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

NORMAN databases in support of WISE and European needs for information on emerging substances

Jaroslav Slobodnik
Environmental Institute, Kos, Slovak Republic

Joint CMA/NORMAN/EAQC-WISE meeting,
Paris, 21 October 2008

Sixth Framework Programme

ENVIRONMENTAL INSTITUTE

EUROWATERNET/WISE

Objectives

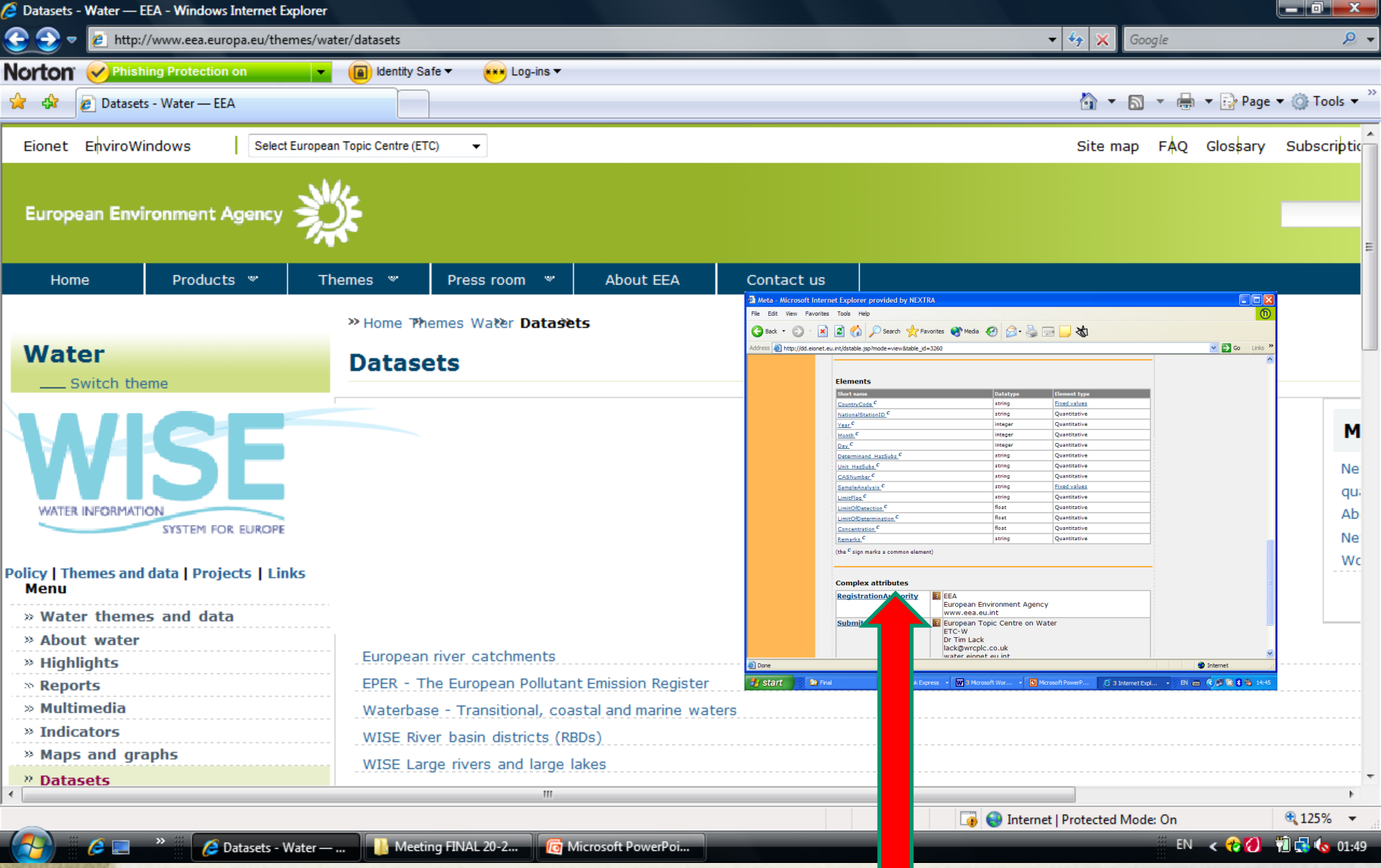
- Harmonisation and streamlining the reporting and information collection needs in line with the EU directives and national obligations;
- Use of the same national data sets for reporting to the EEA and other institutions.

Need for agreement on the:

- Determinands/ Level of data aggregation/ Spatial and temporal resolution/ **Metadata**

Tools to populate WISE – REPORTNET, EUROWATERNET (EIONET-water)

- Water Indicator Report 2003
  - Nutrients/ Oxygen consuming substances/ Hazardous substances (metals)/ Hazardous substances (organics)/ Hazardous substances (pesticides)



Waterbase-Rivers: Quality (637344 records)

The Quality table contains **data on nutrients and organic matter in water** measured at WISE-SoE river monitoring stations. Each station has been assigned a unique Waterbase identifier (WaterbaseID) which can be used to link the Quality data with their respective Stations and Pressures data. Each record has **three special quality assurance fields**. **Their meaning is explained in the QA documentation which can be found in the "Additional information" part.**

NORMAN Databases overall objectives

- Emerging substances in EU 27+ water/air/soil/biota matrices
  - **Platform for bringing existing knowledge together**
  - Framework for systematic elaboration, collection and scientifically sound evaluation of future data

NORMAN FP6 network laboratories monitoring emerging pollutants - Windows Internet Explorer

http://www.norman-network.net/index_php.php?module=public/about_us/home

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Network of reference laboratories for monitoring of emerging environmental pollutants

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About us | Contact Points | Workshops | Databases | QA/QC Issues

- EMPOMAP
- EMPODAT
- EMPOMASS

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WELCOME TO THE NORMAN NETWO

CALL FOR EXPRESSION OF INTEREST

The NORMAN project is funded under the 6th Framework Programme — Priority 6.3 "Global Change and Ecosystems" (Contract N° 018486 - Start da September 2005).

Our focus is on emerging environmental substances. Emerging substances are not necessarily new chemicals. They are substances that have often lon present in the environment but whose presence and significance are only now being elucidated. Data for emerging substances are often scarc measurement methods are often at the research and development stage or have not yet been harmonised at the European level. This makes it difficult to int and compare the results and represents a major difficulty for regulatory bodies in their decision-making.

Our objective is to establish a European network of reference laboratories, research centres and related organisations (including standardisation bodies) i to:

- improve the exchange of information on emerging environmental contaminants

http://www.norman-network.net/index_php.php?module=public/databases/databasex&menu2=public/databases/databases

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NORMAN DATABASES

EMPOMAP: Database of European leading experts, organisations and projects

- **Major goals**
  - Definition of the current state and future needs of research on emerging substances in Europe
  - Help to co-ordinate national research programmes in order to avoid duplication of research
- **Additional features**
  - Targeted identification of experts and stakeholders concerned with a specific emerging pollutant
  - Link to other European databases dealing with related topics (WEKNOW, GEDRI, **METROPOLIS, EUGRIS…)**

EMPOMAP: Database of European leading experts, organisations and projects

- **Publicly available since February 2007**
- **Users invited to register their projects/ organisations/ expertise**
  - No. of registered users - >245 (ca. 140 organizations)
  - Experts – 55 (+8 in draft)
  - Organizations – 24 (+5 in draft)
  - Projects – 100 (+5 in draft)

Norman - Windows Internet Explorer

http://www.ei.sk/norman/empomap/project_show.php

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Emerging Substances – PROJECTS

8 match(es) found to your query

	Project	Contact person: Family name	First name	Mr./Ms.	Country
☐	Endocrine disrupters in Austria's waters – a risk?	Gans	Oliver	Mr.	Austria
☐	Investigation and analysis of Danube sediments and suspended matter to selected organic pollutants	Gans	Oliver	Mr.	Austria
☐	Household dust – an indicator for indoor pollution	Gans	Oliver	Mr.	Austria
☐	Joint Danube Survey I.	Liska	Igor	Mr.	Austria
☐	Organotin compounds in the aquatic environment of Austria	Gans	Oliver	Mr.	Austria
☐	Veterinary antibiotics in animal manure and soils in Austria	Gans	Oliver	Mr.	Austria
☐	Carbamazepine and caffeine – potential screening parameters for groundwater contamination from municipal waste water?	Gans	Oliver	Mr.	Austria
☐	Brominated flame retardants in the aquatic environment	Gans	Oliver	Mr.	Austria

☐ **Select All / Unselect All**

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EAQCWISE | NORMAN Paris 21 ... | Norman - Windows ...

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EMPODAT: Database of occurrence/monitoring data on emerging substances

- Web-database on-line
- Three modules:
  - **Chemical data** including sub-module on **nanoparticles**
  - **Bioassays - monitoring data**
  - **Bioassays - ecotoxicity studies**
- **Data entry**
  - **Data Collection Templates** for bulk data upload - **downloadable**
  - **On-line entry form** for single entries
  - Matrices: **water, sediment, SPM, biota, air**

To submitt a bulk data a set of specific templates has been prepared. For each ecosystem/matrix two templates are available – for individual and for aggregate data template contains several worksheets:

i. Instructions – with basic explanation of each item in worksheets;
ii. Data source – where information about the data provider, laboratory and references should be inserted;
iii. Analysis – to enter information on sampling station, measured values and other relevant metadata;
iv. Analytical method – to enter information about analytical methods used for each determinand.

According to the ecosystem/matrix and type of data (individual/aggregate) an appropriate template should be filled in and sent to the following e-mail address: proj
with copy to slobodnik@ei.sk, for further processing and upload to the web-database.
It is particularly important to fill in all obligatory fields in order to facilitate proper work of the Search function in the database.

Please download the templates relevant for your data:

Ecosystem/matrix	Individual data	Aggregate data	Bioassays data
Water (surface, ground, wastewater)	DCT_WATER-ind-20081004-v9.xls DCT_WATER-ind-20081004-v9.zip	DCT_WATER-aggr-20081004-v9.xls DCT_WATER-aggr-20081004-v9.zip	DCT_BIOASSAYS_Water_20080425_PHE.x DCT_BIOASSAYS_Water_20080425_PHE.z DCT_BIOASSAYS_Ecotoxicity_Studies_200 DCT_BIOASSAYS_Ecotoxicity_Studies_200
Sediments	DCT_SEDIMENTS-ind-20081004-v9.xls DCT_SEDIMENTS-ind-20081004-v9.zip	DCT_SEDIMENTS-aggr_20081004-v9.xls DCT_SEDIMENTS-aggr_20081004-v9.zip	DCT_BIOASSAYS_Sediments_20080425_P DCT_BIOASSAYS_Sediments_20080425_P
Biota	DCT_BIOTA-ind-20081004-v9.xls DCT_BIOTA-ind-20081004-v9.zip	DCT_BIOTA-aggr-20081004-v9.xls DCT_BIOTA-aggr-20081004-v9.zip	
SPM	DCT_SPM-ind-20081004-v9.xls DCT_SPM-ind-20081004-v9.zip	DCT_SPM-aggr_20081004-v9.xls DCT_SPM-aggr_20081004-v9.zip	
Air	DCT_AIR-ind_20081004-v8.xls DCT_AIR-ind_20081004-v8.zip	DCT_AIR-aggr-20081004-v9.xls DCT_AIR-aggr-20081004-v9.zip	

You are logged in as **admin admin** (Username: **admin**)

Add new entry or Edit the database

Select

- (•) Chemical data
- ( ) Bioassays - monitoring data
- ( ) Bioassays - ecotoxicity studies

Next

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http://www.ei.sk/norman_new/empodat/search_show.php

Norman

Fraud monitoring is on

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You are logged in as **Jaroslav Slobodnik** (Username: **js**)

Search

4349 match(es) found to your query

	Determinand/measurand	Concentration	Ecosystem matrices	Sampling site/station	Sampling date
1826	Dibutyl tin ion	3.000 µg/l	Biota - River water	River Saar, barrage Rehlingen	28.07.1997
1858	Dibutyl tin ion	Less than 3 µg/l	Biota - Lake water	Lake Belau	11.09.1997
1785	Dibutyl tin ion	3.000 µg/l	Biota - River water	River Saar, barrage Guedingen	06.08.1996
1572	Dibutyl tin ion	Less than 3 µg/l	Biota - River water	River Elbe, near Prossen	25.08.1999
1636	Dibutyl tin ion	4.000 µg/l	Biota - River water	River Elbe, near Barby	18.08.1999
1700	Dibutyl tin ion	23.000 µg/l	Biota - River water	River Elbe, near Blankenese	14.09.1999
1764	Dibutyl tin ion	Less than 3 µg/l	Biota - River water	River Mulde, near Dessau	01.08.2003
1827	Dibutyl tin ion	Less than 3 µg/l	Biota - River water	River Saar, barrage Rehlingen	20.07.1998
1859	Dibutyl tin ion	Less than 3 µg/l	Biota - Lake water	Lake Belau	16.09.1999
1786	Dibutyl tin ion	3.000 µg/l	Biota - River water	River Saar, barrage Guedingen	27.07.1997
1573	Dibutyl tin ion	Less than 3 µg/l	Biota - River water	River Elbe, near Prossen	11.08.2000

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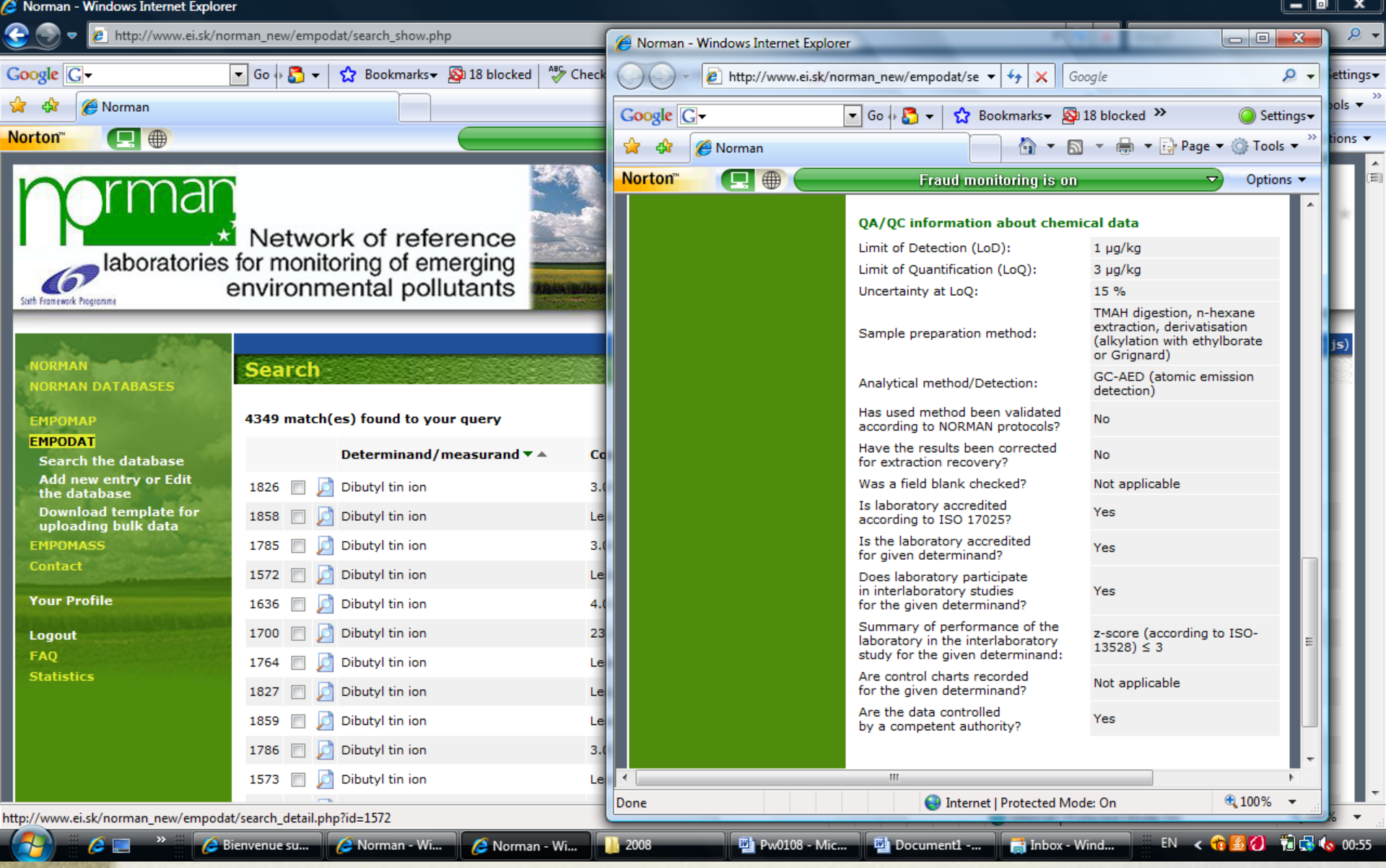
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Determinand/measurand
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1572 Dibutyl tin ion
1636 Dibutyl tin ion
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1573 Dibutyl tin ion
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Fraud monitoring is on
Options
QA/QC information about chemical data
Limit of Detection (LoD): 1 µg/kg
Limit of Quantification (LoQ): 3 µg/kg
Uncertainty at LoQ: 15 %
Sample preparation method: TMAH digestion, n-hexane extraction, derivatisation (alkylation with ethylborate or Grignard)
Analytical method/Detection: GC-AED (atomic emission detection)
Has used method been validated according to NORMAN protocols? No
Have the results been corrected for extraction recovery? No
Was a field blank checked? Not applicable
Is laboratory accredited according to ISO 17025? Yes
Is the laboratory accredited for given determinand? Yes
Does laboratory participate in interlaboratory studies for the given determinand? Yes
Summary of performance of the laboratory in the interlaboratory study for the given determinand: z-score (according to ISO-13528) ≤ 3
Are control charts recorded for the given determinand? Not applicable
Are the data controlled by a competent authority? Yes
Done
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International Office for Water
Capacity building for better water management

INERIS

Implementation of Requirements for Priority Substances within the Context of the Water Framework Directive

Common template for data collection

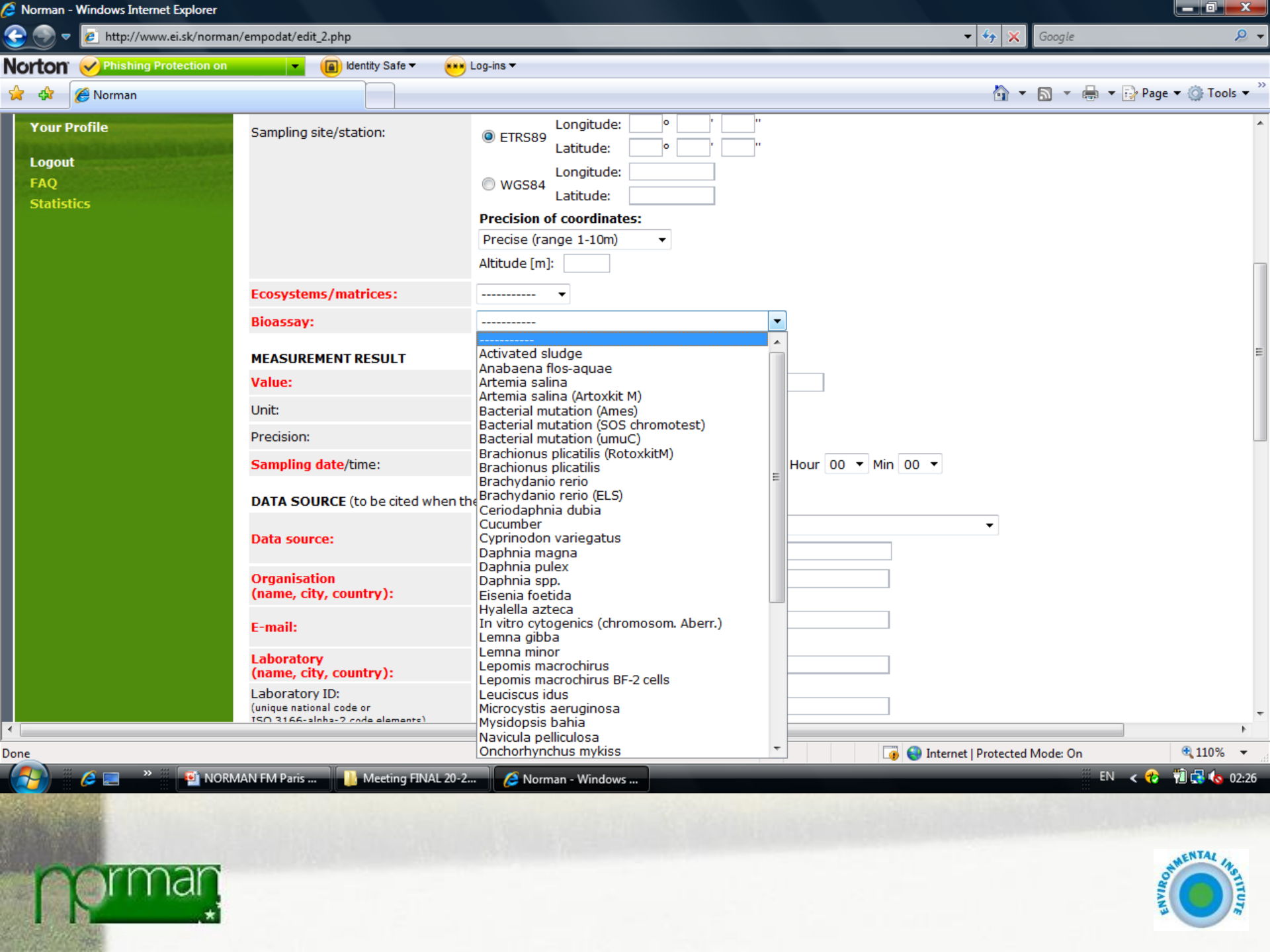
Final version 20th March 2007

+ QA/QC Directive
+ NORMAN VALIDATION
+ EAQC-WISE
+ ICPDR Databases
…..

Contact persons:

Valeria Dulio
T +33 (0) 3 44 55 66 47
F +33 (0) 3 44 55 66 00
e-mail valeria.dulio@ineris.fr

Ing. B. Fribourg-Blanc
T +33 (0) 5 55 11 47 97
F +33 (0) 5 55 11 47 48
E-mail b.fribourg-blanc@oieau.fr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Statistics
Sampling site/station:
ETRS89
Longitude:
Latitude:
WGS84
Longitude:
Latitude:
Precision of coordinates:
Precise (range 1-10m)
Altitude [m]:
Ecosystems/matrices:
Bioassay:
MEASUREMENT RESULT
Value:
Unit:
Precision:
Sampling date/time:
Hour 00 Min 00
DATA SOURCE (to be cited when the
Data source:
Organisation (name, city, country):
E-mail:
Laboratory (name, city, country):
Laboratory ID:
(unique national code or
Activated sludge
Anabaena flos-aquae
Artemia salina
Artemia salina (Artoxkit M)
Bacterial mutation (Ames)
Bacterial mutation (SOS chromotest)
Bacterial mutation (umuC)
Brachionus plicatilis (RotoxkitM)
Brachionus plicatilis
Brachydanio rerio
Brachydanio rerio (ELS)
Ceriodaphnia dubia
Cucumber
Cyprinodon variegatus
Daphnia magna
Daphnia pulex
Daphnia spp.
Eisenia foetida
Hyalella azteca
In vitro cytogenics (chromosom. Aberr.)
Lemna gibba
Lemna minor
Lepomis macrochirus
Lepomis macrochirus BF-2 cells
Leuciscus idus
Microcystis aeruginosa
Mysidopsis bahia
Navicula pelliculosa
Onchorhynchus mykiss
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EMPODAT

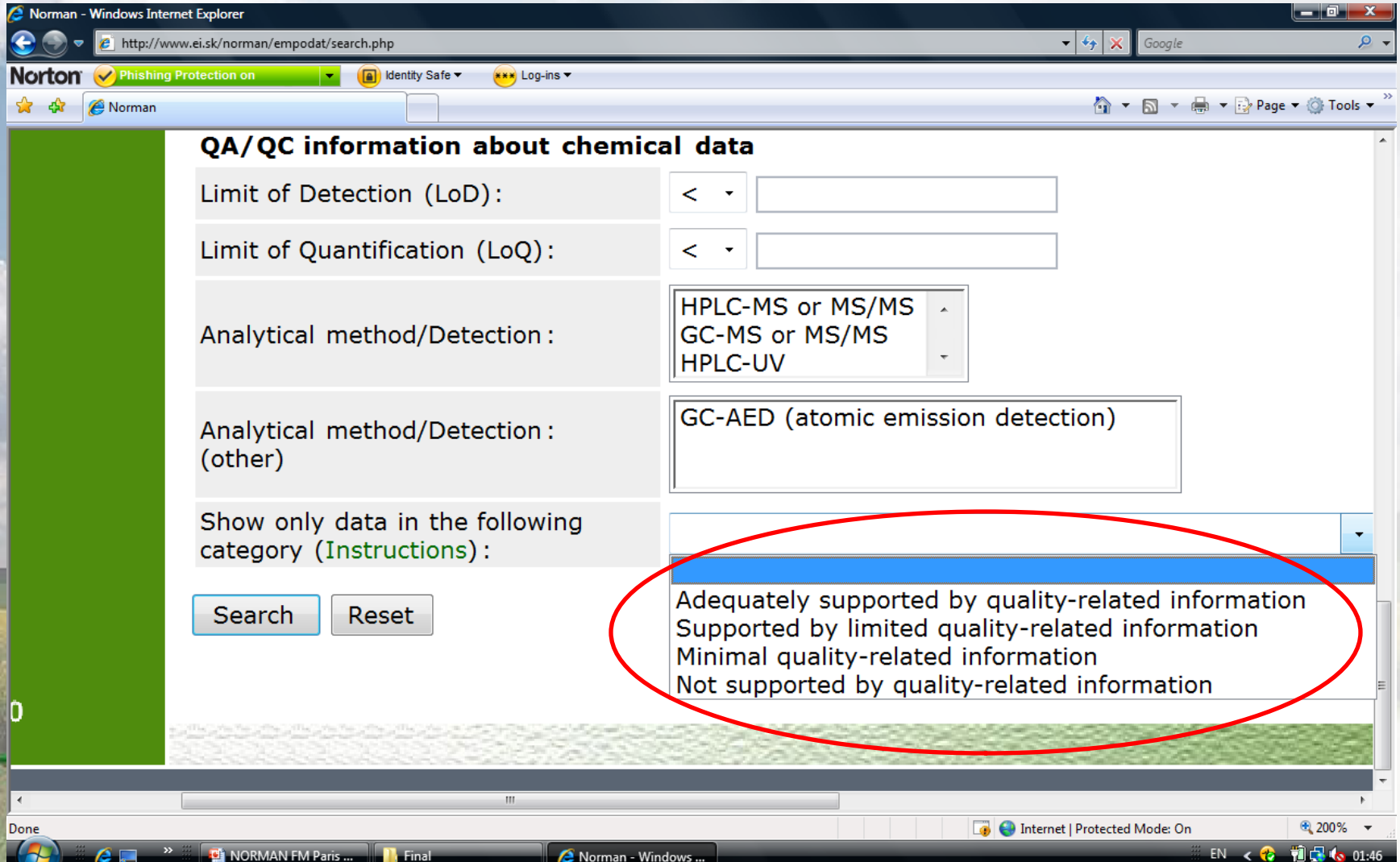
Organization – data provider	Matrix	Data entries uploaded
EI / SHMI (Slovakia)	Surface w. / waste w./ sediments	5067
JRC (Italy)	Surface water	744
IJS (Slovenia)	Surface water	86
UBA (Germany)	Surface w. - marine	180
CSIC (Spain)	Surface w. / sediments	880
FI- IME / German Env. Speciment Bank (Germany)	Biota	1185
ICPDR (Danube Basin)	Surface water	560
TOTAL		**8702**

EMPODAT

Organization – data provider	Matrix	Data in pipeline
UK EA (UK)	Surface w. / ground w. / sediments	734
BRGM (France)	Surface w. /ground w.	648
SYKE (Finland)	Biota / sediments / surface w.	4730
IRSA (Italy)	Surface water / SPM	230
Sweden	Sediments	650
UBA (Germany)	Biota	84
WRI (AQUATERRA Danube Survey)	Sediments - bioassays	817
TOTAL		**7893**

EMPODAT – Data scoring

NEW!!!



No.	Metadata	Information provided	Rating	Minimum requirements - category 3	Minimum requirements - category 2	Minimum requirements - category 1
1	Limit of Detection (LoD)	Filled in	10	10	10	10
		Not filled in	0			
2	Limit of Quantification (LoQ)	Filled in	8		8	8
		Not filled in	0			
3	Uncertainty at LoQ	Filled in	6		6	6
		Not filled in	0			
4	Coverage factor	Filled in	2			2
		Not filled in	0			
5	Analytical method	Filled in	2		2	2
		Not filled in	0			
6	Sample preparation method	Filled in	2		2	2
		Not filled in	0			
7	Has standardised analytical method been used?	Filled in	6			
		Not filled in	0			
8	Has the used method been validated according to one of the NORMAN protocols?	V1 – within laboratory	6	6		
		V2 – between laboratories	8		8	
		V3 - routine	10			10
		No	0			
		Not known	0			

Code	Category	Score
1	Adequately supported by quality-related information	68-92
2	Supported by limited quality-related information	52-67
3	Minimal quality-related information	22-51
4	Not supported by quality-related information	0-21

EMPOMASS: Mass spectral database of unknown and provisionally identified substances

- Web-database on-line
- **Two modules**
  - **GC-MS**
  - **LC-MS-MS**
  - including option of **accurate mass measurement**
- Data entry
  - **Data Collection Templates** for bulk data upload - **downloadable**
  - **On-line entry form** for single entries
  - Matrices: **water, sediment, SPM, biota, air**

Network of reference laboratories for monitoring of emerging environmental pollutants

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Web counter: 1289

UPLOADING BULK DATA

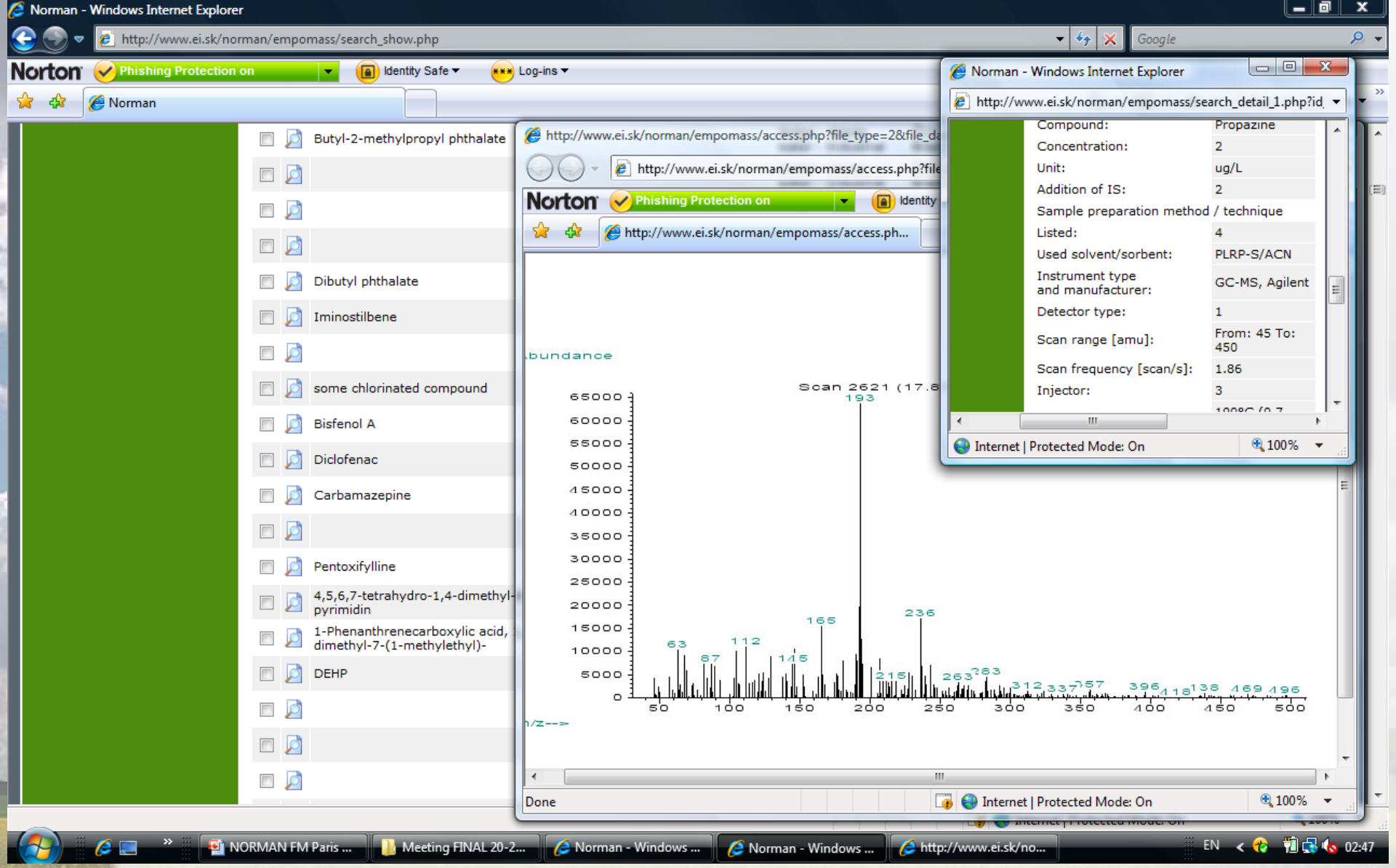
To submit a bulk data a set of specific templates has been prepared. For each ecosystem/matrix template is available, containing several worksheets:

i. Instructions – with basic explanation of each item in worksheets;
ii. Data source – where information about sampling point, data provider, laboratory and references should be inserted;
iii. GC-MS data – to enter information on sampling station, measured values and other relevant metadata;
iv. Analytical method – to enter information about analytical methods used for each substance.

According to the ecosystem/matrix an appropriate template should be filled in and sent to the following e-mail address: projects@ei.sk with copy to slobodnik@ei.sk, for further processing and upload to the web-database. Please note, that mass spectrum charts (*.jpg, *.gif or similar format) and raw chromatograms (*.ms or similar format) should be submitted together with the completed data collection template.
It is particularly important to fill in all obligatory fields in order to facilitate proper work of the Search function in the database.

Please download the templates relevant for your data:

Ecosystem/matrix	GC-MS data
Water (surface, ground, wastewater)	DCT_GC-MS_Water_20080922-v1.xls DCT_GC-MS_Water_20080922-v1.zip
Sediments	DCT_GC-MS_Sediments_20080922-v1.xls DCT_GC-MS_Sediments_20080922-v1.zip
Biota	DCT_GC-MS_Biota_200800922-v1.xls DCT_GC-MS_Biota_200800922-v1.zip
SPM	DCT_GC-MS-SPM_20080922-v1.xls DCT_GC-MS-SPM_20080922-v1.zip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Butyl-2-methylpropyl phthalate
Dibutyl phthalate
Iminostilbene
some chlorinated compound
Bisfenol A
Diclofenac
Carbamazepine
Pentoxifylline
4,5,6,7-tetrahydro-1,4-dimethyl-
pyrimidin
1-Phenanthrenecarboxylic acid,
dimethyl-7-(1-methylethyl)-
DEHP
http://www.ei.sk/norman/empomass/access.php?file_type=2&file_da
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Compound: Propazine
Concentration: 2
Unit: ug/L
Addition of IS: 2
Sample preparation method / technique
Listed: 4
Used solvent/sorbent: PLRP-S/ACN
Instrument type and manufacturer: GC-MS, Agilent
Detector type: 1
Scan range [amu]: From: 45 To: 450
Scan frequency [scan/s]: 1.86
Injector: 3
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Joint Danube Survey

13 August – 26 September 2007, 1600 rkm

- The biggest research river expedition in the world - 11 European countries
- 124 sampling sites (51 on the tributaries)
- **Sampling and analyses programme**
  - Biology – all five BQEs (benthic invertebrates air-lift/K&S; fish EFI+)
  - **Chemistry – > 260 parameters in W/SED/SPM/biota and GC-MS screening**
  - Microbiology – E. coli, Total colifoms, Bacterial abundance/biomass/secondary production, DNA
  - Hydromorphology – 50 km sections + detailed assessment of sampling site
  - Ecotoxicology – *Vibrio fischerii, Lemna minor, Desmodesmus subspicatus*
  - Radiology – $d^{15}N$ and $d^{18}O$ (NO3), ^{222}Rn, $d^{18}O$, $d^{2}H$, ^{3}H (biogeochemistry), ^{137}Cs, ^{90}Sr, ^{226}Ra, ^{228}Ra, ^{40}K, ^{238}U, ^{210}Pb

JOINT DANUBE SURVEY 2

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Future steps

- Further data collection and processing – all EU27+ countries
- **Evaluation of the data from Norman databases**
  - Target substance(s): benchmark values, location, quality of the data, data gaps, etc.
  - **2009**
    - **EQS Directive Annex III substances**
    - **Organic phosphorous flame retardants**
    - **Siloxanes**

Upgrade of the list of NORMAN substances

- **Criteria to be developed by the NORMAN Working Group on Prioritisation**
- Considerations to include:
  - All **OTHER POLLUTANTS** from each MS
  - **Annex III** substances subject to review for possible identification as priority substances or priority hazardous substances – *EQS Directive*
  - **Provisional-PNEC values**

Calculation of EQS at the national level - SK05/IB/EN-01

Organisms	Test	Species	Experimental	QSAR pred.
Fish	acute	*Poecilia reticulata*	> 1000 µg/l	232 µg/L
	prolongated		/	n.a. [a]
Invertebrates	acute	*Daphnia magna*	≥ **170** µg/l	625 µg/L
	chronic	*Daphnia magna*	= 70 µg/l	n.a. [a]
Algae	acute	*Selenastrum capricornutum*	= 6000 µg/l	283 µg/L
	semichronic	*Scenedesmus subspicatus*	= 400 µg/l	n.a. [a]

AA-EQS: 70 µg/L : 50 = 1.4 µg/L → 1.4 µg/L

MAC-EQS: 170 µg/L : 50 = 3.4 µg/L → 3 µg/L

P-PNEC: 232 µg/L : 10,000 = 0.023 µg/L → 0.02 µg/L

Example: 4-Methyl-2,6-di-tert butylphenol

Ranking	Status analyte	CAS #	English name	JDS1 SK	JDS1	TNMN SK	JDS2 SK	JDS2	Safety factor	Source	P-PNEC	AA-EQS	Excess
1	target - SK	5915413	terbutylazine				**0.25**	0.25	1000	L	**0.0032**		**76.6**
2	target - SK	67663	trichloromethane	0.2	1.3	**96**		1.8		L		2.5	**38.4**
3	target - SK	30125634	desethylterbutylazine				**0.097**	0.12	1000	P	**0.0084**		**11.6**
4	target - SK	3115499	nonylphenol-1-carboxylate	0.05			**0.24**	3.4	1000	P	**0.071**		**3.4**
5	target - SK	1582098	trifluralin	**0.1**			0.01	0.01		L		0.03	**3.3**
6	target - SK	193395	indeno[1,2,3-c,d]pyrene			**0.006**		0.021		L		0.002	**3.0**
29	GC-MS - whole Danube	6765395	1-heptadecene		**0.20**					B	**0.00004**		**5508.0**
30	GC-MS - whole Danube	629787	heptadecane		**2.0**			0.11		B	**0.00002**		**5118.8**
31	GC-MS - whole Danube	112801	9-octadecenoic acid		**6.8**			0.32		B	**0.00020**		**1568.8**

SK Prioritisation - 241 compounds evaluated in terms of aquatic exposure and potential ecological effects

Derivation of a Provisional Predicted No Effect Concentration: P-PNEC

Other considerations

- Continue lobbying at DG ENV and DG RESEARCH to make an upload of all data on emerging substances generated within future EU-funded (e.g., FP) projects mandatory

Conclusions

- NORMAN will try to harmonise efforts with:
  - EEA – WISE
  - Reporting/upgrade of DWD
  - REACH
- **Data quality -** close cooperation with international riverine (IKSR, ICPDR, IKSE) or marine environment (OSPAR) protection commissions


QUALITY IS EVERYTHING
As modelers use to say about input data…
JUNK IN - JUNK OUT