



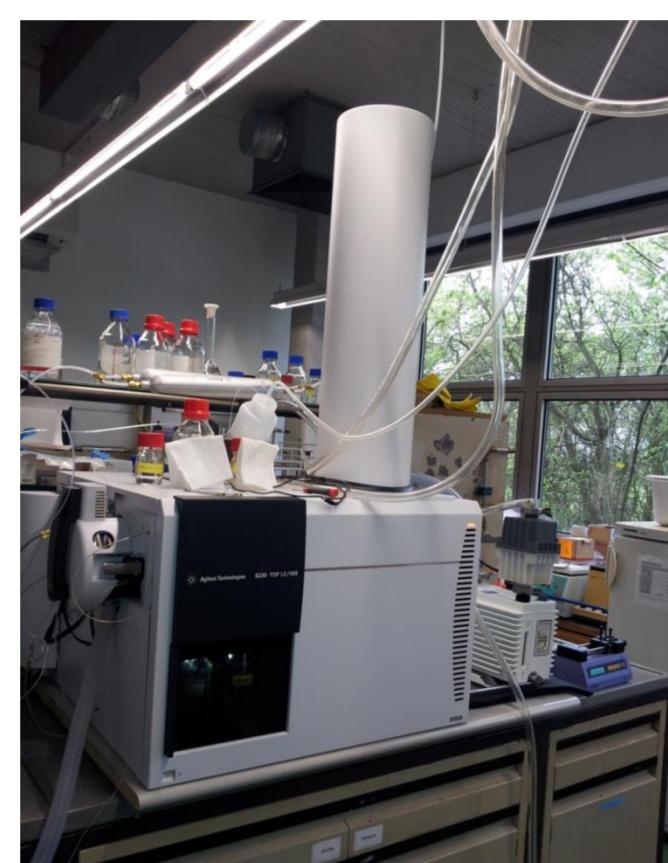
An effective LC-MS strategy of non-target analysis using the database STOFF-IDENT¹

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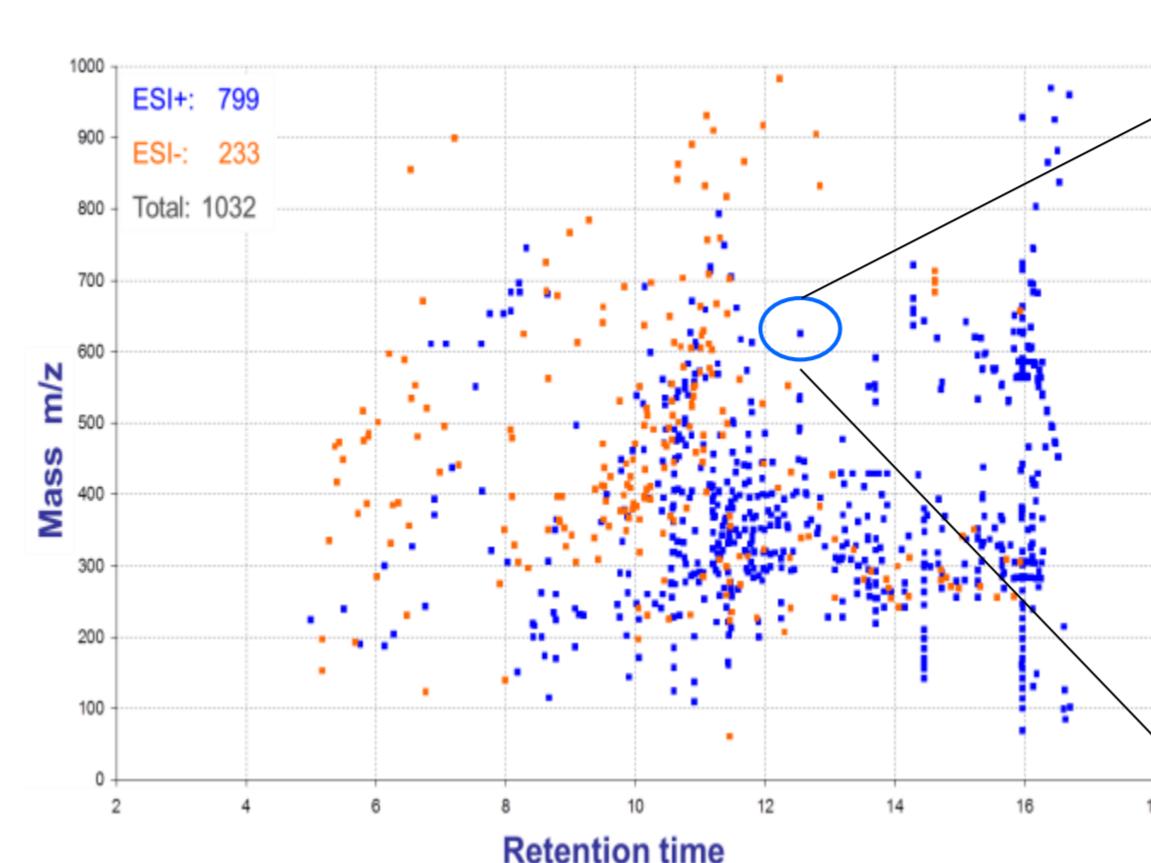


Overview

(HILIC)-RPLC-MS measurement²



Feature finding



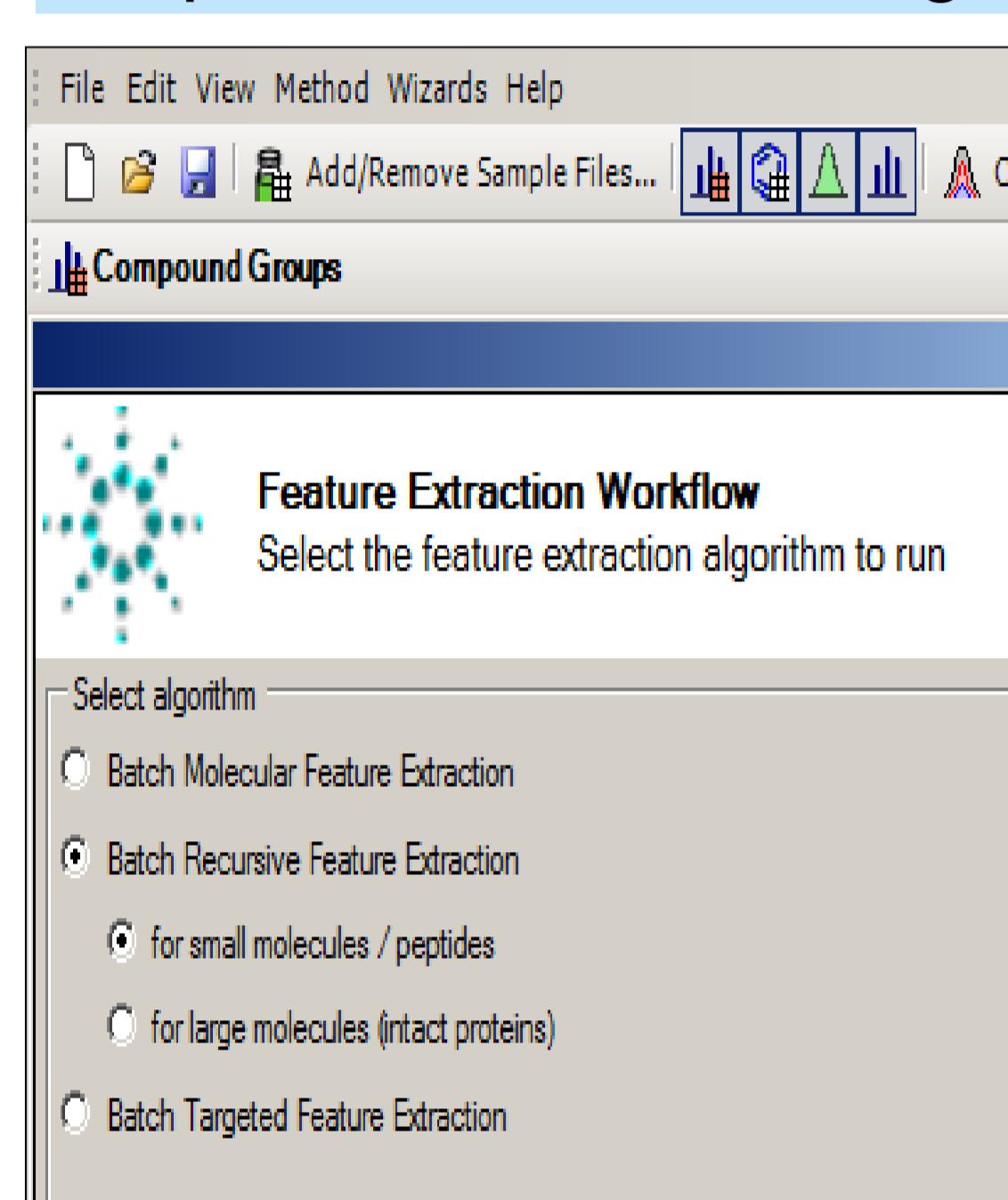
Identification

- accurate mass
- retention time (with RTI)
- retention time (without RTI)

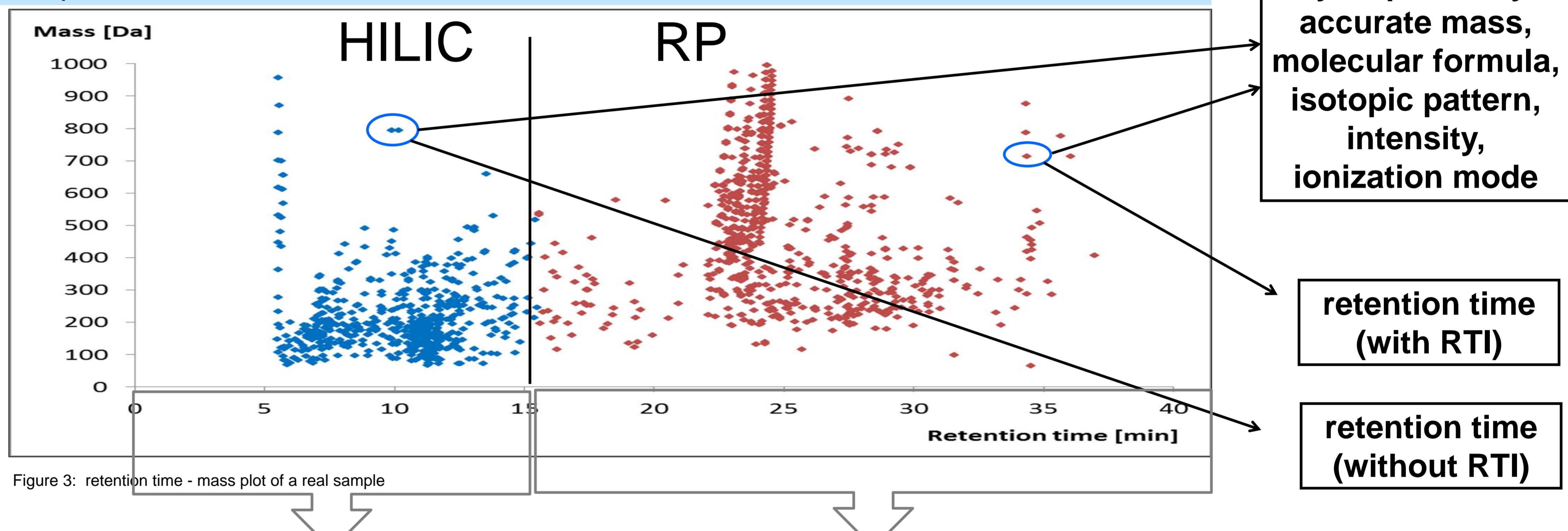
Database:
STOFF-IDENT

Non-target screening workflow³

Step 1 – Feature finding



Step 2 – Feature validation



Step 3 – Database search

Label	Mass
unknown X	236.095
unknown Y	128.1014
unknown Z	253.052

Figure 4: Screenshot of File search part in STOFF-IDENT

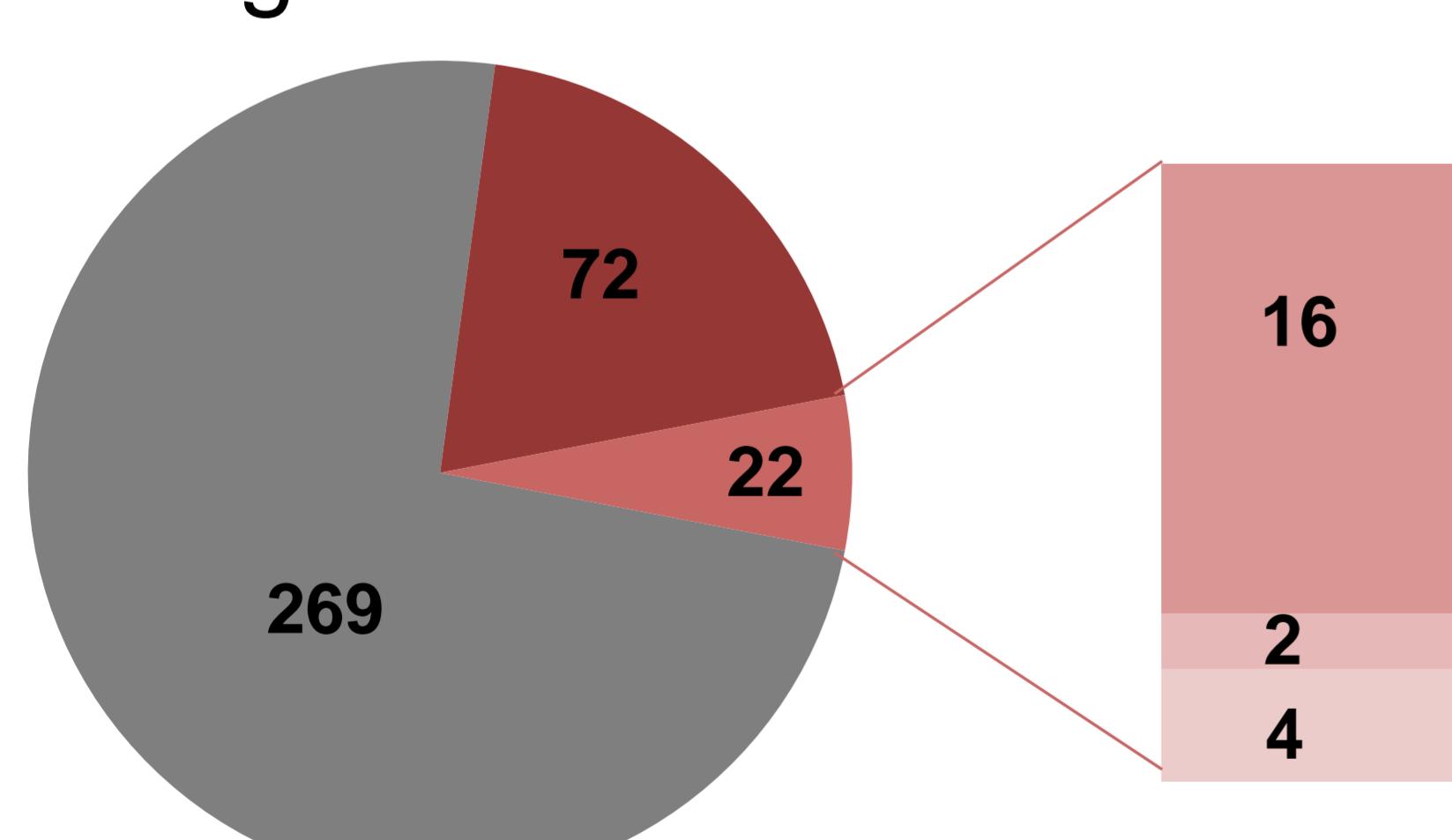
Hidden target screening (RTI)

pH dependency	Target identifier	Best match	Monoisotopic m/z	Δ mass	logD DB	logD RTI	Δ logD (RTI-DB)	Adj. logD RTI	Δ logD (Adj.-DB)	Name
green	Unknown Y	X	164.0950	0.0000	1.32	1.11	-0.21	1.11	-0.21	fenumon
green	Unknown Y		164.0950	0.0000	0.87	1.11	0.24	1.11	0.24	phenethylurea
red	Unknown Y		164.0950	0.0000	-0.78	1.11	1.89	1.11	1.89	N-(4-Aminophenyl)-N-methy

Figure 5: Screenshot of suspected target screening part in STOFF-IDENT

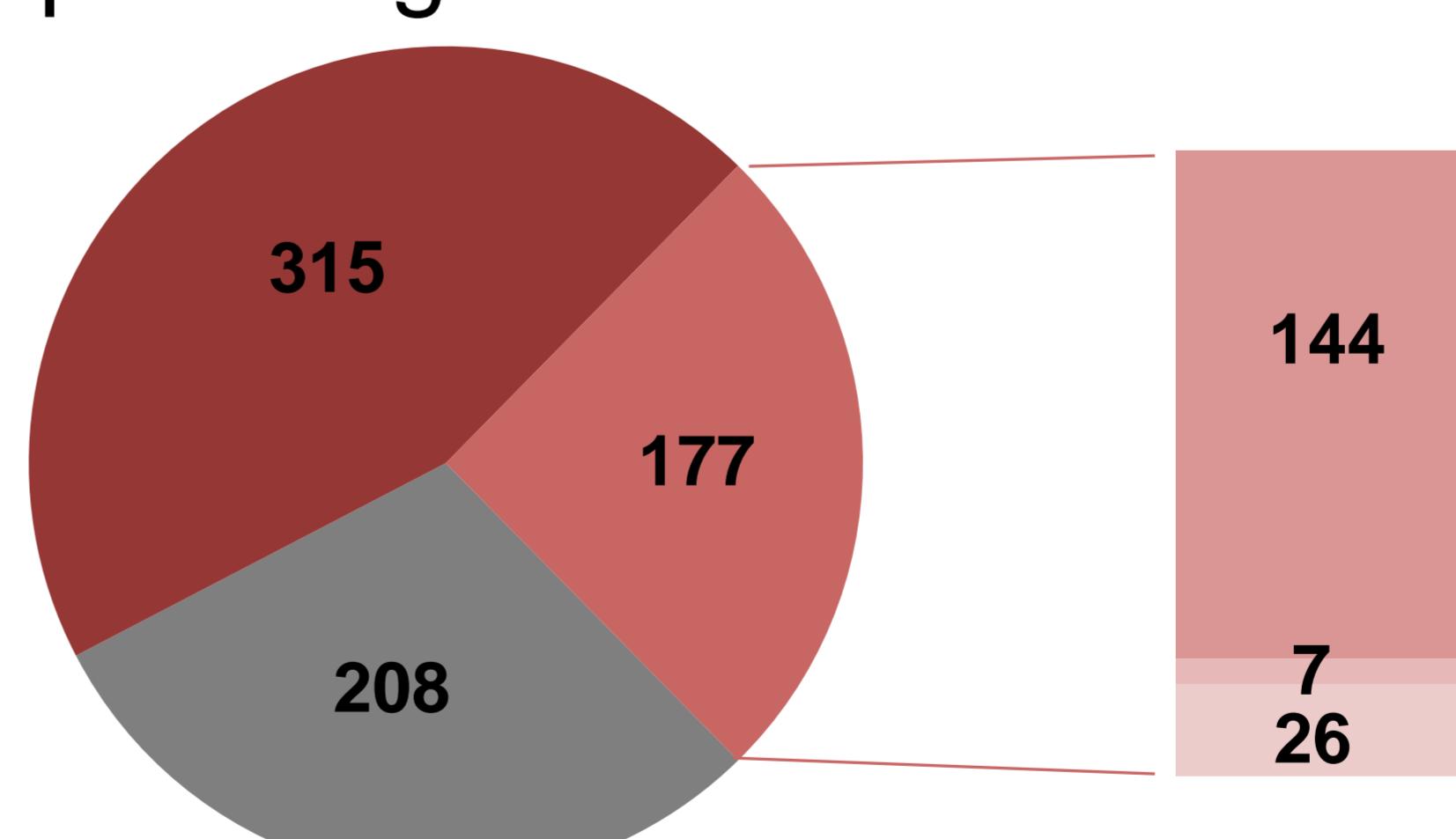
Step 4 – Identification

polar region



- features
- all matches
- "best match" logD < 0
- without standard
- disproved via standard
- identified via standard

nonpolar region



- features
- all matches
- "best match" logD < 0
- without standard
- disproved via standard
- identified via standard

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1: <http://bb-x-stoffident.hswt.de/stoffidentipa/appclean>.

2: G. Greco, et. al, J. Sep. Sci. 36, 1379–1388 (2013)

3: 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