Max Planck Institute
of Molecular Plant Physiology

Metabolomic Approaches for PGR

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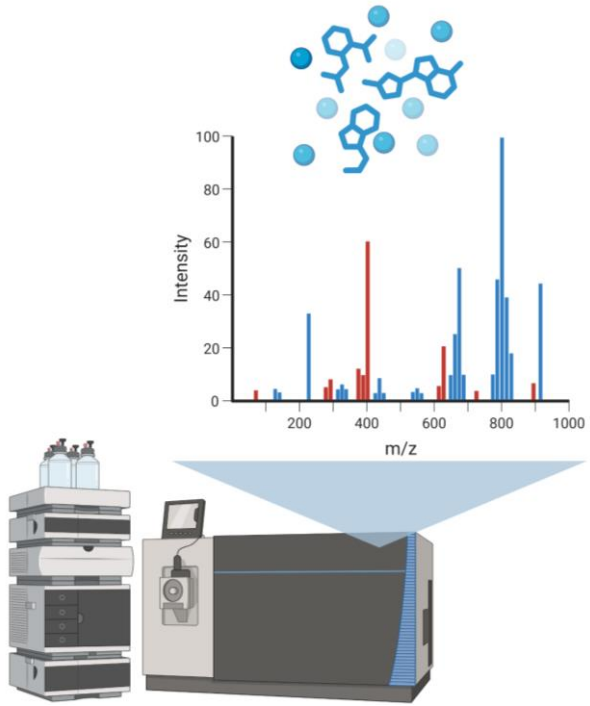
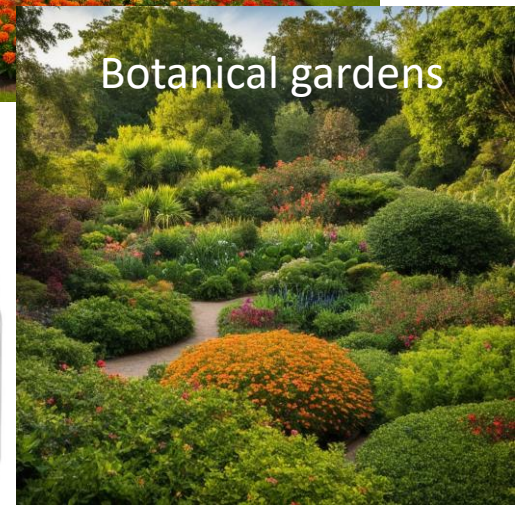
PRO-GRACE
PROMOTING A PLANT GENETIC RESOURCE COMMUNITY FOR EUROPE

Plant genetic resources as a source of variation

- Plant genetic resources (PGR) (wild relatives, seed banks, germplasm collections) hold a vast pool of genetic diversity.
- Metabolomics provides a high-throughput tool to profile metabolites from diverse PGR.

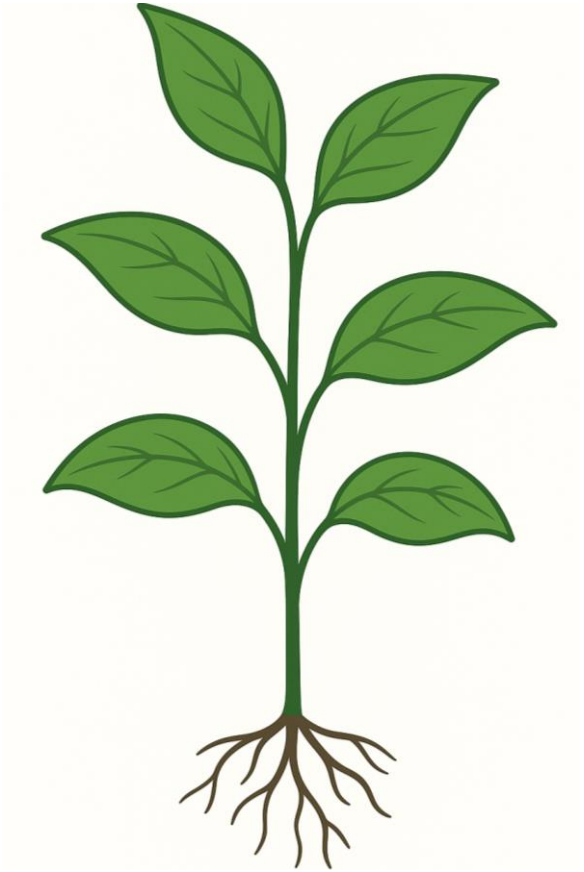




Metabolomics and Plant Metabolism

- **Metabolomics** is an approach of study that involves the comprehensive analysis of small molecules, known as **metabolites**, present in biological samples.

- Metabolomics is usually performed by targeting either a specific cell, a specific tissue, or the entire organism (Shen et al., 2023, Molecular Plant).

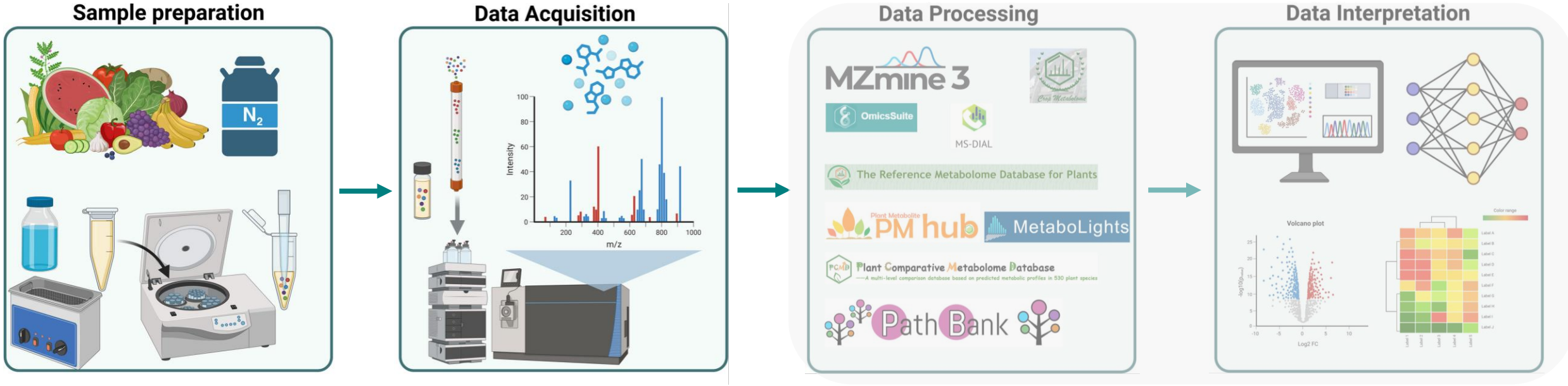


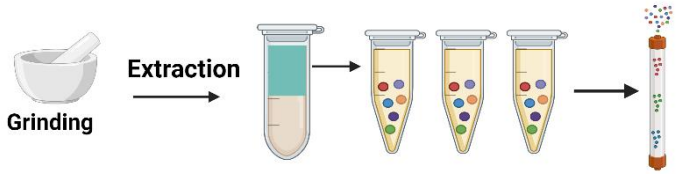
Primary metabolites (Development)
- Fatty acids
- Lipids
- Sugars
- Amino acids
- Others

Secondary metabolites (Environmental Interactions)
- Phenolics
- Terpenes
- Carotenoids
- Flavonoids

Hormones (Regulation)
- Auxins
- Gibberellins
- Jasmonic acids
- Abcisic acid

Metabolomics Approach from Sample Preparation to Data Interpretation





chromatography GC, LC

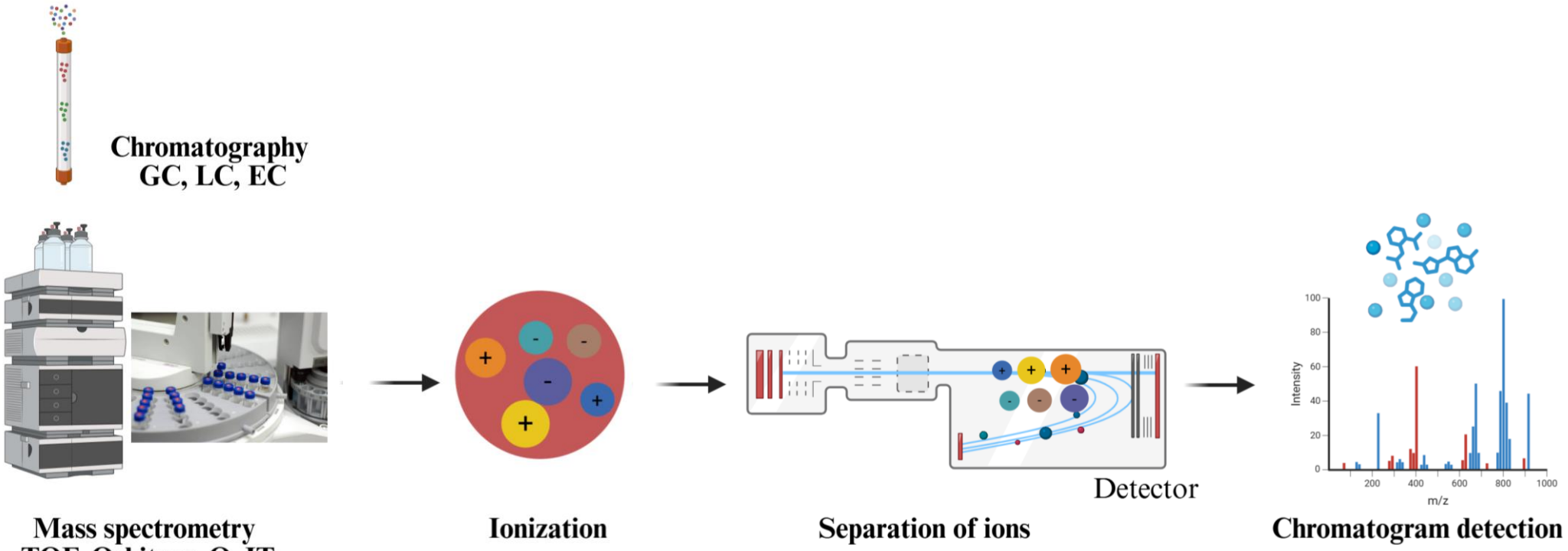
Metabolomics Techniques

- Gas Chromatography Mass Spectrometry (GC-MS)
- Liquid Chromatography Mass Spectrometry (LC-MS)

Mass analyzers are available;

- ✓Quadrupole,
- ✓Time-of-flight (TOF),
- ✓Orbitrap
- ✓Ion trap

- ✓Electrospray ionization (ESI),
- ✓atmospheric pressure chemical ionization (APCI),
- ✓atmospheric pressure photo-ionization (APPI)



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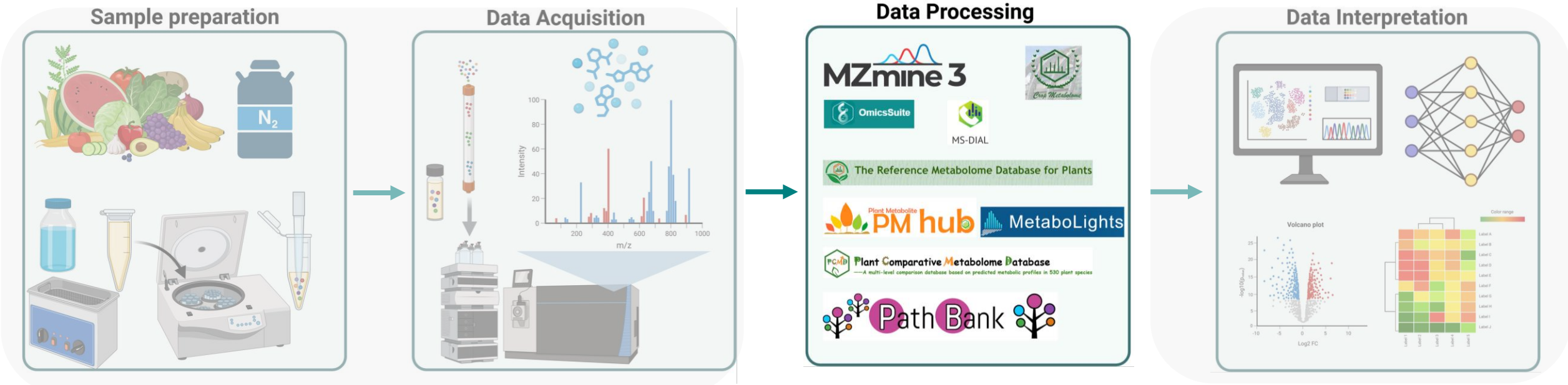
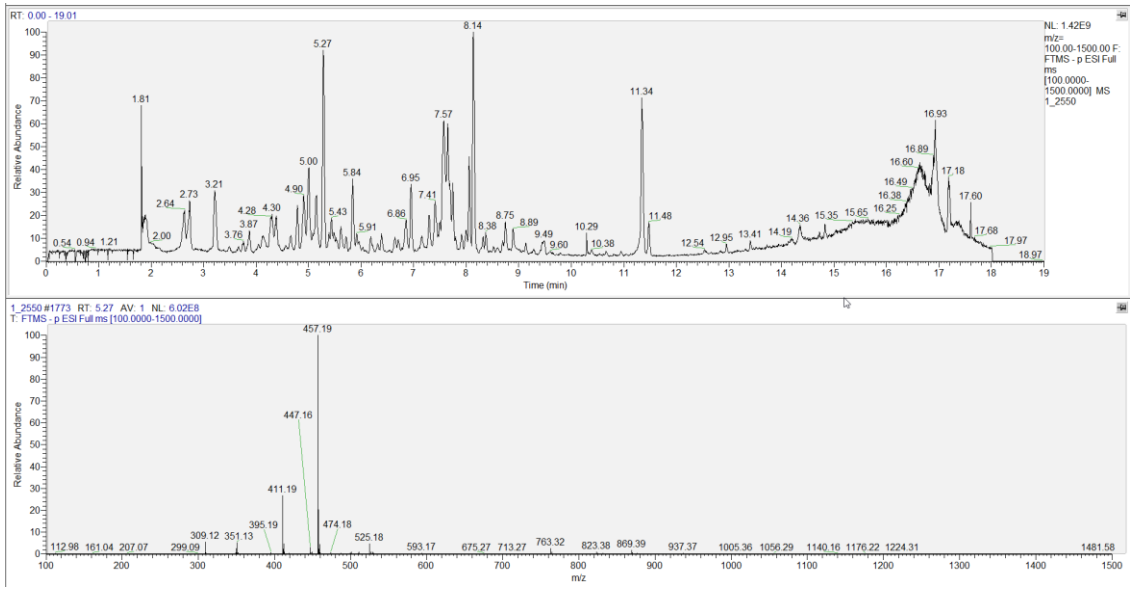
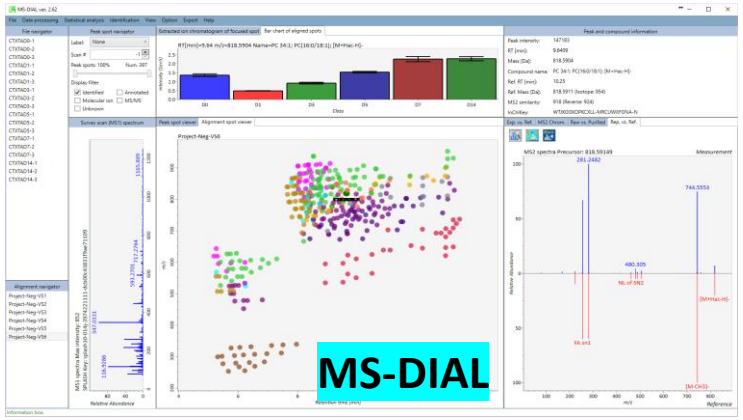
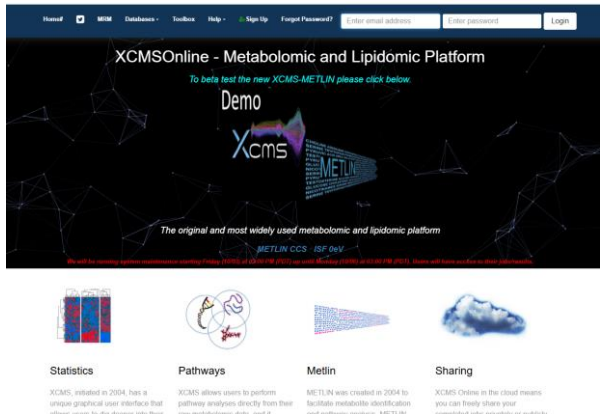


Chromatogram Processing and Data Analysis



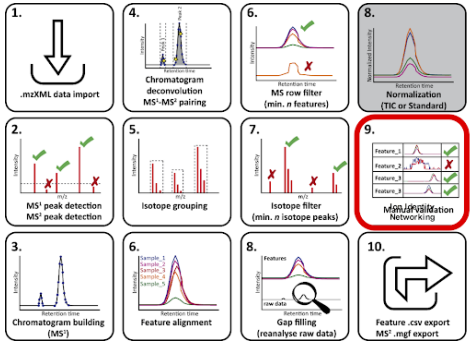
Data pre-processing peak alignment, feature detection





- Several free data processing tools are available to automatically detect mass features generating chromatographic peaks, and compare peak intensities across multiple samples, as a proxy for metabolite concentration.

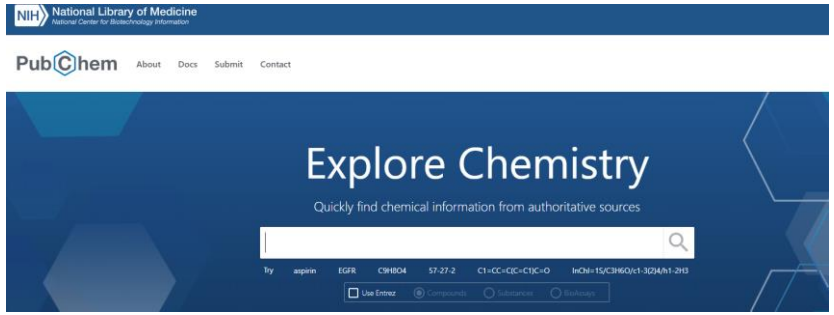
MZmine

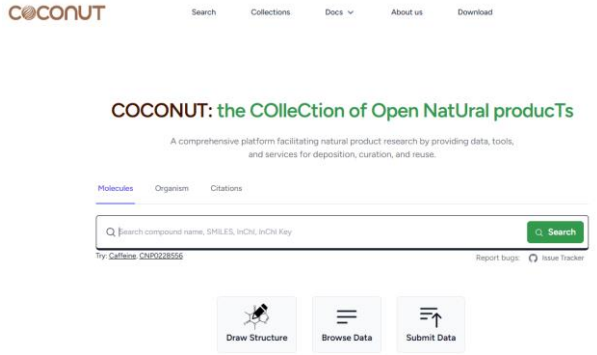


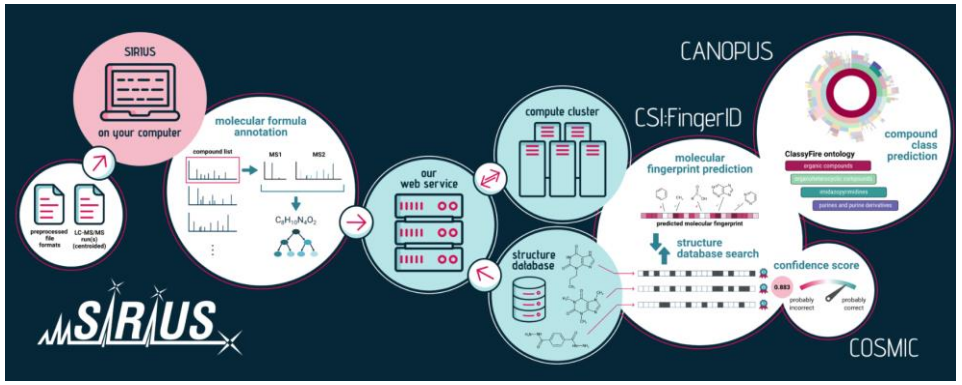
Open MS

- Accurate mass and fragmentation measurements, combined with informative data, are obtained using various software tools for metabolite annotation, including R packages such as;
  - ✓ CAMERA
  - ✓ RAMclust
  - ✓ xMSannotator
  - ✓ MetAssign

Chromatogram Processing and Data Analysis







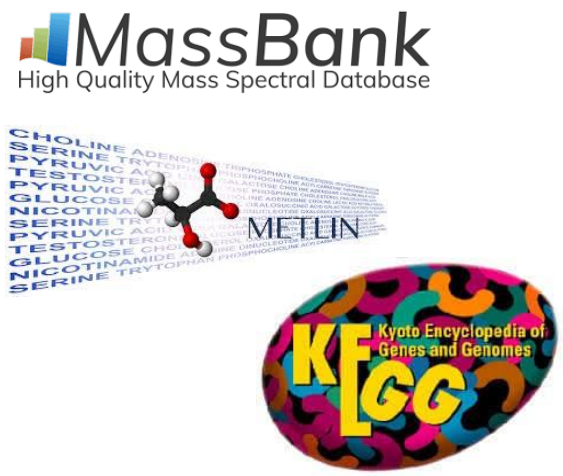
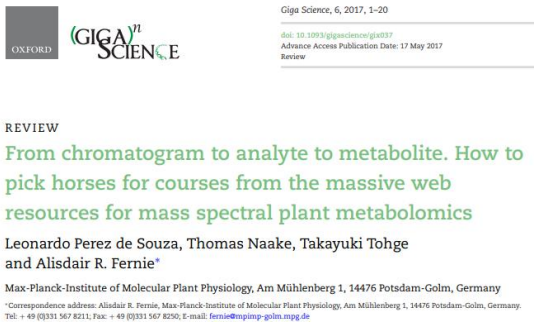


Table 1 The recent metabolomics databases

Metabolomics databases	References	Link	Methodology	Species Scope
LC–MS/GC–MS Centric Databases				
METASPACE-ML	(Wadie et al. 2024)	https://apps.embl.de/metaspacecontext/	LC–MS	Multi-species
MetFrag	(Ruttkies et al. 2016)	https://msbi.ipb-halle.de/MetFrag/	LC–MS/MS	Multi-species
LIPID MAPS	(Conroy et al. 2024)	www.lipidmaps.org	LC–MS, GC–MS	Multi-species
LipidSig 2.0	(Liu et al. 2024)	https://lipidsig.bioinfomics.org/	LC–MS	Multi-species
LipidSuite	(Mohamed and Hill 2021)	http://suite.lipidr.org	LC–MS	Multi-species
COCONUT	(Sorokina et al. 2021)	https://coconut.naturalproducts.net	LC–MS	Multi-species
PathBank 2.0	(Wishart et al. 2024)	https://pathbank.org/	Pathway integration	Multi-species
SCIPDb	(Priya et al. 2023)	http://223.31.159.3/plant_complete/index_orangesunset.php	LC–MS	Multi-species
Multi-Platform Databases (LC–MS, NMR)				
MetaboLights	(Yurekten et al. 2024)	https://www.ebi.ac.uk/metabolights/	LC–MS, GC–MS, NMR	Multi-species
PaintOmics 4	(Liu et al. 2022)	https://paintomics.org/	Multi-omics	Multi-species
RefMetaPlant	(Shi et al. 2024a)	https://www.biosino.org/RefMetaDB/	LC–MS, NMR	Multi-species
OmicsSuite	(Miao et al. 2023)	https://omicssuite.github.io/#/	Multi-omics	Multi-species
ModelSEED	(Seaver et al. 2021)	https://modelseed.org/biochem	Genome-scale modelling	Multi-species
Horticultural Crop-Specific Databases				
TOMATOMET	(Ara et al. 2021)	https://metabolites.in/tomato-fruits/	LC–MS, GC–MS	Tomato
PMhub 1.0	(Tian et al. 2024)	https://pmhub.org.cn/#/	LC–MS	Multi-species
MMHub	(Li et al. 2020)	https://biodb.swu.edu.cn/mmdb/	LC–MS	Mullberry
ArecaceaeMDB	(Yang et al. 2023a)	http://arecaceae-gdb.com/#/	LC–MS	Arecaceae (Palms)
LettuceGDB	(Guo et al. 2023)	https://www.lettucegdb.com/	LC–MS	Lettuce
BoGDB	(Wang et al. 2022)	http://www.bogdb.com/	LC–MS	Brassica oleracea
BnlR	(Yang et al. 2023b)	http://yanglab.hzau.edu.cn/BnlR	LC–MS	Brassica napus
PlantMetSuite	(Liu et al. 2023)	https://plantmetsuite.verygenome.com/	LC–MS	Multi-species
Corriander Genomics Database	(Song et al. 2020)	http://cgdb.bio2db.com/	LC–MS	Corriander and carrot
Metabolite Database for RTB	(Price et al. 2020)	(Supplementary files of the original article)	LC–MS, GC–MS	Banana, cassava, potato, sweet potato, yam
Broad-Spectrum Plant Metabolomics Databases				
Plant Reactome Knowledgebase	(Gupta et al. 2024)	https://plantreactome.gramene.org	Pathway-based	Multi-species
PMN 16	(Hawkins et al. 2025)	https://plantcyc.org/	Pathway-based	Multi-species
MetaCyc	(Caspi et al. 2020)	https://metacyc.org/	Pathway-based	Multi-species
CropMetabolome	(Shi et al. 2024b)	http://www.cropmetabolome.com/	LC–MS, GC–MS	Multiple Crops
Metadb	(Gao et al. 2024)	http://medmetadb.ynau.edu.cn	LC–MS	Multi-species
HypoRiPPAtlas	(Lee et al. 2023)	https://hyporippatlas.npanalysis.org/	LC–MS/MS	Plants and microbes
Databases Emphasizing Secondary Metabolites and Natural Products				
MPOD	(He et al. 2022)	http://medicinalplants.ynau.edu.cn/	LC–MS	Medicinal and food plants
CMAUP	(Zeng et al. 2019)	http://bidd2.nus.edu.sg/CMAUP/	LC–MS	Medicinal plants
Meta-Analysis and Data Integration Tools				
MODMS	(Fang et al. 2023)	https://modms.lzu.edu.cn/	LC–MS, RNA-seq	*Medicago sativa*
PCMD	(Hu et al. 2024)	https://yanglab.hzau.edu.cn/PCMD	LC–MS, GC–MS	Multi-species
The Thing Metabolome Repository family (XMRs)	(Sakurai et al. 2023)	https://metabolites.in/plants/	LC–MS	Multi-species
WikiPathways	(Slenter et al. 2018)	wikipathways.org	Pathway mapping	Multi-species
MDSi	(Li et al. 2023)	http://sky.sxau.edu.cn/MDSi.htm	LC–MS/MS	*Setaria italica*
PEO	(Koh et al. 2024)	https://expression.plant.tools/	LC–MS	Multi-species

Karakas et al., 2025, *Horticulture Advances*


OXFORD
(GIGA)n SCIENCE
Giga Science, 6, 2017, 1–20
doi: 10.1093/gigascience/gix037
Advance Access Publication Date: 17 May 2017
Review

REVIEW

From chromatogram to analyte to metabolite. How to pick horses for courses from the massive web resources for mass spectral plant metabolomics

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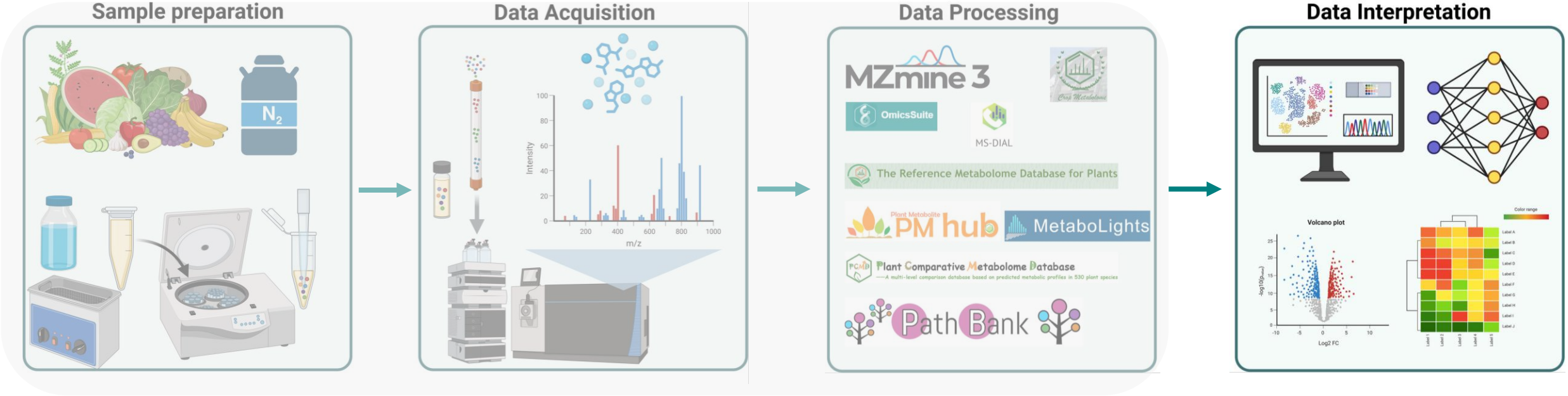
Karakas *et al. Horticulture Advances* (2025) 3:18
https://doi.org/10.1007/s44281-025-00073-8
Horticulture Advances
REVIEW
Open Access

The use of web resources for metabolomics in horticultural crops

Esra Karakas[1], Mustafa Bulut[1] and Alisdair R. Fernie[1*]

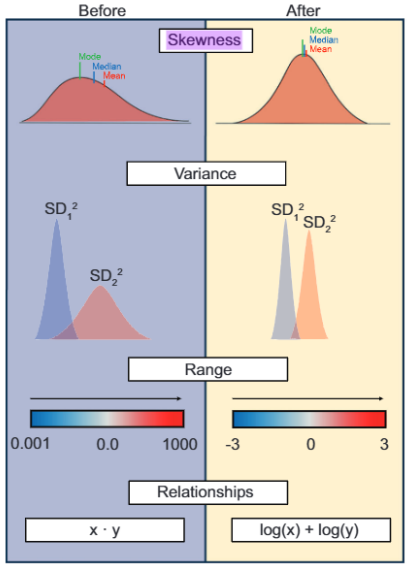
Metabolomics Approach from Sample Preparation to Data Interpretation



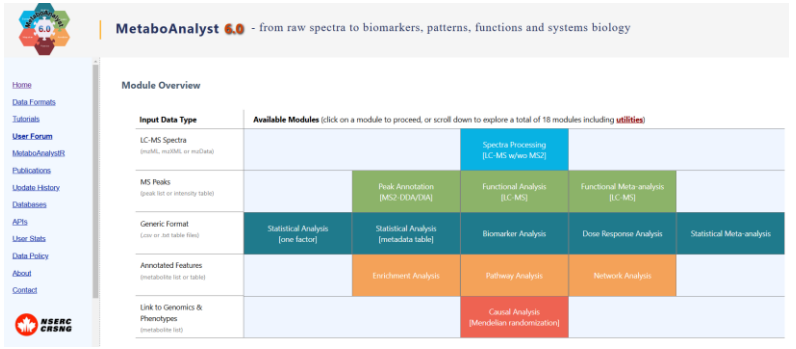
Data Analysis

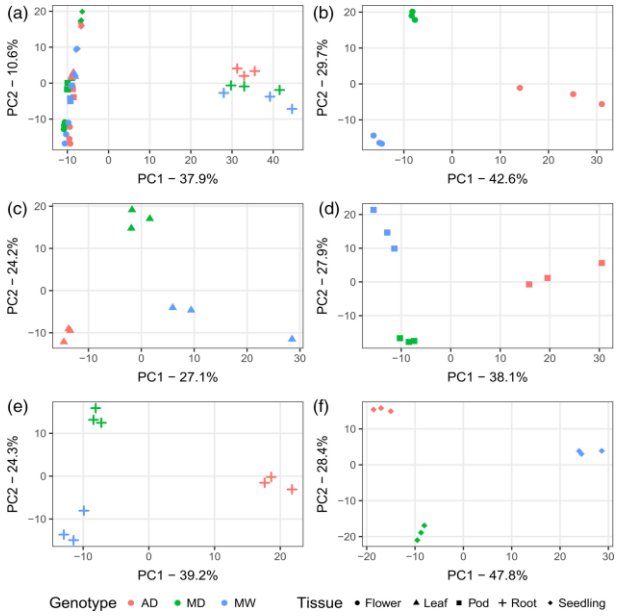
Data normalization
- ✓ Internal standards
- ✓ Median normalization
- ✓ Quality Control (QC) samples

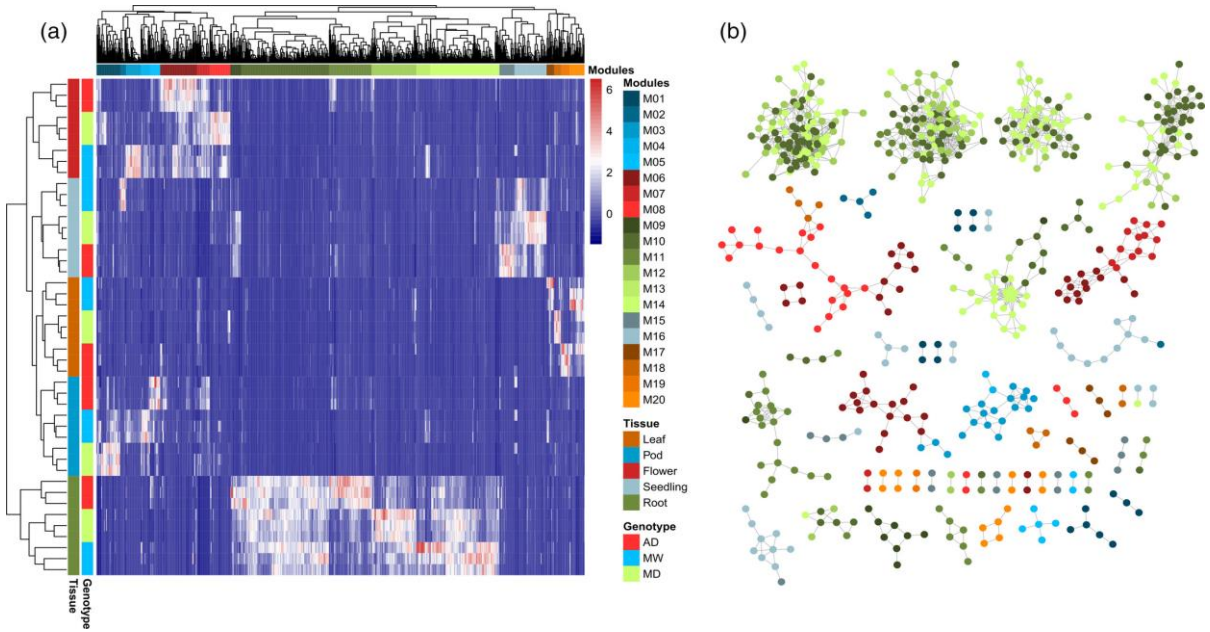
Data Transforming & Scaling
- ✓ Applying log transformation
- ✓ Pareto/auto scaling to reduce skew and make metabolites comparable



Idkowiak et al., 2025, *Nature Communications*

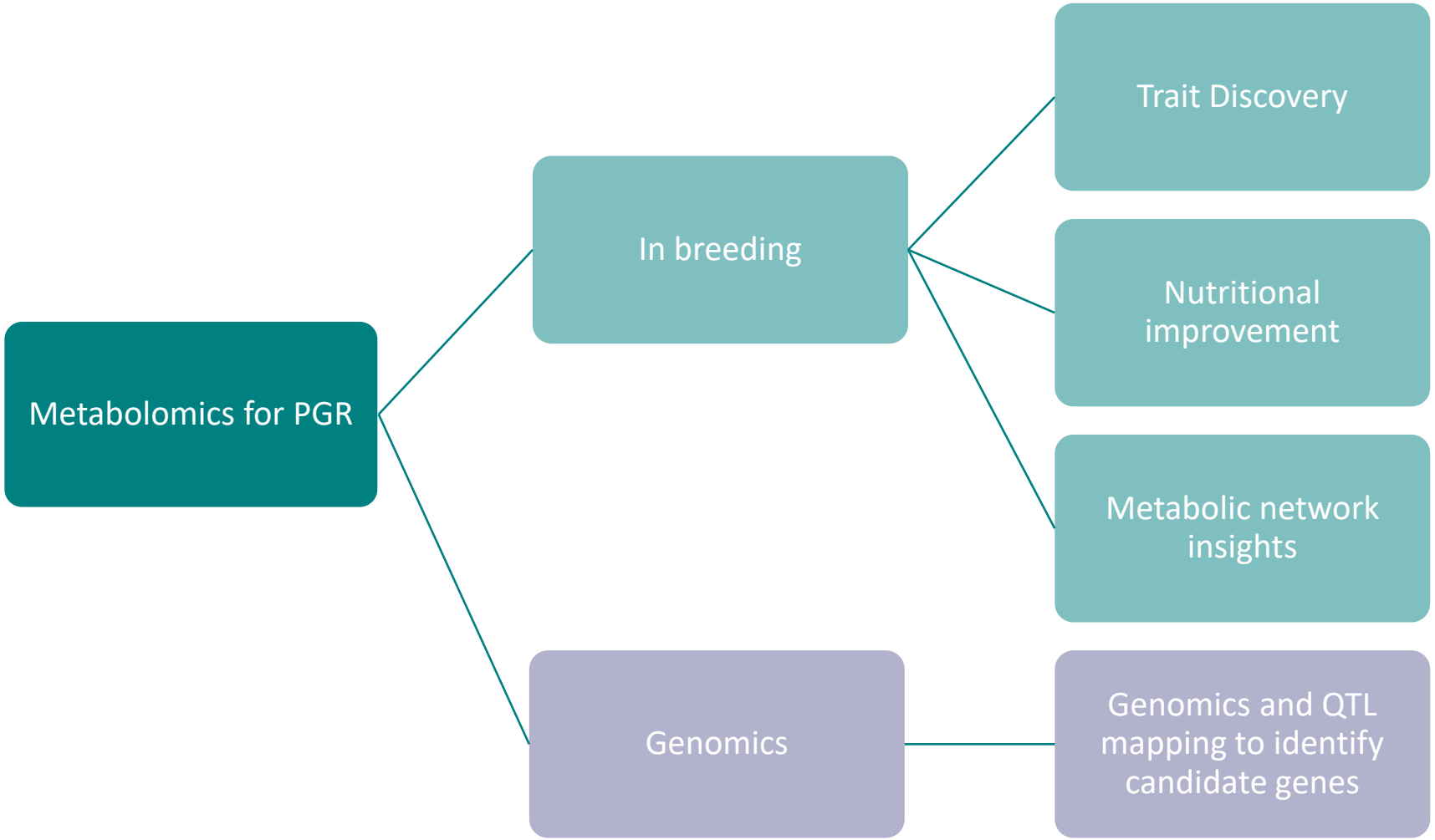






Perez de Souza, 2018, *The Plant Journal*

Applications of Metabolomics for PGR



PRO-GRACE organizers

Thank you for your attention!