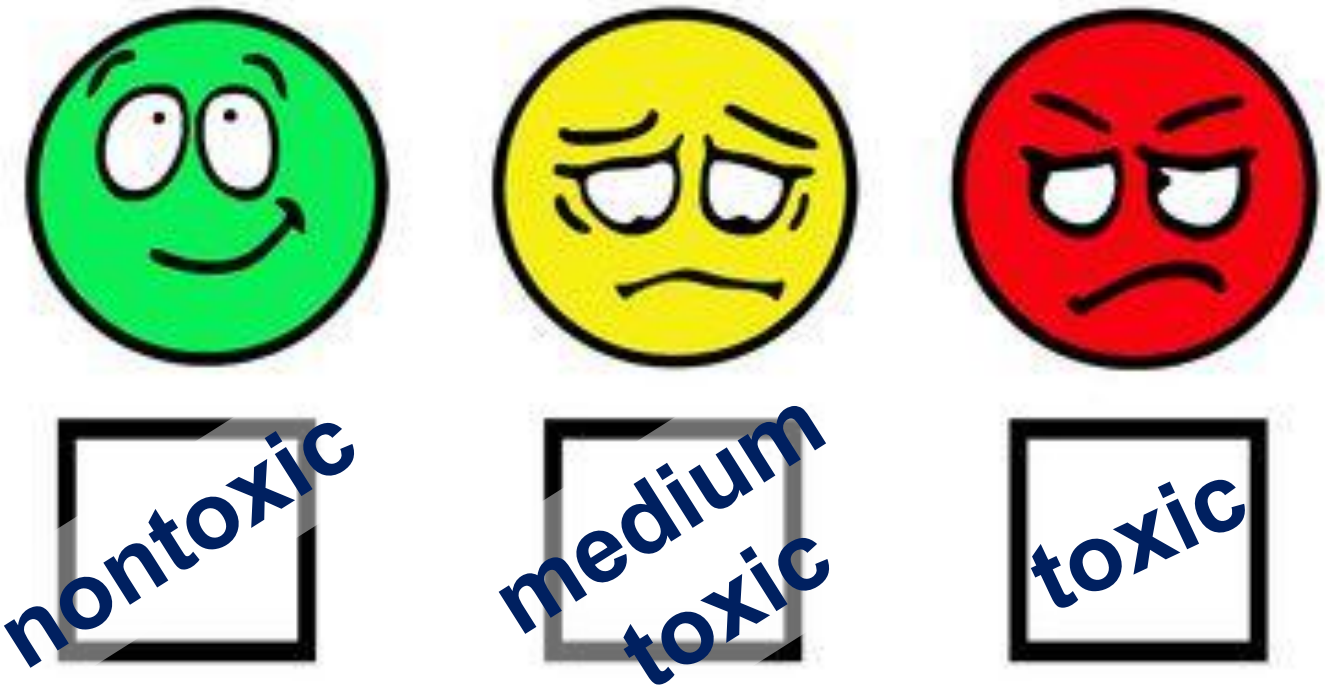
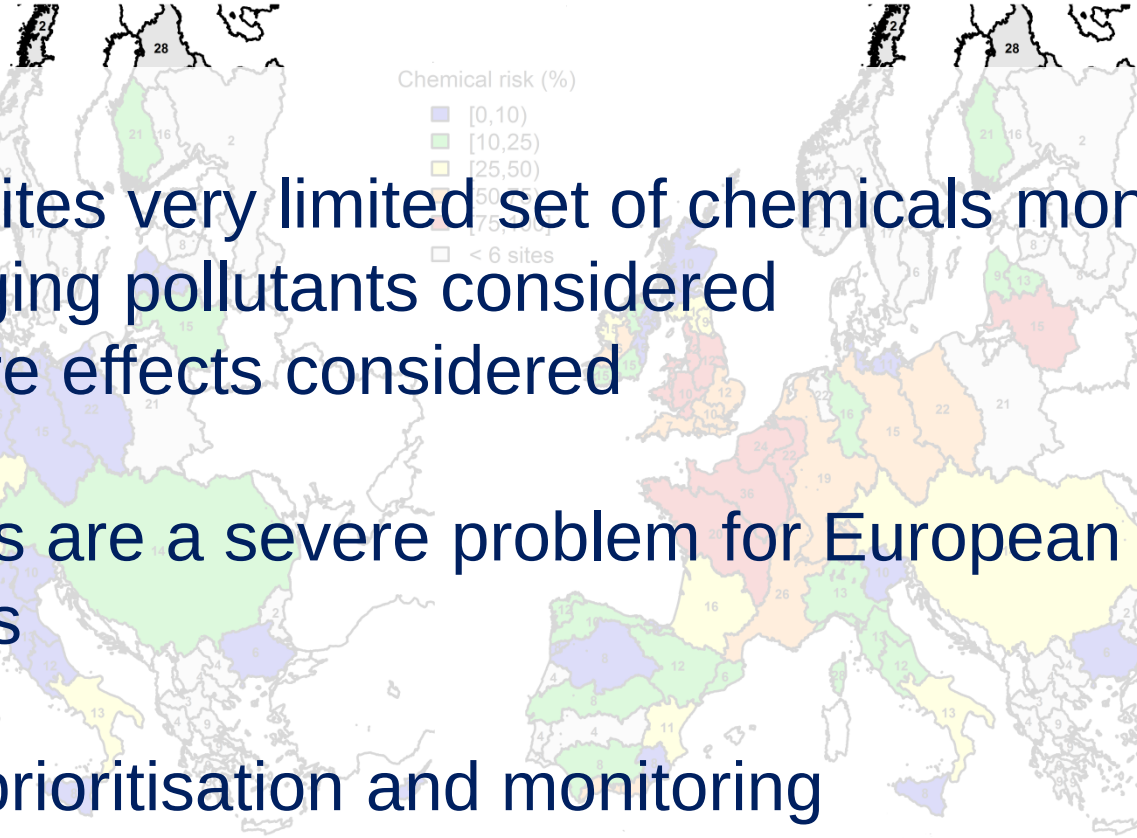


The potential of effect-directed analysis approaches to support prioritisation of chemical contaminants

Werner Brack, UFZ Leipzig

Introduction



but:

- at most sites very limited set of chemicals monitored
- no emerging pollutants considered
- no mixture effects considered

thus:

- chemicals are a severe problem for European water resources

required:

- realistic prioritisation and monitoring

Chemicals monitored in Europe pose acute and chronic risk at 14 and 42 % of the sites, respectively (Malaj et al., 2014, PNAS)

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Introduction

Target analysis of all potentially hazardous chemicals is impossible

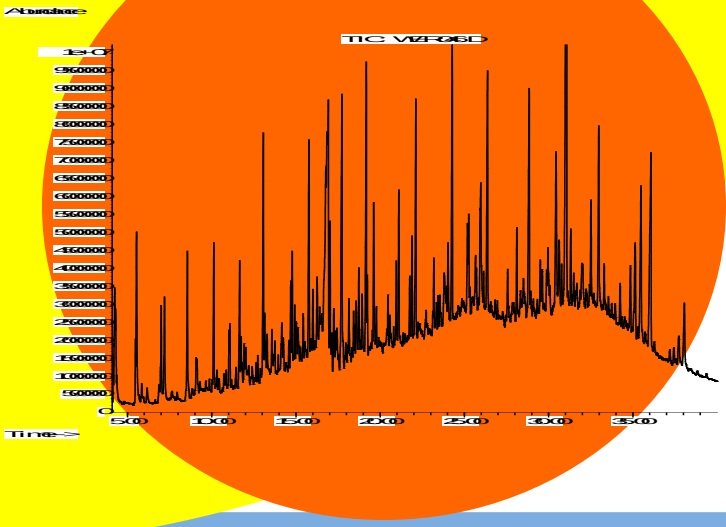
⇒ Need for tools for cumulative assessment of contamination

⇒ Need for prioritisation of drivers of mixture toxicity (Pollutors pay principle)

>88 mio known chemicals (100,000 in daily use)

ten thousands of compounds in environmental samples

few compounds in monitoring e.g. 45 priority pollutants (WFD)



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Approach, Objectives and Level of Implementation

Effect-directed analysis EDA as a site-specific prioritisation tool for effects, fractions (chemical mixtures) and compounds

Multiple-endpoint effect-based monitoring (talk Rolf Altenburger)

⇒ **Prioritisation of effects and sites**

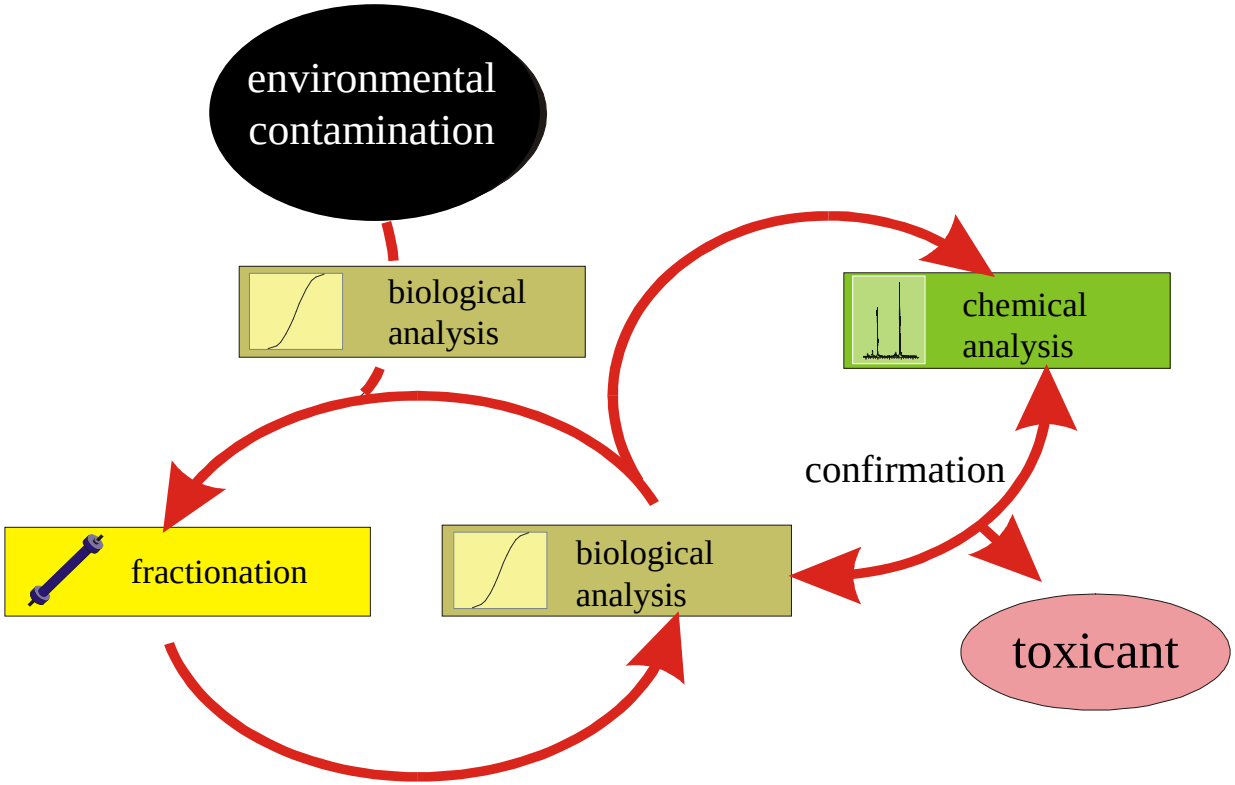
Effect-directed fractionation based on prioritised effects

⇒ **Prioritisation of fractions (chemical mixtures)**

Toxicant identification and confirmation

⇒ **Prioritisation of compounds**

Approach, Objectives and Level of Implementation



Site-specific identification of bad guys

But: often relevance for the larger context

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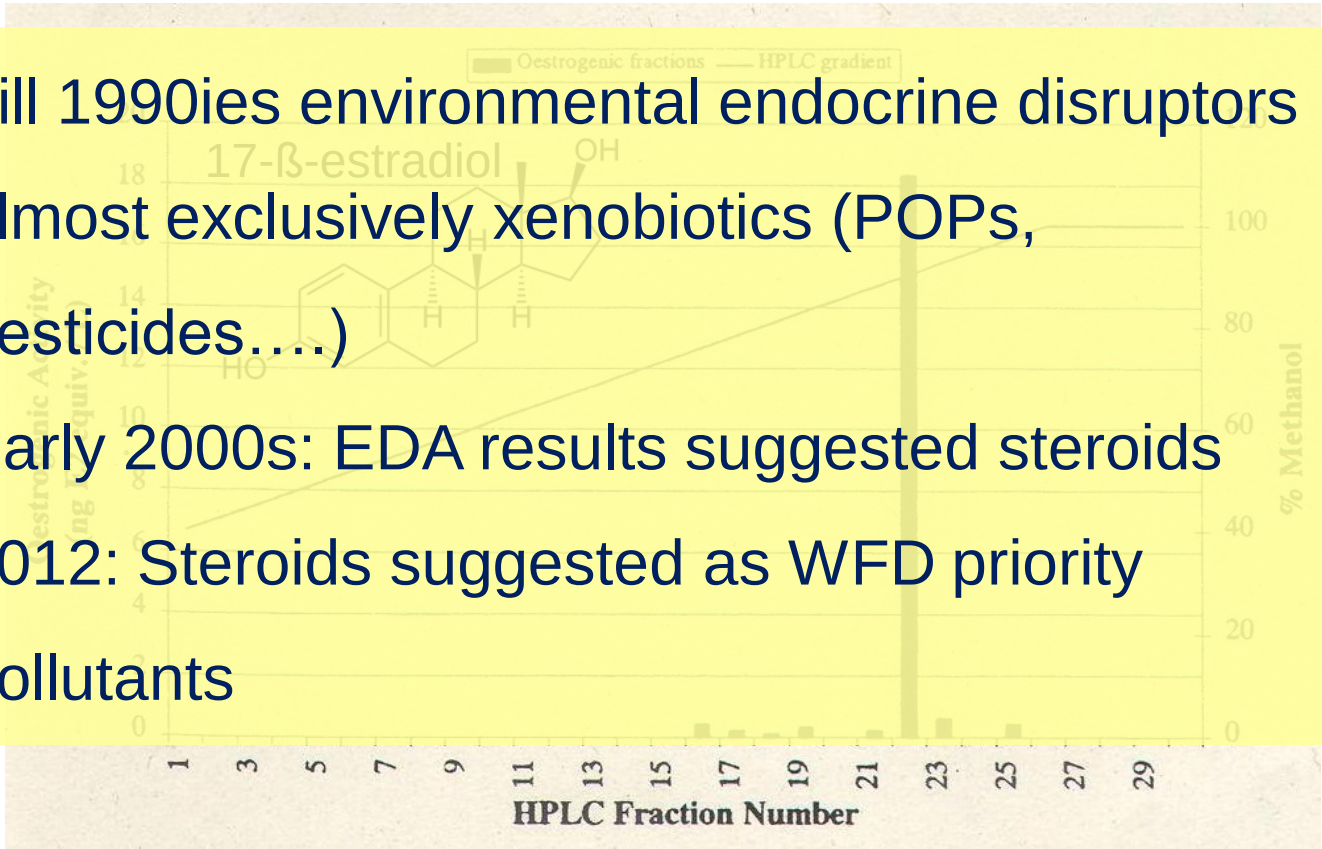
Examples

1) Identification of natural and synthetic steroids with EDA as predominating endocrine disruptors in estuary water, fish bile ect.

- Till 1990ies environmental endocrine disruptors almost exclusively xenobiotics (POPs, pesticides….)
- Early 2000s: EDA results suggested steroids
- 2012: Steroids suggested as WFD priority pollutants



Thomas et al., 2001 ET&C 20:2165

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Examples

2) EDA challenges substances of concern in risk assessment of river sediments

TABLE I

'Substances of concern' in the Rhine River and their assignment to hazard classes

Substances of concern	Hazard class
Cadmium	2
Chromium	1
Copper	1
Mercury	2
Nickel	1
Lead	1
Zinc	1
DDT + DDD + DDE (SUM)	2
Dioxins and Furans	2
HCB	2
PAH (z.B. Benzo(a) pyrene	2
PCB	2
TBT	1
Aldin (Dieldrin, Endrin)	1
γ-HCH	1
Nonyl–phenol compounds	1

metals

non-polar organic compounds

Heise & Förster 2006 Water Air Soil Pollut: Focus 6: 625

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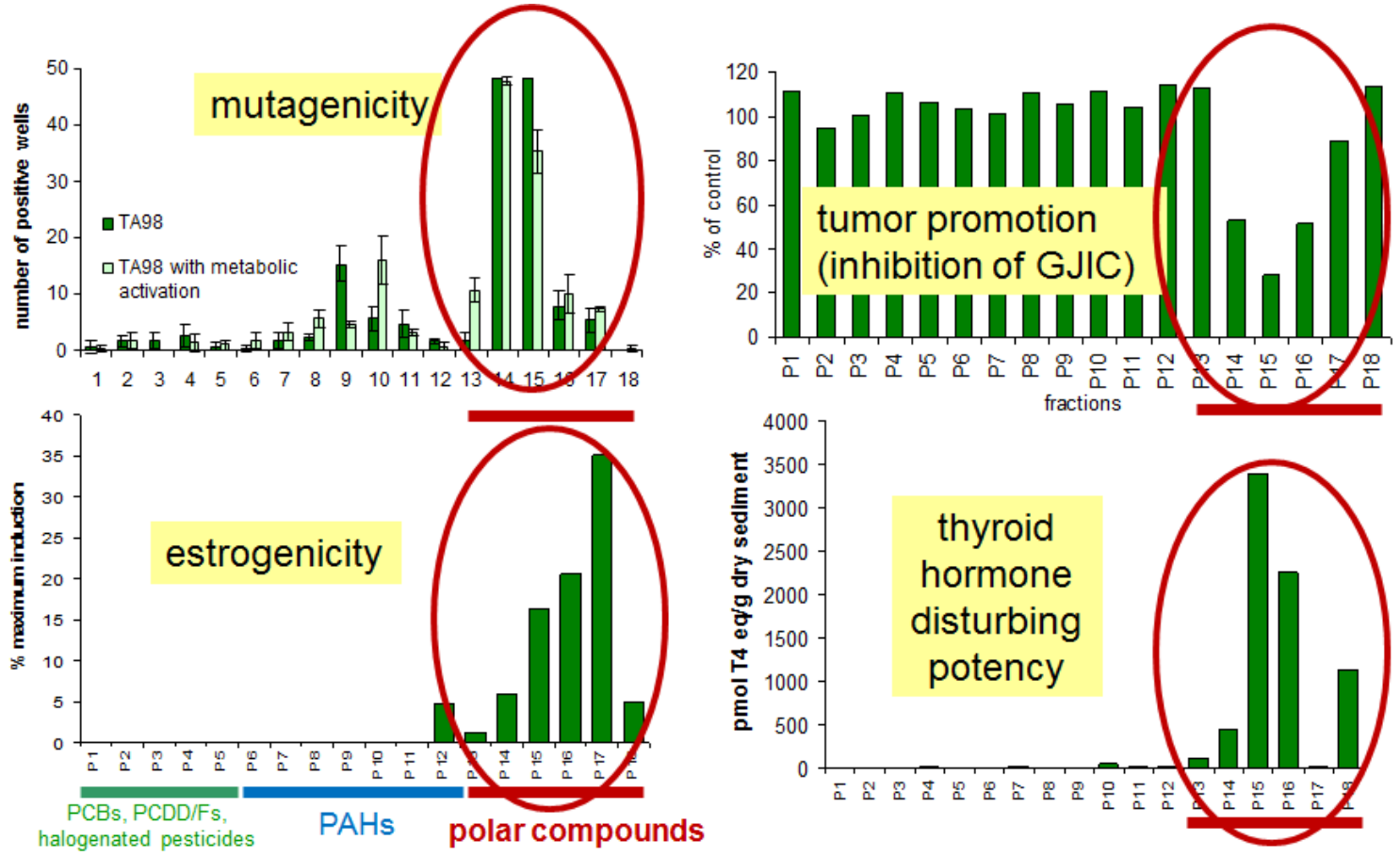
Examples

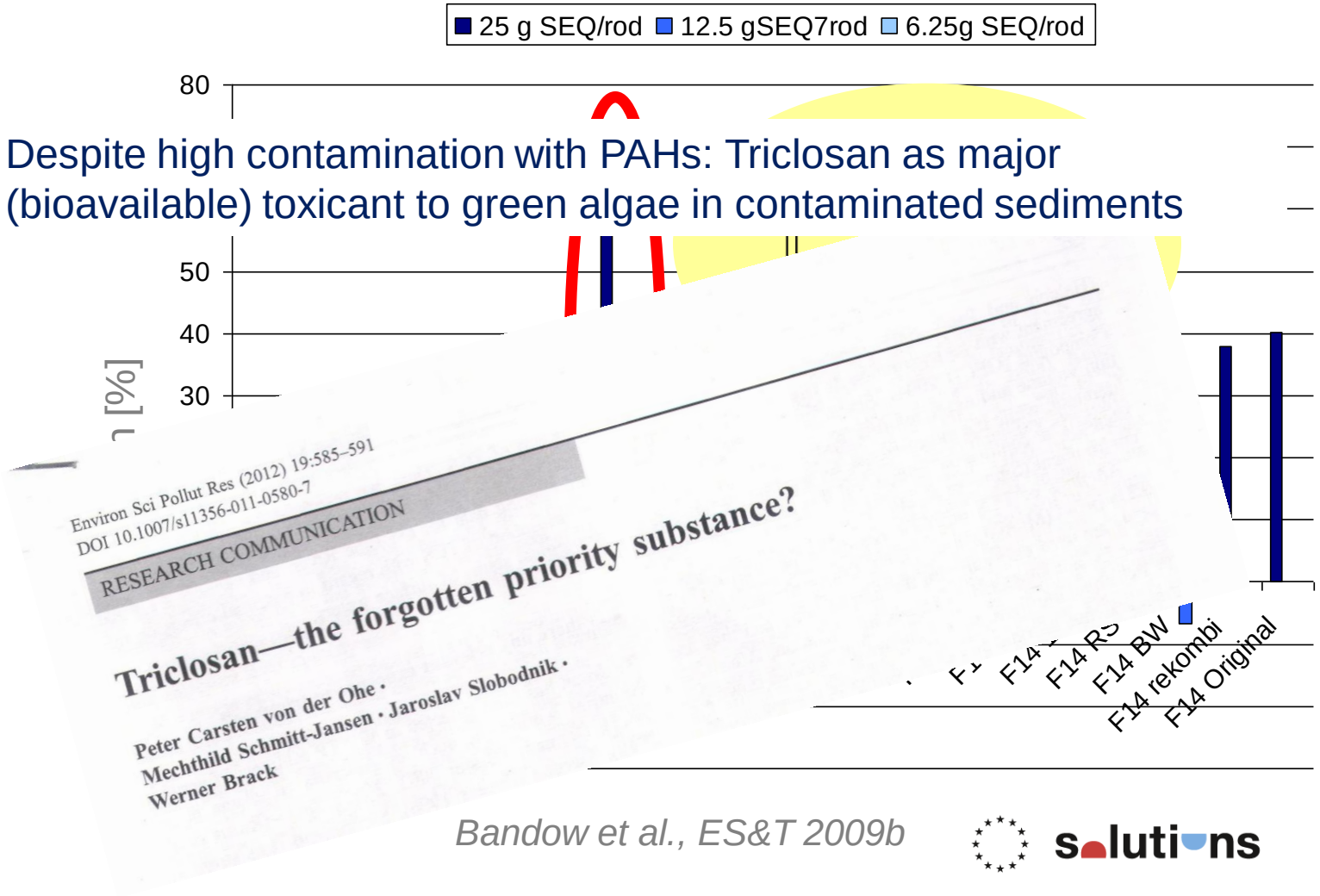
2) EDA challenges substances of concern in risk assessment of several river sediments



Lübcke – von Varel et al. 2011, ES&T

Examples

3) EDA suggests triclosan as candidate for monitoring and prioritisation



Despite high contamination with PAHs: Triclosan as major (bioavailable) toxicant to green algae in contaminated sediments

Environ Sci Pollut Res (2012) 19:585–591
DOI 10.1007/s11356-011-0580-7

RESEARCH COMMUNICATION

Triclosan—the forgotten priority substance?

Peter Carsten von der Ohe · Mechthild Schmitt-Jansen · Jaroslav Slobodnik · Werner Brack

Bandow et al., ES&T 2009b

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Approach, Objectives and **Level of Implementation**

Today: Triggers some discussions and decisions in prioritisation but no official implementation

But: **There is hope**

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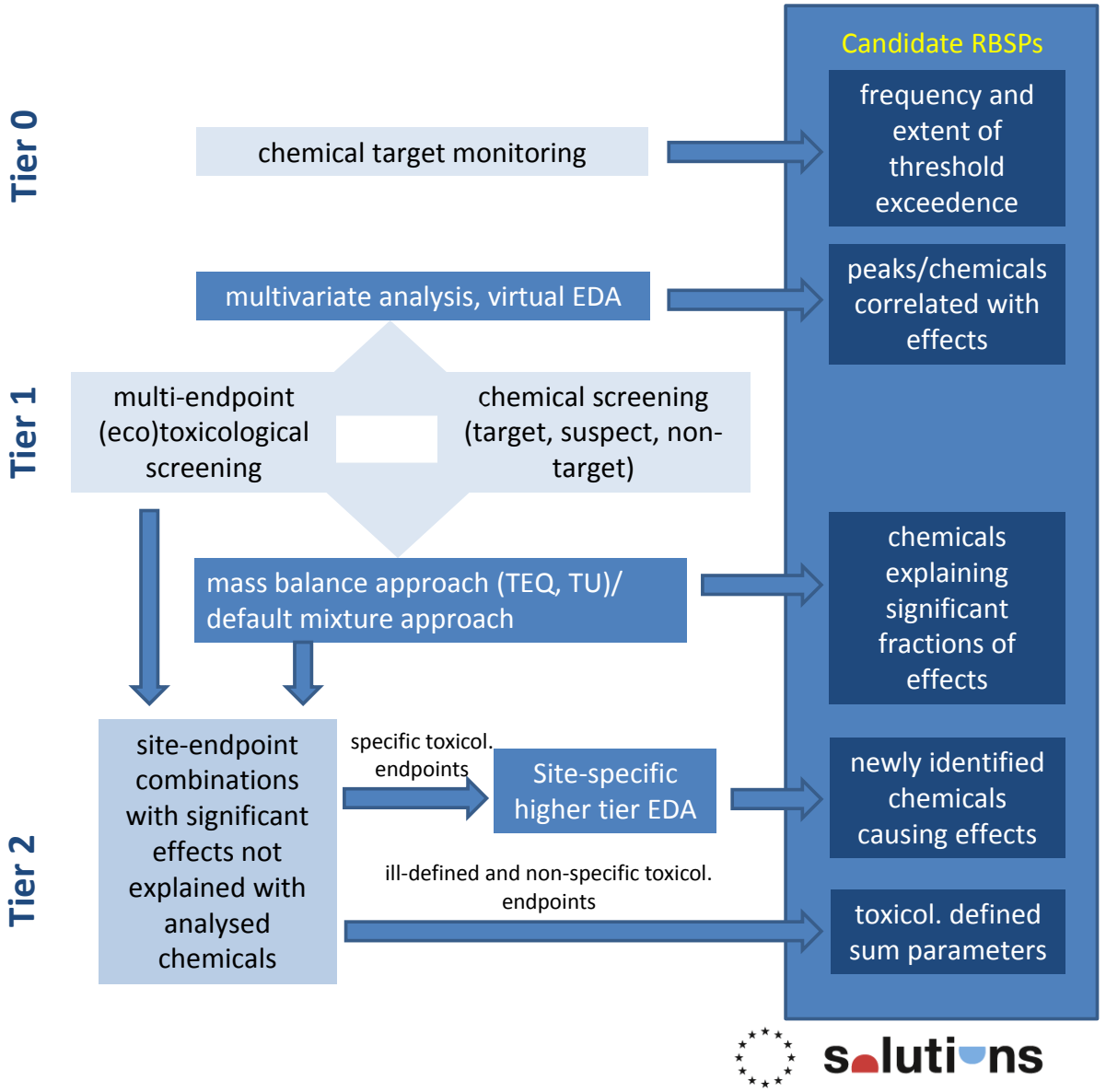
Potential use for prioritisation of chemical contaminants

Suggestion:
Involve EDA as a puzzle piece in a tiered approach of monitoring-based prioritisation



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Innovative aspects

- Prioritisation of what is really there
- Clear effect-orientation
- No bias towards well-known pollutants
- Consideration of unknown and unexpected chemicals
- Effect-based success control of mitigation measures

No replacement of pest by cholera!

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Identified gaps and barriers and proposals for improvement

- no straight-forward approach
- requires interdisciplinary understanding and collaboration
- time-consuming, laborious, not always successful

Inherent limitations:

- relies on enrichment techniques ⇒ broad scale but not infinite
- relies on selected toxicological endpoints (other effects are ignored)
- structure elucidation of unknowns may be very challenging

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Identified gaps and barriers and **proposals for improvement**

- Clearly **define tasks of EDA in an integrated conceptual framework** in concert with effect-based monitoring, chemical screening, „virtual“ EDA...
- **Provide guidance for best practice EDA** (planned in NORMAN WG on EDA)
- **Simplification, acceleration and harmonization** where possible: automated high-throughput approaches, user-friendly software packages to simplify identification
- **Collaborative network and extensive data sharing** on a European or even global scale: NORMAN and SOLUTIONS as important European platforms

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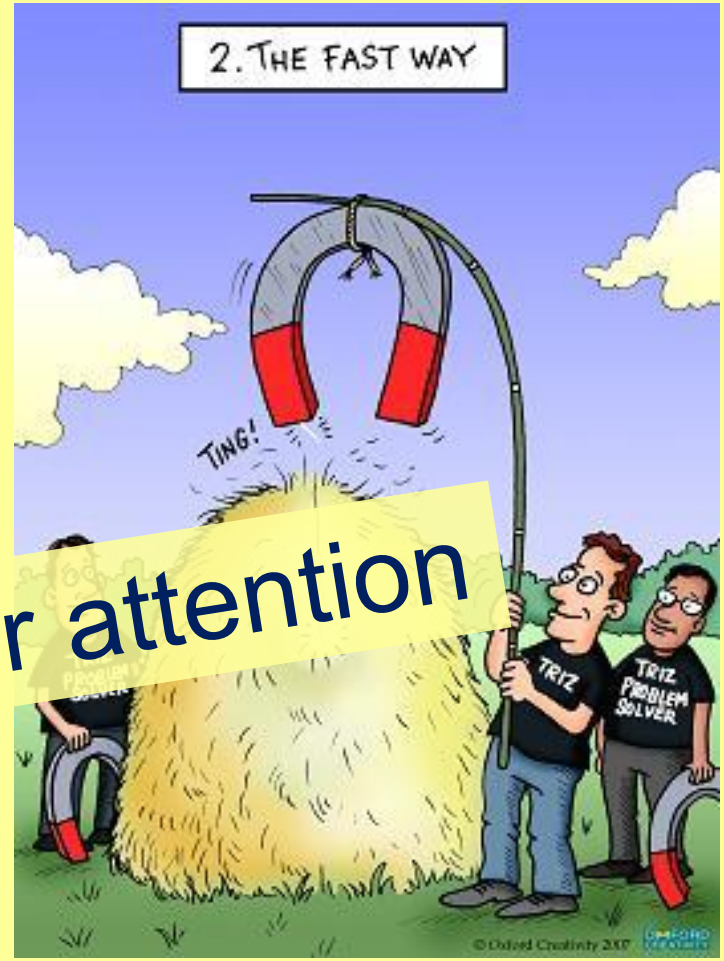

Thanks for your attention

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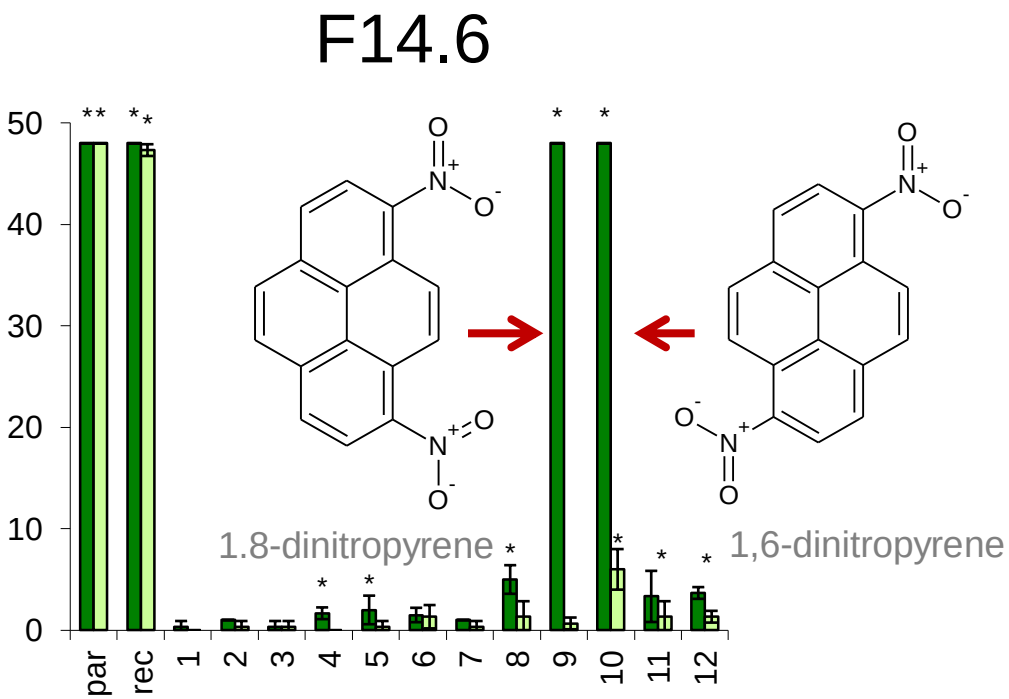
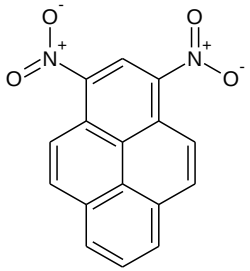
Two fractionation steps later:

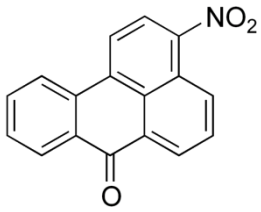


Isolation and quantitative confirmation of 1,8- and 1,6-dinitropyrene as cause of mutagenicity.

Significant contributors to mutagenicity of other fractions:



1,3-dinitropyrene



3-nitrobenz-anthrone

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