Supplementary Information

Distribution and Sources of Aliphatic and Polycyclic Aromatic Hydrocarbons in Surface Sediments of Itajaí-Açu Estuarine System in Brazil

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Table S1. Figures of merit of the analytical procedure for *n*-alkanes

Analyte	Analytical curve equation	R^2	MDL / (μg g^{-1})	MQL / (μg g^{-1})	RSD / %
n-C_7	y = 0.1620x + 0.1358	0.9978	0.23	0.69	5.1
n-C_8	y = 0.2120x + 0.6345	0.9957	0.21	0.63	3.9
n-C_9	y = 0.2345x – 0.2361	0.9995	0.26	0.78	6.3
n-C_{10}	y = 0.1642x + 0.1566	0.9977	0.30	0.90	5.4
n-C_{11}	y = 0.1478x – 0.4056	0.9972	0.15	0.45	10.3
n-C_{12}	y = 0.1525x – 0.5501	0.9904	0.06	0.18	3.0
n-C_{13}	y = 0.2474x – 0.8181	0.9987	0.05	0.15	4.9
n-C_{14}	y = 0.2138x – 0.6048	0.9902	0.30	0.90	8.1
n-C_{15}	y = 0.1770x – 0.0952	0.9946	0.25	0.75	5.6
n-C_{16}	y = 0.2127x – 0.6033	0.9933	0.29	0.87	6.1
n-C_{17}	y = 0.1847x – 0.2168	0.9960	0.20	0.60	4.2
n-C_{18}	y = 0.1899x – 0.3423	0.9913	0.23	0.69	10.2
n-C_{19}	y = 0.2116x – 0.4388	0.9972	0.25	0.75	4.0
n-C_{20}	y = 0.2136x – 0.4269	0.9959	0.33	0.99	6.3
n-C_{21}	y = 0.2031x – 0.4657	0.9991	0.23	0.69	4.1
n-C_{22}	y = 0.1831x – 0.1526	0.9979	0.14	0.42	2.5
n-C_{23}	y = 0.1833x – 0.0891	0.9988	0.07	0.21	2.7
n-C_{24}	y = 0.1925x – 0.1619	0.9991	0.08	0.24	1.2
n-C_{25}	y = 0.1981x – 0.1764	0.9975	0.09	0.27	2.0
n-C_{26}	y = 0.1980x – 0.1208	0.9988	0.08	0.24	1.1
n-C_{27}	y = 0.1956x – 0.1306	0.9995	0.16	0.48	2.4
n-C_{28}	y = 0.1950x – 0.066	0.9993	0.09	0.27	1.3

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Table S1. Figures of merit of the analytical procedure for *n*-alkanes (cont.)

Analyte	Analytical curve equation	R^2	MDL / (μg g^{-1})	MQL / (μg g^{-1})	RSD / %
n-C_{29}	y = 0.1926x – 0.0479	0.9987	0.13	0.39	1.3
n-C_{30}	y = 0.1884x – 0.0688	0.9964	0.10	0.30	1.1
n-C_{31}	y = 0.1831x – 0.0413	0.9974	0.12	0.36	1.0
n-C_{32}	y = 0.1803x – 0.0614	0.9959	0.20	0.60	2.6
n-C_{33}	y = 0.1782x – 0.0457	0.9936	0.10	0.30	2.9
n-C_{34}	y = 0.1725x – 0.038	0.9996	0.12	0.36	1.5
n-C_{35}	y = 0.1646x – 0.0808	0.9996	0.17	0.51	3.8
n-C_{36}	y = 0.1647x – 0.1854	0.9972	0.13	0.39	3.0
n-C_{37}	y = 0.1550x – 0.2619	0.9982	0.20	0.60	5.8
n-C_{38}	y = 0.1798x – 0.7338	0.9975	0.14	0.42	1.6

R^2: coefficient of determination; MDL: method detection limit; MQL: method quantification limit; RSD: relative standard deviation.

Table S2. Concentration levels of *n*-alkane and PAH in sediments of various environments

Parameter	Concentration	Location	Reference
n-Alkanes / (μg g^{-1} d.w.)	0.9-45.6	Laguna Estuarine system, Brazil	1
	1.22-5.57	Babitonga Bay, Brazil	2
	3.32-18.14	Itajaí-AçuRiver mouth, Brazil	2
	0.05-2.44	Mundaú-Manguaba estuarine-lagoon system and Paraíba do Sul River, Brazil	3
	9.9-30.8	SergipeRiver estuarine system, Brazil	4
	0.8-3.2	Mandovi estuary, India	5
	1.6-10.7	Marmugoa harbor, India	5
	3.43-7.06	Pearl river estuary, China	6
	180.8-760.9	XiheRiver, China	7
	0.5-69.7	Itajaí-Açu estuarine system	present work
	34-13,780	Gulf of Fos area, France	8
	1,107-250,094	Laguna Estuarine system, Brazil	1
PAH / (ng g^{-1} d.w.)	2.9-9344.3[a]	Mundaú-Manguaba estuarine-lagoon system and Paraíba do Sul River, Brazil	9
	72.17-277.77[a]	Persian Gulf	10
	7.3-92.8[a]	Patos Lagoon, Brazil	11
	< DL-497.6[a]	Capibaribe Estuarine system, Brazil	12
	< DL-127.3	Sergipe-Alagoas Basin, Brazil	13
	472-16,201	Kaohsiung harbor, Taiwan	14
	3.0-2234.7[a]	Fortaleza, Brazil	15
	60-8680	Santos estuary, southeastern Brazil	16
	63.9-1459.0	Itajaí-Açu estuarine system, Brazil	present work

[a]Stations which only the 16 priority PAH were determined. PAH: polycyclic aromatic hydrocarbons; DL: detection limit.

Table S3. Figures of merit of the analytical procedure for PAH

Analyte	Analytical curve equation	R^2	MDL/ (ng g^{-1})	MQL / (ng g^{-1})	RSD / %
Naphthalene	y = 0.0127x – 0.1366	0.9984	3.6	10.8	5.6
Acenaphtylene	y = 0.0069x – 0.1719	0.9941	9.5	28.5	7.7
Acenapthene	y = 0.012x – 0.2326	0.9941	5.0	15.0	4.8
Fluorene	y = 0.0255x – 0.6333	0.9918	2.1	6.3	4.8
Phenanthrene	y = 0.0171x – 0.3816	0.9985	3.6	10.8	7.6
Anthracene	y = 0.0132x – 0.3013	0.9948	7.1	21.3	7.5
Fluoranthene	y = 0.3123x – 5.3513	0.9940	4.5	13.5	2.8
Pyrene	y = 0.3381x – 5.2187	0.9936	5.6	16.8	3.9
Benzo[*a*]anthracene	y = 0.1433x + 3.9494	0.9925	3.8	11.4	6.3
Crysene	y = 0.2297x – 0.6354	0.9940	5.9	17.7	3.0
Benzo[*b*]fluoranthene	y = 0.0073x – 0.2112	0.9946	5.8	17.4	6.6
Benzo[*k*]fluoranthene	y = 0.0107x – 0.2131	0.9979	5.4	16.2	8.1
Benzo[*a*]pyrene	y = 0.0079x – 0.3382	0.9957	3.7	11.1	13.6
Indeno[1,2,3-*cd*]pyrene	y = 0.0044x – 0.1497	0.9978	5.7	17.1	9.4
Dibenzo[*a, h*]anthracene	y = 0.0102x – 0.3539	0.9973	5.3	15.9	11.8
Benzo[*ghi*]perylene	y = 0.006x – 0.1187	0.9929	5.6	16.8	1.6

R^2: coefficient of determination; MDL: method detection limit; MQL: method quantification limit; RSD: relative standard deviation.

Table S4. Comparison of the concentrations of PAH from sediments of Itajaí-Açu estuarine system with SQGs

Compound	Concentration of PAH / (ng g^{-1} d.w.)				
	TEL[a]	PEL[a]	ERL[b]	ERM[b]	This study
Naphthalene	34.6	391	160	2100	(ND-55.1)
Acenaphthylene	5.87	128	44	640	(ND-37.9)
Acenaphthene	6.0	88.9	16	500	(ND-51.3)
Fluorene	21.2	144	19	540	(ND-38.2)
Phenantrene	86.7	544	240	1500	(ND-276.7)
Anthracene	46.9	245	853	1100	(ND-223.6)
Fluoranthene	113	1494	600	5100	(ND-52.5)
Pyrene	153	1398	665	2600	(ND-58.0)
Benzo[*a*]anthracene	74.8	693	261	1600	ND
Chrysene	108	846	384	2800	ND
Benzo[*b*]fluoranthene	–	–	–	–	–
Benzo[*k*]fluoranthene	–	–	–	–	–
Benzo[*a*]pyrene	88.8	763	430	1600	(ND-68.5)
Indeno[1,2,3-*cd*]pyrene	–	–	–	–	–
Dibenzo[*a,h*]anthracene	6.2	135	63.4	260	ND
Benzo[*ghi*]perylene	–	–	–	–	–
Σ16 PAH	1684	16,770	4000	44,792	(28.4-1237.2)

[a]Threshold effect levels and probable effect levels; [b]effects range-low and effects range-median values. TEL: threshold effects level; PEL: probable effects level; ERL: effects range-low value; ERM: effects range-median value; PAH: polycyclic aromatic hydrocarbons; ND: not detected.

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