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MIGRATION AND DEGRADATION BY VOLATILE COMPOUNDS FROM SCENT LEAF (*Ocimum gratissimum*) ON POLYETHYLENE TEREPHTHALATE PACKAGED WATER

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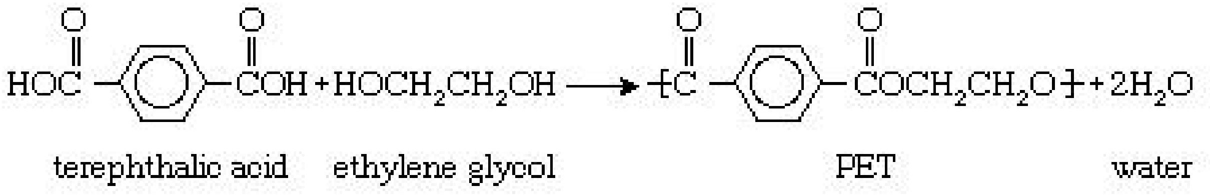
Abstract: Migration and degradation by volatile compounds from scent leaf (*ocimum gratissimum*) on polyethylene terephthalate packaged water was studied using dichloromethane for extraction(solvent extraction) of the analyte from water packaged in polyethylene terephthalate. GC-MS was used to quantify the components. A total of 24 compounds were identified and quantified in the experiment which included: 3 hydrocarbons, 1 polycyclic aromatic hydrocarbon, 5 alcohols, 2 ketones , 4 phthalate, 6 esters, and 3 organic acids. The amount of diisobutyl phthalate(2.20%) followed by 2-decanol (0.00992%), triethyl citrate (0.0429%), hexanedioic acid (0.0264%), 4 – dodecene-6,8,10-triyn-one (0.00233%), squalene (0.0184%) and pyrene (0.0106%). Nitrogen was the only component found in the control, since it was not stored with the scent leaf (*ocimum gratissimum*) . The result showed that polyethylene terephthalate are degraded by volatiles from plants. Hence, bottled and sachet water should be stored separately in homes,offices laboratories etc.

1. INTRODUCTION

Water is one of the most essential commodities needed for the survival of eco-system (Saleh *et al.*, 2001). It is very abundant in nature as its occupies about 70 % of the earth's crust. However, safe drinking water is scarce hence the need for processing, treatment and proper packaging of water before consumption. Despite its relative abundance, good quality drinking water is not readily available to man (Onweluzo andAkuagbazie,2010). According to Ajewole (2010) about 1.2 billion people lack access to portable water worldwideand while only about 30 % of the Nigerian populace have access to clean drinking water.The non availability of good quality drinking water has resulted into a number of health challenges as water is known to be a primary causative agent of many contagious diseases. In developing countries of the world, 80 % of all diseases and over 30 % of deaths are related to drinking water (Onweluzo and Akuagbazie,2010; Olaoye and Onilude, 2009). Research have shown that when clean water and needed hygiene condition are provided, the chances of occurrence of diarrhea, sleeping sickness and guinea worm infestation can be eliminated or prevented by 50, 80 and 100 % respectively (Alhassan and Ujoh, 2012). This insufficiency of water supply has given rise to the involvement of private individuals in the production of packaged drinking water (Pure water) (Dada, 2009). The advent of sachet water has significantly helped in tackling the insecurity associated with household drinking water supply with the renewed global commitments towards the achievement of millennium development goals (MDGs) by 2015 (Ndinwa *et al.,* 2012). Commonly sachet water is known to be safe and instant means of quenching taste. This water is now common in Nigeria, Ghana and other bordering West Africa Countries (Cheabu and Ephraim, 2014). Sachet water is usually consumed without further processing especially during the dry and hot seasons in Nigeria. In addition to the prevalence of sachet water, bottled water are also widely consumed in many parts of the world by the huge number of urban populace due to its pleasant taste, absence of odour and the believe that it is mostly free of germs. Bottled water are also consumed due to water scarcity resulting from natural disaster such as earthquake, tsunami, flood, drought and hurricane or other forms of societal disaster like terrorist attack, war outbreak, sabotage and blockage that are capable of obstructing public and private water supplies for extented period of time (Guler 2007; Guler and Alpaslan, 2009). Constant and periodic assessment of packaged drinking water is needed to satifactorily enlightened the consumers about quality.(Alhassan and Ujoh, 2012; Cheabu and Ephraim 2014). National and international organization standard have been explicitly developed for safe drinking water quality. Virtually all available standards have upper limit for physical, chemical and microbiological properties which when exceeded are dangerous and have the potential of been harmful to the end users. The hygiene of the enviroment and conditions under which majority of the brand of packaged water are produced and stored are faced with a number of uncertainties (Ndinwa *et al*., 2012). According to Aino Pelto-Huikko *et al* (2021) A brand-new office building in Rauma, Finland, was used to study the first five years of PEX-a drinking water pipes in normal use. Both pipe material and water samples from hot and cold-water pipelines were analyzed. Migration of volatile organic compounds (VOC) from the PEX-a pipes into the drinking water was observed to decrease rapidly during the first months. PEX-a material were observed to be deteriorating due to the wearing down of organic antioxidants added into the PEX-a material during the manufacturing of the pipes. Tert-butyl alcohol (TBA) concentrations were said to be high during the first months after commissioning of use. The stagnation time of the drinking water in contact with the PEX-a material before the actual water sample was taken had a severe impact on analyzed migration of organic compounds. Hence, they concluded that the amount of organic compounds able to migrate from materials into the drinking water will increase when the stagnation time is increased. Pelto-Huikko,A *et al* (2021), took the water samples after overnight stagnation. They advised to run water properly before drinking it. Latva, M *et a*l(2017) reported that water quality in Scandinavia has low alkalinity and hardness, and is consequently corrosive to the metallic materials. They said, brass materials used in drinking water systems have been under discussion because of the quantity of the lead and it's sighificant migration into drinking water. Latva, M *et a*l(2017), studied, the use of non-dezincification resistant brass alloy CuZn40Pb2 (CW617N) in drinking water systems in Rauma, Finland by using real-life distribution network built in the office building Technology Center Sytytin.

1.1 Polyethylene terephthalate (PET)

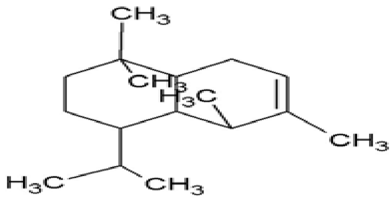
PET is the material most commonly used to make the clear plastic bottles in which bottled/sachet water is sold. The contents of the PET bottle, and temperature at which it is stored, both appear to influence the rate and magnitude of leaching of organic and inorganic compounds from pet bottle (Schmida *et al.*, 2008), PET is produced by the polymerization of ethylene glycol and terephthalic acid. Ethylene glycol is a colourless liquid obtained from ethylene, and terephthalic acid is a crystalline solid obtained from xylene. When heated together under the influence of chemical catalysts, ethylene glycol and terepthalic acid produce PET in the form of a molten, viscous mass that can be spun directly to fibres or solidified for later processing as a plastic. In chemical terms, ethylene glycol is a diol, an alcohol with a molecular structure that contains two hydroxyl (OH) groups, and terephthalic acid is a dicarboxylic aromatic acid, an acid with a molecular structure that contains a large, six-sided carbon (or aromatic) ring and two carboxyl (CO_2H) groups. Under the influence of heat and catalysts, the hydroxyl and carboxyl groups react to form ester (CO-O) groups, which serve as the chemical links joining multiple PET units together into long-chain polymers. Water is also produced as a by-product. The overall reaction can be represented as follows:



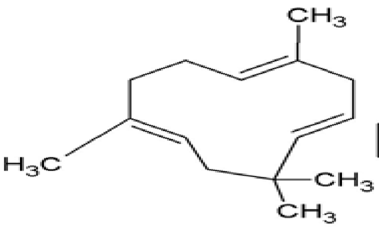
1.2 Ocimum gratissimum

Ocimum gratissimum belong to the *Lamiacae* family and are made up of several species. They are diverse in aroma and flavor and the herb may be used fresh or after drying to flavor foods, or aromatic compounds may be extracted and used for food flavoring and preservation, pharmaceuticals, cosmetics and as a source of natural pesticides (Paton et al., 1999).Ocimum includes annual and perennial herbs, as well as shrubs endemic to the tropical and subtropical regions of Asia, Africa and Central South America (Darrah, 1998).It is a perennial plant that is woody at the base. It has an average height of 1-3m high. The leaves are broad and narrowly ovate, usually 5-13cm long and 3-9cm wide. It is a scented shrub with lime-green fuzzy leaves. (Wagner *et al*., 1999) . Lawrence (1993) and Grayer *et al*. (1996) proposed chemotype classification based on volatile oil (aromatic portion) composition. In this classification they separated basil chemotypes on the basis of the major aromatic compound, whose relative percentage was 20-50% of the total oil. This percentage composition of the essential oil was based on gas chromatographic analysis.*O. gratissimum* is important economically and used as medicine and insecticide and was found to have sedative and anticonvulsant effects. Also, it is used as medicines to treat central nervous system diseases in the tropical part of the world as well as for oil production and as a pot herb (Freire, 2006).The oils are used in the treatment of many ailments, including upper respiratory tract infections, diarrhea, headache, fever, cough, eye problems, skin diseases, and pneumonia. The oil is also a potent antidiabetic agent.In folk medicine, Ocimum gratissimum is extensively used throughout West Africa as a febrifuge, anti- malarial and anti- convulsant. The crushed leaf juice is used in the treatment of convulsion, stomach pain and catarrh. Oil from the leaves have been found to posses antiseptics, antibacterial and antifungal activities. (Pino *et al.*, 1996). In the coastal area of Nigeria, the plant is used in the treatment of epilepsy, (Osifo, 1992), high fever (Oliver 1980) and diarrhea (Oliver, 1980 and Sofowara, 1993). While in the savannah areas decoctions of the leaves are used to treat mental illness (Abdulrahman, 1992).Ocimum gratissimum is used by the Ibos of southern Nigeria in the management of the baby’s cord. It is believed to keep the baby’s cord and wound surface sterile. It is used in the treatment of fungal infections, fever, cold and catarrh. (Iwu, 1986). Clinical trials in creams formulated against dermatological disease have yielded favorable result (Edeoga and Eriata, 2001). Nutritional importance of this plant centers on it’s usefulness as a seasoning because of its aromatic flavor. (Pino *et al.*, 1996).Photochemical evaluation of this plant has shown that it is rich in alkaloid, tannis, phytates, flavonoids and oligosaccharides. It has tolerable cyanogenic content (Ijeh *et al*., 2004). The volatile aromatic oil from the leaves consists mainly of thymol (32-65%) and eugenol; it also contains xanthones, terpenes and lactones (Pino *et al.*, 1996). Characterization of its ethanolic extracts revealed the presence of non – cyclic sesquiterpenes, phenols (Esvanzhuga, 1980).Clinical trials in creams formulated against dermatological disease have yielded favorable result (Edeoga and Eriata, 2001). Nutritional importance of this plant centers on it's usefulness as a seasoning because of its aromatic flavor. (Pino *et al.*, 1996).Aroma of scent leaf (Ocimum gratissimum) has a strong, pungent, sweet and somewhat menthol aroma.

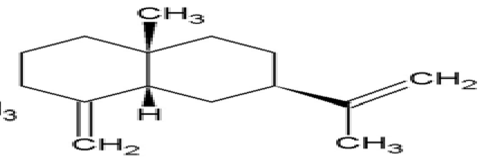
1.1.3 List of Biologically Active Compounds that have been Isolated from *O. Gratissimum*



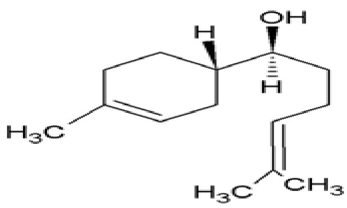
Alpha copaene



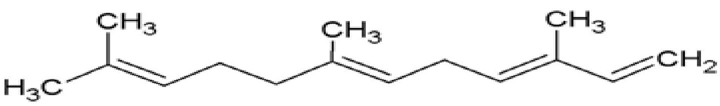
Alpha humelene



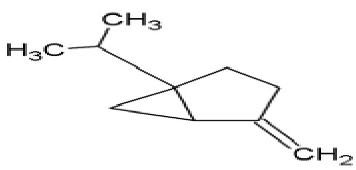
Beta selinene



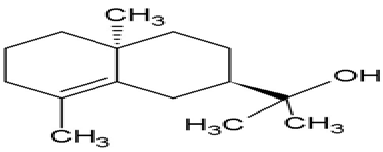
Bisabolo



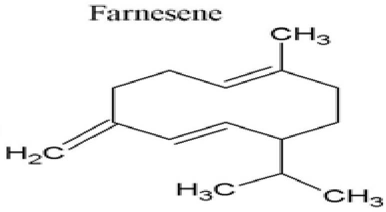
Farnesene



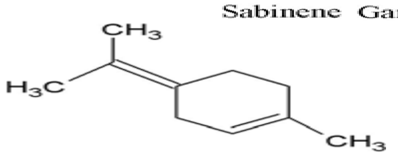
Sabinene



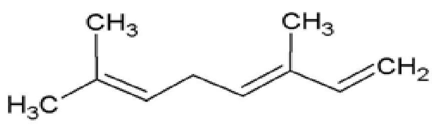
Gamma eudesmol



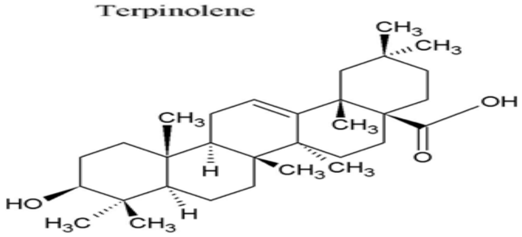
Germacrene D



Terpinolene



Ocimene



Lin *et al.*, (2000). Worked on the effect of temperature on the degradation of the component of the long chain backbone of the polymer system, and finds out that thermal degradation is temperature dependent and it occurs more rapidly at high temperature. Wegelin *et al.*, (2001) worked on the effect of high temperature and UV radiation on the quality of bottled water and discovered that PET degradation product such as terephthalate monomer and dimers were formed on the surface of the bottle with likelihood of leaching. Nawrocki*et al*.,(2002) worked on the leaching of PET containers on bottled and sachet water and find out that time is a dominant factor governing the release of organic substances. Mutsuga *et al*.(2006). Suggested that the formaldehyde and acetaldehyde forming during the polymerization reaction and the hot step process in the bottled water manufacture and discovered that substance relative to additives used in the plastic material processing have been reported in water packaged in PET.Mufeed (2006) reported that bottled water quality are subjected to intensive investigation in many countries in order to evaluate its suitability for consumption and observed that the water may vary from one sources to another based on several parameters such as water sources, types of water purification and storage tanks. Rusz *et al.*, (2006). Studied the effect of sunlight on bottled water and observed an increase in the value of electrical conductivity, total dissolve solid, chemical oxygen demand, nitrate and ammonium ion with increasing exposure time. Amobi *et al.,* (2007) worked on sachet and plastic-bottled water exposed to heat above room temperature to contains cancerous substances and discovered that the heat from the sun could melt some of the substance used in making the polythene bags which is made of synthetic petroleum, since the polythene bag are weather sensitive.

Lena *et al.,(*2007), Suggested that plastic bottles in water and soda bottles can release antimony and bisphenol A, if exposed to heat over a long period of time. Farhoodi *et al*.,(2008) studied the interaction of incubation time with storage temperature on the leaching of DEHP(di(2-ethylhexyl)adipate) from PET bottles and find out that PET bottles may yield endocrine disruptors under conditions of common use, particular with prolong storage and elevated temperature.Montuori *et al.,* (2008), worked on the presence of phthalic acid in water stored in PET bottles and reported that phthalic acid was the most abundant phthalate found in bottled water with a minimum level of 3.50µg/L and also find out that concentrations of phthalates in samples bottled in PET bottles were 20 times higher than those from glass bottles directly analyzed after purchase. Schmida *et al.,* (2008a) worked on the content of polyethylene terephthalate (PET) bottles at varying temperature and discovered that the contents of the PET bottle, and temperature at which it is stored, both appear to influence the rate and magnitude of leaching of organic and inorganic compounds from PET bottle. Schmida *et al.*,(2008b) sought to determine whether solar water disinfectant (SODIS) would promote leaching of phthalate into water in PET bottles and discovered that the content of the bottles and temperature influences the rate of leaching of organic and inorganic compounds from the PET bottles. Bach *et al.*, (2009)tested water bottle after exposure to extreme conditions of high temperature and UV radiation to accelerate the possible migration of substances and find out that genotoxic and estrogenic activities in PET bottle and chemical mixture in bottle water have been reported.Daniel *et al*., (2011) studies the phytochemical analysis and mineral elements composition of *Ocimum basilicum* and discovered that *ocimum gratissimum* contains bioactive compounds and minerals that could enhance the curative process of health.

Amiridau and Voutsa, (2011) worked on the migration of phthalates in food, beverages and bottled drinking water and discovered that endocrine disrupting potential and phthalate such asbenzyl butyl phthalates (BBP), dibutyl phthalate (DBP) and diisobutyl phthalate (DiBP) have been found to elicit estrogenic responses in vitro assays.Sulaiman *et al.,* (2011) worked on the effect of storage temperature and sunlight exposures on the physiological properties of bottled water and find out that exposure to sunlight and temperature at which it is stored causes changes in all physiochemical properties of water in the plastic bottle. Adewole (2014), worked on the proximate and Phytochemical constituents of *Ocimum gratissimum* and discovered that the presence of high secondary metabolites in the leaves are good indication that if the plant is subjected to further research and characterization, bioactive compounds with strong biological activities may be isolated and novel compounds may also be discovered. Yanagimoto, Lee, Ouchi, & Shibamoto. (2002)

showed that volatile chemicals or extracts dissolved in the organic solvent, dichloromethane, can easily be evaluated for their antioxidant potential. Sharkey and Yeh (2001) have shown that plant leaves are a major source of volatile organic compound emitted in the atmosphere. Latva, M.*et al*(2016), studied the influence of altering magnetic field on chemical properties of water, scale formation and morphology using polyethylene and copper pipes located both in a laboratory pilot-system and in an apartment complex formed by five different buildings each having four or five different homes. It was reported that the pilot network, magnetic field reduced calcium scalingby15% in both studied piping materials and the surface film on the copper pipe appeared to be less treaty by the magnetic exposure.

2. MATERIALS AND METHODS

2.1 MATERIALS

Fresh leaves of *Ocimum gratissimum*,Weighing balance, Dessicator, Syringe(10mL),Sachet water, Beaker, Extraction bottle, Petri dish**,**separating funnel

2.2 METHODS

2.2.1 SAMPLE PREPARATION

Fresh leaves of *Ocimum gratissimum* were rinsed with running tap water to remove dust and other impurities. The extract were squeezed from the ground leaves. 55.4g scent leaf was weighed on a weighing balance with which was then kept in a dessicator with the sachet water for 48hrs (two days) at room temperature (30^{o}C).

2.2.2 SAMPLE ANALYSIS

Liquid liquid extraction technique was applied to extract the analyte from the aqueous phase using dichloromethane. It was then taken for GC-MS analysis.

2.3 EQUIPMENT

GAS CHROMATOGRAPH / MASS SPECTROMETER (GC-MS)
MODEL: AGILENT GC 7890B / 5977C TRIPLE AXIS MSD
Oven Condition:
Initial Temperature: 50^{o}C FOR 5mins
Ramp to 310^{o}C @ 15^{o}C/min for 22mins.:
Heater 280^{o}C **Inlet Temperature**
Pressure 40.6psi
Splitless mode
Purge flow 15ml/min at 2min
Septum purge 10.5ml/min
MSD Transfer line Temperature = 300^{o}C
MS Quad Temperature = 180^{o}C

3. RESULTS AND DISCUSSION

3.1 Results

The results obtained are given on the tables 1and 2 below

Table 1. Quantification of compounds identified in the water by GC-MS analysis.

COMPOUNDS	RT(mins)	AMOUNT (%)
2-Decanol	14.2724	0.00992
4-Dodecene-6,8,10-triyn-one	19.6333	0.00233
Hexanedioic acid	16.8259	0.0264
Silane, diethylheptyloxyoctadecyloxy	21.2534	0.0442
Pyrene	16.7444	0.0106
Bis(2-ethylhexyl)ester	16.8259	0.0264
Hexane-3,3-dimethyl	13.6593	0.0118
Triethyl citrate	13.1418	0.00429
2- Ethyl-1-hexanol	12.2483	0.00416
Risperidone	20.3140	0.00106
Diisobutyl phthalate	14.4372	2.20
Squalene	18.6453	0.0184
10-chloro-1-decanol	18.4552	0.00105
Dibutyl phthalate	15.1427	0.7350
3,9-acridinediamine,7-ethoxyl	15.1810	0.00111
2,2,2-trichloroethyl ester	17.4282	0.000948
a-Ethoxypropoinic acid	19.2082	0.00306
Enterodiol	18.0511	0.000825
Dodecane-2,7,10-trimethyl	14.8623	0.0269
Bis(2-methylpropyl) ester	13.0175	0.00236
L-(-)-Arabitol	17.5157	0.00237
Bis(2-ethylhexyl) phthalate	17.9971	0.116
2-(4-methoxyphenyl)propane	17.0285	0.00394
Isobutyl methyl phthalate	13.4005	0.00733

Table 2. Quantification of control identified byGC-MS analysis

COMPOUNDS	RT(mins)	AMOUNT (%)
Nitrogen	5.5726	0.0750
Nitrogen	5.5277	0.0379

3.2 Discussion

After the analysis of the sample, a total of 24 compounds were identified and quantified including: 3 hydrocarbons, 1 polycyclic aromatic hydrocarbon, 5 alcohols, 2 ketones, 4 phthalate,6 esters, and 3 organic acids. The compounds found in greatest amount were Diisobutyl phthalate (2.20%) followed by 2- decanol (0.00992%), triethyl citrate (0.00429%), hexanedioic acid (0.0264%), 4 –dodecene-6,8,10-triyn-one (0.00233%), squalene(0.0184%), and pyrene(0.0106%). Nitrogen was found in the control. Menthol components from the crushed scent leaf which is the main source of the odour and flavour in scent leaf is stable in aqueous solution, hence remains in the solution due to its high lipophilic character.The volatile compounds of the crushed scent leaf aided the degradation of the polyethylene terephthalate thereby leaching different organic compounds into the water packaged in PET which is hazardous to the human health. Farhoodi *et al* (2008) confirmed that the leaching of DEHP (di(2-ethyl hexyl)phthalate along with other phthalates such as isobutyl methyl phthalate(IBMP), dibutyl phthalate(DBP) and diisobutyl phathalate may yield endocrine disruption and may have lasting effects on reproductive functions for both childhood and adult exposures. A Preliminary Study of the Migration of Volatile Components from Crushed Garlic *(Allium sativum)* in to Polyethylene Terephthalates Packaged water was done by Orodu et al (2017). The result showed the presence of fifty three (53) different components which includes phthalates, citrate esters, saturated hydrocarbons, siloxanes, amides and other water soluble volatile compounds from garlic.

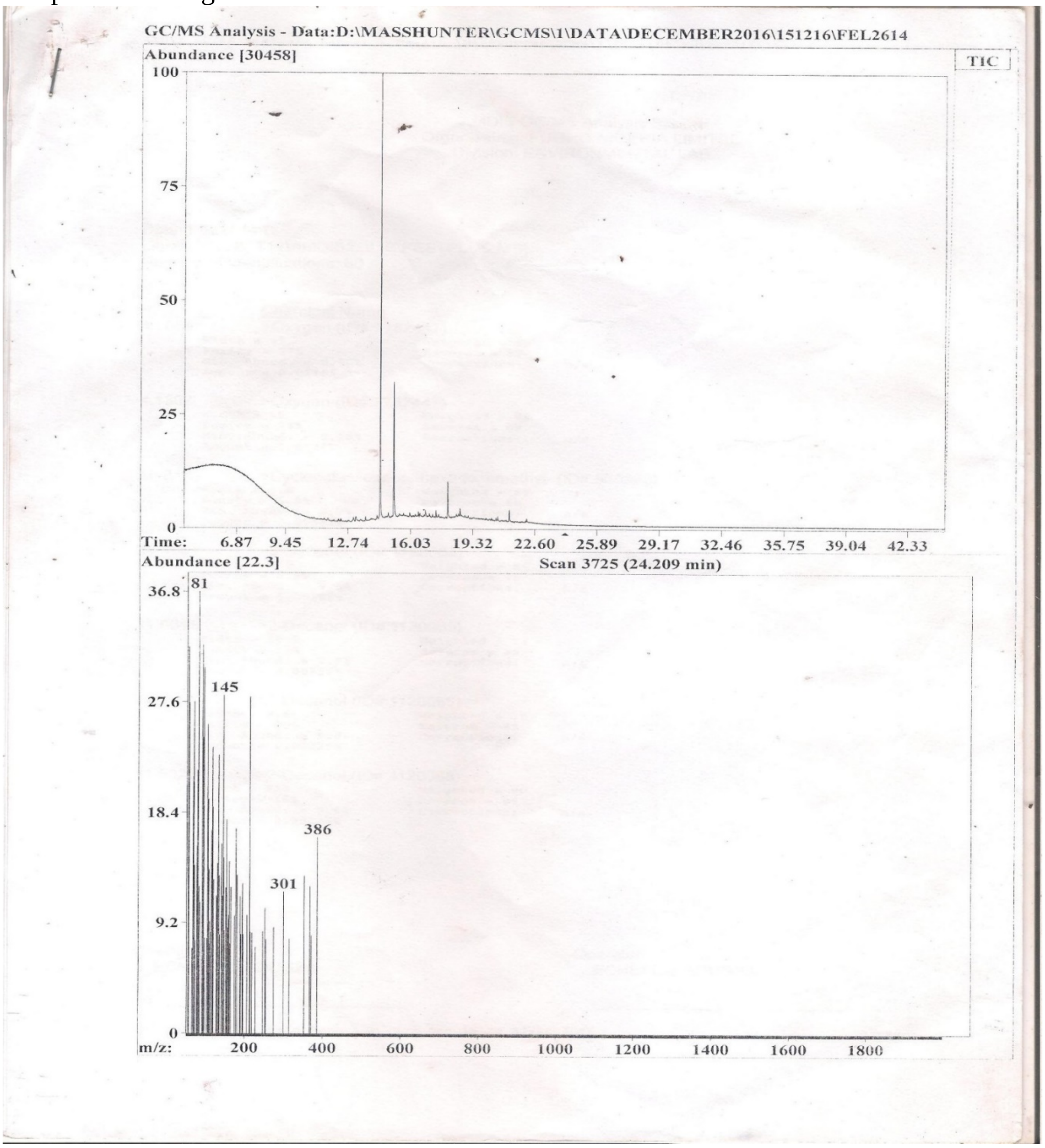


Figure 1 Chromatogram of Analyte obtained by GC-MS analysis

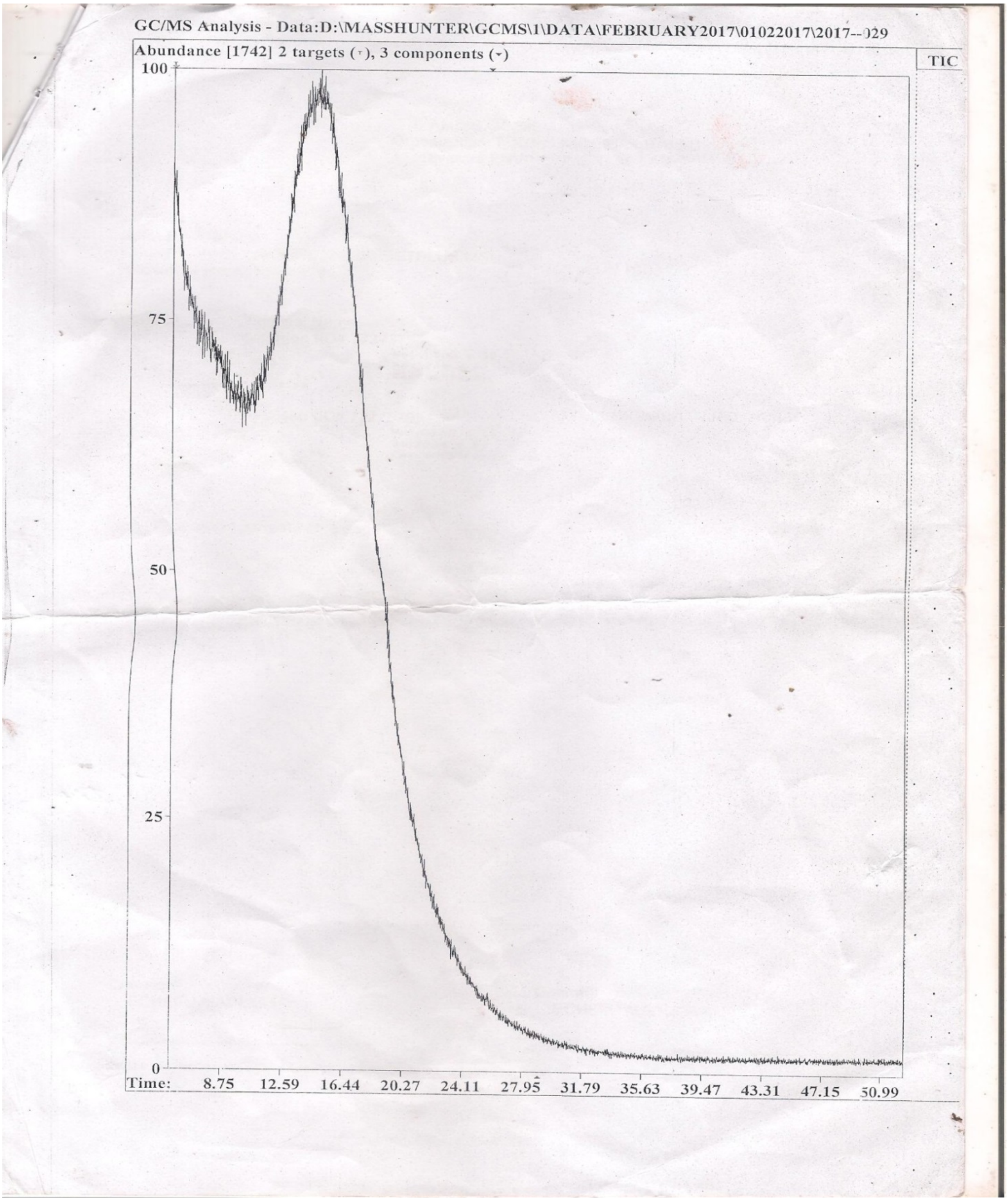


Figure 2 Chromatogram of control obtained by GC-MS analysis

4. Conclusion

GC-MS analysis revealed the presence of leachates from the sachet PET. volatile compounds from crushed scent leaf degraded the polyethylene terephthalate sachet. The volatile compounds of the crushed scent leaf aided the degradation of the polyethylene terephthalate thereby leaching different organic compounds into the water packaged in PET which may be harmful to human health. However, it is important to note that water packaged in polyethylene terephthalate should not be stored with other substances that have volatiles which are capable of degrading the water containers. It is advisable to store polyethylene terephthalate packaged water in less adverse condition.

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