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

NORMAN network on emerging substances: Gathering information on occurrence and environmental effects of emerging substances

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**Executive Secretary of the NORMAN Network*

www.norman-network.net

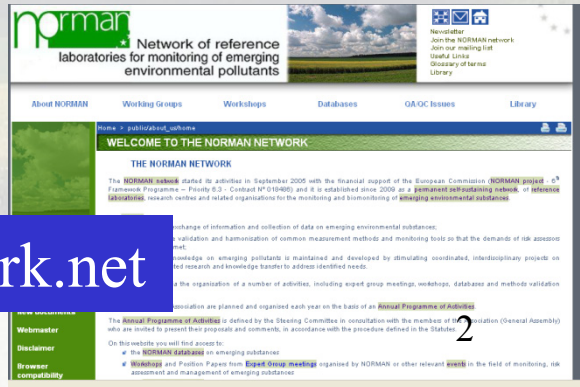
Berlin 5-6 November 2012

NORMAN network – emerging substances

- Network of reference laboratories, research centres and related organisations for monitoring of emerging substances
- >50 members from EU leading organisations (19 European countries and Canada)
- Former EU-funded project, established as a permanent network in 2009

Mission of the NORMAN network:

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



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Environmental contaminants: "knowns and unknowns"

- **"Known knowns": Conventional pollutants e.g. PCBs, metals, PAHs**

  We know how to measure them and we have data to assess the risks

Emerging risks

- **"Known unknowns": Known emerging pollutants: e.g. PFCs, PPCP, nanomaterials**

  We know that they are present in the environment, but we don't know them enough (not enough data to assess the risks)

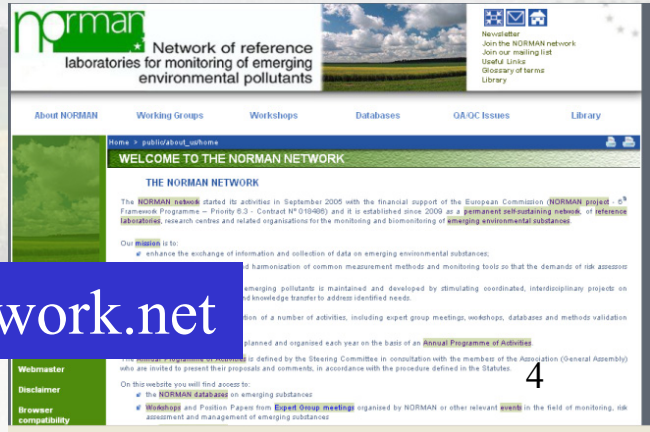
- **"Unknown unknowns" : Unknown emerging pollutants ???:**

  We don't know yet WHAT they are….(next generation emerging contaminants, metabolites and transformation products, suspect of causing effects, including as mixtures)

Adapted from Francis S. Collins, 2008

NORMAN network – emerging substances: key challenge

What are the relevant emerging pollutants ?



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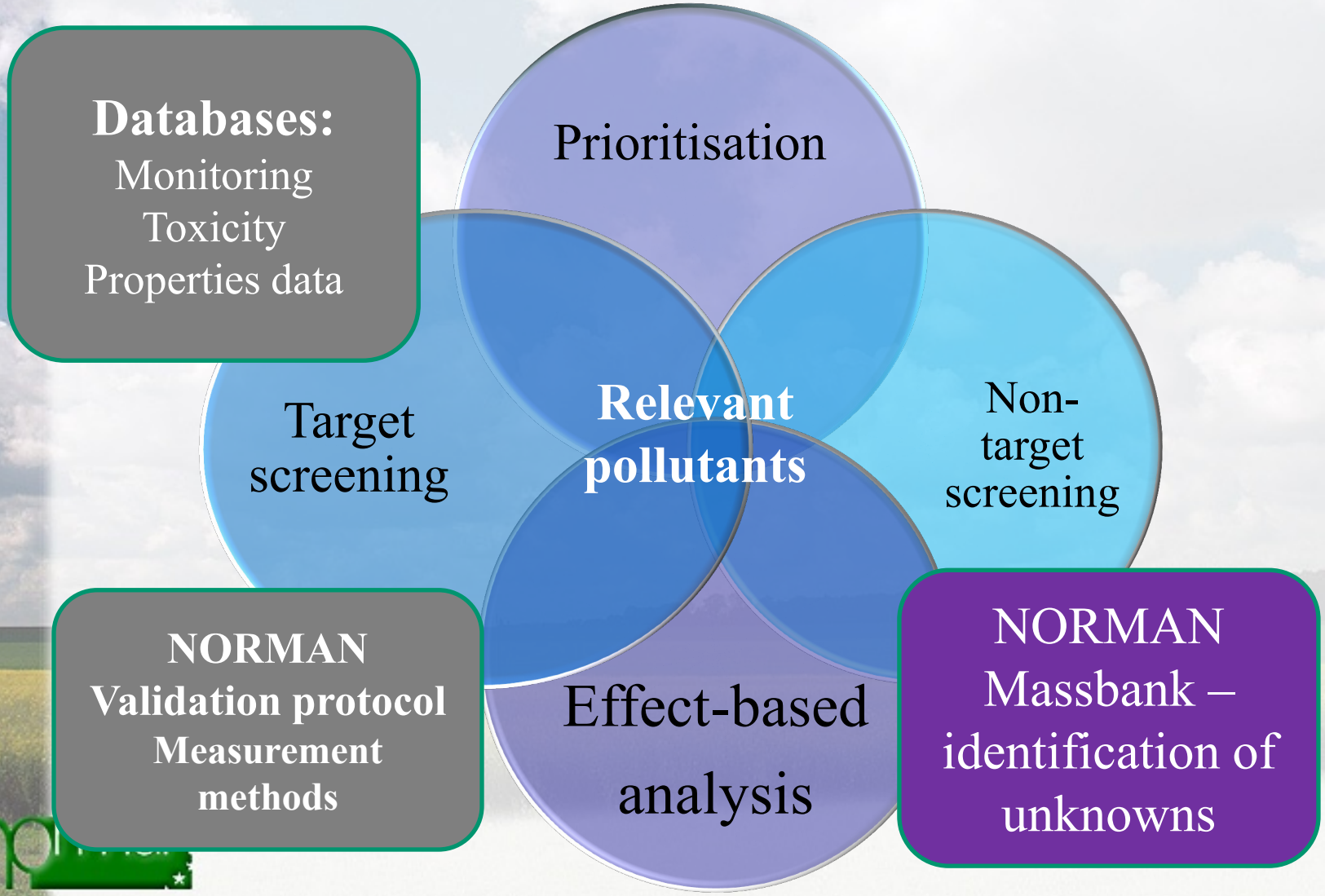
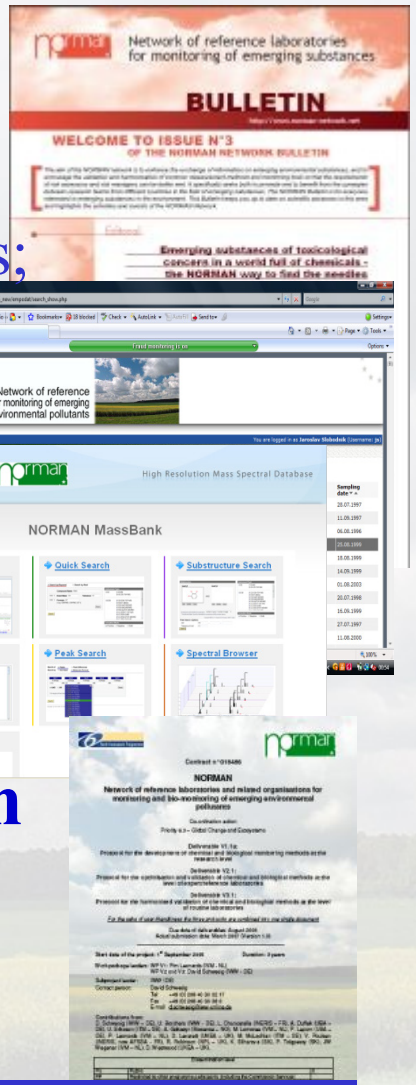
NORMAN activities to identify the relevant emerging pollutants



NORMAN network – emerging substances

- **Working Groups**
  - Prioritisation; Bioassays; Effect-Directed Analysis; Engineered Nanoparticles
- **Databases**
  - EMPODAT: **Occurrence and (eco)toxicity data**;
  - NORMAN **MassBank** : Mass spectra =>> identification of unknowns
- **NORMAN Protocol for methods' validation**
  - Under negotiation at CEN =>> **future CEN TS**
- **NORMAN Bulletin**



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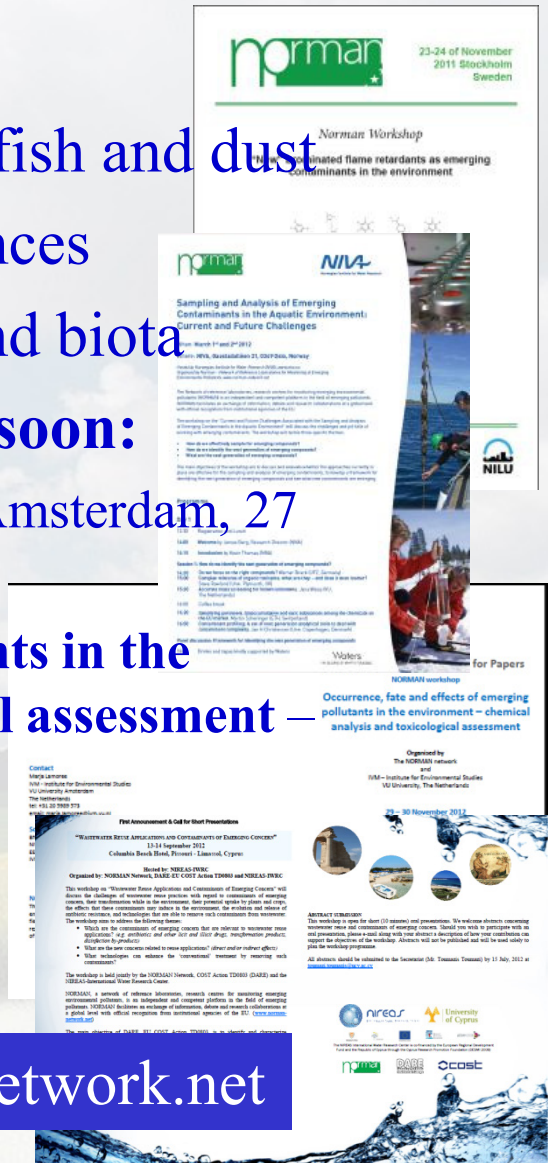
NORMAN network – emerging substances

- **International Interlaboratory Studies, e.g.:**
  - 2012 Organophosphorous FR in sediment, fish and dust
  - 2011 Passive sampling of emerging substances
  - 2010 Perfluorinated compounds in water and biota
- **Thematic international workshops, coming soon:**
  - **MassBank training workshop –** UFZ, EAWAG, Amsterdam, 27 Nov 2012
  - **Occurrence, fate and effects of emerging pollutants in the environment - chemical analysis and toxicological assessment** – IVM, Amsterdam, 29-30 Nov 2012



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Prioritisation of emerging substances

- Emerging substances often **overlooked** with **conventional prioritisation methodologies**

- **DG ENV** exercise for revision of PS list
  - **More than 50% of the substances discarded**
  - **Lack of data** or **insufficient data reliability**

- **NORMAN prioritisation scheme**
  - Designed specifically **for emerging substances**
  - **Knowledge gaps**
  - **Actions needed**

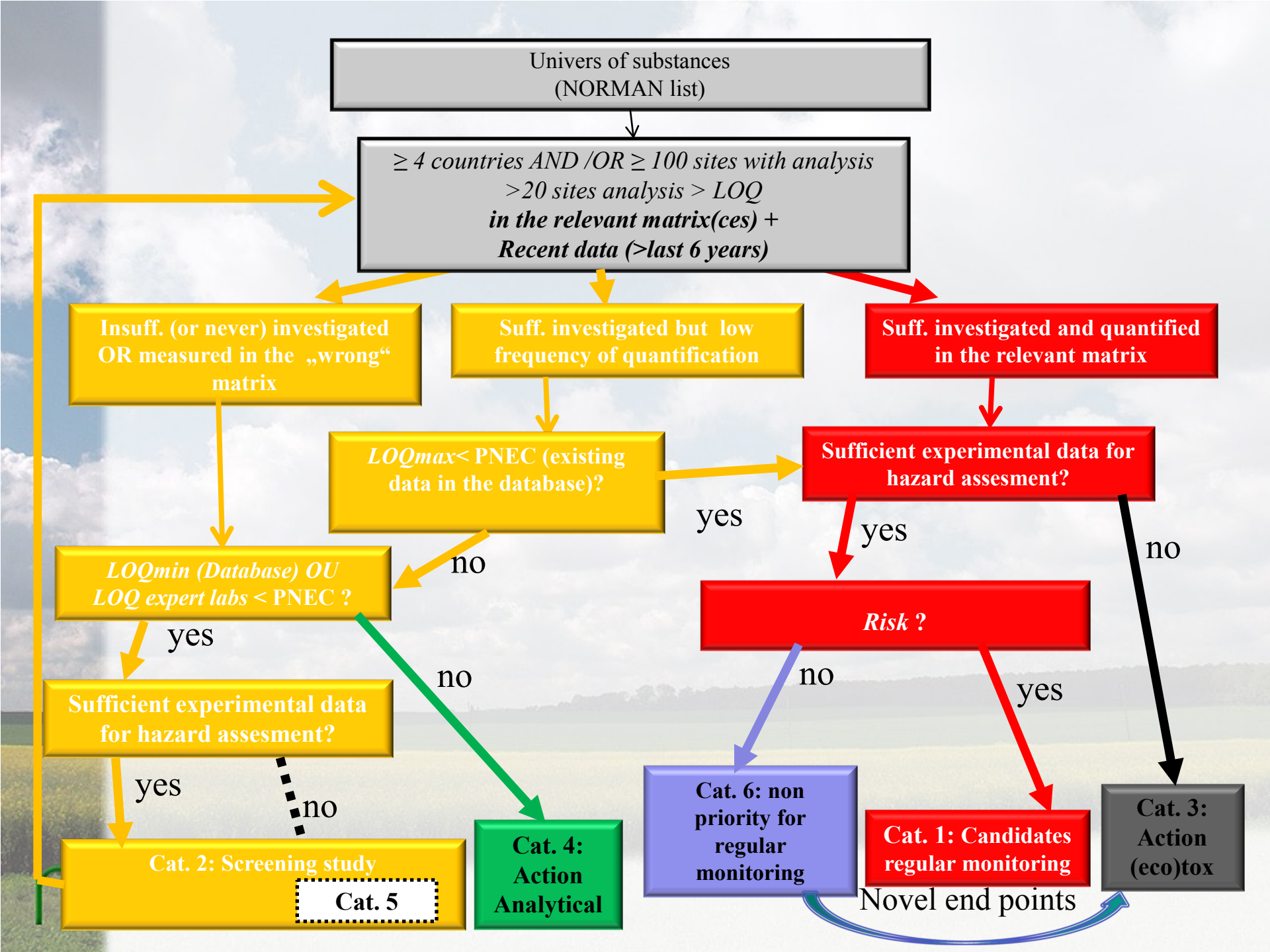
NORMAN Framework for prioritisation of emerging substances

Categorisation - what are the actions needed?

Prioritisation within each category

Why emerging? What are the priorities

1. Sufficient exposure/hazard info - risk: Candidate PS/RBSP
2. Lack of exposure info: Screening campaigns
3. Lack of ecotox info: Hazard assessment (PNEC)
4. LOQ > PNEC/EQS: Improvement of analytical methods
5. Lack of exposure AND ecotox info: Screening AND hazard assessment
6. Sufficient exposure/hazard info – no risk: Reduce monitoring efforts


Univers of substances
(NORMAN list)
≥ 4 countries AND /OR ≥ 100 sites with analysis
>20 sites analysis > LOQ
in the relevant matrix(ces) +
Recent data (>last 6 years)
Insuff. (or never) investigated OR measured in the „wrong“ matrix
Suff. investigated but low frequency of quantification
Suff. investigated and quantified in the relevant matrix
LOQmax< PNEC (existing data in the database)?
Sufficient experimental data for hazard assesment?
yes
yes
no
LOQmin (Database) OU LOQ expert labs < PNEC ?
Risk ?
yes
no
no
yes
Sufficient experimental data for hazard assesment?
yes
no
Cat. 2: Screening study
Cat. 5
Cat. 4: Action Analytical
Cat. 6: non priority for regular monitoring
Cat. 1: Candidates regular monitoring
Cat. 3: Action (eco)tox
Novel end points

NORMAN scheme applied for assessment of 500 substances within FP6 Modelkey project

- Monitoring data provided by: Joint Danube Survey (JDS2) and four regional water authorities (Elbe, Scheldt and Llobregat river basins)

Table 2
Compounds of Category 1 with their Chemical Abstract Number (CAS), the use category (Use), the priority substance number (PS), chronic-based Predicted No-Effect Concentration ($PNEC_{chronic}$), acute-based PNEC ($PNEC_{acute}$), provisional PNEC (P-PNEC), LC50-basis of the P-PNEC (Ref), trophic level used for the P-PNEC (TL), number of sites monitored since 2005 (# of sites>2004), exceedance of the lowest PNEC since 2005 (Exceedance>2004), frequency of exceedance since 2005 (Frequency>2004), priority ranking value (PR) and the river basins monitored (RB). The lowest PNEC value is indicated in bold.

CAS	Compound [a]	Use [b]	PS	$PNEC_{chronic}$ [μg/L]	$PNEC_{acute}$ [μg/L]	P-PNEC [μg/L]	Ref [c]	TL[d]	# of sites >2004	Exceedance >2004	Frequency >2004 [%]	PR	RB[e]
333-41-5	diazinon	P		0.017		**0.0011**	E	D	32	197	88	1.38	L, S
131860-33-8	azoxystrobin	P		2.0		**0.11**	E	A	766	1018	21	1.21	E
5915-41-3	terbutylazine	P		0.22		**0.0032**	E	A	1052	164	64	1.14	D, E, L, S
76-44-8	heptachlor	P			**0.000030**	0.033	P	A	914	2828	3	1.03	D, E, L, S
959-98-8	endosulfan I	P	14	0.0050		**0.00093**	E	F	67	543	51	1.01	D, L, S
72-54-8	4,4′-ddd	P			**0.00064**	0.0090	E	D	994	184	23	0.73	D, E, L, S
330-54-1	diuron	P	13	0.20		**0.0024**	E	A	1082	499	21	0.71	D, E, S
117-81-7	dEHP	I	12	1.3		**0.48**	B	D	1020	4	56	0.66	D, E, S
28159-98-0	irgarol	P		0.0050		**0.0014**	E	A	766	370	13	0.63	E
53-19-0	2,4′-ddd	P			**0.00064**	0.0090	E	D	959	139	8	0.58	E, L, S
15972-60-8	alachlor	P	1	0.30		**0.0045**	E	A	964	149	7	0.57	D, E, L, S
129-00-0	pyrene	I			**0.0046**	0.24	P	D	1082	28	36	0.56	D, E, L, S
891-86-1	endosulfan II	P	14	0.0050		**0.00093**	E	F	548	623	6	0.56	D, E, L, S
35065-29-3	pcb-180	I		**0.000016**		0.00053	P	F	959	106	6	0.56	D, E, L, S
72-55-9	4,4′-DDE	P			**0.00060**	0.030	P	D	994	172	6	0.56	D, E, L, S
1024-57-3	heptachloro epoxide B	P			**0.000030**	0.25	E	D	548	467	4	0.54	D, E, L, S
7012-37-5	pcb-28	I		**0.000032**		0.062	E	A	959	111	4	0.54	D, E, L, S
21725-46-2	cyanazine	P		**0.012**		0.022	E	A	929	116	2	0.52	E, S
886-50-0	terbutryn	P		0.013		**0.0059**	E	A	916	23	32	0.52	D, E, L, S
50-29-3	4,4′-ddt	P	34	0.010		**0.0048**	E	D	994	29	22	0.42	D, E, L, S
51218-45-2	metolachlor	P		0.070		**0.028**	E	A	964	43	20	0.40	D, E, L, S
67129-08-2	metazachlor	P		**0.060**		23	E	D	929	10	18	0.38	E, S
36643-28-4	tributyltin	B	30	0.00020		**0.00016**	E	D	1064	58	18	0.38	D, E, S
122-34-9	simazine	P	29	1.0		**0.18**	E	A	1102	2	24	0.34	D, E, L, S
35065-28-2	pcb-138	I		**0.000025**		0.00060	E	F	959	67	13	0.33	D, E, L, S
35065-27-1	pcb-153	I		**0.000022**		0.00060	E	F	959	82	12	0.32	D, E, L, S

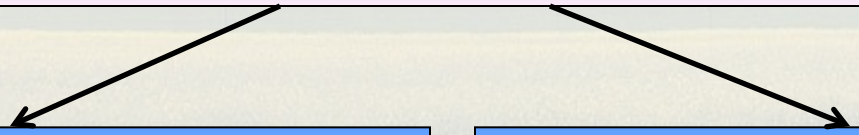
von der Ohe et al. Science of Total Environment 2011

NORMAN scheme applied in France
(ONEMA, Ministry of Ecology, coordinated by INERIS)

- **Watch list: less investigated substances**
- **Prepare future revision of RB specific pollutants list (WFD)**

Ca. 2400 candidates subst.
(700 already part of national monitoring)

TOP PRIORITY subst. :
221 water and 370 in sediment



Ca. 180 subst. Watch list
Nat. monitoring campaign 2012

Priority subst. for improvement of analytical perform. (under way)

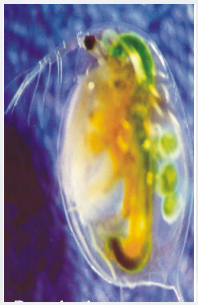
Known unknowns:
NORMAN List of frequently discussed emerging substances : 706 compounds

- Algal toxins
- Anticorrosives
- Antifoaming agents
- Antifouling compounds
- Antioxidants
- Biocides 36 notified
- Bio-terrorism/ sabotage agents
- Complexing agents
- Detergents
- Disinfection by-products (drinking water)
- Flame retardants
- Fragrances
- Gasoline additives
- Industrial solvents
- Nanoparticles
- Perfluoroalkylated compounds
- Personal care products
- Pesticides
- Pharmaceuticals
- UV screening agents
- Wood preservatives

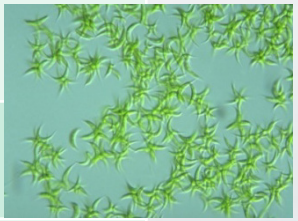
Collected data

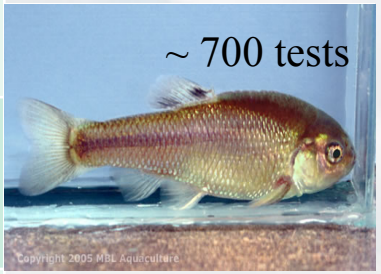
Kow (Source: Exp. data EPI suite >> QSARs via read-across methods)	705/ 707 substances
Koc (Source: Decision tree model (*Sabljic et al. 1995, Sabljic et al. 1996*)	707/ 707 substances
W S (*Exp. Data EPI suite >> read-across via ACF (Kühne 2006)*	707 / 707 substances
Fugacity models (Mackay et al. at 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

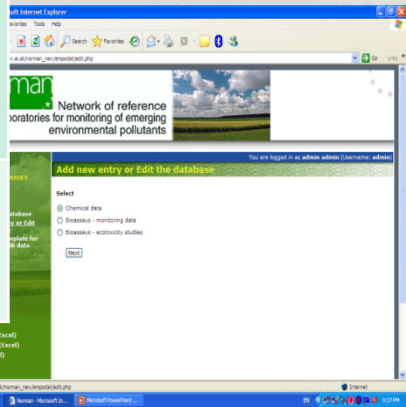
~ 1100 tests



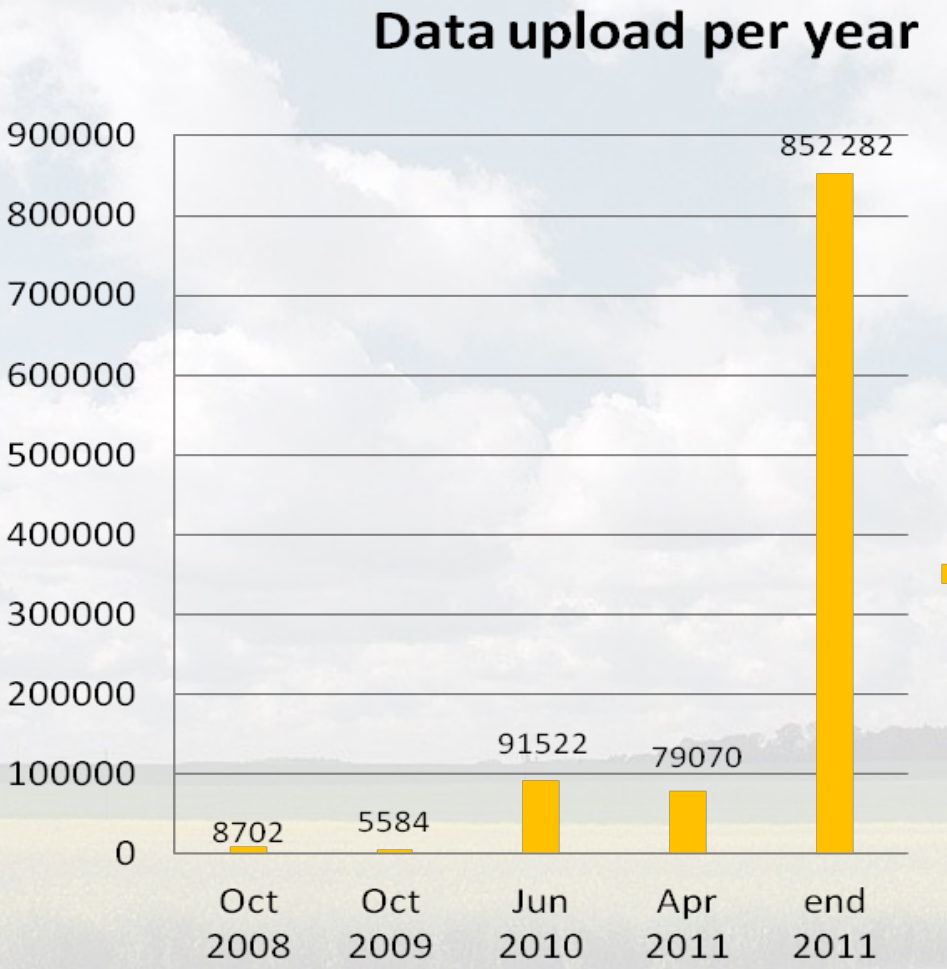
~550 tests





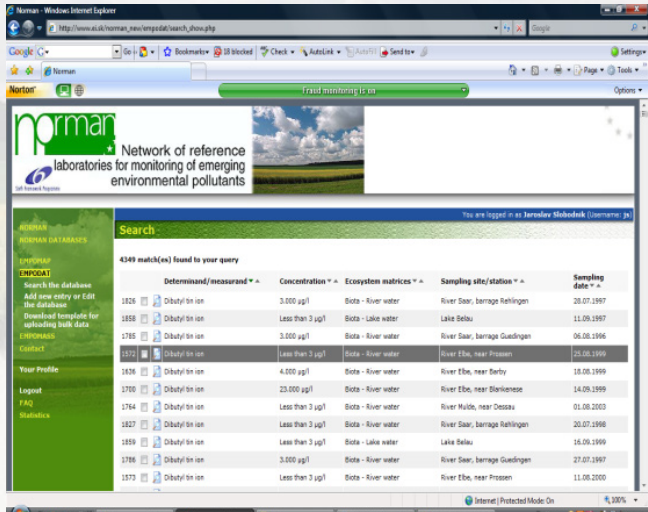


NORMAN EMPODAT database – portal for data on emerging substances (2011)



Examples of uploaded data:

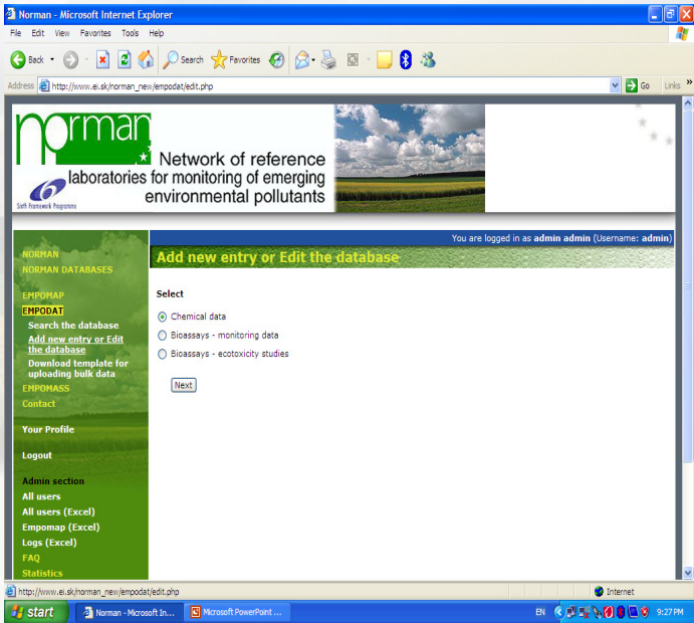
- MODELKEY FP6 project (four river basins)
- Saxony-Anhalt (Germany)
- Danube River Basin (14 countries)
- Rhine River Basin (RIWA)
- Screening studies (Scandinavian countries)



Candidate substances - NORMAN list of emerging substances (update 2011)

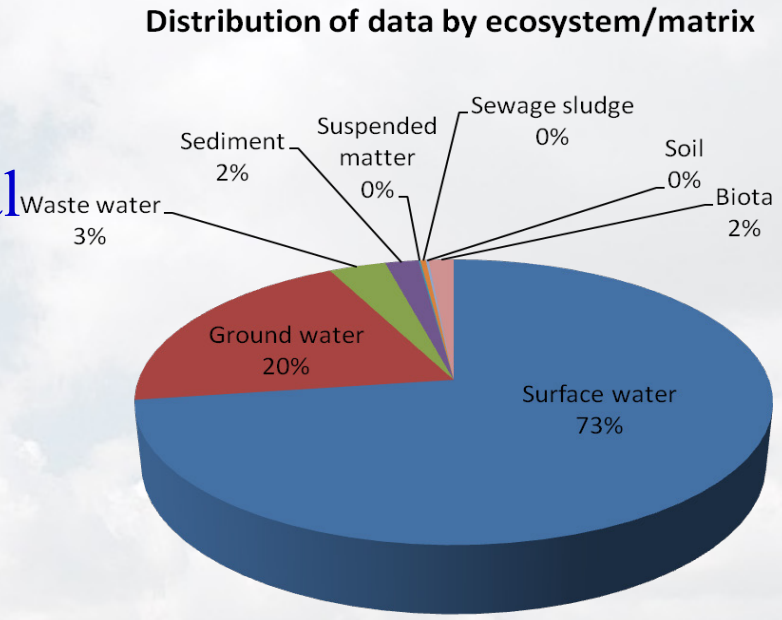
- More than 700 emerging substances (selected in 2011)

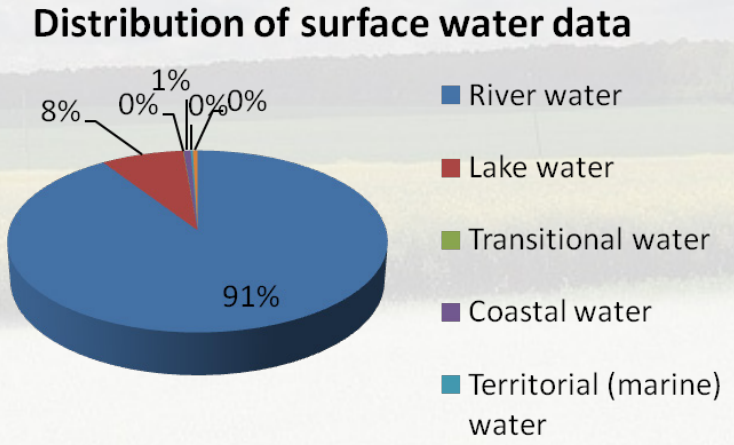
- Data only available for < 50% of the substances !



NORMAN Databases – EMPODAT monitoring data

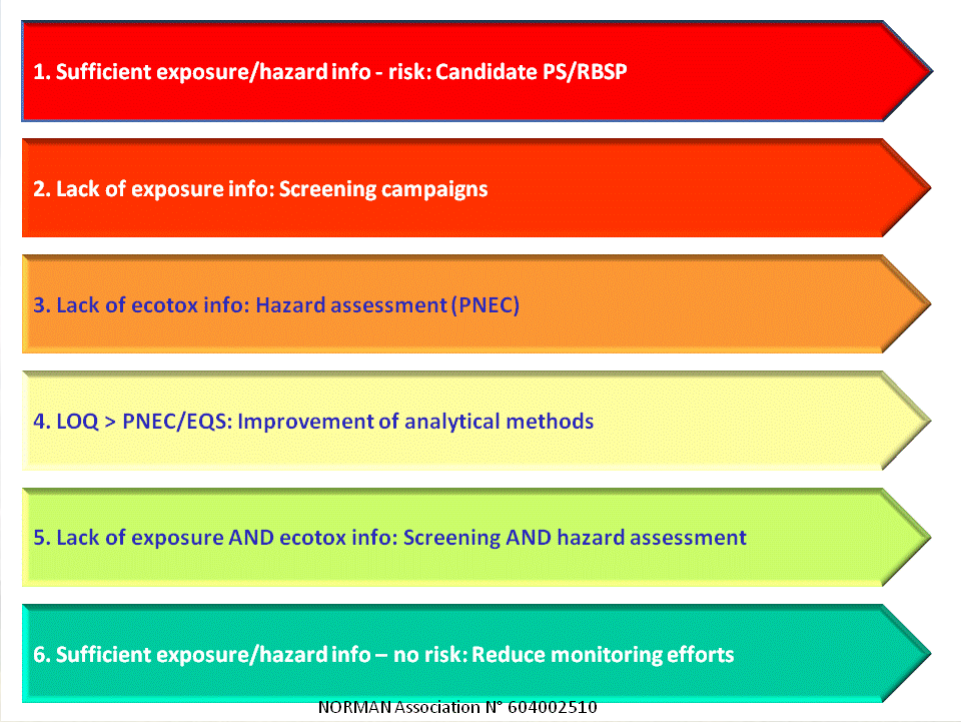
- Designed to store data from research projects and national /EU monitoring campaigns on emerging substances
- Regularly fed with input of the NORMAN members
- **MassBank database** to identify *unknowns* from mass spectrometric data – feeding EMPODAT





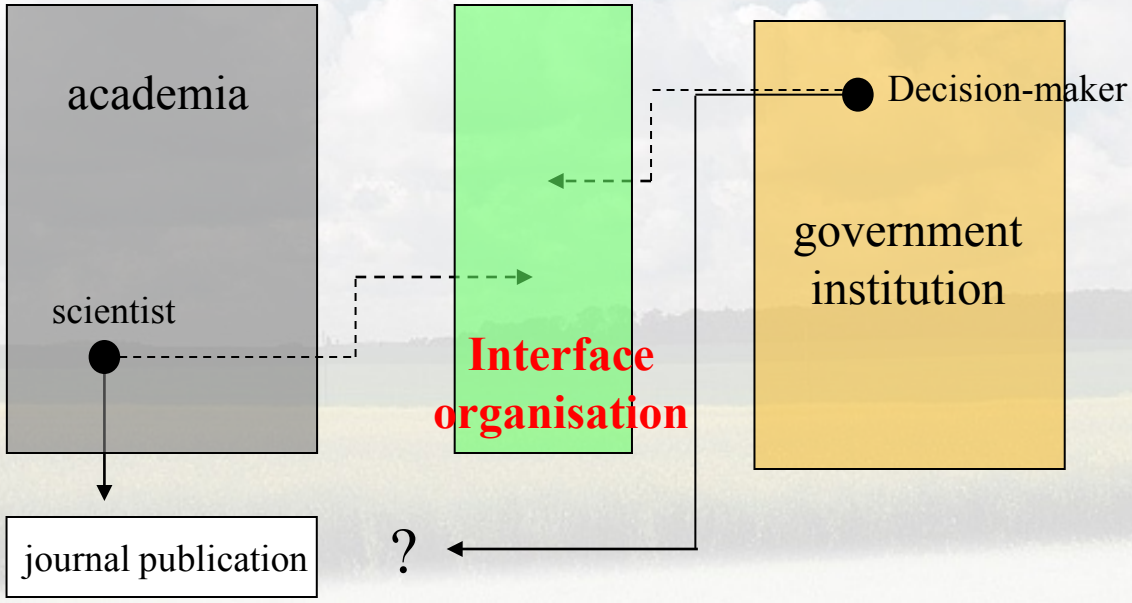
Databases added value

Exploitation of data at EU level =>>
added value for the scientific community and public authorities



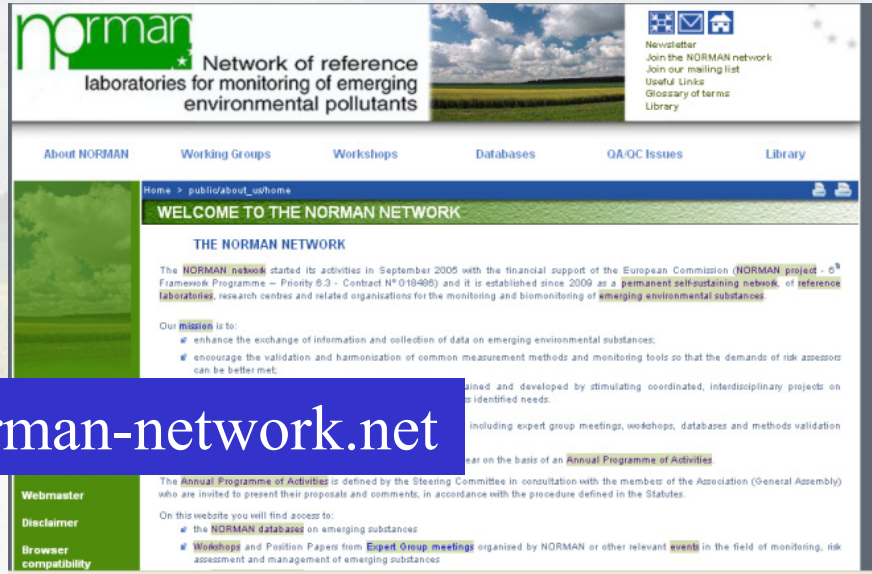
Science-policy interface

- Often a mismatch of objectives and needs…between scientists and decision-makers
- Effective communication needed
- The role of NORMAN as an interface organisation



Adapted from Martin Scheringer , 2011

Thank you for your attention !



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Biocides in the NORMAN list of emerging substances (2011)

- 34 biocides on the NORMAN List
  - 26 for which monitoring data are available (about 94 300 monitoring data - recent data >> 2004, 9% of the total)
    - 7 for which monitoring data from > 4 countries and potential risk is identified (Chlorotoluron , Prometryne , Carbendazine , Triclosan , Terbuthylazine , Diazinon , Terbutryne) + 1 risk non identified
    - 2 (Chlorpyrifos-methyl , Dichlorvos) for which analytical performance need to be improved
    - 16 for which further screening needed: (Imidacloprid , Deltamethrin, N,N-diethyl-m-toluamide, Dichlofluanid , Tolylfluanid, Propiconazole, Thiabendazole, Formaldehyde, Clorophene, Benzothiazole-2-thiol , Chlorothalonil , Clorophene, Malathion , Phoxim, Anthraquinone)

How to identify and prioritise relevant emerging pollutants?

Top-down approaches

Modelling-based
(production and usage
structural properties)

Target monitoring
Toxicity testing
(→ target)

Relevant emerging pollutants

Bottom-up approaches
(non-target screening, EDA
→ non target)

Known vs Unknown
Well investigated *vs* emerging substances

Adapted from Jorge Rodriguez Romero – DG ENV - SOCOPSE Final Conference, Maastricht, 24 – 26 June 2009

MEC 95 and Lowest PNEC to be more conservative

➔ **Lowest PNEC**

- Predict missing acute toxicity data with read-across models (kNN read-across methodology *Schüürmann et al. 2011, EST, DOI:10.1021/es200361r*f)
- Use *Lowest value* of *PNEC acute* (lowest LC50 / 1000) and *PNEC chronic* (lowest NOEC / 100), instead of preferring chronic over acute data *per se*

➔ **MEC 95**

- Take the maximum concentration at each site (MEC *site*)
- Calculate 95th percentile of all MEC*site* values (MEC95)

➔ **Risk ratio**

- MEC 95 / Lowest PNEC

Criteria for allocation of the substances to the 6 action categories

Monitoring data available in relevant matrix(ces) for the given substance :

- *Fugacity models, Kow, Koc, Water solubility*

Level of investigation and evidence of exposure:

- *N° of countries and N° of sites with monitoring data*
- *N° of sites with quantified data*
- *Recent data (after 2004 in this exercise)*

Sufficient performance of analytical methods:

- *Limit of quantification (LOQ) < Lowest PNEC*

Risk of exceedance of the PNEC

- *Max (Predicted) Exposure Conc. (MEC95) / Lowest PNEC >1*