Network of reference laboratories and related organisations for monitoring and bio-monitoring of emerging environmental pollutants

Databases and exchange of monitoring data - experiences from NORMAN

Jaroslav Slobodnik
NORMAN Association
www.norman-network.net

Environmental monitoring of biocides in Europe - from prioritisation to measurements, Berlin, 5-6 November 2012

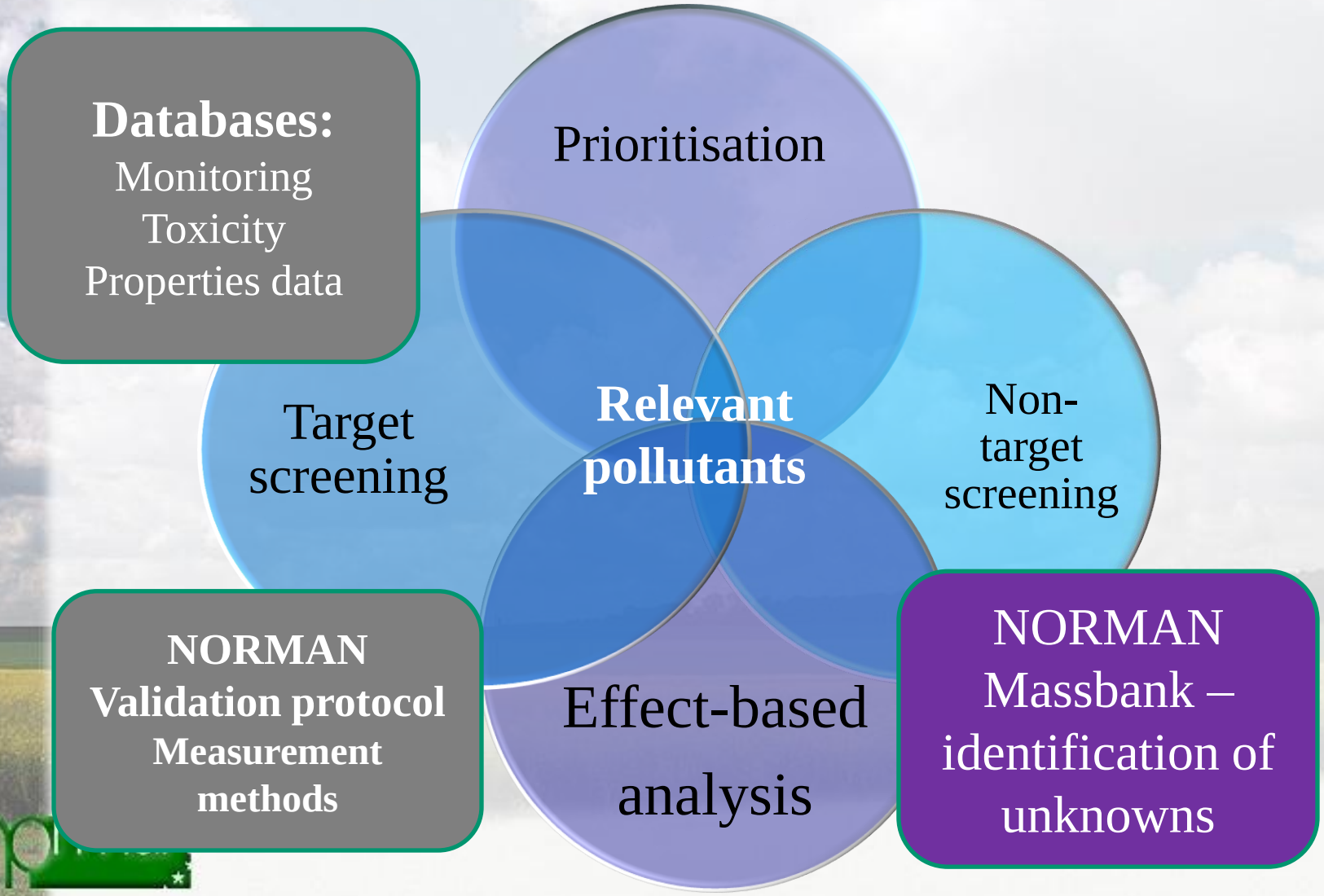
NORMAN network – emerging substances

- Former EU-funded project, established as **a permanent network (NORMAN Association) since 2009**
- >50 members from EU leading organisations (19 European countries and Canada)

Mission:

- **Exchange information** on emerging substances
- Improve **data quality**
- Promote **synergies** among research teams

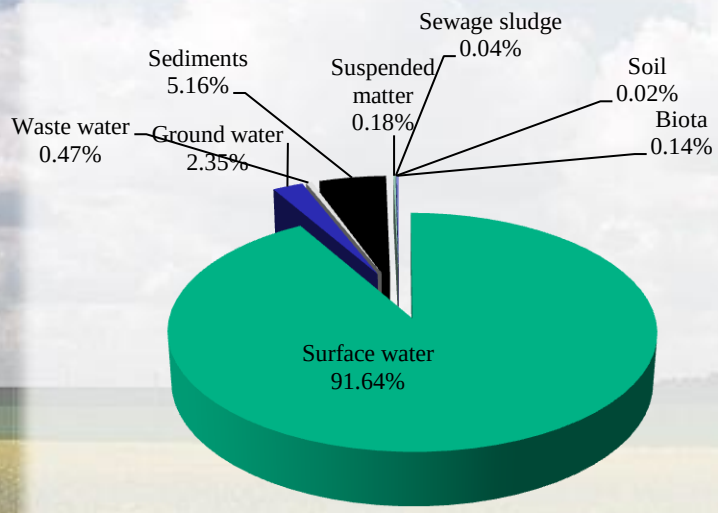
NORMAN activities to identify the relevant emerging pollutants



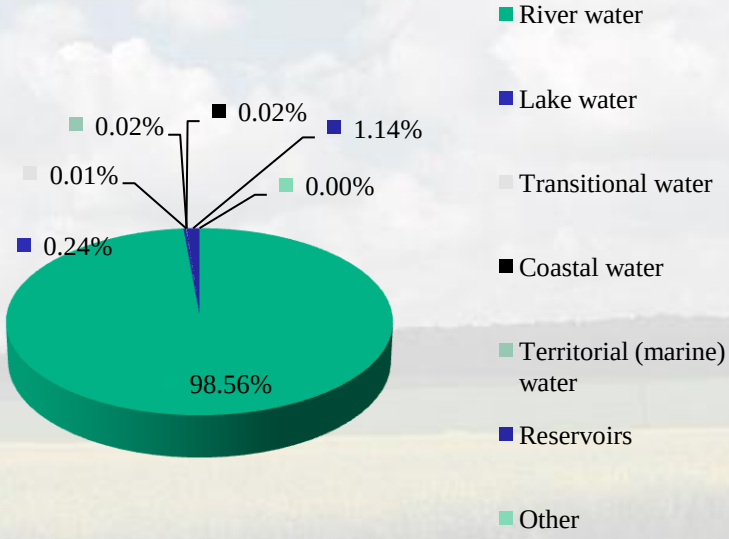
NORMAN Databases – EMPODAT monitoring data

- Designed to store data from research projects and national and EU monitoring campaigns on emerging substances

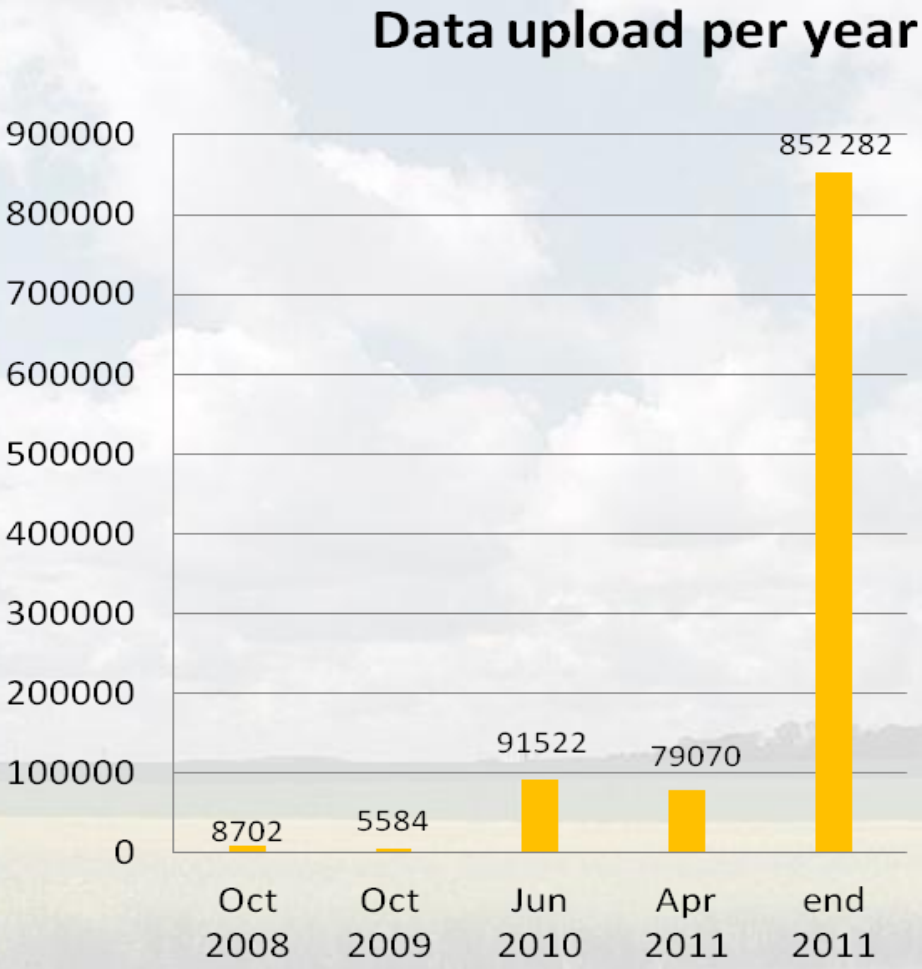
Distribution of data by ecosystem/matrix



Distribution of surface water data

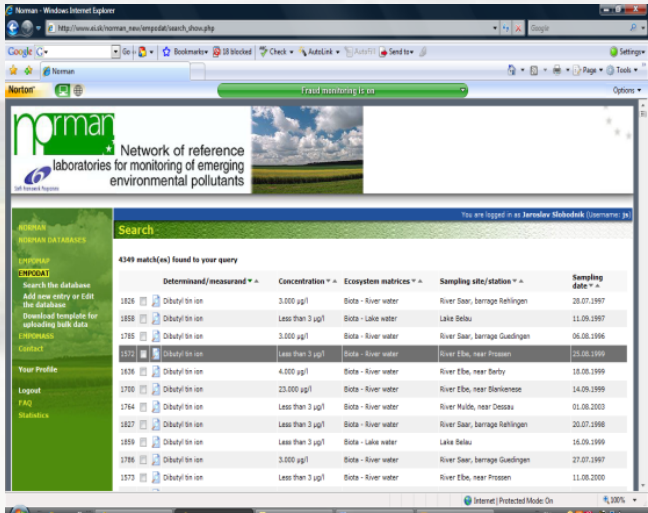


NORMAN EMPODAT database – portal for data on emerging substances (2011)



Examples of uploaded data:

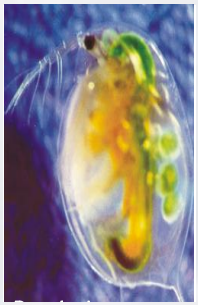
- MODELKEY FP6 project (four river basins)
- Saxony-Anhalt (Germany)
- Danube River Basin (14 countries)
- Rhine River Basin (RIWA)
- Screening studies (Scandinavian countries)



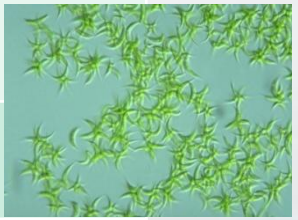
Collected data

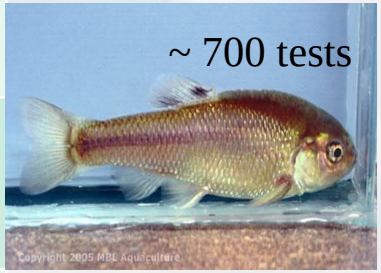
Kow (Source: Exp. data EPI suite >> QSARs via read-across methods)	705/ 707 substances
Koc (Source: Decision tree model (*Sabljic et al. 1995, Sabljic et al. 1996*)	707/ 707 substances
W S (*Exp. Data EPI suite >> read-across via ACF (Kühne 2006)*	707 / 707 substances
Fugacity models (Mackay et al. at 10°C, Level III, emission to water)	568 / 707 substances
PNEC (P-PNEC)water/ sed / biota (Exp. data + kNN read-across Schüürmann et al. 2011, EST DOI:10.1021/es200361r)	693 / 707 substances
Monitoring data (EMPODAT database)	1 037 000 data for 359 substances (NORMAN members)
Limit of Quantification (LOQ water/ sed / biota)	Available in the NORMAN DB + literature search and expert labs for > 300 substances
Classification PBT, vPvB, CMR, ED Int. classification lists; DT50 (Kühne et al. 2007); BCF (EUSES 1996, Dimitrov-Mekenyan (2002)	702 /707 substances

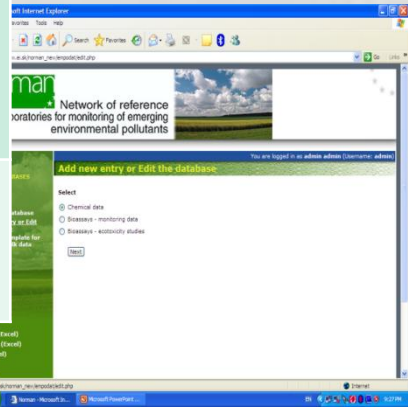
~ 1100 tests



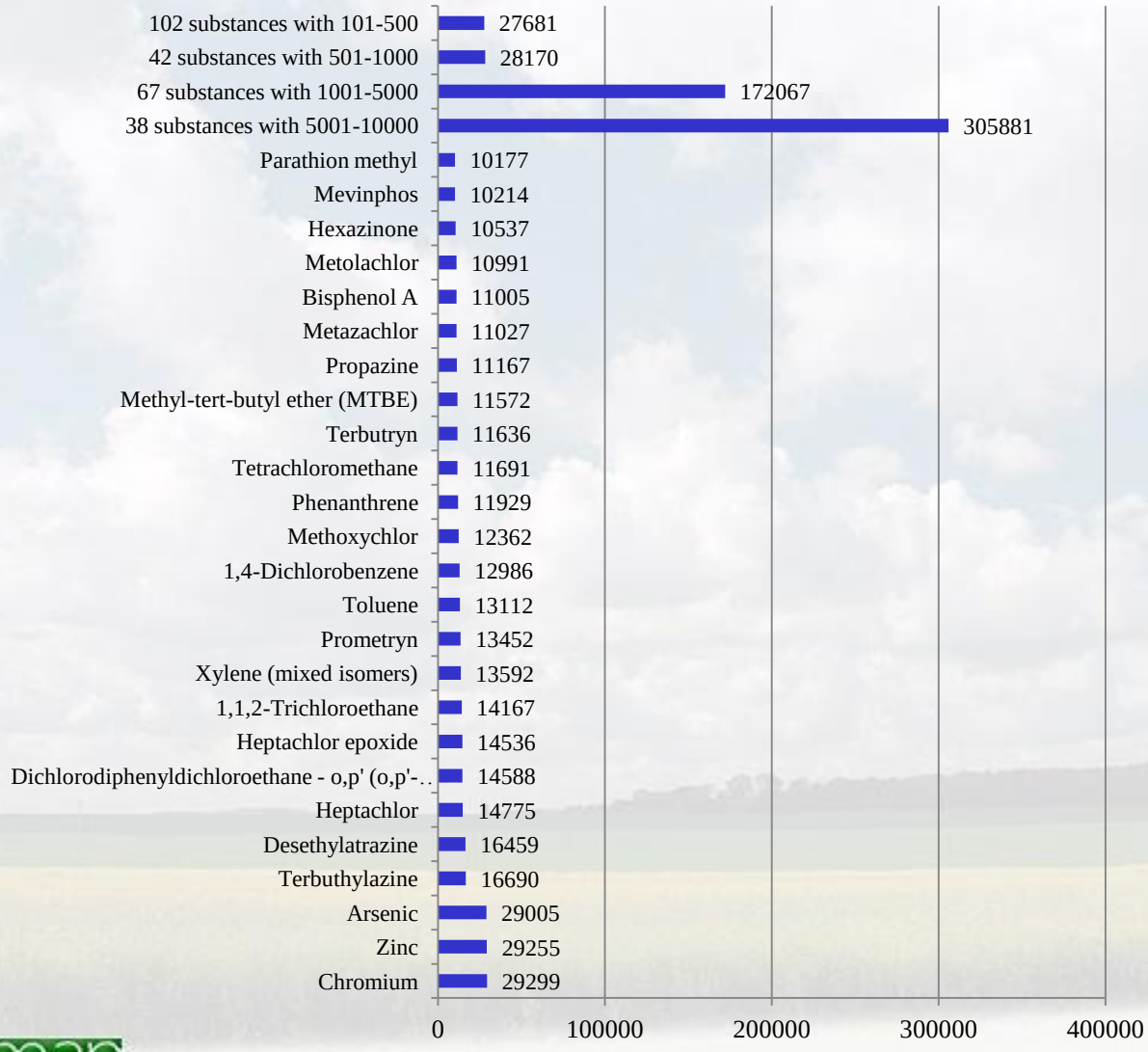
~550 tests







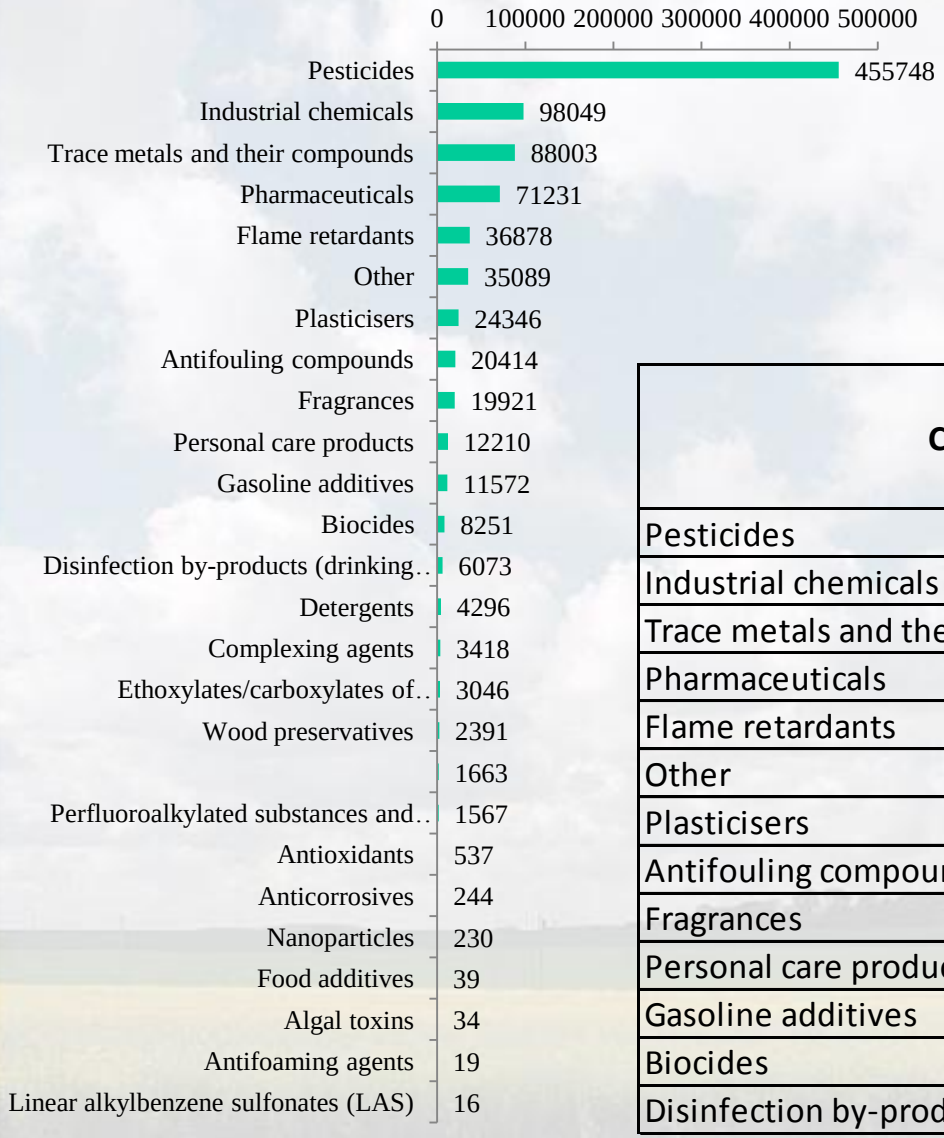
Data entries per substance



Total number of data entries: 905285

Total number of substances: 354

Number of analysis per substance class



Class (class I)	% of the total number of NORMAN data
Pesticides	50,3
Industrial chemicals	10,8
Trace metals and their compounds	9,7
Pharmaceuticals	7,9
Flame retardants	4,1
Other	3,9
Plasticisers	2,7
Antifouling compounds	2,3
Fragrances	2,2
Personal care products	1,3
Gasoline additives	1,3
Biocides	0,9
Disinfection by-products (drinking water)	0,7

Biocides in the NORMAN list of emerging substances (2011)

34 biocides on the NORMAN List

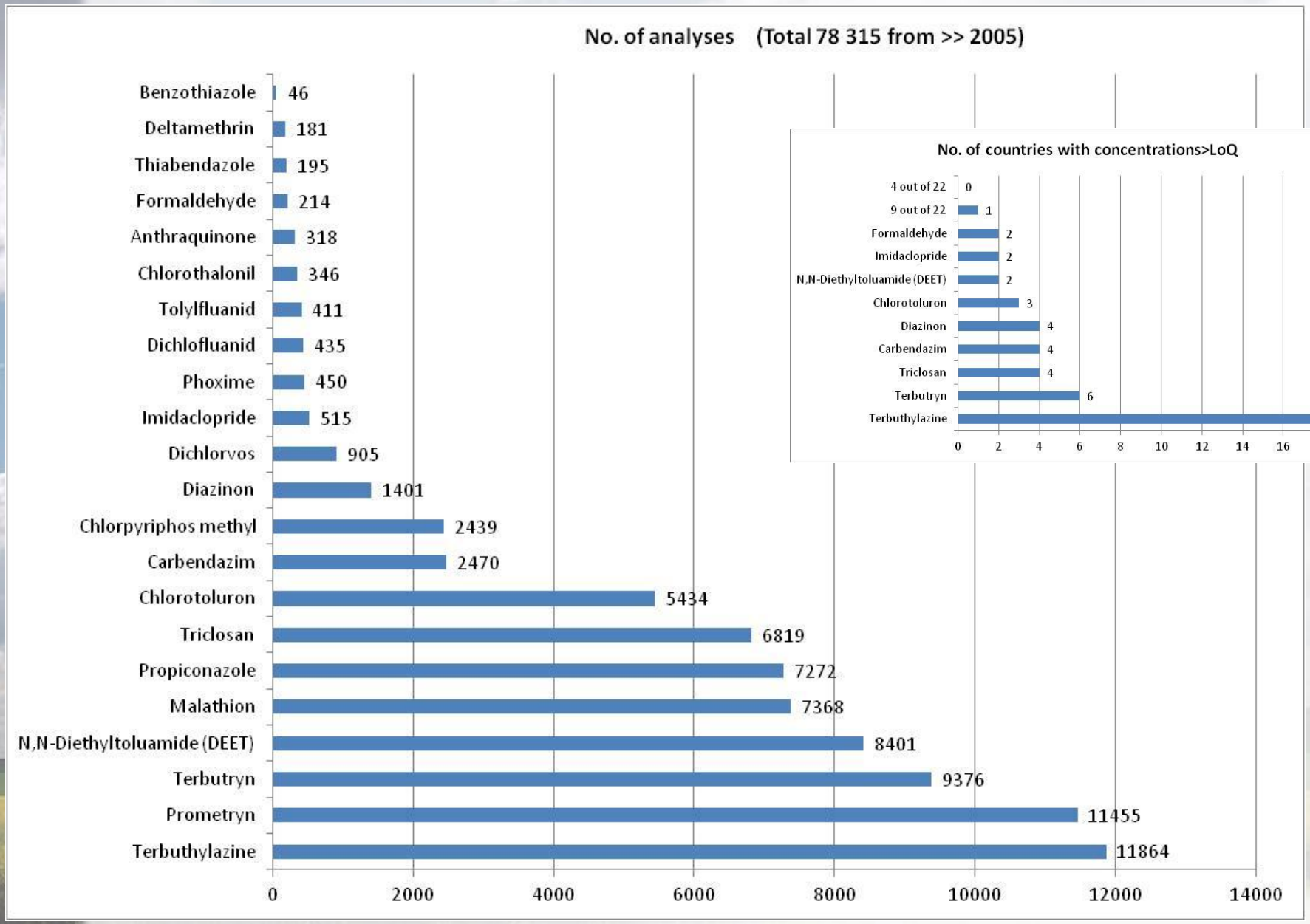
- 22 for which monitoring data are available
  - 78 300 data >> 2005 - 8,5 % of the total (925 000)
  - 97 200 data >> 2000 - 10,5 % of the total

3 for which monitoring data from ≥ 4 countries and potential risk is identified
Terbuthylazine , Diazinon, Terbutryn

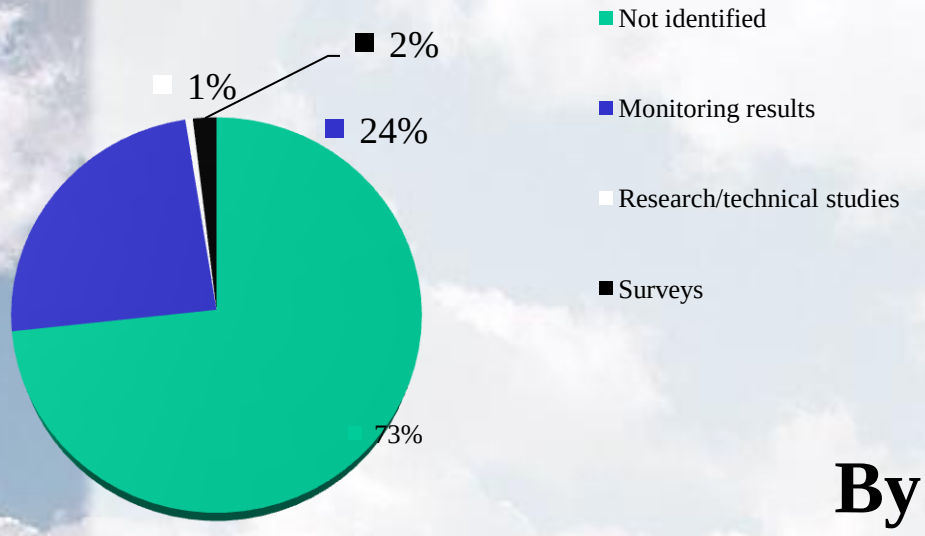
5 for which monitoring data is available from ≥ 4 countries
Terbutylazine, Terbutryn, Triclosan, Carbendazim, Diazinon

17 for which further screening is essential

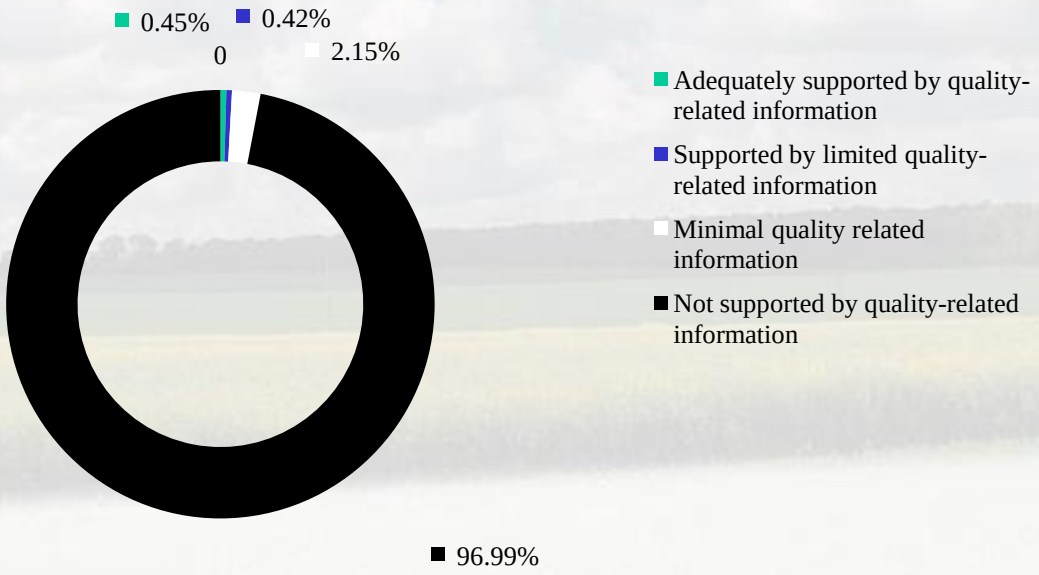
Chlorotoluron, N,N-Diethyltoluamide (DEET), Imidaclopride, Formaldehyde, Prometryn, Malathion, Propiconazole, Dichlorvos, Phoxime, Tolylfluanid, Chlorothalonil, Anthraquinone, Benzothiazole, Chlorpyriphos methyl, Dichlofluanid, Thiabendazole, Deltamethrin


No. of analyses (Total 78 315 from >> 2005)
Benzothiazole 46
Deltamethrin 181
Thiabendazole 195
Formaldehyde 214
Anthraquinone 318
Chlorothalonil 346
Tolylfluanid 411
Dichlofluanid 435
Phoxime 450
Imidaclopride 515
Dichlorvos 905
Diazinon 1401
Chlorpyriphos methyl 2439
Carbendazim 2470
Chlorotoluron 5434
Triclosan 6819
Propiconazole 7272
Malathion 7368
N,N-Diethyltoluamide (DEET) 8401
Terbutryn 9376
Prometryn 11455
Terbuthylazine 11864
0 2000 4000 6000 8000 10000 12000 14000
No. of countries with concentrations>LoQ
4 out of 22 0
9 out of 22 1
Formaldehyde 2
Imidaclopride 2
N,N-Diethyltoluamide (DEET) 2
Chlorotoluron 3
Diazinon 4
Carbendazim 4
Triclosan 4
Terbutryn 6
Terbuthylazine 18
0 2 4 6 8 10 12 14 16 18 20

Origin of data



By QA/QC category



Environ Sci Pollut Res
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

Science of the Total Environment 409 (2011) 2064–2077

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/scitotenv

A new risk assessment approach for the prioritization of 500 classical and emerging organic microcontaminants as potential river basin specific pollutants under the European Water Framework Directive

Peter Carsten von der Ohe [a,*], Valeria Dulio [b], Jaroslav Slobodnik [c], Eric De Deckere [d], Ralph Kühne [e], Ralf-Uwe Ebert [e], Antoni Ginebreda [f], Ward De Cooman [g], Gerrit Schüürmann [e,h], Werner Brack [a]

Trends in Analytical Chemistry, Vol. 30, No. 8, 2011

A harmonized European framework for method validation to support research on emerging pollutants

David Schwesig, Ulrich Borchers, Laure Chancerelle, Valeria Dulio, Ulla Eriksson, Marinella Farré, Anders Goksoyr, Marja Lamoree, Pim Leonards, Peter Lepom, Dean Leverett, Anne O'Neill, Rod Robinson, Katarina Silharova, Jaroslav Slobodnik, PeterTolgyessy, Renaud Tutundjian, Jan-Willem Wegener, David Westwood

Non-target screening

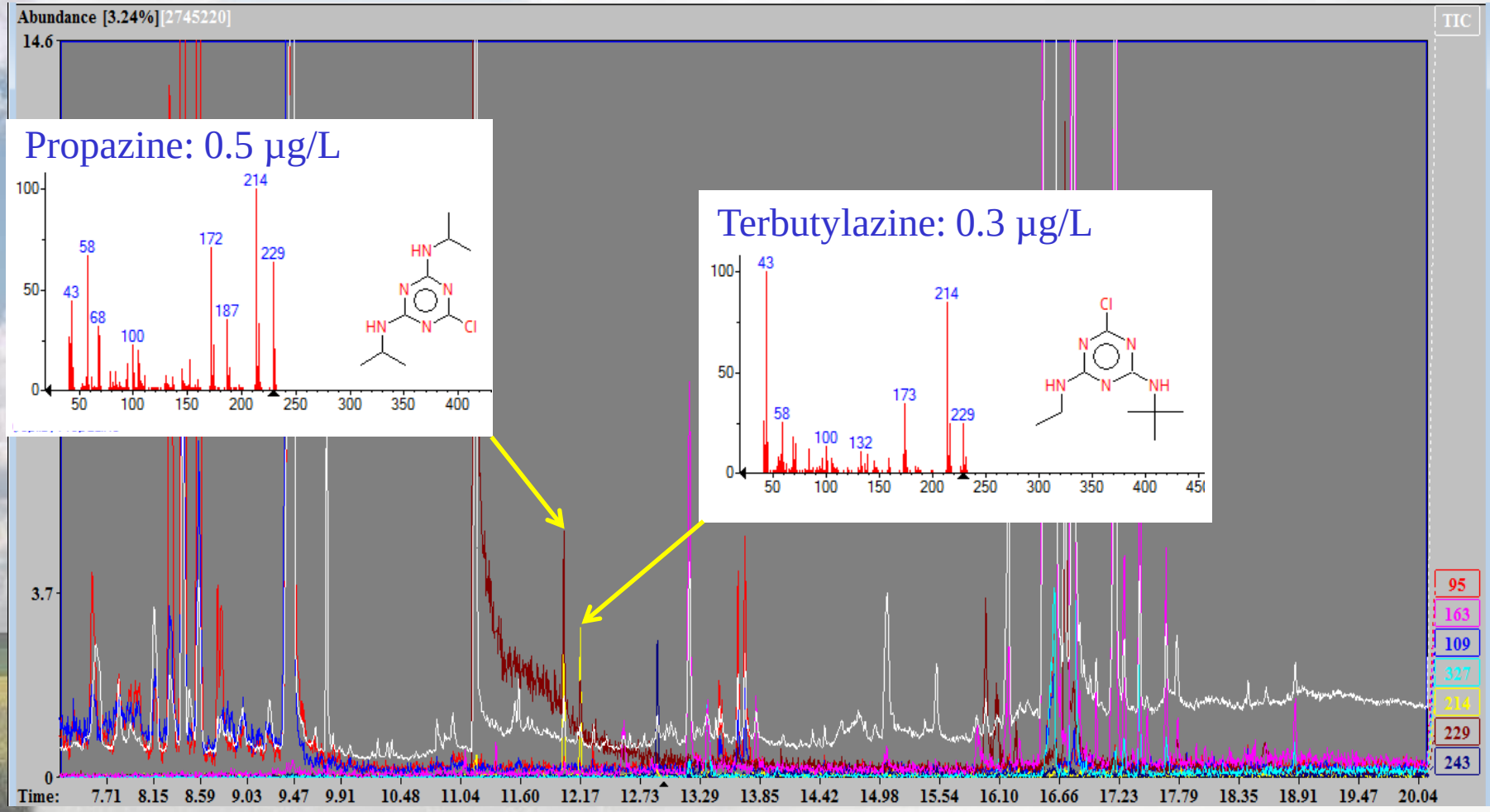
- Samples of water/sediment/biota/soil/air screened with GC-MS and/or LC-accurate mass-MS
- Data stored in NORMAN MassBank
- Provisional identification of substances present in samples
- Derivation of provisional PNECs using QSAR
- Prioritisation based on occurrence and toxicity
- Top listed non-target substances ➡ target monitoring

NORMAN MassBank database

http://massbank.normandata.eu/Massbank

Non-target Screening

Example: Slovak Republic

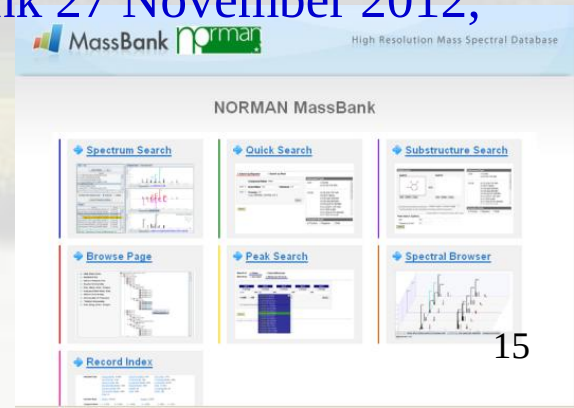


NORMAN MassBank – "let's share the knowns and focus on the unknowns"

- **VISION** =>> bringing together community of environmental chemists and set up of **a common and open access mass spectral database for identification purposes**.

- Upgrade of the former NORMAN EMPOMASS database =>> hosted and maintained by UFZ, Leipzig
- NORMAN joined MassBank consortium (existing global platform *) in 2012
- Members of the NORMAN network committed to provide mass spectra to fill up the database
- Training workshop on the use of NORMAN MassBank 27 November 2012, Amsterdam

*MassBank Horai et al., 2010; www.massbank.jp



MassBank DB Search

Quick Search

Example: atrazine

Home | Spectrum | Quick | Peak | Substructure | Identification | Browser | Batch | Browse | Index | MassBank ID: Go

Search by Keyword Search by Peak

Peak Data

```
174.0542 999
216.1013 222
104.0006 152
132.032 147
96.0552 130
146.0226 122
68.0237 113
79.0052 102
138.077 39
```

* *m/z* and relative intensities(0-999), delimited by a space.

Example1 Example2

Cutoff threshold of relative intensities 5

Number of Results 20

Search

Instrument Type

- EI
  - EI-B
  - EI-EBEB
  - GC-EI-TOF
- ESI
  - ESI-IT-MS/MS
  - ESI-QQ
  - ESI-QqIT-MS/MS
  - ESI-QqQ-MS/MS
  - ESI-QqTOF-MS/MS

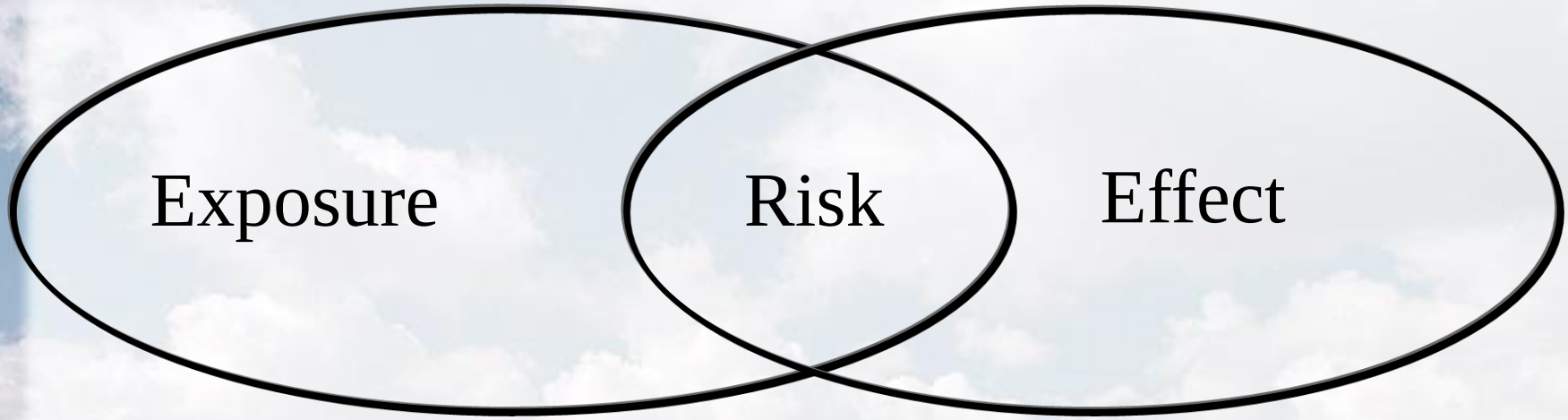
MS Type

All MS MS2 MS3 MS4

Ion Mode

Positive Negative Both

Non-target Screening



Tentatively Identified

Predicted Conc.

MEC_{95}

$\underline{MEC_{95}}$

P-PNEC

Predicted Toxicity

AF 1000

P-PNEC

ARTICLE IN PRESS
Trends in Analytical Chemistry, Vol. xxx, No. x, 2012 Trends

Identification of river basin specific pollutants and derivation of environmental quality standards: A case study in the Slovak Republic☆

Jaroslav Slobodnik, Lea Mrafkova, Mario Carere, Fulvio Ferrara, Bruno Pennelli, Gerrit Schüürmann, Peter Carsten von der Ohe

Prioritisation based on non-target screening: case study in the Slovak Republic

Table 9: Results of prioritisation based on the GC-MS screening data and and (predicted) toxicity data.

No.	CAS	Name	Max. conc.	MEC_{95}[a]	AA-EQS[b]	Source EQS	Lowest PNEC	Ref.[c]	TL[d]	Freq. PNEC[e]	Exceed. PNEC[f]	Priority[g]
1	629-62-9	Pentadecane	1.7	1.5			0.0015	B	A	0.20	1000	1.20
2	544-76-3	Hexadecane	3.6	2.4			0.0015	P	F	0.17	1600	1.17
3	95-16-9	Benzothiazole	30958	4459	2	SK	2	E	D	0.12	2230	1.12
4	57-10-3	Hexadecanoic acid	15	3.7			0.021	B	F	0.53	176	1.03
5	629-50-5	Tridecane	8.0	4.3			0.023	B	F	0.50	187	1.00
6	84-74-2	Di-n-butylphthalate (DBP)	60	22	10	SK	0.74	E	F	0.77	30	0.97
7	117-81-7	DEHP	272	46	1.3	WFD	0.96	B	D	0.63	48	0.83
8	629-59-4	Tetradecane	4.3	2.2			0.0095	B	P	0.25	232	0.75
9	112-40-3	Dodecane	6.8	5.6			0.009	P	D	0.21	622	0.71
10	1002-84-2	Pentadecanoic acid	9.0	7.5			0.04	P	A	0.12	188	0.62
11	544-63-8	Tetradecanoic acid	6.8	1.9			0.05	P	A	0.36	38	0.56
12	4130-42-1	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	10.0	2.6			0.092	B	D	0.36	28	0.56
13	85-68-7	Benzylbutylphthalate (BBP)	6.4	2.7			0.27	E	A	0.22	10	0.42
14	143-07-7	Dodecanoic acid	7.2	3			0.08	P	F	0.20	31	0.40
15	84-69-5	Diisobutyl phthalate	14.0	3.6			0.9	P	F	0.26	4	0.36
16	57-11-4	Octadecanoic acid	2.5	0.76			0.013	B	F	0.15	58	0.35
17	92-52-4	Biphenyl	3.7	1.7	1	SK	0.36	E	D	0.22	5	0.32
18	2091-29-4	9-hexadecenoic acid	7.4	1.8			0.032	B	P	0.12	56	0.32
19	120-72-9	1H-indole	84	34			1	E	D	0.08	34	0.28
20	128-37-0	Methyl-2,6-di-tert butylphenol (BHT)	10	2.6	1.4	SK	1.4	E	D	0.15	1.86	0.25
21	615-22-5	2-(methylthio)-benzothiazole	14.0	3.8			0.31	P	D	0.05	12	0.25
22	1620-98-0	Phenol, 2,6-bis(1,1-dimethylethyl)-4-ethyl-	9.3	5.4			0.59	B	D	0.08	9	0.18
23	334-48-5	Decanoic acid	9.8	0.86			0.26	P	A	0.07	3	0.17
24	17851-53-5	Butyl isobutylphthalate	9.0	6.8			1.2	B	D	0.04	6	0.14
25	80-05-7	Bisphenol-A	208	8	10	SK	4.7	E	F	0.02	2	0.12
26	91-20-3	Naphthalene	982	49	2.4	WFD	6.1	E	F	0.02	8	0.12

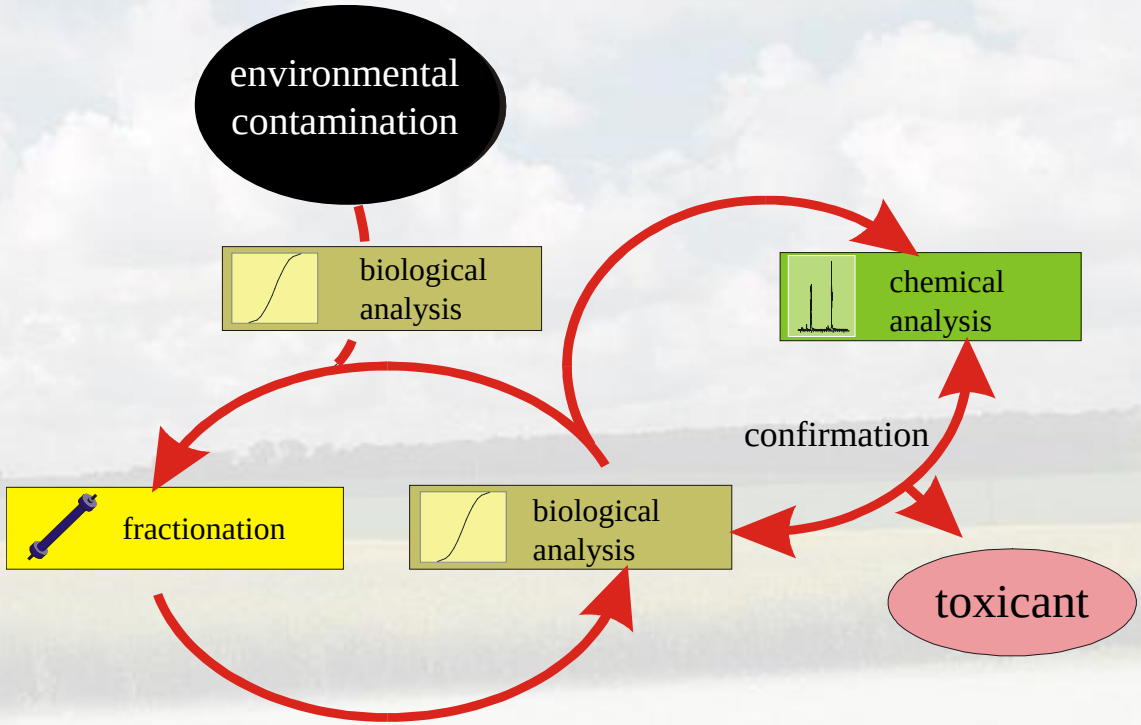
241 compounds evaluated in terms of aquatic exposure and potential ecological effects, **Derivation of a Provisional Predicted No Effect Concentration: P-PNEC using QSAR**

Effect-directed analysis (→ field-based approaches)

Predicted effects based on target monitoring are often different from measured effects

⇒WG on Effect-Directed Analysis (EDA)
⇒EDA-EMERGE project (ITN Marie Curie)

- Effect monitoring at site level
- No *a priori* knowledge on or selection of compounds required
- Applicable to any matrix (water, sediments, biota, …)



SPIN - Substances in Preparations In the Nordic countries - a database that contains "non-confidential" information on substances from the Product Registers of Norway, Sweden, Finland and Denmark

- The database contains **volumes in use for each substance in the four countries** also divided into which industrial branch (NACE) and which product type (UCN).
- The database also has a toolbox called SPIN Exposure Toolbox. The tool is called Use Index. The tool makes it possible to search for a **general indicative exposure of human beings and environment from different chemical uses and a tool indicating widespread use**. It is based on the extensive information stored in the Nordic product registers.

www.spin2000.net

NORMAN Position Paper
Collection, exchange and interpretation of data on emerging substances

- **VISION**
  - **NORMAN should become the primary data source and global one-stop-shop for all issues regarding emerging substances contributing to the creation of the early-warning system for emerging pollutants and subsequent policy actions**
- ***Data collection***
- ***Data quality***
- ***Establishment of a regular and automated data collection scheme***
- ***The use of the data in support of European environmental policies and data collection activities***
- ***Presentation of the data to the public***
- ***Possible contribution to the architecture of the European Integrated Platform for Chemical Monitoring***

Conclusions

- The need to look beyond the traditional target pollutants is now generally recognised as a priority issue in all policy areas
- **It is not possible to develop the necessary knowledge and methodologies solely at the national scale**
  - Need for:
    - Commonly accepted methodology for **prioritisation** of relevant emerging substances and follow -up actions
    - **Harmonisation** of data collection formats
    - Continuous **improvement of analytical expertise and data quality**
    - **Non-target screening** and site-specific **effect-based approaches** to identify toxicants responsible for the observed effects
    - **Inclusion of use data**
    - Formulation of common views of the scientific community on research needs and **priorities for future legislation**
    - **INTERNATIONAL COLLABORATION**

NORMAN – an open access platform where all knowledge on emerging substances can meet

INTERESTED TO COLLABORATE?

www.norman-network.net

EUR 24613 EN - 2010

JRC EUROPEAN COMMISSION

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