Non-target Screening in Drinking Water – An Overview –

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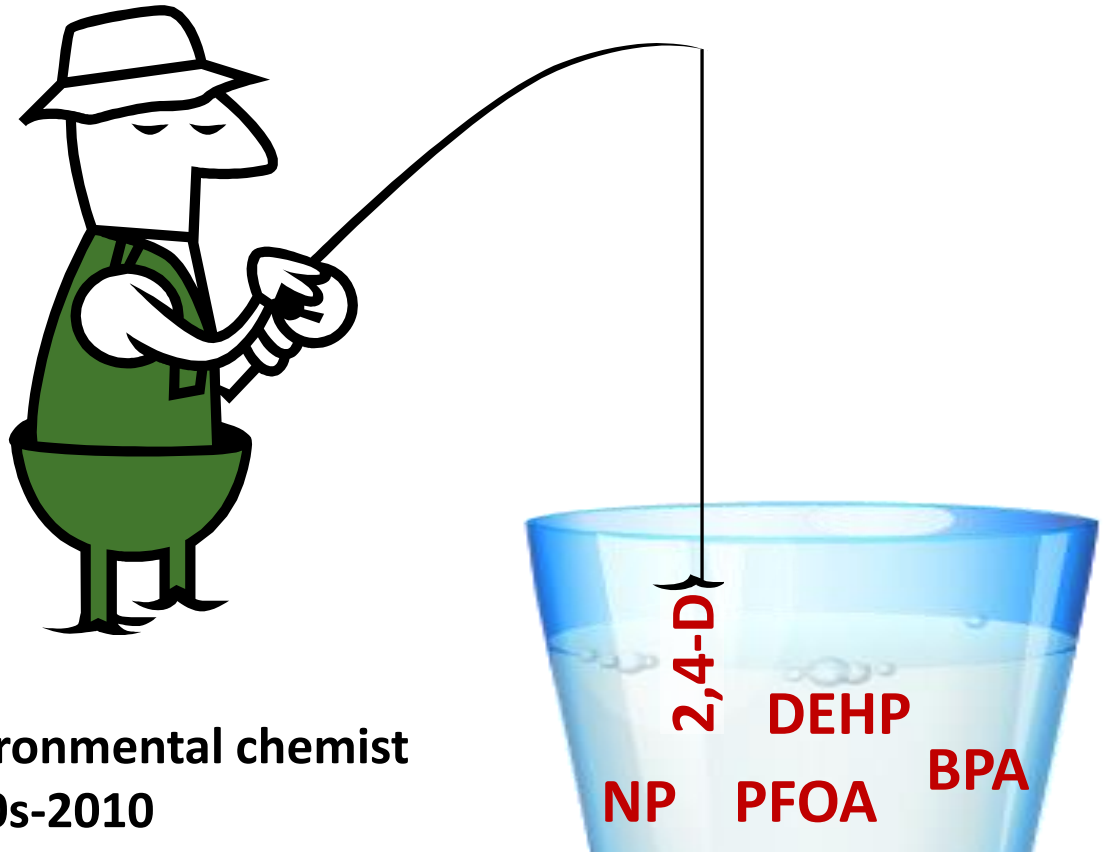
SLU

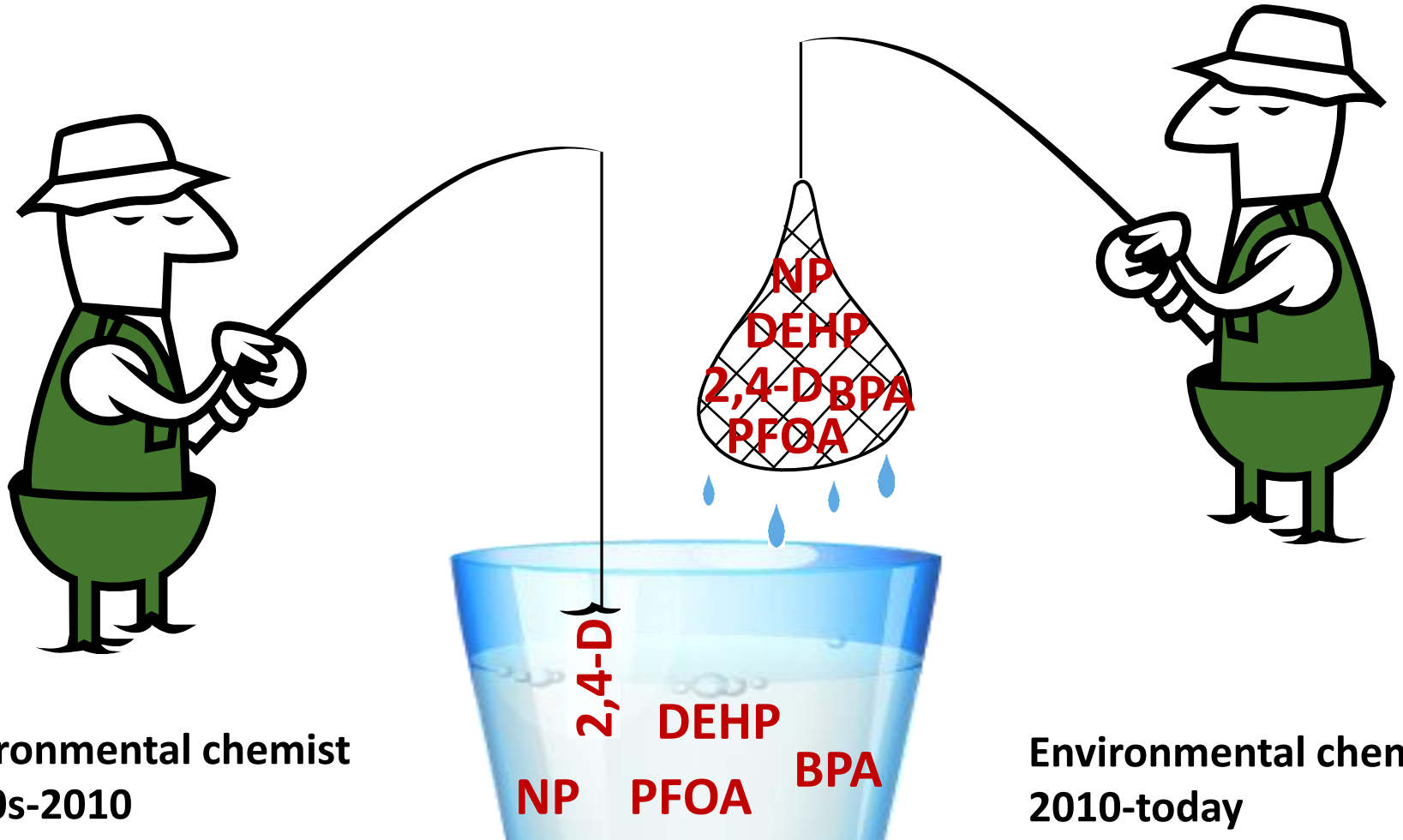
All these chemicals

Progress in Analytical Chemistry



Environmental chemist
1970s-2010

Progress in Analytical Chemistry

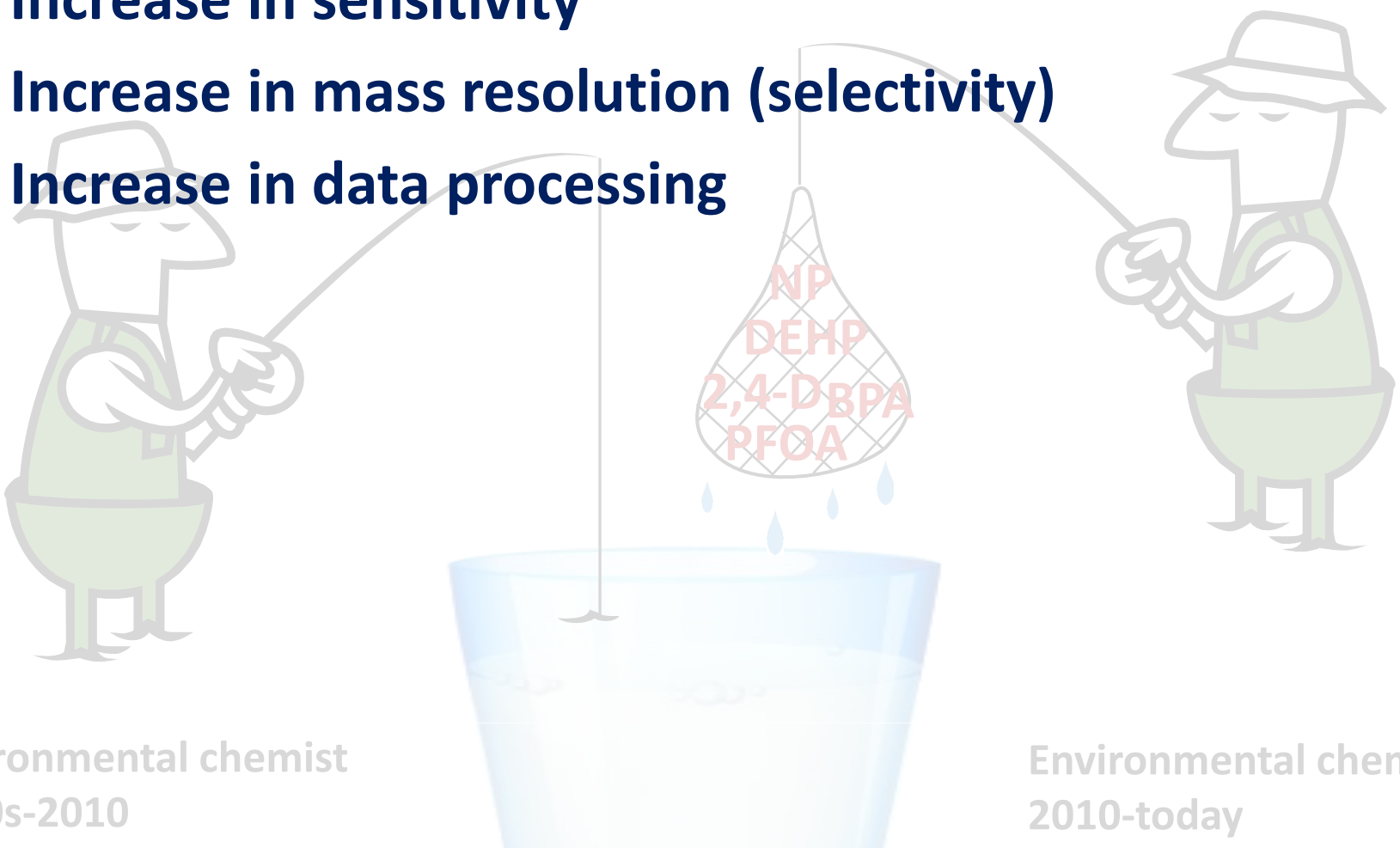


Environmental chemist
1970s-2010

Environmental chemist
2010-today

Progress in Analytical Chemistry

- Increase in chromatographic resolution
- Increase in sensitivity
- Increase in mass resolution (selectivity)
- Increase in data processing

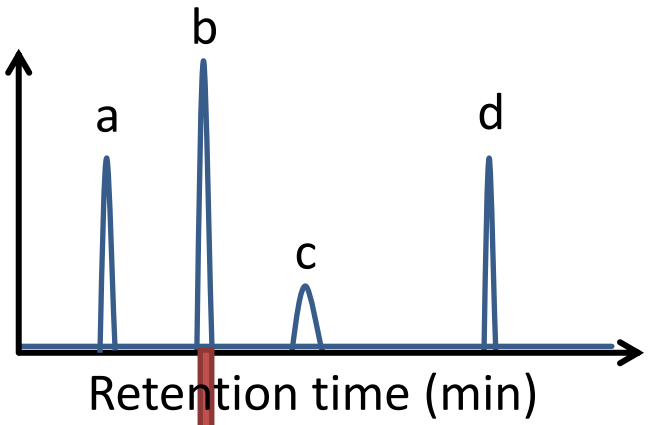


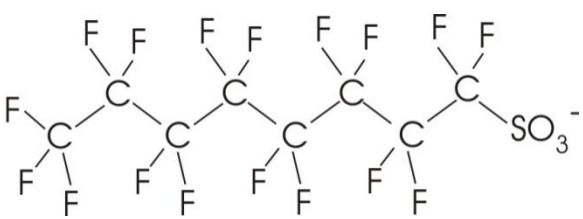
Environmental chemist
1970s-2010

Environmental chemist
2010-today

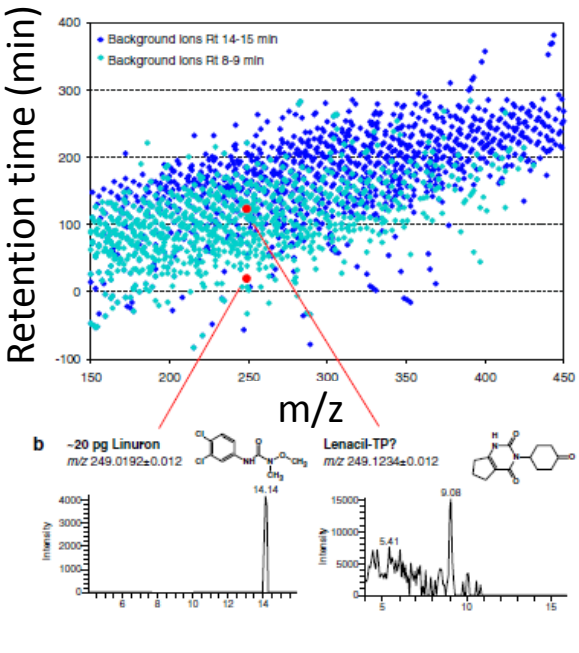
From Target to Non-target Screening

Target analysis





Non-target screening



Krauss, Singer, Hollender. *Anal. Bioanal. Chem.* 2010

Drinking Water Contamination

cirkulation VA-tidskriften

Cirkulation frågar: ”Sårbarheten för de här ämnena är väldigt bekymmersamt”

Publicerat 2012-10-03 07:31

Uppsala Vattens planeringschef Sven Ahlgren är bekymrad över fynden av låga halter PFOS och PFHxS (hexansulfonat) i Uppsalas dricksvatten. Problemet liknar i viss mån det som finns i Tullinge.

UppsalaTidningen

Publicerad 2013-10-10

Försvaret kräver fortsatt utredning av miljögifter

NYHETER Enligt Försvarsmakten är det inget som entydigt pekar på att miljögifterna i Uppsalas dricksvatten kommer från Ärna.

– Utredningarna måste fortsätta, säger Folke Borgh på Försvarsmaktens miljöprövningsenhet.

IVL Svenska Miljöinstitutet

PRESSMEDDELANDE | 2013-12-17

Kemikalier från brandskum fortsätter läcka ut i miljön

Mätningar visar att högfluorerade ämnen, så kallade PFAS, fortsätter att läcka ut från svenska flygplatser. Med dagens minskningstakt kommer det att ta 60-70 år innan halterna i miljön är nere på normala nivåer igen, visar studien från IVL Svenska Miljöinstitutet.

UNT.SE

Akademiska slutar använda egna brunnar

Akademiska sjukhuset slutar använda vatten från de två egna brunnar som förorenats av miljöfarliga perfluorerade alkylsyror.

Publicerad: 29/10/2013

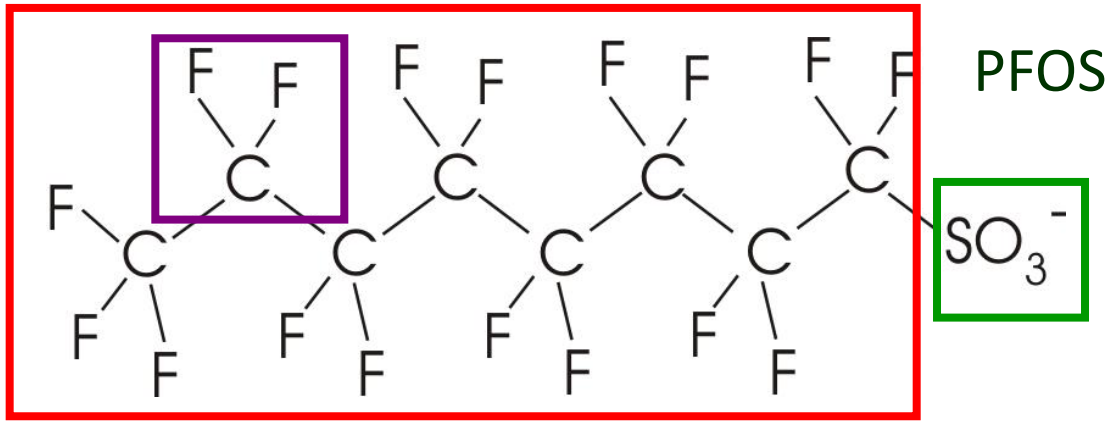
UNT.SE

Låga doser av giftet i dricksvattnet

Dricksvattnet i Knivsta är av god kvalitet fastän den hälsoskadliga kemikalien PFOS har spårats i analyser. Det säger Per Ericsson, vattenexpert på Norrvatten. Men han tycker att man ska undvika att äta mycket fisk fångad i norra Mälaren.

Publicerad: 24/10/2010

Per– and Polyfluoroalkyl Substances (PFASs)



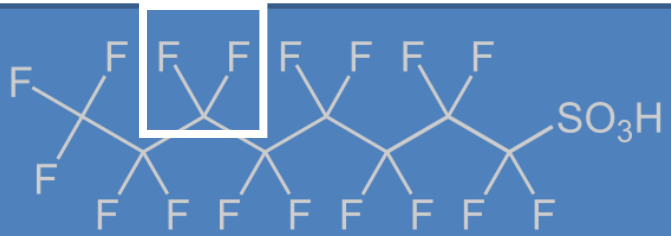
PFOS

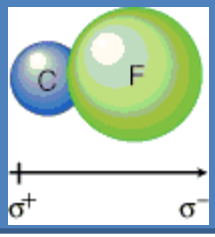
- Unique physicochemical properties
  - C–F → high bond energy
  - Hydrophobic group (their "tails") and hydrophilic group ("their head")
- Wide area of application

Characteristics of PFASs

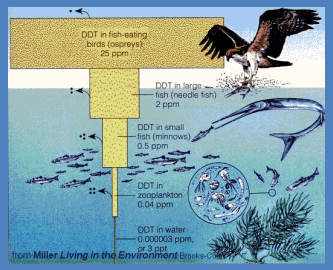
Persistent

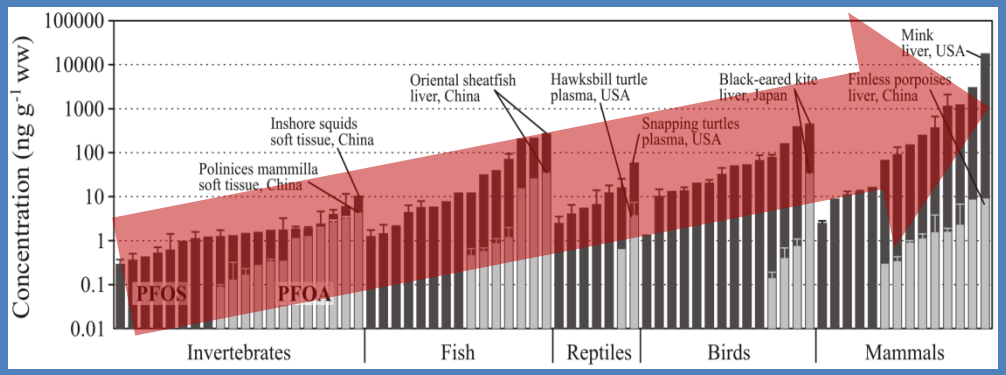
C–F → high bond energy





Bioaccumulation

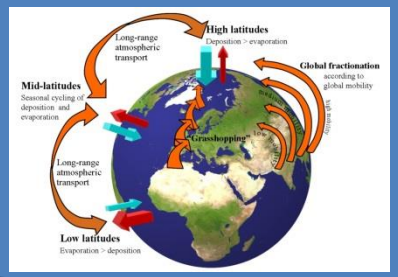


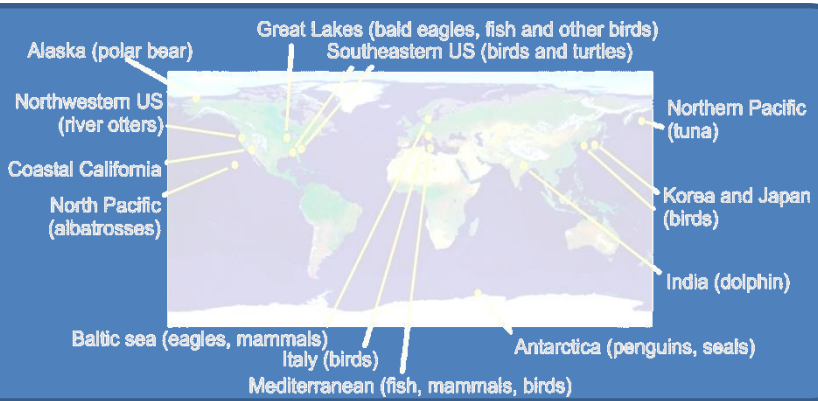


Toxicity

- Accumulates in blood-proteins, half-life in humans of about 8 years
- Is suspected to cause liver, thyroid and pancreatic tumors
- Endocrine disrupting potential

Long-range transport





Characteristics of PFASs

Persistent

C–F → high bond energy

Bioaccumulation

Persistent Organic Pollutants

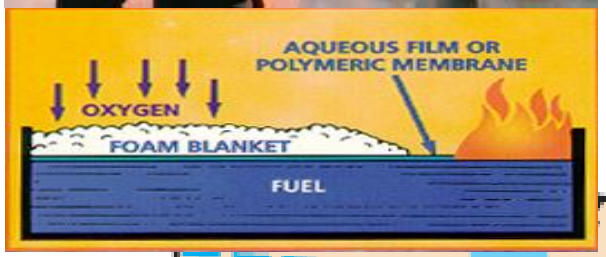
-> PFOS listed in the Stockholm Convention since 2009

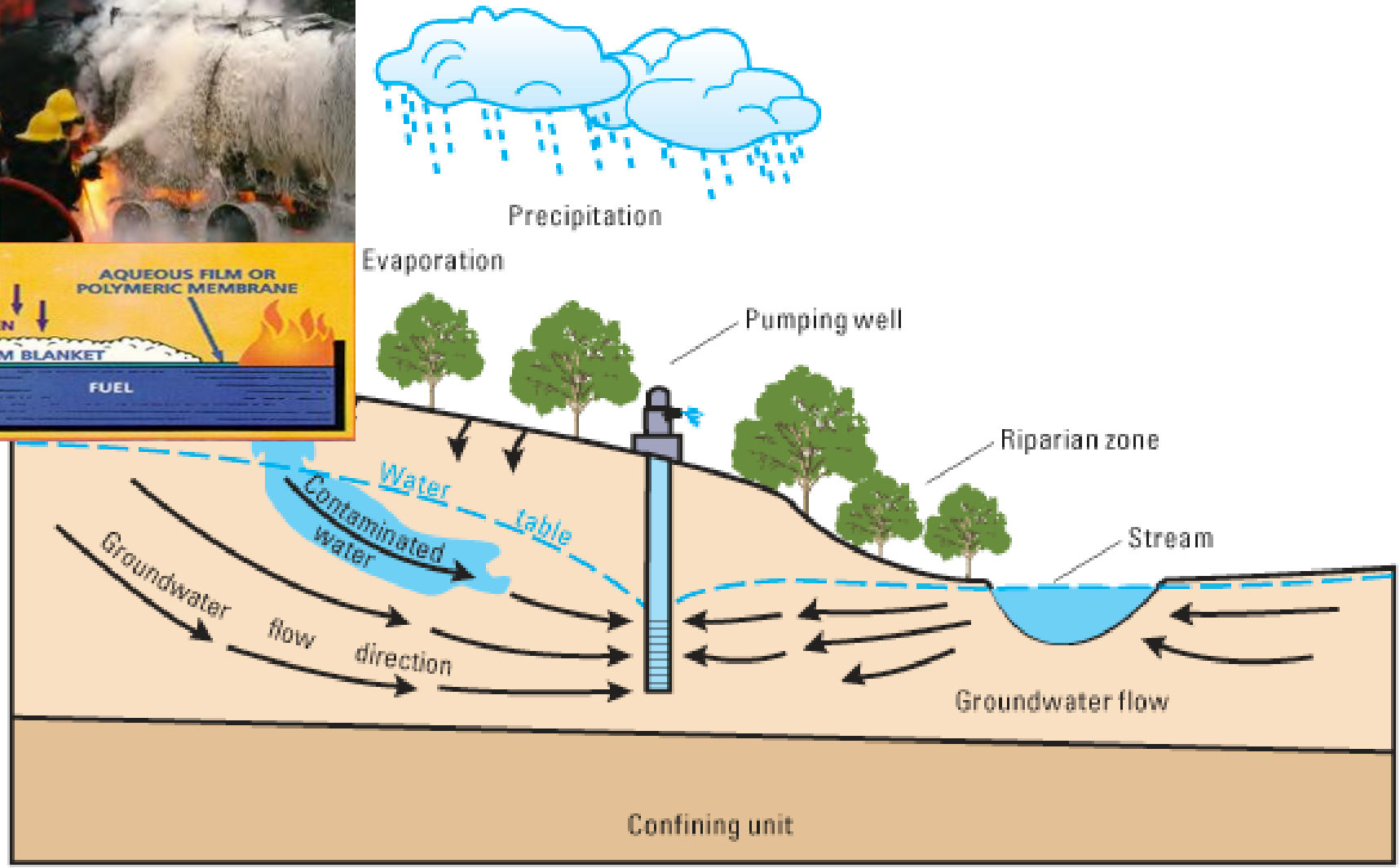
Toxicity

- Accumulates in blood-proteins, half-life in humans of about 8 years
- Is suspected to cause liver, thyroid and pancreatic tumors
- Endocrine disrupting potential

Long-range transport

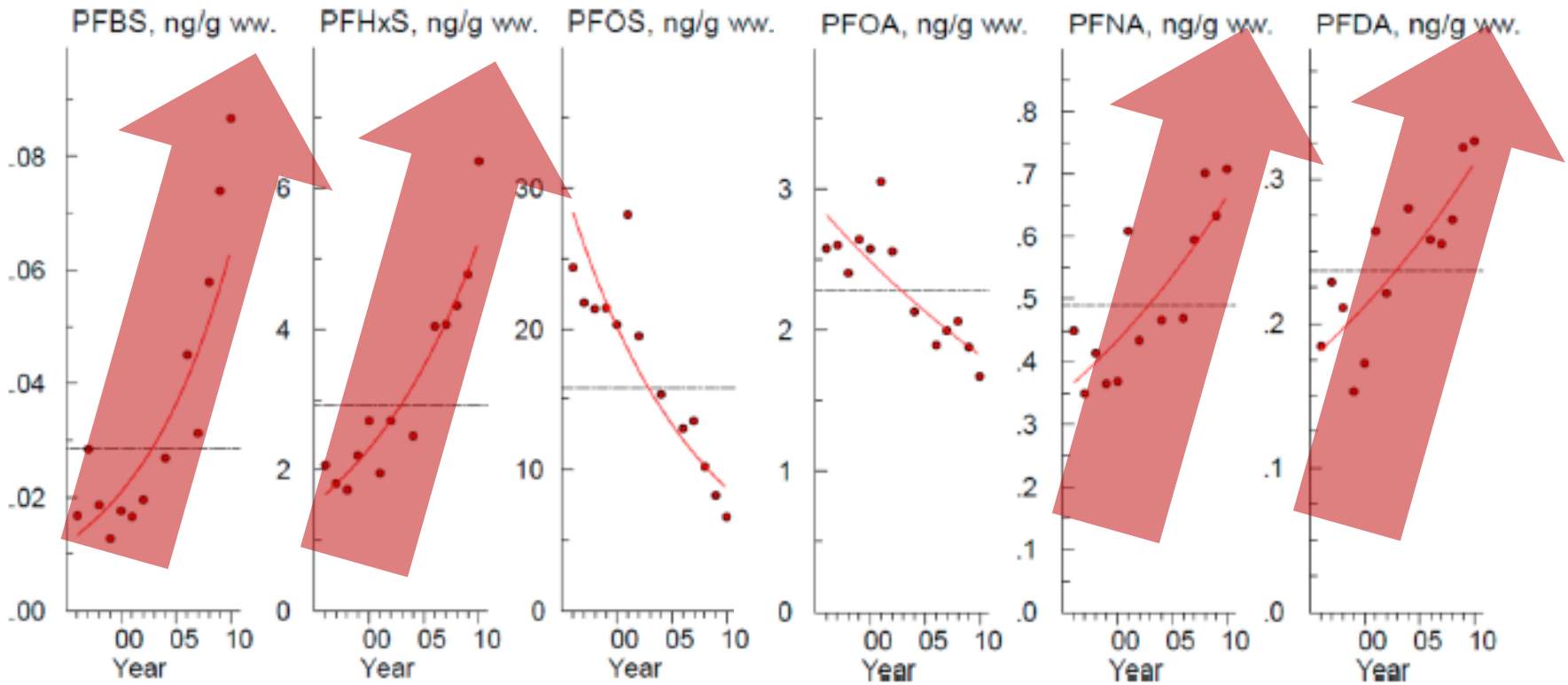
Infiltration of PFAS-contaminated Water





Domagalski, Johnson, 2012, *U.S. Geological Survey Fact Sheet 2012-3004, 4 p.*

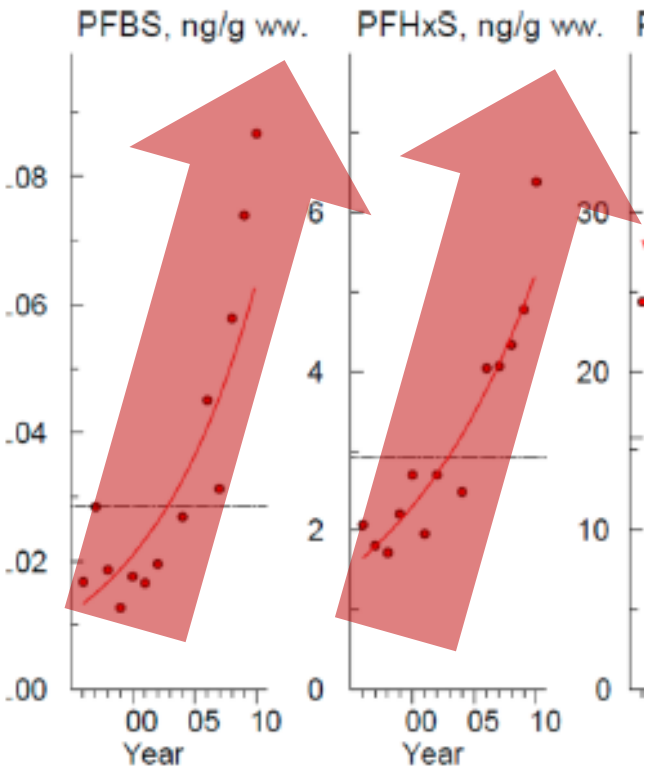
Temporal Trend of PFASs in blood from pregnant Women in Uppsala



Glynn, Berger, Bignert, Ullah, Aune, Lignell, Darnerud , 2012, *Environ Sci Technol*, 46, 9071–9079

Temporal Trend of PFASs in blood from pregnant Women in Uppsala

Too Late!



Glynn, Berger, Bignert, Ullah, Aune, Lignell, Darnerud, 2012, *Environ Sci Technol*, 46, 9071–9079

Early Detection of Hazardous Chemicals in Drinking Water - Safe-Drink

Integrated chemical and toxicological methods for early detection of hazardous chemicals in drinking water

SLU

Karin Wiberg

Agneta Oskarsson

Lutz Ahrens

Stephan Köhler

Meritxell Gros

Rikard Tröger

Uppsala University

Björn Hellman

Mid Sweden University

Erika Wall

Swedish National Food Agency

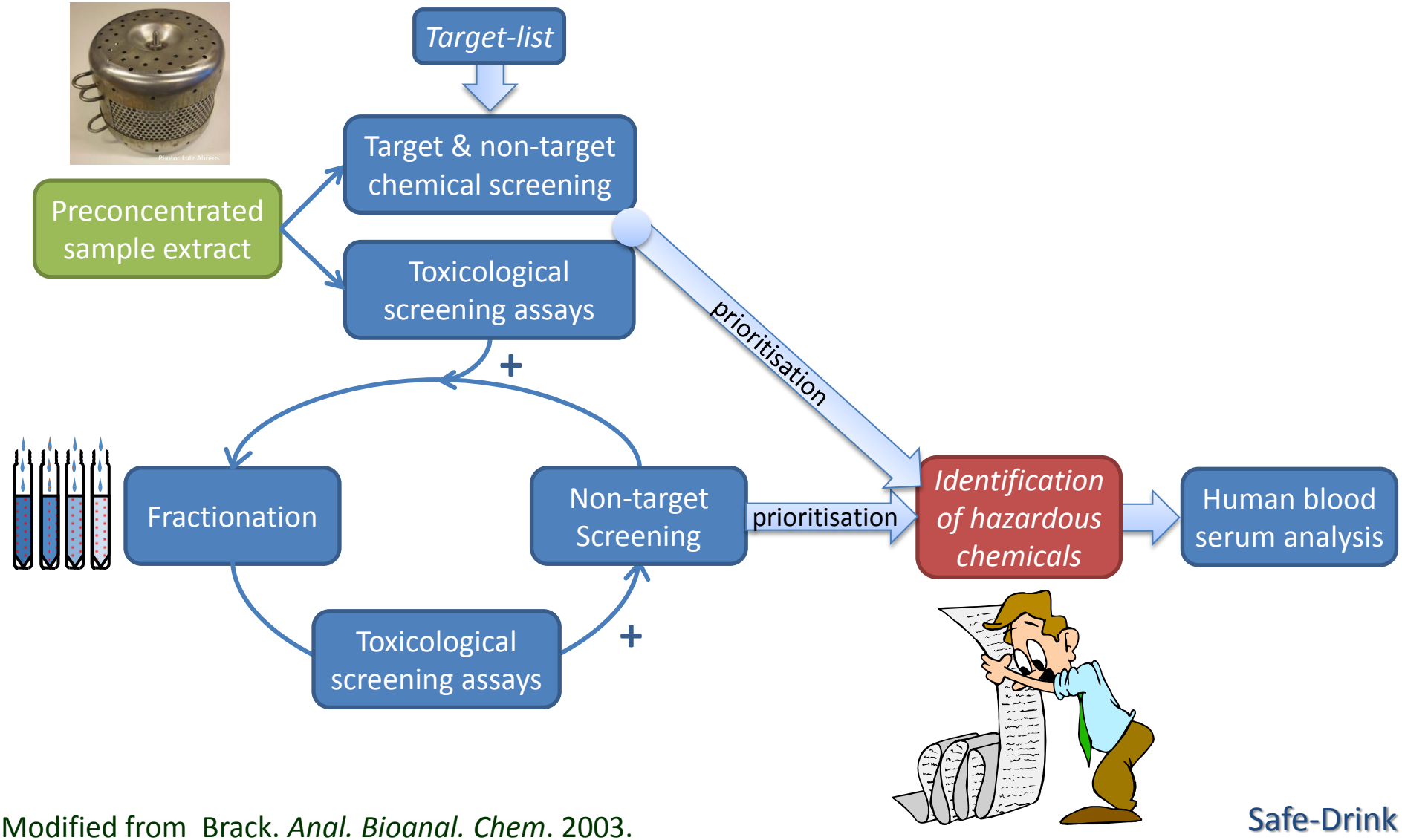
Heidi Pekar

Anders Glynn

Formas

Safe-Drink

Integrated chemical and toxicological method



Modified from Brack. *Anal. Bioanal. Chem*. 2003.

Safe-Drink

Sampling Strategies

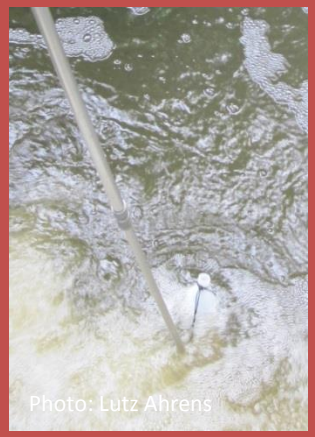
Grab Sampling

VS

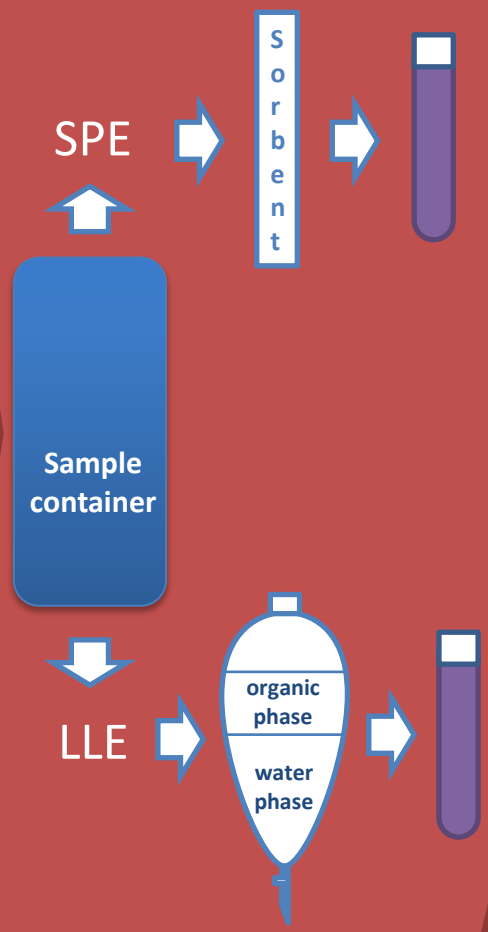
Passive Sampling

Grab Sampling

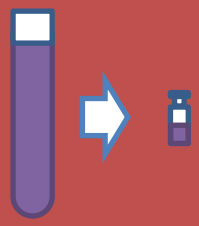
Grab Sampling



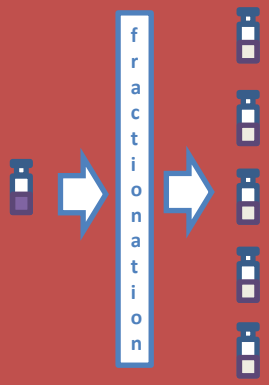
Large Volume Extraction



Concentration



Fractionation

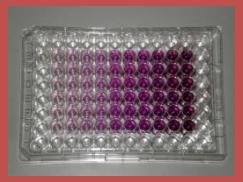


Analysis

Chemical

&

Toxicological



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Passive Sampling

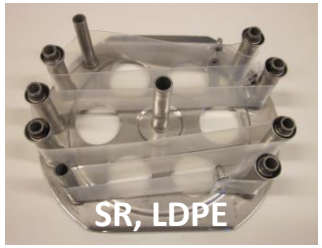
Passive sampling

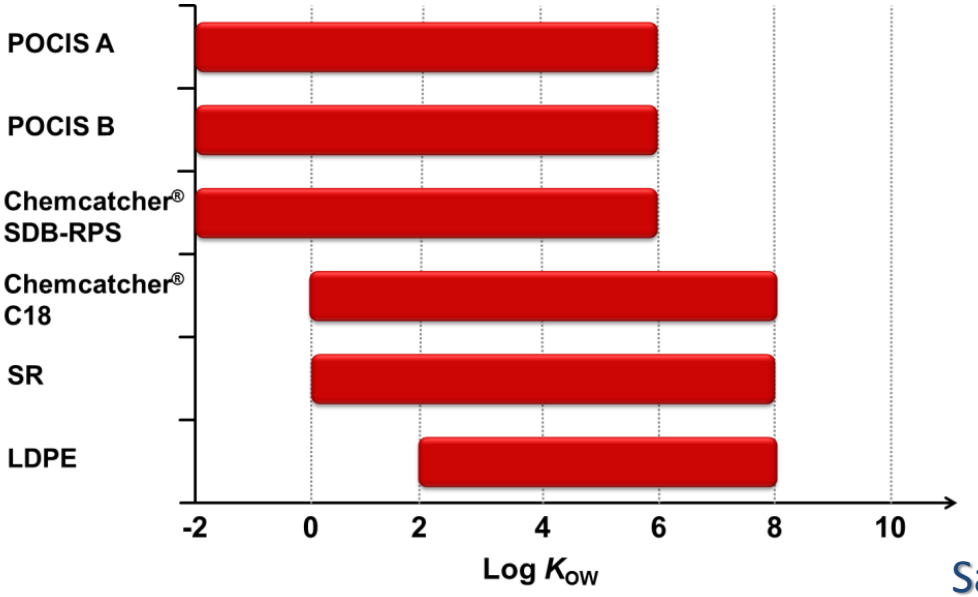
Sorbents

- **Time-integrated sampling for freely dissolved chemicals in water**

Passive Sampler Sorbents

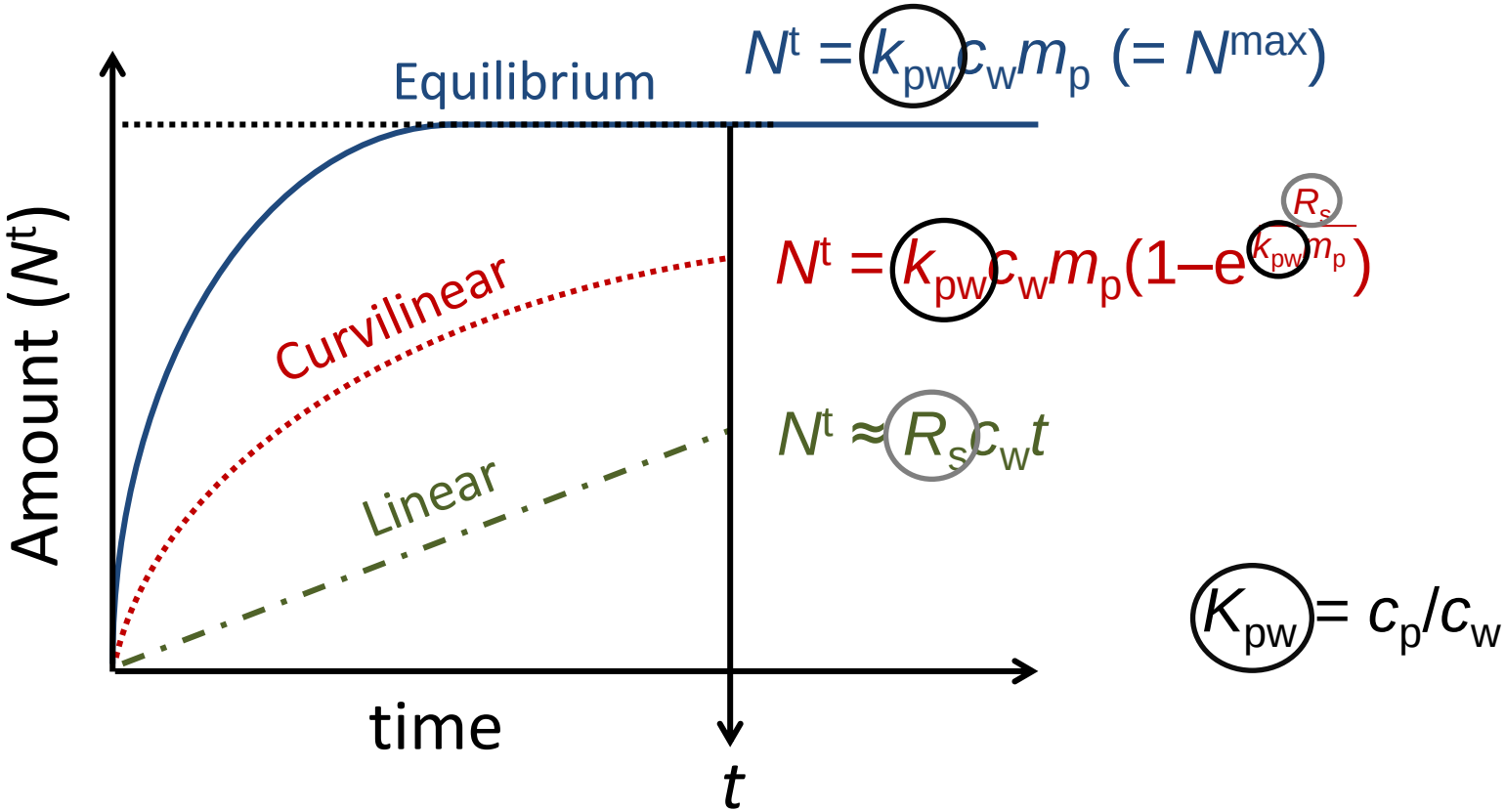
Passive sampler sorbents
Silicone rubber (SR)
Low-density polyethylene (LDPE)
POCIS A: Pharmaceutical-POCIS, (Oasis HLB sorbent)
POCIS B: Pesticide-POCIS, (Isolute ENV+ and Ambersorb 1500)
SDB-RPS: Styrene divinyl benzene Empore™ disk
C18 Empore™ disk





Safe-Drink

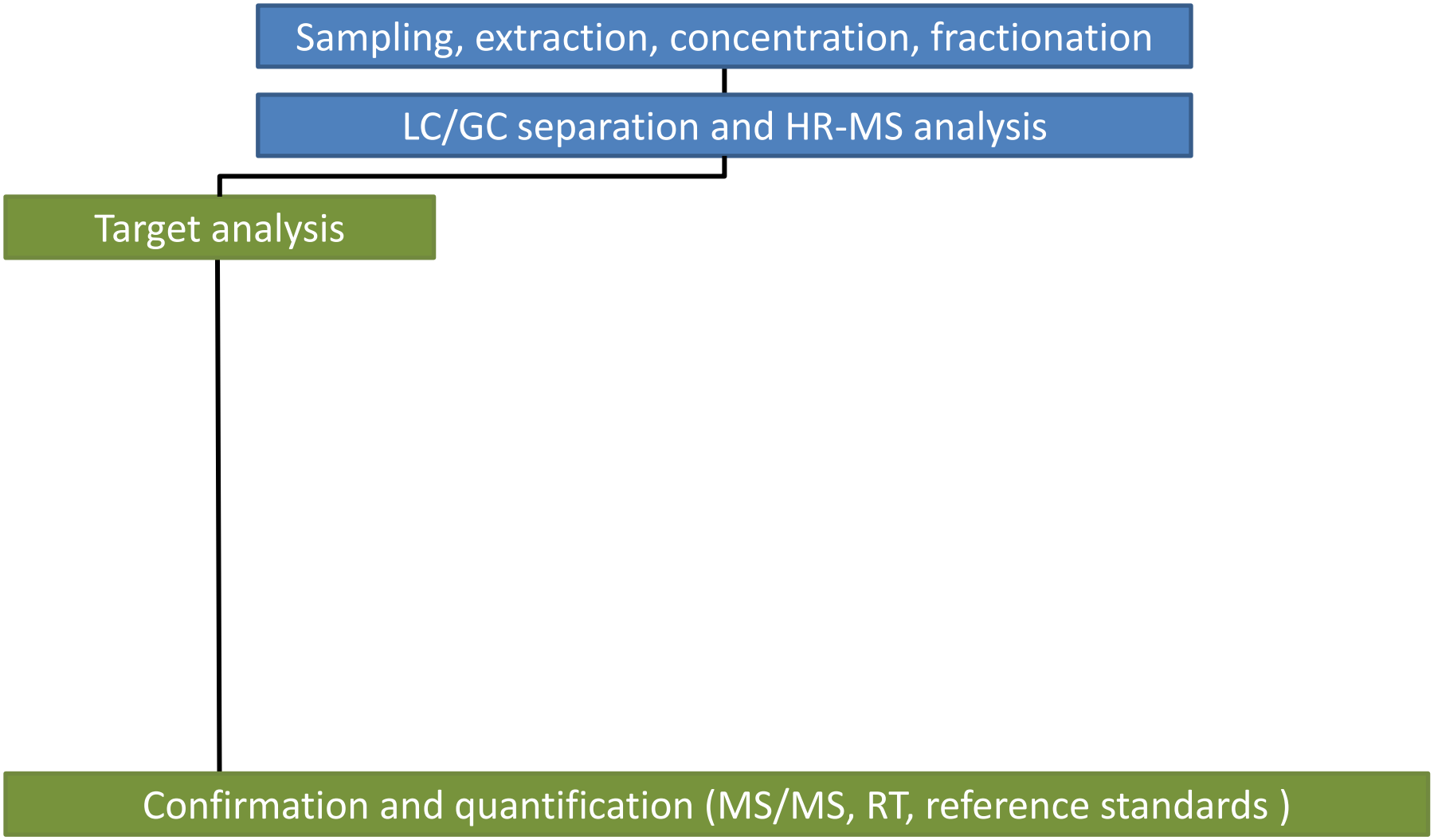
Uptake Process



N^t : amount on the sampler after t days exposure
c_w: free dissolved concentration in water
m_p: sorbent mass per sampler
R_s: sampling rate
c_p: concentration in the sampler

➢ **Affected by environmental conditions (e.g. water temperature)**

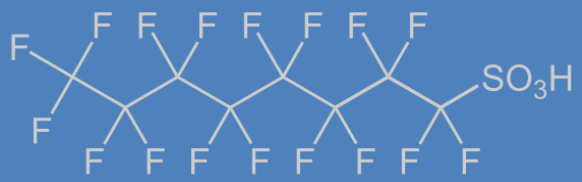
Workflow for Identification



Modified from Krauss, Singer, Hollender. *Anal. Bioanal. Chem.* 2010

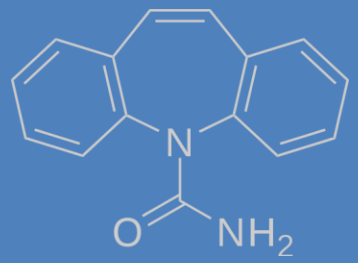
Target Analysis

Perfluoroalkyl Substances (PFASs)



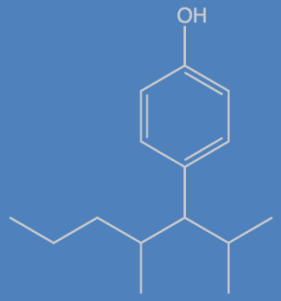
PFOS

Pharmaceuticals



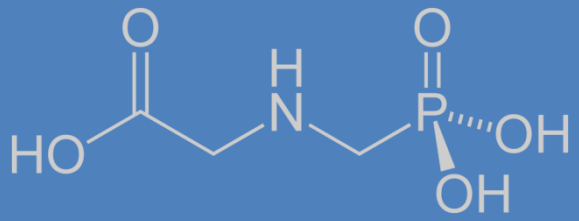
Carbamazepine

Plasticizer



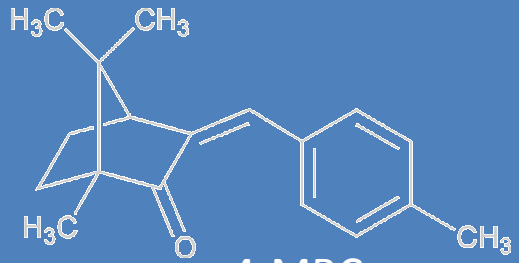
Nonylphenol

Pesticides



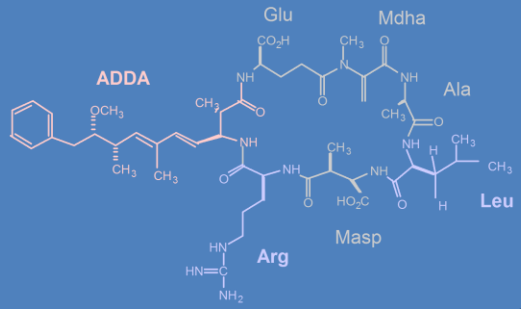
Glyphosate

Personal care products



4-MBC

Algal toxins

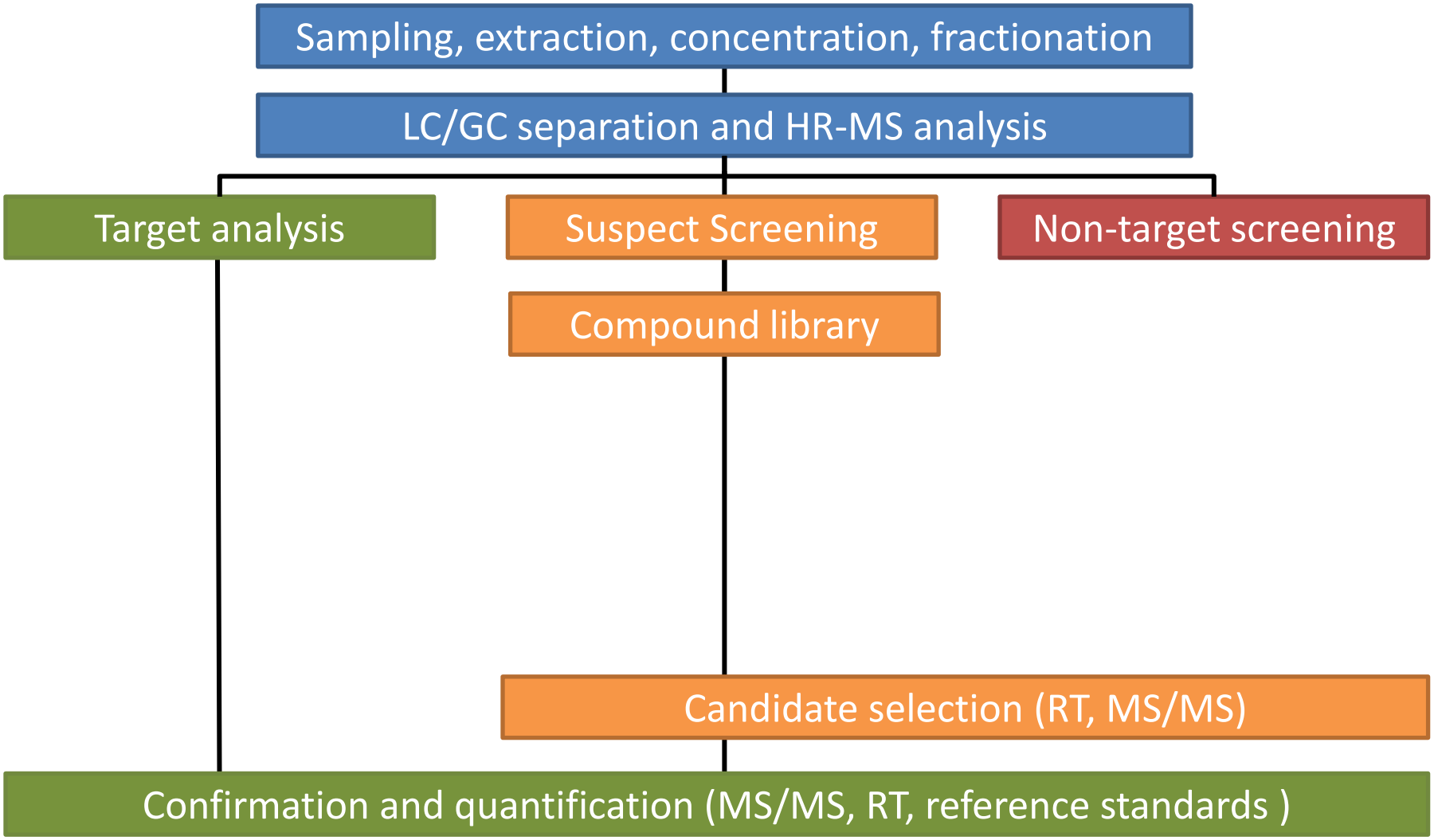


Target Analysis

- >100,000 chemicals in the environment
- Low concentrations
- Mixtures
- Transformation products

Safe-Drink

Workflow for Identification



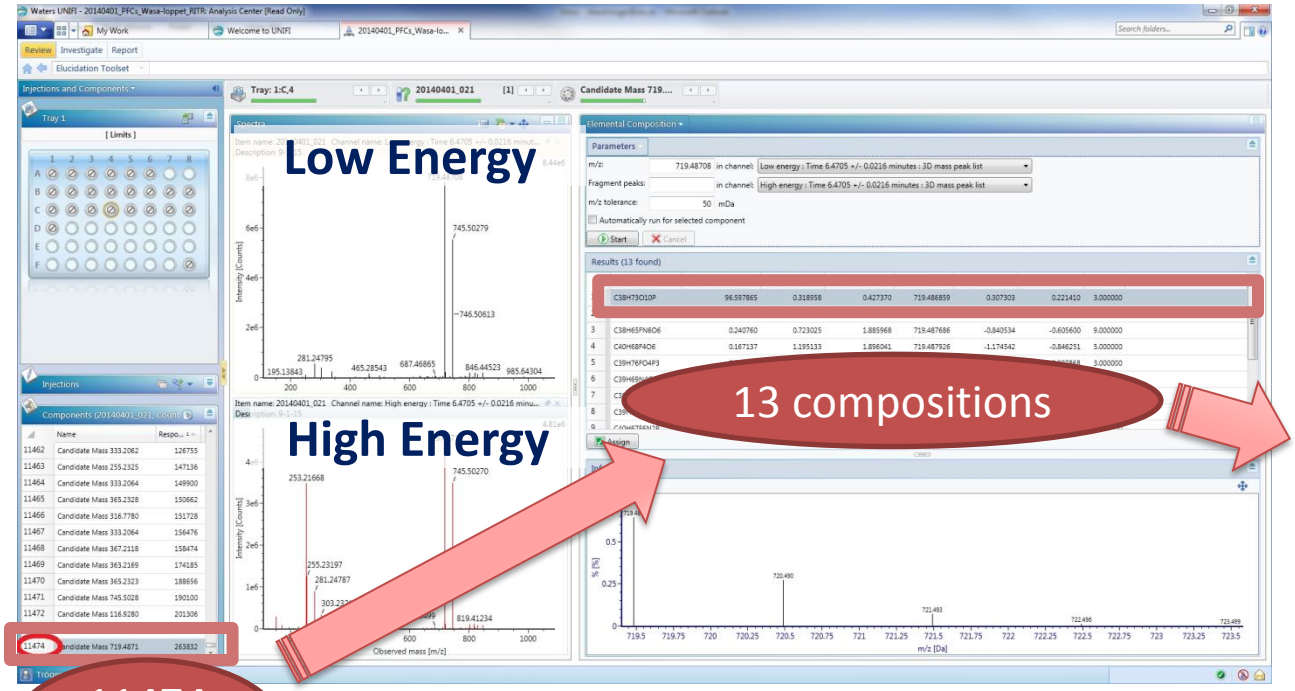
Modified from Krauss, Singer, Hollender. *Anal. Bioanal. Chem.* 2010

Workflow for Identification

Waters: Xevo G2-S QTof MS

Sampling, extraction, concentration, fractionation

LC/GC separation and HR-MS analysis



Non-target screening

Exact mass filtering

Molecular formula (MS isotope/adducts)

Structure (Database search, MS/MS)

Candidate selection (RT, MS/MS)

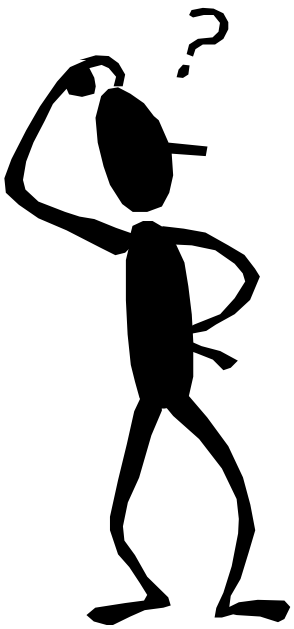
Confirmation and quantification (MS/MS, RT, reference standards)

Modified from Krauss, Singer, Hollender. *Anal. Bioanal. Chem.* 2010

Safe-Drink

Challenges

- **Grab sampling *vs* time-integrated sampling**
  - A sampling strategy for a broad suit of chemicals is needed!
- **Target analysis using multi-compound quantification methods**
- **Non-target screening**
  - >100.000 chemicals in the environment. How to process all the data?
- **Integrated chemical and toxicological approach**
  - Which can we detect? Which are relevant?



Questions?