Navigating nonlinear careers in science

Tomáš Pluskal

CHARLES UNIVERSITY

2004 M.Sc.
Computer science

2015–2020 postdoc
Plant biochemistry

WHITEHEAD INSTITUTE

Specialized metabolism
in non-model plants

From June 2020

Pluskal Group
IOCB Prague

2014 Ph.D.
Molecular biology

OIST

- Cellular metabolism under quiescence in fission yeast
- Metabolomics and mass spectrometry

Dec 2020

Sep 2022

Feb 2026

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peaceful | waterfall | mountain | animal | flower | beauty | drawing | rain | snow | grass | light | spring | aesthetic | bird | water | art | mobile | beautiful flower | sunset | sunrise















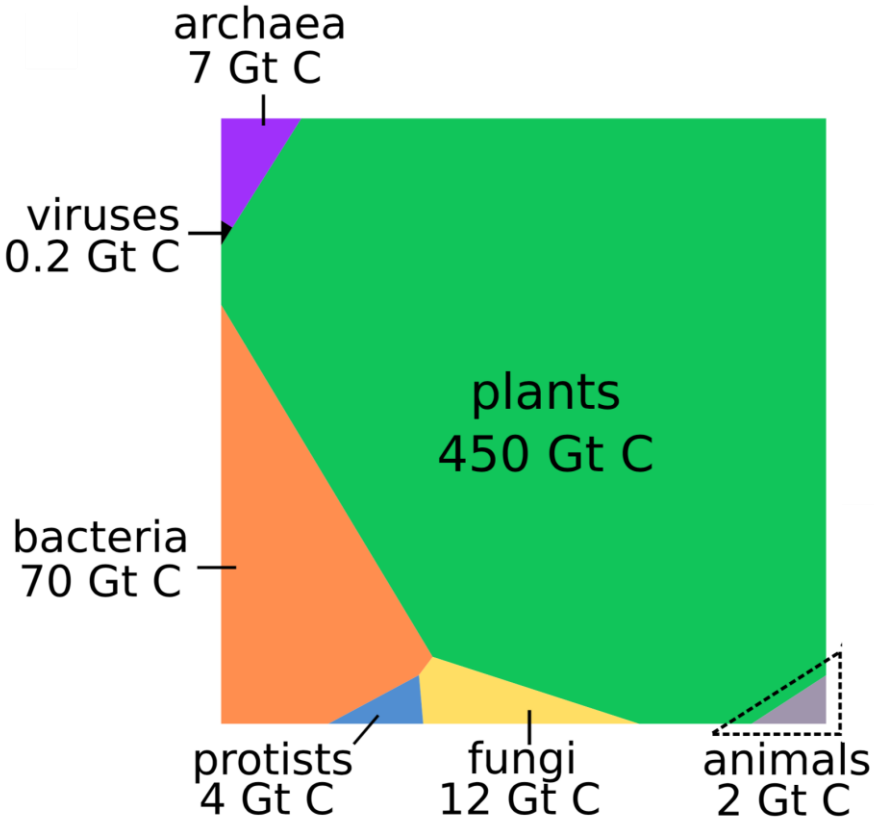






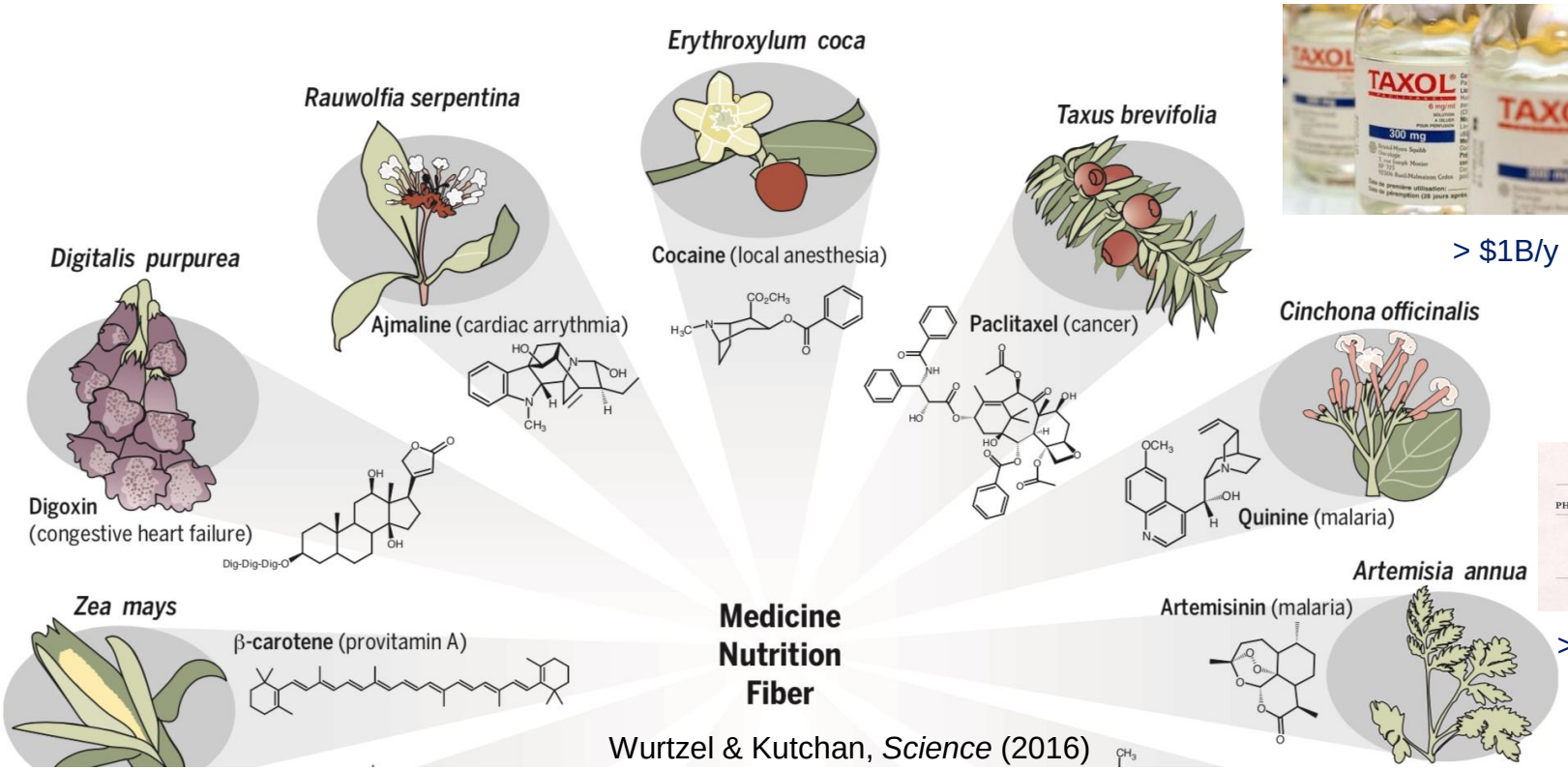



Plants constitute the majority of biomass on Earth



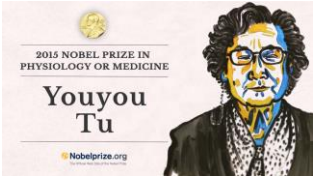
Bar-On et al., *Proc. Natl. Acad. Sci.* 2018

Plants rely entirely on chemistry for defense and adaptation



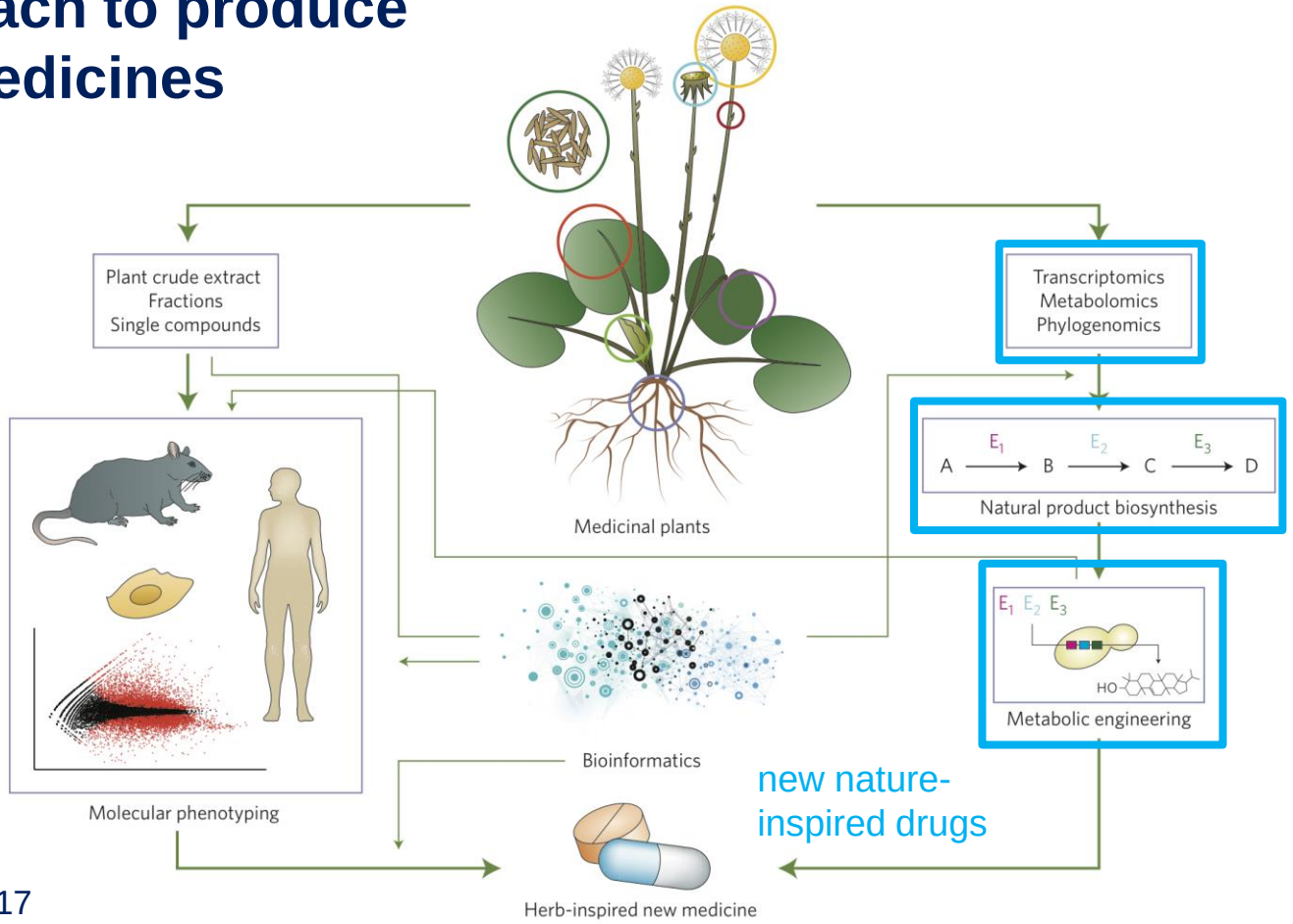
Wurtzel & Kutchan, *Science* (2016)

> $1B/y market



> $500M/y market

A modern approach to produce plant-inspired medicines



Li and Weng, *Nature Plants* 2017

LETTER

doi:10.1038/nature12051

High-level semi-synthetic production of the potent antimalarial artemisinin

C. J. Paddon[1], P. J. Westfall[1]†, D. J. Pitera[1], K... D. R. Polichuk[2], K. H. Teoh[2]†, D. W. Reed[2], G. Dorin[1], K. W. Ellens[2]†, S. Fickes[1], J. Galaz... H. Jiang[1], L. Kizer[1], B. Lieu[1], D. Melis[1], N. Mos... Y. Zhang[2]†, L. Zhao[1], J. Lievense[1]†, P. S. Cov...

SYNTHETIC B...

Compl... in yeas...

Stephanie Gala... Maria Filsinger...

Article

Discovery and eng... alkaloid biosynthe...

https://doi.org/10.1038/s41586-020-2546-8

Received: 19 October 2019

Accepted: 17 June 2020

Published online: 22 July 2020

Check for updates

Article

A microbial supply chain for production of the anti-cancer drug vinblastine

https://doi.org/10.1038/s41586-022-05157-3

Received: 12 April 2021

Accepted: 27 July 2022

Published online: 31 August 2022

Open access

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Jie Zhang[1], Lea G. Hansen[1], Olga Gudich[1], Konrad Viehrig[1], Lærke M. M. Lassen[1], Lars Schrübbers[1], Khem B. Adhikari[1], Paulina Rubaszka[1], Elena Carrasquer-Alvarez[1], Ling Chen[1], Vasil D'Ambrosio[1], Beata L... Konstantina Giannakou[1], Marcos Lalou... Leanne Jade G. Chan[2,3], Mette Kristen... Emily A. Stander[4], Edward Baidoo[2,3], C... Sarah E. O'Connor[4], Vincent Courdava...

nature synthesis

Article

https://doi.org/10.1038/s44160-025-00800-z

Elucidation of the final steps in Taxol biosynthesis and its biotechnological production

Received: 26 August 2024

Accepted: 31 March 2025

Published online: 30 April 2025

Check for updates

Feiyan Liang, Yuman Xie, Chi Zhang, Yong Zhao, Mohammed S. Motawia & Sotirios C. Kampranis

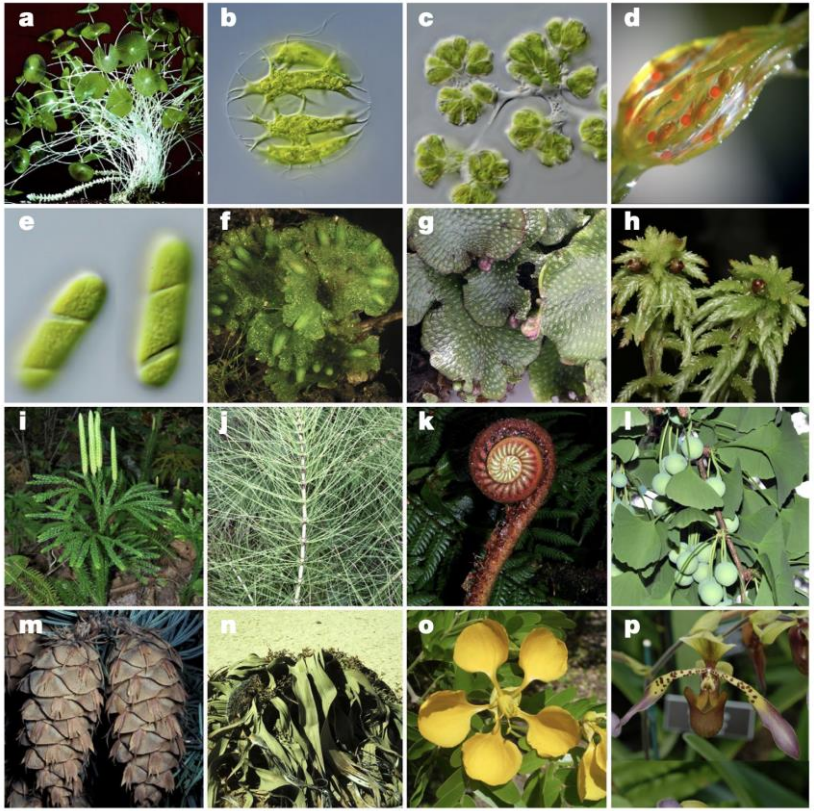
Taxol (paclitaxel) is a widely used anti-cancer drug with a complex biosynthetic pathway that has puzzled biochemists for decades. Owing to inefficient chemical synthesis, Taxol supply depends on costly semi-synthesis. Elucidating the Taxol biosynthesis will solve a long-standing question in biochemistry and enable cost-effective production using biotechnological methods. While recent advances have improved our understanding of the steps leading up to the intermediate baccatin III, the final steps of the pathway remain elusive. Here we use gene co-expression analysis, chemically synthesized intermediates and a stepwise learning-by-building approach to reveal the enzymes that catalyse the final two modifications, that is, C2′α hydroxylation and 3′-N benzoylation, which are essential for Taxol's bioactivity. To replace the current semi-synthetic method of Taxol production, we reconstruct the late pathway in yeast and synthesize Taxol from the readily available intermediate baccatin III. This work provides a complete understanding of Taxol biosynthesis and establishes a foundation for its biotechnological production.

Taxol is among the most commonly used chemotherapeutic drugs, effective in the treatment of breast, ovarian, cervical, nasopharyngeal and non-small cell lung cancer[1]. It exerts its anti-mitotic activity by preventing the disassembly of microtubules[2]. Initially isolated from the inner bark of the mature Pacific yew tree (*Taxus brevifolia*)[3,4], sourcing Taxol from yew trees is not viable owing to its remarkably low content in the bark. Chemical synthesis of Taxol is also inefficient because of its complex chemical structure[5–7]. Consequently, pharmaceutical Taxol is currently produced either from *Taxus* cell culture or by semi-synthesis from more available plant-derived taxoids. Both methods are costly, making Taxol and its derivatives (docetaxel and cabazitaxel) among the highest-priced small molecule active pharmaceutical ingredients[8]. To improve Taxol supply, biotechnological production presents a promising alternative. However, progress has been hindered by incomplete knowledge of the biosynthetic pathway.

The remarkably complex structure of Taxol has prompted intense research into its biosynthesis for over 30 years. The pathway is believed to involve at least 18 biosynthetic steps. Early investigations in the 1990s established the first step as the cyclization of geranylgeranyl diphosphate to the basic diterpene scaffold, taxadiene, by the enzyme taxadiene synthase[9,10]. Subsequent studies revealed several cytochrome P450 (CYP) enzymes that oxidize the taxadiene structure[11–16] and acyltransferases that further decorate the oxygenated taxoids[17–20]. However, further progress was hampered by the lack of comprehensive genomic and transcriptomic information. The recent genome sequencing of two Taxol-producing yew species[21,22] has rekindled efforts to elucidate the Taxol pathway. Several studies have since contributed to understanding the early steps leading to the key intermediate baccatin III[23–27]. These studies revisited earlier proposed biosynthetic schemes, discovering missing oxidase enzymes[23–27], accessory proteins essential

Biochemical Engineering Group, Plant Biochemistry Section, Department of Plant and Environment Sciences, Faculty of Science, University of Copenhagen, Frederiksberg C, Denmark. e-mail: soka@plen.ku.dk

Plants are diverse and complex

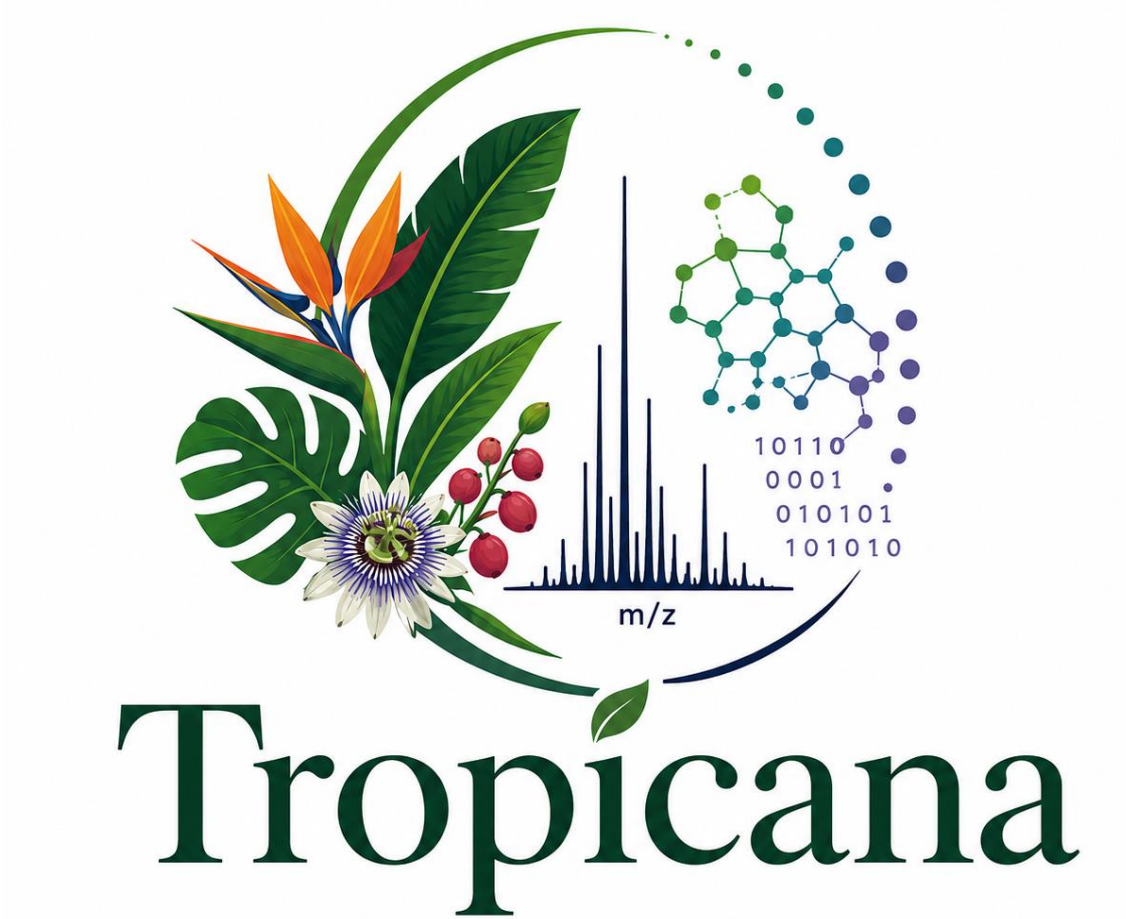


How do we **measure** and **interpret** the complex metabolic diversity in plants?

How do we **elucidate** the biosynthetic enzymes, pathways, or networks?

How can we take advantage of modern **computational** approaches?

Leebens-Mack, J. H. *et al.* One thousand plant transcriptomes and the phylogenomics of green plants. *Nature* **574**, 679–685 (2019)



Logo credit: ChatGPT

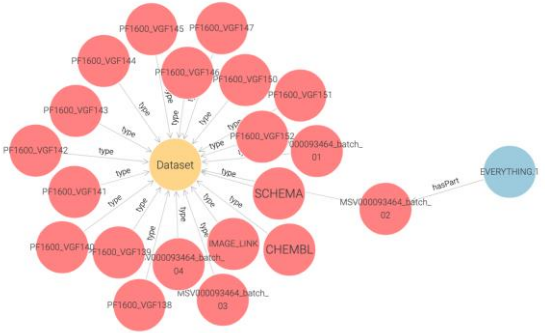
Data collection and organization

Sample collection

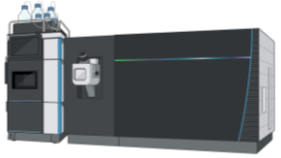
Digital Botanical Gardens Initiative

QField for QGIS

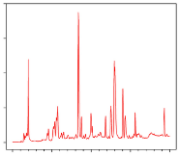
Metadata storage



Knowledge graphs



LC-MS analysis



LC-MS data

BOTANICKÁ ZAHRADA PRAHA

Faculty of Tropical AgriSciences

Prague, CZ
15,000+ species

Vlastimil Rybka

Anežka Daníčková

Royal Botanic Gardens Kew

London, UK
50,000+ species

Melanie-Jayne Howes

unine Université de Neuchâtel

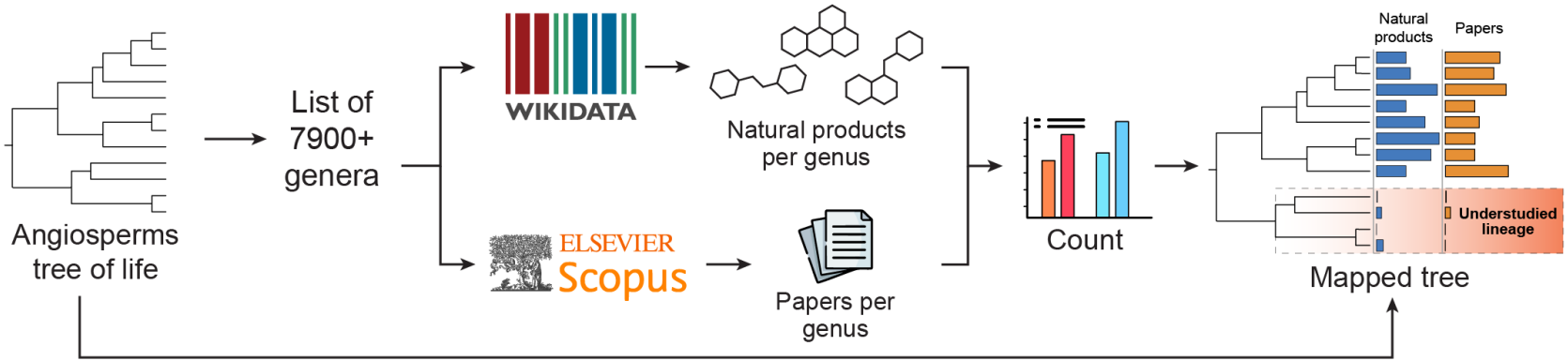
UNI FR

Neuchâtel and Fribourg, CH
10,000+ species

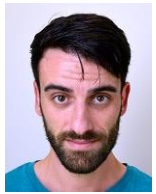
Emmanuel Defossez

Pierre-Marie Allard

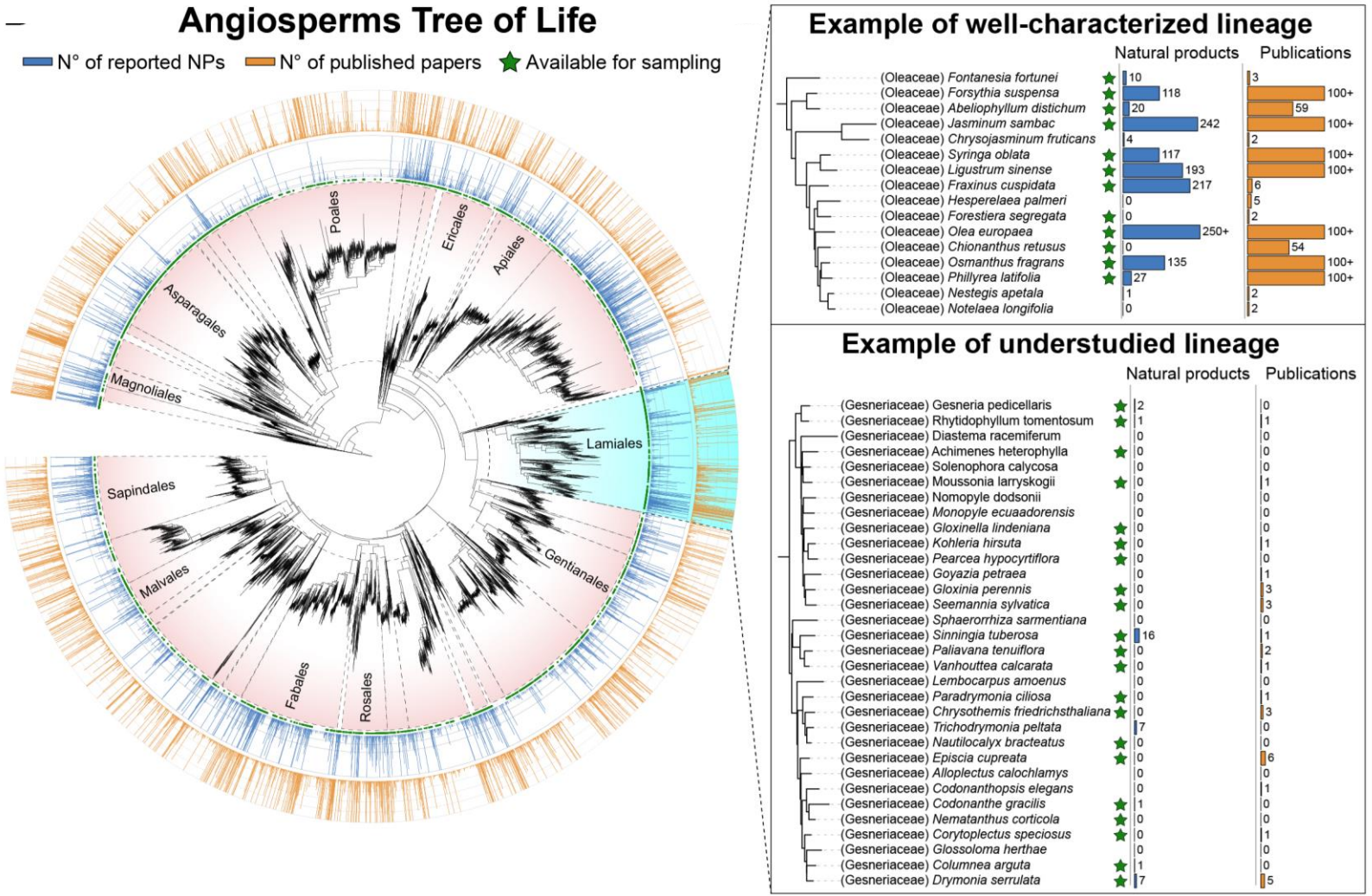
Prioritization of plant species for sampling



Téo Hebra



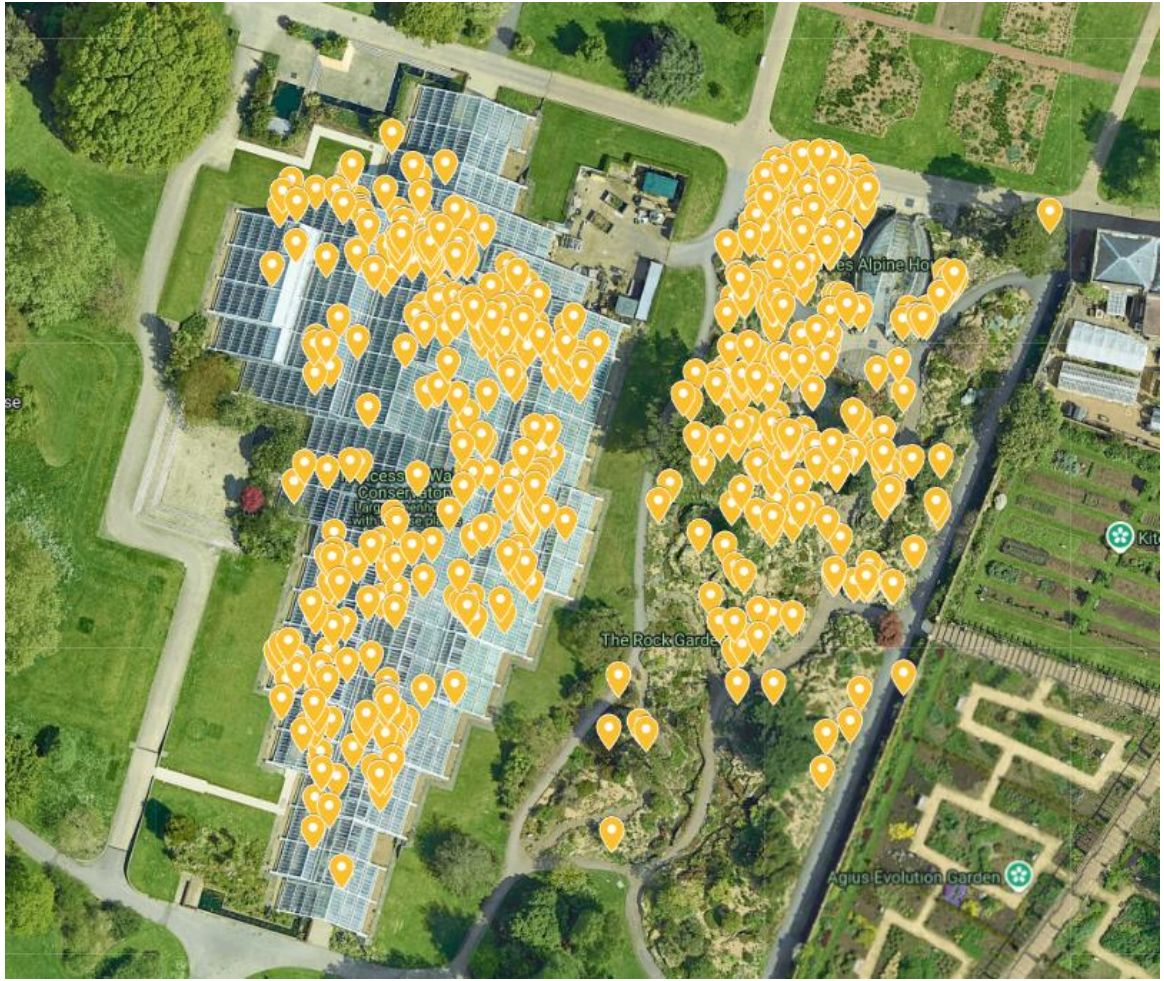
Tito Damiani


Angiosperms Tree of Life
N° of reported NPs
N° of published papers
Available for sampling
Poales
Ericales
Apiales
Asparagales
Magnoliales
Lamiales
Sapindales
Gentianales
Malvales
Fabales
Rosales
Example of well-characterized lineage
Natural products
Publications
(Oleaceae) Fontanesia fortunei 10 3
(Oleaceae) Forsythia suspensa 118 100+
(Oleaceae) Abeliophyllum distichum 20 59
(Oleaceae) Jasminum sambac 242 100+
(Oleaceae) Chrysojasminum fruticans 4 2
(Oleaceae) Syringa oblata 117 100+
(Oleaceae) Ligustrum sinense 193 100+
(Oleaceae) Fraxinus cuspidata 217 6
(Oleaceae) Hesperelaea palmeri 0 5
(Oleaceae) Forestiera segregata 0 2
(Oleaceae) Olea europaea 250+ 100+
(Oleaceae) Chionanthus retusus 0 54
(Oleaceae) Osmanthus fragrans 135 100+
(Oleaceae) Phillyrea latifolia 27 100+
(Oleaceae) Nestegis apetala 1 2
(Oleaceae) Notelaea longifolia 0 2
Example of understudied lineage
Natural products
Publications
(Gesneriaceae) Gesneria pedicellaris 2 0
(Gesneriaceae) Rhytidophyllum tomentosum 1 1
(Gesneriaceae) Diastema racemiferum 0 0
(Gesneriaceae) Achimenes heterophylla 0 0
(Gesneriaceae) Solenophora calycosa 0 0
(Gesneriaceae) Moussonia larryskogii 0 1
(Gesneriaceae) Nomopyle dodsonii 0 0
(Gesneriaceae) Monopyle ecuaadorensis 0 0
(Gesneriaceae) Gloxinella lindeniana 0 0
(Gesneriaceae) Kohleria hirsuta 0 1
(Gesneriaceae) Pearcea hypocyrtiflora 0 0
(Gesneriaceae) Goyazia petraea 0 1
(Gesneriaceae) Gloxinia perennis 0 3
(Gesneriaceae) Seemannia sylvatica 0 3
(Gesneriaceae) Sphaerorrhiza sarmentiana 0 0
(Gesneriaceae) Sinningia tuberosa 16 1
(Gesneriaceae) Paliavana tenuiflora 0 2
(Gesneriaceae) Vanhouttea calcarata 0 1
(Gesneriaceae) Lembocarpus amoenus 0 0
(Gesneriaceae) Paradrymonia ciliosa 0 1
(Gesneriaceae) Chrysothemis friedrichsthaliana 0 3
(Gesneriaceae) Trichodrymonia peltata 7 0
(Gesneriaceae) Nautilocalyx bracteatus 0 0
(Gesneriaceae) Episcia cupreata 0 6
(Gesneriaceae) Alloplectus calochlamys 0 0
(Gesneriaceae) Codonanthopsis elegans 0 1
(Gesneriaceae) Codonanthe gracilis 1 0
(Gesneriaceae) Nematanthus corticola 0 0
(Gesneriaceae) Corytoplectus speciosus 0 1
(Gesneriaceae) Glossoloma herthae 0 0
(Gesneriaceae) Columnea arguta 1 0
(Gesneriaceae) Drymonia serrulata 7 5

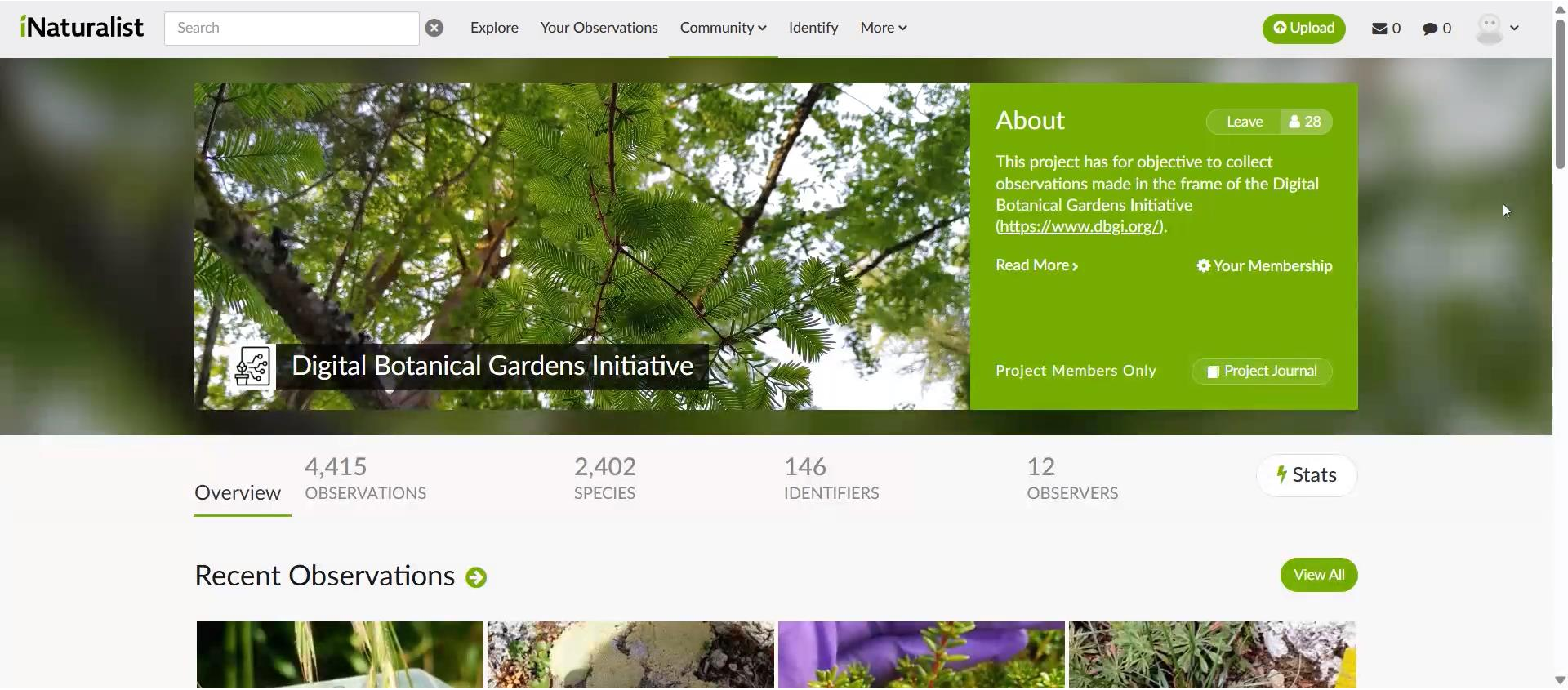
Plant sample collection

~100 samples
per student per day

Kateřina Kučerová



Royal Botanic Gardens Kew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Digital Botanical Gardens Initiative
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28
This project has for objective to collect observations made in the frame of the Digital Botanical Gardens Initiative (https://www.dbgi.org/).
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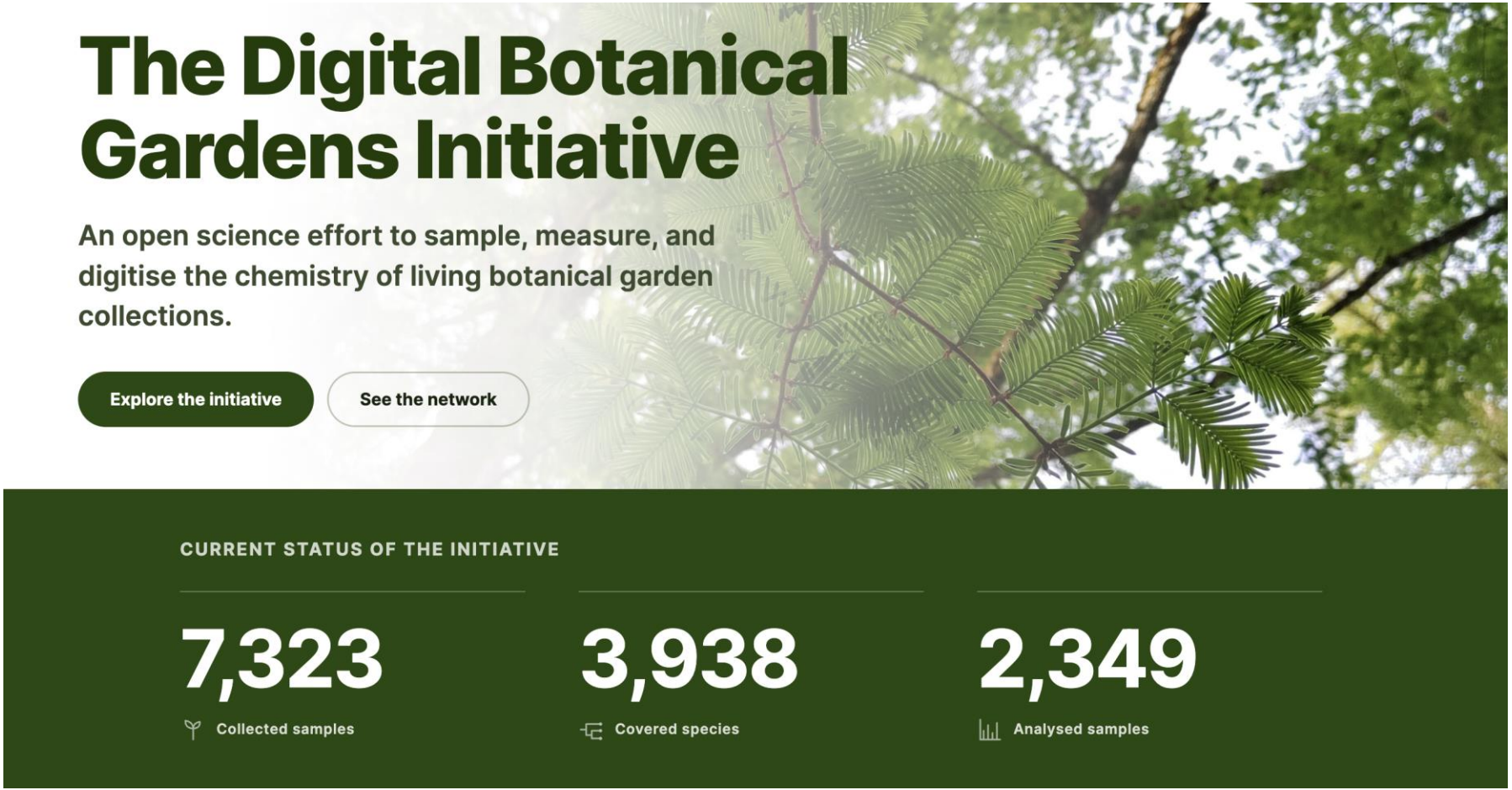
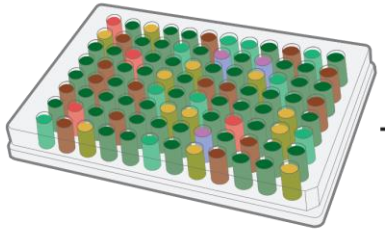
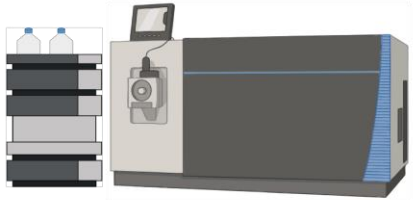
Project Members Only
Project Journal
Overview
4,415
OBSERVATIONS
2,402
SPECIES
146
IDENTIFIERS
12
OBSERVERS
Stats
Recent Observations
View All


The Digital Botanical Gardens Initiative
An open science effort to sample, measure, and digitise the chemistry of living botanical garden collections.
Explore the initiative
See the network
CURRENT STATUS OF THE INITIATIVE
7,323
Collected samples
3,938
Covered species
2,349
Analysed samples

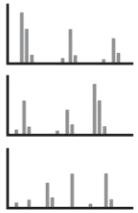
www.dbgi.org



Plant extracts
(n=1110)



LC-MS/MS



MS/MS
spectra

A self-supervised ML model trained on millions of unannotated MS/MS spectra

Mass Spectrometry
Interactive **V**irtual **E**nvironment

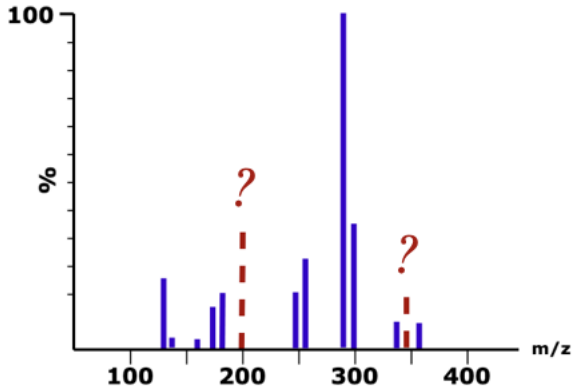
6,275,382,878 raw spectra
(~500 Terabytes)

Self-supervised learning on MS/MS spectra

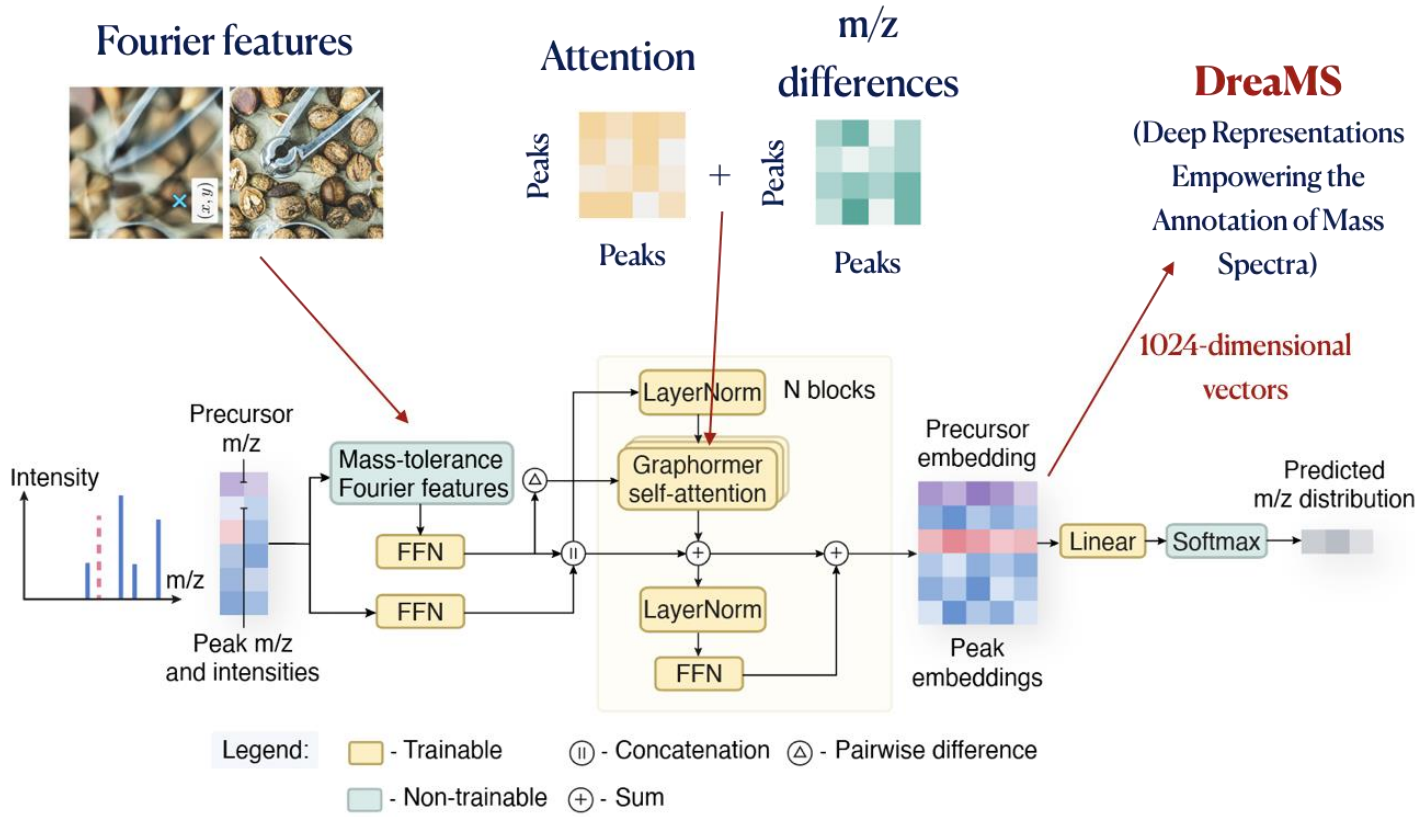
ChatGPT

The quick brown fox jumps over a lazy dog is the most famous ___?___

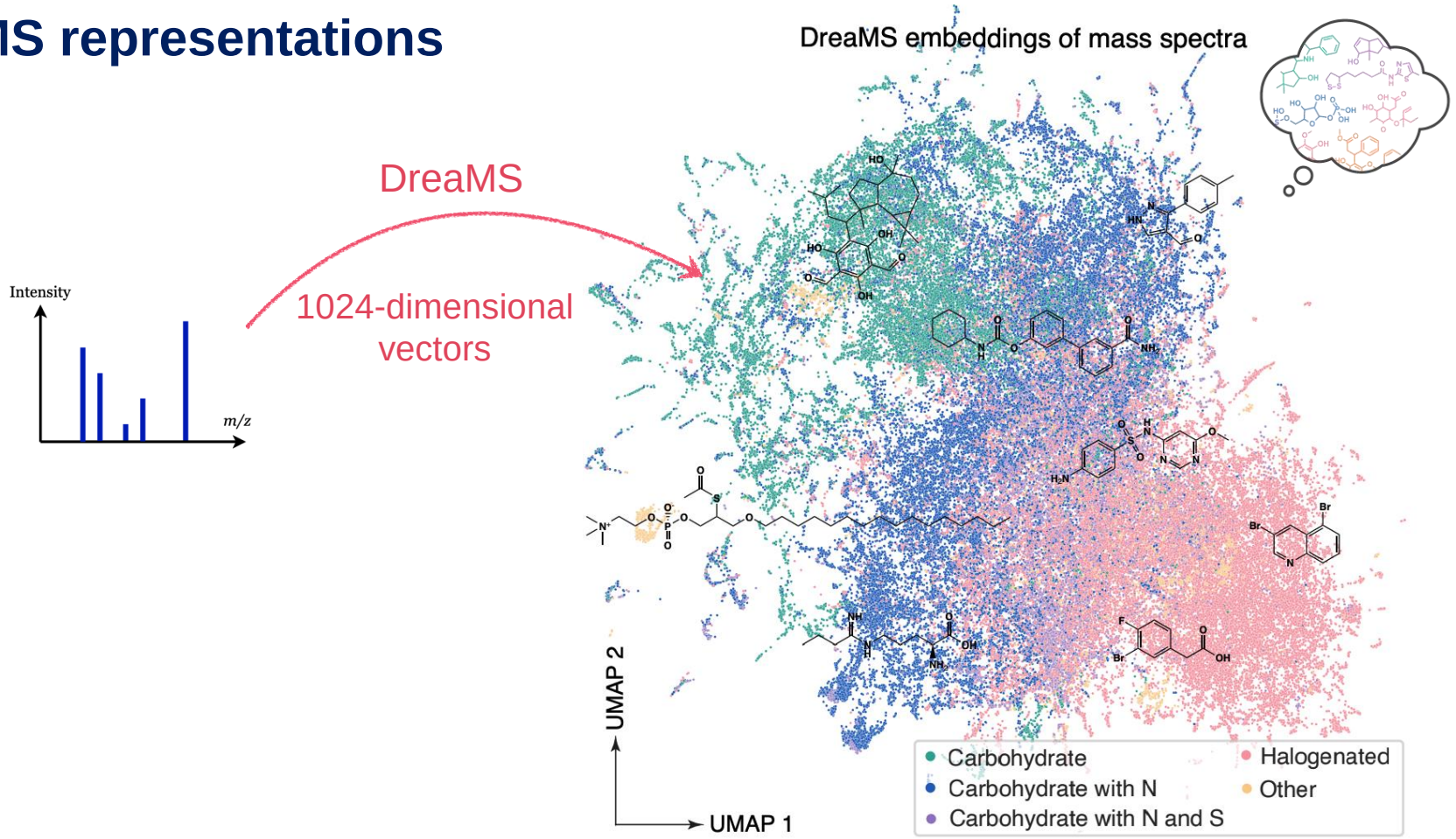
Our approach



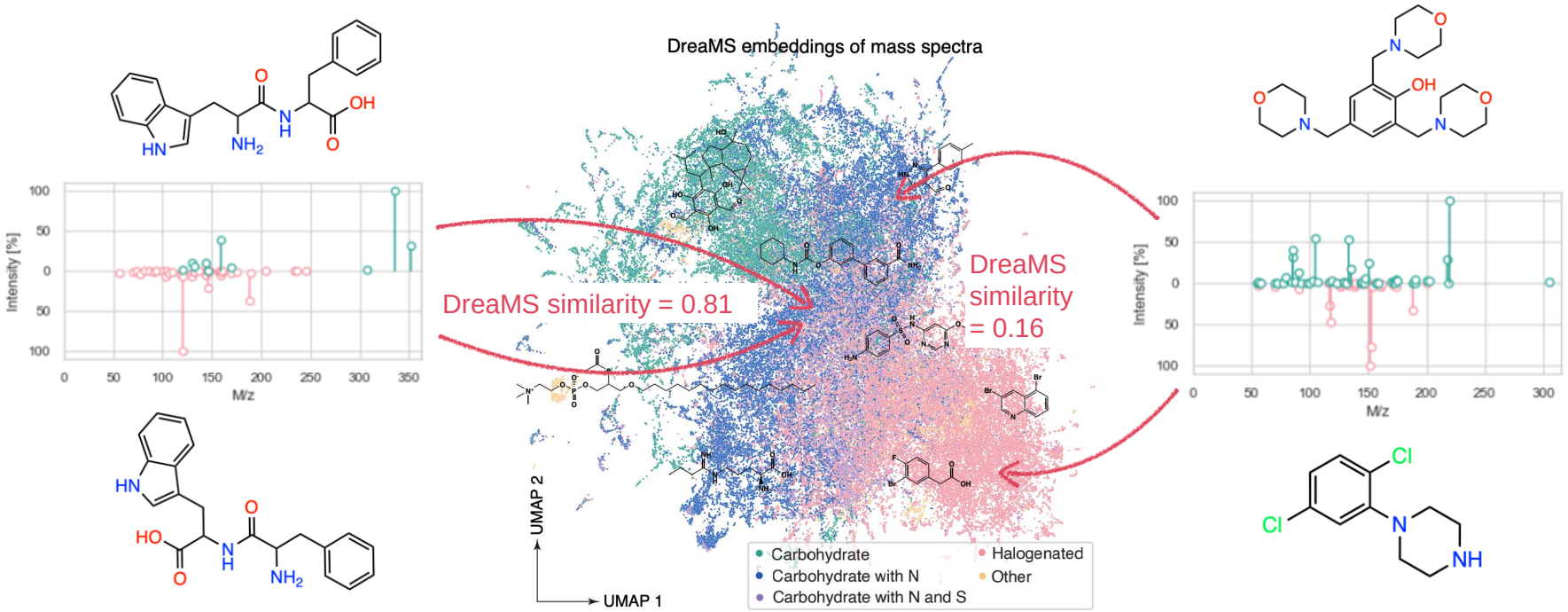
The DreaMS model architecture



DreaMS representations



DreaMS mass spectral similarity

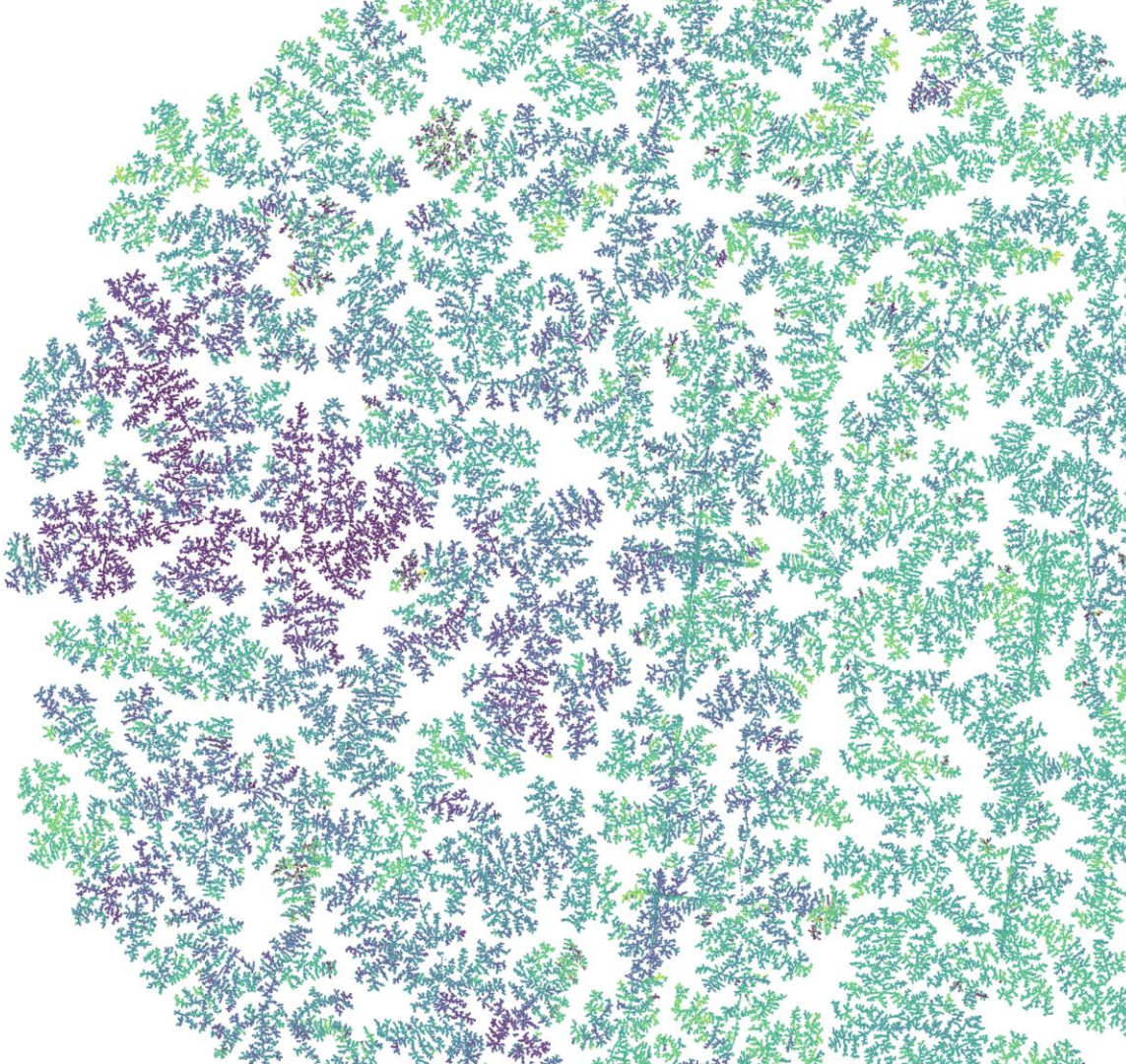


Similar DreaMS representations = similar molecular structures

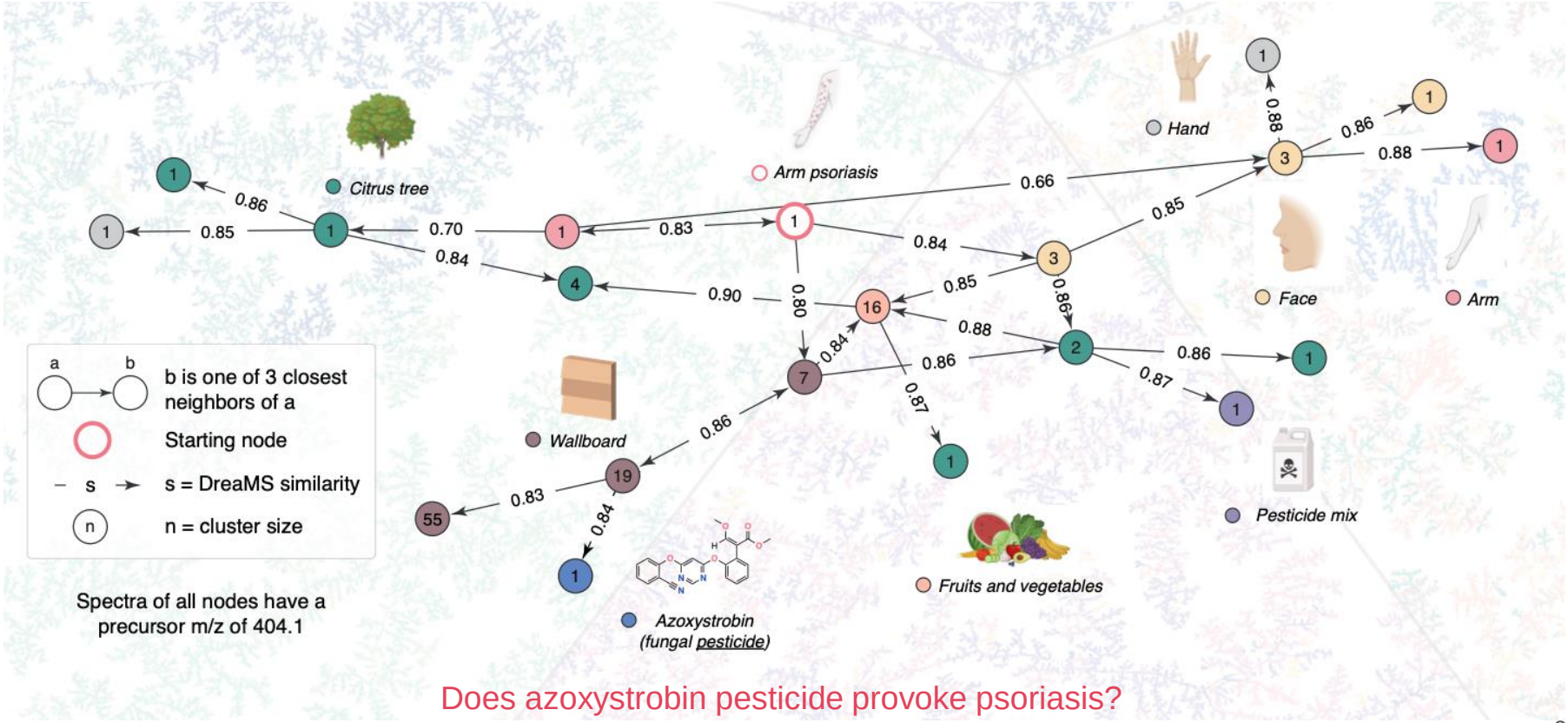
DreaMS Atlas

Molecular network of 200 million mass spectra from MassIVE

“The Internet of mass spectrometry”



DreaMS Atlas can lead to new hypotheses



Does azoxystrobin pesticide provoke psoriasis?

Roman Bushuiev

Anton Bushuiev

Josef Šivic

nature biotechnology

Article

https://doi.org/10.1038/s41587-025-02663-3

Self-supervised learning of molecular representations from millions of tandem mass spectra using DreaMS

Received: 22 April 2024

Accepted: 31 March 2025

Published online: 23 May 2025

Check for updates

Roman Bushuiev[1,2,3], Anton Bushuiev[2,3], Raman Samusevich[1,2], Corinna Brungs[1], Josef Sivic[2] ✉ & Tomáš Pluskal[1] ✉

Characterizing biological and environmental samples at a molecular level primarily uses tandem mass spectroscopy (MS/MS), yet the interpretation of tandem mass spectra from untargeted metabolomics experiments remains a challenge. Existing computational methods for predictions from mass spectra rely on limited spectral libraries and on hard-coded human expertise. Here we introduce a transformer-based neural network pre-trained in a self-supervised way on millions of unannotated tandem mass spectra from our GNPS Experimental Mass Spectra (GeMS) dataset mined from the MassIVE GNPS repository. We show that pre-training our model to predict masked spectral peaks and chromatographic retention orders leads to the emergence of rich representations of molecular structures, which we named Deep Representations Empowering the Annotation of Mass Spectra (DreaMS). Further fine-tuning the neural network yields state-of-the-art performance across a variety of tasks. We make our new dataset and model available to the community and release the DreaMS Atlas—a molecular network of 201 million MS/MS spectra constructed using DreaMS annotations.

The discovery and identification of small molecules and metabolites impacts various scientific fields, including drug development[1], environmental analysis[2] and disease diagnosis[3]. However, only a tiny fraction of natural small molecules have been discovered to date, estimated to be less than 10% of those present in the human body or the entire plant kingdom[4]. Most of the natural chemical space remains unexplored.

Tandem mass spectrometry coupled with liquid chromatography (LC–MS/MS) is an analytical technique for investigating the molecular composition of biological and environmental samples. When analyzing a sample, the LC–MS/MS system separates molecules through liquid chromatography, ionizes them and records their mass-to-charge ratios (m/z), generating a series of mass spectra (referred to as MS^1). Each MS^1 spectrum is acquired at a specific retention time and represents the abundance of ions in terms of their m/z ratios (that is, peaks). Using a technique referred to as data-dependent acquisition, selected ions (referred to as precursor ions) undergo fragmentation, typically using collision-induced dissociation (CID), yielding additional tandem mass spectra (referred to as MS^2 or MS/MS), where signals characterize molecular fragments of a single selected ion. Although MS^2 and deeper MS^n tandem mass spectra constitute the primary source of structural information in mass spectrometry, their interpretation remains challenging. In particular, a mere 2% of MS/MS spectra in an untargeted metabolomics experiment can be annotated with molecular structures using reference spectral libraries[5,6], and less than 10% of MS/MS spectra can typically be annotated using state-of-the-art machine learning tools[7].

Existing methods for the interpretation of mass spectra of small molecules can be classified into three major categories: spectral

Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic. [1]Czech Institute of Informatics, Robotics and Cybernetics, Czech Technical University, Prague, Czech Republic. [2]These authors contributed equally: Roman Bushuiev, Anton Bushuiev. ✉e-mail: josef.sivic@cvut.cz; tomas.pluskal@uochb.cas.cz

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Hlavní stránka Stalo se Domácí Volby Zahraniční Válka na Ukrajině Komentáře Krimi Kultura Ek
Internet a PC AutoMoto Věda Cestování Historie Podcasty a pořady Sport Kvízy Speciály Počas

Fotosoutěž: Nejhezčí zahradní jezírko

Novinky.cz » Věda a školy » Čeští vědci objevují neznámé molekuly s pomocí umělé inteligence

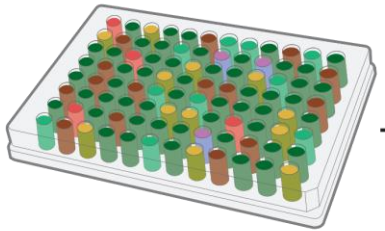
Čeští vědci objevují neznámé molekuly s pomocí umělé inteligence

Lucie Fialová
+ sledovat 121

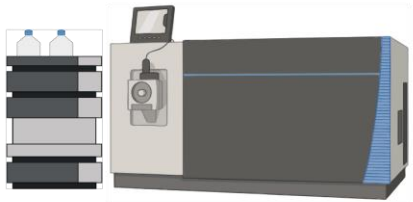
3:51 Poslechněte si tento článek eBook Sdílet 0

30. 5. 2025, 6:41

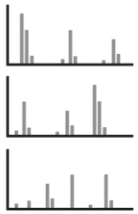
Vědci z Ústavu organické chemie a biochemie Akademie věd ČR (ÚOCHB) a Českého institutu informatiky, robotiky a kybernetiky (CIIRC) ČVUT v Praze vyvinuli s pomocí umělé inteligence nástroj ke hledání zatím neobjevených přírodních molekul. Může pomoci ve vývoji nových léků, šetrnějších pesticidů nebo při zkoumání života ve vesmíru.



Plant extracts
(n=1110)

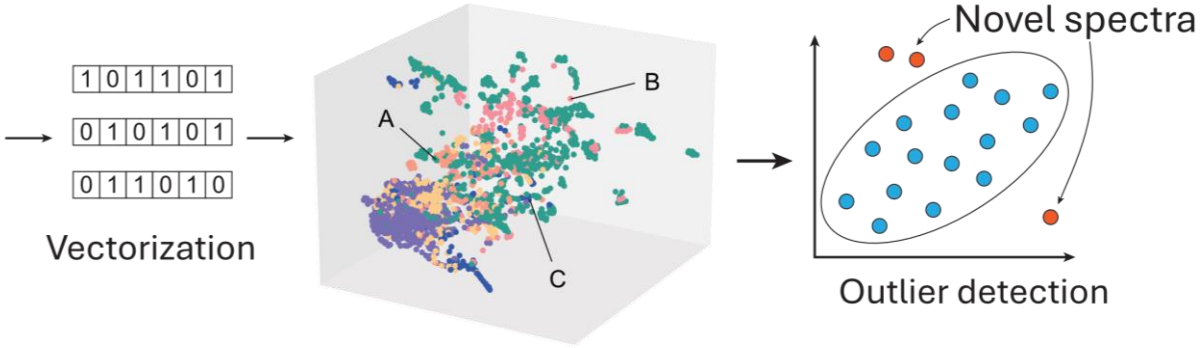


LC-MS/MS



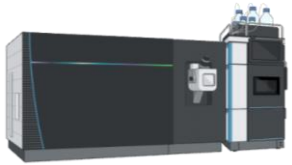
MS/MS
spectra

DreaMS
embedding space



(each dot is an MS feature = molecule)

1,110 samples

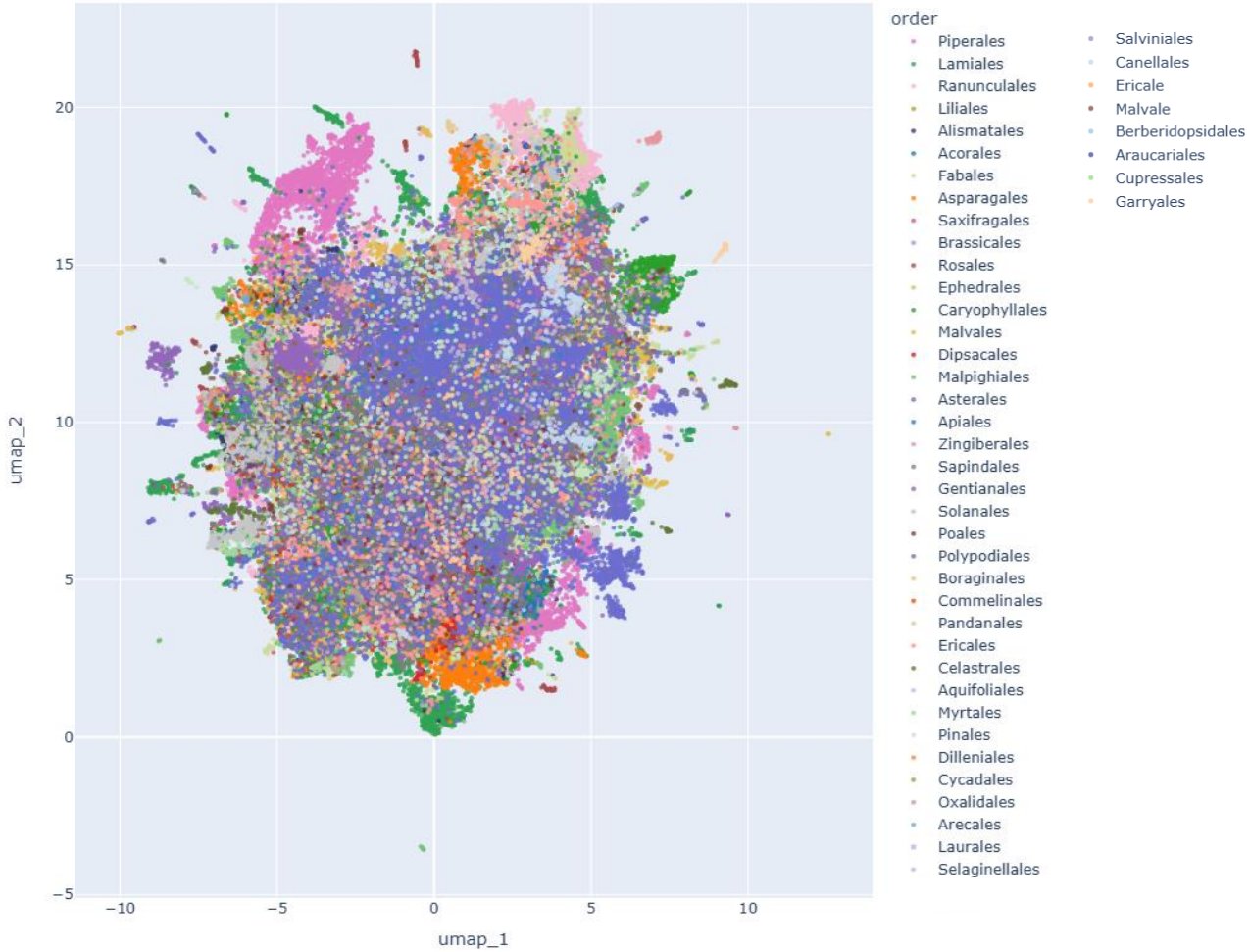


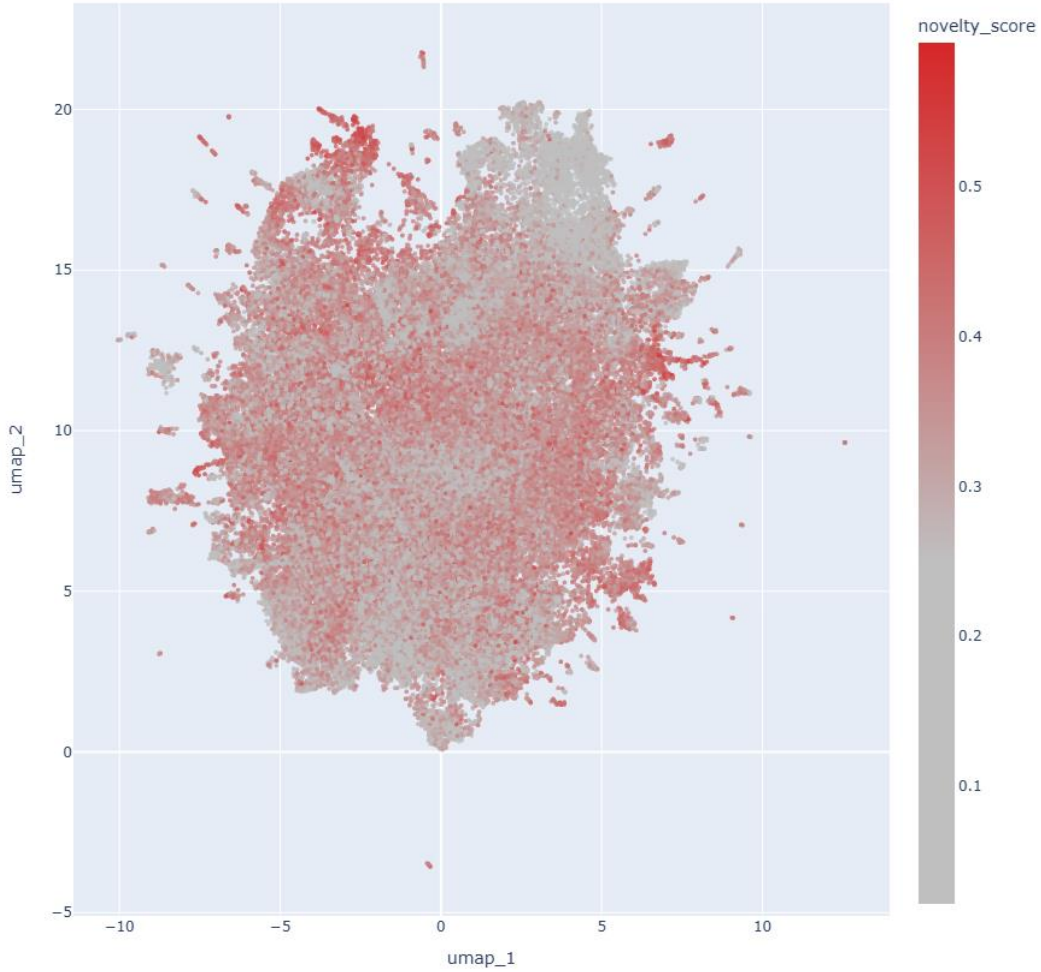
mzmine

92,465 MS features

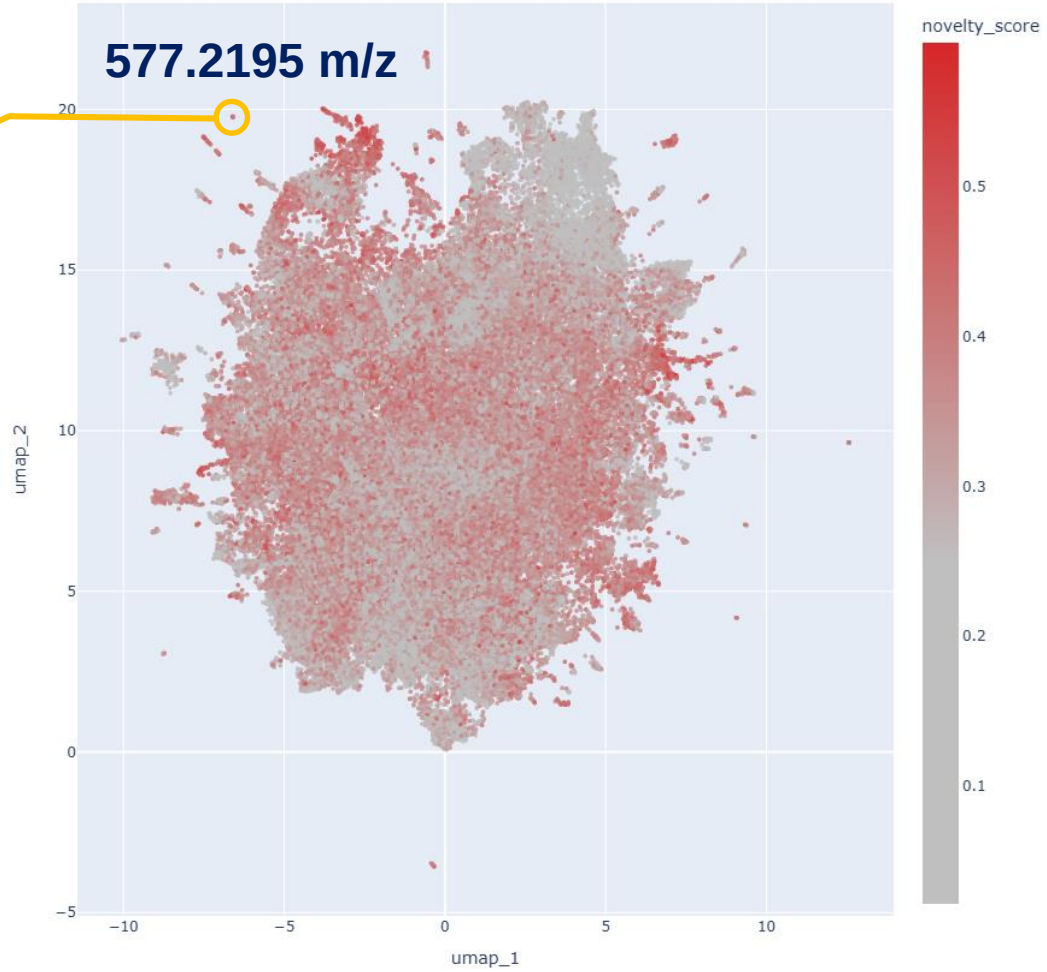
DreaMS

UMAP projection of embeddings

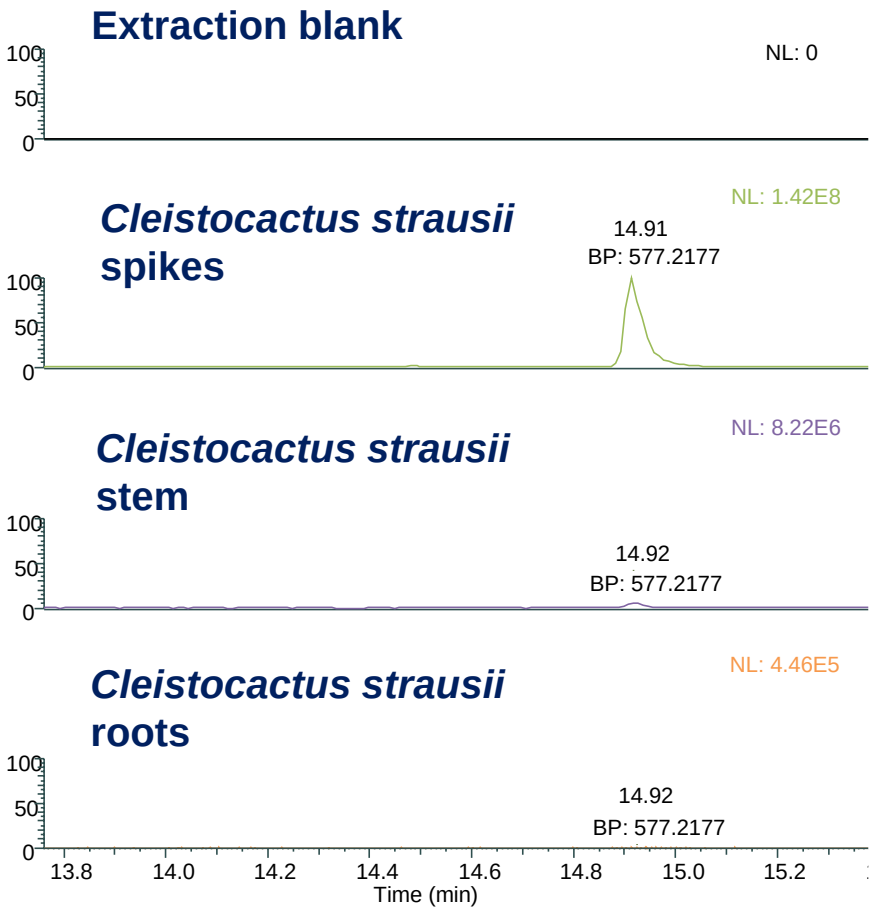


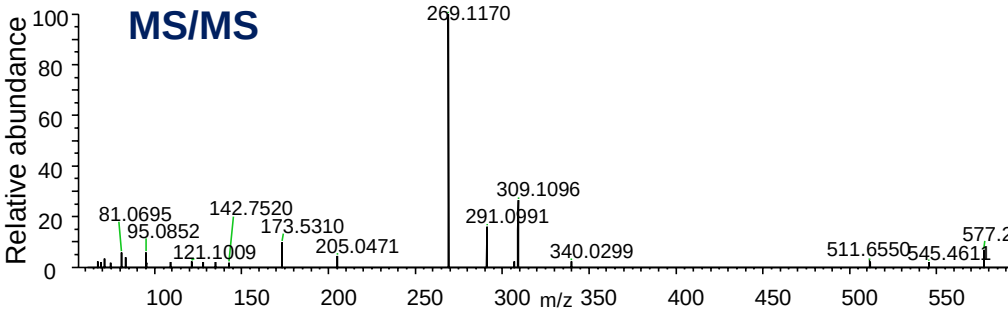

novelty_score
0.5
0.4
0.3
0.2
0.1
umap_2
20
15
10
5
0
−5
−10
−5
0
5
10
umap_1

Cleistocactus strausii



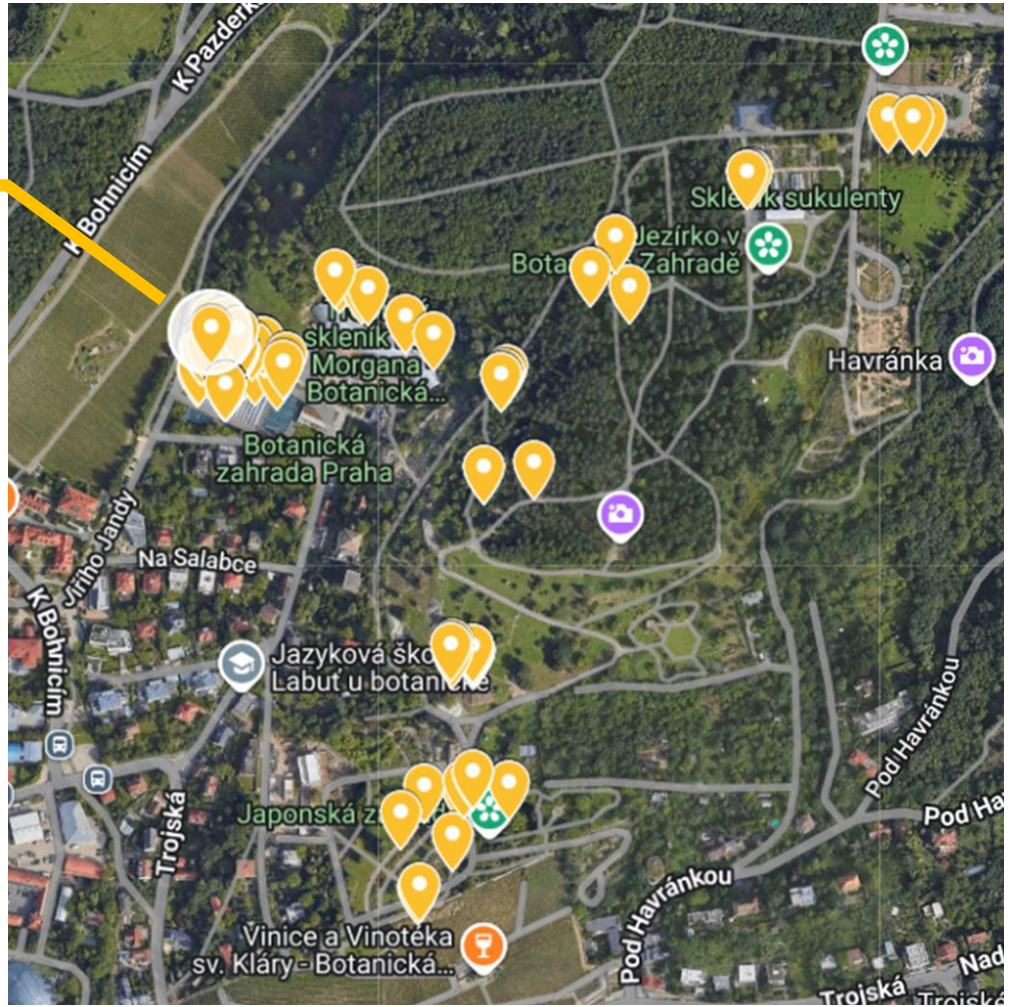
XIC of *m/z* 577.218





iNaturalist

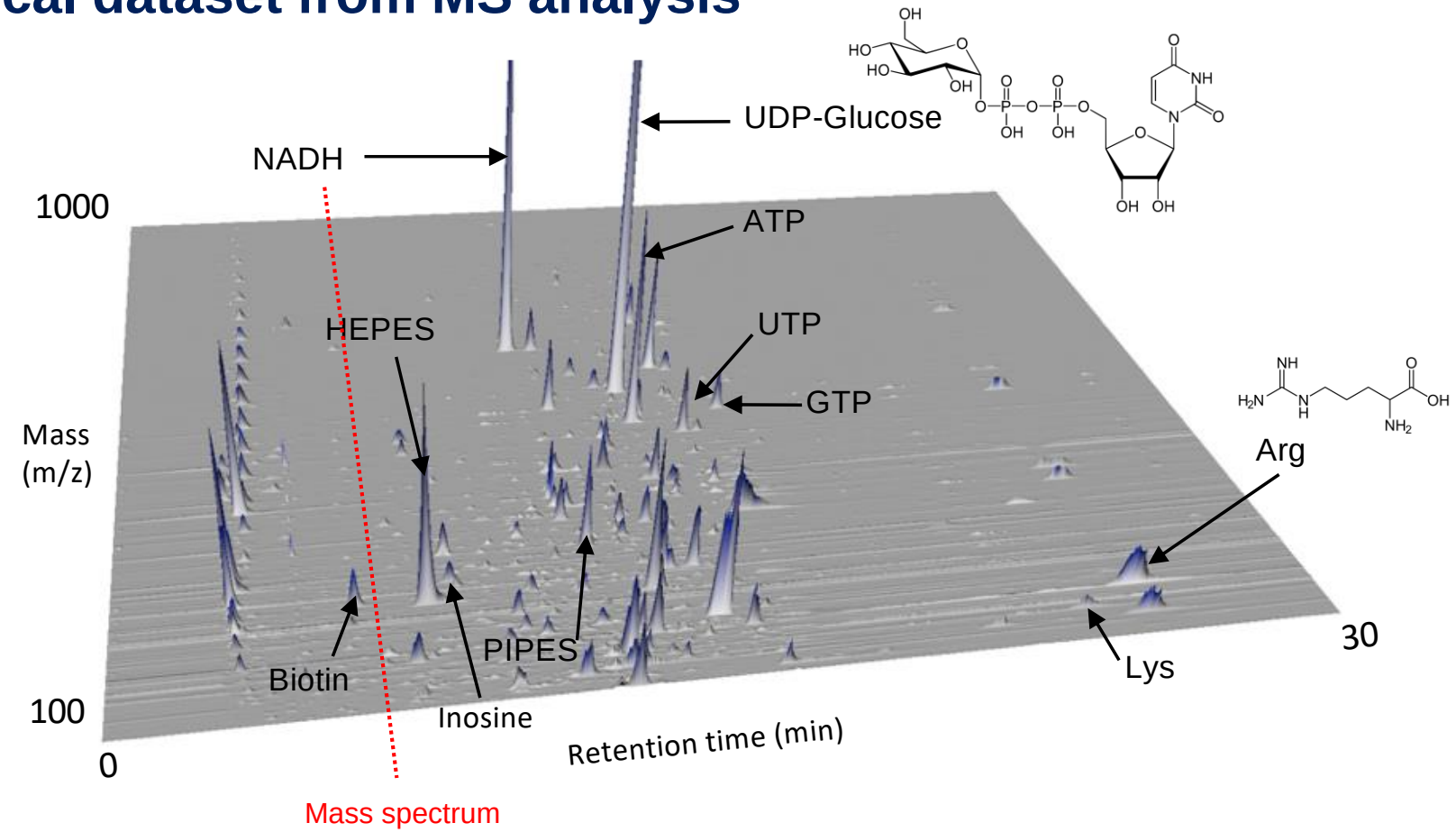
Cleistocactus strausii



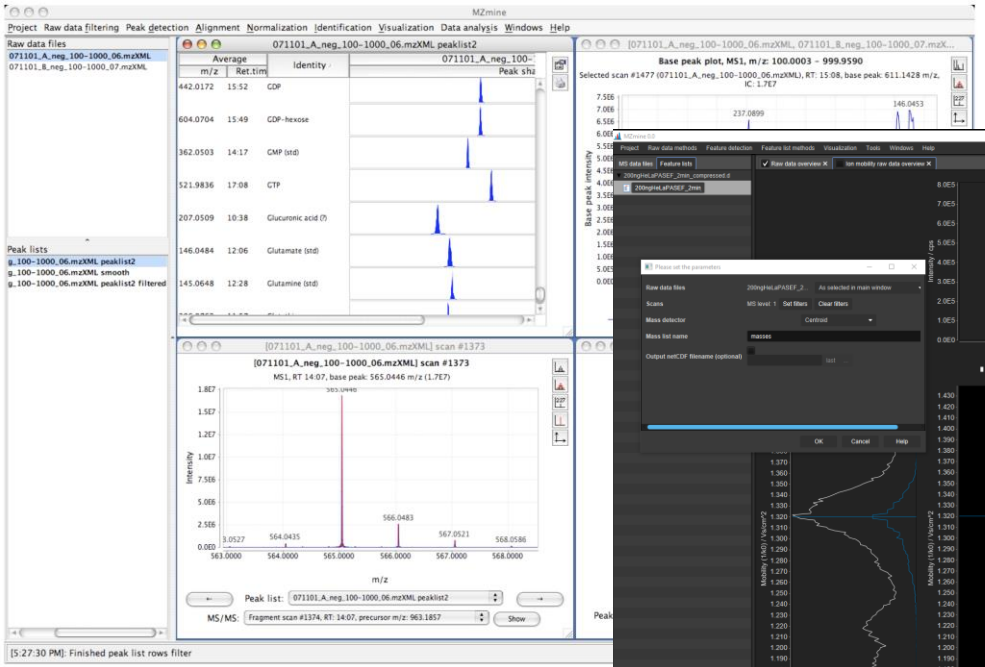
mzmine – how open-source academic software goes commercial

Mass spectrometry – the gold standard for chemical analysis

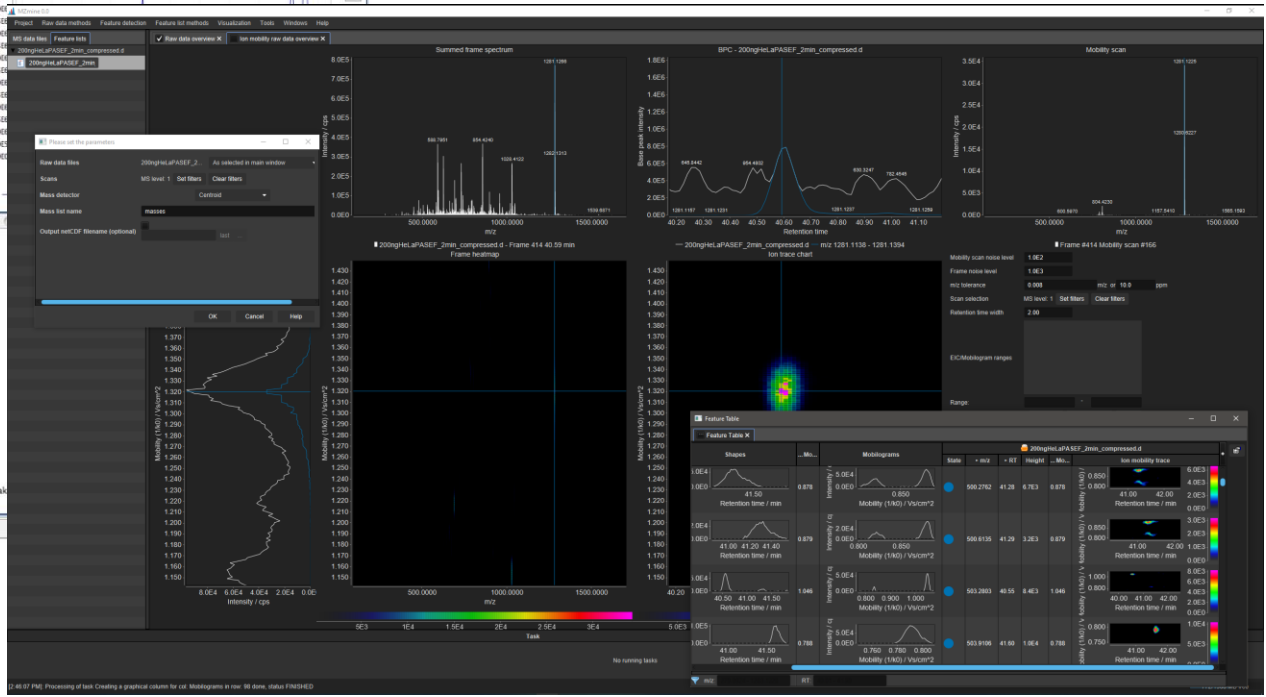
A typical dataset from MS analysis



mzmine is a software to view, process, and interpret MS data

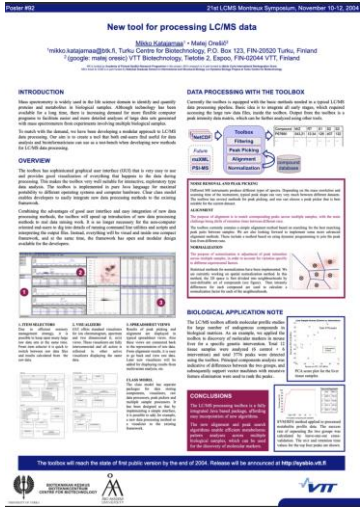


2006



2026

A brief history of mzmine


New tool for processing LC/MS data

2004

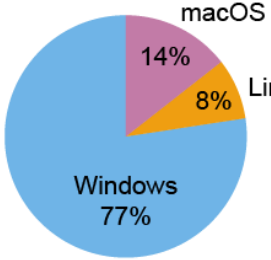
+5 since publication

53 contributors

35 with >500 changed lines

92,000+ downloads

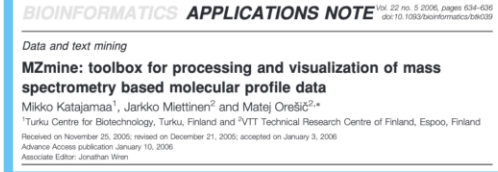
(last 5 years)



mzmine publications

MZmine

2006


BIOINFORMATICS APPLICATIONS NOTE Vol. 22 no. 5 2006, pages 634–636 doi:10.1093/bioinformatics/btk039

Data and text mining

MZmine: toolbox for processing and visualization of mass spectrometry based molecular profile data

Mikko Katajamaa[1], Jarkko Miettinen[2] and Matej Orešič[2,*]

[1]Turku Centre for Biotechnology, Turku, Finland and [2]VTT Technical Research Centre of Finland, Espoo, Finland

Received on November 25, 2005; revised on December 21, 2005; accepted on January 3, 2006

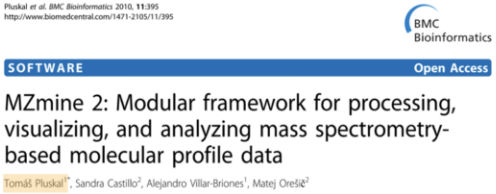
Advance Access publication January 10, 2006

Associate Editor: Jonathan Wren

897 citations

MZmine 2

2011


Pluskal et al. BMC Bioinformatics 2010, 11:395
http://www.biomedcentral.com/1471-2105/11/395

BMC Bioinformatics

SOFTWARE Open Access

MZmine 2: Modular framework for processing, visualizing, and analyzing mass spectrometry-based molecular profile data

Tomáš Pluskal[1*], Sandra Castillo[2], Alejandro Villar-Briones[1], Matej Orešič[2]

3445 citations

MZmine 3

2023


Correspondence | Published: 01 March 2023

Integrative analysis of multimodal mass spectrometry data in MZmine 3

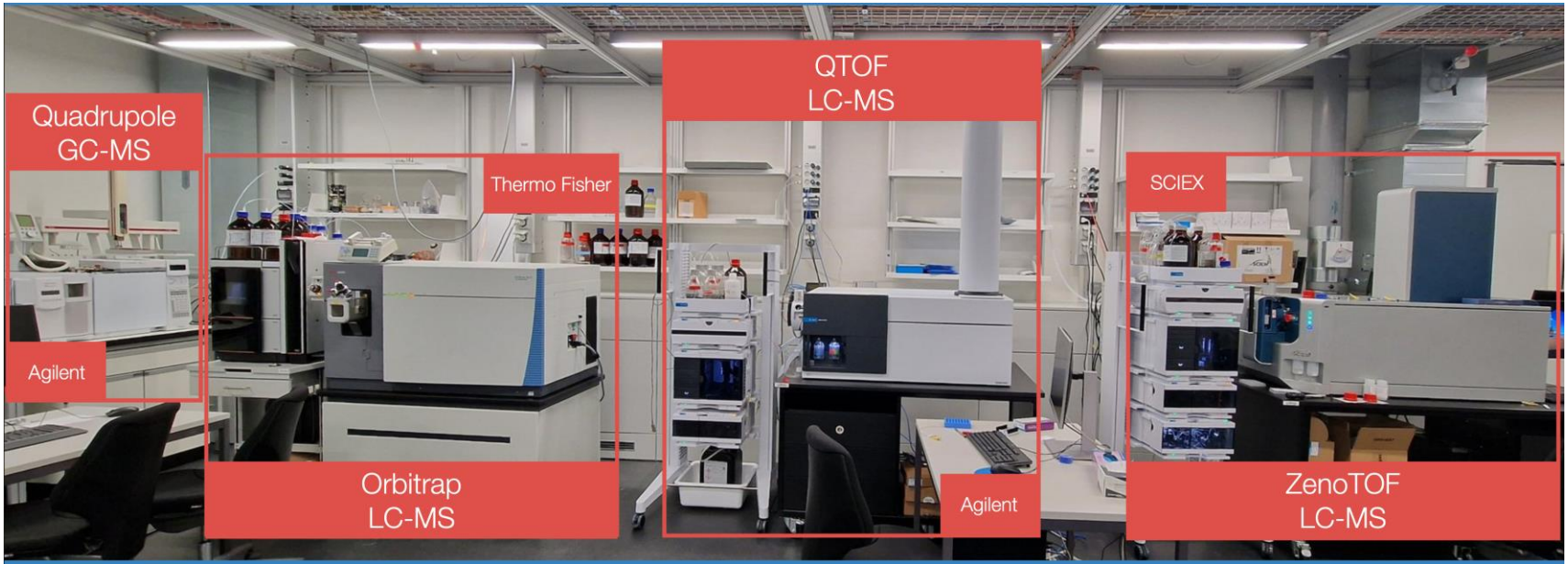
Robin Schmid, Steffen Heuckeroth, Ansgar Korf, Aleksandr Smirnov, Owen Myers, Thomas S. Dyrlund, Roman Bushuiev, Kevin J. Murray, Nils Hoffmann, Miaoshan Lu, Abinesh Sarvepalli, Zheng Zhang, Markus Fleischauer, Kai Dührkop, Mark Wesner, Shawn J. Hoogstra, Edward Rudt, Olena Mokshyna, Corinna Brungs, Kirill Ponomarov, Lana Mutabdžija, Tito Damiani, Chris J. Pudney, Mark Earll, ... Tomáš Pluskal + Show authors

Published March 2023 in *Nature Biotechnology*

mzmine was a huge success in academia, but with little adoption in industry

A typical mass spectrometry lab

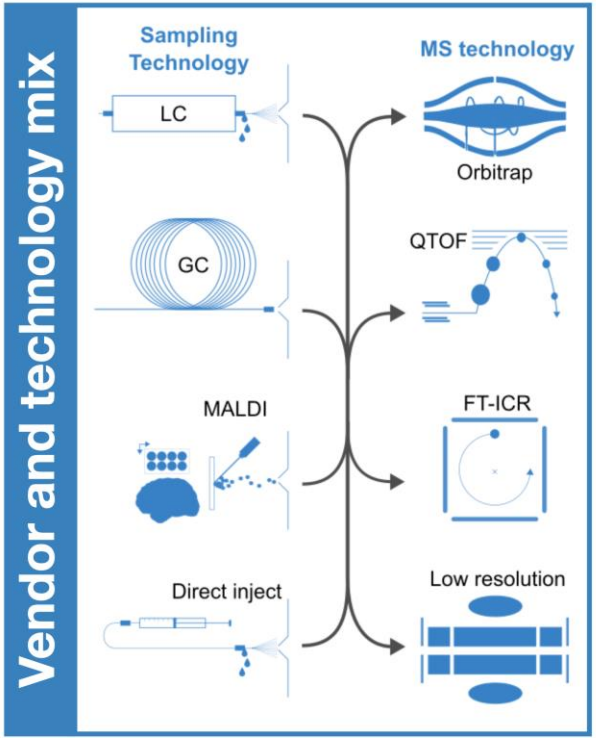
A typical mass spectrometry lab



- Different data types and formats
- Each vendor offers their own closed software solutions
- Customer has to buy multiple software (in total ~100k USD for this lab)
- Customer has to train staff in numerous software

MS: mass spectrometry, **LC**: liquid chromatography, **GC**: gas chromatography, **QTOF**: quadrupole time-of-flight

Our solution

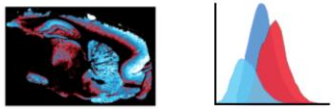


One software for:

- All data types
- All major vendor data formats (Thermo, Bruker, Waters, Agilent, SCiEX, Shimadzu)
- Same easy-to-use user interface for all data
- Scalable and efficient

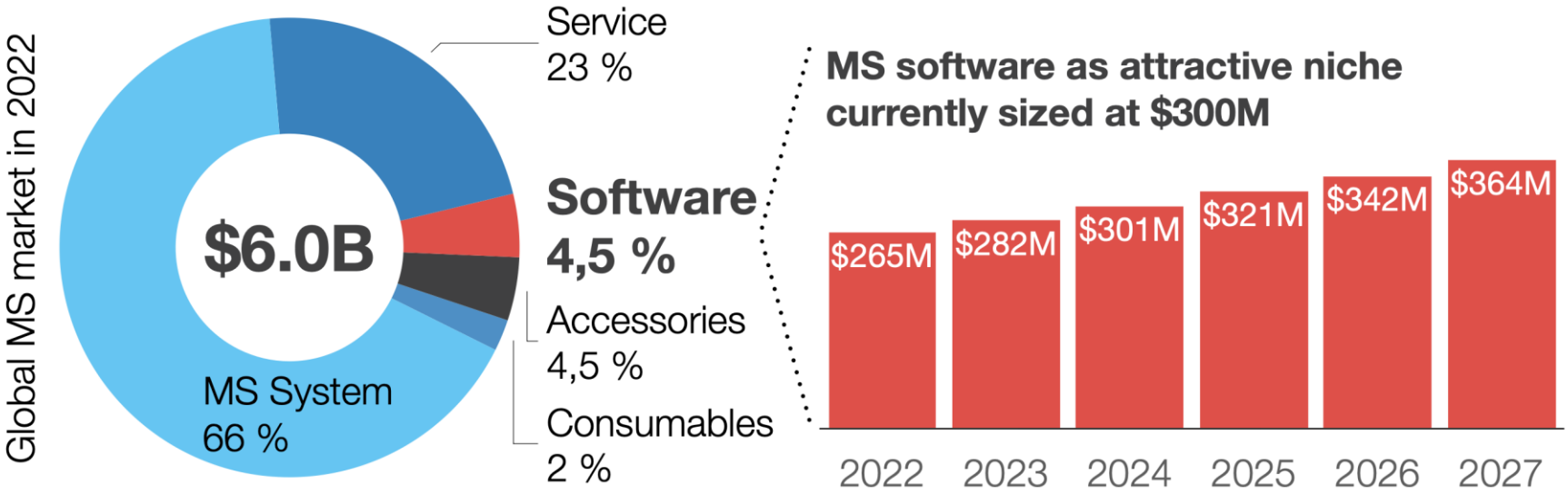
Reduce costs

Reduce training

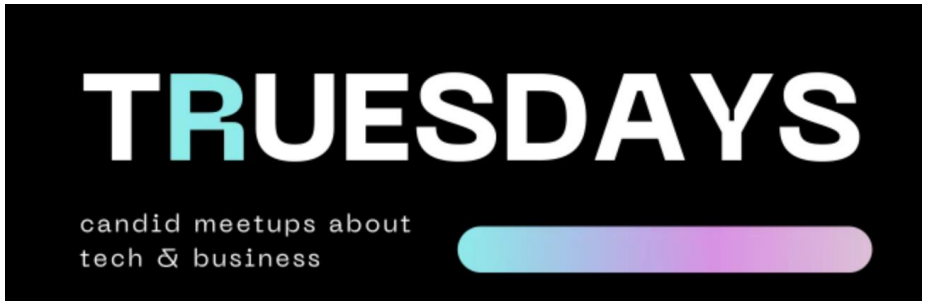


Compare and link modalities

How does the MS software market look like?



What was helpful for us



Our plan and roadmap for investors

June 2022
Release
MZmine 3


Correspondence | Published: 01 March 2023
Integrative analysis of multimodal mass spectrometry data in MZmine 3
Robin Schmid, Steffen Heuckeroth, Anupar Korf, Aleksandr Smirnov, Owen Myers, Thomas S. Dorrestein, Roman Bushuiev, Kevin J. Murray, Nils Hoffmann, Mingxun Lu, Abinesh Sarvepalli, Zheng Zhang, Markus Fleischauer, Kai Dührkop, Mark Wesner, Shawn J. Hoogstra, Edward Rudt, Olena Mokshyna, Corinna Brungs, Kirill Ponomarov, Lana Mutabdžija, Tito Damiani, Chris J. Pudney, Mark Earll, ... Tomáš Pluskal
Nature Biotechnology (2023) | Cite this article

March 2023
Publication of MZmine 3 in Nature Biotechnology

January 2024
Startup MZmine GmbH

April 2024
1. Annual MZmine Meeting at IOCB Prague

Release
MZmine PRO

April 2025
2. Annual MZmine Meeting at IOCB Prague

Release
MZmine ECOSYSTEM

GINKGO BIOWORKS
oloBion
LifeMine
edelris

December 2024
Reach 10 to 50 sold licenses in first year

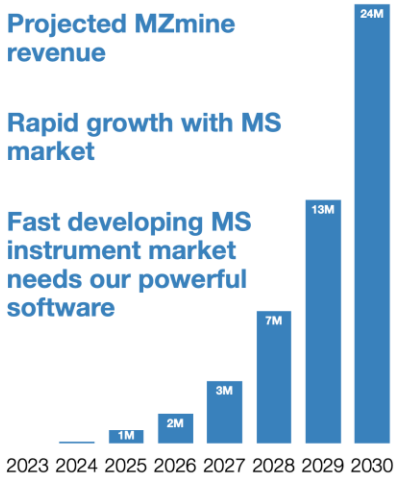
December 2026
Grow business to 100+ sold licenses

December 2029
Grow business to 1000+ sold licenses

Projected MZmine revenue

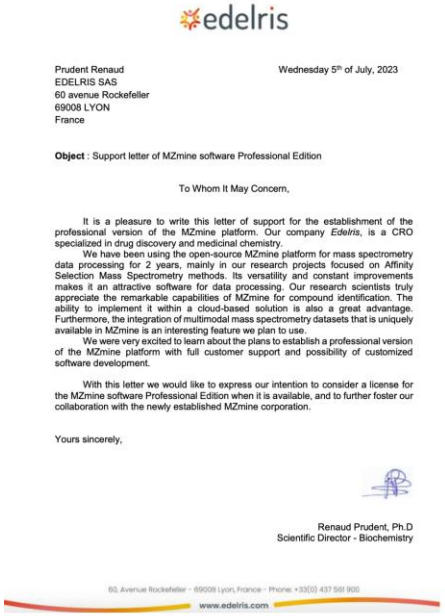
Rapid growth with MS market

Fast developing MS instrument market needs our powerful software



1.5M EUR investment to fund development of enterprise software and execute marketing strategy.

Letters of intent



edelris

Prudent Renaud
EDELRIS SAS
60 avenue Rockefeller
69008 LYON
France

Wednesday 5th of July, 2023

Object : Support letter of MZmine software Professional Edition

To Whom It May Concern,

It is a pleasure to write this letter of support for the establishment of the professional version of the MZmine platform. Our company *Edelris*, is a CRO specialized in drug discovery and medicinal chemistry.

We have been using the open-source MZmine platform for mass spectrometry data processing for 2 years, mainly in our research projects focused on Affinity Selection Mass Spectrometry methods. Its versatility and constant improvements makes it an attractive software for data processing. Our research scientists truly appreciate the remarkable capabilities of MZmine for compound identification. The ability to implement it within a cloud-based solution is also a great advantage. Furthermore, the integration of multimodal mass spectrometry datasets that is uniquely available in MZmine is an interesting feature we plan to use.

We were very excited to learn about the plans to establish a professional version of the MZmine platform with full customer support and possibility of customized software development.

With this letter we would like to express our intention to consider a license for the MZmine software Professional Edition when it is available, and to further foster our collaboration with the newly established MZmine corporation.

Yours sincerely,

Renaud Prudent, Ph.D
Scientific Director - Biochemistry

60, Avenue Rockefeller - 69008 Lyon, France - Phone: +33(0) 437 581 900
www.edelris.com

DocuSign Envelope ID: 6D6DE1AA-CB99-4D32-BFDD-E679F40B40AB

GINKGO BIOWORKS

August 08, 2023

Tomáš Pluskal, IOCB Prague, Group Leader
Ústav Organické Chemie a Biochemie, Flemingovo nám. 2, 160 00 Praha 6, Czech Republic
tomas.pluskal@uochb.cas.cz

Dear Dr. Pluskal,

We are writing to express our deep appreciation for the MZmine platform, our excitement about the upcoming release of MZminePRO, and to express our support of your pursuit of funding for this effort. As a leading biotechnology company in Boston, Ginkgo Bioworks is committed to utilizing synthetic biology to engineer microorganisms for various industries, collaborating with sectors such as agriculture, pharmaceuticals, and consumer goods.

In our metabolomics research, we rely on advanced GC-MS and LC-MS technologies to uncover the secrets of small molecules in biological systems, providing crucial insights into metabolic pathways and biomarkers. To support our metabolomics workflows, we utilize a variety of open source, in-house, and licensed software to cater to our specific project goals.

We have found MZmine to be a critical tool in our data processing, improving our research processes and aiding us in accomplishing our project goals. Therefore, we are eagerly looking forward to the release of MZminePRO, which we believe will provide us with even more advanced tools and capabilities to further enhance our work.

We would like to express our intention to acquire an MZminePRO license upon its release. We firmly believe that integrating MZminePRO into our research processes may significantly contribute to our ongoing metabolomics studies. We anticipate that MZminePRO may open up new opportunities for collaboration and exploration with Ginkgo Bioworks.

We genuinely appreciate your commitment to advancing data analysis in metabolomics and lipidomics through the MZmine project. We look forward to the possibilities that MZminePRO will bring and the potential for further collaboration with Ginkgo Bioworks in the future.

Thank you for your dedication and contributions to the field of metabolomics. We wish you every success with the MZmine project.

Sincerely,

Patrick Boyle

Patrick Boyle
Head of Codebase

27 Drydock Avenue, 8th Floor
Boston, MA 02210 USA
877.HACK.DNA or 877.422.5362
www.ginkgobioworks.com

Metable LLC
1919-1 Tancha, Onna
Okinawa 904-0412
Japan

Subject: Letter of Support and Intent to Purchase Professional Edition of MZmine

Dear Dr. Tomáš Pluskal,

I hope this letter finds you in good health and high spirits. On behalf of Metable LLC, a metabolomics research startup company based in Japan, I am writing to express our heartfelt appreciation and satisfaction with the MZmine platform. Over the last 10 years, I have personally been using MZmine for processing, analysis, and visualization of mass spectrometry data obtained from our metabolomics research projects. In our study investigating changes in blood metabolites associated with human aging and age-related diseases, the software's robust functionality and user-friendly interface have been instrumental in streamlining our data analysis workflows and expediting our research endeavors.

MZmine's powerful data preprocessing capabilities have significantly improved the accuracy and reliability of our peak detection and alignment procedures, allowing us to confidently identify and annotate metabolites of interest. The platform's comprehensive visualization tools have facilitated a deeper understanding of complex mass spectra, enabling our team to extract crucial insights from our experimental data effortlessly.

Metable firmly believes in supporting and collaborating with innovative solutions that contribute to the advancement of scientific research. We are excited to learn about the forthcoming launch of a professional edition of MZmine. The features and enhancements promised in this new edition align perfectly with our evolving research requirements. Therefore, it is our sincere intention to purchase a license of the professional edition as soon as it becomes available on the market.

We commend the dedication and hard work of your team in continuously refining and expanding the capabilities of MZmine. Your commitment to open-source principles and community engagement has been truly commendable and has played a pivotal role in driving advancements in the field of metabolomics.

In conclusion, we extend our gratitude to the entire MZmine team for creating a remarkable platform that has positively impacted our research outcomes. Your efforts are invaluable in empowering researchers worldwide to push the boundaries of metabolomics research. We eagerly await the launch of the professional edition of MZmine and look forward to further collaboration in the future.

Yours sincerely,

Takayuki Teruya, Ph.D.
CEO
Metable LLC

oloBion

Barcelona 27/06/2023

Dear Dr. Tomáš Pluskal,

As CEO of oloBion, I am reaching out to both express our organization's deep appreciation for the MZmine platform and our excitement for the upcoming MZminePRO. Our projects in metabolomics and lipidomics have been greatly enriched by MZmine's robust and flexible feature set, enabling us to achieve our objectives with an efficiency and precision that we had not previously thought possible.

The MZmine platform has already proven to be an indispensable tool in our data processing, facilitating our work and aiding in the accomplishment of our project goals. Our experience with it has not only been positive, but transformative for our research processes.

In our continual pursuit of innovative solutions to enhance our research and development, we were thrilled to learn about your plans to launch a commercial version, MZminePRO. Given our experiences with the current platform, we anticipate that MZminePRO could provide us with even more sophisticated tools, support and capabilities that could dramatically bolster our work.

We are particularly interested in the development of a custom application for ion mobility data from our Agilent 6560 platform. This addition would provide enormous value to our team, as it would significantly enhance our compound identification capabilities.

With this in mind, I am pleased to express oloBion's intention to acquire an MZmine PRO license upon its release. While this letter is a statement of support, it underscores our genuine interest in the platform and our belief in its potential to become an even more integral part of our research processes.

We eagerly anticipate the possibilities MZminePRO will bring and look forward to potentially deepening our collaboration with you in the future.

Thank you for your dedication to improving data analysis in the field of metabolomics and lipidomics. We wish you every success with the MZmine project.

Best regards,

Paolo Bonini, CEO, oloBion

oloBion SLU | Av. Dr. Marañón 8 | c/o Parc Científic de Barcelona (PCB) | 08028 Barcelona
NIF: ES B01593243 | Tel. +34 934 597 786 | info@olobion.ai

Testimonials

Dr. Sebastian Hagenhoff, Dow Chemicals

"During my PhD in Analytical Chemistry I have developed GC-MS and LC-MS methods to analyse a wide variety of environmentally relevant compounds.

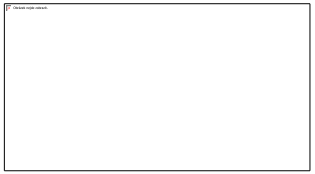
*The enormous **flexibility** of MZmine has allowed me to handle MS data from a **wide variety of analysis techniques** and application areas in **just a single software**, resulting in great time savings.*

*In my current position as Associate Research Scientist I am handling multiple MS Systems from different vendors. Being able to use the same software for all my data analysis has great impact on my daily productivity. In my department, MZmine has proven to be the tool to use when **vendor software fails**."*

2023 – the year of VC investor hunting

I&I BIO

KAYA



Tensor.Ventures

RSJ

High-Tech Gründerfonds

PRESTO VENTURES

DEPO VENTURES

PACE VENTURES

PURPLE VENTURES

impulseventures

ZAKA


P
Prague.bio Conference 2023
PRAGUE BIO
CERTIFICATE
OF EXCELLENCE
1st place
Prague.bio
Conference
2023
This Certificate is proudly awarded to
MZmine
for the most impressive presentation and pitching techniqu
at Prague.bio Conference.
In Prague,
September 26th,
2023
Jana Žaludová
CEO Prague.bio
MORE VIDEOS

Summary of 2023

- Lots of Zoom calls
- Lots of excitement from investors
- Lots of lessons learned
- 0$ investments secured

A revelation – we want to start a company, not a startup

Startup

- Pressure for fast growth, reinvestment in all profits
- Expectation to multiply the initial investment 100-fold in a few years
- Expectation to exit (sell the company) in 5-8 years

Company

- A stable and sustainable business
- Can be a long-term job

mzio

Accelerate Scientific Discoveries

Established Jan 2024 in Bremen, Germany

mzio

CEO, sales, business development, finance, marketing

Dr. Ansgar Korf

Industry

Senior Manager Software R&D, Bruker Daltonics, Germany
Global Product Manager, Bruker Daltonics, Germany
Software Engineer, Bruker Daltonics, Germany

Education

Ph.D. Analytical Chemistry, University of Münster, Germany
M.Sc. Business Chemistry, University of Münster, Germany
B.Sc. Food Chemistry, University of Münster, Germany

1.0 FTE

Product management and software development

Dr. Robin Schmid

Academia

Postdoctoral researcher, IOCB Prague, Czech Republic
Postdoctoral researcher, University of California San Diego, USA

Education

Ph.D. Analytical Chemistry, University of Münster, Germany
M.Sc. Food Chemistry, University of Münster, Germany
B.Sc. Food Chemistry, University of Münster, Germany

1.0 FTE

R&D and software development

Steffen Heuckeroth

Education

Ph.D. candidate Analytical Chemistry,
University of Münster, Germany
M.Sc. Chemistry, University of Münster, Germany
B.Sc. Chemistry, University of Münster, Germany

1.0 FTE

Scientific advisor

Dr. Tomáš Pluskal

Academia

Group Leader, IOCB Prague, Czechia
Helen Hay Whitney Postdoctoral Fellow,
Whitehead Institute for Biomedical Research, MA USA

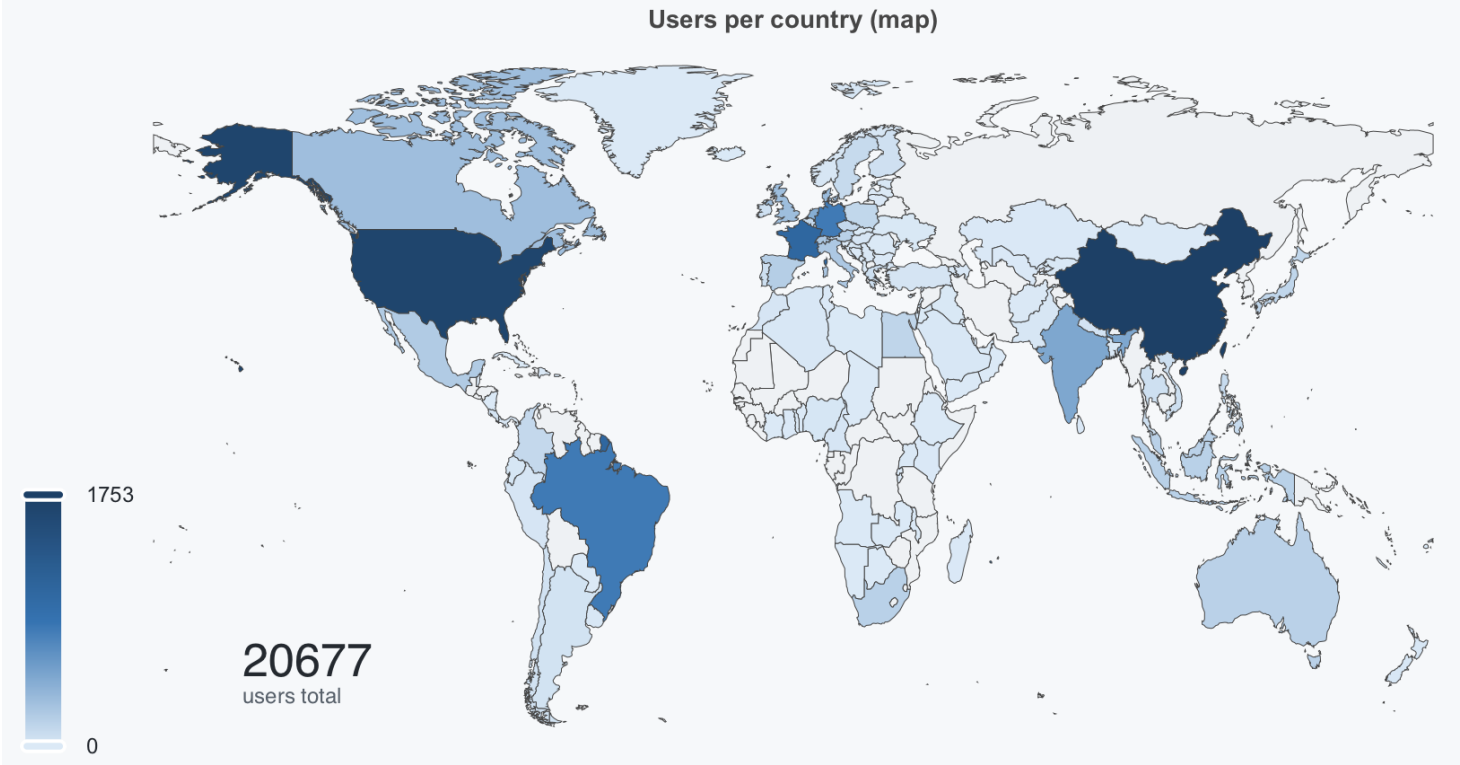
Industry

Scientific Consultant, Ginkgo Bioworks, MA USA
Scientific Consultant, WarpDriveBio, MA USA

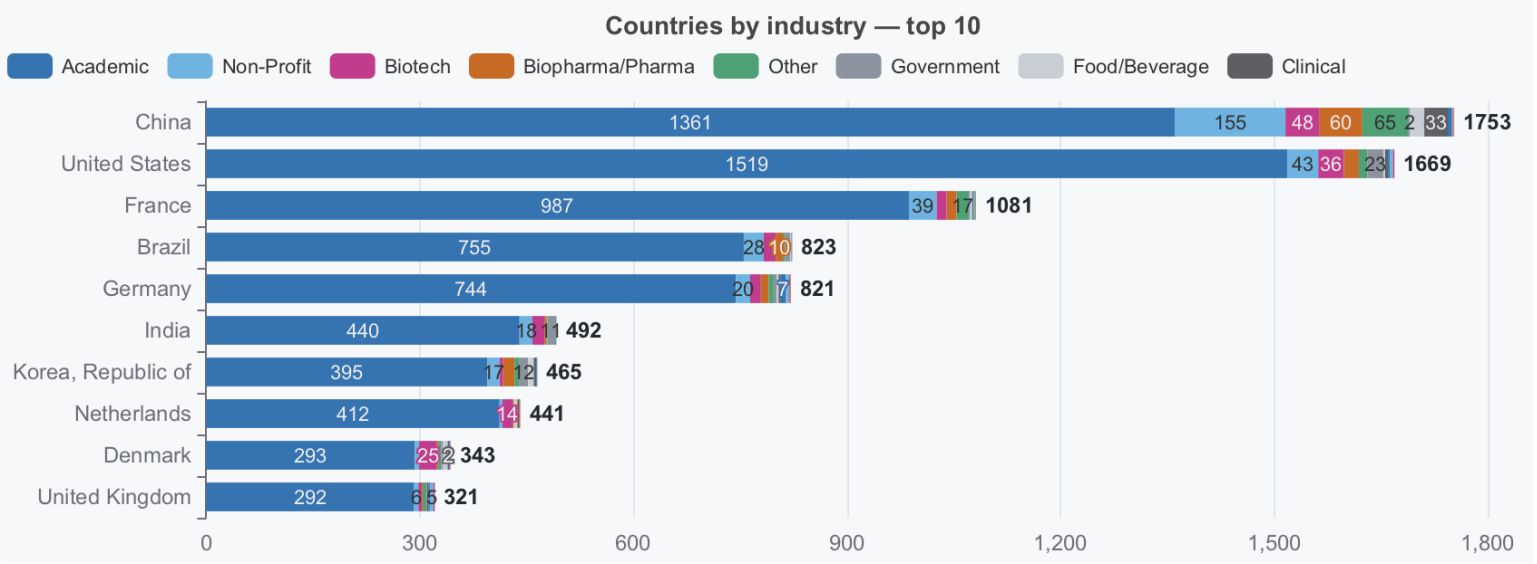
Education

Ph.D. Okinawa Institute of Science and Technology, Japan
M.Sc. Charles University in Prague, Czechia

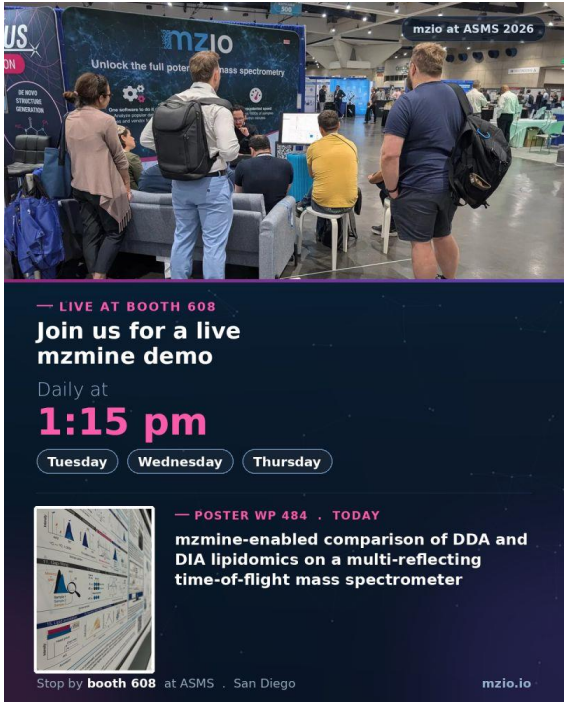
mzmine user statistics (Aug 2026)



mzmine user statistics (Aug 2026)



mzio presence at scientific conferences



Thank you!

mzio

mzmine

Ansgar Korf
Robin Schmid
Steffen Heuckeroth
Tomáš Pluskal

open source

GitHub

mzmine community

IOCB PRAGUE
Institute of Organic Chemistry and Biochemistry
Czech Academy of Sciences

UC San Diego

FRIEDRICH-SCHILLER-UNIVERSITÄT JENA

Whitehead Institute

WESTLAKE UNIVERSITY

OIST

VTT

steno diabetes center

Massachusetts Institute of Technology

UNC CHARLOTTE

UNIVERSITY OF MINNESOTA

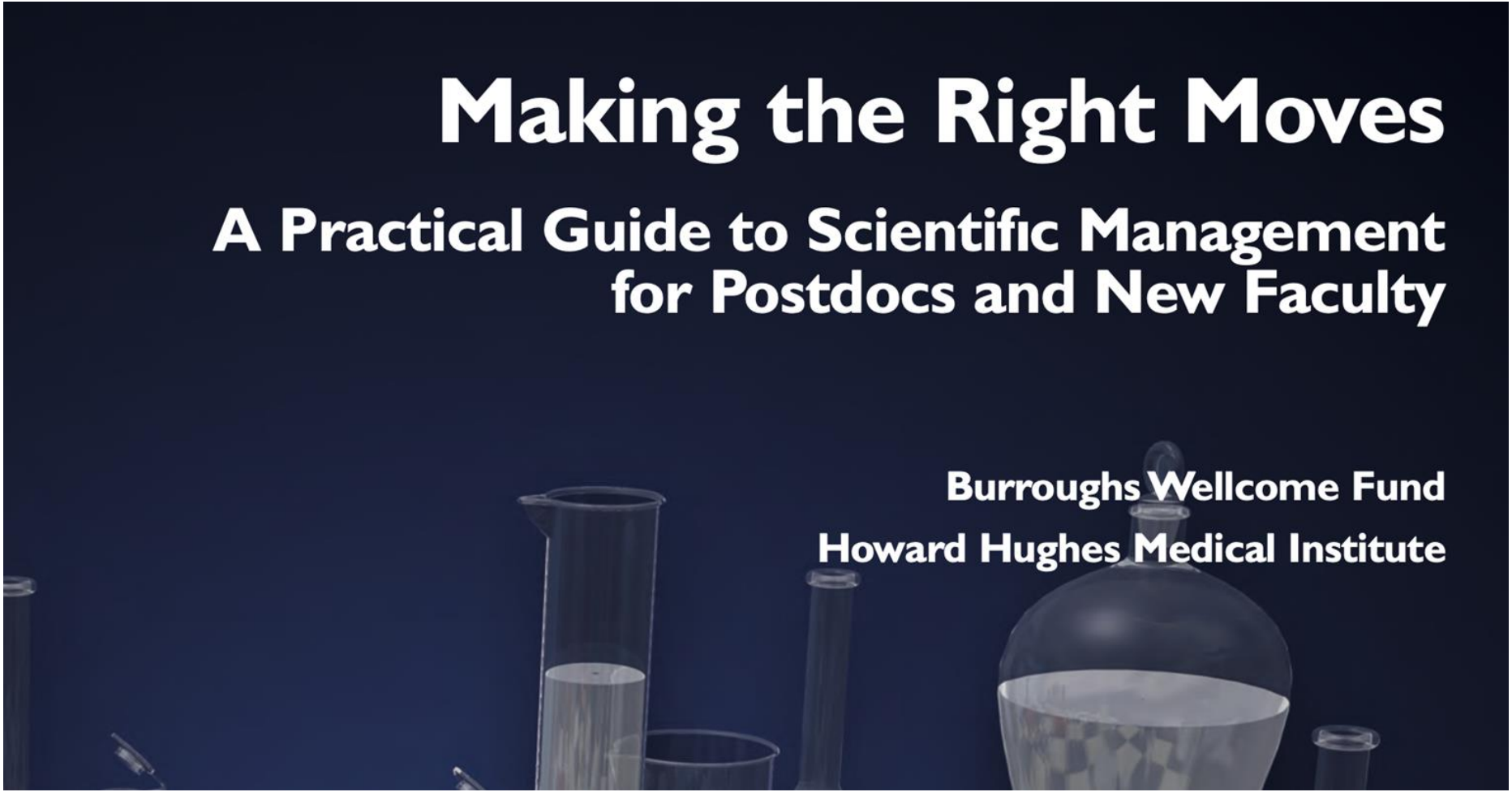
Google

GAČR
CZECH SCIENCE FOUNDATION

i&i Prague
Bio-Innovation Center

And what are YOUR plans after your PhD?

Do think about it!



https://www.bwfund.org/career-tool/making-the-right-moves/

Who is a postdoc?

- ✓ Someone who recently obtained a PhD
  (most institutions have a **post-PhD-years cap**)

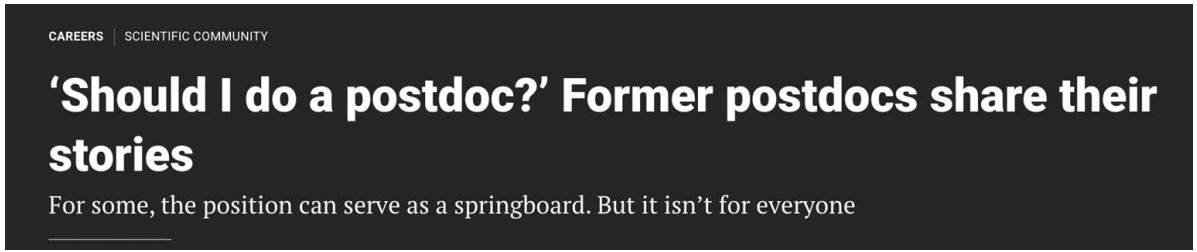
- ✓ Someone who is still in research training
  (a postdoc is **NOT** a job, it is temporary and often underpaid)

Why you should do a postdoc?

✓ Because you want to have an academic research career.

Occasionally also other reasons, mostly wrong:

- Add additional expertise to your skillset
- Try living abroad
- Strengthen your CV
- Have a better salary (compared to your PhD stipend)
- …



https://www.science.org/content/article/should-i-do-postdoc-former-postdocs-share-their-stories

Why you should not do a postdoc

CAREERS | CAREER FABLES

Three bad reasons to do a postdoc

3 FEB 2020 • BY KARIN BODEWITS

1. Your Ph.D. adviser tells you it is a good idea.
2. You think it will increase your market value.
3. A postdoc is the easiest job to get.

CAREERS | CAREER CHOICES

The price of doing a postdoc

10 JAN 2017 • BY DEVIN POWELL

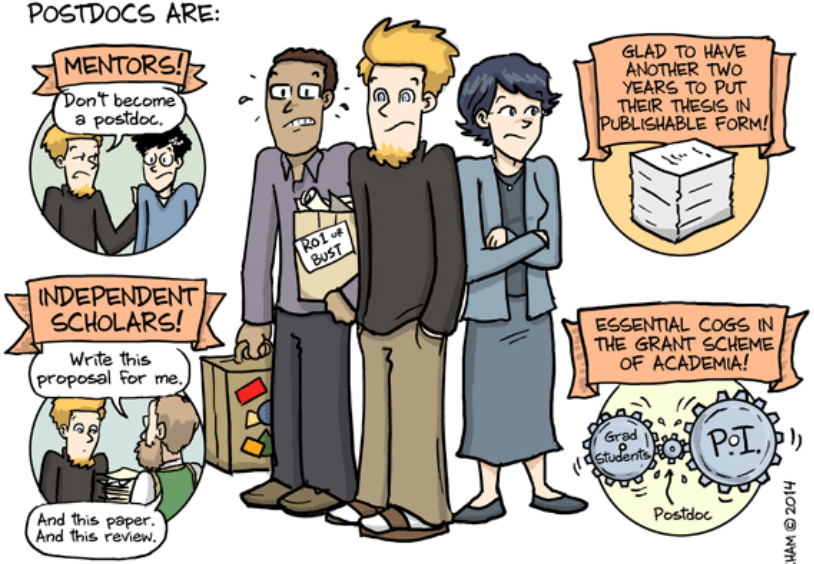
For the overwhelming majority of Ph.D. holders who do not become tenured professors, spending time as a postdoc comes at a hefty price. Compared with peers who started working outside academia immediately after earning their degrees, ex-postdocs make lower wages well into their careers, according to a study published today in *Nature Biotechnology*. On average, they give up about one-fifth of their earning potential in the first 15 years after finishing their doctorates—which, for those who end up in industry, amounts to $239,970.

IT'S NATIONAL

POSTDOC APPRECIATION WEEK!

Celebrate
The Middleman of Academia™

POSTDOCS ARE:



NEXT WEEK: BACK TO BEING UNDERAPPRECIATED!

WWW.PHDCOMICS.COM

How to do a successful postdoc?

- Plan for an **academic research career**
- Have a **stellar CV** (+well formatted)
- **Move** to a different country (mobility is a must)
- Choose your PI and research institution wisely (most Nobel prize winners trained in previous Nobel prize winning labs)
- Change your research domain (more different from your PhD is better)
- Get a **fellowship** (demonstrated ability to secure funding is essential for your career development)

Postdoctoral fellowships

MSCA, HFSP, EMBO, FEBS, Experientia, …

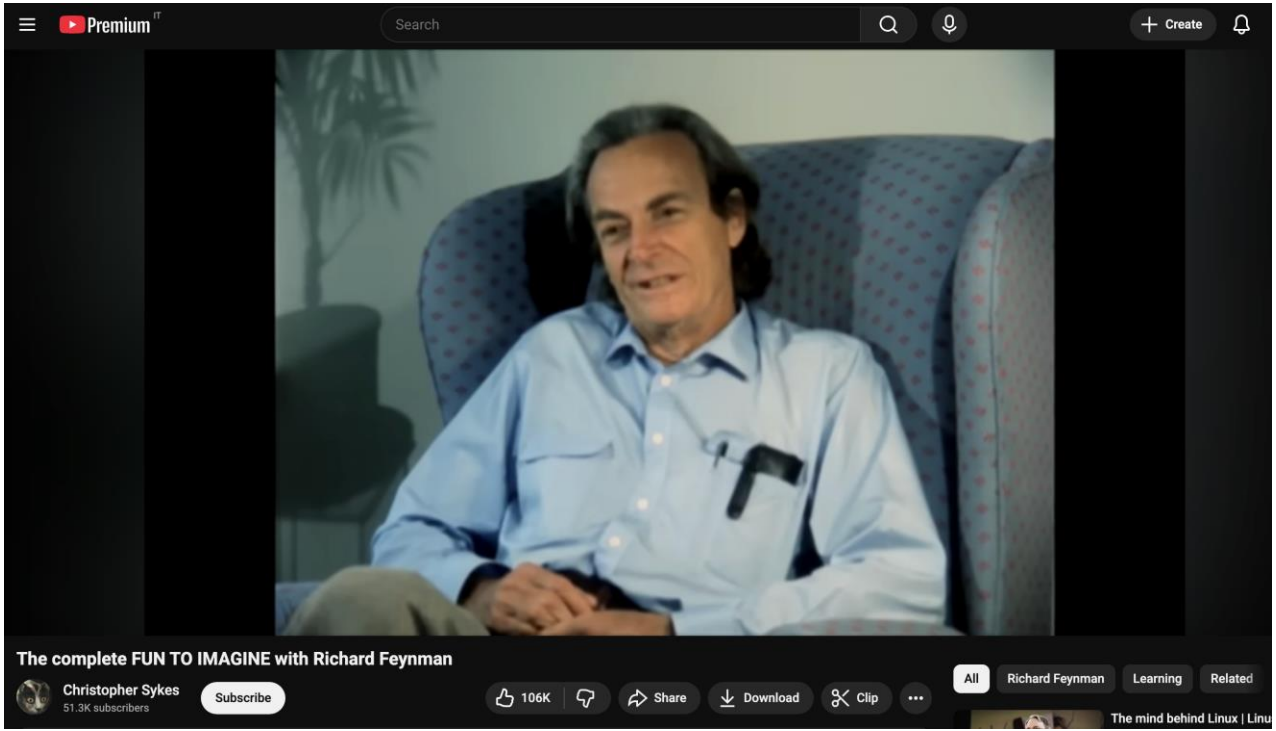
https://www.hfsp.org/sites/default/files/Communications/PRIMER.pdf

“Your success in life will be determined largely by your ability to ***speak***, your ability to ***write***, and the ***quality of your ideas***… in that order.”

— *Patrick Winston*

“Precise language is not the problem. **Clear** language is the problem.”

— Richard Feynman



Who is going to review your fellowship proposal?

Let’s pick a random example…

Reviewer

Reviewer

Write their own grants

Reviewer

Write their own grants

Reviewer

Write their own grants

Reviewer

Write their own grants

Reviewer

Your proposal

Write their own grants

Reviewer

Guess what they care about the least?

Your proposal

So where do reviewers find the time to read your fellowship proposal?

They don’t


gettyimages
Credit: fotostorm
1960329077

The ultimate tip

Be lucky

Luck is a skill

IOCB PRAGUE
Institute of Organic Chemistry and Biochemistry
Czech Academy of Sciences

Pluskal Group
IOCB Prague

www.pluskal-lab.org

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