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Improving data reliability to support marine pollution assessment according to MSFD Descriptor 8 in the European Seas: the contribution of EMODnet Chemistry

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Introduction: According to the Marine Strategy Framework Directive (MSFD, 2008/56/EC), member states of the European Union (EU) had to develop a common approach in environmental monitoring and assessment. Regarding marine pollution assessments, large heterogeneities remain regarding sampling protocols, analytical methods, and quality assurance (QA) and quality control (QC) procedures. Further, data availability for Descriptor 8 (contaminants) was very fragmented in the first cycle of the MSFD. As one of the major EU spatial data infrastructures for providing access to marine data, EMODnet Chemistry has endeavoured to overcome data fragmentation and increase data 'FAIRness' (findable, accessible, interoperable, and reusable).

Methods: Aiming to improve the reliability of marine contaminant data for assessment purposes under the MSFD, detailed QA/QC information was collected using a questionnaire based on the requirements of the European Environment Agency, International Council for the Exploration of the Sea, United Nations Environment Program–Mediterranean Action Plan, and NORMAN Network. The questionnaire was distributed to institutions in 26 countries participating in EMODnet Chemistry.

Results: Information was received from 18 countries on ~90% of the substances included in EU legislation on priority substances. The results indicate an overall good level of laboratory proficiency; however, heterogeneities were observed in sampling protocols (especially for biota) and analytical methods (e.g. for metals), suggesting the potential for increased harmonisation. While laboratory proficiency and equipment depend on institutional resources that may differ among countries, it is fundamental to share detailed QA/QC information associated with data to improve data reliability and re-usability, and to support marine pollution assessment.

Discussion: Enriching data with required metadata and detailed QA/QC is part of the data curation process, which is still an overlooked aspect of the overall scientific research process and is crucial to support a reliable assessment of marine pollution, and ultimately better management of the marine environment.

KEYWORDS

marine pollution, quality control, metadata template, heterogeneous data, Marine Strategy Framework Directive, Regional Sea Conventions, data curation

1 Introduction

Under the Water Framework Directive (WFD, 2000/60/EC) (European Commission, 2000) and Marine Strategy Framework Directive (MSFD, 2008/56/EC) (European Commission, 2008) of the European Union (EU), member states must take measures to maintain or achieve ‘good environmental and ecological status’ (GES) in the European seas. The MSFD, in particular, involves regular assessments of the marine environment, setting objectives and targets for reaching GES, establishing monitoring programmes, and putting in place measures to improve the state of marine waters. The MSFD sets out 11 descriptive indicators that are then articulated in a set of assessment criteria and associated indicators that are used to assess environmental status. In addition, the Barcelona Convention (Mediterranean Sea), Bucharest Convention (Black Sea), Helsinki Convention (HELCOM, Baltic Sea), and OSPAR Convention (North-East Atlantic) have protocols, strategic action plans, and monitoring/assessment programs in place to protect these regional seas against pollution (OSPAR Convention, 1992; Black Sea Commission, 2009; United Nations Environment Programme, 2019; Baltic Marine Environment Protection Commission, 2021). Following the implementation of the MSFD in 2008, member states had to develop and follow a common approach in environmental monitoring and assessment at the level of a given marine region or sub-region. Regarding chemical pollution, as an amendment to the WFD and MSFD, Directive 2013/39/EU on priority substances in the field of water policy (European Commission, 2013) sets the environmental quality standards for priority substances, such as heavy metals (e.g. mercury), polycyclic aromatic hydrocarbons (e.g. benzo[a]pyrene), dioxins and dioxin-

like compounds, brominated diphenylethers, and pesticides (e.g. heptachlor) in water and biota. In 2017, Commission Decision (EU) 2017/848 (European Commission, 2017) laid down the criteria and methodological standards on GES for marine waters and provided the specifications and standardised methods for monitoring and assessment. Despite progress in legislation, it has been reported that the degree of coherence with respect to implementing the requirements of the aforementioned directives and protocols is still relatively low (United Nations Environment Programme/Coordinating Unit for the Mediterranean Action Plan, 2017; Tornero Alvarez and Hanke, 2018; Gorjanc et al., 2020).

The assessment of marine pollution at regional and sub-regional scales required by the MSFD and Regional Sea Conventions (RSCs) follows a 6-year cycle (MSFD, 2008/56/EC) and implies the use of data collected by multiple sources. These data may be heterogeneous with respect to sampling protocols, analytical methods, laboratory proficiency, and quality assurance (QA) and quality control (QC) procedures. For several countries, availability of harmonised, comparable, and accessible data and information was an issue of great concern in the first reporting cycle of the MSFD and for the Quality Status Reports, especially for the Mediterranean and Black seas (Gonzalez Fernandez et al., 2014; United Nations Environment Programme/Coordinating Unit for the Mediterranean Action Plan, 2017; Commission on the Protection of the Black Sea Against Pollution, 2019; Lipizer et al., 2021).

In terms of ocean data management, the adoption of the ‘findable, accessible, interoperable, and reusable’ (FAIR) principles (Wilkinson et al., 2016) has led to considerable improvements in data infrastructures and data sharing (Tanhua et al., 2019). Although the use of common metadata sets, common data/metadata formats, and standard vocabularies aims to guarantee interoperability (Vinci et al., 2017; Giorgetti et al., 2020), pollution data for the marine environment are often incomparable and unsuitable for regional/sub-regional assessments owing to the use of different sampling methods, pre-treatment, analytical techniques, and QA/QC procedures, and/or to limited information on QA/QC (Molina Jack et al., 2020). Lack of information or inadequate QA/

Abbreviations: BODC, British Oceanographic Data Centre; DOI, Digital object identifier; EEA, European Environment Agency; EMODnet, European Marine Observation and Data Network; EU, European Union; EU DG ENV, EU Commission Directorate-General for the Environment; FAIR, Findable, accessible, interoperable, and reusable; GES, Good environmental and ecological status; HELCOM, Helsinki Convention; ICES, International Council for the Exploration of the Sea; LoD, Limit of detection; LoQ, Limit of quantification; MSFD, Marine Strategy Framework Directive; NVS, National Environment Research Council (NERC) Vocabulary Server; QA/QC, Quality assurance/quality control; RSCs, Regional Sea Conventions; UNEP-MAP, United Nations Environment Program-Mediterranean Action Plan; WFD, Water Framework Directive.

1 <https://emodnet.ec.europa.eu/en>.

2 [SeaDataNet - SeaDataNet](#).

QC can also mean that data quality is compromised. For instance, based on a comparison between sampling, analytical, and QA protocols adopted by laboratories in the region of the Adriatic and Ionian seas, Berto et al. (Berto et al., 2020) observed that heavy metal data were highly heterogeneous, highlighting the need to develop common and harmonised protocols for monitoring procedures to be applied for the assessment of GES.

The European Marine Observation and Data Network (EMODnet¹) was setup in 2009 as part of the Blue Growth strategy (European Commission, 2012) to ensure that European marine data across seven discipline-based themes (bathymetry, biology, chemistry, geology, seabed habitats, human activities, and physics) are easily accessible, interoperable, and free from restrictions on use (Martín Míguez et al., 2019). EMODnet Chemistry is the spatial data infrastructure responsible for providing access to marine chemical data (eutrophication, ocean acidification, contaminant, and marine litter data) (Giorgetti et al., 2018). EMODnet Chemistry adopts the FAIR principles and relies on standards, which were established through SeaDataNet², a Pan-European infrastructure for ocean and marine data management (Schaap and Lowry, 2010). EMODnet Chemistry (phase V, 2021–2023) currently involves more than 30 marine research and monitoring institutes and oceanographic data management experts from 26 countries. Data derive from inputs gathered and collated from national monitoring efforts and research activities from all European coastal states (Giorgetti et al., 2018).

Before EMODnet Chemistry was setup, data availability for Descriptor 8 (contaminants) and Descriptor 9 (contaminants in seafood) of the MSFD was very fragmented. Accordingly, efforts have been made within EMODnet Chemistry to i) overcome data fragmentation among institutes; ii) standardise systems to make data 'FAIR'; iii) harmonise vocabulary (from the National Environment Research Council (NERC, United Kingdom) Vocabulary Server, NVS³), parameter units, metadata profiles, and dataset formats; iv) identify similar sampling/analytical protocols and common target species between data originators; and v) develop data validation and QC procedures/guidelines. Despite the need to further improve data reliability and comparability (e.g. via thorough and uniform QC procedures by data originators), much progress has been made and EMODnet Chemistry offers the potential to instil a more harmonised approach among institutes, ultimately leading to a data repository that contains dependable and useful information.

In addition to sample-specific metadata (e.g. sample time and location), contaminant data should be associated with comprehensive information on the sampling/analytical methods and QA/QC procedures performed by data originators (i.e. different laboratories). This information is required for further QC checks performed by data management infrastructures (e.g. EMODnet) and is also useful for comparing data from different institutes. Detailed metadata reporting templates to obtain both sample-specific and general information on contaminant measurements

in the marine environment have been created by the 1) EU Commission Directorate-General for the Environment (EU DG ENV) (with respect to reporting for the WFD)/European Environment Agency (EEA) (with respect to reporting on the state of the environment) (EIONET data dictionary, https://dd.eionet.europa.eu/datasets/latest/WISE-SoE_WaterQualityICM/tables/DisaggregatedData), 2) International Council for the Exploration of the Sea (ICES) (relating to the OSPAR/Helsinki conventions) (International Council for the Exploration of the Sea, 2015), 3) United Nations Environment Program–Mediterranean Action Plan (UNEP–MAP) (relating to the Barcelona Convention) (United Nations Environment Programme, 2021), and 4) NORMAN Network for emerging contaminants (<https://www.norman-network.com/nds/empodat/downloadDCT.php>). With the development of EMODnet Chemistry, there has been an emphasis on attempting to align efforts with these organisations, including the supporting information that is collected with contaminant data.

A first set of QA/QC information was collected from institutes participating in EMODnet Chemistry in 2014 using a questionnaire proposed by the Italian Institute for Environmental Protection and Research to obtain information on sampling/analytical methods and QA/QC procedures for contaminants. The questionnaire was pursuant to ISO 17025:2005 ('General requirements for the competence of testing and calibrating laboratories'), which was, however, updated in 2017 (International Organization for Standardization, 2017). Considering the abovementioned factors along with the increase in data requested for GES assessment, an update/revision of the questionnaire was also needed to improve harmonisation of information and alignment with other initiatives dealing with marine pollution data, ultimately to support the FAIR data principles. With the aims of i) improving the reliability of marine contaminant data for the purpose of GES assessment under the MSFD (i.e. by collecting standardised and harmonised information following consolidated international procedures), ii) identifying improvements to facilitate the FAIR principles and support the implementation of the MSFD, and iii) highlighting the heterogeneities in sampling and analytical methods used by different EU member states, a new EMODnet Chemistry questionnaire was prepared, sent out to participants, and analysed in this study to obtain comprehensive up to date information. First, priorities for non-sample-specific metadata fields in a revised questionnaire (pertaining to contaminants in seawater, sediment, and biota) were determined by comparing the metadata required in the aforementioned data collection templates of the EU DG ENV/EEA, ICES, UNEP–MAP, and NORMAN Network. Then, a revised EMODnet Chemistry questionnaire relating to non-sample-specific metadata fields was created and sent out to participants. The completed questionnaires were subsequently assigned digital object identifiers (DOIs) for use in data submissions to EMODnet Chemistry. Finally, the information from the questionnaires was merged and analysed to determine the main field sampling methods and analytical techniques used for different contaminants to observe differences between laboratories and highlight the importance of having such reference information associated with data.

³ NVS (nerc.ac.uk).

2 Materials and methods

To take account of practices already adopted by European and global frameworks, including the EEA (https://dd.eionet.europa.eu/datasets/latest/WISE-SoE_WaterQualityICM/tables/DisaggregatedData), ICES (*International Council for the Exploration of the Sea, 2015*) (i.e. the data management infrastructure for the RSCs of the Baltic Sea (HELCOM) and North East Atlantic Ocean (OSPAR)), UNEP-MAP (*United Nations Environment Programme, 2021*), and NORMAN (the global network of reference laboratories for the monitoring of emerging environmental substances; <https://www.norman-network.com/nds/empodat/downloadDCT.php>), documents detailing the metadata requirements (pertaining to reporting on contaminants in water, sediment, and biota) of these organisations were collected and compared. The metadata requirements listed in these different documents were merged and organised to distinguish those i) related to water, sediment, and/or biota, and ii) regarded as mandatory, recommended, or optional by the given organisation. Metadata specific to data on litter or rivers/lakes/reservoirs/groundwater, which are outside the scope of this analysis, and generic metadata fields (e.g. 'other') were excluded. To facilitate comparison, metadata fields that had the same or similar labels (i.e. different wording) among organisations were identified, assigned a rephrased metadata term for consistency/comparison, and sorted into groups. Thus, the comparison among metadata requested by the different communities was carried out through a harmonised list and the metadata terms were subsequently ranked first by the number of organisations requiring that information, and then by whether the field was mandatory, recommended, or optional. Finally, the metadata terms referring to non-sample-specific information were highlighted in bold (*Table S1*).

Based on the above evaluation, a questionnaire was developed to collect information regarding laboratory proficiency, QA protocols, and sampling and analytical procedures from data centres contributing contaminant data to the EMODnet Chemistry marine data management infrastructure. Non-sample-specific metadata fields required by three or four organisations were set as mandatory, while others were set as either mandatory or optional. To facilitate the collection of harmonised information and support compilation, searchable drop-down lists (manual input required when the option was not listed) were included for certain fields. Whenever possible, drop-down lists contained standardised options based on the descriptions/full terms of the vocabularies implemented by the British Oceanographic Data Centre (BODC) as part of the NERC vocabulary server (NVS, e.g. P36 codes for the EMODnet Chemistry chemical target groups, S27 codes for chemical substances, and S04 codes for analytical methods) and adopted by the Pan-European infrastructure for ocean and marine data management (SeaDataNet). The use of consolidated standard vocabularies supports coherence among the metadata and data managed by EMODnet Chemistry. Use of the full terms or descriptions of the NVS vocabularies in the drop-down lists aimed to identify gaps in the current vocabulary (e.g. analytical methods not yet coded) to improve the system.

The questionnaire was sent out to 32 scientific institutions and marine monitoring laboratories in 26 European and neighbouring

countries, who represent all of the current institutes contributing contaminant data to EMODnet Chemistry. The questionnaire was sent out via email to the list of contact people of the EMODnet Chemistry network, and these people then forwarded the questionnaires to the laboratory responsible for analysing contaminant data. The compilation of the questionnaire was not mandatory as this was considered an initial phase to ascertain the feasibility of establishing it as a mandatory part of data submissions in the future. As part of EMODnet's long term strategy of providing access to reliable and accurate data, information on methodological protocols and QA/QC needs to be regularly and systematically updated and made available with contaminant data.

3 Results

3.1 Questionnaire template

Based on the prioritised metadata fields from the templates of the EU DG ENV/EEA, ICES, UNEP-MAP, and NORMAN Network (*Table S1*), it was found that 19 metadata fields were required by all 4 organisations, of which 10 were mandatory for all 4 organisations. In contrast, 11 and 30 metadata fields were required by 3 and 2 organisations, respectively. Of these 60 metadata fields, 26 fields (9 for 4 organisations, 4 for 3 organisations, and 13 for 2 organisations) referred to non-sample specific information (e.g. country of reporting organisation and analytical methods used for a given determinand) (*Table S2*).

The questionnaire designed according to the above-mentioned comparison included 65 non-sample-specific metadata fields (9, 4, 13, and 12 fields required by 4, 3, 2, and 1 organisation/s, respectively, plus 27 new fields): 14 related to general laboratory procedure/QA information (collected on the coversheet) and 51 related to each matrix (water, sediment, and biota) in separate sections to obtain comprehensive up to date information from institutes participating in EMODnet Chemistry. *Figure 1* displays examples of the metadata fields included on the coversheet and in the seawater section of the questionnaire, and *Table S3* lists the transposed fields from the seawater, biota, and sediment sections.

3.2 Questionnaire responses

3.2.1 Number and completeness of responses

Forty-two questionnaires were received from 21 institutes (18 countries, *Figure 2*) participating in EMODnet Chemistry (summarised in *Table S4*), which corresponds to a response rate of 66% (i.e. 21/32). As it was not mandatory to complete the questionnaire, this response rate was deemed relatively high, especially considering the time and effort required for its compilation and that institutes do not have the same resources available. Each questionnaire was assigned a DOI to facilitate permanent access of this information. Some institutes included information referring to several laboratories within the same questionnaire; therefore, information was collected from a total of 64 single laboratories, with 46 laboratories providing information

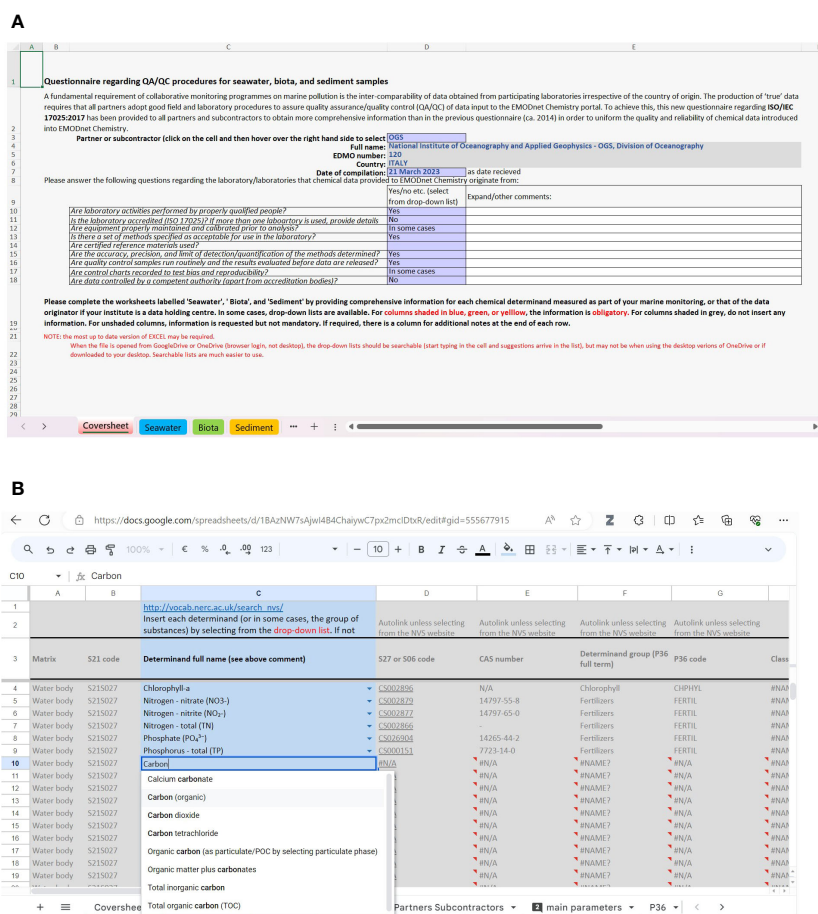


FIGURE 1 Examples of the metadata fields in the questionnaire to obtain non-sample-specific information on contaminants from institutes participating in EMODnet Chemistry. (A) Coversheet completed by OGS and (B) part of the seawater section.

on the seawater matrix, 24 on the biota matrix, and 26 on the sediment matrix (Table S4).

In general, many of the non-auto-filled optional/non-mandatory fields for the seawater, biota, and sediment sections were not completed, which prevented collection of relevant information such as the analytical method citation and the type of reference material used. In addition, some mandatory fields were not completed, especially regarding the actual limit of detection (LoD) and limit of quantification (LoQ) and the method/formula used to determine the LoQ. To highlight the main similarities and differences between EMODnet Chemistry participants with respect to contaminant metadata, the results presented in this section focus on the general laboratory QA information, determinands reported, and field sampling and analytical methods reported, which were completed in all or most cases.

3.2.2 General laboratory QA information

Table 1 summarises the responses to nine QA questions. The comparison indicates that QA procedures are more consolidated and adopted for the analysis of seawater (adopted by 47.8–100% of

laboratories) and sediment (38.5–100%) compared with biota (37.5–87.5%). Despite the variability among the different laboratories, the QA practices reflect an overall good level of proficiency: >87% of respondents reported that laboratory activities are performed by qualified staff and that equipment is properly maintained and calibrated prior to analysis; at least 83% of laboratories have a set of methods specified as acceptable and determine the accuracy, precision, and LoD/LoQ associated with analytical methods; 75.0–84.8% of laboratories routinely run quality control samples; 61.5–75.0% of laboratories record control charts to test bias and reproducibility; >50% of laboratories use certified reference materials; >47% of laboratories are ISO 17025 accredited; and 37.5–47.8% of laboratories have their concentration data controlled by a competent authority.

3.2.3 Determinands reported for seawater, sediment, and biota

Table 2 lists the number of determinands reported in the questionnaires grouped by EMODnet Chemistry target groups (P36 codes, BODC vocabulary). Overall, 395 individual



determinands were reported for all matrices (141 for seawater, 284 for sediment, and 232 for biota), which included approximately 90% of the substances included in Directive 2013/39/EU on priority

substances in the field of water policy. Of the 395 determinands reported, >50% were either hydrocarbons (13.7%), metals and metalloids (12.7%), pesticides and biocides (10.9%),

TABLE 1 Summary of the number (and percentage of the total for each matrix in *italics*) of each response to the coversheet questions (by institute–laboratory; *n* = 46 for seawater, *n* = 24 for biota, and *n* = 26 for sediment).

Matrix	Response	Are laboratory activities performed by properly qualified people?		Is the laboratory accredited (ISO 17025)?		Are equipment properly maintained and calibrated prior to analysis?		Is there a set of methods specified as acceptable for use in the laboratory?		Are certified reference materials used?		Are the accuracy, precision, and limit of detection/quantification of the methods determined?		Are quality control samples run routinely and the results evaluated before data are released?		Are control charts recorded to test bias and reproducibility?		Are data controlled by a competent authority (apart from accreditation bodies)?	
		Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage	Count	Percentage
Seawater	No	0	0.0%	20	43.5%	0	0.0%	0	0.0%	4	8.7%	0	0.0%	1	2.2%	6	13.0%	17	37.0%
	Don't know	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%	0	0.0%	5	10.9%	7	15.2%
	No response given	0	0.0%	0	0.0%	0	0.0%	0	0.0%	2	4.3%	0	0.0%	1	2.2%	0	0.0%	0	0.0%
	In some cases	0	0.0%	4	8.7%	1	2.2%	2	4.3%	12	26.1%	0	0.0%	5	10.9%	4	8.7%	0	0.0%
	Yes	46	100.0%	22	47.8%	45	97.8%	44	95.7%	28	60.9%	46	100.0%	39	84.8%	31	67.4%	22	47.8%
Biota	No	0	0.0%	6	25.0%	0	0.0%	0	0.0%	3	12.5%	0	0.0%	0	0.0%	1	4.2%	7	29.2%
	Don't know	3	12.5%	3	12.5%	3	12.5%	4	16.7%	3	12.5%	3	12.5%	3	12.5%	3	12.5%	8	33.3%
	No response given	0	0.0%	0	0.0%	0	0.0%	0	0.0%	1	4.2%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
	In some cases, or if possible	0	80.0%	2	8.3%	0	0.0%	0	0.0%	5	20.8%	1	4.2%	3	12.5%	2	8.3%	0	0.0%
	Yes	21	87.5%	13	54.2%	21	87.5%	20	83.3%	12	50.0%	20	83.3%	18	75.0%	18	75.0%	9	37.5%
Sediment	No	0	0.0%	10	38.5%	0	0.0%	0	0.0%	2	7.7%	0	0.0%	0	0.0%	3	11.5%	11	42.3%
	Don't know	0	0.0%	0	0.0%	0	0.0%	1	3.8%	1	3.8%	0	0.0%	0	0.0%	2	7.7%	5	19.2%
	No response given	0	0.0%	0	0.0%	0	0.0%	0	0.0%	2	7.7%	0	0.0%	0	0.0%	0	0.0%	0	0.0%
	In some cases, or if possible	0	0.0%	2	7.7%	1	3.8%	1	3.8%	6	23.1%	2	7.7%	4	15.4%	5	19.2%	0	0.0%
	Yes, or assumed yes because accredited	26	100.0%	14	53.8%	25	96.2%	24	92.3%	15	57.7%	24	92.3%	22	84.6%	16	61.5%	10	38.5%

TABLE 2 Number of determinands reported in questionnaires by their EMODnet Chemistry chemical target group (P36 code) for all matrices, seawater, sediment, and biota.

P36	Number of determinands			
	All matrices	Seawater	Sediment	Biota
Acidity	9	9	2	0
Antifoulants	16	2	15	13
Chlorophyll	9	9	0	0
Dissolved gases	4	4	0	0
Fertilisers	13	12	1	1
Hydrocarbons	54	26	42	34
Metals and metalloids	50	20	48	22
Organic matter	6	5	4	1
Pesticides and biocides	43	14	43	40
Polychlorinated biphenyls	25	8	20	24
Radionuclides	10	2	10	2
Silicates	3	2	1	0
NULL (see below)	153	28	98	95
Total:	395	141	284	232
NULL breakdown:				
<i>Biomarkers</i>	<i>1</i>	<i>0</i>	<i>0</i>	<i>1</i>
<i>Carboxylic acids (adipates)</i>	<i>1</i>	<i>0</i>	<i>1</i>	<i>0</i>
<i>Chlorinated paraffins</i>	<i>1</i>	<i>1</i>	<i>1</i>	<i>1</i>
<i>Dioxins and furans</i>	<i>20</i>	<i>0</i>	<i>19</i>	<i>19</i>
<i>Fluorocarbons; perfluorochemicals</i>	<i>32</i>	<i>0</i>	<i>15</i>	<i>24</i>
<i>Terpenes; carotenoids</i>	<i>15</i>	<i>15</i>	<i>0</i>	<i>0</i>
<i>Marine biotoxins</i>	<i>11</i>	<i>0</i>	<i>0</i>	<i>11</i>
<i>Organobromines</i>	<i>27</i>	<i>4</i>	<i>21</i>	<i>24</i>
<i>Organochlorines (general)</i>	<i>12</i>	<i>3</i>	<i>12</i>	<i>11</i>
<i>Organophosphorus flame retardants</i>	<i>12</i>	<i>0</i>	<i>12</i>	<i>0</i>
<i>Halogens</i>	<i>1</i>	<i>1</i>	<i>0</i>	<i>1</i>
<i>Oxides</i>	<i>2</i>	<i>0</i>	<i>2</i>	<i>0</i>
<i>Phenol compounds</i>	<i>4</i>	<i>0</i>	<i>4</i>	<i>2</i>
<i>Cholinesterase inhibitors</i>	<i>2</i>	<i>0</i>	<i>2</i>	<i>0</i>
<i>Phthalates</i>	<i>9</i>	<i>1</i>	<i>9</i>	<i>1</i>
<i>Salinity</i>	<i>2</i>	<i>2</i>	<i>0</i>	<i>0</i>
<i>Sulfates</i>	<i>1</i>	<i>1</i>	<i>0</i>	<i>0</i>
Total:	153	28	98	95

For substances without a P36 code (NULL), the substance groups are shown in italics.

polychlorinated biphenyls (6.3%), antifoulants (4.1%), or fertilisers (3.3%). Of the 38.7% of determinands not currently included in EMODnet Chemistry target groups, >50% were either perfluorochemicals (20.9%), organobromines (17.6%), or dioxins and furans (13.1%).

3.2.4 Field sampling and analytical methods

Table 3 summarises the field sampling methods reported in the questionnaires. Biota samples are collected by eight groups of methods (e.g. nets, by hand, and baited traps), reflecting the numerous different species, whereas seawater samples are mainly

TABLE 3 Summary of questionnaire responses regarding field sampling methods reported for biota, seawater, and sediment matrices.

Matrix	Field sampling method	No. of determinands per field sampling method	No. of laboratories per field sampling method
Biota	Active fishing gear	5	1
Biota	Baited trap	9	1
Biota	Beam trawls	63	4
Biota	Collected by hand or counted by eye (including by diver)	167	6
Biota	Mussel dredge	51	3
Biota	Net (fyke, gill, pelagic, or unspecified)	96	8
Biota	Scraping tool	51	3
Biota and/or seawater	Manual biota samplers	102	15
Biota and/or seawater	Unknown or no response	17	4
Seawater	Continuous water samplers	1	1
Seawater	CTD	45	16
Seawater	Discrete water samplers	114	35
Seawater	Probe or sensor	5	6
Sediment	Corer (box, Gemax, or sediment corer)	186	9
Sediment	Micro-reineck/Reineck corer, Foreshore spatula, or Eckman Grab	125	1
Sediment	Sediment grabs	120	16
<i>Biota</i>	<i>All field sampling methods</i>	<i>232</i>	<i>25</i>
<i>Seawater</i>	<i>All field sampling methods</i>	<i>141</i>	<i>45</i>
<i>Sediment</i>	<i>All field sampling methods</i>	<i>284</i>	<i>26</i>
All matrices	All field sampling methods	395	63

The totals for each matrix are shown in italics.

collected using discrete water samplers and CTDs, and sediment samples are mainly collected using corers and grabs.

Tables 4A, B summarise the questionnaire responses regarding the analytical methods used for determinands within and outside of

the EMODnet Chemistry target groups (P36), respectively (see Tables S5, S6 for full details). For antifoulants, information on 16 determinands were reported by 9 laboratories, who use some kind of gas chromatography. For fertilisers, information on 13 determinands were reported by 27 laboratories, who use 8 different analytical methods, with the main method being colorimetric analysis. For hydrocarbons, 54 determinands were reported by 15 laboratories, who use some kind of gas chromatography or high-performance liquid chromatography. For metals and metalloids, 50 determinands were reported by 17 laboratories, who use 12 different analytical methods, mainly inductively coupled plasma mass spectrometry or some kind of atomic absorption spectrometry. For pesticides and biocides, 43 determinands were reported by 11 laboratories, who use either gas chromatography or liquid chromatography/mass spectrometry. For polychlorinated biphenyls, 25 determinands were reported by 9 laboratories, who use some kind of gas chromatography (Table 4A). For determinands outside of the P36 groups, the main chemical groups were perfluorochemicals (32 determinands reported by 5 laboratories), organobromines (27 determinands reported by 8 laboratories), dioxins (20 determinands were reported by 6 laboratories), and organochlorines (12 determinands reported by 9 laboratories), all of which are analysed using some kind of gas chromatography or liquid chromatography (Table 4B). Overall, 17 different kinds of gas chromatography and liquid chromatography, and 10 different kinds of spectrometry were reported in the questionnaires (Table S6).

3.2.5 LoQs

The questionnaire allowed information on the LoQs of different substances to be collected, which is a mandatory requirement for the EU DG ENV/EEA, ICES, UNEP-MAP, and NORMAN Network (Table S2). Information on the method or formula used to calculate the LoQ was also requested in the questionnaire as this information is useful for determining data comparability. Various methods were reported for determining the LoQ and full details of the LoD/LoQ information reported can be found in the questionnaires (available upon request). Here, a few examples are taken to highlight some inter-laboratory/inter-instrument variations for the same substances. As shown in Figure 3A and Table S7, there was up to three orders of magnitude difference between the LoQs reported for pyrene in seawater between different laboratories for the same analytical method (gas chromatography–mass spectrometry; 0.00002–0.01 µg/L) and an order of magnitude of difference between analytical methods (0.004 µg/L for high-performance liquid chromatography–ultraviolet detector versus 0.01 µg/L for gas chromatography–mass spectrometry). For lead in sediment (Figure 3B; Table S7), the reported LoQs ranged from 0.0002 mg/kg to 25.4 mg/kg, including a range of 0.03–6.0 mg/kg for the same analytical method (atomic absorption spectrometry - graphite furnace). Similarly, for anthracene in biota, the LoQs of laboratories using the same analytical method (gas chromatography–mass spectrometry) ranged from 0.11 µg/kg to 10.0 µg/kg (Figure 3C; Table S7).

TABLE 4A Questionnaire responses regarding the analytical methods used for determinands within the main EMODnet Chemistry chemical target groups (i.e. P36 codes).

Antifoulants	No. of determinands		No. of laboratories	
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS)	14	87.5%	2	22.2%
Gas chromatography–mass spectrometry (GC–MS)	7	43.8%	2	22.2%
Gas chromatography–flame photometric detector	9	56.3%	1	11.1%
Gas chromatography (GC)	4	25.0%	1	11.1%
Gas chromatography–flame ionisation detection	1	6.3%	1	11.1%
Unknown or no response	1	6.3%	1	11.1%
Total for P36	16		9	
Fertilisers				
Colorimetric analysis	11	84.6%	21	77.8%
Carbon/nitrogen (elemental) analyser	3	23.1%	5	18.5%
QuAA Tro continuous flow analyser/autoanalyser	4	30.8%	2	7.4%
Flow-injection analysis	6	46.2%	1	3.7%
Elemental analyser–isotope ratio mass spectrometer	1	7.7%	1	3.7%
Calculated	1	7.7%	1	3.7%
Fluorometry	1	7.7%	1	3.7%
Manual analysis using the phenol and sodium nitro-cyanoferrate method	1	7.7%	1	3.7%
Unknown or no response	7	53.8%	2	7.4%
Total for P36	13		27	
Hydrocarbons				
Gas chromatography–mass spectrometry (GC–MS)	36	66.7%	8	53.3%
Gas chromatography–flame ionisation detection	24	44.4%	4	26.7%
Fluorescence high performance liquid chromatography (HPLC)	17	31.5%	4	26.7%
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS)	26	48.1%	1	6.7%
High-performance liquid chromatography–ultraviolet detector (HPLC–UV)	12	22.2%	1	6.7%
Gas chromatography–electron capture detection	2	3.7%	1	6.7%
Unknown or no response	6	11.1%	2	13.3%
Total for P36	54		15	
Metals and metalloids				
Inductively coupled plasma mass spectrometry (ICP–MS)	21	42.0%	7	41.2%
Atomic Absorption Spectrometry (AAS)	15	30.0%	6	35.3%
Atomic Absorption Spectrometry (AAS) - graphite furnace	9	18.0%	6	35.3%
Atomic Absorption Spectrometry (AAS) - cold vapour	3	6.0%	6	35.3%
Synchrotron X-ray fluorescence	46	92.0%	1	5.9%
Inductively coupled plasma atomic emission spectroscopy (ICP–AES)	9	18.0%	1	5.9%
Atomic fluorescence spectroscopy - cold vapour	3	6.0%	1	5.9%
Ion selective electrode	3	6.0%	1	5.9%
Titration against standardised acid	2	4.0%	1	5.9%

(Continued)

TABLE 4A Continued

Antifoulants	No. of determinands		No. of laboratories	
AMA254 mercury analyser	1	2.0%	1	5.9%
Hydride generation atomic absorption spectrometry	1	2.0%	1	5.9%
Spectrophotometry	1	2.0%	1	5.9%
Unknown or no response	4	8.0%	2	11.8%
Total for P36	50		17	
Pesticides and biocides				
Gas chromatography–electron capture detection	19	44.2%	8	72.7%
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS)	28	65.1%	1	9.1%
Liquid chromatography–tandem (double) mass spectrometry (LC–MSMS) in isotopic dilution	7	16.3%	1	9.1%
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS) or Liquid chromatography–tandem (double) mass spectrometry (LC–MSMS)	7	16.3%	1	9.1%
Gas chromatography–mass spectrometry (GC–MS)	5	11.6%	1	9.1%
High performance liquid chromatography–tandem (double) mass spectrometry (HPLC–MSMS)	3	7.0%	1	9.1%
Unknown or no response	8	18.6%	2	18.2%
Total for P36	43		11	
Polychlorinated biphenyls (PCBs)				
Gas chromatography–electron capture detection	12	48.0%	5	55.6%
Gas chromatography–high resolution mass spectrometry (GC–HRMS)	21	84.0%	3	33.3%
Gas chromatography–mass spectrometry (GC–MS)	9	36.0%	2	22.2%
High resolution gas chromatography–high resolution mass spectrometry (HRGS–HRMS)	3	12.0%	1	11.1%
Total for P36	25		9	

See Tables S5–S6 for full details.

TABLE 4B Questionnaire responses regarding the analytical methods used for the main reported determinands outside of the EMODnet Chemistry target groups (see Tables S5–S6 for full details).

Dioxins	No. of determinands		No. of laboratories	
Gas chromatography–high resolution mass spectrometry (GC–HRMS)	18	90.0%	3	50.0%
Gas chromatography–mass spectrometry (GC–MS)	16	80.0%	1	16.7%
High resolution gas chromatography–high resolution mass spectrometry (HRGS–HRMS)	16	80.0%	1	16.7%
Unknown or no response	1	5.0%	1	16.7%
Total	20		6	
Perfluorochemicals				
Ultra performance liquid chromatography–tandem (double) mass spectrometry (UPLC–MS)	19	59.4%	1	20.0%
High performance liquid chromatography–tandem (double) mass spectrometry (HPLC–MSMS)	14	43.8%	1	20.0%
High resolution gas chromatography–high resolution mass spectrometry (HRGS–HRMS)	7	21.9%	1	20.0%
Liquid chromatography–tandem (double) mass spectrometry (LC–MSMS) in isotopic dilution	2	6.3%	1	20.0%
Unknown or no response	2	6.3%	2	40.0%
Total	32		5	

(Continued)

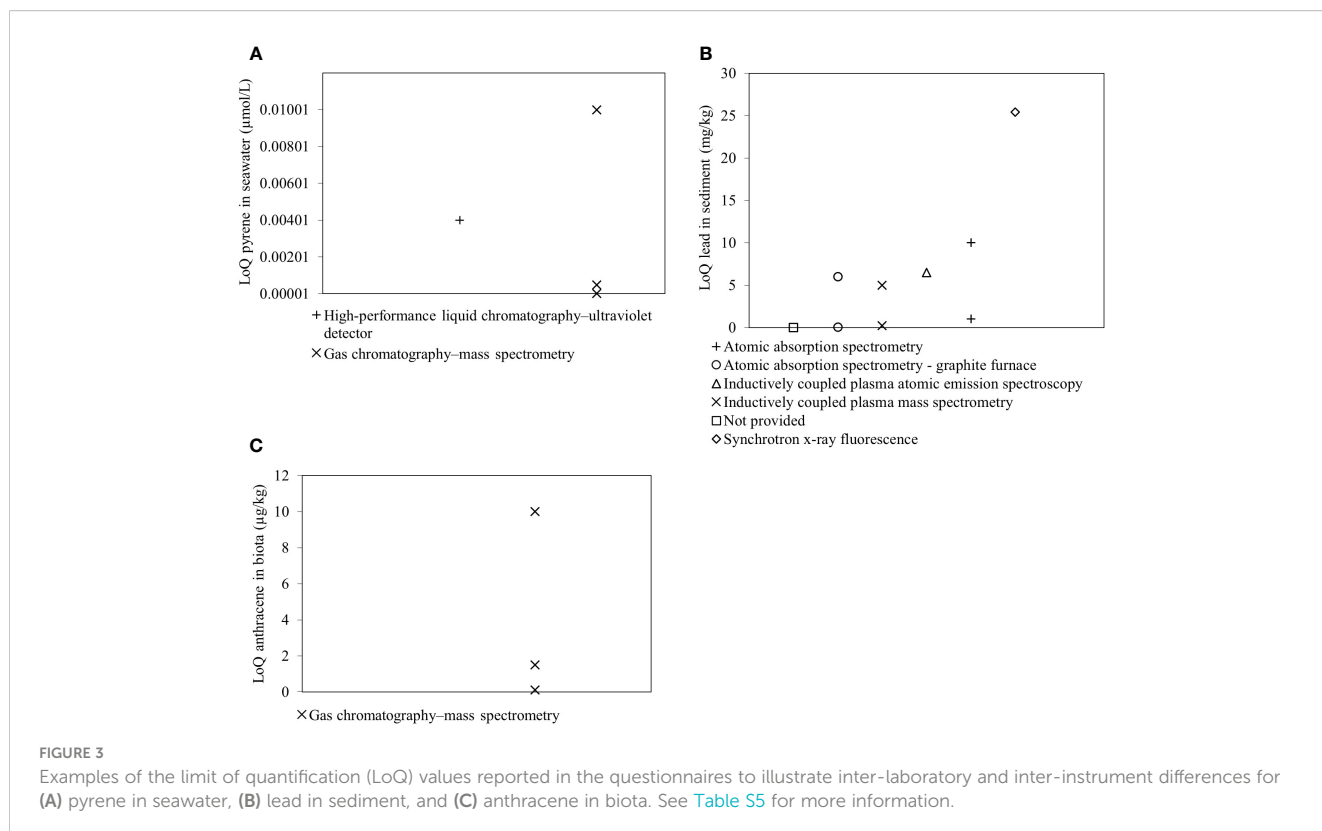
TABLE 4B Continued

Dioxins	No. of determinands		No. of laboratories	
Organobromines				
Gas chromatography–mass spectrometry (GC–MS)	12	44.4%	3	37.5%
High resolution gas chromatography–high resolution mass spectrometry (HRGS–HRMS)	14	51.9%	2	25.0%
Gas chromatography–electron capture detection	9	33.3%	1	12.5%
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS)	4	14.8%	1	12.5%
Liquid chromatography–tandem (double) mass spectrometry (LC–MSMS) in isotopic dilution	3	11.1%	1	12.5%
Unknown or no response	2	7.4%	1	12.5%
Total	27		8	
Organochlorines				
Gas chromatography–electron capture detection	3	25.0%	7	77.8%
Gas chromatography–mass spectrometry (GC–MS)	7	58.3%	2	22.2%
Gas chromatography–tandem (double) mass spectrometry (GC–MSMS)	7	58.3%	1	11.1%
Gas chromatography–flame ionisation detection	1	8.3%	1	11.1%
Unknown or no response	1	8.3%	1	11.1%
Total	12		9	

4 Discussion

The adoption of standard data and metadata models along with the systematic collection and provision of detailed information on methods, laboratory performance, and QA/QC procedures all

contribute to the process of data curation, which emerges as a key data management process when there is an increase in the number of data sources and platforms for data generation (Freitas and Curry, 2016; Yoon et al., 2022). Especially in the field of environmental sciences, improvements in data curation require a



multidisciplinary approach that involves information, communication, and technology (ICT) experts, multidisciplinary marine environmental scientists in charge of data acquisition, and authorities responsible for environmental status assessment. This approach may be greatly supported by strengthening collaboration and dialogue between data managers, data originators, and data users. In this regard, the activities described in this study are the result of a large effort combining (a) requirements in terms of data and metadata from the MSFD community and RSCs, (b) tools and protocols for data management adopted within the EMODnet framework, and (c) information from the laboratories in charge of analysing samples and generating contaminant data.

Based on the templates proposed by several European and global frameworks, the new EMODnet Chemistry questionnaire allowed a rich set of standardised and harmonised information that is required to evaluate data comparability and, therefore, re-usability (Wilkinson et al., 2016) to be collected from 64 laboratories in 18 European countries. Data comparability refers to the possibility to use data from multiple sources and is assisted by information on methodological aspects (from sampling to analysis and laboratory performance) that is available to data users, who can evaluate whether possible methodological heterogeneity may prevent the use of data from different sources. The collection of information through this questionnaire is part of a systematic effort that initially began in 2014 when the first EMODnet questionnaire was sent out to institutes participating in EMODnet Chemistry, thus contributing to EMODnet's long-term strategy of providing access to reliable and accurate information.

Importantly, the use of DOIs makes the EMODnet questionnaires openly available and associates them with data submitted to EMODnet Chemistry, allowing different data users to evaluate data comparability, and improving transparency in data quality, reliability, and fitness for use for assessment purposes. Such transparency is crucial for environmental status assessment in cross-border areas (e.g. at regional and sub-regional scales), as required under the MSFD and by RSCs, whereby data from multiple and heterogeneous sources are needed. The contaminants reported in the questionnaires included approximately 90% of the substances included in Directive 2013/39/EU on priority substances in the field of water policy (European Commission, 2013). Considering that these substances are used to assess marine pollution according to Descriptor 8 of the MSFD, it is essential to collect and evaluate QA/QC information from different laboratories.

Evaluation of the questionnaires highlighted some heterogeneities in laboratory proficiency, analytical techniques, and methods used to calculate the LoQ. Although the questionnaire responses regarding QA procedures indicate an overall good level of laboratory proficiency (Table 1), they also suggest possible improvements. For instance, although 100% of laboratories reported that they have properly qualified people performing laboratory activities for seawater and sediment samples, only 47.8%, 54.2%, and 53.8% of laboratories are ISO 17025 accredited for seawater, sediment, and biota analysis, respectively, and only 60.9%, 50.0%, and 57.7% of laboratories use certified reference materials when analysing contaminant concentrations in seawater, biota, and sediment samples, respectively.

In terms of analytical methods (Section 3.2.3), the results indicate general harmonisation between the laboratories participating in EMODnet Chemistry for hydrocarbons (gas chromatography or high-performance liquid chromatography), antifoulants (some kind of gas chromatography), pesticides and biocides (gas chromatography or liquid chromatography/mass spectrometry), and polychlorinated biphenyls (some kind of gas chromatography). However, 8 different analytical methods were reported for fertilisers (i.e. nitrogen and phosphorus substances) and 12 different analytical methods were reported for metals and metalloids, suggesting the potential for increased harmonisation.

Inter-laboratory/inter-instrument variations in the reported LoQs and LoDs for a given substance were expected and occur because of various factors, such as the analytical technique/instrument used, method used to calculate these values, and accuracy of the calibration curve obtained. In addition, it is also possible that compilation errors could have occurred (e.g. selecting the wrong unit or providing the LoD method instead of the requested LoQ method) due to the complexity of information requested and the expertise required to fill in the questionnaire. Although IUPAC made international recommendations for calculating LoDs and LoQs in 1995 (Currie, 1995), problems (e.g. that there are several possible conceptual approaches to the subject, as confirmed by the examples included in Table S7) associated with the subject of the LoD and LoQ were already outlined by IUPAC in 2002 (Thompson et al., 2002) and are also considered elsewhere (Barwick, 2023). While laboratory proficiency and equipment depend on institutional resources that may differ among countries, improved coherence in LoD/LoQ calculation methods could be a step towards improved harmonisation. Accordingly, the results of the questionnaires suggest that it could be beneficial to recommend and share IUPAC's LoD/LoQ calculation methods between EMODnet participating laboratories.

It is fundamental to understand the complexity and entire cycle of pollution data (from *in situ* sampling to analytical procedures, QA/QC protocols, and data curation) and to have access to accurate and updated metadata and methodological information to allow a coherent assessment of marine environmental status and, ultimately, to take proper actions to limit pollution. This work further extends the approach already proposed for heavy metals in a sub-basin of the Mediterranean Sea (Berto et al., 2020; Molina Jack et al., 2020) by addressing more chemical groups and providing information for all European Seas.

Lastly, even though drop-down lists were included in the questionnaire to facilitate the collection of standard information and to avoid spelling mistakes and the use of wrong terms or variations in the same term for important metadata fields, the issues of typos and incomplete information were still observed for information requiring manual input, representing possible sources of error and inconsistency given the many different countries involved.

5 Conclusions

In this work, rich standardised and harmonised QA/QC information on contaminants was collected at the European level using a dedicated questionnaire, including information requested

by different RSCs and legal frameworks (e.g. WFD and MSFD). Overall, the questionnaire allows standard information to be collected and made available, and promotes interoperability among data infrastructures, thus supporting the FAIR data principles. The information received from 64 laboratories associated with 21 institutes in 18 countries i) highlights disparities in the entire process of contaminant data production, ii) identifies gaps in existing vocabulary terms used to code contaminants, and iii) supports action to be taken to improve the overall data management system. In particular, high levels of heterogeneity were observed in the analytical methods and with respect to performance in terms of LoQs for some substances; however, such heterogeneity could also be due to some compilation errors, highlighting the need for more care to be taken to provide correct information, which will be addressed in a future amended questionnaire. The questionnaire contributes to the need for accurate and comprehensive metadata to improve the reliability of marine contaminant data collected under the MSFD. As a target of improved harmonisation, IUPAC's methods for calculating LoD/LoQ values could be shared within the EMODnet network, which involves 26 European and neighbouring countries. This contribution also highlights the attention, effort, and expertise required to carry out data curation, which is crucial to support a reliable assessment of marine pollution, and ultimately better management of the marine environment. Data curation is still an overlooked aspect of the overall scientific research process and requires multidisciplinary expertise, dedicated staff, and funding. The support provided by EMODnet to the implementation of the MSFD is an ongoing process, whereby those involved learn by doing and the system improves over time.

Lastly, as the EMODnet network also involves countries beyond the EU (e.g. Montenegro, Georgia, and Turkey), the activity described in this study allowed standardised and harmonised information to be collected from institutions outside the EU. Further, the study promotes the sharing of a common understanding on the importance of accurate metadata and QA/QC details. Access to harmonised information represents an important step towards interoperability and FAIRness with respect to pollution data, which are of paramount importance to support the principles of coordinated ecosystem-based management, also at the transboundary level.

Data availability statement

The original contributions presented in the study are included in the article/[Supplementary material](#), further inquiries can be directed to the corresponding author/s.

Ethics statement

Ethical approval was not required for the studies involving humans because it was not applicable to the nature of this study. The studies were conducted in accordance with the local legislation and institutional requirements. The participants provided their written informed consent to participate in this study. This study

was performed as part of the European Marine Observation and Data Network (EMODnet Chemistry) contract between the National Institute of Oceanography and Applied Geophysics (OGS, the coordinating institution) and European Union Executive Agency for SMEs (EASME). All questionnaires were completed by institutes participating in EMODnet Chemistry. This contract requires that (1) data must be free of charge and free of restrictions of use, including in relation to pre-existing rights; and (2) data and data products shall be accompanied by metadata covering at least: (a) ownership; (b) assessment of accuracy and precision according to pre-existing standards in the marine field; and (c) indication of method used for their measurement or construction. Prior to manuscript submission, written consent regarding the publication of either i) laboratory name/s and institute name, ii) institute name only, or iii) country name only was obtained from each institution that completed a questionnaire.

Author contributions

MF: Data curation, Formal analysis, Methodology, Visualization, Writing – original draft, Writing – review & editing. ML: Conceptualization, Supervision, Writing – original draft, Writing – review & editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fmars.2023.1275097/full#supplementary-material>

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