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.

Rationale

With these urgent biodiversity characterization objectives in mind we are setting up the Digital Botanical Gardens Initiative (DBGI), which aims to develop robust and scalable workflows for the digitization of botanical gardens using several approaches. The central one being the use of analytical chemistry strategies to build information-rich chemical maps that will guide researchers focusing on biodiversity characterisation and conservation.

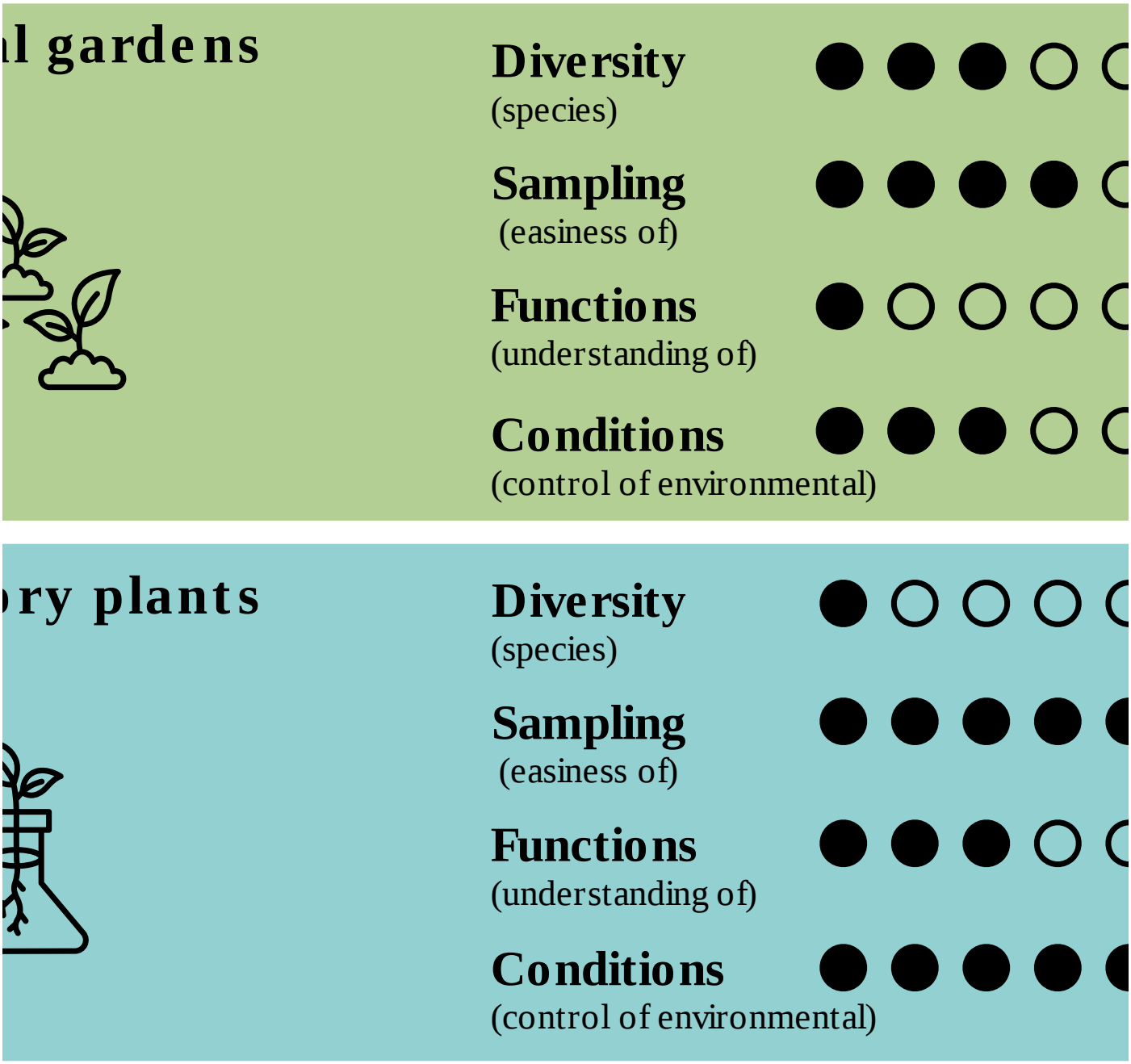

Figure 2: Characteristics of three main plant biodiversity sources for the scientist.

Sampling plants for chemical characterization can be done in three ways, either from natural living collections (botanical gardens), in the wild, or by growing plants in highly controlled settings (See Figure 2. For an overview of the advantages and inconveniences of each biodiversity source). For this first project, the sampling in botanical gardens is the chosen option, as within a very accessible location, thousands of species, which are already identified, labeled and organized, can be readily sampled.

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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

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: H_2O is a liquid

superscript: 2^{10} 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 [7].

Citation by PubMed Central ID [8].

Citation by PubMed ID [**pubmed:30718888?**].

Citation by Wikidata ID [9].

Citation by alias [10].

Manubot plugins provide easier, more convenient visualization of and navigation between citations [8,10,11,**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 3

Figure 4

Figure 5

Figure 6

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-geneticheskih-
        konstruktsiyah"
```

Code block with no syntax highlighting:

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

Figures

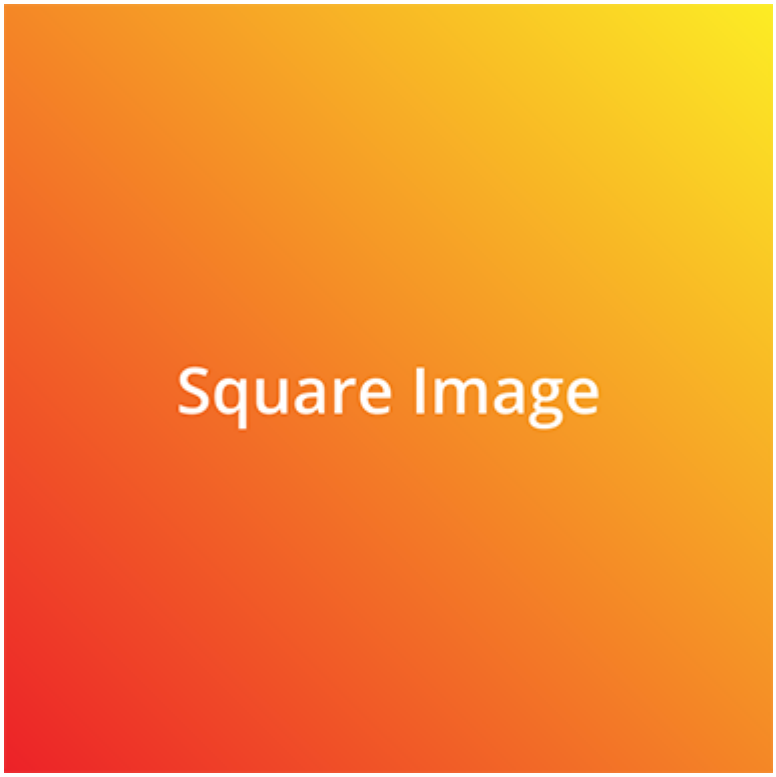

Figure 3: A square image at actual size and with a bottom caption. Loaded from the latest version of image on GitHub.

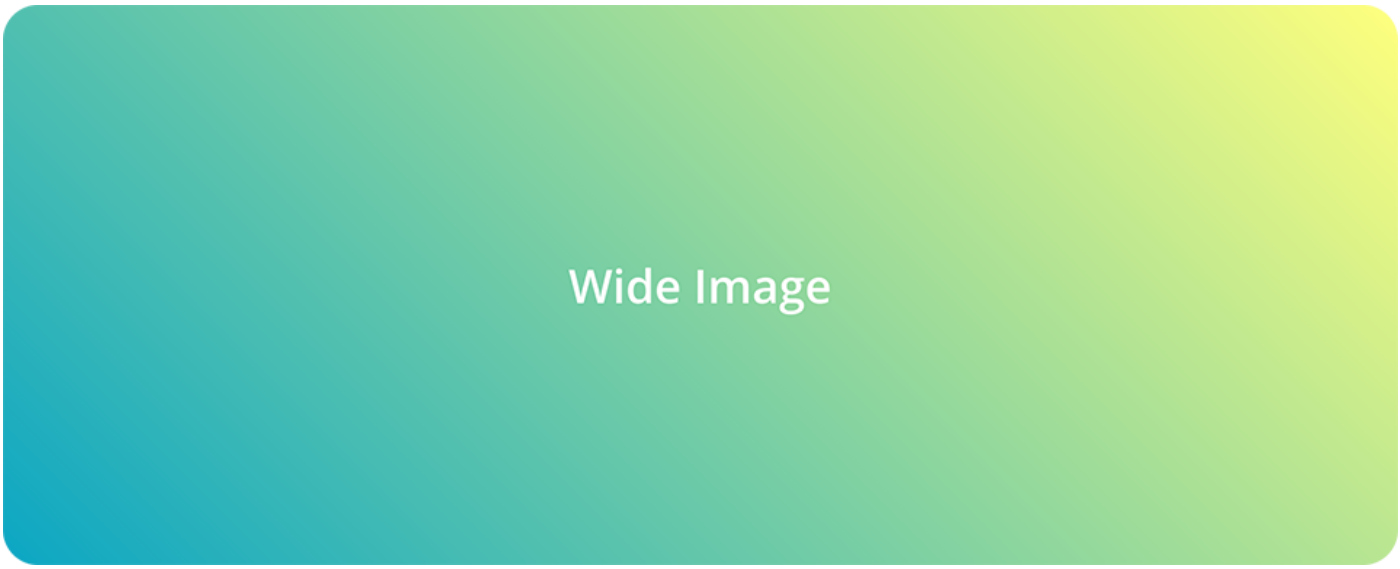

Figure 4: An image too wide to fit within page at full size. Loaded from a specific (hashed) version of the image on GitHub.

Figure 5: A tall image with a specified height. Loaded from a specific (hashed) version of the image on GitHub.

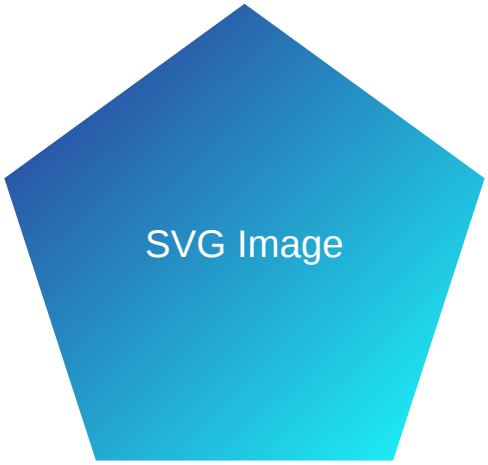

Figure 6: A vector `.svg` image loaded from GitHub. The parameter `sanitize=true` is necessary to properly load SVGs hosted via GitHub URLs. White background specified to serve as a backdrop for transparent sections of the image.

Tables

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

Bowling Scores	**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	3.14159265358979323 846264338327950	28841971693993751 0582097494459230	78164062862089986 2803482534211706	`piday.org`
e	2.71828182845904523 536028747135266	24977572470936999 5957496696762772	40766303535475945 7138217852516642	`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`*.*

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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):

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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:

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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

References

1. **Biodiversity and Ecosystem Functioning**
David Tilman, Forest Isbell, Jane M Cowles
Annual Review of Ecology, Evolution, and Systematics (2014-11-23) https://doi.org/gf5tpq
DOI: 10.1146/annurev-ecolsys-120213-091917

2. **Biodiversity and Ecosystem Functioning: Current Knowledge and Future Challenges**
M Loreau, S Naeem, P Inchausti, J Bengtsson, JP Grime, A Hector, DU Hooper, MA Huston, D Raffaelli, B Schmid, ... DA Wardle
Science (2001-10-26) https://doi.org/cnf65t
DOI: 10.1126/science.1064088 · PMID: 11679658

3. **Linking biodiversity to ecosystem function: implications for conservation ecology**
MW Schwartz, CA Brigham, JD Hoeksema, KG Lyons, MH Mills, PJ van Mantgem
Oecologia (2000-02-23) https://doi.org/cjwdg4
DOI: 10.1007/s004420050035 · PMID: 28308280

4. **Number of species on Earth tagged at 8.7 million**
Lee Sweetlove
Nature (2011-08-23) https://doi.org/djwm2d
DOI: 10.1038/news.2011.498

5. **Global assessment report on biodiversity and ecosystem services of the Intergovernmental Science-Policy Platform on Biodiversity and Ecosystem Services**
IPBES
Zenodo (2019-05-04) https://doi.org/grbxsr
DOI: 10.5281/zenodo.6417333

6. **The misunderstood sixth mass extinction**
Gerardo Ceballos, Paul R Ehrlich
Science (2018-06-08) https://doi.org/ggf4kk
DOI: 10.1126/science.aau0191 · PMID: 29880679

7. **Sci-Hub provides access to nearly all scholarly literature**
Daniel S Himmelstein, Ariel Rodriguez Romero, Jacob G Levernier, Thomas Anthony Munro, Stephen Reid McLaughlin, Bastian Greshake Tzovaras, Casey S Greene
eLife (2018-03-01) https://doi.org/ckcj
DOI: 10.7554/elife.32822 · PMID: 29424689 · PMCID: PMC5832410

8. **Reproducibility of computational workflows is automated using continuous analysis**
Brett K Beaulieu-Jones, Casey S Greene
Nature biotechnology (2017-04) https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6103790/
DOI: 10.1038/nbt.3780 · PMID: 28288103 · PMCID: PMC6103790

9. **Plan S: Accelerating the transition to full and immediate Open Access to scientific publications**
cOAlition S
(2018-09-04) https://www.wikidata.org/wiki/Q56458321

10. **Opportunities and obstacles for deep learning in biology and medicine**
Travers Ching, Daniel S Himmelstein, Brett K Beaulieu-Jones, Alexandr A Kalinin, Brian T Do, Gregory P Way, Enrico Ferrero, Paul-Michael Agapow, Michael Zietz, Michael M Hoffman, ... Casey S Greene

Journal of The Royal Society Interface (2018-04) https://doi.org/gddkhn
DOI: 10.1098/rsif.2017.0387 · PMID: 29618526 · PMCID: PMC5938574

11. **Open collaborative writing with Manubot**
Daniel S Himmelstein, Vincent Rubinetti, David R Slochower, Dongbo Hu, Venkat S Malladi, Casey S Greene, Anthony Gitter
PLOS Computational Biology (2019-06-24) https://doi.org/c7np
DOI: 10.1371/journal.pcbi.1007128 · PMID: 31233491 · PMCID: PMC6611653