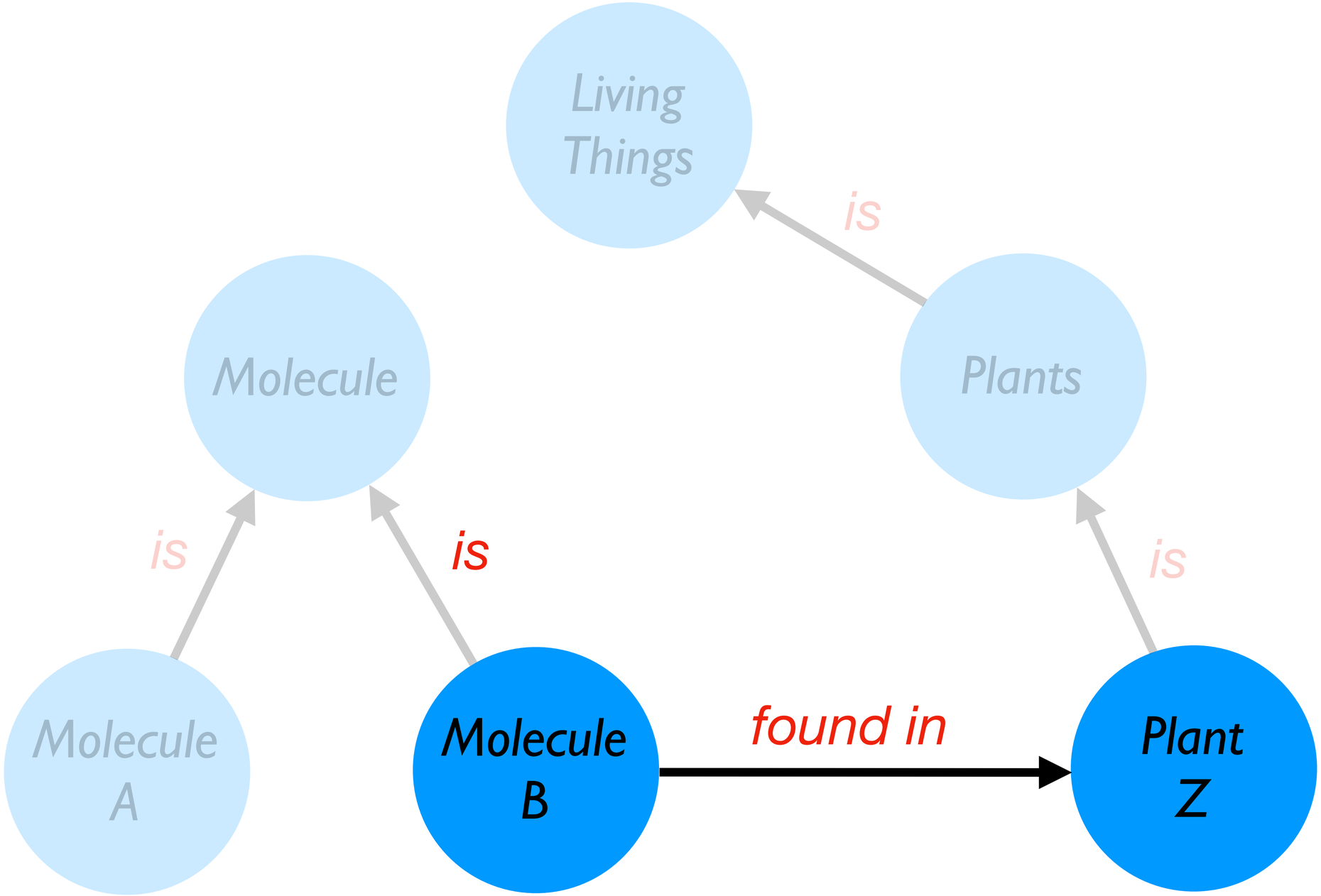
Living Things
is
Molecule
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is
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is
Molecule A
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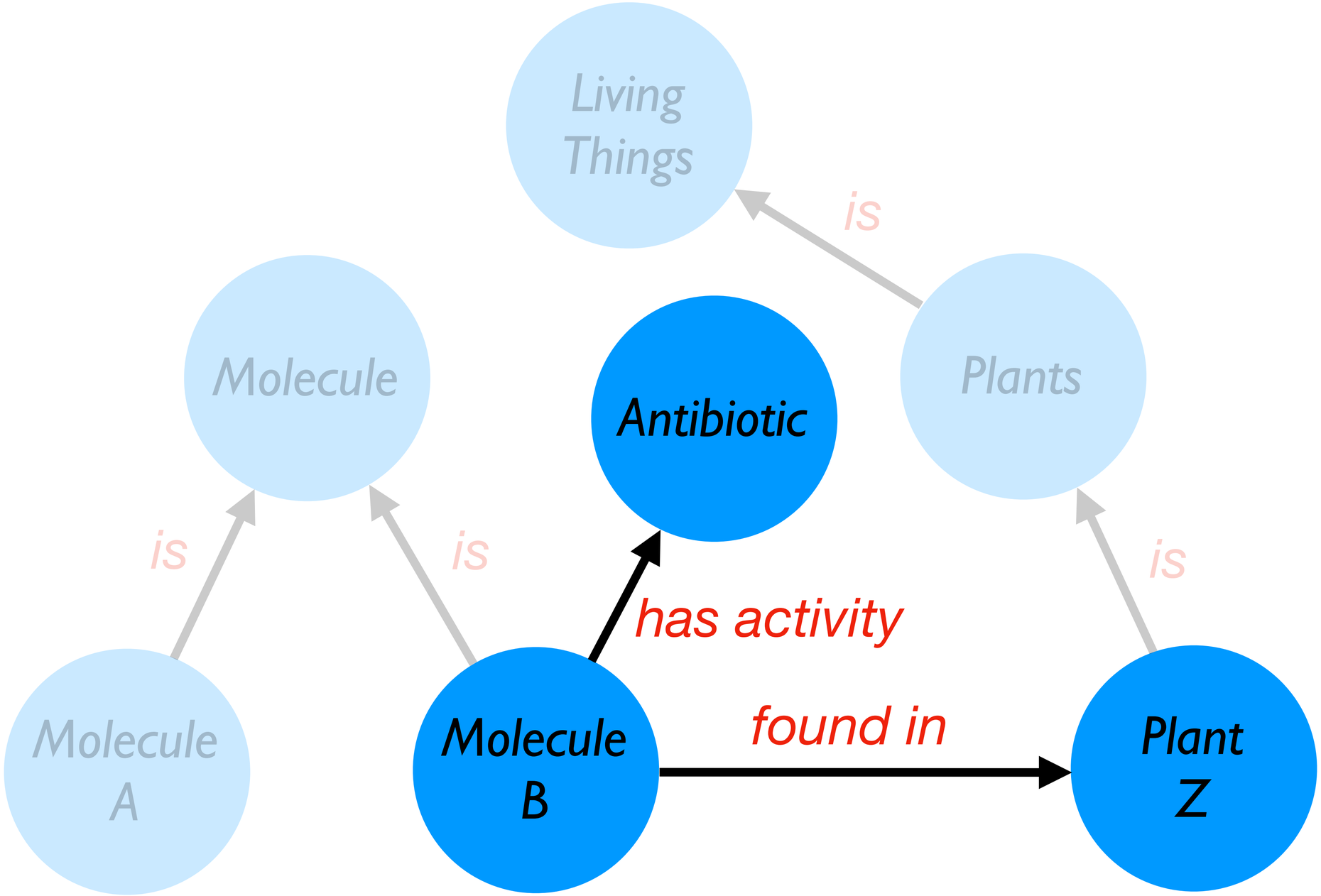
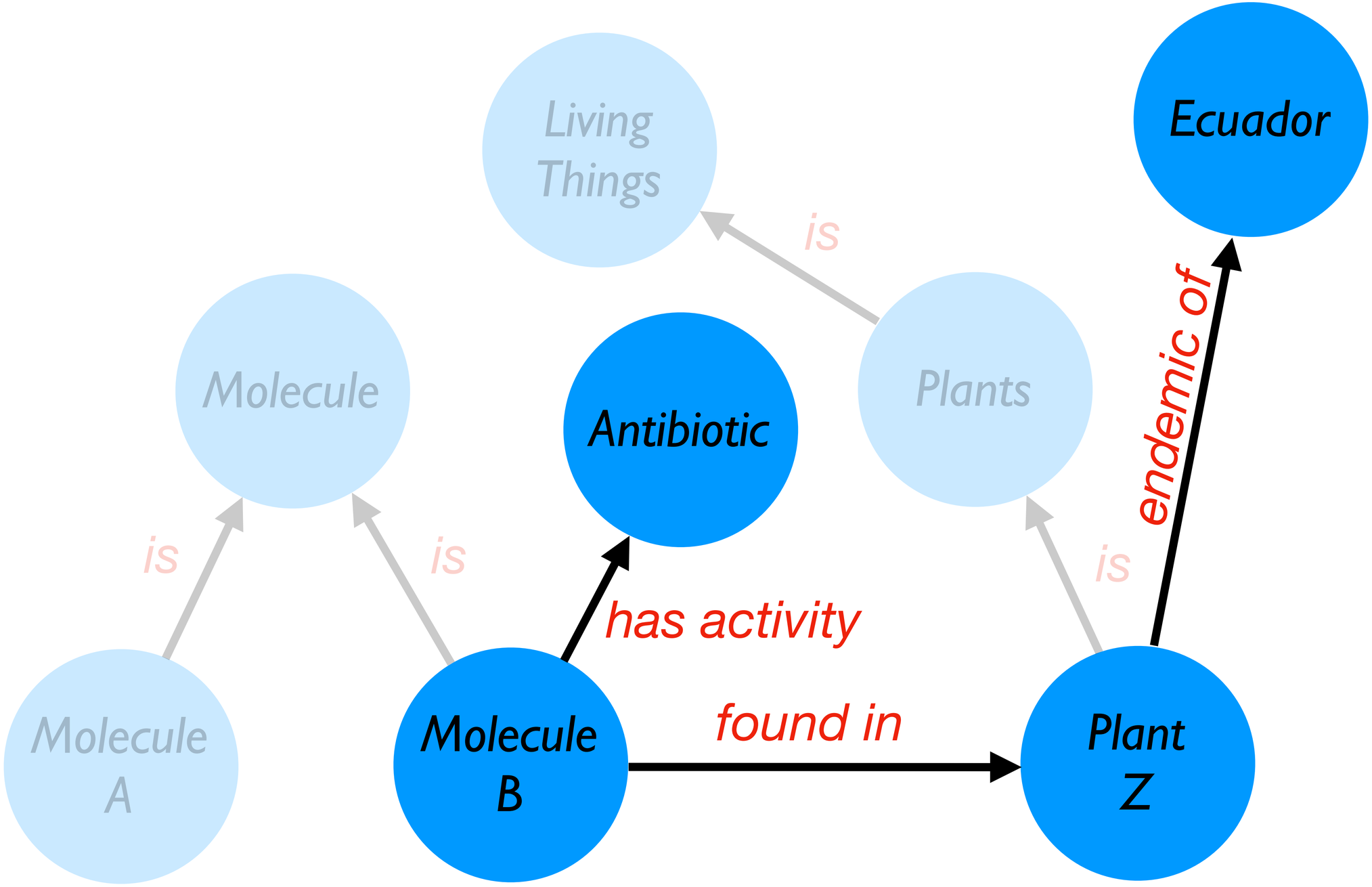
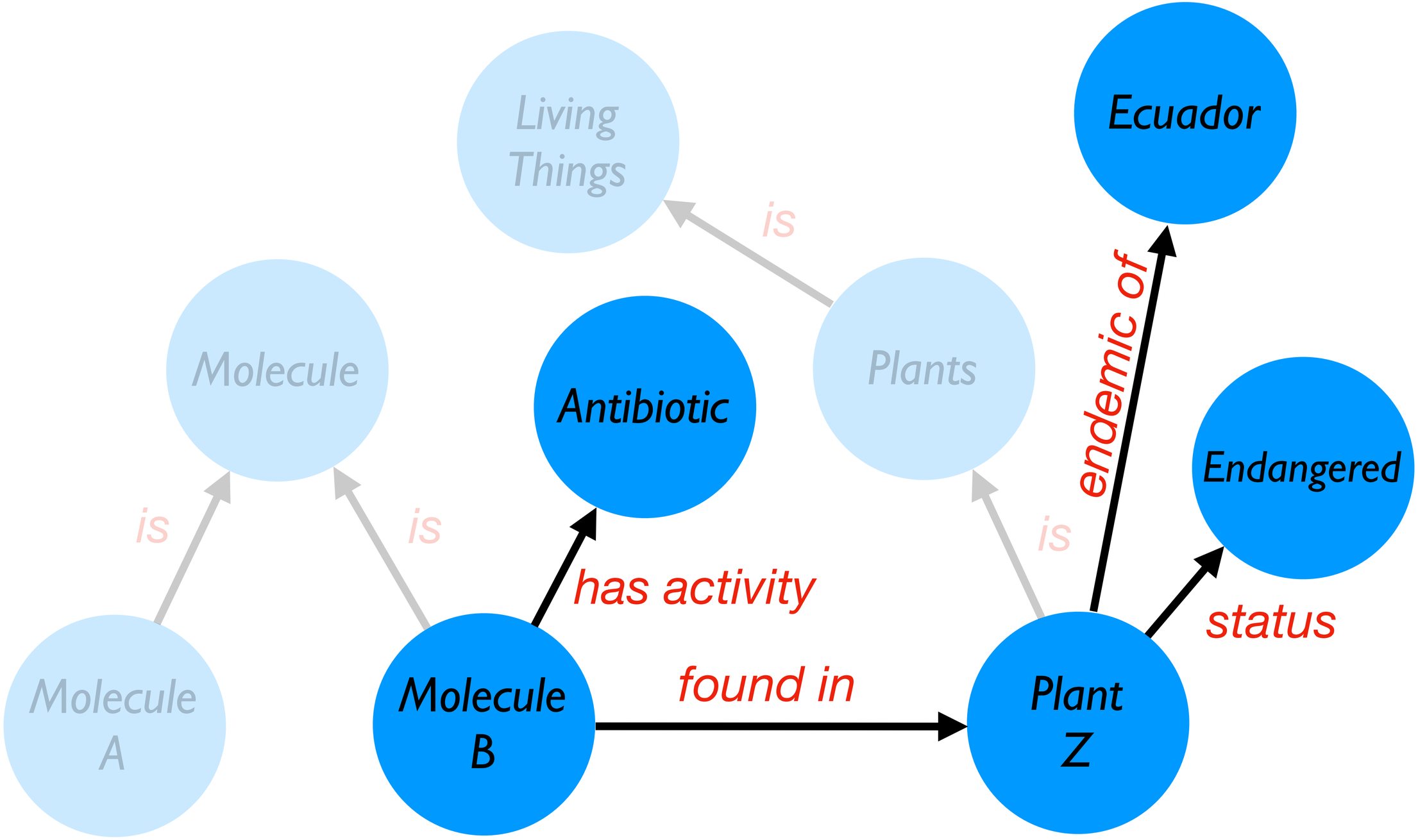
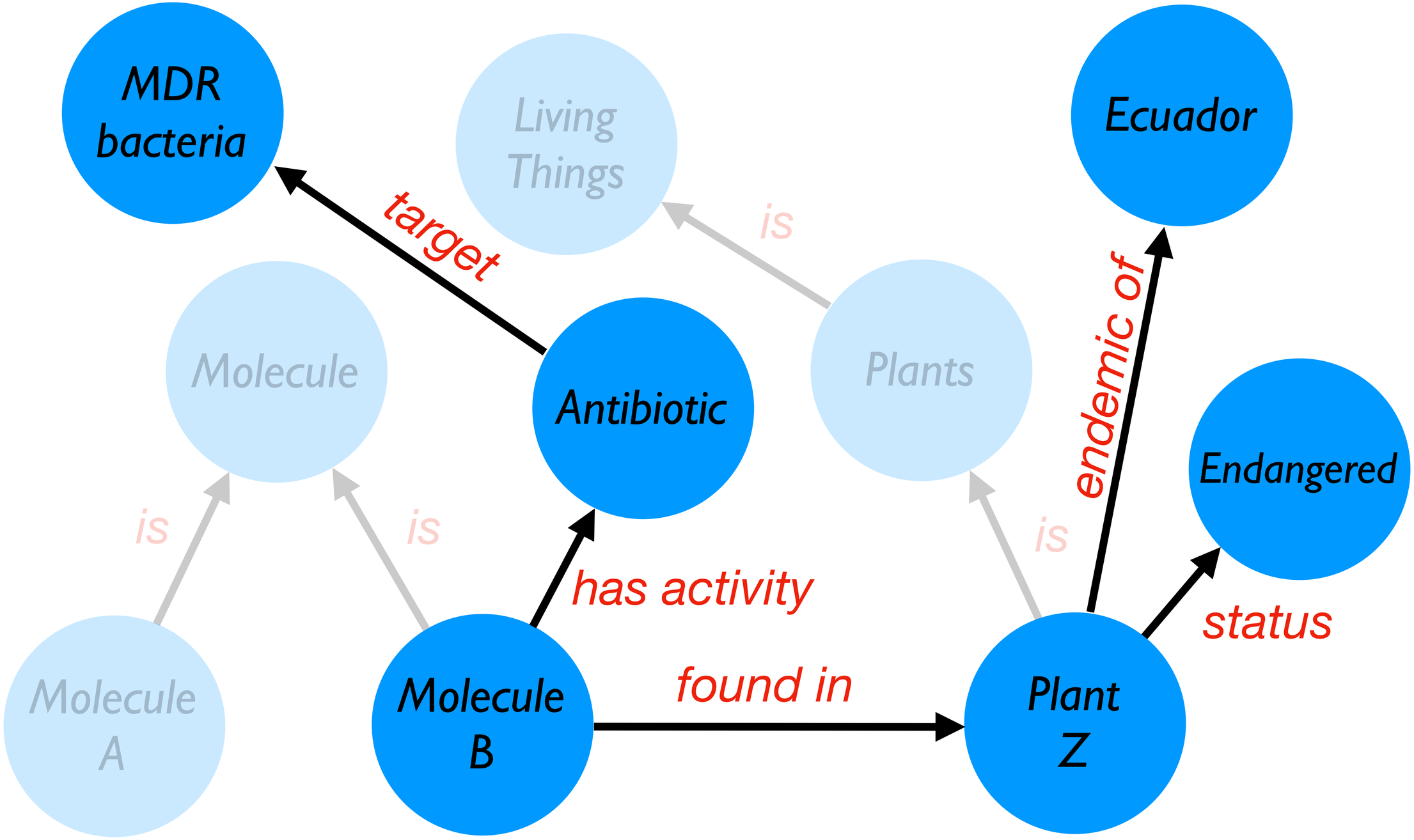
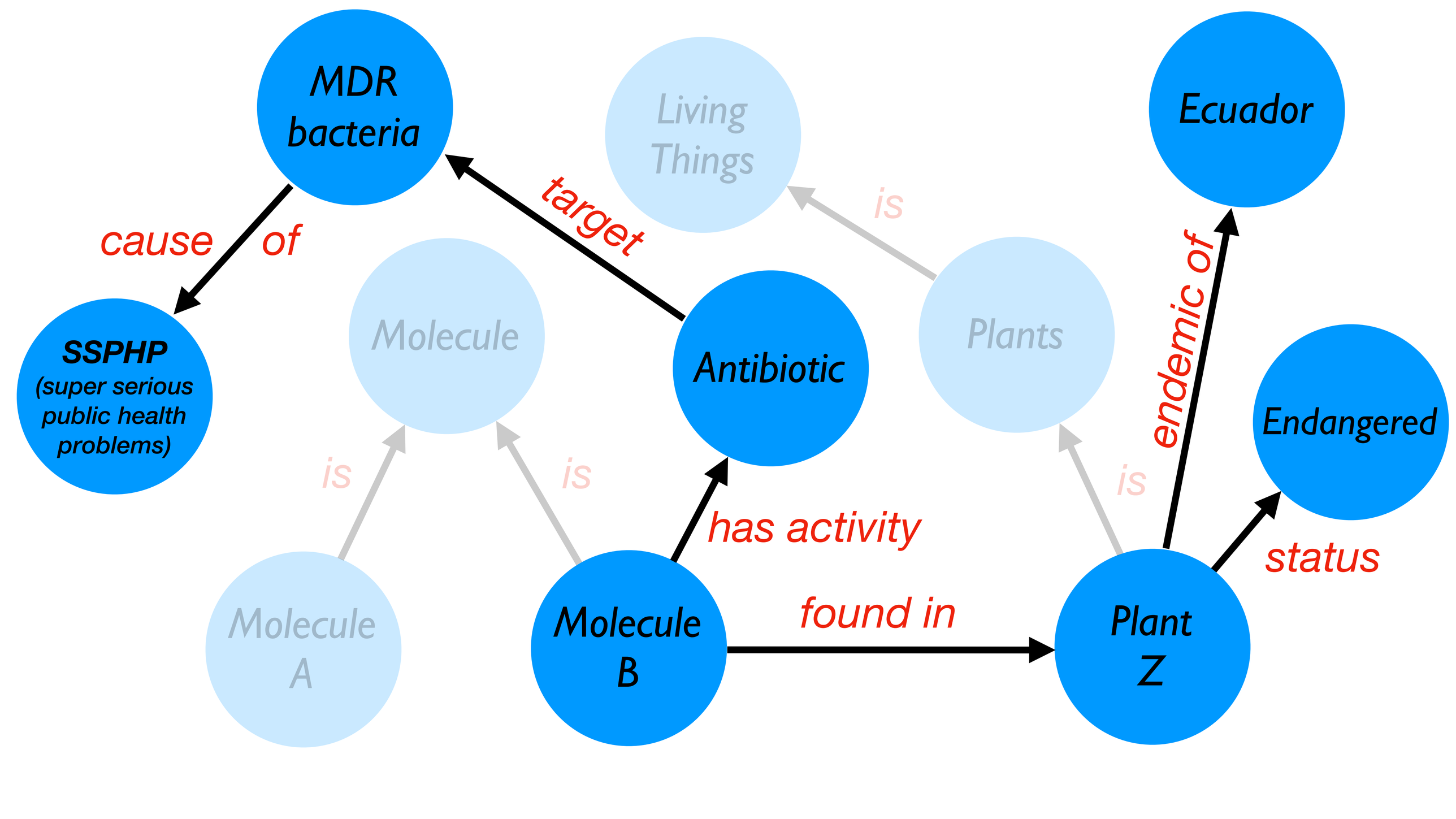
found in
Plant Z


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
is
has activity
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

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TAKING CARE OF FREEDOM

Guido Sauter

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Emmanuel Defossez

Adriano Rutz

Ana Claudia Sima

Déborah Caucheteur

Patrick Ruch

Philipp Von Essen

Pierre-Marie Allard

Tarcisio Mendes de Farias