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Supplementary Materials

Assessment of Artificial Sweeteners as Wastewater Co-Tracers in an Urban Groundwater System of Mexico (Monterrey Metropolitan Area)

Edrick Ramos [1], Diego Padilla-Reyes [1], Abrahan Mora [2], Hector Barrios-Piña [3], Shashi Kant [3] and Jürgen Mahlknecht [1,*]

[1] Escuela de Ingenieria y Ciencias, Tecnologico de Monterrey, Av. Eugenio Garza Sada Sur N° 2501, Monterrey 64849, Nuevo León, Mexico
[2] Escuela de Ingenieria y Ciencias, Tecnologico de Monterrey, Atlixcáyotl 5718, Reserva Territorial Atlixcáyotl, Puebla 72453, Puebla, Mexico
[3] Escuela de Ingenieria y Ciencias, Tecnologico de Monterrey, Av. General Ramón Corona #2514, Col. Nuevo México, Zapopan 45138, Jalisco, Mexico
* Correspondence: jurgen@tec.mx; Tel.: +52-81-1577-9870

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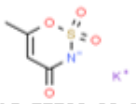
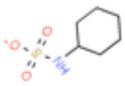
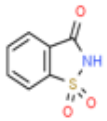
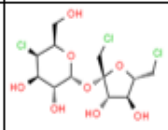
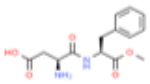
1. Supplementary Materials

1.1 Background on Asws Local Regulation

In Mexico, the use of Asw$_s$ have been regulated for food services and non-alcoholic beverages under the NOM-086-SSA1-1994. Such regulation establishes the use of acesulfame (ACE), aspartame (ASP), cyclamate (CYC), saccharin (SAC), and sucralose (SUC) as synthetic compounds that can substitute (in full or half) the sweetness of natural sugars (e.g., sucrose) [38]. The main chemical descriptions, sweetness equivalent (to sucrose), and global market for five common Asw$_s$ are shown on **Table 1**. Despite such consumption regulation, local normative pertaining drinking water quality (NOM-127-SSA1-1994) and wastewater treatment plant (WWTP) effluent discharges into national waters (NOM-001-ECOL-1996) policies does not consider nor regulate the presence of Asw$_s$ as potential pollutants into aqueous environments. Unlike other contaminants of environmental concern such as agrochemical or industrial residues in urban water systems, the fate and occurrence of Asw$_s$ has been linked to anthropogenic pollution and limited information is available regarding the understanding of possible environmental threats for Mexican water resources. It is of particular concern since at least 96% of the Mexican population consume at least one product made with artificial sweeteners daily [49], resulting in a significant environmental entryway of such sweetening compounds through urban sewage into surface and groundwater resources. The impact of artificial sweeteners in urban groundwater systems is understudied in the Mexican territory.

Table S1. Artificial sweeteners main chemical characteristics, uses, and market locations.

Compound Name	Structure	MW (g/mol)	log K_{ow}	Solubility (mg/L)	Sugar equivalence	Tabletop brand	Uses	Market
Acesulfame k (ACE)	 CAS: 55589-62-3	163.2	-1.33	587,500	100 - 200	Nutra Sweet, Equal, DiabeSugar Sweeny, Sweet-O, Azucar BC, Stevia	Candies, tabletop sweetener, chewing gum, jam, gellatins, baked goods, and dairy products	Asia Europe North America
Cyclamate (CYC)	 CAS:139-05-9	201.22	-2.63	1,000,000	30 - 50	No brand names	Cereal bars, bakery products, vitamins, and dietary supplements, tabletop sweeteners, dairy products	Asia Europe
Saccharin (SAC)	 CAS: 81-06-2	183.18	0.91	4,000	200 - 700	Necta Sweet Sweet'N Low	Fruit based snacks, soft drinks, dried fruit snacks, baked products, jams & jellies, vitamins & dietary supplements, toothpaste	Asia Europe North America
Sucralose (SUC)	 CAS: 56038-13-2	397.64	-1	109,800	600	Splenda	Chewing gum, soft drinks, energy drinks, pastas, cakes, candies, cereal, ice cream & dairy, yogurts, mermelades, vitamins & dietary supplements	North America
Aspartame (ASP)	 CAS: 22839-47-0	201.22	-2.63	1,000,000	180 - 200	Equal Nutra Sweet	Yogurts Soft drinks Pharmaceuticals Gellatins	Asia Europe North America

1.2 Historical climate in the Monterrey Metropolitan Area

Weather data from the MMA region was retrieved from Mexico's National Meteorological Service for Monterrey gauge station #19082 which is currently operating and located in the San Nicolás de los Garza municipality for the period of 1951-2021. Mean annual precipitation reaches 622 mm and 22.7 °C, respectively. Mean monthly precipitation spatiotemporal variation range between 14.1 and 150.6 mm and mean monthly temperature ranging 14.5 to 28.4 °C [29].

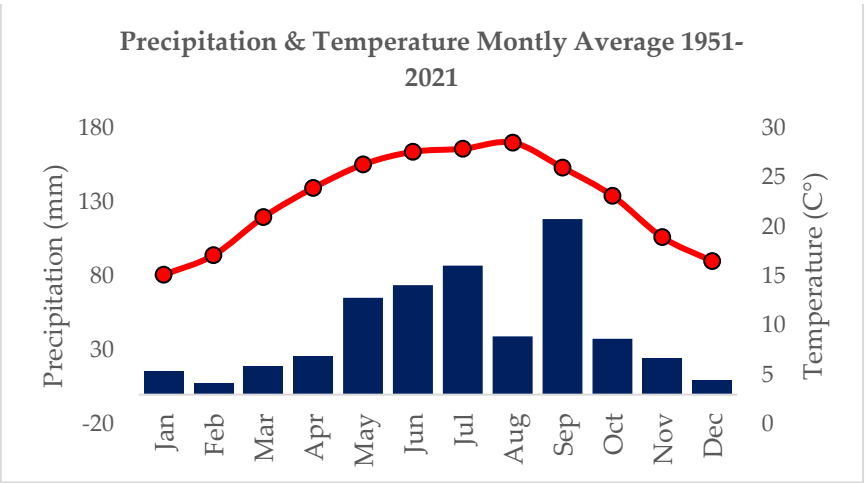


Figure S1. Historical (1951-2021) monthly precipitation and mean monthly temperature on the Monterrey Metropolitan Area (source: http://clicom-mex.cicese.mx.).

1.3 Normality tests

Table S2. Summary of Shapiro Wilk test for normality for chemical parameters measured from MMA sampled wells.

Tests of Normality

	Kolmogorov-Smirnov[a]			Shapiro-Wilk		
	Statistic	df	Sig.	Statis-tic	df	Sig.
Temperature (°C)	0.148	42	0.022	0.953	42	0.084
pH	0.209	42	0.000	0.844	42	0.000
Electrical Con-ductivity (µs/cm)	0.187	42	0.001	0.865	42	0.000
Eh (mV)	0.154	42	0.014	0.911	42	0.003
Dissolved Oxy-gen (mg/L)	0.423	42	0.000	0.250	42	0.000
TDS (mg/L)	0.181	42	0.001	0.848	42	0.000
CO3- (mg/L)	0.161	42	0.008	0.811	42	0.000
HCO3- (mg/L)	0.167	42	0.005	0.774	42	0.000
F- (mg/L)	0.213	42	0.000	0.894	42	0.001
Cl- (mg/L)	0.214	42	0.000	0.794	42	0.000
NO3-N (mg/L)	0.208	42	0.000	0.802	42	0.000
SO4- (mg/L)	0.261	42	0.000	0.800	42	0.000
PO4-P- (mg/L)	0.342	42	0.000	0.737	42	0.000
Ca2+ (mg/L)	0.179	42	0.002	0.858	42	0.000
K+ (mg/L)	0.228	42	0.000	0.845	42	0.000
Mg2+ (mg/L)	0.159	42	0.009	0.750	42	0.000
Na+ (mg/L)	0.224	42	0.000	0.708	42	0.000
Si (mg/L)	0.138	42	0.042	0.946	42	0.045
B (µg/L)	0.211	42	0.000	0.761	42	0.000
Br (µg/L)	0.233	42	0.000	0.646	42	0.000
I (µg/L)	0.300	42	0.000	0.455	42	0.000
Acesulfame (µg/L)	0.248	42	0.000	0.844	42	0.000
Sucralose (µg/L)	0.256	42	0.000	0.700	42	0.000

a. Lilliefors significance correction

1.4 Kruskal Wallis test for Asws seasonal variability

Table S3. Summary of Kruskal Wallis non-parametric test for determining Asws seasonal variability.

Summary of contrast hypothesis

	Null Hypothesis	Test	Sig.	Decision
1	Acesulfame distribution is the same between the Season categories.	Kruskal-Wallis test for independent samples.	0.009	Reject null hypothesis.
2	Sucralose distribution is the same between the Season categories.	Kruskal-Wallis test for independent samples.	0.009	Reject null hypothesis.

Asymptotic differences are shown. The significance level is 0.05.

1.5 Spearman correlation

Table S4. Spearman rank-order correlation matrix.

Parameters	SUC	ACE	I	Br	B	Na+	Mg2+	K+	Ca2+	PO4-	SO4-	NO3-	NO2-	Cl-	F-	HCO3-	TDS	DO	Eh	EC	pH	Temp
Temp	.332*	0.225	.458**	.421**	.471**	.400**	.310*	.363*	0.128	0.070	0.155	.511**	.355*	.497**	.462**	0.055	.378*	-.445**	-.550**	.456**	-0.141	1.000
pH	-.531**	-.732**	-.538**	-.594**	-.493**	-.595**	-0.277	-.468**	-.505**	0.071	-.650**	-.633**	-.532**	-.592**	0.036	-.533**	-.602**	0.211	.516**	-.603**	1.000	
EC	.700**	.768**	.849**	.890**	.832**	.894**	.613**	.672**	.576**	-0.130	.827**	.880**	.888**	.912**	.321*	.727**	.990**	-.371*	-.582**	1.000		
Eh	-.378*	-.488**	-.671**	-.593**	-.666**	-.575**	-.533**	-.421**	-0.268	0.221	-.371*	-.705**	-.505**	-.642**	-.468**	-.347*	-.528**	.377*	1.000			
DO	-0.093	-0.121	-0.205	-0.222	-0.213	-0.230	-0.113	-0.103	-0.171	0.103	-0.288	-0.296	-.444**	-.306*	-.531**	-0.070	-.365*	1.000				
TDS	.679**	.755**	.813**	.868**	.791**	.879**	.594**	.656**	.598**	-0.118	.850**	.844**	.900**	.879**	0.295	.733**	1.000					
HCO3-	.675**	.710**	.685**	.737**	.697**	.737**	.517**	.671**	.581**	-0.028	.649**	.620**	.618**	.697**	-0.131	1.000						
F-	-0.018	0.130	.394**	.328*	.398**	.324*	.484**	0.213	-0.013	-.310*	0.144	.360*	.354*	.352*	1.000							
Cl-	.786**	.844**	.927**	.956**	.934**	.957**	.737**	.774**	.572**	-0.185	.745**	.935**	.833**	1.000								
NO2-	.579**	.661**	.700**	.790**	.719**	.839**	.496**	.562**	.628**	-0.120	.855**	.752**	1.000									
NO3-	.713**	.812**	.892**	.890**	.875**	.867**	.737**	.699**	.490**	-0.132	.707**	1.000										
SO4-	.529**	.727**	.636**	.730**	.621**	.777**	.426**	.510**	.692**	-0.126	1.000											
PO4-	0.036	-0.138	-0.266	-0.213	-0.157	-0.179	-0.215	0.083	-0.069	1.000												
Ca2+	.377*	.575**	.510**	.666**	.551**	.699**	.404**	.506**	1.000													
K+	.757**	.738**	.796**	.834**	.867**	.834**	.769**	1.000														
Mg2+	.552**	.601**	.873**	.803**	.845**	.763**	1.000															
Na+	.771**	.852**	.927**	.983**	.944**	1.000																
B	.751**	.792**	.950**	.955**	1.000																	
Br	.769**	.854**	.951**	1.000																		
I	.764**	.783**	1.000																			
ACE	.732**	1.000																				
SUC	1.000																					

*Correlation is significant at the 0.05 level (two-tailed). **correlation is significant at the 0.001 level (two-tailed)