



Water Quality Assessment and Source Apportionment of Huangpu River Water Pollution in Shanghai City, Eastern China using APCS-MLR

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ABSTRACT

As a result of increasing anthropogenic disturbance, the degradation of the surface water environment has become a key concern for water resource management. Controlling possible pollution sources is necessary for protecting water resources. In this paper, water quality data from online monitoring national control stations were analyzed in terms of pH, Water Temperature (WT), Electrical Conductivity (EC), turbidity (NTU), dissolved oxygen (DO), and concentrations of permanganate index (COD_{Mn}), ammonium nitrogen (NH_3^+-N), total nitrogen (TN), total phosphorus (TP). Principal component analysis/factor analysis (PCA/FA) was employed to qualitatively figure out the potential sources of river water pollution of Huangpu River in Shanghai City, eastern China. An absolute principal component score-multiple linear regression (APCS-MLR) receptor model was used to analyze each source's contribution to the variables affecting water quality quantitatively. The results showed that all observed water quality indices met the quality criteria specified in the Chinese surface water standards, except for TN. Five sources of river water pollution were identified, and their contribution ratios in a descending order were as follows: The meteorological process (26%)>agricultural activities (14%)>industrial sewage (10%)>natural environmental sources (4%)=domestic sewage (4%). Therefore, recommendations for enhancing the quality of surface water resources in this area involve decreasing agricultural pollution and improving the sewage system.

Keywords: Surface water; Water quality; Source apportionment; APCS-MLR model; Huangpu river

INTRODUCTION

As the main source of fresh water on the Earth's surface, rivers play an irreplaceable role in human survival and social development. In recent years, with accelerated urbanization and rapid economic development, river pollution has drawn great attention from the government and the public [1-3]. According to studies, the primary factors responsible for a decrease in river water quality are excessive sewage discharges from industry, households, and agriculture, particularly in developing countries [1,4-6]. When a river is polluted, it can significantly impact the overall water quality of the surrounding aquatic environment because it plays an essential role in the hydrological cycle [7,8]. For this reason, the implementation of accurate source identification and allocation in the management of pollution sources is of paramount importance in assessing

and safeguarding the integrity of water resources [9,10]. According to the Bulletin of Ecology and Environment in China in 2022 (MEEC, 2022), 12.1% of surface water was unsuitable for drinking in 2022, Yangtze River Basin, Pearl River Basin, Zhejiang and Fujian piece of rivers, northwest rivers, and southwest rivers water quality is excellent, the Yellow River Basin, Huaihe River Basin, and Liaohe River Basin water quality is good, the Songhua River Basin and the Haihe River Basin for light contamination. Principal component analysis/factor analysis (PCA/FA) is traditional mathematical and statistical methods. PCA/FA linearly transforms variables using orthogonal transformation. These techniques have a proven efficacy in qualitatively identifying sources of pollution. However, they lack the capacity to accurately determine the precise contributions of sources [11-15]. Positive Matrix Factorization (PMF), chemical mass balance, Unmix, absolute principal component score-multiple

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linear regression (APCS-MLR), and global optimal inverse models which are models use statistical methods and mathematical algorithms to estimate the contributions of different pollutant sources and provide valuable insights into the sources of pollution in soil, air, and water [9,11,15-21]. The APCS-MLR models have been commonly used to quantify pollution sources in different water bodies, such as lakes, rivers coastal water, and groundwater [9,15,18,20,22]. In recent years, numerous researches have demonstrated the stability of these models, however, the APCS-MLR model proves to be more effective in handling data sets with parameter of varying magnitudes analyzed a water quality dataset consisting of 15 parameters collected from eight sampling sites in the tributaries and mainstream of the Min River [9,11,16,17,20,21]. The APCS-MLR model was employed to identify potential sources of pollution and allocate their respective contributions. Similarly, the five sources of river water contamination that identified were as follows, with the contribution ratios listed in descending order: The geogenic process (24%) is more prevalent in the Xinbian River of Anhui Province, Eastern China than agricultural activities (21%), sources related to chicken farming (17%), residential pollution (9%) and transportation pollution (5%) [17]. These studies have important implications for regional water resources management. Shanghai is located in East China, on the West Coast of the Pacific Ocean and the eastern edge of the Asian continent, part of the alluvial plain of the Yangtze River Delta. Previous studies have shown that deteriorated river water quality significantly affects the economic development and the health of people in this area [23,24]. In recent years, the water systems of Shanghai have been greatly improved by the execution of a series of water-management plans. Since 2017, Shanghai has started a new phase of large-scale water environment management. In 2018, the black odor of small and medium-sized rivers was essentially eliminated, and in 2020, the inferior Grade V water bodies were essentially eliminated. In the Huangpu River Waterfront Area Construction Plan (2018-2035), a spatial development strategy of “two cores and multiple nodes” is intended for the area along the Huangpu River, with each portion being staggered and synergistic, and the core functions of finance, innovation, and culture with global competitiveness being built out in a cluster fashion in the most significant sections. Upstream The Xupu Bridge to Dianshan Lake segment strengthens the strategic ecological conservation function basis and effectively integrates the functions of life, recreation, culture, and innovation industry. The core section (Yangpu Bridge to Xupu Bridge) concentrates on carrying the core functions of finance, business, culture, commerce, and recreation of the international metropolis, and provides public activity space with global influence. The downstream section (Wusongkou to Yangpu Bridge) provides development space for innovative functions based on regional transformation and upgrading, and strengthens the integration of ecological and public functions and living functions used the chemical oxygen demand, total phosphorus, dissolved oxygen, ammonium nitrogen and biochemical oxygen demand and showed that after the river remediation work of Yangpu District in 2017, the main pollutants in the river converted from ammonium nitrogen to total phosphorus, indicating that the river remediation improves the self-purification ability of the river, which had a remarkable influence on the water quality [23]. However, no

study has been conducted to characterize online monitoring statistics of the whole river. Therefore, this study selected the Huangpu River, known as the “Mother River of Shanghai,” as the study area, and used mathematical and statistical analysis techniques PCA/FA combined with the APCS-MLR model to

- Evaluate the seasonal characteristics of river water quality in the study area,
- Identify potential sources of primary water elements, and
- Quantify the source inputs and contribution variables for each water quality parameter. The findings of this study are expected to help assess the water quality and potential sources of pollution in the Huangpu River in Shanghai and enable stakeholders to more effectively manage pollutants entrance into the river and improve surface water quality in this area.

MATERIAL AND METHODS

Study Area

Shanghai is located in a longitude belt of 120°52'E to 122°12'E and a latitude belt of 30°40'N to 31°53'N, Shanghai has a four-season, north subtropical monsoon climate with plenty of sunlight and rain. The weather in Shanghai is moderate and muggy, with longer winters and summers than springs and autumns. The city had an average temperature of 17.9°C and 1474.5 mm of precipitation in 2021. Between June and September, there is a concentration of 66.1% of the yearly precipitation. Shanghai's elevation is 2.19 m on average. Shanghai's highest point is DaJinshan Island, which is 103.7 m above sea level [19]. Huangpu River, the upper reaches of which are located in the southwest of Shanghai, flows through Qingpu, Songjiang, Fengxian, Minhang, Xuhui, Huangpu, Hongkou, Yangpu, Pudong New Area, Baoshan and other districts to Wusongkou with a total length of 113.4 kilometers, and the main stream of Huangpu River from Mishidu to Wusongkou is 82.5 kilometers long [19]. Huangpu River is a lake source river network tidal river, is the main source of drinking water, industrial water, agricultural irrigation water in Shanghai, and plays an important role in shipping and other aspects. Additionally, it is also a receiving water body for Shanghai's wastewater discharge, resulting in water pollution. Therefore, the local water resources management department has planned to develop the Huangpu River (the sampling section of the river) in the coming years to better support functional area development (Figure 1). Four sampling sections were shown as follows: “1” stands for Dianfeng, “2” stands for Linjiang, “3” stands for west Minhang border (Songpu Bridge), “4” stands for Wusongkou.

Sampling and Analysis

The study employed water quality data from online monitoring national control stations from January to December 2021 of Wusongkou to investigate the intra-year variable characteristics of the water quality of the Huangpu River. As Wusongkou is the Huangpu River's downstream exit, and because the catchment area encompasses the whole basin, it may represent the features of the water body as a whole and serve as a foundation for determining the primary component findings in the study of the sources of pollution that follows. As a result of the

COVID-19 outbreak resulted in Shanghai's closure control, the study did not include data from 2022. The Huangpu River's pollution sources will be investigated using a total of 60 average online water quality data points covering the first, second, and third 10 days of each month from January to May 2023. From the national monitoring website, information on water quality was obtained. The water quality parameters for investigation in this study included electrical conductivity (EC), dissolved oxygen (DO), water temperature (WT), turbidity (NTU), pH, permanganate index (COD_{Mn}), ammonium nitrogen (NH_3^+-N), total nitrogen (TN), total phosphorus (TP).

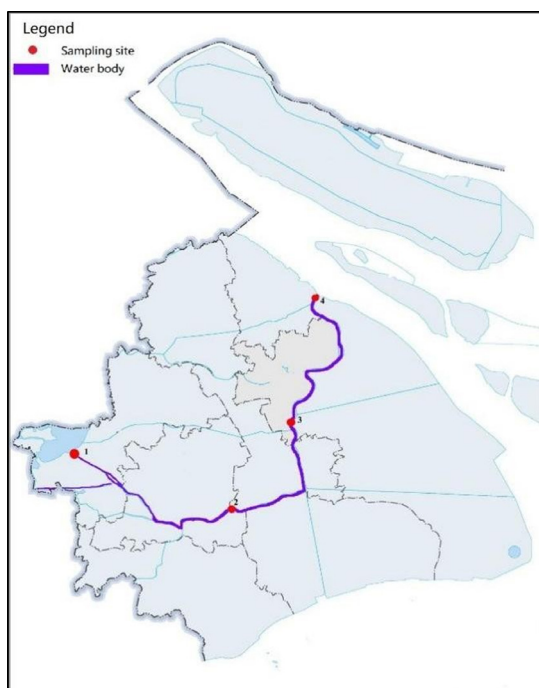


Figure 1: Map of surface water quality sampling sites in Huangpu River of Shanghai, China

PCA-APCS-MLR Model

The APCS-MLR is a receptor model integrating the two statistical methods of APCS and MLR. This model is suggested to quantify the contribution of pollution sources to water quality parameters in the basins based on the PCA model Thurston et al. (1985). The core idea of PCA is dimensionality reduction, which reduces a large number of indicators to a small number of indicators to represent the majority of original materials [12,25]. In order to identify potential factors affecting water quality, PCA was used to analyze each data group that the CA had indicated. By computing the covariance and principal components of separation (PCs), a linear combination of eigenvectors and original variables, PCA may assess the degree of dispersion in water quality data. Closely related to PCA, factor analysis (FA) can be applied in a variety of ways to polarize the loadings of the original variables and obtain new factors, called varifactors (VFs), that more effectively explain the potential information contained in the original variables [26,27].

The data must first be examined for goodness-of-fit to the log-normal distribution using Kolmogorov-Smirnov (K-S) statistics before doing PCA. All of the variables prepared for PCA had log-normal distributions with confidence levels greater than or equal to 95%, according to K-S statistics. To determine whether

the data in this study were suitable for PCA, Kaiser-Meyer-Olkin (KMO) and Bartlett's Test of Sphericity statistical analyses were carried out [8,28,29]. Absolute factor loadings [0.30-0.50], [0.50-0.75], and > 0.75 were considered to be weak, moderate, and strong loadings, respectively. The greater the absolute value of load, the stronger the correlation between water quality parameters and principal components, and the positive and negative signs indicate the positive and negative correlation between them [30].

Principal Component Analysis

PCs are expressed as follows:

$$Z_{ij} = a_{i1}x_{1j} + a_{i2}x_{2j} + \dots + a_{in}x_{nj}$$

where Z is the component score; a is the component loading; x is the measured value of the variable; i is the component number; j is the sample number; and n is the total number of variables. Absolute principal component score-multiple linear regression (APCS-MLR) Principal Component Scores (PCS) calculated by PCA were converted to absolute principal component scores (APCS); then the source contributions to pollutant concentrations could be calculated by using multiple linear regression (MLR):

$$\bar{C}_i = r_{oi} + \sum_{j=1}^n r_{ji}A_{ji}$$

where r_{oi} is the multiple regression constant term for the i pollutant, which means the contribution of the i pollutant from the sources cannot be explained by PCs derived from PCA, r_{ji} is the regression coefficient of the j source for the i parameter, and $r_{ji}A_{ji}$ is the contribution of the j source to the i parameter. The mean value of $r_{ji}A_{ji}$ for all samples represents the mean contribution of the j source. Although the sources represented by the APCS-MLR model can have negative influence on water quality indicators, the Environmental Protection Agency's (EPA) Unmix and PMF models with non-negative restrictions might be perplexing when they show contributions from several sources. According to Gholizadeh et al. (2016), negative contributions can be changed into positive ones in the following ways to help with the quantitative evaluation of source contributions [18]:

$$R_j = \frac{|S_j|}{|S_1| + |S_2| + |S_3| + \dots + |S_n|} \times 100\%$$

where R_j is the contribution ratio of the j source; and $S_1, S_2, S_3,$ and S_n are the contributions of the first, second, third, and n sources, respectively.

RESULTS AND DISCUSSION

Temporal and Spatial Variations in Water Quality

Overall, NH_3-N , TN, and TP are all significant indicators of eutrophication, COD_{Mn} is one of the primary indicators of organic pollution in water bodies, DO is essential for aquatic life and is recognized as a fundamental marker of water quality, and NTU, EC, and pH are significant physicochemical indices [25].

Basic statistics of physicochemical variables of water quality in Huangpu River of the four sampling sites within 5 months are presented in **Table 1**. Generally, TN had relatively high levels compared to National Surface Water Quality Standard of China (GB3838-2002), worse than the Grade V, the mean concentrations of COD_{Mn}, NH₃-N, TP were Grade II of the standard, and DO was Grade I. Only the TN concentration was very poor, indicating that agricultural non-point source pollution is likely to be the main cause of pollution in this river. concentrations ranged from 1.75 mg/L to 4.66 mg/L in 12 months, the mean TN concentration was 2.61 mg/L exceeding the Grade V of the National Surface Water Quality Standard of China (GB3838-2002). The highest mean TN (4.17 mg/L) appeared from January to March. The TN concentration fluctuated greatly in the first 3 months, then decreased gradually from April, and then increased from July to September. TP concentrations were basically stable throughout the year, except for September reached the highest of 0.25 mg/L, mean concentration of TP was 0.15 mg/L within Grade of water quality standard. The mean concentrations of COD_{Mn} and NH₃-N met the Grade II of water quality standard (3.38 mg/L and 0.23 mg/L). Mean concentrations of COD_{Mn} during August to October (August 4.05 mg/L, September 3.70 mg/L, October 4.15 mg/L) were slightly higher than those during the other months, while mean concentrations of NH₃-N during September (0.07 mg/L) and October (0.09 mg/L) were lower. However, it should be noted that NH₃-N in some month is very close to Grade I of the standards (0.15 mg/L). Throughout the year, mean concentrations of COD_{Mn} and TP of Wusongkou water were not fluctuated much, while mean concentrations of NH₃-N and TN fluctuated greatly from January to March.

Table 1: Statistical descriptions of the Huangpu River's water quality (Arithmetic Mean [Mean], Standard Deviation [SD], Coefficient of Variation [CV], and grade of water quality [grade])

Parameters	Mean	SD	CV	Grade
WT(°C)	14.71	5.04	0.34	-
pH	7.77	0.5	0.06	
DO	8.46	1.59	0.19	I
EC/(μS/cm)	623.35	71.36	0.11	-
NTU	96.34	69.27	0.72	-
COD _{Mn} /(mg/L)	3.92	1.72	0.44	II
NH ₃ -N/(mg/L)	0.26	0.18	0.69	II
TP/(mg/L)	0.1	0.04	0.43	II
TN/(mg/L)	3.34	1.49	0.45	worse than V

PCA-APCS-MLR Model

The number of data samples in this study complied with Thurston and Spengler's (1985) recommendation that the degree of freedom of the data set should be greater than 50 in order to get a reliable PCA/FA outcome. Bartlett's p-value for sphericity was 0.000 and the KMO value was 0.629, both of which showed that there were significant correlations between the input parameters. Therefore, source identification in this investigation was attainable using PCA/FA. The first five VFs were obtained in accordance with Kaiser's criteria (eigenvalue great-

er than 1), and they accounted for 86.2% of the total variance. It shows the loadings of each parameter in the five VFs (**Figures 2-3**). The first VF (VF1) showed strong positive loadings (> 0.750, 0.863) on DO, moderate positive loading on NH₃-N (> 0.50, 0.625), and a strong negative loading on WT (< -0.750, -0.958), accounting for 31.6% of the total variance. DO is determined by WT, the NH₃-N concentration is affected by WT. Indeed, nitrification reaction accelerates the consumption of ammonia nitrogen when the temperature rises, which leads to a decrease in NH₃-N concentration in the water environment [31]. Thus, VF1 might represent meteorological sources.

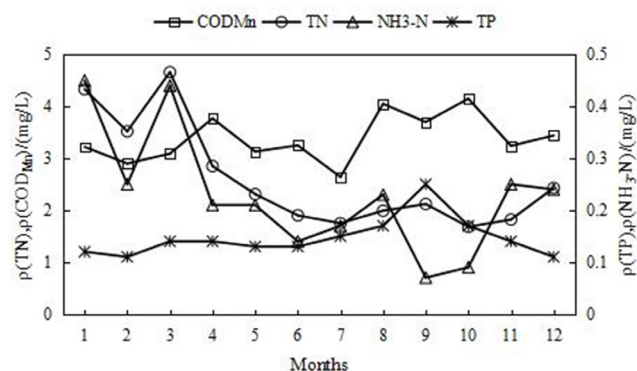


Figure 2: Temporal characteristics of water quality in Wusongkou ("4" sampling site) from January to December in 2021

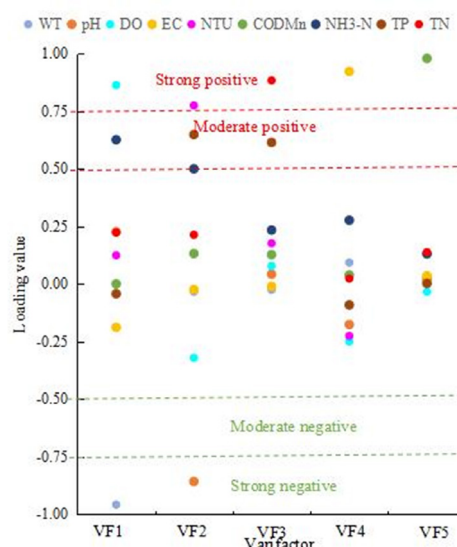


Figure 3: Component loadings for 9 variables following varimax rotation

The second VF (VF2), which occupied 25.9% of the total variance, showed a strong positive loading on NTU (0.775), a strong negative loading on pH (-0.858), and a moderate positive loading on TP (0.648) and NH₃-N (0.500). pH is affected by water temperature, the ion concentration, the activities of aquatic organisms, and the partial pressure of atmospheric carbon dioxide. NTU is calculated by insoluble substances of sediment, planktonic algae, corrosive matter, and colloidal particles suspended in water. Due to the domestic sewage discharge and its rich phosphorus and nitrogen into the water body, which will affect the NTU and pH of the water body, so VF2 could reflect the influence of industrial sewage? The third VF (VF3) accounted 11.4% of the total variance and showed a strong positive loading on TN (0.883) a moderate positive

loading on TP (0.614). TN and TP seem to be primarily more affected by manure and chemical fertilizer application than by domestic and industrial sewage. According to Wang L et al. VF3 could reflect the influence of the activities such as the application of fertilizers in agricultural activities [32]. The fourth VF (VF4) explained 9.9% of the total variance and showed a strong positive loading on EC (0.923). Water contains a variety of dissolved salts present in the form of ions. E is used to predict the total ion concentration or salt content in water [33]. This result indicates that VF4 was mainly related to salt ions in the water it may be attributed to natural ionic group sources from river inflow. Thus, VF4 might represent natural environmental sources. The fifth VF (VF5) explained 7.5% of the total variance and showed a strong positive loading on COD_{Mn} (0.979), and no other factors play strong or moderate relationships with VF5, so this result indicates that VF5 was mainly related to domestic sewage.

The APCS-MLR model was employed to determine the contribution ratio of each source and quantify its contribution to each water quality indicator based on the outcomes of source identification using PCA/FA. According to fig, the determination coefficient (R^2) between the parameters that were observed and those that were predicted ranged from 0.79 to 0.99, with a mean value of 0.87, demonstrating a satisfactory fit between the two values (Figure 4). The APCS-MLR model could therefore accurately estimate source apportionment [18,20,22]. The meteorological process (VF1) had a significant influence on DO, $\text{NH}_3\text{-N}$, and WT, with high contribution ratios for DO (81.9%), $\text{NH}_3\text{-N}$ (40.2%), and WT (39.9%) (Figure 5). The largest contribution to NTU (30.2%) and TP (27.4%) came from industrial sewage (VF2). The contribution ratios from agricultural activities (VF3) application for TP, TN, and COD_{Mn} were 51.6%, 37.8%, and 14.5%, respectively. EC (10.6%) and NTU (8.7%) were primarily caused by natural environmental sources (VF4) in water. Domestic sewage (VF5) made up 30.9% of COD_{Mn} 's contribution. However, the concentrations of some pollutants in the area are still high and additional treatment is needed. Therefore, local governments should take measures to control pollutant emissions from agriculture and industry to improve river water quality in the future [34-38].

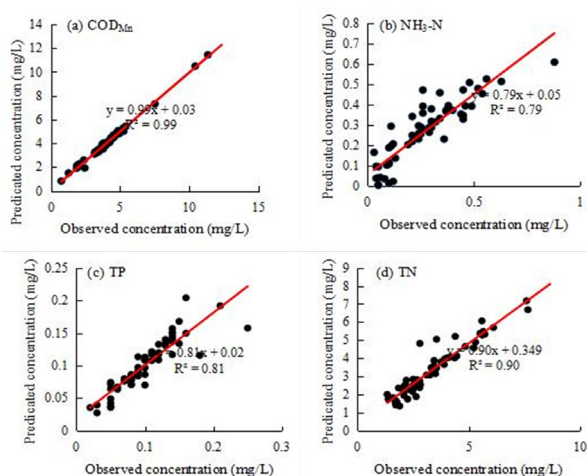


Figure 4: Scatter plots of observed and APCS-MLR-predicted concentrations of water quality

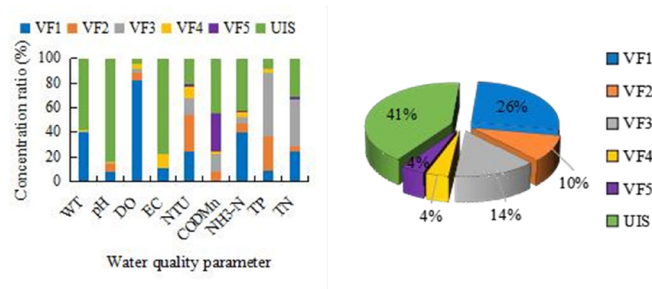


Figure 5: Effects of pollution sources on river water pollution calculated with the APCS-MLR model A) Contributions of sources to each water quality parameters. B) Average contributions of pollution sources

Limitations of this Study

This study involves certain uncertainties since the methods, as well as the data, are limited. Since the lack of water quality data, this study does not provide a clear picture of changes in the temporal scale of the main pollution sources. When further information is available, additional research will be required based on the factors mentioned above.

CONCLUSION

This study used PCA and correlation analysis to extract and identify potential pollution sources in the Huangpu River in Shanghai, China, and the APCS-MLR receptor model partitioned their contribution to each quality variable. Overall, TN was the most important pollution index in the river, which exceeded Class V of China's National Surface Water Quality Standard (GB3838-2002). The results showed that PCA/FA identified five factors responsible for river water quality degradation, accounting for 86.2% of the total variation. The average contribution of weather process, agricultural activity, industrial wastewater, natural environmental sources, and domestic wastewater was 26%, 14%, 10%, 4%, and 4%, respectively. In the Huangpu River, the main pollution sources shifted to weather processes, agricultural activities, and industrial sources, indicating that the area's ecological environment has improved after long-term pollution management and control. In consideration of this, the study provided the following recommendations for improving drainage systems, reinforcing livestock regulations, and reducing agricultural pollution in the study area.

STATEMENT OF ETHICS

This study was conducted following the ethical standards of the Declaration of Helsinki, and the confidentiality of patients' data was respected. Written informed consent was obtained from the participant.

PATIENT CONSENT

The patient has given consent for possible publication of this case report.

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CONFLICT OF INTEREST STATEMENT

No conflict of interest to disclose.

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None.

AUTHOR CONTRIBUTION

All the authors contributed to the study's development. All the authors have reviewed the statistical analysis and validated the manuscript's final version.

DATA AVAILABILITY STATEMENT

All data generated or analysed during this study are included in this article. Further enquiries can be directed to the corresponding author.

PROVENANCE AND PEER REVIEW

Not commissioned, externally peer reviewed.

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