

Distribution and ecological risk of Iodinated and Gadolinium-based contrast agents in an impacted basin of central Mexico

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Abstract

Iodinated X-ray contrast media (ICM) and Gadolinium-based contrast agents (Gd-CAs) are extensively used in medical imaging and are excreted unchanged by patients. However, conventional wastewater treatment plants (WWTPs) are ineffective at removing these compounds, leading to their discharge into surface waters, where they persist due to their recalcitrant nature. Although the presence of both groups of contrast agents in the aquatic environment has been documented, data on their co-occurrence, distribution, and ecological risk in freshwater systems remain scarce. This study addresses this knowledge gap by providing the first comprehensive assessment of the co-occurrence, spatial distribution, and ecological risks of ICM, specifically amidotrizoic acid (DIA), iomeprol (IOM), iopamidol (IOD), and iopromide (IOP), as well as anthropogenic Gd (Gd_{anth} , encompassing all Gd-CAs), in the surface waters of the Atoyac River basin in Mexico. Concentrations of these contaminants ranged from 6.38 ng L^{-1} for Gd_{anth} to $3,700 \text{ ng L}^{-1}$ for IOP, with the highest levels measured near the WWTP discharge sites and areas with a high density of medical facilities. Elevated concentrations were also observed in river sections with fewer upstream medical facilities, suggesting additional sources or transport mechanisms. In the reservoir, the concentrations of IOD and IOP were high across nine sites, ranging from $261.10 \pm 61.20 \text{ ng L}^{-1}$ to $412.20 \pm 48.50 \text{ ng L}^{-1}$. This finding highlights their persistence and resistance to biodegradation in aquatic environments. Interestingly, while ICM and Gd-CAs are released into the river from medical facilities, they did not co-occur in the river waters, indicating distinct environmental behavior and/or sources. Finally, deterministic ecological risk assessments revealed that contrast agents pose no ecological risk to aquatic species. This study is the first to document the co-contamination of ICM and Gd-CAs in river waters and to evaluate their associated ecological risks, providing critical insights into the environmental presence of these medical imaging agents.

Keywords: Iodinated X-ray contrast media, Gd-based contrast agents, anthropogenic Gd, ecological risk assessment, Atoyac River

1. Introduction

Iodinated X-ray contrast media (ICM) and Gadolinium-based contrast agents (Gd-CAs) are a group of chemicals widely used in medical imaging procedures, enabling better visualization of internal organs, blood vessels, and soft tissues (Cheng et al., 2023), as well as identifying neoplastic, inflammatory, and functional abnormalities (Brünjes and Hofmann, 2020). Gd-CAs are stable, hydrophilic organic compounds featuring Gd^{3+} ions at their core, commonly used in gadolinium-enhanced magnetic resonance imaging (MRI) to increase image quality and diagnostic accuracy (Zhang et al., 2024), whereas ICM are commonly used for X-ray imaging of soft tissues. Although the dose of ICM and Gd-CAs administered to the patient vary depending the type of examination (Sengar and Vijayanandan, 2021), the injected dose in a single examination can reach up to 200 g/person per day for ICM (Cheng et al., 2023; Lehmann et al., 2022) and range from 0.03 to 0.1 mmol kg^{-1} for Gd-CAs (Brünjes and Hofmann, 2020; Ibrahim et al., 2018). However, these agents are not metabolized (Brillantino et al., 2020) and are thus excreted intact by patients through feces and/or urine within a few hours (Gao et al., 2023). In freshwater systems, Gd-CAs are often referred to as “anthropogenic Gd (Gd_{anth})”, a term that neither implies the transformation of Gd-CAs nor distinguishes between Gd-CAs and their transformation products (Brünjes and Hofmann, 2020). The geochemical cycling of Gd_{anth} is very similar to that of naturally occurring Gd, with the primary difference being their respective sources (Zhang et al., 2024). Therefore, rare earth elements (REEs) are used to estimate the concentration of natural Gd, and consequently, the levels of Gd_{anth} in freshwater environments. Due to their strong chemical stability (Frenzel et al., 2015; Gao et al., 2023), high hydrophilicity (England et al., 2024; James et al., 2023; Zhang et al., 2019), and resistance to removal in conventional wastewater treatment plants (WWTPs) — a result of poor adsorption onto biosolids and resistance to biological degradation —, contrast agents (including both groups ICM and Gd-CAs) are continuously introduced into surface waters via wastewater effluents (Frenzel et al., 2015; Kulaksız and Bau, 2007; Oluwasola et al., 2022; Ternes and Hirsch, 2000; Watanabe et al., 2016; Xu et al., 2017; Yan et al. 2024). Once in surface waters, they can easily diffuse and be transported due to their high solubility, non-volatility, and persistence (Cheng et al. 2023; Zhang et al. 2019). Consequently, these contaminants have been detected in freshwater environments, such as rivers, lakes, and groundwater, with concentrations ranging from 1.4

ng L⁻¹ to 13.0 µg L⁻¹ (Sengar and Vijayanandan, 2021) for ICM and from 0.1 ng L⁻¹ to 585 ng L⁻¹ for Gd_{anth} (Brünjes and Hofmann, 2020; De Paula Marteleto and Enzweiler, 2021). Despite the recalcitrant nature of these contaminants and the fact that ICM can account for up to 80% of the total pharmaceutical mass load in hospital effluents (Sengar and Vijayanandan, 2021), the occurrence and distribution of ICM and Gd_{anth} in freshwater environments have only been documented in few locations worldwide, including China (Cheng et al., 2023; Gao et al., 2024; Liu et al., 2024a; Xu et al., 2017, Cheng et al., 2025), Vietnam and the Philippines (Watanabe et al., 2016), Germany (Kulaksız and Bau, 2011a; Muenze et al., 2017), Switzerland (Kormos et al., 2011), Brazil (Amorim et al., 2019; De Paula Marteleto and Enzweiler, 2021), Australia (Lawrence, 2010), Austria and Hungary (Kreitsmann and Bau, 2023), and Korea (Lim et al., 2023). Therefore, these compounds are among the least-studied pharmaceutical contaminants globally.

Among ICM, only iopromide (IOP) has been classified as an environmental hazard under the Globally Harmonized System (GHS), labeled with H400 and H410, indicating very high toxicity to aquatic life with long-lasting effects (PubChem, 2025). Moreover, ICM are designed to be biologically inert and thus are expected to exhibit low ecotoxicity (Escudero-Oñate et al., 2017). In this regard, to the best of our knowledge, only a limited number of studies have evaluated this assumption. For example, Steger-Harmann et al. (1999) conducted a series of ecotoxicological tests and found no acute toxic effects of IOP at concentrations up to 10 g L⁻¹ in bacteria (*Vibrio fischeri*, *Pseudomonas putida*), algae (*Scenedesmus subspicatus*), crustaceans (*Daphnid magna*), and fish (*Danio rerio*, *Leuciscus idus*). Similarly, no chronic toxicity was observed in *Daphnid magna* at concentrations up to 1 g L⁻¹. Furthermore, the calculated risk quotient (RQ) of these compounds, considering a standard assessment factor of 100, was extremely low (0.0002), suggesting that IOP poses no significant environmental risk under typical exposure conditions (Steger-Harmann et al., 1999).

Owing to the scarcity of toxicity data, the ecological risk assessments of these compounds in freshwater environments remain limited, with only a few studies conducted globally (Daouk et al., 2016; Kötke et al., 2024; Liu et al., 2020, Sanderson et al., 2003). In general, risk evaluation have primarily conducted using the RQ deterministic approach, based on available toxicity data for specific aquatic species. Although this approach provides

a straightforward method for estimating risk, it has limitations because it does not account for variability and uncertainties in environmental exposure and toxicity data, nor consider population-wide risk factors. Instead, it relies on dose-response toxicity data specific to particular species (Domínguez-Mariani et al., 2004; Dueñas-Moreno et al., 2024a; Rodríguez-Bolaña et al., 2024). Thus, due to the lack of extensive toxicity data for these contrast agents, this approach offers a preliminary assessment of their potential ecological risks. Nevertheless, although ICM are generally considered to pose low acute toxicity to aquatic organisms even at high concentrations, their environmental persistence, bioaccumulation potential, and transformation into potentially harmful byproducts highlight as critical gaps in understanding their long-term ecological risks.

The Atoyac River, located between the states of Puebla and Tlaxcala, is one of the most anthropogenically impacted water bodies of Mexico (CONAHCYT, 2023; Mora et al., 2021). Its surface waters are heavily contaminated by organic and inorganic pollutants, primarily due to the discharge of untreated or inadequately treated urban and industrial wastewater (Mora et al., 2021). Among the sources of contamination, there are the medical facilities that release pharmaceutical compounds (Vázquez Tapia, 2023), including ICM and Gd-CAs. With over 300 medical facilities in Puebla and Tlaxcala (Puebla 2025; Tlaxcala 2015), many of which are situated along the Atoyac River or its tributaries, the contamination of the river is severe. This is particularly concerning given its use for agricultural irrigation and the prevalence of illegal fishing in areas such as the Valsequillo Reservoir (Domínguez-Mariani et al., 2004; Dueñas-Moreno et al., 2024b; Pérez Castresana et al., 2018). Despite these critical issues, there is a notable lack of data on the occurrence and distribution of ICM and Gd-CAs in the Atoyac River and in Mexico as a whole. Furthermore, no prior study has investigated the simultaneous co-contamination and spatial distribution of these two groups of contrast agents in freshwater environments. This knowledge gap is significant, as both groups of contrast agents can persist in the environment and are poorly removed by conventional wastewater treatment processes. Therefore, the analysis of their co-occurrence and spatial patterns can help to improve the understanding of cumulative contamination load, distinguish overlapping sources of pollution, evaluate potential compound interactions, and identify localized hotspots of medical pollution. Such insights are important for informing

environmental risk assessments and guiding targeted mitigation strategies, particularly in highly impacted river systems like the Atoyac River.

Given that both ICM and Gd-CAs originate from similar sources, such as hospitals, laboratories, and medical facilities, we hypothesized that they may co-occur in wastewater-receiving surface waters. Among the ICM, IOP, iopamidol (IOD), iomeprol (IOM), iohexol (IOH), ioversol (IOV), and iobitridol (IOB) are commonly used in medical facilities in the states of Puebla and Tlaxcala (IMSS, 2024), as well as throughout Mexico (Nava et al., 2008). However, this study focused on the occurrence of Gd-CAs, IOM, IOD, IOP, and amidotrizoic acid (DIA) in surface waters of the Atoyac River basin. Although IOH, IOV, and IOB are frequently used in diagnostic imaging globally (Seong et al., 2013, Pinyopornpanish et al., 2025, Kim et al., 2022, Jensen et al., 2011; Lerondeau et al., 2016; Gamboa et al., 2022; Baldo and Pham et al., 2021), these compounds were not measured. However, this does not compromise the validity or relevance of this study, because this is the first effort in evaluating the co-occurrence and co-contamination of two different groups of contrast agents (ICM and Gd-CAs) in a critically impacted watershed. As the first study of its type, our targeted approach provides a foundational understanding of ICM and Gd-CAs occurrence in a region of Mexico and supports the development of future and more comprehensive monitoring efforts that may include a broader range of compounds.

Hence, this study aimed to address the abovementioned gaps by investigating the co-occurrence, co-contamination, and spatial distribution of selected ICM (IOM, IOD, IOP, and DIA) and Gd_{anth} in waters of the Atoyac River basin, a highly anthropogenically impacted region. Further to this, a preliminary ecological risk assessment was conducted using the RQ deterministic method to estimate the potential environmental impacts of these contaminants. The results of this study provide a valuable database to bridge the knowledge gap regarding contrast agent contamination in surface waters and offer critical insights for developing water quality criteria and improving wastewater treatment technologies capable of removing these contaminants in treated wastewater.

2. Material and Methods

2.1. Study area

The Atoyac River basin lies in central Mexico, within the states of Puebla and Tlaxcala. Spanning 4,130 km², it is located within the Trans-Mexican Volcanic Belt, bordered by three stratovolcanoes: Popocatepetl, Iztaccíhuatl, and Malinche. The basin is 2,160 m above sea level and its climate comprises a rainy season from May to October and a dry season from December to March, with average annual temperature and precipitation of 16.4 °C and 955 mm, respectively. The Atoyac River originates at the foothills of the Iztaccíhuatl Volcano. From there, the river flows through the Puebla-Tlaxcala valley with initially good water quality (Dueñas-Moreno et al., 2024a; Mora et al., 2021). However, as it flows, the river is heavily impacted by the discharge of untreated municipal and industrial wastewater. Its tributaries further contribute to the contamination, carrying substantial amounts of organic and inorganic pollutants (Martínez-Tavera et al., 2017; Pérez Castresana et al., 2018; Rodríguez-Espinosa et al., 2018). Before reaching the urban area of Puebla City, the Atoyac River joins with the heavily polluted Zahuapan River, which flows from the Tlaxcala state and is the main tributary of the Atoyac River (**Fig. 1**). Before the confluence, the polluted water from both rivers is used to irrigate agricultural lands. Downstream Puebla City, the river splits, with one branch supplying irrigation water to agricultural lands in Ocoyucan Municipality, while the main branch flows into the Valsequillo Reservoir. This reservoir stores excess water during the rainy season and later distributes it downstream to Irrigation District “030-Valsequillo”.

The Atoyac River is also impacted by wastewater from medical facilities. Although most hospitals treat their effluents or discharge them into urban channels for further treatment in municipal WWTPs, the processes in these plants are insufficient to remove pharmaceutical compounds. Therefore, these compounds are discharged into the Atoyac River mainstream, being their final fate the Valsequillo reservoir, the peri-urban croplands irrigated with polluted river waters, and probably, the groundwater of the irrigated area.

2.2.Sampling

To assess the contribution of hospitals to the presence of contrast agents in waters of the Atoyac River basin, 29 surface water samples were collected in April 2022. These were collected from various locations, including the Atoyac River before its confluence with the Zahuapan River (seven samples), the Zahuapan River itself (six samples), and the Atoyac River after the confluence (seven samples). In addition, nine surface water samples were collected in the Valsequillo Reservoir (**Fig. 1**). The samples were collected at approximately 0.5 m depth from the middle of the river watercourse and transferred to 1 L amber glass bottles. The bottles were placed in ice-filled coolers, transported to the laboratory, and stored at 4 °C. Physicochemical parameters, including temperature, pH, dissolved oxygen (DO) concentrations, electrical conductivity (EC), and total dissolved solids (TDS) concentrations, were measured *in situ* using a pre-calibrated YSI Pro-Quatro multiparameter instrument (Xylem, USA). The concentrations of SO_4^{2-} , NO_3^- , and NH_4^+ were measured by ion chromatography, whereas the chemical oxygen demand (COD) was measured within 24 hours of sample collection, following the APHA 5220-D method ([APHA, 2017](#)).

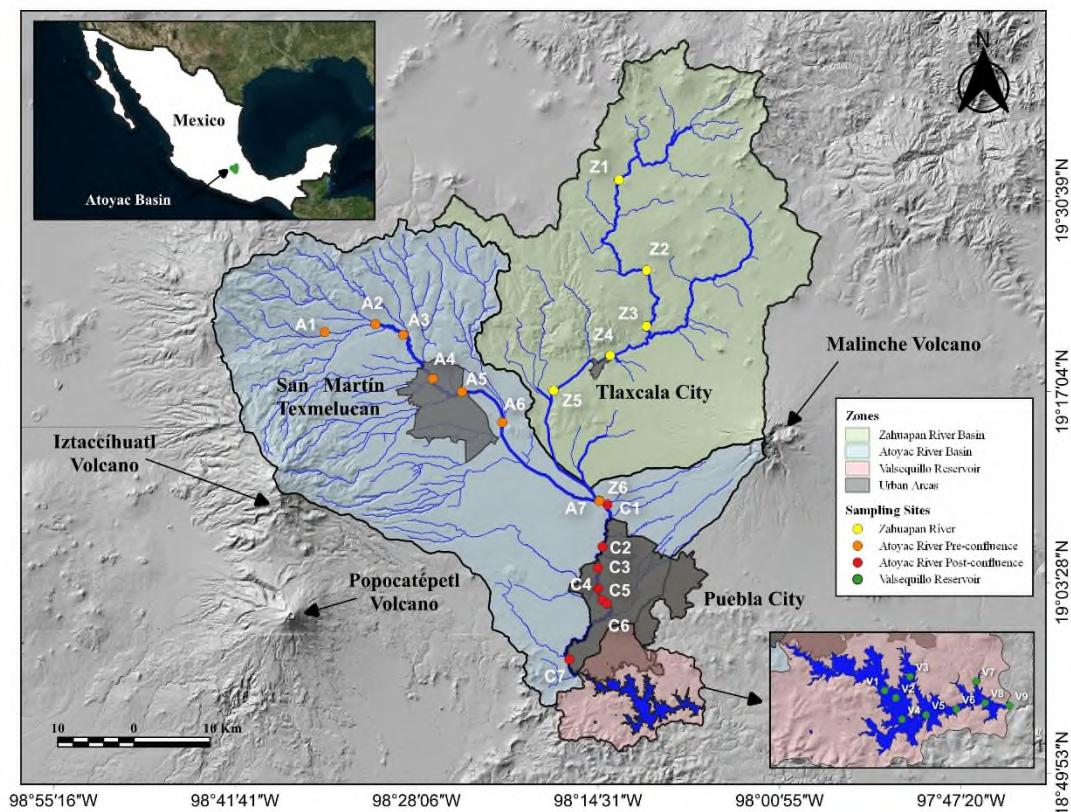


Fig. 1. Map of the Atoyac River basin illustrating the sampling sites

2.3. Sample analysis

2.3.1. Iodinated Contrast Media (ICM)

The water samples for ICM measures, including IOM, IOD, IOP, and DIA, were analyzed at the TZW: DVGW Technology Water Center in Germany. In brief, these contrast media were quantified by single-sample analysis using high-performance liquid chromatography with tandem mass spectrometry (HPLC/MS-MS) following the DIN EN ISO 21676:2022–01 method ([DINENISO21676:2022-01, 2022](#)) by direct measurement using an in-line injection system (ILIS), which corrects the error due to the injection volume. IOD-d3, DIA-d6, desmethoxy IOP, and IOM-d3 (10.0 μL of a 0.10 mg L^{-1} solution in methanol) were added as internal standards. The analysis was conducted using an HPLC-system 1290 from Agilent with an API 6500+ Qtrap mass spectrometer from Sciex. The analytical column used was a Kinetex 2.6 μm EVO C18 (100 $\text{\AA}$, 150 x 2.1 mm) from

Phenomenex. An injection volume of 100 μL was analyzed with a flow rate of 0.25 mL min^{-1} . In addition, 1 mM aqueous ammonium acetate solution with 0.1% formic acid and 1 mM ammonium acetate in methanol with 0.1% formic acid were used as eluents. The mass transitions used for identification and quantification of the ICM were m/z 631.7 $\rightarrow$ 360.9 and 631.7 $\rightarrow$ 233.0 for DIA, m/z 777.6 $\rightarrow$ 686.5 and 777.6 $\rightarrow$ 404.8 for IOM, m/z 777.6 $\rightarrow$ 558.8 and 777.6 $\rightarrow$ 386.9 for IOD, and m/z 791.6 $\rightarrow$ 572.8 and 791.6 $\rightarrow$ 558.7 for IOP. Only if the retention time was correct and both mass transitions yielded the same quantitative result within a range of less than 10%, the compound was regarded as identified and the quantitative results were reported. It is important to mention that for IOP two peaks were obtained, and both peaks were used for quantification. A typical chromatogram highlighting the retention time and the peaks for IOD, IOM, IOP, and DIA during the analysis is presented in the Supplementary Material, **Fig. S1**.

The Quality Assurance and Quality Control (QA/QC) process included comprehensive method validation to ensure reliable and accurate results. Key aspects of validation involved assessing recovery rates from extraction procedures, calibration linearity, measurement precision, reproducibility, and matrix effects. Standards for calibration curves and QA/QC samples were prepared from a 1 mg L^{-1} certificate solution (in methanol) from Campro Scientific (Berlin, Germany). These were prepared by adding an aliquot of this solution to Milli-Q water. Linearity was checked in a concentration range between 10 and 1,000 ng L^{-1} . In this range, the calibration was found to be linear with a correlation coefficient ≥ 0.999 for all measured ICM. Limits of detection (LOD) were determined following the German standard DIN 32645:2008–11 ([DIN32645:2008-11, 2008](#)). The precision was assessed through the relative standard deviation (RSD), which was calculated from the results of a five-fold analysis of several samples at concentrations of 50 ng L^{-1} . To correct intensity variations, several samples were spiked with internal standards. Overall, twenty samples were run in each batch, with a QA/QC sample (a spiked sample with defined concentration) at the beginning and end of each batch. As a rule, the variation in concentration of these samples was less than 10%. Each measurement sequence also incorporated calibration with analytical standards across ten calibration points. In addition, blanks (Milli-Q water without the target analyte) were analyzed within each sequence. The results of these quality control samples were monitored using control charts to ensure instrument stability over time. During

the method validation, it was proven that matrix effects were of minor relevance. The values of the LOD, limits of quantification (LOQ), and the RSD (%) determined for ICM during the analysis are reported in the Supplementary Material, **Table S1**.

2.3.2. Rare Earth Elements (REEs), Al, and Fe

The analysis of Al, Fe, and REEs was conducted at Actlabs in Ancaster, Canada. Unfiltered water samples (100 mL) underwent aqua regia digestion in the laboratory, using 2 mL of concentrated HNO₃ and 5 mL of concentrated HCl. The mixture was heated to 90 °C until the sample volume was reduced to approximately 15–20 mL, following the guidelines of USEPA Method 3005A (USEPA, 2024). Once digested, the samples were filtered using Whatman 41 filters and diluted to a final volume of 100 mL with deionized water. The processed samples were then analyzed using a Perkin Elmer Sciex ELAN 9000 ICP-MS instrument. Calibration and instrument accuracy were verified by measuring blank samples and standard solutions alongside the test samples. All blank samples showed values below the detection limits for each element tested. The detection limit for all REEs was 1.0 ng L⁻¹.

2.4. Calculation of anthropogenic Gd

Gd_{anth} represented the total of all Gd-CAs that are present in waters of the Atoyac River basin. Since Gd_{anth} relies on total Gd for its estimation, it was calculated only in the water of the Atoyac River (A1–A7 and C1–C7), where Gd was detected. For this, the REE patterns were normalized to Post-Archean Average Australian Shale (PAAS) (McLennan, 1989). In the REE shale-normalized distributions (REE_{SN}), the presence of Gd_{anth} is indicated by a distinct positive anomaly or deviation in Gd concentrations compared to those of other REEs. In this study, the Gd anomalies (Gd_{SN}/Gd_{SN}^{*}) were interpolated from the shale-normalized concentrations of two neighboring REEs (Sm and Nd), as depicted in the **Eq. 1**. The use of Sm and Nd results in lower Gd_{SN}/Gd_{SN}^{*} ratios compared to those obtained using the traditional Sm and Tb approach; however, this former approach provides a more representative estimate of background Gd levels and yields values that more accurately reflect natural Gd concentrations (Kulaksız and Bau, 2007). Therefore, given the low Gd_{SN}/Gd_{SN}^{*} ratios and the facts that Gd behaves similarly to light REEs (LREEs) and no heavy REEs (HREEs) were included in the estimation of background Gd (Kulaksız and Bau,

2011b), a positive Gd anomaly was identified by a $Gd_{SN}/Gd_{SN}^* > 1.0$. Using Gd_{SN} derived from Eq. 1, the natural background Gd concentration (Gd^*) was determined through Eq. 2. Then, Gd_{anth} was estimated through the Eq. 3.

$$Gd_{SN}/Gd_{SN}^* = Gd_{SN}/10^{(2 \log Sm - \log Nd)} \quad (1)$$

$$Gd^* = Gd_{SN}^* \times Gd_{PAAS} \quad (2)$$

$$Gd_{anth} = Gd_{total} - Gd^* \quad (3)$$

where SN is the PAAS-normalized value, * denotes the geological background value, and Gd_{PAAS} represents the Gd concentration in the PAAS (4.66 mg Kg⁻¹) (McLennan, 1989).

2.5. Potential Ecological Risk Assessment

Given the limited availability of experimental toxicity data for contrast agents (Steger-Hartmann et al., 1999; Borgmann et al., 2005; González et al., 2005), the ecological risk assessment in waters of the Atoyac River basin was conducted using the deterministic RQ approach. This assessment considered three trophic levels: fish, crustaceans, and algae. RQ values for each compound at each sampling site where they were detected, and for each trophic level, were calculated by dividing the measured environmental concentration (MEC) by the predicted no-effect concentration (PNEC). Since the discharge of contrast agents into river systems is a continuous process, chronic toxicity data were considered more appropriate for evaluating long-term ecological risks (Mendoza et al., 2015). Accordingly, PNEC values were derived from available chronic toxicity values (ChV) of contrast agents for aquatic species—fish, daphnid, and green algae—representing the previously mentioned trophic levels, applying an assessment factor of 10 to account for interspecies variability and ecosystem sensitivity (EC, 2003). The ChV were extracted from the Ecological Structure Activity Relationships Program (ECOSAR, version 2.2, USEPA) (ECOSAR, 2025), which estimates chronic toxicity for various aquatic organisms based on chemical structure and functional class. ECOSAR serves as a valuable tool for environmental risk assessment, particularly when experimental data are limited. The extracted ChV and the resulting PNEC for each compound and aquatic organism are listed in Table S2. Finally, the calculated RQ values were categorized as follows: low risk ($RQ < 0.1$), medium risk ($0.1 \leq RQ < 1.0$), and high risk ($RQ \geq 1.0$).

2.6. Statistical analysis

Nonparametric Spearman correlation analyses were conducted using Statistica 10.0 software to examine significant correlations between various contrast agents and measured physicochemical parameters. Sampling sites with values below the LOD for any given variable were excluded from individual pairwise correlation calculations. Results from this analysis were considered statistically significant at confidence levels of 95% ($p < 0.05$), 99% ($p < 0.01$), and 99.9% ($p < 0.001$).

3. Results and discussion

3.1. Water quality

The water quality of the Atoyac River basin was determined using field-measured physicochemical parameters, specifically pH, EC, DO concentration, and COD. The behavior of each of these parameters along the basin is shown in **Fig. 2 a-d** (refer to **Table S3** for data). Given the absence of urban settlements and industrial corridors at the first sampling sites of the Atoyac River (A1–A3) (**Fig. 1**), the physicochemical parameters indicated good water quality at those sites. However, just downstream of San Martín Texmelucan (A4), the Atoyac River shows signs of contamination due to the discharge of urban and industrial wastewater. Similarly, although the first sampling site of the Zahuapan River (Z1) appears pristine due to its distance from urban settlements and industrial areas, intensive agricultural and livestock activities significantly affect its water quality, as reflected in most of the physicochemical parameters (**Fig. 2 a-d**).

In general, pH values along these rivers ranged from 7.45 to 8.15 (**Fig. 2a**), with an increase of above 8.0 in some sites (Z3, A3, A4, C4, C5, and C7). This increase can be attributed to the discharge of poorly treated wastewater from several textile industries, which commonly contain dyes, alkalis, and other pollutants ([Martinez-Tavera et al., 2017](#)). Similarly, EC (ranging between $114.20 \mu\text{S cm}^{-1}$ and $1,341.0 \mu\text{S cm}^{-1}$) increased drastically downstream (**Fig. 2b**), likely due to the discharge of industrial wastewater and urban sewage, resulting in elevated levels of dissolved ions from both organic and inorganic waste ([Dueñas-Moreno et al., 2024b](#)).

Low COD values were observed at the initial sampling sites of the Zahuapan (Z1–Z3: 41.50 mg L⁻¹ – 52.0 mg L⁻¹) and Atoyac (A1–A4: 18.50 mg L⁻¹ – 29.50 mg L⁻¹) rivers (**Fig. 2c**). These sites are in rural areas with low population density, which likely contributes to the lower levels of organic and inorganic pollutants. However, COD levels increased markedly downstream, with higher values recorded at sites Z4 (138.50 mg L⁻¹) and A7 (239.50 mg L⁻¹). The most severe pollution, in terms of COD, was detected in the Atoyac River post-confluence with the Zahuapan River, where COD values ranged from 178.0 mg L⁻¹ to 1,608.50 mg L⁻¹. This sharp increase in COD levels after sites Z3 and A4 could be attributed to the presence of industrial corridors and urban centers along the riverbanks, including San Martín Texmelucan, Tlaxcala City, and Puebla City. These areas are home to industries such as polymer manufacturing, textiles, automotive components, electronics, and chemicals, many of which discharge untreated or poorly treated wastewater directly into the river. The highest COD value was recorded at site C3 (1,608.50 mg L⁻¹), significantly exceeding the downstream average of 193.20 ± 19.30 mg L⁻¹ (C1–C7 excluding C3). This peak may be the result of a specific industrial discharge upstream of site C3 during sampling. Notably, COD levels dropped substantially at site C4 (166.50 mg L⁻¹), likely due to dilution by inputs of other tributaries. Previous reports have also highlighted the declining water quality in this sector of the river, which has deteriorated year after year, underscoring the urgency of addressing pollution from industrial and urban sources (Covarrubias-López et al., 2023; Hernandez-Ramirez et al., 2019; Martinez-Tavera et al., 2017; Mora et al., 2021; Muñoz-Nava et al., 2012; Pérez Castresana et al., 2018).

The concentrations of DO decreased drastically downstream of both rivers (**Fig. 2d**), especially in the Atoyac River, where DO levels dropped from 8.38 mg L⁻¹ to 0.30 mg L⁻¹. In the Zahuapan River, the DO concentrations were already low at the first sampling site (2.33 mg L⁻¹), likely due to upstream agricultural and livestock activities near Z1. However, the discharges of industrial and municipal wastewater along the waterway are likely contributing to the further decrease in DO, with concentrations dropping to 0.61 mg L⁻¹ near the confluence with the Atoyac River. Downstream the confluence, the anoxic conditions remain in the river, with values ranging between 0.39 mg L⁻¹ and 1.27 mg L⁻¹. The anoxic conditions of both rivers are linked to high oxygen consumption due to the aerobic bacterial degradation

of organic matter in wastewater, which exceeds the reaeration rates (Dueñas-Moreno, et al. 2024b).

Although the Valsequillo Reservoir receives poor-quality water from the Atoyac River, its high hydraulic retention time (321 days) (Tabla-Hernandez et al., 2020) allows it to function as a waste stabilization pond, degrading some organic pollutants. This resulted in a COD reduction of up to 3.5-fold (from 87.0 mg L⁻¹ to 25.0 mg L⁻¹) and an 18.1-fold increase in DO concentrations (from 0.10 mg L⁻¹ to 1.81 mg L⁻¹) throughout the reservoir. However, despite the increase in DO, it remained low (1.72 mg L⁻¹ near the dam wall) due to the small turbulence of surface waters, which limits the water–atmosphere interaction and consequently, the oxygen dissolution. In addition, the decomposition of organic matter accumulated in the reservoir, as well as the nutrient loads coming from agricultural runoff and wastewater discharges in the area, can deplete the DO because microorganisms consume it to break down organic material (Mangas-Ramírez and Elías-Gutiérrez, 2004; Mora et al., 2021).

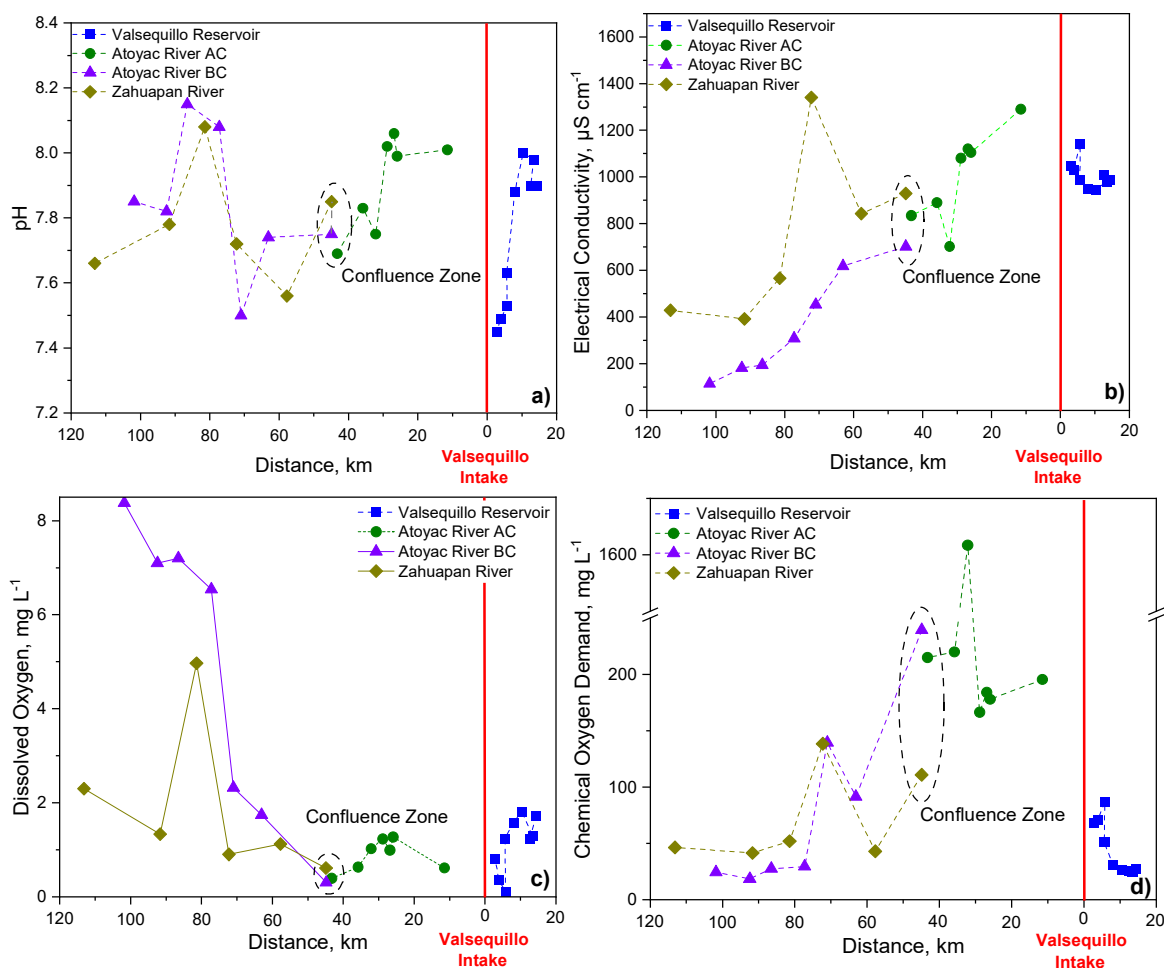


Fig. 2. Spatial distribution of pH (a), EC (b), DO (c), and COD (d) in surface waters of the Atoyac River. The x-axis indicates the distance of each sampling site from the entrance of the Valsequillo Reservoir.

3.2. Occurrence of Al, Fe, and REEs in waters

Gadolinium is part of the REEs group and can be found in surface water due to the water-rock interaction (Qian et al., 2022). However, the natural signature of this element in contaminated water bodies may be altered due to the widespread use of Gd-CAs in magnetic resonance imaging exams, which contaminate surface waters receiving wastewater effluents from medical facilities (Brünjes and Hofmann, 2020; De Paula Marteleto and Enzweiler, 2021; Inoue et al., 2020). Therefore, the total amount of Gd in anthropogenically impacted surface water comprises Gd^* and Gd_{anth} , being the last mainly related to Gd-CAs (Zhang et

al. 2024). The concentrations of Al, Fe, and REEs along the studied rivers, as well as the Gd anomalies (Gd_{SN}/Gd_{SN}^*), Gd^* , Gd_{anth} , and their relative proportion compared to total Gd ($\%Gd_{anth}$), are displayed in **Table S4**. According to the results, Al and Fe, along with Gd, were mostly detected in the sampling sites of the Atoyac River pre- and post-confluence, suggesting a significant co-occurrence of these three elements in river waters. This is supported by the strong significant positive correlations found between Gd and Al ($r = 0.85$ and $p < 0.001$) and between Gd and Fe ($r = 0.70$ and $p < 0.01$), as depicted in **Fig. 3a**. This co-occurrence can be attributed to the mineral colloids of Fe and Al (Fe- and Al-oxyhydroxides), which strongly scavenge REEs due to their large specific surface area (De Moraes and Ladeira, 2021; Liu et al., 2024b). Additionally, the adsorption capacity of these mineral colloids increases significantly with the pH and the organic matter content in waters (Han et al., 2023; Mora et al., 2020), which are intrinsic features of the studied rivers. In general, these findings are consistent with studies on the co-occurrence of REEs with Al and Fe in waters, concluding that Fe and Al mineral colloids play an important role in the abundance and transport of REEs (Han et al., 2023; Mora et al., 2020; Pietralonga et al., 2017; Pokrovsky et al., 2006; Verplanck et al., 1999).

Regarding the occurrence of all REEs, middle REEs (MREEs, including Sm, Eu, Gd, Tb, Dy, and Ho) and HREEs (including Er, Tm, Yb, and Lu) were not detected in the Zahuapan River, except for Dy and Er, which were found at site Z4, along with Fe and Al. This may be related to the low suspended load transported by the Zahuapan River, which in turn depends on the river flow. In fact, the average lower flow rate of the Zahuapan River ($1.28 \text{ m}^3 \text{ s}^{-1}$) (CONAGUA, 2020a), compared to that of the Atoyac River before and after confluence (from $2.21 \text{ m}^3 \text{ s}^{-1}$ to $3.88 \text{ m}^3 \text{ s}^{-1}$, respectively) (CONAGUA, 2020b), may favor the sedimentation of suspended sediments, which may contain considerable amounts of inorganic and organic material, including Al- and Fe-oxyhydroxides and associated MREEs and HREEs.

In the Valsequillo reservoir, almost all REEs were not detected in surface water, with only a few LREEs (La, Ce, and Nd) quantified at several sites (V2, V3, and V8). Fe and Al were only detected at site V3, suggesting that sedimentation of organic and inorganic material determines the abundance of these elements in those lentic waters. Despite the high amount of organic and inorganic material received by this reservoir (up to 24.31 ton d^{-1}) (CONAGUA

2020a; 2020b), the extended residence time and low flow (Tabla-Hernandez et al., 2020) may promote the sedimentation of this material (including silts, clays, sands, oxyhydroxides, and particulate organic matter), thereby limiting the presence of Al, Fe, and REEs in surface waters.

3.3. Anthropogenic Gd

The REE_{SN} in surface waters of the Atoyac River basin are shown in **Fig. 3b**. Since the measured REE concentrations in the Zahuapan River and Valsequillo Reservoir were below the LOD at almost all sampling sites (**Table S4**), the diagrams of these river sections were not included. According to the results, these diagrams show a slight positive Gd anomaly at sampling sites A6, A7, C2, C3, C4, C5, C6, and C7, with Gd_{SN}/Gd_{SN}^* values ranging from 1.02 (C1 and C7) to 1.27 (A6). Although several authors have suggested that Gd anomalies close to 1.0 indicate the absence of Gd_{anth}, other studies propose that the presence of Gd_{anth} can be considered when Gd anomalies are greater than 1.0, particularly when using Sm and Nd for calculating baseline Gd, given that this approach provides a more representative estimate of background Gd levels (Kulaksız and Bau, 2007). Therefore, since HREEs (such as Tb) were not included in the estimation of geogenic Gd, and the fact that Gd behaves similar to other LREEs, this study considers that Gd anomalies greater than 1.0 indicate the presence of Gd_{anth} (Kulaksız and Bau, 2011b).

The quantification of Gd_{anth} levels at sampling sites A6, A7, C2, C3, C4, C5, C6, and C7 yielded values ranging from 6.38 ng L⁻¹ (C7) to 201.14 ng L⁻¹ (C3). These concentrations represent between 1.96 % and 21.02 % of the total Gd detected in the Atoyac River, as displayed in **Fig. 3c**. The relative percentage of Gd_{anth} (% Gd_{anth}) remained below 15% at most sites, except for sites A6, C3, and C5, with the highest percentage recorded at A6 (21.02%). Even though the total Gd concentrations measured in the pre-confluence sites of the Atoyac River (A1–A7) were almost similar, Gd_{anth} was first detected at site A6, downstream of the urban area of San Martín Texmelucan, with a concentration of up to 59.07 ng L⁻¹. This was the highest concentration obtained in the pre-confluence region, suggesting that the WWTP “Tepetitla”, which uses waste stabilization ponds and is located approximately 15 m upstream of this sampling site, can be a source of this contaminant.

However, at site A7, the concentration of Gd_{anth} decreased to 7.24 ng L^{-1} , likely due to sedimentation of inorganic material.

The sampling sites with the highest Gd_{anth} levels after the confluence were C3, C4, and C5. This pattern agrees with the location of the major medical facilities and large hospitals located along the Atoyac River main channel in Puebla City, which discharge wastewater effluents into the river mainstream (**Fig. 4d**). Otherwise, the following sampling sites (C6 and C7) showed a decrease in the concentration of Gd_{anth} , although the concentrations of total Gd remained similar to those found in the rest of the sampling sites.

The positive Gd anomalies observed in this study ($Gd_{SN}/Gd_{SN}^* < 1.27$) were significantly lower than those reported in other studies, where Gd anomalies often exceeded 1.20, showing a notable peak in the REE_{SN} distribution pattern. These lower Gd anomalies may be influenced by hydrological characteristics, such as the low flow that promotes the sedimentation of suspended material, and the substantial tributary discharges into the river, which can dilute the Gd_{anth} (Hissler et al., 2015; Martin et al., 2021). In addition, the low quantity of magnetic resonance scanners in hospitals of this region may also account for the low concentrations of Gd_{anth} observed in the Atoyac River compared with other studies.

Overall, the concentrations of Gd_{anth} estimated at most of the sampling sites of the Atoyac River were higher than those reported in the Thames River (2.67 ng L^{-1}) and the Danube River in Germany (4.25 ng L^{-1}) (Kulaksız and Bau, 2011b), but comparable to those found in the Rao, Xin, Fu, Ganjiang, and Xiushui rivers in China ($6.2 - 37.2 \text{ ng L}^{-1}$) (Liu et al., 2024a), the Paranoá Lake in Brazil ($0.06 - 34.30 \text{ ng L}^{-1}$) (Amorim et al., 2019), the Brisbane River in Australia ($0.5 - 36.0 \text{ ng L}^{-1}$) (Lawrence, 2010), the Wulka River and Lake Neusied in Austria and Hungary (265.6 and $36.8 - 48.9 \text{ ng L}^{-1}$) (Kreitsmann and Bau, 2023), the Suyong River basin in Korea (42.5 ng L^{-1}) (Lim et al., 2023), the Rhine-Meuse Delta in the Netherlands ($10 - 80 \text{ ng L}^{-1}$) (Klaver et al., 2014), and the Yongding River and Chaobai River in China ($1.5 - 127.2 \text{ ng L}^{-1}$) (Gao et al., 2024). Instead, the Gd_{anth} levels in the Atoyac River were lower than those found in the low-discharge Havel River in Germany (492.3 ng L^{-1}), which receives treated wastewater effluents (Kulaksız and Bau, 2011b), and in the reservoirs of the University of Campinas Campus and Chico Mendes Lake in Brazil ($1.9 -$

585 ng L⁻¹), which receive sewage from pipelines of local hospitals and medical laboratories (De Paula Marteleto and Enzweiler, 2021).

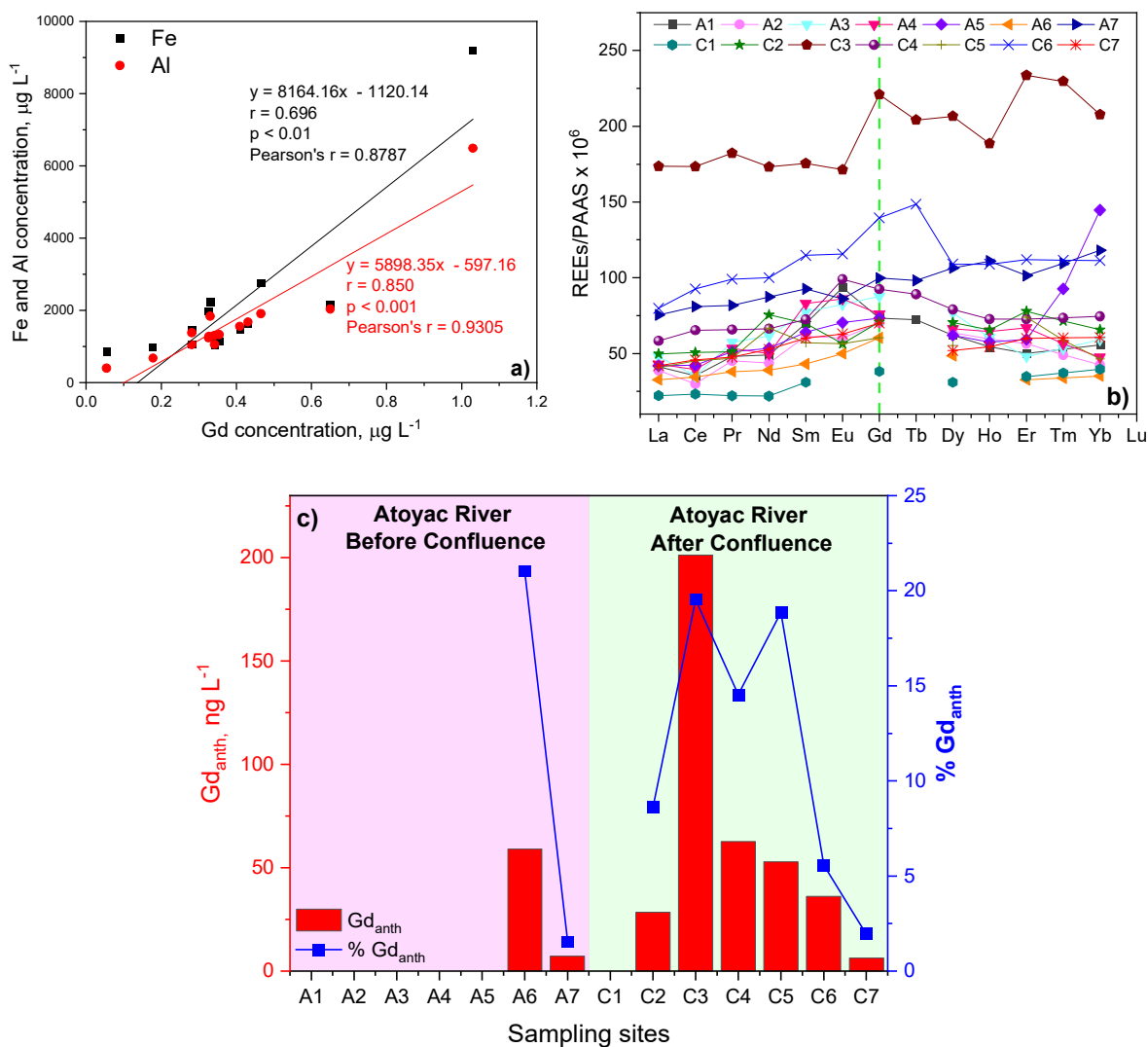


Fig. 3. Correlations between total Gd concentrations and Al and Fe concentrations (a), REE shale-normalized distributions (b), and concentrations of Gd_{anth} and % Gd_{anth} in surface water samples from the Atoyac River (c).

3.4. Occurrence of ICM

Among the investigated ICM, only DIA was not detected in any of the collected samples. Therefore, the results and discussion will focus on the remaining contrast media.

Fig. 4 a-d shows the occurrence and spatial distribution of IOM, IOD, and IOP in surface water samples of the Atoyac River basin (refer to **Table S5** for data). IOP, IOD, and IOM were detected in 83%, 79%, and 10% of the total samples, respectively. Thus, IOP and IOD were the most frequently detected ICM. The site A4 was the first location in the Atoyac River where ICM were detected (IOD 34 ng L⁻¹), suggesting that the first sampling sites of the Atoyac River remain free of this type of contamination (**Fig. 4a**). However, the Zahuapan River shows signs of contamination by wastewater from hospital facilities at site Z2 (IOP 44 ng L⁻¹), a site located very close to its headwaters (**Fig 4b**).

The composition of ICM varied depending on the river or the specific section of the river. IOM was detected in the Zahuapan River at sampling sites Z3, Z4, and Z6 (**Fig 4b**), and was detected neither in the Atoyac River pre-confluence nor post-confluence (**Fig 4d**). This may suggest a dilution due to increased tributary inflow and/or decomposition downstream, as well as the low use of IOM in hospitals and other medical facilities in Puebla City. Meanwhile, IOP was frequently detected at the Zahuapan River and the Atoyac River pre-confluence, accounting for between 0% – 100% and 0% – 81.1% of the total ICM (in % w/w), respectively. IOD was detected at several sampling sites in the Zahuapan River (downstream site Z4) and in the Atoyac River before confluence (downstream site A4), accounting for between 0% – 18.1% and 0% – 100% of the total ICM in the Zahuapan and Atoyac, respectively. The concentrations of IOD and IOP increased downstream in the Zahuapan River, whereas the concentration of IOP increased from 32 ng L⁻¹ to 210 ng L⁻¹ at site A7. This pattern is consistent with the presence of urban centers downstream both rivers, particularly from sites A5 – A7 in the Atoyac (San Martín Texmelucan City) and from sites Z4 – Z6 in the Zahuapan (Tlaxcala City), as well as the presence of medical facilities and WWTPs in these urban centers (**Fig 4 a-b**).

Both IOD and IOP were detected at all sampling sites of the Atoyac River post-confluence (C1–C7), ranging between 110 ng L⁻¹ and 1,300 ng L⁻¹ for IOD and between 450 ng L⁻¹ and 3,700 ng L⁻¹ for IOP. At sampling site C1, the concentrations of both contrast media increased compared to those observed in the last sampling sites of the Atoyac River before confluence (A7) and the Zahuapan River (Z6). Nevertheless, as depicted in **Fig. 4 a-b**, the concentrations of these ICM predominantly increased downstream, with the highest concentration of IOD and IOP found at C7 (1,300.0 and 3,700.0 ng L⁻¹, respectively). Overall,

these concentration patterns of both ICM may be attributed to the presence of several large hospitals located close to the Atoyac River mainstream in Puebla City (**Fig. 4d**), which discharge their wastewater effluents into the Atoyac main channel. At site C7, where both IOD and IOP exhibited the highest concentrations, the primary source of ICM contamination is likely the “Atoyac Sur” WWTP, given that this plant is located just a few meters upstream of this site.

While the total ICM concentration varied along the mainstream of the studied rivers, the IOD and IOP levels in the reservoir remained almost unchanged, indicating minimal decomposition, as shown in **Fig. 4c**. In the reservoir, IOD concentrations ranged from 190 ng L⁻¹ to 390 ng L⁻¹ (mean 261 ± 61 ng L⁻¹), accounting for between 29.7% and 48.2% of the total ICM. Similarly, IOP concentrations ranged from 350 ng L⁻¹ to 490 ng L⁻¹ (mean 412 ± 49 ng L⁻¹), contributing from 52% to 70% of the total ICM. Despite this reservoir functioning as a wastewater stabilization pond, these findings suggest that ICM are not readily degraded under natural conditions, highlighting their persistence and recalcitrant nature in the water environment. This agrees with the fact that ICM are challenging to remove in WWTPs due to their resistance to biological degradation (Yan et al., 2024). Thus, since the Atoyac River receives wastewater coming from hospitals and medical facilities (Dueñas-Moreno et al., 2024a; 2024b), these contaminants are transported through this river due to their high water solubility and low volatility (Cheng et al., 2023), and then became accumulated in the reservoir waters, where they remain undegraded.

Overall, the concentrations of IOD, IOM, and IOP found in the Atoyac River were significantly higher than those reported in other rivers such as the Yangtze River in China, which presented mean concentrations of 26.0 ng L⁻¹ for IOD, 3.2 ng L⁻¹ for IOM, and 7.4 ng L⁻¹ for IOP (Cheng et al., 2023). Despite the ICM concentrations in the Yangtze River were much lower than those observed in the Atoyac River, it is noteworthy that the Yangtze is one of the world’s largest rivers, with an average flow of 31,000 m³ s⁻¹, four orders of magnitude higher than that of the Atoyac (3.88 m³ s⁻¹). Consequently, the ICM fluxes transported by the Yangtze are approximately two orders of magnitude higher than those of the Atoyac River, a fact that agrees with the large extension of the Yangtze basin (1.8 million km²), which is much larger than the Atoyac River basin (4,130 km²).

Other studies reporting ICM levels in surface water bodies include those conducted in the Taihu Lake and the Huangpu River in China, which found concentrations of IOD, IOM, and IOP lower than those found in the present study. Overall, the mean levels of these ICM ranged from 1.4 ng L⁻¹ to 126 ng L⁻¹ and from 1.9 ng L⁻¹ to 27.6 ng L⁻¹ in the Taihu Lake and the Huangpu River, respectively (Xu et al., 2017). Another study conducted downstream of the Bode River in central Germany, which is impacted by seven WWTP discharges, reported mean concentrations of IOD and IOP much lower than those observed in this study. These ranged from 0.13 ng L⁻¹ to 1.63 ng L⁻¹ for IOD and from 0.42 ng L⁻¹ to 0.52 ng L⁻¹ for IOP (Muenze et al., 2017).

Although those studies reported ICM concentrations lower than those found in the Atoyac River waters, other studies have documented ICM concentrations similar to those found in this study. For example, IOD levels in the Atoyac River were comparable to those in the surface waters of Hanoi, Vietnam (median values up to 120 ng L⁻¹) and Manila, Philippines (49 ng L⁻¹) (Watanabe et al., 2016). Similarly, IOD (mean value up to 160 ng L⁻¹) and IOP (mean value up to 83 ng L⁻¹) found in the Rhine River, Switzerland, were not much different from those found in this study. Nonetheless, the levels of IOM found in the Rhine River and Lake Constance were much higher than those found in the Atoyac River, being up to 150 ng L⁻¹ and 1,450 ng L⁻¹, respectively (Kormos et al. 2011).

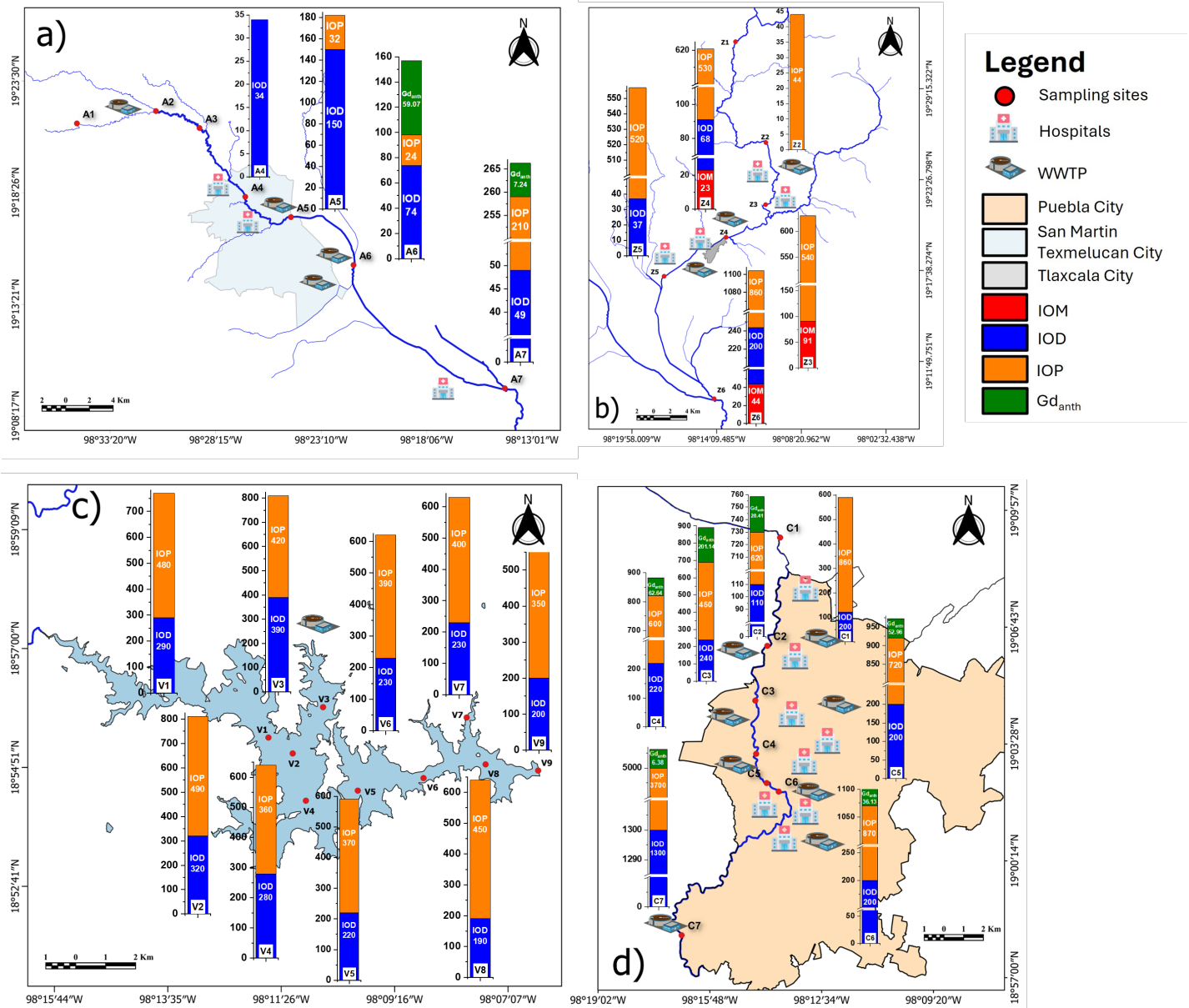


Fig. 4. Spatial distribution of contrast agent concentrations along the Atoyac River pre-confluence (a), the Zahuapan River (b), the Valsequillo Reservoir (c), and the Atoyac River post-confluence (d). The data are available in **Tables S4–S5**.

3.5. Correlations between variables and co-contamination of contrast agents.

Table 1 shows the Spearman rank-order correlations between the variables measured in the Atoyac River system (including river and reservoir waters). IOM was excluded because it was detected at only three sites. Briefly, the COD showed highly significant negative and positive correlations with DO and NH_4^+ , respectively, indicating that the DO abundance and thereby the nitrification process are limited due to the high levels of biodegradable organic matter. The TDS showed significant positive correlations with EC, COD, SO_4^{2-} , NO_3^- , and NH_4^+ , suggesting that the dissolved solids contained in waters are mainly originated from the discharge of wastewater effluents rather than the weathering processes within the basin. Otherwise, the DO concentrations showed significant negative correlations with EC, COD, TDS, SO_4^{2-} , NO_3^- , and NH_4^+ , indicating that increased wastewater contamination leads to lower DO levels in waters.

Regarding ICM, IOD and IOP showed a significant positive correlation with TDS, indicating their anthropogenic nature. However, these contaminants correlated neither with the COD concentrations nor with each other. This lack of correlation between ICM with COD is consistent with other studies that did not find correlations between ICM concentrations and dissolved organic carbon ([Cheng et al., 2023](#)). This suggests that, although both contaminants originate from wastewater effluents, ICM are not present in the pool of wastewater containing high COD levels, which mainly comes from urban and industrial discharges. In fact, these contaminants may mainly come from other types of wastewater, such as those generated by hospitals, medical laboratories, and healthcare facilities. Similarly, the lack of correlation between IOD and IOP in river waters may be due to the varying usage of each contrast medium in hospitals, as well as the frequency of X-ray analyses in medical facilities. Despite the lack of correlation between ICM and DOC, ICM appear to be correlated with the inorganic nitrogen pool in the river waters. IOD showed a highly significant positive correlation with NO_3^- ($p < 0.001$), whereas IOP was positively correlated with NH_4^+ ($p < 0.05$). This agrees with other studies, which revealed through machine learning techniques that total nitrogen (TN) and ammonia (NH_3) were the most influential indicators affecting the occurrence of ICM in lacustrine surface waters ([Cheng et al., 2025](#)). Conversely, despite the lack of correlations between some ICM, studies have found highly significant positive correlations between IOM, IOD, and IOP in waters of the Yangtze River basin, which may

be related to a higher population density and the large number of hospitals and medical centers in that region of China (Cheng et al., 2023).

It is important to note that, although Gd and Gd_{anth} were found in the most polluted sites where ICM also showed their highest concentrations, neither Gd nor Gd_{anth} correlated with other variables (except for the correlation between Gd and Al and Fe concentrations, which was discussed previously), including the concentrations of ICM. One of the main causes of this lack of correlation can be the low quantity of Gd_{anth} found and the low detection frequency of Gd in river waters, which was lower (48.2%) than those of IOD (79.3%) and IOP (82.7%). These low levels of Gd_{anth} and the low Gd detection frequencies may mask possible correlations between water quality parameters and other hospital-derived contaminants with Gd-CAs, which may require further investigation, especially in potential sources such as hospital sewer lines (Weissbrodt et al., 2009). Another possible explanation for the lack of correlation between ICM and Gd-CAs is their use in different medical imaging analysis. Although these chemicals are widely used in medical imaging, ICM are used in X-ray analysis, whereas Gd-CAs are used in magnetic resonance imaging, a technique requiring sophisticated scanners that are unavailable in most hospitals and healthcare centers in Puebla and Tlaxcala states. In addition, the concentration of these contaminants in surface waters can vary widely depending on the number of patients undergoing medical imaging analysis, the differences in usage patterns in medical facilities, and the efficiency of treatments in WWTPs. Moreover, other chemical processes, such as Gd scavenging onto inorganic minerals and subsequent sedimentation of this material, may also account for the lack of co-occurrence and thereby the lack of correlations between these contaminants.

Table 1. Spearman rank-order correlation matrix showing the correlation coefficients between the Gd, Gd_{anth}, ICM and the physicochemical parameters in waters of the Atoyac River basin. (*) denotes $p < 0.05$, (**) denotes $p < 0.01$, and (***) denotes $p < 0.001$.

	Gd	Gd _{anth}	IOD	IOP	pH	EC	DO	COD	TDS	SO ₄ ²⁻	NO ₃ ⁻	NH ₄ ⁺	Fe	Al
Gd	1												**	***
Gd_{anth}	0.204	1												
IOD	0.158	0.180	1			**			*	*	***			
IOP	-0.012	-0.452	0.121	1		**			**			*		
pH	0.317	-0.096	-0.083	0.376	1		*						*	*
EC	-0.004	-0.407	0.528	0.522	-0.042	1	***		***	***	***	**		
DO	0.064	0.690	-0.235	-0.404	0.389	-0.652	1	***	***	*	**	**		
COD	0.199	-0.214	-0.088	0.375	-0.191	0.341	-0.658	1	*			***	*	
TDS	-0.052	-0.491	0.483	0.584	-0.040	0.986	-0.659	0.378	1	***	**	***		
SO₄²⁻	0.050	-0.048	0.501	0.156	0.111	0.738	-0.399	0.306	0.738	1	**	**		
NO₃⁻	0.200	0.168	0.652	-0.246	-0.234	0.588	-0.502	0.028	0.525	0.494	1			
NH₄⁺	0.154	-0.167	0.177	0.449	0.022	0.572	-0.543	0.581	0.621	0.560	0.189	1		
Fe	0.696	-0.119	0.140	0.231	0.539	0.020	-0.085	0.553	0.064	0.342	0.066	0.419	1	***
Al	0.850	0.190	0.105	0.346	0.546	-0.026	0.009	0.428	0.008	0.251	-0.095	0.354	0.928	1

3.6. Potential ecological risk assessment and environmental implications

The potential ecological risk posed by the occurrence of IOM, IOD, IOP, and Gd_{anth} in the Atoyac River basin to aquatic organisms was evaluated using the deterministic RQ approach. To ensure a comprehensive assessment and a more integrative understanding of the potential impacts of these contaminants on the aquatic ecosystem, representative species from three common trophic levels—fish, daphnid (crustaceans), and green algae (algae)—were selected as test organisms. It is important to highlight that aquatic organisms do not distinguish between Gd^* and Gd_{anth} , because they are sensitive to the cumulative effects of Gd ($Gd_{anth} + Gd^*$). As shown in **Fig. 5a**, chronic ecological risks appear to be negligible, given the absence of overlap between the MECs of contrast agents and their corresponding ChVs estimated using ECOSAR. There is approximately a difference of three order of magnitude between the MEC and the effect concentrations at which 10% of the most sensitive species would be affected in 5% of the cases (i.e., the 10th percentile effect concentration exceeded at the 95th percentile frequency). The probability of the highest observed MEC exceeding the 10th percentile of ChV for fish, daphnid, or green algae is estimated to be 0%. Therefore, this suggests that chronic toxicity risks under current environmental conditions are unlikely. However, these values should be interpreted with caution, due to the inherent limitations and uncertainties associated with ECOSAR-predicted toxicity data, which are based on structure–activity relationships rather than empirical testing. Therefore, future studies should include experimental toxicity testing and broader datasets to corroborate these findings and improve the robustness of the risk assessment.

As expected, based on the previous discussion, the RQ values for contrast agents along the Atoyac River basin were below 0.1, indicating low environmental risk (see **Fig. 5b**; refer to **Table S6** for data). The results show that MECs were from 4 to 9 orders of magnitude lower than the corresponding effect concentrations, suggesting no significant environmental risk to aquatic organisms in any of the studied sectors, based on ECOSAR estimates and the quantified MECs for contrast agents. Notably, the highest RQ values for ICM, including IOD and IOP, were observed at site C7, the last sampling site in Puebla City, located just downstream of a WWTP (**Fig. 4d**). In contrast, the combined effect of Gd^* and Gd_{anth} (total Gd) triggered the highest RQ values in almost all sampling sites of the Atoyac River pre- and post-confluence, with the peak observed at site C3. In fact, the Atoyac River after its

confluence with the Zahuapan River, specifically in the urban area Puebla, displayed the highest RQ values for both Gd and ICM in the basin. This result aligns closely with previous reports, highlighting that this section of the river is the most impacted by anthropogenic activities (Dueñas-Moreno et al., 2024a; 2024b; Hernandez-Ramirez et al., 2019; Martinez-Tavera et al., 2017; Mora et al., 2021). On average, the order of susceptibility among the three studied trophic levels was green algae $\geq$ daphnid $\geq$ fish.

The assessment of the ecological risk of contrast agents in other worldwide water bodies is very limited. Nonetheless, the RQ values estimated in this study were similar to previously reported data in surface waters of some countries such as Portugal (1.81×10^{-4} for IOP) (Kötke et al., 2024), China ($\sim 1.0 \times 10^{-4}$ for IOP) (Liu et al., 2020), Switzerland (~ 0.10 for Gd) (Daouk et al., 2016), and Germany (1.82×10^{-5} for IOP) (Kötke et al., 2019). It is noteworthy that, given the limited availability of toxicity data for aquatic organisms concerning these contaminants, the deterministic RQ values estimated in this study only provide a preliminary indication of potential ecological risks as a screening tool. Although ECOSAR can serve as a reliable first approximation, particularly in light of validation studies showing an 87–90% agreement between ECOSAR predictions and measured toxicity data across more than 2,000 chemicals, with fewer than 3% false negatives (Sanderson et al., 2003), these values should be interpreted with caution, as they do not account for the variability and uncertainty in exposure concentrations and biological effects (Yang et al., 2023). Therefore, further research involving a broader range of ecotoxicity data and probabilistic risk assessments is needed to refine these estimates and improve the reliability of the conclusions. Finally, although there is currently no potential ecological risk, the levels of Gd-CAs and ICM found in the Atoyac River basin underscore the need for targeted strategies to improve the removal of these contrast agents, particularly in wastewater originating from medical facilities and hospitals. Given that the waters of the Atoyac River basin are primarily used for irrigation in croplands, and considering that ICM are highly recalcitrant to biodegradation, these contrast agents (including Gd) may accumulate in agricultural soils and be transferred to crops.

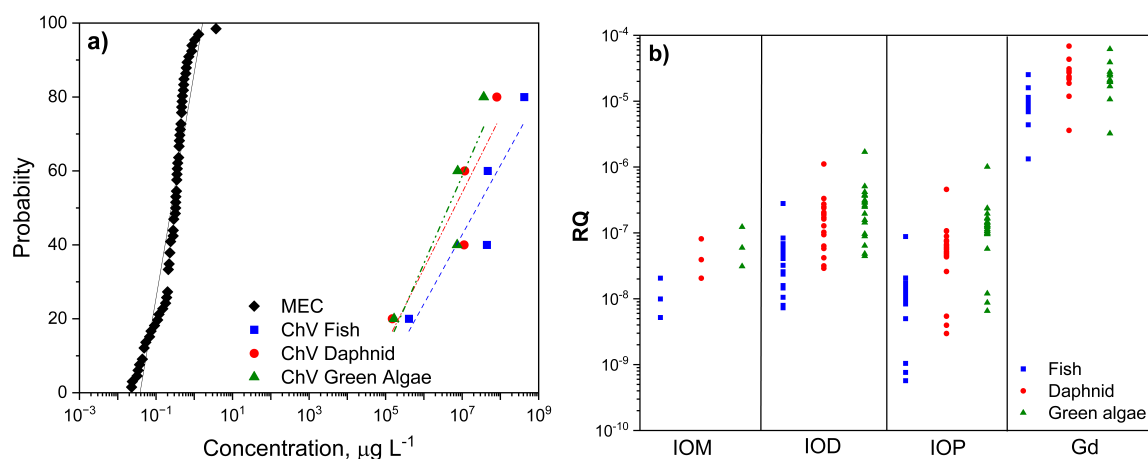


Fig 5. Percentile distribution of MECs of contrast agents along the basin, as well as ChV for fish, daphnid, and green algae estimated using ECOSAR modeling **(a)**. RQ values estimated for IOM, IOD, IOP, and Gd across the sampling sites in the Atoyac River basin **(b)**.

4. Conclusions

This study provides the first comprehensive investigation into the co-occurrence, distribution, and ecological risks of two groups of contrast agents, the ICM and Gd-CAs. Key findings reveal that the concentrations of contrast agents ranged from 6.38 ng L⁻¹ to 3,700 ng L⁻¹ for Gd_{anth} and IOP, with the highest detection frequencies observed for IOP (83%) and IOD (79%). A major concern is the persistence and high concentrations of IOP (412 ± 49 ng L⁻¹) and IOD (261 ± 61 ng L⁻¹) in the Valsequillo Reservoir, which underscore their recalcitrant nature in the environment. Contrary to expectations, no correlation was found between Gd or Gd_{anth} and ICM, disproving their co-occurrence in the study system. This likely results from limited MRI use in the region, as indicated by the low Gd_{anth} levels. In addition, deterministic ecological risk assessments indicated that these contrast agents do not pose a significant risk to aquatic species; however, further evaluation is recommended when more toxicity data become available, given the limitations of the method. As the first study on contrast agent contamination in Mexican surface waters, it establishes a critical baseline for future monitoring and underscores the urgent need for improved wastewater treatment and regulatory measures to mitigate the release of these persistent contaminants. Similarly, this dataset provides a point of reference against which future sampling campaigns in the area

and other surface water bodies in Mexico can be compared. Given that the contamination of the Atoyac River has been proven to increase year after year, these results of the year 2022 are a valuable contribution to understanding the environmental footprint of hospital-derived contrast agents, providing a solid foundation for longitudinal environmental assessments in the region and establishing a first database to which future measures can be compared.

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Data availability statement

Data is available from the authors upon request

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Distribution and ecological risk of Iodinated and Gadolinium-based contrast agents in an impacted basin of central Mexico

Supplementary information

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Materials and methods

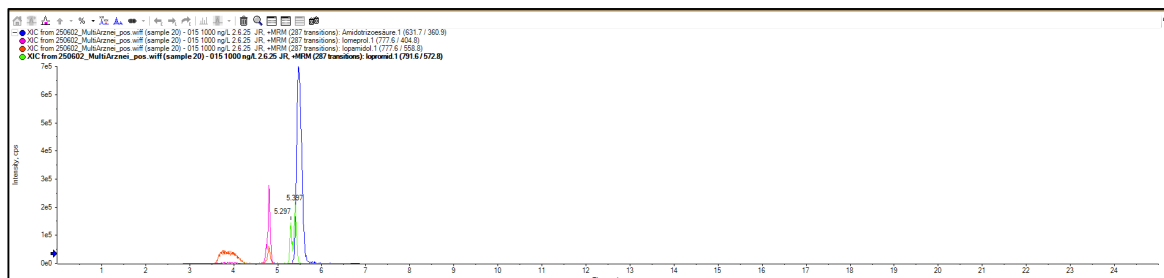


Fig. S1. Typical chromatogram showing the retention time (RT) and the peaks for iopamidol (IOD), iomeprol (IOM), iopromide (IOP), and amidotrizoic acid (DIA) (from left to right). For IOP, two peaks were obtained, and both were used for quantification

Table S1. Limits of detection (LOD), limits of quantification (LOQ), and the relative standard deviation (RSD) determined during the analysis of the ICM

ICM	LOD (ng L ⁻¹)	LOQ (ng L ⁻¹)	RSD (%)
DIA	2.4	8.4	4.1
IOM	2.2	7.6	3.5
IOD	1.8	6.3	3.0
IOP	2.4	8.5	3.9

Table S2. Extracted chronic toxicity values (ChV) from the Ecological Structure–Activity Relationships Program (ECOSAR, version 2.2, USEPA) (ECOSAR, 2025) for contrast agents, along with the resulting predicted no-effect concentration (PNEC) for each compound across three trophic levels.

Contrast Agent	ChV, fish (µg L ⁻¹)	PNEC, fish (µg L ⁻¹)	ChV, daphnid (µg L ⁻¹)	PNEC, daphnid (µg L ⁻¹)	ChV, green algae (µg L ⁻¹)	PNEC, green algae (µg L ⁻¹)
Iomeprol (IOM)	4.42×10^7	4.42×10^6	1.12×10^7	1.12×10^6	7.40×10^6	7.40×10^5
Iopamidol (IOD)	4.65×10^7	4.65×10^6	1.17×10^7	1.17×10^6	7.67×10^6	7.67×10^5
Iopromide (IOP)	4.20×10^8	4.20×10^7	8.08×10^7	8.08×10^6	3.67×10^7	3.67×10^6
Gd (as Gd-CAS)	4.06×10^5	4.06×10^4	1.50×10^5	1.50×10^4	1.67×10^5	1.67×10^4

Results and discussion

Table S3. Physicochemical parameters of the waters of the Atoyac and Zahuapan Rivers as well as Valsequillo Reservoir.

Sampling site	Temp, °C	pH	EC, μScm^{-1}	DO, mgL^{-1}	TDS, mgL^{-1}	COD, mgL^{-1}	SO_4^{2-} , mgL^{-1}	NO_3^- , mgL^{-1}	NH_4^+ , mgL^{-1}
Zahuapan River									
Z1	16.3	7.66	427.9	2.3	335.4	46.5	3.46	0.34	8.65
Z2	15.4	7.78	392.1	1.33	311.36	41.5	11.7	1.39	1.66
Z3	16.6	8.08	566.0	4.97	435.5	52.0	26.9	1.34	5.90
Z4	17.8	7.72	1341	0.9	1007.5	138.5	34.9	1.62	14.24
Z5	18.9	7.56	843.0	1.12	624.0	43.0	35.6	0.59	18.30
Z6	21.2	7.85	929.0	0.61	650.0	111.0	34.2	0.79	22.85
Atoyac River before confluence									
A1	9.0	7.85	114.2	8.38	106.6	24.5	2.8	0.07	1.64
A2	11.9	7.82	181.5	7.1	157.3	18.5	3.55	0.26	1.17
A3	12.6	8.15	193.7	7.2	164.4	27.5	4.36	0.33	2.30
A4	14.7	8.08	308.4	6.54	249.6	29.5	8.56	0.61	3.86
A5	16.6	7.5	452.9	2.32	351.0	139.5	17.4	0.43	11.92
A6	16.4	7.74	618.0	1.74	481.0	91.5	84.7	0.68	10.30
A7	19.3	7.75	702.0	0.3	507.0	239.5	53.6	1.24	15.30
Atoyac River after confluence									
C1	20.9	7.69	834.0	0.39	585.0	215.0	47.6	1.40	19.18
C2	19.3	7.83	890.0	0.63	598.0	220.0	62.4	1.19	14.01
C3	18.8	7.75	702.0	1.02	468.0	1608.5	65.1	1.82	20.13
C4	19.2	8.02	1080.0	1.23	786.5	166.5	78.3	1.20	15.98
C5	20.7	8.06	1120.0	0.99	793.0	184.0	84.1	0.87	19.06
C6	20.6	7.99	1105.0	1.27	786.5	178.0	79.2	0.68	23.44
C7	22.0	8.01	1290.0	0.61	890.5	195.5	115	0.89	26.85
Valsequillo Reservoir									
V1	21.8	7.45	1048.0	0.81	728.0	68.5	78.1	272.96	4.55
V2	22.3	7.49	1031.0	0.35	708.5	71.5	76.4	97.03	13.14
V3	25.3	7.53	1143.0	0.1	734.5	87.0	70.2	235.60	10.60
V4	22.7	7.63	989.0	1.24	669.5	51.5	78	30.38	19.27
V5	22.6	7.88	948.0	1.58	643.5	31.0	78.4	35.05	15.94
V6	23.2	8.0	946.0	1.81	637.0	26.5	78	30.64	16.40
V7	24.9	7.98	981.0	1.29	637.0	25.0	77.4	54.37	7.94
V8	25.6	7.9	1008.0	1.23	650.0	26.0	77.8	30.29	12.05
V9	24.7	7.9	990.0	1.72	643.5	27.0	77.3	18.05	16.74

Remarks: EC: Electrical Conductivity, DO: Dissolved Oxygen, TDS: Total Dissolved Solid, COD: Chemical Oxygen Demand

Table S4. Concentrations of REEs, Al, and Fe across the Atoyac River Basin. All concentrations are expressed in ng L⁻¹ unless otherwise noted

Sampling Site	La	Ce	Pr	Nd	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm*	Yb	Lu	Fe, $\mu\text{g L}^{-1}$	Al, $\mu\text{g L}^{-1}$	Gd_{SN}/Gd_{SN}^*	Gd*	Gd _{anth} (Gd-CAs)	%Gd _{anth}
Z1	239	457	75	106	BDL	BDL	54	BDL	BDL	BDL	BDL	BDL	BDL	BDL	870	401	-	-	-	-
Z2	245	412	66	236	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	392	-	-	-	-
Z3	87	199	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
Z4	710	131	92	269	BDL	BDL	BDL	BDL	66	BDL	55	BDL	BDL	BDL	530	334	-	-	-	-
Z5	785	1,690	BDL	54	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
Z6	2,270	533	BDL	105	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
A1	1,580	2,810	424	1,660	388	101	342	56	290	54	143	21.4	157	BDL	1,280	1,310	0.74	465.11	0.00	-
A2	1,480	2,380	398	1,480	341	65	327	BDL	298	59	161	19.9	120	BDL	1,260	1,280	0.81	402.95	0.00	-
A3	1,830	2,810	506	2,090	430	89	409	BDL	360	60	137	21.6	167	BDL	1,460	1,560	0.90	453.72	0.00	-
A4	1,640	3,140	471	1,690	461	93	354	BDL	310	64	191	22.9	134	BDL	1,150	1,330	0.55	644.93	0.00	-
A5	1,600	3,370	452	1,810	356	76	342	BDL	290	57	169	37.5	408	BDL	1,060	1,060	0.95	359.10	0.00	-
A6	1,250	2,740	336	1,320	239	54	281	BDL	227	BDL	93	13.7	99	BDL	1,070	1,050	1.27	221.93	59.07	21.02
A7	2,880	6,450	722	2,960	514	93	465	76	498	110	289	44.3	333	BDL	2,750	1,910	1.02	457.76	7.24	1.56
C1	848	1,850	195	742	172	BDL	178	BDL	145	BDL	99	15.0	112	BDL	980	682	0.87	204.48	0.00	-
C2	1,900	4,030	452	2,560	388	61	330	BDL	330	65	222	29.0	185	BDL	2,240	1,840	1.09	301.59	28.41	8.61
C3	6,630	1,380	1,610	5,870	974	185	1,030	158	967	187	666	93.0	586	BDL	9,200	6,490	1.24	828.86	201.14	19.53
C4	2,230	5,200	581	2,250	402	107	431	69	370	72	207	29.8	210	BDL	1,640	1,680	1.17	368.36	62.64	14.53
C5	1,550	3,590	413	2,260	317	61	281	BDL	258	BDL	211	23.8	131	BDL	1,460	1,380	1.23	228.04	52.96	18.85
C6	3,050	7,380	875	3,390	637	125	650	115	510	108	319	45.2	314	BDL	2,160	2,040	1.06	613.87	36.13	5.56
C7	1,600	3,650	420	1,790	334	68	326	BDL	243	54	171	24.4	171	BDL	1,970	1,240	1.02	319.62	6.38	1.96
V1	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V2	52	81	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V3	217	332	BDL	54	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	590	425	-	-	-	-
V4	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V5	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V6	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V7	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V8	BDL	55	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-
V9	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	BDL	-	-	-	-

Remarks: Tm*: Interpolated TM concentration based on Er and Yb concentration (Kulaksız and Bau, 2011), with exception of C3 which shows the Tm concentration. $\sum\text{REE}$ = Sum of REE including Tm*. Gd_{SN}/Gd_{SN}^* = Gadolinium anomaly calculated according to **Eq. 1** (Material and Methods Section). Gd_{anth} ($\mu\text{g L}^{-1}$) = Anthropogenic Gd concentration according to **Eqs. 2-3** (Material and Methods Section). % Gd_{anth} = Anthropogenic Gd content as a percentage of total Gd. BDL (Below Detection Limit).

Table S5. Iodinated Contrast Media concentration along (ng L⁻¹) the sampling sites of the
Atoyac River Basin

Sampling Site	IOM	IOD	IOP	DIA
Z1	BDL	BDL	BDL	BDL
Z2	BDL	BDL	44	BDL
Z3	91	BDL	540	BDL
Z4	23	68	530	BDL
Z5	BDL	37	520	BDL
Z6	44	200	860	BDL
A1	BDL	BDL	BDL	BDL
A2	BDL	BDL	BDL	BDL
A3	BDL	BDL	BDL	BDL
A4	BDL	34	BDL	BDL
A5	BDL	150	32	BDL
A6	BDL	74	24	BDL
A7	BDL	49	210	BDL
C1	BDL	120	470	BDL
C2	BDL	110	620	BDL
C3	BDL	240	450	BDL
C4	BDL	220	600	BDL
C5	BDL	200	720	BDL
C6	BDL	200	870	BDL
C7	BDL	1,300	3,700	BDL
V1	BDL	290	480	BDL
V2	BDL	320	490	BDL
V3	BDL	390	420	BDL
V4	BDL	280	360	BDL
V5	BDL	220	370	BDL
V6	BDL	230	390	BDL
V7	BDL	230	400	BDL
V8	BDL	190	450	BDL
V9	BDL	200	350	BDL

Remarks: BDL (Below Detection Limit)

Table S6. Risk Quotient (RQ) values estimated for IOM, IOD, IOP, and Gd (Gd_{anth} + Gd*) at each sampling site in the surface water of the Atoyac River Basin for three common trophic levels: fish, crustaceans (daphnids), and algae (green algae).

Site	IOM			IOD			IOP			Gd (Gd _{anth} + Gd*)		
	RQ Fish	RQ Daphnid	RQ Green algae	RQ Fish	RQ Daphnid	RQ Green algae	RQ Fish	RQ Daphnid	RQ Green algae	RQ Fish	RQ Daphnid	RQ Green algae
Z1	NA	NA	NA	NA	NA	NA	NA	NA	NA	1.33×10^{-6}	3.60×10^{-6}	3.23×10^{-6}
Z2	NA	NA	NA	NA	NA	NA	1.05×10^{-9}	5.45×10^{-9}	1.20×10^{-8}	NA	NA	NA
Z3	2.06×10^{-8}	8.13×10^{-8}	1.23×10^{-7}	NA	NA	NA	1.29×10^{-8}	6.68×10^{-8}	1.47×10^{-7}	NA	NA	NA
Z4	5.20×10^{-9}	2.05×10^{-8}	3.11×10^{-8}	1.46×10^{-8}	5.81×10^{-8}	8.87×10^{-8}	1.26×10^{-8}	6.56×10^{-8}	1.44×10^{-7}	NA	NA	NA
Z5				7.96×10^{-9}	3.16×10^{-8}	4.82×10^{-8}	1.24×10^{-8}	6.44×10^{-8}	1.42×10^{-7}	NA	NA	NA
Z6	9.95×10^{-9}	3.93×10^{-8}	5.95×10^{-8}	4.30×10^{-8}	1.71×10^{-7}	2.61×10^{-7}	2.05×10^{-8}	1.06×10^{-7}	2.34×10^{-7}	NA	NA	NA
A1	NA	NA	NA	NA	NA	NA	NA	NA	NA	8.42×10^{-6}	2.28×10^{-5}	2.05×10^{-5}
A2	NA	NA	NA	NA	NA	NA	NA	NA	NA	8.05×10^{-6}	2.18×10^{-5}	1.96×10^{-5}
A3	NA	NA	NA	NA	NA	NA	NA	NA	NA	1.01×10^{-5}	2.73×10^{-5}	2.45×10^{-5}
A4	NA	NA	NA	7.31×10^{-9}	2.91×10^{-8}	4.43×10^{-8}	NA	NA	NA	8.72×10^{-6}	2.36×10^{-5}	2.12×10^{-5}
A5	NA	NA	NA	3.23×10^{-8}	1.28×10^{-7}	1.96×10^{-7}	7.62×10^{-10}	3.96×10^{-9}	8.72×10^{-9}	8.42×10^{-6}	2.28×10^{-5}	2.05×10^{-5}
A6	NA	NA	NA	1.59×10^{-8}	6.32×10^{-8}	9.65×10^{-8}	5.71×10^{-10}	2.97×10^{-9}	6.54×10^{-9}	6.92×10^{-6}	1.87×10^{-5}	1.68×10^{-5}
A7	NA	NA	NA	1.05×10^{-8}	4.19×10^{-8}	6.39×10^{-8}	5.00×10^{-9}	2.60×10^{-8}	5.72×10^{-8}	1.15×10^{-5}	3.10×10^{-5}	2.78×10^{-5}
C1	NA	NA	NA	2.58×10^{-8}	1.03×10^{-7}	1.56×10^{-7}	1.12×10^{-8}	5.82×10^{-8}	1.28×10^{-7}	4.38×10^{-6}	1.19×10^{-5}	1.07×10^{-5}
C2	NA	NA	NA	2.37×10^{-8}	9.40×10^{-8}	1.43×10^{-7}	1.48×10^{-8}	7.67×10^{-8}	1.69×10^{-7}	8.13×10^{-6}	2.20×10^{-5}	1.98×10^{-5}
C3	NA	NA	NA	5.16×10^{-8}	2.05×10^{-7}	3.13×10^{-7}	1.07×10^{-8}	5.57×10^{-8}	1.23×10^{-7}	2.54×10^{-5}	6.87×10^{-5}	6.17×10^{-5}
C4	NA	NA	NA	4.73×10^{-8}	1.88×10^{-7}	2.87×10^{-7}	1.43×10^{-8}	7.43×10^{-8}	1.63×10^{-7}	1.06×10^{-5}	2.87×10^{-5}	2.58×10^{-5}
C5	NA	NA	NA	4.30×10^{-8}	1.71×10^{-7}	2.61×10^{-7}	1.71×10^{-8}	8.91×10^{-8}	1.96×10^{-7}	6.92×10^{-6}	1.87×10^{-5}	1.68×10^{-5}
C6	NA	NA	NA	4.30×10^{-8}	1.71×10^{-7}	2.61×10^{-7}	2.07×10^{-8}	1.08×10^{-7}	2.37×10^{-7}	1.60×10^{-5}	4.33×10^{-5}	3.89×10^{-5}
C7	NA	NA	NA	2.80×10^{-7}	1.11×10^{-6}	1.69×10^{-6}	8.81×10^{-8}	4.58×10^{-7}	1.01×10^{-6}	8.03×10^{-6}	2.17×10^{-5}	1.95×10^{-5}
V1	NA	NA	NA	6.24×10^{-8}	2.48×10^{-7}	3.78×10^{-7}	1.14×10^{-8}	5.94×10^{-8}	1.31×10^{-7}	NA	NA	NA
V2	NA	NA	NA	6.88×10^{-8}	2.74×10^{-7}	4.17×10^{-7}	1.17×10^{-8}	6.06×10^{-8}	1.34×10^{-7}	NA	NA	NA
V3	NA	NA	NA	8.39×10^{-8}	3.33×10^{-7}	5.08×10^{-7}	1.00×10^{-8}	5.20×10^{-8}	1.14×10^{-7}	NA	NA	NA
V4	NA	NA	NA	6.02×10^{-8}	2.39×10^{-7}	3.65×10^{-7}	8.57×10^{-9}	4.46×10^{-8}	9.81×10^{-8}	NA	NA	NA
V5	NA	NA	NA	4.73×10^{-8}	1.88×10^{-7}	2.87×10^{-7}	8.81×10^{-9}	4.58×10^{-8}	1.01×10^{-7}	NA	NA	NA
V6	NA	NA	NA	4.95×10^{-8}	1.97×10^{-7}	3.00×10^{-7}	9.29×10^{-9}	4.83×10^{-8}	1.06×10^{-7}	NA	NA	NA
V7	NA	NA	NA	4.95×10^{-8}	1.97×10^{-7}	3.00×10^{-7}	9.52×10^{-9}	4.95×10^{-8}	1.09×10^{-7}	NA	NA	NA
V8	NA	NA	NA	4.09×10^{-8}	1.62×10^{-7}	2.48×10^{-7}	1.07×10^{-8}	5.57×10^{-8}	1.23×10^{-7}	NA	NA	NA
V9	NA	NA	NA	4.30×10^{-8}	1.71×10^{-7}	2.61×10^{-7}	8.33×10^{-9}	4.33×10^{-8}	9.54×10^{-8}	NA	NA	NA

Remarks: NA: No available

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