



Data analysis strategies with the use of STOFF-IDENT (SI) and DAIOS

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Background

- The comparison of the non-target screening (NTS) results among different laboratories is currently difficult due to the use of different databases and reference standards
- Data analysis and substance identification is currently possible, but with extensive manual effort
- Currently there is no harmonised NTS-Workflow
- The integration of databases and tools is required

Results / Outlook

- A structured method is created
- Comparability of results from different laboratories is possible by using a common workflow
- Establishment of a procedure for the identification of Trace Organic Substances in aquatic environments
- Effective use of necessary tools for data analysis on the working platform **FOR-IDENT**

Methods

RPLC-HRMS(MS) (HILIC)-RPLC-HRMS
TOF
Q-TOF



or



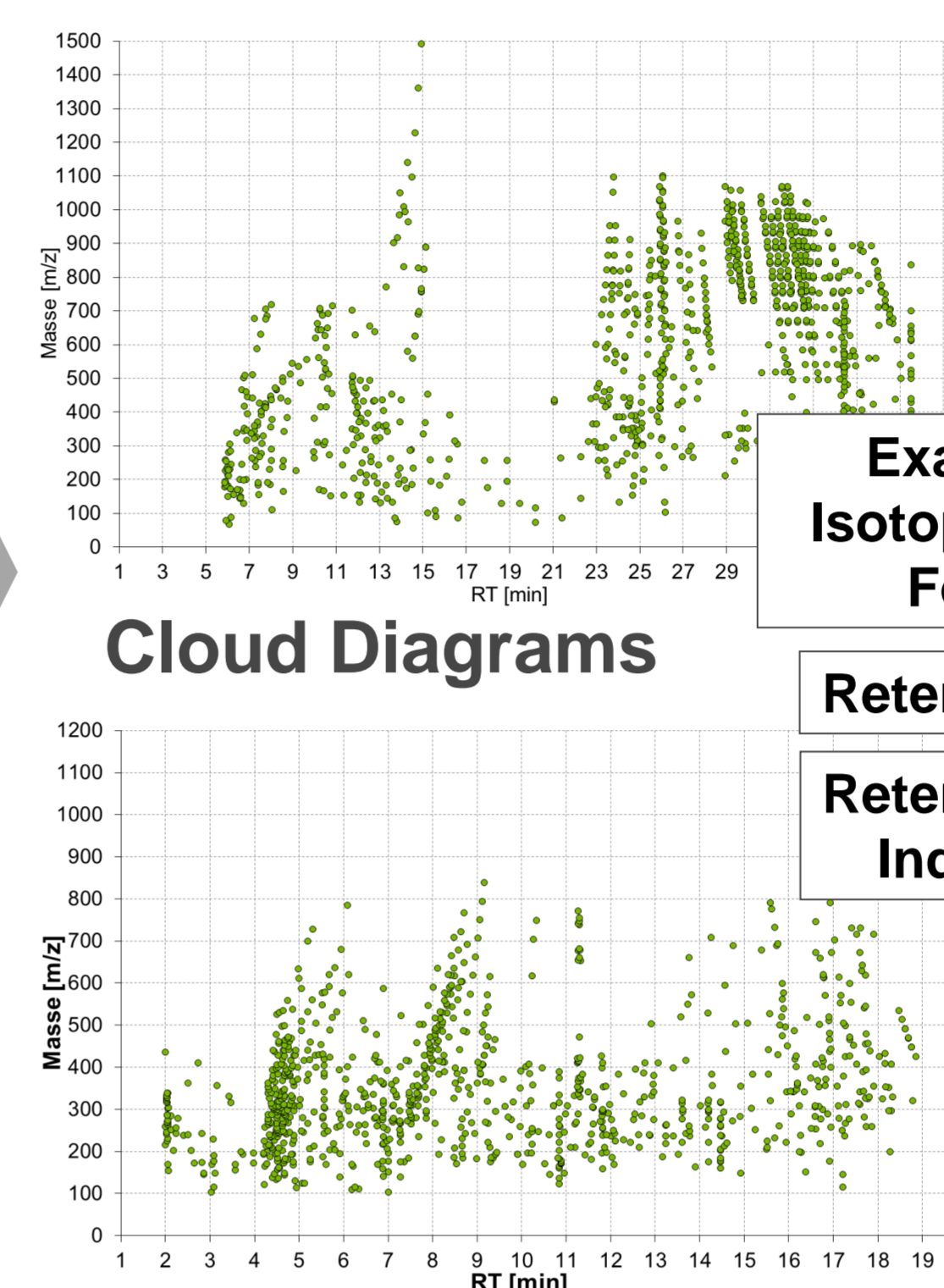
Analysis using standardized NTS-Workflows

Feature Finding
Feature Validation

Database Supported
Substance
Identification

Database:
STOFF-IDENT

Database:
DAIOS



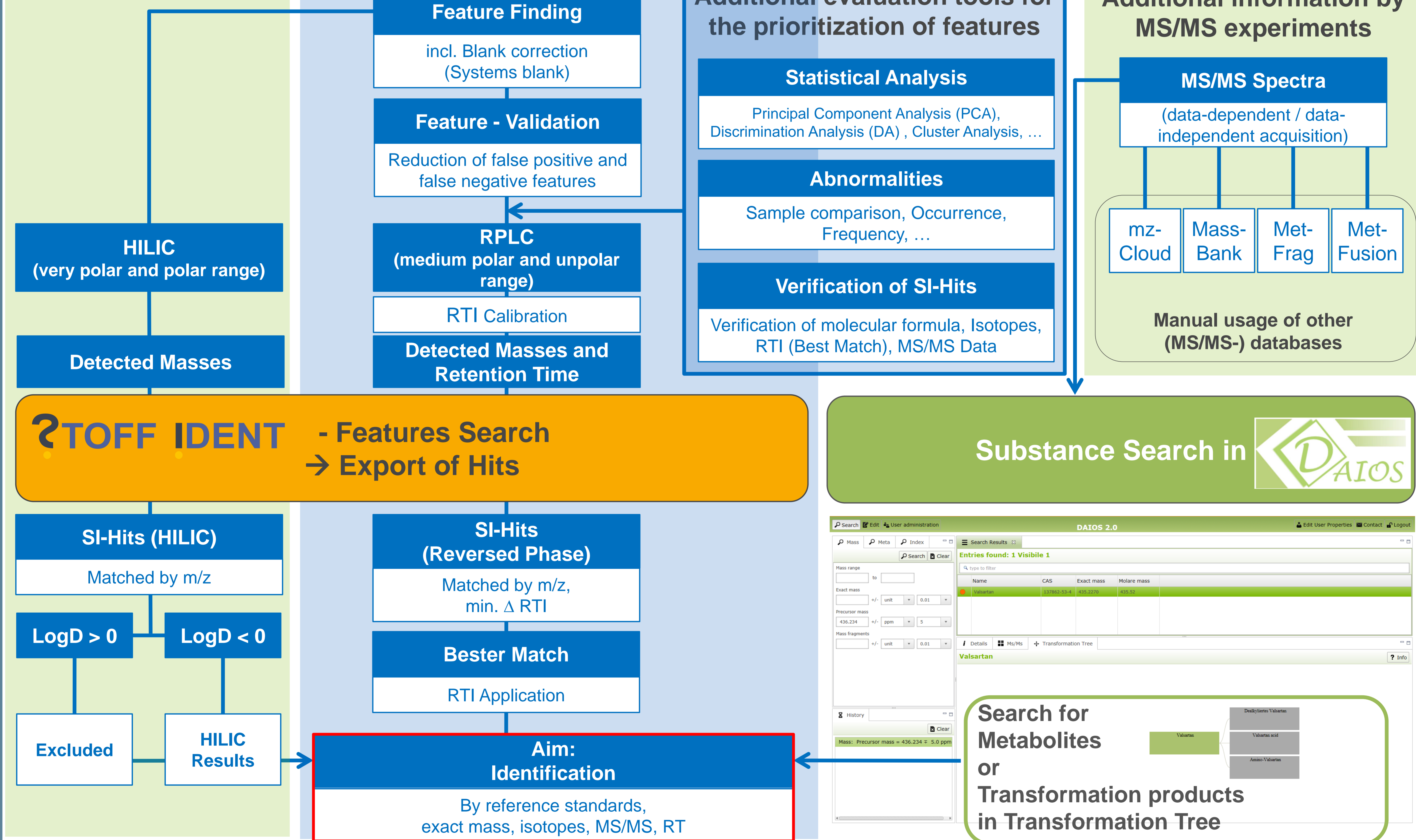
Non-Target Screening Workflows

Additional information by HILIC-HRMS

RPLC-HRMS(/MS)

Additional evaluation tools for the prioritization of features

Additional information by MS/MS experiments



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