

Which Organism Can be the New Rising Star?

- Selection Support by Informatic and Metabolomic Tools -

Prof. Dr. Ludger Wessjohann

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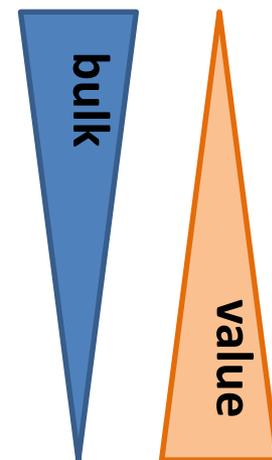
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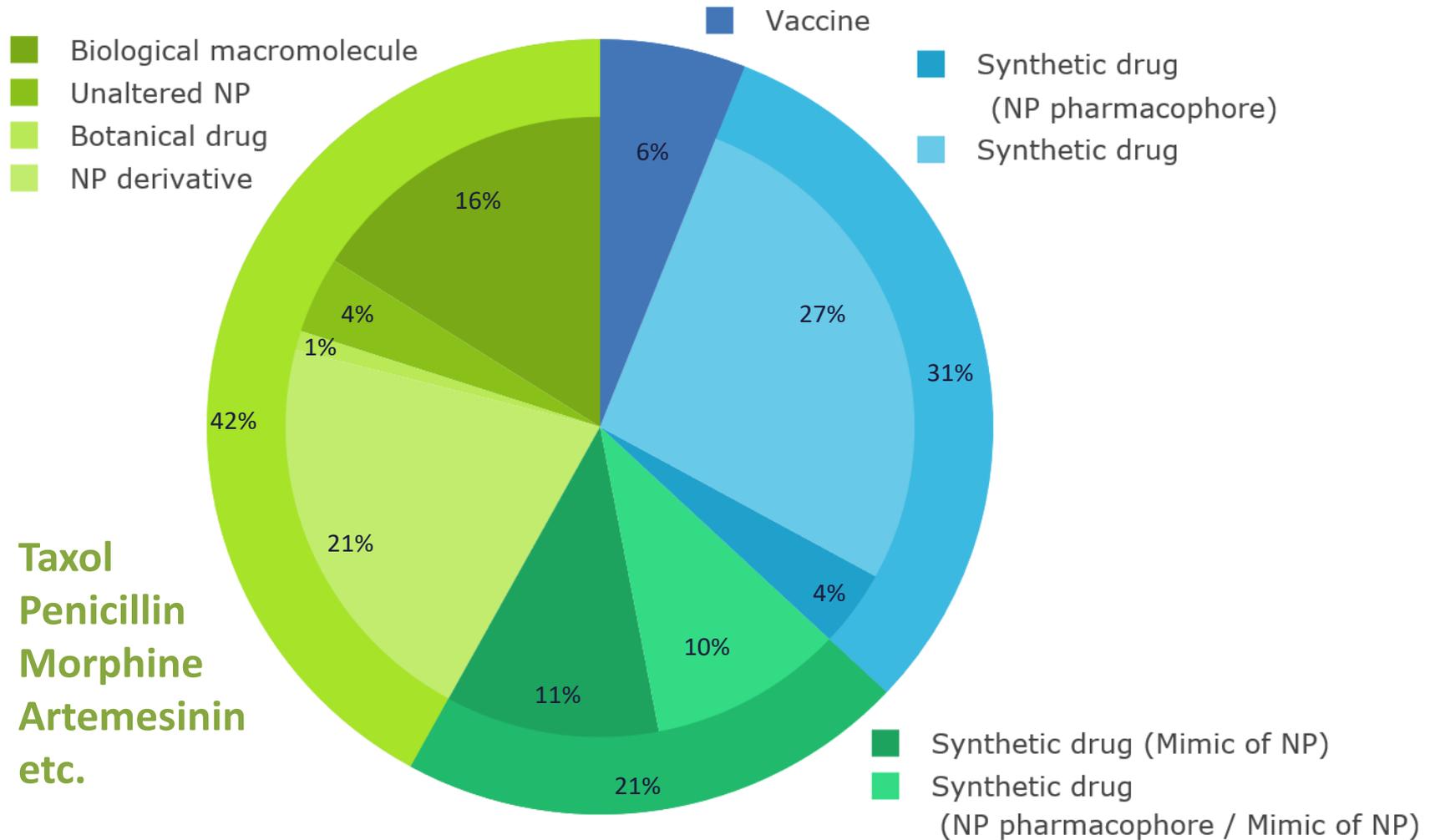
Why are
Plants & Chemistry
Relevant
for Bioeconomy,
Biodiversity and
the Earth System?

*The commercial and ecological
value of an organism is mostly
defined by its chemical phenotype*

Examples:

- Biopolymers like lignin and cellulose for structure
- Starch and oil for food, feed and industrial use
- Proteins and vitamins for nutrition
- Colors (look, beauty), flavor & fragrance (smell/taste)
- Medicinal constituents





Adapted from Newman *et al.*, *J Nat prod*, 2016, 79, 629-661.

starting point: selection of the natural source

classical way

selection based on / focused on

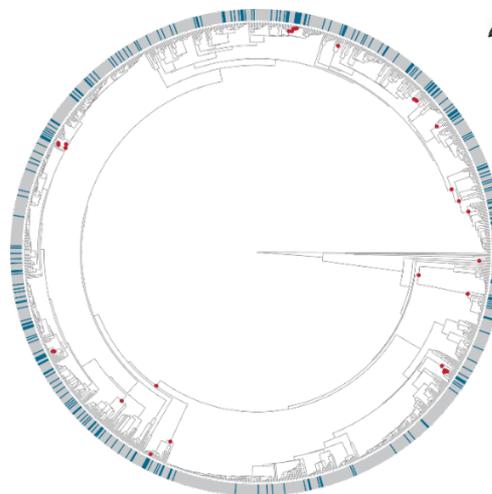
- accessibility / personal preference
- chemical compounds
- natural source families / genera
- known activities (traditional medicine)



<https://www.nabu.de/tiere-und-pflanzen/aktionen-und-projekte/vogel-des-jahres/2012-dohle/14188.html>

our approach

selection based on extensive overview of natural sources, their natural products and activities



<https://www.nabu.de/tiere-und-pflanzen/aktionen-und-projekte/vogel-des-jahres/2012-dohle/14199.html>

How can we achieve a global overview?



7

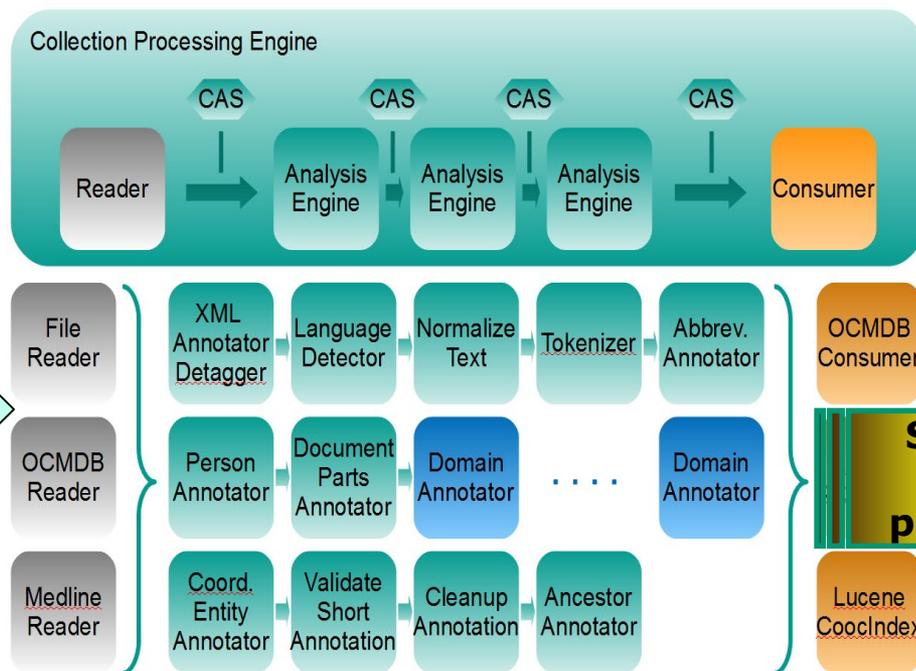
- **It is an illusion to be able to preserve all organisms and their chemistry** (i.e. the biological & chemical diversity).
[Music analog: You can not keep all composers/musicians alive forever]
- **We can preserve the important information instead:**
sequences & **chemical structures** [the music and recordings]
- **How can we have an unbiased look from a global perspective?**
[Avoid biases: classical European or modern Angloamerican composers/musicians]
- Limited resources: **Where do we have to look for maximum effect?**
[how do we select the best composers/musicians worth of recording]
- Dwindling resources: **Where do we have to look before it is too late?**
[which relevant composer/musician dies next]

Do you think these questions are answered or can be answered currently?



Can
New Technologies
aid
Old Processes?

Smart Data from Big Data



OntoChem's OCMiner/SkyWalker®

www.ontochem.com

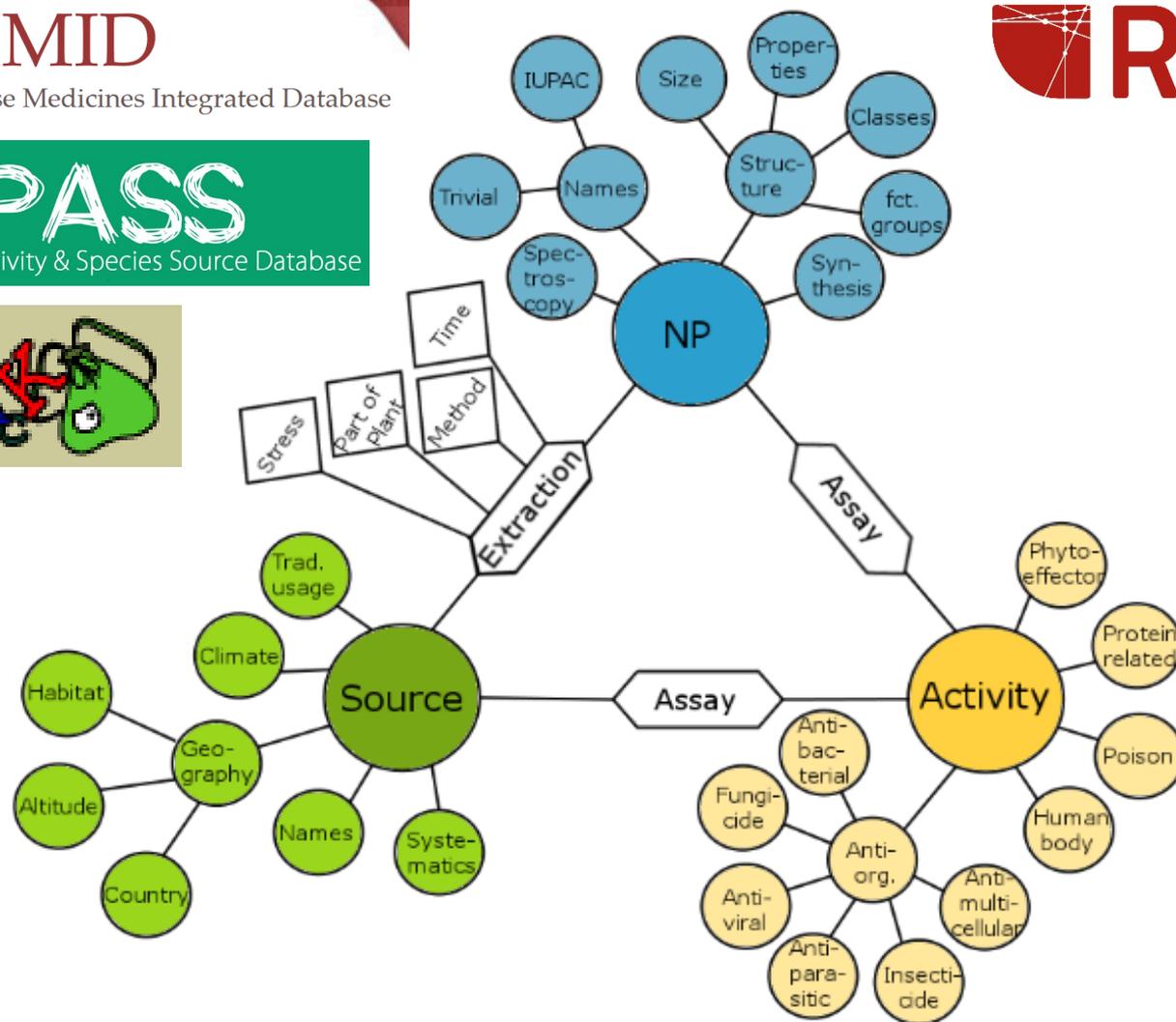
Not only a google for chemistry - better

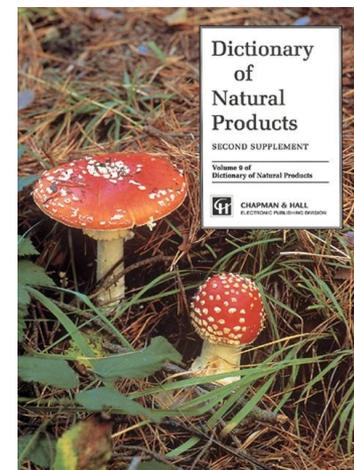
TCMID

Traditional Chinese Medicines Integrated Database

NPASS

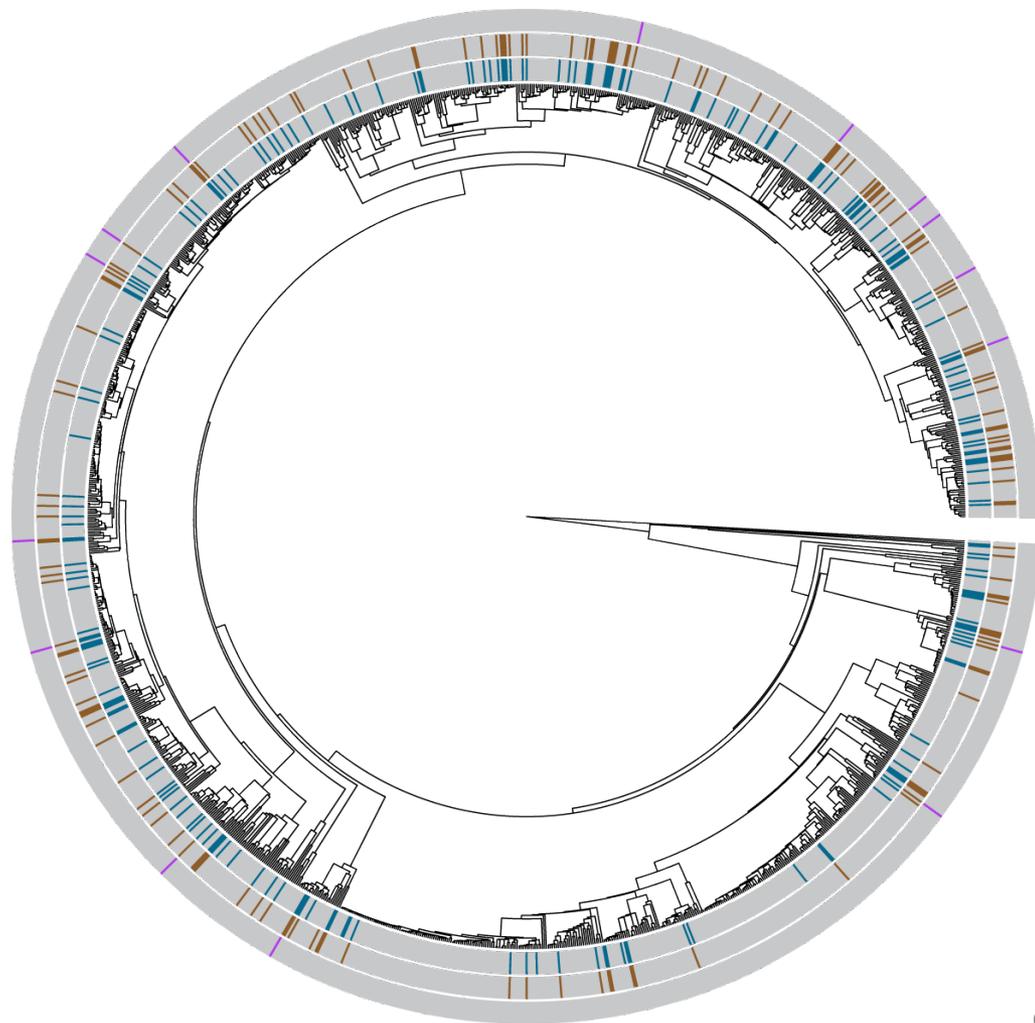
Natural Product Activity & Species Source Database





All
databases
are biased!!

Selected Bioactivities vs. Genus (example:Java)



Phylogeny: Flora of
Java (1396 genera
ca. 750'000 pubs.)

Reported NP Activities:

Anti-infective

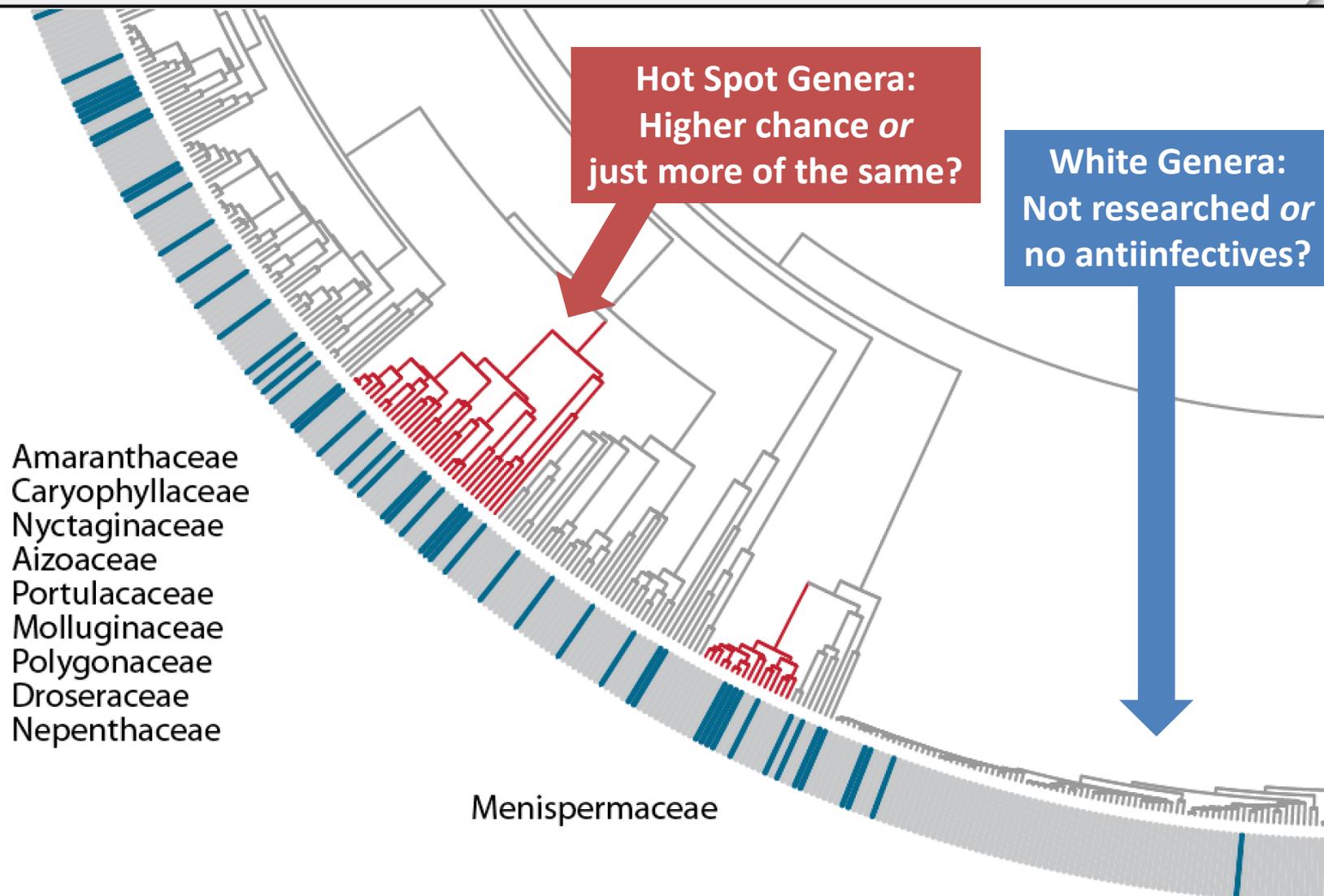
Cardiovascular

Anticancer

PNAS 2020

coop. A. Müllner-Riehl, J. Schnitzler – U. Leipzig

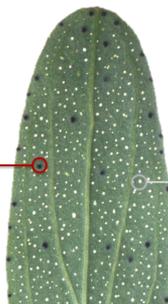
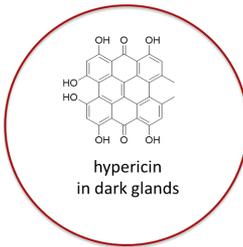
Antiinfectives vs. Genus (example:Java)



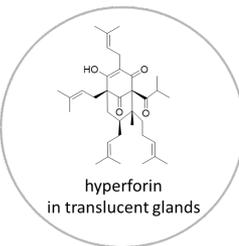
From Virtuality to Reality



naphthodianthrone



phloroglucinols



- 21 different *Hypericum* species
- cultivated in the greenhouses of IPK, IPB, BG Berlin
- comparison by metabolomic approaches



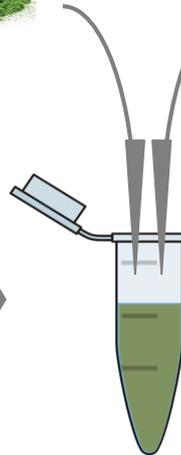
NMR metabolomics

Sample preparation

15



40 mg

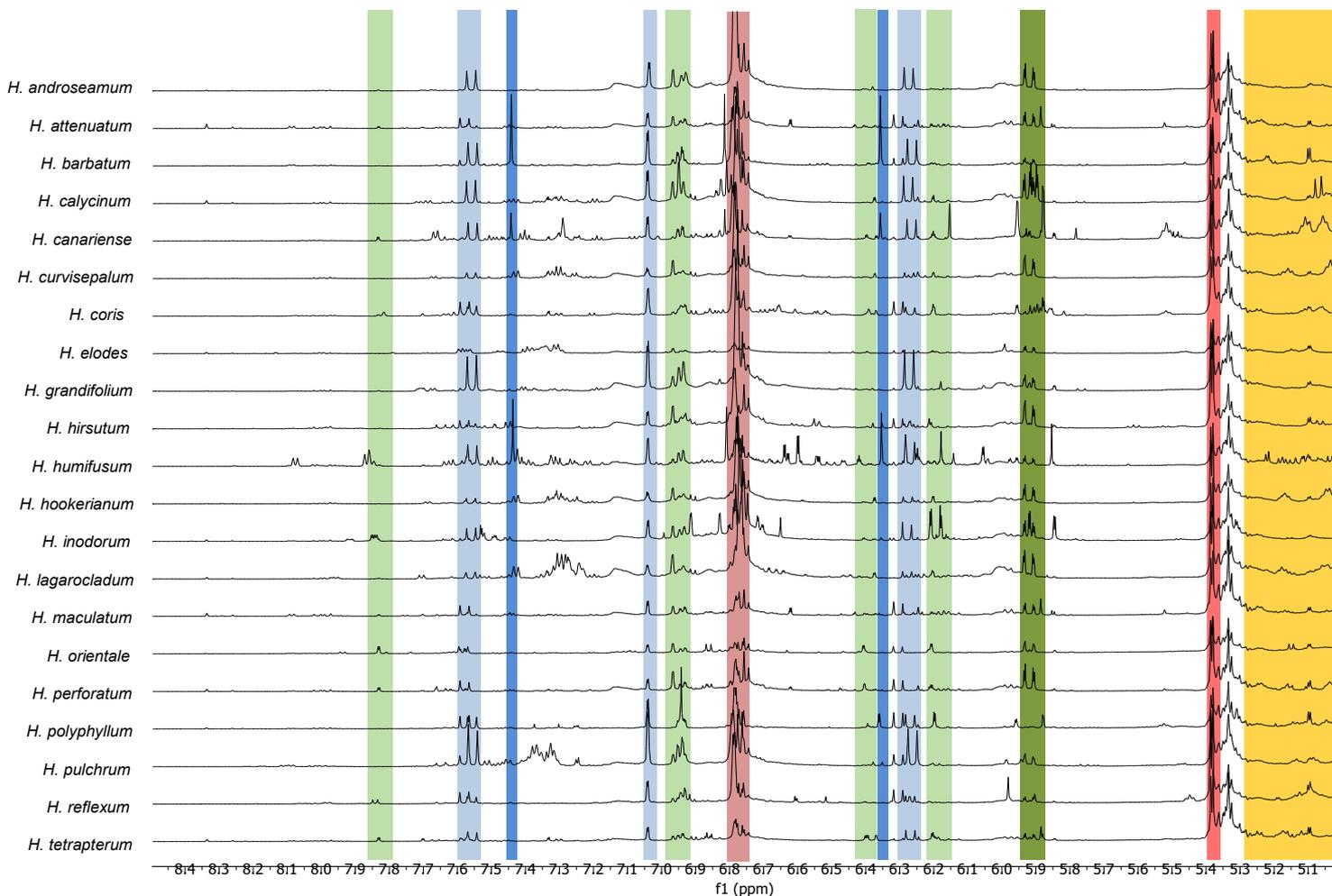


ultrasonication

CD₃OD
+HMDS



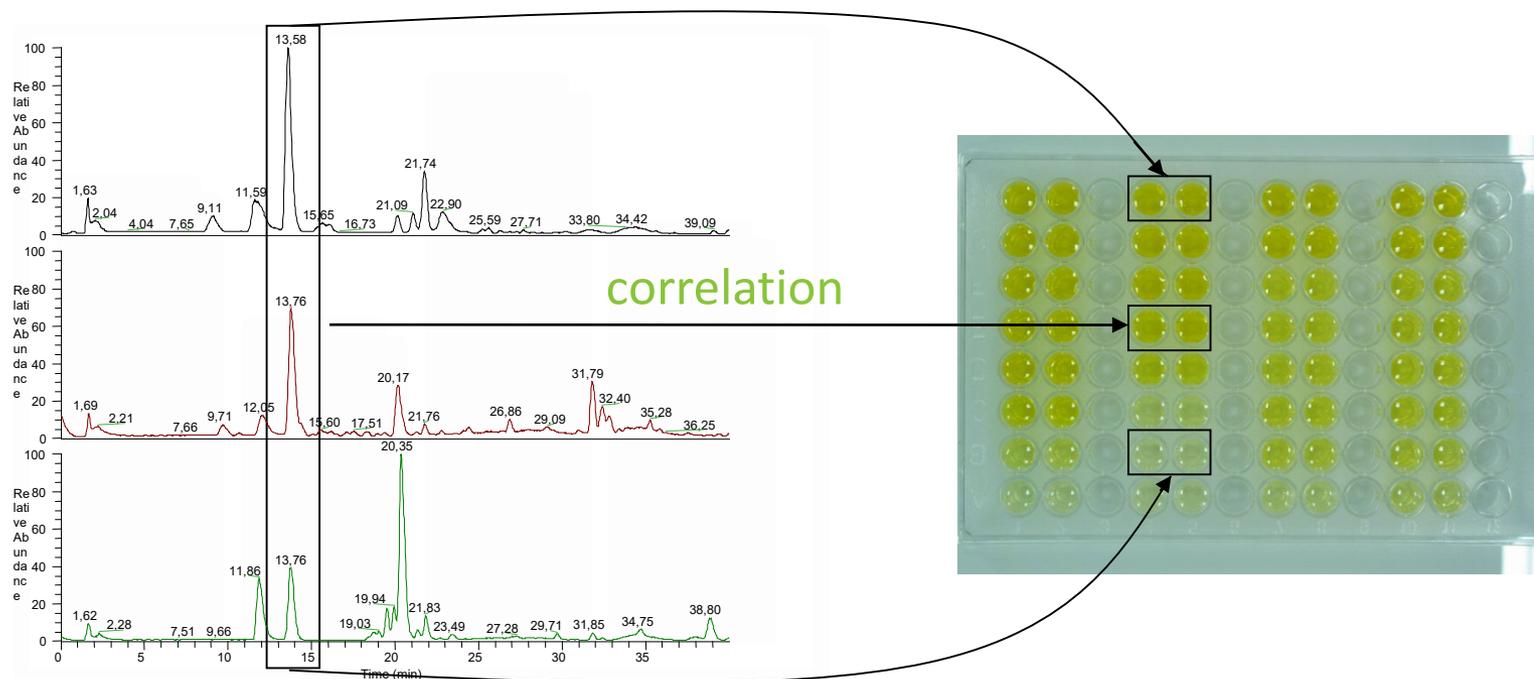
600 MHz



- quercetin derivatives
- chlorogenic acid
- mangiferin
- shikimic acid
- catechin / epicatechin
- sucrose
- polyprenylated
- phloroglucinols

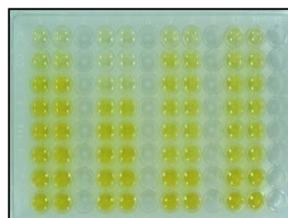
Discriminant metabolites from Principal Component Analysis are restricted to chemical shift > 5 ppm

- correlation of metabolic profiles (LC, MS etc.) and bioactivity
- identification of activity-relevant metabolites
- from complex mixtures: crude extracts, fractions, synthetic libraries

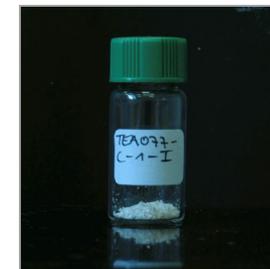


Herbal medicines/
Phytoextracts

Bioassay

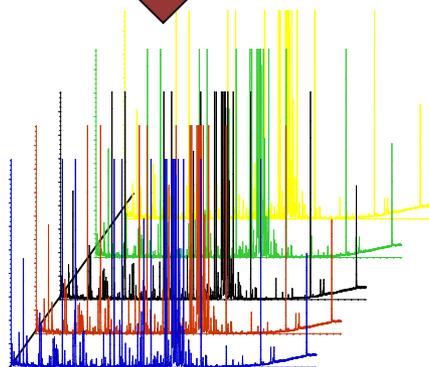
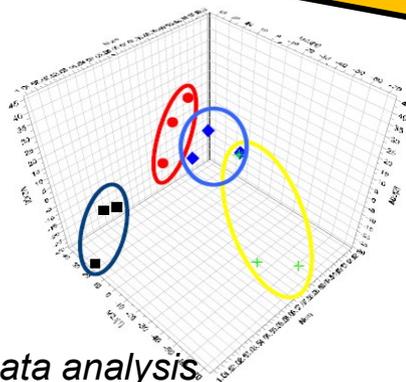


Correlation

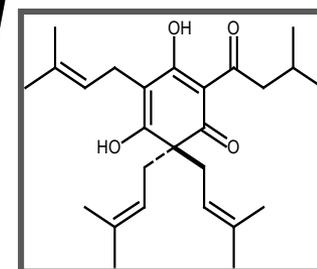


Isolation

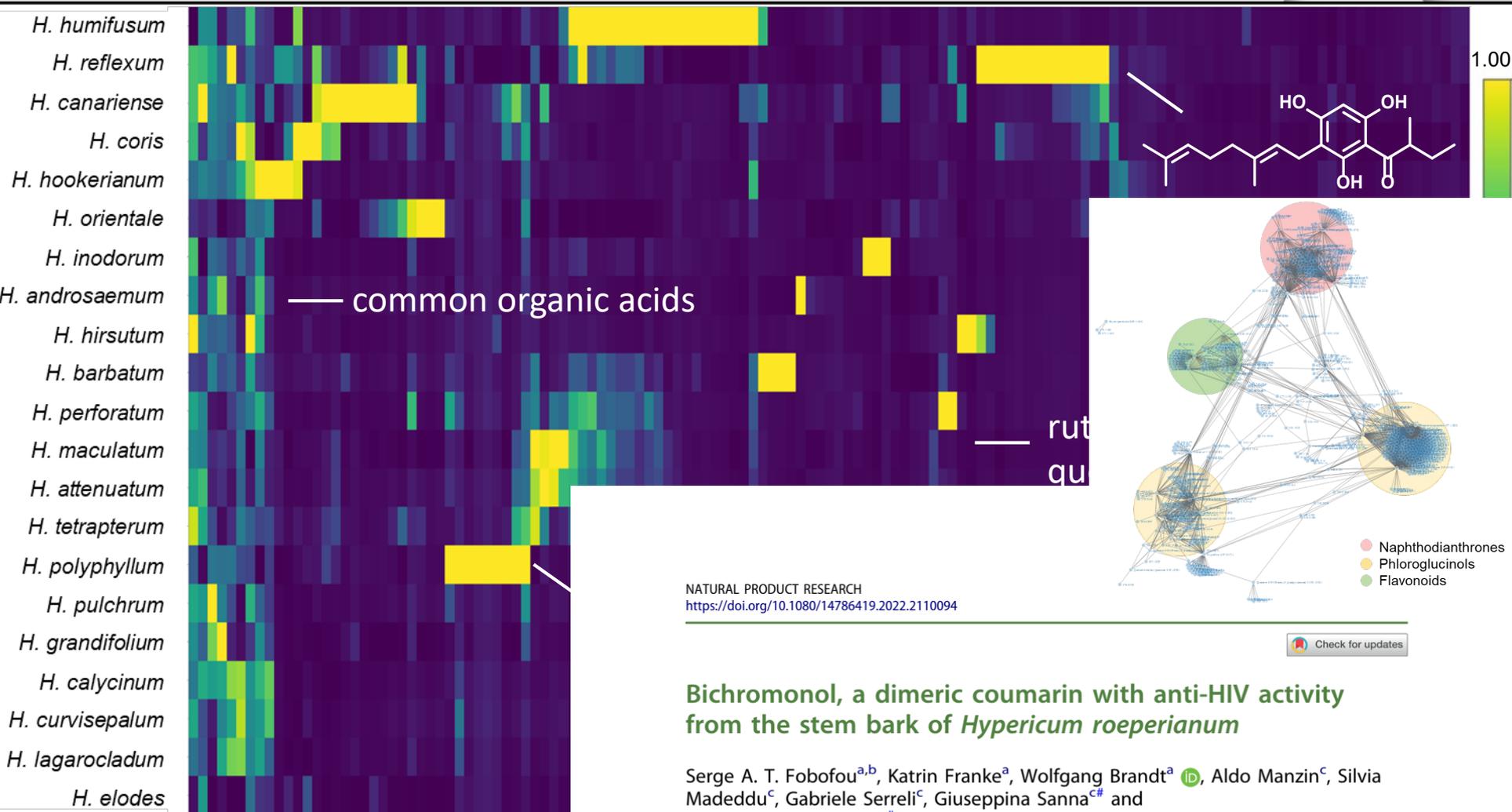
For film see:
<https://av.tib.eu/media/50351>

Metabolomic fingerprints
(LC-MS, LC-NMR or GC-MS)Data analysis
(PCA, HCA)

Target Finding:
 Proteomics
 ABPP etc.

Structure
elucidation

Metabolites Heatmap



Bichromonol, a dimeric coumarin with anti-HIV activity from the stem bark of *Hypericum roeperianum*

Serge A. T. Fobofou^{a,b}, Katrin Franke^a, Wolfgang Brandt^a , Aldo Manzin^c, Silvia Madeddu^c, Gabriele Serrelli^c, Giuseppina Sanna^{c#} and Ludger A. Wessjohann^{a#}

Do you remember some questions from the beginning?

- Limited resources: **Where do we have to look for maximum effect?**
[how do we select the best composers/musicians worth of recording]
- Dwindling resources: **Where do we have to look before it is too late?**
[which relevant composer/musician dies next]



What is the biggest inhibitor of efficient bilateral research?

Bureaucracy! (only then follows money, lack of experts)

- Most threatening for research: Negative impacts of inefficient CBD, Nagoya rules
- Currently: we cooperate only with countries who have very efficient access granting procedures, or which have not yet ratified the rules.
- Biodiversity loss is much faster than bureaucracy and research!
Thus generating ecological and economic benefit from it is reduced by bureaucracy.

Suggestion (wish) for Vietnam:

- For all research in non-protected areas there should be a simple registration model for Vietnamese-German cooperation teams.
- Fast & Preserves all benefits, if one day commercialization becomes an issue

Let's continue to move forward together

.... now modernized



**Excursion in a Northern Vietnam hill tribe region
with Prof. Tran Van Sung (front), VAST, ca. 2008**

Let's continue to walk the road of science together

