ABUAD INTERNATIONAL JOURNAL OF NATURAL AND APPLIED SCIENCES
ISSN: 2955-1021
AIJNAS 2022, Volume 2, Issue 2, pp 59–65
https://doi.org/10.53982/aijnas.2022.0202.02-j

https://journals.abuad.edu.ng/index.php/aijnas

Organic Compound Composition in Sachet and Bottled Potable Water Produced in Southwest Ado Ekiti, Nigeria

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Abstract
Organic pollutants are pollutants that are organic in nature, and usually contain carbon bonded with other elements covalently. These compounds are toxic and or carcinogenic in nature. Their presence in water in large quantities causes considerable and widespread concern. Sachet, and bottled potable waters are generally consumed in the southwest, Ado-Ekiti capital city, as drinking water. In this study, the composition of organic compounds was investigated in ten water samples -sachets and bottles, purchased from different potable water-producing plants in Ado-Ekiti environs. By using a separatory funnel with a liquid-liquid extraction system of 50mL:50mL n-Hexane: Dichloromethane, organic compounds were extracted from the water samples. These extracts were analyzed using ultraviolet-visible spectrophotometry, which determined that the wavelength of maximum absorption (λmax) of the organic compounds present in all the water samples occurred at 222 nm. The organic compounds were identified using Gas Chromatography-Mass Spectrometry. The composite water sample obtained from the sachet water revealed sixteen (16) organic compounds, while ten (10) were found in the bottled water composite sample. The common organic compounds found in both the sachet and bottled waters were: Neophytadiene, Hexadecanoic acid, Eicosadiene, Cyclotrisiloxane, and Tetrasiloxane. Organic compounds found only in the composite bottled water samples were Dodecanoic acid, Octadecadienoic acid, Octadecenoic, Methyl stearate, Benzisothiazol-3-amine, and Arsenous acid. Apart from the toxic organic compounds, the identification of Arsenous acid in bottled water is quite worrisome, because most elites in the society drink bottled water. In the composite sachet water sample, other organic compounds found include Copaene, Cubebene, Caryophyllene, Humulene, Naphthalene, Caryophyllene oxide, Tetradecyne, Caffeine, Methyl Hexadecenoic acid, Hexadec-9-enoate, p-Camhorene, Octadecatrienenoic acid, Supraene, and Hexamethyl Cyclotrisiloxane. In general, most of these organic compounds have plant origin but their presence in potable water is undesirable and therefore regarded as contaminants and harmful. The water producing plants need to incorporate effective organic purification systems to remove the organic compounds considered as harmful contaminants in the drinking waters.
Keywords: *sachet and bottled water, ultraviolet-visible spectrophotometry, Gas Chromatography-Mass Spectrometry and organic compounds.*

INTRODUCTION

Water quality assessment is one of the most crucial indices to ensuring public health safety for the consumption of drinking water. Constant evaluation of drinking water quality in terms of heavy metals and toxic substances is vital (Ehya and Marbouti 2016). Water contamination has diverse complications on the well-being of both plants and animals across the board (Ojo & Onasanya 2013). Ailments linked to contaminated water pose a serious burden on human health (WHO 2017); thus, the assessment of potable water is of great significance in preventing health issues. Drinking water is sourced commonly from wells, rivers, lakes, reservoirs, ponds etc. The variety of sources of water poses the utmost risk to human health because of contamination from these sources. Water pollutants are mainly heavy metals, microorganisms, fertilizers, and thousands of toxic organic compounds. Organic pollutants are pollutants that are organic in nature, and usually contain carbon bonded with other elements covalently. These compounds are toxic and or carcinogenic in nature. When present in large quantities in water, they cause considerable and widespread concern. Rivers serve as a hotspot for organic pollutant loading, particularly those in lowland regions (Burton and Pitt, 2001). Organic water pollutants generally include detergents, disinfection by-products (having"down-the-drain" applications), food processing waste, insecticides and herbicides, petroleum hydrocarbons and lubricants, and fuel combustion by products (from storm water regarded as persistent organic pollutants, POPs) (Burton and Pitt, 2001). Many pieces of evidence exist regarding water-bodies pollution by organic pollutants. In drinking water, concentration rarely exceeds 20 mg/L. Some organic pollutants including polychlorinated dibenzo-p-dioxins and polychlorinated dibenzofurans (PCDD/Fs), antibiotics, herbicides, and bisphenol A (BPA), have drawn significant attention by environmental researchers. However, other organic pollutants considered low priority pollutants may be in the form of nutrient or dissolved materials including phosphates, nitrate, sulphate, ammonium nitrate, nitrite, etc (Burton and Pitt, 2001).

Available oxygen in water is reduced by organic pollutants. This affects water organisms by causing reduced fitness or death from asphyxiation. Effects also include increased turbidity (especially by petroleum-related wastes) of the water, which reduces the available light for photosynthetic organisms and potentially leading to its death (Akinwumi &Oderinde 2013). It can also settle on the benthic and alters its characteristics.

There are numerous reasons for monitoring and controlling organic pollutants in the environment, especially in the body of water consumed by humans as drinking water. This is because these substances are dangerous to human health and the environment. In general, organic chemical pollutants affecting human health are regulated by legal limits such as WHO Guidelines for Drinking-Water Quality, EPA National Primary Drinking Water Regulations, water quality standards in waterworks law, environmental standards, and wastewater standards (Tsuchiya, Y, 2019). Pollution by organic chemicals in the aquatic environment occurs by various mechanisms. Naturally occurring organic chemicals produced by aquatic micro organisms, such as 2-methylisoborneol and geosmin, which have an earthy-musty odor, and microcystin, which shows hepatotoxicity, contaminate surface water such as rivers, lakes and reservoirs. Industrial waste containing artificial chemicals flows into and contaminates many water areas. Volatile organic compounds (VOCs), pesticides, phenolic compounds, phthalates, and nitrogen-containing compounds, are often detected in polluted water (Tsuchiya, Y, 2019). VOCs such as trichloroethylene, tetrachloroethylene and 1,1,1-trichloroethane, are most often found in ground water. Dioxins, and poly nuclear aromatic hydrocarbons (PAHs), produced during the combustion of organic materials, are also found in surface water. On the other hand, chlorination by-products such as trihalomethanes (THMs), haloacetic acids and MX, which are produced during the water purification process by reaction of chlorine and organic materials, are found in drinking water. In the WHO Guidelines for Drinking-Water Quality, levels are set for 28 organic constituents (i.emicrocystin-LR, chlorinated alkanes, chlorinated ethenes, aromatic hydrocarbons, chlorinated benzenes and miscellaneous), 33 pesticides, and 9 disinfectant by-products, due to their health effects on humans. In recent years, occurrence of PPCPs (pharmaceutical and personal care products) and perfluoroalkyl acids (PFAs, i.e. PFOS and PFOA) in aquatic environment has been recognized as emerging issues in environmental chemistry (Tsuchiya, Y, 2019). Since harm caused by the ingestion and use of contaminated water are on the increase, there is a need to investigate the pollution level of organic compounds in the water we consume, especially by water-producing companies in our local communities.

MATERIALS AND METHODS

Study area data

Ado-Ekiti (Longitude 7.6124° N, 5.2371° E Latitude) is the capital city of Ekiti State, a mountainous area in the South West region of Nigeria. In Ado-Ekiti, the wet season is warm, over bearing, and dreary, while the dry season is hot, damp, and partly cloudy. Over the course of the year, the temperature typically varies from 64°F (17.8°C) to 90°F (32.2°C) and is rarely below 58°F (14.4°C) or above 95°F (35°C). The temperature hovers around 34°C (61.2°F) during the day and at night, and it feels like 22°C (39.6°F). In November, when the water samples were taken, Ado-Ekiti gets 44.24mm of rain and approximately 16 rainy days in the month. Humidity is close to 72% and temperature near 29°C (84°F).

Sample collection and preparation

In this study, five (5) bottled and five (5) sachet waters were sampled in a way that covers the whole capital city distribution system. The water samples (1000 ml) were bought from different potable water-producing plants in Ado-Ekiti environs. The collected samples were also kept in accordance with standard methods for water and wastewater. The collected water samples were transported to the analytical lab in ice box.

Sample preparations using liquid-liquid extraction for organic pollutant analysis

Liquid-Liquid extraction procedure was employed in the extraction of organic compounds from the water samples using a separatory funnel and solvent system 50mL:50 mL n-Hexane: Dichloromethane as extractant according to the procedure outlined by Akinwumi and Oderinde, (2013). The sachet water samples were filtered through a membrane filter with 0.45 μm pore size before extraction procedures. Water sample of 100 mL was poured into a separating funnel and 100 mL of organic solvent (50 mL:50 mL – hexane: dichloromethane) added while the mixture was subjected to thorough shaking for almost 45 minutes. The extract was poured into a beaker, left for few minutes to evaporate, and then the remaining unevaporated extract filtered using cotton wool as a separating medium in a pasture pipette. Excess anhydrous sodium tetraoxosulphate (VI) (Na_2SO_4) was added to absorb the remaining water in the sample and this was combined into a vial bottle, usually up to 2 mL, ready for Gas Chromatography analysis.

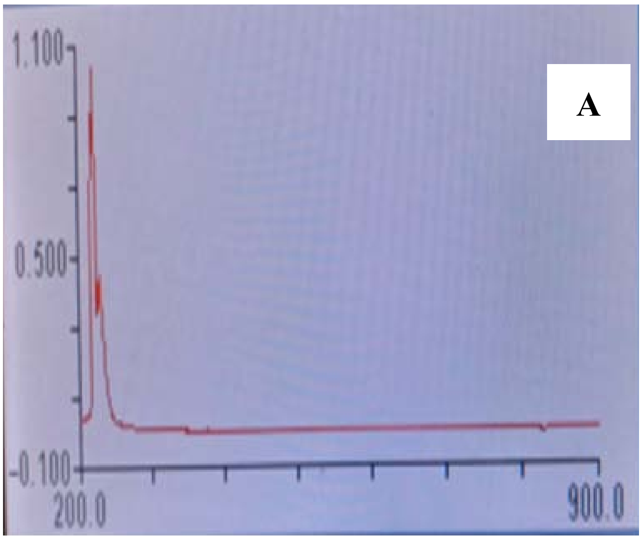
Characterization of extracted organic contaminants

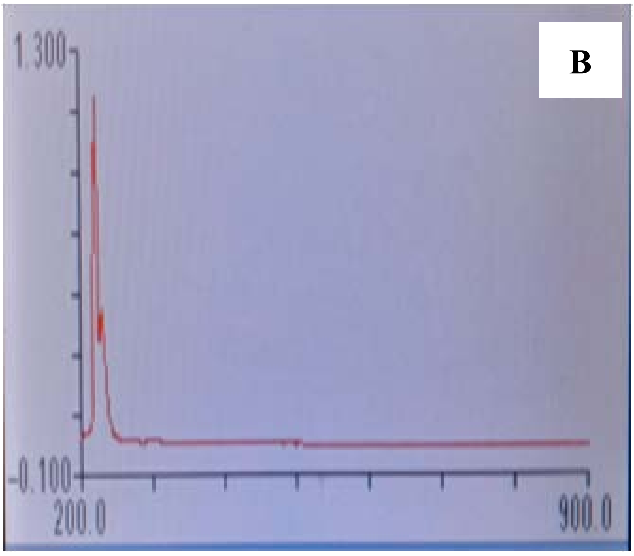
Extracted organic compoundswere identified using Gas Chromatography-Mass Spectrometry (GC-MS). Gas Chromatography analyses were performed with a Hewlett-Packard 7890 series Gas Chromatograph equipped with 5975C Mass Spectrometer detector usingsplit less injection mode with a pulse pressure of 5.9818psi. Chromatographic separation was carried out using a polar column (30 m length, 0.32 mm i.d., and 0.25 µm film thickness). The oven temperature was 250°C for 31 minutes followed by temperature programmed to 200°C at 17°C/min. Helium was used as carrier gas.

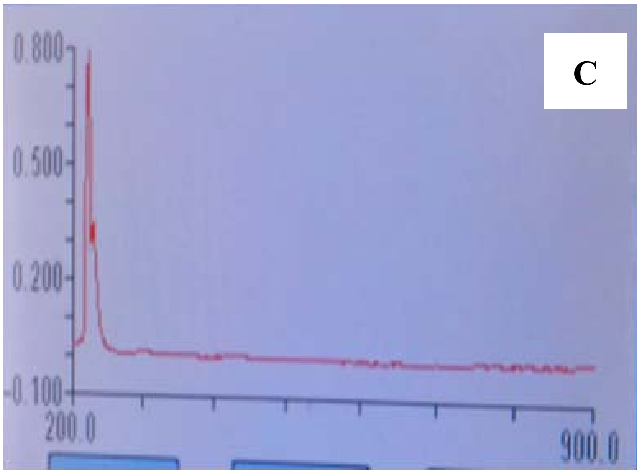
The water sample was subjected to ultra violet spectrophotometry to determine the wave length of maximum absorption (λmax), which characterized the organic compounds present in the water samples, and also suggested the chromophore likely present in the organic compounds.

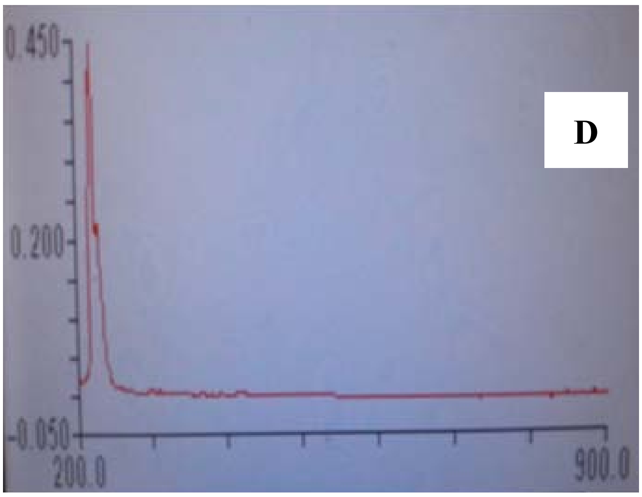
RESULTS

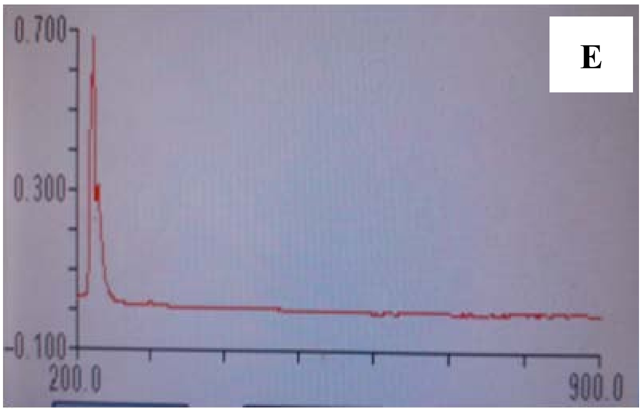
Ultra Violet Spectrophotometry Analysis











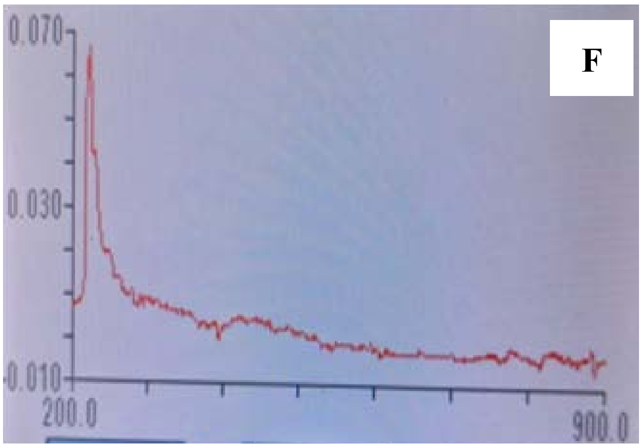
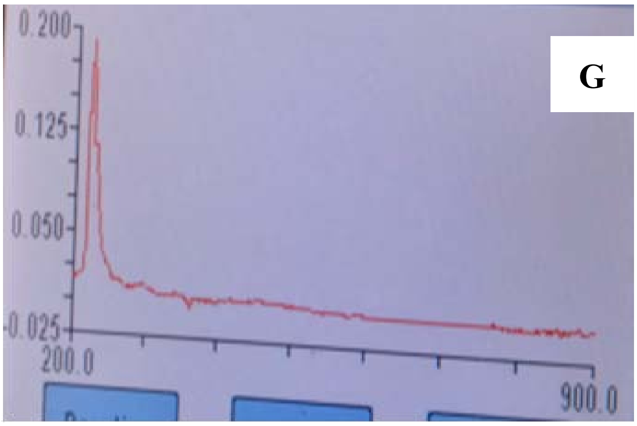
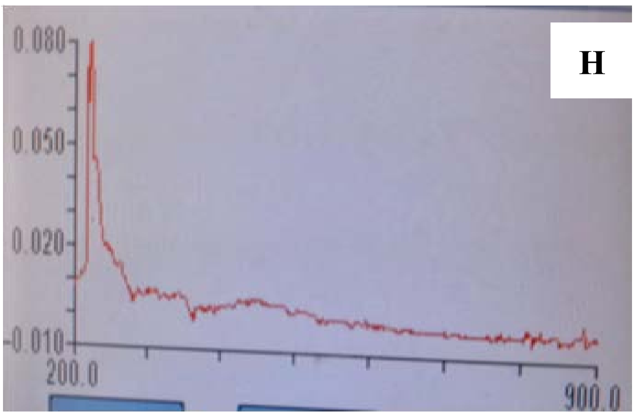
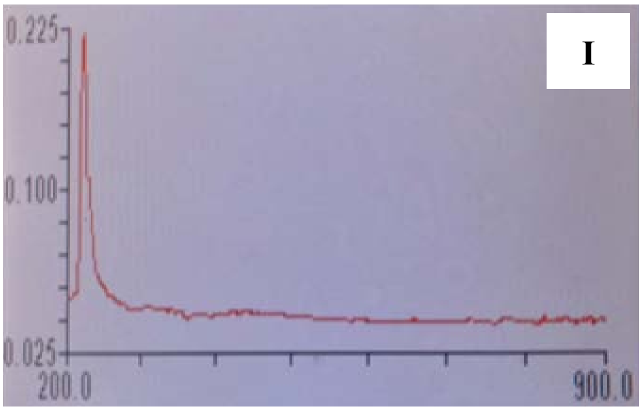


Figure 1: Utraviolet Spectral for water samples A-F showing Wavelength of Maximum Absorption (λmax)







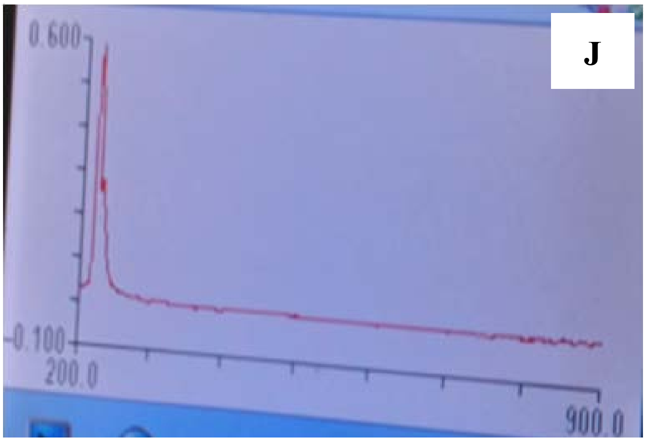


Figure 2: Utraviolet Spectral for water samples G-J showing Wavelength of Maximum Absorption (λmax)

GC-MS Analysis of composite sachet and bottles water samples

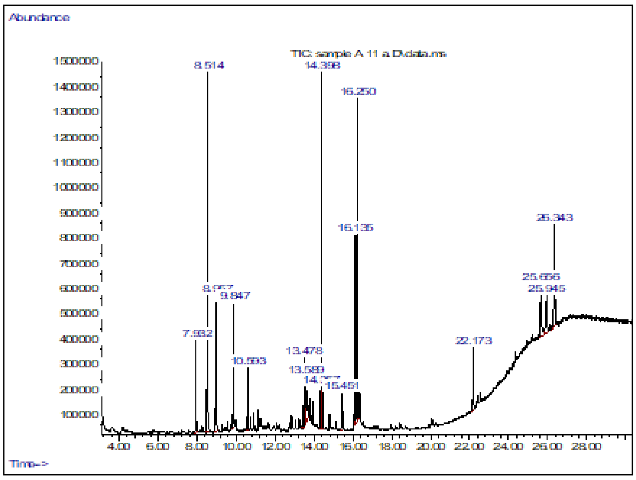


Figure 3: Chromatogram of composite sachet water samples

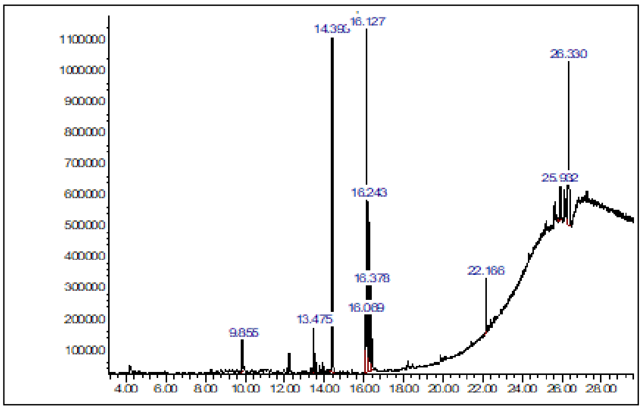


Figure 4: Chromatogram of composite bottled water samples

Table 1: Organic compounds detected in composite sachet water sample

PEAK NUMBER	RETENTION TIME (RT)	PEAK AREA (%)	COMPOUND
1	7.933	4.35	Copaene , Cubebene
2	8.511	16.59	Caryophyllene
3	8.958	6.28	Humulene
4	9.845	4.95	Naphthalene
5	10.594	2.97	Caryophyllene oxide
6	13.478	2.27	Neophytadiene, Hexadecyne Tetradecyne
7	13.587	3.95	Caffeine
8	14.359	1.49	Hexadecenoic acid, Methyl hexadec-9-enoate
9	14.399	15.71	Hexadecanoic acid
10	15.452	1.77	p-Camphorene
11	16.133	8.26	Octadecatrienoic acid
12	16.247	12.99	Eicosadiene
13	22.175	3.07	Supraene
14	25.654	4.27	Cyclotrisiloxane
15	25.946	3.92	HexamethylCyclotrisiloxane
16	26.341	7.16	Tetrasiloxane

Table 2: Organic compounds detected in composite bottled water sample

PEAK NUMBER	RETENTION TIME (RT)	PEAK AREA (%)	COMPOUND
1	9.856	2.29	Dodecanoic acid
2	13.478	2.34	Neophytadiene
3	14.394	21.68	Hexadecanoic acid
4	16.070	3.34	Octadecadienoic acid
5	16.127	24.98	Octadecenoic acid
6	16.242	13.01	Eicosadiene
7	16.379	6.64	Methyl stearate
8	22.164	3.51	Benzisothiazol-3-amine, Cyclotrisiloxane
9	25.935	3.42	Tetrasiloxane
10	26.330	18.78	Arsenous acid,

DISCUSSION

Organic contaminats determined by ultraviolet spectrophotometer

Evaluation of the chromophores of the organic compounds present in the sachet and bottled water samples were determined using the UV spectrophotometry according to Figures 1 and 2. It was observed that the chromophores of the compounds absorbed at wavelength of maximum absorption (λmax) of 222 nm for all the water samples. This common chromophore at λmax = 222 nm suggests the presence of conjugated dienes (loudon5ech15sec02.pdf, 2010), and also indicated that the groundwater source used by all the ten water producing companies in Ado-Ekiti is contaminated with similar organic compositions obtained from the same water table since no variation was observed.

Organic compounds determined by gas chromatography mass spectrometer

The chromatograms obtained from the composite water samples via gas chromatography mass spectrometry (GC-MS) were presented in Figures 3 and 4. Organic compounds found in the water samples were listed in Tables 1 and 2. Accordingly, sixteen (16) organic compounds were found in the sachet water composite sample while ten (10) were determined in the bottled water composite sample. The following organic compounds were found common in both the sachet and bottled waters: Neophytadiene, Hexadecanoic acid, Eicosadiene, Cyclotrisiloxane, and Tetrasiloxane. Neophytadiene is a diterpene that is 3-methylidenehexadec-1-ene substituted at positions 7, 11 and 15 by a methyl group. It has a role as an anti-inflammatory agent, an antimicrobial agent, a plant metabolite and an algal metabolite. It is an alkene and a diterpene. Neophytadiene is a natural product found in Gynura japonica, Tageteslucida, and other organisms. (National Center for Biotechnology Information, 2022). 1,4-Eicosadiene is a natural product found in Paronychia Kapela (National Center for Biotechnology Information, 2022). Palmitic Acid or hexadecanoic acid in IUPAC nomenclature is a saturated long-chain fatty acid with a 16-carbon backbone. Palmitic acid is found naturally in palm oil and palm kernel oil, as well as in butter, cheese, milk and meat. Palmitic acid is a metabolite found in Escherichia coli (strain K12, MG1655). Palmitic acid is a metabolite found in the aging mouse brain (National Center for Biotechnology Information, 2022). Cyclotrisiloxane is a cyclosiloxane, which are a class of silicone material. They are volatile and often used as a solvent. The three main commercial varieties are octamethylcyclotetrasiloxane

(D4), decamethylcyclopentasiloxane (D5) and dodecamethylcyclohexasiloxane (D6) (National Center for Biotechnology Information, 2022). Tetrasiloxane is an unbranched siloxane. (National Center for Biotechnology Information, 2022). A siloxane is a functional group in organosilicon chemistry with the Si−O−Si linkage. The parent siloxanes include the oligomeric and polymeric hydrides with the formulae $H(OSiH_2)_nOH$ and $(OSiH_2)_n$. The siloxane functional group forms the backbone of silicones, the premier example of which is polydimethylsiloxane. The functional group R_3SiO- (where the three Rs may be different) is called siloxy. Siloxanes are man made and have many commercial and industrial applications because of the compounds' hydrophobicity, low thermal conductivity, and high flexibility (Röshe, L. *et al,* 2003). Other organic compounds found only in the composite bottled water samples are: Dodecanoic acid, Octadecadienoic acid, Octadecenoic, Methyl stearate, Benzisothiazol-3-amine, and Arsenous acid. The presence of Arsenous acid is quite worrisome, especially when found in bottled water that most elites in the society drinks. Arsenous acid (or arsenious acid) is the inorganic compound with the formula H_3AsO_3. It is known to occur in aqueous solutions, but it has not been isolated as a pure material, although this fact does not detract from the significance of $As(OH)_3$. (Munoz-Hernandez, M.-A., 1994). Arsenic-containing compounds are highly toxic and carcinogenic. The anhydride form of arsenous acid, arsenic trioxide, is used as a herbicide, pesticide, and rodenticide (Harrington, C. *et al,* 1997; Abiodun A. Ojo *et al,* 2013). In the composite sachet water sample, other organic compounds found include Copaene, Cubebene, Caryophyllene, Humulene, Naphthalene, Caryophyllene oxide, Tetradecyne, Caffeine, Methyl Hexadecenoic acid, Hexadec-9-enoate, p-Camhorene, Octadecatrienenoic acid, Supraene, and Hexamethyl Cyclotrisiloxane. In general, most of these organic compounds have plant origin but their presence in potable water is undesirable and therefore regarded as contaminants and harmful. The water producing plants need to incorporate effective organic purification systems to remove these organic compounds, which are harmful contaminants from these drinking waters.

CONCLUSION

This study was carried out on ten drinking water samples (sachet and bottled) obtained from the southwestern city ofAdo-Ekiti in Nigeria. The UV-Visible analysis revealed a common organic chromophore having wavelength of maximum absorption (λmax) of 222 nm, likely to be conjugated dienes, for all the water samples. This evidence also suggested that the ground water source used by the ten water-producing companies had similar chromophore composition in its organic structure, from similar water table source. The sachet and bottled waters were found to have common organic compounds consisting of Neophytadiene, Hexadecanoic acid, Eicosadiene, Cyclotrisiloxane, and Tetrasiloxane. In addition to these, the composite bottled water samples contained Dodecanoic acid, Octadecadienoic acid, Octadecenoic, Methyl stearate, Benzisothiazol-3-amine, and Arsenous acid. The presence of Arsenous acid is quite worrisome, especially when found in bottled water that most elites in the society drinks. In the composite sachet water sample, other organic compounds found include Copaene, Cubebene, Caryophyllene, Humulene, Naphthalene, Caryophyllene oxide, Tetradecyne, Caffeine, Methyl Hexadecenoic acid, Hexadec-9-enoate, p-Camhorene, Octadecatrienenoic acid, Supraene, and HexamethylCyclotrisiloxane. The presence of a wide varieties of organic contaminants in both the sachet and bottled water composite samples suggest that the water producing companies need to invest in better water purification system in order to remove all the undesired chemical compounds, organic and inorganic materials, as well as biological contaminants from these drinking waters.

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