



New strategies and workflows in the 'Hidden-Target Screening' approach

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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 workflows, databases and reference standards
- Compound Databases with huge amount of molecules are available open-access but mostly without categorization by research area
- Analytical databases for special instruments or instrument manufacturers are available open-access but not linked to compound databases or others
- Data analysis and substance identification is therefore currently possible, but with extensive manual effort
- Currently there is no harmonised NTS-Workflow
- The integration of databases and tools is required

Methods

(HILIC)-RPLC-HRMS (ToF or Q-ToF)

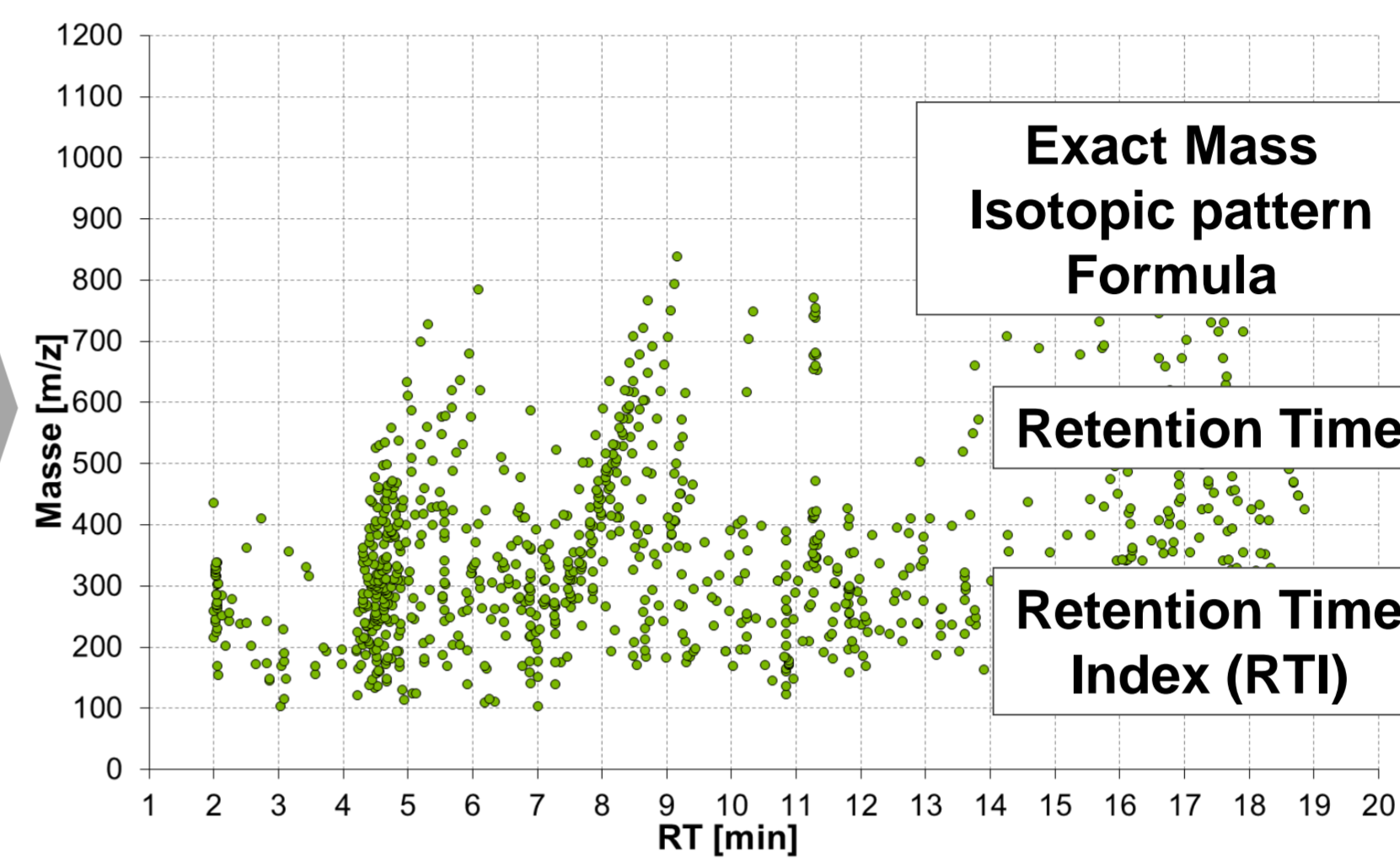


Analysis using standardized NTS-Workflows

Feature Finding
Feature Validation

Database Supported
Substance
Identification

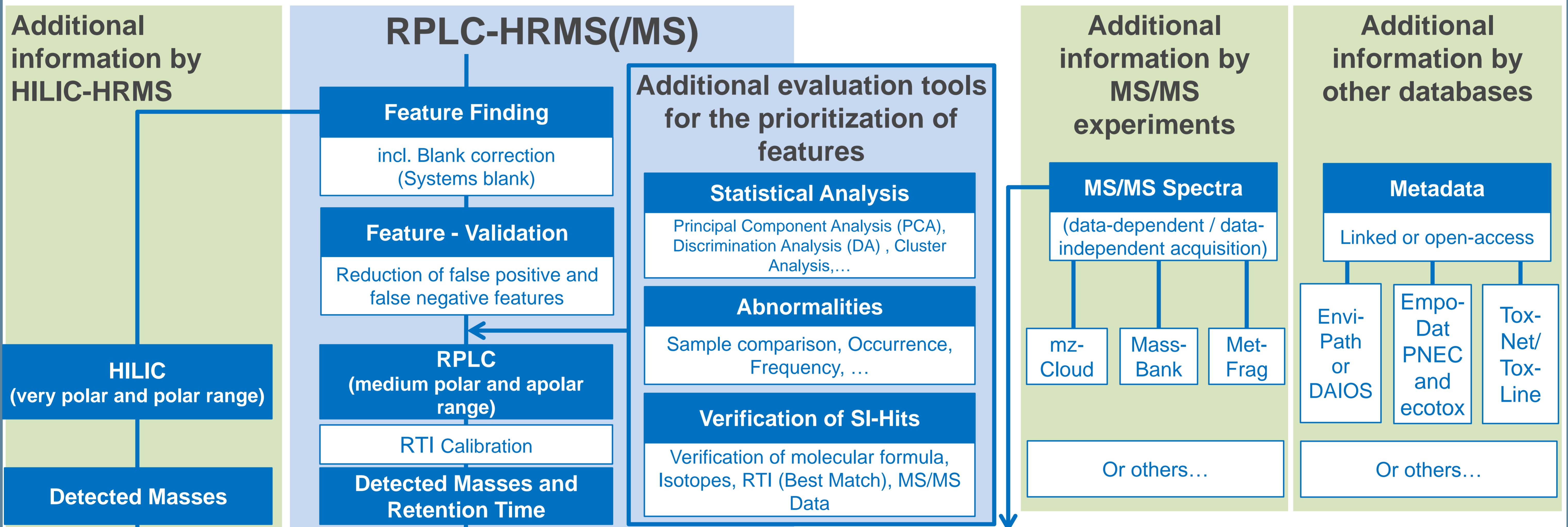
Cloud Diagram



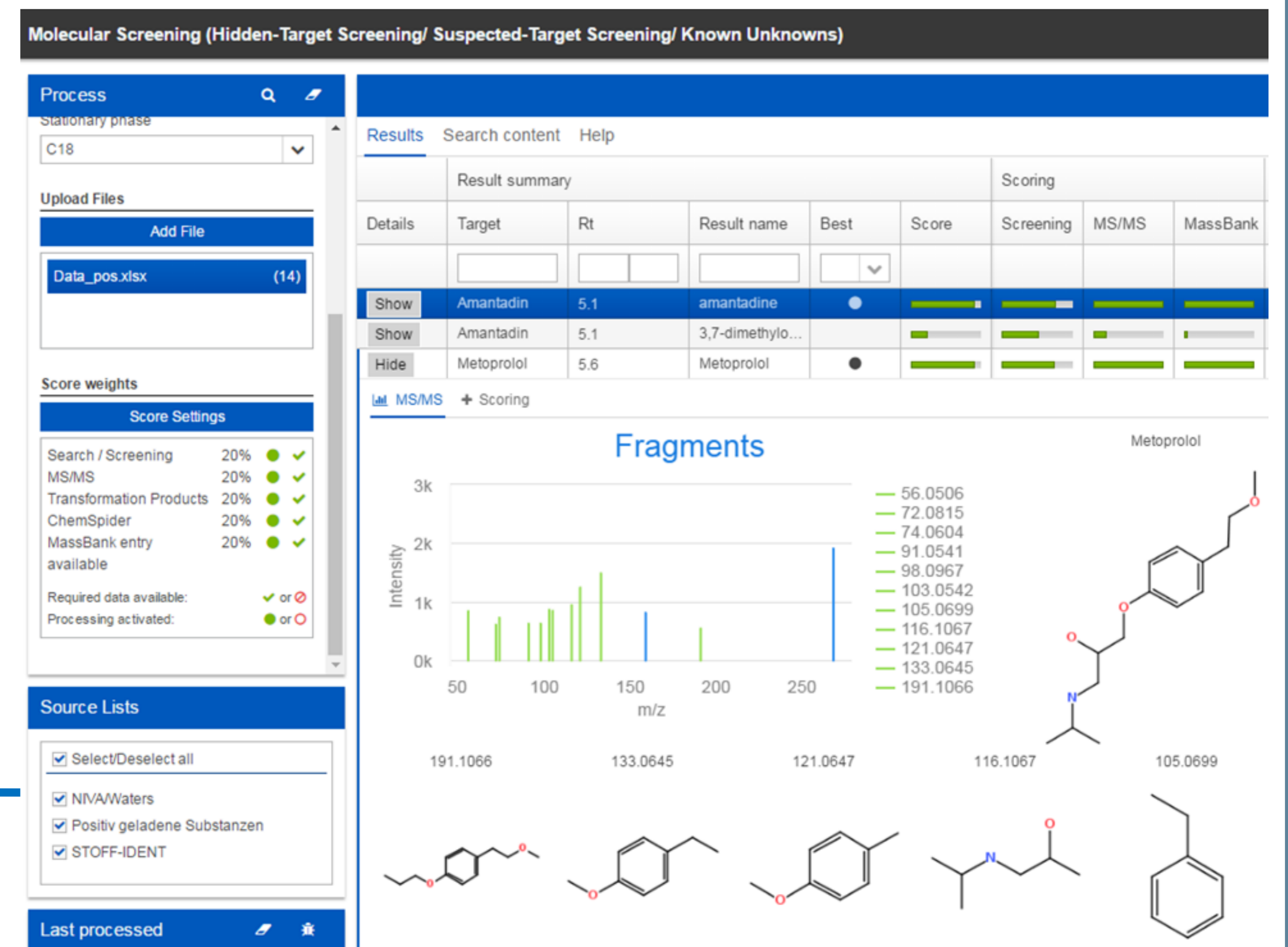
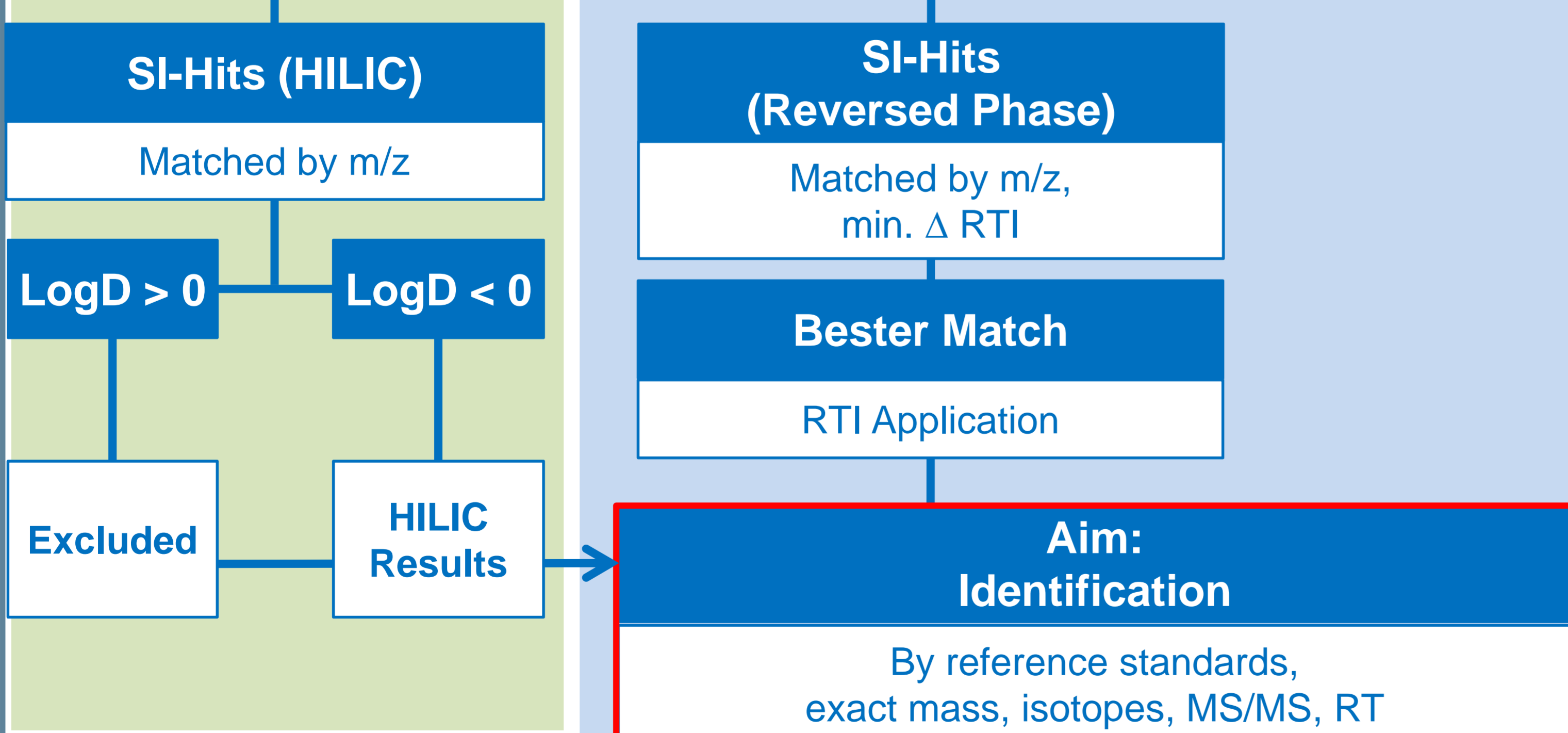
Database:

FOR-IDENT
(incl.
STOFF-
IDENT, RTI,
analytical
databases)

Hidden-Target Screening Workflows



? TOFF IDENT - Features Search
→ Export of Hits



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