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Investigating the chemical impact of human-related activities on the Red Sea marine environment utilizing High Resolution Mass Spectrometry

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Abstract: A baseline study was conducted in the Red Sea marine environment, where sediments were collected, aiming to investigate the long-term impact of anthropogenic activities, and provide useful insights to legislative parties in the framework of the Marine and Coastal Environment Protection Initiative (MCEP). Generic sample preparation protocols were implemented for the extraction of as many semi-polar to polar, LC-amenable emerging contaminants (ECs) and a hybrid trapped ion mobility tandem high-resolution mass spectrometric technique was utilized. Subsequently, wide-scope target and suspect screening of more than 3,100 ECs was conducted. A total of 51 ECs from 7 distinct chemical classes were determined. The highest chemical burden was determined in Jeddah Mena and Jeddah Lagoon regions, with cumulative concentrations of ECs reaching up to 2.24mg/kg d.w. and 5.80mg/kg d.w., respectively. Risk assessment showed that 8 compounds were at high environmental risk, highlighting the significance of their comprehensive monitoring. This study aims to set the baseline of chemical pollution in the study area and act as a reference for future research.

Keywords: HRMS, sediments, target/suspect screening, risk assessment, WWTPs

1. Introduction

Despite the economic and environmental importance of the Red Sea to the Middle East and North Africa (MENA) regions, the pollution status of its marine environment and especially the occurrence and distribution of emerging contaminants (ECs), have not been studied extensively. This study aims to set the baseline of pollution in the Red Sea marine environment based on the determination and prioritization of ECs.

Literature suggests that previously conducted research mainly targeted heavy metals and GC-amenable compounds, both in seawater[1,2] and sediments[3,4].. A state-of-the-art trapped ion mobility spectrometry tandem high-resolution mass spectrometry (TIMS-HRMS) method was employed herein, further enhancing research novelty.

This is the first geographically comprehensive survey of contaminants in the Saudi Arabian coastal zone, including the most important hotspot coastal marine areas, and involving the utilization of HRMS. Sediment samples were gathered, the analysis of which reflects on the long-term chemical encumbrance of the study area by anthropogenic activities. Wastewater treatment plants (WWTPs), port facilities, maritime traffic, industrial operations, aquacultures and urban runoffs comprise the main sources of marine pollution in the region. An ecotoxicological risk assessment was also conducted, aiming to prioritize detected substances.

2. Materials and methods

A sampling campaign was carried out from June 9th to July 6th by the Hellenic Centre for Marine Research (HCMR) with research vessel (R/V) “Aegaeo” throughout the coastal zone of the Red Sea, Saudi Arabia. Sediments were collected from distinct regions, representing the hotspot areas affected by various anthropogenic activities.

Collected samples were immediately stored in the freezer (-20ºC) and transferred to the lab for analysis. A previously reported generic sample preparation method was implemented[5].Raw data were treated through strict identification criteria were applied, taking full advantage of ion mobility implementation, minimizing false positive determinations, thus increasing confidence levels.

3. Results and discussion

A total of 55 ECs were determined, belonging to 7 distinct chemical groups. The most chemically encumbered regions, regarding the number and cumulative

concentration of analytes, were Jeddah Mena and Jeddah Lagoon with a total of 30 and 21 detected ECs, respectively. In Jeddah Mena, the highest cumulative concentration of chemicals was calculated for PPPs and PCPs, equaling 1.40mg/kg d.w. and 704μg/kg d.w., respectively. PCPs and PFAS were detected predominantly in Jeddah Lagoon, in cumulative concentration levels reaching up to 5.80 and 2.53mg/kg d.w., respectively.

A total of 18 PHRs were determined along the coastal areas of the Red Sea, mainly in the Jeddah Mena, Jeddah Lagoon and Al-Wajh regions, in concentration levels reaching up to 1.00mg/kg d.w. A total of 7 PFAS were determined in almost all sampling points. Their highest cumulative concentrations were observed in Jeddah Mena and Jeddah Lagoon stations, equaling 2.97mg/kg d.w. and 593μg/kg d.w., respectively. Perfluorooctanesulfonic acid (PFOS) (FoD=48%) exhibited the highest concentration levels in the study area, reaching up to 1.41mg/kg d.w. The highest calculated concentration was determined in NI2 sampling station, Jeddah Lagoons, possibly due to wastewater effluents. PFOS has also been reported in the past, in seawater samples collected from distinct areas of the Indian Ocean[7,8]. Although PFOS is currently being regulated in EU countries[9], no specific legislation exists in the Kingdom of Saudi Arabia.

Regarding PPPs & TPs, only a few compounds were determined, possibly due to limited cultivations in the Red Sea coastal area. The highest cumulative concentration of pesticides was determined in the Jeddah Mena, equal to 2.24mg/kg d.w.

A suspect screening of more than 500 SRFs was also conducted, aiming to expand the investigated chemical domain. A total of 4 suspect compounds were detected, namely C11-LAS, C12-LAS, C13-LAS and AES-C12 (n=2). These compounds have also been determined in wastewater effluents in past datasets[10].

A comprehensive risk assessment was conducted, aiming to prioritize detected compounds. Substances with risk quotient (RQ) values greater than 1 demonstrate high-risk, endangering sea bottom quality and marine biota. High-risk analytes are presented in **Table 1**.

Table 1. High-risk compounds in seawater samples

Analyte Name	FoD	FoE	EoE	RQ
Fenbendazole	0.96	0.96	0.50	2.42
Mercaptobenzothiazole	0.62	0.48	0.50	1.60
Dinoterb	0.52	0.52	0.50	1.54
Perfluorooctanesulfonic acid (PFOS)	0.48	0.48	0.50	1.46
Benzyl butyl phthalate (BBP)	0.38	0.38	0.50	1.26
Salicylic acid	1.00	0.02	0.20	1.22
Flumequine	0.50	0.08	0.50	1.08
Octocrylene	0.54	0.00	0.50	1.04

4. Conclusions and future prospects

In this study, a wide-scope target and suspect screening of ECs was conducted, investigating the occurrence of thousands of analytes, aiming to assess the environmental quality status of the Red Sea area. Determined compounds were prioritized through risk evaluation, based on PNEC values. Ecotoxicological risk assessment indicated that a total of 8 compounds exhibited high-risk potential, suggesting that environmental legislation should be established.

In the future, retrospective analysis and non-target screening should be conducted for the determination of new ECs.

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