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Assessment of Polycyclic Aromatic Hydrocarbon Contamination in Goan River Water: Toxicity and Persistence Concerns

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Abstract

The study focuses on the determination of polycyclic aromatic hydrocarbons (PAHs) in the Goan rivers. Certain locations along Goan rivers were strategically selected and analysed for the collected water samples in order to determine the concentration and distribution of the PAH contaminants in it. In the samples, Acenaphthene were discovered to be present in significant concentrations that allowed us to infer that it is persistent in the environment. Pyrene was also detected in high concentrations especially in water samples collected near sediments signifying heavy contamination that may have been a result of industrial effluents and/or urban runoff. However, benzo[a]pyrene, a known carcinogen, has been found at various levels; its occurrence raises concern as it implies its potential long term environmental as well as public health hazards if consumed by the human body. These findings highlight the need for continuous monitoring and mitigation measures to be taken in order to control sources of pollution in the river bodies and preserve these rivers within the Goan region from potential damage being caused.

Keywords: *Polycyclic Aromatic Hydrocarbons, Acenaphthene, Pyrene, Benzo[a]pyrene and Goan river.*

1. Introduction

Goan rivers play a vital role in maintaining ecological balance by supporting the state's diverse flora and fauna while serving as an essential water source for local communities (Goans), agricultural irrigation, and various industries. However, these rivers have recently been experiencing increasing environmental stress due to several anthropogenic activities, including mining, deforestation, urban development, agriculture, and port activities. These activities have led to the introduction of contaminants and toxins into the river systems, posing significant threats to aquatic life (such as fish, eels, and prawns), human health, and the overall stability of the Goan ecosystem maintained by these rivers.

As we investigate the toxins polluting these rivers, it is important to highlight that a major source of pollution arises from *coal tar*. This by-product is typically generated from the burning of coal or various petrogenic and mining-related activities. Coal tar is a significant source of polycyclic aromatic hydrocarbons (PAHs), which are commonly found in river bodies [1]. PAHs are a group of organic, semi-

volatile compounds containing more than two fused aromatic rings. They are characterized by high environmental stability and low biodegradation rates [2]. These properties allow PAHs to settle as sediments and accumulate over time, posing a serious threat to aquatic life and the people dependent on these water sources. PAHs can enter river systems from multiple sources, including industrial effluents, urban drainage, coal, petroleum, and wood combustion, as well as petrogenic activities like oil spills and road construction. Additionally, pyrolytic processes, such as biomass or fossil fuel burning, further contribute to PAH contamination [3].

In sediments, the presence of higher molecular weight PAHs typically indicates a pyrolytic origin. Their persistence in river sediments, resulting from both natural and anthropogenic sources, raises significant concerns, as PAHs can undergo microbial degradation, photolysis, and oxidation. Among fish species [4], exposure to PAHs has been linked to bone abnormalities observed in Pacific herring, pink salmon, and sea bass. Notably, PAH toxicity has persisted for years after initial contamination episodes, highlighting the need for thorough environmental impact studies. Additionally, some PAHs are classified as carcinogenic and mutagenic, posing a threat to wildlife and potentially entering the human food chain.

In a recent study, two *E. schistose* sea snakes were collected from the intertidal region of Caranzalem Beach, Goa, for analysis [5]. Their gut contents, liver, and kidney tissues were examined for PAHs and *n*-alkanes, revealing significant concentrations of both pollutants in their bodies.

The current study aims to identify, and analyse various pollutants present in samples strategically collected from Goan rivers. These contaminants may pose risks to human health, particularly for those relying on river water for household use. By assessing these pollutants, we seek to provide insights into their potential hazards and emphasize the urgent need for mitigation measures to protect public health.

2. Methods

The study was conducted in the river bodies of Goa, India. Sampling sites were selected based on their proximal distance from potential sources of contamination, including - industrial effluent outlets, urban runoff points, and natural river flow areas. The selection criteria aimed to capture a comprehensive view of pollutant distribution across Goan rivers.

2.1 Sample Collection: As part of the study to evaluate the extent of contamination in rivers within Goa, India; water samples were collected from several strategic points across five Goan rivers spanning areas proximal to pollution sources. Sample collection was carried out in photic zones (i.e. the above 200 meters of river) of river sites. The site selection included a variety of potential contamination origins, contributing to a better assessment of the distribution patterns as well as contaminant concentration within these ecological settings (Figure 1 and Figure 2).

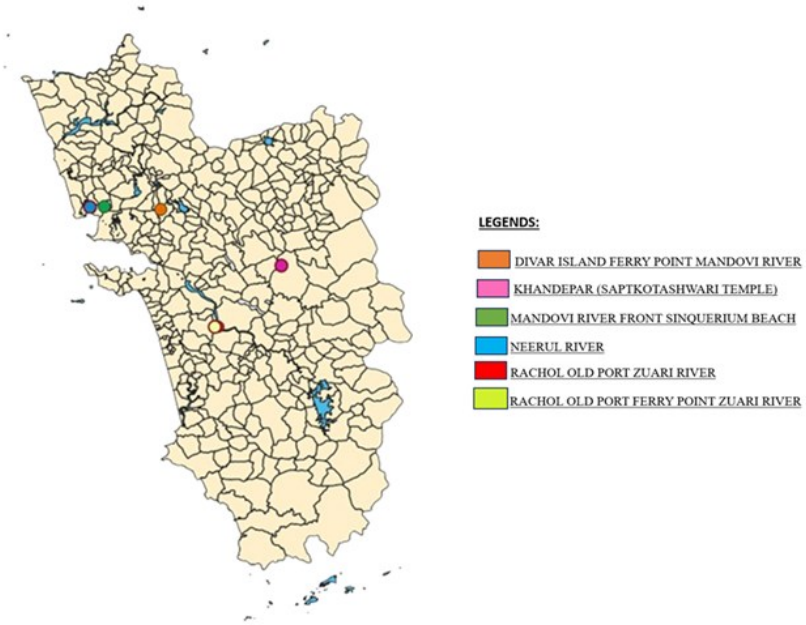

Figure 1. Geology map of the Goan river. Add reference

Figure 2. Sites for water sample collection: **A)** Orange marker represents the site of sample collection at Ferry Point Divar Island **B)** Pink marker represents the site of sample collection at khandepar river saptakoteshwar temple **C)** Green marker represents the site of sample collection at Mandovi River Front **D)** Blue marker represents the site of sample collection at Nerul river near Aguada Fort **E)** Red marker represents the site of sample collection at Rachol Old Port Zuari River Front **F)** Yellow Marker represents sample collected from Rachol ferry point Zuari River.

The steps were followed in order to collect river water samples from the various locations in Goa. In this case, pre-cleaned bottles of 500 mL were used as sample containers fitted with hard-plastic caps for preventing contamination and degradation of target compounds. To prepare

them for sampling, all bottles were rinsed with water (distilled) three times using water obtained from the sampling site. The bottle opening was upstream to prevent contamination from surface materials and debris. During sampling, care was taken not to disturb the sedimentary material. After filling, a small air gap was made by punching a small hole in the bottle so that thermal expansion can occur and then tightly closed with the lid and to equalise pressure for sample integrity. Each bottle contained details such as the date and place where it had been sampled. These samples were put into a cooler to maintain at a temperature around 4°C and transported within twenty-four hours to avoid PAHs decay during transit time till they reached the laboratory for analysis. The areas chosen for sampling included those close to possible sources of pollution such as industrial effluents, urban runoff points and sites with natural riverine flow in order to have a better understanding of PAH distribution in Goa's riverine ecosystems.

To extract organic compounds from water samples, the sample was first prepared by filtering to remove any particulate matter. An appropriate volume of ethyl acetate, i.e.30 ml with the 100 ml volume of the water sample, was then measured and added to a separating funnel containing the water sample. The funnel was securely closed with the stopper, followed by shaking it vigorously to ensure thorough mixing of the aqueous and organic phases. The funnel was allowed to stand until the two layers separated, with ethyl acetate forming the upper layer. The lower aqueous layer was carefully drained into a separate container, leaving the ethyl acetate layer behind.

2.2 Analysis: In the laboratory, water samples were filtered to remove particulate matter and were extracted with ethyl acetate using a separating funnel, such that it separated into an organic phase containing PAHs. The organic phase was concentrated followed by the PAH's being characterised by the High-Performance Liquid Chromatography (HPLC) and Mass Spectrometry (WATERS CORPORATION) that allowed the retention time and even fragmentation patterns of PAHs to be identified.

2.2.1. Chromatography: High-Performance Liquid Chromatography (HPLC) was the primary instrumentation technique in the methodology, employed for the detection and subsequent analysis of PAHs. It was undertaken systematically to avoid any errors in the analysis. First, water or sediment samples were taken in clean pre washed bottles so that no contamination occurred. For water samples, particulates were removed by filtration, while sediment and biological samples were solvent extracted with ethyl acetate. The extract was concentrated if this was required. The HPLC system employed a reversed phase i.e. C18 column as stationary phase for separation. The mobile phase composition was water: acetonitrile (50%: 50%). The flow rate was maintained at 1.5 mL/min and the column had a constant temperature of 40°C to facilitate separation. Detection was done using a PDA detector (photodiode array) based on the types of PAHs being analysed. Injections of the samples were made by introducing prepared extracts of between 10 µL into the HPLC system which had been calibrated and equilibrated prior. The analysis was mainly concerned with the retention times for various compounds and quantitation of these compounds.

2.3 *In silico* Analysis: Further, to analyse the impact of these PAHs on the human body, an in silico ADME analysis was run to understand various pathways the effect these toxins if consumed by humans as these Goan rivers are used as a source of daily purpose water in local households. An ADME search was run using SWISSDOCK, an online software which offers SwissADME, for in silico analysis of contaminants [6, 7]. A molecular structure and smiles code was retrieved from the databases and run for its structure based ADME analysis in an online platform, SWISSDOCK [8-10].

3. Result and Discussion

3.1 High Performance Liquid Chromatography (HPLC) analysis: The samples showed nearly similar peaks that were detected at 190 nm on the PDA i.e. Photodiode Array Detector. The chromatograms, obtained from the chromatographic analysis, provided consistent peaks at specific retention times, particularly around 1.4–1.5 minutes and 2.6–2.7 minutes, suggesting the presence of recurring compounds across all the water samples. The peak around 1.4–1.5 minutes may represent small aromatic compounds or phenol derivatives, which are known to elute early on a C18 column due to their moderate hydrophobicity and strong UV absorbance (Figure 3 and Table 1). The peak at 2.6–2.7 minutes could indicate a slightly larger aromatic or possibly a light PAHs, common in environmental water samples due to pollution sources. The absorbance at 190 nm suggests these compounds have significant UV absorbance, which is characteristic of conjugated systems like aromatics.

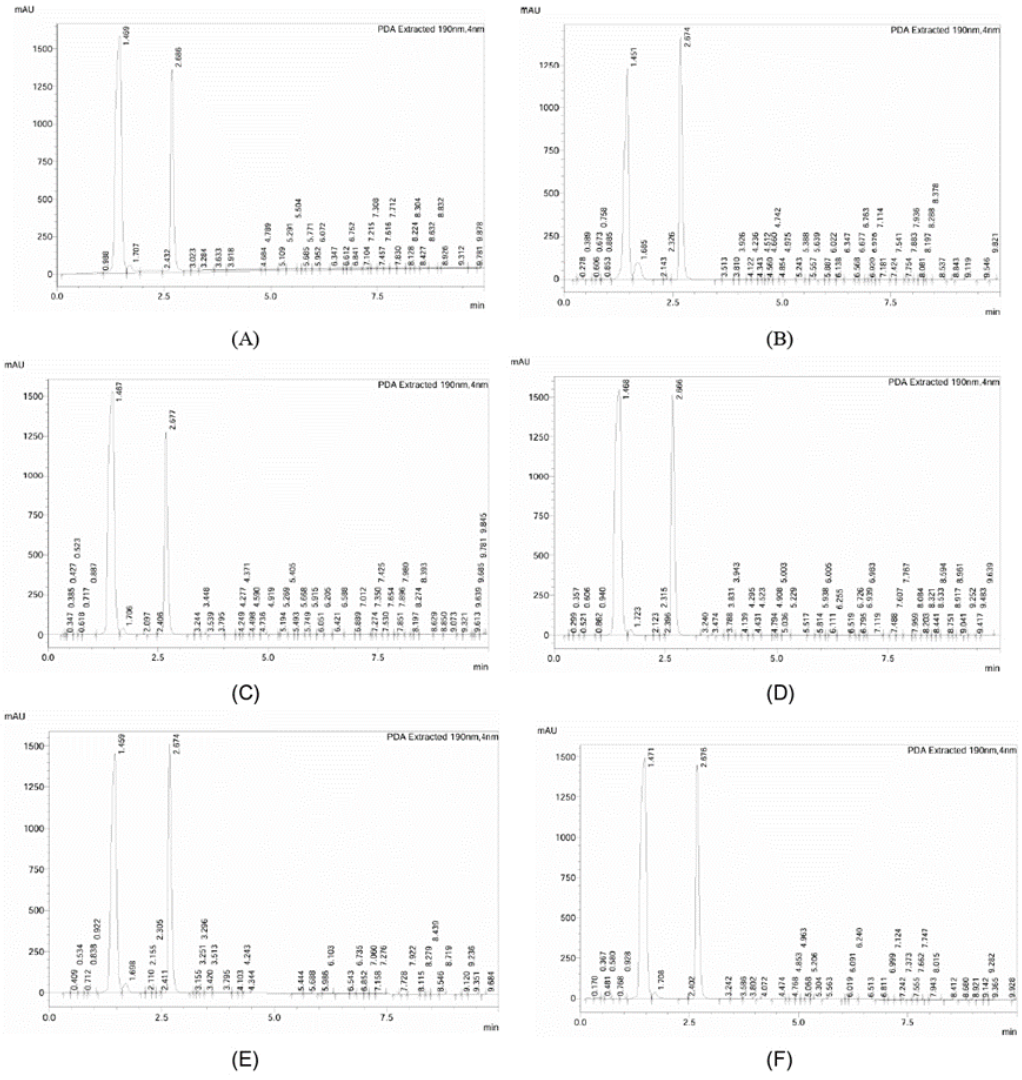

Figure 3. HPLC graphs of river water samples. Figure A is the Chromatogram obtained from the water sample collected from the Deewar island banks of Mandovi River. Figure B and D is the chromatogram obtained from the Khandepar river and Nerul river. Figure C is the subsequent

sample obtained from the Mandovi river. Figure E and F are the chromatograms obtained from the water sample collected from Zuari river, strategically collected from two different locations.

Table 1. HPLC peaks with retention time (in min).

Chromatogram	Peak 1 (min)	Peak 2 (min)	Peak 3 (min)	Peak 4 (min)	Peak 5 (min)	Other Peaks
Chromatogram 1	1.471	2.676	3.242	4.072	5.206	6.240, 7.124, 8.015, 9.928
Chromatogram 2	1.459	2.674	3.155	4.243	5.444	6.103, 7.276, 8.546, 9.684
Chromatogram 3	1.487	2.678	3.167	4.27	5.432	6.219, 7.330, 8.128, 9.741
Chromatogram 4	1.48	2.673	3.162	4.265	5.426	6.215, 7.325, 8.124, 9.735
Chromatogram 5	1.466	2.671	3.15	4.23	5.41	6.200, 7.302, 8.102, 9.710
Chromatogram 6	1.471	2.676	3.155	4.243	5.444	6.211, 7.315, 8.120, 9.724

For the spectroscopic technique, mass spectroscopy was employed. It is a sophisticated technique that allows the ionisation, fragmentation and analysis of the molecule based on their mass to charge ratio. Some ion peaks were obtained as 155.25, 203.45, 253.21, 300.4, 400.2, 597.7, 607.6 m/z (Figure 4 and Table 2). On subsequent interpretations of the graph, three compounds emerged as major constituents in the river sample collected from Goa. The constituents were pyrene, benzo[a]pyrene and acenaphthene with mass recorded in the spectrometer and identified to be potential pollutants in the river body. The World Health Organization (WHO) has specified guideline values for benzo[a]pyrene that are of health significance in drinking water as 0.7 µg/l [11]. Further on referring Environmental Protection Agency, the relative exposure limit for Acenaphthene 0.1mg/m3. The relative potency of pyrene and benzo[a]pyrene were described as 0.8 and 1 respectively in WHO guidelines for drinking water quality [12].

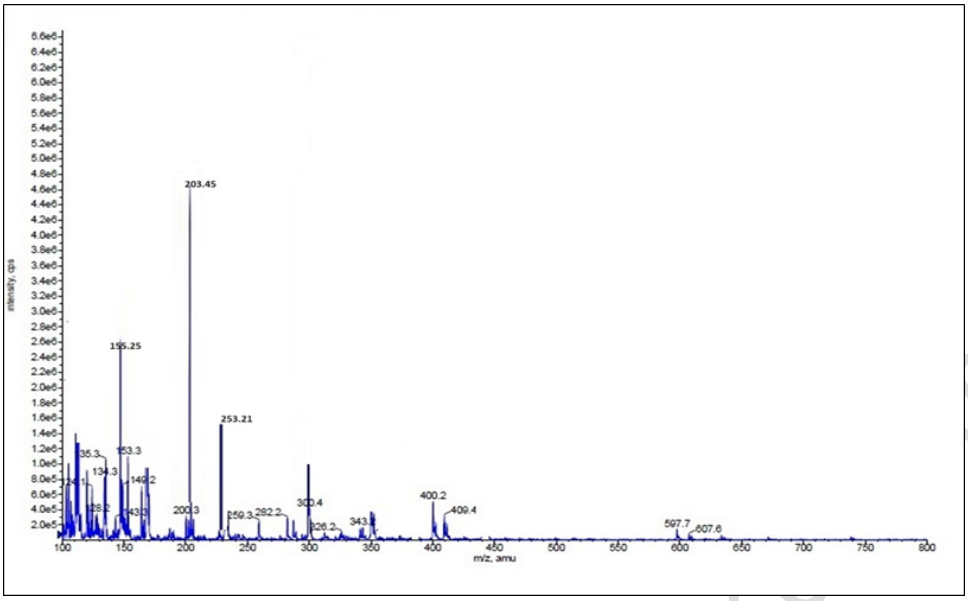

Figure 4. Mass spectra of Goan river sample.

Table 2. Mass spectrometer and HPLC data interpretations.

Compound Name	Molecular Weight (g/mol)	m/z Peak in MS	HPLC Retention Time	Description
Acenaphthene [13]	154.21	~154	Short to Moderate Retention Time	Smallest PAH, likely eluting before others.
Pyrene [14]	202.25	~202	Moderate Retention Time	Intermediate PAH, likely eluting after acenaphthene.
Benzo[a]pyrene [15]	252.31	~252	Longer Retention Time	Largest PAH, likely eluting last due to more hydrophobicity.

3.2 *In silico* Analysis: Further, to analyse the impact of these PAHs on the human body an *in silico* ADME analysis was run to understand various pathways. Toxic components, such as PAHs undergo various toxicodynamic pathways on administration. Hence, an ADME study of these chemical helps enhance the toxicological profile. An ADME search was run using SWISSDOCK, an online software which offers SwissADME, for *in silico* analysis of contaminants and following as results were discovered as given in Table 3.

Table 3. SwissDock ADME results.

Parameter	**Pyrene**	**Benzo[a]pyrene**	**Acenaphthene**
Canonical SMILES	c1cc2ccc3c4c2c(c1)ccc4ccc3	c1ccc2c(c1)c1ccc3c4c1c(c2)ccc4ccc3	c1cc2cccc3c2c(c1)cc3
Formula	$C_{16}H_{10}$	$C_{20}H_{12}$	$C_{12}H_{10}$
Molecular Weight (MW)	202.25	252.31	154.21
Number of Heavy Atoms	16	20	12
Number of Aromatic Heavy Atoms	16	20	10
Fraction Csp3	0	0	0.17
Number of Rotatable Bonds	0	0	0
Number of H-bond Acceptors	0	0	0
Number of H-bond Donors	0	0	0
Molar Refractivity (MR)	70.15	87.65	51.77
Topological Polar Surface Area (TPSA)	0	0	0
iLOGP	2.45	2.8	2.23
XLOGP3	4.88	5.97	3.92
WLOGP	4.58	5.74	2.94
MLOGP	5.56	6.32	4.44
Silicos-IT Log P	4.81	5.8	3.99

Consensus Log P	4.46	5.33	3.5
ESOL Log S	-4.91	-5.91	-3.88
ESOL Solubility (mg/ml)	2.50×10^{-3}	3.14×10^{-4}	2.02×10^{-2}
ESOL Solubility (mol/l)	1.23×10^{-5}	1.24×10^{-6}	1.31×10^{-4}
ESOL Class	Moderately soluble	Moderately soluble	Soluble
Ali Log S	-4.62	-5.75	-3.62
Ali Solubility (mg/ml)	4.91×10^{-3}	4.53×10^{-4}	3.71×10^{-2}
Ali Solubility (mol/l)	2.43×10^{-5}	1.79×10^{-6}	2.40×10^{-4}
Ali Class	Moderately soluble	Moderately soluble	Soluble
Silicos-IT LogSw	-6.59	-8.26	-4.61
Silicos-IT Solubility (mg/ml)	5.22×10^{-5}	1.38×10^{-6}	3.80×10^{-3}
Silicos-IT Solubility (mol/l)	2.58×10^{-7}	5.46×10^{-9}	2.47×10^{-5}
Silicos-IT Class	Poorly soluble	Poorly soluble	Moderately soluble
GI Absorption	Low	Low	Low
BBB Permanent	No	No	Yes
Pgp Substrate	No	No	Yes
CYP1A2 Inhibitor	Yes	Yes	Yes
CYP2C19 Inhibitor	No	No	No
CYP2C9 Inhibitor	No	No	No

CYP2D6 Inhibitor	No	No	No
CYP3A4 Inhibitor	No	No	No
Log Kp (cm/s)	-4.07	-3.6	-4.46
Lipinski # Violations	1	1	1
Ghose # Violations	0	1	1
Veber # Violations	0	0	0
Egan # Violations	0	0	0
Muegge # Violations	1	2	2
Bioavailability Score	0.55	0.55	0.55
PAINS # Alerts	0	0	0
Brenk # Alerts	1	2	2
Lead Likeness # Violations	0	0	0
Synthetic Accessibility	1	1	1

The ADME data for pyrene shows a lot of important features about the physicochemical properties, lipophilicity, solubility, pharmacokinetics, and drug-likeness. The molecular weight of pyrene is 202.25 g/mol with fully aromatic structure making it highly lipophilic as evidenced by an averaged Log Po/w value of 4.46. This high lipophilicity indicates that pyrene rather gets dissolved in fats than water as evidenced by its poor/moderate aqueous solubility. Pyrene has a low gastrointestinal absorption and does not easily cross blood-brain barrier suggesting that it may have challenges reaching central nervous system (CNS) and oral bioavailability problems, respectively. It does not act as a p-glycoprotein substrate implying its distribution and excretion could be influenced by this factor. Nonetheless, within this pathway, pyrene serves as an inhibitor to CYP1A2 which is involved in drug metabolism thus leading to possible interactions with other drugs metabolised along this pathway. The drug likeliness criterion is the total addition of the molecular physicochemical properties that are characteristic of drugs. This criterion can be used to determine the safety of the chemical compound that may be administered [16]. Some of the PAHs may be ingested orally by drinking the river water, therefore, the *in silico* analysis of these compounds in terms of

administration can be conducted through the drug-likeliness criteria. Despite satisfying most of the drug-likeness criteria, one Lipinski's rule is violated because Pyrene has a high MLOGP (Molecular Logarithm of the Partition Coefficient) value which may influence its drug-like behaviour. Additionally, Pyrene is flagged by Brenk's alert system as a PAHs; a structural feature often associated with toxicological concerns.

Taking benzo[a]pyrene ($C_{20}H_{12}$), as a very aromatic molecule with Molecular Weight 252.31 g/mol and has all of their heavy atoms are highly oriented from the rings. This molecule is perfectly rigid, there are no rotatable bonds at all and it has neither hydrogen bond acceptors or donors which suggest a low capability for forming "hydrogen" bonds from other molecules (this would probably impact the affinity to biological targets). Its molar refractivity of 87.65 cm^3/mole (indicating it is highly unsaturated and aromatic). It is even more hydrophobic, with a topological polar surface area (TPSA) of 0.00 $Å^2$. Considering lipophilicity of the compound, the Log Po/w value varies and is characterised by an average level 5.33 obtained as a consensus. Therefore, the benzo[a]pyrene compound is more likely to be partitioned into lipids, which might be considered cell membranes, as opposed to an aqueous environment. Water solubility ratio for the compound is annotated by a consensus Log S with very low values. When evaluating solubility rate from the data, it can be classified as moderately to poorly soluble, with solubility ranging from 3.14 x 10^{-4} mg/ml to 1.38 x 10^{-6} mg/ml, depending on the method.
Benzo[a]pyrene satisfies some drug-likeness criteria but violates Lipinski's rule due to a MLOGP is greater than 4.15 and Ghöse 's rule due to a WLOGP (Weighted Logarithm of the Partition Coefficient) is greater than 5.6. It also violates Muegge's criteria due to having a high XLOGP3 (eXtra-logP version 3) and a low number of heteroatoms. The estimated bioavailability of 0.55 suggests moderate oral bioavailability. According to medicinal chemistry analysis, benzo[a]pyrene has two alerts because PAHs have a poor safety profile, raising concerns regarding mutagenicity and carcinogenicity. The synthetic accessibility score is 1.00, which classifies it as easy to synthesise.

Further, acenaphthene, a PAH with a molecular formula of $C_{12}H_{10}$ and has a molecular mass 154.21 g/mol; it is observed that it has a minimum number of SP^3 hybridised carbons (0.17) and lacks hydrogen donor and acceptor respectively, and a lower molar refractivity (2.77), while the TPSA (0.00$Å^2$), which measure the polar surface area of a molecule and allows evaluation of chemical reactions, indicates a non-polar compound. The different methods (iLOGP: 2.23, XLOGP3: 3.92, WLOGP: 2.94, MLOGP: 4.44 and SILICOS-IT: 3.99) gave AF differing Log P values: 3.50. Overall, acenaphthene appears to be a fairly lipophilic molecule, one of the defining features of a PAH. Log S values for the solubility of acenaphthene are different and indicate the moderate solubility. Pharmacokinetically, acenaphthene is a low gastrointestinal absorbed molecule that gets classified as BBB (Blood-Brain Barrier) permeant (crossing into central nervous system), substrate of p-glycoprotein (p-gp), and inhibits CYP1A2 but does not inhibit CYP2C19 or CYP2C9 or CYP2D6 or CYP3A4. Skin permeability is low (Log Kp = -4.46 cm/s). Similar to the above two compounds, when considering aspects of drug-likeness, acenaphthene represents violation to Lipinski's Rule (MLOGP > 4.15). It violates Ghose's criteria for druglikeness, as it has an overall molecular weight < 160. It also violates Muegge components of druglikeness, with violations in molecular weight and heteroatom content. However, acenaphthene adheres to Veber's and Egan's rules. Acenaphthene's bioavailability score is 0.55, which indicates moderate oral bioavailability.

Through ADME analysis by SWISSDOCK, it was found that acenaphthene and pyrene have low water solubility, while benzo[a]pyrene is fat-soluble. These PAHs exhibit poor

gastrointestinal absorption, except for moderate blood-brain barrier permeability, along with relatively high lipophilicity and inhibition levels of cytochrome P450 enzyme (e.g., CYP1A2 inhibitor). Although all compounds meet some drug-likeness criteria, they violate at least one or more of Lipinski's, Ghose's, or Muegge rules, indicating concerns over potential toxicity and bioavailability for each compound.

4. Conclusion

The investigation followed a preliminary detection of contaminants in river water through an HPLC profile for each sample collected. Detection of the compounds was achieved based on their retention time using HPLC, followed by precise molecular mass identification by mass spectrometry. Further, MS results confirmed the presence of some PAHs, i.e. Benzo[a]pyrene, Pyrene and Acenaphthene. The presence of PAHs in water bodies is linked to a number of possible ecological hazards as well as human exposure pathways. Because of their toxicity to aquatic life, carcinogenicity, and propensity for bioaccumulation, it is concerning to find certain compounds in water bodies. PAHs can have long-term consequences on aquatic ecosystems, including mutagenic and endocrine-disrupting effects, even at low levels. Human exposure can occur by the intake of polluted aquatic creatures, cutaneous absorption, or ingestion of contaminated water. *In silico* analysis by SWISSDOCK revealed some toxicity concerns of this PAHs. Pyrene is highly lipophilic, it is a contaminant in fatty tissues and sediments. Further, its low gastrointestinal absorption and poor blood-brain barrier penetration suggest that it has limited systemic toxicity but extensive environmental persistence. Benzo[a]pyrene, which was found in certain quantities, is a carcinogenic pollutant. Acenaphthene, another key PAH found in this study, bearing intermediate properties, is relatively stable and persistent in the environment. This emphasises the necessity of extensive profiling for PAHs, as even lower levels can exert long-term effects where they persist. The moderate solubility and lipophilicity of acenaphthene allow it to accumulate in sediments or biotic tissues of river organisms, potentially exposing a range of organisms over time. PAHs indicate long-term sources of combustion processes and industrial activities. Its identification shows the importance of extensive monitoring studies of the river in order to determine the accumulation of the contaminant and future analysis of the impact dynamics of the PAHs on the ecosystem.

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All authors listed on this manuscript have made substantial contributions to its creation and are accountable for all aspects of the work. Each author has participated in the following aspects of the research and manuscript preparation:

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- **Investigation:** MB, CA, RB
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