Workshop on
Non-Target Screening
Towards the harmonisation of methods for
non-target screening of environmental samples

Organised jointly by the NORMAN Network and SOLUTIONS

Organisers
Juliane Hollender & Emma Schymanski, Eawag (Host Institute)
Jaroslav Slobodnik, EI
Martin Krauss & Tobias Schulze, UFZ

Eawag's Focus & Numbers

- **Research subjects are water and aquatic ecosystems.**
- **Eawag is committed to an ecological, economical and socially responsible management of water**
- **Bridging theory and practice**

Employees (61 % CH, 31 % EU)

- **200 scientists**
  (70% natural sciences, 25% engineering, 5% social sciences)
- **150 PhD students**
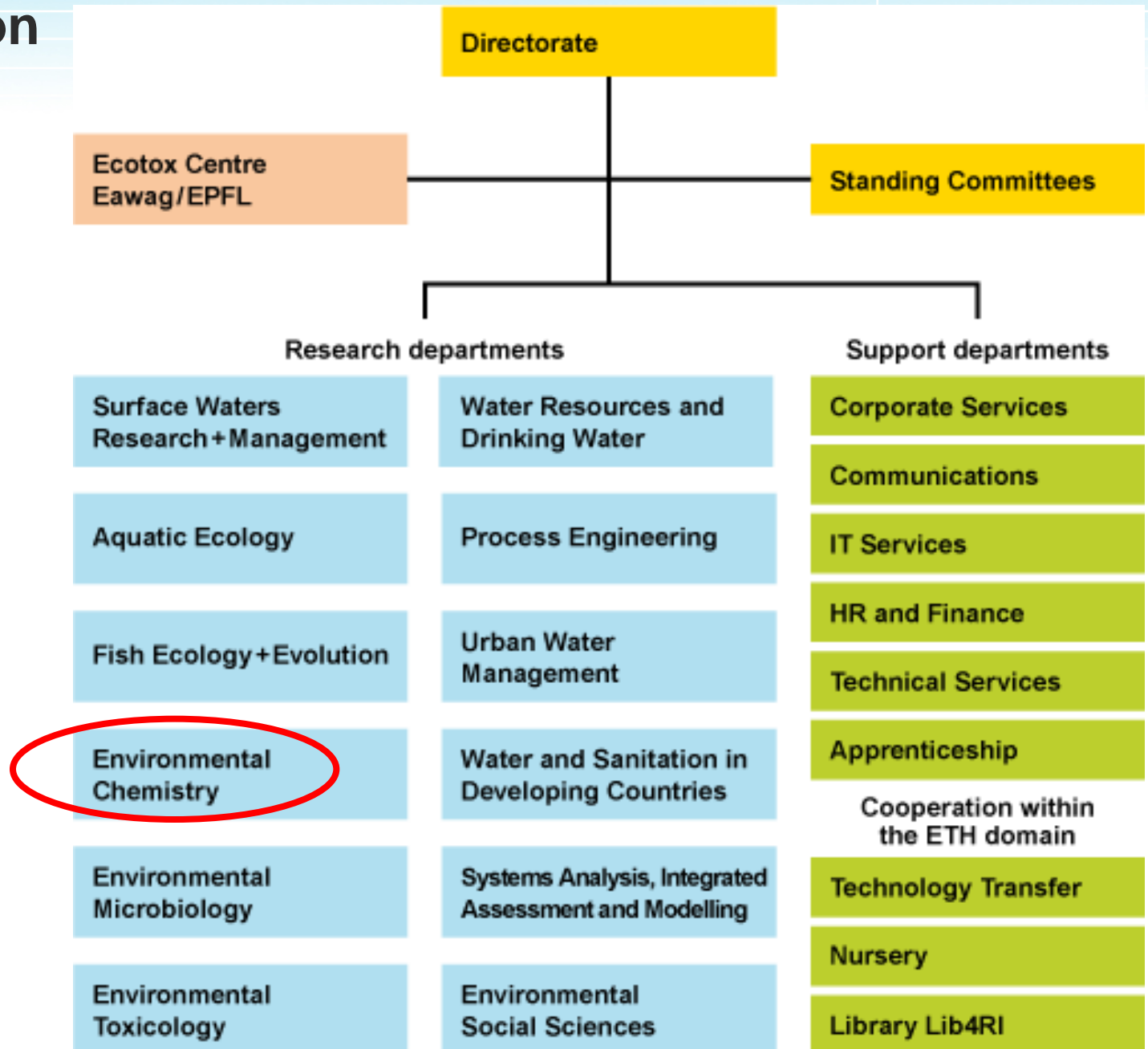- **150 technical and administrative employees**

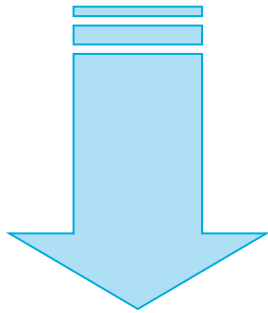**Kastanienbaum**   **Dübendorf**

Organisation
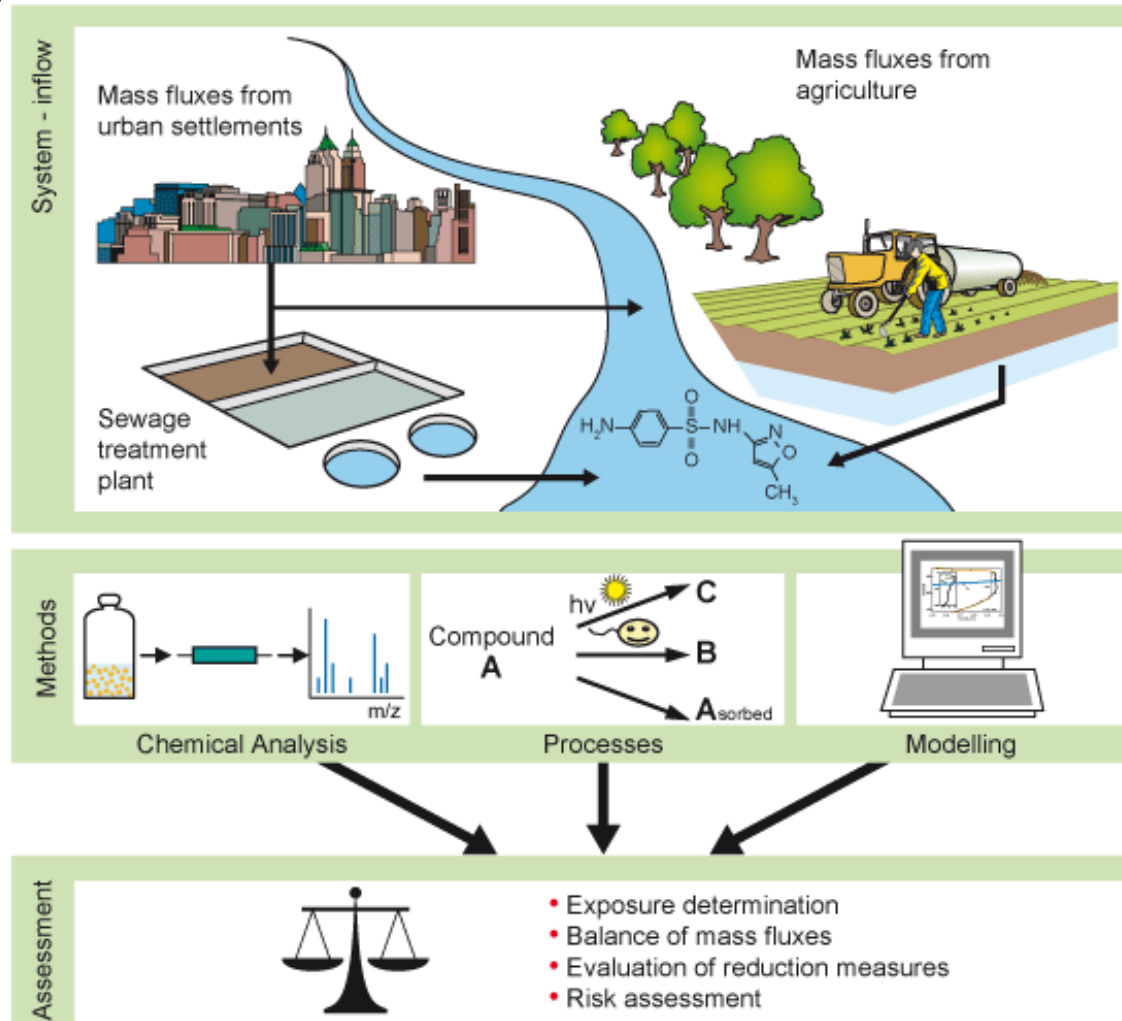
Uchem - overall aim of our research

mechanistic understanding of the exposure and fate

➢ of organic (micro)pollutants

➢ in the natural & engineered aquatic environment

Basis for
- ❖ risk assessment
- ❖ mitigation measures
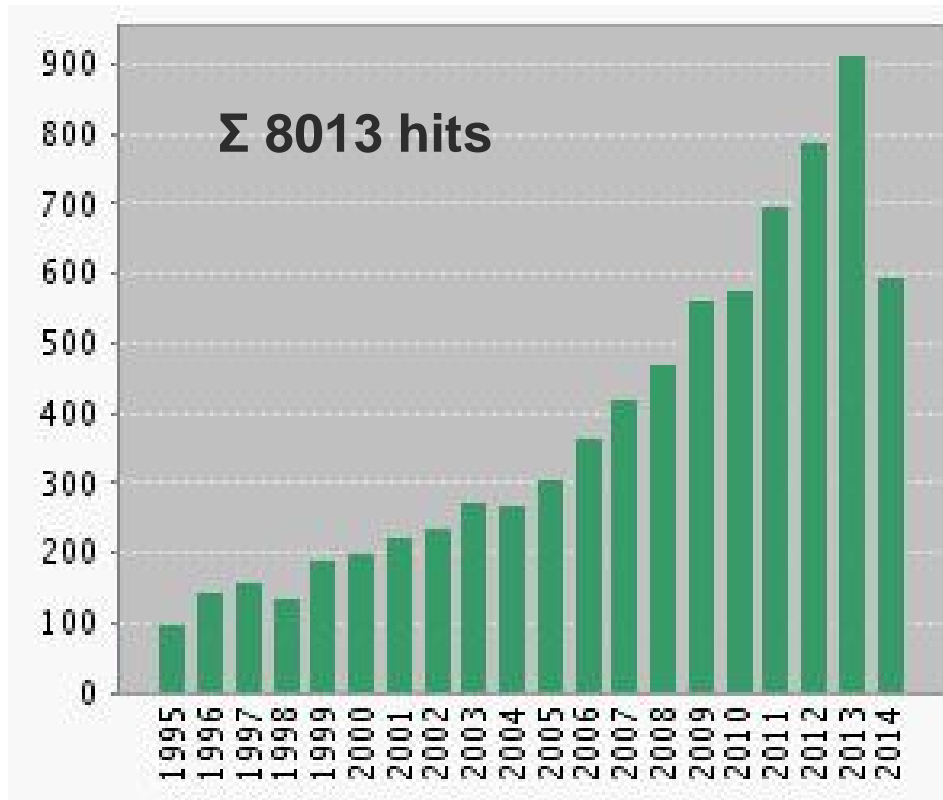- ❖ Improvement of water quality

Increasing interest in non-target analysis

Search for publications in web of science (11 September 2014)

Nontarget or non-target* & mass spectrometry

Progress in analytical instrumentation enables non-target screening

- Increase in chromatographic resolution (UHPLC, GCxGC, LCxLC)
- Increase in sensitivity
- Increase in mass resolution (selectivity)
- Improved MS/MS strategies (fast detectors, data-dependent/-independent analysis)
- Increase in data processing (more data, databases & computer tools)
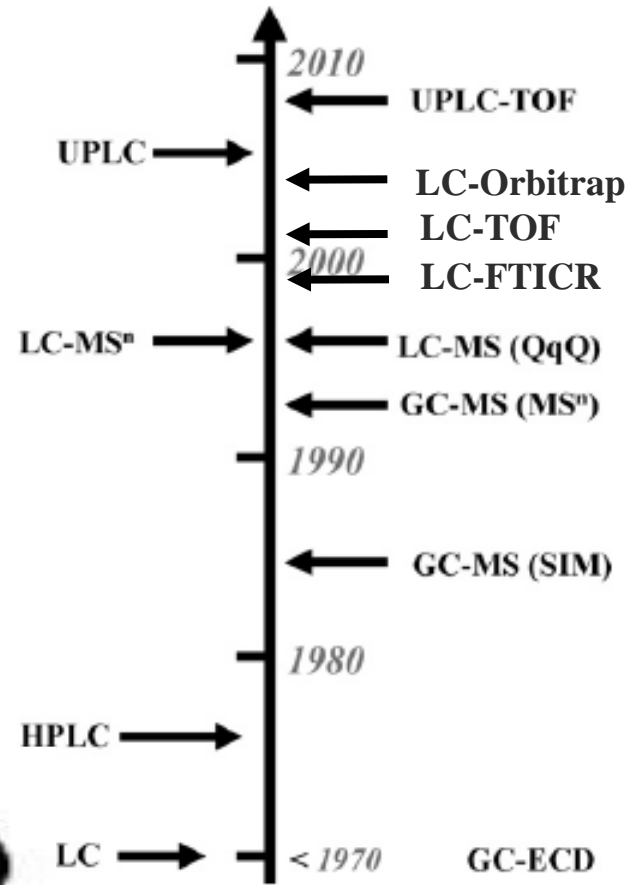
➔ **Chemical transparent environment?**
➔ **Early warning system for emerging contaminants?**

modified from De Brabander et al. J. Chromatogr. A 2009

Open Questions – Discussion points at ICCE 2011
Satellite event on non-target screening at Eawag

Environmental applications

- **How can non-target screening be implemented in the practice**
- **How much confirmation is necessary for an unequivocal identification?**
  Reference compound or NMR indispensable? Definition of identification points?

Computational and analytical tools

- **Which computer tools and databases are suitable for high-throughput and high qualitative identification?**
- **What can we learn from metabolomics or other disciplines?**
- **Which additional analytical strategies are suitable for improving identification?**
  chromatography, ionization, derivatization, H/D exchange

Effect-directed analysis and transformation products

- **Can the identification procedure be simplified for transformation products because of prior knowledge (suspect screening)?**
- **How can non-target identification effectively be combined with effect tests to EDA strategies?**

Some success…

NORMAN Collaborative Non-target Screening Trial

Rhine monitoring stations

Solutions for prioritisation, assessment and management of emerging contaminants

Goals of workshop

- Overview on current trends and future developments of non-target screening

- Discussion on harmonisation of non-target screening workflows

- Preparation for opinion paper/guidance document

Schedule of the Day – Tuesday September 16

First Session

Time	Title	Presenter	Institute
13:00	**Welcome and setting the scene**	Juliane Hollender	Eawag
13:05	Suspect and non-target screening approaches for GC-MS	Peter Haglund	Umea
13:30	Suspect and non-target screening approaches for LC-MS	Heinz Singer	Eawag
13:55	Summary of the Collaborative Screening Trial	Jaroslav Slobodnik	EI
14:20	Non-target Approaches: A US Perspective	Lee Ferguson	Duke Uni
15:00	**Coffee Break until 15:30**		

Schedule of the Day – Tuesday September 16

Second Session

Time	Title	Presenter	Institute
15:30	Use and Benefits of GC(APCI)-QTOF-MS	Juan Sancho	UJI
15:50	Spectral Information and Identification Confidence	Emma Schymanski	Eawag
16:10	In silico fragmentation and reference information	Christoph Ruttkies	IPB
16:30	Comparison of approaches for retention prediction	Martin Krauss	UFZ
16:50	**Short Break until 17:00**		

Schedule of the Day – Tuesday September 16

Third Session

Time	Title	Presenter	Institute
17:00	Screening using databases: STOFF-IDENT	Manfred Sengl	LfU
17:10	Screening using databases: DAIOS	Wolfgang Schulz	LW
17:20	Incorporating market data and use pattern	Stellan Fischer	KEMI
17:40	Inclusion of toxicity information	Ralph Kühne	UFZ
18:00	Discussion; end of Day 1	Juliane Hollender	Eawag
19:00	**Common BBQ at aQa Sponsored by Eawag**		

Schedule of the Day – Wednesday September 17

Discussion of Strategies

Time	Title	Presenter	Institute
09:00	Statistical approaches for data-mining and non-target selection	Drazenka Stipanicev	CW
09:20	Time series analysis of the Rhine at Basel	Matthias Ruff	Eawag
09:40	Stealing ideas from metaolomics data exchange repositories	Steffen Neumann	IPB
10:00	Advanced spectral processing and management	Robert Mistrik	HighChem
10:20	NORMAN Digital Storage - archiving raw environmental mass spectral data for future analysis and assessment	Tobias Schulze	UFZ
10:40	**Coffee Break**		
11:15	Prioritisation and non-target screening	Jaroslav Slobodnik	EI
11:45	Discussion on harmonisation potential and future needs	Chair: Peter Haglund	Umea
12:45	**Workshop Wrap-up**	Juliane Hollender	Eawag

Schedule of the Day – Wednesday September 17

Dinner