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LC-HRMS-based metabolomics as a tool to develop analytical methods: How to choose the best extraction protocol when it comes to untargeted analysis?

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Context

In the current poster, different computational and graphical tools applied to LC-HRMS-based untargeted analysis are presented. These tools are used to compare 5 different extraction protocols developed to perform exhaustive untargeted analysis of formulated pesticides residues and microbial metabolites in soil. The comparisons are based on 4 analytical and contextual criteria: (1) the coverage of different types/families of compounds, (2) the quantitative performance, (3) the repeatability, and (4) the capacity to discriminate between contaminated and non-contaminated soils. Each of these tools needs specific usage precautions and presents advantages, limitations and complementarities with the other suggested tools.

The toolbox

Performance

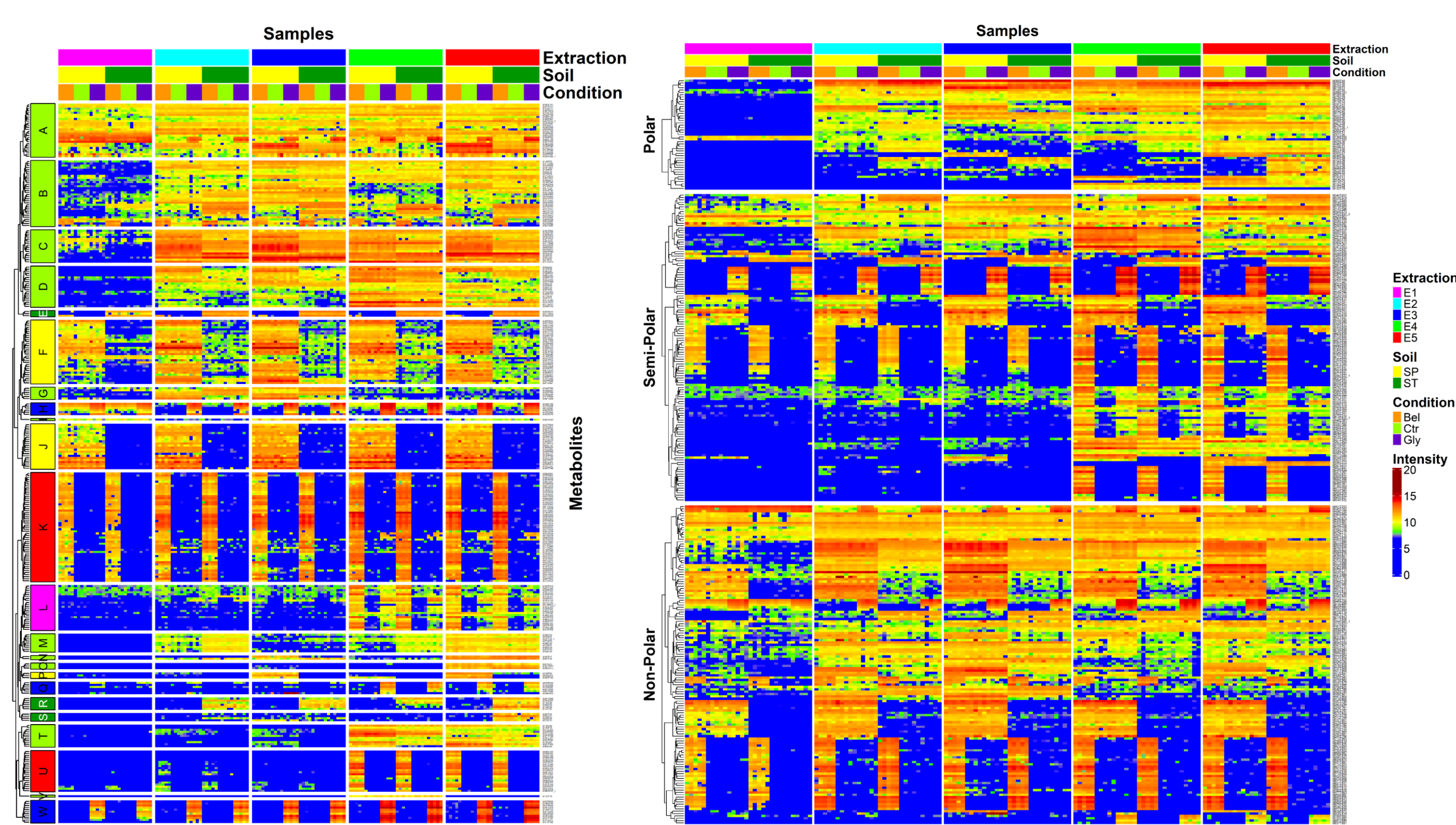


Heatmap + HCA Dendrogram

Adjustable parameters:

- ✓ Distance measuring method and clustering algorithm
- ✓ Metadata organization (based on experimental design)
- ✓ Intensity scale and color contrasts
- ✓ Configuration architecture (holistic, polarity- or origins-segmented, etc.)

Advantages	Limitations
✓ Exhaustive 3D cartography of data	✗ Needs removal of ionization redundancies
✓ Compounds annotation is not mandatory	✗ No information on chemical families

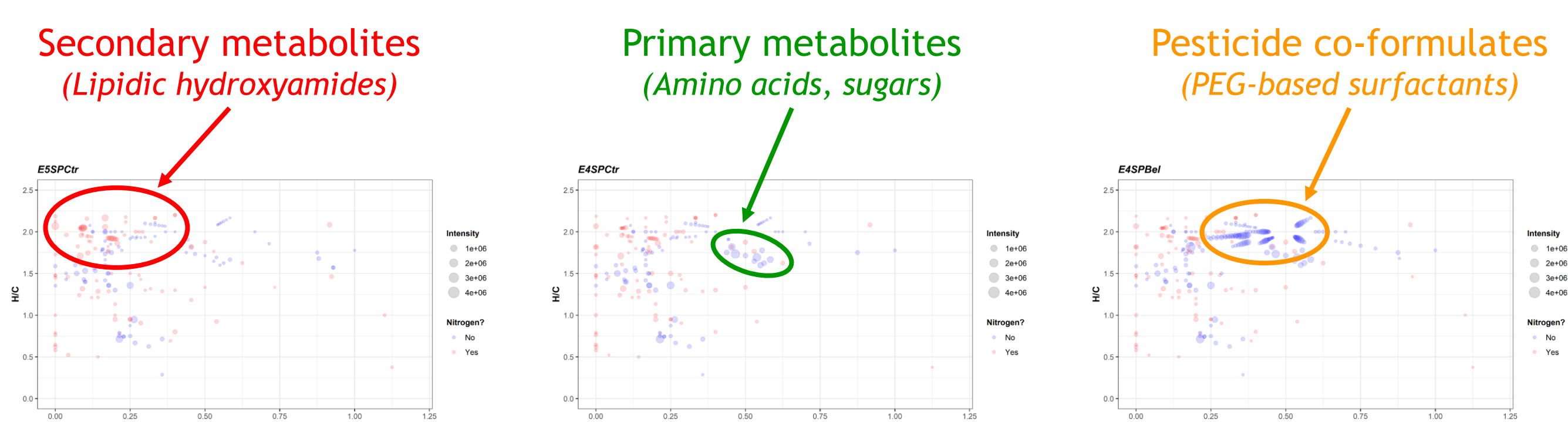


Van Krevelen Diagram

Mandatory precautions:

- ✓ Molecular formula annotation (level 4) is needed
- ✓ Needs removal of ionization redundancies (advantage to have LC coupling to HRMS)
- ✓ Intensity scaling needs to be carefully optimized

Advantages	Limitations
✓ Chemical families coverage assessment	✗ Non-exhaustive cartography
✓ Revealing heteroatoms-specific families	✗ Results quality depends on HRMS power



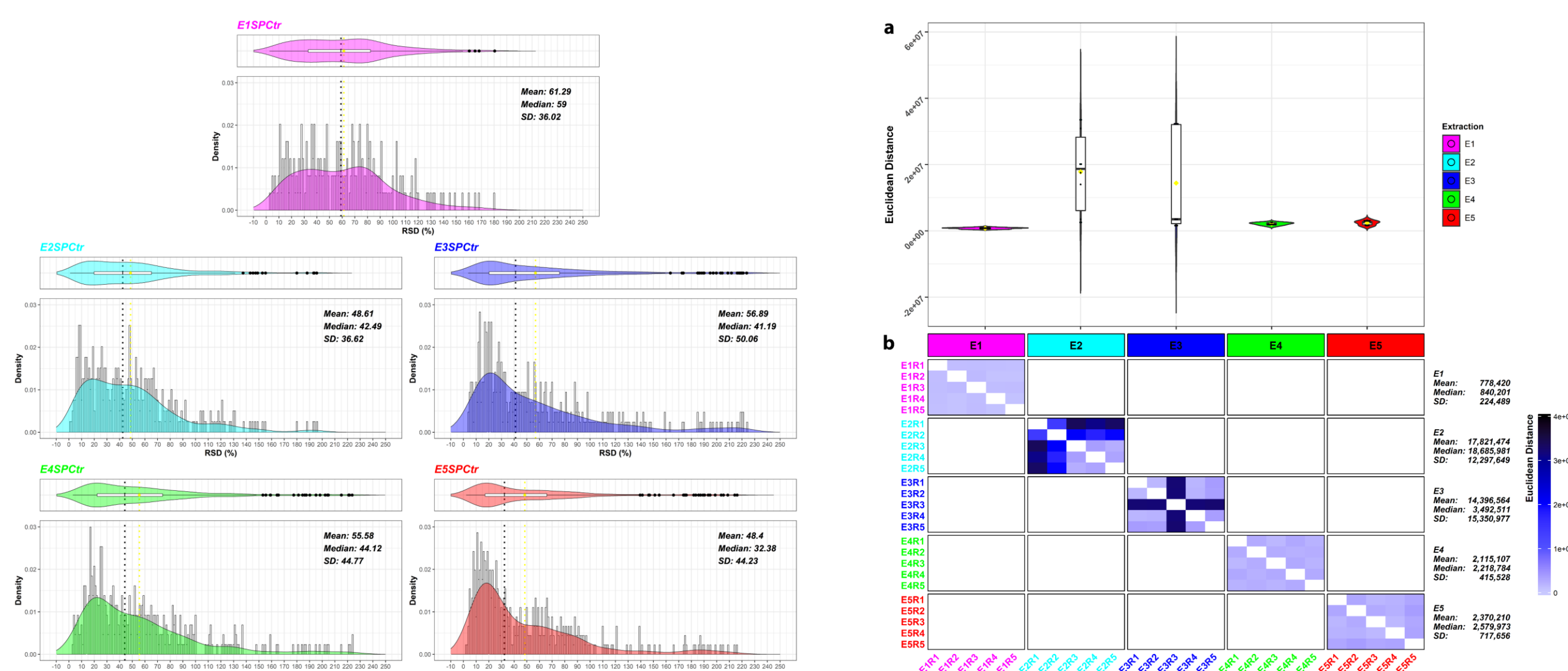
Repeatability



All ions-RSDs vs. Euclidean Distances

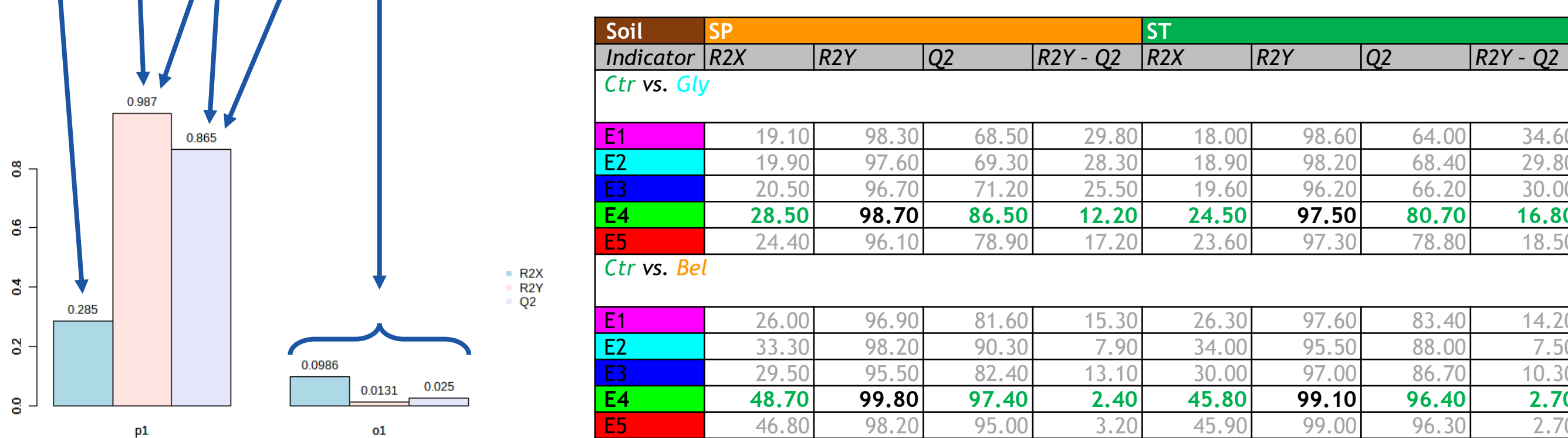
Mandatory precautions:

- All ions-RSDs
 - ✓ Adjusting noise to zero to avoid insignificant amplification of RSDs
- Euclidean Distances
 - ✓ Standardizing ion intensities to avoid "size effects" (e.g. logarithmic transformations)



Discrimination Power

R²X: Percentage of the explained variation that is causing the discrimination
R²Y: Correlation between the discrimination and the tested factor (*here: contamination*)
R²Y - Q²: Significance of the discrimination (overfitting assessment)
Q²: Discrimination predictivity: The chance (in %) to reliably determine the sample type
o_i: Systemic variations that are orthogonal to the tested factor



For more information

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LC-HRMS-Driven Computational Toolbox to Assess Extraction Protocols Dedicated to Untargeted Analysis: How to Ease Analyzing Pesticide-Contaminated Soils?

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Web Networks

