

# 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... ✕

### 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.

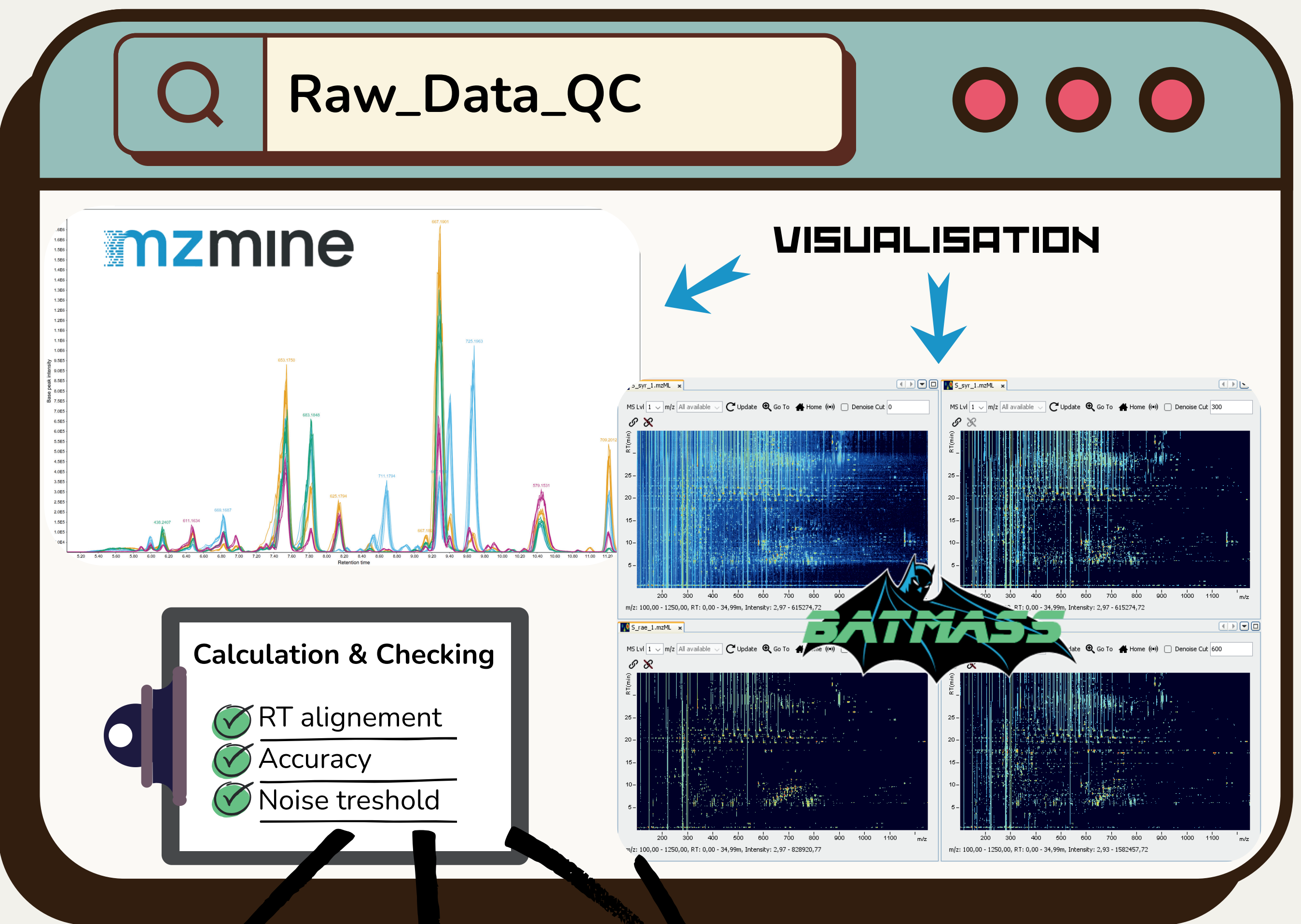
\*HMPC = Committee on Herbal Medicinal Products (European Medicines Agency)

## Aim of our study ✕ ⊖

Use an **untargeted approach** to:

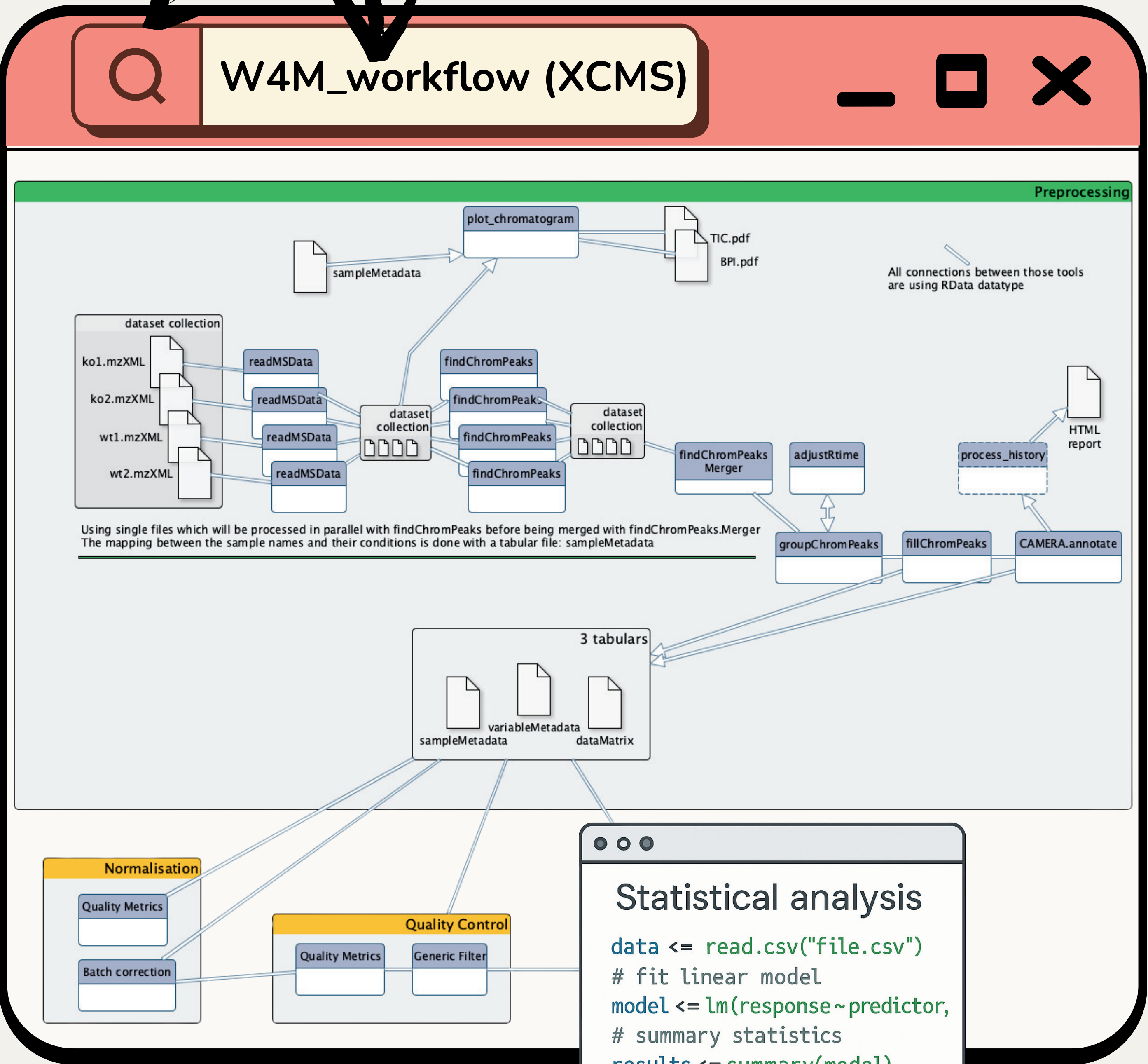
- ✓ Distinguish the 4 *Sideritis* species
- ✓ Rank their characteristic metabolites
- ✓ Prioritize potentially novel & bioactive compounds

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

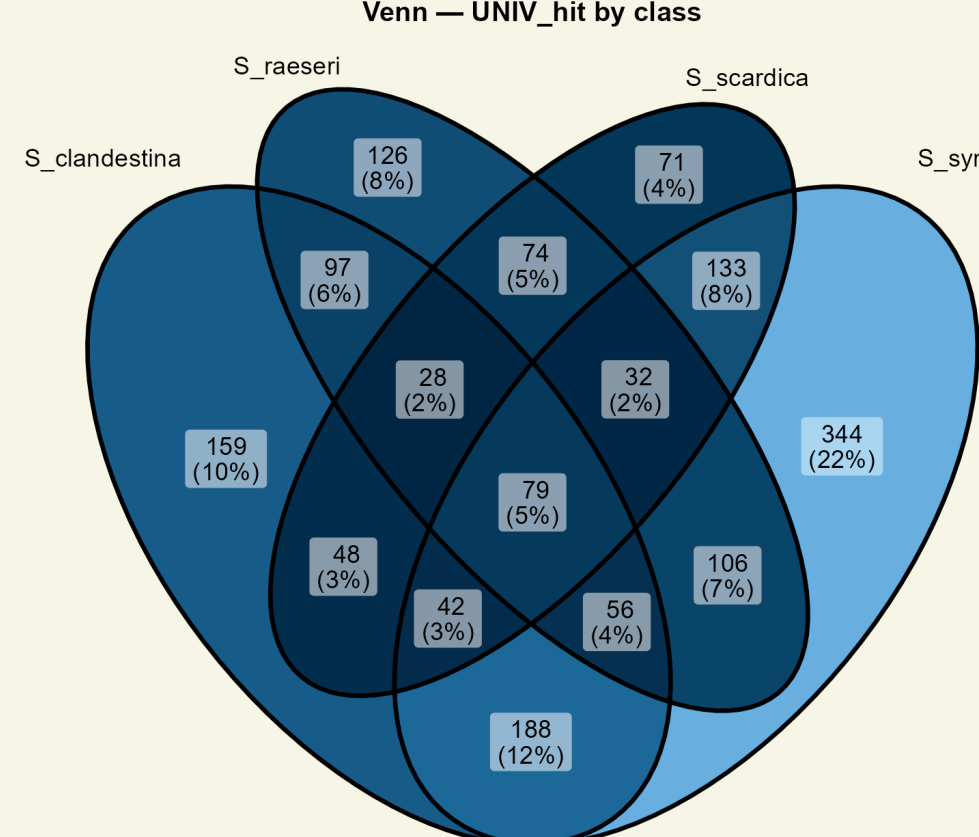
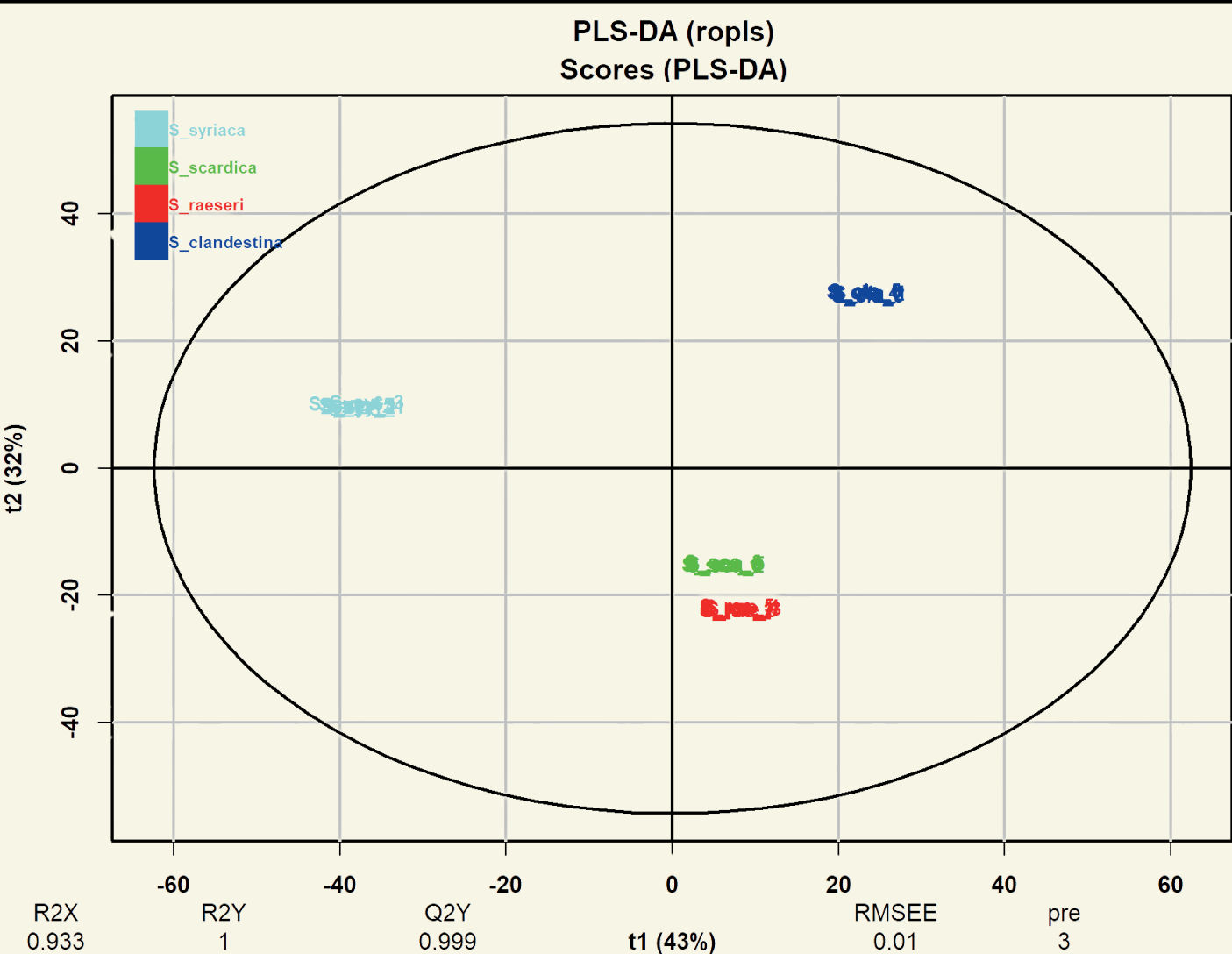


DDA (IDA) acquisition mode

Polarity : + & -



## Statistics\_POSITIVE



**UNIV\_hit\_c\_Def**

The feature is class "c" specific (significant difference & sufficient magnitude).

3 conditions:

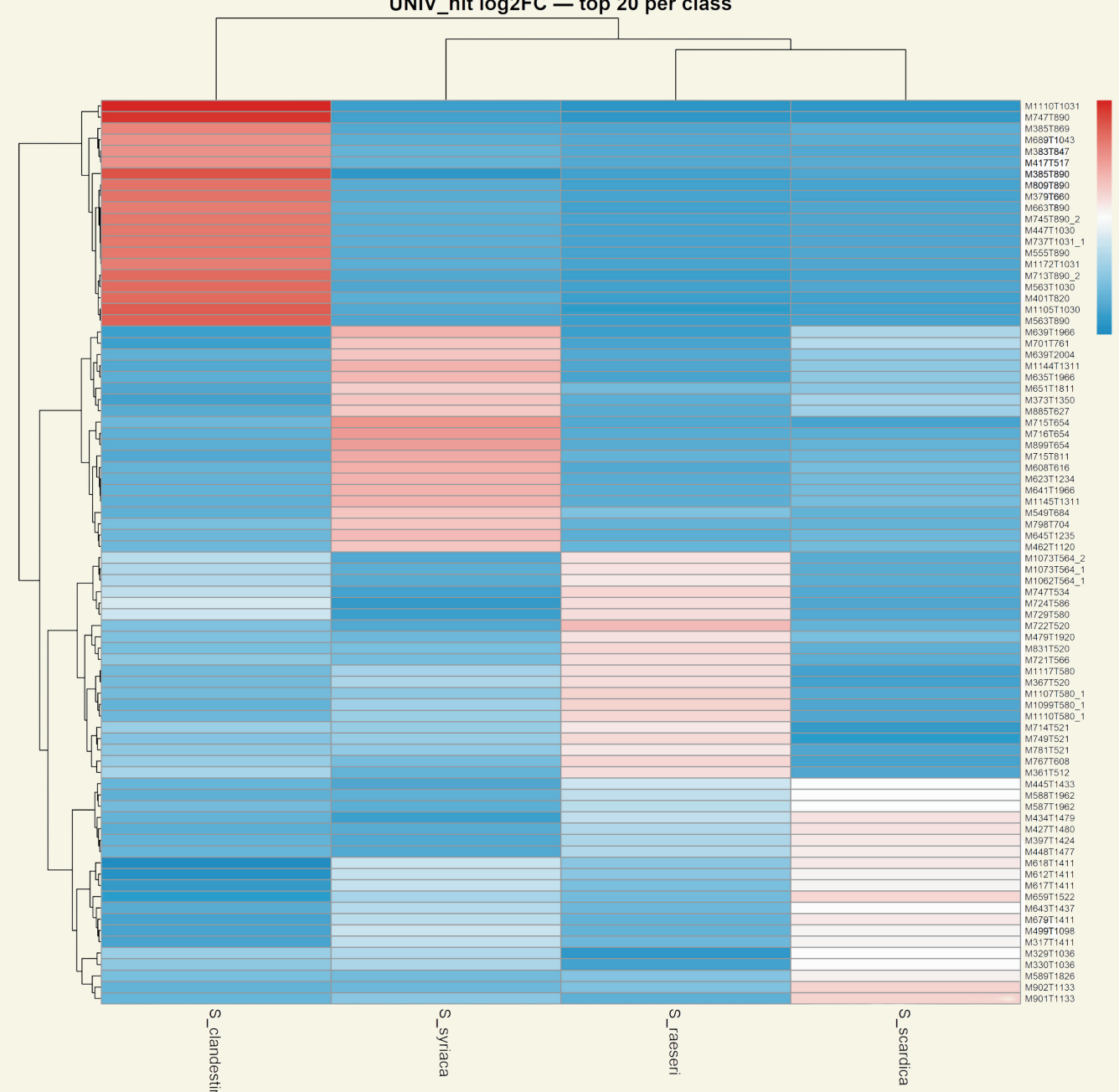
1. Global significance:  $q_{global} \leq \alpha$
2. Post-hoc OVR significance (c vs REST):  $q_{c,OVR} \leq \alpha$  (pairs involving c, aggregated by intersection/pmax).
3. Effect size:  $|\log_2 FC_c| \geq \log_2 FC$

$\log_2 FC_c$  definition:  $\log_2(\text{center}(\text{class } c) / \text{center}(\text{REST}))$

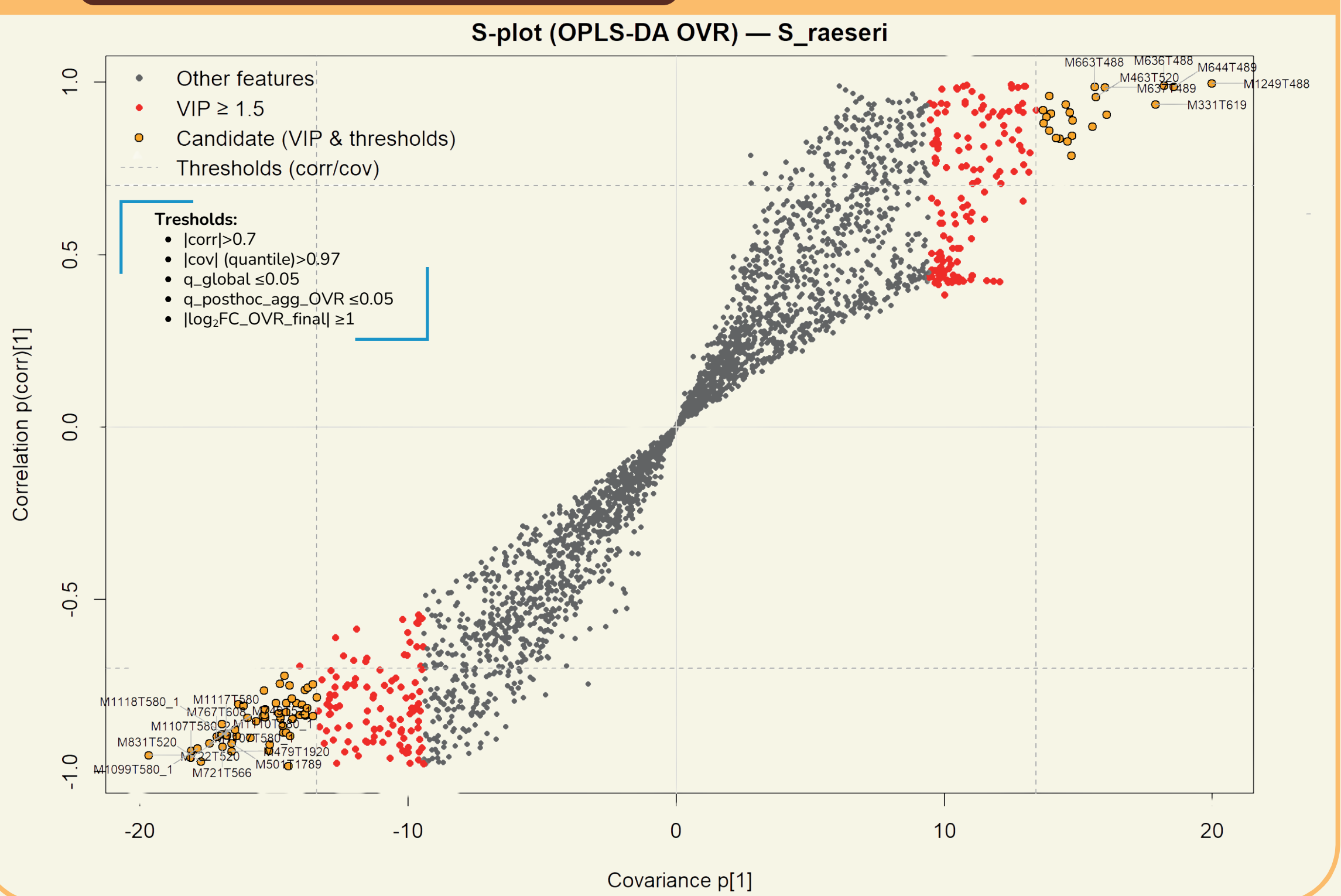
- Parametric route (ANOVA/Welch): geometric mean
- Non-parametric route (Kruskal-Wallis): median.

Parameters:

- $\alpha=0.05$  (FDR-adjusted q-values);  $FC=2$ .



## S-Plot\_S\_raeseri



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Poster created with canva.com

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