Analytical techniques, (non-target) screening workflows and monitoring tools - *'Getting control of PMT and vPvM substances under REACH'*

Third PMT Workshop 25th/26th March 2021

partially developed at TECHNISCHE UNIVERSITÄT MÜNCHEN

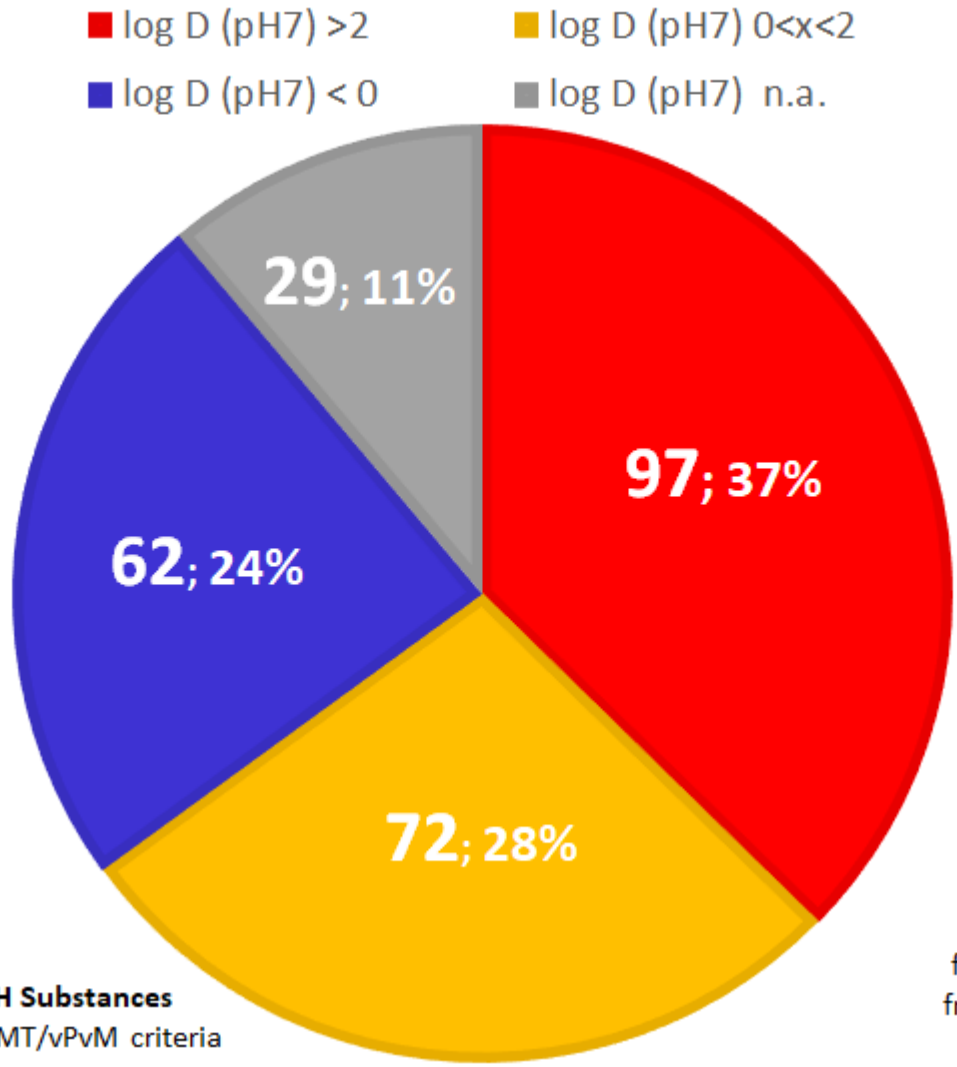
Thomas Letzel
AFIN-TS GmbH

Getting control of PMT and vPvM substances under REACH

Looking for:

- Organic Molecules like PMT/vPvM Substances
- (Non-Target) Screening Workflows
- Monitoring Tools
- Sustainable and Robust Analytical Platform for ‚NTS in Routine Analysis‘

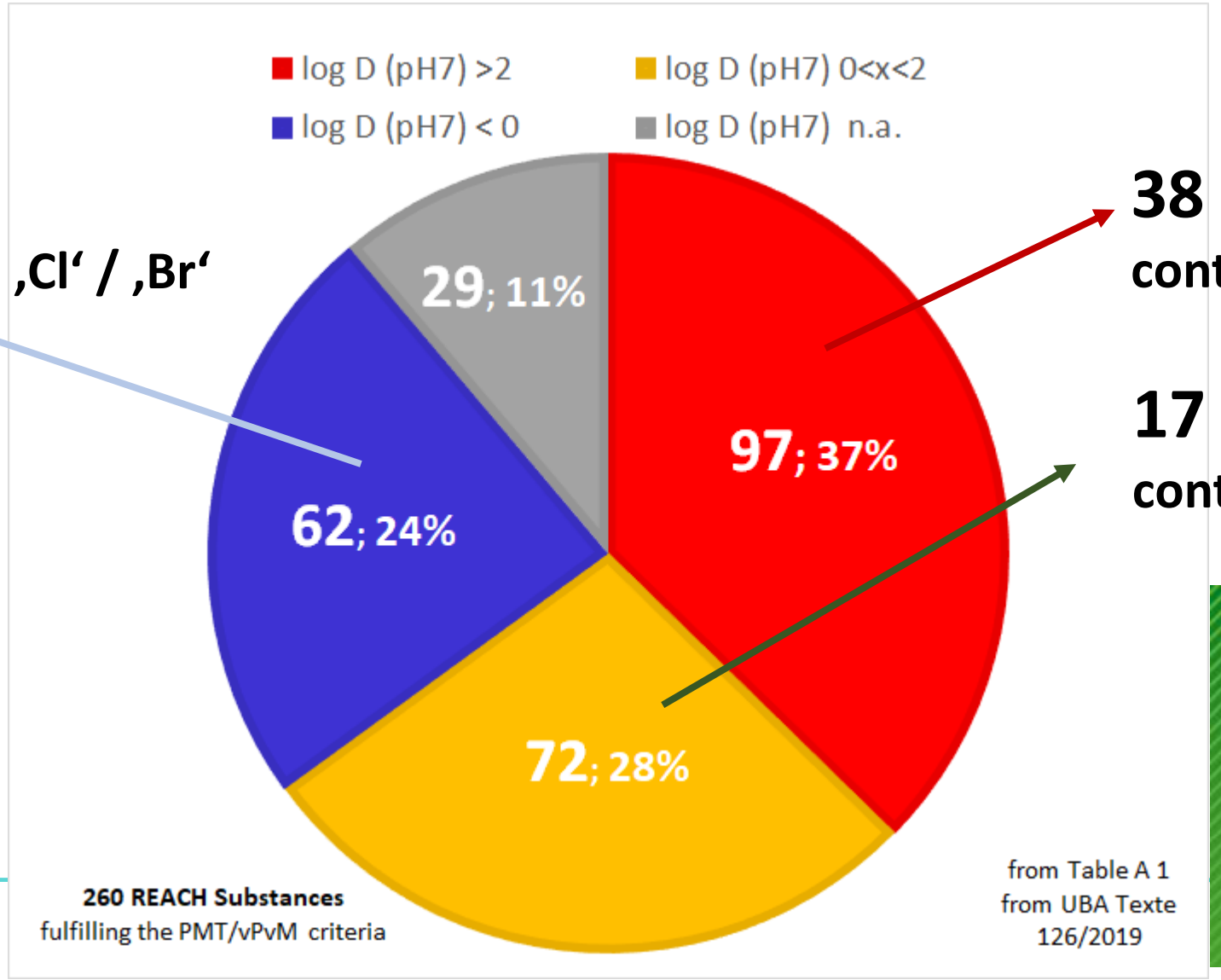
Organic Molecules (in the PMT/vPvM list)



260 REACH Substances
fulfilling the PMT/vPvM criteria

from Table A 1
from UBA Texte
126/2019

Organic Molecules (in the PMT/vPvM list)



4

containing ‚Cl' / ‚Br'

38

containing ‚Cl' / ‚Br'

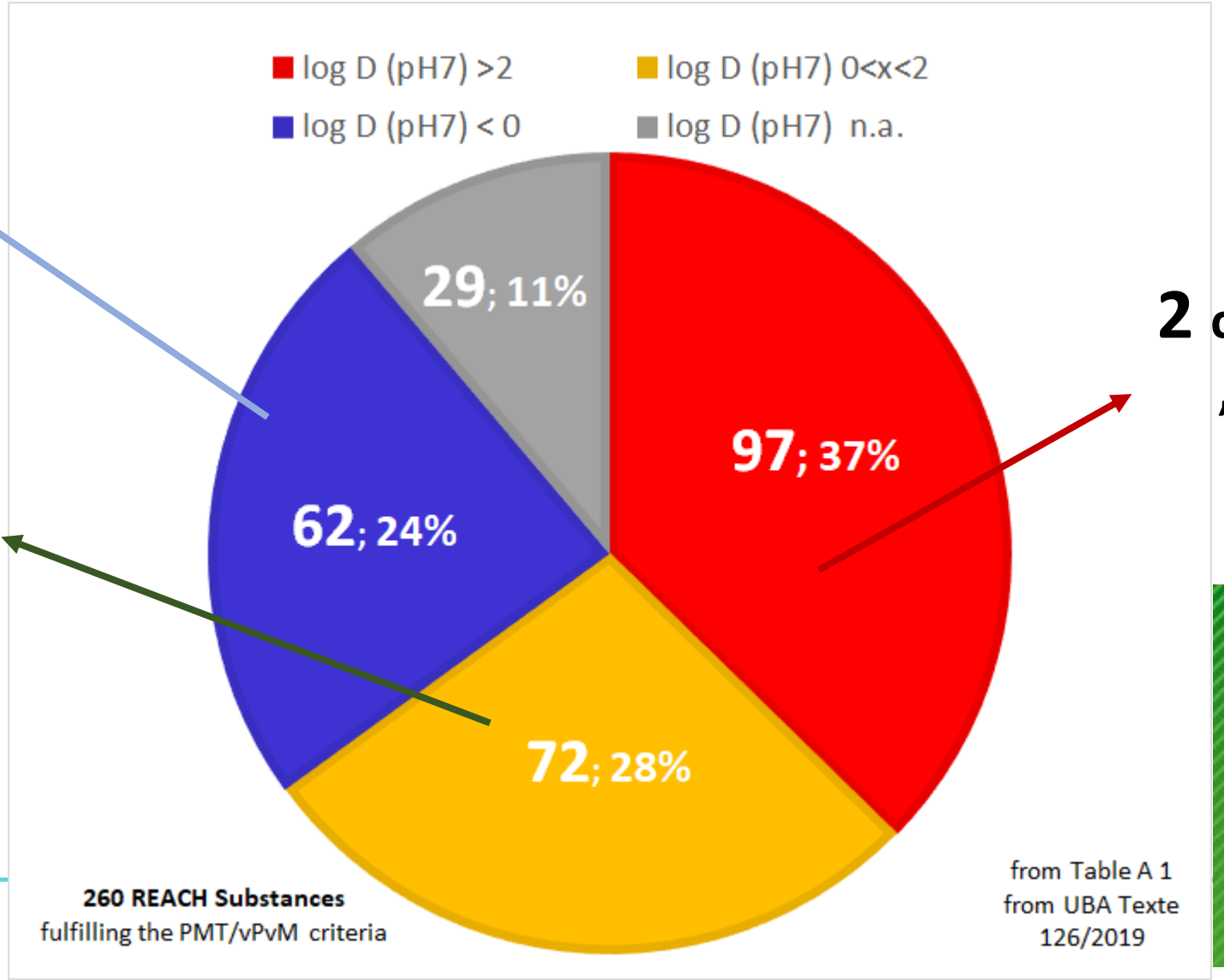
17

containing ‚Cl' / ‚Br'

Organic Molecules (in the PMT/vPvM list)

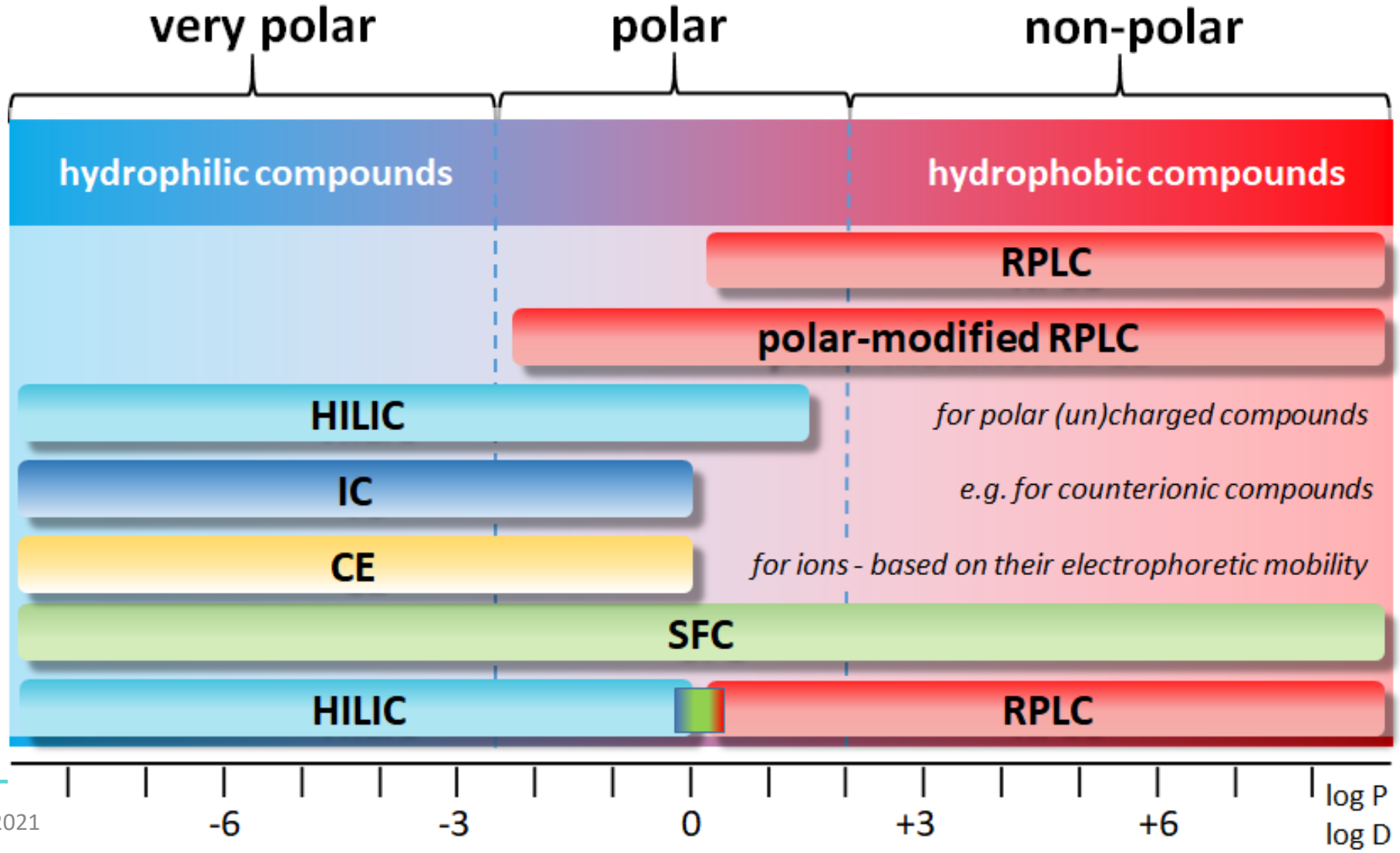
33 containing ‚Amino‘/ ‚Acid‘

18 containing ‚Amino‘ / ‚Acid‘ (mostly anilins)



2 containing ‚Amino‘ / ‚Acid‘

Liquid Phase Separation Techniques

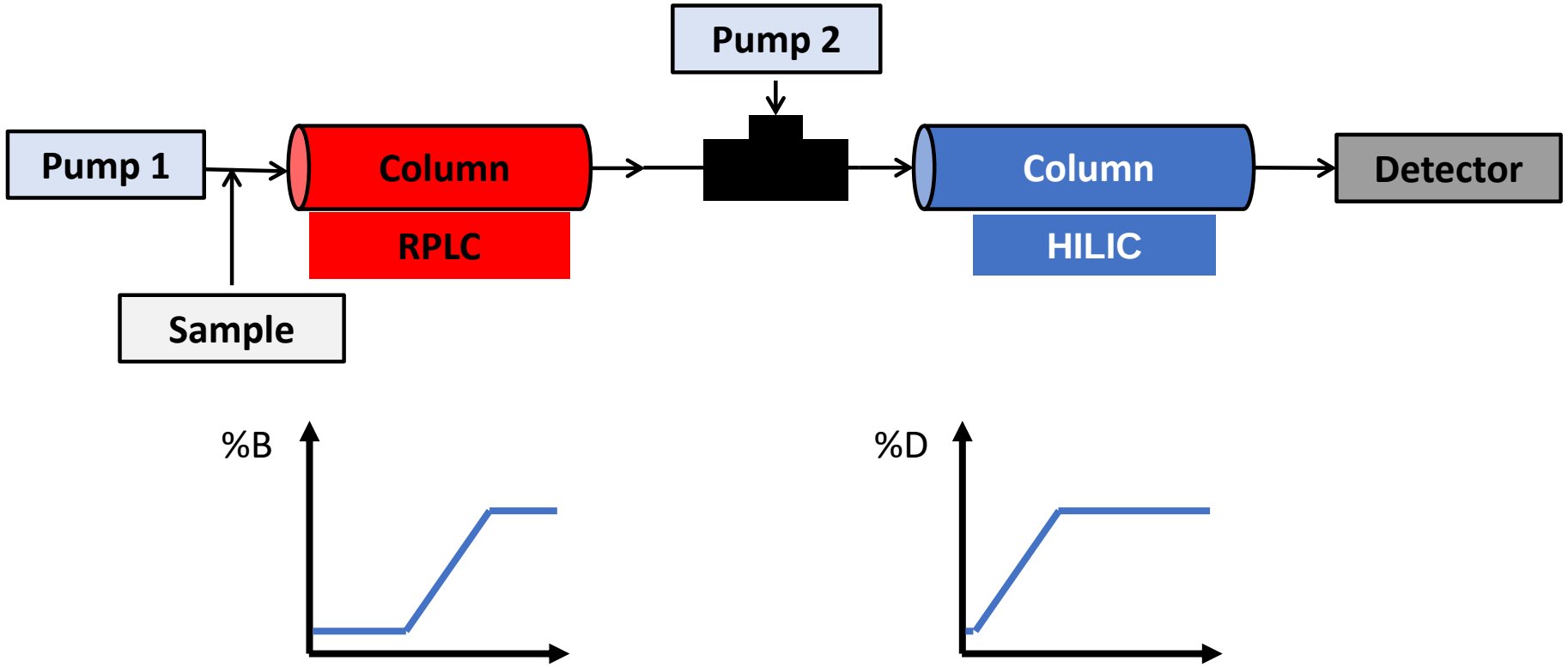


S. Bieber et al. **2017,** *Analytical Chemistry*, *89 (15)*, 7907-7914.

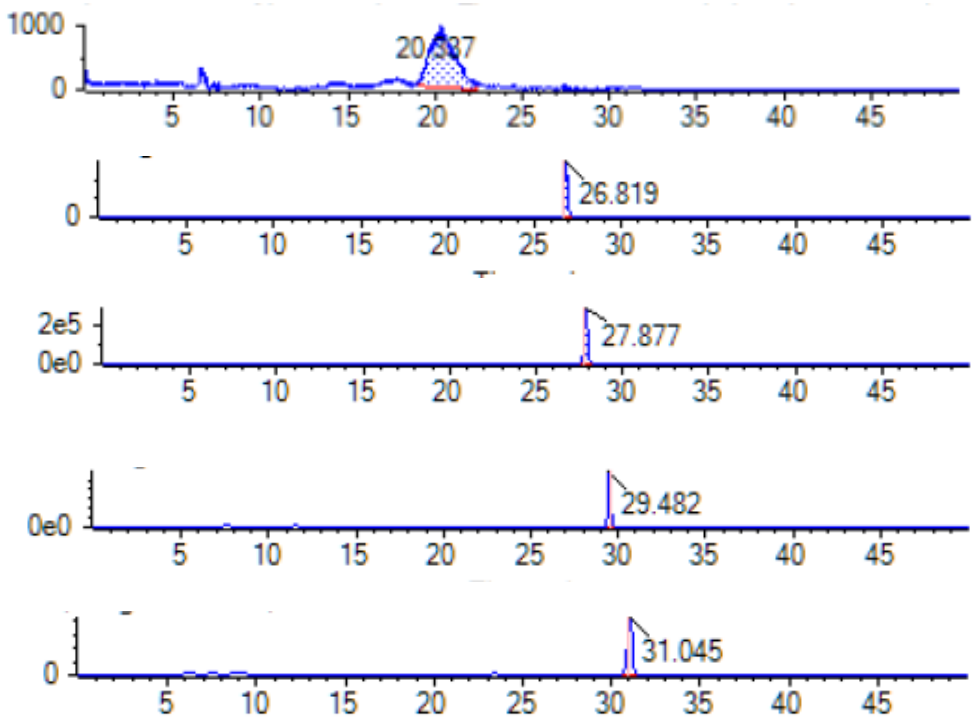
S. Bieber and T. Letzel **2018**, LCGC Europe 31 (11), 602-608.

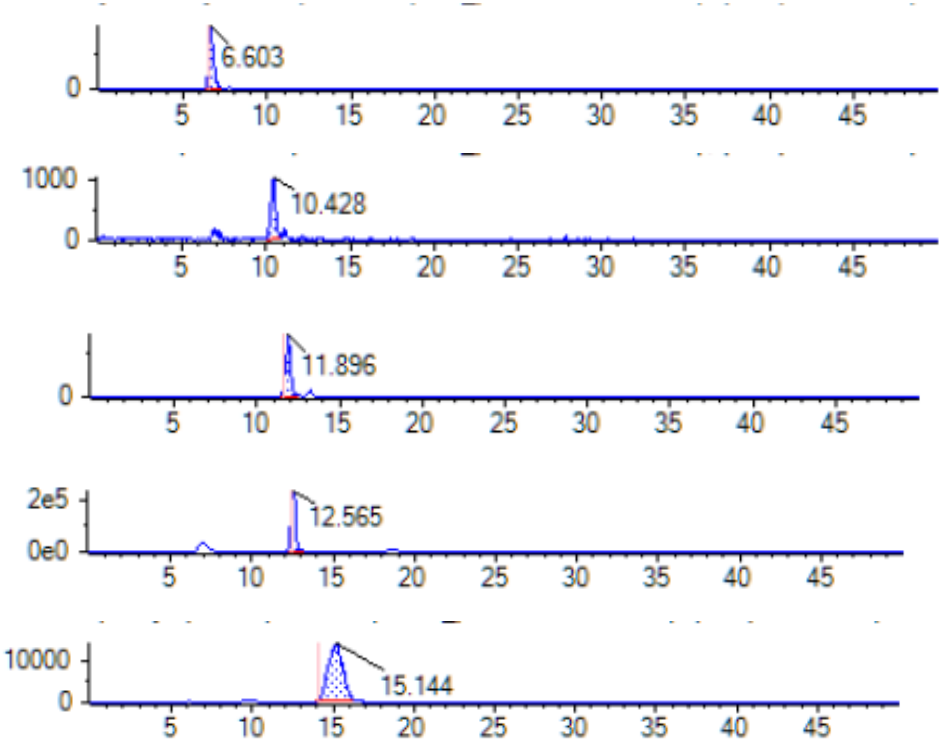
S. Bieber and T. Letzel **2020**, AFIN-TS Forum (1), 1-10.

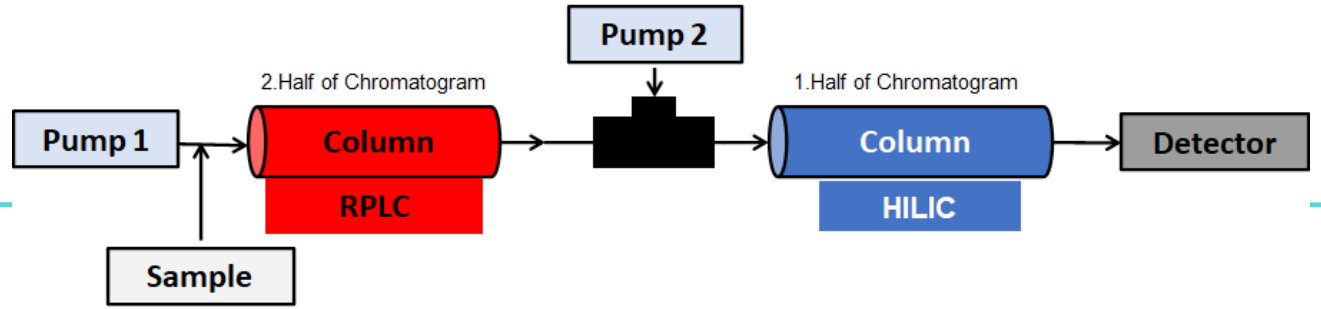
Polarity-Extended Liquid Chromatography



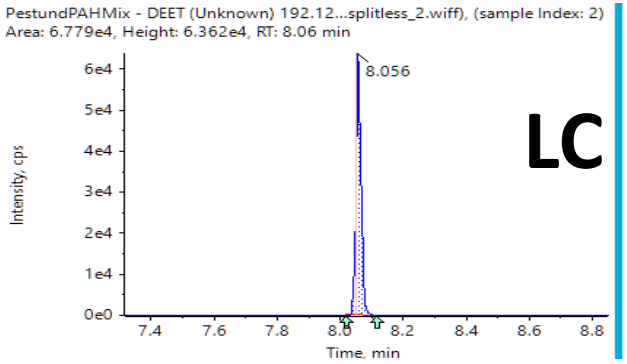
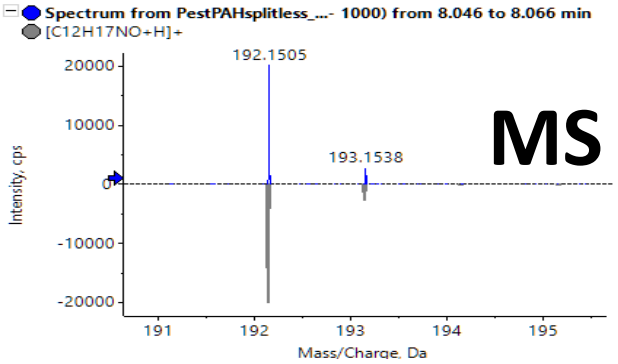
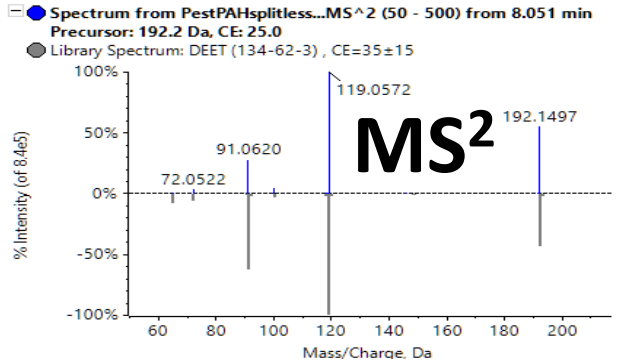
RPLC-HILIC-ESI-MS/MS (using target analysis)



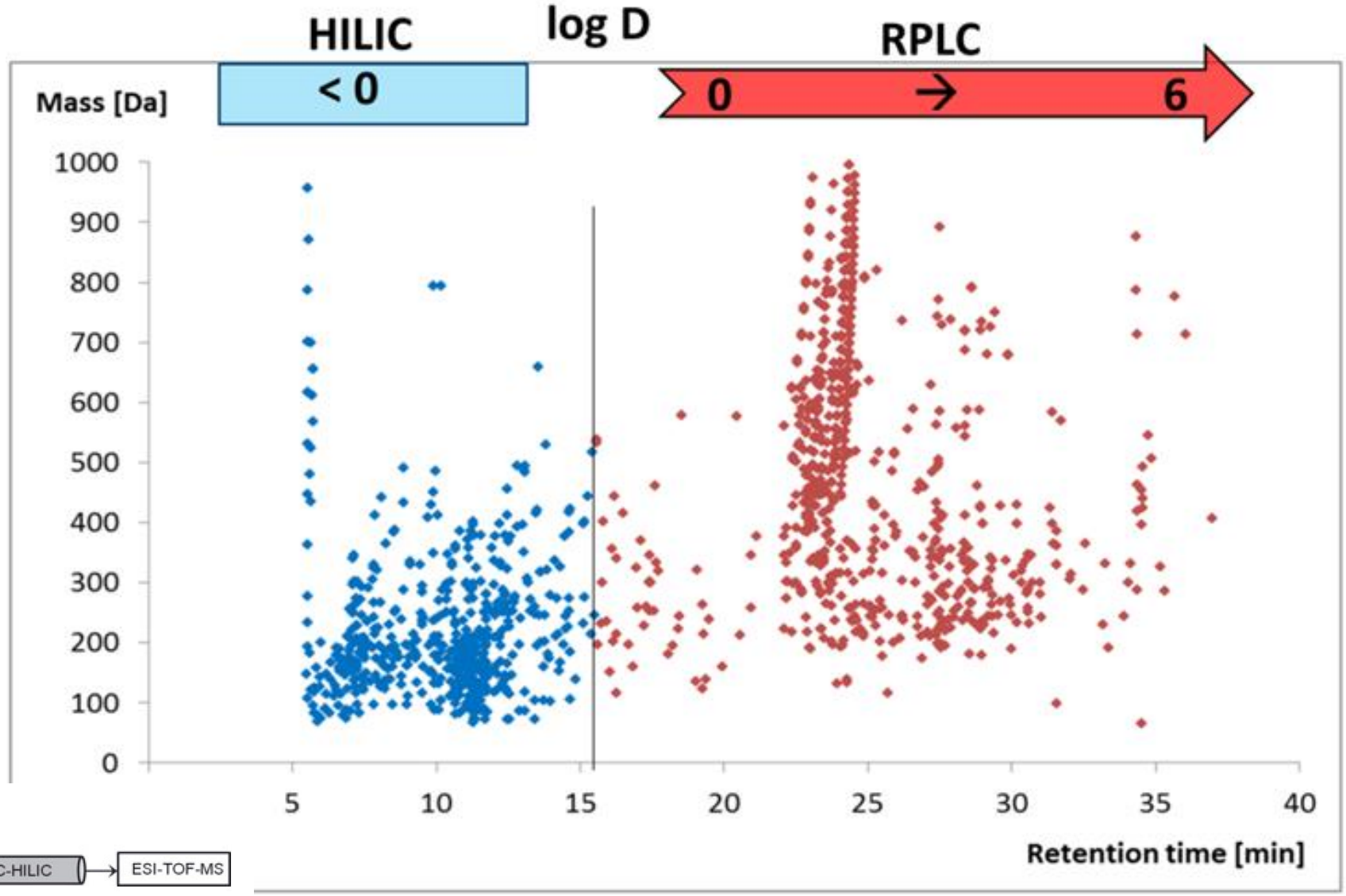




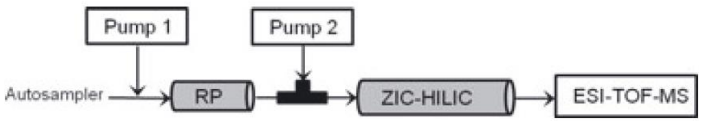
Instrumental Analysis in Routine

Analytical Technique				
Analytical Parameter	Retention time	Signal (ion) intensity	Accurate mass, Isotopic pattern	Fragment spectrum
Quality Assurance	RT deviation, FWHM	Signal deviation, Signal response	Mass deviation, mass accuracy	Mass deviation, mass accuracy
Physico-Chemical Parameter	logD value Hydrophobicity	Sensitivity	Empirical formula	Structural information

Polarity-Extended Liquid Chromatography



G. Greco et al. **2013**, J. of Separation Science 36 (8), 1279-1388.

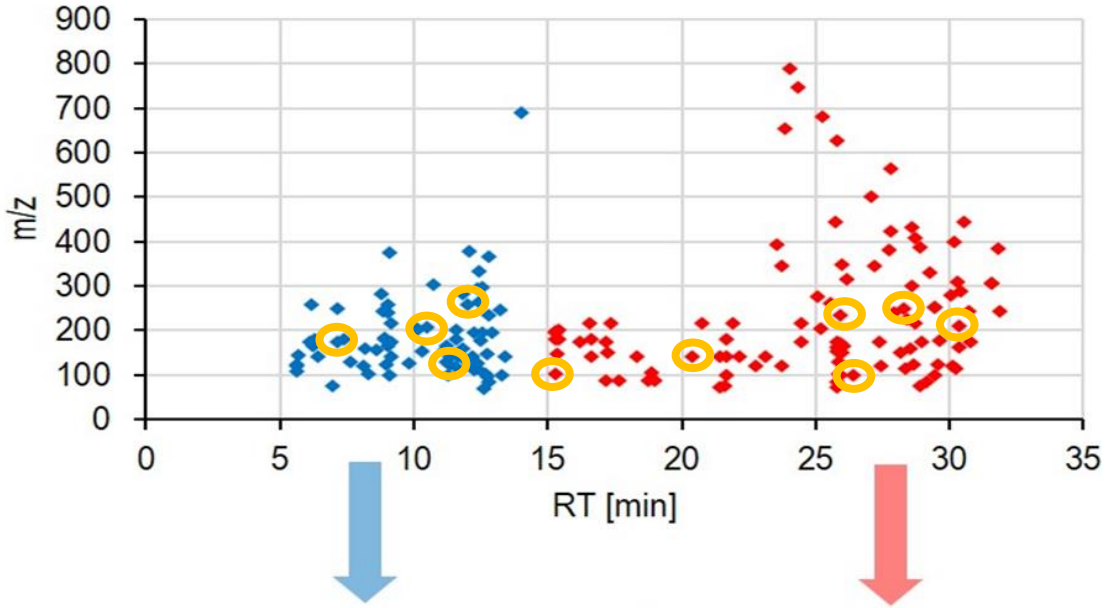


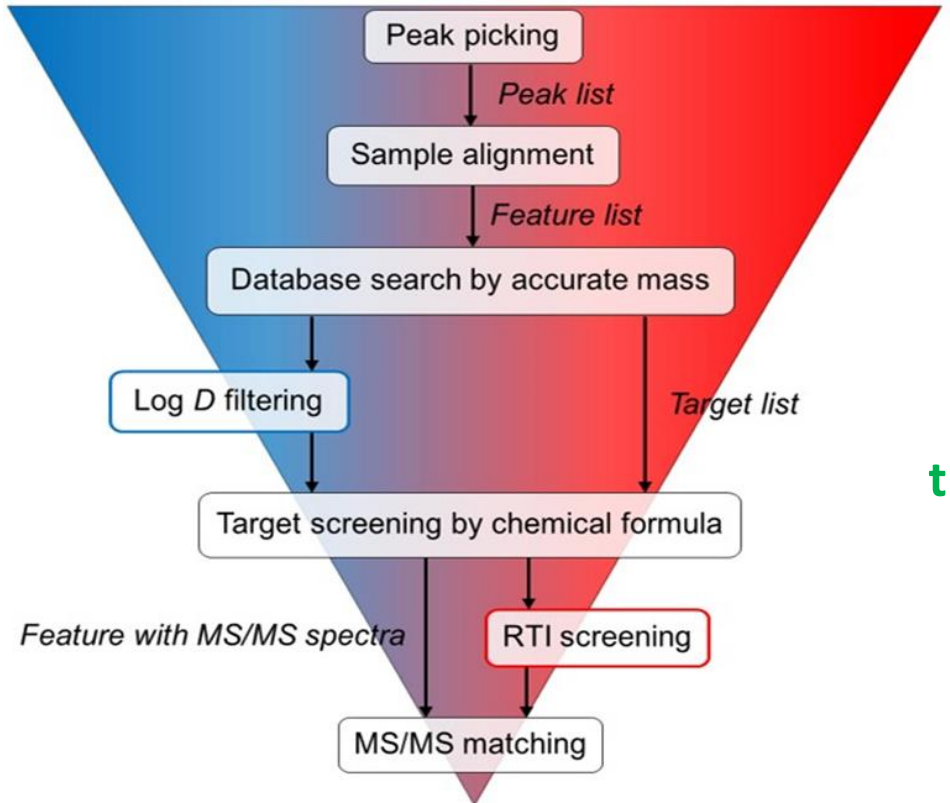
S. Bieber et al. **2017,** *Analytical Chemistry*, *89 (15)*, 7907-7914.

S. Bieber and T. Letzel **2020**, AFIN-TS Forum (1), 1-10.

NTS (data handling) in Routine

NTS = Non-Target Screening





Data Preprocessing

↓

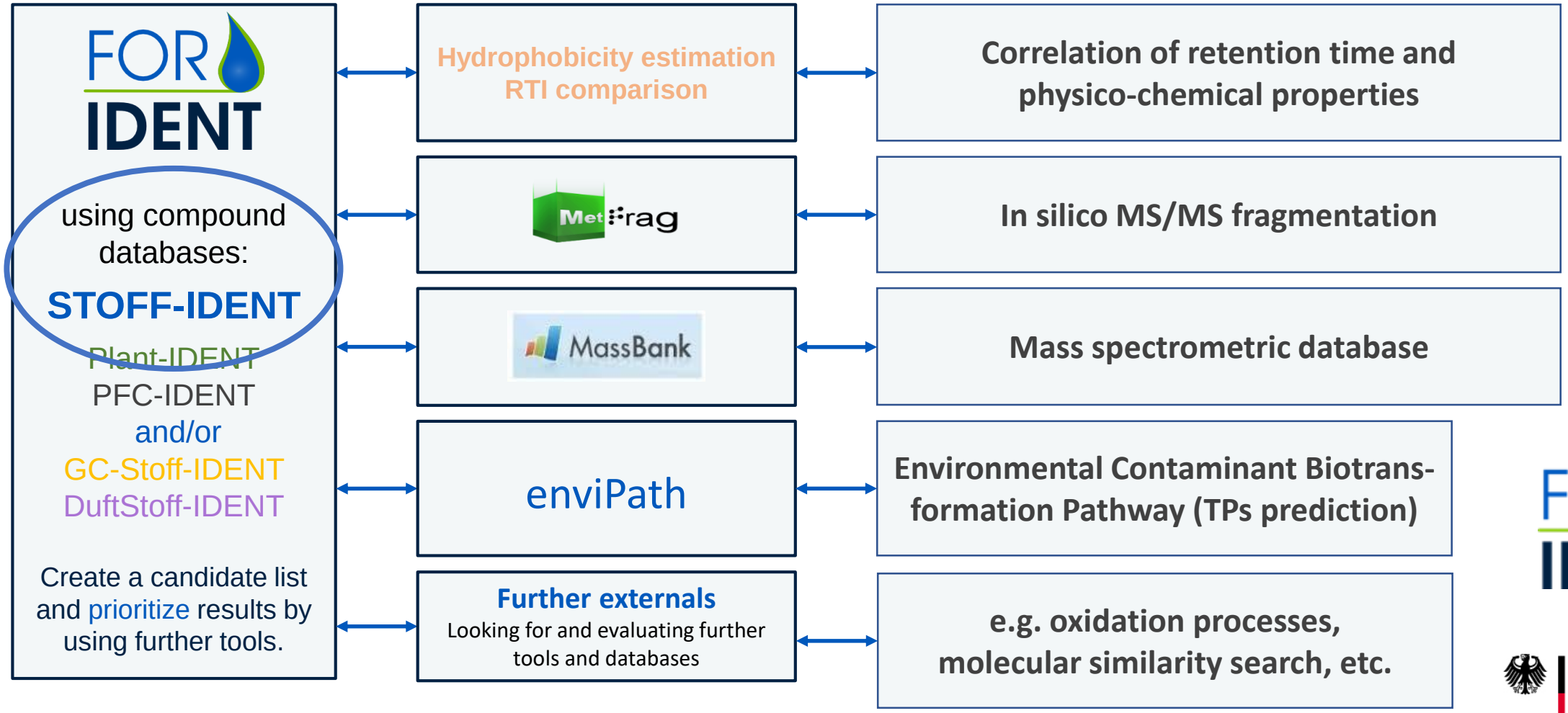
Features (mass@RT)

↓

Data Processing using Vendor Solutions and the Advanced Workflow Platform FOR-IDENT

S. Minkus et al. **2021,** *Joint Danube Survey 4 Report*, in press.

Open Access NTS Priorization Workflow



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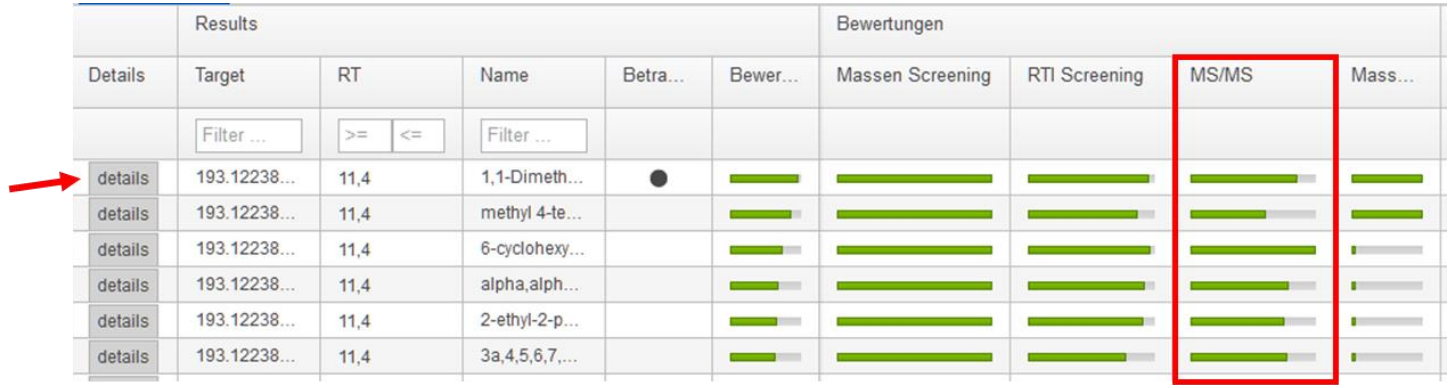
FOR-IDENT Priorization

- Automated data evaluation
- Comparison of data with **database entries**
- Scoring based on:
  - Accurate Mass
  - Retention Time
    (neg. logD filter vs. RTI)
  - MS/MS coverage
    (in silico fragmentation tool)
  - MassBank entries



	Results					Bewertungen			
Details	Target	RT	Name	Betra...	Bewer...	Massen Screening	RTI Screening	MS/MS	Mass...
	Filter ...	>= <=	Filter ...						
details	193.12238...	11,4	1,1-Dimeth...	●					
details	193.12238...	11,4	methyl 4-te...						
details	193.12238...	11,4	6-cyclohexy...						
details	193.12238...	11,4	alpha,alph...						
details	193.12238...	11,4	2-ethyl-2-p...						
details	193.12238...	11,4	3a,4,5,6,7,...						

	Results					Bewertungen			
Details	Target	RT	Name	Betra...	Bewer...	Massen Screening	RTI Screening	MS/MS	Mass...
	Filter ...	>= <=	Filter ...						
details	193.12238...	11,4	1,1-Dimeth...	●					

+ Scoring MS/MS

Prozess	Score	Gewicht	Gewichteter Score
Massen Screening	1.0	0.25	0.25
RTI Screening	0.96	0.25	0.24
MSMS	0.85	0.25	0.21
Massbank	1.0	0.25	0.25
Gesamt			**0.95**

Screening PMT/vPvM – ‘Research’ Solutions

Anal Bioanal Chem (2015) 407:6237–6255
DOI 10.1007/s00216-015-8681-7

REVIEW

2015

Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis

Emma L. Schymanski[1] · Heinz P. Singer[1] · Jaroslav Slobodnik[2] · Ildiko M. Ipolyi[2] · Peter Oswald[2] · Martin Krauss[3] · Tobias Schulze[3] · Peter Haglund[4] · Thomas Letzel[5] · Sylvia Grosse[5] · Nikolaos S. Thomaidis[6] · Anna Bletsou[6] · Christian Zwiener[7] · María Ibáñez[8] · Tania Portolés[8] · Ronald de Boer[9] · Malcolm J. Reid[10] · Matthias Onghena[11] · Uwe Kunkel[12] · Wolfgang Schulz[13] · Amélie Guillon[14] · Naïke Noyon[14] · Gaëla Leroy[15] · Philippe Bados[16] · Sara Bogialli[17] · Draženka Stipaničev[18] · Pawel Rostkowski[19] · Juliane Hollender[1,20]

analytical chemistry

Article

pubs.acs.org/ac

2017

RPLC-HILIC and SFC with Mass Spectrometry: Polarity-Extended Organic Molecule Screening in Environmental (Water) Samples

Stefan Bieber, Giorgia Greco,† Sylvia Grosse, and Thomas Letzel*

Analytical Methods

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
View Journal

2021

(Very) polar organic compounds in the Danube river basin: Non-target screening workflow and prioritization strategy for extracting highly confident features

Received 00th January 20xx,
Accepted 00th January 20xx

Susanne Minkus[a,b], Stefan Bieber[b] and Thomas Letzel[a,b*]

Analytical and Bioanalytical Chemistry (2020) 412:4953–4966
https://doi.org/10.1007/s00216-020-02743-0

RESEARCH PAPER

2020

Optimized hidden target screening for very polar molecules in surface waters including a compound database inquiry

Susanne Minkus[1,2] · Sylvia Grosse[1,3] · Stefan Bieber[2] · Sofia Veloutsou[1,4] · Thomas Letzel[1,2]

Rüdel *et al. Environ Sci Eur* (2020) 32:5
https://doi.org/10.1186/s12302-019-0286-x

2020

Environmental Sciences Europe

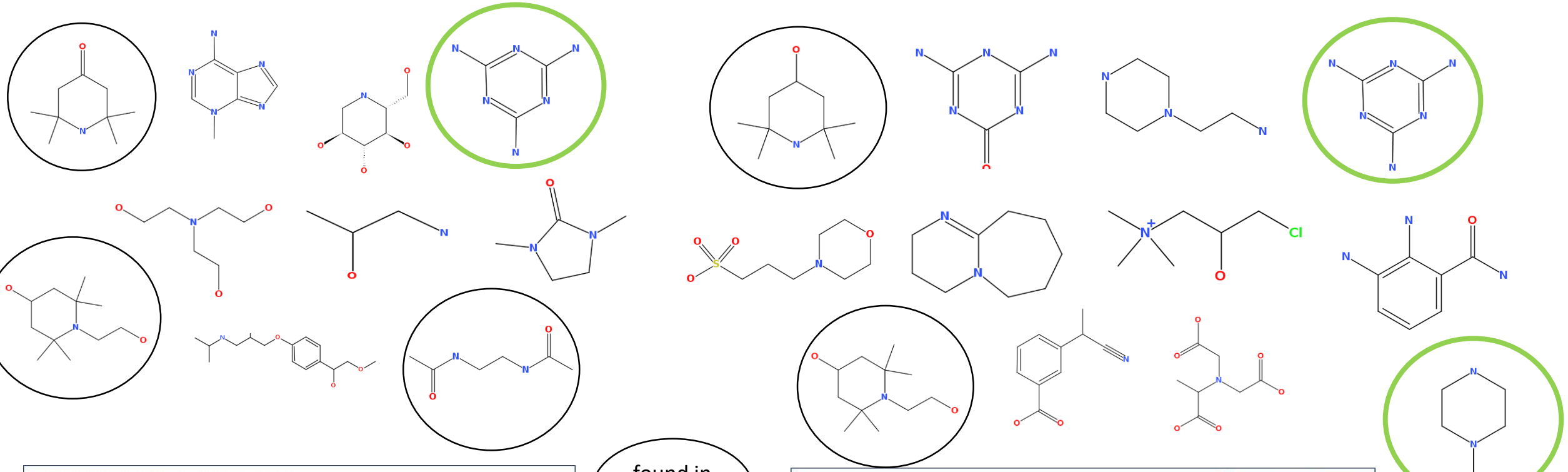
COMMENTARY Open Access

Persistent, mobile and toxic substances in the environment: a spotlight on current research and regulatory activities

Heinz Rüdel[1*], Wolfgang Körner[2], Thomas Letzel[3], Michael Neumann[4], Karsten Nödler[5] and Thorsten Reemtsma[6,7]

Further Literature regarding this topic see-> https://afin-ts.de/literatur/?lang=en

‘REACH’-contained suggestions (in surface waters)



found in more studies

and in PMT/vPvM list

Analytical and Bioanalytical Chemistry (2020) 412:4953–4966
https://doi.org/10.1007/s00216-020-02743-0

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Analytical Methods

ROYAL SOCIETY OF CHEMISTRY

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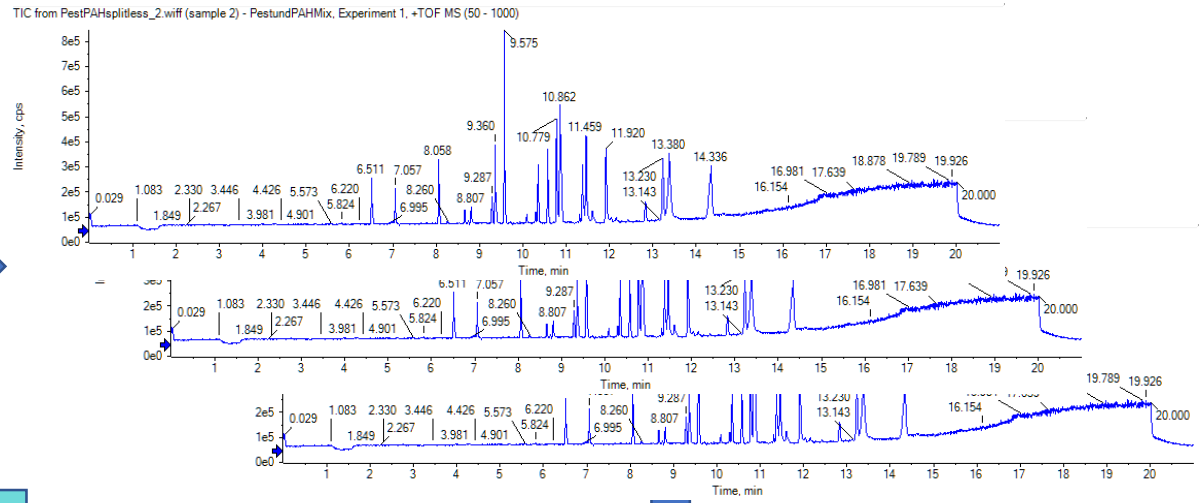
Structure Source: https://water.for-ident.org/

Non-Target Screening Data Evaluation

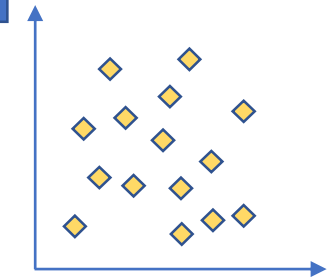
Separation

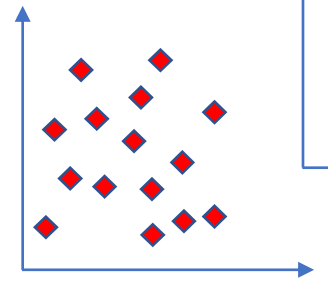
Ionization

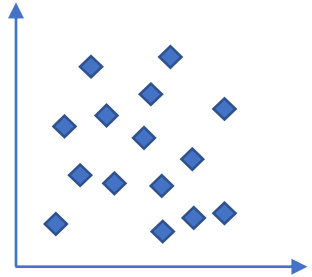
(LC-)MS/MS

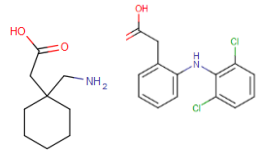


Peak picking
Feature alignment





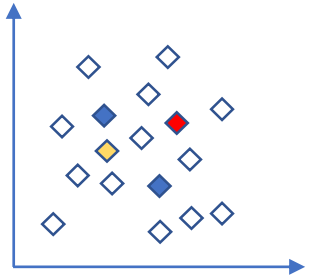


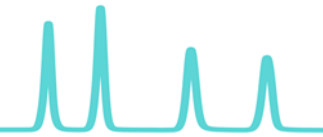


Identification

Statistical handling

- PCA
- Trend detection
- Cluster analysis
- …..





Perspective

- **Wanted**

As many as possible interested institutions supporting our established sustainable analytical process and having samples for our analytical lab (and our data analysis)

- **Offered**

Own lab capacities (from AFIN-TS) and aditionally partner consulting
to establish the Target- and NTS- strategies also in their analytical labs

- **Needed**

Networks for connecting as many as possible international labs that realize this polarity-extended type of analysis and want to have inter-laboratory solutions

Contact us at: info@afin-ts.de and see further details at: www.afin-ts.de