EMODnet Chemistry

Quality Control steps and dataset formats for EMODnet Chemistry Contaminant aggregated datasets

M. Lipizer, M.E. Molina Jack and A. Giorgetti (OGS), L. Buga (NIMRD), K. Wesslander (SMHI), J. Gatti (IFREMER), A. K. Østrem (IMR), A. Iona and M. Tsompanou (HCMR), M. M. Larsen (AU), R. Schlitzer (AWI)

Date: 08/04/2021

Citation: M. Lipizer, M.E. Molina Jack, A. Giorgetti, L. Buga, K. Wesslander, J. Gatti, A. K. Østrem, A. Iona, M. Tsompanou, M. M. Larsen, R. Schlitzer, 2021, Quality Control steps and dataset formats for EMODnet Chemistry Contaminant aggregated datasets, 08.04.2021, 20 pp., DOI 10.6092/8b52e8d7-dc92-4305-9337-7634a5cae3f4

Content:

1. Introduction

EMODnet Chemistry aims to provide access to marine chemistry data sets and derived data products concerning eutrophication, ocean acidification, contaminants and marine litter. The chemicals chosen are relevant for the Marine Strategy Framework Directive (MSFD). Parameter names are based on P01, BODC Parameter Usage Vocabulary, which is available at: http://seadatanet.maris2.nl/bandit/browse_step.php. Each measurement value has a quality flag indicator, based on the standard SeaDataNet scheme (L20 SEADATANET MEASURAND QUALIFIER FLAGS[1]). This document describes the steps of data and metadata validation needed to achieve the standardised, harmonised and validated datasets concerning **contaminants in the marine environment**, in water, sediment and biota matrices. EMODnet Chemistry is focused on the parameter groups listed in the table below. The links between P36 (Terms based on the EU MSFD used by the EMODNET chemistry lot to provide coarse granularity groupings of the chemical parameters it covers) and P02 (terms describing fine-grained related groups of measurement phenomena designed to be used in dataset discovery interfaces) are in the process of revision as more experience is gained in the field. The updated links are available here: http://vocab.nerc.ac.uk/collection/P36/current/

P36 Code	P36 Parameter groups	P02 Code	P02 Parameter discovery vocabulary
ANTIFL	Antifoulants	OMBI	Organometallic species concentration parameters in biota
		OMPW	Organometallic and organometalloid species concentration parameters in sediments
		OMWC	Organometallic and organometalloid species concentration parameters in water bodies
HCARBS	Hydrocarbons	AQYN	Concentration of alkenes and alkynes in the water column
		BCAH	Concentration of polycyclic aromatic hydrocarbons (PAHs) in biota
		DALK	Concentration of alkanes in the water column
		OHWC	Concentration of other hydrocarbons in the water column

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=

		PCAH	Concentration of polycyclic aromatic hydrocarbons (PAHs) in suspended particulate material
		PCHW	Concentration of polycyclic aromatic hydrocarbons (PAHs) in the water column
		SALK	Concentration of aliphatic hydrocarbons in sediment samples
		SCAH	Concentration of polycyclic aromatic hydrocarbons (PAHs) in sediment samples
HVYMTL	Heavy metals	BCMT	Metal concentrations in biota
		MDBO	Trace metalloid concentrations in biota
		MDPW	Trace metalloid concentrations in sediment pore water
		MDWD	Dissolved trace metalloid and inorganic selenium concentrations in water bodies
		MDWP	Particulate trace metalloid and inorganic selenium concentrations in water bodies
		MTPW	Metal concentrations in sediment pore waters
		MTWC	Colloidal metal concentrations in the water column
		MTWD	Dissolved metal concentrations in the water column
		MTWP	Particulate metal concentrations in the water column
		MTWT	Total metal concentrations in water bodies
PCBSXX	Polychlorinated biphenyls	BCPB	Concentration of polychlorobiphenyls (PCBs) in biota
		PPCB	Concentration of polychlorobiphenyls (PCBs) in suspended particulate material
		PPWC	Concentration of polychlorobiphenyls (PCBs) in the water column
		SPCB	Concentration of polychlorobiphenyls (PCBs) in sediment samples
PESTB	Pesticides and biocides	PEBI	Pesticide concentrations in biota
		PESD	Pesticide concentrations in sediment
		PEWB	Pesticide concentrations in water bodies
RADNUC	Radionuclides	BRAD	Radioactivity in biota
		SRAD	Geological sample radioactivity
		WRAD	Radioactivity in water bodies
OTHERS	Other contaminants	BCOC	Concentration of other organic contaminants in biota
		PCOC	Concentration of other organic contaminants in suspended particulate material
		SCOC	Concentration of other organic contaminants in sediment samples
		WCOC	Concentration of other organic contaminants in the water column

2. Validation steps

A step-wise approach is carried out to obtain validated regional aggregated datasets, taking into account the large heterogeneity in matrices (seawater total, filtered, unfiltered samples; different size classes of sediment; different biota taxa, target organs, size, ...), in parameters measured by the different laboratories all over Europe, in analytical protocols used, in measurement units as well as in monitoring frequency and purposes. The multiple combinations of the above - mentioned variables results in a huge list of parameters included in the datasets, often with limited temporal – spatial distribution for single parameters. Additionally, there is not enough knowledge on concentration ranges for the specific variables in the different areas. As a consequence, the applied validation procedure involves[2]:

- metadata completeness and dataset format control
    - check of consistency of primary variables, especially in sediment and biota datasets
    - separation of data related to different matrices into different dataset collections
- harmonization of unit and parameter naming
- check of quality flagging of data and metadata
- checks for inconsistent measurement units
- checks for clearly impossible data ranges (ex. Different orders of magnitude)

The results of validation are reported to data originators to evaluate, revise and eventually correct encountered issues. Part of the validation process can be carried out using ODV standard interface, while part requires the use of the harmonized, transposed and decomposed matrix and the handling outside ODV. The use of ODV transposed and decomposed matrix enables to filter per substance, matrix characteristics, analytical method, …

[2] This approach derives in part to activities carried out in the framework of the project HarmoNIA (Harmonization and Networking for contaminant assessment in the Ionian and Adriatic Seas, https://harmonia.adrioninterreg.eu/) financed by Interreg ADRION (2018-2020).

3. Metadata completeness and dataset format control

Metadata availability:

In order to be correctly used, data of contaminants need to be accompanied by relevant metadata associated to the datasets:

- For water: Depth (if time series),
- For sediment: Depth below seabed (if time series); additionally, proportion of sizes of particles, Parameters related to granularity, water content, organic matter content, thickness of sediment properties and sedimentation rates. 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.
- For biota: parameters related to the sample (biota sizes, sample ids, sex, life stage…), water and lipid contents, wet weight, depth…

Furthermore, temporal and spatial (position, sampling depth, station bottom depth) information must be available otherwise data cannot be used.

Dataset format check:

EMODnet Chemistry regional aggregated datasets are available as “extended-ODV” spreadsheet file, that contains data plus almost all metadata associated. Up to seven types of aggregated datasets can be expected from each region:

- Time-series for each matrix (water, sediment and biota)
- Profiles for each matrix (water, sediment and biota)
- Biota datasets with the sample identification as the primary data variable

During the import phase (CDI+ODV files) with ODV software, some automatic file format checks are performed and different types of collections are generated:

- Ocean depth profiles: Primary variable will be depth (DEPHPR01 or ADEPZZ01), so the collection may be primarily for water. It is necessary to be careful because if there are profiles of biota, this collection would contain them. If there are parameters related to biota in the collection, the stations that contain biota can be filtered with the station filter described below in step 2. Additionally, if there are parameters related to sediment, this would be an indication of profiles related to sediment with the wrong primary variable attribution; in that case, stations have to be filtered, primary variable changed to COREDIST and merge with the collection related to sediment profiles.
- Sediment depth profiles: Primary variable will be depth below seabed (COREDIST), so the collection would be related to sediment.
- Time Series: Primary variable will be time. This collection may contain parameters related to water, sediment and biota.
- Sample-ID primary variable collection: If data originators have used sample -ID as the primary variable for biota datasets, an additional collection would be created.

Additional checks needed:

An additional check could be necessary to investigate if biota data should rather be in the time series collection. This check consists in looking at the number of depths, and if it's a profile with only one depth, check how other biota data from this EDMO code have been submitted. Contact with data originator is needed to evaluate to check the dataset type.

It might happen that during the import phase more than one collection of sediment or water is created, due to a different primary variable and or units. Examples:

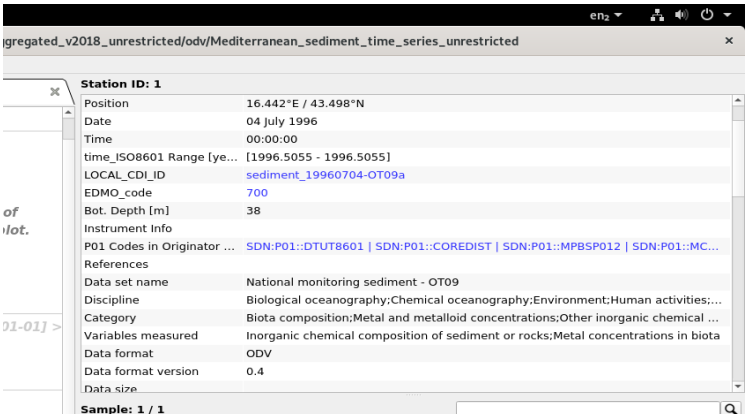
- Sediment profiles, with COREDIST in as primary variables but given in different units (metres or centimetres). In this case, it is necessary to harmonise units for depth, the preferred unit is **metres**.
- Ocean profiles, with different primary variables, DEPHPR01 and ADEPZZ01, that can be considered equivalent, so DEPHPR01 can be edited into ADEPZZ01 for the whole collection.

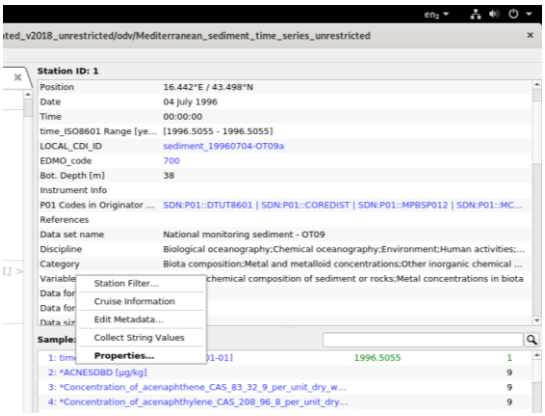
There is a functionality inside ODV to aggregate them performing previously the transformation needed. It is necessary to add the data variables from the second collection to the main collection. This can be done through the properties of the collection→ data variables → new→ add from another collection. Then you start with the import dialog in the option “add/replace station data”. For water, depth variables can be associated without any transformation (as they are in the same units and considered equivalent parameters). For sediment, it is necessary to convert the primary variable during the import to have the same units in the three collections.

For timeseries, parameters related to the three matrices must be splitted, using the filter for the metadata field “variables measured” (using the station filter described in step 2). Export stations related to biota, sediment and water. Open each of the new created collections, delete the empty variables and export the collection using the option to obtain SDN harmonized ODV collection. Some parameters of the collection may belong to other matrix if the station samples multiple matrices.

Format and content controls roadmap:

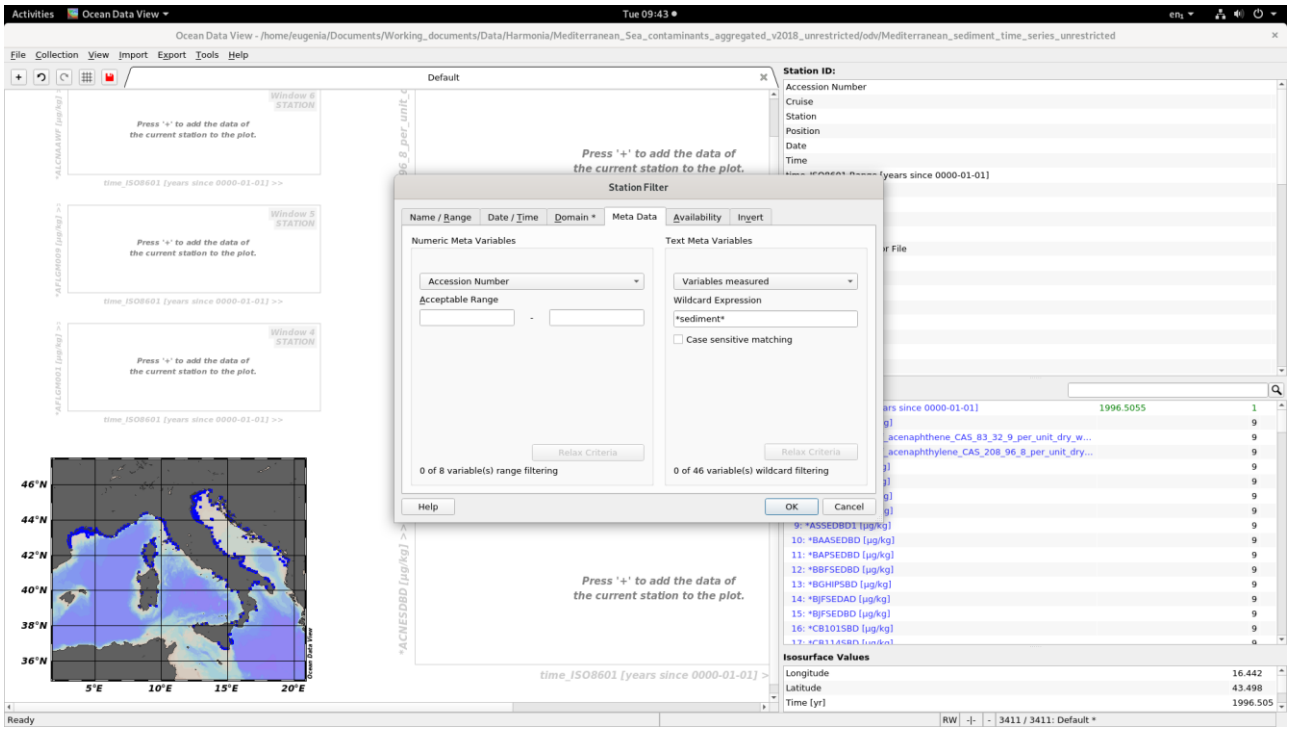
1. Check P02 present in the collection: Right-click in metadata field “variables measured”, select collect string values. Copy and paste in a text or spreadsheet file. Check if all P02s are related to the collection being analysed.



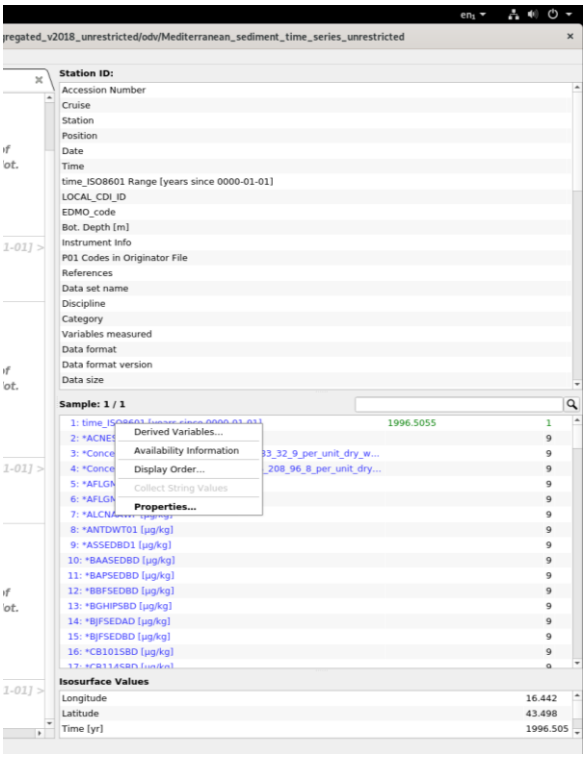


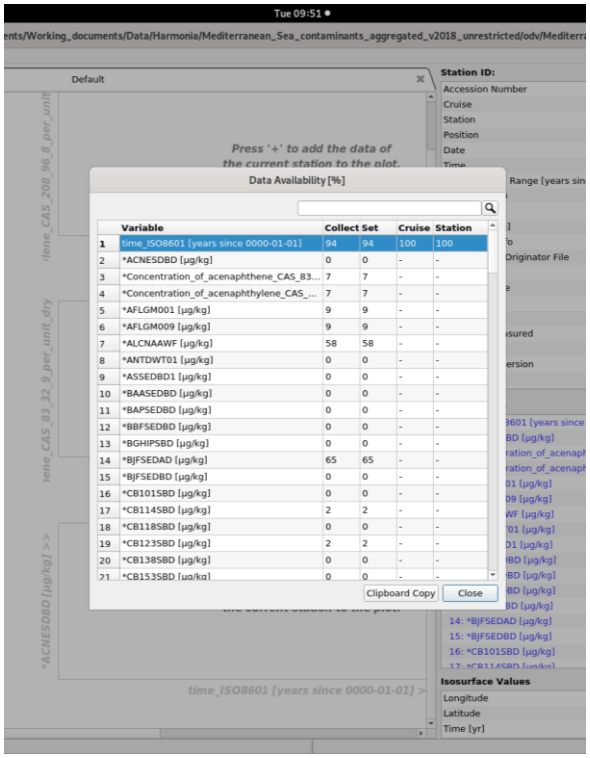
2. If any P02 is not related to the matrix/collection that is being prepared or to split collections that belong to different matrices: Right-click in metadata field “variables measured”, select “station filter”. Inside station filter window select “meta data” sheet and within text meta variables select “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. For water, if the filter is "*water col* || *water bod*", it will avoid getting parameters related to sediment pore waters.

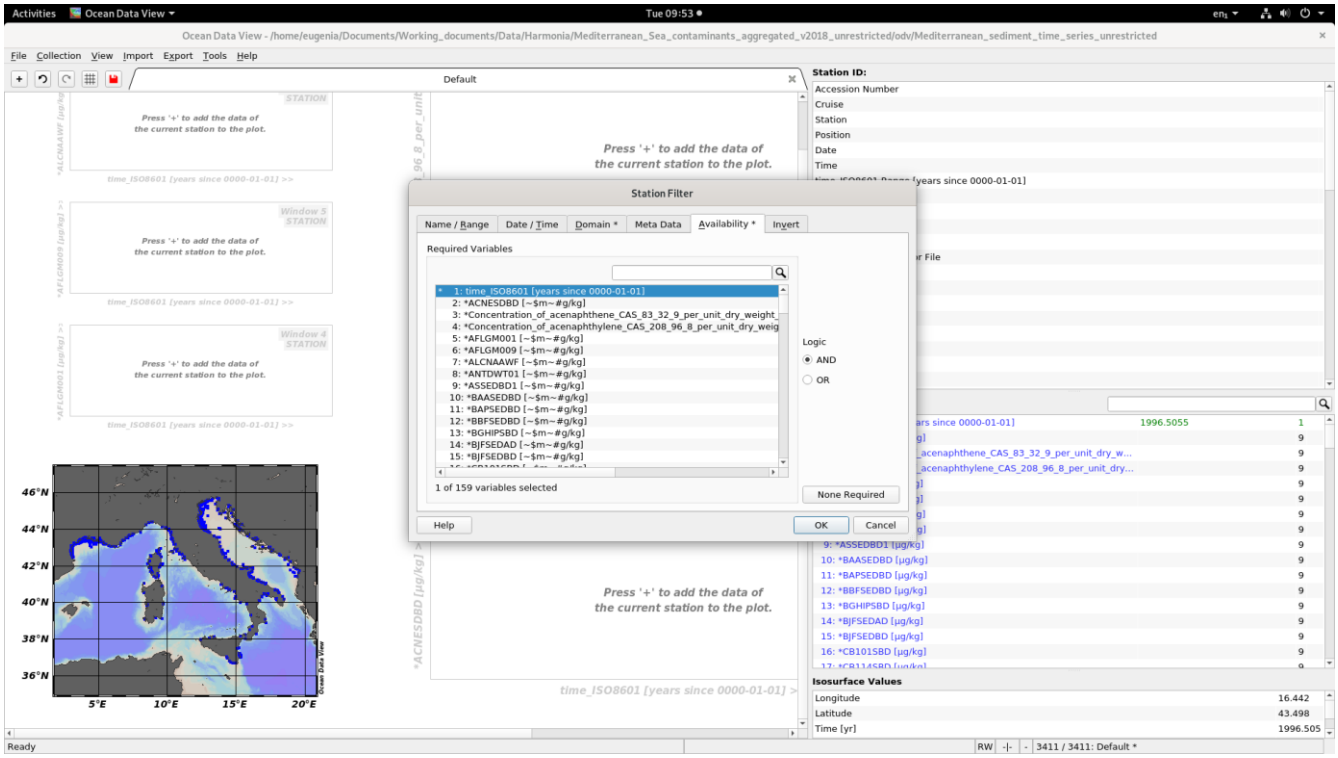


3. Export the stations and variables related to the previous filter.
4. Check if the primary variable is present in the whole collection. Right-click in the primary variable field, select availability information. If the percentage is not 100% for the primary variable, check if there is another P01 that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



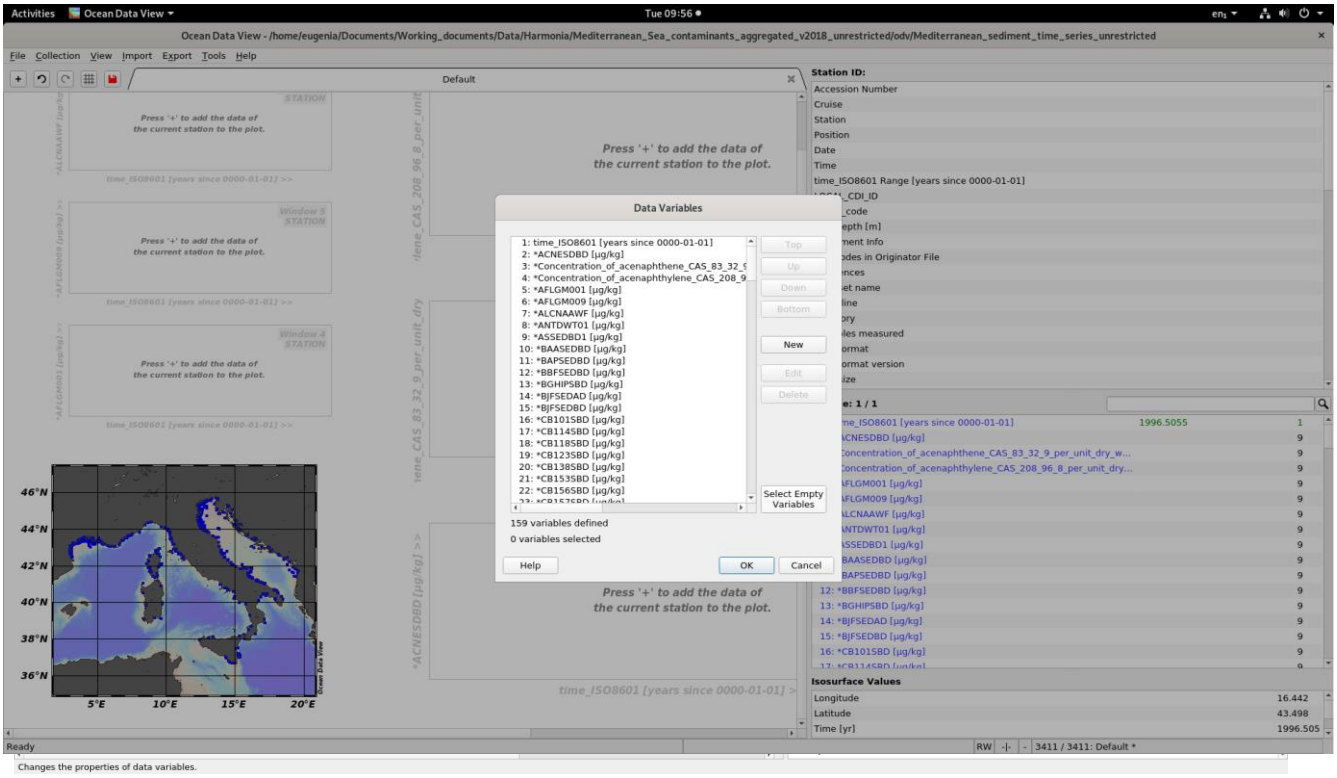


5. If primary variable is not 100% present, you can filter which stations don't contain the parameter associated to the primary variable. Right-click in metadata field "variables measured", select "station filter". Inside station filter window select "availability" and choose the primary variable as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



6. Check if there are empty variables in the whole collection. In the window collection, inside properties, data variables, select empty variables. If there' s any empty variable for the whole collection, they should be inspected in order to verify any possible errors deriving from import into ODV. Only if it is confirmed that these are empty, they can be deleted.

7. Check if there are variables that do not correspond to the matrix (i.e. depth in sediment instead of depth below seabed). See the parameters list on the right part of ODV; one by one with the cursor over each variable the name can be visualized, taking note of which of them are not suitable in the collection. Parameters related to water are usually in units /L (but not always). Parameters related to sediment or biota are usually in units /kg. It is necessary to be careful with the end of the parameters list that contain parameters related to the sample and not to contaminants measurements.

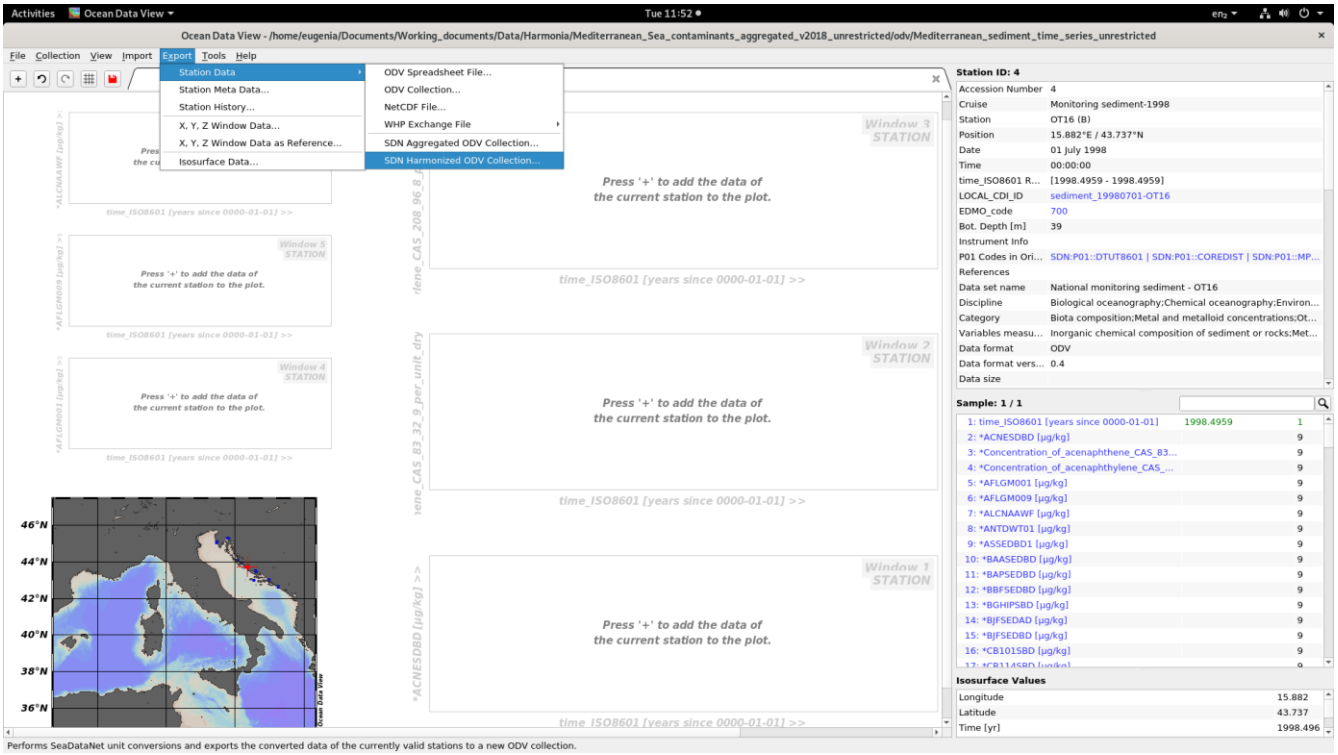

Activities
Ocean Data View
Tue 09:56
Ocean Data View - /home/eugenia/Documents/Working_documents/Data/Harmonia/Mediterranean_Sea_contaminants_aggregated_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted
File Collection View Import Export Tools Help
Default
Press '+' to add the data of the current station to the plot.
Data Variables
1: time_ISO8601 [years since 0000-01-01]
2: *ACNESDBD [µg/kg]
3: *Concentration_of_acenaphthene_CAS_83_32_9_per_unit_dry_weight
4: *Concentration_of_acenaphthylene_CAS_208_96_8_per_unit_dry_weight
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]
16: *CB101SBD [µg/kg]
17: *CB114SBD [µg/kg]
18: *CB118SBD [µg/kg]
19: *CB123SBD [µg/kg]
20: *CB138SBD [µg/kg]
21: *CB153SBD [µg/kg]
22: *CB156SBD [µg/kg]
Top
Up
Down
Bottom
New
Edit
Delete
Select Empty Variables
159 variables defined
0 variables selected
Help
OK
Cancel
Station ID:
Accession Number
Cruise
Station
Position
Date
Time
time_ISO8601 Range [years since 0000-01-01]
Isosurface Values
Longitude 16.442
Latitude 43.498
Time [yr] 1996.505
46°N
44°N
42°N
40°N
38°N
36°N
5°E
10°E
15°E
20°E
Ready
Changes the properties of data variables.


Activities
Ocean Data View
Tue 10:10
Ocean Data View - /home/eugenia/Documents/Working_documents/Data/Harmonia/Mediterranean_Sea_contaminants_aggregated_v2018_unrestricted/odv/Mediterranean_sediment_time_series_unrestricted
File Collection View Import Export Tools Help
Default
Press '+' to add the data of the current station to the plot.
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
46°N
44°N
42°N
40°N
38°N
36°N
5°E
10°E
15°E
20°E
Ready

4. Harmonization of unit and parameter naming

The next step involves harmonising the collection in terms of units and P01 parameters. In order to harmonize measurement units, a bibliographic analysis of most widely used measurement units for classes of contaminants in the different matrices has been performed. EU directives (2013/39/UE; Comm. Dec. EU 2017/848) have been considered to define short list of «preferred units» and to establish, when possible, conversion factors.

Ocean Data View (ODV) allows to harmonize (i.e. performs unit conversion, merges the same P01 expressed by different local names and keeps track of “harmonized” variables) and to allow easier retrieval of variable names from P01 standard codes.



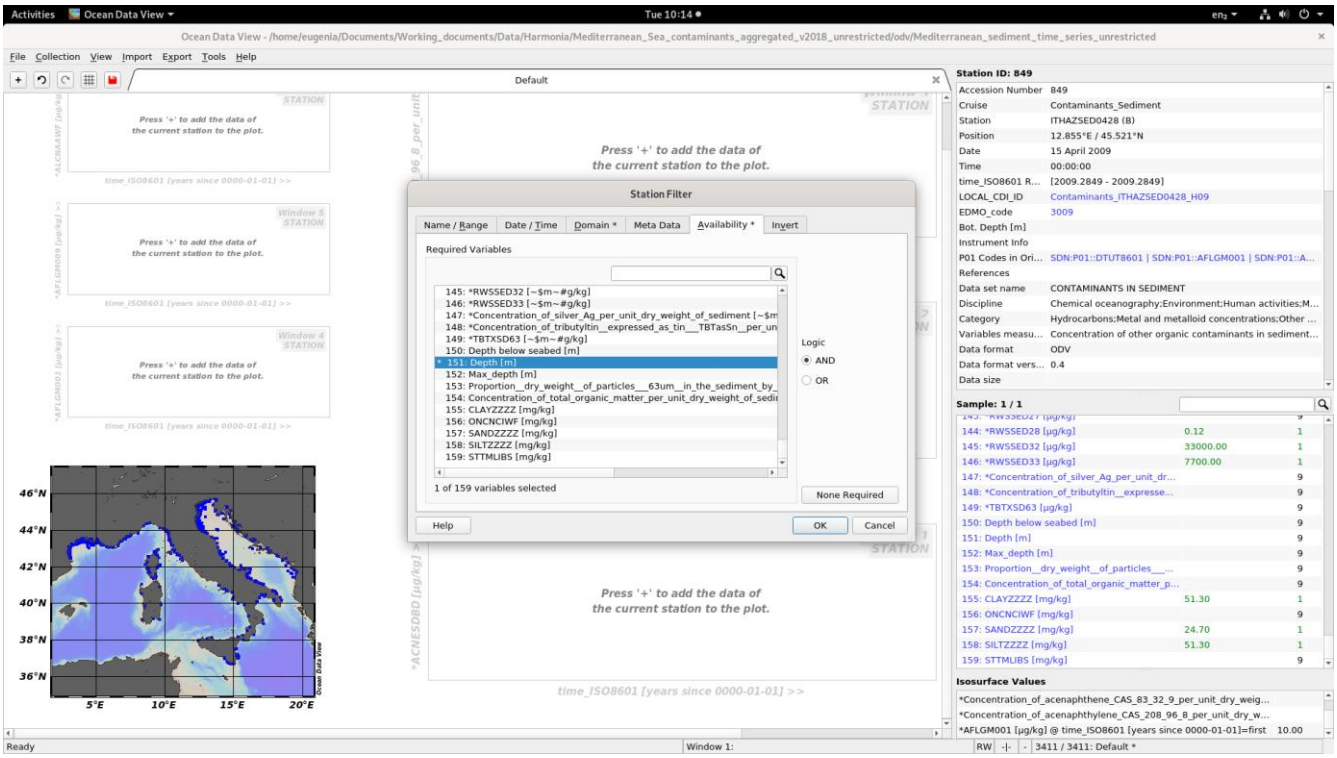
1. Check at the end of the variable list if there is any non-harmonized variable that is not linked with contaminants data (i.e. chlorophyll data…). It is better to avoid exporting additional parameters related to other themes (e.g. eutrophication). However, this step needs to be carefully performed because there may be a set of parameters at the end of the list that are related to the sample (e.g. sediment size and porosity, water content, …) and not to contaminants measurements, which need however to be maintained in the collection. Try to avoid deleting this kind of parameters:

- For water: Depth (if time series), pH, Salinity, Temperature, Transparency Depth, Dissolved Oxygen
- For sediment: Depth below seabed (if time series), Proportion of sizes of particles, Parameters related to granularity, water content, organic matter content, thickness of sediment properties and sedimentation taxes...
- For biota: parameters related to the sample (biota sizes, sample ids, sex, life stage…), water and lipid contents, wet weight, depth…

Regarding time-series collections, sometimes there is more than one parameter related to the sampling depth (with equivalent P01s or same P01 in different units). In this case the parameters should be merged.

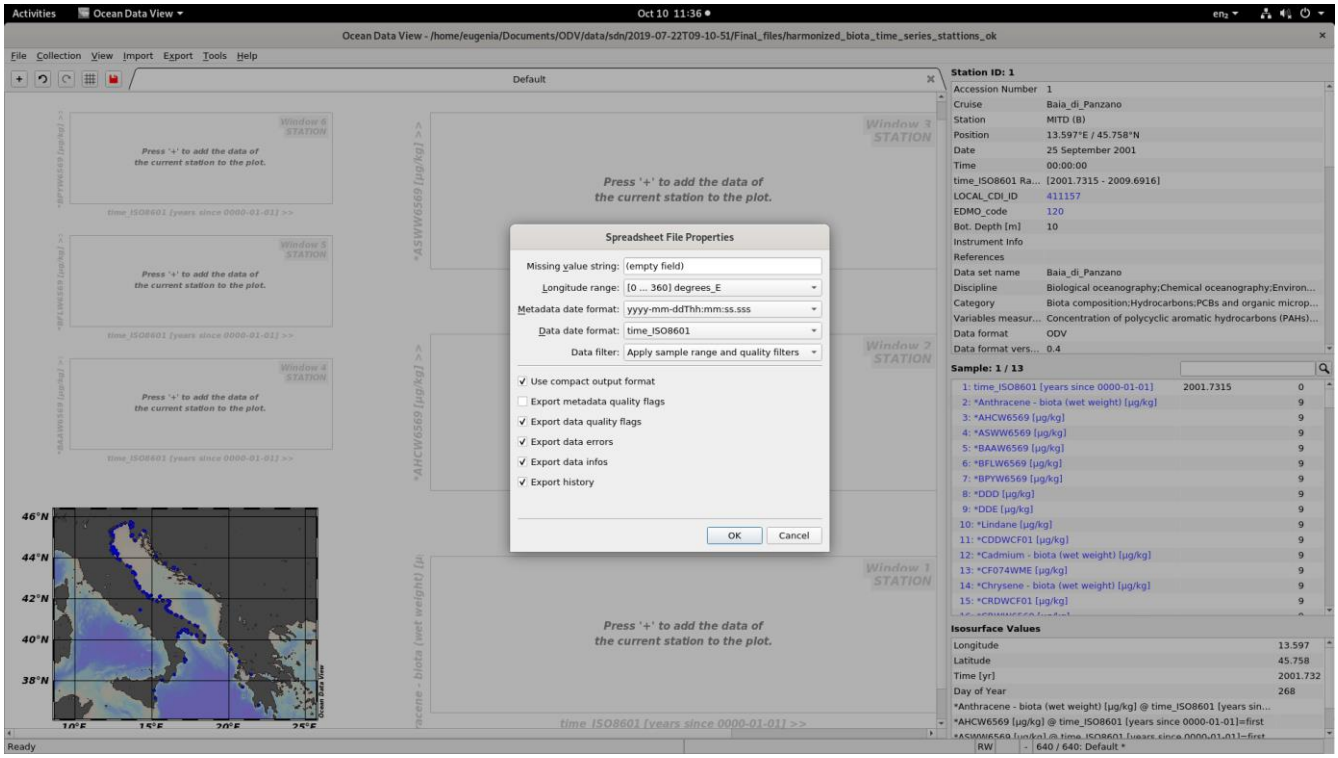
2. Once the parameters collection is “clean” and all parameters are supposed to belong to the matrix, a final check can be done. Open again the station filter, and in the availability sheet, choose “OR” and select only related to contaminants, not to the sample (i.e. depth, sample_id, composition of the sample….). It is possible to have stations in the collection that contain only parameters related to the sampling and not contaminants and these stations have to be avoided. Export the final clean selection of stations. A double check before the export can be performed inverting the selection of the stations and making sure that the “discarded stations” don’t contain parameters related to contaminants.
3. If there are still stations that contain potential wrong variables, contact the originators. In the station filter, choosing the sheet “availability”, choose the variable to check.

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



4. If there are variables in different units, there is a functionality inside ODV to aggregate them performing previously the transformation needed.
5. For contaminant in sediment only measurements till 10 cm depth (COREDIST=0.1 m) are useful. During the final spreadsheet export, this can be done exporting values with the data filter as function of the range, choosing values from 0 – 0.10 for COREDIST parameters.

6. Check manually inside ODV or outside using a script that variables related to contaminants with value=0, have a QF=6 (under LOD)



5. Check of quality flagging of data and metadata

Check values of quality flags on data and metadata and modifications according to SDN standards:

- In case of empty cells → QF=9
- In case of values = 0 for contaminant concentrations → QF=6

Negative values should be carefully inspected:

- in case of negative values (**not related** to P01 that can have negative values, and **different from** missing values: -9999, -999, ...) --> QF=4
- in cases of P01 admitting negative values, originator Quality Flagging should be maintained, unless scientific evidence suggests modification

6. Checks for inconsistent measurement units

When using the harmonized, transposed and decomposed matrix outside ODV, it is possible to select all parameters related to “concentration” variables and check for inconsistent measurement units (e.g. Kg, meters, °C for concentrations) and attribute the proper QF.

7. Checks for clearly impossible data ranges (ex. Different orders of magnitude)

Due to the multiple combinations of matrices, chemical substances and analytical methods, the resulting list of variables included in the datasets is huge. There is not enough information about the concentration ranges for the specific variables in the different areas. With this in mind, visual inspection of data is carried out in order to check for clearly impossible data ranges (ex. different orders of magnitude). Suspect data are flagged according to SDN standards and data originators must be contacted.

8. Dataset output formats

Data collections for marine contaminants are available in two formats:

- as SeaDataNet ODV csv spreadsheet format, which can be easily handled and visualised with ODV Software (More information can be found at www.seadatanet.org/Software/ODV);
- as transposed and decomposed csv spreadsheet format.

SeaDataNet ODV csv spreadsheet format

The fundamental data model underlying the format is the spreadsheet: i.e. a collection of rows each having the same fixed number of columns. There are three different types of columns:

- · Metadata columns
- · Primary variable data columns (one column for the value plus one for the qualifying flag)
- · Data columns

Further details on standard Data Transport Formats are provided here (https://archimer.ifremer.fr/doc/00454/56547/)

Transposed and decomposed csv spreadsheet format

Due to high heterogeneity and complexity of data on marine contaminants, to assist data processing and selection of specific information such as chemical substance, matrix characteristics, biological entity, basis of determination, etc., connected to each single variable, EMODnet Chemistry provides as additional dataset format the “transposed and decomposed” csv spreadsheet format. This dataset format, as the standard ODV csv format, contains metadata and data together.

The differences consist in:

- data on concentrations of chemical substances are transposed, which results in one column containing the parameter names (i.e. P01 codes) and one column with the concentration value
- P01 terms are decomposed into the different subcomponents (namely parameter entity name, parameter statistic, substance name, matrix characteristics, biological entity names, analytical method, ...), when available

The transposed and decomposed format allows users to independently filter and aggregate data according to their specific needs. As some information (eg. station name, bottom depth, water depth, …) is present both in the metadata and data, some information can be either present twice or available only as data or as metadata. The list of column names with description and example is available in the table below. All vocabularies are available here: https://vocab.seadatanet.org/search.

Column names	Description	Example
Cruise	Name of the cruise	148
Station*	Code of monitoring station	TZ-8-S
yyyy-mm-ddThh:mm:ss.sss	time	2014-09-27T11:00:00
Longitude [degrees_east]	Longitude	18.741
Latitude [degrees_north]	Latitude	42.474
LOCAL_CDI_ID	LOCAL_CDI_ID	SED148_3/v1
EDMO_code	Originator code	2432
Bot. Depth [m]	Bottom depth of the station	34
Instrument Info	Information on sampling device	sediment grabs
References	References	https://cdi.seadatanet.org/report/edmo/2432/SED148_3/v1
Datum	Geodetic Datum	World Geodetic System 84 (4326)
Water depth [m]	Water column depth	33.8
Depth reference	Depth reference	sea level (D08)
Minimum instrument depth [m]	Minimum instrument depth [m]	
Maximum instrument depth [m]	Maximum instrument depth [m]	
Instrument / gear type	Sampling and analytical instrument	sediment grabs (50)|inductively-coupled plasma mass spectrometers (LAB15)|rulers (LAB29)
Station name*	Station name	TZ-8-S
Originator	Originator	Institute of Marine Biology (IMBK) (2432)
Project name	Project name	Monitoring program of the state of coastal sea ecosystem of Montenegro (12207)
EDMED references	EDMED references	Monitoring of contaminants in Montenegrin coastal areas 2009-2015 (6820)
Access restriction	Access restriction	SeaDataNet licence (LS)
CDI-record id	CDI-record id	2676153

Sample identifier	Sample identifier	500
Subsample identifier	Subsample identifier	500.1
ODV internal sample number	ODV internal sample number	1
Depth below seabed [m]	Depth below seabed [m]	0
QV:SEADATANET	Quality Value (according to SEADATANET)	1
Value	Value of parameter indicated by S06	270
QV:SEADATANET	Quality Value (according to SEADATANET)	0
Units	Measerurement Units	ug/kg
P01_conceptid	P01 code	CD04ICP3
P01_preflabel	BODC Parameter usage vocabulary	Concentration standard deviation of cadmium {Cd CAS 7440-43-9} per unit mass of the water body [dissolved plus reactive particulate <0.4/0.45um phase] by filtration, acidification and inductively-coupled plasma mass spectrometry
S06_preflabel	Parameter entity names	Concentration
S07_preflabel	Parameter statistic	standard deviation
S27_preflabel	BODC substances	cadmium
S27_altlabel	short name	Cd
CAS no	Chemical Abstracts Service number	7440-43-9
S02_preflabel	Where/what relationships	per unit mass of the
S26_preflabel	BODC matrices	water body [dissolved plus reactive particulate <0.4/0.45um phase]
S25_preflabel	Biological entity names	Dinophysis caudata (ITIS: 9939: WoRMS 109612)
S03_preflabel	Sample preparation	filtration, acidification
S04_preflabel	Analytical method	inductively-coupled plasma mass spectrometry

S05_preflabel	Data processing	volume computation from mass and mean density
S21_preflabel	Sphere names	water body

*** duplicate information, however sometimes not exactly matching**
****duplicate information, however sometimes not exactly matching (due to decimal rounding)**