

# Supplementary Material

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9 **TEXT S1: Extraction and fractionation of total lipid extract (TLE)**

10 The collected samples were wrapped with aluminum foil, sealed in zip-lock bags, transferred to  
11 the lab, and were dried at  $\leq 40$  °C for 3 to 4 days. Powdered sediment samples (50 g) were  
12 homogenized with unsaturated silica, packed into stainless steel cells, and introduced via Buchi  
13 Speed Extractor E-914 for lipid extraction. Using a solution of dichloromethane (DCM) and  
14 methanol (93:7), the extractor was configured to operate for two cycles at 100 °C and 70 bar  
15 pressure for maximal organic content recovery. The obtained extract was then thoroughly  
16 concentrated at 30 °C using a Buchi P-6 Multivapor. The total extract was loaded into a glass  
17 column comprising 2 cm of glass wool and 17 cm of silica gel with 2 mL of hexane. 20 mL of  
18 hexane was used to separate the saturated hydrocarbon component from the total extract. The  
19 recovered saturated fraction was condensed with dry N<sub>2</sub> gas to a volume of 0.5 mL. Subsequently,  
20 this concentrated saturated hydrocarbon fraction was treated with activated copper beads for sulfur  
21 removal. Similarly, the aromatic fraction was eluted by 80 mL solution of Hexane and DCM (4:1),  
22 condensed completely with dry N<sub>2</sub> gas and dissolved with 0.5 mL of DCM (Behera et al., 2022;  
23 Ajay et al., 2021).

24 **Text S2: Information about GC-MS parameters and quantitative method for *n*-alkanes,**  
25 **UCM, hopanes and PAHs.**

26 The fractionated aliquots were analysed with gas chromatography mass spectrometry (GC-MS;  
27 Agilent 7890B/5977 MSD) following the methodology described in Behera et al., (2022). Non-  
28 polar capillary column (HP5-MS, 30 m × 250 μm × 0.25 μm) was employed and helium was used  
29 as the carrier gas. We have used splitless mode of injection (inlet temperature 320 °C) and up to 1  
30 μL of sample volume. The GC oven was programmed with an initial temperature of 40 °C, hold  
31 for 2 minutes, and then finally increased to 320°C at the rate of 4°C/minute. The flow velocity of

32 helium gas in the column was maintained at 1.4 cm<sup>2</sup>/sec. The MSD conditions included 70 eV of  
33 EI ionization source, 45–600 amu of mass range, 2341 V of multiplier voltage, ion source  
34 temperature at 230 °C. The *n*-alkanes were identified by matching the characteristic mass spectra  
35 with the available literature and NIST library. Authentic standard (analytical standard *n*-C<sub>8</sub> to *n*-  
36 C<sub>40</sub> (Sigma–Aldrich, Aldrich Chemical Co. (SIGMA-40147-U))) was prepared at different  
37 concentrations (10 µg/mL, 20 µg/mL, 40 µg/mL, 60 µg/mL, 80 µg/mL, 100 µg/mL and 160  
38 µg/mL) for quantitative identification of the *n*-alkanes. The concentration of total aliphatic  
39 hydrocarbons present within each given sample was meticulously determined by the total area of  
40 the chromatogram of the aliphatic fraction. To delineate the proportion of Unresolved Complex  
41 Mixture (UCM), a methodical subtraction of the sum total of unidentified peaks in the aliphatic  
42 fraction, apart from the resolved aliphatic hydrocarbons, and the characteristic peaks  
43 corresponding to *n*-alkanes, pristane, and phytane was conducted. The hopanes (m/z 191) were  
44 quantified by comparing the integrated peak area of the selected ion with the peak area of analytical  
45 reference standard 17β(H), 21β(H)-Hopane solution (SIGMA-07562). To quantify the PAHs,  
46 present in the samples, an external calibration curve was developed for the analytical standards  
47 using varying concentrations (n=8), including Sigma CRM47930 PAH mix (100, 200, 300, 400,  
48 600, 800, 1200, 1600 ng/mL). Various *n*-alkane parameters/indices were calculated in order to  
49 quantify and comprehend the different sources contributing to the organic content of the system  
50 (Table 1).

### 51 **Text S3: Quality control and quality assurance**

52 *n*-Hexane, DCM, and methanol of HPLC-grade (Merck, Darmstadt, Germany) were utilized  
53 for sample processing. Prior to extraction, samples were spiked with an internal standard (5-  
54 cholestane) to determine the efficacy of the protocol, which resulted in between 84 and 90 percent

55 recovery. Methods for GC/MS quality control included frequent system adjustments, tunes, and  
56 method blanks (*n*-hexane). Between each pair of samples, procedural blanks were performed, and  
57 no contamination was detected. Alongside sediment samples, a triplicate extraction of powdered  
58 pre-combusted sand (500 °C for 8 hours) was performed to rule out any background signals. In  
59 addition, blank samples of reagents were tested for contamination and to improve the precision of  
60 the experimental results. To prepare for sample extraction, a recovery experiment was conducted,  
61 and the samples were enriched with deuterated analytical standards, including 5 $\alpha$ -cholestane-  
62 2,2,4,4-d<sub>4</sub> (Sigma, 747505) and Pyrene-d<sub>10</sub> (Sigma, 490695). The average recovery rates of  
63 internal standards across all samples were between 86% to 98%. The limit of detection (LOD) for  
64 *n*-alkanes, hopanes and PAHs, was 0.001  $\mu\text{g/g}$ , 0.02 ng/g, and 0.38 ng/g. The limit of detection  
65 (LOD) for alkanes was 0.5  $\mu\text{g/g}$ , whereas that for hopanes and PAHs was 0.68 ng/g and 1.14 ng/g  
66 respectively. The precision of aliphatic hydrocarbon measurement was found to be 90%, as  
67 determined by the acceptable range (of values within 15% of the mean). Remarkably, the precision  
68 of the measurement for PAHs and petroleum biomarkers (hopanes) was even higher, with 100%  
69 of the data points meeting this standard. Moreover, the determination of target hydrocarbon  
70 concentrations in the sediment reference material (IAEA-417) was deemed satisfactory, as the  
71 recoveries were in accordance with the certified values within a range of  $\pm 35\%$ . Such results  
72 signify the reliability and accuracy of the analytical methodology employed in this study.

#### 73 **Text S4: Statistical analysis**

74 Principal component analysis (PCA) was utilized in this study, which was conducted using Origin  
75 Pro 10.0. (Origin Lab. Corp., Northampton, MA). Similar samples tend to cluster together, and the  
76 degree of difference between groups and clusters is indicated through this analysis. The spatial  
77 interpolation of hydrocarbons concentration and indices was performed using the inverse distance

78 weighted (IDW) technique in geographic information system. The distribution maps were  
79 generated using ArcGIS software package – ArcMap (version 10.8.0.12790).

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81 **Supplementary Table S1:** The hopanes identified in the study with their respective diagnostic  
82 ions.

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<b>Serial No.</b>	<b>Retention Time (min.)</b>	<b>Compound Name</b>	<b>Diagnostic Ions</b>
1.	63.59	18 $\alpha$ (H)-22,29,30-trisnorneohopane	191, 370
2.	64.99	17 $\alpha$ (H)-22,29,30-trisnorhopane	191, 370
3.	68.13	17 $\alpha$ (H), 21 $\beta$ (H) C <sub>29</sub> hopane	191, 398
4.	69.23	Hop-17(21)-ene	191, 231, 367, 410
5.	70.04-70.75	17 $\alpha$ (H), 21 $\beta$ (H) C <sub>30</sub> hopane	191, 412
6.	72.26-72.614	C <sub>31</sub> homohopanes (22S, 22R)	191,426
7.	73.52-74.67	C <sub>32</sub> homohopanes (22S, 22R)	191, 440
8.	75.77-76.71	C <sub>33</sub> homohopanes (22S, 22R)	191, 454
9.	77.51-78.57	C <sub>34</sub> homohopanes (22S, 22R)	191, 470
10.	79.51-80.58	C <sub>35</sub> homohopanes (22S, 22R)	191, 484

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99 **Supplementary Table S2:** The PAHs identified in the study with their respective diagnostic ions

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Serial No.	Compound	Composition	No of rings	Ions (m/z)
1.	Phenanthrene (Ph)	C <sub>14</sub> H <sub>10</sub>	3	178
2.	Fluoranthene (Fla)	C <sub>16</sub> H <sub>10</sub>	4	202
3.	Pyrene (Py)	C <sub>16</sub> H <sub>10</sub>	4	202
4.	Benz[a]anthracene (BaA)	C <sub>18</sub> H <sub>12</sub>	4	228
5.	Chrysene (Chr)	C <sub>18</sub> H <sub>12</sub>	4	228
6.	Benzo[b]fluoranthene (BbF)	C <sub>20</sub> H <sub>12</sub>	5	252
7.	Benzo[k]fluoranthene (BkF)	C <sub>20</sub> H <sub>12</sub>	5	252
8.	Benzo[a]pyrene (BaP)	C <sub>20</sub> H <sub>12</sub>	5	252
9.	Benzo[g,h,i]perylene (Bpe)	C <sub>22</sub> H <sub>12</sub>	6	276
10.	Indeno[1,2,3-c,d]pyrene (Ipy)	C <sub>22</sub> H <sub>12</sub>	6	276
11.	Dibenzofuran	C <sub>12</sub> H <sub>8</sub> O	3	168
12.	Benzonaphthofuran	C <sub>16</sub> H <sub>10</sub> O	4	218

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113 **Table S3:** Compilation of diverse investigations detailing the concentrations (in  $\mu\text{g/g}$ ) of the *n*-  
114 alkanes.

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<b>Location</b>	<b><math>\Sigma n</math>-alkanes (<math>\mu\text{g/g}</math>)</b>	<b>References</b>
Krishna-Godavari Basin, India	269.50-449.90	Mani et al., 2016
Kharg Island, SW Iran	19.75-49.25	Akhbarizadeh et al., 2016
Capibaribe Estuarine System, Brazil	N.D.-9.47	Maciel et al., 2016
Bohai Sea, China	0.88-3.48	Li et al., 2015
Northern Persian Gulf	N.D.-1.71	Mohebbi-Nozar et al., 2015
Bohai Bay	6.3-535	Zhou et al., 2014
Barataria Bay, Gulf of Mexico	219.06-77399	Kirman et al., 2016
Gulf of Mexico	0.05-535000	Sammarco et al., 2013
Khmiss Tunisian Coast, Mediterran Sea	1020-2320	Ines et al., 2013
Cross River and Estuary System, SE Nigeria	0.05-1179	Pisani et al., 2013

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122 **Table S4:** Compilation of diverse investigations detailing the concentrations (in ng/g) of the  
123 hopanes.

<b>Location</b>	<b><math>\Sigma</math>Hopanes (ng/g)</b>	<b>References</b>
Mandovi Estuary, India	2.2-681.3	Bulbul et al., 2021
Caspian Sea, Iran	429.3-21691.1	Shirnesan et al., 2016
Paranagua Bay, South Brazil	40.2-197.7	Garcia et al., 2019
Persian Gulf	88-568	Jafarabadi et al., 2017
Astamudi Estuary, India	N.D.-363.2	Bulbul et al., 2022

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143 **Table S5:** Compilation of diverse investigations detailing the concentrations (in ng/g) of the  
144 PAHs.

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<b>Location</b>	<b>ΣPAHs (ng/g)</b>	<b>References</b>
Timor Sea, Australia	1.8-11.2	Burns and Jones, 2016
Luan River Estuary, China	5.1-545.12	Zhang et al., 2016
Kharg Island, SW, Iran	29.5-253.3	Akhbarizadeh et al., 2016
Northern Gulf of Mexico	68-158	Adhikari et al., 2016
Yangtze River Estuary, China	27.2-621.6	Wang et al., 2016
South China Sea	24-647	Kaiser et al., 2015
Barataria Bay, Gulf of Mexico	233-390835	Kirman et al., 2016
Pearl River Estuary, China	126.08-3828.58	Zhang et al., 2015
Pearl River Estuary, Daya Bay and northern South China Sea	248-2089	Yuan et al., 2015
Imam Khomeini Port, Persian Gulf, Iran	2885.8-5482.23	Abdolahi et al., 2013
Vembar Islands Group, Gulf of Mannar, India	0.36-15.98	Pradhap et al., 2021

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