Template for inputting passive sampling data into EMPODAT

Status and progress

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How can PS data in a common repository be useful?

- Tangible and common objectives are needed

- Possible uses for the PS scientist:
  - «Validation» of PS data with data from other PS
  - Combining data from PS with data from other monitoring/sampling techniques, e.g. superimposing PS data with biota monitoring data
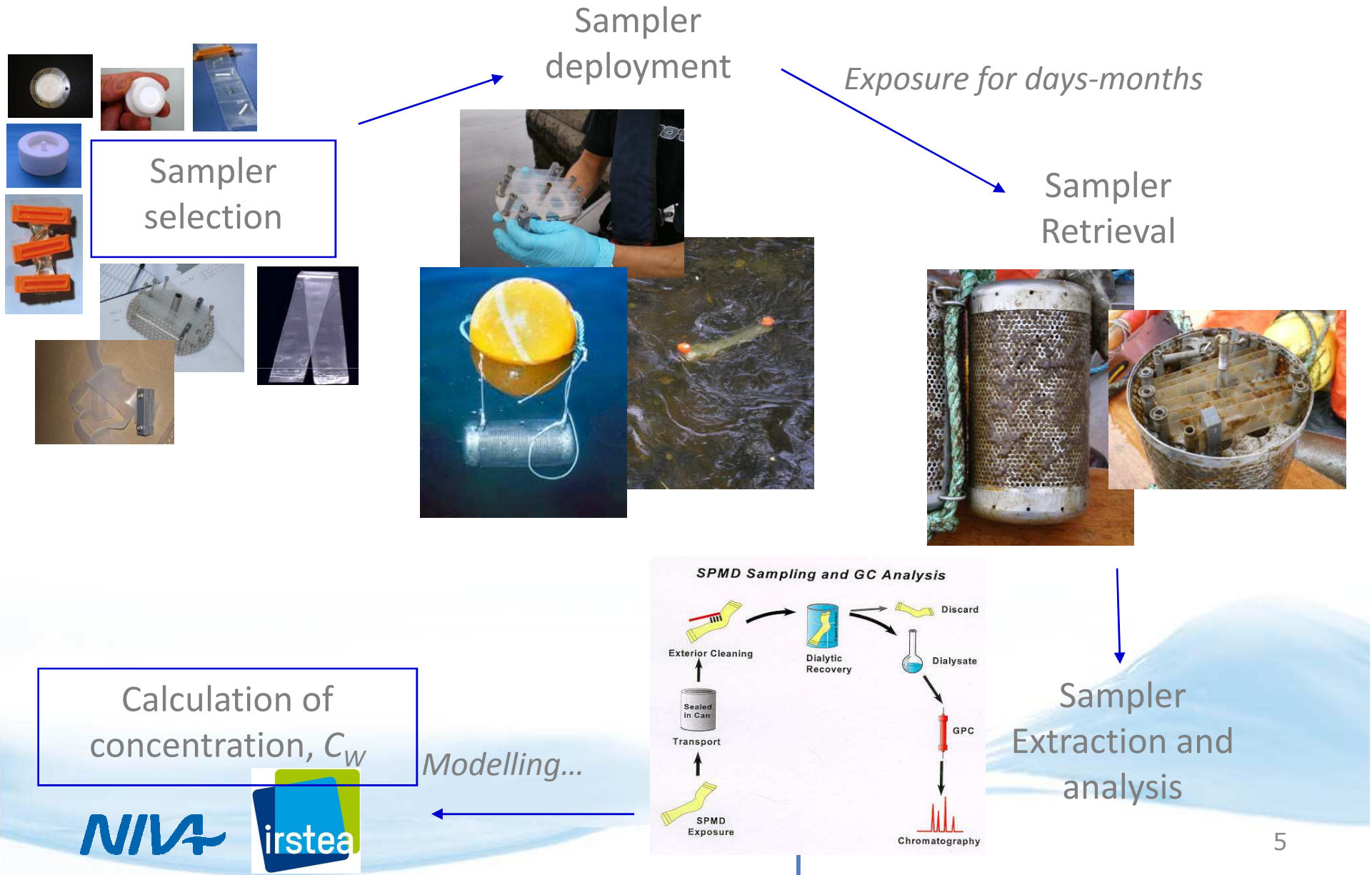
How can PS data in a common repository be useful?

- Current uses of the EMPODAT database*

  - Finding environmental occurence data for chemicals on the NORMAN list of suspect chemicals

  - Finding environmental occurence data for chemicals identified through REACH

  - Prioritisation of substances that may need further investigation at national level

*According to the participants to the cross working group activity workshop in Prague, September 2016
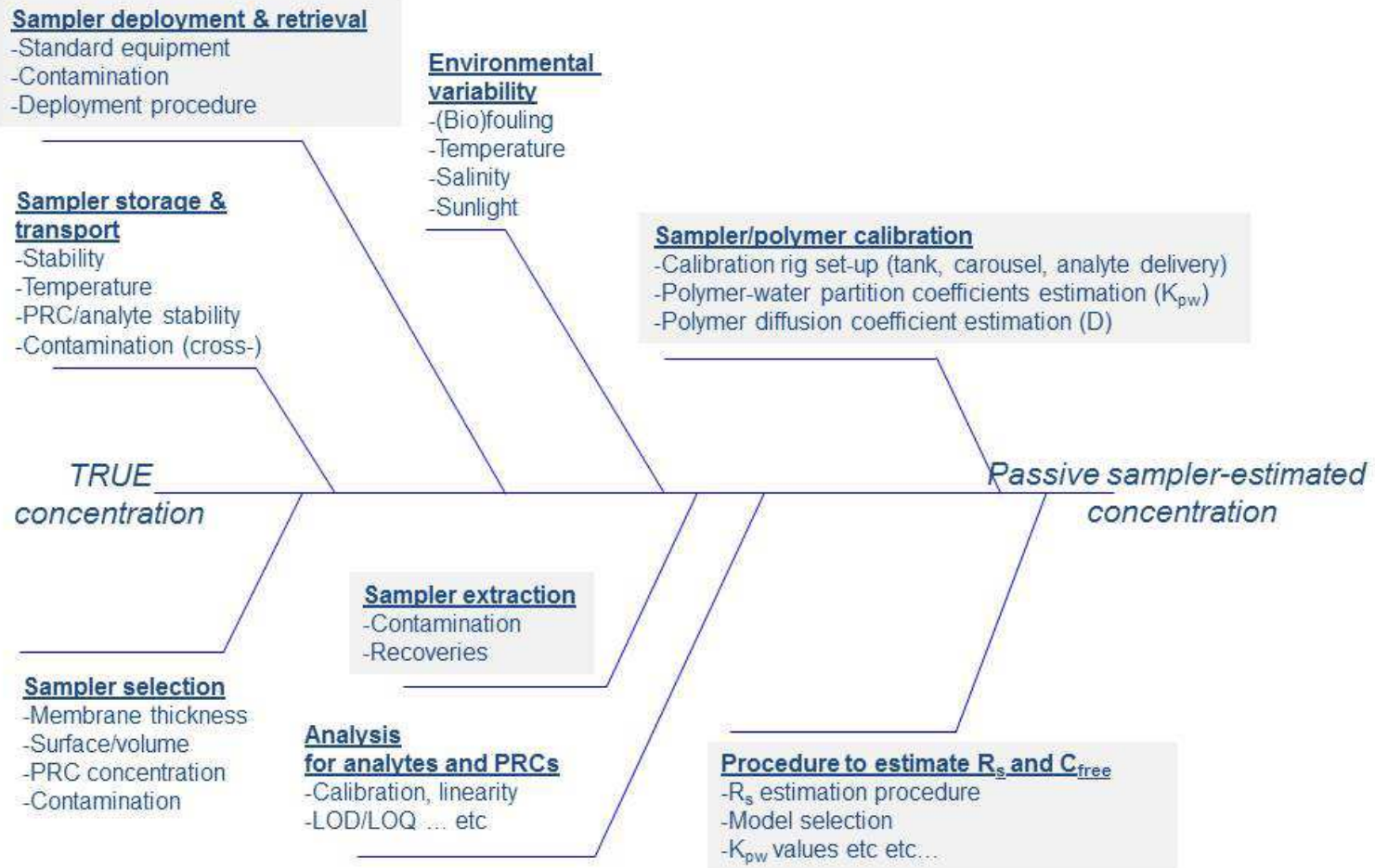
Status for a common repository for passive sampling data

- JDS-3 data sheets
  - Sufficiently comprehensive
  - But focused on specific passive samplers
- Work to be completed in 2017
- Cater for different users of these data:
  - External users not likely to be interested by metadata
  - PS users likely needing metadata
- Quality criteria should be established based on
  - Passive sampling process
  - Data representativeness
- Required metadata and PS information
  - → Need not to deter people willing to input data
  - → Need work on (i) quality criteria and (ii) supporting information needs

The passive sampling process

Sampler
deployment

Exposure for days-months

Sampler
selection

Sampler
Retrieval

Calculation of
concentration, C_W

Modelling…

Sampler
Extraction and
analysis

SPMD Sampling and GC Analysis

Exterior Cleaning

Dialytic
Recovery

Discard

Dialysate

Sealed
in Can

Transport

GPC

SPMD
Exposure

Chromatography

The passive sampling process

Sampler deployment & retrieval
-Standard equipment
-Contamination
-Deployment procedure

Environmental variability
-(Bio)fouling
-Temperature
-Salinity
-Sunlight

Sampler storage & transport
-Stability
-Temperature
-PRC/analyte stability
-Contamination (cross-)

Sampler/polymer calibration
-Calibration rig set-up (tank, carousel, analyte delivery)
-Polymer-water partition coefficients estimation (K_{pw})
-Polymer diffusion coefficient estimation (D)

TRUE concentration

Passive sampler-estimated concentration

Sampler extraction
-Contamination
-Recoveries

Sampler selection
-Membrane thickness
-Surface/volume
-PRC concentration
-Contamination

Analysis for analytes and PRCs
-Calibration, linearity
-LOD/LOQ ... etc

Procedure to estimate R_s and C_{free}
-R_s estimation procedure
-Model selection
-K_{pw} values etc etc...
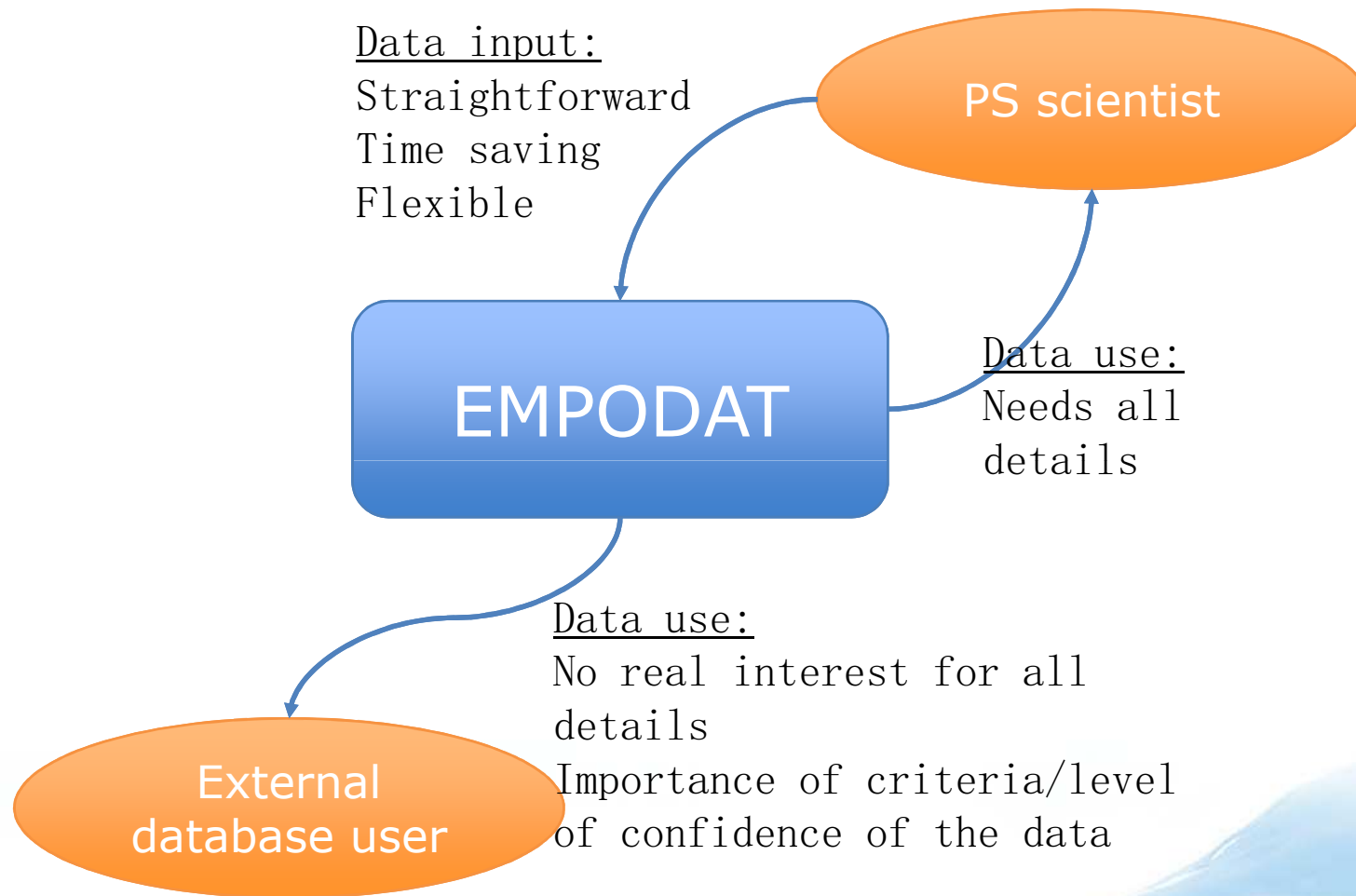
PS data acquisition for the JDS-3

Module for passive sampling

Data reporting	
Mass of contaminant of interest in exposed sampler (ng/sampler)	Need for system for linking contaminant/PRC data for exposed samplers to prep/field controls
Mass of contaminants in preparation blanks/controls	Drop down menu for contaminant, drop down menu for PRCs
Mass of contaminants in field blanks/controls	how do we report when replication is used?
Mass of PRCs in prep and field controls	
Mass of PRCs in exposed samplers	
Freely dissolved concentration of contaminant of interest in water (ng/L)	
Calculation of concentration in water	Different procedure for polar and hydrophobic samplers
For polar and ionised chemicals	
Sampling rates (Rs)	source? Publication, lab-based Rs, field-calibrated, Sampler assumed to be "insensitive to flow rate"
	Assumes linear uptake?
	Use of PRCs with polar samplers e.g. pocis? How are the PRCs used?
For hydrophobic compounds	
Polymer-water or sampler-water partition coefficients for contaminants	Source?, exact values, Do we need a database of published values (Smedes et al., 2009, Gilbert et al., 2016)
Polymer-water or sampler-water partition coefficients for PRCs	Source?, exact values
	if not available need to explain how values were obtained
	For very hydrophobic compounds (PBDEs), values not likely available
Model used to estimate in situ exchange kinetics from PRC dissipation?	Use of nonlinear least square method for sil or ldpe etc etc, 20:80
Use of equation to calculate concentration in water irrespective of how far the sampler is from	We need the ability to expand the list of possible models etc
	Perhaps user-based development (e.g. to add Ksw data into database…, adding new values as they emerge)
Possibility to correct data for temperature and salinity?	If temperature was recorded, how much did it deviate from 20 degC?
ref to report or publication	

Status of passive sampling and data availability

- Highest level of confidence for non-polar substances sampled with absorption-based passive samplers
  - Mostly for compounds not on the NORMAN list of emerging substances

- Lower level of confidence for polar samplers
  - Wider variety of sampler configuration
  - Need for flexibility: Possibility to «add» types of passive samplers?
  - More likely to have data available for input to EMPODAT

User-database interaction

Data input:
Straightforward
Time saving
Flexible

PS scientist

EMPODAT

Data use:
Needs all
details

External
database user

Data use:
No real interest for all
details
Importance of criteria/level
of confidence of the data

Final remarks

- ## A graphical user interface
  - Superimposing data from different monitoring tools to investigate spatial variations and trends in concentrations

- ## Ability to re-process the raw data at a later stage?
  - Standardisation
  - Availability of new/improved polymer calibration data and models for estimting sampling rates

- ## Same template for different databases?
  - National databases (e.g. http://vannmiljo.miljodirektoratet.no/), database at RECETOX, AQUAREF?, ICES database …
  - Requirement to transfer data to NORMAN after a certain period of time?