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Multi-Elemental Contamination and Historic Record in Sediments from the Santos-Cubatão Estuarine System, Brazil

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Table S1. Concentrations (average ± standard deviation, n=2) of major, minor and trace elements (in mg kg^{-1}, unless otherwise indicated) determined for the reference material LKSD-3 (CANMET) and the in-house standard DST6 (Acme Analytical Laboratories) by ICP-MS

	Reference value	Our value	Recovery / (%)		Reference value	Our value	Recovery / (%)
Li	25 ± 2	28.8 ± 1.2	115.2	As	27 ± 2	22.9 ± 0.8	84.8
Be*	3.3	3.0 ± 0.0	90.9	Rb	78 ± 10	77.6 ± 0.8	99.5
Na (%)	1.72 ± 0.07	1.75 ± 0.00	101.7	Sr	240 ± 42	272 ± 3	113.3
Mg (%)	1.20 ± 0.06	1.14 ± 0.07	95.0	Y	30 ± 10	26.6 ± 0.1	88.7
Al (%)	6.61 ± 0.21	6.55 ± 0.27	99.1	Zr*	50.1	62.2 ± 1.2	124.2
P	1090 ± 40	1146 ± 8	105.1	Nb*	8.11	9.16 ± 0.11	112.9
S (%)	0.14 ± 0.03	0.17 ± 0.01	121.4	Mo*	12.70	12.8 ± 0.1	100.8
K (%)	1.84 ± 0.07	1.66 ± 0.02	90.2	Ag	2.7 ± 0.11	2.67 ± 18	98.9
Ca (%)	1.64 ± 0.14	1.77 ± 0.01	107.9	Cd*	5.60	5.66 ± 0.01	101.1
Sc	13 ± 2	12.6 ± 0.5	96.9	Sn	3 ± 2	2.1 ± 0.0	70.0
Ti	3330 ± 330	3195 ± 21	95.9	Sb	1.3 ± 0.1	1.27 ± 0.01	97.7
V	82 ± 8	84.1 ± 1.6	102.6	Cs	2.3 ± 0.3	2.6 ± 0.1	113.0
Cr	87 ± 8	76.5 ± 0.7	87.9	Hf	4.8 ± 0.7	3.6 ± 0.1	75.0
Mn	1440 ± 80	1472 ± 4	102.2	Ta	0.7 ± 0.1	0.96 ± 0.10	137.1
Fe (%)	4.0 ± 0.2	4.21 ± 0.02	105.3	Pb	29 ± 3	33.7 ± 1.3	116.2
Co	30 ± 2	32.6 ± 0.3	108.7	Bi*	4.70	4.86 ± 0.07	103.4
Ni	47 ± 5	49.4 ± 2	105.1	Th	11.4 ± 0.7	11.6 ± 0.0	101.8
Cu	35 ± 3	38.1 ± 0.0	108.9	U	4.6 ± 0.5	4.6 ± 0.0	100.0
Zn	152 ± 14	167 ± 1.5	109.9				
Ga	17 ± 4	16.85 ± 0.03	99.1				

*DST6 (in-house standard).

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Table S2. Correlation coefficients calculated for concentrations of select elements, grain-size and LOI (550 °C) in a sediment core from the Morrão River (n=32, entire data). Marked correlations are significant at $p < 0.05$

	Li	Na	Mg	Al	S	K	Ti	V	As	Rb	Mo	Cs	Silt	Clay	Sand	LOI
Li	1.00															
Na	–0.20	1.00														
Mg	0.06	**0.62**	1.00													
Al	**0.96**	–0.09	0.13	1.00												
S	**0.45**	**0.35**	0.33	**0.51**	1.00											
K	**0.93**	–0.20	0.11	**0.90**	**0.40**	1.00										
Ti	**0.91**	–0.26	0.06	**0.89**	0.29	**0.86**	1.00									
V	**0.59**	–0.21	0.24	**0.61**	0.11	**0.64**	**0.53**	1.00								
As	**0.38**	0.19	0.33	**0.41**	**0.75**	**0.36**	0.24	0.23	1.00							
Rb	**0.78**	–0.31	–0.03	**0.73**	0.21	**0.88**	**0.72**	**0.66**	0.16	1.00						
Mo	0.31	0.16	0.06	0.31	**0.76**	0.24	0.04	–0.03	**0.63**	0.14	1.00					
Cs	**0.80**	0.09	0.17	**0.86**	**0.65**	**0.77**	**0.58**	**0.54**	**0.53**	**0.64**	**0.58**	1.00				
Silt	0.06	0.16	–0.28	0.15	–0.01	–0.06	–0.06	–0.09	–0.36	–0.14	0.09	0.22	1.00			
Clay	**–0.51**	0.05	**–0.51**	**–0.47**	**–0.51**	**–0.64**	**–0.52**	**–0.46**	**–0.55**	**–0.59**	–0.28	**–0.42**	**0.62**	1.00		
Sand	0.02	–0.15	0.32	–0.07	0.08	0.14	0.13	0.15	**0.40**	0.21	–0.05	–0.14	**–0.99**	**–0.70**	1.00	
LOI	–0.08	**0.49**	**0.59**	0.00	**0.38**	0.01	–0.12	–0.01	0.35	–0.01	0.27	0.13	–0.32	–0.34	0.34	1.00

Table S3. Correlation coefficients calculated for concentrations of elements associated with the phosphorous or iron in the 0-90 cm depth in a sediment core from the Morrão River (n = 15). Marked correlations are significant at $p < 0.05$

	Elements associated with phosphorous														Elements associated with iron											
	Be	P	Ca	Sc	Co	Cu	Sr	Y	Zr	Nb	Hf	Ta	Th	U	Cr	Mn	Fe	Ni	Zn	Ga	Ag	Cd	Sn	Sb	Pb	Bi
Be	1.00																									
P	**0.95**	**1.00**																								
Ca	**0.96**	**0.98**	1.00																							
Sc	**0.91**	**0.90**	**0.94**	1.00																						
Co	**0.76**	**0.83**	**0.77**	**0.68**	1.00																					
Cu	**0.76**	**0.80**	**0.82**	**0.79**	**0.85**	1.00																				
Sr	**0.86**	**0.91**	**0.90**	**0.77**	**0.68**	**0.60**	1.00																			
Y	**0.78**	**0.84**	**0.83**	**0.67**	**0.63**	0.50	**0.97**	1.00																		
Zr	**0.92**	**0.90**	**0.92**	**0.85**	**0.90**	**0.85**	**0.81**	**0.76**	1.00																	
Nb	**0.94**	**0.94**	**0.95**	**0.91**	**0.88**	**0.89**	**0.81**	**0.73**	**0.98**	1.00																
Hf	**0.93**	**0.91**	**0.93**	**0.87**	**0.90**	**0.85**	**0.80**	**0.74**	**1.00**	**0.98**	1.00															
Ta	**0.92**	**0.92**	**0.93**	**0.90**	**0.90**	**0.90**	**0.78**	**0.71**	**0.98**	**0.99**	**0.99**	1.00														
Th	**0.88**	**0.90**	**0.89**	**0.78**	**0.83**	**0.69**	**0.93**	**0.93**	**0.93**	**0.89**	**0.91**	**0.88**	1.00													
U	**0.74**	**0.81**	**0.75**	**0.65**	**0.56**	0.42	**0.91**	**0.86**	**0.64**	**0.66**	**0.64**	**0.63**	**0.83**	1.00												
Cr	0.38	**0.56**	0.47	0.27	0.50	0.28	**0.73**	**0.79**	0.43	0.40	0.39	0.39	**0.68**	**0.78**	1.00											
Mn	**0.52**	**0.63**	**0.56**	0.40	**0.85**	**0.64**	**0.62**	**0.65**	**0.73**	**0.67**	**0.69**	**0.69**	**0.77**	**0.56**	**0.74**	1.00										
Fe	0.47	**0.59**	**0.54**	0.36	**0.81**	**0.62**	**0.60**	**0.63**	**0.69**	**0.63**	**0.65**	**0.66**	**0.74**	**0.55**	**0.77**	**0.99**	1.00									
Ni	**0.60**	**0.71**	**0.67**	**0.53**	**0.86**	**0.75**	**0.71**	**0.70**	**0.78**	**0.73**	**0.74**	**0.76**	**0.83**	**0.64**	**0.73**	**0.94**	**0.94**	1.00								
Zn	0.21	0.19	0.25	0.13	0.25	0.40	0.22	0.19	0.30	0.25	0.26	0.25	0.32	0.18	0.19	0.34	0.40	0.49	1.00							
Ga	–0.03	0.05	–0.02	–0.15	0.21	–0.15	0.29	0.40	0.10	–0.01	0.06	0.00	0.37	0.42	**0.68**	**0.56**	**0.56**	0.47	0.14	1.00						
Ag	–0.01	0.20	0.15	0.07	0.32	0.22	0.26	0.28	0.15	0.18	0.13	0.21	0.28	0.38	**0.66**	**0.57**	**0.64**	**0.57**	0.25	0.36	1.00					
Cd	–0.20	–0.08	–0.09	–0.25	–0.26	–0.34	0.27	0.36	–0.23	–0.28	–0.28	–0.29	0.11	0.39	**0.63**	0.10	0.18	0.17	0.26	**0.55**	0.47	1.00				
Sn	0.06	0.13	0.11	0.20	0.23	0.34	–0.06	–0.03	0.11	0.19	0.11	0.21	0.00	–0.11	0.02	0.19	0.18	0.20	0.09	–0.28	0.44	–0.19	1.00			
Sb	0.31	0.40	0.38	0.21	**0.60**	0.45	0.48	**0.55**	0.54	0.44	0.48	0.47	**0.65**	0.45	**0.69**	**0.85**	**0.89**	**0.87**	**0.67**	**0.60**	**0.65**	0.38	0.20	1.00		
Pb	0.10	0.16	0.18	0.10	0.31	0.38	0.16	0.21	0.25	0.21	0.21	0.24	0.30	0.15	0.34	0.48	**0.53**	**0.58**	**0.83**	0.23	**0.56**	0.31	**0.52**	**0.79**	1.00	
Bi	–0.08	–0.10	–0.04	–0.10	0.04	0.21	–0.08	–0.03	0.05	–0.02	0.00	0.00	0.05	–0.15	0.01	0.19	0.25	0.32	**0.88**	0.07	0.22	0.23	0.35	**0.59**	**0.89**	1.00