EMODnet
European Marine Observation and Data Network

Your gateway to marine data in Europe

EMODnet Chemistry: Open and trusted data, products, and services for understanding the evolution of marine water quality

Ocean Best Practices Workshop
October 2023

M. A. French
C. Altobelli
A. Giorgetti
E. Kubin
M. Lipizer
M. E. Molina Jack

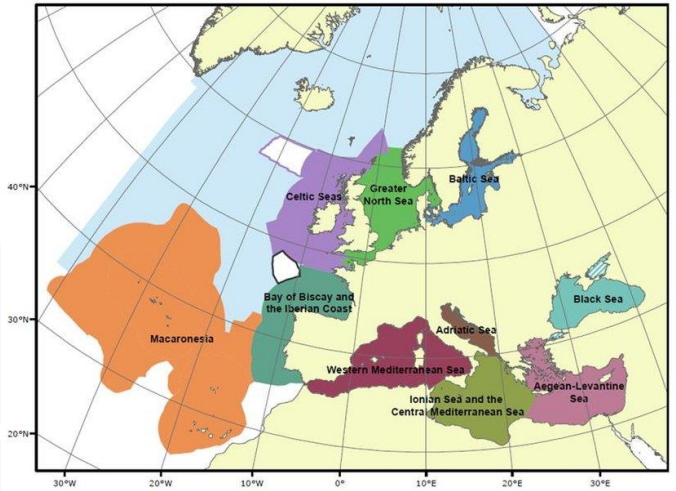
OGS

The European Marine Observation and Data Network (EMODnet) is financed by the European Union under Regulation (EU) No 508/2014 of the European Parliament and of the Council of 15 May 2014 on the European Maritime and Fisheries Fund.

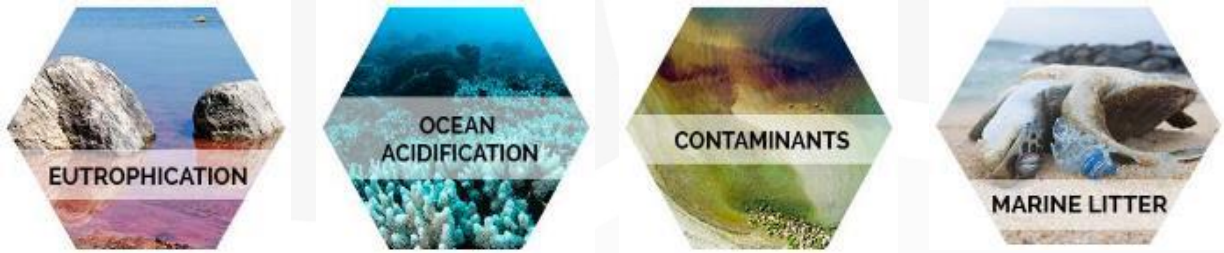
EMODnet Chemistry

The European Marine Observation and Data Network (EMODnet) has 7 themes:

- Bathymetry
- Biology
- **Chemistry**
- Geology
- Human Activities
- Physics
- Seabed Habitats.



EMODnet Chemistry: goal of facilitating the discoverability, accessibility, and usability of marine chemical datasets and derived data products on:



Contributing to descriptors:

- 5 (eutrophication),
- 8 (chemical pollution),
- 9 (contaminants in seafood), and
- 10 (marine litter)

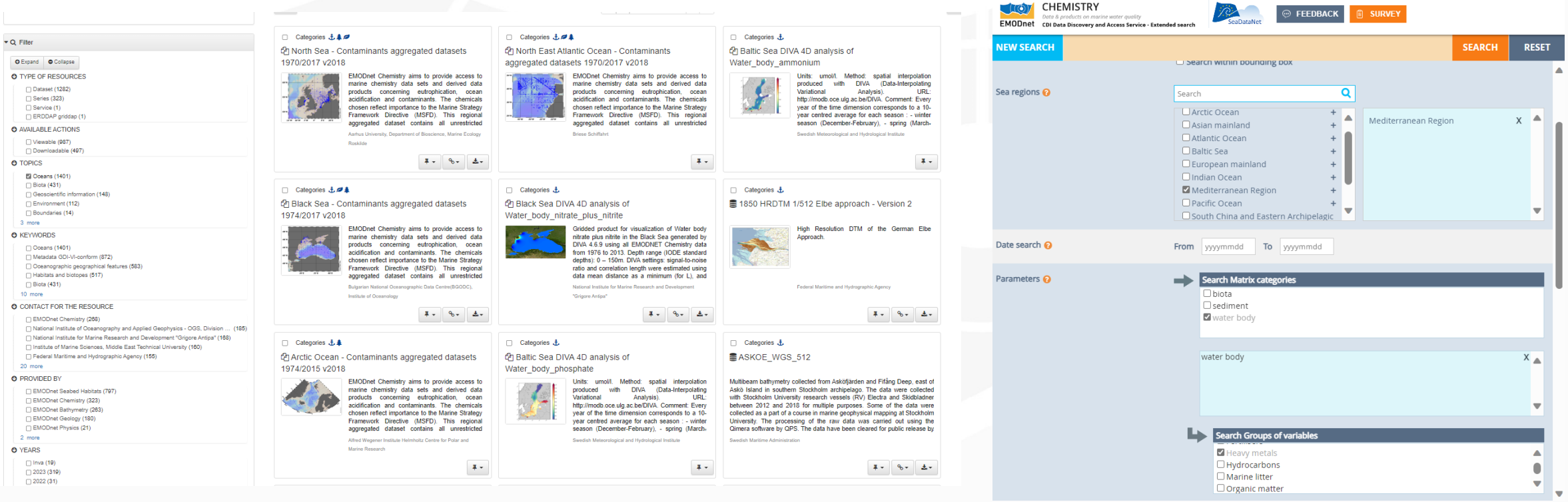
of the **Marine Strategy Framework Directive** (MSFD)

Datasets and data products

A huge amount of complex and heterogeneous data corresponding to:

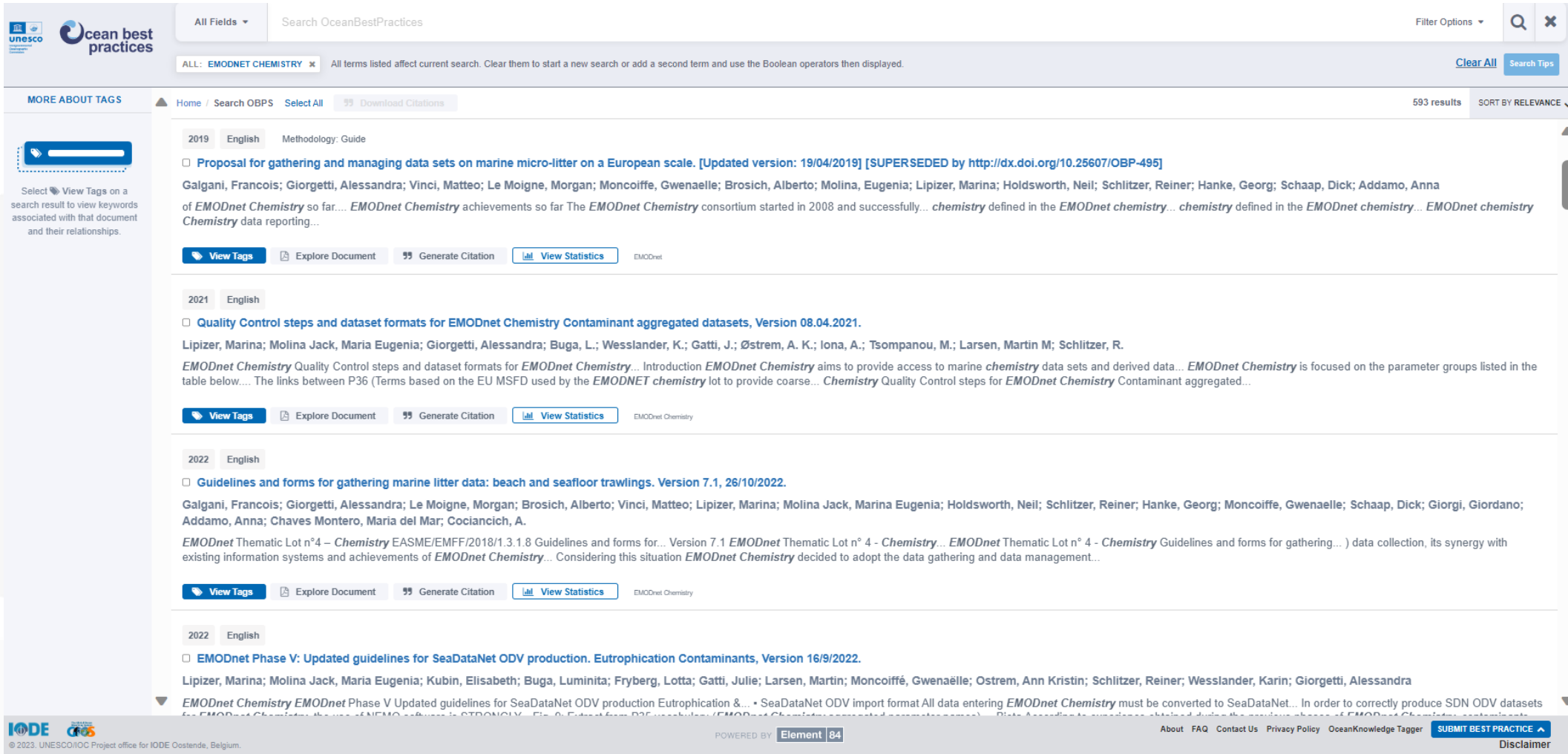
- seawater,
- biota, and
- sediment are managed to prepare:

Standardised, harmonised, and quality-controlled **data collections** and derived **data products** on marine water quality

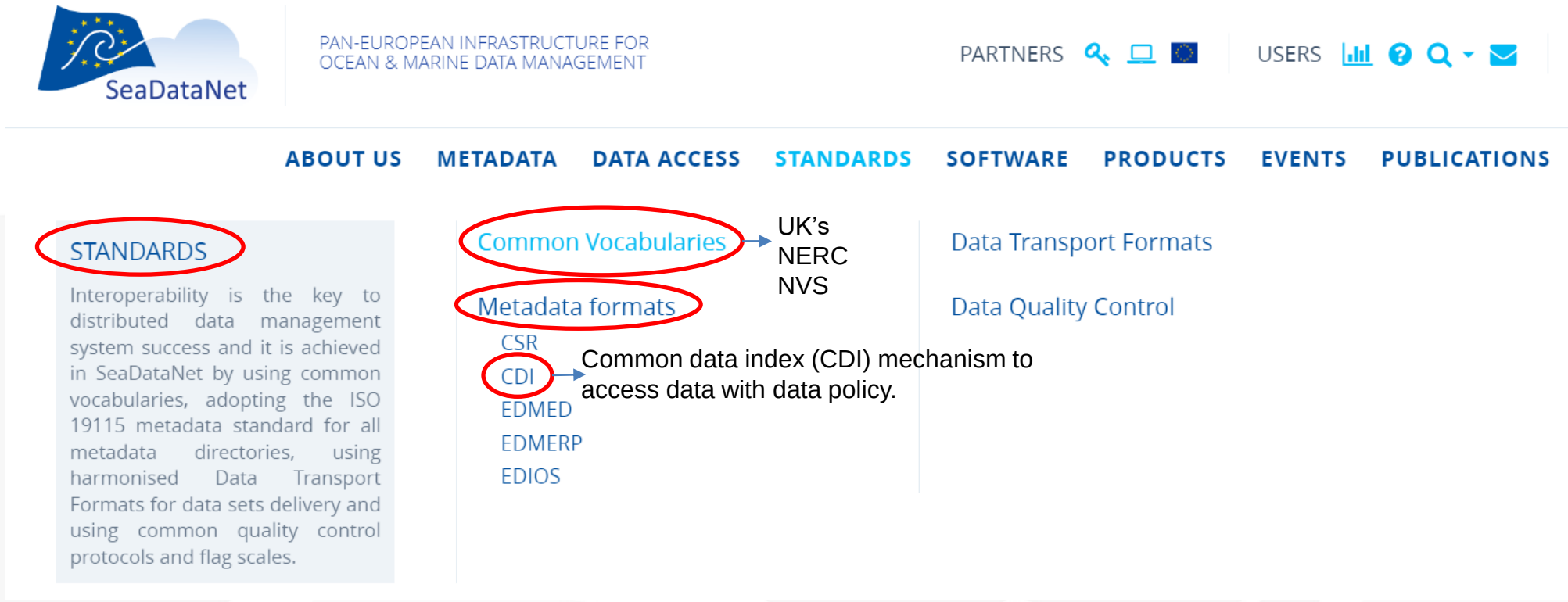


Data preparation and validation

OBP repository contains **guideline documents** on data preparation and quality control procedures for contaminants, eutrophication, acidification, and marine litter



Data preparation



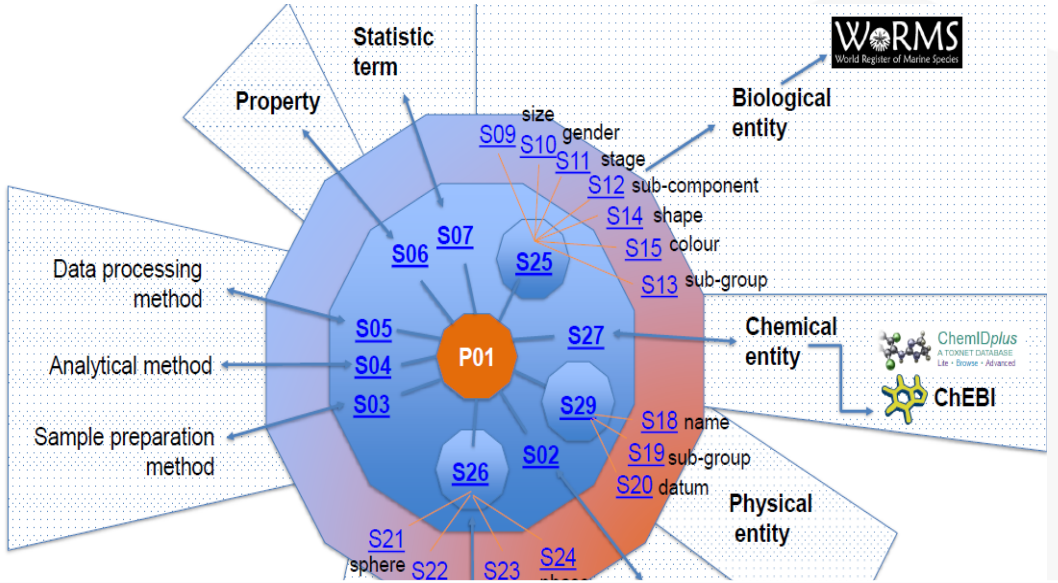
Software tools are also used for metadata and data formatting, data exchange, and visualisation.

NERC Vocabulary Server (NVS)

Common vocabularies for the metadata fields of a dataset include:

- L05 codes (device categories, e.g., CTD),
- L06 codes (platform categories, e.g., research vessel), and
- P02 (parameter discovery vocabulary)

P01 codes describe information associated with a sample and are comprised of other vocabularies:

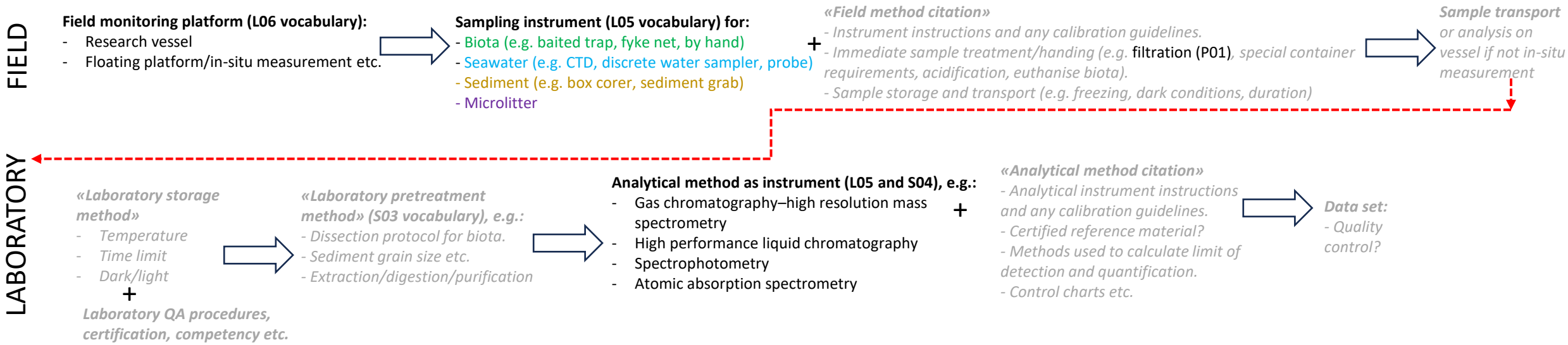


PBXXICP2	Concentration of lead {Pb CAS 7439-92-1} per unit volume of the water body [particulate >0.4/0.45um phase] by acid leaching of filter residue and inductively-coupled plasma mass spectrometry
PBUFICXX	Concentration of lead {Pb CAS 7439-92-1} per unit volume of the water body [dissolved plus reactive particulate phase] by acidification and inductively-coupled plasma mass spectrometry
MTWD0046	Concentration of lead {Pb CAS 7439-92-1} per unit volume of the water body [dissolved plus reactive particulate <0.4/0.45um phase]
PBUFWC02	Concentration of lead {Pb CAS 7439-92-1} per unit volume of the water body [dissolved plus reactive particulate phase]

Data flow

Considerable **data flow** has implications for harmonisation and quality control procedures owing to **differences in methods and discrepancies between the supporting information** that is collected (or lost).

This data flow starts with the collection of samples in the field to which relevant vocabulary can be assigned…


FIELD
Field monitoring platform (L06 vocabulary):
- Research vessel
- Floating platform/in-situ measurement etc.
Sampling instrument (L05 vocabulary) for:
- Biota (e.g. baited trap, fyke net, by hand)
- Seawater (e.g. CTD, discrete water sampler, probe)
- Sediment (e.g. box corer, sediment grab)
- Microlitter
+
«Field method citation»
- Instrument instructions and any calibration guidelines.
- Immediate sample treatment/handing (e.g. filtration (P01), special container requirements, acidification, euthanise biota).
- Sample storage and transport (e.g. freezing, dark conditions, duration)
Sample transport or analysis on vessel if not in-situ measurement
LABORATORY
«Laboratory storage method»
- Temperature
- Time limit
- Dark/light
+
Laboratory QA procedures, certification, competency etc.
«Laboratory pretreatment method» (S03 vocabulary), e.g.:
- Dissection protocol for biota.
- Sediment grain size etc.
- Extraction/digestion/purification
Analytical method as instrument (L05 and S04), e.g.:
- Gas chromatography–high resolution mass spectrometry
- High performance liquid chromatography
- Spectrophotometry
- Atomic absorption spectrometry
+
«Analytical method citation»
- Analytical instrument instructions and any calibration guidelines.
- Certified reference material?
- Methods used to calculate limit of detection and quantification.
- Control charts etc.
Data set:
- Quality control?

Addressing gaps

To improve:

- transparency in data quality,
- reliability, and
- comparability,

a new element was recently incorporated into the data flow process:

a “**questionnaire**” that provides a **record of field and laboratory information** for the chemical parameters submitted by a data originator.

Developed based on a comparison of **non-sample specific terms** in the **data collection templates** of:

- UNEP/MAP MEDPOL,
- ICES (for OSPAR and HELCOM),
- WISE-6,
- JRC (for the Water Framework Directive, WFD), and
- NORMAN Network for emerging contaminants.

Questionnaires

Cover sheet - general questions on laboratory proficiency and quality assurance (QA)

Worksheets - biota, seawater, and sediment - field and laboratory information inserted for each chemical parameter using drop down lists.

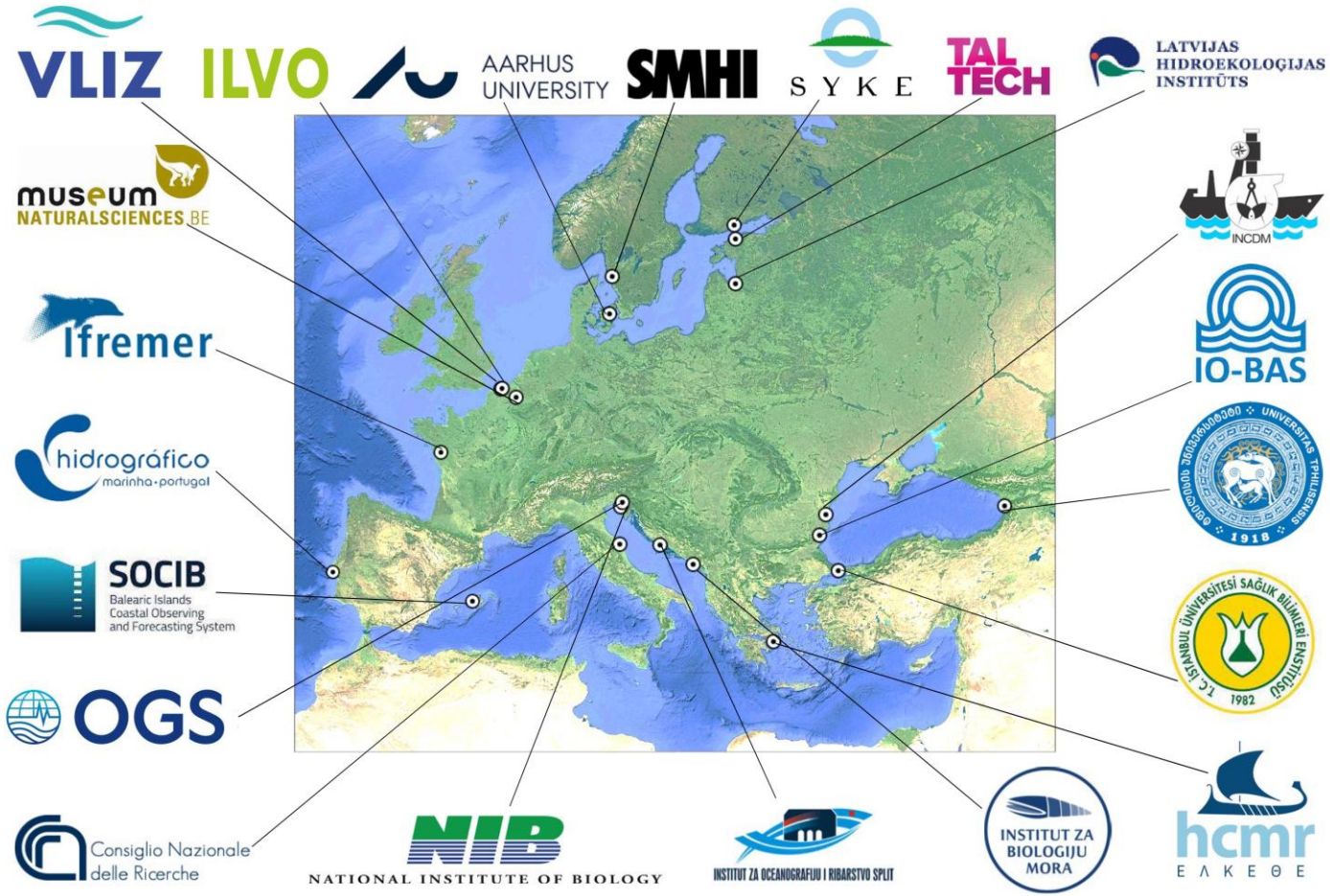
Y4 | fx filtration, incubation

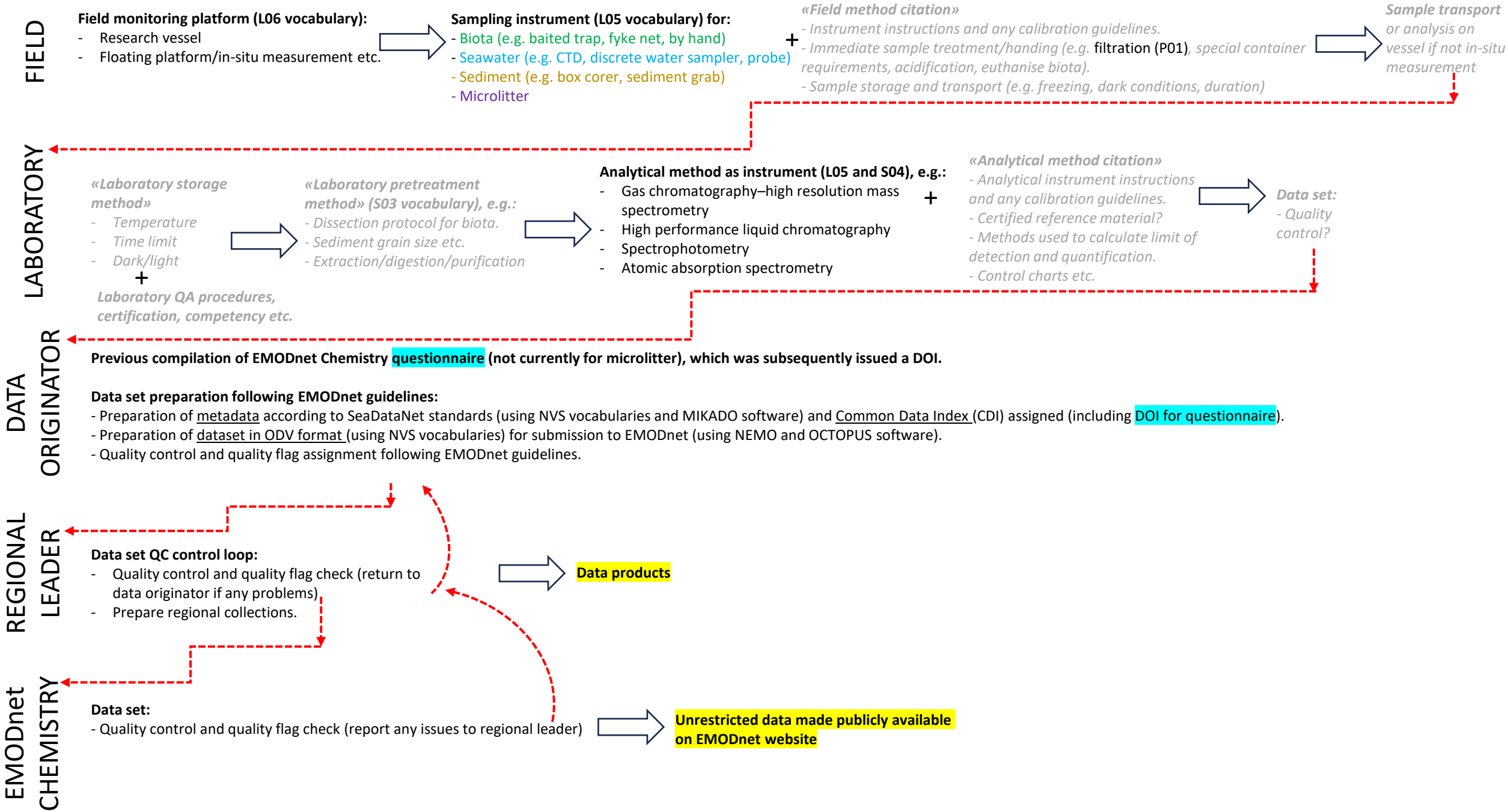
	Y	Z	AA	AB	AC	AD	AE
1	http://vocab.nerc.ac.uk/search_nvs/	Autolink unless	http://vocab.nerc.ac.uk/search_	Autolink unless	If available, insert a	Select yes or	Insert a relevant protocol if the analytical
2	Select from the drop-down list (definitions are provided on the worksheet 'main S03 sample		Select the analytical method from the drop-down list or search the		citation for the	no from the	method has been validated according to it
3	**Sample preparation (pre-treatment/extraction/digestion)**	**S03 code**	**Analytical method**	**S04 code**	**Analytical method citation**	**Is a standardised analytical method used?**	**Protocol used to validate analytical method**
4	filtration, incubation	S03107	fluorometry	S04185	Lorenzen C, Jeffrey	Yes	ISPRA, SIBM (2010) Metodologie di studio
5	filtration	S0393	Colorimetric analysis	S04136	Hansen, H.P.,	Yes	GO-SHIP Repeat Hydrography Nutrient
6	filtration	S0393	Colorimetric analysis	S04136	Hansen, H.P.,	Yes	GO-SHIP Repeat Hydrography Nutrient
7	filtration, persulphate oxidation	#N/A	Colorimetric analysis	S04136		Yes	ISPRA, SIBM (2010) Metodologie di studio
8	filtration	S0393	Colorimetric analysis	S04136	Hansen, H.P.,	Yes	GO-SHIP Repeat Hydrography Nutrient
9	filtration, persulphate oxidation	#N/A	Colorimetric analysis	S04136		Yes	ISPRA, SIBM (2010) Metodologie di studio
10		#N/A		#N/A			
11		#N/A		#N/A			
12		#N/A		#N/A			
13		#N/A		#N/A			
14		#N/A		#N/A			
15		#N/A		#N/A			
16		#N/A		#N/A			
17		#N/A		#N/A			
18		#N/A		#N/A			
19		#N/A		#N/A			

Questionnaires

Questionnaires were collected from 63 laboratories associated with 21 institutes.

- each was assigned a DOI that is included in the CDI record for data submissions.

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- Analytical instrument instructions and any calibration guidelines.
- Certified reference material?
- Methods used to calculate limit of detection and quantification.
- Control charts etc.
Data set:
- Quality control?
DATA ORIGINATOR
Previous compilation of EMODnet Chemistry questionnaire (not currently for microlitter), which was subsequently issued a DOI.
Data set preparation following EMODnet guidelines:
- Preparation of metadata according to SeaDataNet standards (using NVS vocabularies and MIKADO software) and Common Data Index (CDI) assigned (including DOI for questionnaire).
- Preparation of dataset in ODV format (using NVS vocabularies) for submission to EMODnet (using NEMO and OCTOPUS software).
- Quality control and quality flag assignment following EMODnet guidelines.
REGIONAL LEADER
Data set QC control loop:
- Quality control and quality flag check (return to data originator if any problems)
- Prepare regional collections.
Data products
EMODnet CHEMISTRY
Data set:
- Quality control and quality flag check (report any issues to regional leader)
Unrestricted data made publicly available on EMODnet website

Closing remarks

- **EMODnet Chemistry** facilitates the accessibility of chemical **data collections** and derived **data products**
- **Data flow** has implications for harmonisation and quality control procedures
- Addressing gaps - fundamental to improve **transparency in data quality**, reliability, comparability
- Ultimate aim: to obtain open and trusted data and data products on marine water quality to support **harmonised environmental status assessment**
- For more information on the development and results of the questionnaire – a paper titled "**Improving data reliability to support marine pollution assessment according to MSFD Descriptor 8 in the European Seas: the contribution of EMODnet Chemistry**" will be published soon in Frontiers in Marine Pollution.

Thank you!

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