1. General Notes

These guidelines are based on a number of inputs to the EMODNET Chemical pilot project, which are acknowledged at the end of this document. It should be noted that to compare small amounts of chemical sample measurements in the same area, over time is a difficult exercise. The challenge of doing this for different instruments, with different techniques, from different institutes, over a much wider area is a challenge in order of magnitudes. This document is provided as a guideline only to demonstrate some of the basic principles that will need to be addressed in order to make the data in the EMODNET Portal as useful as possible.

This is a living document and will develop over the period of the project, so please check back for updates on a regular basis.

2. Data guidelines

I. General to all matrices

Missing Values

A number of data items in this manual are mandatory to report. We strongly recommend that the data centres adhere to this, however in cases where there are missing values the data record should still be included. This is because EMODNET should provide a comprehensive inventory of all data that has been collected, regardless of quality. It is however recommended that data records with incomplete information are appropriately flagged in the ODV data files.

Use of CAS numbers

There are many overlapping chemical synonyms, official corrections to CAS (Chemical Abstract Service) numbers by CAS, and errors for chemicals on some internet sites. Using CAS as a standard ensures traceability.

Intercalibrations

Participation in intercalibrations such as QUASIMEME should be a reoccurring exercise to ensure accreditation is achieved and maintained. Participation should be reported with the monitoring data.

Reference Materials

Running control charts should be standard procedure. Reporting the laboratory's standard value for a certified reference material enables assessors to evaluate the ability of the laboratory to determine the concentration in monitoring samples, especially when the laboratory does not take part in intercalibrations.

NOTE: OSPAR MIME has recently adopted a proposal to phase out the reporting of certified reference materials in favour of including the uncertainty of each value.

Uncertainty

Uncertainty of the value should be reported. If uncertainty is reported, then the method of calculation must also be reported.

Temporal accuracy

For historical data – where the dates were not accurately registered, it is acceptable to provide the value with no month or day. This should be flagged in the quality flag system.

Code lists

See section on Controlled Vocabularies
Data must comply with the accepted code lists and fields marked as mandatory must be supplied with legal values.

Cruise ID's

Must be unique within data reported by a distinct organisation for a specific dataset.

Basis (of determination)

Basis is mandatory for all organic and inorganic contaminants in sediment, seawater and biota. Note that basis forms a component of the P011 vocabulary.

The same basis and unit should be consistently reported for yearly trend series. Unit vs Basis are checked against year-1 submission to flag changes in reported Basis, which can influence the quality of trend analysis.

See also Basis Calculation conversion.

Depth

Depth of samples should be reported. If reported, lower depth cannot be greater than upper depth.

II. Meta-data requirements

Purpose of Monitoring

Purpose of monitoring is mandatory since not all types of monitoring samples can be combined in a trend series. For example, samples taken for a one-off research survey would be excluded from a 10 year temporal trend analysis. Therefore meta-data information is needed and will create a warning if not reported. See SeaDataNet vocabulary (C342) Monitoring activity rationale.

Station Names

This must be reported for monitoring data. Both OSPAR and HELCOM use the ICES Station Dictionary to control their meta-data information regarding stations. This allows the grouping of samples over a period of time for trend analysis. Although stations can in theory be identified by their coordinates, it is often very difficult to reconcile over a period of time due to station/species drift, changes to monitoring programme sampling procedures and other factors.

Sampling method and instrument

To ensure comparability, sampling method should be reported. In addition, the instrument of sampling must also be reported, see SeaDataNet list (L051) sample collector categories.

Method of Analysis

This must be reported. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Method of Filtration for trace metals

This must be reported for water column. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Method of chemical extraction

This must be reported for sediment data. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Limit of detection/limit of determination

Report the limit of detection for the parameter concerned according to the method of analysis used. The value must be reported in the units for the parameter concerned, and on the appropriate basis of determination.

The limit of detection, or LOD, is defined as that concentration of analyte which yields an analytical response equal to three times the standard deviation of the complete procedural blank - or a sample with a very low concentration of the analyte (as sometimes spiking is necessary in order for a response to be detectable).

III. Biota

Species

Species must match to the European Register of Marine Species (ERMS) or ITIS (Taxonomic Information System). Ordinarily, the taxonomic list that was used should be reported with the species.

Check maximum range for age, length and weight of species for outliers.

Number of Individuals

Number of individuals in a biota sample is mandatory. The number of individuals required to comprise a "sample" is/should be defined by the monitoring programme.

Length and Weight

Check length and weight parameter values reported for a whole organism against parameter values reported in their respective tissue. With shellfish, consistently report if the whole organism includes the shell.

Tissue

Reporting the tissue (or fraction of tissue) is mandatory. This is an element of the parameter in the SeaDataNet P011 vocabulary. When pooling tissue, report the number included.

IV. Water

Method of Filtration for trace metals

This must be reported for water column. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Suspended Particulate Matter (SPM)

When reporting metal concentration in suspended particulate matter, report the metal concentration on a dry weight basis and also report the total concentration of suspended matter.

V. Sediment

Method of chemical extraction

This must be reported for sediment data. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Grain Size

When reporting a metal concentration, it is mandatory to report the fraction analysed, i.e., the grain size of the fractionated sample. This is an element of the parameter in the SeaDataNet P011 vocabulary.

Normalisers

When reporting metals, the reporting of normalisers (organic carbon, aluminium) and dry weight % are also mandatory. See Normalisation.

3. Controlled Vocabularies

The SeaDataNet vocabularies will be the provider of lists and definitions for the EMODNET Chemical pilot.

VI. Parameters

Detailed parameters are defined in the SDN P011 list, and further mapping information is available on the EMODNET chemical extranet.

P021 list:
http://seadatanet.maris2.nl/v_bodc_vocab/search.asp?name=(P011)%20BODC+Parameter+Usage+Vocabulary&l=P011

EMODNET Chemical Parameter mapping:
http://nodc.ogs.trieste.it/emodoc/Parameter_mappings_P011.xls

Data submitters should note that the parameter defined in the P011 list is not a single entity but really a combination of elements, that together make up a parameter in this context. Simply explained:

[Measurement] + [Chemical] + [Unit] + [Matrix] + [Phase] + [Method] + =

P011 parameter term =

"Concentration of mercury (Hg) per unit dry weight of biota {Mytilus galloprovincialis (ITIS: 79456: WoRMS 140481) [Subcomponent: flesh]}"

NOTE: Data submitters should therefore take special care that the P011 terms they map to are correct and where necessary propose new terms to P011 to account for parameter combinations not already in existence. DO NOT MAP TO A 'NEAR' MATCH

Special care should be taken when reporting parameters expressed as ions, for example Tributyltin can be expressed as an ion (CAS 36643-28-4).

VII. Units

Units are defined in the SDN P061 list, the mapping of these units to the parameter grouping (P021) has been made available on the EMODNET chemical extranet.

P021 -> P061
http://nodc.ogs.trieste.it/emodoc/EMODNET_Parameter_Units_P021_P061new.xls

Parameters should be reported in the preferred unit selected for the EMODNET Chemical pilot. In cases where this is not possible, the original unit should be reported with supporting information, such as basis of determination (wet weight, dry weight) that will allow proper interpretation of the data.

4. Normalisation (by sampling matrix)

When attempting to assess the concentration of parameters from different geographical areas, it is essential that these data are comparable. Minimising the natural variation in time and space due to confounding factors is achieved via normalisation which can be done by various methods. Thus, when reporting contaminant data in environmental matrices it is critical to also report cofactor data and key method information to enable interpretation.

I. Sediment

When analysing parameters in sediment, concentrations should be expressed as dry matter or accompanied by dry weight content since the variable adhering water is not part of the sediment. The second equally or more important issue is that contaminants in sediments are primarily bound to the fine material and sand grains are essentially diluting the sample. The same concentration of a toxic compound in sandy sediment has a much higher risk than when sorbed to a clay-like sediment. Therefore it is a prerequisite to consider the composition of sediment with regard to the sorption capacity when assessing the quality of sediments on a spatial or time scale. This can be done by normalising the measured concentrations using cofactors that represent the properties of sediment in terms of uptake capacity. Cofactors that can be used are the aluminum or lithium content when it concerns heavy metals and organic carbon for organic contaminants.

Another widely used method is testing sediment samples of similar composition by removal of sand particles. Typically the sieved fraction of less than 63 or 20µm is analysed. The obtained fine fraction has a composition that varies much less in time and space than the original samples. In a spatial sense normalisation still compares apples and pears, but, without normalisation, apples and elephants are compared.

II. Biota

Concentrations in biological tissues can be expressed in several ways. In general, concentrations are expressed on fresh weight, dry weight or lipid weight. The basis is entirely dependent on the goal. For food consumption it makes perfect sense to express concentrations on a fresh weight basis as this is what is actually taken up by the consumer. Exposure of, for instance, marine mammals could also be approached in this fashion. Comparing environmental concentrations or performing trend analysis is an entirely different matter. In that case, one will try to limit the differences caused by factors that are inherent to tissues or species.

One major factor is the lipid content. Lipid contents may vary considerably within individuals of the same population and across populations. Contaminants, such as organic substances, are associated with lipids and one runs the risk of observing differences purely based on differences in the lipid content when concentrations are expressed on a fresh weight basis. If the objective is to assess the environmental status of a region, the evolution in time of contaminants or to compare the same species across different regions, it is absolutely essential that any variability or differences caused by a factor such as the lipid content is taken out of the picture.

Another example is the water content of shellfish, a parameter that tends to vary considerably due to the processing of shellfish samples. To compensate for this, shellfish contaminant data is generally expressed, for environmental purposes, on a dry weight basis. Finally, in any program a common policy regarding reporting units is essential and will be linked to the purpose of the program (health protection, trend analysis, environmental status assessment). Essential information such as the lipid content and dry weight content, should always accompany the data.

III. Water

Water concentrations may be reported as dissolved concentrations (filtered) or as total concentrations. This needs to be clearly defined for the sample and suspended matter content should also be reported to facilitate interpretation.

5. Acknowledgements

With thanks for guidance and input from:

ICES Marine Chemistry Working Group (MCWG)
http://www.ices.dk/workinggroups/ViewWorkingGroup.aspx?ID=20

OSPAR Monitoring and Assessment Group (OSPAR MON/MIME)
http://www.ospar.org/

SeaDataNet Technical Task Team
http://www.seadatanet.org/

HELCOM Monitoring and Assessment (MONAS)
http://www.helcom.fi/groups/monas/CombineManual/en_GB/Contents/

ICES Data Centre
http://www.ices.dk/datacentre

QUASIMEME
http://www.quasimeme.org/

Biological Effects Quality Assurance in Monitoring Programmes (BEQUALM
http://www.bequalm.org/QA_programme.htm

1. Basis calculation conversion

Logic for Fat Weight Percentage (FATWT%), Lipid weight percentage (LIPIDWT%) and Extractable-lipid percentage (EXLIP%).

If FATWT% is reported use else if LIPIDWT% is reported use it else if EXLIP% is reported use it. FATWT% and LIPIDWT% are comparable, but EXLIP% should have a lower priority.

Case 1: dry weight (D): metals, organotins, organochlorines and PAHs in bivalve soft body tissues

WHEN 'D' is reported THEN @VALUE

WHEN 'W' is reported THEN @VALUE*(100/DRYWT%)

(if DRYWT% is missing, NULL is reported)

WHEN 'L' is reported THEN VALUE*(FATWT%/DRYWT%)

(if FATWT% is missing, use LIPIDWT%, if LIPIDWT% is missing use EXLIP%, otherwise NULL)

Case 2: wet weight (W): metals and organochlorines, organotins in fish muscle and tail muscle (crustaceans), metals and organotins in fish liver

WHEN 'W' is reported THEN @VALUE

WHEN 'L' is reported THEN @VALUE*(FATWT%/100)

(if FATWT% is missing, use LIPIDWT%,if LIPIDWT% is missing use EXLIP%, otherwise NULL)

WHEN 'D' is reported THEN @VALUE*(DRYWT%/100)

Case 3: lipid weight (L): organochlorines in fish liver

WHEN 'L' is reported THEN @VALUE

WHEN 'W' is reported THEN @VALUE*(100/FATWT%)

(if FATWT% is missing, use LIPIDWT%,if LIPIDWT% is missing use EXLIP%, otherwise NULL)

WHEN 'D' is reported THEN @VALUE*(DRYWT%/FATWT%)

(If FATWT% is missing,use LIPIDWT%,if LIPIDWT% is missing use EXLIP%, otherwise NULL)

2. Document Version History

21 May 2010

V1.1 First version developed by ICES released to EMODNET Chemical Portal

3 June 2010

V1.2

- New text under 3.VII Units
- Added new text concerning missing values under 2. I