

FROM FOLK REMEDY TO DISCOVERY: AN HPLC-HRMS UNTARGETED METABOLOMICS WORKFLOW UNVEIL SPECIES-SPECIFIC METABOLITES IN SIDERITIS HERBA

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A quick brief before we begin... X

Sideritis herba (Ironwort)

Aerial parts of 4 species (*S. scardica*, *S. clandestina*, *S. raeseri*, *S. syriaca*).

Traditional use (HMPC*)

Relieve coughs (colds) & mild GI discomfort (infusions/decoctions).

Knowledge Gap

Despite many studies, **phytochemistry is incomplete**

Need for **untargeted metabolomics**
+ **dereplication** to explore chemical diversity.

*HMPC = Committee on Herbal Medicinal Products (European Medicines Agency)

Aim of our study X -

Use an **untargeted approach** to:

- Distinguish the 4 *Sideritis* species
- Rank their characteristic metabolites
- Prioritize potentially novel & bioactive compounds

How? By using **multivariate statistics** & **molecular networking**



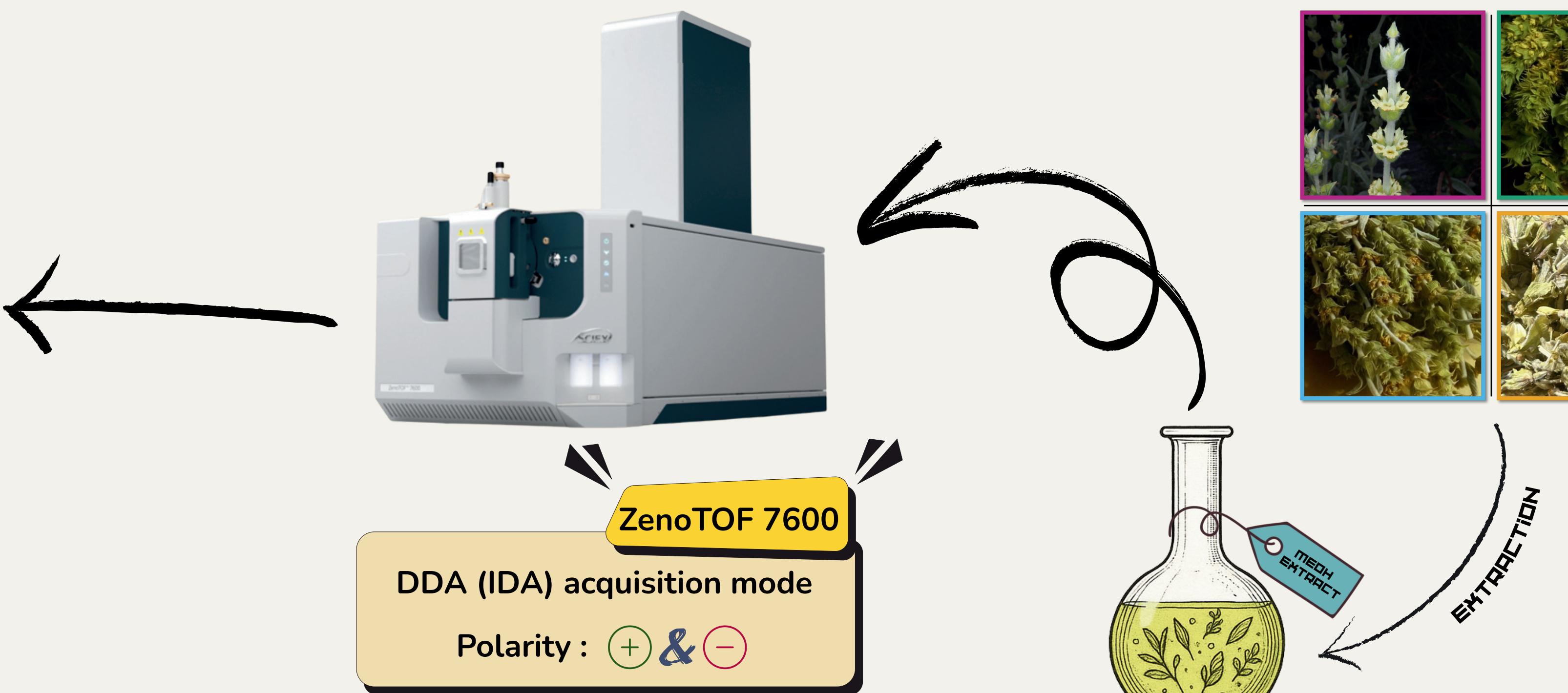
Raw_Data_QC

mzmine

Calculation & Checking

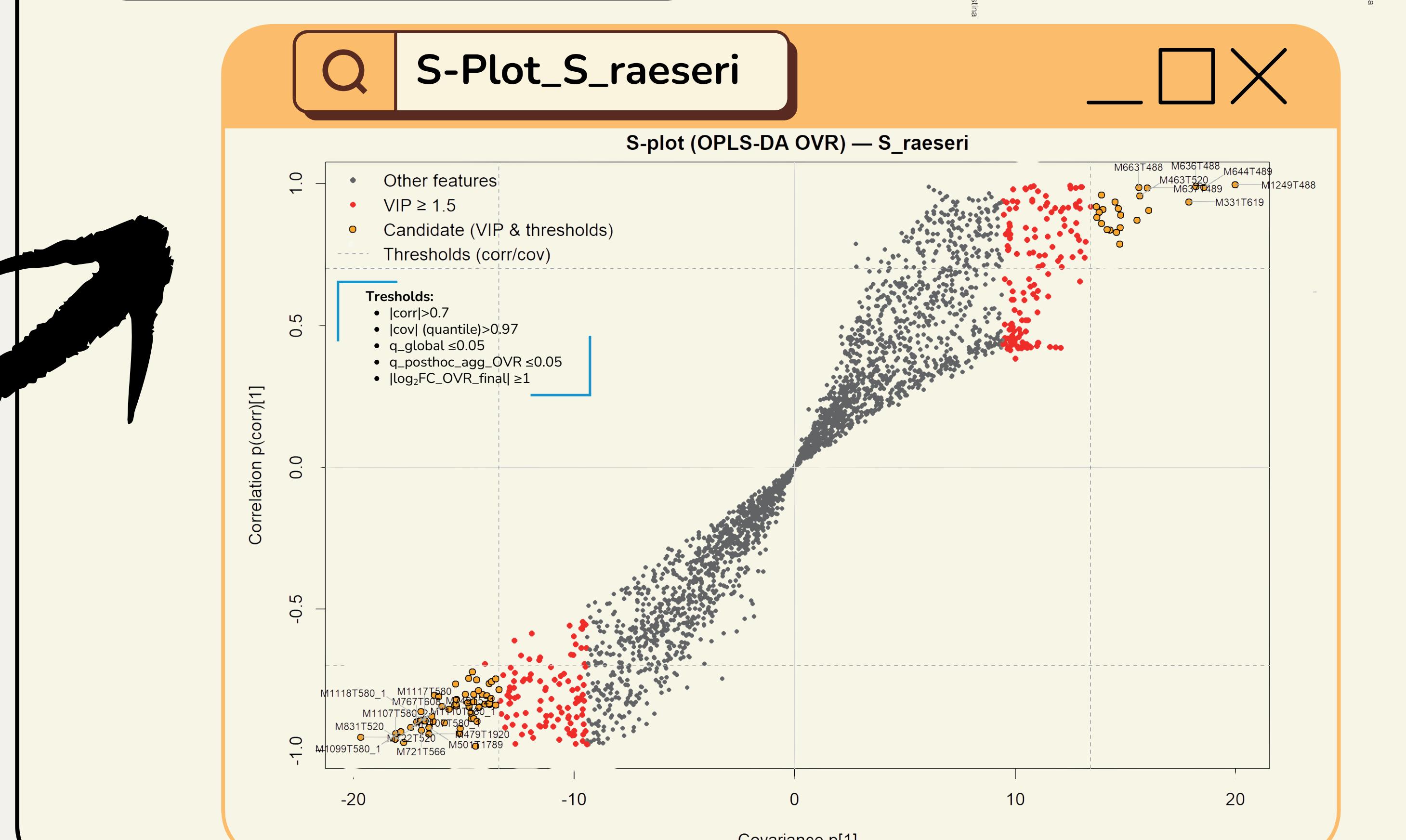
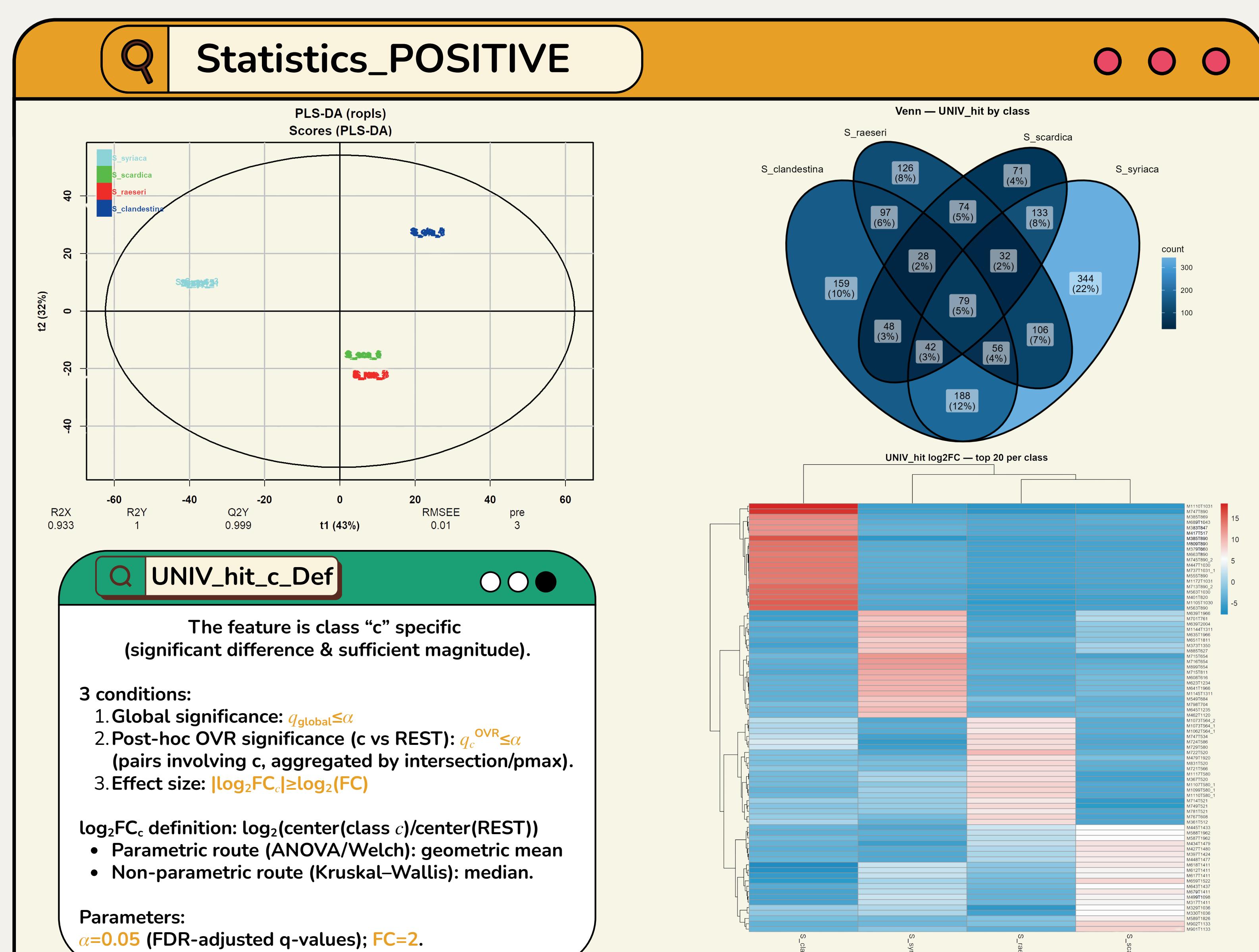
- RT alignment
- Accuracy
- Noise threshold

Visualisation



W4M_workflow (XCMS)

Preprocessing



Acknowledgement

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Poster created with canva.com

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