Interreg
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European Regional Development Fund - Instrument for Pre-Accession II Fund

HarmoNIA

Harmonization and Networking for
contaminant assessment in the Ionian and
Adriatic Seas

Deliverable T1.1.3 Methodological proposal for data Quality Control procedures

Work Package T1 - Sharing best practices for transnational harmonization for EQSD implementation and link with UNEP/MAP MEDPOL Programme and Offshore Protocol of Barcelona Convention

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July 2019

How to cite: M. Giani, M. Kralj, M.E. Molina Jack, M. Lipizer – OGS, G. Giorgi, A. Rotini – ISPRA, D. Ivankovic, I. Ujevic, S. Matijević – IOF, H. Kaberi, J. Hatzianestis, C. Zeri, S. Iona - HCMR, M. Fafandjel, N. Mikac – RBI, B. Cermelj, O. Bajt - NIB 2020 WPT1 HarmoNIA Deliverable T1.1.3 - Methodological proposal for data Quality Control procedures doi: 10.6092/db6877bc-9ebd-4d7d-bc15-fd5997e4fc63

Content:

1. Introduction

The aim of this work is to provide common and agreed guidelines to improve the Quality Control (QC) of data on the concentrations of contaminants (trace metals and PAHs) in marine sediments, which are managed by large marine data infrastructures (eg. SeaDataCloud, EMODnet) or which are not yet Quality Controlled according to common procedures. The Guidelines are developed in the framework of Interreg ADRION HarmoNIA project and are focused on the Adriatic – Ionian Region. The overall approach represents, nevertheless, a framework which can be adapted to other marine areas, with proper background information.
The QC procedure involves an overall dataset format check, which will be described in the Annex and the data Quality Control, described below. The overall dataset format check includes also the evaluation of the availability of relevant metadata.

EMODnet Chemistry data have been used to identify the most common problems encountered when merging datasets deriving from different institutions and to propose the main targets of data Quality Control procedures. Two kinds of datasets of contaminants in sediments were downloaded from EMODnet Chemistry:

- Profiles
- Time Series

This distinction derives from the originator’s choice during the preparation of the data set (Figure 1) according to SeaDataNet/SeaDataCloud protocols and tools.

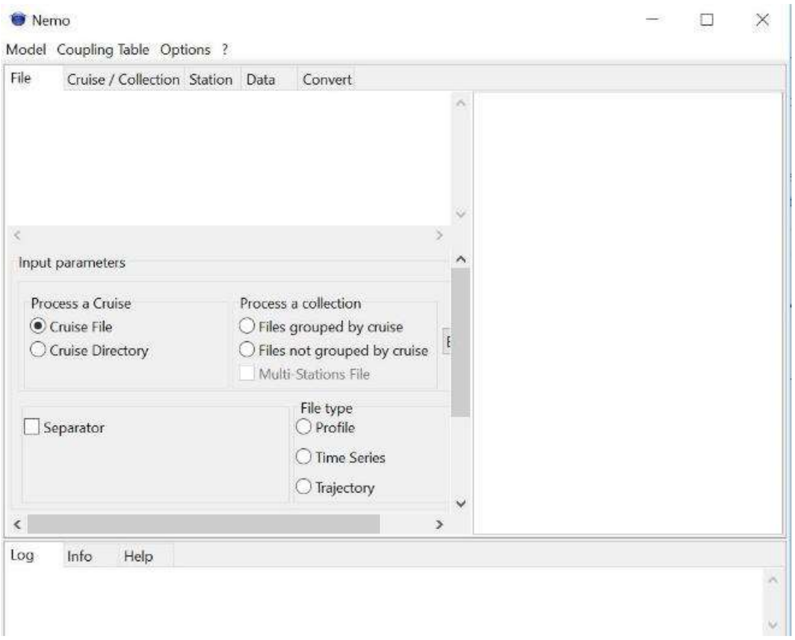

Figure 1. Example of dataset formatting tool NEMO available through SeaDataCloud and the selection of “File type”.

Profile data refer to surface sediments and to samples taken at different depth layers below the sediment-water interface.

Time series data refer to sediments sampled at different times in the same site.

The following dataset was made available through EMODnet Chemistry on December 2018 and was used for this document:

- Mediterranean Sea - Contaminants aggregated datasets 1974/2017 v2018 which contains restricted and unrestricted data. Please cite unrestricted data: Mediterranean Sea - Contaminants aggregated datasets 1974/2017 v2018 doi: 10.6092/k3yj-6a02

In this report, data available from scientific literature from the Eastern Mediterranean Sea were used to derive the ranges to be used for the QC. Those ranges were applied for the QC of data from the Adriatic Sea, Ionian Sea, Sicily Channel, Aegean Sea and Cretan Sea available through EMODnet Chemistry. The Longitude limits were set from 12 to 27 °E and the Latitude limits from 34° to 45.7 °N.

These data are only for internal use by the HarmoNIA project.

2. Quality Control approach

The QC procedure is proposed for a selected set of contaminants, in particular for a selection of trace metals and of PAHs (polycyclic aromatic hydrocarbons). The procedure is based on the following steps:

1-**Geographical check:** Only the data for coastal and offshore sediments of Adriatic Sea, Ionian Sea, Cretan Sea and Aegean Sea were considered. Transitional environments as lagoons and inner rivers mouths were not considered.

2-**Units check:** Consistency with adopted units in relation to the matrix: µg kg^{1} dw for sediments.

3- **Selection of the analyte:** According to the specific parameter names (P01 SeaDataNet vocabulary) which contain details on granulometry size classes (< 2 mm, < 63 µm) and instrumental methods if possible.

4- **Check of methods for analyte quantification**: When 90%-100% of the data lie below or are equal to LOD or LOQ, the data set was considered not useful in this exercise, even though may be still compliant with EQSD. This approach was used in particular for metals which are always quantifiable with modern analytical methods.

5- **Range check:** Check if values fall within a defined range of expected variability and if they are out of range re-check data with originators before the validation, in order to assign appropriate Quality Flag (QF) according SeaDataNet standards (Table 1).

The regional ranges for the QC were established on the basis of on existing data published in the scientific literature for the Eastern Mediterranean Sea similarly to the approach used for chemical oceanographic data (UNESCO, 2010). This ranges were applied to check the data made available through EMODnet Chemistry.

Criteria for the range definition are:

- the value should be **equal or higher** than the minimum value of regional background concentration (RBC_{min}) and Regional Minimum Concentration for Offshore sediments (RMinCO) for the Eastern Mediterranean based on all relevant background concentrations reported in the scientific literature.
- the value should be **equal or lower** than the maximum value of Regional coastal maximum concentration (RMaxC), regional maximum Offshore concentration(RMaxCO) and Regional maximum Background Concentration (RBCmax) derived for Eastern Mediterranean area.
- data with “zero” value are not acceptable → in these cases “0” value should be substituted with the appropriate LOD or LOQ value, when possible, and they should be labeled with the SeaDataNet QF 6 “value below detection limit” or Q “value below limit of quantification”.

Table 1: List of Quality Flags (QF) adopted according to SeaDataNet (L20 SEADATANET MEASURAND QUALIFIER FLAGS[1]).

QF Code	QF name	QF definition
0	no quality control	No quality control procedures have been applied to the data value. This is the initial status for all data values entering the working archive.
1	good value	Good quality data value that is not part of any identified malfunction and has been verified as consistent with real phenomena during the quality control process.
2	probably good value	Data value that is probably consistent with real phenomena but this is unconfirmed or data value forming part of a malfunction that is considered too small to affect the overall quality of the data object of which it is a part.
3	probably bad value	Data value recognised as unusual during quality control that forms part of a feature that is probably inconsistent with real phenomena.
4	bad value	An obviously erroneous data value.
5	changed value	Data value adjusted during quality control. Best practice strongly recommends that the value before the change be preserved in the data or its accompanying metadata.
6	value below detection	The level of the measured phenomenon was less than the limit of detection (LoD) for the method employed to measure it. The accompanying value is the detection limit for the technique or zero if that value is unknown.
7	value in excess	The level of the measured phenomenon was too large to be quantified by the technique employed to measure it. The accompanying value is the measurement limit for the technique.

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[1] http://seadatanet.maris2.nl/v_bodc_vocab_v2/browse.asp?order=conceptid&formname=search&screen=0&lib=l20&v0_0=&v1_0=conceptid%2Cpreflabel%2Caltlabel%2Cdefinition%2Cmodified&v2_0=0&v0_1=&v1_1=conceptid&v2_1=3&v0_2=&v1_2=preflabel&v2_2=3&v0_3=&v1_3=altlabel&v2_3=3&v0_4=&v1_4=modified&v2_4=9&v0_5=&v1_5=modified&v2_5=10&x=19&y=22&v1_6=&v2_6=&v1_7=&v2_7=

8	interpolated value	This value has been derived by interpolation from other values in the data object.
9	missing value	The data value is missing. There should be no accompanying value in ODV format files. The accompanying value in SeaDataNet NetCDF data must be the absent data representation specified by the _FillValue parameter attribute and lie outside the range of data not flagged bad (4) or probably bad (3).
A	value phenomenon uncertain	There is uncertainty in the description of the measured phenomenon associated with the value such as chemical species or biological entity.
Q	value below limit of quantification	The level of the measured phenomenon was less than the limit of quantification (LoQ). The accompanying value is the limit of quantification for the analytical method or zero if that value is unknown.

6-Relevant metadata availability check: In some cases, relevant metadata were missing e.g., Bottom depth, thickness of the sampled sediment, depth of the sediment layer, coordinates.
The availability of proper metadata is of fundamental relevance for the QC check and also for its improvement. Without bottom depths, it is not possible to distinguish deep sediments from the costal shallower sediments, where contaminant ranges are much different and make a specific QC.

7-Availability of useful data for normalization procedures: Check of information useful for the normalization e.g. grain size, organic carbon content, aluminium content.

Definitions adopted in present report:

Background Concentration (BC): The concentration of a contaminant at a “pristine” or “remote” site based on contemporary or historical data (OSPAR/ICES, 2004; UNEP/MAP, 2011).

Regional Background Concentration (RBC): Background concentration of the contaminant in the sediments for the Mediterranean, with a specific focus on the eastern basin (Adriatic Sea, Ionian Sea, Sicily Channel, Aegean Sea, Cretan Sea). The RBC were derived from the data available in the scientific literature. A range of variability was reported as RBCmin-RBCmax for the investigated area due to the different geochemical provinces.

Regional Maximum Concentration (RMaxC): Maximum concentration reported in scientific literature for contaminated coastal sediments in the Eastern Mediterranean (Adriatic Sea, Ionian Sea, Sicily Channel, Aegean Sea, Cretan Sea).

Regional Minimum Concentration (RMinC): Minimum concentration reported in scientific literature for contaminated coastal sediments in the Eastern Mediterranean (Adriatic Sea, Ionian Sea, Aegean Sea, Cretan Sea).

Regional Maximum Concentration for Offshore sediments (RMaxCO): Maximum concentration reported in scientific literature for offshore sediments in the Eastern Mediterranean (Adriatic Sea, Ionian Sea, Sicily Channel, Aegean Sea, Cretan Sea)

Regional Minimum Concentration for Offshore sediments (RMinCO): Minimum concentration reported in scientific literature for offshore sediments in the Eastern Mediterranean (Adriatic Sea, Ionian Sea, Sicily Channel, Aegean Sea, Cretan Sea)

Limit of detection (LOD): This is the output signal or concentration value above which it can be affirmed, with a stated level of confidence that a sample is different from a blank sample containing no determinant of interest (Commission Directive 2009/90/EC).

Limit of quantification (LOQ): This is a stated multiple of the limit of detection at a concentration of the determinant that can reasonably be determined with an acceptable level of accuracy and precision. The limit of quantification can be calculated using an appropriate standard or sample, and may be obtained from the lowest calibration point on the calibration curve, excluding the blank (Commission Directive 2009/90/EC).

Skewness: Statistical parameter that measures the deviation of the distribution from symmetry. If the skewness is clearly different from 0, then the distribution is asymmetrical, while normal distributions are perfectly symmetrical.

Kurtosis: Statistical parameter that measures the "peakedness" of a distribution. If the *kurtosis* is clearly different than 0, then the distribution is either flatter or more peaked than normal; the *kurtosis* of the normal distribution is 0.

3. Quality Control for trace metals

The approach used to define minimum and maximum concentrations in order to perform “range checks” is described below.
Background concentrations were used in order to assess the lowest concentrations expected to be present in the sediments. These concentrations should represent the concentration that would be expected in a “pristine” or “remote” site based on contemporary or historical data (OSPAR/ICES, 2004; UNEP/MAP, 2011).
Among the different methods to define a background concentration, the geochemical method was used (Dung et al., 2013) which is based on mean or median values of trace metals in sediment layers of core samples that are assumed to have a pre-industrial origin.
Due to atmospheric fall out, riverine discharges and point sources pollution from coastal cities and industrial plants it is not reliable to consider a surface sediment of a pristine area as uncontaminated by human activities during the industrial period. In the present work, background concentrations are derived from subsurface sediment concentrations, which according to sedimentation rates or the dating of the sediment core, can be considered as representative of the pre-industrialization period.
For trace metals, Regional Background Concentrations (RBC) were obtained by sediment profiles available for the Eastern Mediterranean, as explained below.
However, only a limited variety of sedimentological environments is represented by cores used for the estimates of RBC, due to the paucity of the samplings. Therefore to take into account the natural variability of the sedimentological environments,

we considered also the range of concentrations found in offshore (deep) surface sediments (RMinCO-RMaxCO) which, due to a higher spatial coverage, represent a wider spectrum.

Table 2 summarizes some of the RBC available from the scientific literature for trace metals in sediments of the Mediterranean area.

For the target elements only the data resulting from analytical methods capable to determine the total concentration in the sediment were considered. Specifically, X ray fluorescence spectroscopy (Lucchini et al, 2003 and Karageorgis et al., 2005) applied to the solid bulk sediment matrix, or atomic absorption spectroscopy (FAAS; GFAAS; CVASS) and emission spectroscopy (ICP, ICPMS) applied to the solution obtained from total dissolution of the bulk sediment by strong acid mixtures containing HF, in teflon bombs (after heating or digestion in microwave oven), guarantee a correct measure of the total concentrations of trace metals (Acquavita et al, 2018; Aloupi & Angelidis, 2001; Angelidis &aloupi, 1995; Angelidis et al., 2011; Buccolieri et al., 2006; Covelli & Fontolan, 1997; Giani et al., 1994; Giordano et al, 1992, De Lazzari et al., 2004; Ilijanic et al 2014; Lopes-Rocha et al., 2017). In one of the considered studies, Hg was determined by direct thermal treatment of the solid sample, preconcentration on an amalgamator, desorption and determination by AAS (Buccolieri et al., 2006). Moreover, only concentrations determined on unsieved sediments or sieved at 2 mm were taken into account, as the sieved sediment (<63 µm) is characterized by a higher metal concentration with respect to the original sediment. This was necessary to obtain comparable range estimates of the RBC for both the offshore and the coastal sediments.

Furthermore, only offshore cores or cores from marine areas relatively far from direct pollution source were considered. Lagoons and river delta sediments were not considered as they represent highly human perturbed environment also during preindustrial period.

The importance of considering only methods allowing the quantification of the total concentrations of elements in the sediments is evident when considering that the concentration of trace metals present in the residual fraction of the sediments, which include the elements bound to the crystal lattice of minerals, usually increased from coastal “polluted” sediments towards offshore “unpolluted” sediments (Angelidis, 2005). As an example using selective extractions, the residual fraction for some trace metals was found to increase from 16.5% to 67.5% for As, from 22.8% to 54.3% for Cr, from 13.2 to 82.1% for Zn in the transition from coastal to offshore sediments (Angelidis, 2005). In non-polluted sediments of the continental shelf the residual fraction plays a predominant role in the partitioning of all trace elements (human related or natural), although some metals are more strongly lattice-related than others (Angelidis, 2005).

Table 2: Regional Background Concentrations (RBC) for Mediterranean sediments

Element	Units	RBC		Med [1]	MAd, SAd[2]*		NAd, Mad, SAd [3]		MAd, SAd [4]		NAd [5]	NAd [7]	WMed [8]		EMed [9]
		Min	Max		Min	Max	Min	Max	Min	Max			Min	Max	
Cd	mg kg^{-1} dw	**0.07**	**0.57**	0.085	0.20	0.57	-	-	-	-	-	-	0.07	0.08	0.124
Hg	mg kg^{-1} dw	**0.02**	**0.08**	0.053	0.02	0.03	-	-	-	-	0.07	-	0.04	0.08	
Pb	mg kg^{-1} dw	**10.0**	**116**	16.95	15.4	18.4	10	23	16	34	18.9	116	15	18.1	13.8
As	mg kg^{-1} dw	**4.3**	**19.1**	-	4.3	19.1	-	-	5	10	-	-	-	-	
Cr	mg kg^{-1} dw	**57**	**178**	-	123	150	57	152	84	178	141	80	62	63.9	
Cu	mg kg^{-1} dw	**11.3**	**49**	-	20.2	37.3	12	30	29	37	-	16	11.3	25.8	49.3
Ni	mg kg^{-1} dw	**16.9**	**181**	-	126	181	23	103	67	173	-	148	16.9	46.9	
Zn	mg kg^{-1} dw	**41.5**	**103**	-	69	84	54	95	90	103	-	72	57	84.1	41.5
Co	mg kg^{-1} dw	**12**	**28**	-	19.7	28.2	-	-	12	22	-	-			-
V	mg kg^{-1} dw	**82**	**109**	-	-	-	-	-	84	109	-	-	82	108.3	-
Sedimentation rate	mm yr^{-1}				1.8	3.1	0.67	5.2	-		1-2 [6]	1-2.5	0.4-0.6		0.17
Core section	cm				14	28	older than 1910		200	Holocene	40-80	49-51 (ISO45)	2.5	8.5	3-12
Silt+clay	%				87	100	41	100			95-98	67	50	69.61	-
Corg	%				-	-	0.3	1.5	-	-	-	0.38	0.24	0.44	-

*ranges derived from the data provided by the authors

[1]UNEP-MAP 2016; [2]Ilijanic et al., 2014; [3]Lopes-Rocha et al., 2017; [4]Lucchini et al,. 2003; [5] Giani et al., 1994;

[6] derived from Frignani et al., 2005; [7]Covelli &Fontolan, 1995; [8]Berto et al., 2006; [9] median calculated from Angelidis et al, 2011

Med: Mediterranean; WMed: Western Mediterranean;Emed: Eastern Mediterranean; NAd: Northern Adriatic; MAd: Mid Adriatic; SAd: Southern Adriatic

The LODs reported in the considered studies were:
0.02-0.13 µg kg^{-1} for Cd (Acquavita et al., 2018; Aloupi & Angelidis, 2001;); 0.01-0.4 µg kg^{-1} (LOQ) for Hg (Giani et al., 1994; Giordano et al., 1992; Acquavita et al., 2018), 0.02-5 µg kg^{-1} for Pb (Aloupi & Angelidis, 2001; Acquavita et al.,2018; Giani et al., 1994; Giordano et al., 1992;); 0.25 as LOQ for As (Acquavita et al., 2018); 0.04-2.5 µg $kg^{-1}$for Cr, 0.5 [1] (LOQ)-5 µg $kg^{-1}$for Cu, 2 µg kg^{-1} (LOQ) for Ni; 2-12.5 µg kg^{-1} (LOQ) for Zn (Acquavita et al., 2018).
All the reported accuracies for the target trace metals were within ±10% from the certified values (Acquavita et al., 2018; Aloupi & Angelidis, 2001; Buccolieri et al., 2006; Dolenc et al., 1998; Giordano et al, 1992, Giani et al., 1994; Lucchini et al., 2003; Karageorgis et. 2005; Ilijanic et al., 2014; Lopes-Rocha et al., 2017b;), with 2 exceptions for Cd (Acquavita et al., 2018) and for Pb (Lopes_Rocha, 2017b). The reproducibility, reported in the same studies were less than 5% for Cd, As, Cu, Co and V, less than 6% for Cr, less than 8% for Zn, and less than 10% for Pb and Hg.
A cumulative error (analytical + sampling) in the determination of a trace metal in a sediment was assumed to be ±10% (Birch et al., 2001).
Table 3 summarizes the range of metal concentrations reported for the eastern Mediterranean surface offshore sediments. Most of the considered sediment samples were collected at depths ranging from 165 to 2200 m, except one core that was collected at ~70-80 m depth (Karageorgis et al., 2005).
Concentrations lower than the limit defined as the minimum value between RBC_{min} and RMinCO, multiplied by 0.9 to take into account an analytical 10 % error, were considered “to be re-checked”, this means that they should be controlled with the data originator e.g. there could be errors in the measurement units or in their conversion or in the analytical methods adopted.
For the determination of upper limit of concentrations in offshore environment the Regional Maximum Concentrations in Offshore sediments (RMaxCO) were considered for the Quality Check, only data collected far from estuarine areas, >10 nautical miles from the coast, at depth deeper than 70 m were used.
The Regional Minimum concentrations found in offshore sediments (RMinCO, Table 3) can be compared to the Regional Background minima derived from the cores (Table 2). For some elements as Cd, Hg, Zn and Co the lowest concentrations in

offshore sediments are "slightly" lower than the RBC$_{min}$ (-14, -32 %, -7%, and -17%, respectively). These differences could arise from grain size differences but there are not sufficient data available on the granulometry to ascertain this aspect. For these elements, the RMinCO were considered as the lower limit for the Quality Check (Table 5).

Table 3. Trace metals concentrations in offshore sediments of the eastern Mediterranean Sea.

Element	**Units**	**Offshore sediments**		**EMed[1]** (Thermaikos gulf)		**EMed[2]**		**Ionian sea[3]**		**MAd & SAd[4]**		**MAd & SAd[5]**	
		RMinCO	RMaxCO	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cd	mg kg^{-1} dw	**0.06**	**0.26**			0.12	0.26			0.06	0.14		
Hg	mg kg^{-1} dw	**0.013**	**0.419**					0.07	0.13	0.013	0.106	0.02	0.419
Pb	mg kg^{-1} dw	**5**	**71.4**	17	41	14.8	38.4	55.2	71.4	14.9	24.5	5	18
As	mg kg^{-1} dw	**1**	**32**									1	32
Cr	mg kg^{-1} dw	**53**	**276**					75.2	102.8	112	276	53	246
Cu	mg kg^{-1} dw	**2**	**60**	2	27	36.1	60	46.1	52.3	19.3	44.5	9.8	44.9
Ni	mg kg^{-1} dw	**49**	**323**	76	162			53.7	97.1	109	323	49	264
Zn	mg kg^{-1} dw	**34**	**124**	34	105	41.3	82.6	97.1	124	61	112	38	101
Co	mg kg^{-1} dw	**10**	**25**									10	25
V	mg kg^{-1} dw	**4**	**142**	4	106							50	142
Sediment section	cm			0	19	0	2	0	5	0	2	0	5
Stations selected				IP-30				9, 15, 16, 18, 19		SAPit1-2,Jabuka,Palagruza		Mad & Sad stations	
Bottom depth	m			~70-80		2800		400	2200	169.8	1041.4		~1000
Silt+clay	%			relict sand		pelitic muds				84.1	100		
Sedimentation rate	mm yr^{-1}			1.8						1.8	3.1		

EMed: eastern Mediterranean; MAd:MiddleAdriatic; SAd:Southern Adriatic

[1]Karageorgis et al, 2005 ;[2]Angelidis et al. 2011; [3]Buccolieri et al., 2006; [4]Ilijanic et al., 2017; [5]Dolenc et al., 1998

For Pb, As, Cr, Cu and V, the concentrations in offshore sediments are from 2 to 21 times lower than the RBC$_{min}$ (Table 1). This could be due to grain size heterogeneity, as the lowest concentrations for Cu, Zn and V were found in relict sand of Thermaikos gulf, in the North Aegean Sea. Values as low as 2 mg kg^{-1} dw for Cu and 10 mg kg^{-1} dw for Zn were reported by De Lazzari et al. (2004) for the Northern and Mid Adriatic Sea.

In the case of Ni the RBC$_{min}$ is lower than the RMinCO found in offshore sediments and, therefore, these values are considered as the lowest expected concentrations for the Quality Check (Table 5).

In the case of Cr the minimum concentrations is found in coastal sediments, therefore the RMinC was chosen for the Quality check (Table 4).

Table 4 summarizes the range of metal concentrations reported since 1992 for contaminated surface coastal sediments in the Eastern Mediterranean. The publications considered represent only a selection from the available scientific literature, based on the analytical methods applied, sediment pre-treatment and regional availability of data for target trace metals.

The highest value was considered as the upper limit, Regional Maximum concentration (RMaxC) (Table 4). A maximum error (analytical + sampling) in the determination of the metal concentrations in a sediment was assumed to be ±10% (Birch et al., 2001). Concentrations higher than this upper limit +10% were considered "to be re-checked" this means that they should be verified with the data originators e.g. there could be errors in the measurement units or in their conversion.

Table 4. Ranges of metal concentrations in coastal sediments of the Eastern Mediterranean Sea.

Element	Unit	Coastal sediments		Trieste Harbor and Isonzo R. mouth[1]		Adriatic-Ionian harbors[2]		Mytilene harbor[3]		Rhodes harbor[4]		Thermaikos Gulf[5]		WNAd[6]	
		RMinC	RMaxC	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Cd	mg kg^{-1} dw	0.03	18.2	0.16	18.2	0.13	0.25	0.17	0.495	0.03	0.17	-	-	-	-
Hg	mg kg^{-1} dw	0.11	6.18	0.54	6.18	0.11	0.40	-	-	-	-	-	-	-	-
Pb	mg kg^{-1} dw	19	230	24	170	19	68	32.7	93	77.1	230	26	128	9	30
As	mg kg^{-1} dw	6.6	18.2	6.6	18.2	-	-	-	-	-	-	-	-	-	-
Cr	mg kg^{-1} dw	19.4	180	73	171	-	-	83	154	19.4	118	-	-	26	180
Cu	mg kg^{-1} dw	14	101	23	70	-	-	21	86.2	31.5	101	38	61	14	47
Ni	mg kg^{-1} dw	23	231	62	231	-	-	-	-	-	-	124	255	23	87
Zn	mg kg^{-1} dw	59	339	100	339	-	-	74.1	230	59	242	84	229	65	137
Co	mg kg^{-1} dw	-	-	-	-	-	-	-	-	-	-	-	-	-	-
V	mg kg^{-1} dw	72	175	72	124	-	-	-	-	-	-	112	175	-	-
Stations selected				A0-4, TS1-3, IS1-2		Ta, Br, Ba, Man, Ter*		1-12		all except SD		IP1, IP17, IP38		Nad	
Corg	%	0.67	4.8	0.91	1.48	0.9	1.34	1.31	4.8	0.67	2.74	-	-	0.5	1.7
Silt+clay	%	3.2	99.8	97.8	87.8	-	-	3.2	96.66	3.5	23	95.8	99.8	42	99

*Ta:Taranto, Br:brindisi, Ba: Bari, Man: Manfredonia; Ter: Termoli

[1] Acquavita et al., 2018; [2]Giordano et al., 1992; [3]Aloupi&Angelidis, 2001;[4]Angelidis et al., 1995; [5]Karageorgis et al., 2005; [6]Lopes-Rocha et al., 2017b

The minimum value of all RBC$_{min}$ (Table 2), RMinCO (Table 3) and RMinC (Table 4) was taken as the lower limit for the Quality Check of the data and reported in Table 5.
The maximum value of all the RBC$_{max}$ (Table 2), RMAxCO (Table 3) and RMaxC (Table 4) was taken as the upper limit for the Quality Check of the data and reported in Table 5.

In Table 5 the ranges used for the quality check of the trace metals in sediments of the EMed are compared with the ranges from an extensive monitoring of sediments in the NW Mediterranean French coast (RNO, 1998). The selected ranges result quite comparable for Cd, Hg, Pb, Cu and Zn. The Zn maximum is about 2 fold higher in the Marseille area (RNO, 1998) which could be due to a higher level of pollution.

For the Quality Check of offshore sediments, the ranges could be more restricted taking into consideration only the ranges that could be derived from Tables 2 and 3. However this control was not performed due to the limited number of data on offshore sediments for the area of interest and to the lack of bottom depths in the metadata for a high number of data.

Table 5. Ranges used for the quality check of the trace metals in sediments in the EMed and comparison with ranges in WMed coastal sediments.

Element	**Units**		**EMed**			**WMed**[2]	
			Min	Max		Min	Max
Cd	mg kg^{-1} dw	RMinCO	0.06	18.2	RMaxC	<0.1	3.6
Hg	mg kg^{-1} dw	RMinCO	0.013	6.18	RMaxC	0.01	4.9
Pb	mg kg^{-1} dw	RMinCO	5	230	RMaxC	9.5	321
As	mg kg^{-1} dw	RMinCO	1	18.2	RMaxC	na	na
Cr	mg kg^{-1} dw	RMinC	19.4	276	RMaxCO	na	na
Cu	mg kg^{-1} dw	RMinCO	2	101	RMaxC	2.5	208
Ni	mg kg^{-1} dw	RBC_{min}	16.9	323	RMaxCO	na	na
Zn	mg kg^{-1} dw	RMinCO	34	339	RMaxC	21	741
Co	mg kg^{-1} dw	RMinCO	10	28.2	RMaxCO[1]	na	na
V	mg kg^{-1} dw	RMinCO	4	175	RMaxC	na	na

na: data not available [1]no data available for coastal sediments [2]RNO, 1998

4. Quality Control for organic pollutants: PAHs

Background concentrations for man-made substances (e.g, polychlorinated biphenyl, PCB) should be regarded as zero, however for the PAH there can be natural sources petrogenic or due to combustion (fires) which determine a non-zero level also in pre-industrial time. In this case the background level was estimated for the Mediterranean area as described below.

The background level was derived by the concentrations in deep cores (Table 6) obtained from scientific literature available since 1993. As the cores are representative of a limited variety of sedimentological environments, offshore (deep) surface sediments were considered to define the regional ranges of concentrations in areas subject to contamination (Table 7). The considered publications represent only a selection from the available literature, based on the applied analytical methods, sediment pre-treatment and regional availability of data for each polycyclic aromatic compound.

The minimum value between the RBC_{min} and RMinCO was considered as the lower limit to check the data of organic pollutants (Table 9).

The maximum concentrations for the Quality Check were derived by the Regional Maximum Concentration (RMaxC) reported for contaminated coastal areas of the Eastern Mediterranean as harbors and river mouths (Table 8).

Table 6. Regional background concentrations of PAH compounds in sediments of the Mediterranean Sea.

Compound	Unit	RBC		Mediterranean[1]	OSPAR-BC[2,3]	Ustica Island [4]	Elefsis bay [5]		WNAd [6]		Trieste Gulf [7]
		Min	Max								
Naphthalene	µg kg^{-1} dw	4.00	13.25	4	5	-	-	-	-	-	13.25
Acenaphthene	µg kg^{-1} dw	0.20	0.80	0.38	-	bdl	0.2	0.8			0.48
Acenaphtylene	µg kg^{-1} dw	0.50	1.23	0.5	-	-	-	-	-	-	1.23
Fluorene	µg kg^{-1} dw	bdl-0.60	1.67	0.75	-	1.67	0.6	1	bdl	bdl	1.59
Phenanthrene	µg kg^{-1} dw	3.30	15.20	4.55	4.0	3.67	7.3	3.3	9.9	15.2	3.49
Anthracene	µg kg^{-1} dw	0.20	1.50	0.8	1.0	-	1.3	0.3	1.1	1.5	0.2
Fluoranthene	µg kg^{-1} dw	0.83	15.50	5.6	7.5	1.33	9.3	1.9	15.5	14.5	0.83
Pyrene	µg kg^{-1} dw	1.54	11.60	10.28	6	1.67	7.4	2.5	9.6	11.6	1.54
Benzo[a]anthracene	µg kg^{-1} dw	bdl-1.7	8.90	3.45	3.5	bdl	1.7	8.9	-	-	3.55
Chrysene	µg kg^{-1} dw	bdl-1.07	9.50	1.3	4	bdl	9	1.7	9.5	3.9	1.07
Benzo[a]pyrene	µg kg^{-1} dw	bdl-1.6	9.70	2.55	4	bdl	3.5	1.6	9.0	9.7	2.28
Benzo[ghi]perylene	µg kg^{-1} dw	bdl-1.09	18.90	3.5	3.5	bdl	-	-	17.3	18.9	1.09
Indeno[1,2,3-cd]pyrene	µg kg^{-1} dw	bdl-0.2	12.70	1.7	-	bdl	0.2	6.1	bdl	12.7	1.35
Dibenzo[ah]anthracene	µg kg^{-1} dw	bdl-0.18	2.40	0.18	-	bdl	0.2	0.7	2.3	2.4	bdl**
Perylene	µg kg^{-1} dw	0.60	2.40	-	-	-	2.4	0.6	-	-	-
Benzo[b]fluoranthene	µg kg^{-1} dw	bdl	-	-	-	bdl	-	-	-	-	-
Dibenzothiophene	µg kg^{-1} dw	-	-	-	-	-	-	-	-	-	-
Benzo[k]fluoranthene	µg kg^{-1} dw	-	-	-	-	-	-	-	-	-	-
Stations selected							K	I	53	62	GT2
Core section	cm					>=8.5 cm	30-32	33-35	30-35	30-35	315
Sedimentation rate	mm yr^{-1}					0.4-0.6	2		~2 *	~2 *	1.2-1.8
Organic carbon	%					0.28	1.41	0.64	-	-	1.2

*derived fom Frignani et al., 2005 bdl: below detection limit; NAd: Northern Adriatic **the 0.00 value was assumed to be bdl

[1]UNEP-MAP, 2011; [2]UNEP-MAP, 2016; [3]OSPAR, 2009 ;[4]Berto et al., 2009; [5]Hatzianestis et al., 2004; [6]Caricchia et al., 1993; [7]Notar et al., 2001

PAHs can be determined in the sediments with a variable percent of error depending on the compound. Unfortunately, the recoveries, accuracies, precisions and LODs are usually not reported for the single compounds but as a range for the whole class of analyzed PAHs or for subgroups depending on the number of aromatic rings.

The PAHs in the studies used for the selection of background levels and the ranges in offshore and coastal sediments were extracted from sediments with a solvent mixture (n-hexane, hexane/acetone, or dichloromethane/methanol) usually with a Soxhlet apparatus (Bihari et al., 2006; Botsou & Hatzianetsis, 2012, Cardellicchio et al., 2007; Caricchia et al., 1993; Gogou et al., 2000; Hatzianestis et al., 2006; Tsapakis et al., 2010). In few cases the extraction was carried out with methylene chloride by Accelerated Solvent Extraction (ASE) (Mandić &Vrančić, 2017) or by ASE and Supercritical Fluid Extraction (Notar et al., 2001). After the purification of the extracts, the PAHs were determined usually by GC-MS (Botsou & Hatzianestis, 2012, Cardellicchio et al 2007; Gogou et al, 2000; Hatzianestis et al, 2006; Mandić & Vrančić , 2017; Notar et al, 2001; Tsapakis et al., 2010), or by HPLC with a fluorescence detector (Berto et al., 2009; Caricchia et al., 1993) or with a fluorescence and UV detector (Bihari et al., 2006).

Detection limits were usually not reported for each compound but as ranges for all the PAHs. Reported values ranged from 0.05 to 0.1 µg kg^{-1} (Bihari et al. 2006); from 0.06 to 3.45 µg kg^{-1} (Notar et al., 2001); from 0.6 to 9 µg kg^{-1} (Cardellicchio et al., 2007), from 0.03 to 0.1 µg kg^{-1} (Botsou & Hatzianestis, 2012). Berto et al. (2009) reported for all 15 investigated PAHs a detection limit of 0.5 µg kg^{-1}.

Reported recoveries of PAHs were: 77-97% (Notar et al, 2001), 77-91% Cardellicchio et al., 2007; 79-108% (Bihari et al., 2006); 62-95 % (Botsou & Hatizanestis, 2012), >80% (Hatzianestis et al., 2006), 82-92% (Berto et al., 2009), 60.28-100.00% (Gogou et al., 2000). The precision of the analytical determination was 7-19 % (Notar et al., 2001), 5-15% (Cardellicchio et al., 2007), 1.7-6.3% (Botsou et al., 2012), <15% (Berto et al., 2009).

Usually, the lowest recoveries were obtained for the PAHs with low molecular weights. For comparison, we considered the USGS (Unites States Geophysical Survey) report on PAH determination (Olson et al., 2004) where RSD of 10% were reported for CRMs. Overall, we assumed an error of ±15% in the single PAH determination. Therefore the concentrations below the lowest limit, 0.85* min (RBC_{min}, RMinCO), were considered “to be re-checked” this means that they should be controlled with the data originator e.g. there could be errors in the measurement units or in their conversion.

Table 7. Range of concentrations of PAH compounds in offshore sediments of the Mediterranean Sea.

Compound	Unit	Offshore sediments		Mediterranean[1] deep sediments	Cretan Sea[2]		MAd[3]	
		RMinCO	RMaxCO		min	max	min	max
Naphthalene	µg kg^{-1} dw	0.22	2.13	-	-	-	0.22	2.13
Acenaphthene	µg kg^{-1} dw	bdl, 0.20	1.05	1.05	-	-	bdl	0.2
Acenaphtylene	µg kg^{-1} dw	bdl, 0.15	0.33	0.33	-	-	bdl	0.15
Fluorene	µg kg^{-1} dw	0.18	0.45	0.45	-	-	0.18	0.43
Phenanthrene	µg kg^{-1} dw	0.74	7.21	3.95	0.74	4.18	1.13	7.21
Anthracene	µg kg^{-1} dw	0.04	1.56	1.56	0.04	0.32	0.17	0.27
Fluoranthene	µg kg^{-1} dw	0.73	11.1	6.7	1.13	11.1	0.73	3.27
Pyrene	µg kg^{-1} dw	0.5	6.35	2.1	0.5	6.35	0.77	3.13
Benzo[a]anthracene	µg kg^{-1} dw	0.2	47.39	1.28	0.36	4.82	0.2	47.39
Chrysene	µg kg^{-1} dw	0.25	7.3	6.64	0.97	7.3	0.25	5.15
Benzo[a]pyrene	µg kg^{-1} dw	0.25	6.65	3.71	0.54	6.65	0.25	2.04
Benzo[ghi]perylene	µg kg^{-1} dw	0.51	8.91	3.25	1.11	8.91	0.51	4.03
Indeno[1,2,3-cd]pyrene	µg kg^{-1} dw	1.07	9.85	4.49	1.39	9.85	1.07	7.18
Dibenzo[ah]anthracene	µg kg^{-1} dw	0.17	2.46	1.37	0.37	2.46	0.17	1.07
Perylene	µg kg^{-1} dw	0.28	18.35	-	0.43	18.35	0.28	3.1
Benzo[b]fluoranthene	µg kg^{-1} dw	8.32	-	8.32	-	-	-	-
Dibenzothiophene	µg kg^{-1} dw	0.15	0.71	-	-	-	0.15	0.71
Benzo[k]fluoranthene	µg kg^{-1} dw	6.03	-	6.03	-	-	-	-
Stations selected					all		S4-S7	
Sampled section	cm				0	1	not specified (top)	
Organic carbon	%				0.3	0.82		
Bottom depth	m				100	1570	78	175

[1] UNEP/MAP 2011; [2] Gogou et al., 2000; [3] Mandic&Vrancic, 2017

bdl: below detection limit; MAd: Middle Adriatic

Table 8. Range of concentrations of PAH compounds in coastal sediments (harbors and rivers prodeltas) of the Eastern Mediterranean Sea.

		Coastal sediments		WNAd[1]		WNAd[2]		NAd[3]		ENAd[4]		Ionian Sea[5]		EMed[6]		EMed[7]	
Compound	Unit			Po prodelta		Po delta, Ancona		Gulf of Trieste		Rovinj harbor		Taranto harbor		Greece coast		Greece coast	
		RMinC	RMaxC	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max	Min	Max
Naphthalene	μg kg^{-1} dw	bdl-3.11	76.3	-	-	bdl	47.9	3.11	76.3	bdl	bdl	15	56	-	-	-	-
Acenaphthene	μg kg^{-1} dw	bdl-0.1	256	-	-	bdl	31.3	-	-	bdl	bdl	26	83	0.1	256	-	-
Acenaphtylene	μg kg^{-1} dw	bdl-0.1	69.6	-	-	bdl	7.9	1.12	10.2	bdl	bdl			0.1	69.6	-	-
Fluorene	μg kg^{-1} dw	<0.1	172	3	6.9	bdl	6.4	0.76	4.64	bdl	bdl	4	69	0.8	172	<0.1	5
Phenanthrene	μg kg^{-1} dw	0.2	1571	18.7	41.8	-	-	6.43	50.31	4.28	1412	27	673	6.4	1571	0.2	13.1
Anthracene	μg kg^{-1} dw	bdl-<0.1	765	3.2	7.6	-	-	0.83	11.35	bdl	765	7	109	0.7	93.4	<0.1	4.6
Fluoranthene	μg kg^{-1} dw	bdl-0.1	3089	34.7	55.8	bdl	76.2	1.64	69.53	bdl	2758	39	1351	6.6	3089	0.1	21
Pyrene	μg kg^{-1} dw	bdl-0.1	2427	25.8	48.1	bdl	73.7	2.04	64.38	bdl	1149	37	1163	7	2427	0.1	19.7
Benzo[a]anthracene	μg kg^{-1} dw	<0.1	1888	-	-	-	-	1.56	40.94	4.76	1265	22	781	4.6	1888	<0.1	20.2
Chrysene	μg kg^{-1} dw	bdl-1.69	2327	20	42.5	-	-	1.69	51.48	bdl	1128	20	713	5.5	2327	-	-
Benzo[a]pyrene	μg kg^{-1} dw	bdl-<0.1	2756	6.7	36.9	bdl	125.8	0.83	53.31	2.06	141.89	28	1180	6.1	2756	<0.1	17.1
Benzo[ghi]perylene	μg kg^{-1} dw	bdl-<0.1	1924	27.1	51.4	bdl	67.9	1.36	59.09	bdl	1015	32	1160	5.9	1924	<0.1	25.1
Indeno[1,2,3-cd]pyrene	μg kg^{-1} dw	bdl-<0.1	1944	18.9	29.4	bdl	47.9	1	42.21	bdl	1158	29	1445	8.8	1944	<0.1	19.6
Dibenzo[ah]anthracene	μg kg^{-1} dw	bdl-0.33	1379	3.9	6	bdl	12	0.33	10.11	bdl	1379	17	631	1	402	-	-
Perylene	μg kg^{-1} dw	1.7	678	-	-	-	-	-	-	-	-	-	-	1.7	678	-	-
Benzo[b]fluoranthene	μg kg^{-1} dw	<0.1	3807	25.0	40.4	-	-	-	-	-	-	-	-	16.8	3807	<0.1	15.8
Dibenzothiophene	μg kg^{-1} dw	0.7	93.4	-	-	-	-	-	-	-	-	-	-	0.7	93.4	-	-
Benzo[k]fluoranthene	μg kg^{-1} dw	<0.1	16.6	11.6	16.6	-	-	-	-	-	-	-	-	-	-	<0.1	6.3
Stations selected				53, 57, 68		all		all		all		all		all		all	
Sampled section	cm			0	5	not specified		0	2	not specified		0	5	not specified		0	10
Organic carbon	%			-	-	-		0.18	1.32	-	-	-	-	-	-	-	-

[1]Caricchia et al., 1993; [2]Magi et al. 2002; Nota et al, 2001; [4]Bihari et al., 2006; [5]Cardellicchio et al., 2007; [6]Botsou&Hatzianestis, 2012; [7]Tsapakis et al., 2010

NAd: Northern Adriatic; Med: Mediterranean; bdl: below detection limit

Maximum concentrations reported from contaminated sediments, collected in coastal areas under elevated anthropogenic pressure as harbors and riverine prodeltas, were used to determine the higher limit (Regional Maximum Concentration, RMaxC) for the expected concentration range in the Eastern Mediterranean sediments.

Overall, we assumed an error of ±15% in the single PAH determination. Therefore, concentrations higher than 1.15*RMaxC were considered "to be re-checked" this means that they should be controlled with the data originators e.g. there could be errors in the measurement units or in their conversion.

The minimum value of all RBC_{min} (Table 6), RMinCO (Table 7) and RMinC (Table 8) was taken as the lower limit for the Quality Check of the data and reported in Table 9.

The maximunm value of all RBC_{max} (Table 6), RMaxCO (Table 7) and RmaxC (Table 8) was taken as the upper limit for the Quality Check of the data and reported in Table 9.

The range proposed for the Quality Check of the PAHs concentration in the Eastern Mediterranean Sea sediments are summarized in Table 9. For the Quality Check of offshore sediments the range can be more restricted taking into consideration only the range that can be derived from Tables 6 and 7. The control was not performed due to the limited data in offshore sediments and to the lack of bottom depths in the metadata for a high number of data.

Table 9. Ranges used for the quality check of the PAHs in sediments in the EMed and comparison with ranges in WMed coastal sediments.

Compound	Unit		EMed			WMed[1]	
			Min	Max		Min	Max
Naphthalene	μg kg^{-1} dw	RMinCO	0.22	76.3	RMaxC	-	-
Acenaphthene	μg kg^{-1} dw	RMinC	0.1	256	RMaxC	-	-
Acenaphtylene	μg kg^{-1} dw	RMinC	0.1	69.6	RMaxC	-	-
Fluorene	μg kg^{-1} dw	RMinC	0.1	172	RMaxC	-	-
Phenanthrene	μg kg^{-1} dw	RMinC	0.2	1571	RMaxC	-	-
Anthracene	μg kg^{-1} dw	RMinCO	0.04	765	RMaxC	-	-
Fluoranthene	μg kg^{-1} dw	RMinC	0.1	3089	RMaxC	4.5	8200
Pyrene	μg kg^{-1} dw	RMinC	0.1	2427	RMaxC	-	-
Benzo[a]anthracene	μg kg^{-1} dw	RMinC	0.1	1888	RMaxC	-	-
Chrysene	μg kg^{-1} dw	RMinCO	0.25	2327	RMaxC	-	-
Benzo[a]pyrene	μg kg^{-1} dw	RMinC	0.1	2756	RMaxC	<1	2340
Benzo[ghi]perylene	μg kg^{-1} dw	RMinC	0.1	1924	RMaxC	<1	2525
Indeno[1,2,3-cd]pyrene	μg kg^{-1} dw	RMinC	0.1	1944	RMaxC	<1	1900
Dibenzo[ah]anthracene	μg kg^{-1} dw	RMinCO	0.17	1379	RMaxC	-	-
Perylene	μg kg^{-1} dw	RMinCO	0.28	678	RMaxC	-	-
Benzo[b]fluoranthene	μg kg^{-1} dw	RMinC	0.1	3807	RMaxC	<1	2790
Dibenzothiophene	μg kg^{-1} dw	RMinCO	0.15	93.4	RMaxC	-	-
Benzo[k]fluoranthene	μg kg^{-1} dw	RMinC	0.1	-		<1	1320

[1]RNO, 1998 Med: Mediterranean

5. Application of Quality Control methodological proposal on EMODnet Chemistry data

5.1. Trace metals: Cd, Pb, Hg, and Cu

The procedure for Quality Control of data archived in EMODnet Chemistry was tested for some trace metals as Cd, Pb and Hg which are commonly monitored in the sediments.

Cadmium (Cd) - Sediment Profiles Dataset
The data with the following 6 P01 labels were present in the datasets and were considered:

ConceptID	Preferred label
MTSDM001	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of sediment <63um by inductively-coupled plasma mass spectrometry
CONCDS01	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of sediment <2000um
CONCDS02	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of sediment <63um
MCDSP012	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of sediment
GEOLSACD	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of geological sample
CDCNAAWF	Concentration of cadmium {Cd CAS 7440-43-9} per unit dry weight of sediment <63um by wet sieving, acid digestion and atomic absorption spectroscopy

At least 2 labels are unclear or potentially misleading:
it is unclear which is the difference between MCDSP012 and GEOLSACD

Data not considered:
14 data from Varano lagoon, CNR, Institute of Marine Science (ISMAR, Lesina) as these sediments are located in transitional waters which are not considered for this specific Project.
19 data from CEREGE were outside the area of interest

Data to be “rechecked”:
8 data were with values “0” but they were correctly flagged with 6 “value below detection limit”
8 data from OGS, Cruise: Ferriera. Date 2009-04-05 Presented an incongruence in the units “µg/kg”, as the term in the P01 catalogue was:
CDXXISPW Concentration of cadmium {Cd CAS 7440-43-9} per unit volume of the sediment pore water [dissolved plus reactive particulate <0.4/0.45um phase] by in-situ pore water sampling, filtration, chelation, solvent extraction and atomic absorption spectroscopy

45 data from Institute of Marine Biology (IMBK) had all 0 values with Quality Flag "1" this should be changed to "6"
47 data from IEO/Murcia Oceanographic Centre had a Longitude >355 and their geographical position could not be identified.

271 data were considered usable (Table 10) and represented in figures 2 and 3.

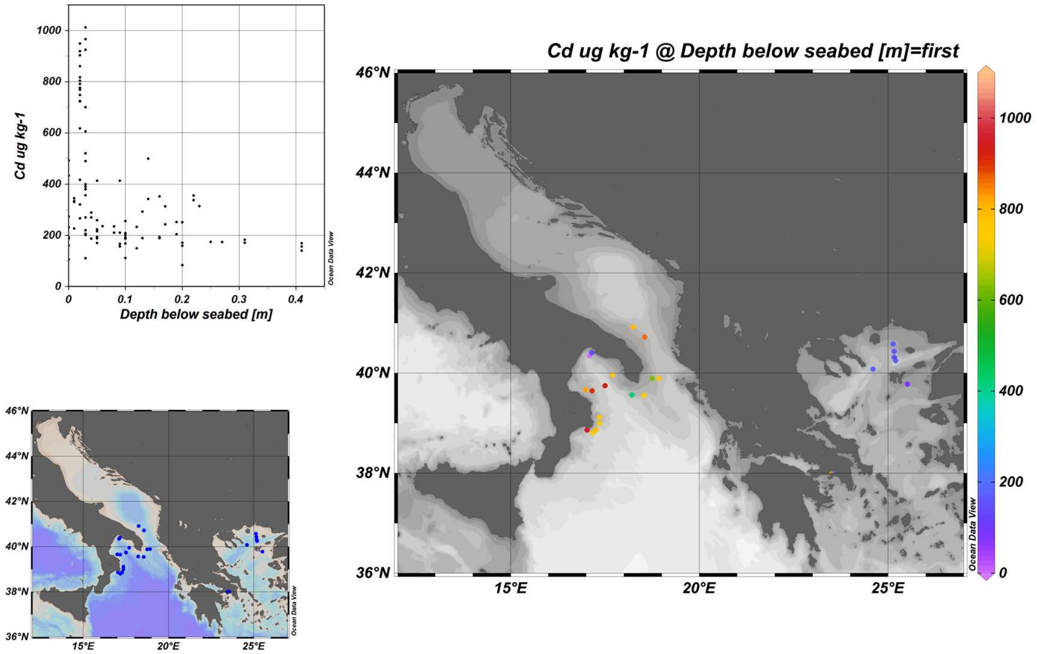

Figure 2. Cadmium (Cd) concentrations in surface sediments (right) and below the sediment-water interface (left).

Table 10. Descriptive statistics for the sediment profiles data set of cadmium (Cd) and comparison with the limits for the Quality Check (green color: within the limits, red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	270	455	152	15	2250	34	1270	520.1	1.5	1.6		
Water depth [m]	126	624	213	20	2250	43	1500	646.7	0.8	-0.5		
Depth below seabed [m]	270	0.1	0.0	0.0	0.4	0.0	0.2	0.1	1.8	2.6		
Cd [µg kg^{-1}]	271	472	313	0.0	2583	156	914	371	1.6	4.3	54	20020

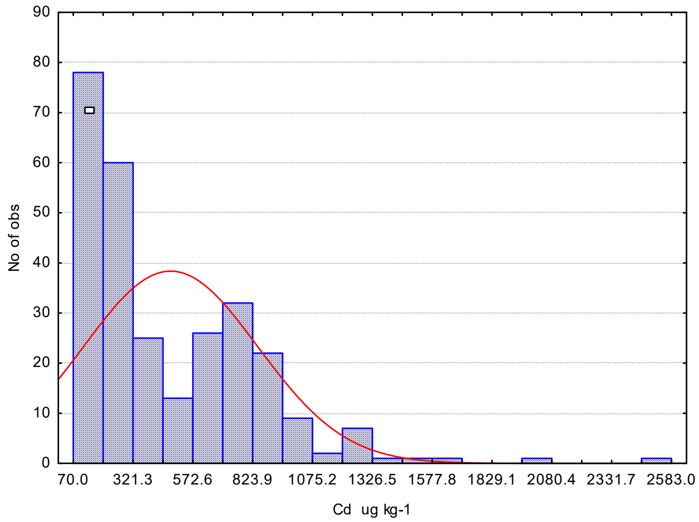

Figure 3: Frequency distribution of Cd concentrations from the sediment profile data set after exclusion of the data considered to be “re-checked”.

Cadmium (Cd) – Sediment time series Dataset

2757 data were available for the area of interest (Table 11) and are presented in Figures 4, 5 and 6.

However, metadata are not complete and should be re-checked as there is no indication of bottom depth or station depth for 2530 data.

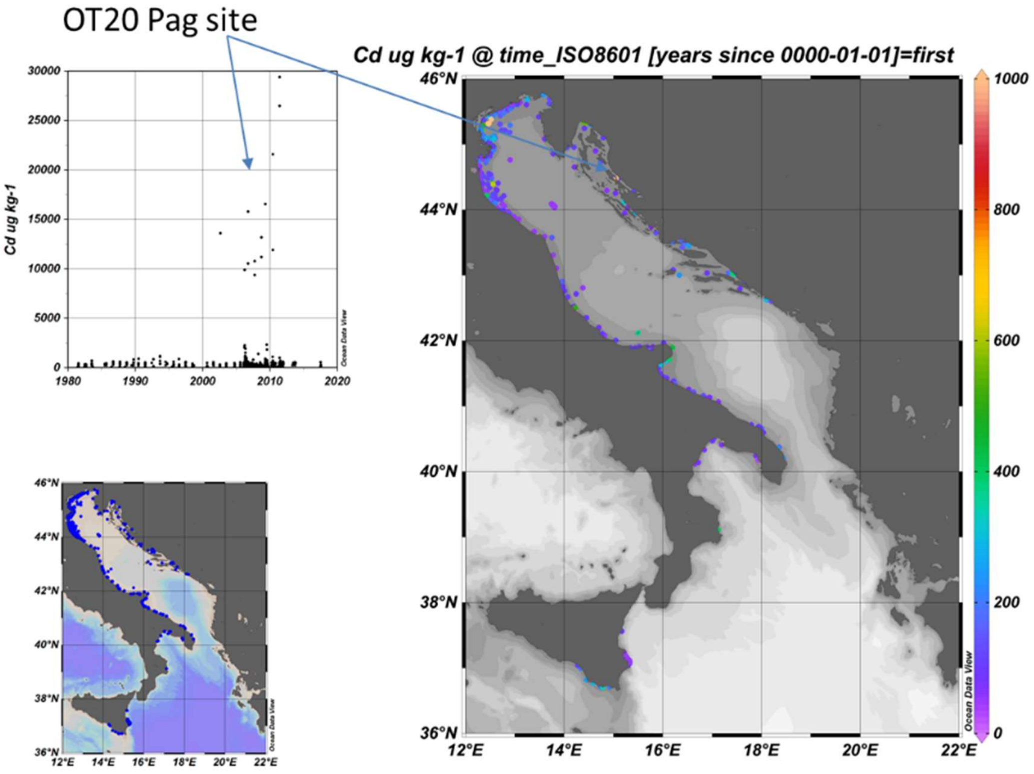

Figure 4. Cadmium (Cd) concentrations in surface sediments (right) and the data distribution as a function of the time (left). This analysis allowed us to recognize

that data of OT20 Pag site were too high, as this is an unpolluted area, and it was found that these data refer to Cu concentrations in sediments and not to Cd.

Data to be "re-checked"

Referring to the 1370 data below the lower limit reported in Table 10 of which 1360 data are equal to 50 µg kg^{-1} (ISPRA) and 502 are flagged with "6", while the rest with "1".

All these data seem to represent the LOD of the analytical method applied.

The fact that such a high number of data for a wide spatial area are at the level of the detection limit or below, means that probably the method of dissolution of the sediment was not based on a total digestion with hydrofluoric acid. Unfortunately, not sufficient information is available in the metadata to ascertain this hypothesis. Other 8 values (ISPRA) fall between 1 µg kg^{-1} and <50 µg kg^{-1}, and 2 data (Institute of Oceanography and Fisheries and ISPRA) fall between 50 µg kg^{-1} and 54 µg kg^{-1} (RMinCO', Table 11).

Data visualization (Fig. 4) allowed to recognise that the values higher than the upper limit of 20020 µg kg-1, and those ranging from 9369 µg kg-1 to 29410 µg kg-1 collected at the same station, were very suspicious. A careful checking by the data originator allowed us to understand that this data were results for Cu and not for Cd.

Table 11. Descriptive statistics for the time series data set of cadmium (Cd) in sediments and comparison with the limits for the Quality Check (red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90.	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	227	50.9	38.0	2.0	105.0	23.0	105.0	32.2	0.7	-0.9		
Water depth [m]	227	50.9	38.0	2.0	105.0	23.0	105.0	32.2	0.7	-0.9		
Cd [µg kg^{-1}]	2757	213.4	60.0	1.0	29410	50.0	308.5	1143.6	17.6	352.8	54	20020

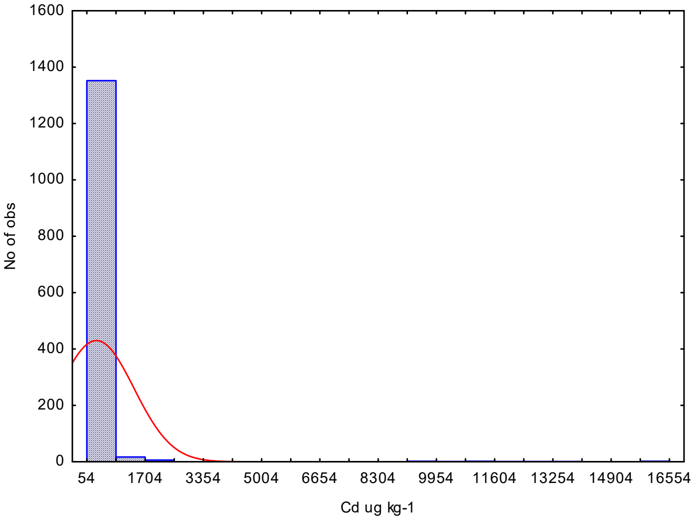

Figure 5. Frequency distribution of Cd concentrations in sediment time series data set after exclusion of the data considered to be "re-checked".

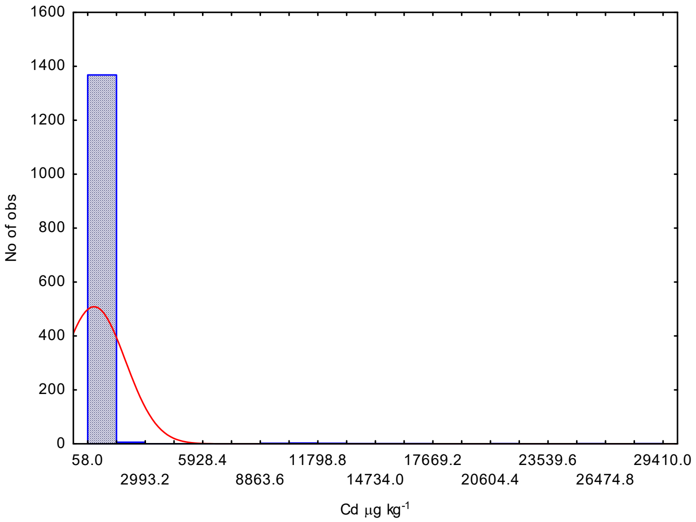

Figure 6. Frequency distribution of Cd concentrations in sediment time series data set after exclusion of the data considered to be "re-checked" only for the lower limit.

LEAD (Pb) - Sediment Profiles Dataset
The data with the following 8 types of P01 labels were present in the data set and were considered:

ConceptID	Preferred label
MTSDM004	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment <63um by inductively-coupled plasma mass spectrometry
CONPBS01	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment <2000um
MPBSP012	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment
GEOLSAPB	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of geological sample
PBCNXTXT	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment by compression into pellets and X-ray fluorescence
PBCNPEXT	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment by acid digestion and inductively-coupled plasma atomic emission spectroscopy
PBCNAAWF	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment <63um by wet sieving, acid digestion and atomic absorption spectroscopy
CONPBS02	Concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment <63um

At least 4 labels are unclear or potentially misleading:
It is unclear which is the difference between MPBSP012 and GEOLSAPB

Moreover, the lack of information about the mixture used in the acid digestion is confusing, because only the adoption of a mixture containing HF in sealed teflon containers in a microwave oven can assure the total dissolution of the sediment sample.

Data not considered:
14 data from CNR, Institute of Marine Science (ISMAR Lesina) were from Varano lagoon (Varano_POR_PUGLIA_Pr)
40 data from CNR, Institute of Marine Science (ISMAR Lesina) were from Varano lagoon (ELTCON)
129 data from CNR, Istituto di Scienze Marine (Sezione di Venezia - ex IBM) were from the Po river
9 data from CEREGE were outside the area of interest

Data to be re-checked:
47 data from IEO/Murcia Oceanographic Centre had a Longitude >355 and it was not possible to identify the position of the stations
45 data from Institute of Marine Biology (IMBK) all concentrations different from 0 were in the range between 0.01 and 0.76 μg kg^{-1} i.e. from 6.6*10^3 to 5*10^5 fold lower than the RMinCO (Table 5)
8 data from OGS, Cruise: Ferriera. Date 2009-04-05 presented an incongruence in the units μg/kg as the term in the P01 catalogue was PBXXISPW Concentration of lead {Pb CAS 7439-92-1} per unit volume of the sediment pore water [dissolved plus reactive particulate <0.4/0.45 μm phase] by in-situ pore water sampling, filtration, chelation, solvent extraction and atomic absorption spectroscopy

1154 data were considered usable (Table 12) and are represented in the figures 7 and 8.

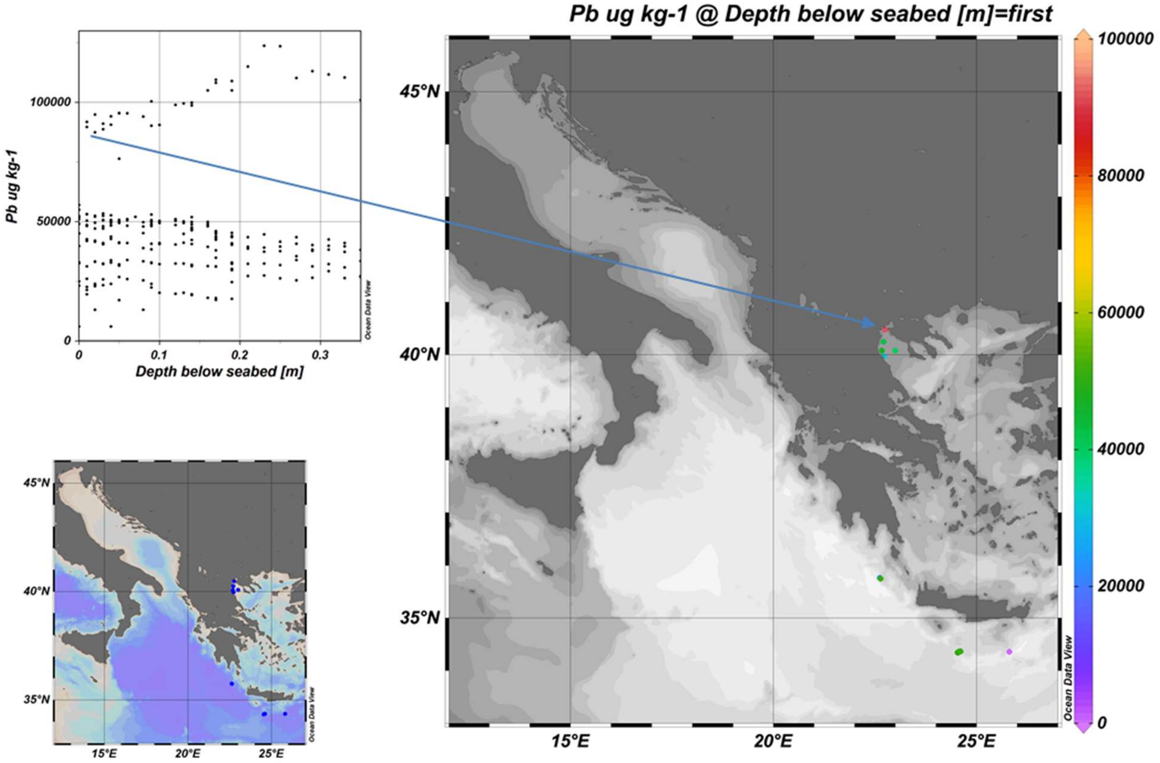

Figure 7. Lead (Pb) concentrations in surface sediments (right) and below the seabed (left).

Table 12. Descriptive statistics for the sediment profile data set of lead (Pb) in sediments and comparison with the limits for the Quality Check (red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Minimum	Maximum	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	1154	208	55	5	3450	15	599	496	4	21		
Water depth [m]	399	388	63	20	3450	30	1300	765	3	6		
Depth below seabed [m]	1154	0.2	0.1	0.0	1.3	0.0	0.4	0	2	8		
Pb [µg kg^{-1}]	1154	33261	25620	0	373900	12890	51000	33733	5	42	4500	253000

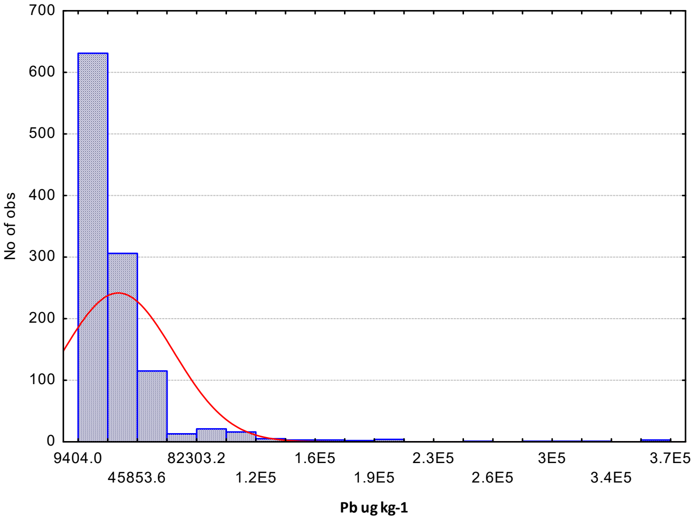

Figure 8. Frequency distribution of Pb concentrations from the sediment profile data set after exclusion of the data considered to be "re-checked"

Lead (Pb) - Sediment Time series Dataset

2756 data were in the area of interest (Table 13) and are represented in Figures 9, 10 and 11.

For 2538 data no bottom depth or station depth or water depth was indicated in the metadata (ISPRA-Institute for Environmental Protection and Research).

Data to be re-checked:

87 data fall below the lower limit RMinCo (table 4), of these, 24 values are equal to1000 µg kg^{-1} with QF 6 (ISPRA-Institute for Environmental Protection and Research) 1 value is equal to 1000 µg kg^{-1} with QF 1.

There seems to be an incongruence as there are 812 values all equal to 5000 µg kg^{-1} labelled with QF 1 (ISPRA). It seems suspect that there are so many identical values. If this is the LOD for that dataset (higher than 1000 µg kg^{-1} which is indicated as the LOD), the values should be flagged accordingly.

However, in any case the reported values are much lower than the RBC$_{min}$ (Table 2) and also with respect to the RMinCO in offshore sediments (Table 3). The difference could be related to uncomplete dissolution method used for the determination of the total lead concentration. However, no information is available in the metadata to ascertain this hypothesis.

The other potential explanation of the differences could be the comparison between the range found in unsieved sediments with those found in the fine fraction, as the

ISPRA data refers to concentration of lead {Pb CAS 7439-92-1} per unit dry weight of sediment <63um by wet sieving, acid digestion and atomic absorption spectroscopy. This, anyway, would not be a reasonable explanation as trace metals, and in particular Pb, are usually more concentrated in the finer fraction (< 63 µm).

It is to remark that the reported values, higher than the RMaxC (Table 5), derive from potentially hot spot areas, subject to elevated anthropogenic pollution. Pb concentrations up to 388 mg kg^{-1} and 637 mg kg^{-1} have been reported in Trieste harbor (Cibic et al., 2017) and Rijeka Harbor (Cukrov et al., 2011), respectively. In Ierissos Gulf (Aegean Sea), concentrations up to 586 and 2233.1 mg kg^{-1} have been reported by Sakellariadou (1987) and Stamatis et al (2002), respectively. Only after a careful check with the originators, and the availability of a QC data set, it could be decided if the upper limits for coastal area of the region of interest should be increased, possibly calculating them with a statistical method.

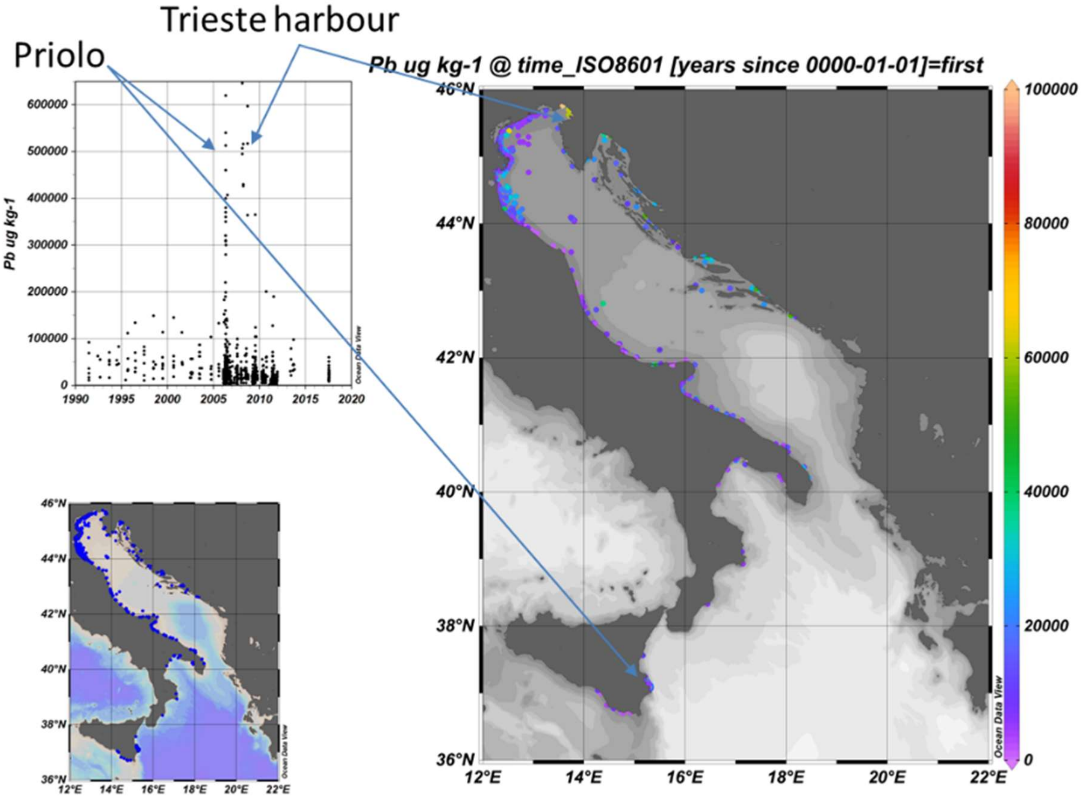

Figure 9. Lead (Pb) concentrations in surface sediments (right) and the data distribution as a function of the time (left).

Table 13. Descriptive statistics for the time series data set of lead (Pb) in sediments and comparison with the limits for the Quality Check (red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	**Valid N**	**Mean**	**Median**	**Min**	**Max**	**Percentile 10**	**Percentile 90**	**Std.Dev.**	**Skewness**	**Kurtosis**	**RBCmin'**	**RMaxC'**
Bot. Depth [m]	218	48.3	38.0	2.0	105.0	13.0	105.0	32.2	0.8	-0.7		
Water depth [m]	218	48.3	38.0	2.0	105.0	12.5	105.0	32.2	0.8	-0.7		
Pb [µg kg^{-1}]	2755	22916.0	14000.0	232	646000	5000	38720	46869	8.1	77.2	4500	253000

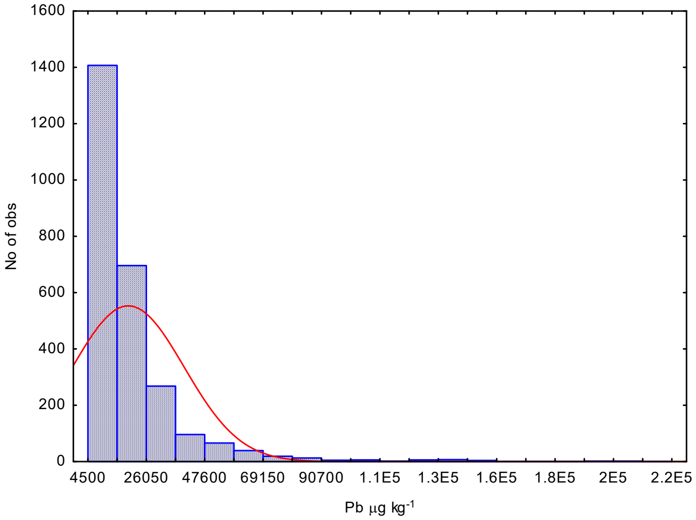

Figure 10. Frequency distribution of Pb concentrations from the sediment profile data set after exclusion of the data considered to be "re-checked".

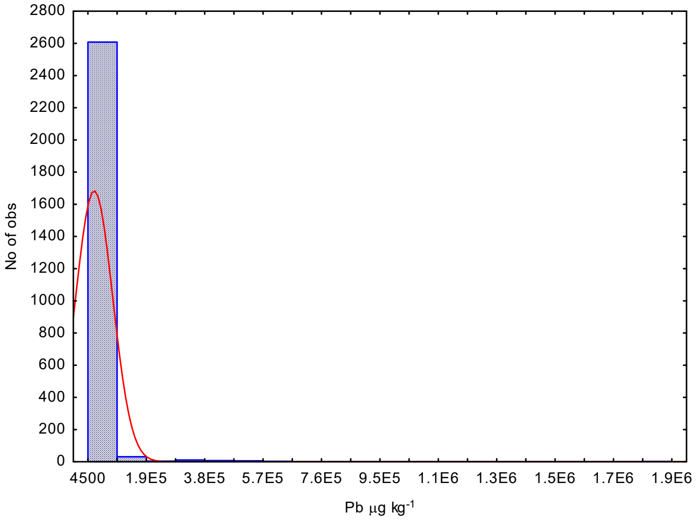

Figure 11. Frequency distribution of Pb concentrations from the sediment profile data set after exclusion of the data considered to be "re-checked" only for the lower limit.

Mercury (Hg) - Sediment Profiles Dataset

The data with the following 4 types of P01 labels were considered:

ConceptID	Preferred label
MTSDM005	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit dry weight of sediment <63um by inductively-coupled plasma mass spectrometry
CONHGS01	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit dry weight of sediment <2000um
MHGSP012	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit dry weight of sediment
HGCNCFXT	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit dry weight of sediment by cold vapour atomic absorption spectroscopy

Not considered:
7 data from Varano lagoon, CNR, Institute of Marine Science (ISMAR) (Lesina)
40 data from CNR, Institute of Marine Science (ISMAR, Lesina) almost all data (37) were 0 and only 3 data were >0, which were classified as “to be re-checked” or labelled with QF6.
129 data from CNR, Istituto di Scienze Marine (Sezione di Venezia - ex IBM) were from inner Po river

Data considered “to be re-checked”:
47 data from IEO/ Murcia Oceanographic Centre had a Longitude >355 and therefore their geographical position could be not determined, moreover they were all referring to a “Depth below seabed [m]” of 5, which seems unrealistic.
45 data all with values equal to 0 or $<10^{-5} \div 10^{-6}$ µg kg^{-1} from Institute of Marine Biology (IMBK) as they are orders of magnitude below the lower limit (Table 5)
27 data (IAMC_MSFD_2015_sedim) have values higher (range: 138815-141081 µg kg^{-1}) than the upper limit of the RMaxC (Table 5). It is to be noted that all these data were related to sediments sampled in a contaminated area (Augusta) and therefore could be due to a hot spot of extremely high pollution.
No value was below the lower limit (Table 5) 0.9* RBC (0.02 mg kg^{-1}) = 0.018 mg kg^{-1}

287 data were considered usable (Table 14) and are represented in figures 12, 13 and 14.

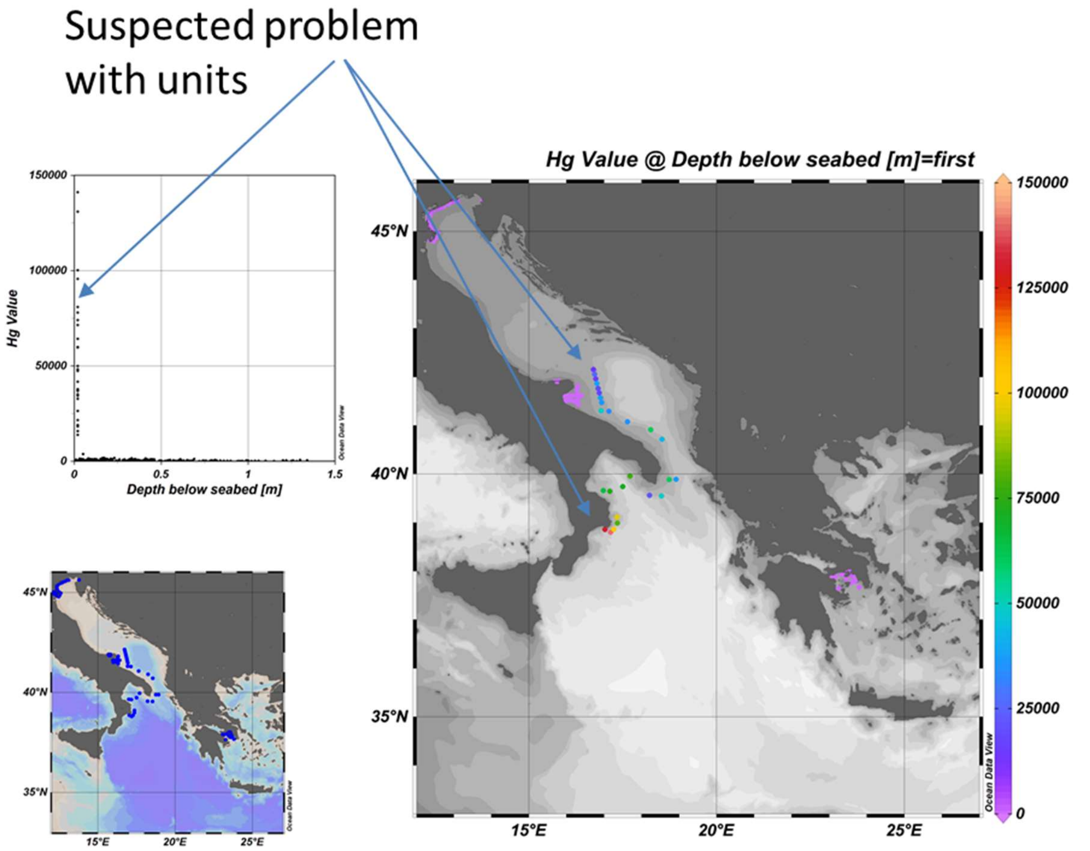
Suspected problem with units

Figure 12. Mercury (Hg) concentrations in surface sediments (right) and below the seabed (left).

Table 14. Descriptive statistics for the sediment profile data set of mercury (Hg) in sediments and comparison with the limits for the Quality Check (green color: within the limits, red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	287	71.75	16.00	5	1886	11	145	190.1	5.2	35.1		
Water depth [m]	38	89.11	72.00	17	400	17	210	93.1	2.2	5.1		
Depth below seabed [m]	287	0.30	0.17	0.01	1.34	0.02	0.82	0.32	1.28	0.86		
Hg [μg kg^{-1}]	287	5466	230	20	141081	80	1650	18784	4	22	11.7	6798

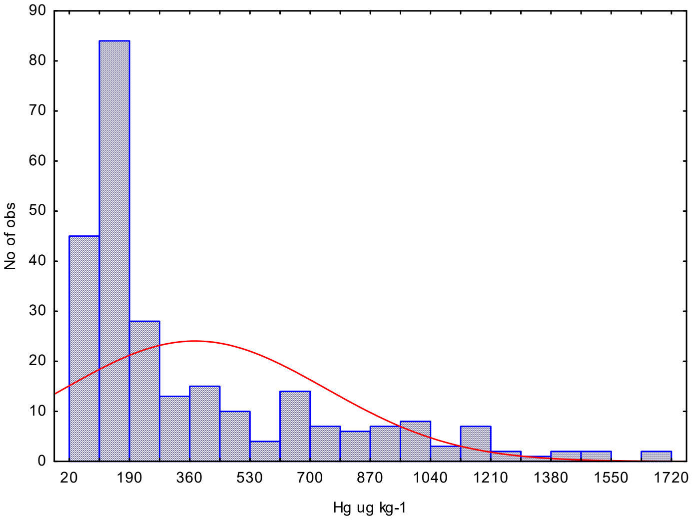

Figure 13. Frequency distribution of Hg concentrations from the sediment profile data set after exclusion of the data considered to be “re-checked”.

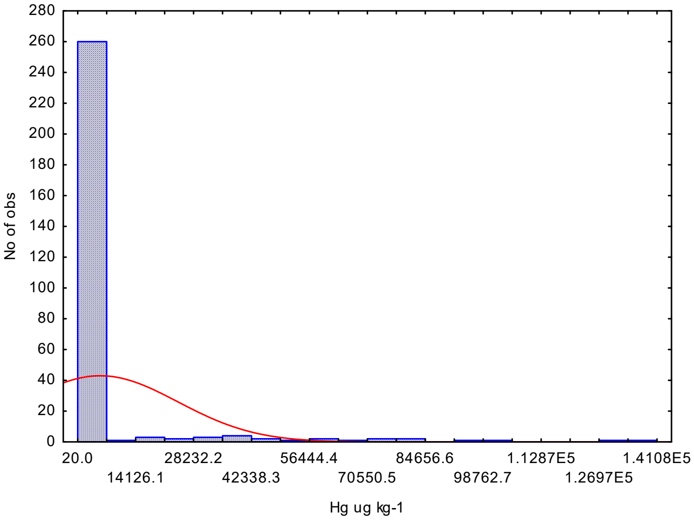

Figure 14. Frequency distribution of Hg concentrations from the sediment profile data set after exclusion of the data considered to be “re-checked”only for the lower limit.

The concentrations of the 22 data in the Ionian Sea, from CNR of Italy - Institute for Marine and Coastal Environment (IAMC Sezione Capo Granitola), exceed the upper limit set for Quality Check (Table 5). These values range from 32752 to 141081 µg kg^{-1} and are related to sediments sampled at depth ranging from 111-1886 m. The deep sediments therefore present concentrations from 1600 to 7000 fold higher than RBC$_{min}$. These data should be re-checked.

Mercury (Hg) - Sediment time series dataset

2561 data were available for the area of interest (Table 15) and are represented in the figures 15, 16 and 17.

No bottom depth metadata or station depth for 2514 data

Data to be re-checked:
29 values (ISPRA) are below the lower limit and should be re-checked of these 19 values are equal to 1 µg kg^{-1} (QF 6) and 10 values are between 1 µg kg^{-1} and 10 µg kg^{-1}

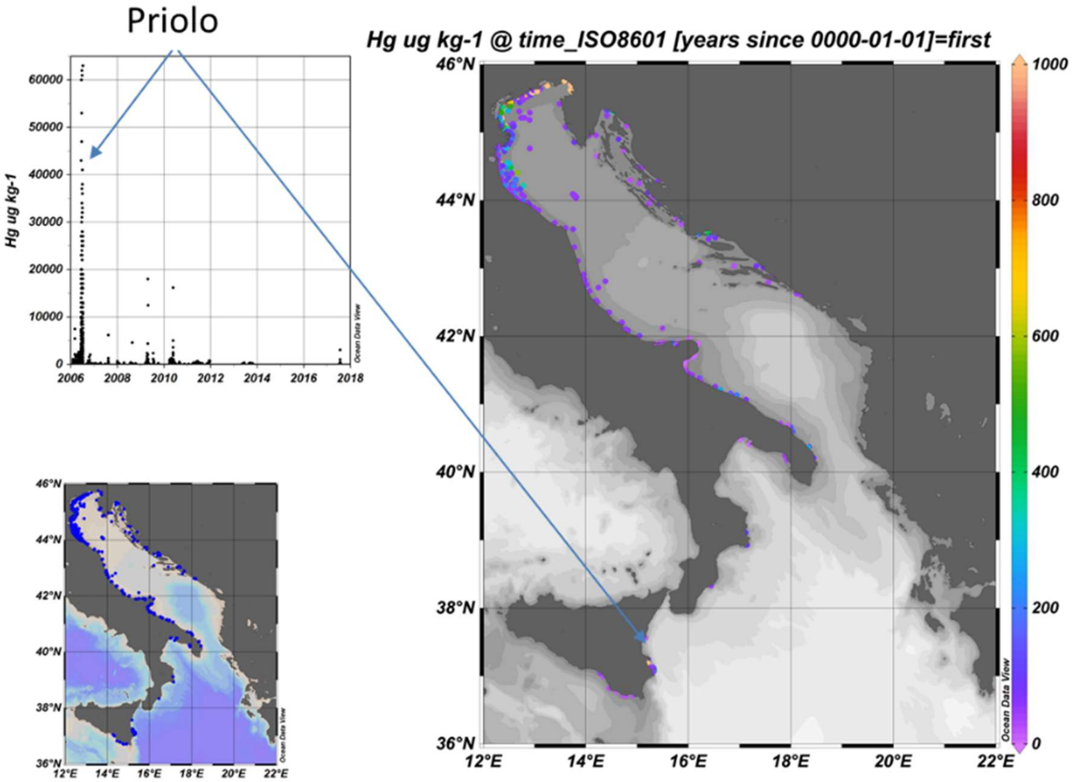

Figure 15. Mercury (Hg) concentrations in surface sediments (right) and the data distribution as a function of the time (left).

133 values (ISPRA) which are higher than the lower limit (RMinCO', Table 5) are from the "hot spot" site of Priolo in Sicily and range from 6800 µg kg^{-1} to 63000 µg kg^{-1}.
3 values (ISPRA-Institute for Environmental Protection and Research) are from Porto Buso, Porto Nogaro, baia di Panzano in the North Eastern Adriatic sea where a high contamination derived from a cinnabar mining activity through the Isonzo river. In this area Hg concentrations in sediments up to 23300 µg kg^{-1} have been reported (Covelli et al., 2001).

As the Concentration of total mercury {total_Hg CAS 7439-97-6} are expressed per unit dry weight of sediment <63 µm (by wet sieving, acid digestion, stannous chloride reduction and cold vapour atomic fluorescence spectrophotometry) the higher concentration with respect to the range set for the Quality Check could be due to a highly polluted site but also to the Hg enrichment in the fine sediment fraction (<63 μm).

Table 15. Descriptive statistics for the time series data set of mercury (Hg) in sediments and comparison with the limits for the Quality Check (red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Maximum	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	47	39.3	42.0	2.0	102.0	3.0	71.0	26.1	0.3	-0.4		
Water depth [m]	47	39.3	42.0	2.0	102.0	3.0	71.0	26.1	0.3	-0.4		
Hg [ug kg^{-1}]	2561	1290.2	100.0	1.0	63000.0	50.0	1700.0	4880.7	6.7	58.3	11.7	6798

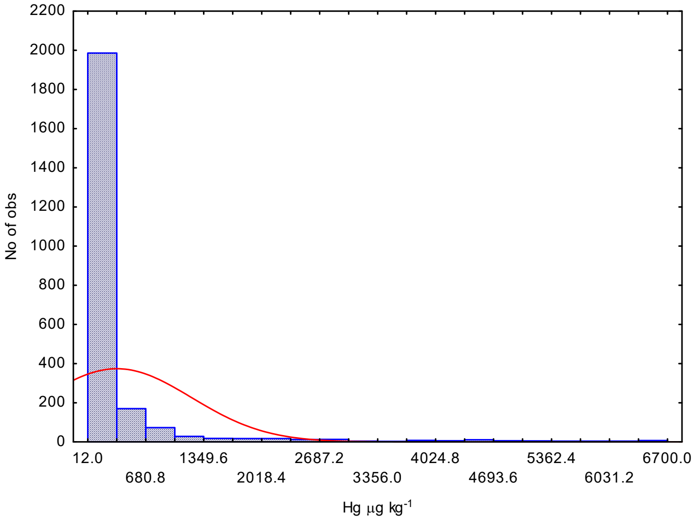

Figure 16. Frequency distribution of Hg concentrations from the sediment time series data set after exclusion of the data considered to be “re-checked”.

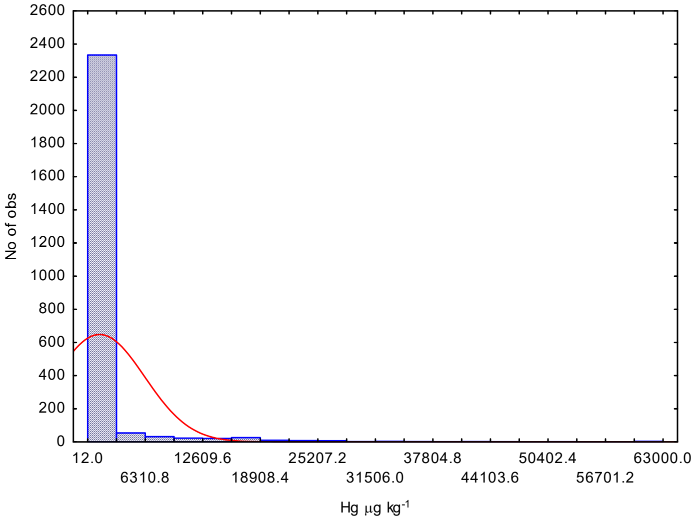

Figure 17. Frequency distribution of Hg concentrations from the sediment time series data set after exclusion of the data considered to be “re-checked” only for the lower limit.

Copper (Cu) - Sediment Profiles Dataset

The data with the following labels were present in the data set and were considered:

ConceptID	Preferred label
GEOLSACU	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of geological sample
CUCNAAWF	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of sediment <63um by wet sieving, acid digestion and atomic absorption spectroscopy
CUCNPEXT	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of sediment by acid digestion and inductively-coupled plasma atomic emission spectroscopy
CUCNXTXT	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of sediment by compression into pellets and X-ray fluorescence
MCUSP012	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of sediment
RWSSED30	Concentration of copper {Cu CAS 7440-50-8} per unit dry weight of sediment <63um

Data not considered:
Thirteen (13) data Varano_POR_PUGLIA_Pr from CNR, Institute of Marine Science (ISMAR) (Lesina) were from Varano lagoon
Thirtyeight (38) data ELTCON from CNR, Institute of Marine Science (ISMAR, Lesina) were from Varano lagoon
6 data from CEREGE were outside the area of interest

Data to be "re-checked":
45 data Institute of Marine Biology (IMBK) as all of the values were < 0.58 μg kg^{-1} ie. more than 3400 folds lower than the than RMinCO and more than 19000 folds lower than the RBC_{min} (Table 5) .
8 data from OGS, Cruise: Ferriera - Date 2009-04-05 have incongruence in the units as they are expressed as μg/kg but the P01 refers to the concentration of Cu in pore waters [dissolved plus reactive particulate <0.4/0.45 μm phase] by in-situ pore water sampling, filtration, chelation, solvent extraction and atomic absorption spectroscopy

A total of 780 data were considered usable (Table 16) and are presented in figures 18 and 19.

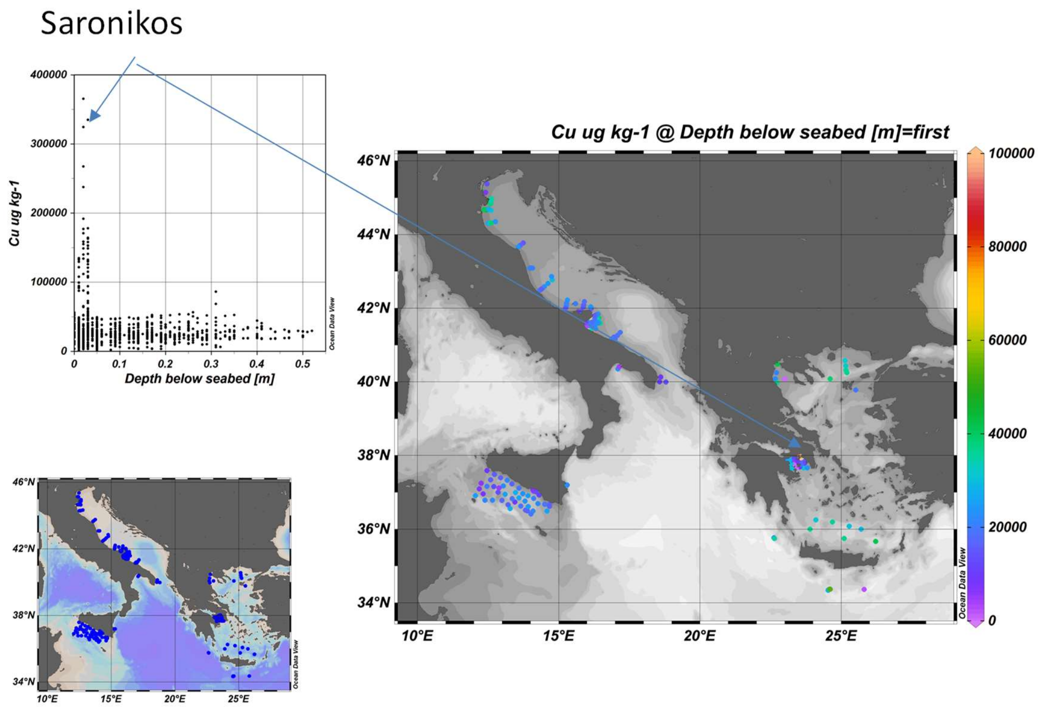

Figure 18. Copper (Cu) concentrations in surface sediments (right) and below the seabed (left).

Table 16. Descriptive statistics for the sediment profile data set of copper (Cu) in sediments and comparison with the limits for the Quality Check (green color: within the limits). RMinCO' and RMaxC' are the limits reported in Table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	779	244	55	11	3450	23	599	554	3.9	16.7		
Water depth [m]	344	407	63	30	3450	50	1300	781	2.6	6.0		
Depth below seabed [m]	779	0.1	0.1	0.0	0.5	0.0	0.3	0.1	1.1	0.6		
Cu [µg kg^{-1}]	779	25323	24200	2000	49900	12787	39000	10064	0.2	-0.3	1800	111100

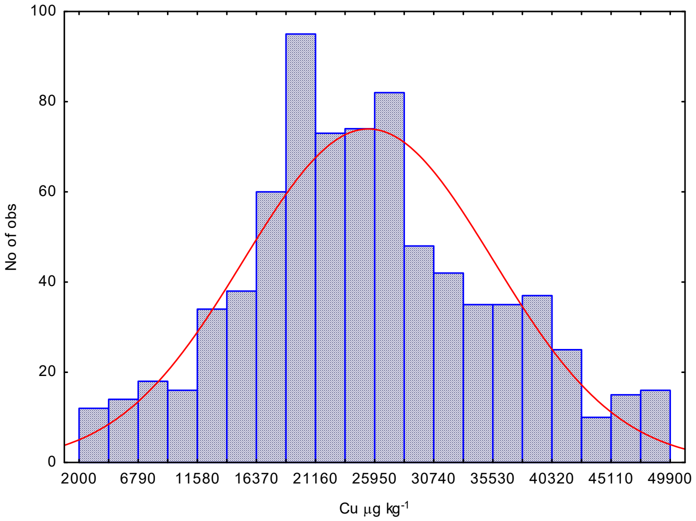

Figure 19. Frequency distribution of Cu concentrations from the sediment profile data set.

Copper (Cu) - Sediment Time series Dataset

2595 data were available for the area of interest (Table 17) and are presented in figures 20, 21 and 22.
No bottom depth or station depth is available for 2393 data.

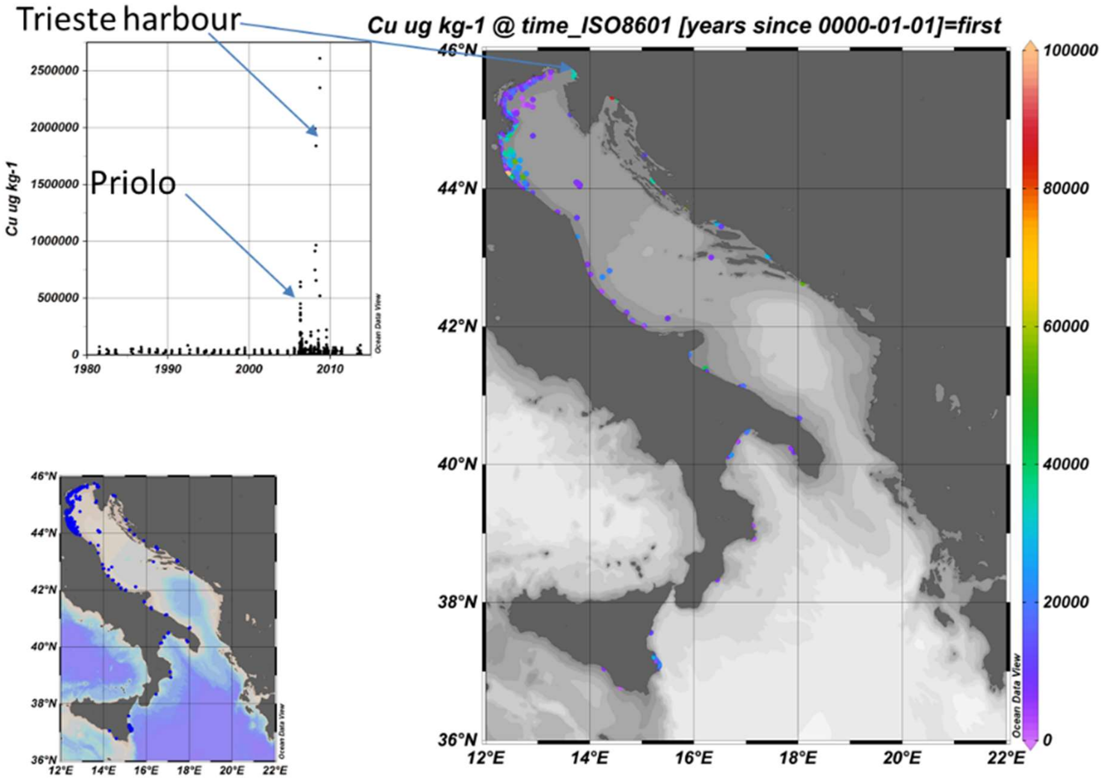

Figure 20. Copper (Cu) concentrations in surface sediments (right) and the data distribution as a function of the time (left).

Data considered to be "re-checked":
92 data (ISPRA) are lower than the RMinCO' (Table 16) and ranged from 42.6 to 1760 µg kg^{-1}. Many of these values were repeated (19 values=500 µg kg^{-1}; 12 value =1500 µg kg^{-1};12 values =1600 µg kg^{-1}, 8 values =1700 µg kg^{-1}) and seemed to be LOD values but were flagged with 1.
39 data higher than RMaxC' (Table 16) ranging from 115610 to 2610000 µg kg^{-1} of these 16 were from Priolo (ISPRA) ranging from 125000 to 640000 µg kg^{-1}; 2 from Cesenatico harbor (116000 µg kg^{-1} and 137400 µg kg^{-1}, ISPRA); 9 Ravenna offshore area (Agostino A, Garibaldi A, Antonella, 115610-800110 µg kg^{-1}, ISPRA); 9 from Trieste harbor (OGS) ranging from 519000 µg kg^{-1} to 2610000 µg kg^{-1}; 1 from Split and 1from Zadar (142440 and 212870 µg kg^{-1}, Institute of Oceanography and Fisheries).

Presumably some of these potential "outliers" are from hot spot sites where higher concentrations of Cu can be found in the sediments whereas other are presumably doubtful data. Moreover it has to be noticed that the ISPRA data of Cu refers to the concentration of Cu per unit dry weight of sediment <63 µm (by wet sieving, acid digestion and atomic absorption spectroscopy) therefore the Cu could be enriched in the fine sediment fraction with respect to the RMaxC that was set on the basis of concentrations determined on the not sieved sediments.

Table 17. Descriptive statistics for the time series data set of copper (Cu) in sediments and comparison with the limits for the Quality Check (green color: within the limits, red color: out of the limits). RMinCO' and RMaxC' are the limits reported in table 5 multiplied by 0.90 and 1.10, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	202	50.3	38.0	2.0	105.0	13.0	105.0	34.2	0.7	-1.0		
Water depth [m]	202	50.3	38.0	2.0	105.0	12.5	105.0	34.2	0.7	-1.0		
Cu [µg kg^{-1}]	2595	26855.5	18000	42.7	2610000	3300.0	37600.0	98908.2	18.6	407.3	1800	111100

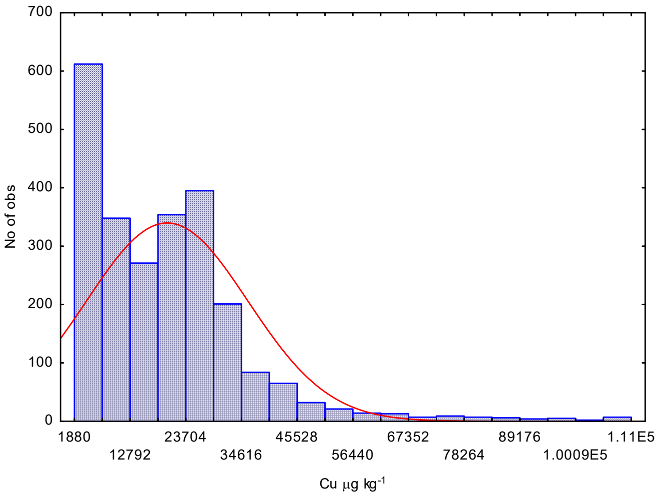

Figure 21. Frequency distribution of Cu concentrations from the sediment time series data set after exclusion of the data considered to be “re-checked”.

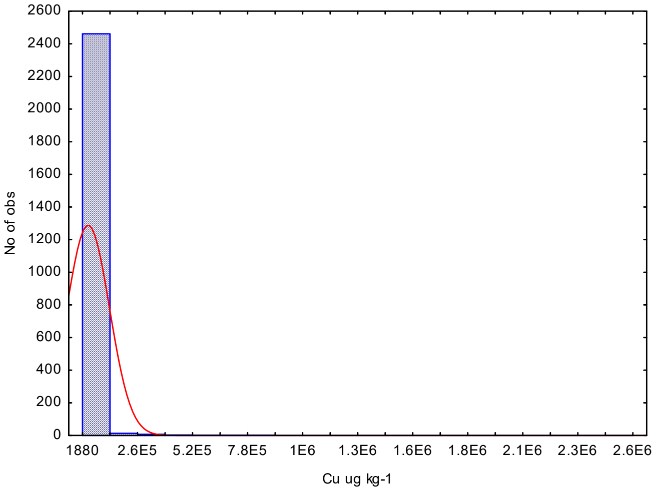

Figure 22. Frequency distribution of Cu concentrations from the sediment time series data set after exclusion of the data considered to be “re-checked” only for the lower limit.

5.2. PAHs: anthracene and benzo[a]pyrene

The procedure for the Quality Control of data on polycyclic aromatic hydrocarbons archived in EMODnet Chemistry was tested for some compounds as benzo[a]pyrene and anthracene which are commonly monitored in the sediments and which are usually present in detectable concentrations.

Anthracene - Sediment profiles dataset

The data with the following 3 types of P01 labels were considered:

ConceptID	Preferred label
ANTDWT01	Concentration of anthracene {CAS 120-12-7} per unit dry weight of sediment <2000um
HDCCZN01	Concentration of anthracene {CAS 120-12-7} per unit dry weight of sediment
HDCCAN01	Concentration of anthracene {CAS 120-12-7} per unit dry weight of sediment <63um by fluorescence high performance liquid chromatography (HPLC)

Data not considered:
129 Data from CNR, Istituto di Scienze Marine (Sezione di Venezia - ex IBM) Lambro (were outside of the area of interest
4 data from CNR, Institute of Marine Science (ISMAR, Lesina) were in lagoons (POR_PUGLIA_Project_s)

Data to be re-checked:
47 data from IEO/ Murcia Oceanographic Centre had longitudes >355 and it was not possible to identify the geographical position of the stations

112 data were considered usable for the area of interest (Table 18) and are represented in figures 23 and 24.

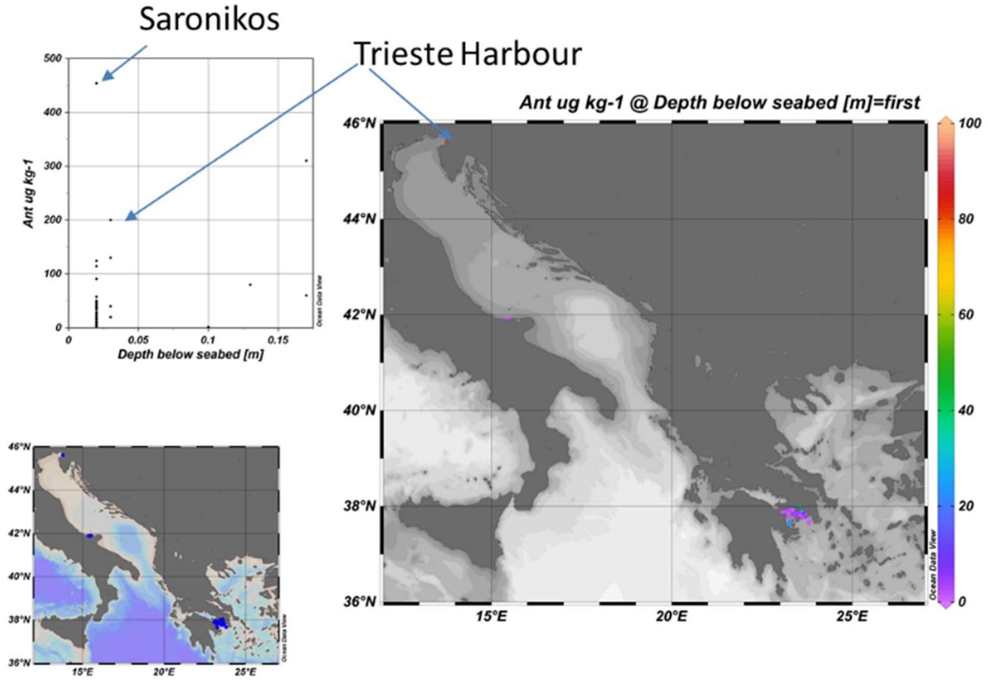

Figure 23. Anthracene (Ant) concentrations in surface sediments (right) and below the seabed (left).

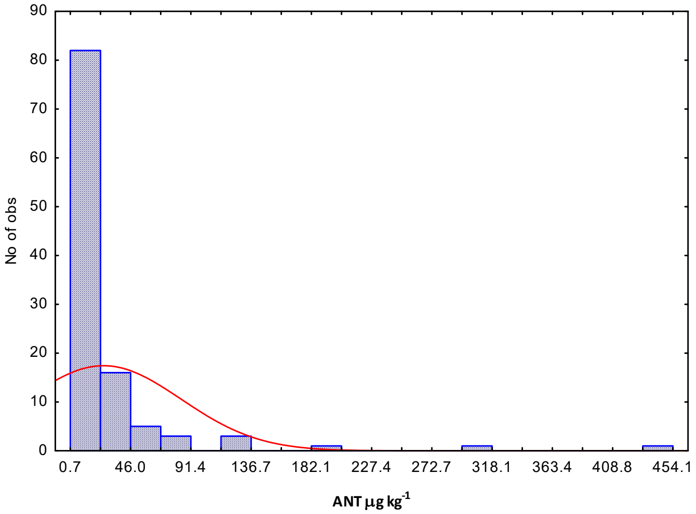

Figure 24. Frequency distribution of Anthracene (Ant) concentrations from the sediment profiles dataset.

Table 18. Descriptive statistics for the sediment profile data set of Anthracene (ANT) in sediments and comparison with the limits for the Quality Check (green color: within the limits). RMinCO’ and RMaxC’ are the limits reported in Table 9 multiplied by 0.85 and 1.15, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	112	71	33	11	400	15	195	83	2.5	7.1		
Water depth [m]	85	89	73	17	400	19	215	88	2.3	5.4		
Depth below seabed [m]	112	0.0	0.0	0.0	0.2	0.0	0.2	0.1	2.0	2.6		
ANT [µg kg-1]	112	25.5	4.8	**0.7**	**454.1**	1.5	50.0	58.1	5.1	31.6	0.034	879.8

Anthracene - Sediment time series dataset

2249 data available for the area of interest (Table 19) and are represented in figures 25 and 26.

No bottom depth and no water depth associated with the available data from ISPRA.

Data considered “to be re-checked”:

1730 values = 7.5 µg kg^{-1} with QF 1 They presumably represent the LOD and should have the QF 6

Data considered “to be rechecked”:
4 values lower than lower limit all with QF 6 (3 values = 0.01 µg kg^{-} and 1 value = 0)
2 values higher than the upper limit from Priolo site (913 µg kg^{-1} and 1700 µg kg^{-1})

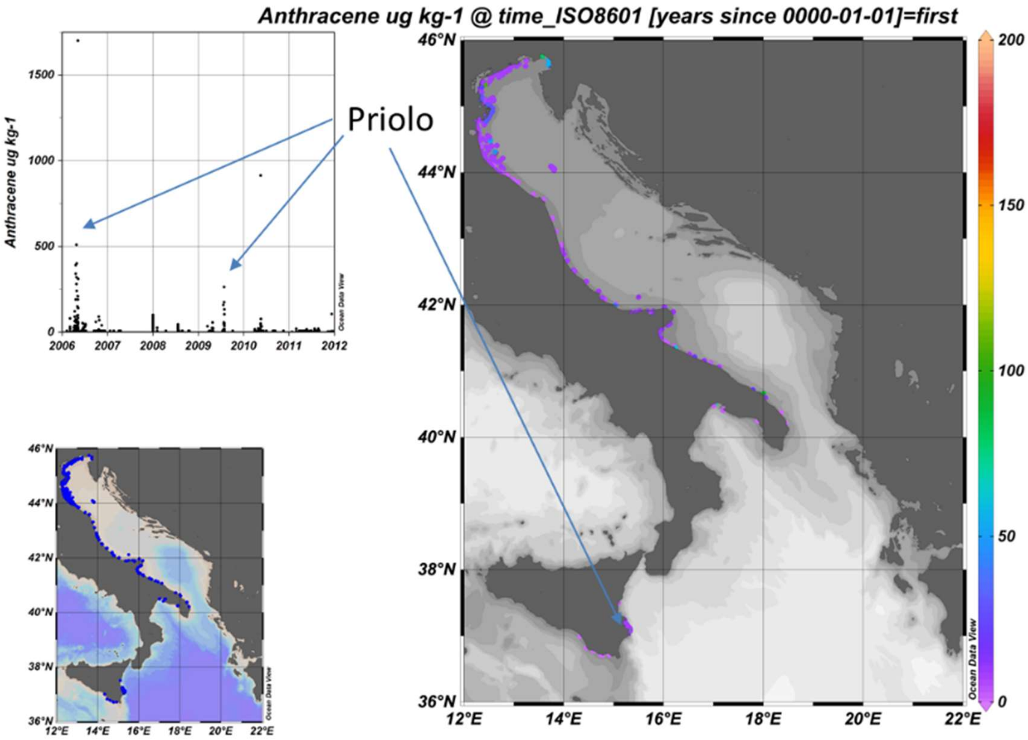

Figure 25. Anthracene (Ant) concentrations in surface sediments (right) and the data distribution as a function of the time (left).

Table 19. Descriptive statistics for the time series data set of Anthracene in sediments and comparison with the limits for the QC (red color: out of the limits). RMinCO' and RMaxC' are the limits reported in table 9 multiplied by 0.85 and 1.15, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	0					0.0	0.0					
Water depth [m]	0					0.0	0.0					
ANT [µg kg^{-1}]	2249	15.1	7.5	0.0	1700.0	7.5	30.0	48.7	22.9	699.6	0.034	879.8

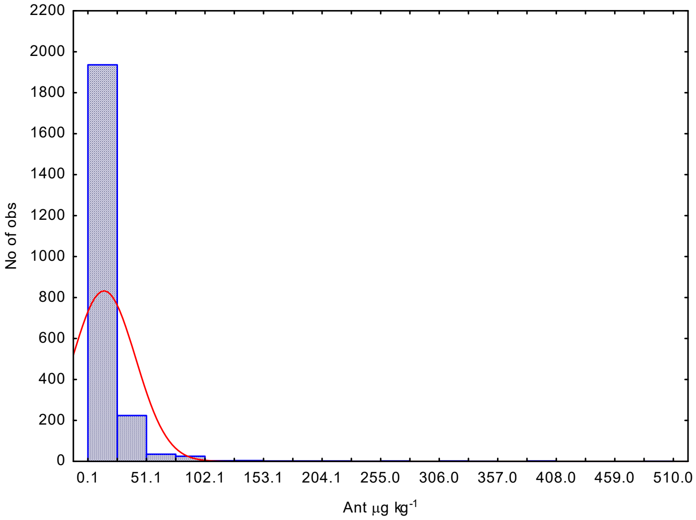

Figure 26. Frequency distribution of Anthracene (Ant) concentrations from the sediment time series dataset after exclusion of the data considered to be "re-checked".

Benzo[a]pyrene – Sediment profile dataset

The data with the following 3 types of P01 labels were considered:

ConceptID	Preferred label
BAPSEDBD	Concentration of benzo(a)pyrene {CAS 50-32-8} per unit dry weight of sediment <2000um
HDCCZAPY	Concentration of benzo(a)pyrene {CAS 50-32-8} per unit dry weight of sediment
CPAHSD07	Concentration of benzo(a)pyrene {CAS 50-32-8} per unit dry weight of sediment <63um

Data not considered:
3 data from Varano Lagoon (ISMAR, Lesina)
7 data from Varano lagoon (CNR, ISMAR, Lesina, POR_PUGLIA_Project_s)

Data considered "to be re-checked":
47 data from IEO data with longitudes >355, all with Depth below seabed [m]=5

85 data were considered usable in the area of interest (Table 20) and are represented in figures 27 and 28.

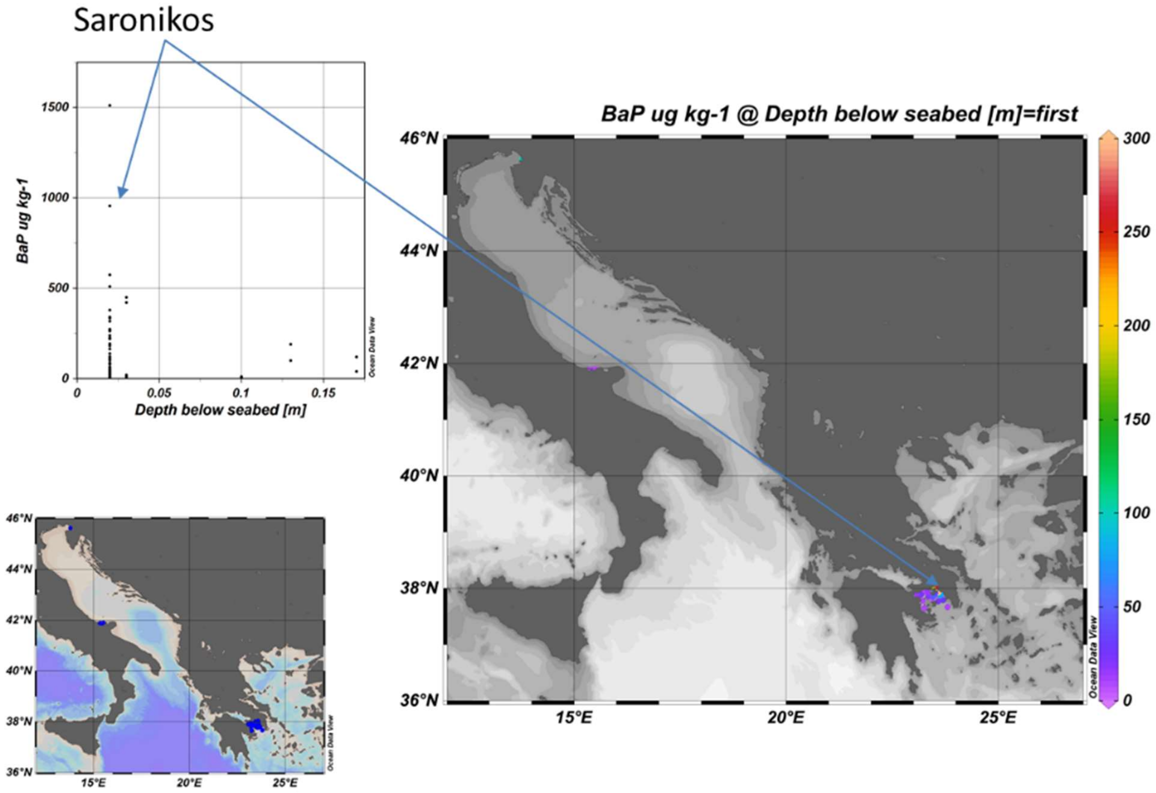

Figure 27. Benzo[a]pyrene (BaP) concentrations in surface sediments (right) and below the seabed (left).

Table 20. Descriptive statistics for the sediment profile data set of benzo[a]pyrene (BaP) in sediments and comparison with the limits for the Quality Check (green color: within the limits). RMinCO' and RMaxC' are the limits reported in Table 9 multiplied by 0.85 and 1.15, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	85	89	73	17	400	19	215	88	2.3	5.4		
Water depth [m]	85	89	73	17	400	19	215	88	2.3	5.4		
Depth below seabed [m]	85	0.0	0.0	0.0	0.2	0.0	0.0	0.0	4.5	19.2		
BaP [[µg kg-1]	85	122.3	34.9	**0.40**	**1511.9**	7.3	334.4	220.5	4.0	20.2	0.09	3069.4

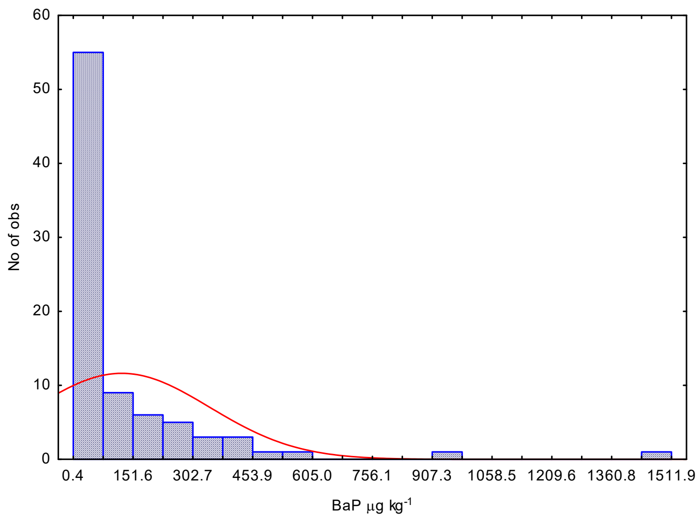

Figure 28. Frequency distribution of Benzo[a] pyrene (BaP) concentrations from the sediment profiles dataset.

Benzo[a]pyrene - Sediment time series dataset

2313 data were available for the area of interest (Table 21) and are represented in figures 29 and 30.

Some problem with metadata were identified: 71 data bottom depth =0 but water depth >0

2243 data no bottom depth, no station depth

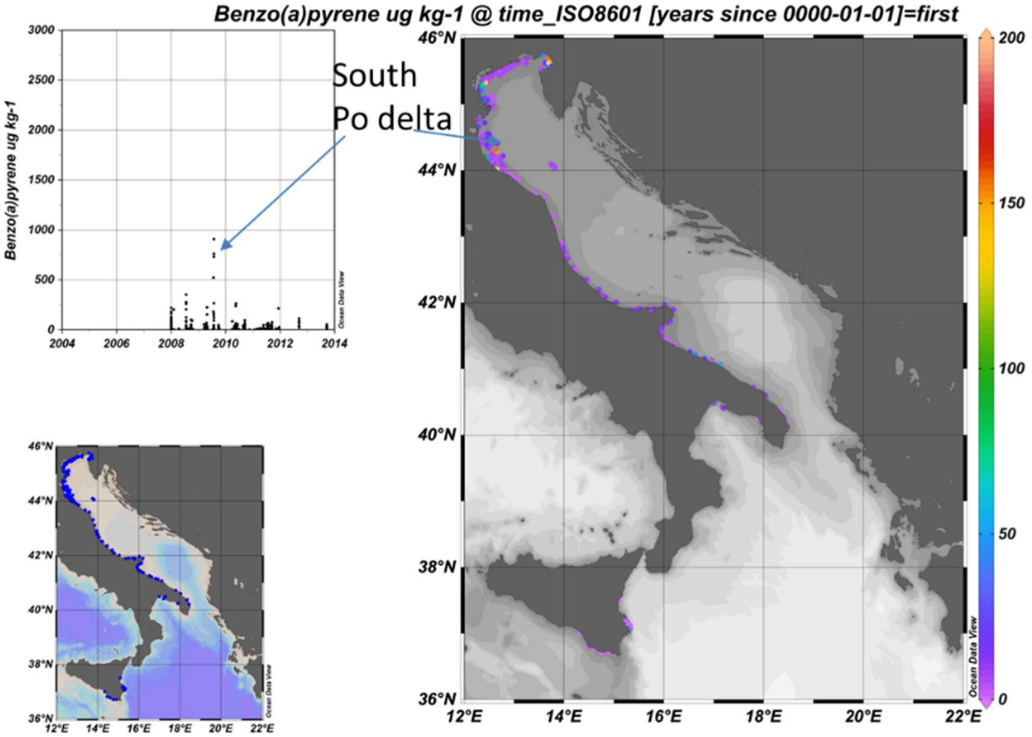

Figure 29. Benzo[a]pyrene (BaP) concentrations in surface sediments (right) and the data distribution as a function of the time (left).

Data considered to be "re-checked":

209 data below the RMinCO reported in Table 20.

143 values (ISPRA) are =0.01 μg kg^{-1} which presumably is the LOD, but only 2 are flagged with QF=6 the rest with QF=1

6 values (ISPRA) =0 but only 1 flagged with 6

14 values (ISPRA) were =0.02 μg kg^{-1} which presumably could be another LOD but were with QF =1.

Table 21. Descriptive statistics for the time series data set of Benzo[a]pyrene in sediments and comparison with the limits for the QC (green color: within the limits, red color: out of the limits). RMinCO' and RMaxC' are the limits reported in Table 9 multiplied by 0.85 and 1.15, respectively.

All data	Valid N	Mean	Median	Min	Max	Percentile 10	Percentile 90	Std.Dev.	Skewness	Kurtosis	RMinCO'	RMaxC'
Bot. Depth [m]	70	0.0	0.0	0.0	0.0	0.0	0.0	0.0				
Water depth [m]	70	15.7	16.0	2.0	24.0	2.0	24.0	7.1	-0.8	-0.4		
B(a)P [μg kg^{-1}]	2313	29.1	5.0	0.0	2900	0.3	56.0	103.2	14.0	304.2	0.21	3169.4

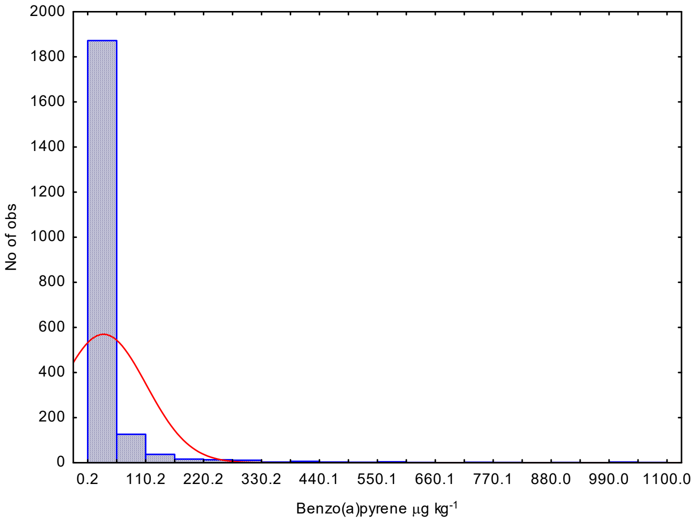

Figure 30. Frequency distribution of Benzo[a]pyrene (BaP) concentrations from the sediment time series dataset after exclusion of the data considered to be "re-checked".

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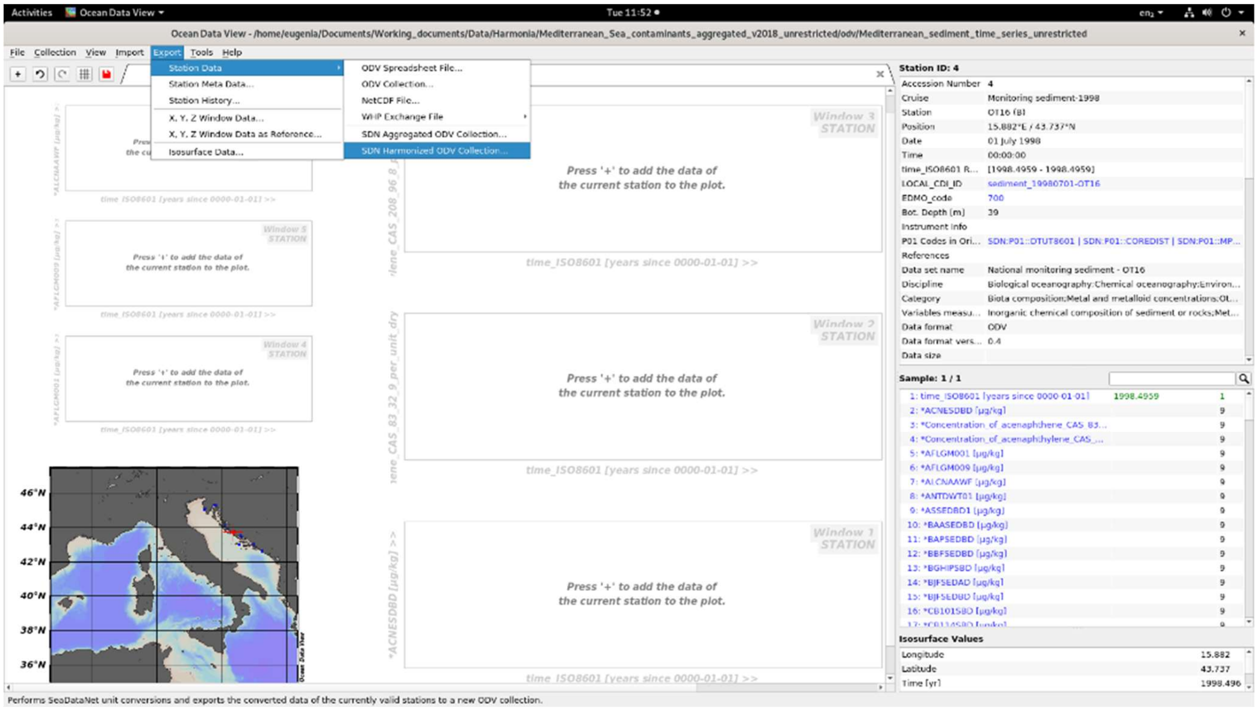
Annex: Dataset metadata and format check

Metadata availability:
One important result of the exercise of data QC on the available EMODnet Chemistry aggregated regional dataset of contaminants in the sediment is the need of relevant metadata associated to the datasets:

- Due to heterogeneity in grain size, missing information on grain size, as well as lack of indication of station depth and of sample thickness strongly affect QC of contaminants in the sediment matrix.
- Organic carbon and grain size are relevant supplementary data required for QC and for the application of normalization procedures.

Dataset format check:
Data collated within HarmoNIA partnership are available through a sub-regional buffer, that will be formatted and quality controlled in order to be used for products development, in the framework of the project. This buffer contains all data collated within HarmoNIA project (restricted + unrestricted) and non-restricted data collated by EMODnet Chemistry in the Adriatic-Ionian sub-region. The format of the collection is an “extended-ODV” spreadsheet file, that contains data plus almost all metadata associated.

Once the collection is opened with ODV software, the first step is to harmonise the collection in terms of units and P01 parameters. To carry out this step, ODV software contains a functionality that aggregates the same P01s present in the whole collection and harmonizes the units when possible:



Ocean Data View - /home/eugenia/Documents/Working_documents/Data/Harmonia/Mediterranean_Sea_contaminants_aggregated_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted

Station ID: 4

Accession Number	4
Cruise	Monitoring sediment-1998
Station	OT16 (B)
Position	15.882°E / 43.737°N
Date	01 July 1998
Time	00:00:00
time_ISO8601 R...	[1998.4959 - 1998.4959]
LOCAL_CDI_ID	sediment_19980701-OT16
EDMO_code	700
Bot. Depth [m]	39
Instrument Info	
P01 Codes in Ori...	SDN:P01::DTUT8601 | SDN:P01::COREDIST | SDN:P01::MP...
References	
Data set name	National monitoring sediment - OT16
Discipline	Biological oceanography:Chemical oceanography:Environ...
Category	Biota composition;Metal and metalloid concentrations;Ot...
Variables measu...	Inorganic chemical composition of sediment or rocks;Met...
Data format	ODV
Data format vers...	0.4
Data size	

Sample: 1 / 1

1: time_ISO8601 [years since 0000-01-01]	1998.4959	1
2: *ACNESDBD [µg/kg]		9
3: *Concentration_of_acenaphthene_CAS_83...		9
4: *Concentration_of_acenaphthylene_CAS_...		9
5: *AFLGM001 [µg/kg]		9
6: *AFLGM009 [µg/kg]		9
7: *ALCNAAWF [µg/kg]		9
8: *ANTDWT01 [µg/kg]		9
9: *ASSEDBD1 [µg/kg]		9
10: *BAASEDBD [µg/kg]		9
11: *BAPSEDBD [µg/kg]		9
12: *BBFSEDBD [µg/kg]		9
13: *BGHIPSBD [µg/kg]		9
14: *BJFSEDAD [µg/kg]		9
15: *BJFSEDBD [µg/kg]		9
16: *CB101SBD [µg/kg]		9

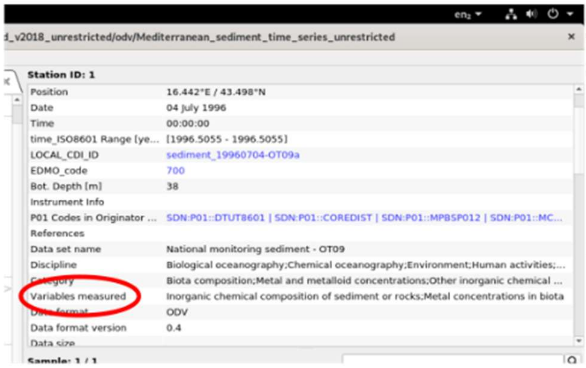
Isosurface Values

Longitude	15.882
Latitude	43.737
Time [yr]	1998.496

Performs SeaDataNet unit conversions and exports the converted data of the currently valid stations to a new ODV collection.

After the harmonisation of the collection, some format and content controls can be performed.

1. Check P02 present in the collection: Right-click in metadata field “variables measured”, select collect string values. Copy and paste in a text or spreadsheet file. Check if all P02s are related to the collection

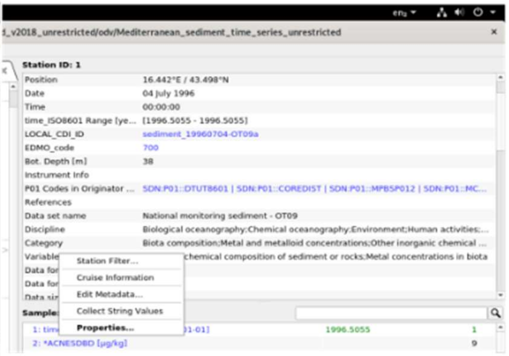


d_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted

Station ID: 1

Position	16.442°E / 43.498°N
Date	04 July 1996
Time	00:00:00
time_ISO8601 Range [ye...	[1996.5055 - 1996.5055]
LOCAL_CDI_ID	sediment_19960704-OT09a
EDMO_code	700
Bot. Depth [m]	38
Instrument Info	
P01 Codes in Originator ...	SDN:P01::DTUT8601 | SDN:P01::COREDIST | SDN:P01::MPBSP012 | SDN:P01::MC...
References	
Data set name	National monitoring sediment - OT09
Discipline	Biological oceanography;Chemical oceanography;Environment;Human activities;...
Category	Biota composition;Metal and metalloid concentrations;Other inorganic chemical ...
Variables measured	Inorganic chemical composition of sediment or rocks;Metal concentrations in biota
Data format	ODV
Data format version	0.4
Data size	

Sample: 1 / 1



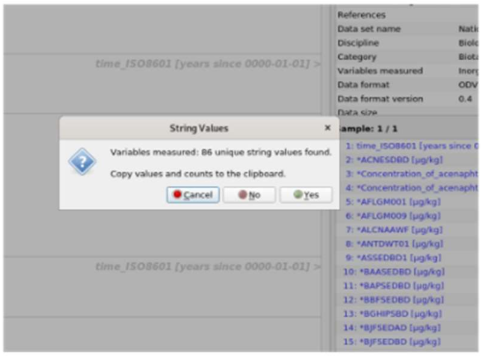
d_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted

Station ID: 1

Position	16.442°E / 43.498°N
Date	04 July 1996
Time	00:00:00
time_ISO8601 Range [ye...	[1996.5055 - 1996.5055]
LOCAL_CDI_ID	sediment_19960704-OT09a
EDMO_code	700
Bot. Depth [m]	38
Instrument Info	
P01 Codes in Originator ...	SDN:P01::DTUT8601 | SDN:P01::COREDIST | SDN:P01::MPBSP012 | SDN:P01::MC...
References	
Data set name	National monitoring sediment - OT09
Discipline	Biological oceanography;Chemical oceanography;Environment;Human activities;...
Category	Biota composition;Metal and metalloid concentrations;Other inorganic chemical ...
Variable	chemical composition of sediment or rocks;Metal concentrations in biota

Sample:

1: tim 01-01] 1996.5055 1
2: *ACNESDBD [µg/kg] 9



String Values

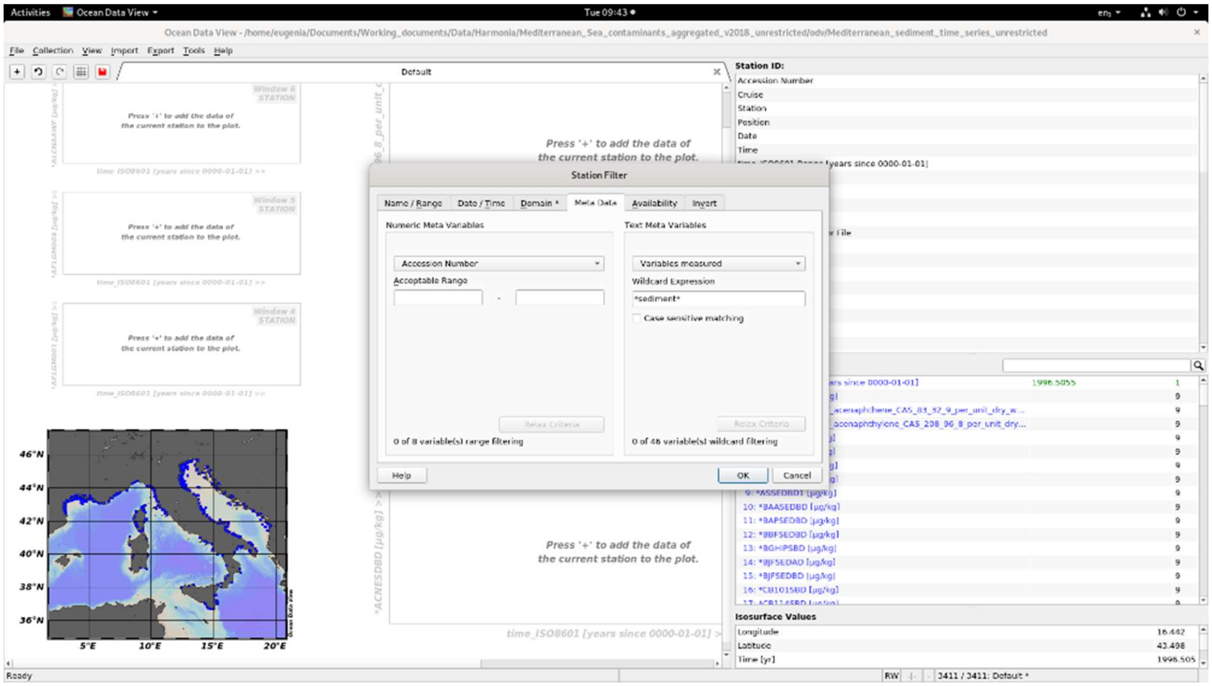
Variables measured: 86 unique string values found.

Copy values and counts to the clipboard.

Sample: 1 / 1

1: time_ISO8601 [years since
2: *ACNESDBD [µg/kg]
3: *Concentration_of_acenapht
4: *Concentration_of_acenapht
5: *AFLGM001 [µg/kg]
6: *AFLGM009 [µg/kg]
7: *ALCNAAWF [µg/kg]
8: *ANTDWT01 [µg/kg]
9: *ASSEDBD1 [µg/kg]
10: *BAASEDBD [µg/kg]
11: *BAPSEDBD [µg/kg]
12: *BBFSEDBD [µg/kg]
13: *BGHIPSBD [µg/kg]
14: *BJFSEDAD [µg/kg]
15: *BJFSEDBD [µg/kg]

2. If any P02 is not related to the matrix/collection that is being prepared: Right-click in metadata field “variables measured”, select “station filter”. Inside station filter window select “meta data” sheet and within text meta variables select “variables measured”. Write the keyword related to your collection: water, sediment or biota with * before and after the key word. If there is more than one keyword separate them with || as ODV general guidelines establish.



Station Filter

Numeric Meta Variables: Accession Number

Acceptable Range: -

0 of 8 variable(s) range filtering

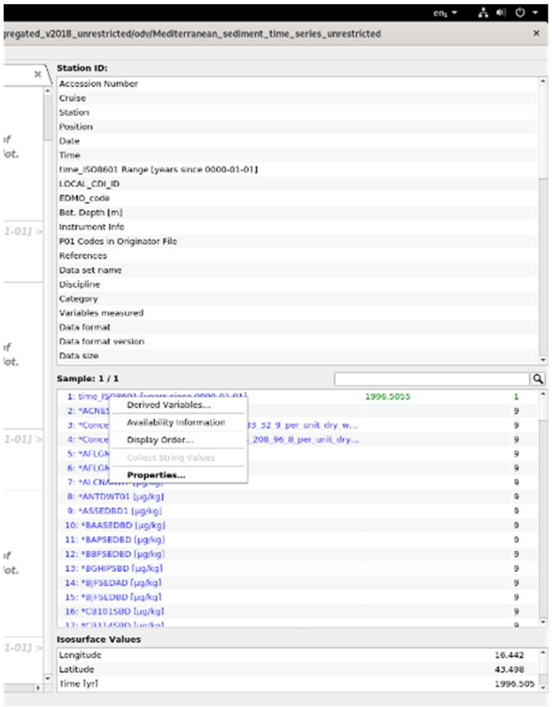
Text Meta Variables: Variables measured

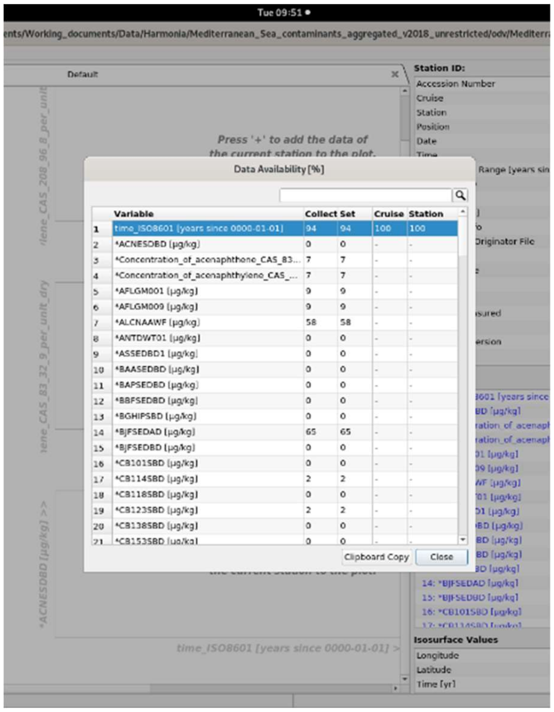
Wildcard Expression: *sediment*

☐ Case sensitive matching

0 of 48 variable(s) wildcard filtering

3. Check if the primary variable is present in the whole collection. Right-click in the primary variable field, select availability information. If the percentage is not 100% for the primary variable, check if there is another P01 that is the primary variable (sample_id; depth instead of coredist for sediment profiles…).

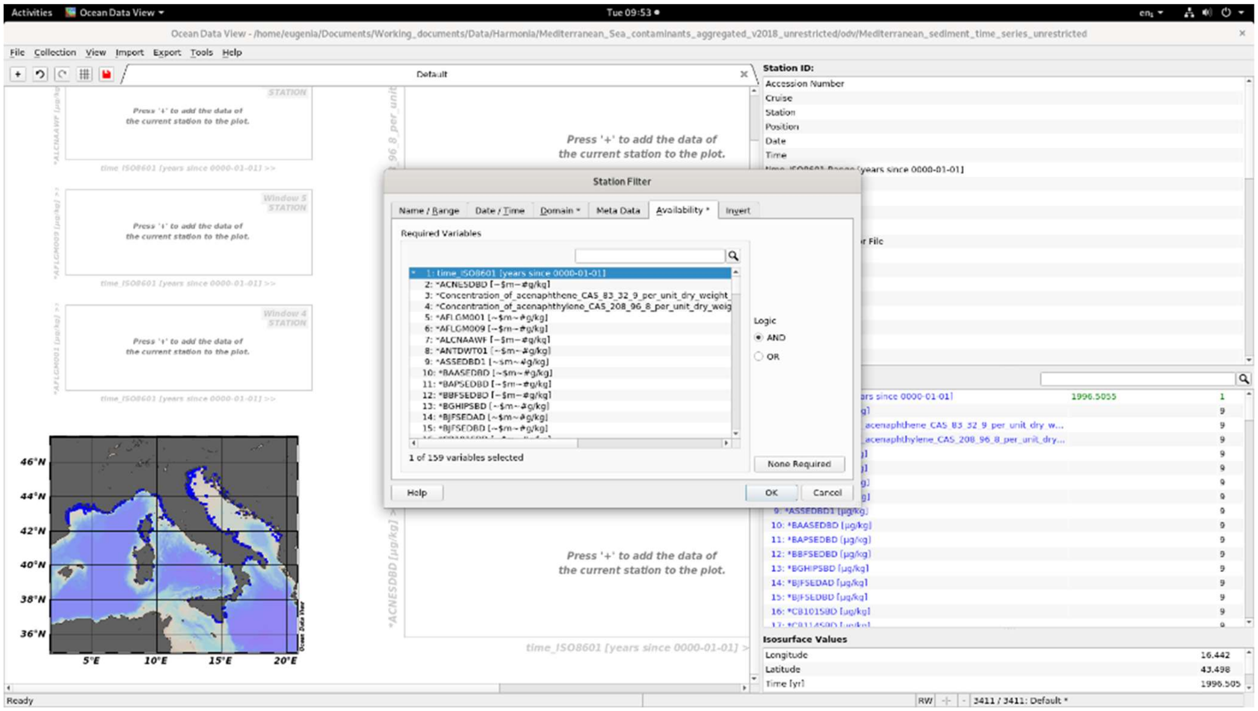




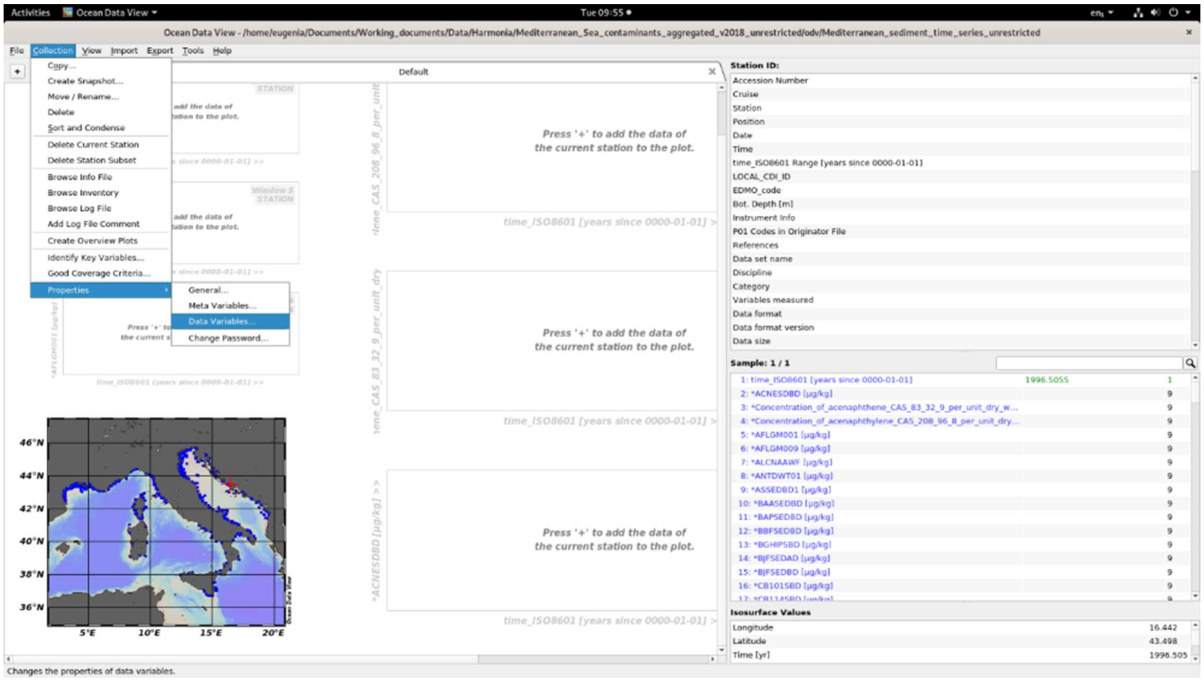
Data Availability [%]

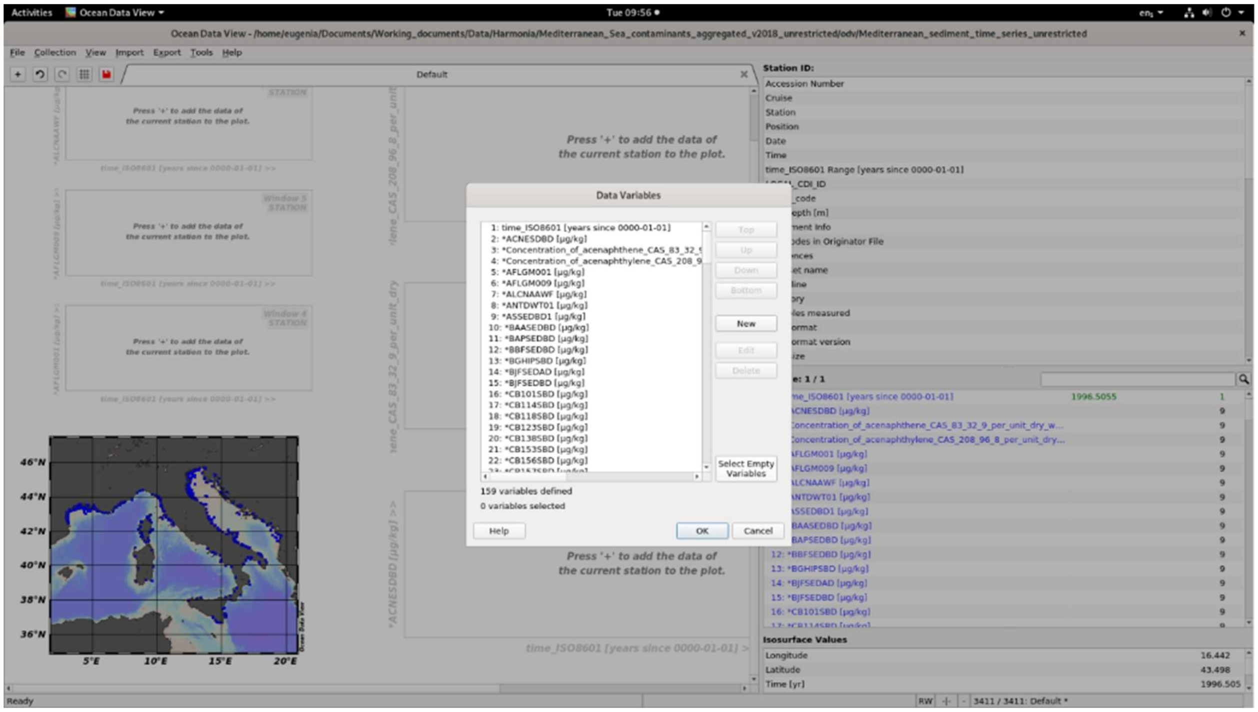
	Variable	Collect	Set	Cruise	Station
1	time_ISO8601 [years since 0000-01-01]	94	94	100	100
2	*ACNESDBD [µg/kg]	0	0	-	-
3	*Concentration_of_acenaphthene_CAS_83…	7	7	-	-
4	*Concentration_of_acenaphthylene_CAS_…	7	7	-	-
5	*AFLGM001 [µg/kg]	9	9	-	-
6	*AFLGM009 [µg/kg]	9	9	-	-
7	*ALCNAAWF [µg/kg]	58	58	-	-
8	*ANTDWT01 [µg/kg]	0	0	-	-
9	*ASSEDBD1 [µg/kg]	0	0	-	-
10	*BAASEDBD [µg/kg]	0	0	-	-
11	*BAPSEDBD [µg/kg]	0	0	-	-
12	*BBFSEDBD [µg/kg]	0	0	-	-
13	*BGHIPSBD [µg/kg]	0	0	-	-
14	*BJFSEDAD [µg/kg]	65	65	-	-
15	*BJFSEDBD [µg/kg]	0	0	-	-
16	*CB101SBD [µg/kg]	0	0	-	-
17	*CB114SBD [µg/kg]	2	2	-	-
18	*CB118SBD [µg/kg]	0	0	-	-
19	*CB123SBD [µg/kg]	2	2	-	-
20	*CB138SBD [µg/kg]	0	0	-	-
21	*CB153SBD [µg/kg]	0	0	-	-

4. If primary variable is not 100% present you can filter which stations don't contain the parameter associated to the primary variable. Right-click in metadata field "variables measured", select "station filter". Inside station filter window select "availability" and choose the primary variable as required variable. Select invert selection in the invert sheet and stations without the correct primary variable will be displayed.

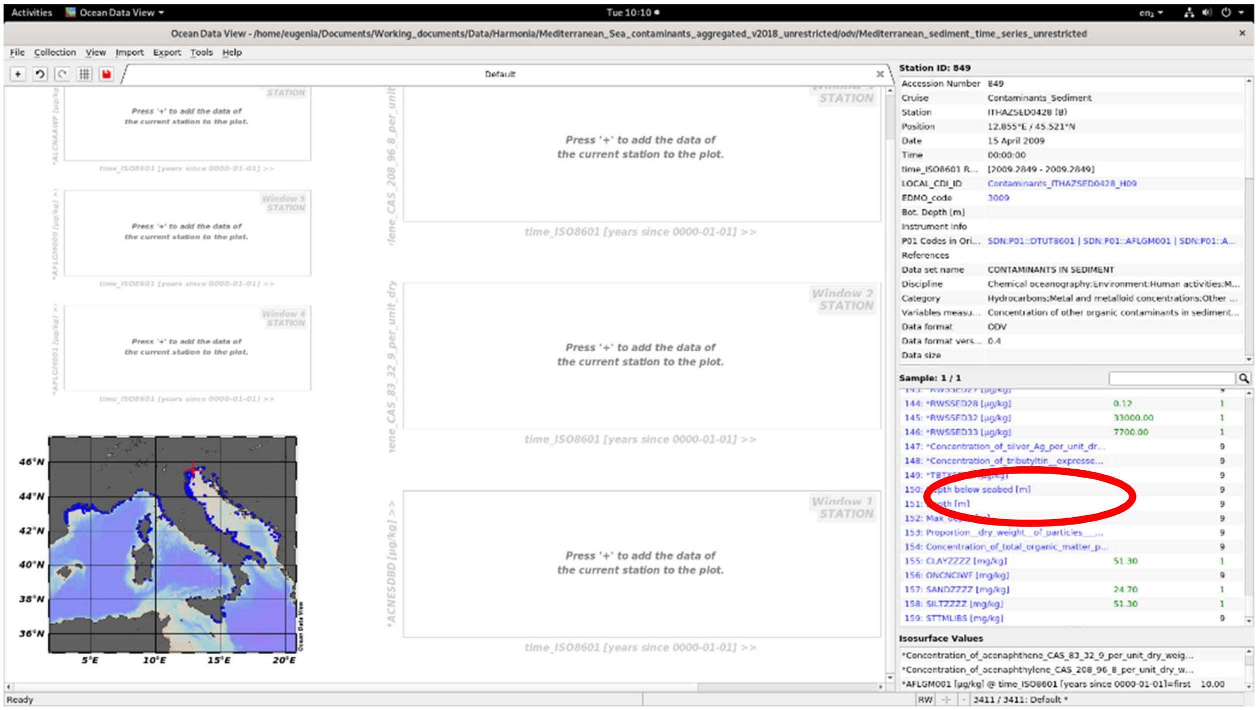


5. Check if there are empty variables in the whole collection. In the window collection, inside properties, data variables, select empty variables. If there is any empty variable for the whole collection, it can be deleted.





6. Check if there are variables that do not correspond to the matrix (i.e. depth in sediment instead of depth below seabed).



Ocean Data View - /home/eugenia/Documents/Working_documents/Data/Harmonia/Mediterranean_Sea_contaminants_aggregated_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted

Station ID: 849

Accession Number	849
Cruise	Contaminants_Sediment
Station	ITHAZSED0428 (B)
Position	12.855°E / 45.521°N
Date	15 April 2009
Time	00:00:00
time_ISO8601 R...	[2009.2849 - 2009.2849]
LOCAL_CDI_ID	Contaminants_ITHAZSED0428_H09
EDMO_code	3009
Bot. Depth (m)	
Instrument Info	
P01 Codes in Ori...	SDN:P01::DTUT8601 | SDN:P01::AFLGM001 | SDN:P01::A...
References	
Data set name	CONTAMINANTS IN SEDIMENT
Discipline	Chemical oceanography:Environment:Human activities:M...
Category	Hydrocarbons:Metal and metalloid concentrations:Other ...
Variables measu...	Concentration of other organic contaminants in sediment...
Data format	ODV
Data format vers...	0.4
Data size	

Sample: 1 / 1

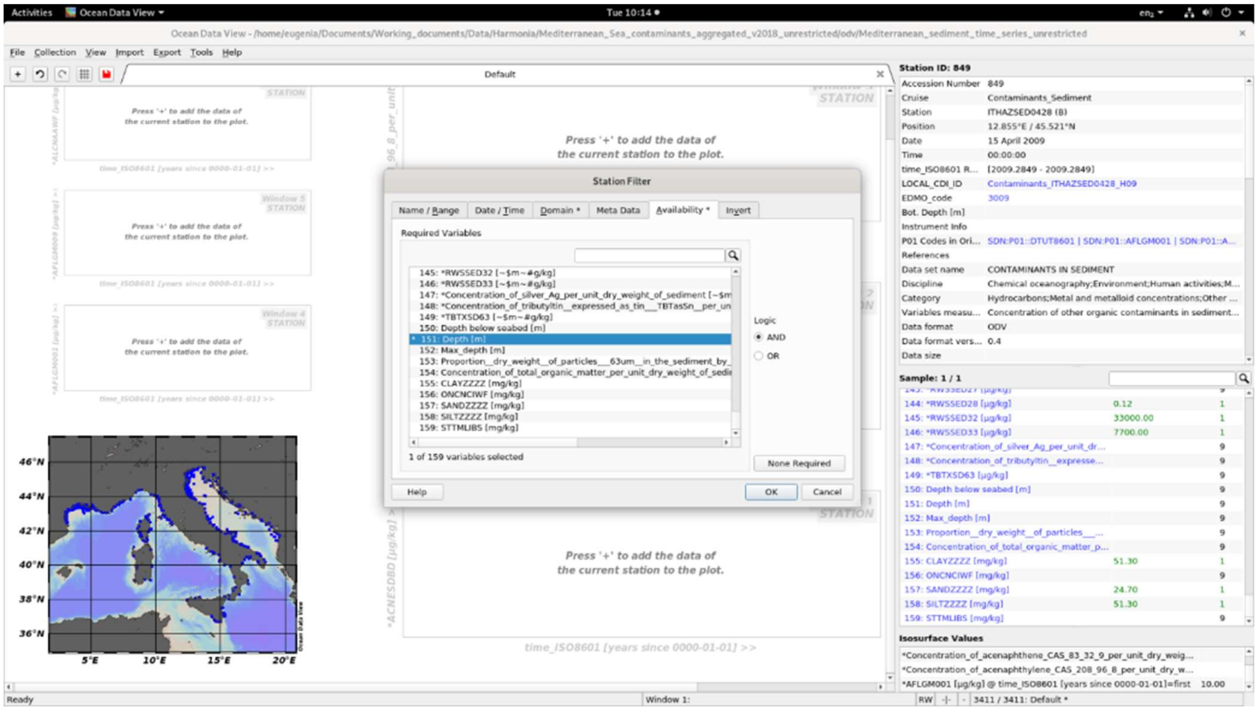
144: *RWSSED28 [µg/kg]	0.12	1
145: *RWSSED32 [µg/kg]	33000.00	1
146: *RWSSED33 [µg/kg]	7700.00	1
147: *Concentration_of_silver_Ag_per_unit_dr...		9
148: *Concentration_of_tributyltin__expresse...		9
149: *TBTX[illegible] [µg/kg]		9
150: [illegible]pth below seabed [m]		9
151: [illegible]pth [m]		9
152: Max [illegible]		9
153: Proportion__dry_weight__of_particles___...		9
154: Concentration_of_total_organic_matter_p...		9
155: CLAYZZZZ [mg/kg]	51.30	1
156: ONCNCIWF [mg/kg]		9
157: SANDZZZZ [mg/kg]	24.70	1
158: SILTZZZZ [mg/kg]	51.30	1
159: STTMLIBS [mg/kg]		9

Isosurface Values

*Concentration_of_acenaphthene_CAS_83_32_9_per_unit_dry_weig...
*Concentration_of_acenaphthylene_CAS_208_96_8_per_unit_dry_w...
*AFLGM001 [µg/kg] @ time_ISO8601 [years since 0000-01-01]=first 10.00

RW 3411 / 3411: Default *

7. Check which stations have the potential wrong variable and contact the originators. In the station filter, choosing the sheet "availability", choose the variable to check.



Station Filter

Name / Range | Date / Time | Domain * | Meta Data | Availability * | Invert

Required Variables

145: *RWSSED32 [~$m~#g/kg]
146: *RWSSED33 [~$m~#g/kg]
147: *Concentration_of_silver_Ag_per_unit_dry_weight_of_sediment [~$m
148: *Concentration_of_tributyltin__expressed_as_tin___TBTasSn__per_un
149: *TBTXSD63 [~$m~#g/kg]
150: Depth below seabed [m]
* 151: Depth [m]
152: Max_depth [m]
153: Proportion__dry_weight__of_particles___63um__in_the_sediment_by_
154: Concentration_of_total_organic_matter_per_unit_dry_weight_of_sedi
155: CLAYZZZZ [mg/kg]
156: ONCNCIWF [mg/kg]
157: SANDZZZZ [mg/kg]
158: SILTZZZZ [mg/kg]
159: STTMLIBS [mg/kg]

1 of 159 variables selected

Logic
● AND
○ OR

None Required | Help | OK | Cancel

Station ID: 849

Accession Number	849
Cruise	Contaminants_Sediment
Station	ITHAZSED0428 (B)
Position	12.855°E / 45.521°N
Date	15 April 2009
Time	00:00:00
time_ISO8601 R...	[2009.2849 - 2009.2849]
LOCAL_CDI_ID	Contaminants_ITHAZSED0428_H09
EDMO_code	3009
Bot. Depth [m]	
Instrument Info	
P01 Codes in Ori...	SDN:P01::DTUT8601 | SDN:P01::AFLGM001 | SDN:P01::A...
References	
Data set name	CONTAMINANTS IN SEDIMENT
Discipline	Chemical oceanography;Environment;Human activities;M...
Category	Hydrocarbons;Metal and metalloid concentrations;Other ...
Variables measu...	Concentration of other organic contaminants in sediment...
Data format	ODV
Data format vers...	0.4
Data size	

Sample: 1 / 1

144: *RWSSED28 [µg/kg]	0.12	1
145: *RWSSED32 [µg/kg]	33000.00	1
146: *RWSSED33 [µg/kg]	7700.00	1
147: *Concentration_of_silver_Ag_per_unit_dr...		9
148: *Concentration_of_tributyltin__expresse...		9
149: *TBTXSD63 [µg/kg]		9
150: Depth below seabed [m]		9
151: Depth [m]		9
152: Max_depth [m]		9
153: Proportion__dry_weight__of_particles___...		9
154: Concentration_of_total_organic_matter_p...		9
155: CLAYZZZZ [mg/kg]	51.30	1
156: ONCNCIWF [mg/kg]		9
157: SANDZZZZ [mg/kg]	24.70	1
158: SILTZZZZ [mg/kg]	51.30	1
159: STTMLIBS [mg/kg]		9

Isosurface Values

*Concentration_of_acenaphthene_CAS_83_32_9_per_unit_dry_weig...
*Concentration_of_acenaphthylene_CAS_208_96_8_per_unit_dry_w...
*AFLGM001 [µg/kg] @ time_ISO8601 [years since 0000-01-01]=first 10.00

RW | -\|- | - | 3411 / 3411: Default *

Station ID: 131

Accession Number	131
Cruise	Monitoring sediment-2013
Station	OT26a (B)
Position	13.671°E / 45.129°N
Date	26 September 2013
Time	00:00:00
time_ISO8601 R...	[2013.7342 - 2013.7342]
LOCAL_CDI_ID	sediment_20130926-OT26a
EDMO_code	700
Bot. Depth [m]	2
Instrument Info	
P01 Codes in Ori...	SDN:P01::DTUT8601 | SDN:P01::COREDIST | SDN:P01::MP...
References	
Data set name	National monitoring sediment - OT26
Discipline	Biological oceanography;Chemical oceanography;Environ...
Category	Biota composition;Metal and metalloid concentrations;Ot...
Variables measu...	Inorganic chemical composition of sediment or rocks;Met...
Data format	ODV
Data format vers...	0.4
Data size	

Sample: 1 / 1

144: *RWSSED28 [µg/kg]		9
145: *RWSSED32 [µg/kg]		9
146: *RWSSED33 [µg/kg]		9
147: *Concentration_of_silver_Ag_per_unit_dr...		9
148: *Concentration_of_tributyltin__expresse...		9
149: *TBTXSD63 [µg/kg]		9
150: Depth below seabed [m]	2.00	0
151: Depth [m]	2.00	1
152: Max_depth [m]		9
153: Proportion__dry_weight__of_particles___...		9
154: Concentration_of_total_organic_matter_p...		9
155: CLAYZZZZ [mg/kg]		9
156: ONCNCIWF [mg/kg]		9
157: SANDZZZZ [mg/kg]		9
158: SILTZZZZ [mg/kg]		9
159: STTMLIBS [mg/kg]		9

Isosurface Values

*Concentration_of_acenaphthene_CAS_83_32_9_per_unit_dry_weig...
*Concentration_of_acenaphthylene_CAS_208_96_8_per_unit_dry_w...
*AFLGM001 [µg/kg] @ time_ISO8601 [years since 0000-01-01]=first

RW | | S | 121 / 3411: Default *

It is very important for sediment samples to have the sampled depth (depth below seabed)

8. Check at the end of the variable list if there is any non-harmonized variable that is not linked with contaminants data (i.e. chlorophyll data…). It is better to avoid exporting these parameters but all those variables like the last ones in the image above are very relevant for sampling details and further conversions so they have to be in the collection.