

The Digital Botanical Gardens Initiative

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Abstract

The Digital Botanical Gardens Initiative (DBGI) ambitions to explore innovative solutions for the collection, management and sharing of digital information acquired on living botanical collections. A particular focus will be placed on the large scale characterization of the chemodiversity of living plants collections through mass spectrometric approaches. The acquired data will be structured, organized and connected with relevant metadata through semantic web technology. The gathered knowledge will then inform ecosystem functioning research and orient biodiversity conservation projects. The DBGI initially aims to take advantage of the readily available living collections of Swiss botanical gardens to establish robust and scalable chemo- and biodiversity digitisation workflows. The ultimate goal is to apply these approaches in the field and at the global scale in wild ecosystems.

Goals

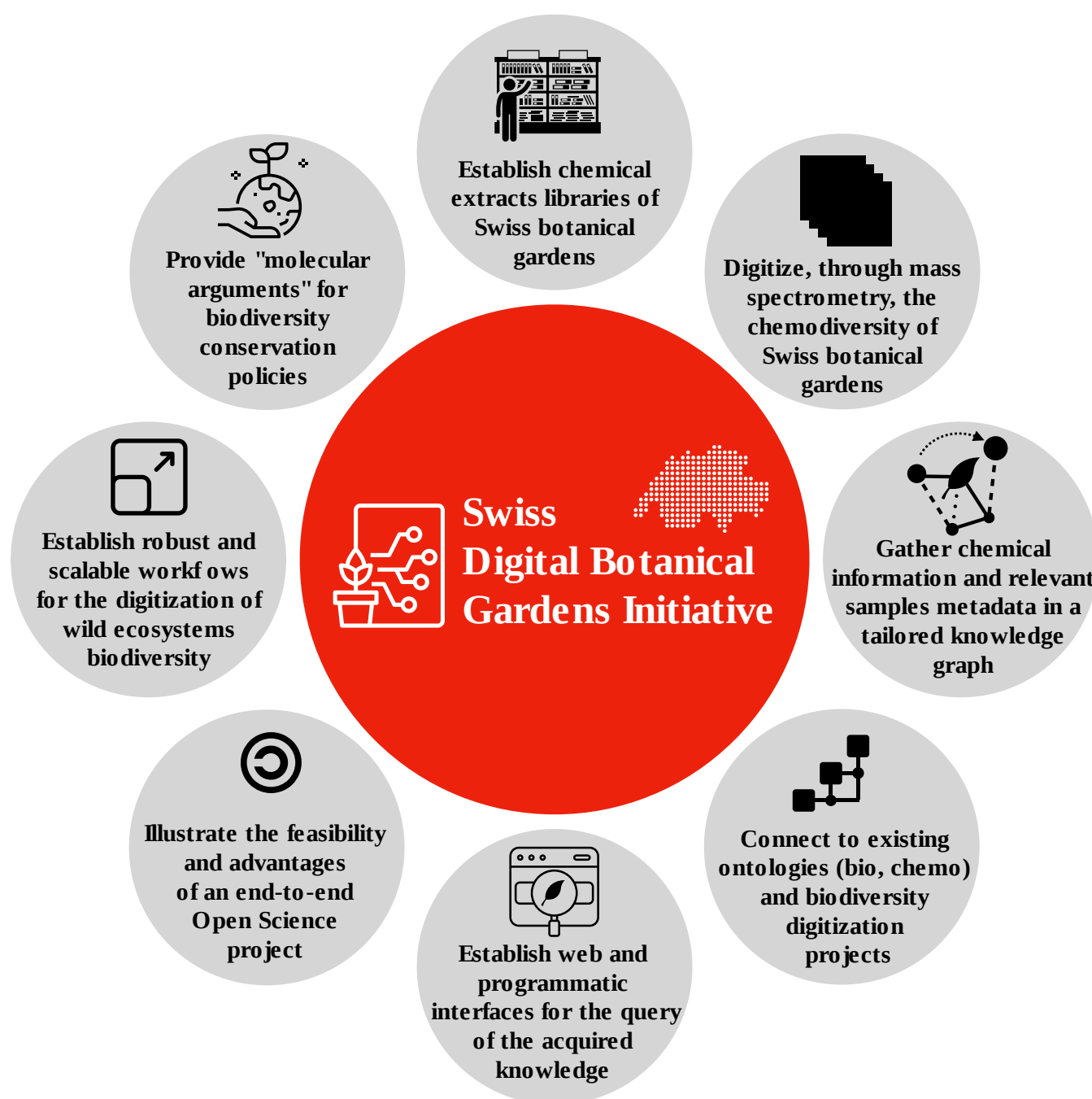


Figure 1: Main goals of the Digital Botanical Gardens Initiative.

The main goals of the DBGI are resumed in Figure 1. Some details are given hereafter:

1. Establish chemical extracts libraries of Swiss botanical gardens. These chemical libraries can be considered as complementary to herbarium samples. They are easily conserved over time and in a reasonable space. They represent the chemical diversity of a sample. They can be easily aliquoted. They can be screened for bioassays.

2. Digitize, through mass spectrometry, the chemodiversity of Swiss botanical gardens. Here high-resolution mass spectrometry is considered as a digital scanner allowing to capture the chemical fingerprint of the profiled sample. State-of-the-art computational metabolomics solutions are used to organize and annotate the acquired spectra with molecular data.

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

Chemical information acquired at the previous step (spectra and chemical structures) are connected to relevant samples metadata (taxonomy, phenology, geolocalisation, time of collection etc.). For this semantic web technologies (namely the RDF data model) are employed and a tailored knowledge graph is established.

4. Connect to existing ontologies (bio, chemo) and biodiversity digitization projects. Chemical and biological objects of the graph are connected to relevant pre-established ontologies (e.g. ChEBI, Plants Ontology) and data graphs (e.g. Wikidata). Connection with complementary biodiversity digitization efforts will be done (e.g. BiCIKL <https://bicikl-project.eu/>, Dissco <https://www.dissco.eu/>)

5. Establish web and programmatic interfaces for the query of the acquired knowledge. A web interface will allow a convenient access to the data acquired within the framework of the project. A dashboard will allow simple visualizations (e.g. pie charts, barplots, treemap) to interpret the data. In addition a SPARQL endpoint and an application programming interface (API) will allow retrieval of data programmatically.

6. Illustrate the feasibility and advantages of an end-to-end Open Science project. The DBGI will strictly follow the Open Science guidelines by using open-source software and making available the acquired data and scripts under an open license agreement. In addition the DBGI results will be published at the moment they are acquired (previous to formal publication or even pre-prints) thus following the Open Notebook Science concepts.

7. Establish robust and scalable workflows for the digitization of wild ecosystems biodiversity. The DBGI, albeit ambitious, is a pilot project. The future objective is to propose digitization workflows for the characterization of the wild ecosystems chemodiversity, on a global scale.

8. Provide “molecular arguments” for biodiversity conservation policies. The ultimate goal of DBGI is to use all the gathered metabolic information to support, extend or implement conservation efforts worldwide. We believe that by providing chemical maps of the landscape it will be possible to contribute to the prioritization of conservation and restoration targets . In other words, by establishing large scale chemical maps we expect to provide “molecular arguments” to biodiversity conservation endeavors (e.g. “This piece of land has a high content of antibacterial scaffolds.” or “This place might be poor in species diversity but rich in a rare chemodiversity”).

Background and context

Biodiversity is a major determinant of ecosystem stability [1]. Hundreds of studies spanning terrestrial and aquatic ecosystems support that higher levels of biodiversity, in all its forms, promote better ecosystem functions, such as carbon sequestration, underpinning human well-being [2,3]. Sadly, earth is experiencing a major biodiversity crisis and of the estimated nine million species of fungi, plants, and animals have been described [4], about a million species are currently at risk of extinction and may go extinct before the end of the century [5]. One major issue is that more than 80% of the estimated biodiversity still awaits to be described. We are in fact facing what is now called the Anthropocene extinction (sixth mass extinction). [6] In order to try to deviate from these alarming trends, all possible efforts must be made by the responsible (i.e. our species) for the conservation of biodiversity. For this, the characterisation and documentation of biodiversity is a fundamental prerequisite. Over 3.5 billion years of evolution, natural selection, the craftsman of biodiversity, has created an overwhelming array of molecular entities. Myriad compounds are produced by all living organisms from bacteria to whales, forming the backbone of the ever-growing tree of life. Through the lens of chemistry, every species, biotic interaction, and community, reveals a unique ensemble of molecular structures: the metabolome. These chemical assemblages are a valuable, yet largely unexplored reflection of biodiversity and ecosystem functioning. To go beyond the simple quantitative representation of biodiversity provided by species inventories, and to reinforce our understanding of links between biodiversity and ecosystem functioning, we see chemical diversity as an alternative and highly complementary view of the diversity of our planet's ecosystems.

This manuscript is a template (aka "rootstock") for [Manubot](#), a tool for writing scholarly manuscripts. Use this template as a starting point for your manuscript.

The rest of this document is a full list of formatting elements/features supported by Manubot. Compare the input (`.md` files in the `/content` directory) to the output you see below.

Basic formatting

Bold text

Semi-bold text

Centered text

Right-aligned text

Italic text

Combined *italics* and **bold**

~~Strikethrough~~

1. Ordered list item
2. Ordered list item
 - a. Sub-item
 - b. Sub-item
 - i. Sub-sub-item
3. Ordered list item

a. Sub-item

- List item
- List item
- List item

subscript: H₂O is a liquid

superscript: 2¹⁰ is 1024.

[unicode superscripts](#)⁰¹²³⁴⁵⁶⁷⁸⁹

[unicode subscripts](#)₀₁₂₃₄₅₆₇₈₉

A long paragraph of text. Lorem ipsum dolor sit amet, consectetur adipiscing elit, sed do eiusmod tempor incididunt ut labore et dolore magna aliqua. Ut enim ad minim veniam, quis nostrud exercitation ullamco laboris nisi ut aliquip ex ea commodo consequat. Duis aute irure dolor in reprehenderit in voluptate velit esse cillum dolore eu fugiat nulla pariatur. Excepteur sint occaecat cupidatat non proident, sunt in culpa qui officia deserunt mollit anim id est laborum.

Putting each sentence on its own line has numerous benefits with regard to [editing](#) and [version control](#).

Line break without starting a new paragraph by putting two spaces at end of line.

Document organization

Document section headings:

Heading 1

Heading 2

Heading 3

Heading 4

Heading 5

Heading 6

A heading centered on its own printed page

Horizontal rule:

Heading 1's are recommended to be reserved for the title of the manuscript.

Heading 2's are recommended for broad sections such as *Abstract*, *Methods*, *Conclusion*, etc.

Heading 3's and Heading 4's are recommended for sub-sections.

Links

Bare URL link: <https://manubot.org>

[Long link with lots of words and stuff and junk and bleep and blah and stuff and other stuff and more stuff yeah](#)

[Link with text](#)

[Link with hover text](#)

[Link by reference](#)

Citations

Citation by DOI [[1](#)].

Citation by PubMed Central ID [[2](#)].

Citation by PubMed ID [[pubmed:30718888?](#)].

Citation by Wikidata ID [[3](#)].

Citation by alias [[4](#)].

Manubot plugins provide easier, more convenient visualization of and navigation between citations [[2](#),[4](#),[5](#),[pubmed:30718888?](#)].

Citation tags (i.e. aliases) can be defined in their own paragraphs using Markdown's reference link syntax:

Referencing figures, tables, equations

Figure [2](#)

Figure [3](#)

Figure [4](#)

Figure [5](#)

Table [1](#)

Equation [1](#)

Equation [2](#)

Quotes and code

Quoted text

Quoted block of text

Two roads diverged in a wood, and I—
I took the one less traveled by,
And that has made all the difference.

Code `in the middle` of normal text, aka `inline code`.

Code block with Python syntax highlighting:

```
from manubot.cite.doi import expand_short_doi

def test_expand_short_doi():
    doi = expand_short_doi("10/c3bp")
    # a string too long to fit within page:
    assert doi == "10.25313/2524-2695-2018-3-vliyanie-enhansera-copia-i-
insulyatora-gypsy-na-sintez-ernk-modifikatsii-hromatina-i-
svyazyvanie-insulyatornyh-belkov-vtransfetsirovannyh-geneticheskikh-
konstruktsiyah"
```

Code block with no syntax highlighting:

```
Exporting HTML manuscript
Exporting DOCX manuscript
Exporting PDF manuscript
```

Figures



Figure 2: A square image at actual size and with a bottom caption. Loaded from the latest version of image on GitHub.



Figure 3: An image too wide to fit within page at full size. Loaded from a specific (hashed) version of the image on GitHub.



Figure 4: A tall image with a specified height. Loaded from a specific (hashed) version of the image on GitHub.



Figure 5: A vector `.svg` image loaded from GitHub. The parameter `sanitize=true` is necessary to properly load SVGs hosted via GitHub URLs. White background specified to serve as a backdrop for transparent sections of the image.

Tables

Table 1: A table with a top caption and specified relative column widths.

<i>Bowling Scores</i>	Jane	John	Alice	Bob
Game 1	150	187	210	105
Game 2	98	202	197	102
Game 3	123	180	238	134

Table 2: A table too wide to fit within page.

	Digits 1-33	Digits 34-66	Digits 67-99	Ref.
pi	3.14159265358979323846264338327950	288419716939937510582097494459230	781640628620899862803482534211706	piday.org
e	2.71828182845904523536028747135266	249775724709369995957496696762772	407663035354759457138217852516642	nasa.gov

Table 3: A table with merged cells using the `attributes` plugin.

	Colors	
Size	Text Color	Background Color
big	blue	orange
small	black	white

Equations

A LaTeX equation:

$$\int_0^\infty e^{-x^2} dx = \frac{\sqrt{\pi}}{2} \tag{1}$$

An equation too long to fit within page:

$$x = a + b + c + d + e + f + g + h + i + j + k + l + m + n + o + p + q + r + s + t + u + v + w + x + y + z + 1 + 2 + 3 + 4 + 5 + 6 + 7 + 8 + 9 \tag{2}$$

Special

⚠ WARNING The following features are only supported and intended for `.html` and `.pdf` exports. Journals are not likely to support them, and they may not display correctly when converted to other formats such as `.docx`.

LINK STYLED AS A BUTTON

Adding arbitrary HTML attributes to an element using Pandoc's attribute syntax:

Manubot Manubot Manubot Manubot Manubot. Manubot Manubot Manubot Manubot. Manubot Manubot Manubot. Manubot Manubot. Manubot.

Adding arbitrary HTML attributes to an element with the Manubot `attributes` plugin (more flexible than Pandoc's method in terms of which elements you can add attributes to):

Manubot Manubot Manubot Manubot Manubot. Manubot Manubot Manubot Manubot. Manubot Manubot Manubot. Manubot Manubot. Manubot.

Available background colors for text, images, code, banners, etc:

white lightgrey grey darkgrey black lightred lightyellow lightgreen lightblue lightpurple red orange yellow green blue purple

Using the [Font Awesome](#) icon set:

✓ ? ★ 🔔 ✖ …



Light Grey Banner

useful for *general information* - manubot.org



Blue Banner

useful for *important information* - manubot.org



Light Red Banner

useful for *warnings* - manubot.org

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