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Data Article

Spatial distribution of organic and inorganic contaminants in Ria de Aveiro Lagoon: A fundamental baseline dataset

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A B S T R A C T

This paper presents baseline data of sediments characterization from Ria de Aveiro lagoon (Portugal). Twenty-two intertidal surface sediments were collected and analysed for their pseudo-total content of 25 major and trace elements and for their total content of PAHs (Sum16) and PCBs (Sum13). The fine fraction percentage and total organic carbon content were also determined. Ria de Aveiro Lagoon has been the target of several studies during the last decades, and it has been pointed out as a hot spot in terms of contamination García-Seoane et al., 2016. Nevertheless, data about sediments contamination is mostly focused on Hg Lillebø et al.,2011, and in a specific area of the lagoon Grilo et al., 2013, and there is not a clear and global picture about the spatial distribution of other elements, and especially of organic contaminants. Thus, this baseline dataset is of utmost importance for researchers and planners and it can be used to monitor the effect of disturbances, such as: dredging activities; hydrodynamic changes (either due to

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human activities or extreme events); external inputs (new discharges from industries and wastewater plants, etc).

Specifications Table

Subject	Environmental Sciences
Specific subject area	Environmental Chemistry; Geochemistry
Type of data	Tables, Figures
How data were acquired	Analytical instrumentation: Elemental Analyser EA1112, Thermmo Finningan (for Total Organic Carbon); ICP-MS 7700 series, Agilent Technologies (for major and trace elements determination); GC-MS QP5050A, Shimadzu Corporation (for PAHs and PCBs analysis). Software: ArcGis (version 9.3); IBM SPSS Statistics (version 25)
Data format	Raw, Analysed
Parameters for data collection	Intertidal surface sediments were collected in 22 sampling stations from Ria de Aveiro lagoon. Sampling locations were chosen in order to obtain a spatial distribution along the lagoon. An higher density of samples were taken from the most contaminated area (Laranjo bay and Esteiro de Estarreja). Each point corresponds to a composite sample. Samples were freeze-dried and sieved (<1mm).
Description of data collection	Fine fraction (<63 µm) and organic carbon (elemental analysis) were determined for a general characterization of samples. PAHs and PCBs were solvent extracted and quantified by GC-MS after appropriate clean-up. Major and trace elements were determined by ICP-MS after microwave digestion. Descriptive statistics was obtained for each parameter analysed using SPSS, and spatial distribution maps were obtained using ArcGis Software.
Data source location	Ria de Aveiro Lagoon, Aveiro, Portugal 40°40′56″N 8°40′5″W
Data accessibility	With the article

Value of the Data

- This data is useful for clearly understand the spatial distribution of contaminants and sediment's properties of Ria de Aveiro lagoon.
- This data will help researchers on planning for further research studies within this area and for comparison studies (temporal and spatial).
- This baseline dataset can be used to monitor the effect of disturbances, such as: dredging activities; hydrodynamic changes (either due to human activities or extreme events); external inputs (new discharges from industries and wastewater plants, etc).

1. Data

Fig. 1 shows the location of Ria de Aveiro Lagoon, as well as the location of the twenty-two samples collected. Tables 1–3 shows the coordinates of sampled sites, as well as their characterization regarding fine fraction percentage, total organic carbon content (OC), sum of 16 PAHs and of 13 PCBs (and of the seven considered indicators), major and trace elements concentration. Descriptive statistics (minimum, maximum, median, and mean values) is also shown. Figs. 2–4 shows the spatial distribution for some selected contaminants (PAHs, PCBs, As). The class limits correspond to the minimum, the quartiles (25, 50, and 75), and the maximum value.

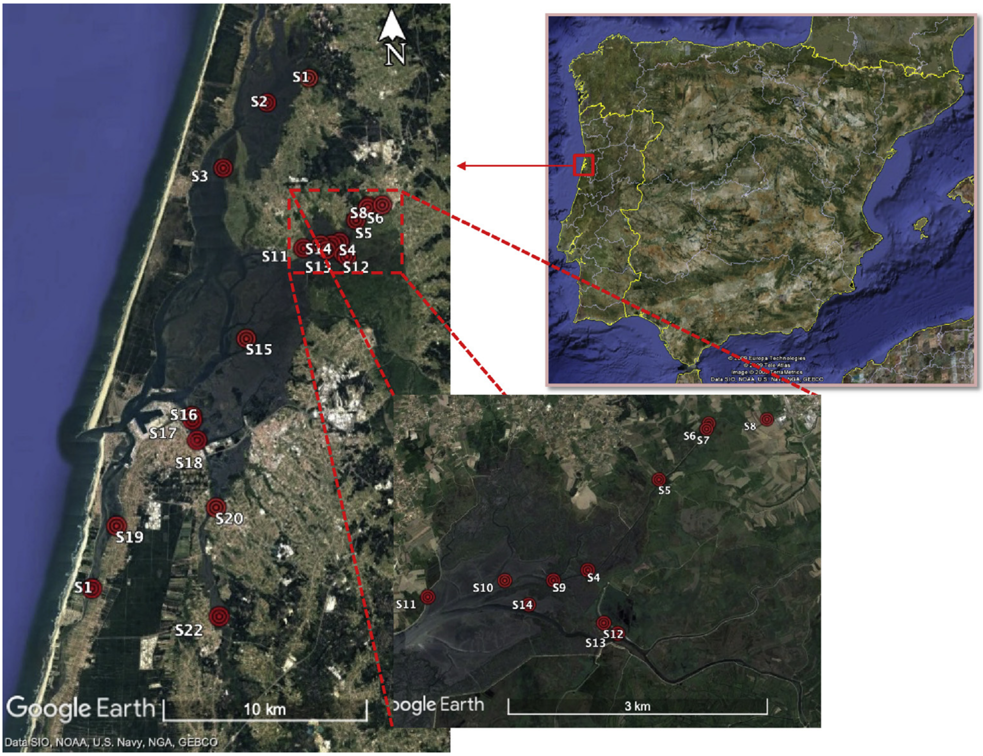

Fig. 1. Location of Ria de Aveiro Lagoon, as well as the location of the twenty-two samples collected.

Table 1
Sampling location coordinates (UTM 29N), percentage of fine fraction and organic carbon (OC), PAHs (SumPAHs), PCBs (SumPCBs) content. The sum of the 7 indicator PCBs is also presented (Sum 7PCBs). Descriptive statistics (minimum, maximum, median, and mean) is also shown.

Site	m	p	Fine Fraction (%)	OC (%)	SumPAHs (μg/kg)	SumPCBs (μg/kg)	Sum7PCBs (μg/kg)
S1	531586.2	4518208.52	92.3	3.13	69.2	1.6	0.96
S2	529330.7	4516839.17	66.1	2.78	50.6	1.0	0.44
S3	527051.1	4513180.93	82.8	4.30	142	1.3	1.0
S4	533307.9	4508928.53	63.9	2.57	224	7.7	5.9
S5	534171.8	4510101.84	–	3.93	1232	26	21
S6	534786.6	4510796.98	–	5.08	358	52	39
S7	534815	4510876.93	–	2.22	221	53	40
S8	535570.7	4510916.62	15.7	1.02	346	–	–
S9	532893.4	4508808.98	43.8	2.36	543	4.0	2.7
S10	532305	4508822.93	50.3	1.96	137	8.0	5.7
S11	531389.9	4508639.63	53.5	2.53	219	1.5	1.1
S12	533517.1	4508267.94	47.4	2.67	269	5.2	3.5
S13	533685.3	4508134.82	64.7	3.07	206	6.4	3.7
S14	532609.4	4508512.26	69.6	3.93	111	4.6	3.5
S15	528465.5	4503868.97	44.7	2.41	75.4	1.4	1.3
S16	525760.1	4499902.84	70.8	1.97	266	1.2	0.99
S17	525776.6	4499704.86	52.4	1.61	107	1.7	1.5
S18	526051.4	4498655.37	75.6	3.01	134	3.2	2.1
S19	522112.3	4494471.92	38.1	1.34	86.2	0.56	0.46
S20	527104.8	4495233.02	66.8	1.48	77.1	1.5	1.2
S21	520981.9	4491396.3	24.1	0.99	36.9	0.41	0.41
S22	527382.9	4489898.1	90.3	2.55	252	1.2	0.85

(*continued on next page*)

Table 1 (*continued*)

Site	m	p	Fine Fraction (%)	OC (%)	SumPAHs (μg/kg)	SumPCBs (μg/kg)	Sum7PCBs (μg/kg)
Min.	–	–	15.7	0.99	36.9	0.41	0.41
Max.	–	–	92.3	5.08	1232	53	40
Median	–	–	63.9	2.54	174	1.7	1.5
Mean	–	–	58.6	2.57	235	8.7	6.5

2. Experimental design, materials, and methods

During decades effluents from the Estarreja Chemical Complex (ECC) were directly discharged in the Ria de Aveiro lagoon through a system of ditches. “Esteiro de Estarreja” was the main channel, that received effluents in the past. The untreated effluents were rich in aromatic based and chlorine compounds (PCBs, HCB), as a result of the plants of production of nitrobenzene, aniline, polyvinyl chloride, aromatic isocyanate-based polymers, and in toxic elements such as As, Hg, Pb and Zn [6]. Consequently, most of the discharged contaminants are settled in the “Esteiro” channel, as well as in the inner basin where this channel discharges, the Laranjo Basin [1–7]. The Antuã river, that drains in the area of Laranjo, has also been pointed as a source of contamination [8]. Despite sampling locations have been chosen in order to obtain a spatial distribution along the lagoon, an higher density of samples were taken from the most contaminated area (Laranjo bay and Esteiro de Estarreja).

Table 2
Major elements concentration (mg/kg) in Ria de Aveiro sediment samples. Descriptive statistics (minimum, maximum, median, and mean) is also shown.

Site	Al	Ca	Fe	K	Mg	Na
S1	30612	3115	36656	6721	8619	12334
S2	16054	5283	17667	4208	5942	11066
S3	21891	4555	25863	5567	8487	17428
S4	15917	1906	13719	2962	4393	5957
S5	19646	2716	16914	3285	5377	7382
S6	18572	2957	19288	2829	4526	6121
S7	11402	1727	13514	1842	2689	2511
S8	26271	1716	28086	3959	4818	6782
S9	13530	2640	15737	2848	4107	8336
S10	15393	2966	16603	3186	4511	8452
S11	14828	1609	13668	3225	4639	8227
S12	8531	2086	13836	1418	2567	1417
S13	24921	3364	23934	3985	5431	10151
S14	23599	3553	23395	4634	6310	11773
S15	12883	4763	16529	3534	4993	8158
S16	15638	5919	17598	4410	6255	10326
S17	12231	6237	15484	3653	4940	7048
S18	18908	10357	22693	4983	7001	9798
S19	7625	1138	9049	1946	2830	3802
S20	15489	3957	16205	4084	5108	7347
S21	4835	1699	6438	1589	2292	3231
S22	26153	2175	25730	7489	7488	10498
Min.	4835	1138	6438	1418	2292	1417
Max.	30612	10357	36656	7489	8619	17428
Median	12778	2962	16758	3594	4966	8192
Mean	17042	3474	18573	3744	5151	8098

Table 3
Trace elements concentration (mg/kg) in Ria de Aveiro sediment samples. Descriptive statistics (minimum, maximum, median, and mean) is also shown.

Site	As	Ba	Be	Cd	Co	Cr	Cu	Li	Mn	Mo
S1	23.4	49.5	1.55	3.1	9.28	48.7	96.1	85.7	267	1.6
S2	17.6	29.2	3.17	0.86	7.23	24.3	22.4	57.0	164	1.4
S3	22.1	40.3	2.51	0.83	7.85	30.1	25.4	68.1	184	2.2
S4	136	18.3	1.02	2.6	8.5	21.4	60.6	39.0	96.6	3.5
S5	136	27.6	1.61	2.29	9.15	42.2	78.5	49.6	121	6.2
S6	256	46.3	1.03	1.76	7.14	41.2	88.9	45.1	108	1.0
S7	197	40.9	0.48	1.13	4.85	30.9	61.3	25.7	66.2	0.79
S8	63.0	69.7	1.07	1.35	8.47	47.9	69.2	51.6	154	1.4
S9	55.4	26.3	2.06	1.7	6.38	23.2	40.8	54.5	92.2	0.74
S10	46.1	27.8	3.51	1.0	5.94	26.3	35.6	62.5	110	0.85
S11	27.2	24.4	1.59	0.79	5.03	19.3	25.3	48.4	101	0.57
S12	76.8	49.2	0.03	0.34	3.30	28.9	43.7	18.4	126	0.83
S13	104	46.4	<0.10	1.9	9.54	49.8	79.4	64.2	120	1.2
S14	67.5	41.5	2.07	1.2	8.04	34.7	46.0	70.4	153	1.0
S15	16.4	27.0	<0.1	0.41	5.75	20.5	18.8	43.2	119	1.0
S16	14.3	30.9	1.71	0.32	6.10	24.9	20.6	59.6	142	1.4
S17	12.4	27.4	<0.10	0.28	4.89	21.0	14.8	39.0	118	0.71
S18	15.7	42.8	2.08	0.37	6.18	29.6	26.5	63.7	172	2.1
S19	5.70	13.5	0.66	0.13	2.34	11.7	8.42	23.2	71.4	0.42
S20	10.1	26.9	1.42	0.26	4.16	20.0	19.0	42.6	108	0.94
S21	4.60	10.7	<0.10	0.10	2.00	8.20	7.00	13.1	52.1	1.4
S22	12.7	35.8	2.65	0.27	6.41	38.6	22.0	46.5	149	1.1
Min.	4.60	10.7	.03	0.10	2.00	8.20	7.00	13.1	52.1	0.42
Max.	256	69.7	3.51	3.1	9.54	49.8	96.1	85.7	267	6.2
Median	25.3	30.0	1.50	0.84	6.28	27.6	31.1	49.0	120	1.1
Mean	60.0	34.2	1.38	1.0	6.30	29.2	41.4	48.7	127	1.5

Site	Ni	Pb	Sb	Sn	Tl	V	W	Zn
S1	30.1	31.6	0.17	4.43	0.68	38.1	1.7	1270
S2	20.8	24.4	0.11	0.76	0.51	26.3	0.12	415
S3	24.7	31.7	0.14	2.31	0.52	34.4	0.32	332
S4	21.0	49.7	0.10	1.4	0.6	17.1	1.6	424
S5	72.1	61.2	0.22	3.20	0.91	25.5	2.18	704
S6	68.1	64.8	0.15	3.04	0.73	22.2	0.62	680
S7	57.0	59.6	0.13	2.32	0.39	17.2	0.42	411
S8	28.2	76.9	0.36	7.41	0.39	33.5	1.63	359
S9	20.4	35.0	0.40	0.99	0.48	20.6	0.52	354
S10	25.0	35.6	0.23	1.35	0.49	23.6	0.21	286
S11	16.3	27.4	0.06	0.75	0.31	19.2	0.21	195
S12	126	67.6	1.09	3.46	0.16	20.4	1.55	335
S13	30.9	58.4	0.34	1.71	0.59	36.0	0.42	589
S14	26.1	52.0	0.26	1.18	0.60	32.5	0.37	364
S15	16.4	41.8	0.22	1.12	0.43	22.6	0.28	120
S16	20.1	37.0	0.13	0.74	0.46	25.8	0.24	134
S17	15.6	27.6	0.21	1.45	0.43	22.3	0.24	99.5
S18	20.0	34.4	0.14	1.59	0.42	29.5	0.43	132
S19	3.31	11.6	0.07	0.62	0.18	12.0	0.20	42.3
S20	10.3	24.9	0.11	1.17	0.34	19.7	0.15	79.0
S21	6.90	8.00	0.04	1.4	0.10	8.00	0.80	36.4
S22	19.9	27.8	0.04	1.66	0.45	28.0	0.11	72.5
Min.	3.31	8.00	0.04	0.62	0.10	8.00	0.11	36.4
Max.	126	76.9	1.1	7.4	0.91	38.1	2.2	1270
Median	20.9	35.3	0.14	1.4	0.46	23.1	0.40	334
Mean	30.8	40.4	0.21	2.0	0.46	24.3	0.65	338

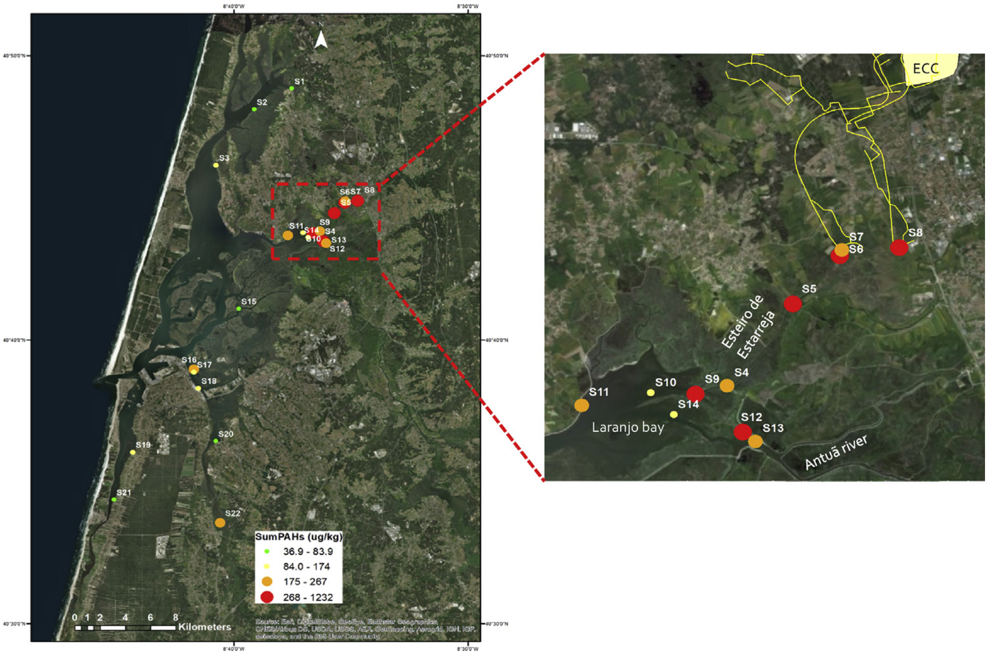

Fig. 2. Spatial distribution of PAHs (sum16) in sediments from Ria de Aveiro lagoon. The class limits correspond to the minimum, the quartiles (25, 50, and 75) and the maximum value. The yellow lines are the channels and ditches formerly used to release contaminated effluents from the chemical complex (ECC).

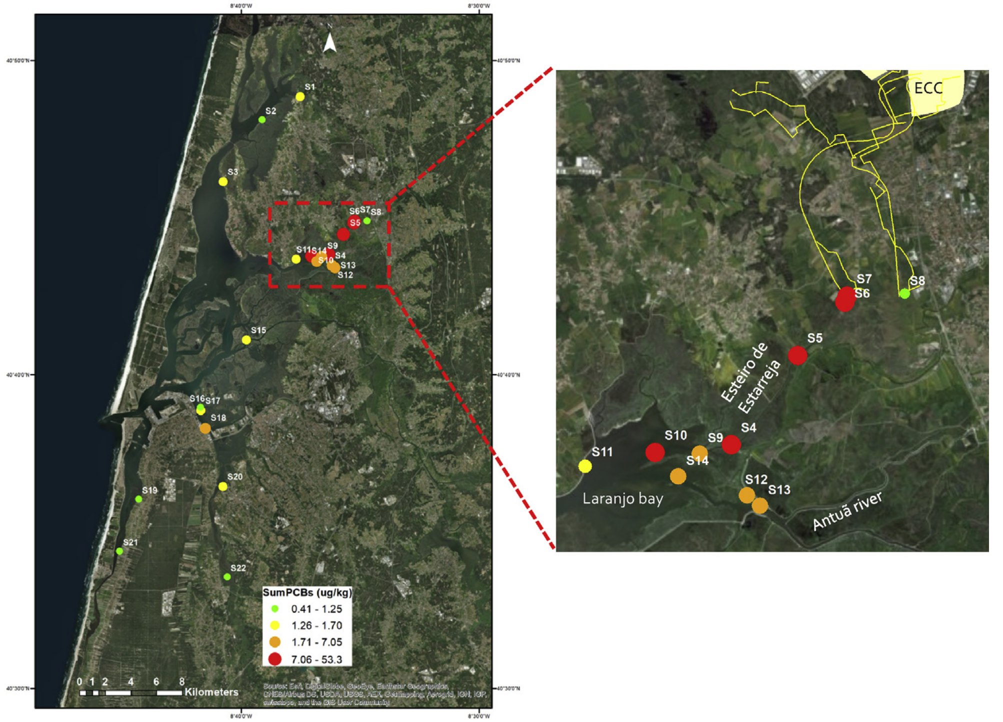

Fig. 3. Spatial distribution of PCBs (sum13) in sediments from Ria de Aveiro lagoon. The class limits correspond to the minimum, the quartiles (25, 50, and 75) and the maximum value. The yellow lines are the channels and ditches formerly used to release contaminated effluents from the chemical complex (ECC).

Intertidal surface sediments (0–5 cm depth), were collected in 22 sampling stations from Ria de Aveiro lagoon, during the spring of 2008. Each sample consisted in a combination of three randomly collected sub-samples, pooled together with the purpose to account for within-site variability. Samples were freeze-dried and sieved to <1 mm. Fine fraction (<63 μm) and total organic carbon (TOC) were determined as described by Rada et al. [8].

PAHs and PCBs were Soxhlet-extracted with a hexane/acetone mixture (2:1) and cleaned up, following the USEPA methodologies, as described previously by the authors [5,9]. Determinations of 16 individual PAHs (acenaphthene, acenaphthylene, anthracene, benzo(a)anthracene, benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(ghi)perylene, benzo(a)pyrene, chrysene, dibenzo(ah) anthracene, fluoranthene, fluorene, indeno(1,2,3-cd)pyrene, naphthalene, phenanthrene, and pyrene), and 13 PCBs (congeners 18, 28, 31, 44, 52, 101, 118, 138, 149, 153, 170, 180, and 194) were performed by GC-MS following the USEPA 8270 method, as previously described by the authors [5,9]. The pseudo-total concentration of major and trace elements was determined by ICP-MS after microwave digestion with a mixture of nitric acid and hydrochloric acid (3:1), following the method 3051A from USEPA [10]. The extracts were analysed for 24 chemical elements: Li, Be, Na, Mg, Al, K, Ca, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, As, Mo, Cd, Sn, Sb, Ba, W, Tl and Pb. The accuracy and the precision of the analytical methods was performed by including replicates, procedure blanks, and certified reference materials in each analytical batch. For inorganic elements, replicate analysis of the soil gave an uncertainty of <10%, whereas for organic contaminants the uncertainty was <25%. The results of blanks analysis were always below detection limit and recoveries of reference material were within the certified value.

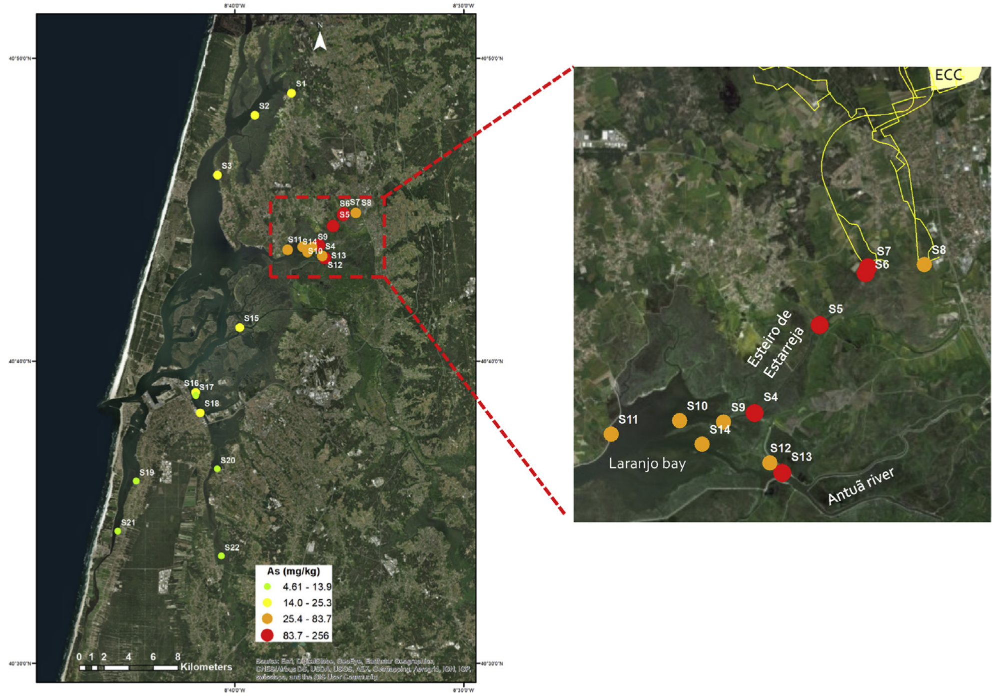

Fig. 4. Spatial distribution of As in sediments from Ria de Aveiro lagoon. The class limits correspond to the minimum, the quartiles (25, 50, and 75) and the maximum value. The yellow lines are the channels and ditches formerly used to release contaminated effluents from the chemical complex (ECC).

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Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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