



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**

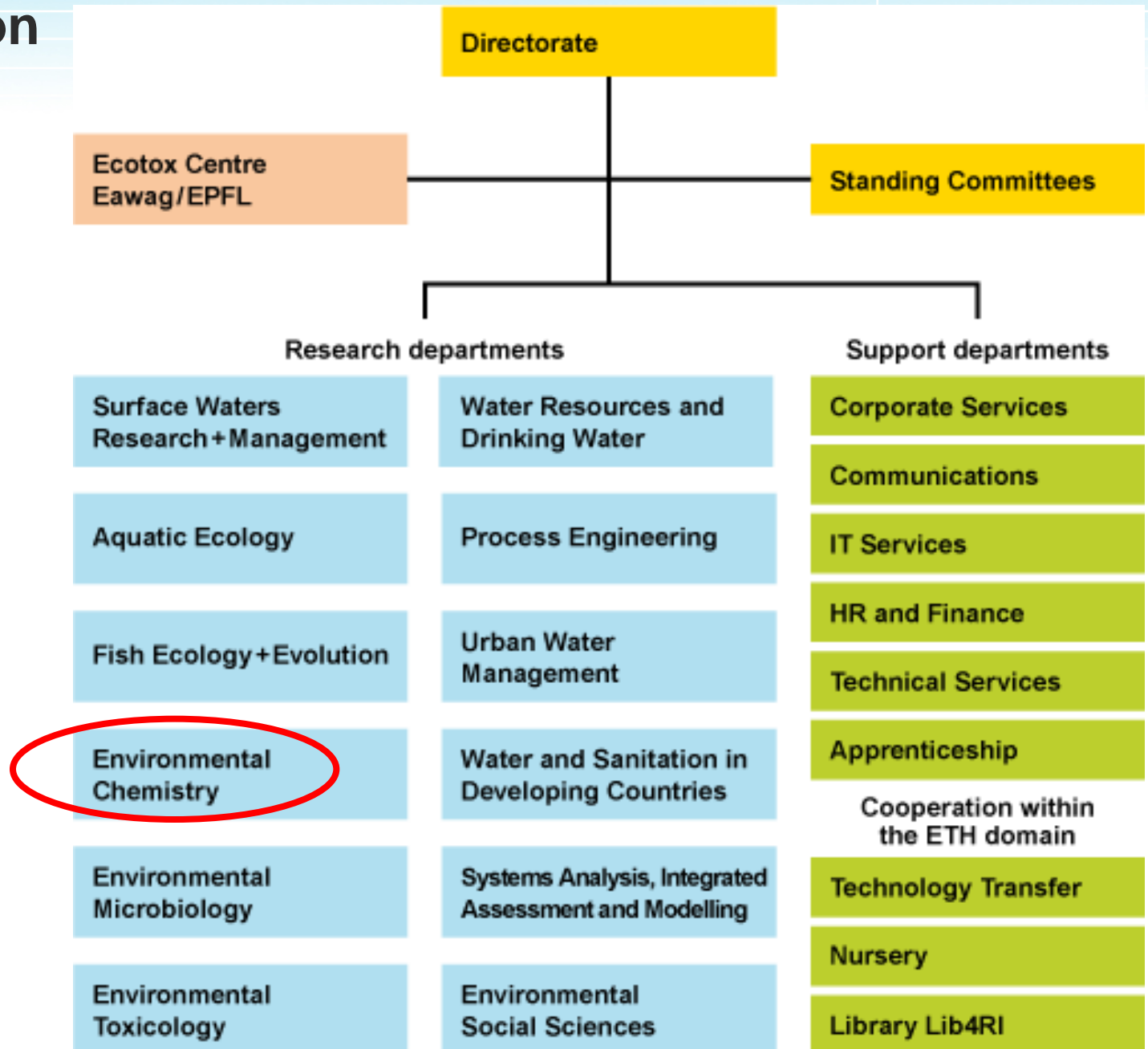
**Kastanienbaum**



**Dübendorf**



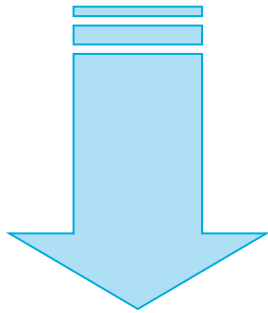
# Organisation



# Uchem - overall aim of our research

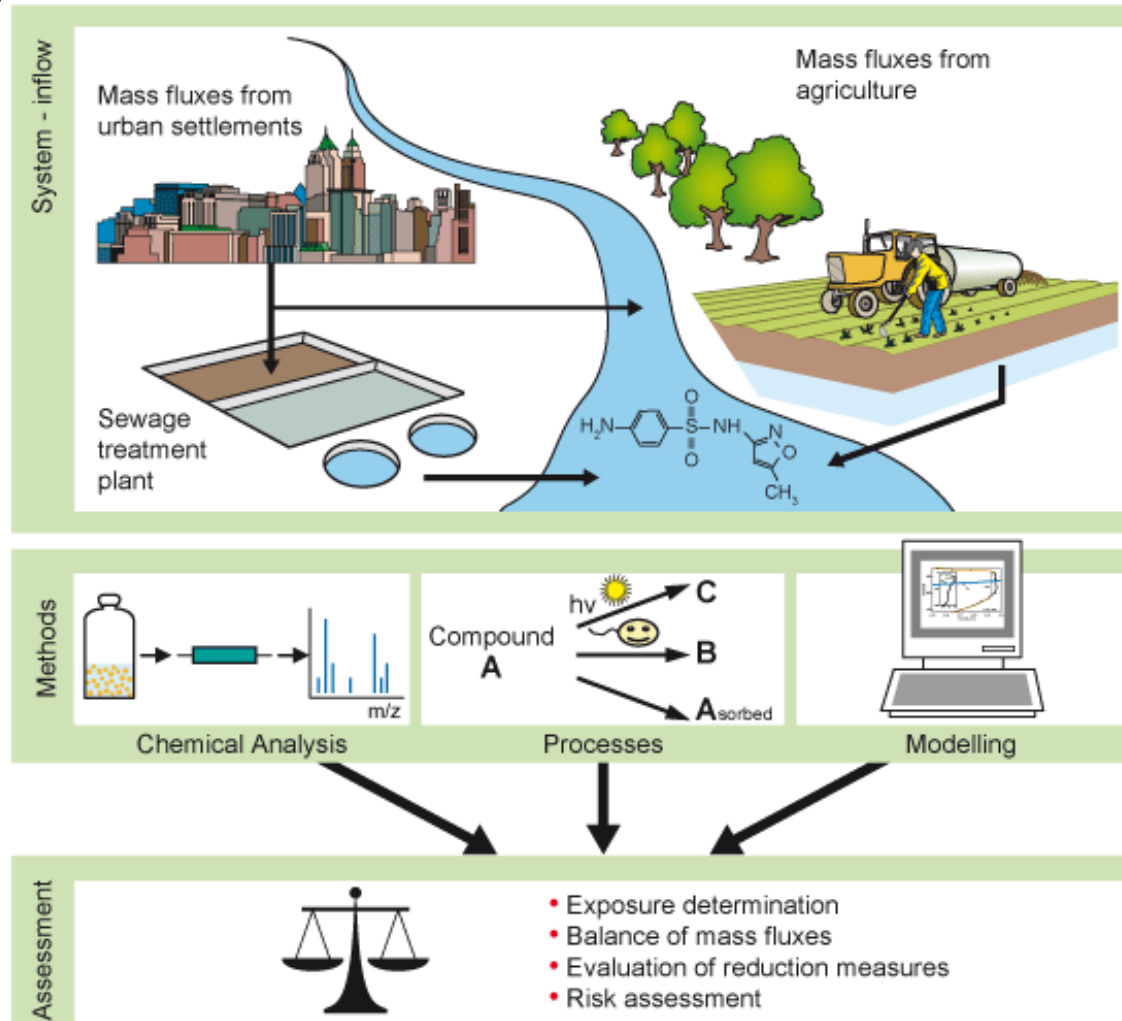
mechanistic understanding of the exposure and fate

- of organic (micro)pollutants
- in the natural & engineered aquatic environment



Basis for

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

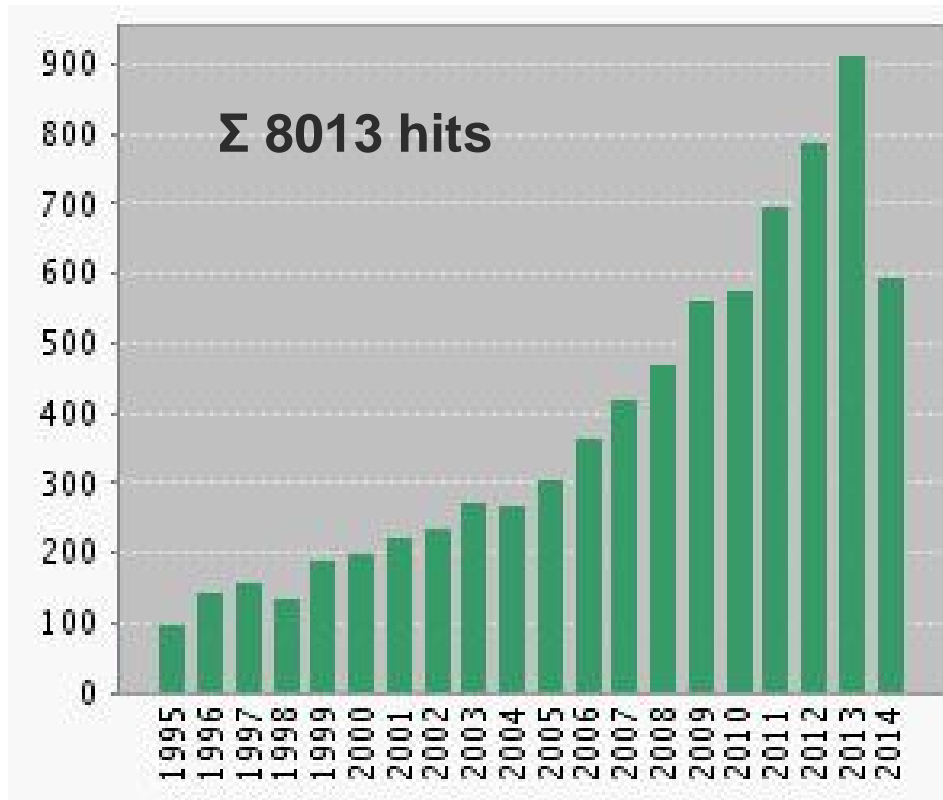


# Increasing interest in non-target analysis

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

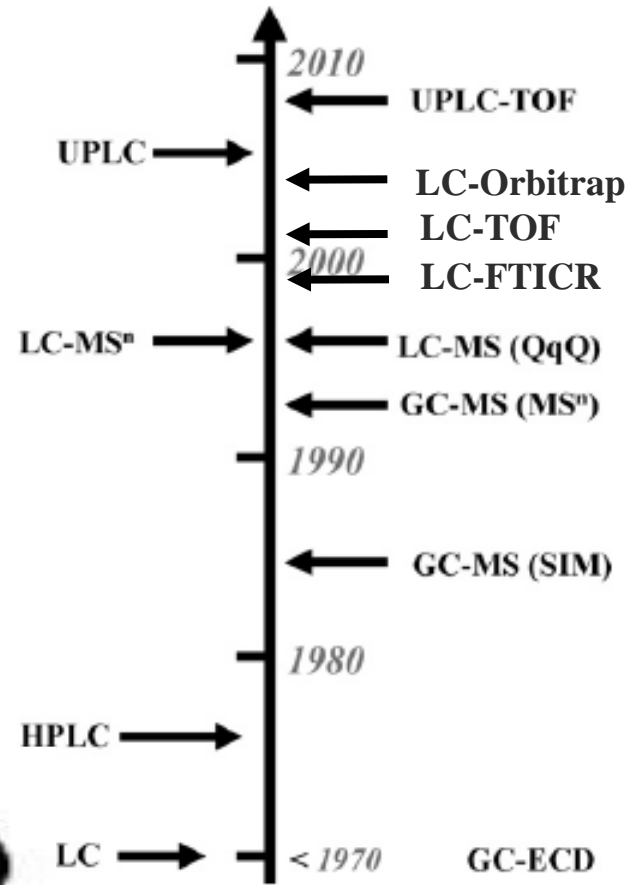
## Nontarget or non-target\* & mass spectrometry

Number  
of papers



# 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?**

# 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...

ENVIRONMENTAL  
Science & Technology

Viewpoint  
pubs.acs.org/est



Contents lists available at ScienceDirect

Environmental Pollution

journal homepage: www.elsevier.com/locate/

ENVIRONMENTAL  
Science & Technology

Identifying Small Molecules via High Resolution Mass Spectrometry: Gas Chromatography Method

Confidence

Emma L. Heinz P.

Searching for unknown substances



NORMAN Collaborative Non-target Screening Trial

M.I. Cervera, T. Po

At very low concentrations, organic micropollutants in natural waters can be hazardous to aquatic organisms. Owing to technical constraints, analytical methods have so far been confined to the detection of a relatively small number of known compounds. With new methods, previously undetected substances can also be identified.

...ton, New York 13446, United States  
... Oceanographic Institution, Woods Hole, Massa

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Received in revised form 24 July 2013  
Accepted 27 July 2013

Keywords:  
Nontarget screening  
Suspect screening  
High resolution mass spectrometry  
Polar contaminants  
WWT effluent

To detect and identify suspected and formerly unknown effluent, we established a screening procedure based on spectrometry (LC-HRMS) with stepwise identification searches a list of 2160 suspected site-specific and documented amenable to LC-HRMS. After searching chromatograms positive detections were stepwise excluded by retention patterns, ionization behavior and HRMS/MS spectra. In selected based on distinctive isotope patterns and intermediate evaluation. Six suspected and five nontarget chemicals previously reported as environmental pollutants.

Chemosphere 85 (2011) 1211-1219

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Keywords:  
Fruits and vegetables

ENVIRONMENTAL  
Science & Technology

Strategies for Wastewater Spectrometry  
Emma L. Schyns  
Michael A. Stairs

Supporting info



Rhine monitoring stations

ABSTRACT: While contaminants and transformation products, which cannot be captured by target analysis alone. High accuracy, high resolution mass spectrometric data were explored with novel untargeted data processing approaches (emission, nontarget, and WYCOSS) to complement an extensive target analysis in usual 'all in one' measurements. On average 1.2% of

mass spectrometry (GC-TOF) utilized as method for rapid fruit and vegetable matrices identification of the analytes, tomatoes and carrots) high QICHERS procedure responses over GC-TOF MS.

solutions

Solutions for prioritisation, assessment and management of emerging contaminants

trace substances in water analysis

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## 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
<b>13:00</b>	<b>Welcome and setting the scene</b>	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
<b>15:00</b>	<b>Coffee Break until 15:30</b>		

# 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
<b>16:50</b>	<b>Short Break until 17:00</b>		

# 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
<b>19:00</b>	<b>Common BBQ at aQa Sponsored by Eawag</b>		

# 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
<b>10:40</b>	<b>Coffee Break</b>		
11:15	Prioritisation and non-target screening	Jaroslav Slobodnik	EI
11:45	Discussion on harmonisation potential and future needs	Chair: Peter Haglund	Umea
<b>12:45</b>	<b>Workshop Wrap-up</b>	Juliane Hollender	Eawag

# Schedule of the Day – Wednesday September 17

Dinner