Supplementary Materials

Are Mangroves and Lagoons Safe? A Global Assessment of PAH Pollution, Sources, and Ecological Risks

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Text 1 Principal Component Analysis – Multiple Linear Regression (PCA-MLR) Calculations

Principal Component Analysis (PCA) is a dimensionality reduction technique that transforms correlated variables, such as PAH concentrations, into a set of uncorrelated principal components (PCs) that represent dominant pollution sources. Multiple Linear Regression (MLR) is then used to model the relationship between the dependent variable (total PAHs) and independent variables (source-related PAH tracers or PCA scores). The PCA-MLR approach uses the following regression equation:

$$X = T \times L \qquad (Eq.S1)$$

Where: X is the concentration matrix, T is the factor score matrix, and L is the factor loading matrix. A key advantage of the PCA-MLR method is its ability to identify pollution sources without prior knowledge of all potential sources or their specific profiles (1, 2). The calculations were performed using Origin software 2021.

Text S2 Risk quotient (RQ) Calculations

According to (3), the ecological risk associated with PAHs in mangrove and lagoon waters can be evaluated using the Risk Quotient (RQ) method, as shown in $(Eq.S2)$:

$$RQ = \frac{C_{PAHs}}{C_{QV}} \qquad (Eq.S2)$$

Where C_{PAHs} denotes the concentration of specific PAHs present in water (ng/L), and C_{QV} represents the associated quality values of those PAHs in water (ng/L) (4). The quality values include negligible concentrations (NCs) and maximum permissible concentrations (MPCs) of PAHs in the water. The RQ_{NCs} and RQ_{MPCs} are determined as follows:

$$RQ_{NCs} = \frac{C_{PAHs}}{C_{QV(NCs)}} \qquad (Eq.S3)$$

$$RQ_{MPCs} = \frac{C_{PAHs}}{C_{QV(MPCs)}} \qquad (Eq.S4)$$

where $C_{QV(NCs)}$ signifies the quality values corresponding to the negligible concentrations NCs of PAHs, while $C_{QV(MPCs)}$ denotes the quality values associated with the maximum permissible concentrations MPCs of PAHs in water. The calculations for $RQ_{\sum PAHs}$, $RQ_{\sum PAHs(NCs)}$, and $RQ_{\sum PAHs(MPCs)}$ can be obtained using the following equations (5):

$$RQ_{\sum PAHs} = \sum_{i=1}^{16} RQ_i \quad RQ_i \geq 1 \qquad (Eq.S5)$$

$$RQ_{\sum PAHs(NCs)} = \sum_{i=1}^{16} RQ_{(NCs)} \quad RQ_{(NCs)} \geq 1 \qquad (Eq.S6)$$

$$RQ_{\sum PAHs(MPCs)} = \sum_{i=1}^{16} RQ_{(MPCs)} \quad RQ_{(MPCs)} \geq 1 \qquad (Eq.S7)$$

Text S3 Toxicity equivalency quotient of BaP (TEQ_{BaP}) Calculations

According to (6), the ecological risk of carcinogenic PAHs in water and sediment in mangroves can be derived using the total BaP toxicity equivalent quotient (TEQcarc), using the following equation:

$$TEQPAHs = \sum TEQi = \sum (Ci * TEFj) \qquad (Eq.S8)$$

The TEF values used are as follows: NaP, Acp, Acy, Flu, Phe, Flu, and Pyr = 0.001; Ant, Chr, and BghiP = 0.01; BaA, BbF, BkF, and InP = 0.1; and BaP and DahA = 1. Due to the lack of TEF for other PAHs, their TEF value were calculated using the following formula:

$$TEF = (-5.99\,E{-}03) + (Mw \times 1.40\,E{-}05) + (H_v \times 6.42\,E{-}05) + (BP \times 5.92\,E{-}06) - (\log Vp \times 1.48\,E{-}04) \qquad (Eq.S9)$$

where M_w represents the molecular weight (g/mol), H_v denotes enthalpy of vaporization (kJ/mol), BP indicates the boiling point (°C), and $\log V_p$ represents the vapor pressure (mmHg); E−03 stands for 10^{-3}

Text S4 m-ERM-q Calculations

According to (7), the mean quotients for all PAHs detected in the lagoon were calculated as follows:

$$m{-}ERM{-}q = \sum(Ci/ERMi)/n \qquad (Eq.S10)$$

In this context, Ci denotes the concentration of each PAH, ERMi is the ERM value for the corresponding PAH target, and *n* denotes the total number of PAHs. m-ERM-q was categorized into four levels based on their probability of toxicity, as obtained from the literature (8).

Text S5 BSAF Calculations

According to (9), the biota-sediment accumulation factors (BSAFs) denotes the ratio of the PAH concentration in the organism to that in the sediment, as shown below:

$$BSAF = \frac{C_o/f_l}{C_s/f_{soc}} \qquad (Eq.S11)$$

In this context, (C_o) represents the PAH concentration in the organism on a wet weight basis, (f_l) is the lipid content of the wet tissue, (C_s) denotes the PAH concentration in the sediment on a dry weight basis, and (f_{soc}) represents the total organic carbon content of the dry sediment.

Text S6 Excess lifetime cancer risk (ELCR) Calculations

According to (9), the Excess lifetime cancer risk (ELCR) evaluates the increased carcinogenic risk relative to a hypothetical background, considering overall PAH dietary intake expressed as total-BaP, as shown below:

$$ELCR = 1000 \times \frac{BaP_{TEF} \times DI \times CSF}{BW} \qquad (Eq.S12)$$

In this context, the human dietary intake (DI) is assumed to be 0.2 kg of food per day, with a body weight (BW) of 70 kg for an individual. The oral BaP cancer slope factor (CSF) used is 1 per mg/kg/day.

Text S7 Translocation Factor Calculations

According to (10), the Translocation Factor evaluates the transfer of PAHs from the root to the leaf in mangrove plants, as shown below:

$$TF = \frac{C_{leaf}}{C_{root}} \qquad (Eq.S13)$$

Where C_{leaf} denotes the PAH concentration in the leaf, and C_{root} denotes the PAH concentration in the root.

Table S1 Diagnostic Ratios of PAHs in Water During Wet and Dry Seasons in the Lagos Lagoon (LA-Lag)

Sampling sites	**FL/FL+PYR**		**ANT/ANT+PH**	
	Wet	Dry	Wet	Dry
Ilaje	0.59	0.62	0.46	0.38
Iddo	0.97	0.65	0.94	0.44
Atlas Cove	0.64	0.65	0.59	0.49
Apapa	0.15	0.16	0.66	0.59

FL / FL + PY = Fluoranthene/Fluoranthene + Pyrene , AN/ AN + PH = Anthracene/Anthracene + Phenanthrene

FL / FL+ PYR > 0.5 indicates pyrogenic PAH origin and the ratio < 0.4 indicate petrogenic origin.
ANT / ANT + PHE < 0.1 indicate petrogenic origin and the ratio > 0.1 indicates pyrogenic origin (11)

Table S2 Sediment Quality Guidelines and Associated Percentage Incidence of Adverse Effects

Compounds	**Abbreviations**	**Guidelines**				**% incidence of effects**		
		TEL	**PEL**	**ERL**	**ERM**	**<ERL**	**ERL-ERM**	**>ERM**
Naphthalene	NAP	34.6	391	160	2100	16	41	88.9
Acenaphthene	ACE	6.71	88.9	16	500	20	32.4	84.2
Acenaphthylene	ACY	5.87	128	44	640	14.3	17.9	100
Fluorene	FLU	21.2	144	19	540	27.3	36.5	86.7
Phenanthrene	PHE	86.7	544	240	1500	18.5	46.2	90.3
Anthracene	ANT	46.9	245	85.3	1100	25	44.2	85.2
Fluoranthene	FLT	113	1494	600	5100	20.6	63.6	92.3
Pyrene	PYR	153	1398	665	2600	17.2	53.1	87.5
Benzo[a]anthracene	BaA	74.8	693	261	1600	21.1	43.8	92.6
Chrysene	CHR	108	846	384	2800	19	45	88.5
Benzo[a]pyrene	BaP	88.8	763	430	1600	10.3	63	80
Dibenzo[a,h]anthracene	DahA	6.22	135	63.4	260	11.5	54.4	66.7
ΣSum of 16 PAHs		1684	16770	4022	44792	14.3	36.1	85

Threshold effect level (TEL)/probable effect level (PEL) values and effect range low (ERL)/effect range mean (ERM) values in ng/g with % incidence of effects (12).

Table S3 Varimax-Rotated Component Matrix from PCA-MLR of 11 PAHs in Sediments from Estero de Urias (EUL)

Variables	**PC1 (43.2%)**	**PC2 (38.4%)**	**PC3 (18.4%)**
NAP	0.03	0.24	**3.82**
FLU	**2.04**	0.09	0.45
PHE	0.45	**0.78**	**0.93**
AN	0.21	0.36	0.09
FLUR	-0.18	-5.8	-1.08
PYR	0.6	**4.08**	0.48
CHRY	0.33	**3.41**	0.32
BbF	**1.04**	0.13	0.31
BaP	-4.8	-4.1	-1.47
BgP	0.43	0.15	-0.89
IN	**3.08**	-0.57	-2.03
Estimated sources	Diesel exhaust emissions	coal combustion	crude oil spills
Source Contribution	47.2%	17.4%	35.4%

Note: Values > 0.5 are in bold

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