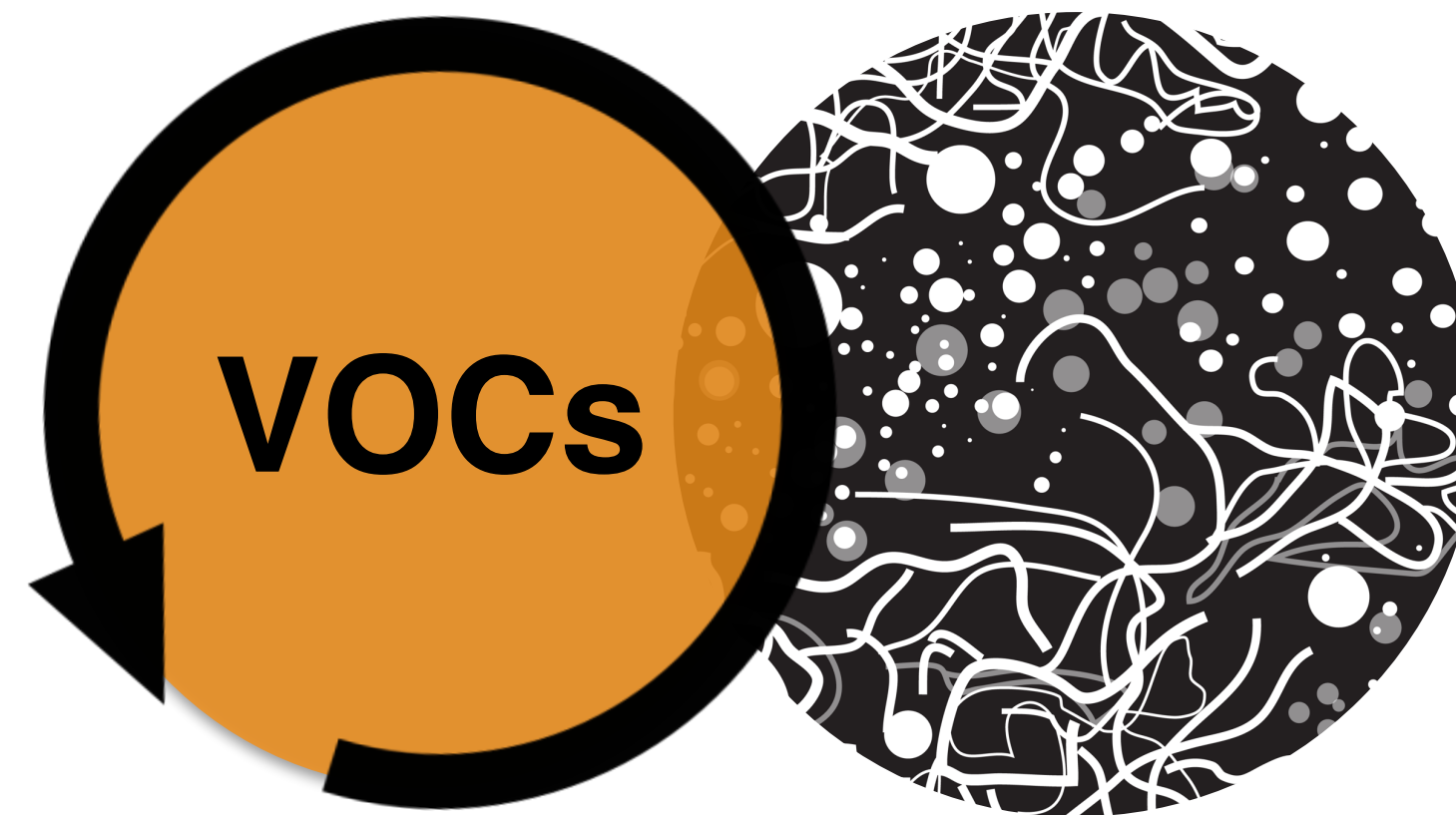


# Microbial Volatile Organic Compounds

important but overlooked in microbial systems studies



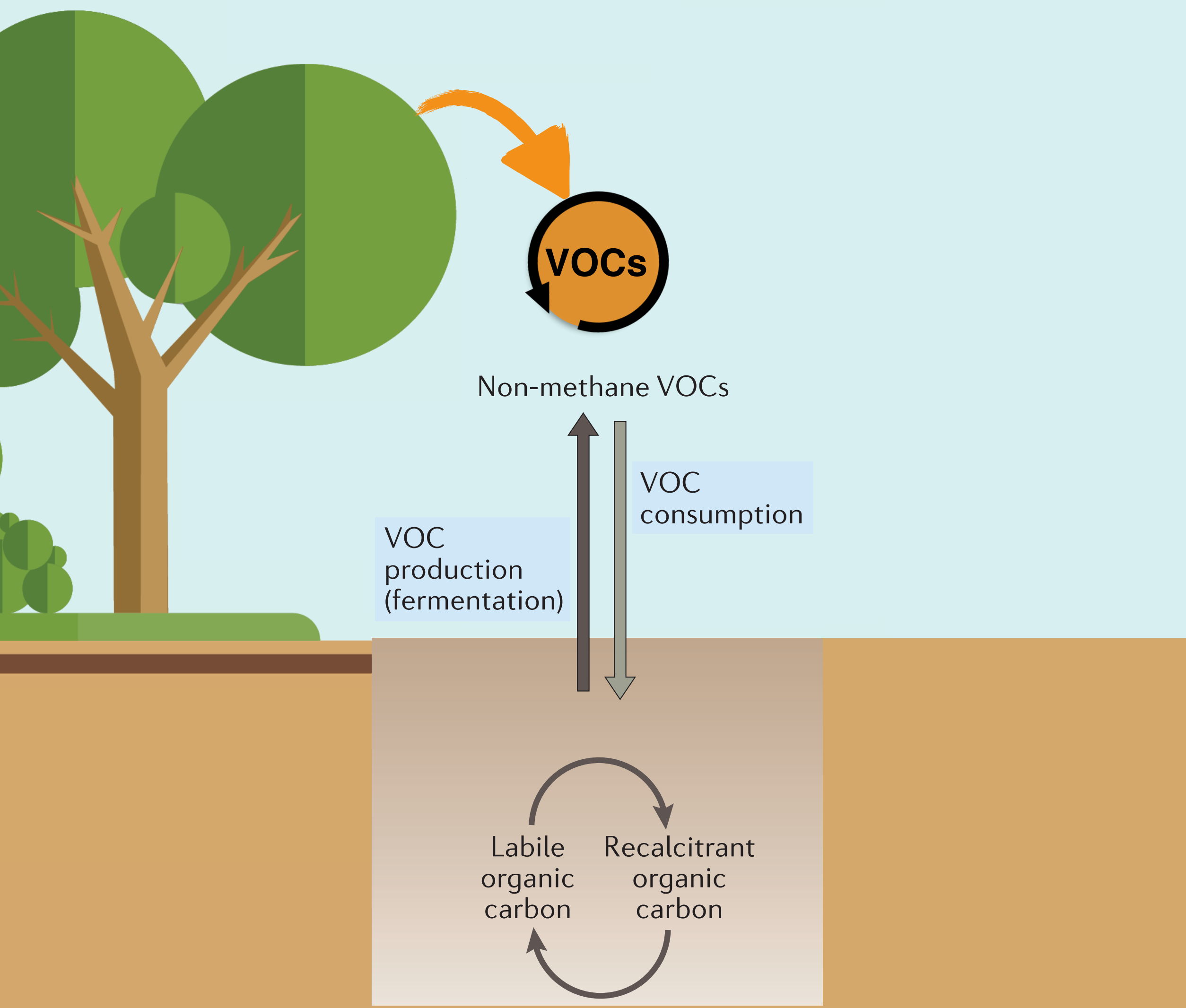
**Laura Meredith**, Malak Tfaily, Parker Geffre, Kelsey Graves,  
Kristina Riemer, Linnea Honeker | University of Arizona



Jordan Krechmer | Aerodyne Research, Inc.

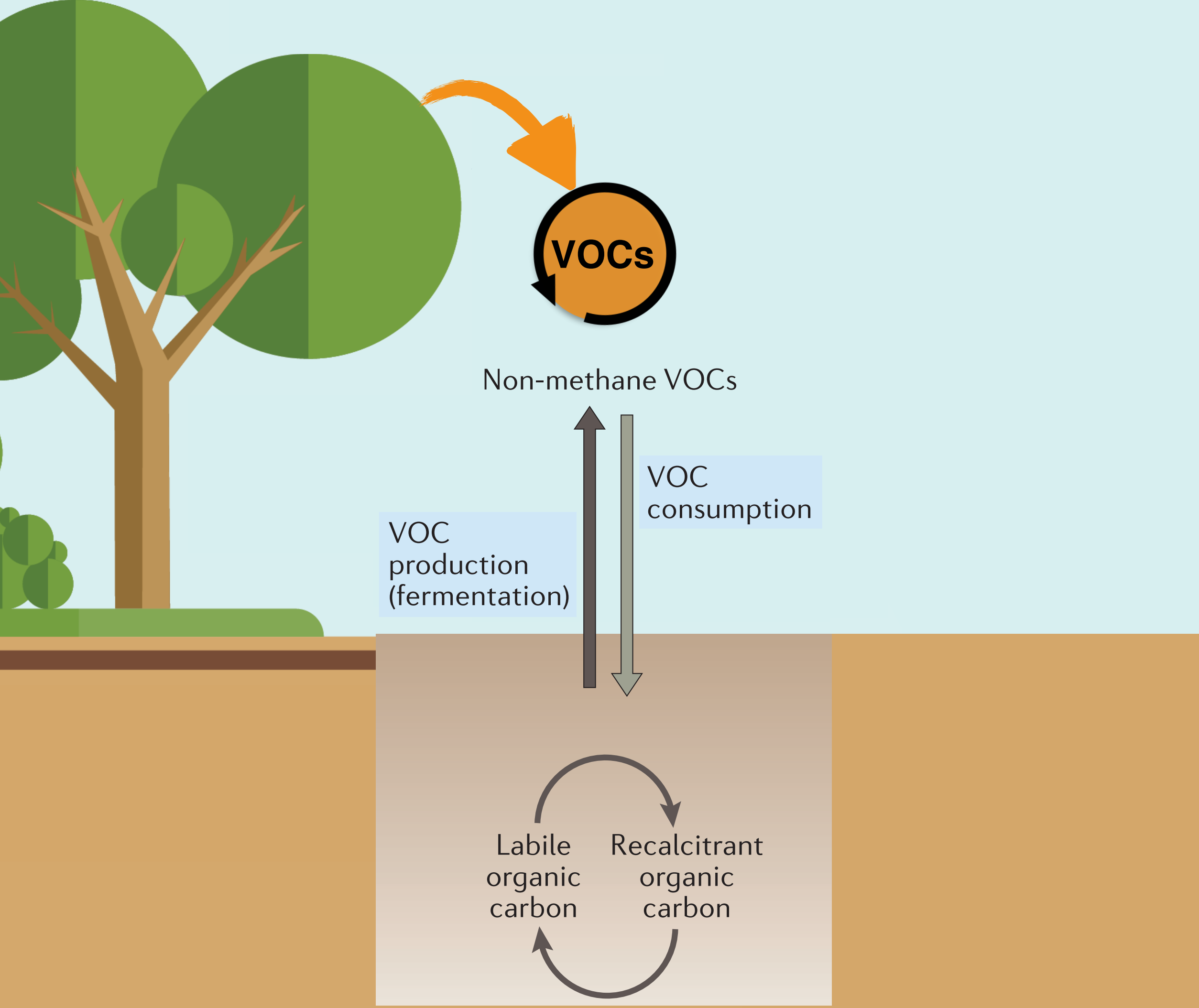


**Volatile organic compounds (VOCs)**  
**are produced and consumed by microbes,**

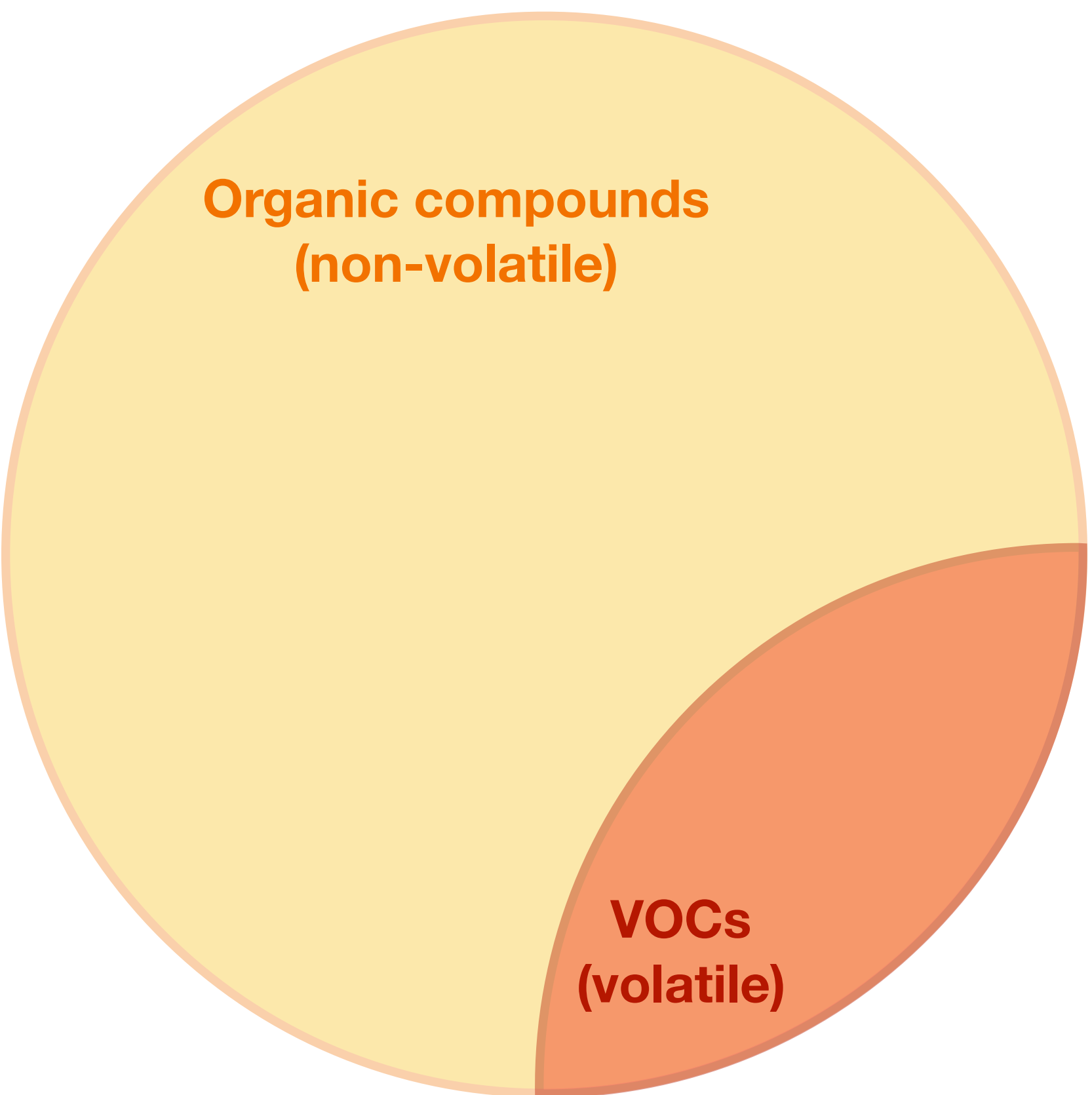


**Peñuelas et al., (2014) Plant, Cell & Environment**  
**Fierer (2017) Nature Reviews Microbiology**

**Volatile organic compounds (VOCs)**  
**are produced and consumed by microbes, yet metabolomics studies commonly**  
**overlook volatile metabolites**



**Peñuelas et al., (2014)** Plant, Cell & Environment  
**Fierer (2017)** Nature Reviews Microbiology

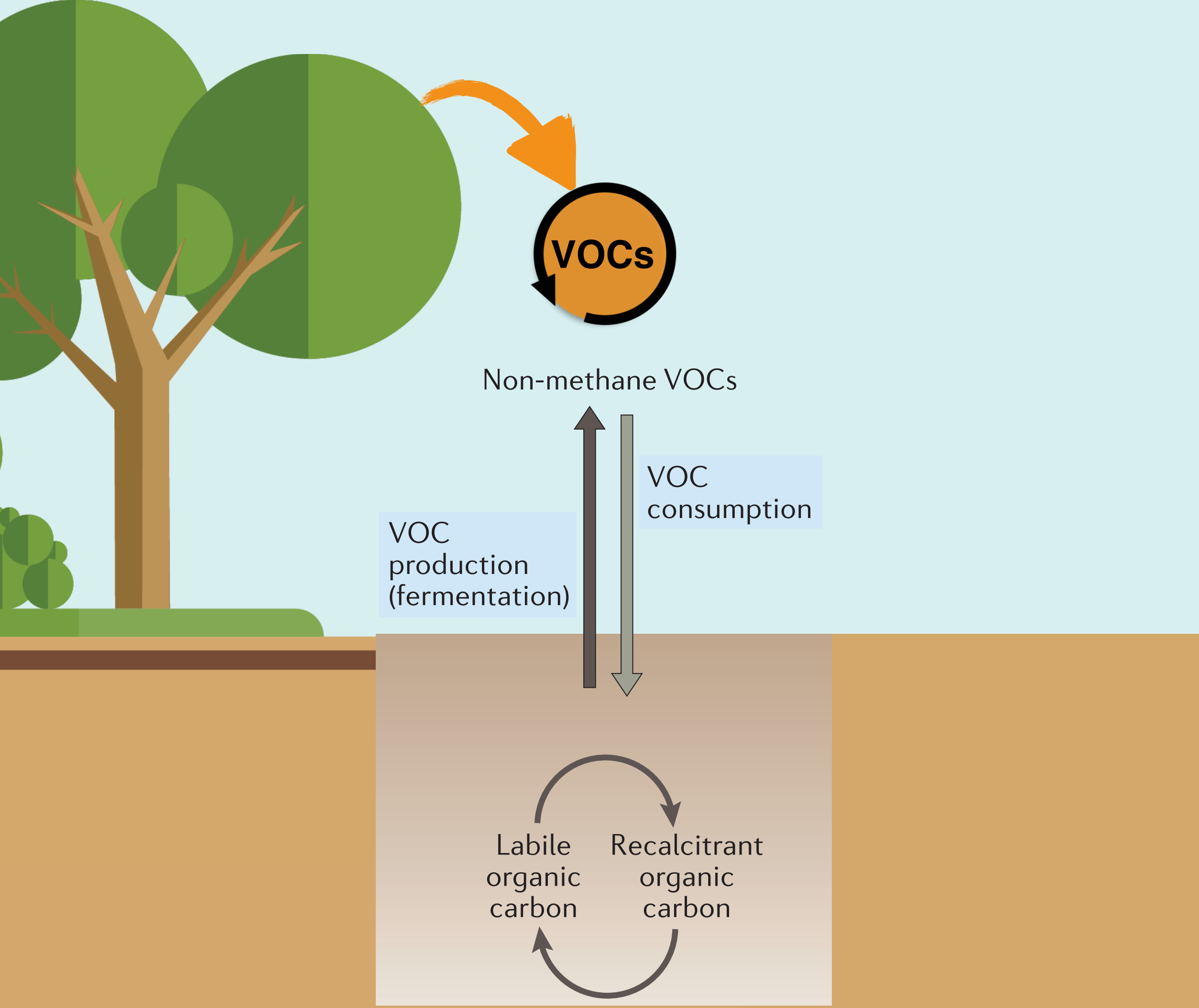


**Meredith and Tfaily (2022)**  
Trends in Microbiology

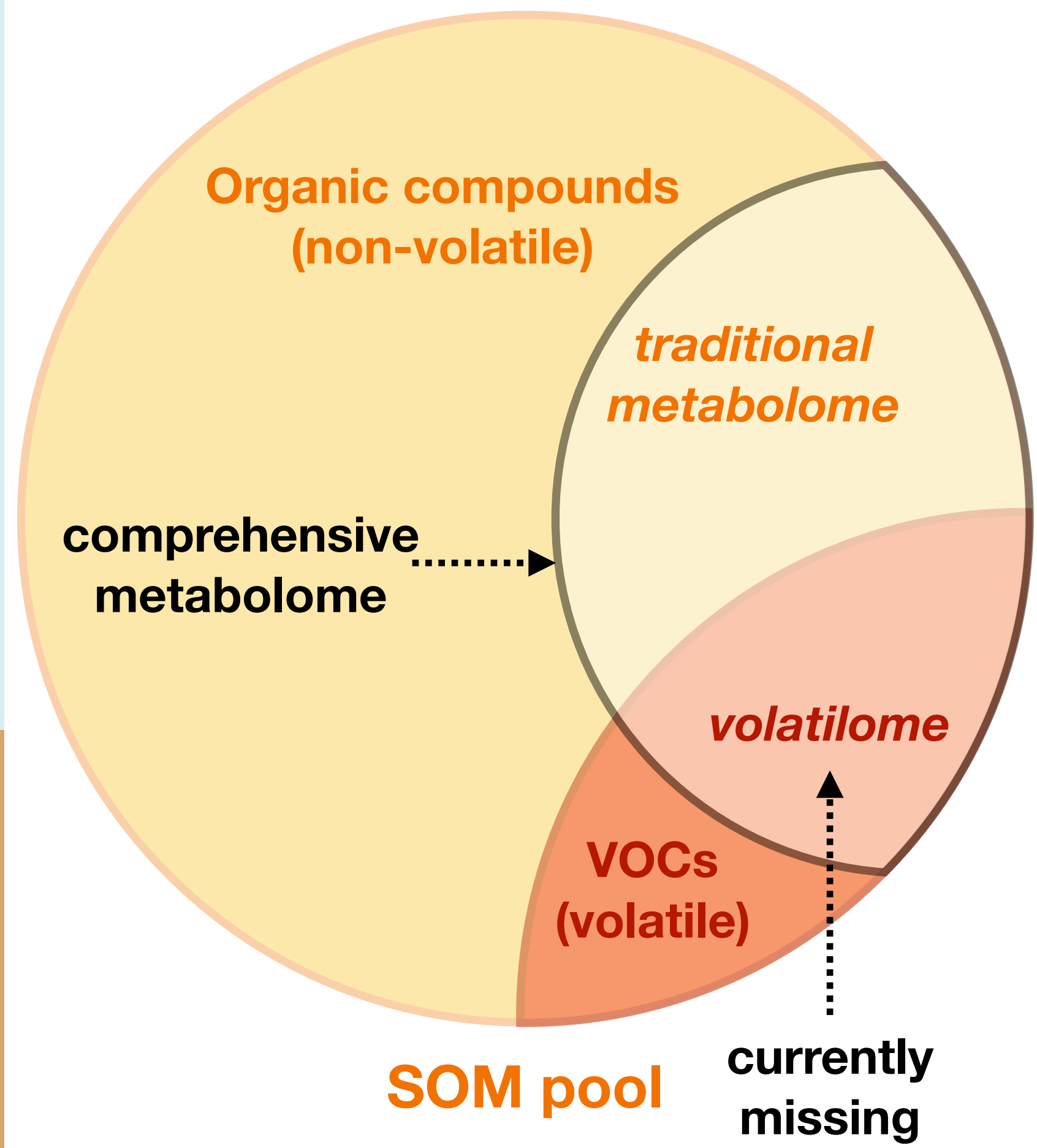


Malak Tfaily

**Volatile organic compounds (VOCs)**  
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**Meredith and Tfaily (2022)**  
**Trends in Microbiology**

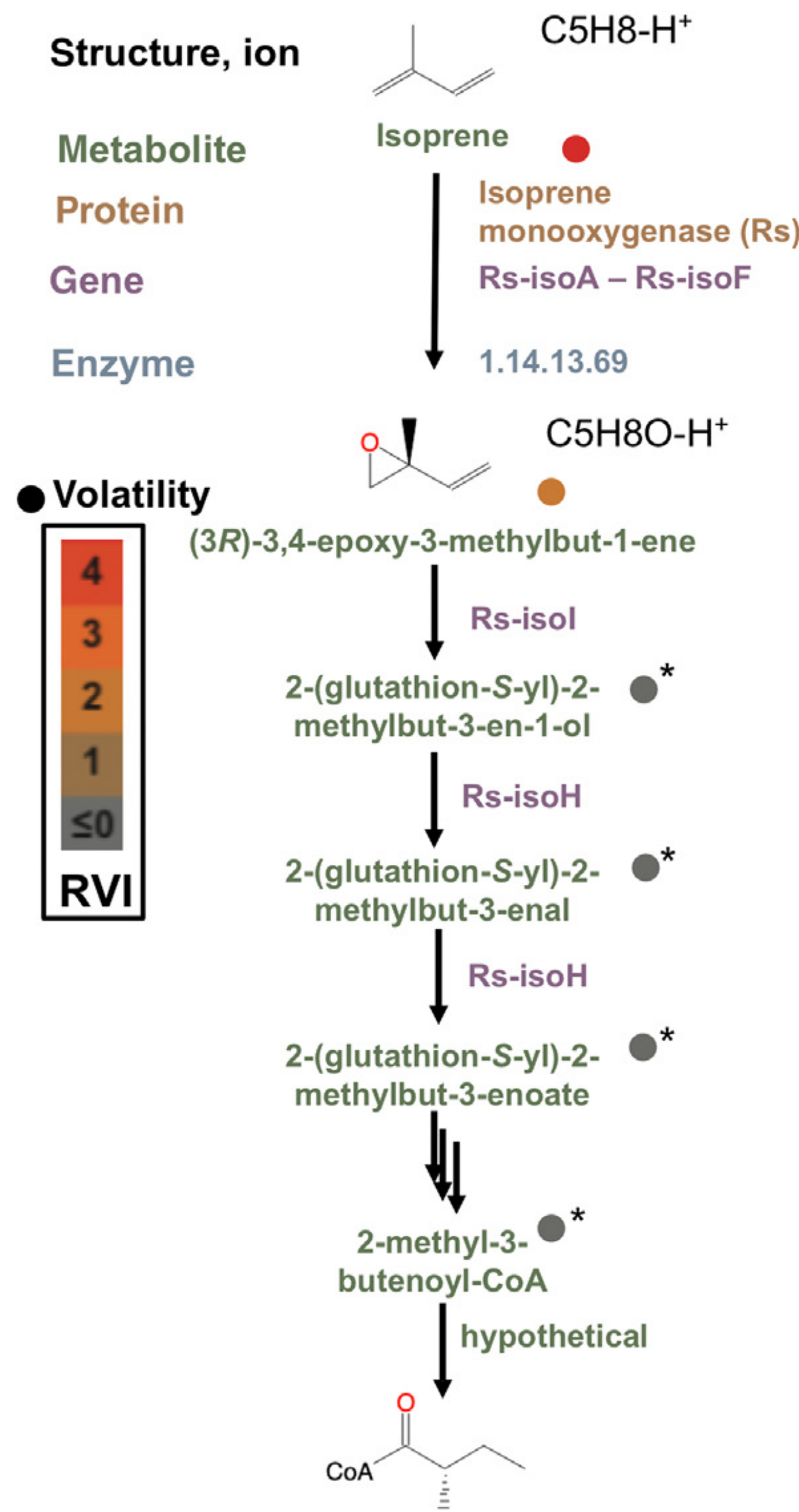


Malak Tfaily



# Estimating metabolite volatility along pathways may explain observational gaps,

ISOPRENE DEGRADATION



Volatility

4

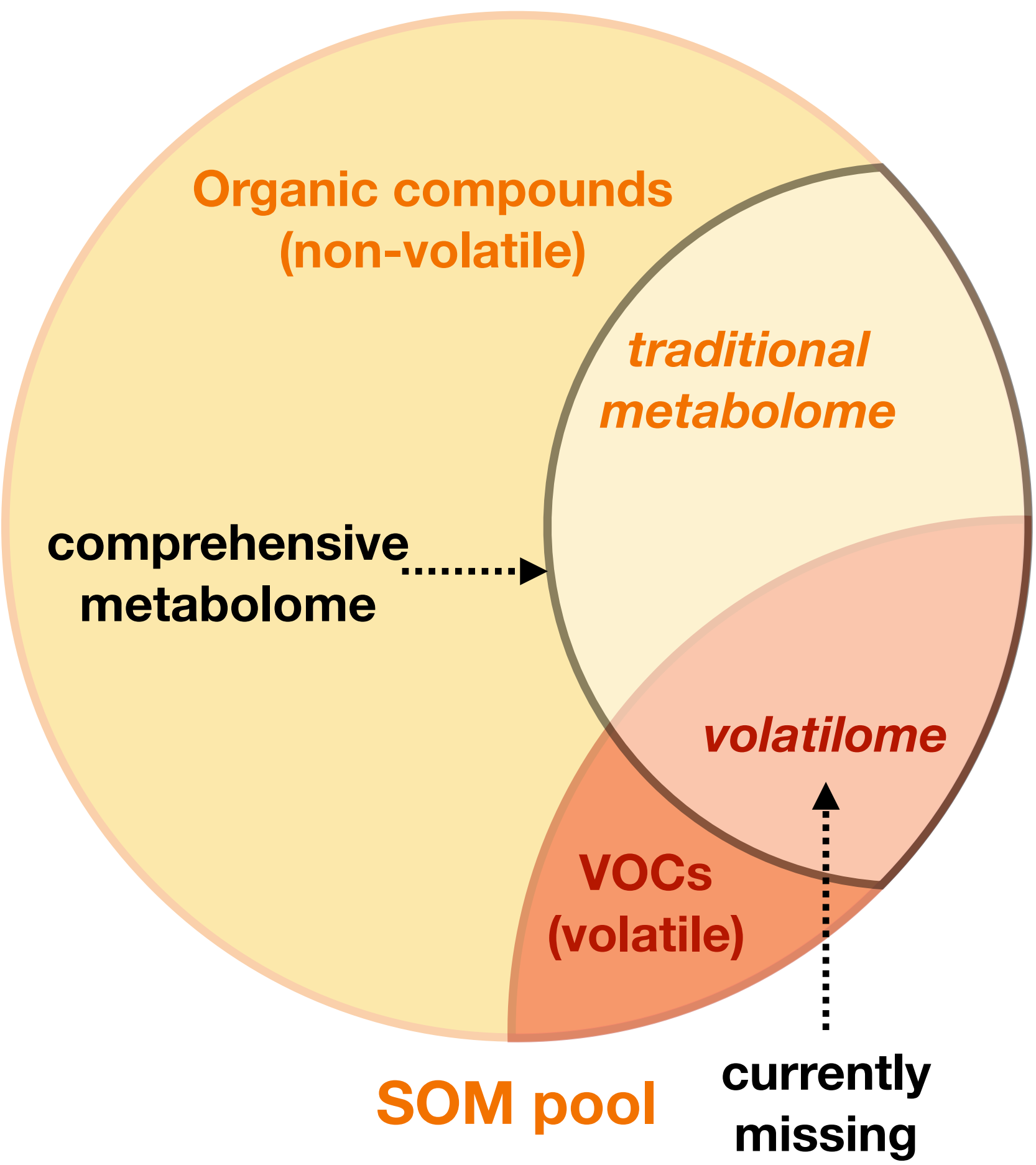
3

2

1

≤0

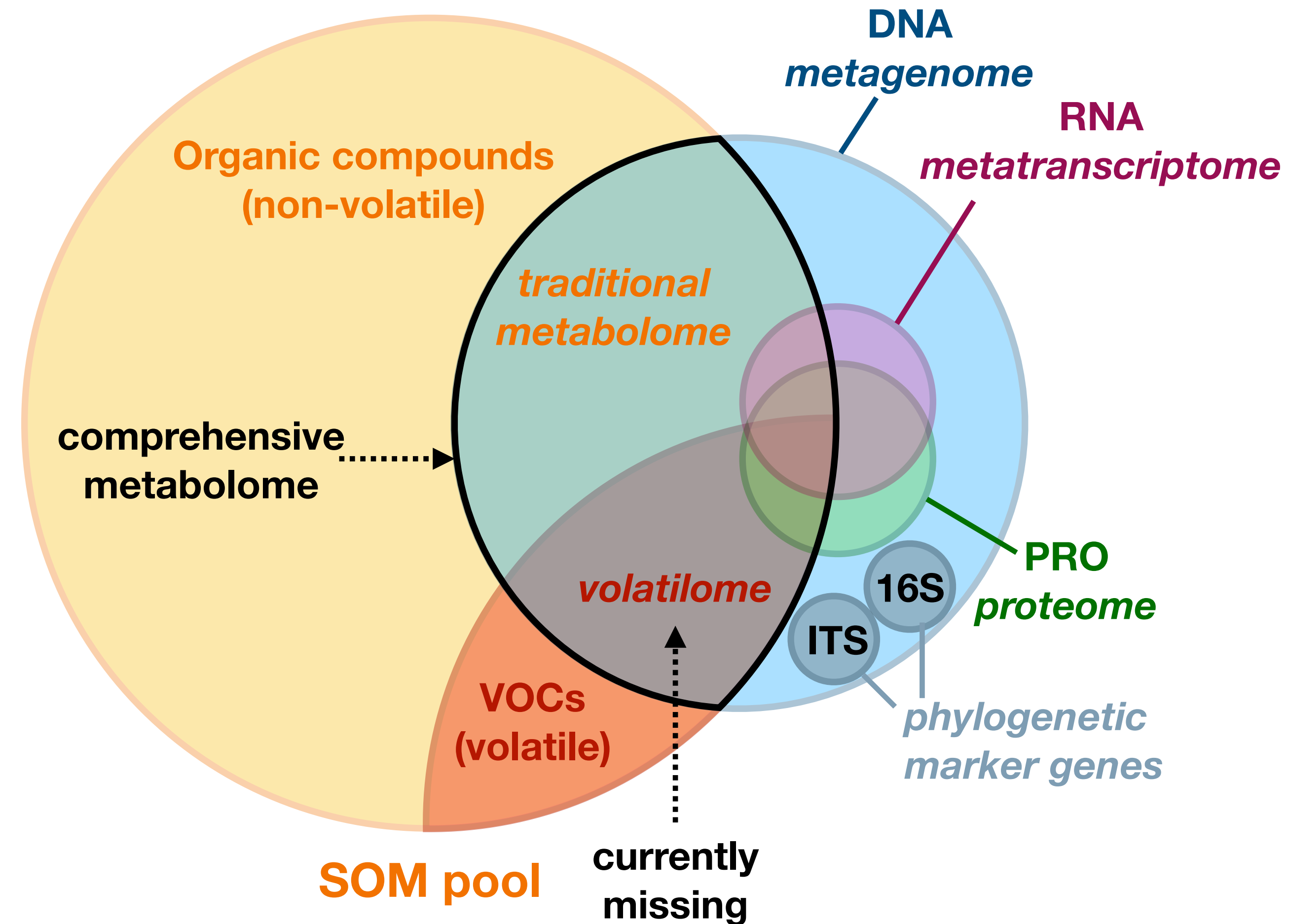
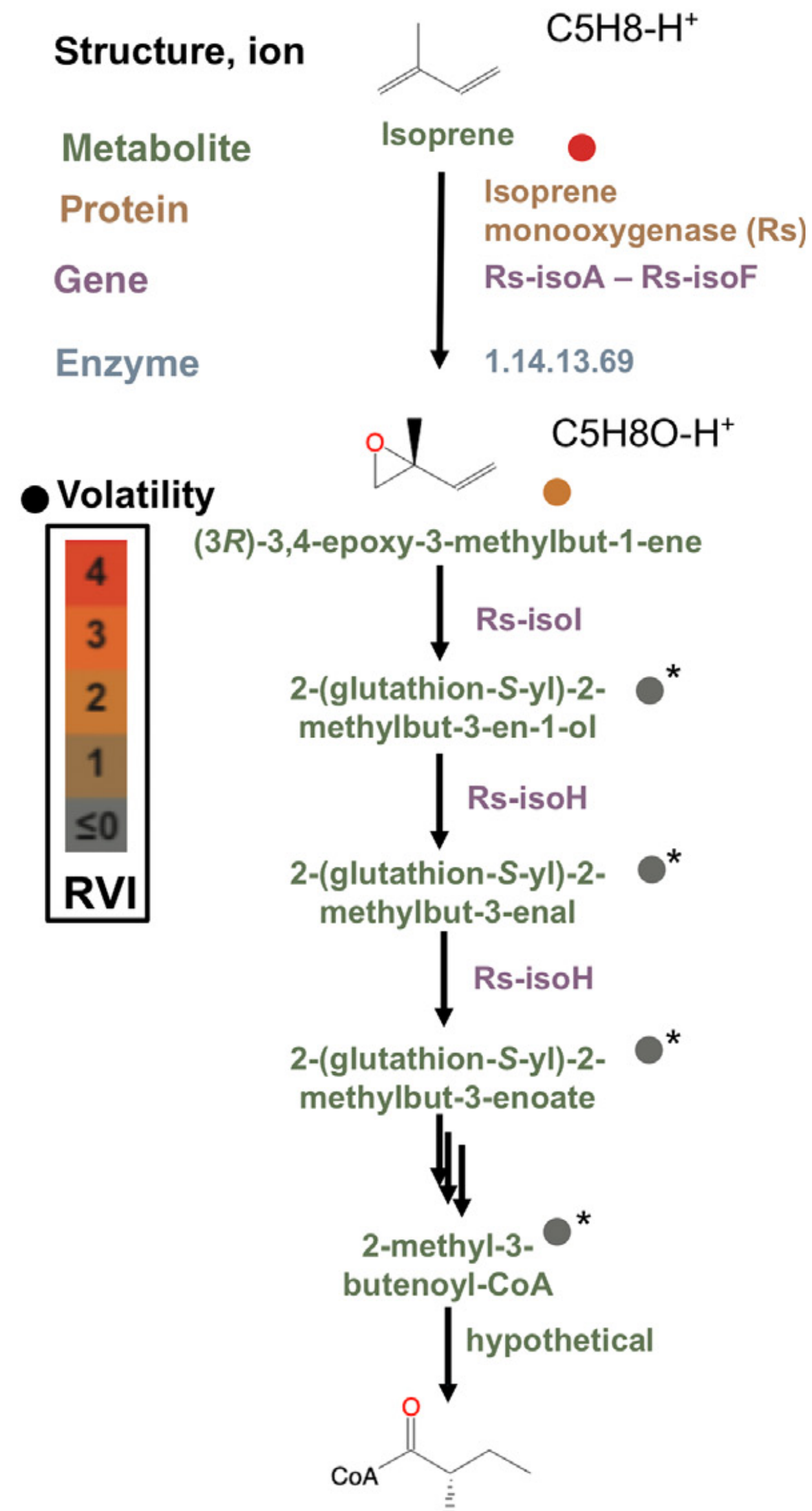
RVI



Malak Tfaily

Meredith and Tfaily (2022)  
Trends in Microbiology

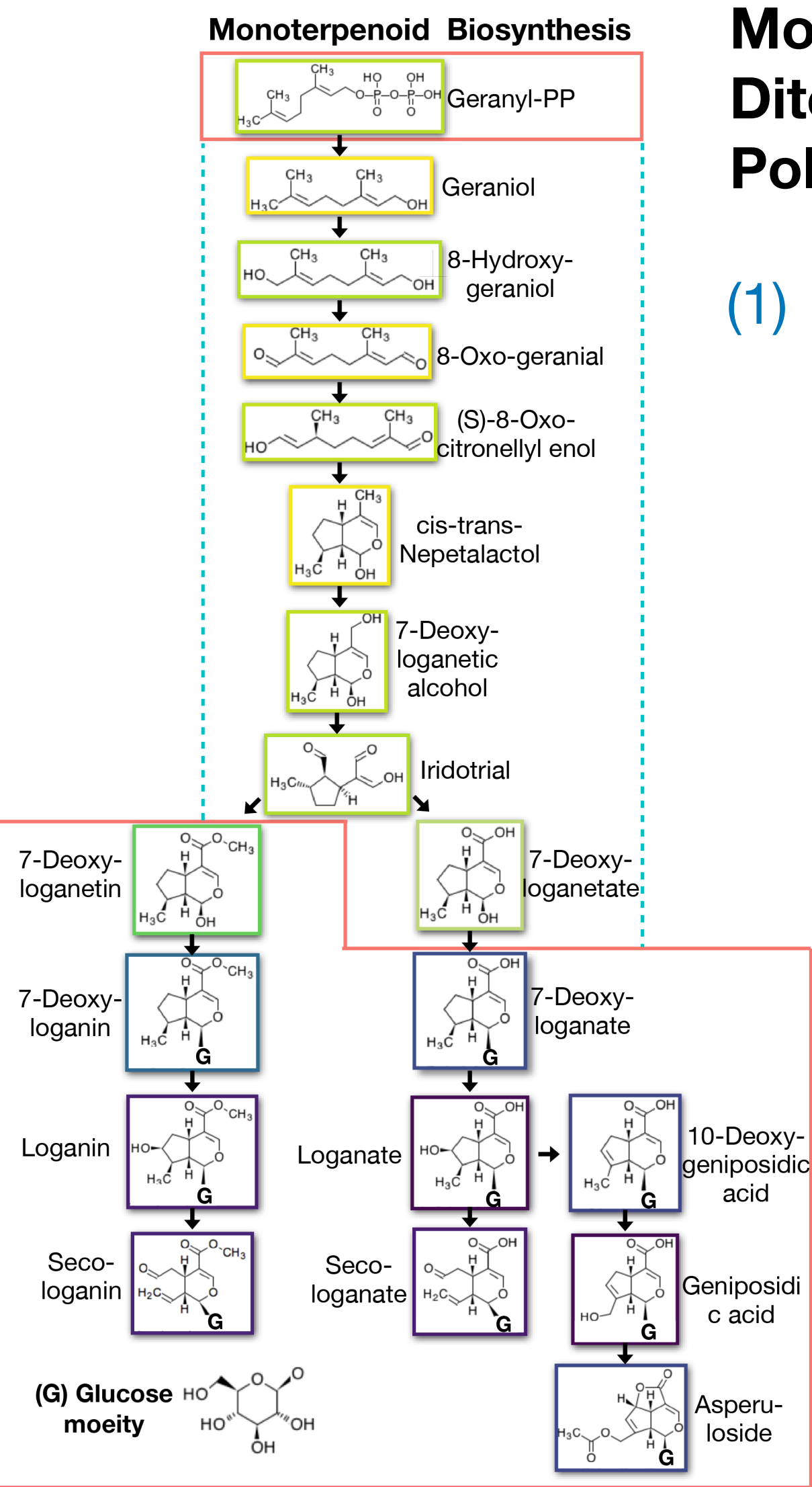
**Estimating metabolite volatility along pathways may explain observational gaps, and motivate more complete integration of -omics data to study microbial systems**





# Do current metabolic approaches underrepresent volatile metabolites?

hypothesis: compounds with higher volatility will be disproportionately undetected



## Monoterpenoid Biosynthesis Diterpenoid Biosynthesis Polycyclic Aromatic Hydrocarbon Degradation

(1) Considered 3 pathways containing VOCs



Linnea Honeker



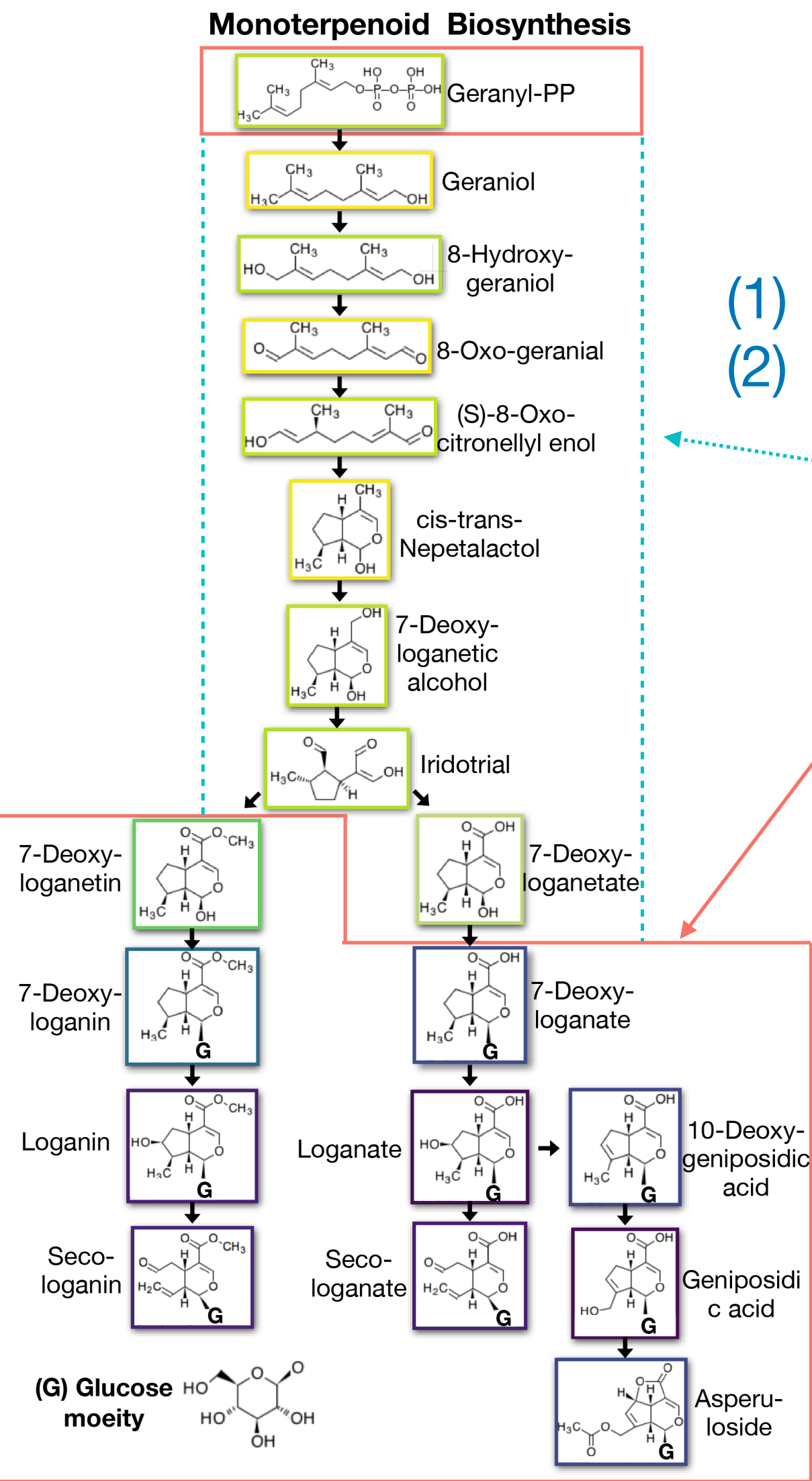
Jordan Krechmer



Kelsey Graves

# Do current metabolic approaches underrepresent volatile metabolites?

hypothesis: compounds with higher volatility will be disproportionately undetected



- (1) Considered 3 pathways containing VOCs
- (2) Metabolite detected in peat metabolome?



Detected



Not-detected

NMR: nuclear magnetic resonance;  
GC-EI-MS: gas chromatography electron-ionization MS;  
FT-ICR-MS: fourier-transform ion cyclotron resonance MS.



Linnea Honeker



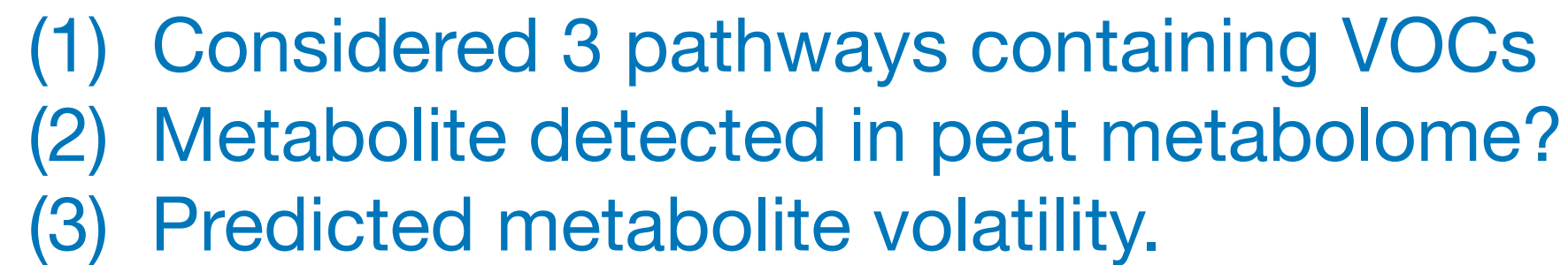
Jordan Krechmer



Kelsey Graves



hypothesis: compounds with higher volatility will be disproportionately undetected



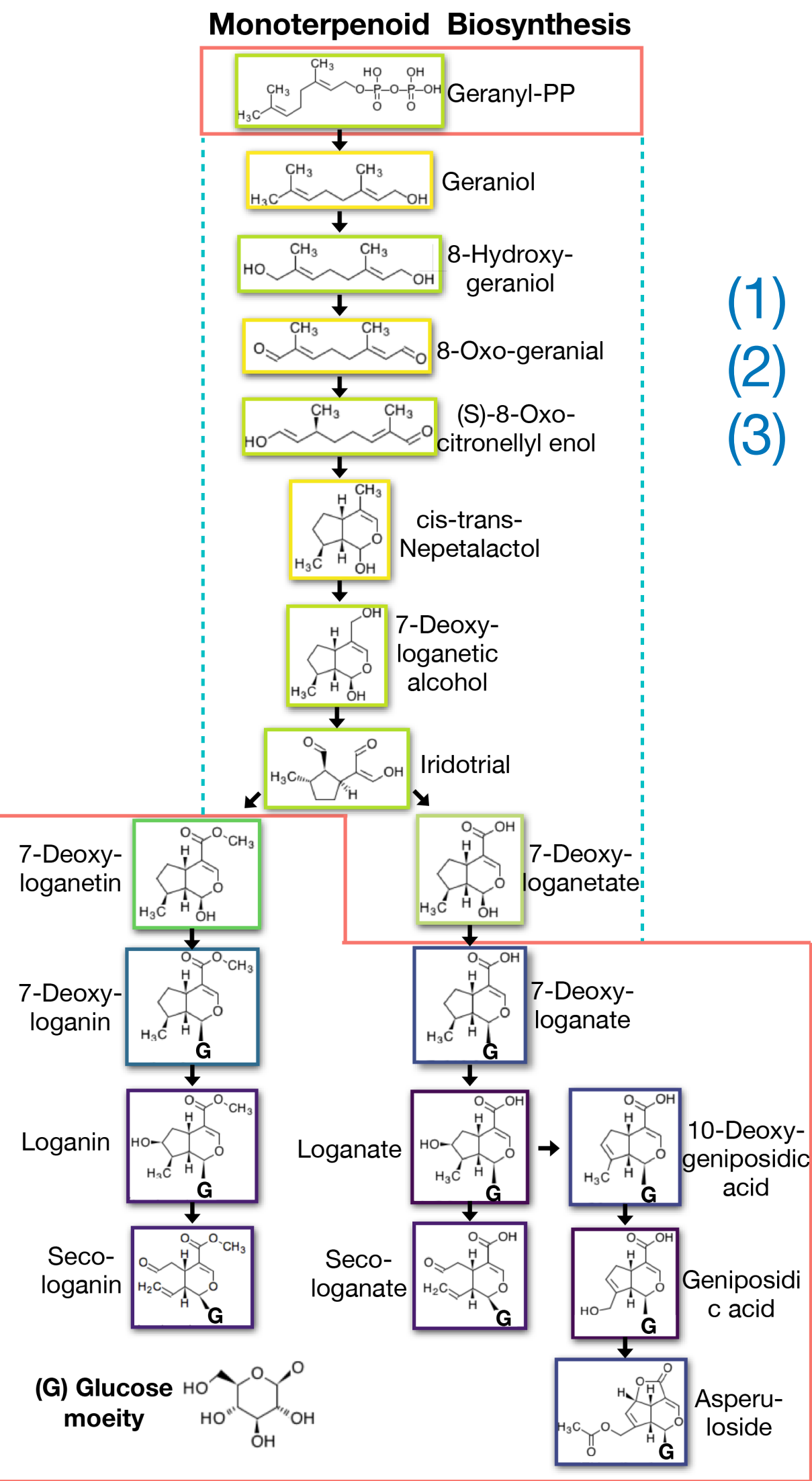
SIMPOL.1 method & gas phase partitioning  
Pankow and Asher (2008) *Atmospheric Chemistry and Physics*  
Donahue et al. (2006) *Environ. Sci. Technol.*



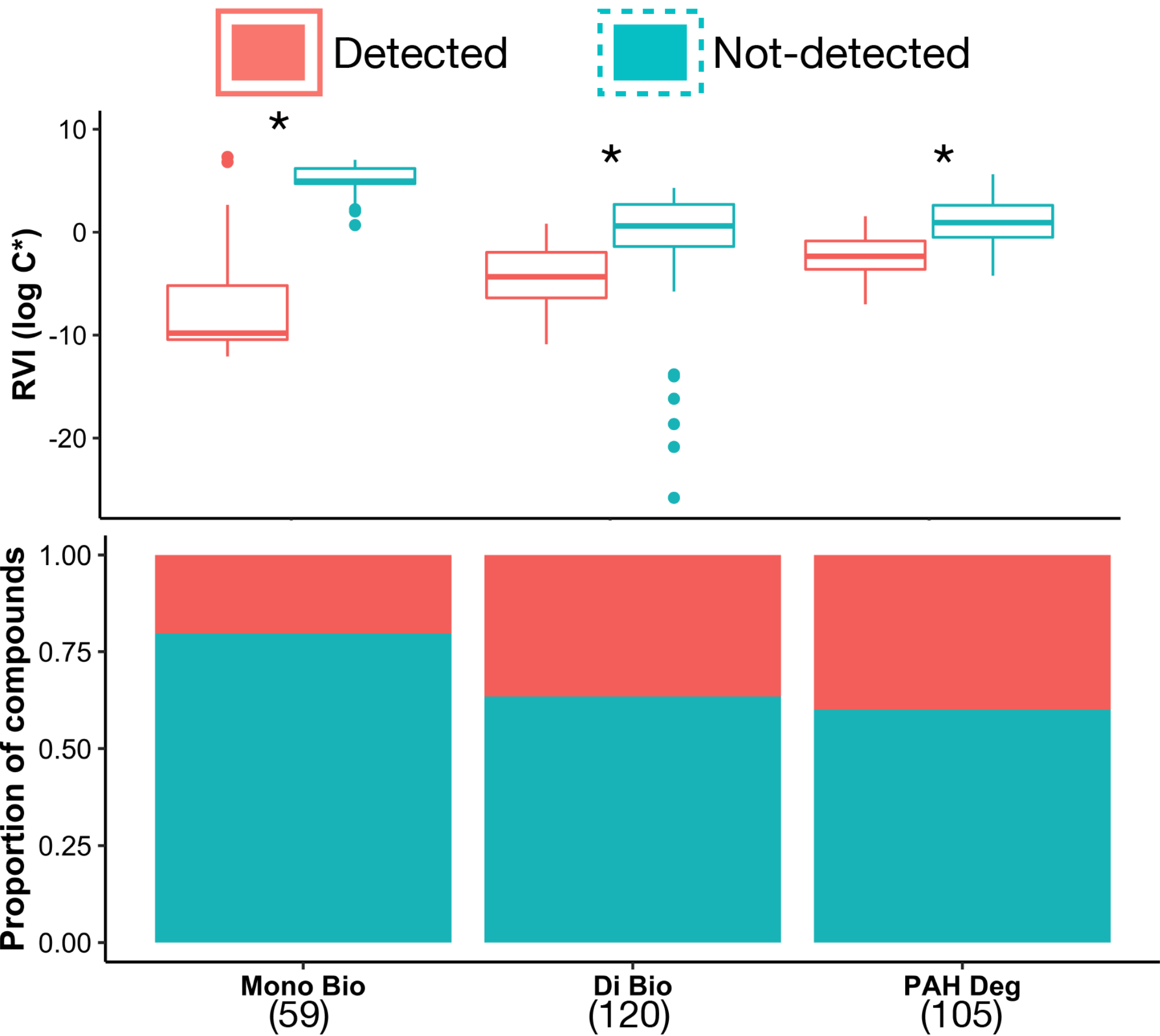
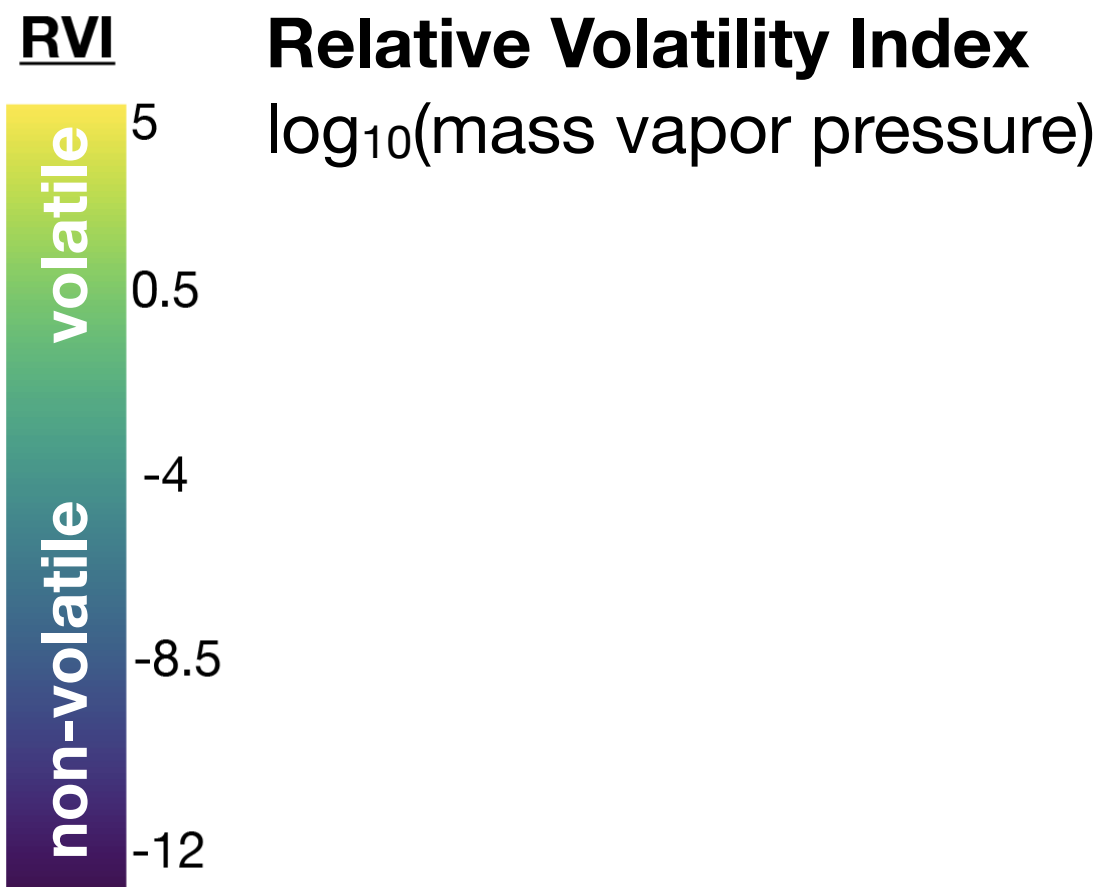
**Honeker et al., (2021)**  
Frontiers in Environmental Sciences

# Do current metabolic approaches underrepresent volatile metabolites?

We find evidence that compounds with higher volatility are disproportionately undetected



- (1) Considered 3 pathways containing VOCs
- (2) Metabolite detected in peat metabolome?
- (3) Predicted metabolite volatility.

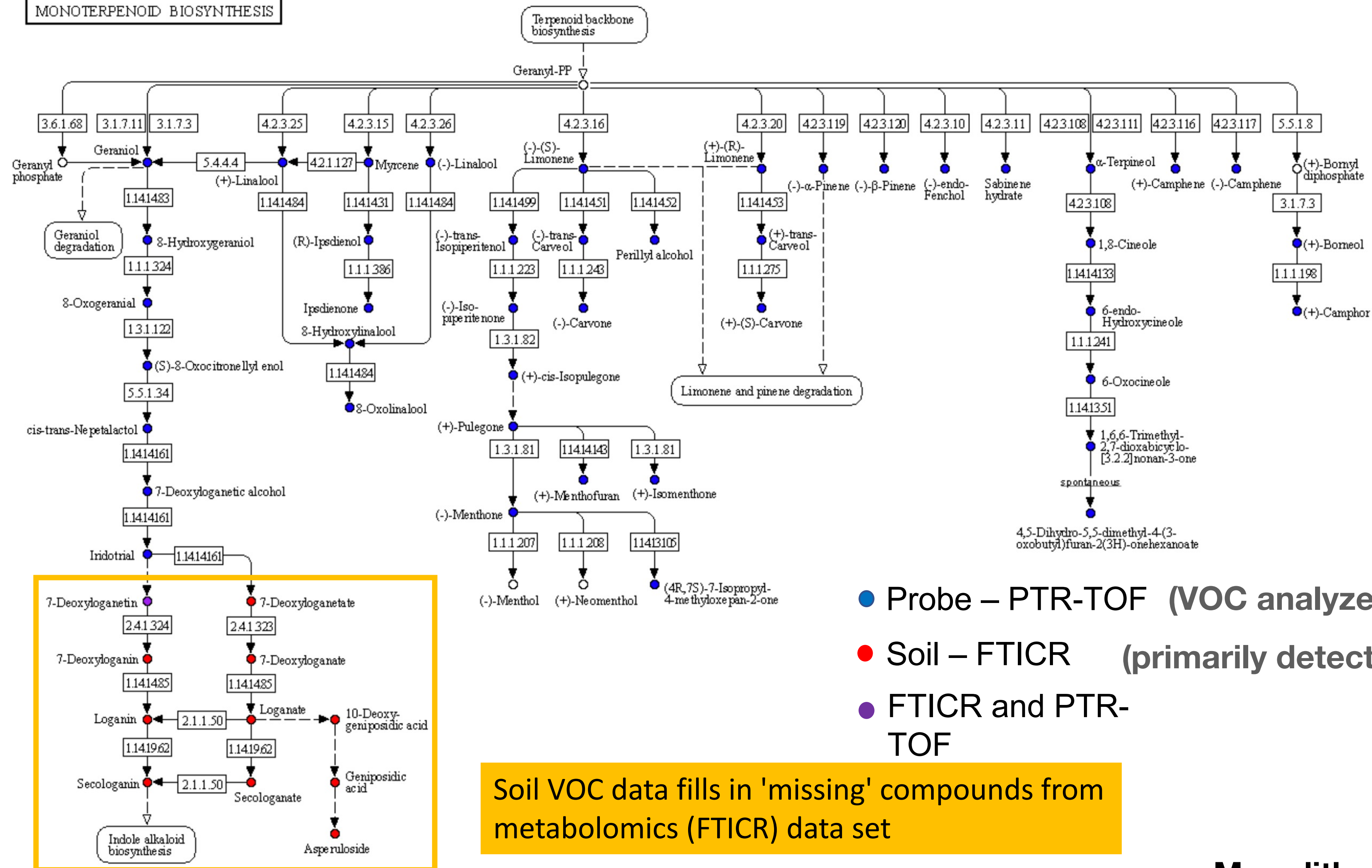




# Compounds with higher volatility are disproportionately undetected

## Potential to fill in 'missing' compounds with VOC measurement methods

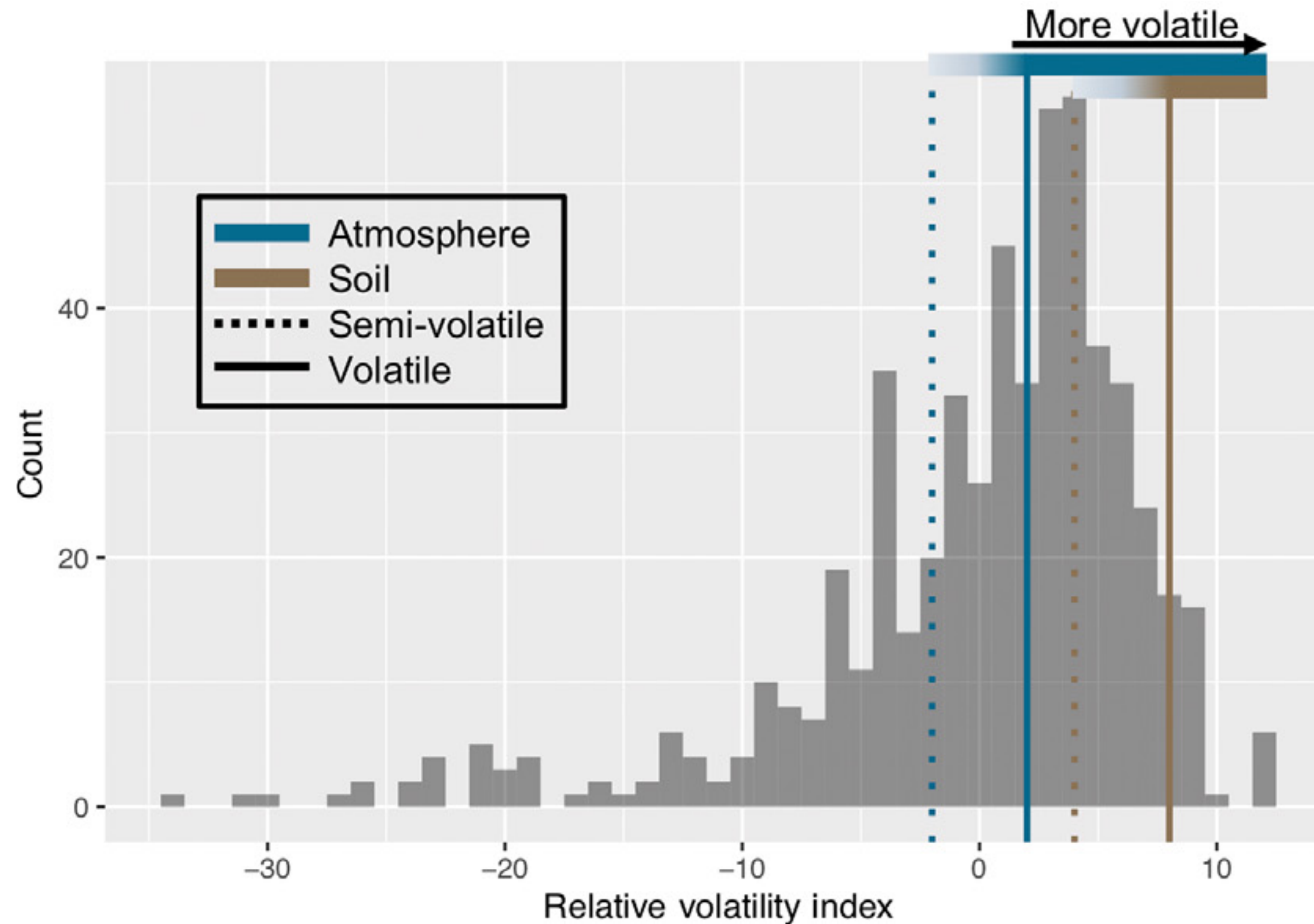
### MONOTERPENOID BIOSYNTHESIS



Meredith et al., unpublished data

# Compounds with higher volatility are disproportionately undetected

A significant number of metabolites may be volatile in soil...





but thresholds for partitioning to gas phase in soil are uncertain.



# Volatility prediction pipeline for metabolomics studies

Predict presence of volatile metabolites in biological systems

 Product ▾ Team Enterprise Explore ▾ Marketplace Pricing ▾  / Sign in Sign up

 Meredith-Lab

Overview Repositories Projects Packages People

Type ▾ Language ▾ Sort ▾

**binder\_volcalc** Public

Repo to hold input files to create a My Binder instances that enables interactive use of volcalc R package

R

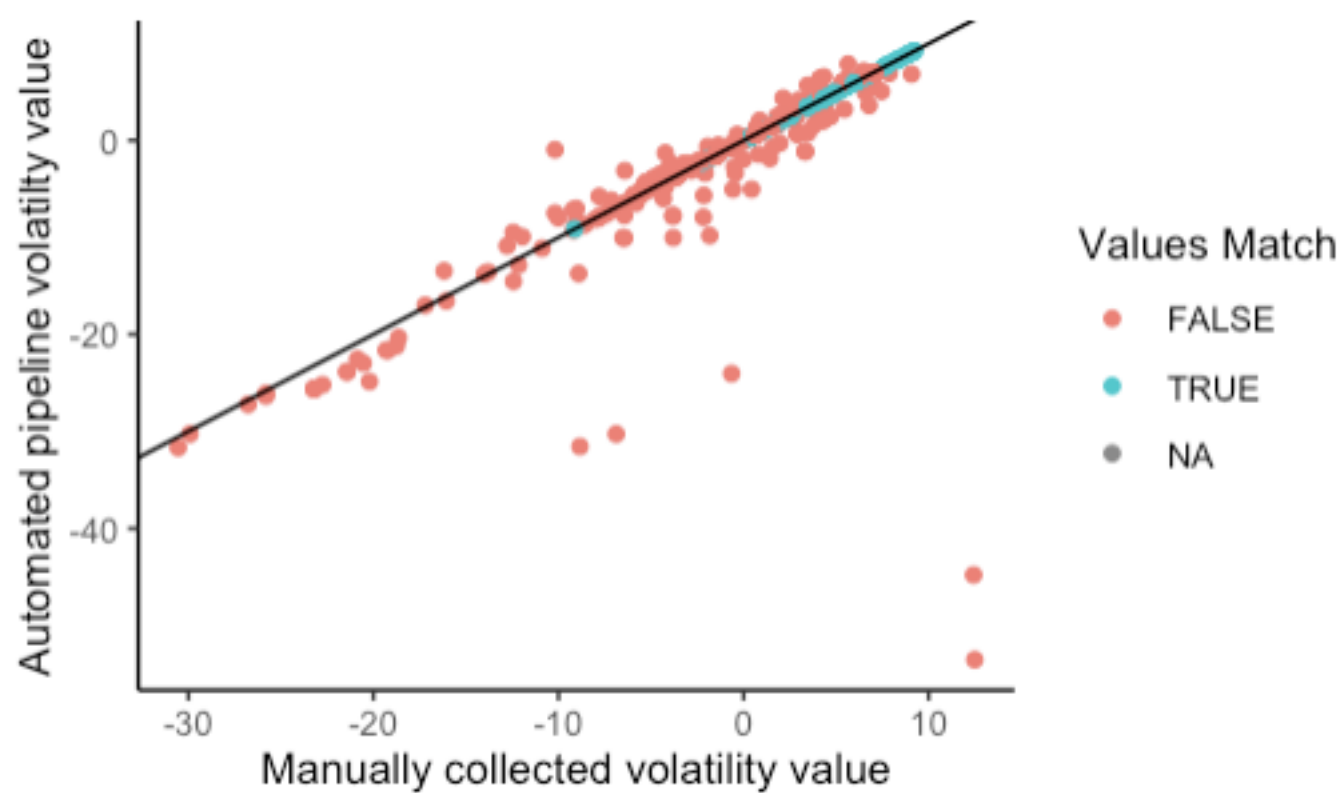
1

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Updated on Apr 15



Kristina Riemer



Parker Geffre

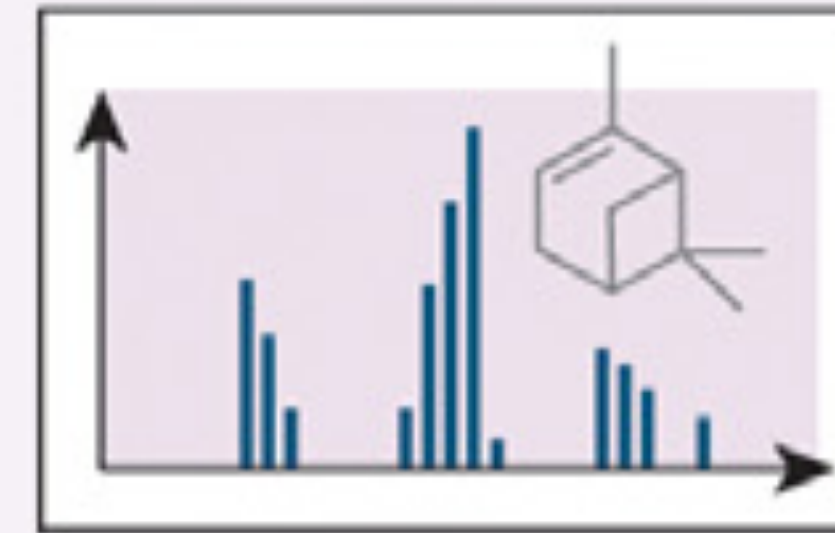
Meredith et al., in prep

# Vision: leverage unifying and contrasting features of volatilomics and multi-omics

Build on areas of common strength

ANALYTICS & INTERPRETATION	DATA INTEGRATION
(C) Unifying features: leverage to improve tools & knowledge	

## VOCs & Metabolites



- Feature detection
- Formula assignment
- Tentative structure
- Putative ID
- Metabolite identification
- **Volatility prediction**

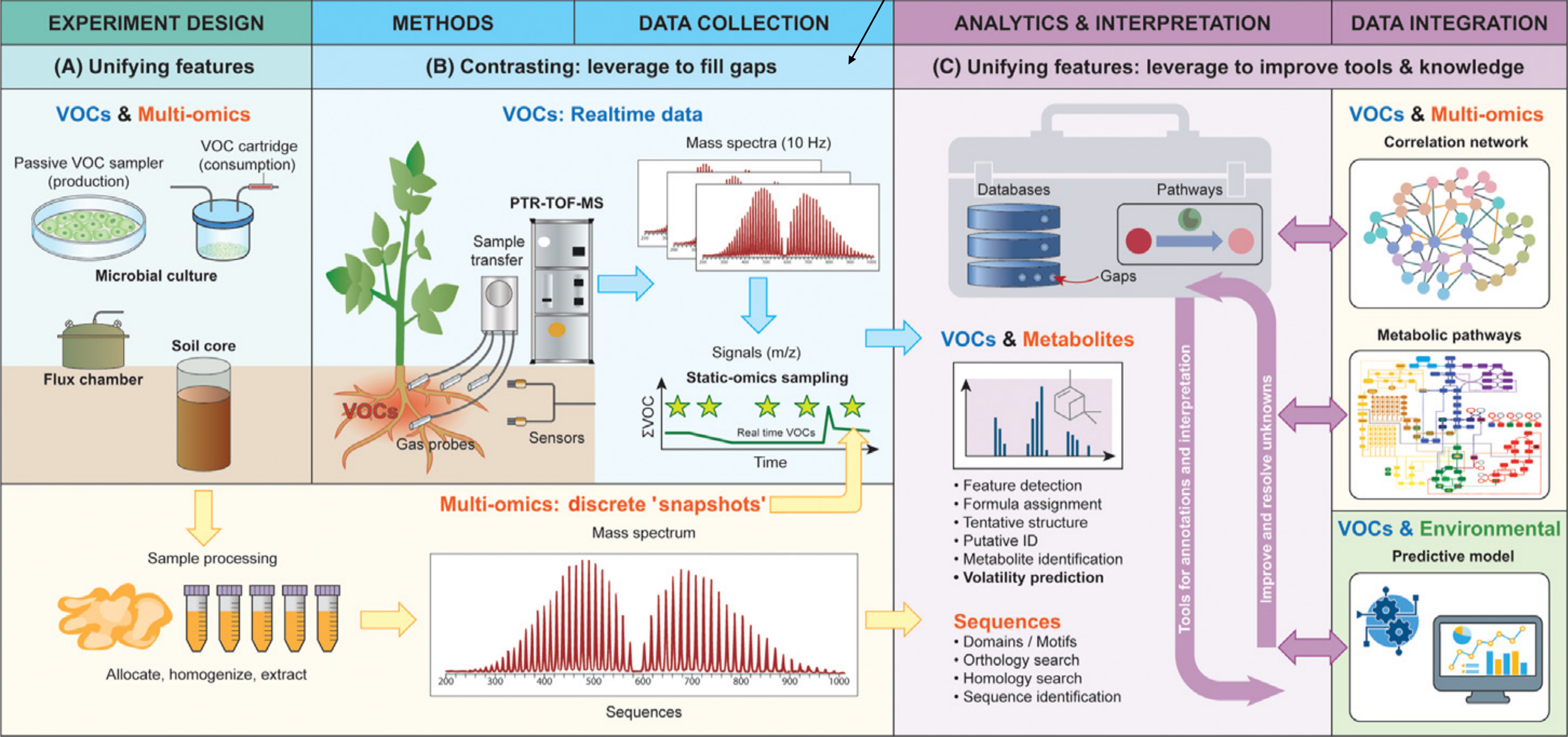
## Sequences

- Domains / Motifs
- Orthology search
- Homology search
- Sequence identification



# Vision: leverage unifying and contrasting features of volatilomics and multi-omics

Build on areas of common strength and leverage contrasts to fill gaps






# Thank you!

Postdoc Position Available!  
Please, get in touch if interested!



*Aerodyne Research*

Signals in the Soil #2034192  
CAREER #2045332

**Laura Meredith**  
laurameredith@arizona.edu  
 @DrLauraMeredith