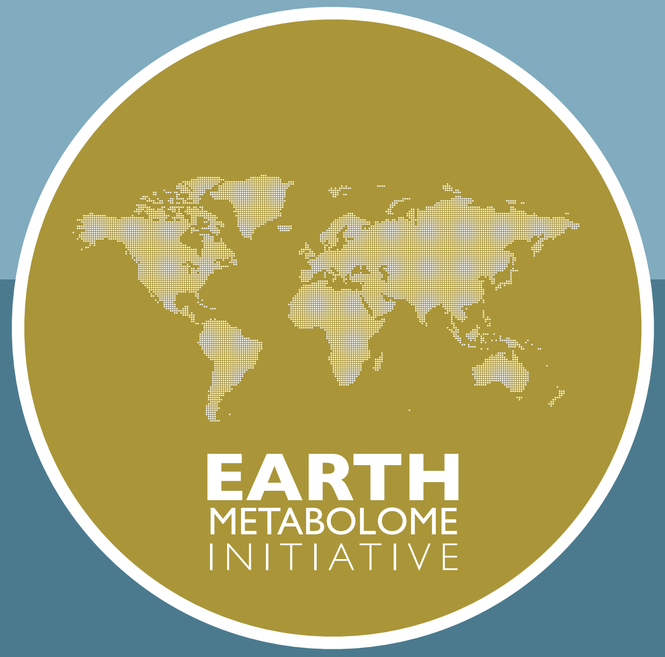
Digital Botanical Gardens & Earth Metabolome : two aligned iniatives

https://doi.org/10.5281/zenodo.7662428

Swiss Digital Botanical Gardens Initiative

A massive undertaking ...

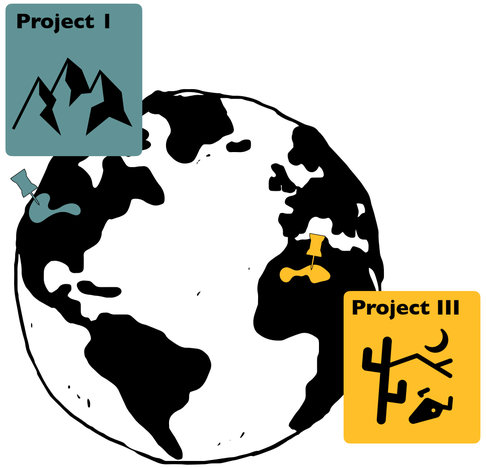


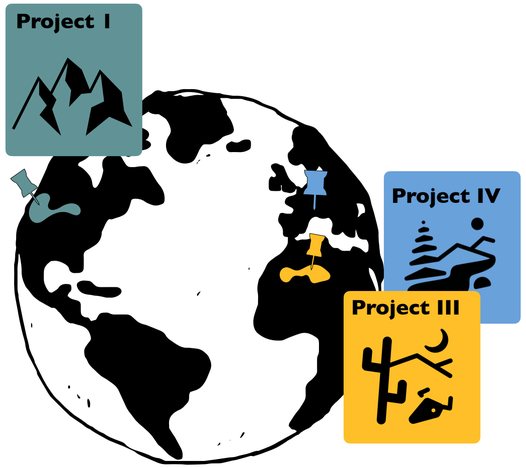
Profile the metabolic content of all currently known species on Earth.

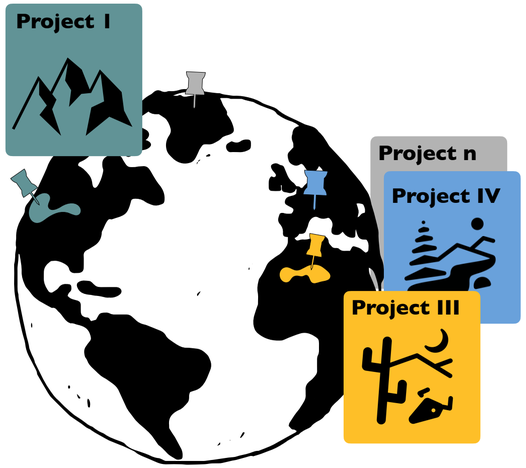
... with three objectives

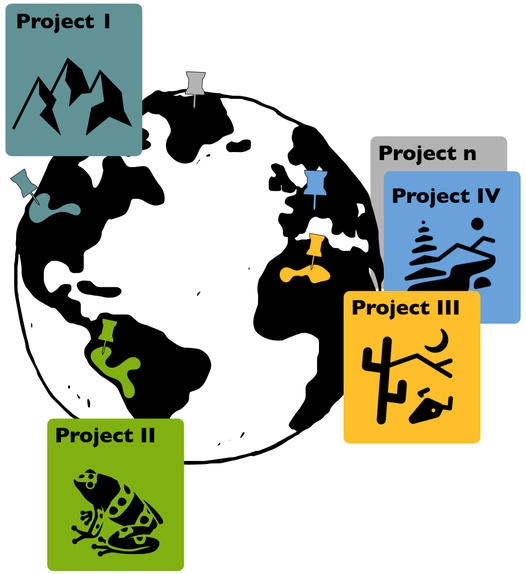
- *Protect biodiversity*
- *Benefit human society*
- *Explore and understand the chemical foundations of the biosphere*

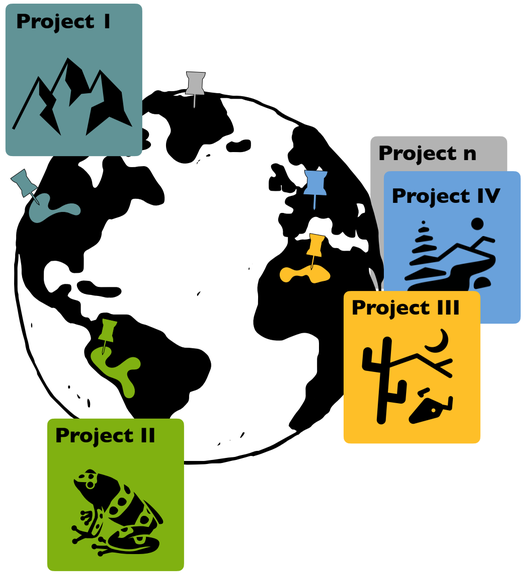
Project I


Project I
Project III

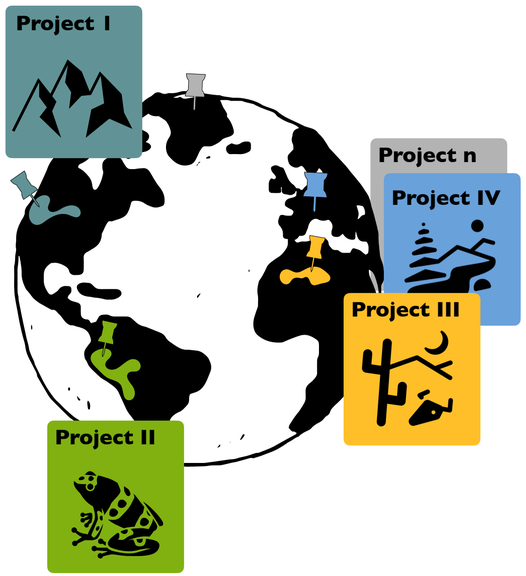

Project I
Project IV
Project III


Project I
Project n
Project IV
Project III


Project I
Project n
Project IV
Project III
Project II

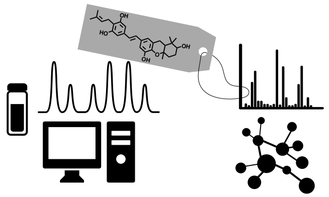

Project I
Project n
Project IV
Project III
Project II

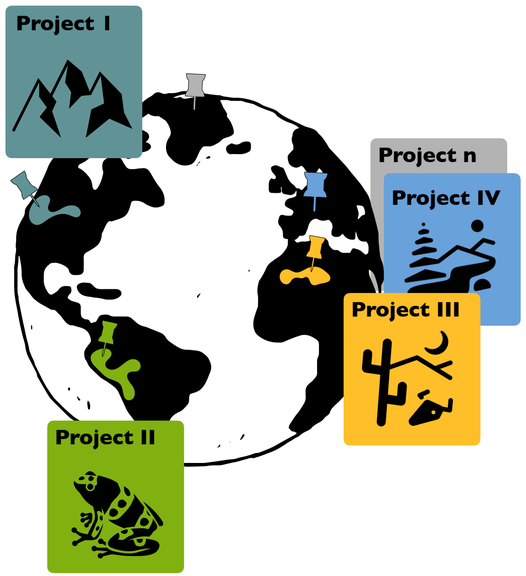
Accessing chemodiversity



Accessing chemodiversity

Knowledge acquisition

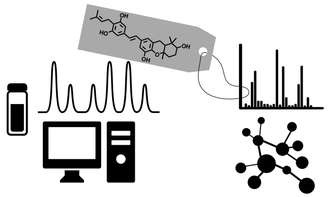


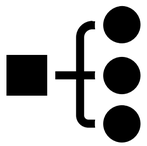


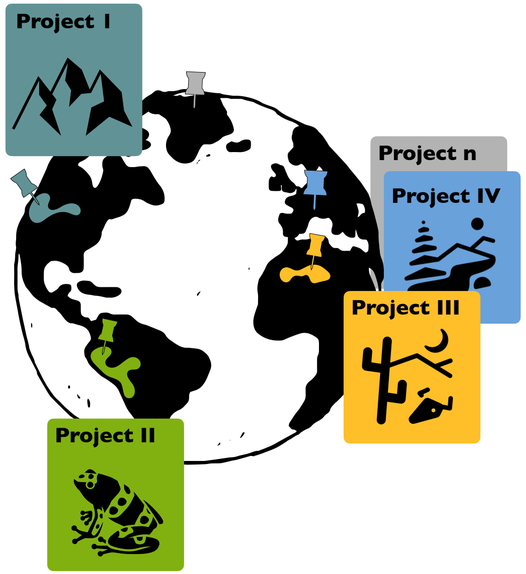
Accessing chemodiversity

Knowledge acquisition

Knowledge organisation





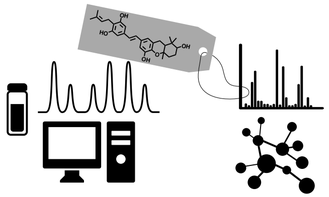


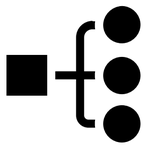
Accessing chemodiversity

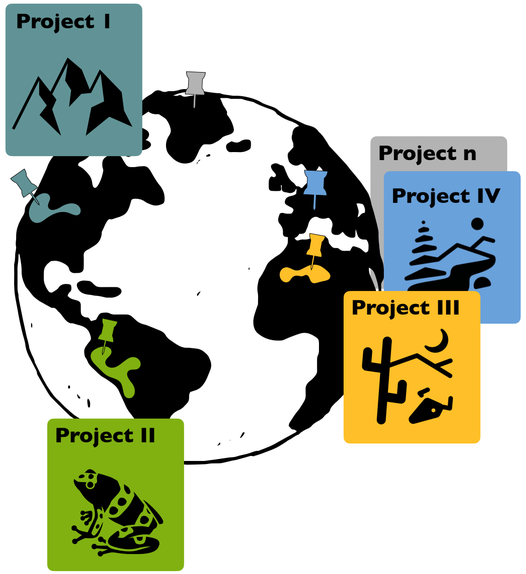
Knowledge acquisition

Knowledge organisation

Knowledge dissemination

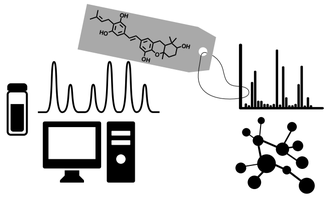




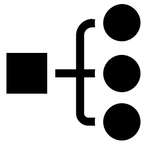


Accessing chemodiversity

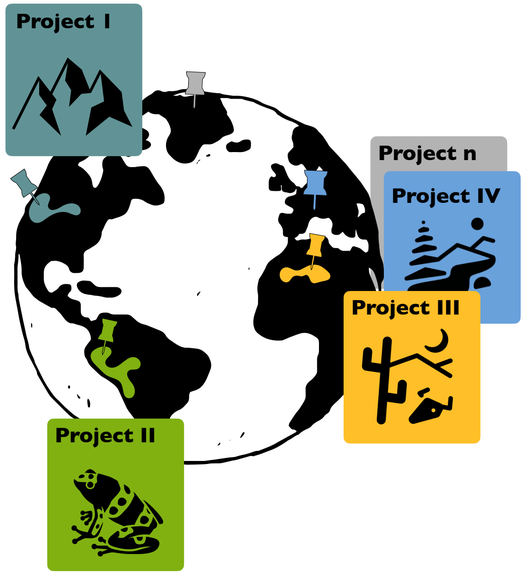
Knowledge acquisition



Knowledge organisation



Knowledge dissemination



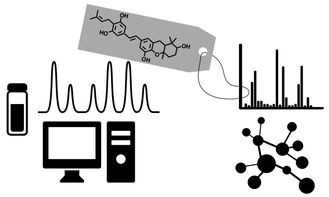
EARTH METABOLOME KNOWLEDGE BASE

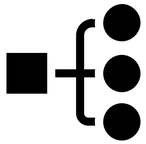
Accessing chemodiversity

Knowledge acquisition

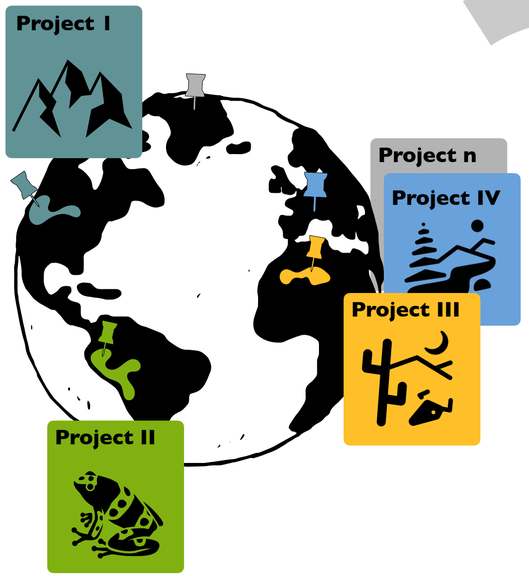
Knowledge organisation

Knowledge dissemination





BUILDING KNOWLEDGE



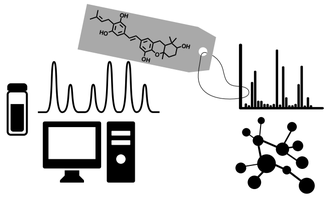
EARTH METABOLOME KNOWLEDGE BASE

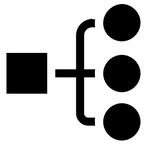
Accessing chemodiversity

Knowledge acquisition

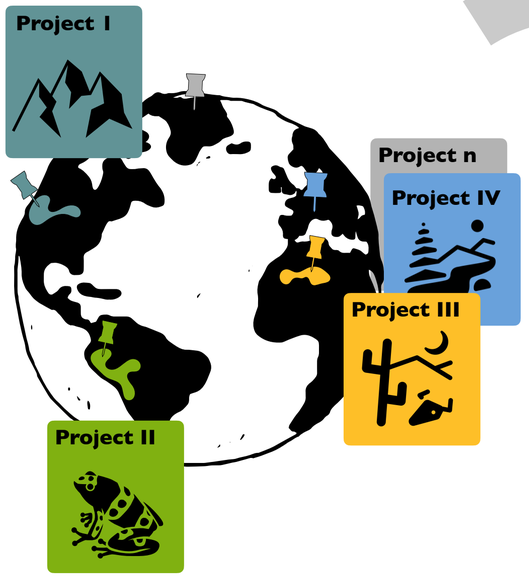
Knowledge organisation

Knowledge dissemination





BUILDING KNOWLEDGE



EARTH METABOLOME KNOWLEDGE BASE

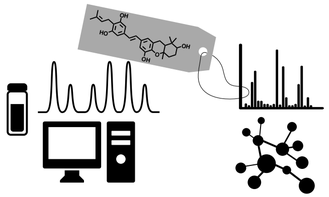
User community
Researchers, policy makers, industry, national parks, curators, public etc.

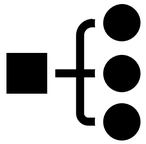
Accessing chemodiversity

Knowledge acquisition

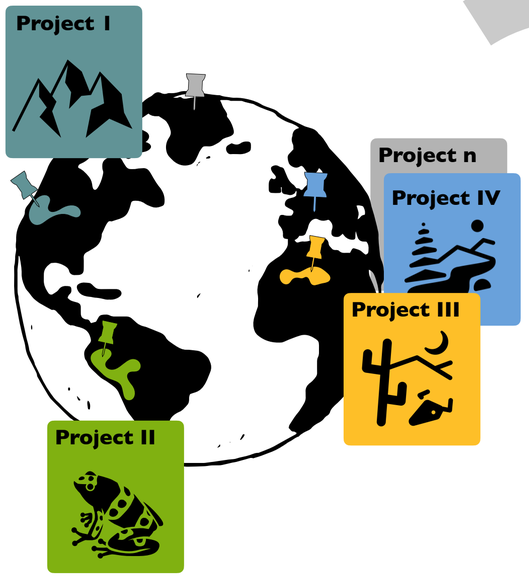
Knowledge organisation

Knowledge dissemination



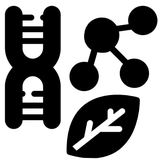


BUILDING KNOWLEDGE



EARTH METABOLOME KNOWLEDGE BASE

User community
Researchers, policy makers, industry, national parks, curators, public etc.



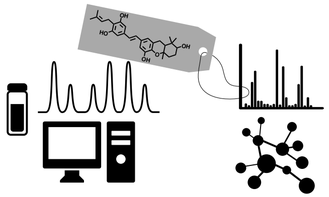
Advance life sciences

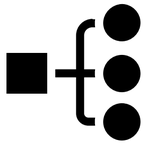
Accessing chemodiversity

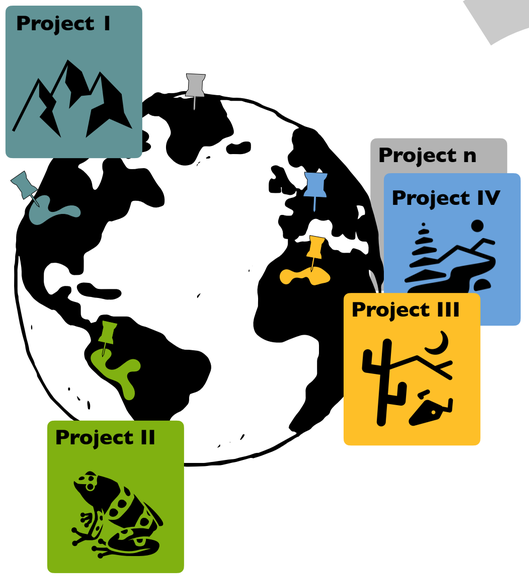
Knowledge acquisition

Knowledge organisation

Knowledge dissemination





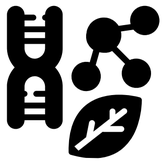


BUILDING KNOWLEDGE

EARTH METABOLOME KNOWLEDGE BASE

User community
Researchers, policy makers, industry, national parks, curators, public etc.

Benefit human society



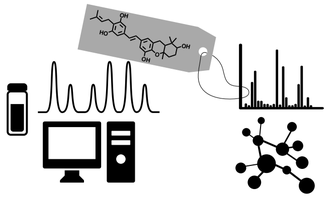
Advance life sciences

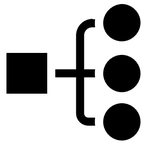
Accessing chemodiversity

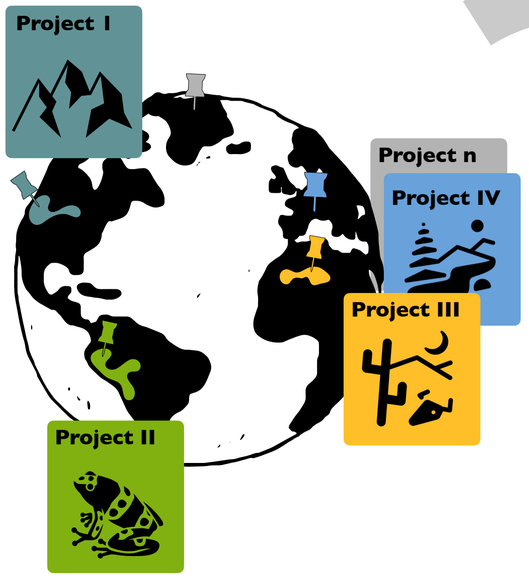
Knowledge acquisition

Knowledge organisation

Knowledge dissemination







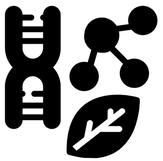
BUILDING KNOWLEDGE

EARTH METABOLOME KNOWLEDGE BASE

User community
Researchers, policy makers, industry, national parks, curators, public etc.

Protect biodiversity

Benefit human society



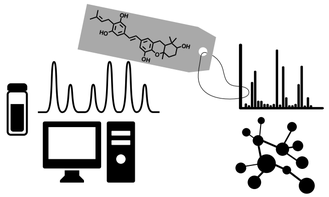
Advance life sciences

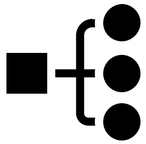
Accessing chemodiversity

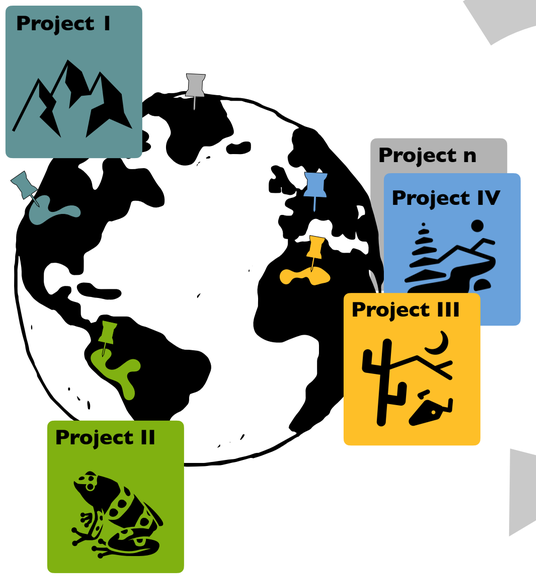
Knowledge acquisition

Knowledge organisation

Knowledge dissemination





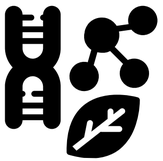


BUILDING KNOWLEDGE

EARTH METABOLOME KNOWLEDGE BASE

MAKING IMPACT

User community
Researchers, policy makers, industry, national parks, curators, public etc.



Protect biodiversity

Benefit human society

Advance life sciences

How do we participate in conservation & restoration ?

- we document biodiversity at novel scales (through the metabolome)
- we develop "molecular arguments" for conservation
- we implement "pay to see" mechanisms for the private sector leading to conservation initiatives including protected areas and co-developed measures for land management
- we develop novel chemodiversity metrics to quantify the impact of conservation & restoration projects

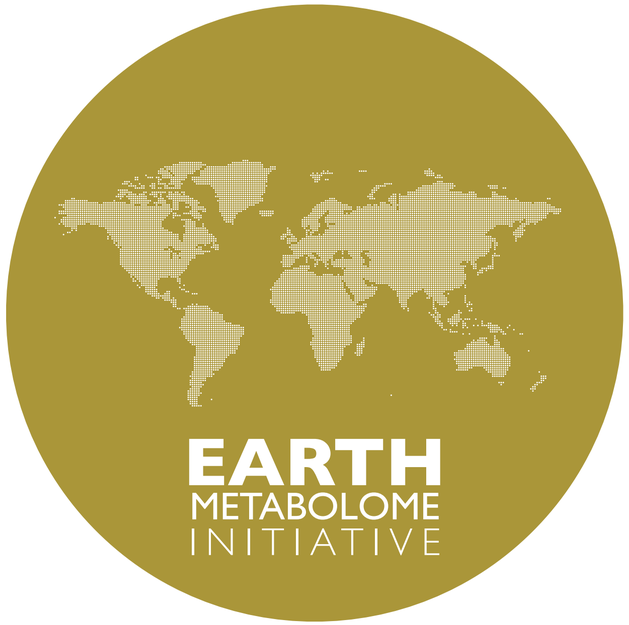
How do we benefit human society ?

- we build, for now and for the next generations, a fully Open Knowledge base documenting the chemistry of Life
- we facilitate the discovery of novel therapeutics from Nature
- we propose and support novel solutions for sustainable food production

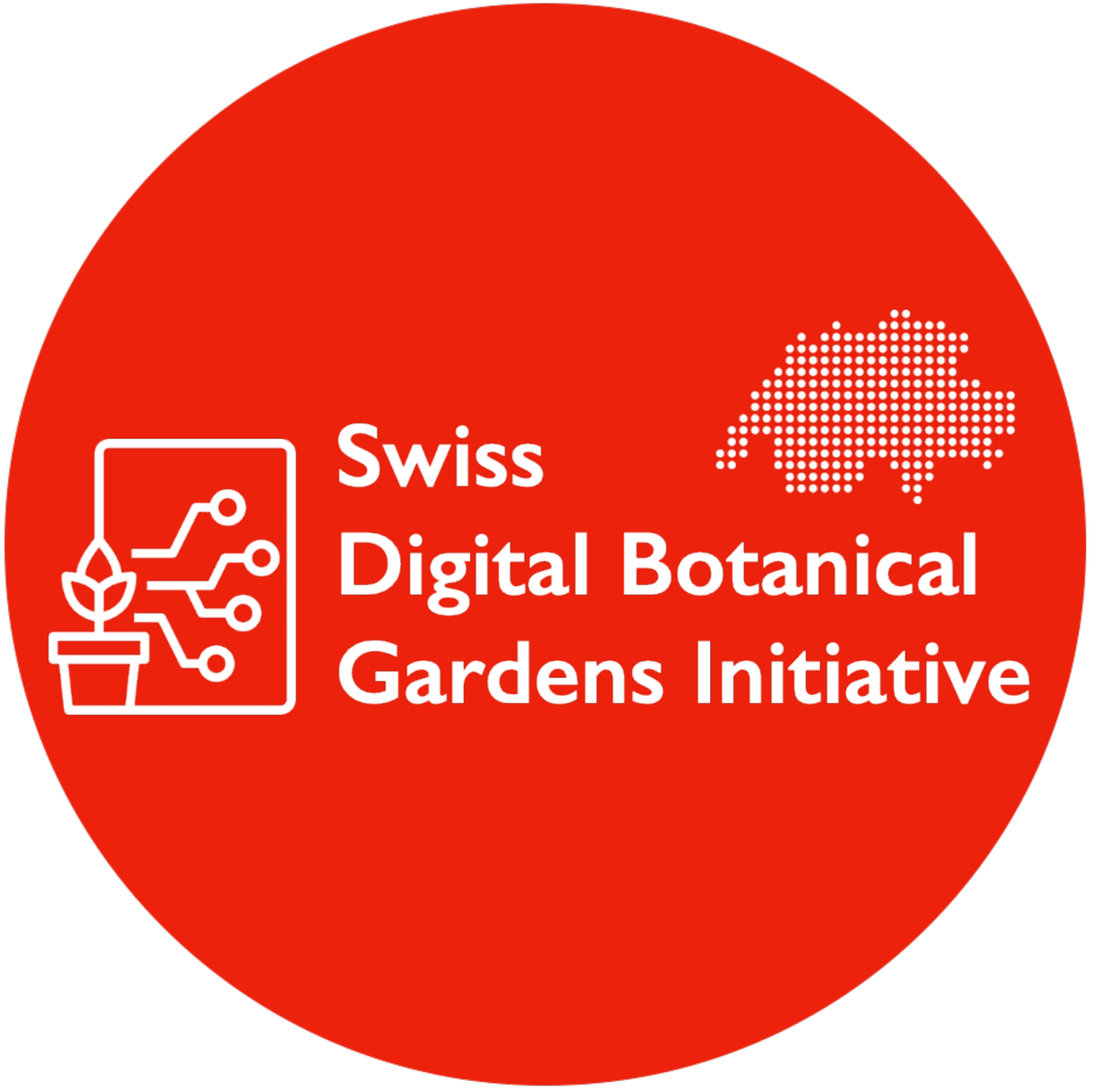
How do we uncover the chemical networks of the biosphere?

- we establish a global molecular map of the Earth's metabolome
- we interlink novel molecular knowledge with biological and ecological open research datasets (e.g. biotic interactions, species distribution, genomics, biological activities)
- we shape evolutionary models of the metabolome
- we anticipate unknown chemistries

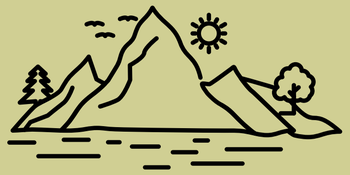
So what is the EMI ?



An Open Science initiative and a global effort to profile the metabolic content of all currently known species on our planet (~2.3 million species). We are building the required computational, scientific and organisational architecture to establish the network of ressources and humans to advance in this massive undertaking. The EMI will explore the chemical foundations of Life for a better human society within a thriving biosphere.


Swiss
Digital Botanical
Gardens Initiative

Wild ecosystems



Diversity (species) ●●●●●

Sampling (easiness of) ●○○○○

Functions (understanding of) ●○○○○

Conditions (control of environmental) ●○○○○

Botanical gardens

Diversity (species) ●●●○○

Sampling (easiness of) ●●●●○

Functions (understanding of) ●○○○○

Conditions (control of environmental) ●●●○○

Laboratory plants

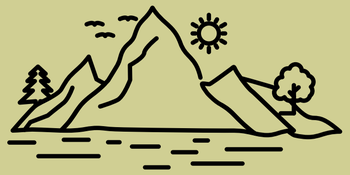
Diversity (species) ●○○○○

Sampling (easiness of) ●●●●●

Functions (understanding of) ●●●○○

Conditions (control of environmental) ●●●●●

Wild ecosystems



Diversity (species) ●●●●●

Sampling (easiness of) ●○○○○

Functions (understanding of) ●○○○○

Conditions (control of environmental) ●○○○○

Botanical gardens

Diversity (species) ●●●○○

Sampling (easiness of) ●●●●○

Functions (understanding of) ●○○○○

Conditions (control of environmental) ●●●○○

Laboratory plants

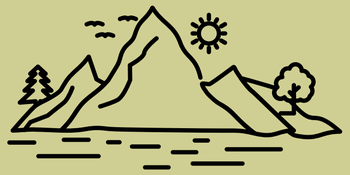
Diversity (species) ●○○○○

Sampling (easiness of) ●●●●●

Functions (understanding of) ●●●○○

Conditions (control of environmental) ●●●●●

Wild ecosystems



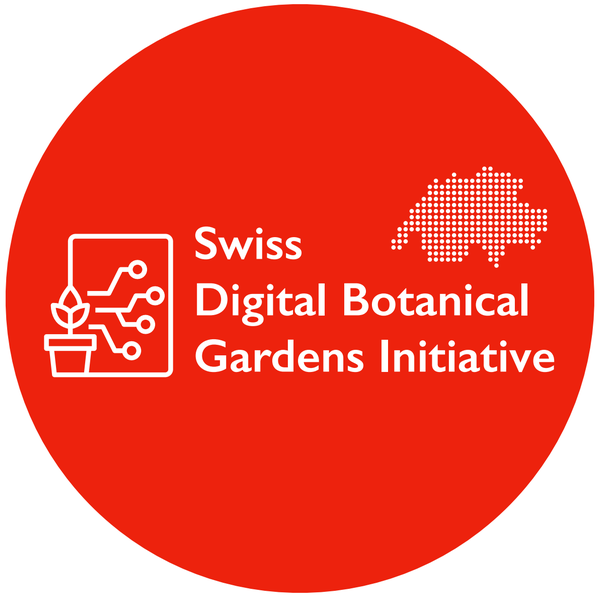
Diversity (species)	●●●●●
Sampling (easiness of)	●○○○○
Functions (understanding of)	●○○○○
Conditions (control of environmental)	●○○○○

Botanical gardens

Diversity (species)	●●●○○
Sampling (easiness of)	●●●●○
Functions (understanding of)	●○○○○
Conditions (control of environmental)	●●●○○

Laboratory plants

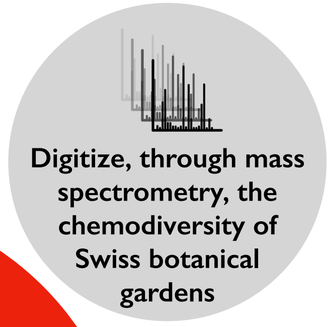
Diversity (species)	●○○○○
Sampling (easiness of)	●●●●●
Functions (understanding of)	●●●○○
Conditions (control of environmental)	●●●●●


Swiss
Digital Botanical
Gardens Initiative

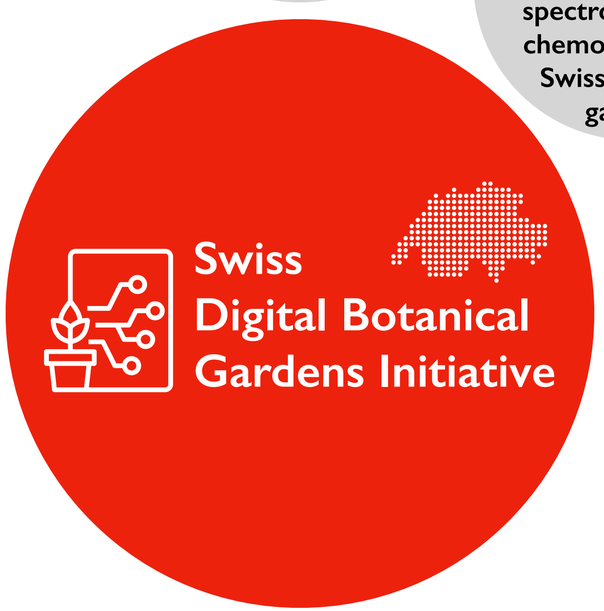
Establish chemical extracts libraries of Swiss botanical gardens

Swiss Digital Botanical Gardens Initiative

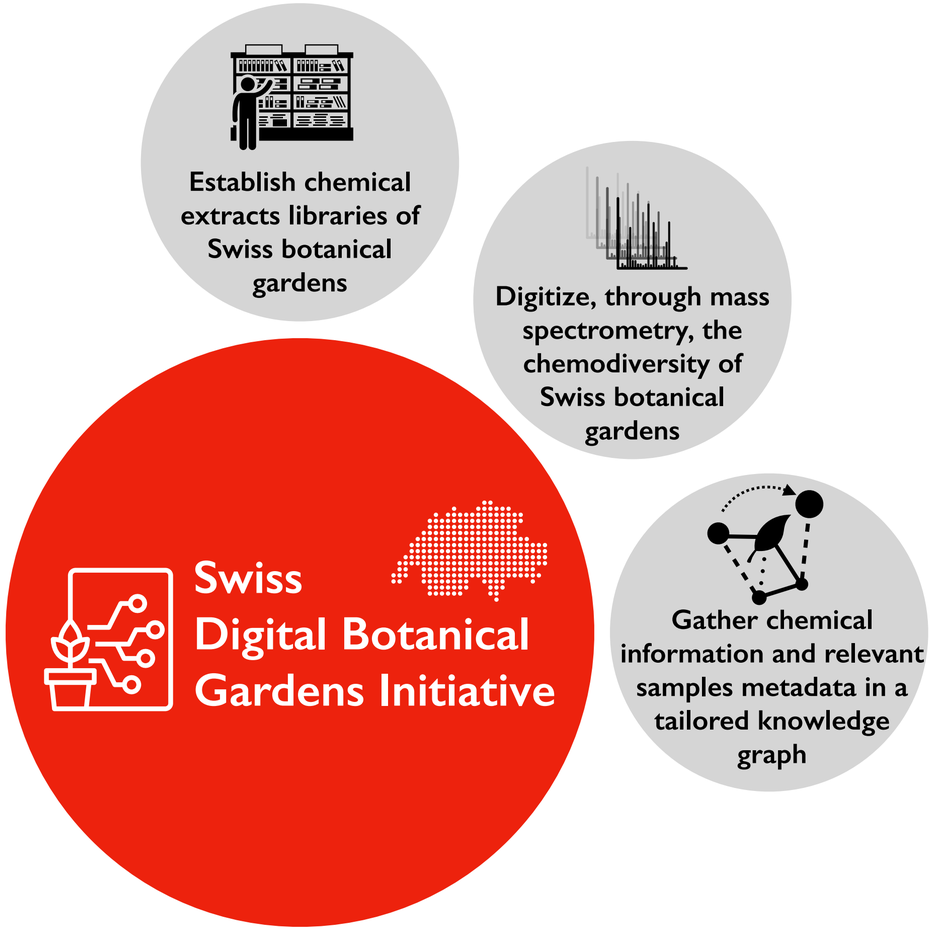
Establish chemical extracts libraries of Swiss botanical gardens

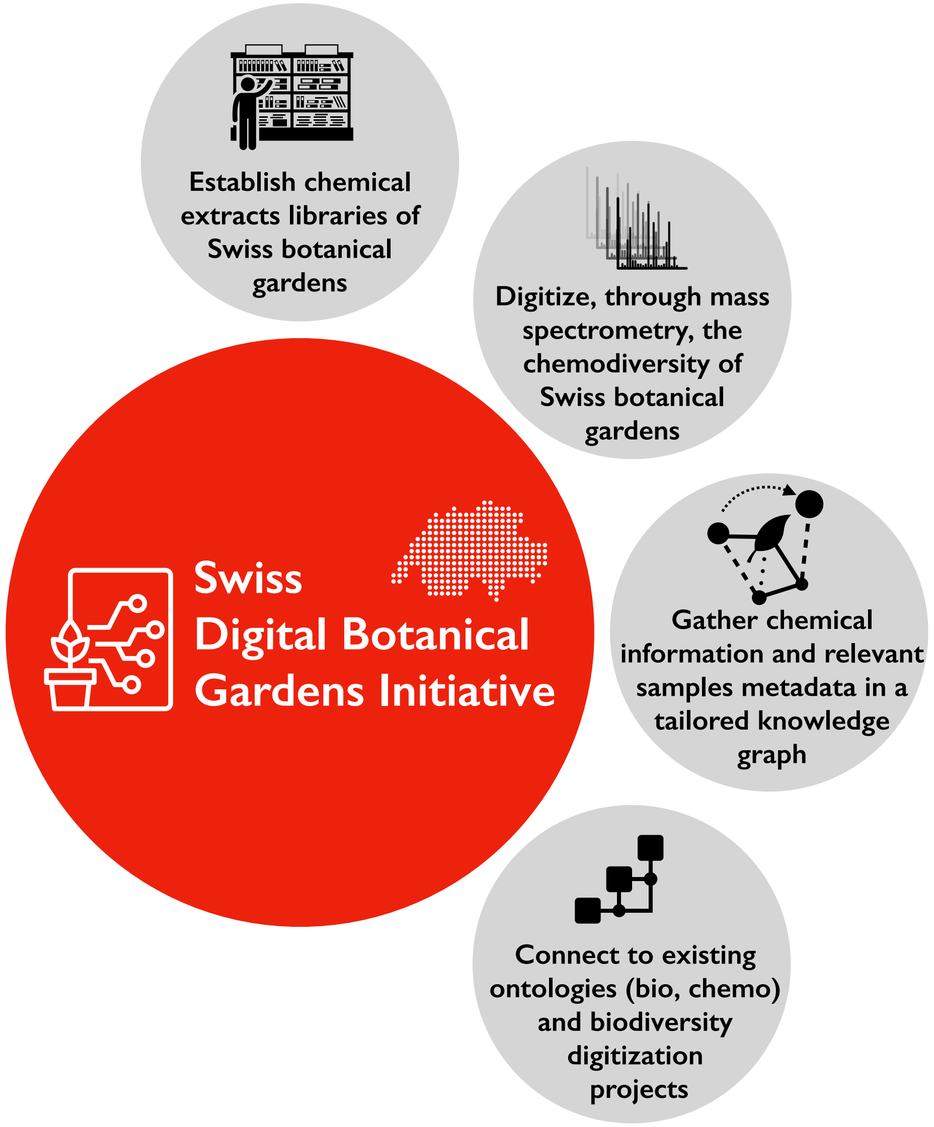


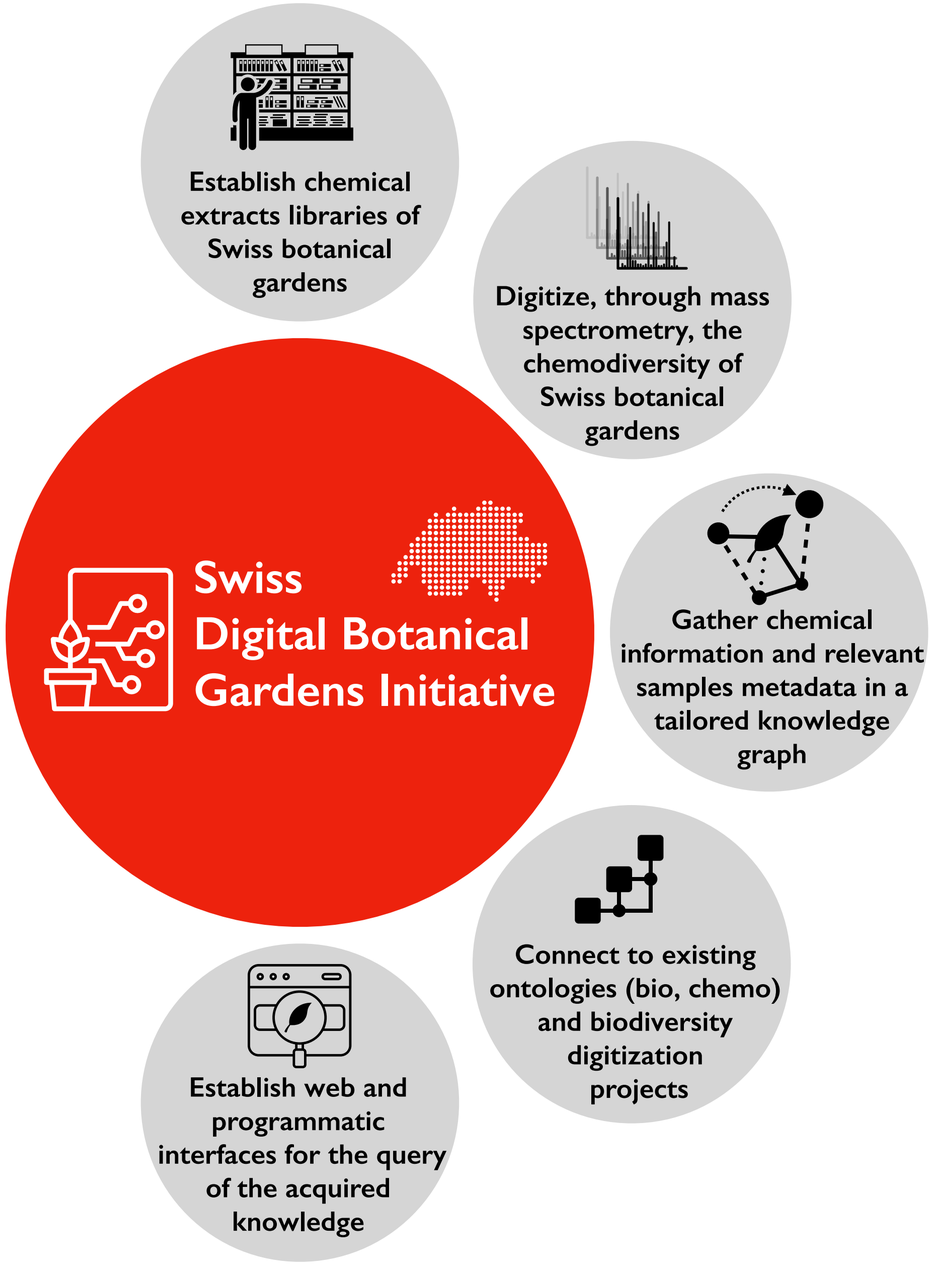
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens



Swiss Digital Botanical Gardens Initiative


Establish chemical extracts libraries of Swiss botanical gardens
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Swiss
Digital Botanical
Gardens Initiative


Establish chemical extracts libraries of Swiss botanical gardens
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens
Swiss Digital Botanical Gardens Initiative
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Connect to existing ontologies (bio, chemo) and biodiversity digitization projects


Establish chemical extracts libraries of Swiss botanical gardens
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens
Swiss Digital Botanical Gardens Initiative
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Connect to existing ontologies (bio, chemo) and biodiversity digitization projects
Establish web and programmatic interfaces for the query of the acquired knowledge

Swiss Digital Botanical Gardens Initiative

Establish chemical extracts libraries of Swiss botanical gardens

Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens

Gather chemical information and relevant samples metadata in a tailored knowledge graph

Connect to existing ontologies (bio, chemo) and biodiversity digitization projects

Establish web and programmatic interfaces for the query of the acquired knowledge

Illustrate the feasibility and advantages of an end-to-end Open Science project

Swiss Digital Botanical Gardens Initiative

Establish chemical extracts libraries of Swiss botanical gardens

Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens

Gather chemical information and relevant samples metadata in a tailored knowledge graph

Connect to existing ontologies (bio, chemo) and biodiversity digitization projects

Establish web and programmatic interfaces for the query of the acquired knowledge

Illustrate the feasibility and advantages of an end-to-end Open Science project

Establish robust and scalable workflows for the digitization of wildlife ecosystems biodiversity

Swiss Digital Botanical Gardens Initiative

Establish chemical extracts libraries of Swiss botanical gardens

Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens

Gather chemical information and relevant samples metadata in a tailored knowledge graph

Connect to existing ontologies (bio, chemo) and biodiversity digitization projects

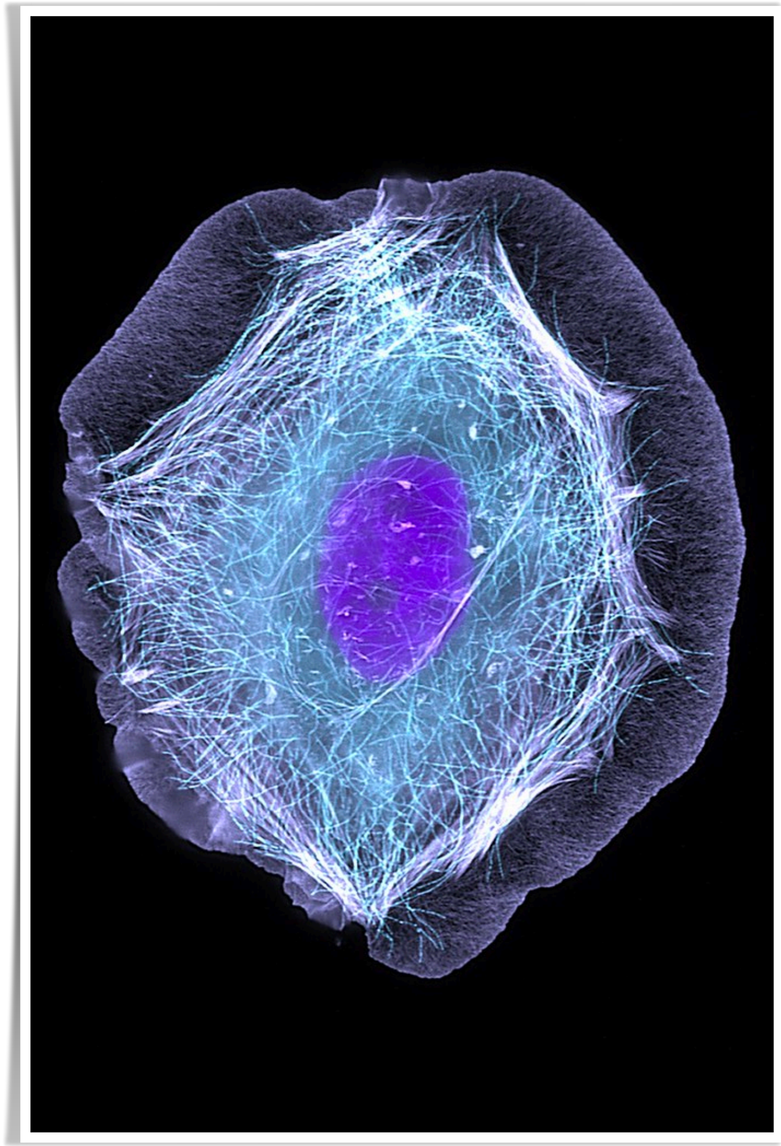
Establish web and programmatic interfaces for the query of the acquired knowledge

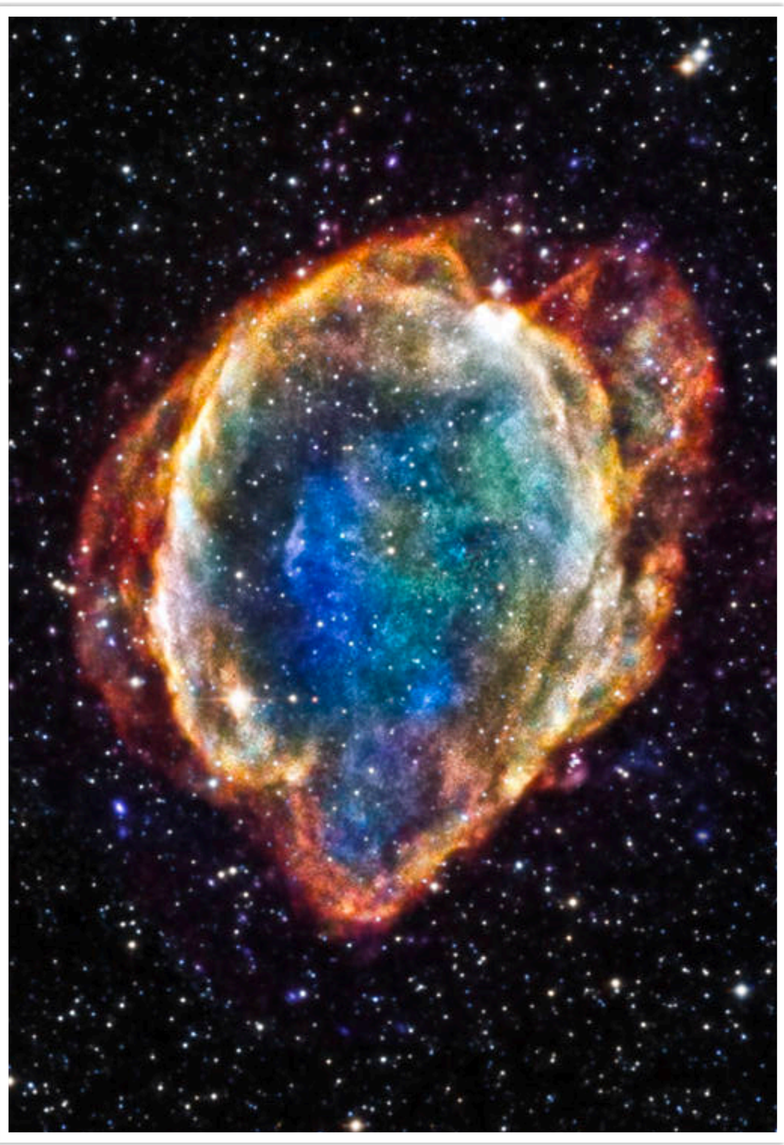
Illustrate the feasibility and advantages of an end-to-end Open Science project

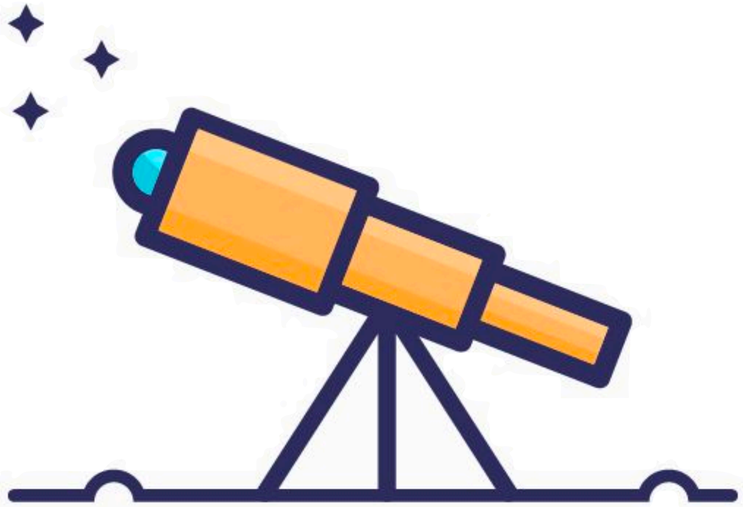
Establish robust and scalable workflows for the digitization of wildlife ecosystems biodiversity

Provide "molecular arguments" for biodiversity conservation policies

Establish chemical extracts libraries of Swiss botanical gardens
Provide "molecular arguments" for biodiversity conservation policies
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens
Swiss Digital Botanical Gardens Initiative
Establish robust and scalable workflows for the digitization of wildlife ecosystems biodiversity
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Illustrate the feasibility and advantages of an end-to-end Open Science project
Establish web and programmatic interfaces for the query of the acquired knowledge
Connect to existing ontologies (bio, chemo) and biodiversity digitization projects

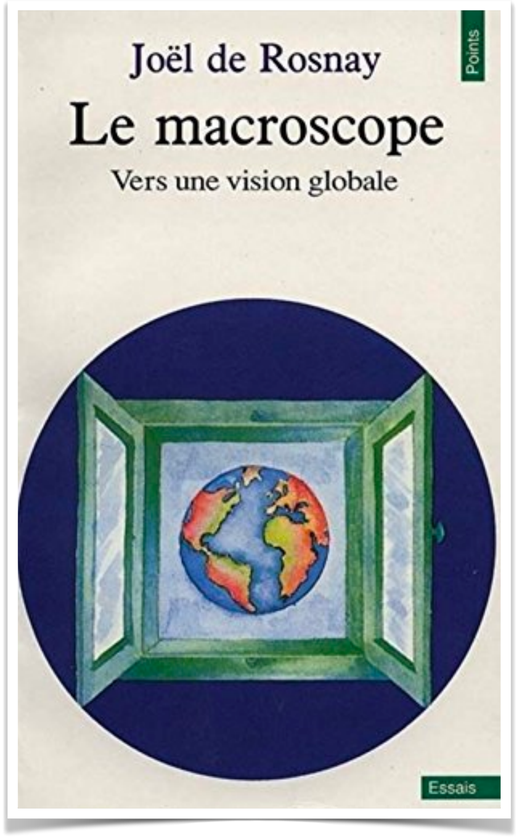






Théorie des systèmes et communication

Joël de Rosnay
LE MACROSCOPE :
VERS UNE VISION GLOBALE
Paris, Le Seuil, 1975, 35 F.

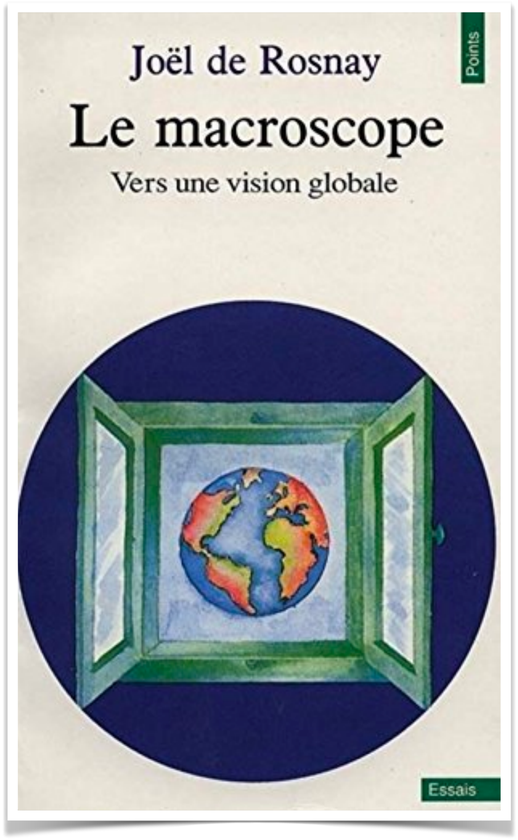


infinitely small: observable by a microscope
infinitely big: observable by a telescope
infinitely complex: observable by a **macroscope***

*a symbolic instrument made of methods and techniques taken from multiple fields

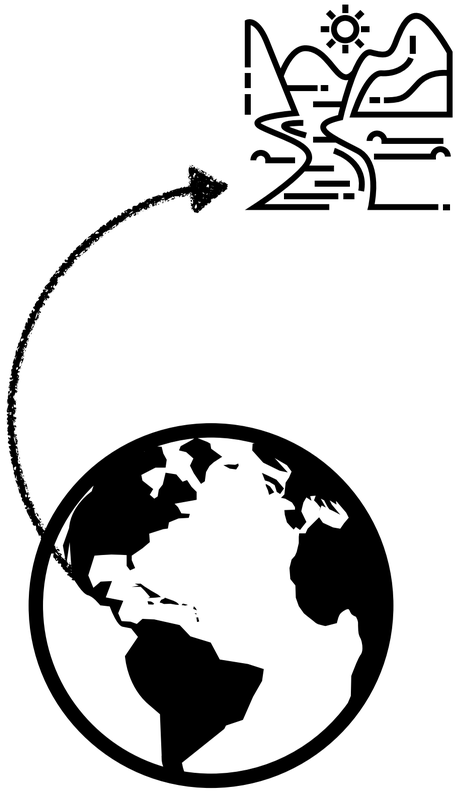
Théorie des systèmes et communication

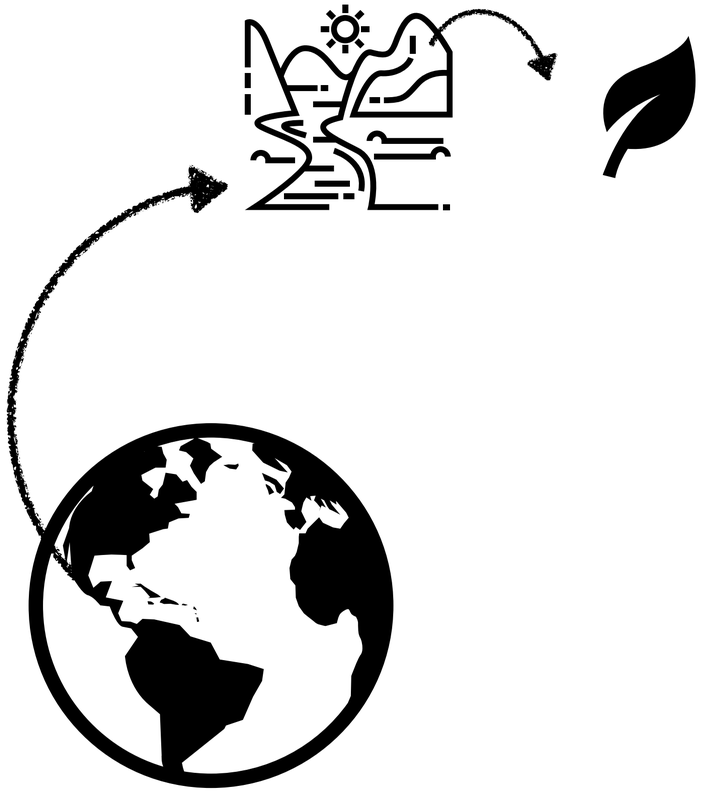
Joël de Rosnay
LE MACROSCOPE :
VERS UNE VISION GLOBALE
Paris, Le Seuil, 1975, 35 F.

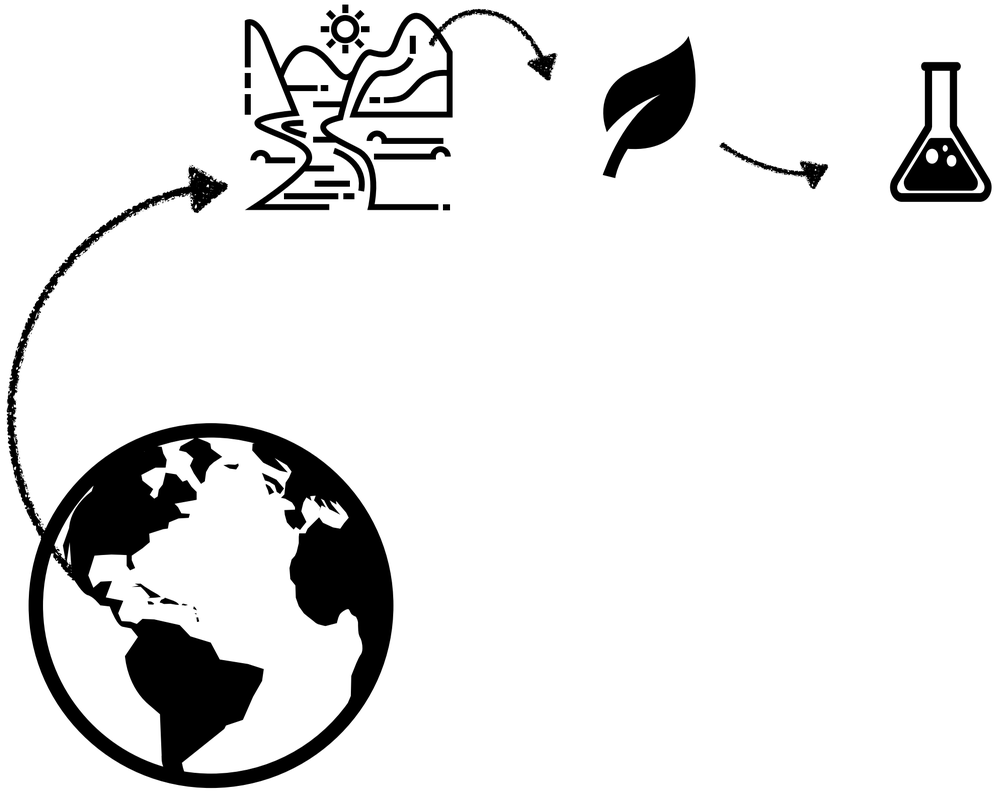


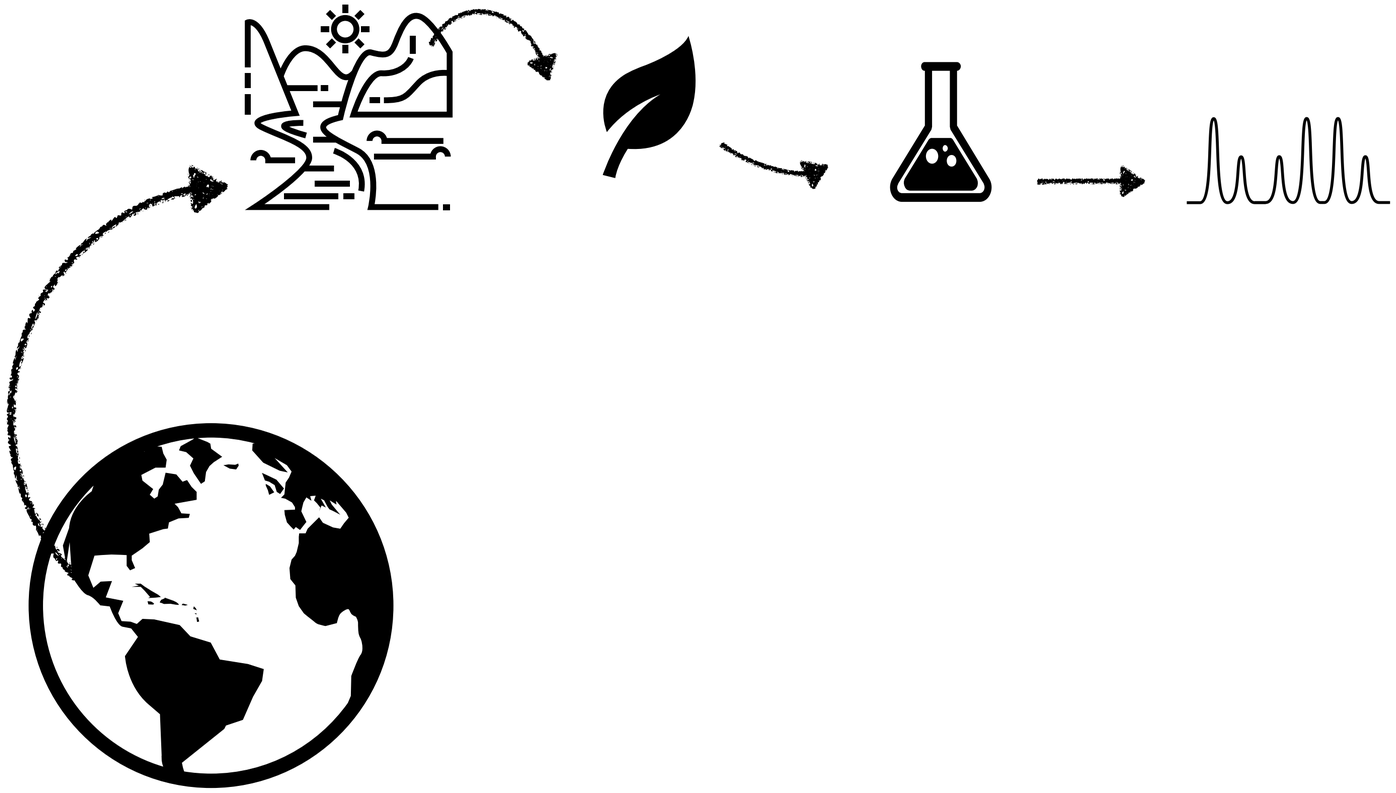
infinitely small: observable by a microscope
infinitely big: observable by a telescope
infinitely complex: observable by a **macroscope***

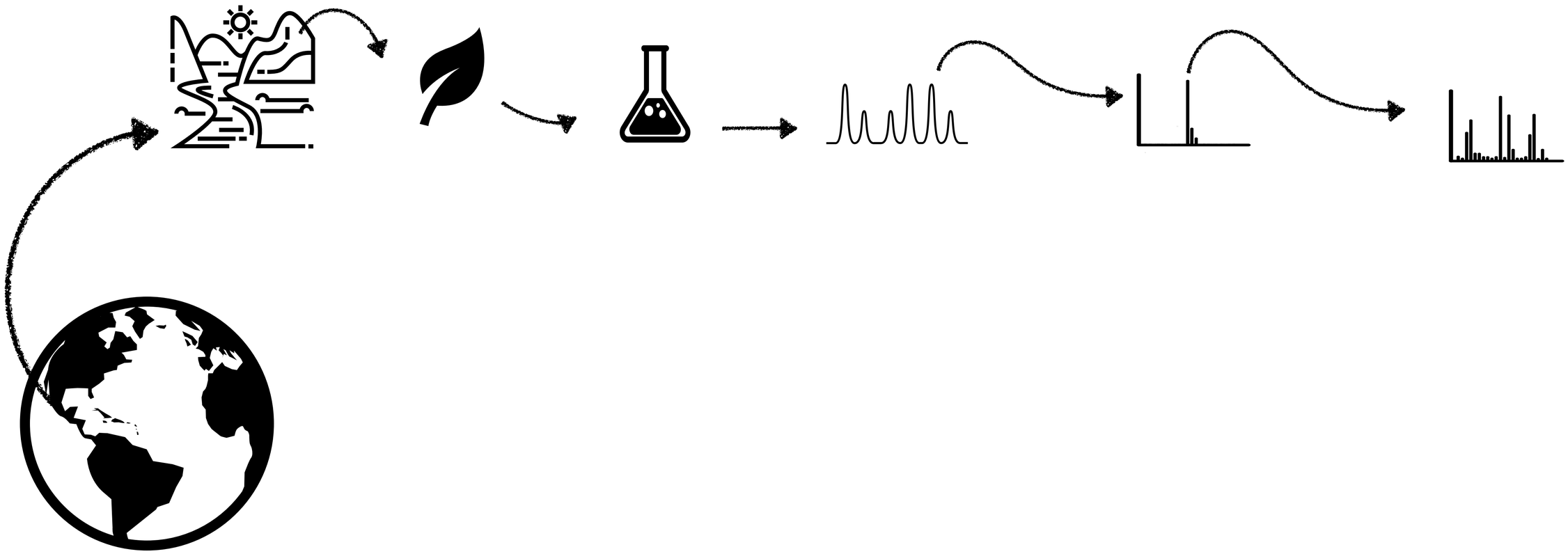
*a symbolic instrument made of methods and techniques taken from multiple fields

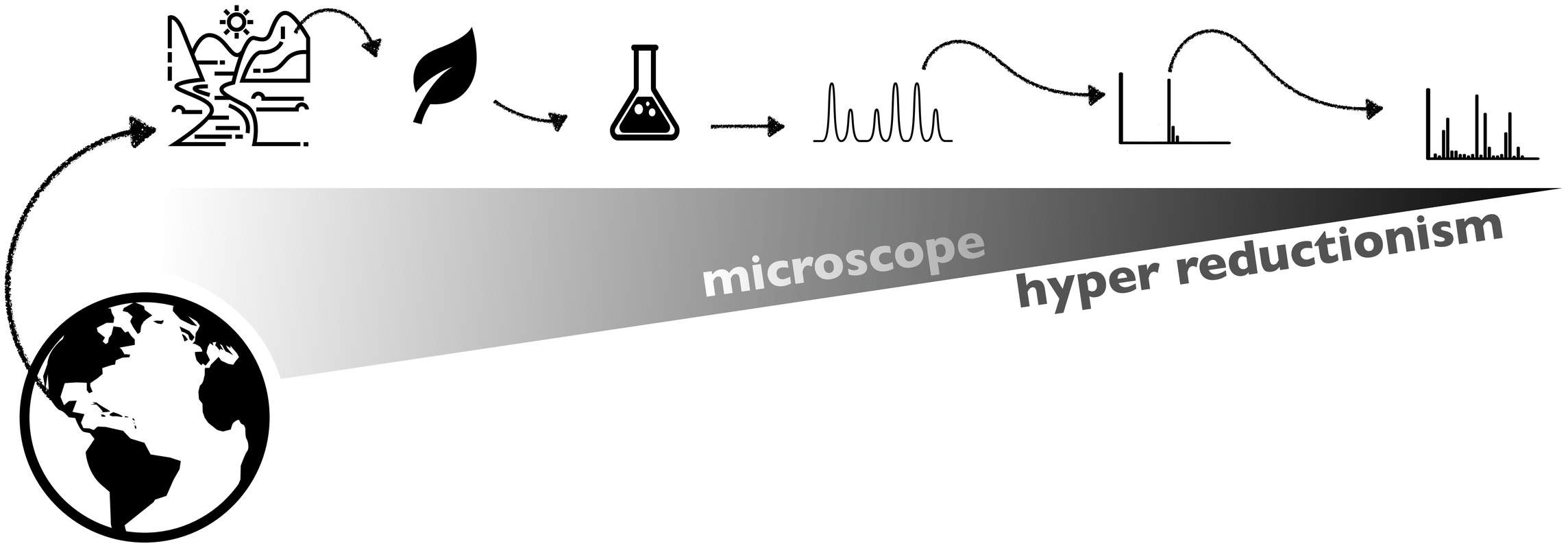


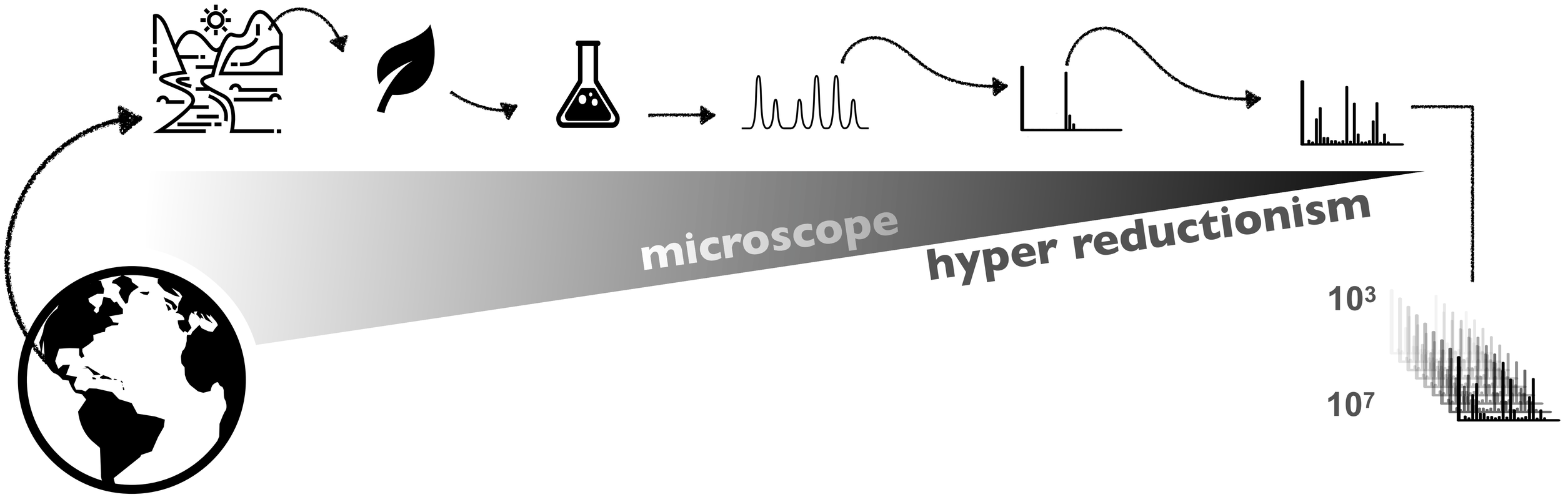


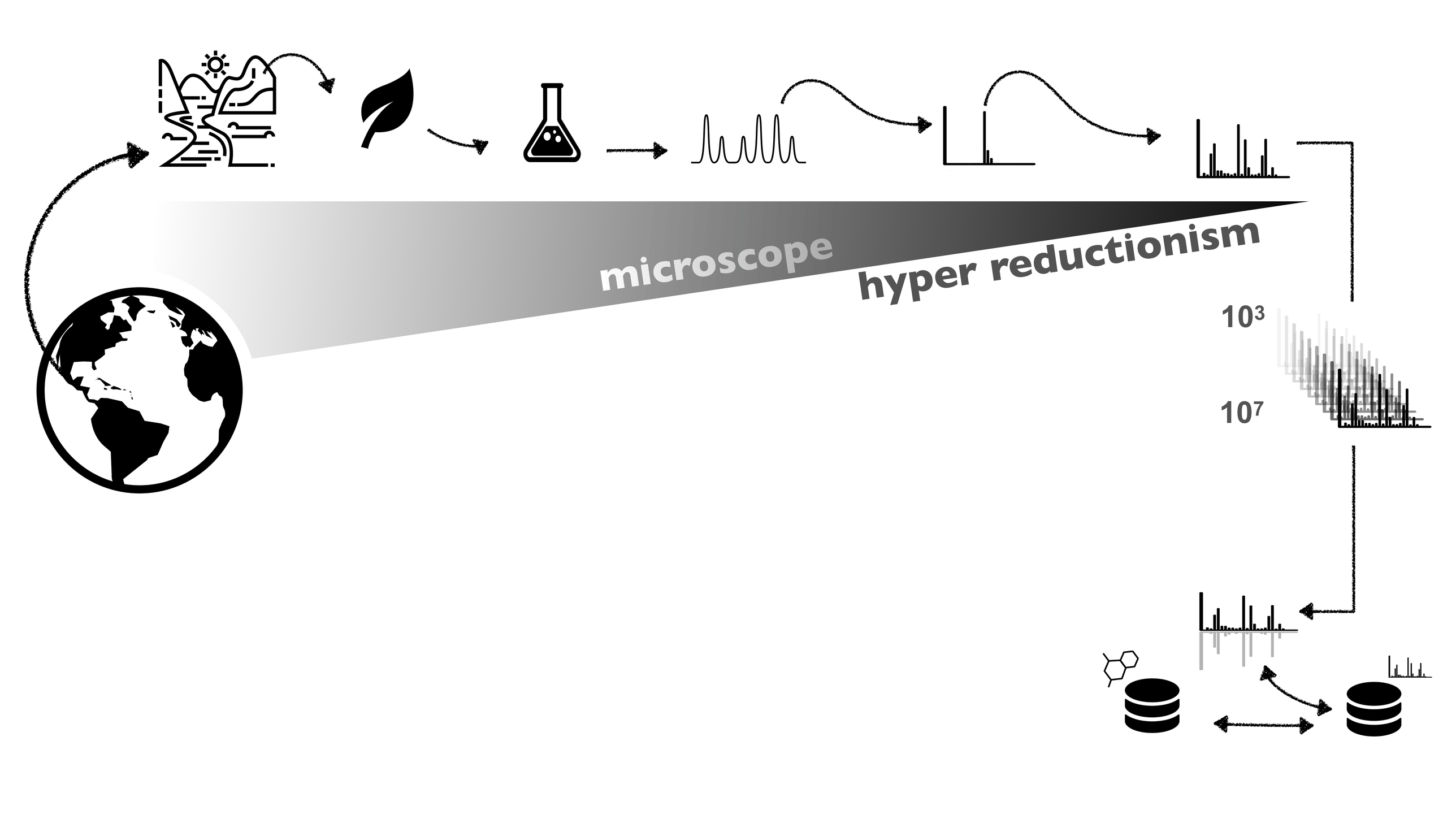


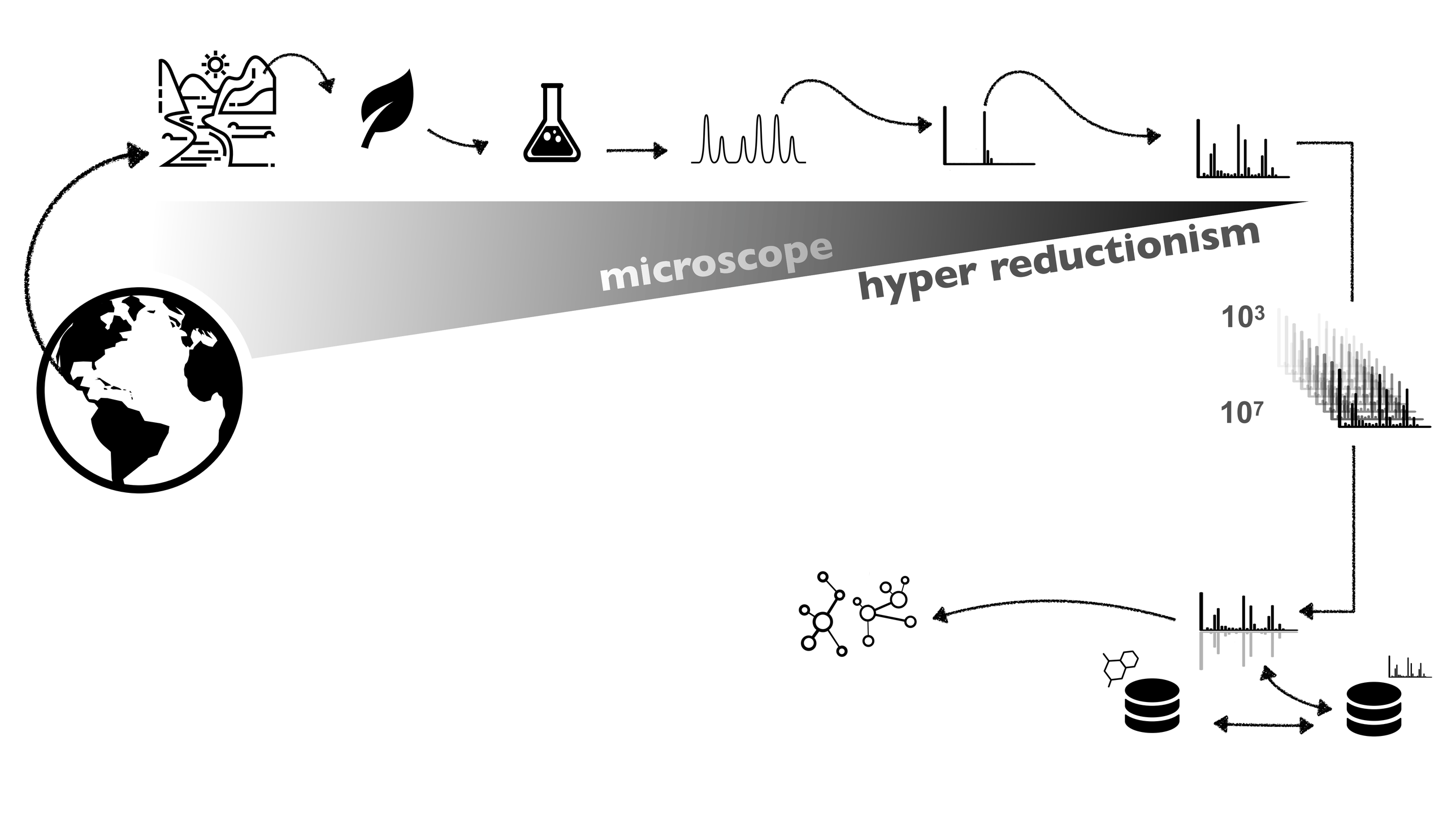


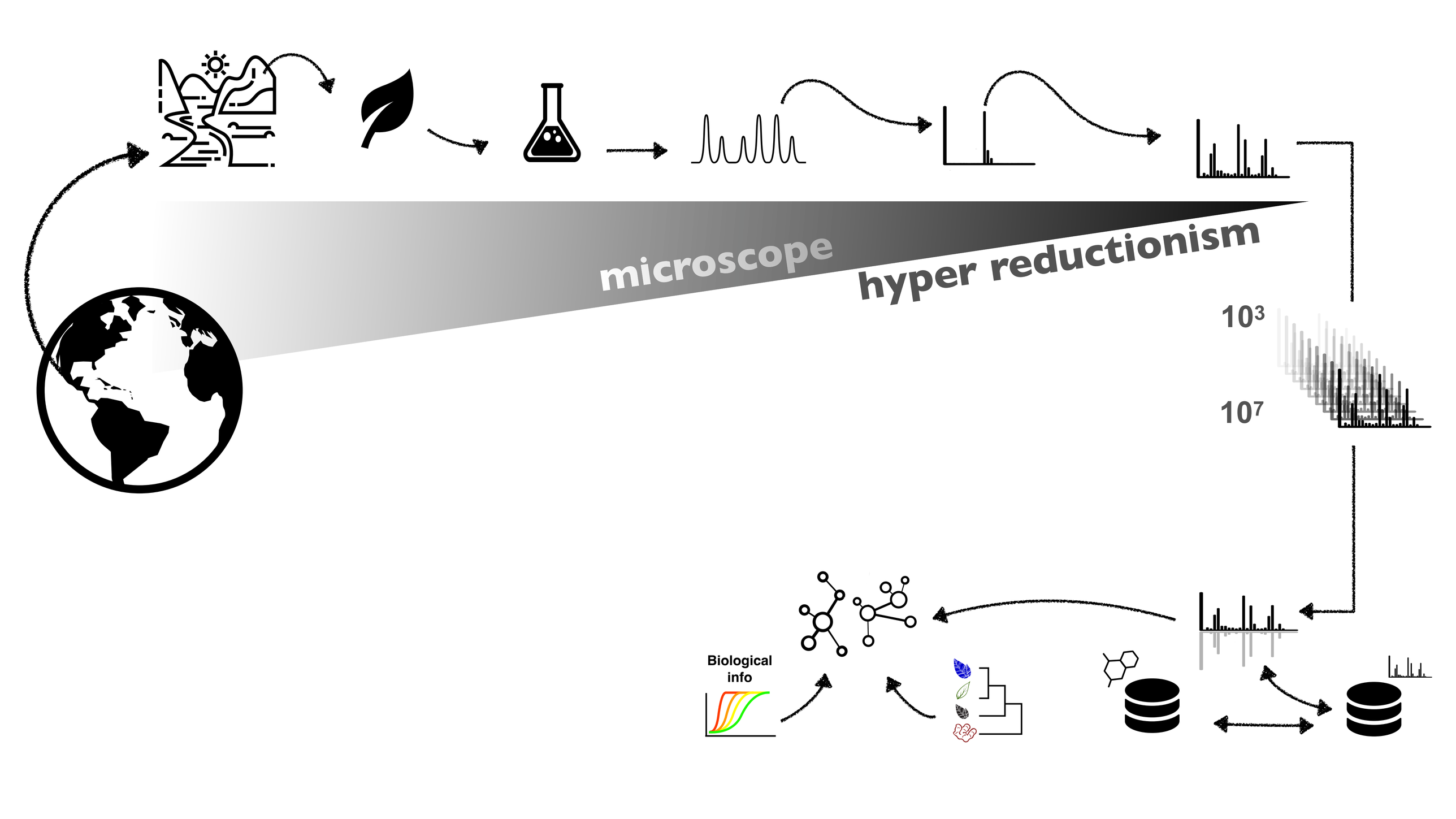


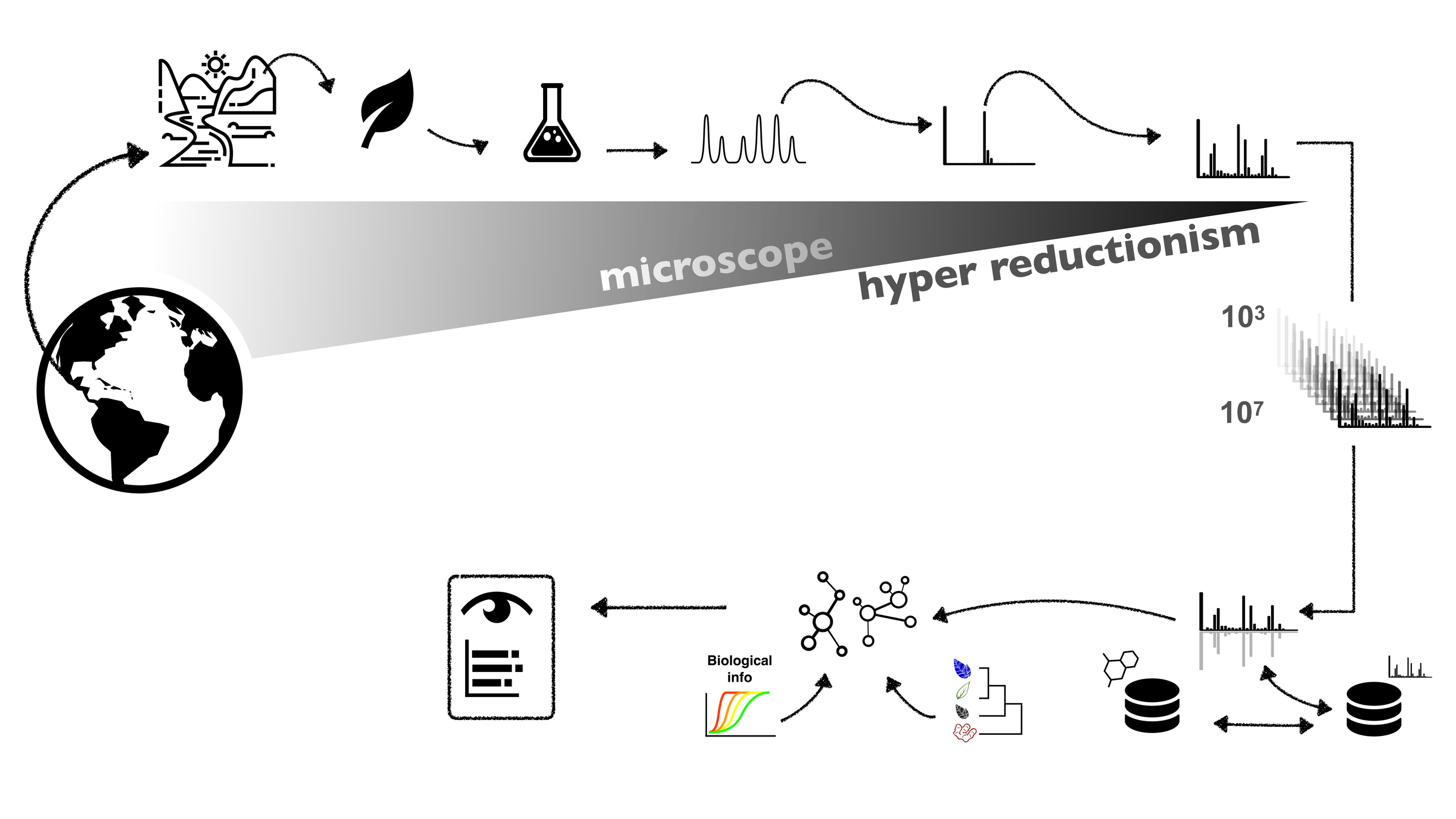

microscope
hyper reductionism

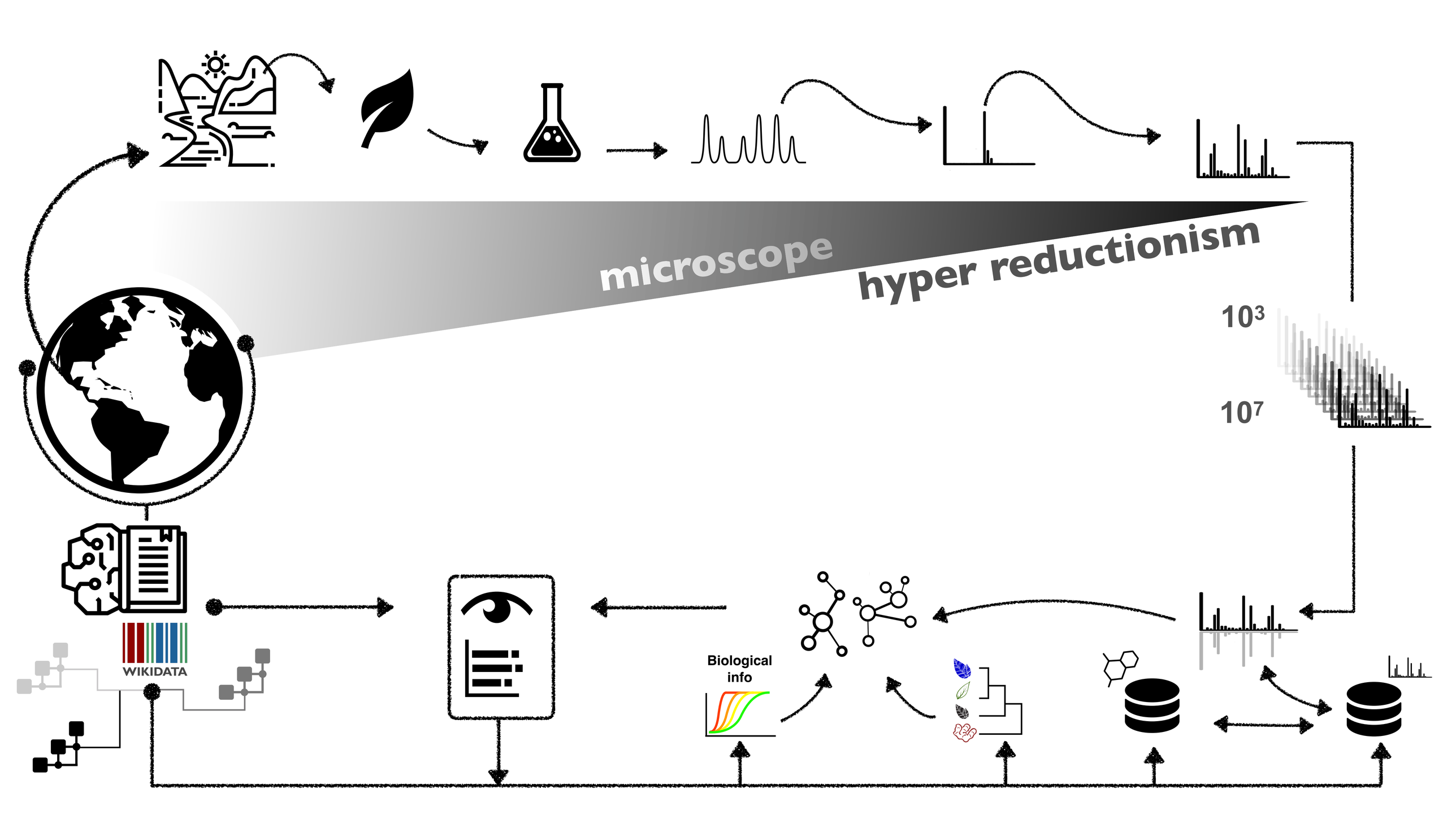

microscope
hyper reductionism
10^3
10^7

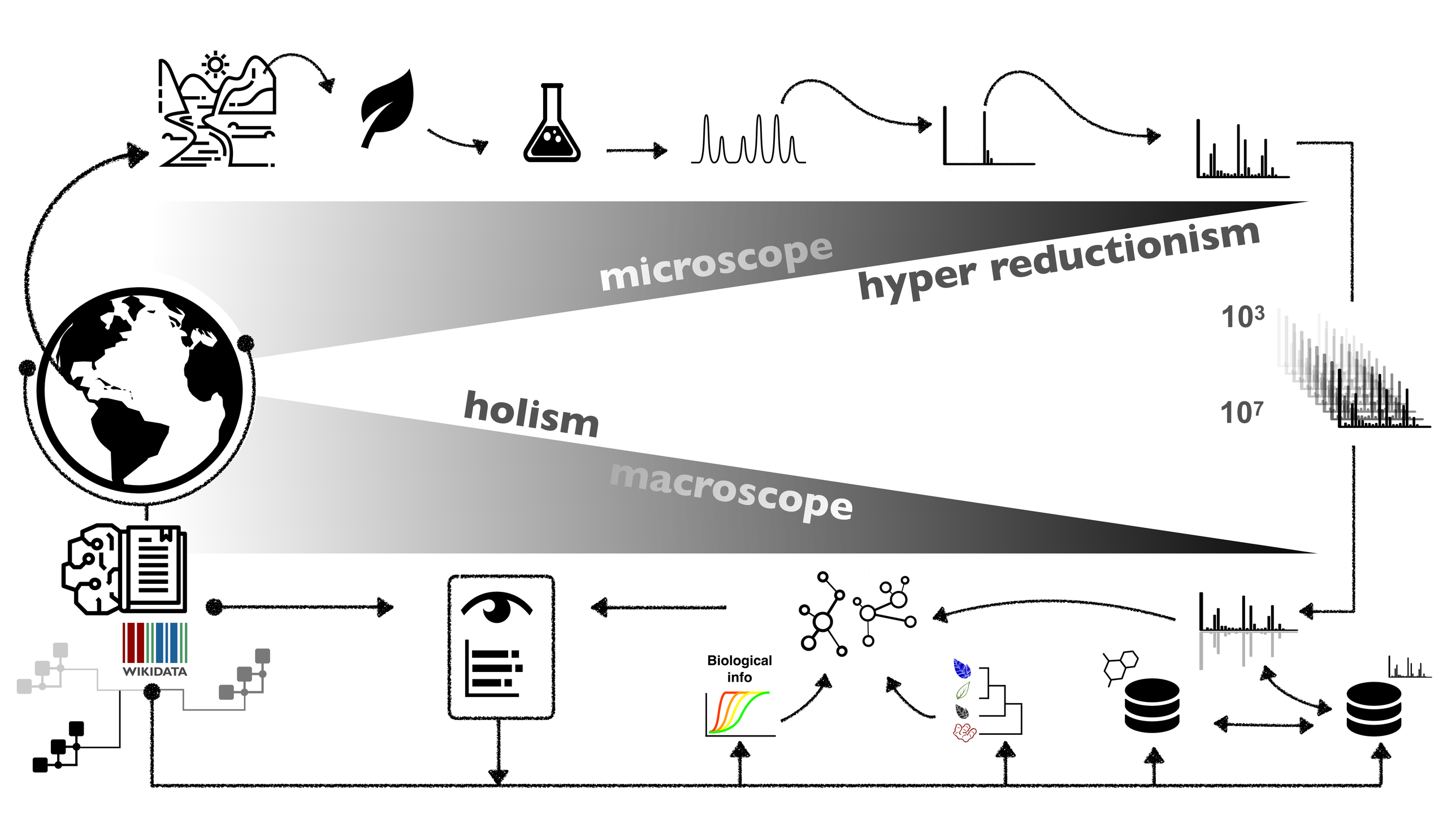

microscope
hyper reductionism
10^3
10^7

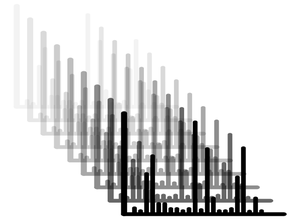

microscope
hyper reductionism
10^3
10^7

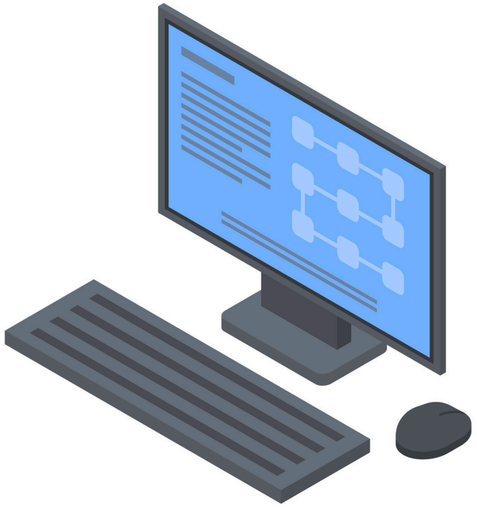

microscope
hyper reductionism
10^3
10^7
Biological info


microscope
hyper reductionism
10^3
10^7
Biological info

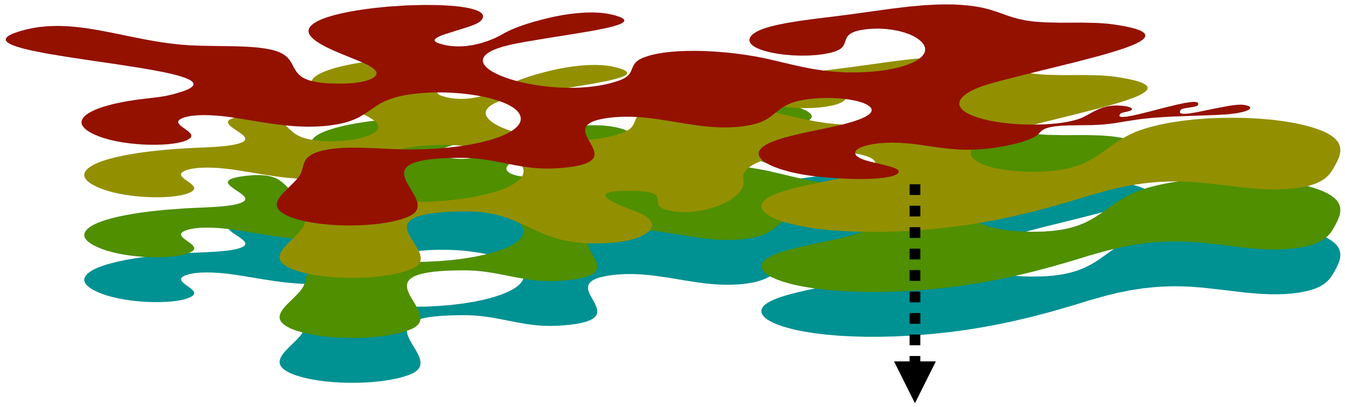

microscope
hyper reductionism
10^3
10^7
WIKIDATA
Biological info


microscope
hyper reductionism
holism
macroscope
10^3
10^7
WIKIDATA
Biological info





Stacking metabolomes for a single species



Specimen sampled in several conditions (e.g. environmental conditions, organ, life stage)

Challenges

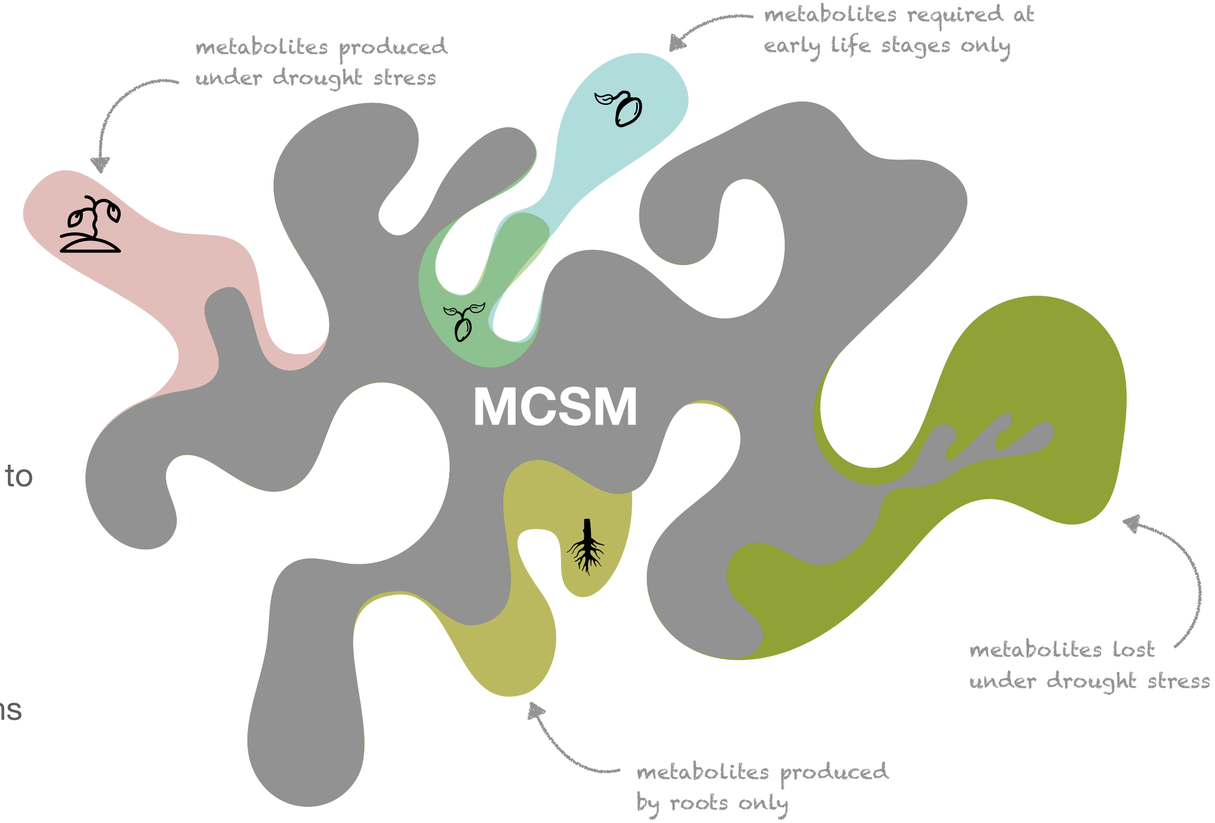
In large scale sequencing initiative ***one*** sequenced sample is enough to capture the genetic potential of the whole species.
In metabolomics, sampling at different life stages, different organs or in different environmental conditions will lead to different metabolic profiles. This is both a weakness (in terms of required experiments) and an incredible strength.

Opportunities

Concept of **MCSM**
Maximum **C**ommon **S**ub-**M**etabolome and its branches

Just like Maximum Common Substructures calculations in chemoinformatics, we propose the concept Maximum Common Sub-Metabolome. This is possible thanks to *i)* Knowledge Graph based structure *ii)* unconventional alignement approaches (e.g vectorizing spectral information at the sample level)

This MCSM will:
- capture the most stable metabolic fingerprint of a species
- inform on biosynthetic pathways invested in or shut down under several conditions
- the higher the number of layers, the more robust the MCSM
- can be applied at any taxa levels an even across the total Earth Metabolome
- can be compared across conditions

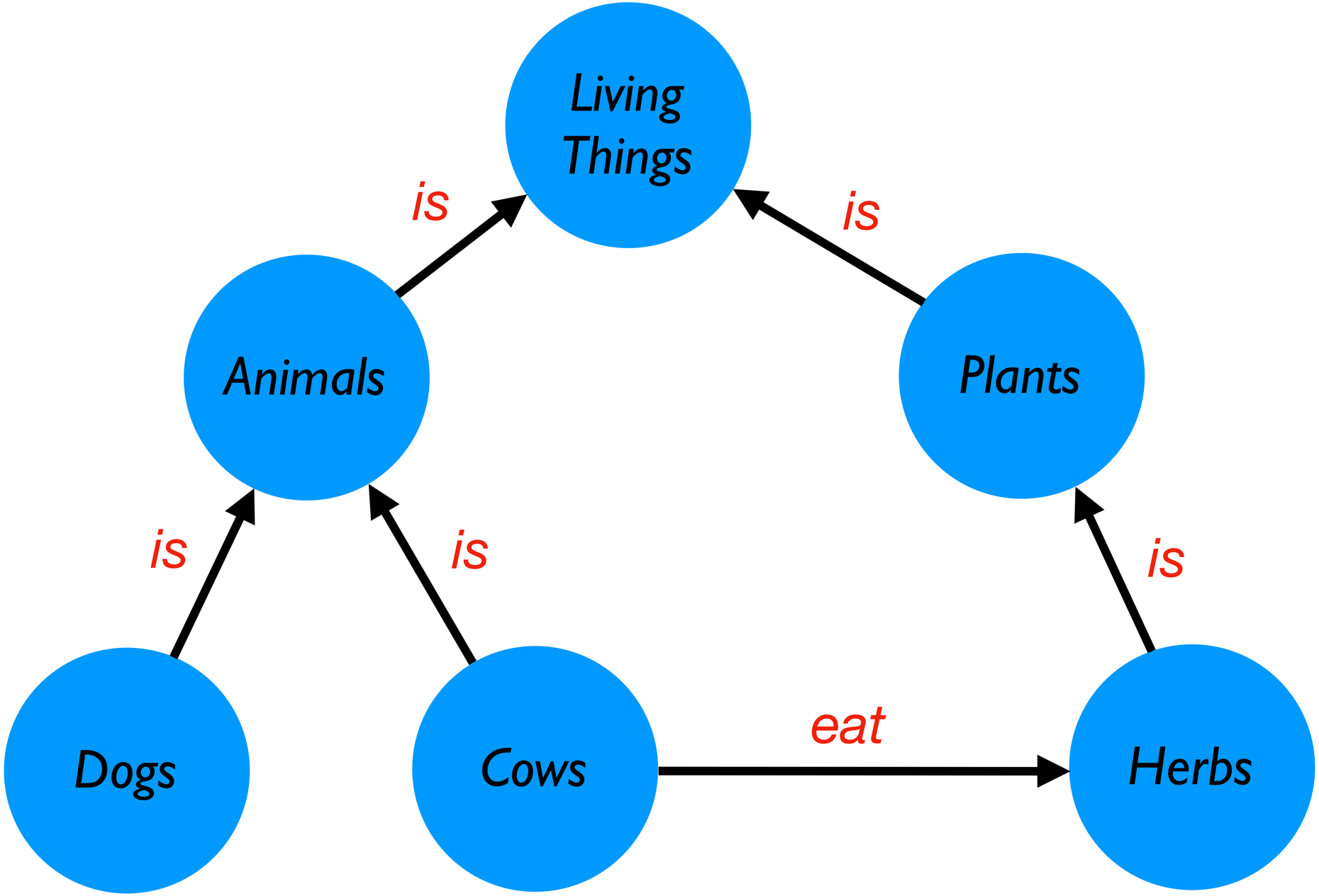


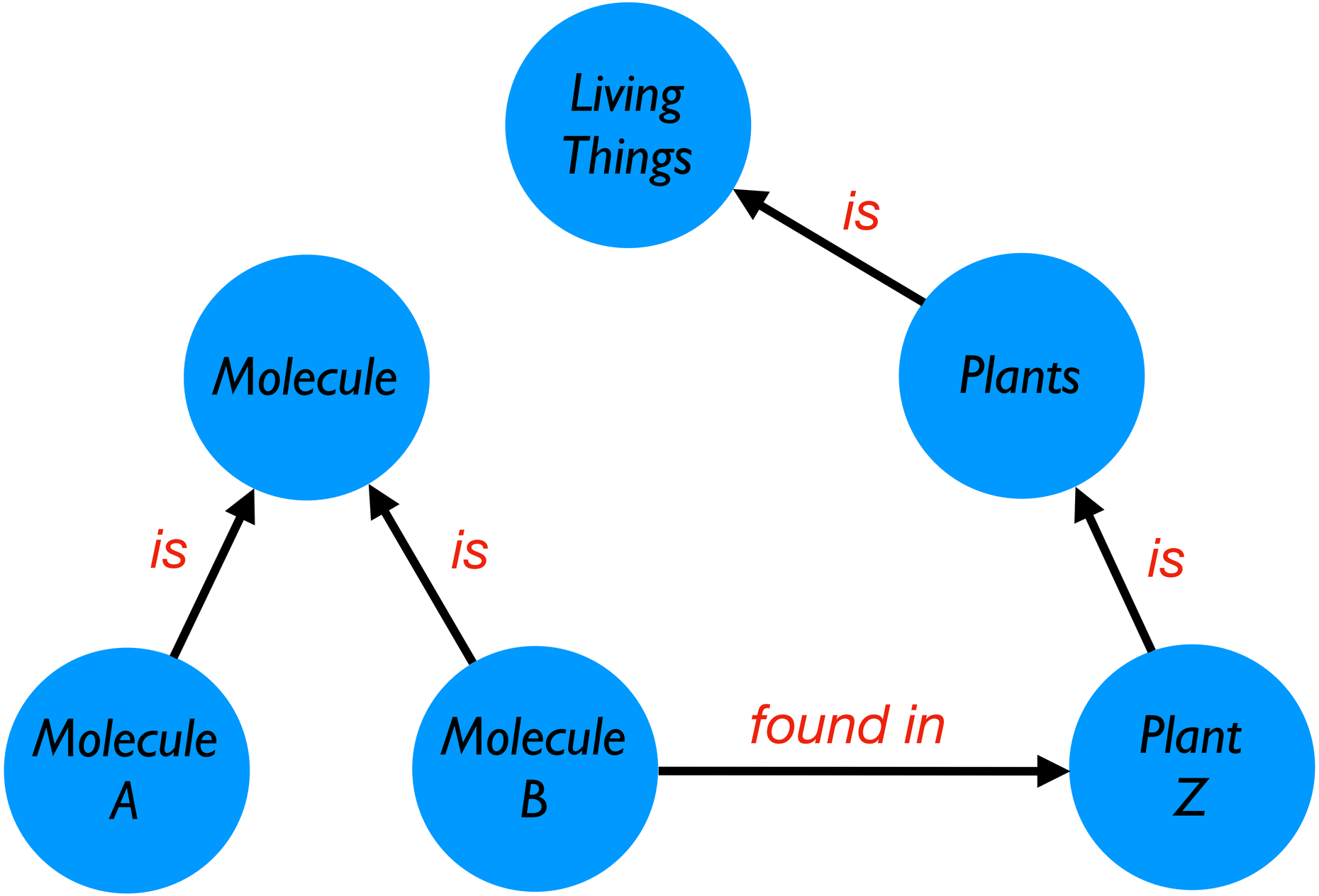
Swiss
Digital Botanical
Gardens Initiative
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Connect to existing ontologies (bio, chemo) and biodiversity digitization projects
Establish web and programmatic interfaces for the query of the acquired knowledge
Illustrate the feasibility and advantages of an end-to-end Open Science project
Establish robust and scalable workflows for the digitization of wildlife ecosystems biodiversity
Provide "molecular arguments" for biodiversity conservation policies
Establish chemical extracts libraries of Swiss botanical gardens
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens

What

is a

Knowledge Graph ?


Living Things
is
is
Animals
Plants
is
is
is
Dogs
Cows
eat
Herbs


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

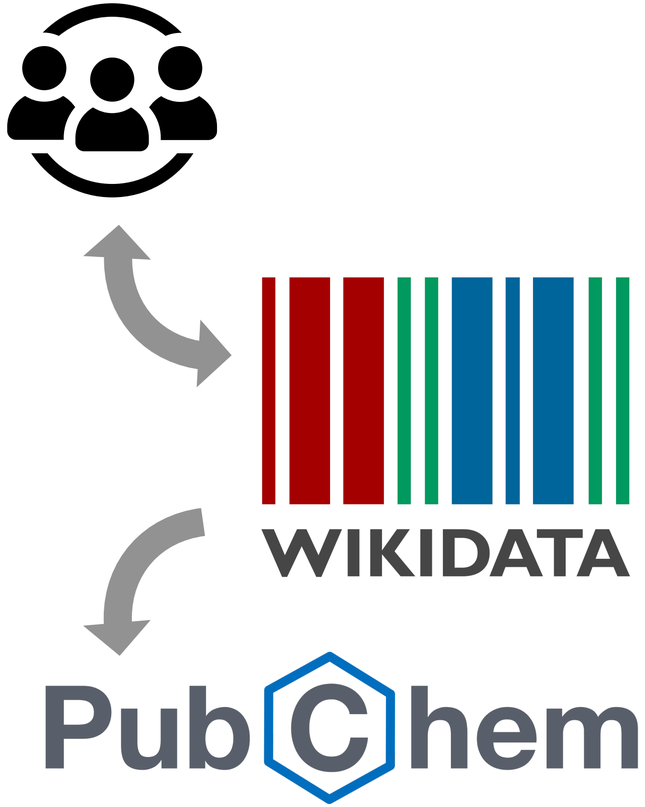
eLife

TOOLS AND RESOURCES

The LOTUS initiative for open knowledge management in natural products research

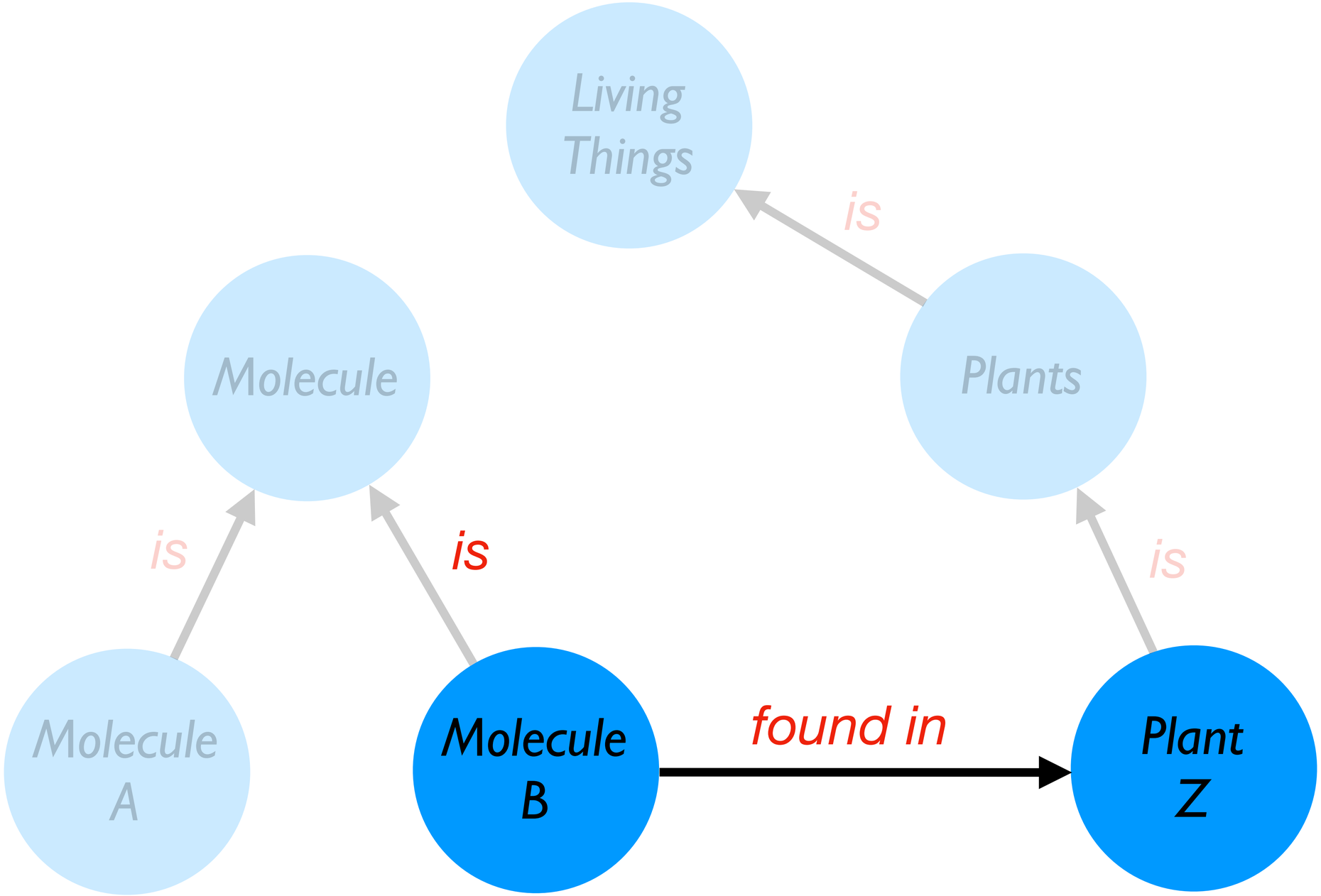
Adriano Rutz[1,2], Maria Sorokina[3], Jakub Galgonek[4], Daniel Mietchen[5,6,7], Egon Willighagen[8], Arnaud Gaudry[1,2], James G Graham[9,10], Ralf Stephan[11], Roderic Page[12], Jiří Vondrášek[4], Christoph Steinbeck[3], Guido F Pauli[9,10], Jean-Luc Wolfender[1,2], Jonathan Bisson[9,10]*, Pierre-Marie Allard[1,2,13]*

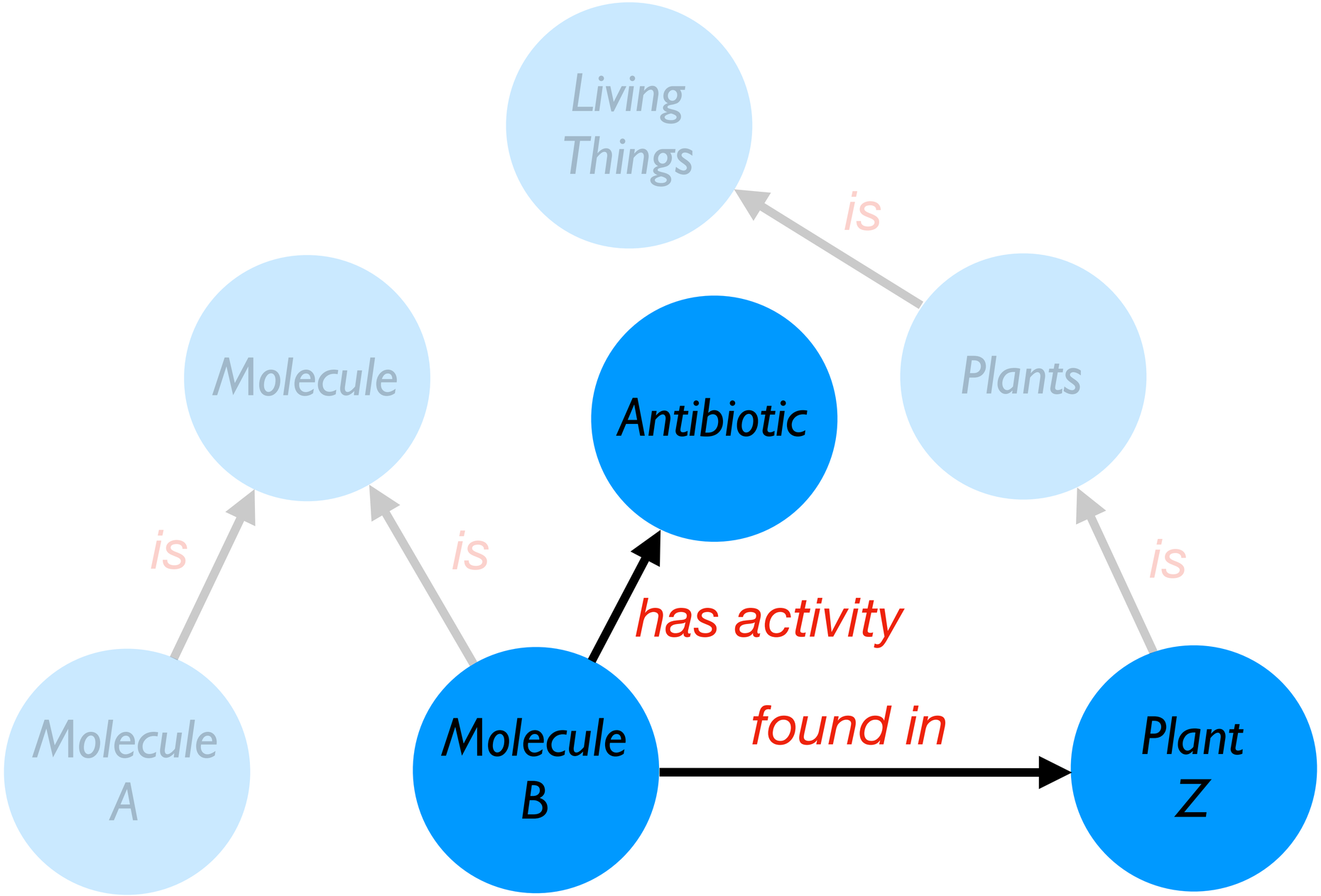
https://doi.org/10.7554/eLife.70780

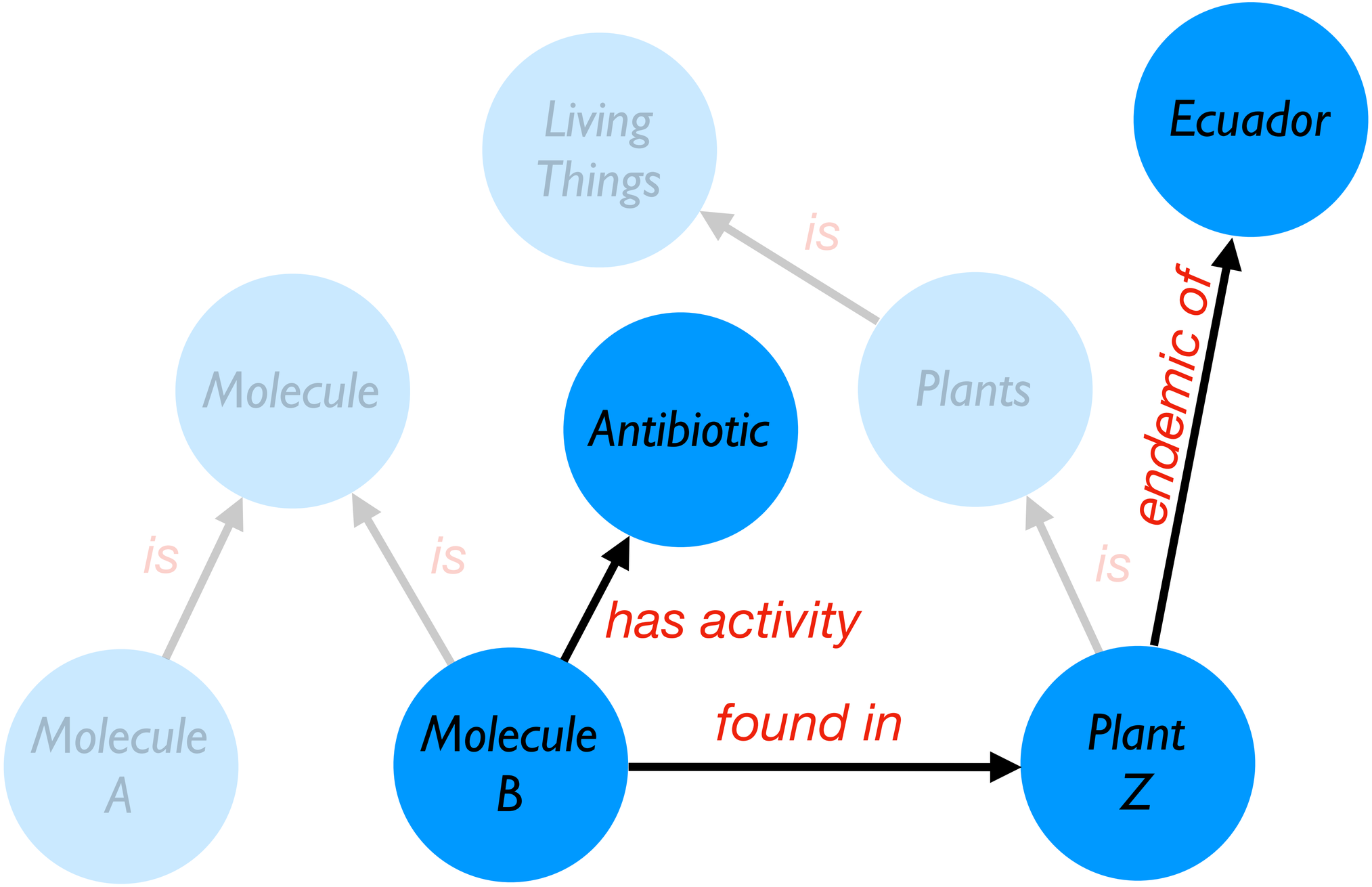


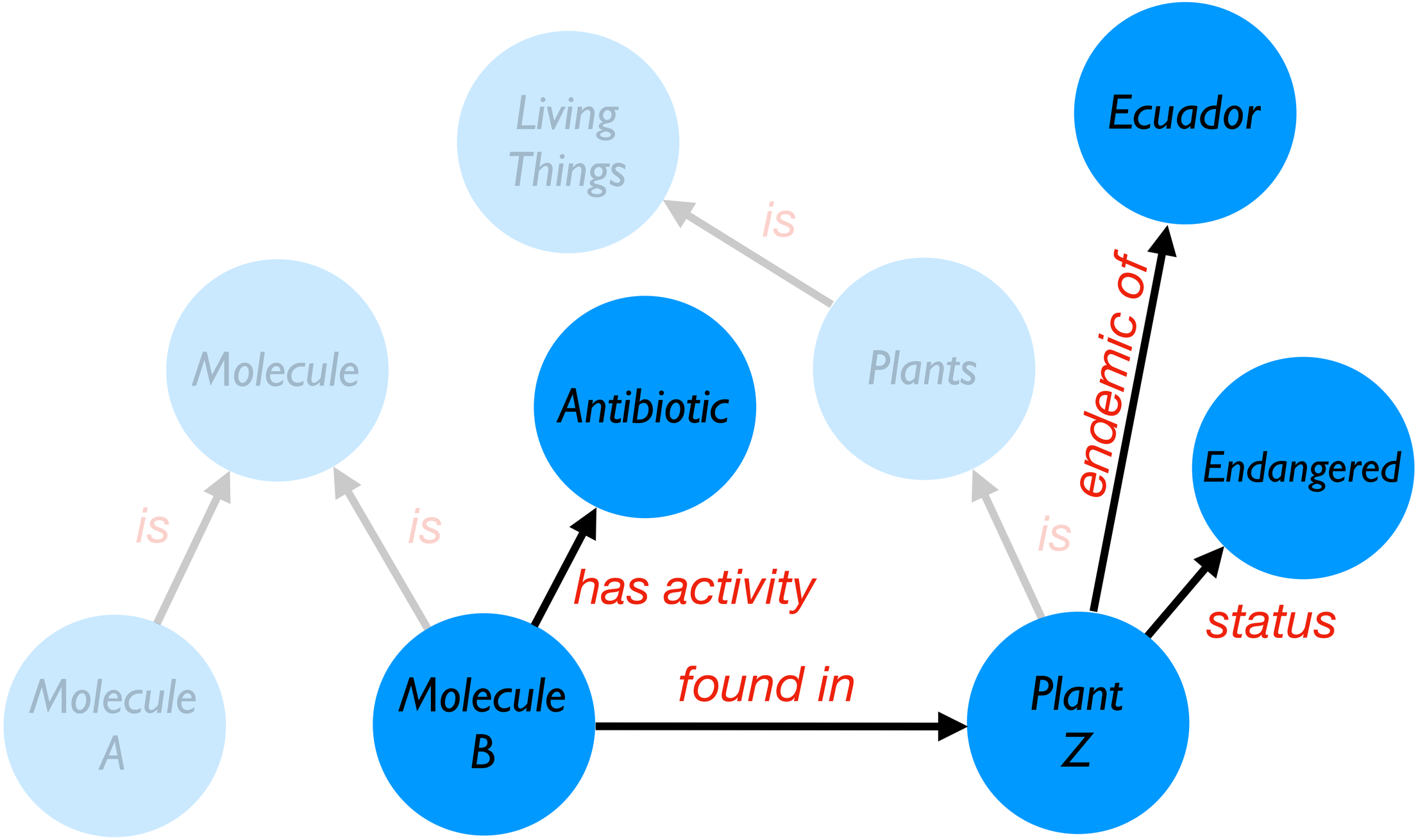
microscope
macroscope

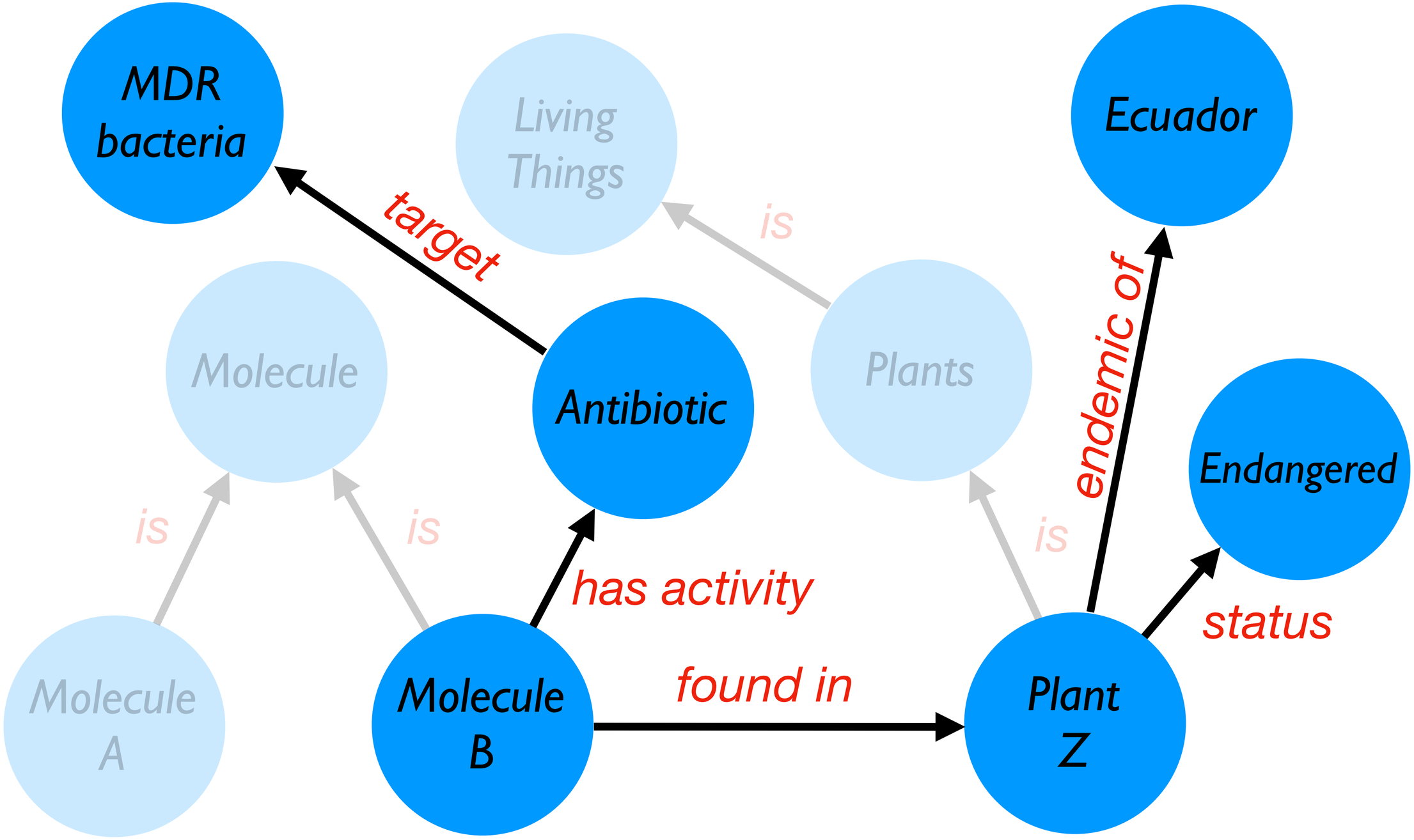
Molecule
found in
Organism

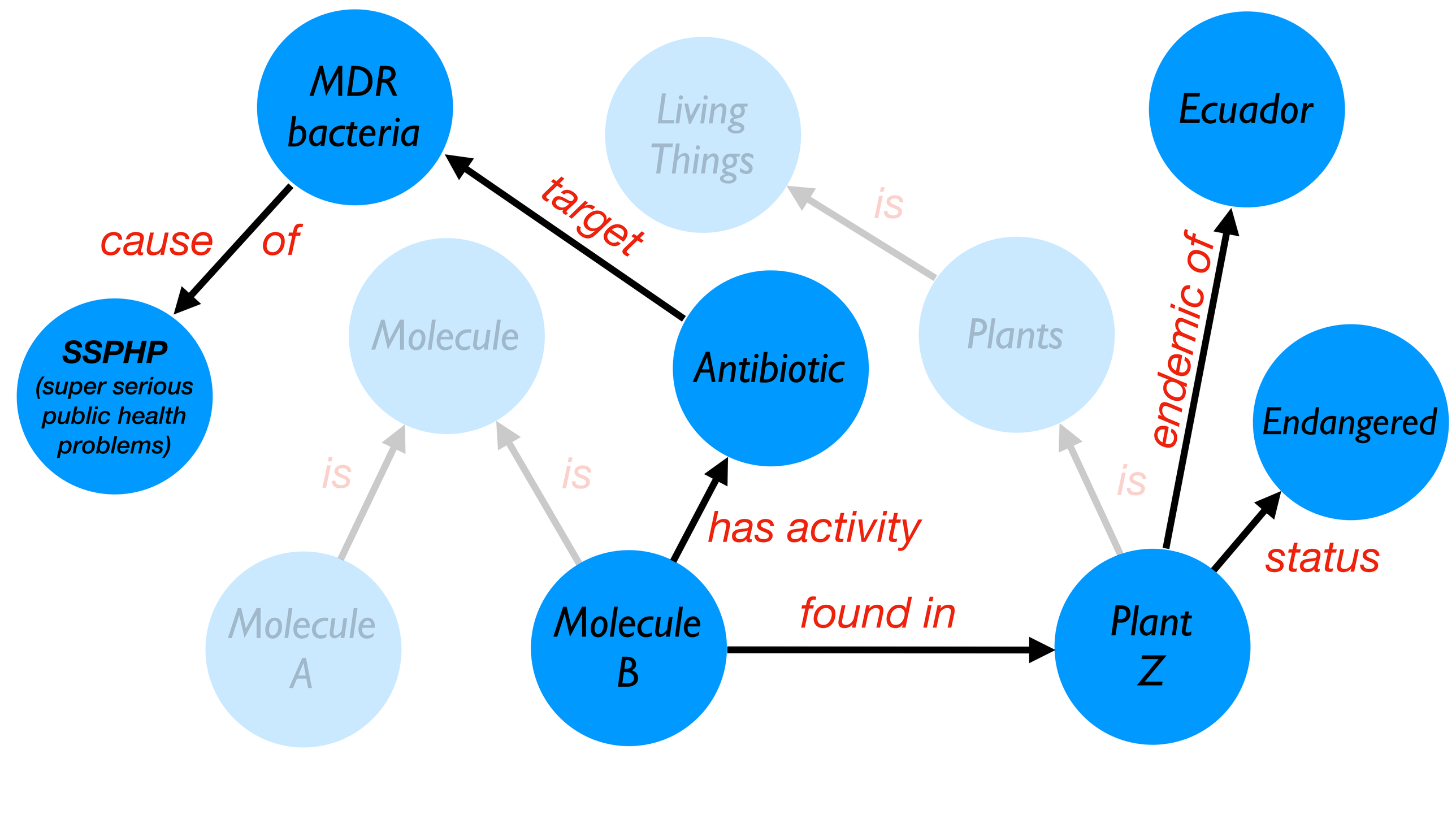

Living Things
is
Molecule
Plants
is
is
is
Molecule A
Molecule B
found in
Plant Z


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


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

Active repository

Local

pf_dbgi · Common ENPKG KG between PF and DBGI d

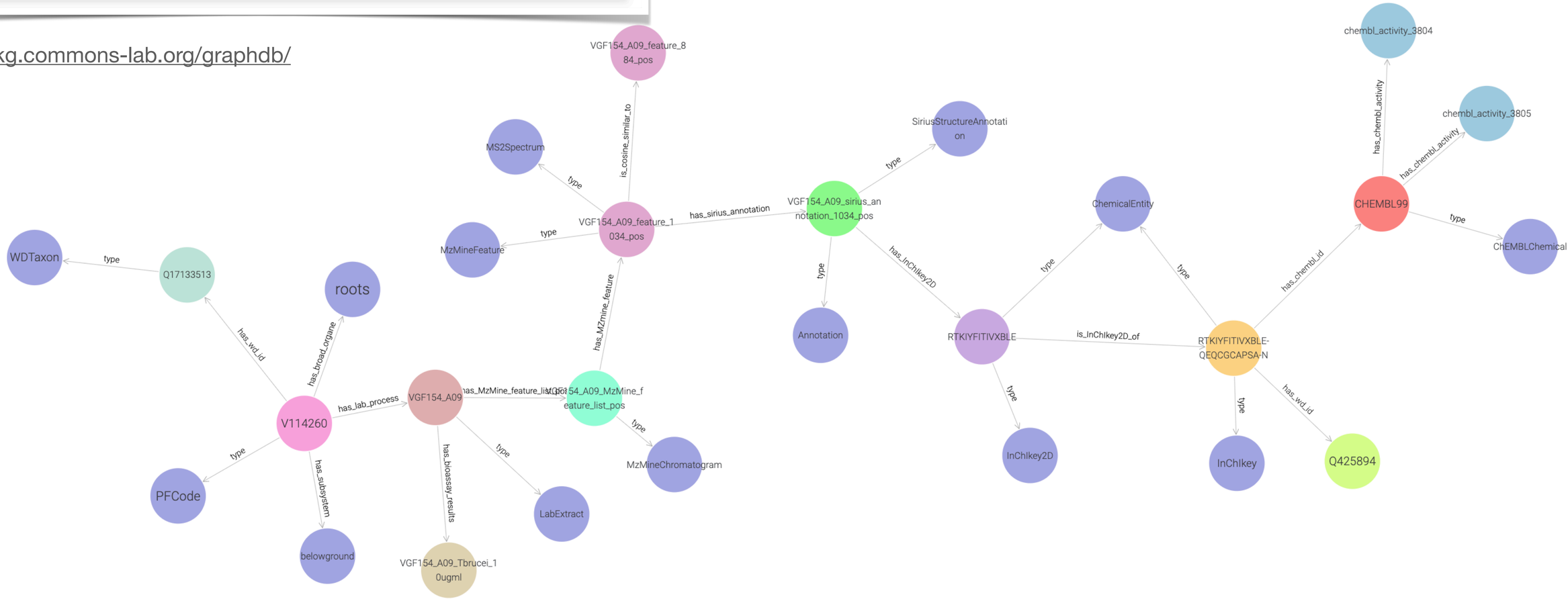
total statements
30,617,014

27,711,418 explicit
2,905,596 inferred
1.10 expansion ratio

Import RDF data

Export RDF data

https://enpkg.commons-lab.org/graphdb/



Swiss
Digital Botanical
Gardens Initiative
Illustrate the feasibility and advantages of an end-to-end Open Science project
Establish chemical extracts libraries of Swiss botanical gardens
Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens
Gather chemical information and relevant samples metadata in a tailored knowledge graph
Connect to existing ontologies (bio, chemo) and biodiversity digitization projects
Establish web and programmatic interfaces for the query of the acquired knowledge
Establish robust and scalable workflows for the digitization of wildlife ecosystems biodiversity
Provide "molecular arguments" for biodiversity conservation policies

https://notes.andymatuschak.org/z21cgR9K3UcQ5a7yPsj2RUim3oM2TzdBByZu

"*Working with the garage door up*" is a good definition of the concept of Open Notebook Science.

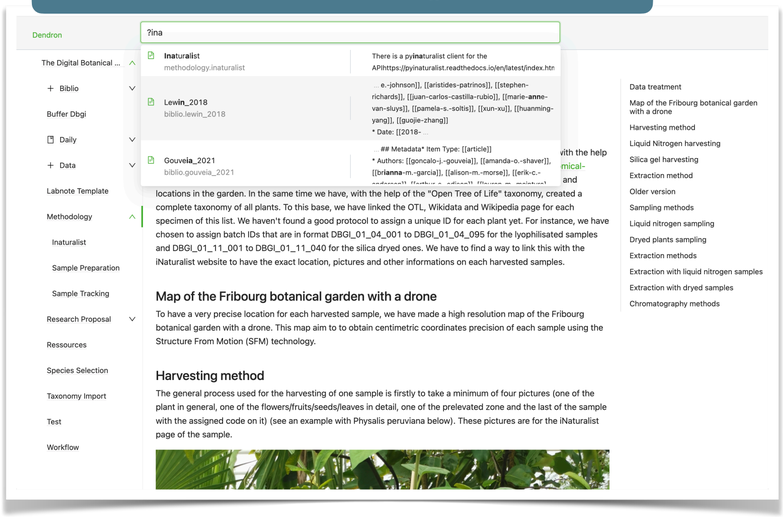
Everything is shared from the beginning of the research project.
Early ideas.
Early results.
Every bit of code.
Of course this will also imply that poorly written code and sketchy ideas will be shared.

Open Science principles and practices are central to the EMI, as they help to ensure that the research is transparent, reproducible, and collaborative. This includes making data and research findings openly available, and allowing the participation of researchers from a wide range of disciplines. It's not just open access publications. It's Open Notebook Science.

What's that ? "***Working with the garage door up***" could be a good definition of the concepts of ***Open Notebook Science***.

Everything is shared from the beginning of the research project. Early ideas. Early results. Every bit of code.
This also implies that poorly written code and sketchy ideas will be shared ... but they are available to be improved upon !

Ideas and daily notes



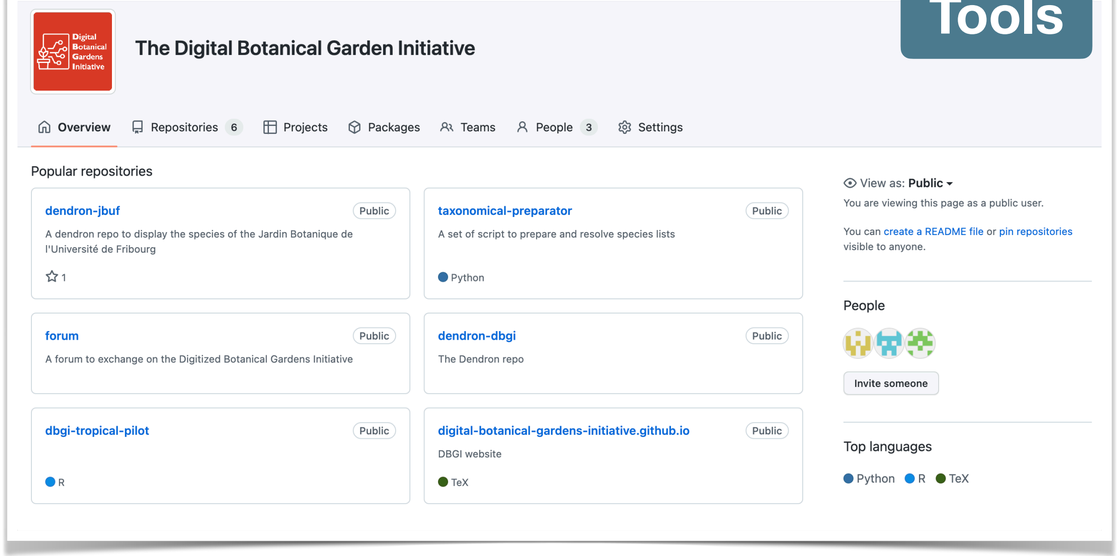
DENDRON

Notes organization via Dendron

- shareable across collaborators
- versioned on Github
- published as website

👉 https://www.dbgi.org/dendron-dbgi/

Tools



Code versioning on Github

👉 https://github.com/digital-botanical-gardens-initiative

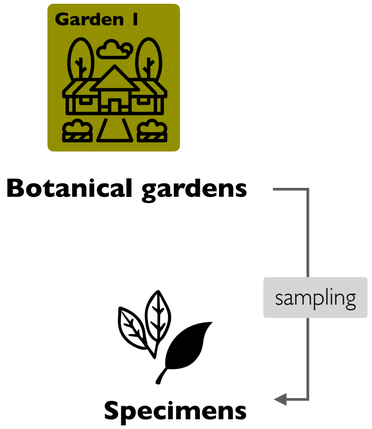
Data and research outcomes

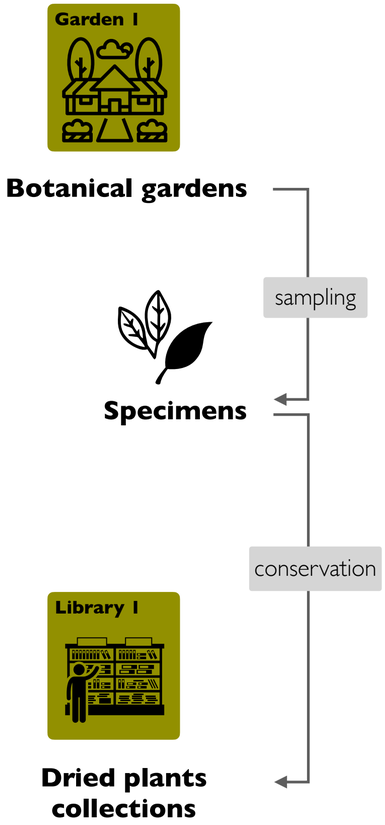
👉 https://zenodo.org/communities/earth-metabolome/

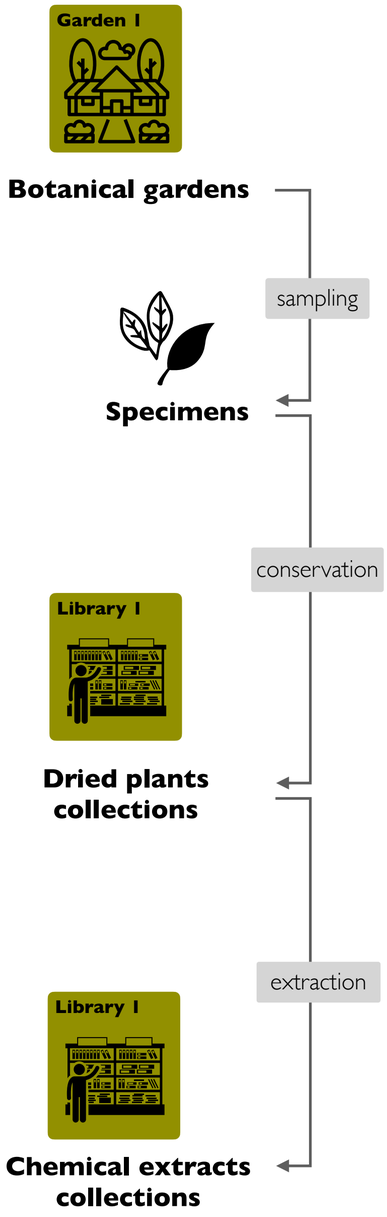
Note: most links are now for the DBGI (a pilot of EMI focussing on botanical gardens)

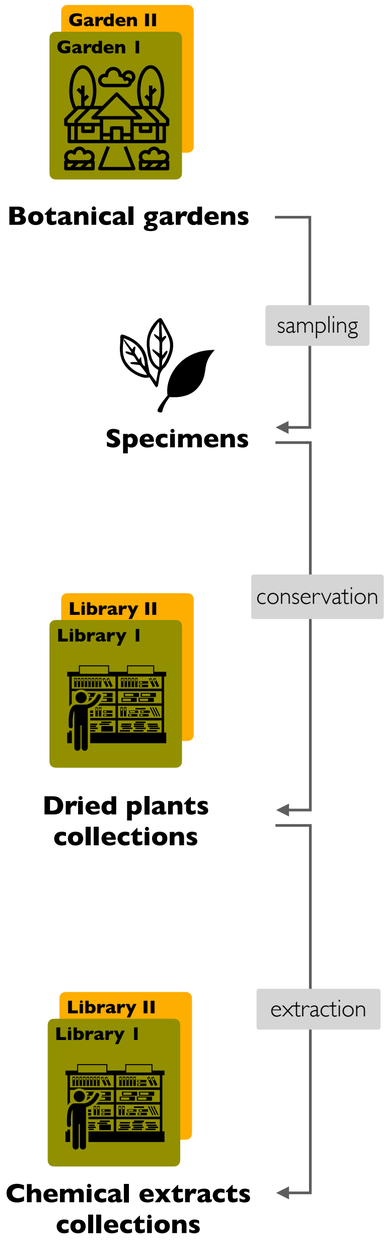
In practice, how did we start ?

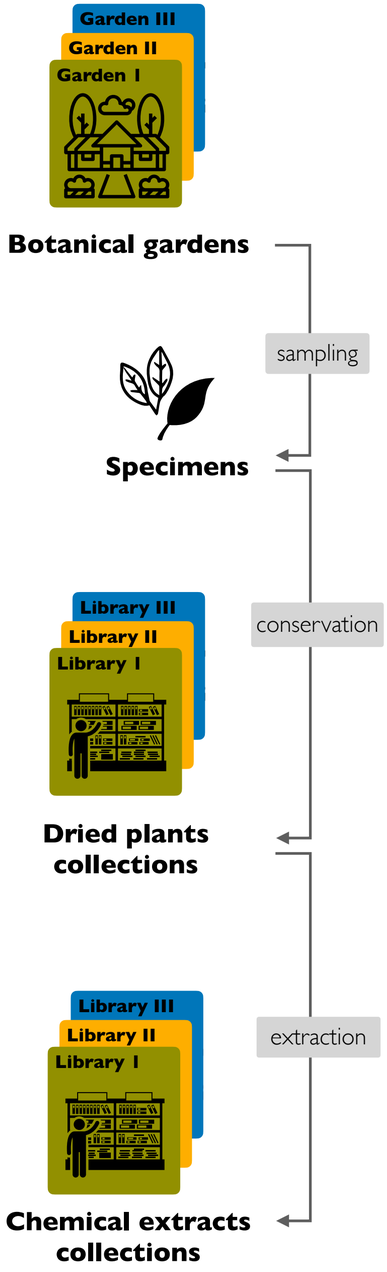
Botanical gardens

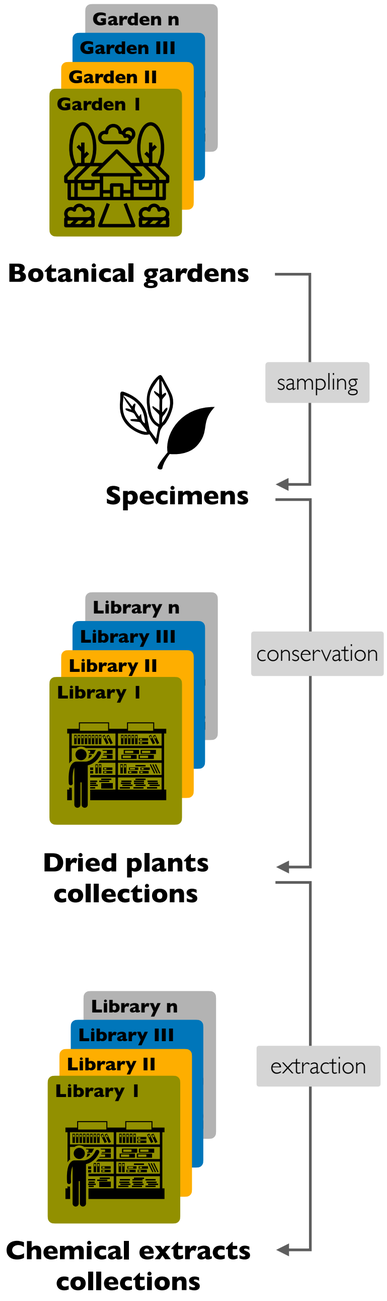

Garden 1
Botanical gardens
sampling
Specimens


Garden 1
Botanical gardens
sampling
Specimens
conservation
Library 1
Dried plants collections


Garden I
Botanical gardens
sampling
Specimens
conservation
Library I
Dried plants collections
extraction
Library I
Chemical extracts collections


Garden II
Garden I
Botanical gardens
sampling
Specimens
conservation
Library II
Library I
Dried plants collections
extraction
Library II
Library I
Chemical extracts collections


Garden III
Garden II
Garden I
Botanical gardens
sampling
Specimens
Library III
Library II
Library I
conservation
Dried plants collections
Library III
Library II
Library I
extraction
Chemical extracts collections


Garden n
Garden III
Garden II
Garden I
Botanical gardens
sampling
Specimens
Library n
Library III
Library II
Library I
conservation
Dried plants collections
Library n
Library III
Library II
Library I
extraction
Chemical extracts collections

physical objects

Botanical gardens

sampling

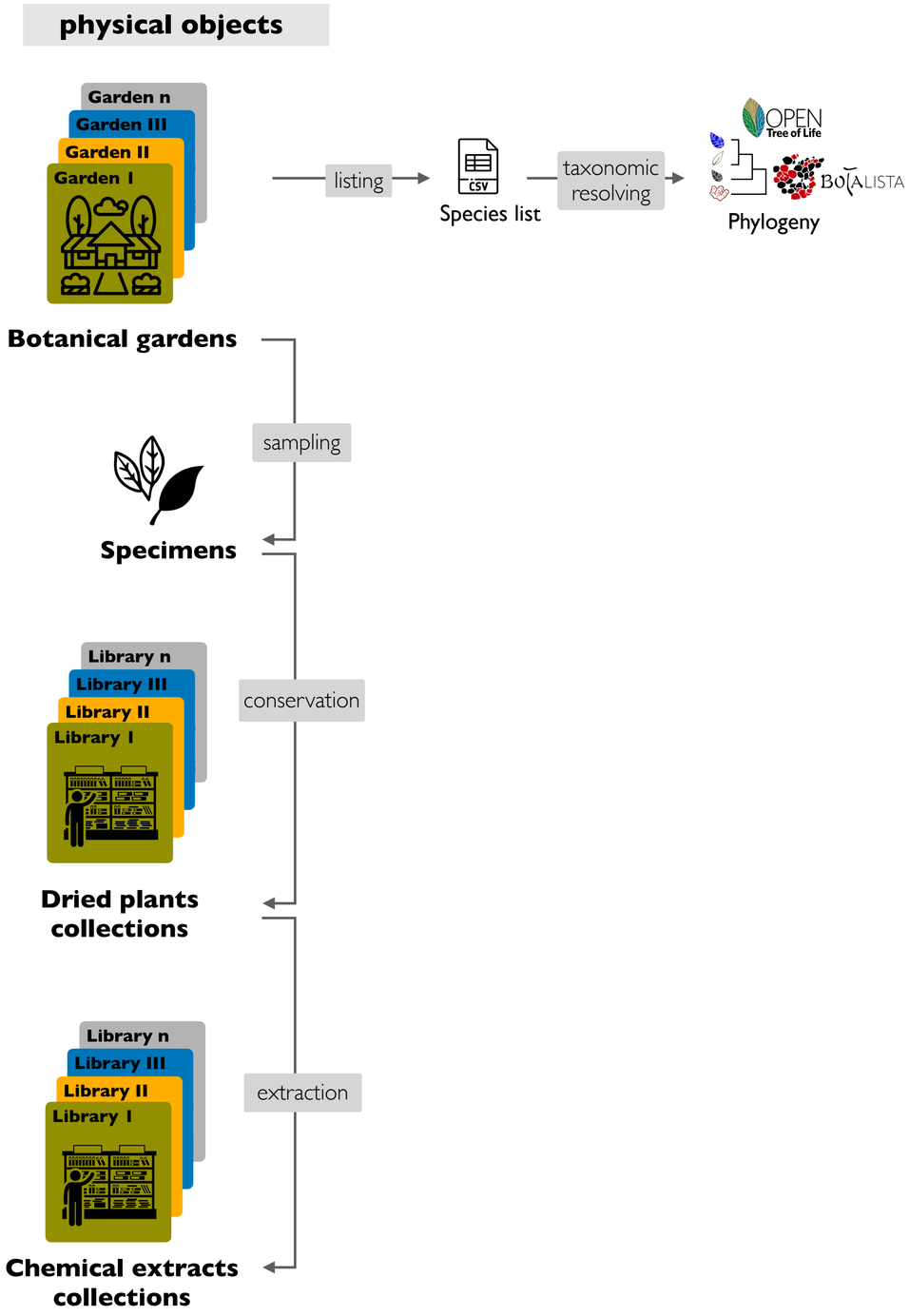
Specimens

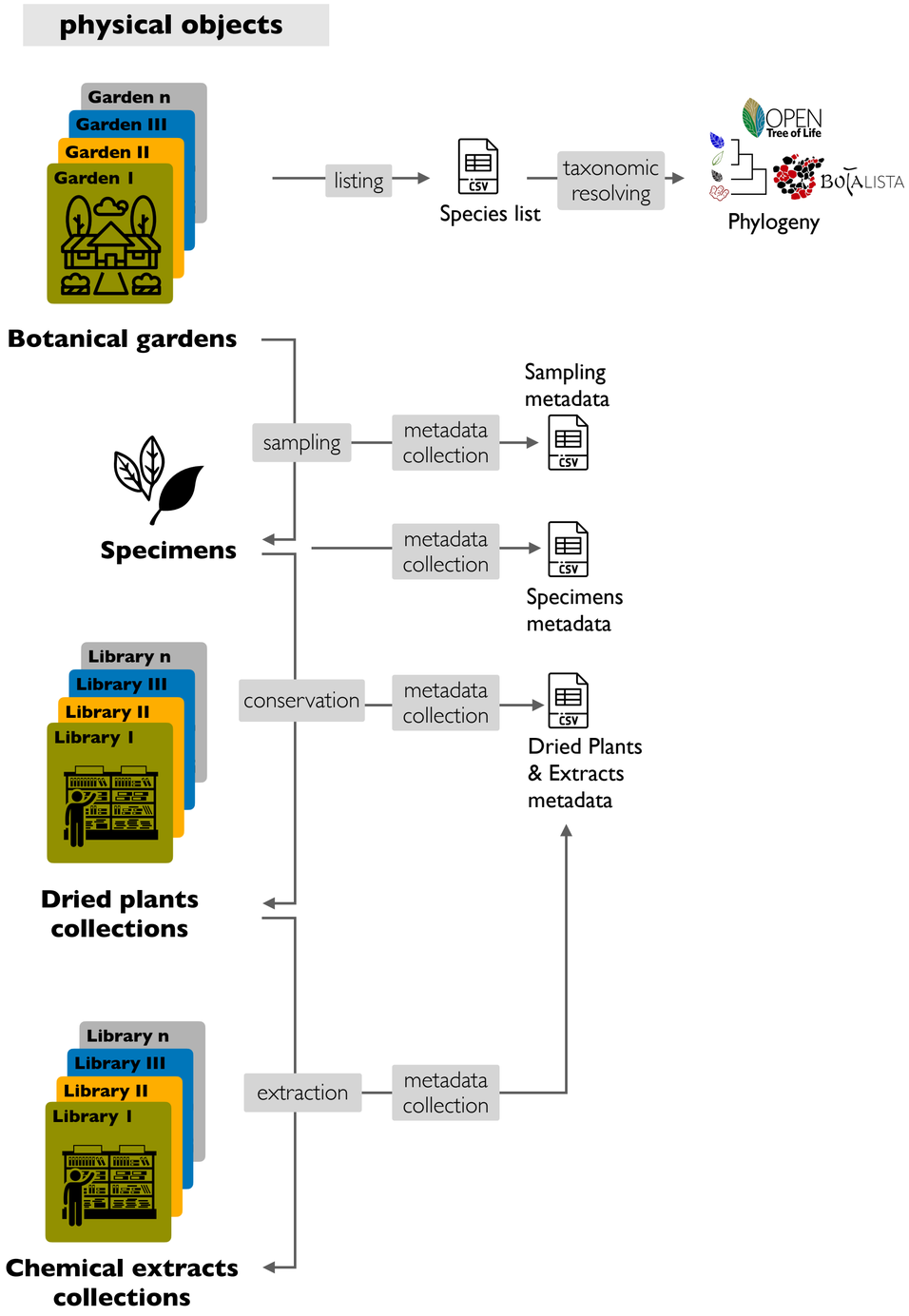
conservation

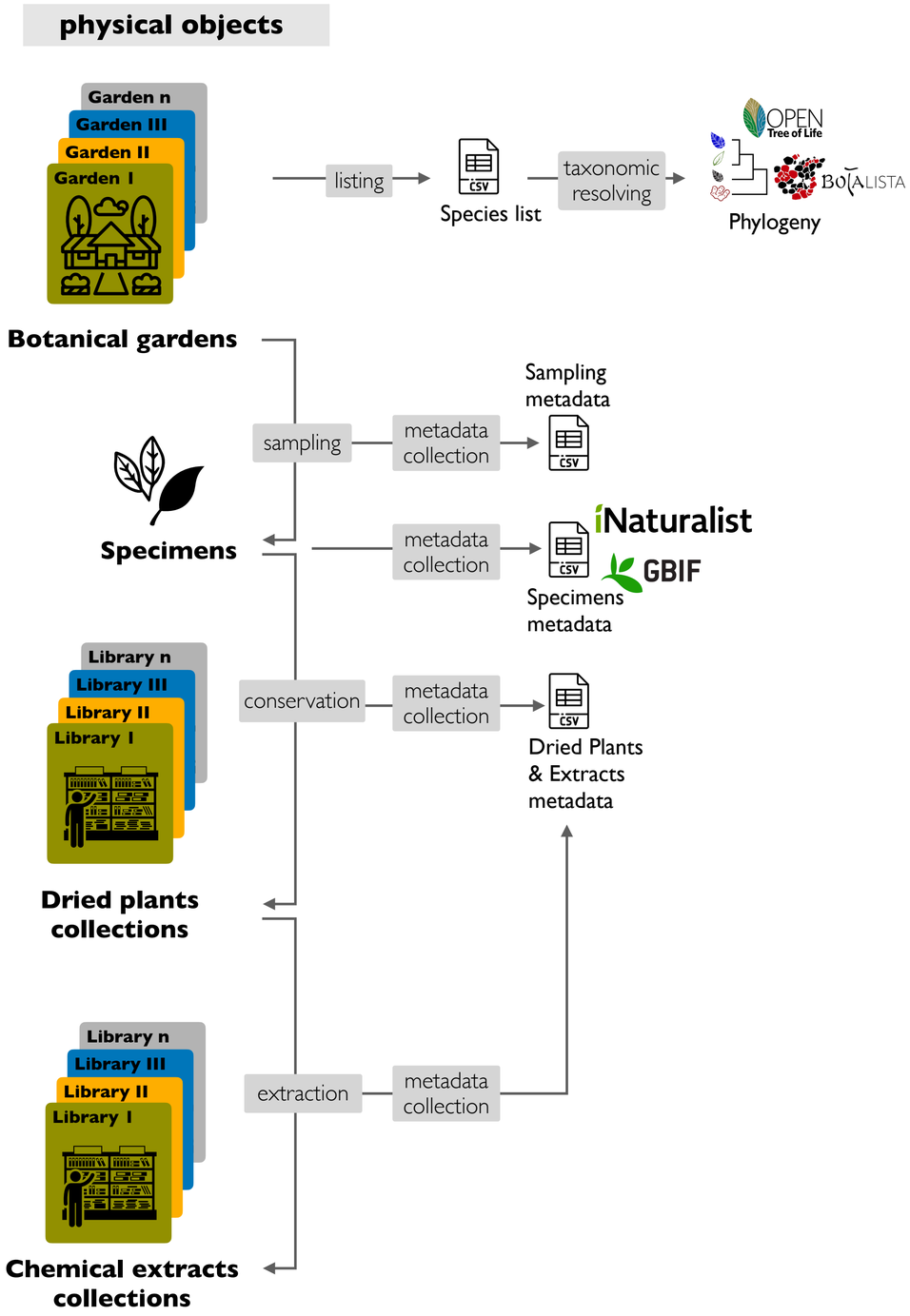
Dried plants collections

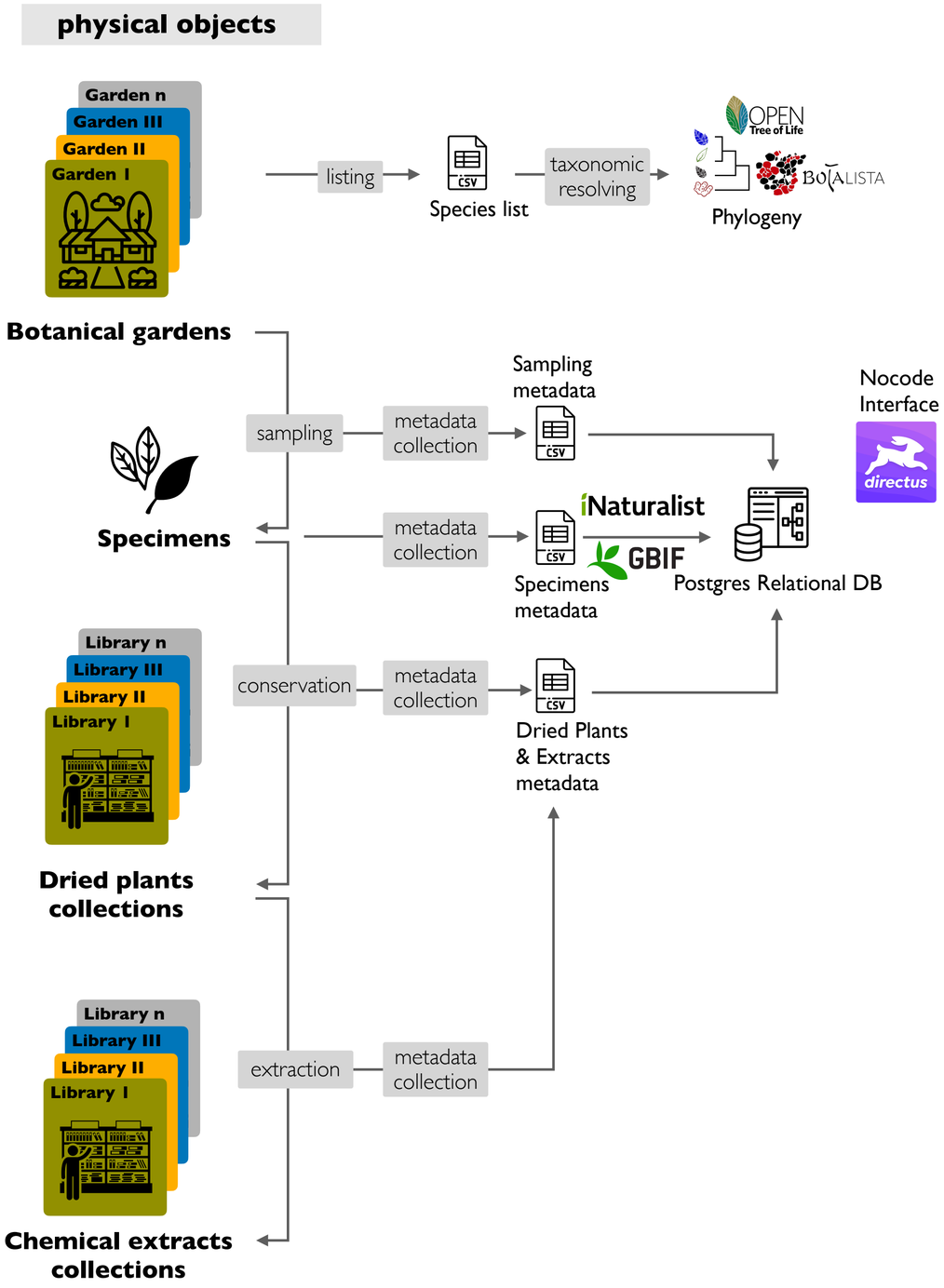
extraction

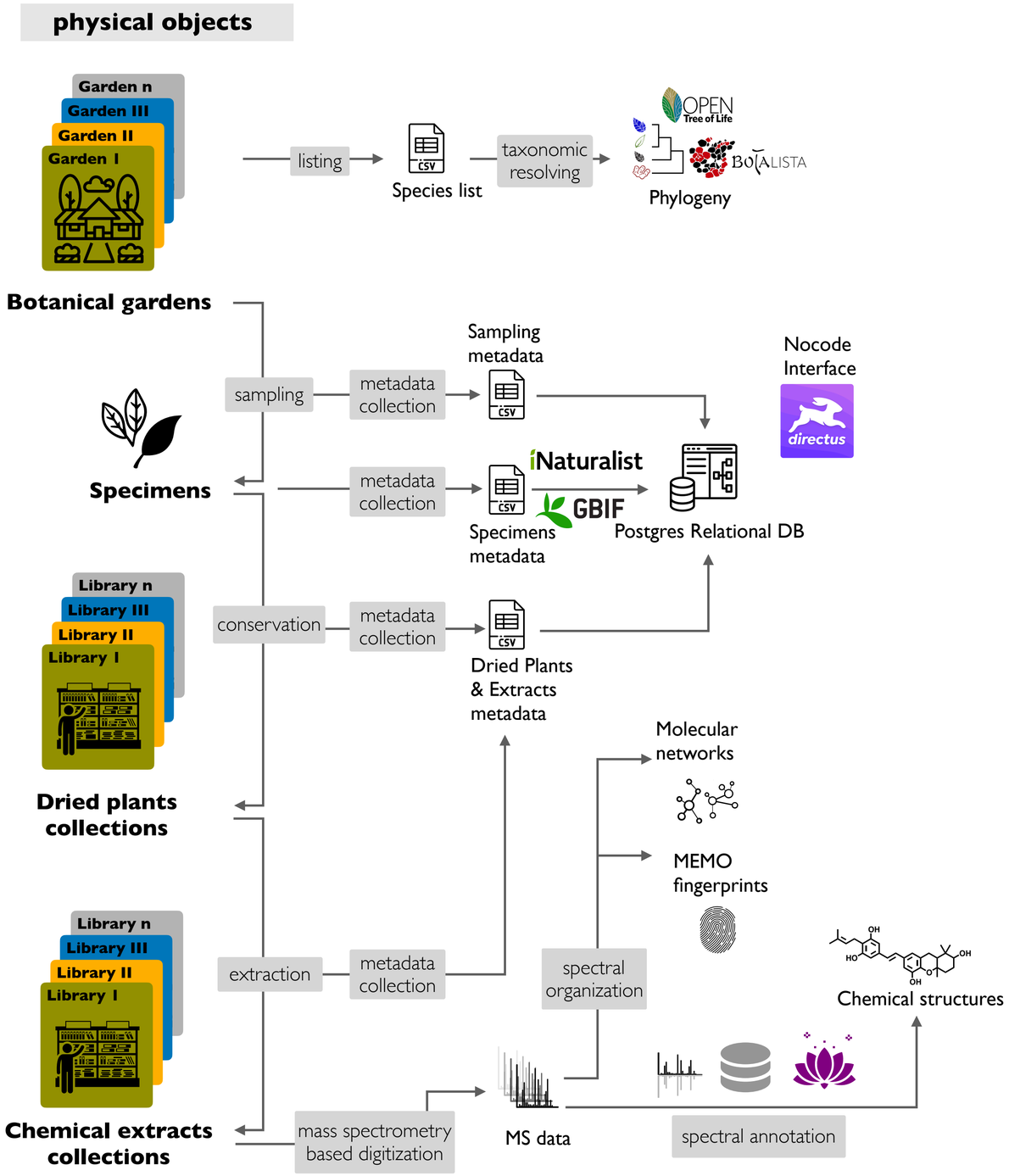
Chemical extracts collections

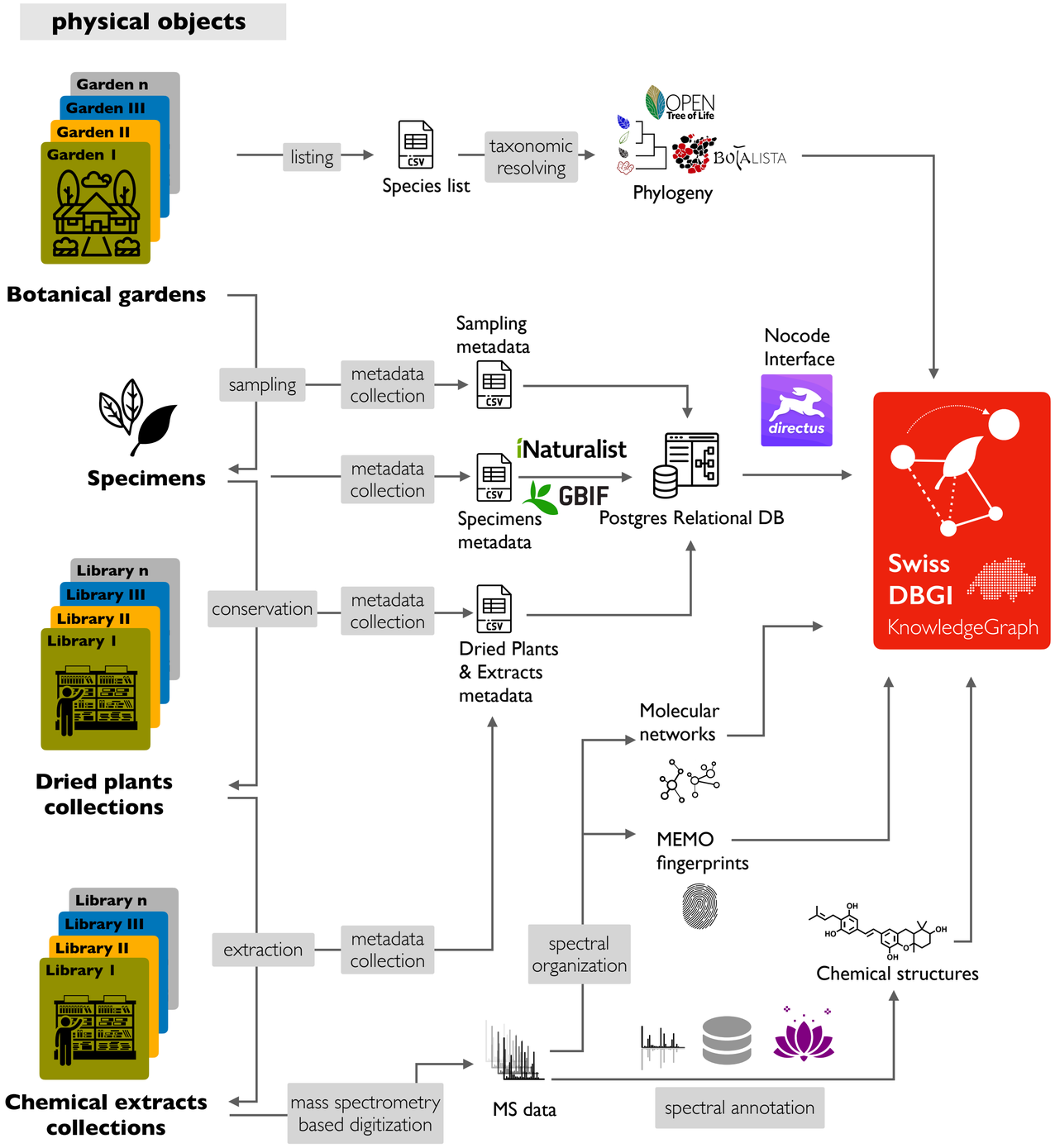

physical objects
Garden n
Garden III
Garden II
Garden I
listing
CSV
Species list
taxonomic resolving
OPEN Tree of Life
BOTALISTA
Phylogeny
Botanical gardens
sampling
Specimens
Library n
Library III
Library II
Library I
conservation
Dried plants collections
Library n
Library III
Library II
Library I
extraction
Chemical extracts collections

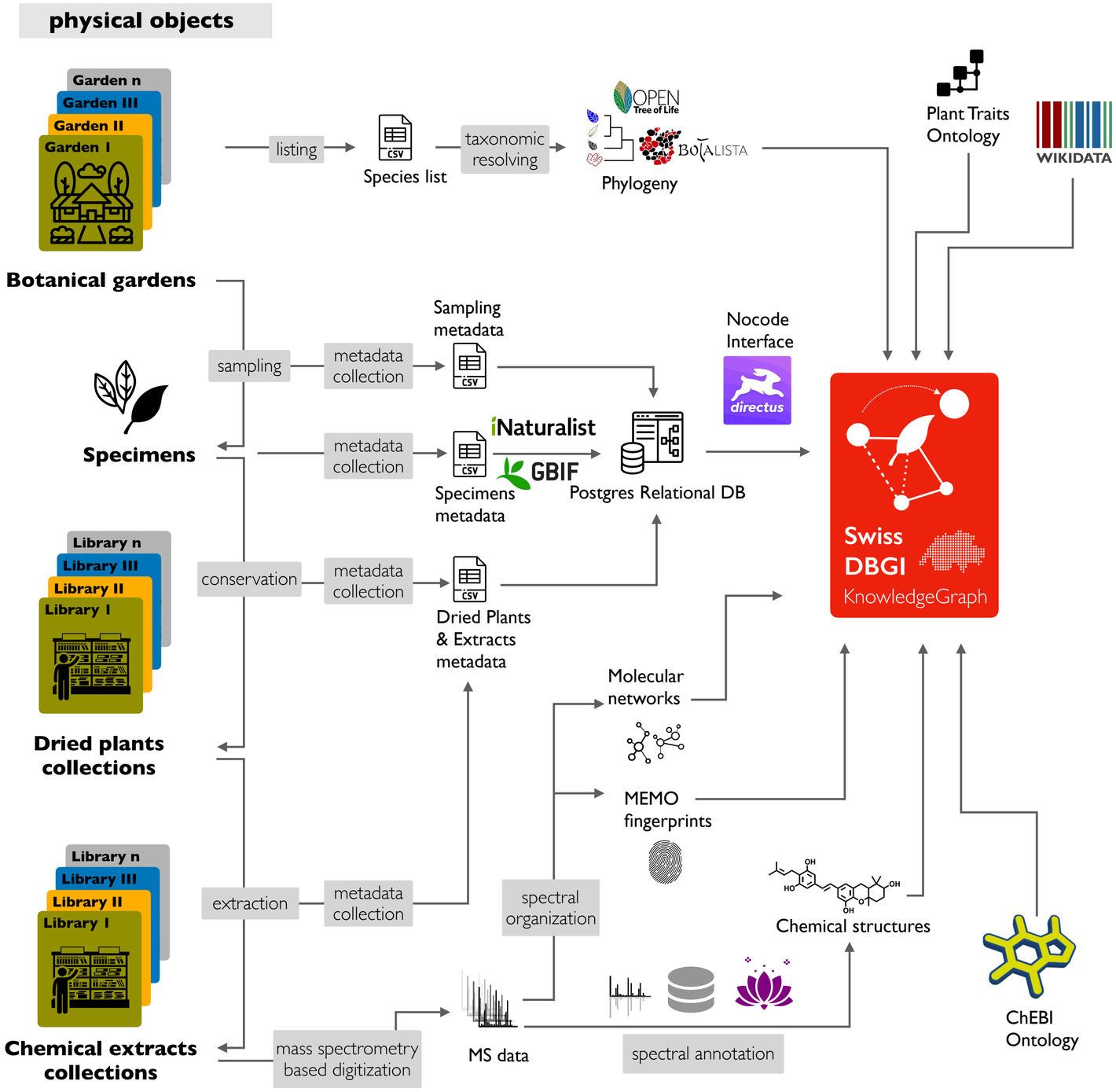

physical objects
Garden n
Garden III
Garden II
Garden I
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Botanical gardens
sampling
metadata collection
Sampling metadata
Specimens
metadata collection
Specimens metadata
Library n
Library III
Library II
Library I
conservation
metadata collection
Dried Plants & Extracts metadata
Dried plants collections
Library n
Library III
Library II
Library I
extraction
metadata collection
Chemical extracts collections

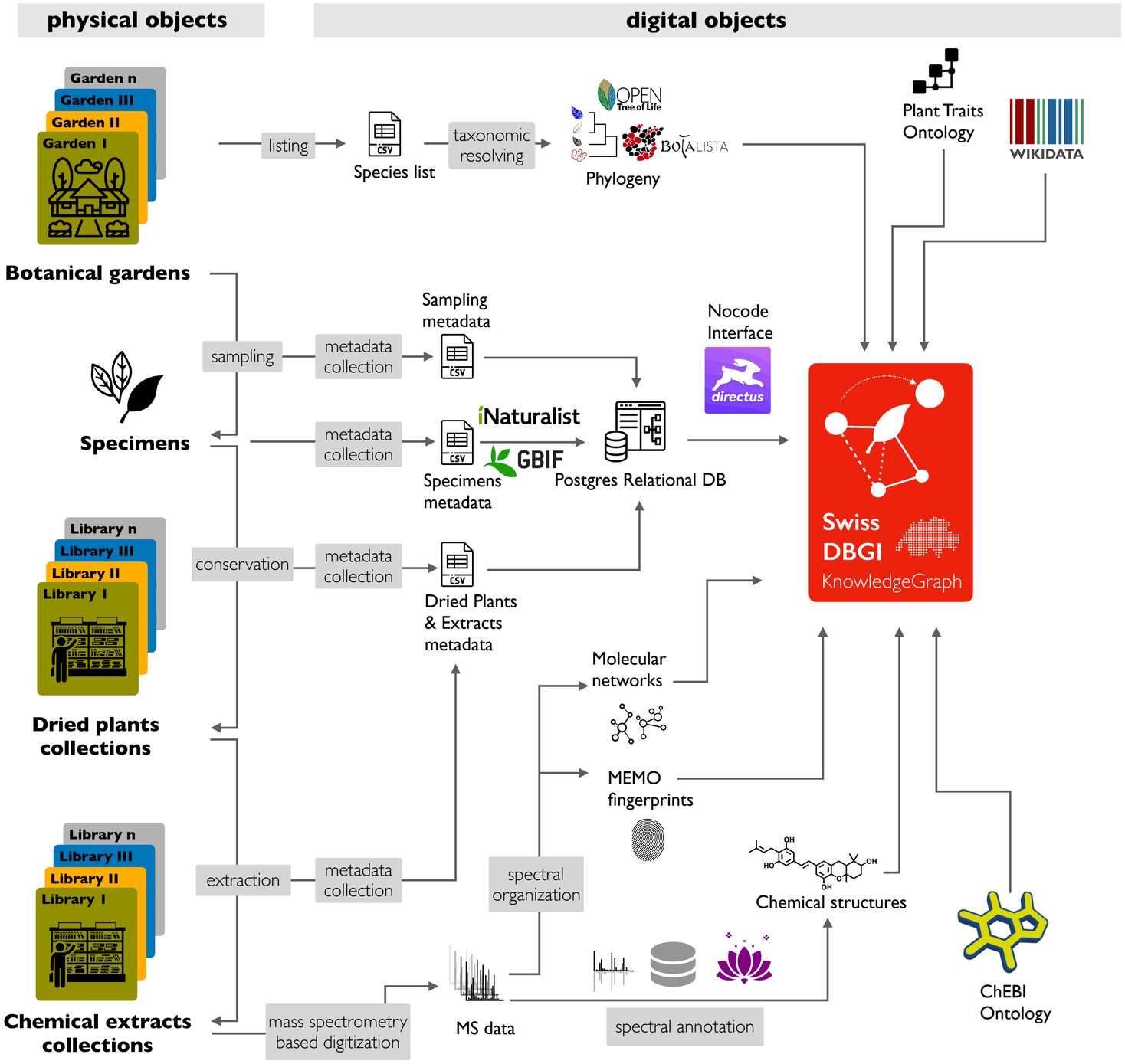

physical objects
Garden n
Garden III
Garden II
Garden I
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Botanical gardens
sampling
metadata collection
Sampling metadata
Specimens
metadata collection
iNaturalist
GBIF
Specimens metadata
Library n
Library III
Library II
Library I
conservation
metadata collection
Dried Plants & Extracts metadata
Dried plants collections
Library n
Library III
Library II
Library I
extraction
metadata collection
Chemical extracts collections

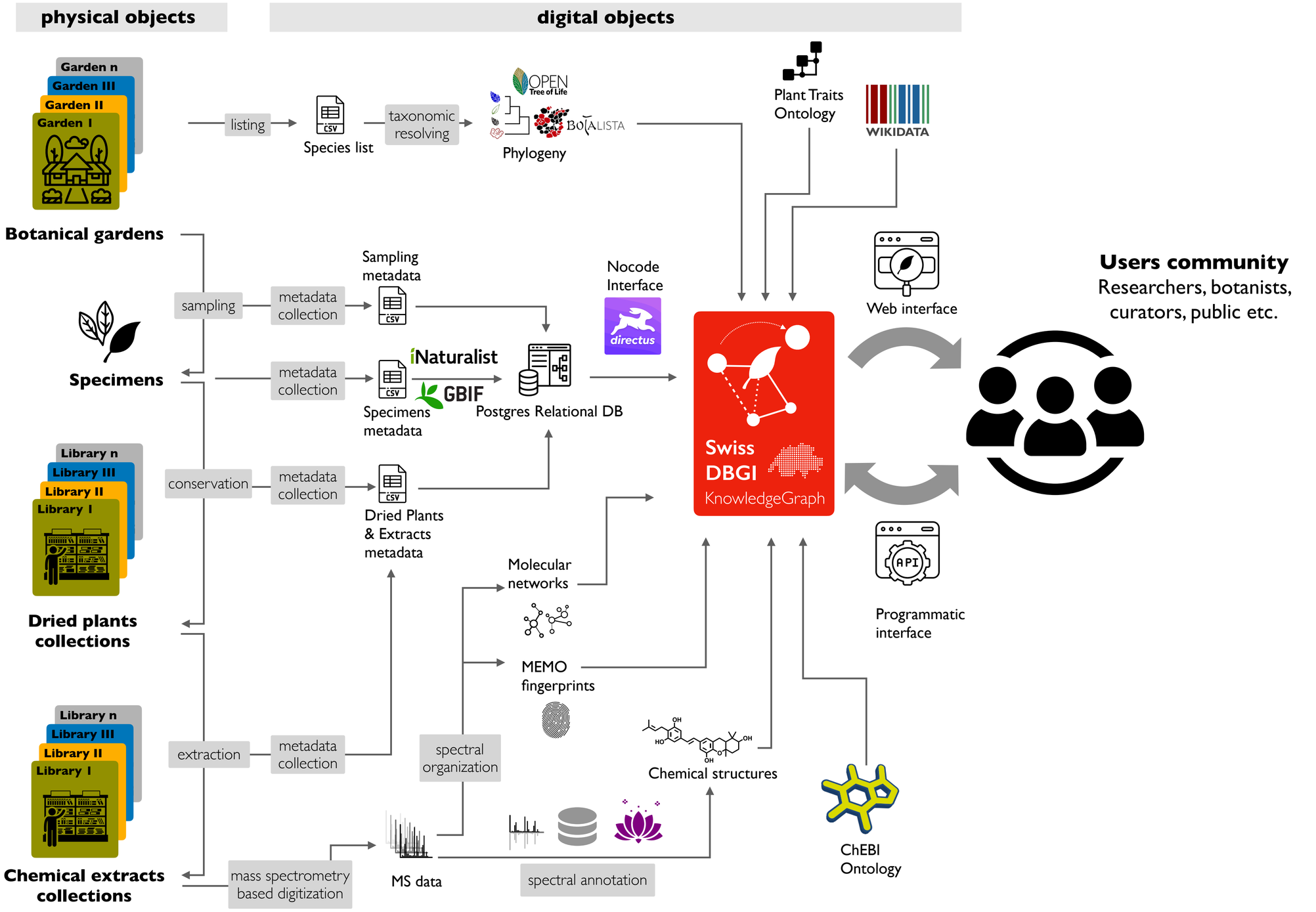

physical objects
Garden n
Garden III
Garden II
Garden I
Botanical gardens
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Specimens
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
metadata collection
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Library n
Library III
Library II
Library I
Dried plants collections
conservation
metadata collection
Dried Plants & Extracts metadata
Library n
Library III
Library II
Library I
Chemical extracts collections
extraction
metadata collection


physical objects
Garden n
Garden III
Garden II
Garden I
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Botanical gardens
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
Specimens
metadata collection
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Library n
Library III
Library II
Library I
conservation
metadata collection
Dried Plants & Extracts metadata
Dried plants collections
Molecular networks
MEMO fingerprints
Library n
Library III
Library II
Library I
extraction
metadata collection
spectral organization
Chemical structures
mass spectrometry based digitization
MS data
spectral annotation
Chemical extracts collections


physical objects
Garden n
Garden III
Garden II
Garden I
Botanical gardens
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Specimens
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
metadata collection
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Swiss DBGI KnowledgeGraph
Library n
Library III
Library II
Library I
Dried plants collections
conservation
metadata collection
Dried Plants & Extracts metadata
Molecular networks
MEMO fingerprints
Chemical structures
Library n
Library III
Library II
Library I
Chemical extracts collections
extraction
metadata collection
spectral organization
mass spectrometry based digitization
MS data
spectral annotation


physical objects
Garden n
Garden III
Garden II
Garden I
Botanical gardens
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Plant Traits Ontology
WIKIDATA
Specimens
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
metadata collection
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Swiss DBGI KnowledgeGraph
Library n
Library III
Library II
Library I
Dried plants collections
conservation
metadata collection
Dried Plants & Extracts metadata
Molecular networks
MEMO fingerprints
Chemical extracts collections
extraction
metadata collection
spectral organization
Chemical structures
ChEBI Ontology
mass spectrometry based digitization
MS data
spectral annotation


physical objects
digital objects
Garden n
Garden III
Garden II
Garden I
Botanical gardens
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Plant Traits Ontology
WIKIDATA
Specimens
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Swiss DBGI KnowledgeGraph
Library n
Library III
Library II
Library I
Dried plants collections
conservation
Dried Plants & Extracts metadata
Molecular networks
MEMO fingerprints
Chemical extracts collections
extraction
spectral organization
Chemical structures
ChEBI Ontology
mass spectrometry based digitization
MS data
spectral annotation


physical objects
digital objects
Garden n
Garden III
Garden II
Garden I
Botanical gardens
listing
Species list
taxonomic resolving
OPEN Tree of Life
BOLALISTA
Phylogeny
Plant Traits Ontology
WIKIDATA
Web interface
Users community
Researchers, botanists, curators, public etc.
sampling
metadata collection
Sampling metadata
Nocode Interface
directus
Specimens
iNaturalist
GBIF
Specimens metadata
Postgres Relational DB
Swiss DBGI KnowledgeGraph
Library n
Library III
Library II
Library I
Dried plants collections
conservation
Dried Plants & Extracts metadata
Molecular networks
MEMO fingerprints
API
Programmatic interface
Chemical extracts collections
extraction
spectral organization
Chemical structures
ChEBI Ontology
mass spectrometry based digitization
MS data
spectral annotation