

EMODnet Chemistry 3

Various issues

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OGS





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European Marine
Observation and
Data Network

Various issues

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Issues:

- ⦿ High resolution DIVA maps for nutrients near river mouths
- ⦿ Proposal of revised mapping SDN flag 5 to ODV flag scale
- ⦿ Preferred units for P01 of contaminants and criteria for Data QC for contaminants
- ⦿ Contaminant buffer analysis and new ODV tool:



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Objectives:

High resolution DIVA maps for nutrients near river mouths

Issues:

- ⦿ Which parameters to map?
- ⦿ Domain extent? Distance along-shore and from the shore?

Proposal:

- ⦿ Priority 1: DIN, PO₄, SiO₂

From the proposal: "number of high resolution DIVA maps for nutrients in the coastal zone/along the coast near river mouths"

- ~~⦿ From the shore: according to WFD: 1 nautical mile (lost of important information)~~
- ⦿ Based on SDN salinity fields (see examples)

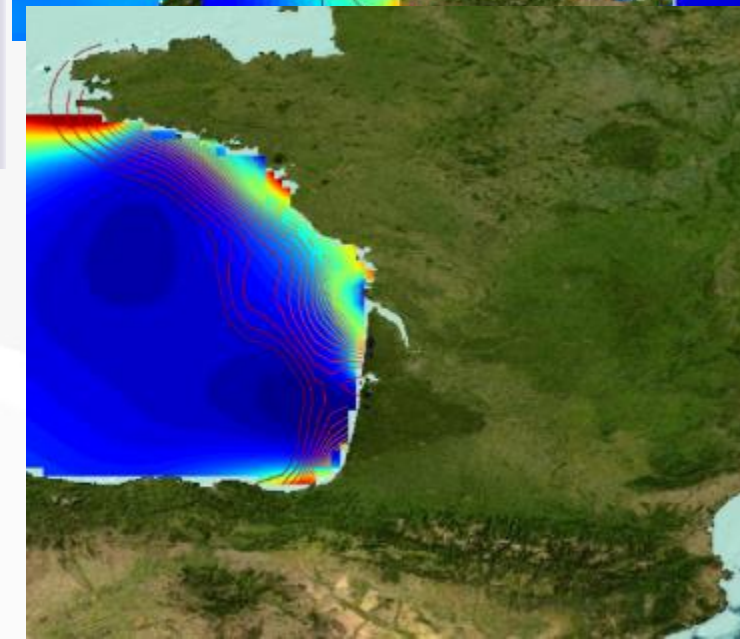
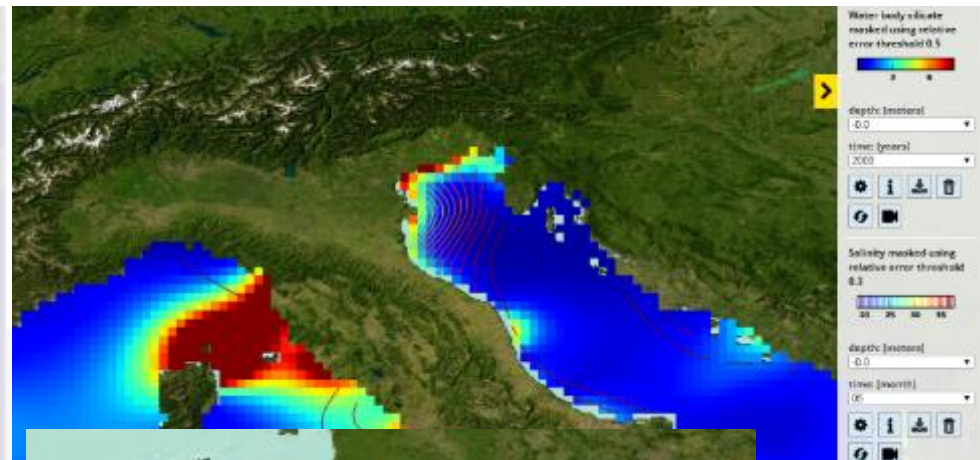
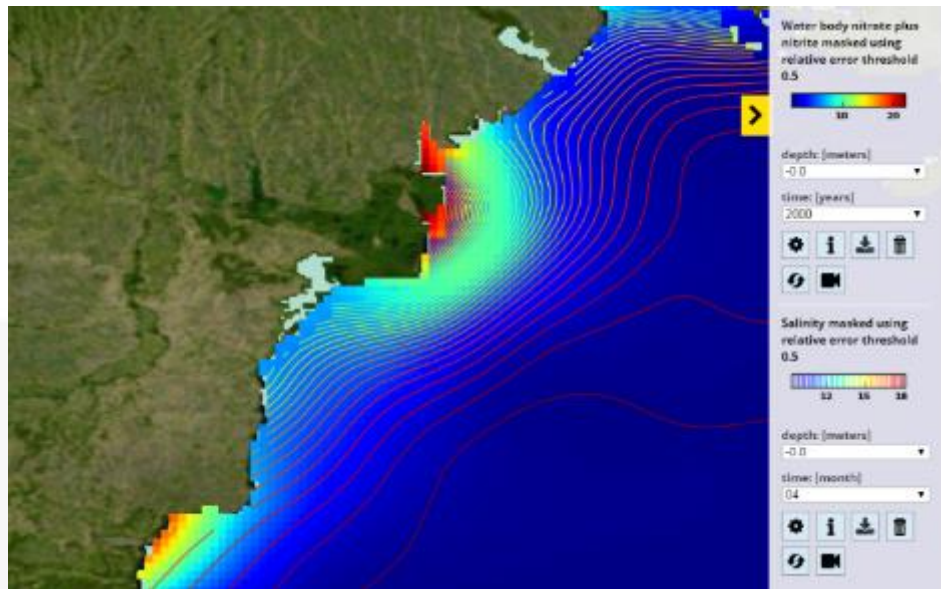


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Examples: spring (April/May) salinity fields -SDN





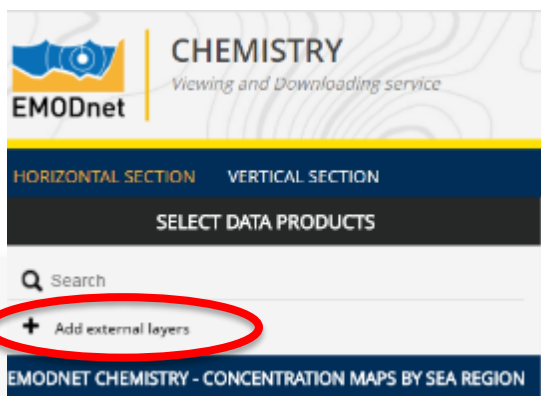
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To add salinity fields from Oceanbrowser:

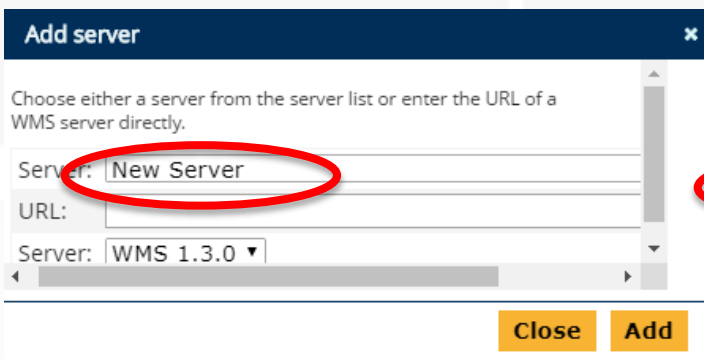
<http://ec.oceanbrowser.net/emodnet/#0>

1. Click on Add external layers

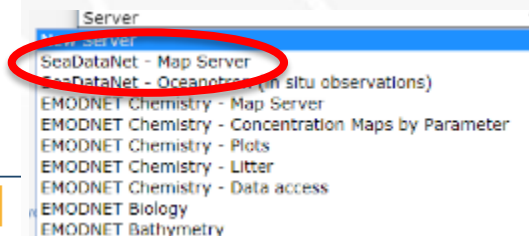


1

2. Click on New Server – SeaDataNet-Map Server

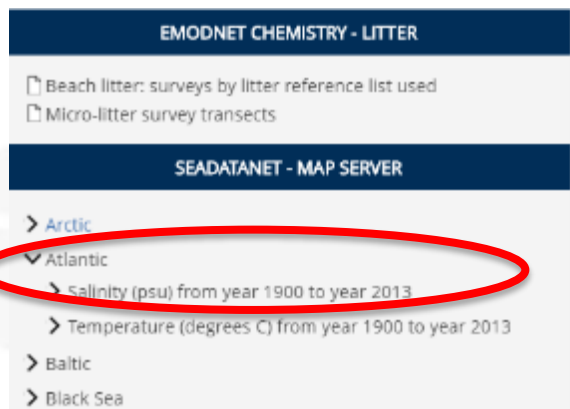


2



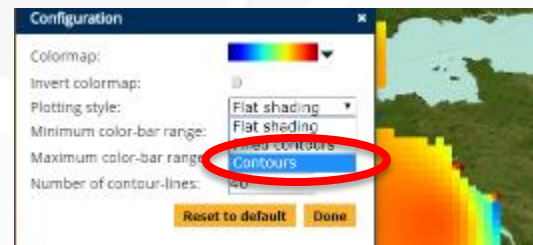
3. Go to the very end of the page on SEADATANET-MAP SERVER

Choose the region and field of interest (salinity)



3

4. Change the Configuration of Salinity to «Contours» to obtain what I showed (previous slide)



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Objectives:

High resolution DIVA maps for nutrients near river mouths

Issues:

- Map resolution?

- Time extent?

- Running mean?

Proposal:

Now:

- Atlantic: 0.1 degree
- Arctic:
- Baltic: 0.1 degree
- BlackSea = 0.05 degree
- Mediterranean: 0.125 degree
- North:

Proposal:

- 0.05 degree to correctly represent the gradient at river mouths
- Running mean 6-years; Priority: recent period; Seasonal basis



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Objectives: High resolution DIVA maps for nutrients near river mouths

The screenshot displays the QGIS 2.18.22 interface with the following components:

- Menu Bar:** Project, Edit, View, Layer, Settings, Plugins, Vector, Raster, Database, Web, MMQGIS, Processing, Help.
- Toolbar:** Standard GIS tools for navigation, editing, and analysis.
- Browser Panel:** Shows the project structure with folders for Project home, Home, Favourites, and data sources like DB2, MSSQL, and PostGIS.
- Statistics Panel:** Displays a table for the selected layer 'Harmonia_Sampling_sites_example'.

Statistic	Value
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- Layers Panel:** Lists the loaded layers:
 - Mappa_completa_HARMONIA_data
 - Waterbase_tcm_v12_Stations_EIONET
 - Large_rivers
 - SurfaceWaterBody
 - coastalWaterBody
 - lakeWaterBody
 - riverWaterBody
 - territorialWaters
 - transitionalWaterBody
- Log Messages Panel:** Located at the bottom of the interface.

The main map area shows a map of Europe with a network of rivers and coastal features. The 'Large_rivers' layer is highlighted in blue, and the 'SurfaceWaterBody' layer is expanded to show various water body types.

Proposal of revised mapping SDN flag 5 to ODV flag scale (feedback needed from R. Schlitzer)

Current mapping:	ODV	SDN
no quality control	1	0
good value	0	1
probably good value	0	2
probably bad value	4	3
bad value	8	4
changed value	1	5
value below detection	1	6
value in excess	1	7
interpoalted value	1	8
missing value	1	9
value phenomenon uncertain	1	A
value below limit of quantification	1	Q

Proposal:	ODV	SDN
no quality control	1	0
good value	0	1
probably good value	0	2
probably bad value	4	3
bad value	8	4
changed value	0	5
value below detection	0	6
value in excess	1	7
interpolated value	1	8
missing value	1	9
value phenomenon uncertain	1	A
value below limit of quantification	1	Q

	ODV	SDN
good quality	0	1
unknown quality	1	0
questionable quality	4	3
bad quality	8	4

Decision needed!

5	changed value	changed	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.	5
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Preferred units for P01 of contaminants and criteria for Data QC for contaminants (and not only):

- Analysis of P06 («data storage units») associated to P01 on contaminants in First Contaminant buffer (File from DICK). Total of 8667 lines (due to combinations of P01-P06)!
- 36 different P06

- (Seleziona tutto)
- Becquerels per kilogram
- Becquerels per litre
- Becquerels per square metre
- Days
- Decibars
- Degrees Celsius
- Dimensionless
- Grams per gram
- Grams per kilogram
- Kilograms
- Kilograms per cubic metre
- Metres
- Micrograms per gram
- Micrograms per kilogram

- Micrograms per litre
- Micromoles per kilogram
- Micromoles per litre
- Millibecquerels per litre
- Milligrams per gram
- Milligrams per kilogram
- Milligrams per litre
- Millilitres per litre
- Millimoles per litre
- Nanograms per gram
- Nanograms per kilogram
- Nanograms per litre

- Nanomoles per kilogram
- Nanomoles per litre
- Nephelometric Turbidity Units
- NULL
- Parts per billion
- Parts per million
- Parts per million by volume
- Parts per thousand
- Parts per thousand per hour
- Percent



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New ODV tool developed by R. Schlitzer:

- Converts P06 measurement units to short list of «**preferred units**» according to EU directives (2013/39/UE; Comm. Dec. EU 2017/848)
- From 36 different P06 to 5!**

UUKG	Micrograms per kilogram
UGPL	Micrograms per litre
BQSM	Becquerels per square metre
UBQK	Becquerels per kilogram
UBQL	Becquerels per litre



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Criteria for Data QC for contaminants (and not only):

Check of measurement units and search for doubtful or impossible units using reference table

Check for "NULL":

p06	p06_text	p01_text
SRAD	NULL	Activity of caesium-137 {137Cs CAS 10045-97-3} per unit dry weight of sediment by gamma spectroscopy
UPDS	NULL	Concentration of aluminium {Al CAS 7429-90-5} per unit dry weight of sediment
UPTC	NULL	Concentration of aluminium {Al CAS 7429-90-5} per unit dry weight of sediment <63um by wet sieving, acid digestion and atomic absorption spectroscopy
UPGL	NULL	Concentration of copper {Cu CAS 7440-50-8} per unit volume of the water body [dissolved plus reactive particulate phase]
NGPL	NULL	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit volume of the water body [dissolved plus reactive particulate <0.4/0.45um phase] by filtration and cold vapour atomic absorption spectroscopy
BCMT	NULL	Concentration of total mercury {total_Hg CAS 7439-97-6} per unit wet weight of biota {Clupea harengus (ITIS: 161722: WoRMS 126417) [Subcomponent: liver]}



	Currently used P06
UBQK	Becquerels per kilogram
UBQL	Becquerels per litre
BQSM	Becquerels per square metre
UTAA	Days
UPDB	Decibars
UPAA	Degrees Celsius
UUUU	Dimensionless
GPRG	Grams per gram
UGKG	Grams per kilogram
KGXX	Kilograms
UKMC	Kilograms per cubic metre
ULAA	Metres
UGGR	Micrograms per gram
UUKG	Micrograms per kilogram
UGPL	Micrograms per litre
KGUM	Micromoles per kilogram
UPOX	Micromoles per litre
UMBQ	Millibecquerels per litre
MGPG	Milligrams per gram
UMKG	Milligrams per kilogram
UMGL	Milligrams per litre
UMLL	Millilitres per litre
MMPL	Millimoles per litre
NGPG	Nanograms per gram
NGKG	Nanograms per kilogram
UNGL	Nanograms per litre
KGNM	Nanomoles per kilogram
UPNM	Nanomoles per litre
USTU	Nephelometric Turbidity Units
UPPB	Parts per billion
UPPM	Parts per million
UMLV	Parts per million by volume
UPPT	Parts per thousand
UPTH	Parts per thousand per hour
UPCT	Percent



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Criteria for Data QC for contaminants (and not only):

ODV tool to convert units into Preferred units should help in identifying this kind of mistake as P01 with units not in the table are not converted

	Currently used P06		Preferred unit
UBQK	Becquerels per kilogram	UBQK	Becquerels per kilogram
UBQL	Becquerels per litre	UBQL	Becquerels per litre
BQSM	Becquerels per square metre	BQSM	Becquerels per square metre
UTAA	Days		
UPDB	Decibars		
UPAA	Degrees Celsius		
UUUU	Dimensionless		
GPRG	Grams per gram	UUKG	Micrograms per kilogram
UGKG	Grams per kilogram	UUKG	Micrograms per kilogram
KGXX	Kilograms		
UKMC	Kilograms per cubic metre	UGPL	Micrograms per litre
ULAA	Metres		
UGGR	Micrograms per gram	UUKG	Micrograms per kilogram
UUKG	Micrograms per kilogram	UUKG	Micrograms per kilogram
UGPL	Micrograms per litre	UGPL	Micrograms per litre
KGUM	Micromoles per kilogram	UUKG	Micrograms per kilogram
UPOX	Micromoles per litre	UGPL	Micrograms per litre
UMBQ	Millibecquerels per litre	UBQL	Becquerels per litre
MGPG	Milligrams per gram	UUKG	Micrograms per kilogram
UMKG	Milligrams per kilogram	UUKG	Micrograms per kilogram
UMGL	Milligrams per litre	UGPL	Micrograms per litre
UMLL	Millilitres per litre		?
MMPL	Millimoles per litre	UGPL	Micrograms per litre
NGPG	Nanograms per gram	UUKG	Micrograms per kilogram
NGKG	Nanograms per kilogram	UUKG	Micrograms per kilogram
UNGL	Nanograms per litre	UGPL	Micrograms per litre
KGNM	Nanomoles per kilogram	UUKG	Micrograms per kilogram
UPNM	Nanomoles per litre	UGPL	Micrograms per litre
USTU	Nephelometric Turbidity Units		
UPPB	Parts per billion	UUKG	Micrograms per kilogram
UPPM	Parts per million	UUKG	Micrograms per kilogram
UMLV	Parts per million by volume	UGPL	Micrograms per litre
UPPT	Parts per thousand	UUKG	Micrograms per kilogram
UPTH	Parts per thousand per hour		
UPCT	Percent	UPCT	Percent

Criteria for Data QC for contaminants (and not only):

- ⦿ What is missing from the conversion now:
 - ⦿ All conversion from “moles/ μ moles...” to mg as conversion factors depend on the specific substance
 - ⦿ Conversions from “mass” to “volume” for water matrix (ex. Below) as they coincide with what defined for sediment

p01	p01_text	p06	p06_text
DDEPPAF1	Concentration of 4,4'-dichlorodiphenyldichloroethylene {p,p'-DDE CAS 72-55-9} per unit volume of the water body [dissolved plus reactive particulate <unknown phase]	NGKG	Nanograms per kilogram
DDEPPAF1	Concentration of 4,4'-dichlorodiphenyldichloroethylene {p,p'-DDE CAS 72-55-9} per unit volume of the water body [dissolved plus reactive particulate <unknown phase]	UGPL	Micrograms per litre
DDEPPAF1	Concentration of 4,4'-dichlorodiphenyldichloroethylene {p,p'-DDE CAS 72-55-9} per unit volume of the water body [dissolved plus reactive particulate <unknown phase]	UMKG	Milligrams per kilogram
DDEPPAF1	Concentration of 4,4'-dichlorodiphenyldichloroethylene {p,p'-DDE CAS 72-55-9} per unit volume of the water body [dissolved plus reactive particulate <unknown phase]	UNGL	Nanograms per litre



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Left overs:

Currently used P06

UBQK	Becquerels per kilogram	UBQK
UBQL	Becquerels per litre	UBQL
BQSM	Becquerels per square metre	BQSM
UTAA	Days	
UPDB	Decibars	
UPAA	Degrees Celsius	
UUUU	Dimensionless	
GPRG	Grams per gram	UUKG
UGKG	Grams per kilogram	UUKG
KGXX	Kilograms	
UKMC	Kilograms per cubic metre	UGPL
ULAA	Metres	
UGGR	Micrograms per gram	UUKG
UUKG	Micrograms per kilogram	UUKG
UGPL	Micrograms per litre	UGPL
KGUM	Micromoles per kilogram	UUKG
UPOX	Micromoles per litre	UGPL
UMBQ	Millibecquerels per litre	UBQL
MGPG	Milligrams per gram	UUKG
UMKG	Milligrams per kilogram	UUKG
UMGL	Milligrams per litre	UGPL
UMLL	Millilitres per litre	
MMPL	Millimoles per litre	UGPL
NGPG	Nanograms per gram	UUKG
NGKG	Nanograms per kilogram	UUKG
UNGL	Nanograms per litre	UGPL
KGNM	Nanomoles per kilogram	UUKG
UPNM	Nanomoles per litre	UGPL
USTU	Nephelometric Turbidity Units	
UPPB	Parts per billion	UUKG
UPPM	Parts per million	UUKG
UMLV	Parts per million by volume	UGPL
UPPT	Parts per thousand	UUKG
UPTH	Parts per thousand per hour	
UPCT	Percent	UPCT
NULL	NULL	

Preferred unit

Becquerels per kilogram
Becquerels per litre
Becquerels per square metre
Micrograms per kilogram
Micrograms per kilogram
Micrograms per litre
Micrograms per kilogram
Micrograms per kilogram
Micrograms per litre
Micrograms per litre
Micrograms per kilogram
Micrograms per kilogram
Micrograms per kilogram
Micrograms per litre
?
Micrograms per litre
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Micrograms per litre
Micrograms per kilogram
Micrograms per litre
Micrograms per kilogram
Micrograms per kilogram
Micrograms per litre
Micrograms per kilogram



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Contaminant buffer analysis and new ODV tool:

Outcomes from activities carried out for HarmoNIA project:

- 🎯 Data buffer contains variables indicated as P01-conceptId together with other «labels/local names»
(more user-friendly BUT arbitrary-not homogeneous)

Data set name: 09M-P-007 - Cap d'Orne - Contaminants

Sample: 1 / 11

1: time_ISO8601 [years since 000...	1979.2740
2: ZNWW6569 [µg/kg]	
3: DryWt_Zn_Mytilus_edulis [µg/...	
4: DryWt_Zn_Crassostrea_gigas [...]	
5: Dieldrin_Boops_Flesh [µg/kg]	
6: Dieldrin_Mullus_Flesh [µg/kg]	
7: pp_DDE_Boops_Flesh [µg/kg]	
8: pp_DDE_Mullus_Flesh [µg/kg]	
9: pp_DDD_Boops_Flesh [µg/kg]	
10: pp_DDD_Mullus_Flesh [µg/kg]	
11: pp_DDT_Boops_Flesh [µg/kg]	
12: pp_DDT_Mullus_Flesh [µg/kg]	
13: g-HCH_Boops_Flesh [µg/kg]	
14: g-HCH_Mullus_Flesh [µg/kg]	
15: α-HCH_Mullus_Flesh [µg/kg]	
16: W2931223 [µg/kg]	
17: W2931198 [µg/kg]	



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New ODV tool: proposed approach:

Harmonization steps for contaminants:

- 1) ODV converts (where possible) measurement units to “preferred units” and merges different “labels (local names)” to the same P01
- 2) Mark in red **P01** that after the process are not in the preferred unit
- 3) Exclude columns with no data, QF=9 (missing values)

Data set name: 091-P-007 - Cap d'Orne - Contaminants

Sample: 1 / 11

1: time_ISO8601 [years since 000...	1979.2740
2: ZNWW6569 [µg/kg]	
3: DryWt_Zn_Mytilus_edulis [µg/...	
4: DryWt_Zn_Crassostrea_gigas [...	
5: Dieldrin_Boops_Flesh [µg/kg]	
6: Dieldrin_Mullus_Flesh [µg/kg]	
7: pp_DDE_Boops_Flesh [µg/kg]	
8: pp_DDE_Mullus_Flesh [µg/kg]	
9: pp_DDD_Boops_Flesh [µg/kg]	
10: pp_DDD_Mullus_Flesh [µg/kg]	
11: pp_DDT_Boops_Flesh [µg/kg]	
12: pp_DDT_Mullus_Flesh [µg/kg]	
13: g-HCH_Boops_Flesh [µg/kg]	
14: g-HCH_Mullus_Flesh [µg/kg]	
15: α-HCH_Mullus_Flesh [µg/kg]	
16: W2931223 [µg/kg]	
17: W2931198 [µg/kg]	



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New ODV tool: proposed approach:

Export steps for contaminants:

- 1) Add option to transpose to row format
- 2) Insert P01-ConceptID and full label as label **to**
harmonize column headers
- 3) Split P01 in sub-components

[[Data set name: 094-P-007 - Cap d'Ijoux - Contaminants]]

Sample: 1 / 11

1: time_ISO8601 [years since 000...	1979.2740
2: ZNWW6569 [µg/kg]	
3: DryWt_Zn_Mytilus_edulis [µg/...	
4: DryWt_Zn_Crassostrea_gigas [...]	
5: Dieldrin_Boops_Flesh [µg/kg]	
6: Dieldrin_Mullus_Flesh [µg/kg]	
7: pp_DDE_Boops_Flesh [µg/kg]	
8: pp_DDE_Mullus_Flesh [µg/kg]	
9: pp_DDD_Boops_Flesh [µg/kg]	
10: pp_DDD_Mullus_Flesh [µg/kg]	
11: pp_DDT_Boops_Flesh [µg/kg]	
12: pp_DDT_Mullus_Flesh [µg/kg]	
13: g-HCH_Boops_Flesh [µg/kg]	
14: g-HCH_Mullus_Flesh [µg/kg]	
15: α-HCH_Mullus_Flesh [µg/kg]	
16: W2931223 [µg/kg]	
17: W2931198 [µg/kg]	