

LC-MS Workflow of non-target and suspected-target screening including the Database STOFF-IDENT¹

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Overview



Non-target screening workflow

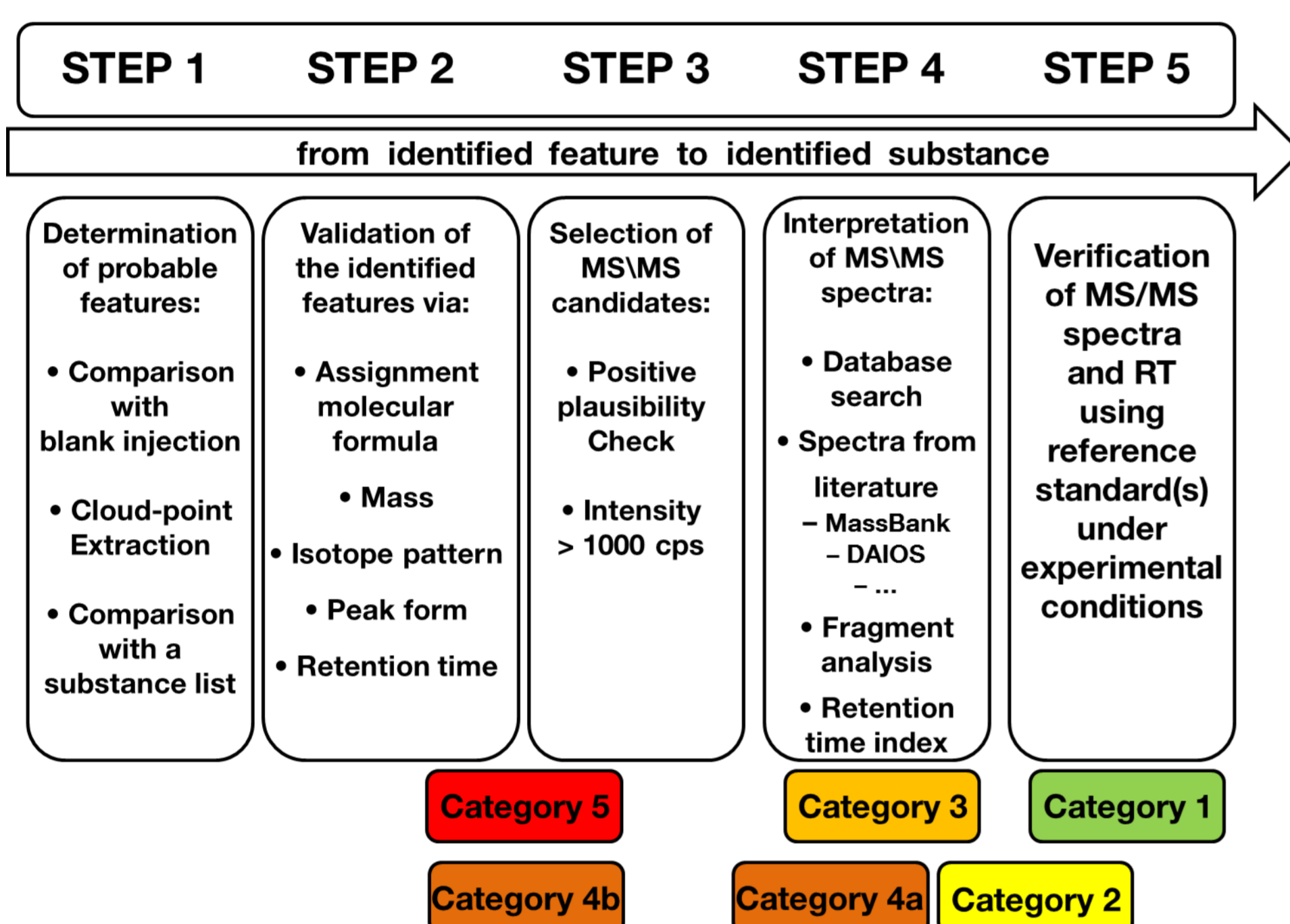


Figure 1: Identification workflow, incl. categorisation of results [2]

Step 1 – feature finding

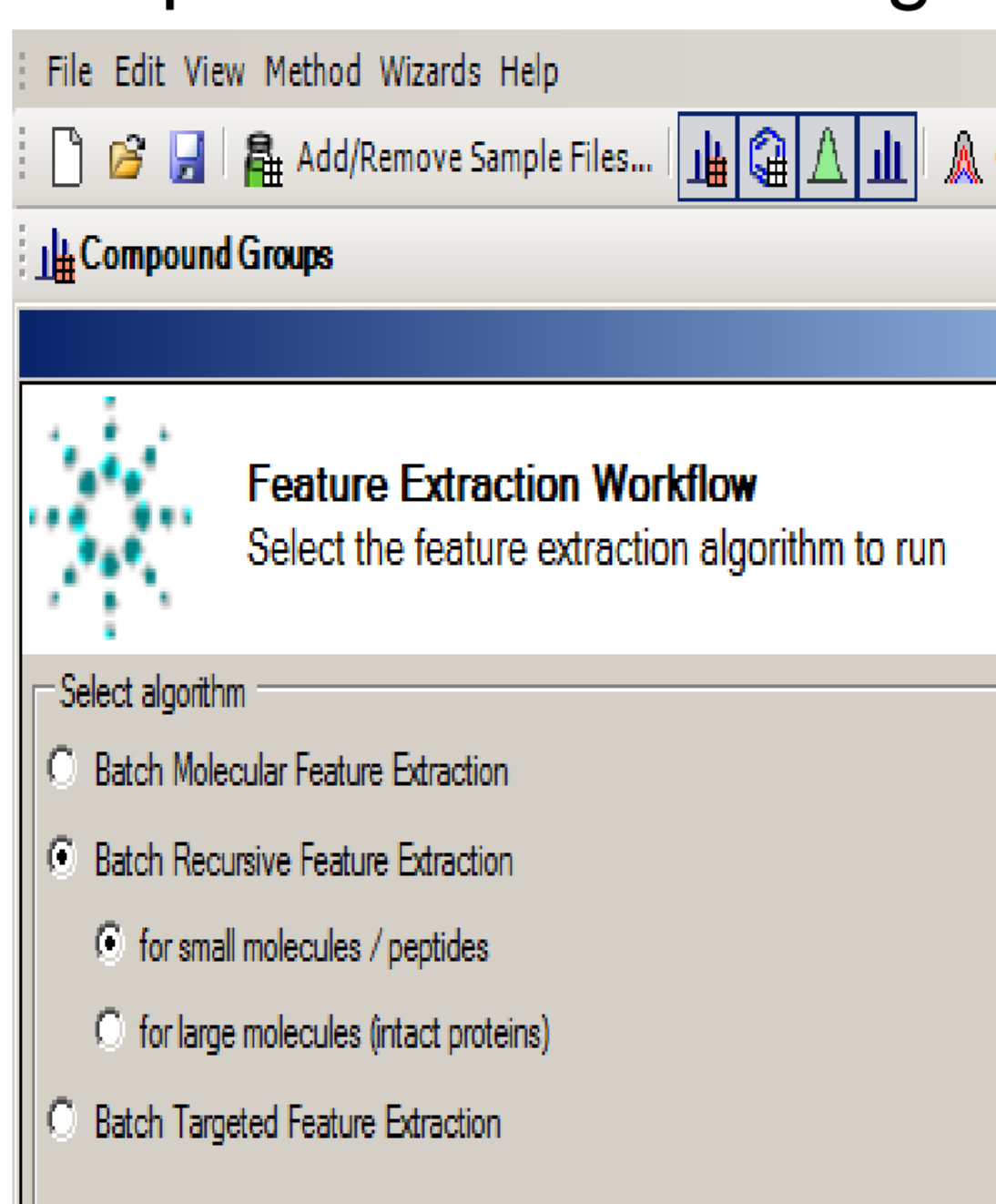


Figure 2: example of feature finding program

Step 2 – feature validation

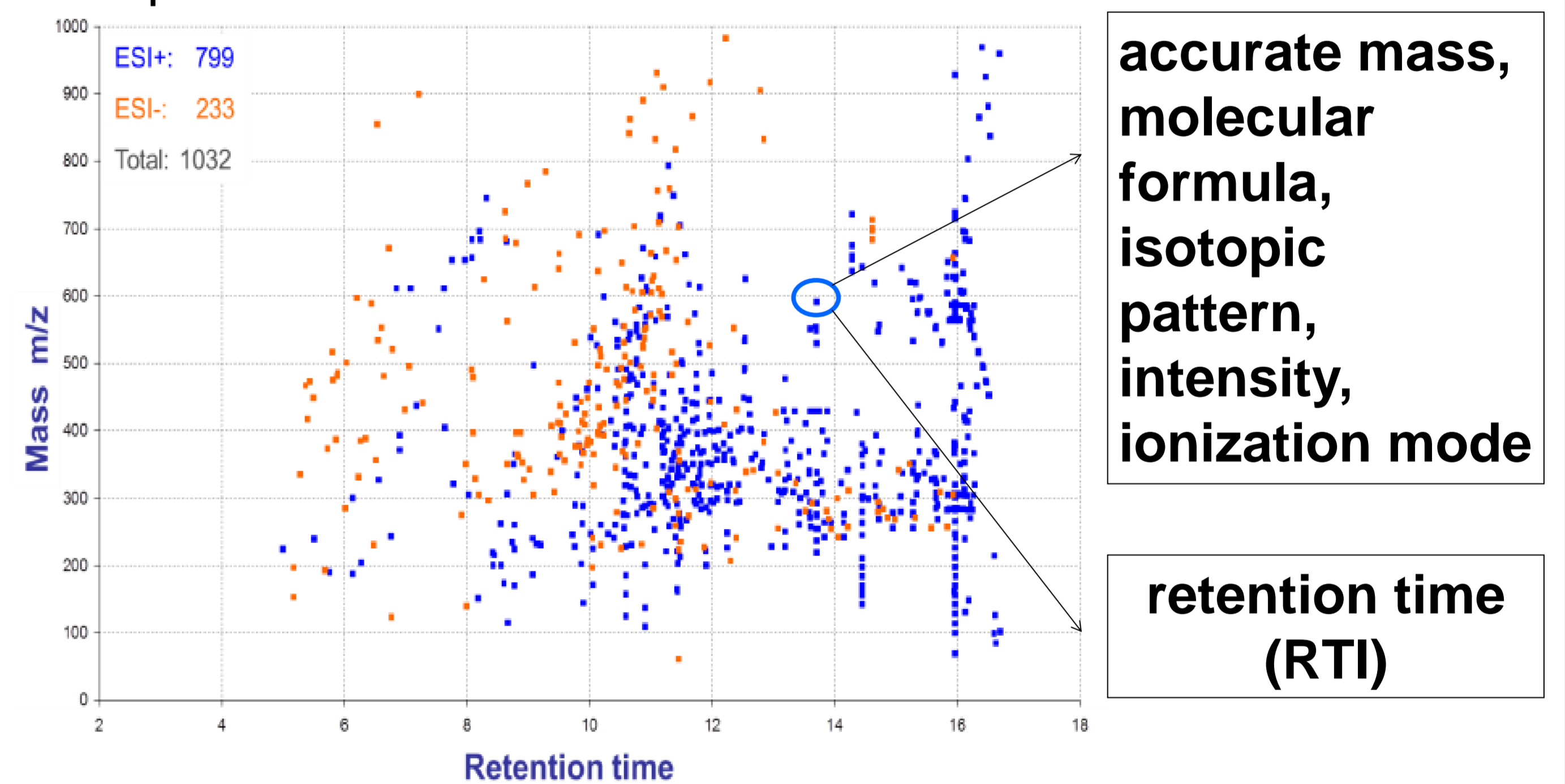


Figure 3: mass - retention time plot of a real sample

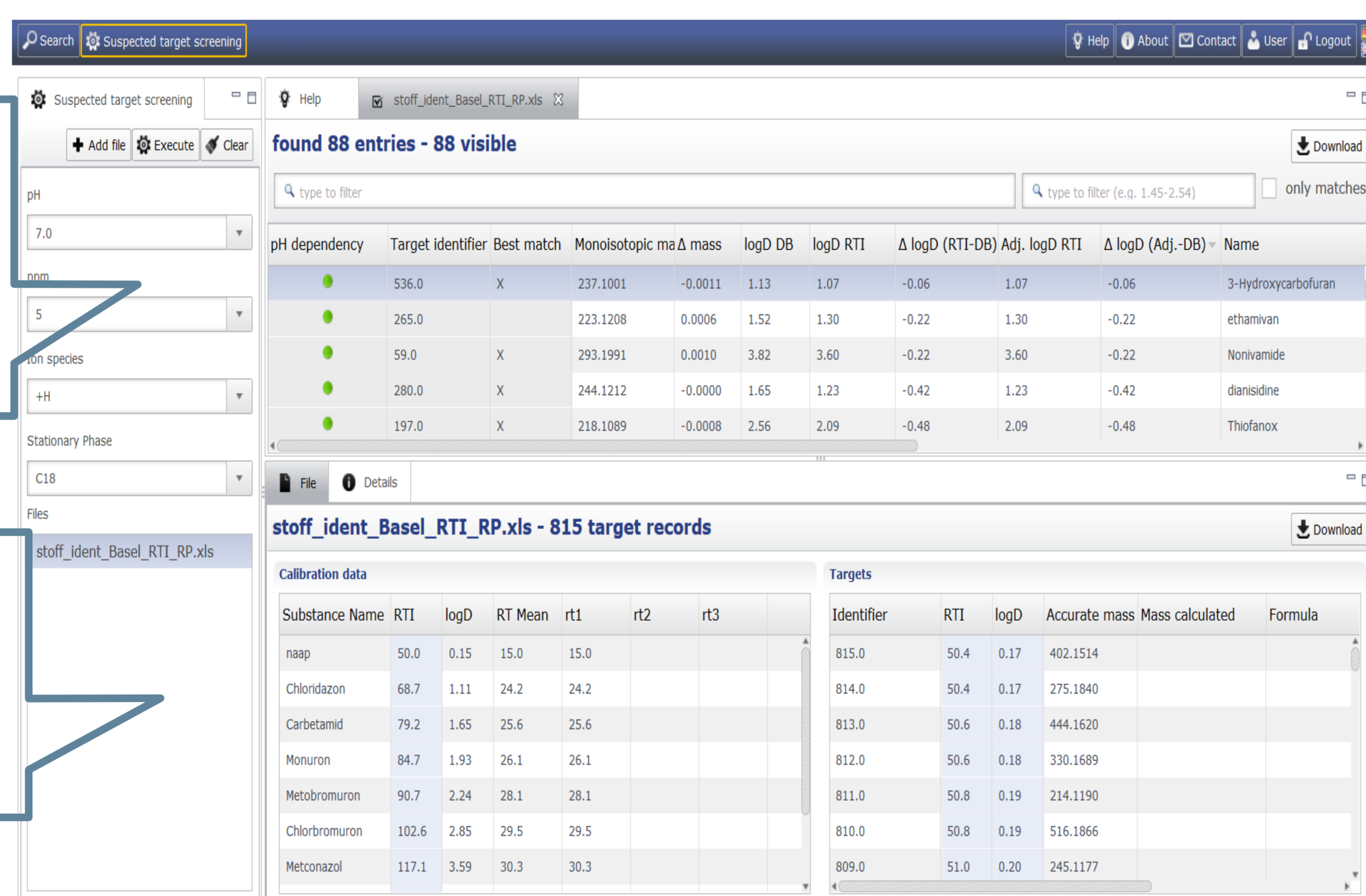


Figure 4: Screenshot of the database STOFF-IDENT

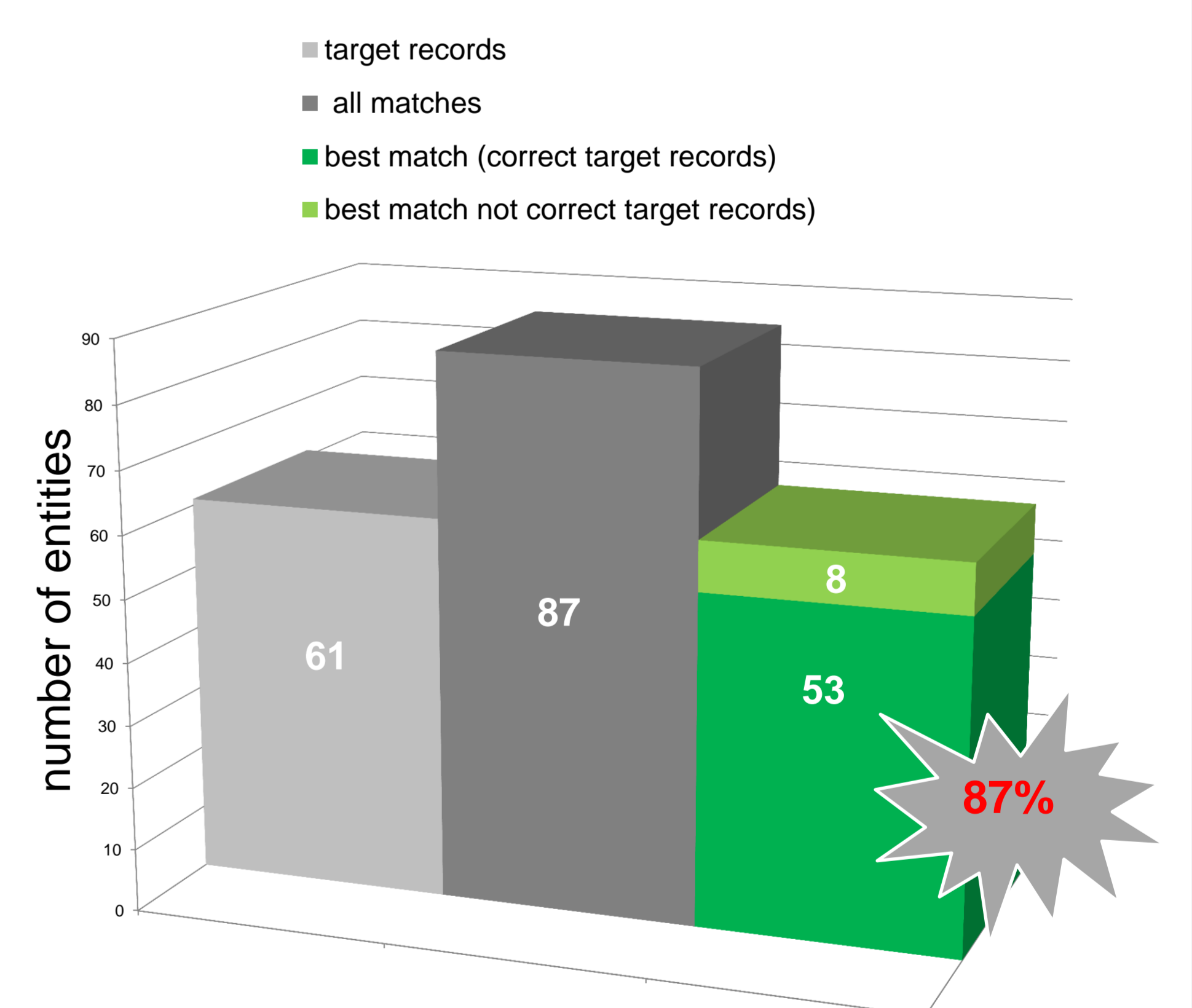


Figure 5: Validation of the STOFF-IDENT database with known targets

Perspective

New data workout strategies could be developed for **non target and suspected target screening techniques** using the observed data from HRMS (i.e. **empirical formula**) and normalized retention time (i.e. **logD**). Thereby free software tools like **RTI** and **STOFF-IDENT** can be applied for efficient data analysis. The database STOFF-IDENT thereby allows to identify so called '**Known Unknowns**' in a first strategy to clarify the 'cloud' of **initially 'Unknowns'**.

Acknowledgement

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¹: <http://bb-x-stoffident.hswt.de/stoffidentjpa/appclean>. 2: Lucke, T., Letzel, M., Schulz, W., Sengl, M. und Letzel, T. (2014) In a class of its own; Organic Molecule Identification in water using LC-MS(MS); Steps from "unknown" to "identified". lab & more 4.14