

University of Modena and Reggio Emilia

PhD School in AgriFood Sciences, Technologies
And Biotechnologies

**Safety evaluation of commercial flexible
packaging materials via exposure assessment
of Non-Listed and Non-Intentionally-Added-
Substances**

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Keep calm and carry on

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**Safety evaluation of commercial flexible packaging materials via
exposure assessment of Non-listed and Non-Intentionally Added
Substances**

Abstract

Increased attention has been placed in the last years on safety of food packaging materials. Often the mere presence of substances, even in minute quantity, not specifically addressed by the existing legislation (such as inks components or plastics manufacturing by-products) is perceived as “risky” and may trigger food contamination alarms. However, most of the conclusions that are drawn regarding the potential risk represented by these substances are based on default consumers’ exposure figures, i.e. assuming that each consumer would eat one kilo of food per day, where the concerned substance migrates at its highest rate, and this for the entire consumer’s life. This is in fact an unrealistic assumption which greatly over-estimates the actual exposure of consumers to the said substances. In 2005 the four major European Associations representing the plastic packaging industries, i.e. the *European Plastics Converters Association*, *Plastics Europe*, *Flexible Packaging Europe* and *CEFIC-Food Contact Additives* panel, started a project aimed at developing a tool capable to better estimate the actual

consumers exposure to non-regulated and non-intentionally added substances, which are present in plastic food packaging. This exercise, known as “Matrix Project” ended in 2011. It was based on food intake data of five European Countries (Italy, UK, France, Germany and Spain), as well as packaging use data collected by contracted market research companies, and resulted into a calculation tool which can provide a better estimation of the actual exposure to these substances.

The thesis shows insights on the exposure concept, as applied to food contact materials, and also how the Matrix tool can be used in practice to assess the risk from non-regulated and non-intentionally added substances migrating from them.

A number of examples of risk assessment were provided, as applied to commercial flexible packaging materials, especially multi-layers both composed entirely by plastics and combination of plastic and other materials (paper, aluminum, adhesives), printed and non-printed.

**Valutazione della sicurezza di materiali commerciali di imballaggio,
attraverso la valutazione dell'esposizione di sostanze non listate e
non intenzionalmente aggiunte**

Abstract

Negli ultimi anni è stata posta maggiore attenzione in materia di sicurezza dei materiali di imballaggio alimentare. Spesso la sola presenza di sostanze, anche in minima quantità, non specificamente valutate dalla normativa vigente (come componenti inchiostri o sotto prodotti di produzione) è percepito come "rischio" e può attivare allarmi riguardo contaminazione degli alimenti. Tuttavia la maggior parte delle conclusioni che vengono tratte per quanto riguarda il rischio potenziale rappresentato da tali sostanze sono basate su valori di esposizione predefiniti dei consumatori, i.e. assumendo che ogni consumatore dovrebbe mangiare un chilo di cibo al giorno, in cui la sostanza in questione migra al suo tasso più alto, e questo per l'intera vita del consumatore. Questo è in fatti un presupposto realistico che ha notevolmente una sovra stima dell'effettiva esposizione dei consumatori alle sostanze suddette. Nel 2005 le quattro principali Associazioni europee che rappresentano le industrie di imballaggio di plastica, ossia *European Plastics Converters Association, Plastics Europe, Flexible Packaging Europe* and *CEFIC-Food Contact Additives*, hanno avviato

un progetto volto a sviluppare uno strumento in grado di valutare meglio l'effettiva esposizione dei consumatori di sostanze non regolamentate non intenzionalmente aggiunte, che sono presenti in un imballaggio di plastica per alimenti. Questo esercizio, noto come "Progetto Matrix" si è concluso nel 2011. Esso si basa su dati di assunzione di cibo di cinque Paesi europei (Italia, Regno Unito, Francia, Germania e Spagna), nonché i dati di utilizzo di imballaggio raccolti da società di ricerche di mercato, e ha portato allo sviluppo di uno strumento di calcolo che può fornire una migliore stima dell'effettiva esposizione a queste sostanze.

La tesi mostra approfondimenti sul concetto di esposizione, applicato ai materiali a contatto con alimenti, e come Matrix può essere utilizzato in pratica per valutare il rischio di sostanze non regolamentate e non intenzionalmente aggiunte che possono migrare dall'imballaggio all'alimento.

Sono forniti inoltre un certo numero di esempi di valutazione del rischio, applicato a materiali commerciali d'imballaggio flessibili, in particolare materiale multi-strato sia composto interamente da plastica che composto da una combinazione di plastica e altri materiali (carta, alluminio, adesivi), stampati e non.

PREFACE

The work presented in this PhD thesis has been mainly carried out in collaboration with the University of Modena and Reggio Emilia, at the research center of **Sealed Air corporation** -Passirana di Rho Italy- under the direction of Dario Dainelli -*Regulatory Affairs Director*- and the supervision of Stefania Torella -*Senior Analyst*- and Maria Grazia Guerini -*Regulatory Affairs Expert*.

A fruitful part of this PhD research has been done thanks to the collaboration with IRCpack s.r.l with the precious help of Valter Rocchelli, and thanks also to Giflex - *Italian Association of Manufacturers of Flexible Packaging* - and his President Italo Vailati. Giflex has provided the possibility to work by applying the Matrix exposure tool to the data that they have obtained from a project conducted at IRCpack.

In the following pages we will present an overview of the experiments dealing with transfer of substances from packaging material into foodstuffs; subsequently an overview of the Matrix project will provide the background of the theoretical consideration that have been applied through this work. The exposure evaluation approach proposed by the *Matrix project* was used in the course of this work for the risk assessment of Non-Intentionally-Added-Substances (**NIAS**) or Non-Listed-Substances (**NLS**).

1. INTRODUCTION

Packaging material may be a contamination source of food due to the migration of chemicals and additives in certain conditions of application. Polymers contain free monomers of various chemical nature (whether they are homo-polymers or co-polymers), that may be transmitted to food, along with a variety of volatile, semi-volatile or non-volatile “additives”. These substances may be present intentionally in the polymeric matrix, such as coloring agents, fillers, plasticizers, light stabilizers, antioxidants etc. or their presence may be unintentional, for example in the case of impurities, breakdown of polymers or additives during processing, reaction products, but also residues and oils in adhesives or in printing inks, or compounds adsorbed during storage.

The manufacturers of Plastic Food Contact Materials and Articles always exert great attention to ensuring consumers safety through constant control of their products. It however may happen that the mere presence of substances, even in minute quantity, of **NIAS** or **NLS** is perceived as “risky” and may trigger food contamination alarms.

To control potentially harmful contamination and protect the consumers health a full regulatory framework has been developed by the Italian and EU authorities. The most recent regulation that consolidates all previous directives and regulations on plastic food-contact materials, and implement some significant changes, was issued in 2011, being

Regulation (EU) No 10/2011 on Plastic Materials and Articles Intended to come into Contact with Food—commonly referred to as the Plastics Implementing Measure (*PIM*). Such regulation was published in the Official Journal of the European Union on January 15th, 2011 and came into force on February 4th, 2011. The *PIM* regulation replaced the previously existing Plastics *Directive* (2002/72/EC) and its amendments, as well as various Directives on migration testing. Because of its legal nature, *Regulation (EU) 10/2011* became directly applicable in all of the EU Member states as of May 1st, 2011.

Due to the introduction of numerous substantive changes, as well as modifications to the migration testing scheme to the existing food a suitable transition time has been provided; in fact such Regulation will be fully in place as from January 1st, 2016.

Under the provisions of the Regulation, a number of substances present in food contact plastics are exempted from the requirement to be included in the Community positive list (Union list) according to the article 6. The substances exempted of positive listing are various and include solvents, colorants, Polymer Production Aids (PPA's), Aids to Polymerization (AP's), oligomers and the “Non-Intentionally-Added-Substances”. The non-listed substances are subject to the provisions of Article 3 of the Framework *Regulation (EC) No 1935/2004* that applies to all food contact materials. Article 3 states that exposure to substances

from food contact material should not pose a risk to human health. For non-listed substances this should be demonstrated through a risk assessment and documented in the internal supporting documentation package to the Declaration of Compliance. Article 19 of the Regulation articulates the need for a risk assessment for non-listed substances in accordance with internationally recognized scientific principles on risk assessment [1].

2. AIM OF STUDY

In 2005 the four major European Association representing the plastic packaging industries, i.e. the European Plastics Converters Association, Plastics Europe, Flexible Packaging Europe and CEFIC - Food Contact Additives panel, started a project aimed at developing a tool capable to better estimate the consumers actual exposure to non regulated and non intentionally added substances, which are present in plastic food packaging. This exercise, known as “*Matrix Project*” ended in 2010. It was based on food intake data of five European Countries (Italy, France, Germany, Spain and UK), as well as packaging use data collected by contracted market research companies, and resulted into a calculation tool which can provide a better estimation of the actual exposure to these substances.

The aims of this study are the following:

- to analyze and identify the NIAS and NLS compounds that could migrate from commercially available flexible packaging materials, provided by **Giflex** -*Italian Association of Manufacturers of Flexible Packaging*- into food. This task was accomplished through **GC-MS** analysis in a semi-quantitative mode;
- to assess any potential health risk from these substances, through the exposure evaluation approach proposed by the *Matrix*

approach;

- to provide insights on the exposure concept, as applied to food contact materials, showing in a very practice way how the Matrix tool can be used to assess the risk from NIAS and NLS migrating from them.

3. CHEMICAL MIGRATION INTO FOOD

The packaging material has the prime function to protect food from contamination and spoilage by external agents such as pests, odors, micro-organisms, light and oxygen, but at the same time the packaging is a source of contamination from chemical through migration of components. Due this latter function packaging is beneficial and necessary to guarantee the shelf-life of food products.

Is very important that food contact material (FCM) does not transfer substances to the foodstuff that may represent a risk for the health, however for many years no tools were available to determine whether the substances that migrate to food may or may not be regarded as a source of risk. The reason for that resided in the absence of systems that were capable to estimate the exposure of consumers to these substances. Food and beverages can be very aggressive products and may interact strongly with materials that they are in contact, releasing chemical constituents even in minute amounts. The chemical migration into food is very important and it can represent a critical issue because it can have an impact on the food safety, as well as food quality. Exposure represents the measure of the potential risk associated to migrating substances; the mere presence of a substance does not tell much about the potential risk if isn't known the occurrence of that substance in the diet that is ingested daily by a consumer. As concerns the impact on the

food quality level, the migrating substances may for instance impart odors to the food packed reducing by this way consumer appeal.

3.1. Migration definition and mechanistic

“Migration” in English and many other languages, derives from the latin verb *Migrare*- prime meaning, to remove or depart (to another place), and the noun *Migratio*- prime meaning, removal or changing of habitation. In the modern language the word was extended to cover physical and chemical science to describe the movement of small particles – atoms, ions, molecules- within a relatively static matrix or across the boundary, especially under the influence of an electric field. A wider definition of Migration is the following: *Migration of chemical substances is a mass transfer from an external source into food by sub-microscopic process.*

As a general rule, the effects of migration are not desirable and the material migrating is often described as a contaminant. Migrant describes a substance which undergoes migration in a particular situation. [2]

Is it important to understand the factors that control chemical migration, and they can be summarized as follows:

- composition of the packaging material;
- the nature and extent of contact;

- the nature of the food;
- the temperature of contact;
- the duration of contact.

3.1.1. Composition of the packaging material

Food contact materials are generally classified into ten main categories as reported below:

1. plastics, including varnishes and coatings;
2. paper and board;
3. metals and alloys;
4. glass;
5. regenerated cellulose;
6. ceramics;
7. elastomers and rubbers;
8. paraffin waxes and micro-crystalline waxes;
9. wood, including cork;
10. textile products.

Plastics in particular have an interest, especially considering the fact that many paper and board packages are laminated to plastics as the food contact surface and most metal cans are lacquered inside with polymeric coatings to protect the metal from the food.

The intrinsic properties of the packaging material itself are important

consideration and the extent of any migration depends first on the concentration of the chemical in the packaging. It is very important to consider also the mobility of a chemical in the packaging material, which depends on the size and shape of the molecule, on interaction it experiences with the material, and on the intrinsic resistance to mass transfer that the material presents. It is assumed that the chemical is compatible with the material. If the chemical is not compatible with the material then it could give higher migration. The migration and its mathematical modeling is a very wide subject, but in order to have a general understanding it is helpful to consider three general cases:

- impermeable materials: material absolute barrier such as metals, glass and ceramics;
- permeable materials: such as plastics, rubbers and elastomers. The material offers some limited resistance to migration but this can occur from the surface as well as from the interior of the material. The resistance to mass transfer depends on the structure, density, crystallinity, etc., of the material;
- porous materials: paper and board materials with a heterogeneous, open network of fibres with large air spaces or channels. Migration can occur rather rapidly with the little hindrance offered.

The chemicals present in the food contact materials are substances

originate from a number of sources, such as:

- known ingredients used to make the basic packaging materials of plastics paper;
- chemicals used to convert or fabricate the basic packaging material into its finished form (i.e. inks and adhesives);
- known or unknown isomers, impurities and transformation products of these known ingredients;
- unknown substances/contaminants in the raw materials used, and especially those in the feedstock if materials are recycled;
- unexpected or unknown substances originating from the last two categories in this list are what have become known as NIAS.

3.1.2. The nature and extent of contact

We can consider different factors that determine the nature and the extent of any contact with the food. This depends mainly on the physical properties of the food, in fact for instance, solid foods make only limited contact, while liquids make more extensive contact; but it is also related to the size as well as the shape of the pack.

Another very important factor to consider is the presence of a barrier layer. The same physical-chemical phenomena that regulate the permeation of gases or moisture in food through packaging materials may be invoked to explain chemical migration.

The barrier layer may delay or prevent migration if the chemical that may migrate is located in one layer of the packaging material behind a barrier layer. This is quite common situation with modern multi-laminate packaging materials where in fact inks, adhesive, or one or more of the laminate plies are not directly in contact with the food.

3.1.3. The nature of the food

Another important parameter that shall be considered is the nature of the food that is in direct contact with the packaging. Packaging users shall in fact ensure that the packaging materials that they use are compatible with the food that it is intended to be contained in them.

It is important for two reasons: Physical interactions and Solubility.

Physical interactions: it may occur between food and its packaging, leading to an accelerated release of chemicals substances.

For instance fats and oils may interact with certain plastics that leads to swelling of the plastics and leaching of substances from the plastic.

Solubility: the nature of the food has a certain influence on chemical migration because it determines the solubility of any packaging constituent in that food. This influences the amount of migration that may occur.

3.1.4. The temperature of contact

Is important also to consider the temperature of the contact because as all chemical and physical reactions the migration of chemicals is accelerated by heat.

Certain kind of packing materials are used under a very wide range of temperature conditions: storage in frozen conditions, refrigerated conditions, room temperature, to boiling, pasteurization and sterilization, microwaving and even cooking or baking in the pack itself.

3.1.5. The duration of contact

The time in terms of contact duration for common packaging can vary widely:

- Minutes (i.e. take-away foods);
- Hours (i.e. fresh bakery, sandwiches);
- Days (i.e. fruit and vegetable, meat, poultry);
- Weeks (i.e. cheese);
- Months and years (canned foods, drinks, frozen foods etc.).

The kinetics of migration are, to first approximation, first order in that the extent of migration increases according to the square-root of the time of contact: $M \propto t^{1/2}$. [3]

3.2. Chemical migration from non-plastic food contact materials

3.2.1. Chemical migration from food packaging inks and varnishes

Printing inks are used on food packaging materials to provide information to consumers as well as for marketing purposes. The consumers as well as the producers and retailers of packed products, want and need information printed on the surface of the packaging for different reasons as:

- to differentiate between products;
- to give the necessary information about the product (dietary details and advice on how to store and prepare the food);
- to make the purchaser interested.

Printing inks, including varnishes, are applied by printing or varnishing processes, such as flexography, offset, gravure printing and roller varnishing.

Varnishing or over-varnishing, also referred to as coating, is a finishing process where rollers apply a thin transparent layer of varnish or lacquer on the printed material. Its purpose is to protect the print from smearing and scratching, to improve gloss and to even the surface. Varnish is a kind of ink without colorant. It is sometimes also applied to the food contact surface in order to improve resistance towards moisture and fat.

Could be different issues related to the processes to print on food

packages. In general the manufacturer applies prints to the outer surface of a food packaging, so they are not intended to make direct contact with food. However, low molecular substances may migrate through the packaging material into the food.

Different kinds of plastics provides different barrier to migration, while fibrous materials do not normally act as barriers to migrants. In particular solvents migrate more easily than other substances. [4]

Most kinds of plastics do not act as barrier to migrant, in particular solvents travel easily through packages made of paperboard or plastics. The printing inks may migrate also onto the internal surface in contact with food through off-set migration.

Further, packaging material can be equipped with printed labels, such as in the case of PET bottles, or PS trays and cups.

Finally, the use of recycled paper can imply that inks may be present within the bulk material. One of the most recent concerns regarding recycled paper is the presence of mineral oil. Due to the non-discriminatory recycling of food contact paper and board used in other applications, mineral oils will mix into the bulk material even if mineral oils are not used on food packaging materials. Of course, the migration of printing inks depends on the material properties.

Many different compounds can be used in printing such as inks and inks components (colorants, binders, solvents, additives) varnishes etc.; thus

the possibility of packed food becoming contaminated by one of the mentioned components needs to be controlled [4] [5].

3.2.1.1. Regulations of inks

Switzerland is the first country that issued a positive list for printing inks (in force since March 2010), which contains more than 5000 substances.

In the EU food contact materials are regulated under the *EU Framework Regulation EC 1935/2004* on materials and articles intended to come into contact with food, which allows for further regulation being made on printing inks.

Whilst European harmonized legislation does not specifically cover printing inks in their supplied form, there are some legislative instruments which impact on materials and articles intended for direct contact with food, whilst being printed on the non-food-contact side.

In 2011 the European Printing Ink Association (EuPIA) has issued updated guidelines relating to the non-food contact surface of food packaging materials and articles, to take account of recent EU regulatory changes, i.e. *Regulation EU 10/2011*.

The updated guideline replaces September 2009 protocols and applies to printing inks, coatings and varnishes applied to any material or article intended to come into contact with foodstuffs. Inks, once printed and dried/cured, on the non-food-contact side of a packaging material in

contact with food become a component of this packaging and this packaging has to comply with all applicable legislation, including the requirements of Article 3.

EuPIA recommended to ensure traceability during ink manufacturing analogous to the requirements as set out in Article 17 of *Regulation 1935/2004* : the traceability of printed materials and articles will allow to facilitate control, to recall defective products, to convey information to consumers and, attribute responsibility. *Regulation (EU) 10/2011* contains a positive list of substances authorized for use in the manufacture of plastics. Packaging inks in their supply form are not in the scope of this Regulation, as they may be subject to other EU or national rules, but printed plastic materials and articles are indeed covered by the Regulation. Consequently if ink components are included in the positive list of the said Regulation, any limitation placed on them such as specific migration limits SMLs or maximum content (QM) must be met, and where there is the presence of dual use additives in the inks, the legal provisions must also be followed.

Regulation (EC) No 2023/2006 sets out rules on Good Manufacturing Practice for the production of food contact articles. This Regulation contains an Annex referring to printing inks applied to the non-food-contact surface of food packaging as well as to the storage of printed articles. In summary, even if the ink manufacturer does not have an

independent responsibility for the formulation and application of the inks, a strong cooperation between ink manufacturer and the rest of the supply chain shall be implemented to allow meeting the legal responsibilities. The cooperation between ink manufacturer and converter is best managed when detailed information about the substrate, type of food packed, printing and converting process parameters, storage and treatment conditions are provided to the ink manufacturer, that in his turn is enabled to formulate inks that comply with the legal requirements. [6] [7]

3.2.1.2. Set-Off and its investigation

Set-off occurs when printed surfaces of packaging material come into contact with the food contact side. Such may be the case during stacking or rolling of food contact materials that are printed on the outside.

Invisible set-off is not easily detected at the printing house. A study on plasticizers by Aurela and Ohra-aho [8] showed that the set-off phenomenon considerably increased migration into food when the substrate was a high barrier material and migration through the substrate was low.

Researchers from the US Food and Drug Authority (FDA) published a new method on May 1st, 2013 in the peer-reviewed scientific journal *Food Additives & Contaminants: Part A* that allows screening food

contact surfaces of packaging for set-off contamination with photoinitiators [9]. Photoinitiators are used to promote polymerization processes or the curing of printing inks in the presence of light. The method developed by Bentayeb and colleagues does not require previous preparation of the sample and therefore allows a high sample throughput. They found the two photoinitiators 4-phenylbenzophenone (CAS 2128-93-0) and Speedcure 7005 (CAS 1182753-56-5) to be more susceptible to set-off than other photoinitiators. The same was true for darker (i.e. green and grey) over lighter colors.

A method to identify spots of invisible set-off of inks and lacquers on the food-contact surface of a food packaging material has been developed by Bradley *et al.* [10].

The authors use optical means to excite and observe luminescence from invisible set-off. In their model experiments with several resins applied on different substrates they have achieved a level of detection of 20 mg per cm² of sheet surface, which seems rather high for level of set-off that are often considerably lower.

3.2.2. Chemical migration from food packaging adhesives

Different types of adhesives can be used to manufacture materials and articles for food packaging. The many different types of adhesives and the wide variety of ways in which they can be used influence the

potential for migration of chemicals into the packaged food.

In most cases adhesives could contain additives to provide them specific characteristics.

These additives could include carriers (water or organic solvents), plasticisers, tackifiers, thickeners and fillers, surfactants, biocides and fungicides, catalysts, pH modifiers, emulsifiers, waxes and antioxidants.

A variety of different substances, thus, might migrate into food:

- Solvents used as carriers for solvent-based adhesives;
- Residues of incomplete polymerization;
- Degradation products and reaction by-products of chemically reactive systems that could be retained in the adhesive and
- Any additives used to impart the chemical characteristics of the adhesive.[11]

The adhesive may be:

- water/solvent based: the *solvent based adhesives*, applied as organic solutions, are mainly used in flexible lamination and occasionally are used in some labeling solutions. The *water based adhesives* are mainly used in production of paper and cardboard food packaging applications; they are applied as aqueous solutions, dispersion or emulsions (i.e. starches, dextrans, animal glues, polyvinyl acetate and ethylene vinyl acetate co-polymer emulsions);

- hot-melt: are solvent free adhesives and they are used in a variety of manufacturing processes such as bookbinding, product assembly, box and carton heat sealing (i.e. ethylene vinyl acetate (EVA) copolymers, styrene-isoprene-styrene (SIS) copolymers, styrene-butadiene-styrene (SBS) copolymers; ethylene ethyl acrylate copolymers (EEA), polyurethane reactive); [12]
- cold-seal adhesives: also called self-seal adhesives or cohesive as they have the particular characteristics of sticking only to themselves. The predominant ingredient of the formulation is the natural rubber latex, but usually manufactures add tackifying resins, plasticizers, extenders, or other ingredients in order to modify the adhesive characteristics of the final product. Cold seal adhesives are used in a wide range of applications like for instance to form wrappers for food items and especially for confectionery; [13][14]
- heat-seal adhesives: Heat-sealing adhesives are thermoplastic materials that can be coated onto substrate surfaces and later reactivated by heat and pressure. They may be used in the sealing of peelable lidding and they differ in function from hot-melt adhesives in that they are heated to melt in situ. The main function of heatseals is to seal in the product, usually to prevent spillage during transportation. Indirect contact may result in migration into

the foodstuff but this will be dependent on the barrier properties of the food packaging material to which the label is applied; [4]

- pressure sensitive: this type of adhesives are commonly used in labels may be placed directly onto the foodstuff or onto a food packaging material. Migration into the foodstuff could happen depending on the barrier properties of the food packaging material to which the label is applied;
- chemically reactive systems: polyurethanes and epoxy adhesives are polymerised in situ and therefore residues of incomplete polymerisation may remain un-reacted and may then migrate into a foodstuff in contact. [15]

These adhesives are most commonly used to laminate flexible materials; epoxy resins may also be used as laminating adhesives. Investigations into the use of epoxy-based adhesives by Bonnell and Lawson [16] suggested that they are not commonly used in food packaging applications. Aromatic Isocyanate-based adhesive originate Primary Aromatic Amine (PAA) as a by-product. Migration of PAA needs to be controlled as they are assigned a “not detectable” SML.

- Tie-layers: are used in some multilayer materials to bond dissimilar resins together in order to combine properties of different materials. Tie layers are chemically modified resins which have chemical groups attached to the base resin. Typically

the chemical added to the polymer is Maleic anhydride, that attached to the polymer by a free radical reaction usually by reactive extrusion in a twin screw extruder. The anhydride group is able to be chemically attacked by polar groups on one polymer, while the polymeric part, being non polar, can bond with a non polar resin. Tie layers are widely used in plastic co-extruded multilayers; they can be based on modified: HDPE, EVA, LDPE and LDPE.

3.2.2.1. Regulation on adhesives

On February 5th, 2013 FEICA, the Industry Association of the European Sealant and Adhesives Industries, published a guidance document on the food contact status declaration for adhesives. The document aims to provide guidance to such extent that manufacturers following it can demonstrate compliance with *Regulation EC 1935/2004*. It summarizes the relevance of *Regulation EC 1935/2004*, *2023/2006* and *10/2011* for adhesives and gives insight into European national legislation. Adhesives are not regulated specifically under European Union law, however general regulations and good manufacturing practices (GMPs) applying to all food contact packaging materials have to comply with. [17] As in the case of inks, substances composing adhesives, that are listed under *Reg. EU 10/2011*, shall meet the restrictions of the said Regulation

whenever applicable.

3.3. Inks and Varnishes some final considerations

1. Substances that are present in inks and adhesives, and are also present in the positive list of Regulation (EU) 10/2011, shall fulfill the limitations set by the said Regulations, should such limitations be assigned.
2. Substances that constitute inks and adhesives but one not present in the Regulation's positive list shall be regarded as NLS, and as such they can be treated with a risks assessment approach, as those provided by Matrix.
3. Breakdown products and decomposition or reaction products, except those (such as Primary Aromatic Amine) that are listed under the Regulation's positive list, shall be regarded as NIAS and treated with the risk assessment method provided by Matrix.

4. REGULATION OF FOOD CONTACT MATERIALS IN EUROPE

Although in Europe national legislation and community level legislation continue to coexist, at the community level various Directives and Regulations have been issued to harmonize the regulatory approach. While Regulations are directly effective in Member States, Directives need to be transposed by National Parliaments on the basis of the countries' law in order to become effective. At the Community level, food contact materials are generally regulated under the EU “Framework Regulation” *EC 1935/2004*. The Framework Regulation covers all food contact materials including packaging, machinery and kitchen ware. According to Art.3 of the Framework regulation no food contact materials shall “transfer constituents into food at levels that endanger human health” (*Art. 3 EC 1935/2004*). Such articles are supported by *Regulation 2023/2006* on Good Manufacturing Practice (*EC 2023/2006*). Safety is estimated through the risk of migration, overall using a worst case scenario in which each citizen is expected to consume one kilogram of fatty food per day. The Framework Regulation further allows for specific requirements on the seventeen individual food contact materials. Six such kind of specific requirements have been adopted (see Table 4.1).

The specific regulation on plastic materials and articles intended to come into contact with foodstuffs (*EC 10/2011*) contains a positive list of monomers and additives that can be used in plastic food contact materials. The regulation addresses mono and multilayer plastic articles, as well as coatings on plastic and gaskets of glass jar closures.

Regulation EC 1895/2005 regulates the epoxy resin derivatives BADGE (Bisphenol A diglycidyl ether), BFDGE (Bisphenol F diglycidyl ether) and NOGE (Novolac glycidyl ether) in coated materials, plastics and adhesives. Two approaches regulate the use of recycled plastic in food contact materials. First approach: plastic depolymerized into monomers or oligomers have to meet the same requirements as virgin materials under *EC 10/2011*. Second approach: in case of plastic mechanically recycled and transformed into pellets a Regulation foresees an individual authorization for the recycling process to be carried out by the European Food and Safety Authority (EFSA) (*EC 282/2008*)[20].

Regenerated cellulose film is regulated under *Directive 2007/42/EC* which contains a positive list of substances that can be used for its manufacturing. Further, printed surfaces may not come into contact with food stuffs.

Active and intelligent packaging are also generally regulated under the framework regulation *EC 1935/2004*. In accordance with the framework regulation, they may only release substances into the food that are

regulated as food additives or food flavorings. Further, Regulation *EC 450/2009* sets additional safety requirements for active and intelligent packaging. A product containing active and intelligent packaging has to be accompanied by a declaration of compliance including consumer information at the retail stage [18].

Ceramics have not been individually regulated but in *Directive 84/500/EC* migration limits have been set for cadmium and lead, heavy metals known to migrate commonly at low levels. This regulation is currently under revision by the EU commission.

Under European community law, not for all packaging materials specific regulation has been adopted as already discussed. There are for example no specific regulation for printing inks, waxes, paper and board and resins other than those covered under regulation *EC 1895/2005* (for entire list see *EC 1935/2004*). A report issued by EFSA contains an inventory of substances commonly used in non-plastic food packaging. This report forms a basis for future legislation (see Annex 1, EFSA report on non-plastics food contact materials), and more specific requirements are to be expected in the next years.

Regarding printing inks, as already explained into 3.2.1.1 paragraph, in the Swiss Confederation a positive list for printing inks containing over 5000 substances has been in force since March 2010 (last updated May 2011). However, not all of the compounds on this list have been assessed

for their safety.

Finally, it has to be considered that while certain food contact materials, resins, coatings and adhesives are only partially covered by EU regulation, some may be specifically covered in the national legislation of member states. Efforts of harmonization will continue to take place and replace remaining national legislation with community level regulation. [19] [20]

General Regulations on FCM	
Regulation EC 1935/2004 (on materials and articles intended to come into contact with food)	
Regulation EC 2023/2006 (on Good Manufacturing Practices)	
Specific Materials	
Ceramics	Directive 84/500/EEC
Epoxy Resins	Regulation EC 1895/2005
Regenerated Cellulose Film	Directive 2007/42/EC
Recycled Plastics Material	Regulation EC 282/2008
Active and Intelligent Packaging	Regulation EC 450/2009
Plastics	Regulation EU 10/2011
Specific Regulation	
Regulation EU 321/2011 (restricting the use of bisphenol A in polycarbonate infant feeding bottles)	

Regulation EU 284/2011 (import procedures for polyamide and melamine plastic kitchenware from China and Hong Kong)	
Regulation EC 1895/2005 (restricting the use of certain epoxy resins)	
Directive 93/11/EEC (regulating the release of N-nitrosamines and N-nitrosatable substances from rubber teats and soothers)	

Table 4.1 - EU Legislation overview

4.1. Regulation EU (10/2011)

A Regulation that consolidates all previous directives and regulations on plastic food-contact materials and implements some significant changes, was enacted in 2011 in the European Union (EU). Regulation (EU) No 10/2011 on Plastic Materials and Articles Intended to Come into Contact with Food—commonly named **PIM Plastics Implementing Measure**—was published in the *Official Journal of the European Union* on January 15, 2011.

The Regulations, consists of 6 chapters with 23 articles and six annexes and applied as from 1 May 2011.

One significant change compared to the previous *Directive 2002/72EC* (and its amendments) consists of the scope of this regulation, which has been enlarged and now also addresses plastic layers which are part of multi-material materials and articles (i.e. liquid beverages cartons..). The

PIM applies to all plastics, coated and non coated, plastic mono and multi layers and plastic coatings forming gaskets in lids and closures. Plastics materials and articles used in the Food Industry i.e. containers, food storage tanks, conveyor belt etc. and to kitchen utensils such as cups, dishes cutlery, inner walls and shelves of a refrigerator etc. are included in the scope of the Regulation.

Out of scope of this Regulation are: ion exchange resins, rubbers and silicones although these materials are macromolecular substances obtained by polymerisation processes.

Articles 5 establishes that only authorized substances, so only the substances included in the Union list, are permitted for use in plastics (unless they are eligible for exemption under the "functional barrier" provision). It contains: Monomers and other starting materials, additives excluding colorants, Polymer Production Aids excluding solvents, and macromolecules obtained by microbial fermentation used to produce particular bio-polymer.

Article 11 establishes Specific migration limits: plastics materials and articles shall not transfer their constituent to foods in quantities exceeding the specific migration limits (SML) set out in Annex I. Those specific migration limits (SML) are expressed in mg of substances per kg of food (mg/kg or ppm). For substances for which no specific migration limit or other restrictions are provided in Annex I, a global migration of

60 mg/kg shall apply.

Article 12 establishes Overall migration limit : plastic materials and articles shall not transfer their constituents to food simulants in quantities exceeding 10 milligrams of total constituents released per dm² of food contact surface (mg/dm²).

Important changes regarding the food simulants used for migration test have been introduced in annex III. Water is considered now as a food and not as a food simulant. However testing can be performed into water only for plastic materials intended to come into contact with water.

New simulants provided from PIM are described as follows:

- **Simulant A:** the default simulant for non-acidic, non-alcoholic foods changes from water to 10% ethanol;
- **Simulant B:** the simulant for acidic foods remains as 3% acetic acid;
- **Simulant C:** the simulant for alcoholic foods is 20% ethanol;
- **Simulant D1:** the simulant for dairy, cloudy, and high-alcohol beverages is 50% ethanol.;
- **Simulant D2:** with regard to fatty foods, for which olive oil is currently used as the simulant, the new simulant is vegetable oil ;
- **Simulant E:** the PIM introduces a new dry food simulant – *poly(2,6-diphenyl-p-phenylene oxide)*, commonly known as Tenax – for use in SML testing only, previously used as an alternative /

substitute oil for migration overall at high temperatures.

For materials not yet come into contact with foodstuffs, compliance with the specific migration limits or global can also be determined by analysis of screening.

Screening test can be content analysis or extraction analysis, analysis of migration in simulants substitutes , easier to analyze than those "official" (for example isooctane instead of olive oil).

Article 19 introduces the innovative concept of risk assessment and it reads as follows: “Compliance with Article 3 of *Regulation (EC) No 1935/2004* of substances referred to in Articles 6(1), 6(2), 6(4), 6(5) and 14(2) of this Regulation which are not covered by an inclusion in Annex I to this Regulation shall be assessed in accordance with internationally recognised scientific principles on risk assessment”. Article 19 and its news will be analyzed in depth into the following chapter Risk assessment. [21].

5. RISK ASSESSMENT

As required by Article 19 of the European Commission *Regulation (EU) No 10/2011* the risk of non-listed substances has to be assessed.

According to that, the substances that shall be subjected to risk assessment are the following:

- Polymeric Production aids;
- Colorants and Solvents;
- NIAS;
- Aids to Polymerization;
- Additives approved at national law, pending inclusion in the Union List;
- Substances not listed in the Union list or the provisional list in a multi-material multi-layer material or article, as components of a plastic layer which is not in direct contact with food and is separated from the food by a functional barrier.

The fact that the wording used by the legislators includes the concept of “internationally recognized principles on risk assessment”, if on one hand represents a considerable opening to assessment methods that have never been explored in the European Union up to now, on the other hand leaves full responsibility to the Food Contact Material manufacturer for an appropriate utilization of such methods and the consequent conclusions that may be drawn on the safety of the product that is

introduced in the market. At the moment of publishing of the Regulation any such method existed, and only with the development of Matrix a first tool have been made available for the risk assessment. Whether or not this may be seen as an “internationally recognized method” depends to a great extent on its utilization and outcomes. Another method that has been made available in the latest years consists of the FACET method.

FACET = Flavourings, Additives (food), Contact materials, Exposure Task, it's a tool aimed at assessing dietary exposure to food chemicals in populations of consumers in Europe. The software contains databases of chemical concentrations for flavourings and additives, chemical occurrence data, industry data on retail packaging composition, and food consumption diaries.

These databases are combined in probabilistic dietary exposure models that estimate exposure in different populations of consumers in the EU.

A comparative study of exposure assessment obtained by using Matrix or FACET may be carried out in the future.

Article 19, in addition, intrinsically recognizes that the regulatory approach based on positive lists may not be appropriate for each single component of the food contact materials and articles, because of its length, costs associated to applications, and difficulty of controls. Being the responsibility of risk assessment entirely on manufacturing stakeholders, this would allow control authorities to exert their duties

through checks of supporting documentation, as provided in Art. 16 of Regulation 1935/2004, where such exercise shall be recorded.

5.1. Risk assessment terminology

Before going through the complex contest of Risk assessment we need to report here some important definitions.

Risk analysis is relatively simple in principle but in practice it is extremely complex as key factors are basically difficult to define.

The European Food Safety Authority (EFSA) asked its Scientific Committee to develop an opinion on the use of risk assessment terminology and how increased harmonisation across its Scientific Committee and Panels could reduce ambiguity and improve the consistency and clarity of its technical risk assessments to risk managers, consumers and the wider scientific and stakeholder community [*EFSA Journal 2012;10(5):2664*]. The aim of this opinion is to review EFSA's use of terminology, to identify possible reasons for differences in the use of language and terms, to identify where harmonisation is possible within and across the very wide food safety areas of EFSA's responsibility and to contribute to collaborative international work to improve the harmonisation of risk assessment terminology.

The international use of defined terminology for risk assessment is driven by three standard-setting organisations, the *Codex Alimentarius*

Commission (CAC) in relation to food safety, the *World Organisation for Animal Health (OIE, Office International des Epizooties)* and the *International Plant Protection Convention (IPPC)* for plant health, under the Agreement on the Application of *Sanitary and Phytosanitary Measures (SPS Agreement)* of the *World Trade Organisation (WTO)* of which the European Union is a member.

Even if the risk assessment term would be the same, the definition may differ among CAC, OIE and IPPC. As concerns the food safety we will report here below the Key terms in risk assessment as defined by CAC in relation to food safety. Some CAC definitions are further expanded in FAO/WHO references -*Food and Agriculture Organization of the United Nations and the World Health Organization-*, which are included here.

- **HAZARD:** a biological, chemical or physical agent in, or condition of, food with the potential to cause an adverse health effect (CAC, 2011) ; A biological, chemical or physical agent in, or condition of, a good with the potential to cause an adverse health effect (FAO/WHO, 2008).
- **RISK:** A function of the probability of an adverse health effect and the severity of that effect, consequential to a hazard(s) in food (CAC, 2011).
- **RISK ANALYSIS:** A process consisting of three components: risk assessment, risk management and risk communication. (CAC,

2011)

- **RISK ASSESSMENT:** A scientifically based process consisting of the following steps: (i) hazard identification, (ii) hazard characterization, (iii) exposure assessment, and (iv) risk characterization (CAC, 2011).

Qualitative Risk Assessment: A risk assessment based on data which, while forming an inadequate basis for numerical risk estimations, nonetheless, when conditioned by prior expert knowledge and identification of attendant uncertainties permits risk ranking or separation into descriptive categories of risk. (FAO/WHO, 2008).

Quantitative Risk Assessment: A risk assessment that provides numerical expressions of risk and indication of the attendant uncertainties (FAO/WHO, 2008).

- **EXPOSURE ASSESSMENT:** The qualitative and/or quantitative evaluation of the likely intake of biological, chemical, and physical agents via food as well as exposures from other sources if relevant (CAC, 2011).

SAFETY ASSESSMENT: is defined by CAC as a scientifically-based process consisting of: 1) the determination of a NOEL (No Observed Effect Level) for a chemical, biological, or physical agent from animal feeding studies and other scientific considerations; 2) the subsequent

application of safety factors to establish an ADI (acceptable daily intake) or a tolerable daily intake (TDI); and 3) comparison of the ADI or TDI with probable exposure to the agent (CAC, 2011. In: Risk analysis principles applied by the Codex Committee on Food Additives and the Codex Committee on Contaminants in Foods).

6. MATRIX PROJECT

The Matrix project is a tool capable to assess potential risks from NIAS/NLS in the light of *Art. 3 of Reg. 1935/2004* and *Art. 19 of Reg. (EU) 10/2011*. It was jointly initiated, financed and supported by CeficFCA -Food contact Additives-, European Plastics Converters (EuPC), Flexible Packaging Europe (FPE) and Plastics Europe.

The project resulted in data sets for *Italy, France, Germany, Spain* and *United Kingdom* on packaging surface to which consumers are exposed per plastic material group and per consumed food group: “**Exposure Surface** or “**S**”.

If we fix a “**Tolerable Exposure Level (TEL)**” = 10µg/p/day (Detection Limit to assess presence of a Functional Barrier in *Reg. 10/2011* is 10 µg/kg food; if a single consumer eats 1 kg of food per day, this translates into a 10 µg/p/d) we can obtain the respective Level Of Interest LOI as cutoff criteria for further risk assessment for NIAS

$$E [\mu\text{g}/\text{person}/\text{day}] = M [\mu\text{g}/\text{dm}^2] \times S [\text{dm}^2/\text{person}/\text{day}]$$

Being “**S**” the surface of the material to which consumer are exposed in their daily diet, and “**M**” the migration of a substance, Exposure “**E**” to such substance can be calculated as:

$$LOI [\mu\text{g}/\text{dm}^2] = TEL [\mu\text{g}/\text{person}/\text{day}] / S [\text{dm}^2/\text{person}/\text{day}]$$

The value of **migration** at **TEL** is defined **Level Of Interest** : the level of migration of a migrant in food below which no assessment is needed.

Substances that are detected at **E**>10 µg/person/day would require full risk assessment, while substances at **E**< 10 µg/person/day are deemed not to pose risk to health, therefore no risk assessment is requested. In order to apply the LOI, it must be demonstrated that the non-assessed substances are not in nano-form and they are not CMR (Carcinogen, Mutagen or Toxic to Reproduction) or do not contain structural alerts that may originate CMR breakdown.

For the materials to which the exposure is low to negligible ($S < 0.1$; LOI > 100), it is suggested to apply a conventional LOI of 100.

Data required for exposure assessments are commonly referred as *fingerprints*. The term “fingerprints” stands for chromatograms (GC or HPLC) obtained under standardized conditions when investigating or screening the migration of medium to high molecular weight substances from food contact plastics with complex or unknown composition.

From the GC or HPLC analysis all major detectable migrants are identified; these substances can be assessed semi-quantitatively over a suitable internal standard (IS). By using a combination of substances added as IS at known concentrations and a library of molecular weight, commercially available, the detected substances can be identified in their chemical structure and concentration.

Peaks identification is normally provided with a matching ratio, in percent, which indicates the probability that the relevant peak can be attributed to the substance identified by the library. Matching ratios above 70% are normally trustable; this means that substances provided with matching ratios equal or above that value have a high probability to correspond to the chemical species identified by the library, while those with matching value below 70% should be seen as not fully identified.

From the fingerprint usually not all migrants can be identified unambiguously but in most cases they can be grouped in substance classes typical for the polymeric matrix, e.g. oligomers, typical degradation products of additives etc.

It is worth mentioning that the identification of the substance would allow assigning or at least hypothetically assuming the class of risk to which such substance would belong, e.g. whether it contains functionalities that would make it a CMR .

If the screening method based on fingerprints indicates that an unambiguous identification of the migrating species as well as their quantitative assessment is needed, then a full quantitative GC or HPLC analysis shall be carried out.

Best cases to investigate the composition of the fingerprint are when full compositional information on the recipe as well as samples (analytical quantities) of all raw materials (monomers, additives, polymer

production aids, catalysts, etc. if possible pure chemical species) are available and can be tested individually. In this situation the identification and full traceability of each peak at 10 ppb detection limit and below can be achieved.

In cases where neither sample recipe nor constituent samples are at hand, the identification of many but not all peaks in the fingerprints can be achieved by isolating the corresponding substances through preparative chromatography and applying micro-analytical characterization methods like IR and NMR as well as MS/MS and further method coupling.

This approach is rather time consuming and analytically difficult, and it may be worth being done only in case that presence of critical substances is suspected.

In this research work, the identification of the *fingerprints* needed to perform the risk assessment of NIAS of 43 food packaging, was made via GC-MS analysis as described in paragraph 7.2.

The use of the Matrix approach to perform the risk assessment of NIAS is explained into paragraph 6.1.

The packaging materials surfaces that are used for calculating exposure are reported in the matrices relative to the countries surveyed (Matrices_IT_FR_UK_DE_ES.xls); As these tables cannot be reported here for their size, that make them difficult to be read, here below is an excerpt of it:

contact with packaging materials, mean of all respondents, in distribution	1 aluminium foil	2 paper	3 PET (polyester ethylene terephthalate)	4 Other mono-substrate plastic	5 Other mono-substrate non-plastic	6 VULCANISATE or LDPE and blends with LDPE	7 LDPE	8 multi-layer copolymers (EVA, EMA, EAA, EEA)	9 other PE based blends	10 HDPE
01. Alcoholic Beverages	0	0	0	0	0.666	0	0	0	0	0
02. Non-alcoholic beverages	0	0	0	0	0.31	0	0	0	0	0.027
03. Concentrates of juices	0	0	0	0	0	0	0	0	0	0
04. Liquid coffee or tea	0	0	0	0.007	0.003	0	0	0	0	0
05. Dry beverage powders	0	0.05	0	0	0.016	0	0	0	0	0.001
06. Breakfast cereals and bars	0	0	0	0.016	0	0	0	0	0	0
07. Cereal flour	0	0.2	0	0	0	0	0	0	0	0
08. Dough	0	0	0	0	0	0	0	0	0	0
09. Bread	0	0.08	0	0	0	0.084	0.17	0	0.084	0
10. Dry rice and pasta	0	0.14	0	0	0	0	0.06	0	0	0.007

Table 6.1 - Excerpt of the Matrix table elaborated on the basis of food/packaging contact data for Italy

Matrix tables are available in a CD-ROM or files that can be provided upon request to European Plastic Converters Association 71 Avenue de Cortenbergh, B-1000 Brussels, Belgium

Such surfaces have been derived by combining dietary intake data available in nutrition research studies in the Countries of interest, with packaging presence in the market, that was obtained by market research companies contracted by the Matrix steering committee (*Euromonitor* for IT, FR, UK and ES, and *GVM* for DE.) [23]

6.1. How the Matrix approach can be used in practice

In order to use the Matrix approach in practice for the evaluation of the risk assessment of NIAS and NLS, we can proceed with three fundamental steps:

➤ **STEP 1: GC-MS analysis** of *VOC (Volatile Organic Compound)*, *semi-VOC* and *non-VOC* following the Analytical screening method protocol described into the paragraph 7.2.

➤ **STEP 2: SELECT THE CORRESPONDING SURFACE OF THE MODEL PACKAGING**

Choice from the Matrix table the packaging type closest to the structure under examination and selecting the one resulting in highest exposure to provide a conservative estimation of exposure. This makes possible to choose the solution that leads to over-estimation.

➤ **STEP 3: CALCULATION**

Calculate the Exposure (*Avg & Max*) multiplying the quantities extracted (**M**) in - **Step1**- by the corresponding S value as resulting from the sum of all surfaces in contact with the selected packaging type for each country, using the “*S-Average*” Tables from Matrix. It shall be noticed that such method of calculation will consider each selected packaging material as it is in contact with the whole diet.

From the results obtained, check if the Max Exposure calculated of **NIAS** and **NLS** is higher or lower than the TEL= 10 µg/person/day; thus, the Risk of substances at higher level can be assessed via literature data or on the basis of toxicological existing classification.

The substances with specific limitation present in the positive list provided from European community are not assessed via Exposure, as it is recognised that the current legislation system provides a sufficient and conservative protection of consumers health.

7. MATERIALS AND METHODS

7.1. Determination of potential migrants in commercial flexible packaging

Forty-three different structures of flexible packaging taken from standard production of *Giflex* associated members have been tested:

- Materials: plastics films, paper, uncoated and coated Aluminium;
- Structures: mono-layer, 2 layers (duplex), 3 layers (triplex); sometimes the core layer can be composed by more than one resins (tie/core/tie or tie/abuse/core/abuse/tie) ;
- Printing: external, internal;
- Inks: different series of solvent based, roto and flexo inks;
- Lamination: outline, in line, solvent and solvent-less adhesives.

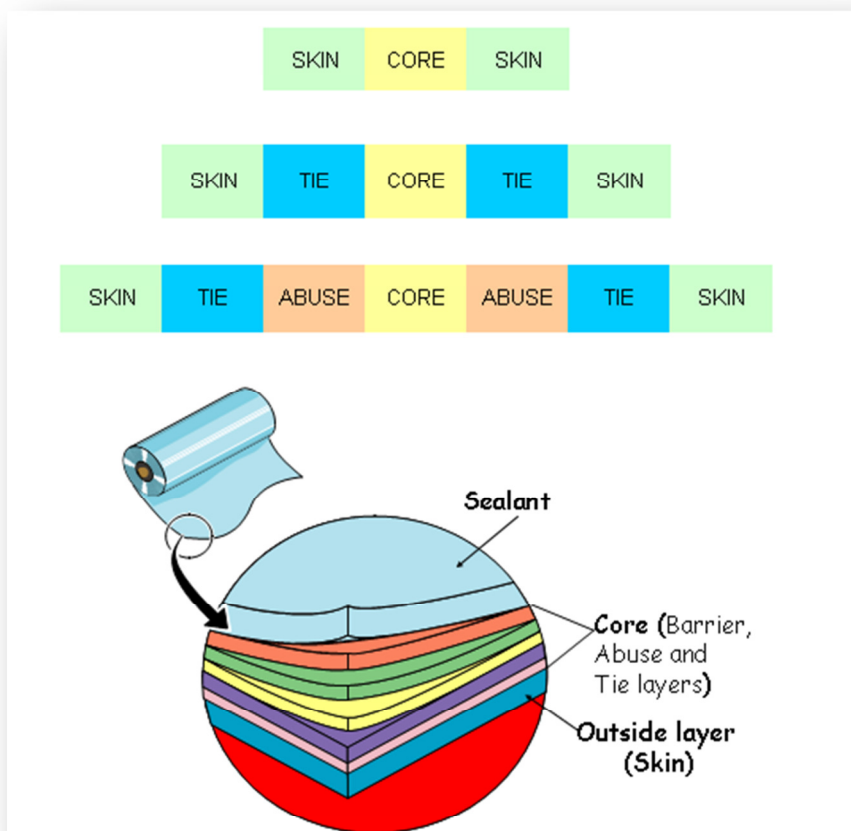


Figure 7.1 - General structure of packaging material

In Table 7.1 it has been reported the 43 materials used for the experimental trials, each of them codified with a number.

To identify any potential migrants in the samples tested, a methodology has been used, as described in the following section, provided from *IRCPack Lab s.r.l Italy*.

Samples Number	Chemical structure				Corresponding surface of the model packaging chosen from the Matrix spreadsheet
	Layer 1	Layer 2	Layer 3	Layer 4	
1	PET	Aluminum	PE		PLASTIC/ALU/PE
2	PET	Aluminum	PET	PE	PLASTIC/ALU/PLASTIC/PE
3	PAPER	Aluminum	PE		CARTA/ALU/PLASTIC
4	PAPER	Aluminum	PE		CARTA/ALU/PLASTIC
5	PET	Aluminum	OPA	PE	OTHER COMBINATION NON PLASTIC/PLASTIC
6	PET	PET siox	CASTPP		OTHER PLASTIC/PP
7	OPPacr/acr				OPP
8	OPA	CASTPP			OTHER PLASTIC/PP
9	PET	PE-EVOH-PE			OTHER PLASTIC/PE
10	PET	PE-EVOH-PE			OTHER PLASTIC/PE
11	PET pvdc	PE			OTHER PLASTIC/PE
12	PETmet	PE			OTHER PLASTIC/PE
13	OPPcoex				OPP
14	PET	Aluminum	PE		PLASTIC/ALU/PE
15	PET met	PE			OTHER PLASTIC/PE
16	PAPER	Aluminum	PE		CARTA/ALU/PLASTIC
17	OPA	PE			OPA/PE
18	PET	Aluminum	PE		PLASTIC/ALU/PE
19	OPPcoex				OPP
20	PET	PE			OTHER PLASTIC/PE
21	OPPpvdc/acr				OPP
22	PAPER	OPP coex			PAPER/PLASTIC
23	PETmet	OPP coex			PLASTIC/OPP
24	OPPcoex				OPP
25	Aluminum	PAPER			ALU/PAPER
26	PAPER	Aluminum			PAPER/ALU
27	PAPER	OPP			PAPER/PLASTIC
28	PET	Aluminum	PE		PLASTIC/ALU/PE
29	PET	Aluminum	PE		PLASTIC/ALU/PE
30	OPPcoex	Aluminum	PE		PLASTIC/ALU/PE
31	CASTPP	PP/EVOH/PP			OTHER PLASTIC/PP
32	PA	PP	PE		OTHER PLASTIC/PE
33	PE	PA/EVOH	PE		PLASTIC/PA/PE
34	PE	EVA	PE-EVOH-PE	IONOMER	OTHER PLASTIC/OTHER PLASTIC
35	OPPmet	OPPcoex			OPP/OPP
36	OPPmet white				OPP
37	PAPER	Aluminum			PAPER/ALU
38	OPA	PE			OPA/PE
39	OPPmet				OPP
40	OPP-pvdc/lts				OPP
41	PETpvdc	PE			OTHER PLASTIC/PE
42	PET	PE			OTHER PLASTIC/PE
43	PET	PETmet	PE		OTHER PLASTIC/PE

Table 7.1 - 43 Giflex structures tested by GC-MS Analysis

7.2. Analytical screening method: identification and semi-quantitative evaluation of volatile, semi-volatile and non volatile organic compounds

Objective:

The objective of the study was to identify and evaluate (semi-quantitative) the organic compounds present in the materials coming in the contact with food to evaluate the potential contamination.

The monitoring was performed through *Agilent 7890A - GC/MSD 5975C system* using three sampling methods:

- **First level screening:** static head space for *volatile* and *semi-volatile* compounds;
- **Second level screening:** solvent extraction for *semi-volatile* and *non volatile* compounds;
- **Third level screening:** internal washing for *semi-volatile* and *volatile* compounds (fast method).



Figure 7.2 - Agilent 7890A - GC/MSD 5975C

7.2.1. First level screening: identification and semi-quantitative evaluation of *volatile* and *semi-volatile* compounds

- Sample preparation: prepare a material specimen of 1 dm² and put it into an head space vial;
- Internal standard: close the vial and add 1 µl of internal standard solution (chlorobenzene in methanol: concentration= 2,8 µg/µl = 2,8 µg/1dm²).

The sampling of the volatile and semi-volatile organic compounds has been carried out by static head space, followed by GC/MS analysis:

Automated head space sampler:

Vial conditioning: 30 minutes at 125°C

Quantity to draw for the injection: 1 ml

Syringe temperature: 100°C

Washing the syringe post injection

Gas chromatographic conditions:

Column: Restek 624sil MS, length 30 meters, internal diameter 0,25 mm-film 1,4µm;

Helium flow: 1,2 ml/min constant flow

Injector temperature: 250°C

Type of injection: split, split ratio 1:10

Oven: 50°C for 2 minutes->5°C/minute -> 100°C -> 7,5°C/minute -> 280°C for 4 minutes.

Acquisition parameters MSD:

Acquisition mode: SCAN

Low mass 35 -> high mass 350

Solvent delay: 2 minutes

Semi-quantitative evaluation of compounds finding in the head space: adding an internal standard allows a semi-quantitative estimation of the compounds related to the chromatographic peaks displayed, applying the response factor of the internal standard.

Thus, the value of each compounds can be calculated as follows:

$Compound \mu\text{g}/\text{dm}^2 = \text{Area (TIC) compound} * 2,8 / \text{internal standard area}$
(chlorobenzene)

7.2.2. Second level screening: identification and semi-quantitative evaluation *semi-volatile* and *not volatile* compounds

- Sample preparation: prepare a material specimen of 1dm^2 , cut it in strips and put them into vial; adding 10 ml of n-hexane inside the vial ;
- Internal standard: add 25 μl of internal standard solution into the vial containing 10 ml of n-hexane; and 1 dm^2 of specimen; (dipropyl phtalate in hexane: concentration: $1\mu\text{g}/\mu\text{l} = 25 \mu\text{g}/1\text{dm}^2$)
- Extraction: ultra sound for 30 minutes plus one night at room temperature;

Gas chromatographic conditions:

Column: HP 5 MS length 30 meter, internal diameter 0,25 mm- film 0,25 μm ;

Helium flow: 1,2 ml/min constant flow

Injector temperature: 300°C

Type of injection: splitless (1 μl)

Oven: 50°C for 2 minutes -> 10°C/minute -> 100°C -> 15°C/minute -> 300°C for 25 minutes

Acquisition parameters MSD:

Acquisition mode: SCAN

Low mass 45 -> high mass 350

At 10 minutes low mass 50 -> high mass 550

At 20 minutes low mass 50 -> high mass 700

Solvent delay: 5 minutes

Semi-quantitative evaluation of compounds found in the solvent extraction: adding an internal standard allows a semi-quantitative estimation of the compounds related to the chromatographic peaks displayed, applying the response factor of the internal standard.

Thus, the value of each compounds can be calculated as follows:

*Compound $\mu\text{g}/\text{dm}^2 = \text{Area (TIC) compound} * 25 / \text{internal standard area (dipropyl phtalate)}$.*

7.2.2. Third level screening: identification and semi-quantitative evaluation of *semi-volatile* and non volatile compounds on the internal side of the specimen

- Sample preparation: prepare a bag of 2 dm² or use a cell with a exposed surface of 2 dm²;
- Solvent: measure 10 ml of n-hexane;
- Internal washing: cut a triangle from the bag in order to put inside the solvent (n-hexane); seal the area of the bag opened by the cut and get the bag on one side of it, keep the contact for 10 minutes

for each side at room temperature.

Solvent recovery from the bag: recover the solvent and put it inside a flask of 10 ml and make up to the mark with n-hexane if needed.

Internal standard: add 25 μl of the internal standard inside the flask containing 10 ml of n-hexane recovered from the bag, shake up.

(dipropyl phtalate in hexane : concentration: $1\mu\text{g}/\mu\text{l} = 25\mu\text{g}/2\text{dm}^2$).

The washing solvent has be analyzed through GC/MS as already described into the previous section.

Semi-quantitative evaluation of compounds found into the washing solvent: adding an internal standard allows a semi-quantitative estimation of the compounds related to the chromatographic peaks displayed, applying the response factor of the internal standard.

Thus, the value of each compounds can be calculated as follows:

*Compound $\mu\text{g}/\text{dm}^2 = \text{area (TIC) compound} * 12,5 / \text{area internal standard (dipropyl phtalate)}$*

Compounds identification was carried out by a comparison of the spectra with libraries present in the instrument's software (*NIST* and *WILEY*).

8. RESULTS

8.1. Extraction's results of 43 flexible packaging materials analyzed by GC-MS

Here below are reported the mass spectra (forest of peaks) of the 43 structures tested by GC-MS:

- *Volatile* and *semi-volatile* organic compounds results -**head space**-
- *Semi-volatile* and *non-volatile* organic compounds results -**total extract**-
- *Semi-volatile* and *non-volatile* organic compounds results -**internal surface**-

In details, into the identification tables are reported the following details:

- Peak retention time (TR), which appears also on the chromatogram;
- Identification obtained through comparison with the concerned mass spectra peaks and those present in the library (*WILEY275K*), managed by the analytical system software;
- Matching ratio= quality or coincidence index between the sample spectrum and that one in the library (maximum 100- acceptable ≥ 70);
- Semi-quantitative evaluation: methods are not quantitative; an approximate evaluation of the concentration is expressed in

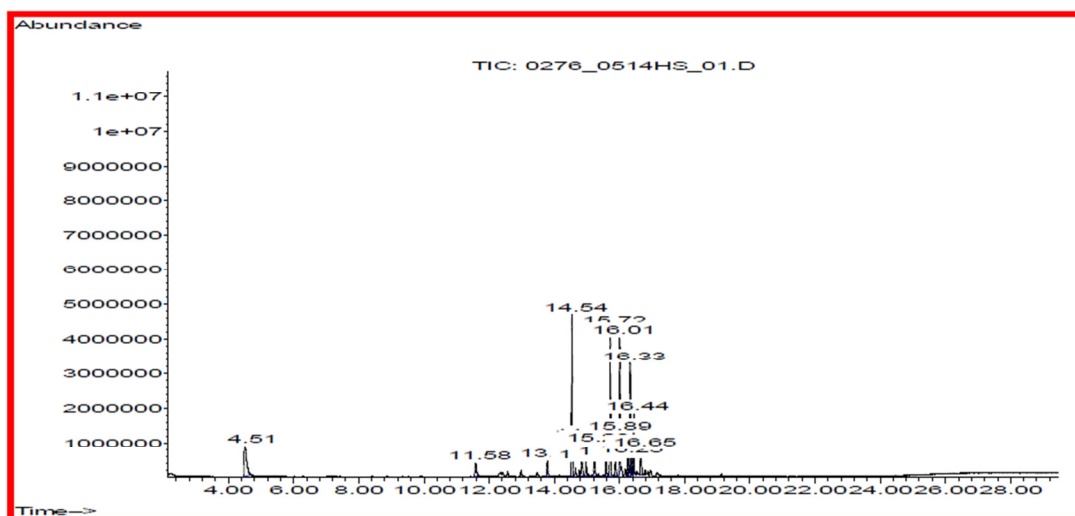
$\mu\text{g}/\text{dm}^2$ using the internal standard as reference (also for “not identified” peaks).

“Not identified “ means that the relative spectrum is not comparable with any spectra present in the Libraries.

In many cases we report the main ions of the spectrum.

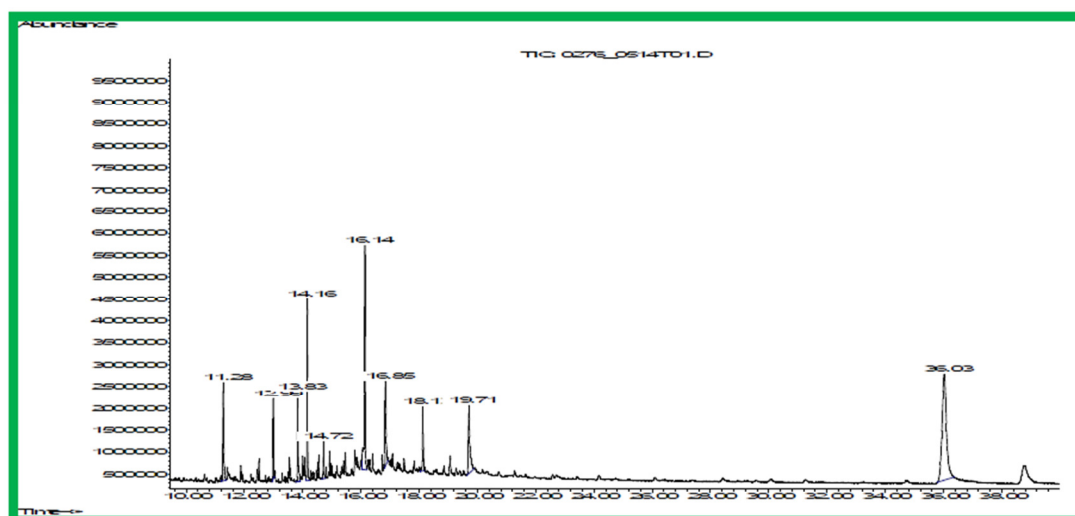
Peaks identified as Siloxane are probably pollutants of the analytical system coming from the closure septum of the vial.

SAMPLE 1: PET/ALUMINUM/PE



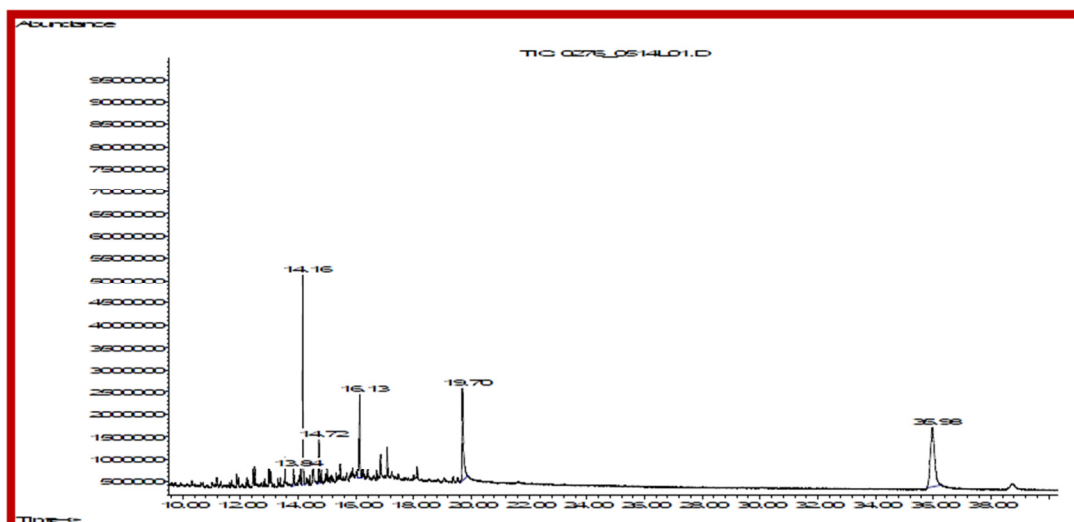
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.51	Ethyl acetate	90	-
11.58	Benzene, chloro (internal standard)	94	2,8
from 13.80 to 16.65	Aliphatic saturated hydrocarbons	>80	87

Table 8.1 - Sample 1: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.28	Benzene, 2,4-diisocyanato-1-methyl	87	17
12.99	Octadecane	97	8,2
13.83	Not identified (m/z = 84,99,111,173)	-	15
14.16	Di propyl phthalate (internal standard)	94	25
14.72	Not identified (m/z = 97,126,155,173)	-	5,2
16.14	Tributyl acetylacrylate	87	42
16.85	Oleamide	90	18
18.13	Analytical system contaminant	-	-
19.71	Erucamide	87	24
36.03	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	78	108

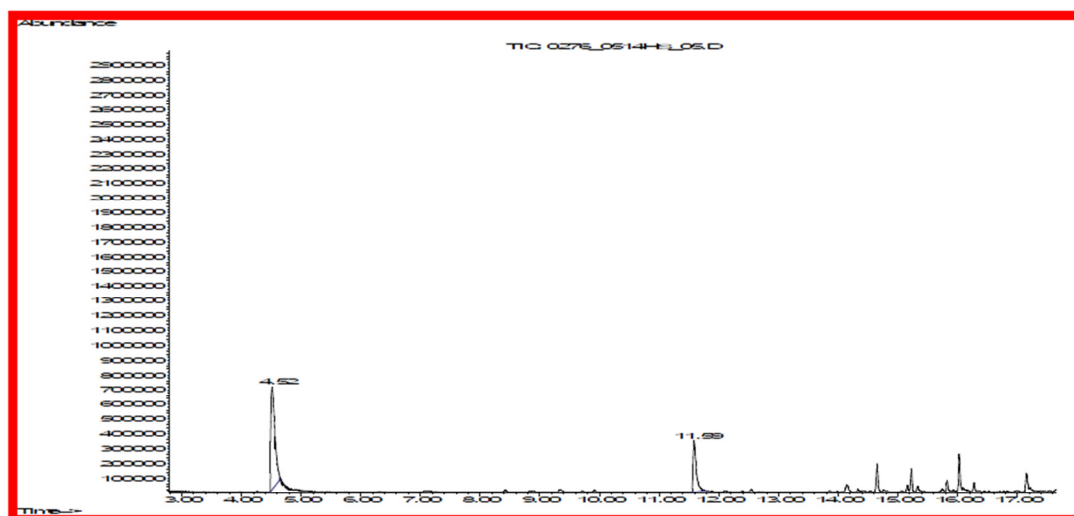
Table 8.2 - Sample 1: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.84	Not identified (m/z = 84,99,111,173)	-	2,0
14.16	Di propyl phthalate (internal standard)	94	12,5
14.72	Not identified (m/z = 97,126,155,173)	-	2,7
16.13	Tributyl acetylcitrate	90	7,0
19.70	Erucamide	87	14
35.98	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester	78	26

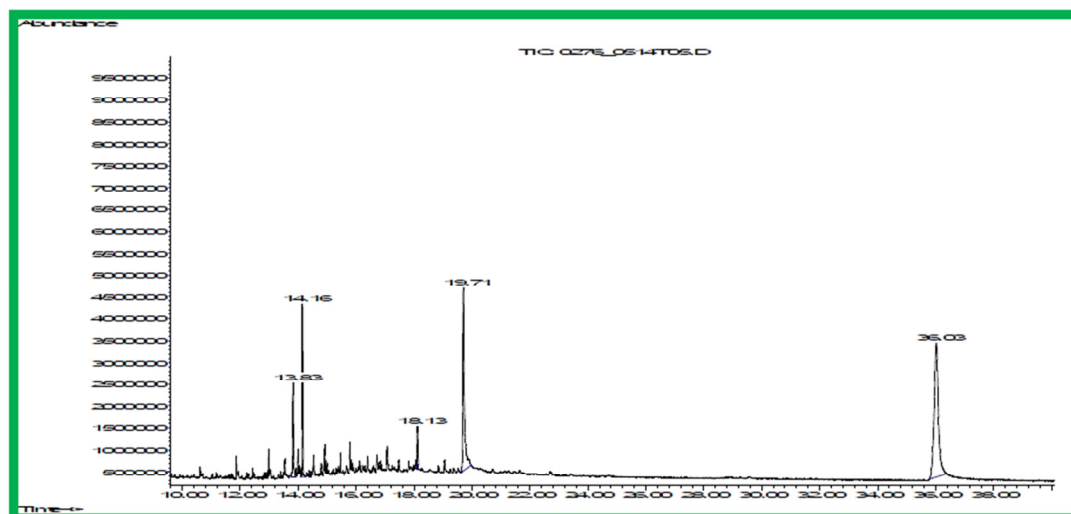
Table 8.3 - Sample 1: Internal surface

SAMPLE 2: PET/ALUMINUM/PET/PE



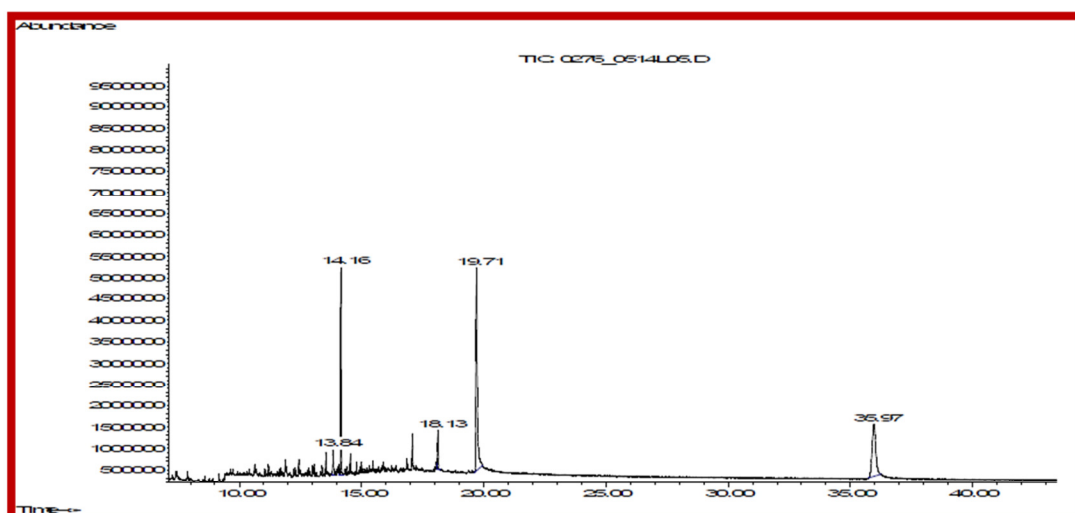
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.52	Ethyl acetate	83	7,4
11.59	Benzene, chloro (internal standard)	94	2,8

Table 8.4 - Sample 2: Head space



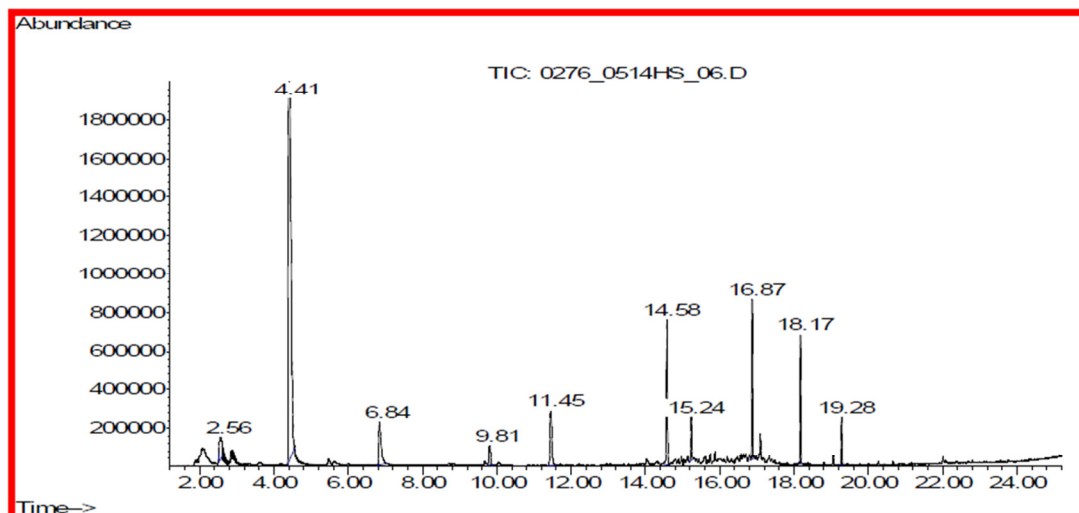
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.83	Not identified (m/z = 84,99,111,173)	-	17
14.16	Di propyl phthalate (internal standard)	94	25
18.13	Analytical system contaminant	-	-
19.71	Erucamide	87	68
36.03	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	78	137

Table 8.5 - Sample 2: Total extract



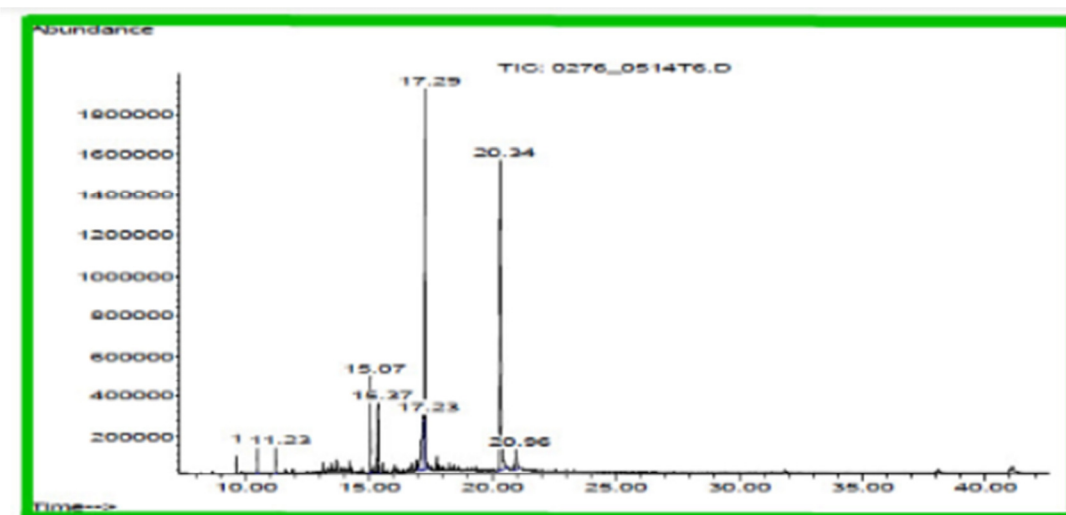
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.84	Not identified (m/z = 84,99,111,173)	-	2,6
14.16	Di propyl phthalate (internal standard)	94	12,5
18.13	Analytical system contaminant	-	-
19.71	Erucamide	87	30
35.97	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	78	23

Table 8.6 - Sample 2: Internal surface

SAMPLE 3: PAPER/ALUMINUM/PE

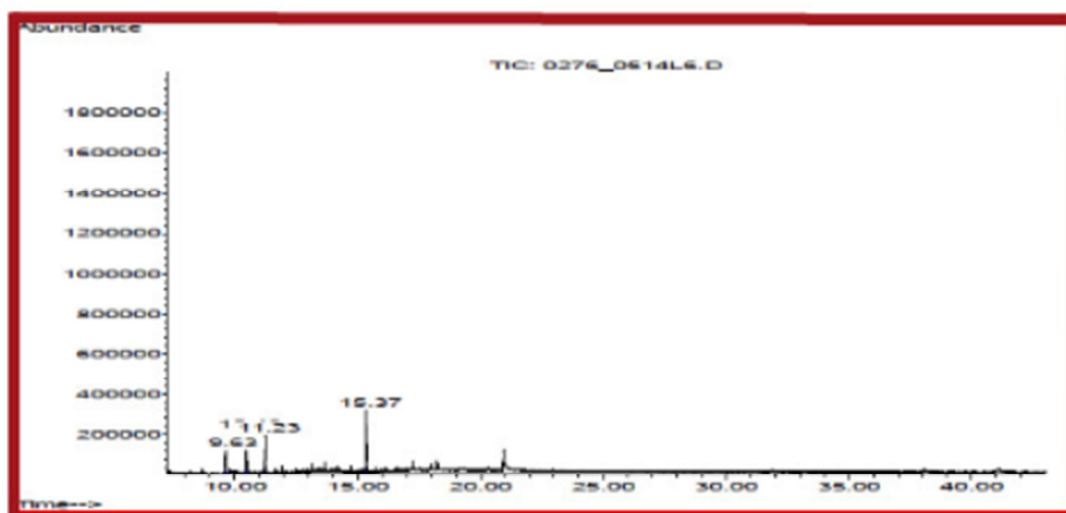
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.56	ethanol	80	1,7
4.41	ethyl acetate	83	31,2
6.84	n-propyl acetate	80	3,1
9.81	siloxane	-	1,0
11.45	Benzene, chloro (internal standard)	94	2,8
14.58	siloxane	-	4,4
15.24	decane	94	1,1
16.87	undecane	91	3,6
18.17	dodecane	91	2,8
19.28	tridecane	94	1,0

Table 8.7 - Sample 3: Head space



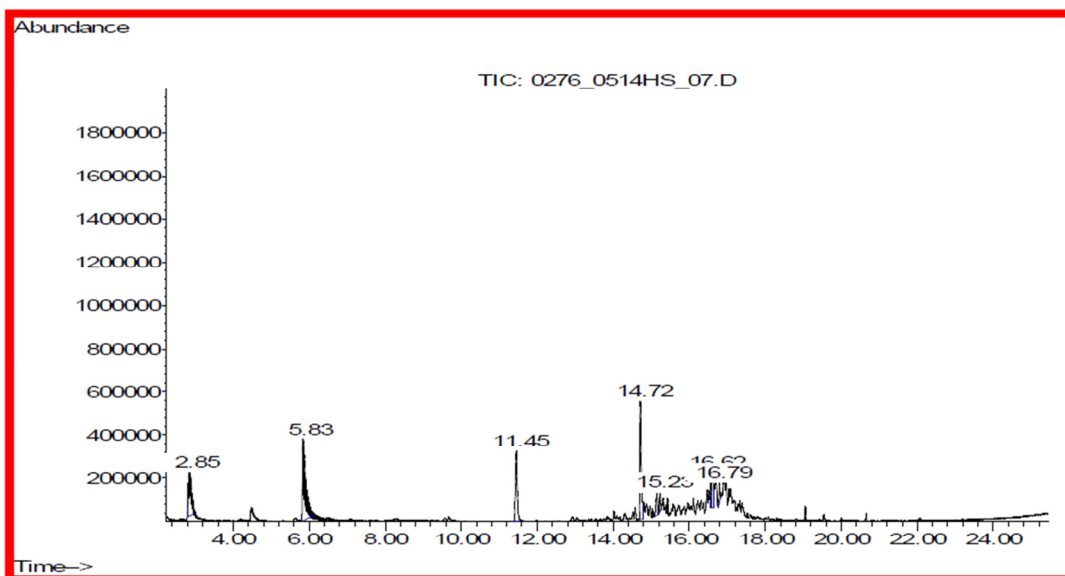
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
9.63	undecane	94	9
10.48	dodecane	94	11
11.23	tridecane	94	10
15.07	not identified (m/z = 84,99,111,173)	-	39
15.36	Dipropyl phthalate (internal standard)	98	25
17.29	acetyl tributyl citrate	80	258
20.34	not identified (m/z = 99,171,127)	-	215

Table 8.8 - Sample 3: Total extract



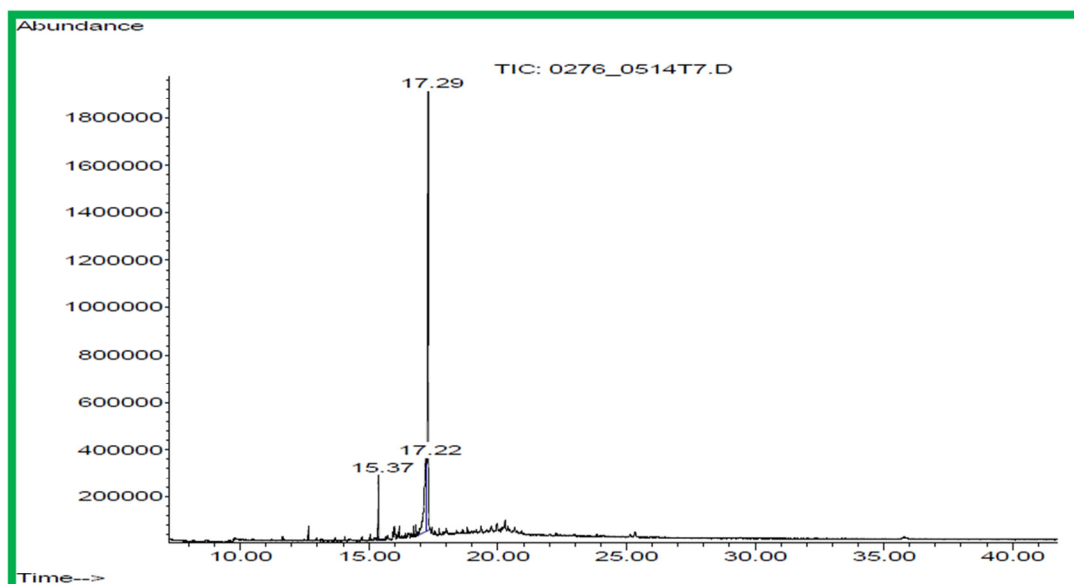
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
9.63	undecane	94	6
10.48	dodecane	94	9
11.23	tridecane	94	8
15.37	Dipropyl phthalate (internal standard)	98	12,5

Table 8.9 - Sample 3: Internal surface

SAMPLE 4: PAPER/ALUMINUM/PE

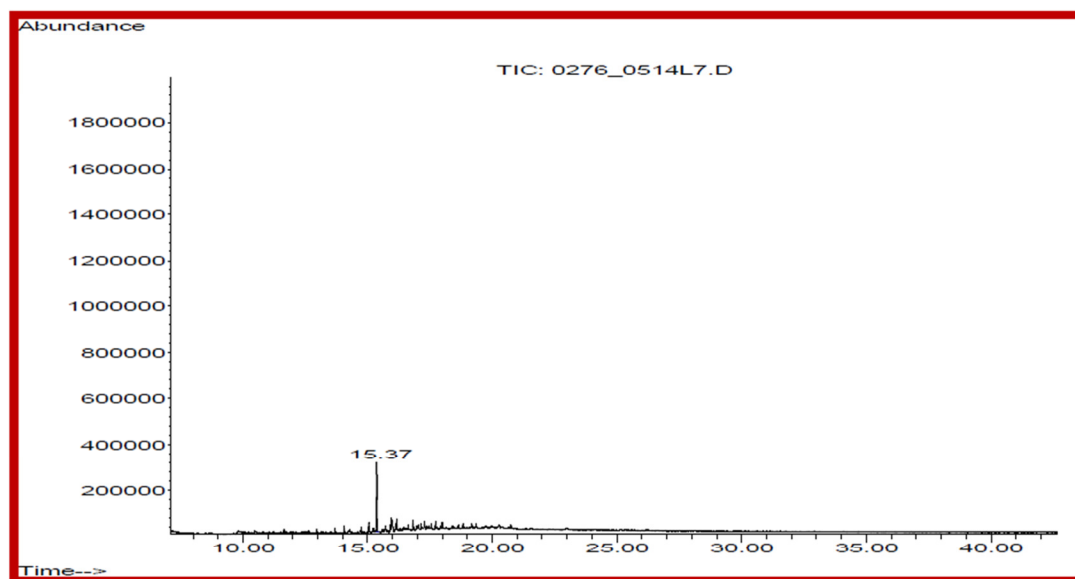
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2,85	iso-propanol	80	2,9
5,83	ethylacetate	83	5,4
11,45	Benzene, chloro (internal standard)	97	2,8
14,72	benzaldehyde	95	3,4
15,23	aliphatic hydrocarbon	-	0,5
16,62	aliphatic hydrocarbon	-	1,4
16,79	aliphatic hydrocarbon	-	0,4

Table 8.10 - Sample 4: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15,37	Dipropyl phthalate (internal standard)	98	25
17,29	acetyl tributyl citrate	91	277

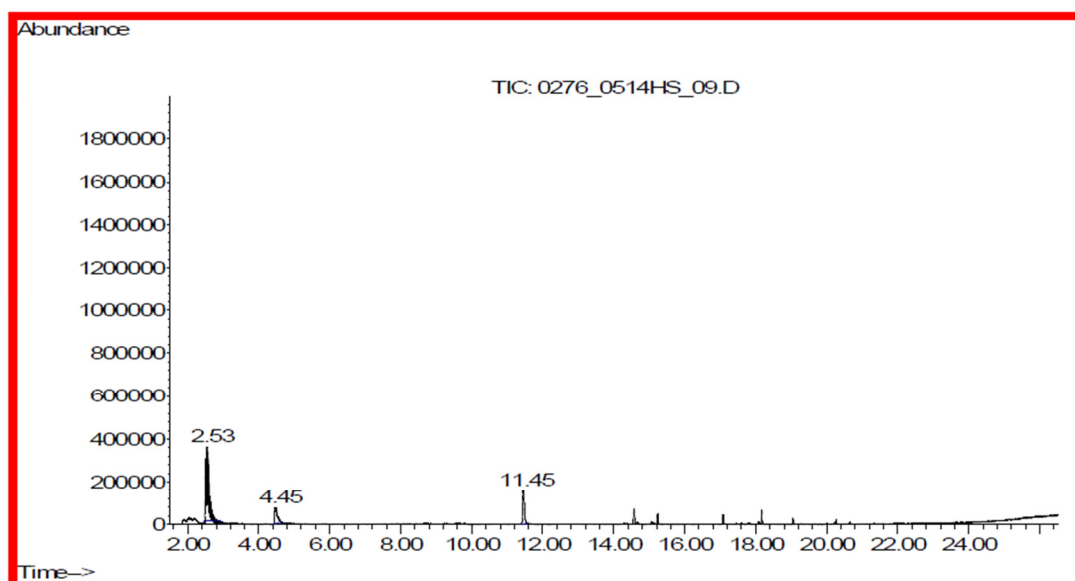
Table 8.11 - Sample 4: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5

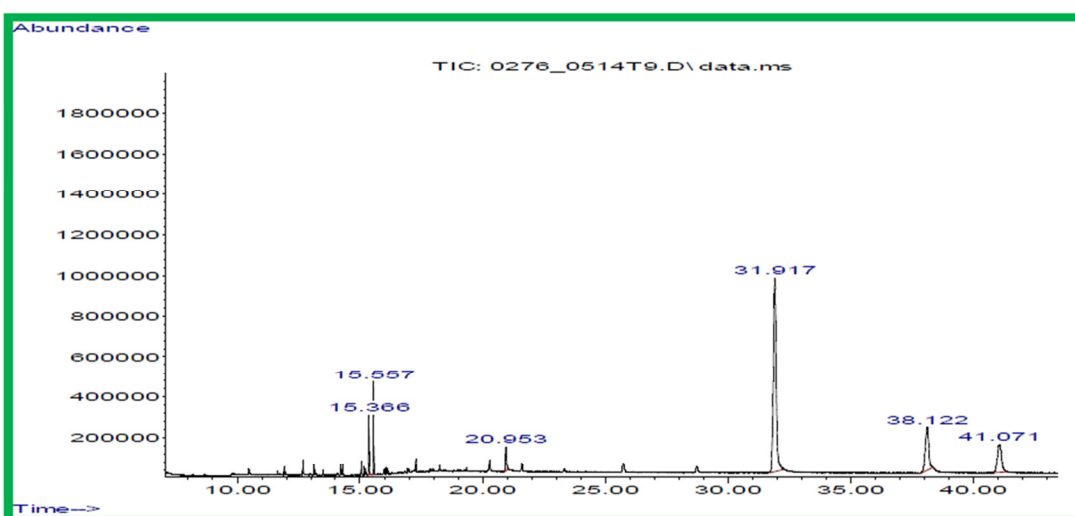
Table 8.12 - Sample 4: Internal surface

SAMPLE 5: PAPER/ALUMINUM/PE



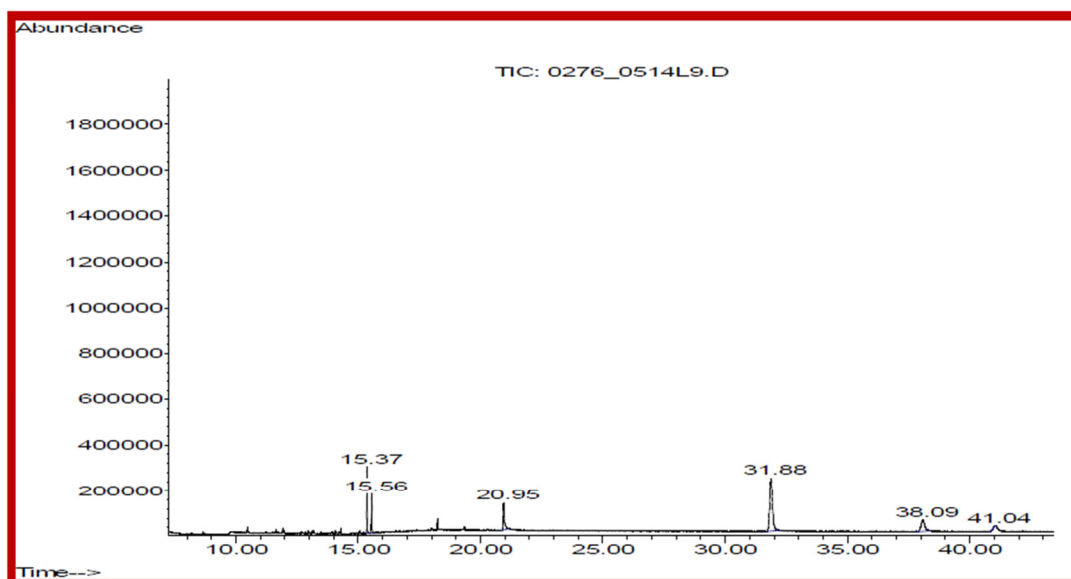
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.53	ethanol	80	7,8
4.45	ethyl acetate	83	2,2
11.45	Benzene, chloro (internal standard)	97	2,8

Table 8.13 - Sample 5: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	25
15.56	not identified (m/z=55,82,111,129)	-	44
20.95	erucamide	95	25
31.92	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	473
38.12	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	94	130
41.07	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	101

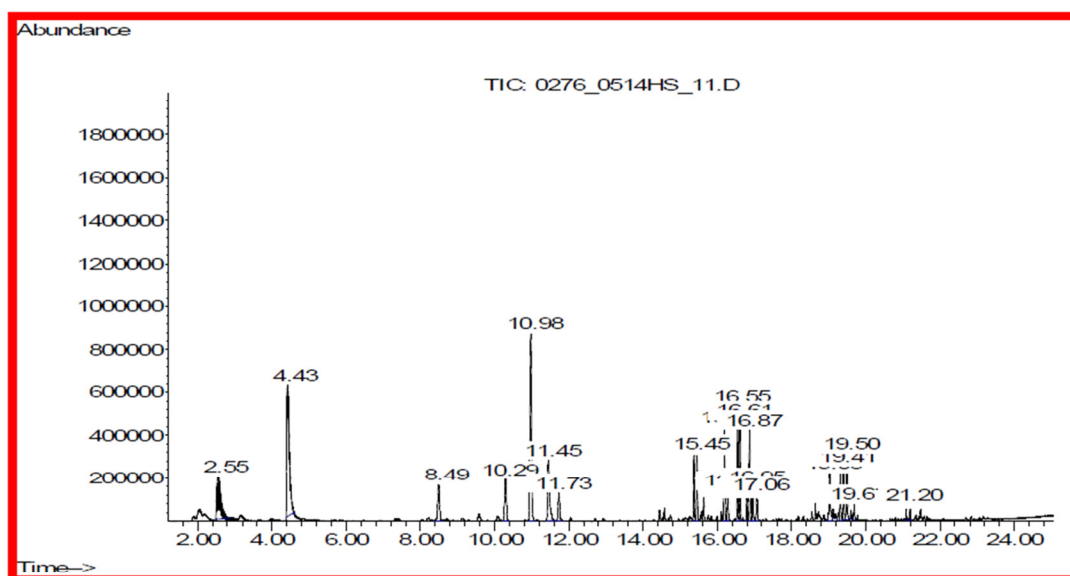
Table 8.14 - Sample 5: Total extract



TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5
15.56	not identified (m/z=55,82,111,129)	-	8,2
20.95	Erucamide	83	15
31.88	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	57
38.09	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	16
41.04	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	8,8

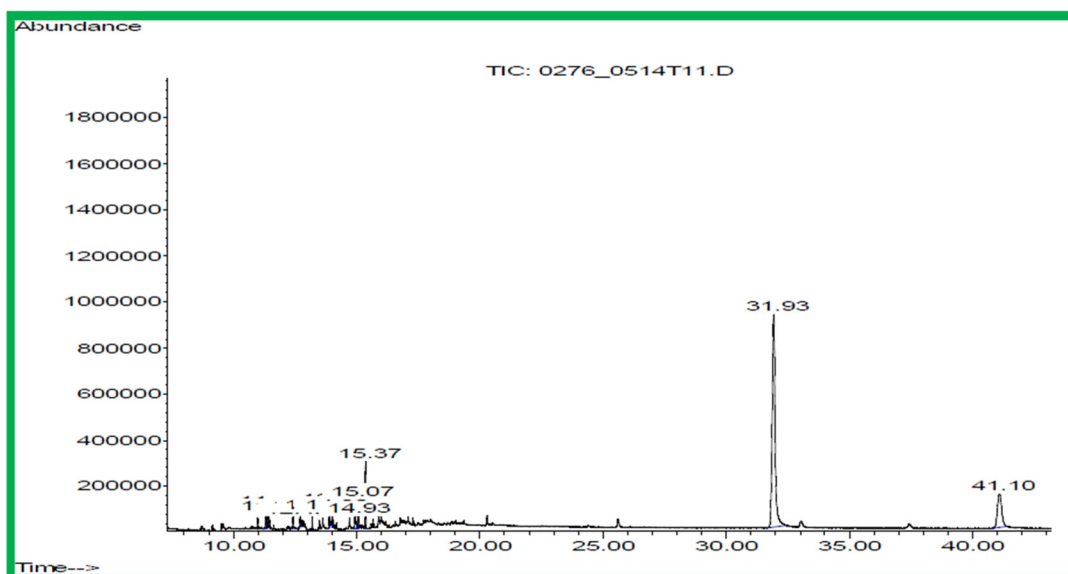
Table 8.15 - Sample 5: Internal surface

SAMPLE 6: PET/PETsiox/CASTPP



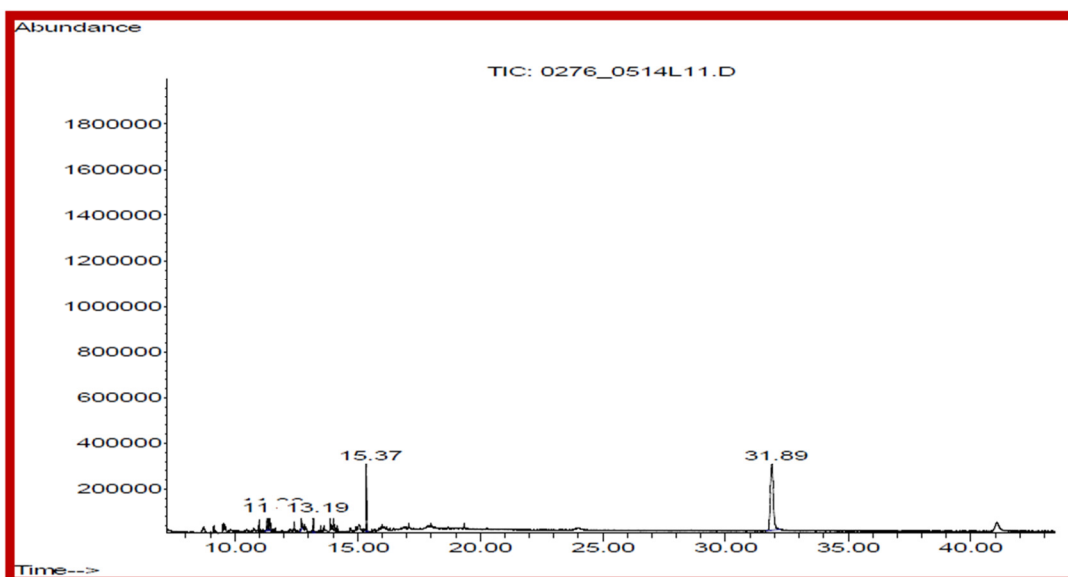
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.55	ethanol	80	3,5
4.43	ethyl acetate	83	8,2
8.49	heptane, 4-methyl-	91	1,6
10.29	heptane, 2,4-dimethyl-	87	1,6
10.98	2,4-dimethyl-1-heptene	87	7,0
11.45	Benzene, chloro (internal standard)	97	2,8
11.73	octane, 4-methyl-	91	1,1
from 15.37 to 21.20	aliphatic hydrocarbon	-	20

Table 8.16 - Sample 6: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
from 11.31 to 15.07	aliphatic hydrocarbon	-	85
15.37	Dipropyl phthalate (internal standard)	98	25
31.93	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	462
41.10	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	105

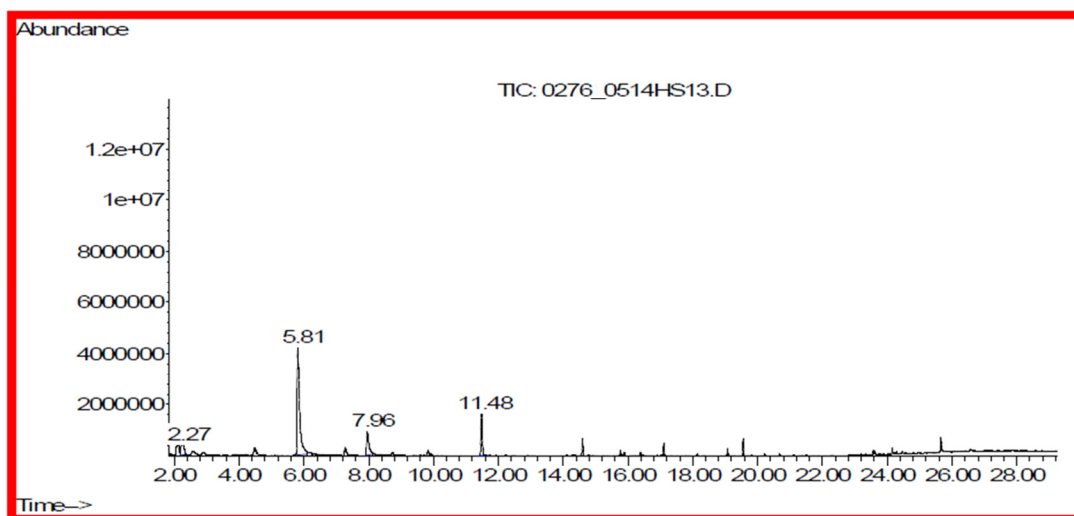
Table 8.17 - Sample 6: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
from 11.31 to 13.19	aliphatic hydrocarbon	-	16
15.37	Dipropyl phthalate (internal standard)	98	12,5
31.89	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	71

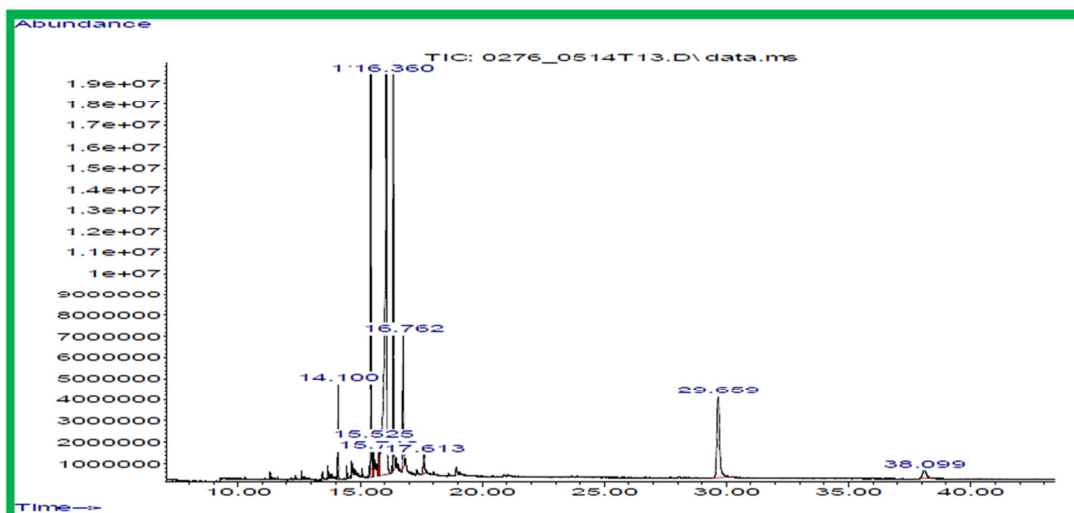
Table 8.18 - Sample 6: Internal surface

SAMPLE 7: OPPacr/acr



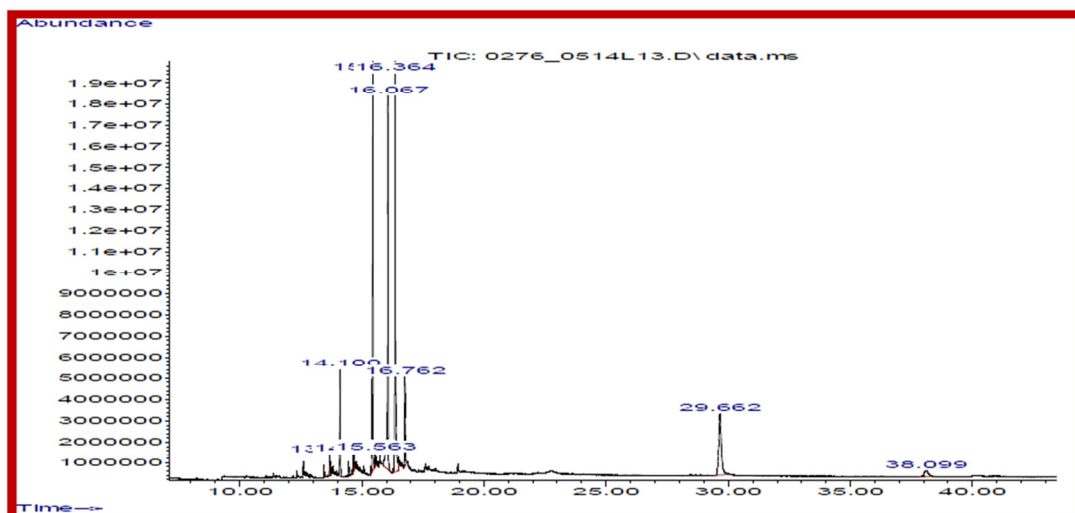
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.27	2-methyl, 1-propene	70	1,6
5.81	methoxypropanol	80	12
7.96	ethoxypropanol	83	2,3
11.48	Benzene, chloro (internal standard)	94	2,8

Table 8.19 - Sample 7: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.10	Dipropyl phthalate (internal standard)	98	25
15.44	Decanedioic acid, di butylester	91	127
15.53	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	10
16.08	acetyl tributyl citrate	80	653
16.36	di-2-ethylhexyl adipate	90	227
16.76	Oleamide	89	41
17.61	2-ethylhexyl diphenyl phosphate	91	10
29.66	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	118
38.10	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	17

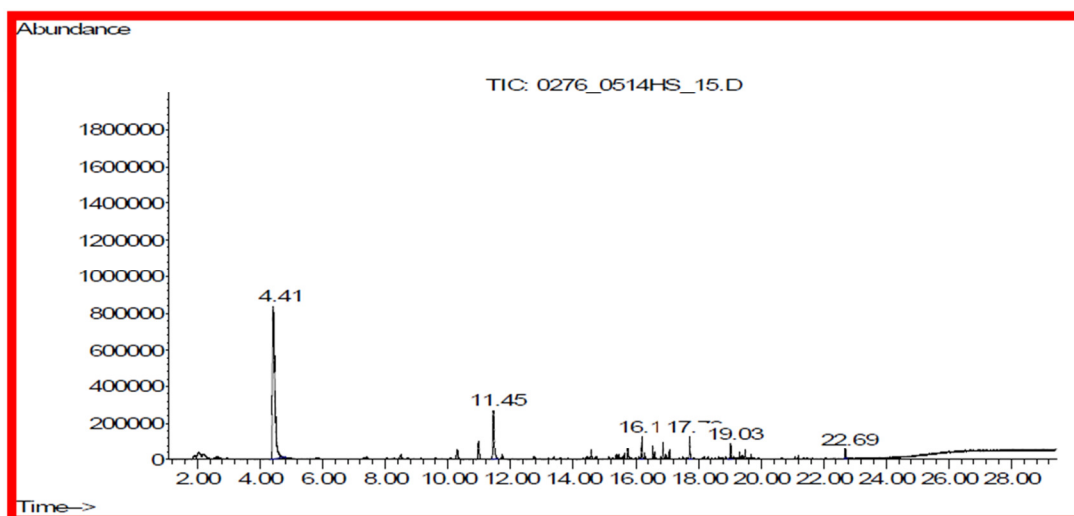
Table 8.20 - Sample 7: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.68	aliphatic hydrocarbon	-	0,7
14.10	Dipropyl phthalate (internal standard)	98	12,5
14.66	aliphatic hydrocarbon	-	1,7
14.69	aliphatic hydrocarbon	-	1,6
15.45	Decanedioic acid, di butylester	91	81
15.56	aliphatic hydrocarbon	-	1,1
16.07	acetyl tributyl citrate	80	56
16.36	di-2-ethylhexyl adipate	90	167
16.76	Oleamide	89	13
29.66	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	38
38.10	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	6,1

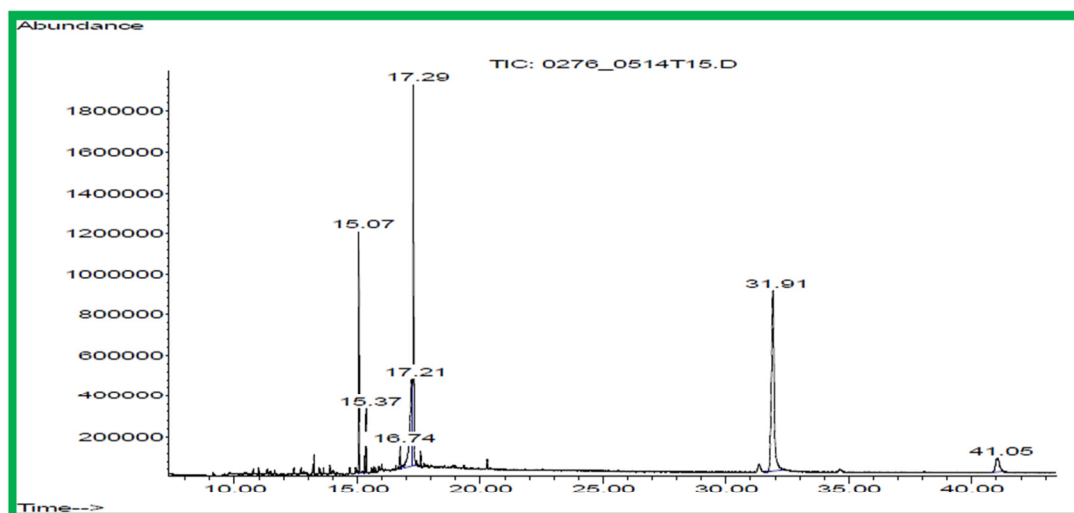
Table 8.21 - Sample 7: Internal surface

SAMPLE 8: OPA/CASTPP



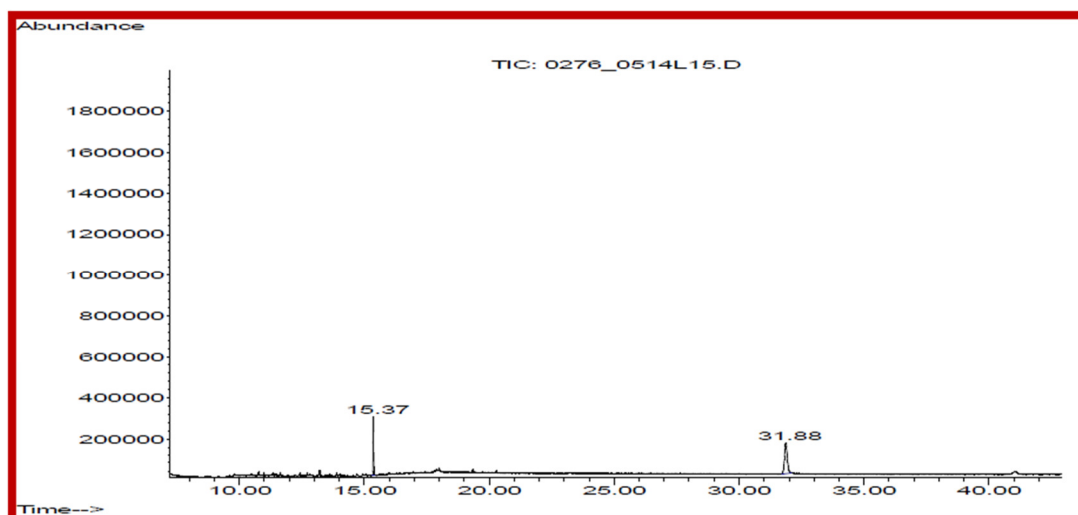
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.41	ethyl acetate	83	13,5
11.45	Benzene, chloro (internal standard)	94	2,8
16.19	aliphatic hydrocarbon	-	0,7
17.72	siloxane	-	0,6
19.03	aliphatic hydrocarbon	-	0,6
22.69	not identified (m/z = 84,99,111,173)	-	0,3

Table 8.22 - Sample 8: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.07	not identified (m/z =99,111,173)	-	108
15.36	Dipropyl phthalate (internal standard)	98	25
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	11
17.29	acetyl tributyl citrate	80	513
31.91	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	399
41.05	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	45

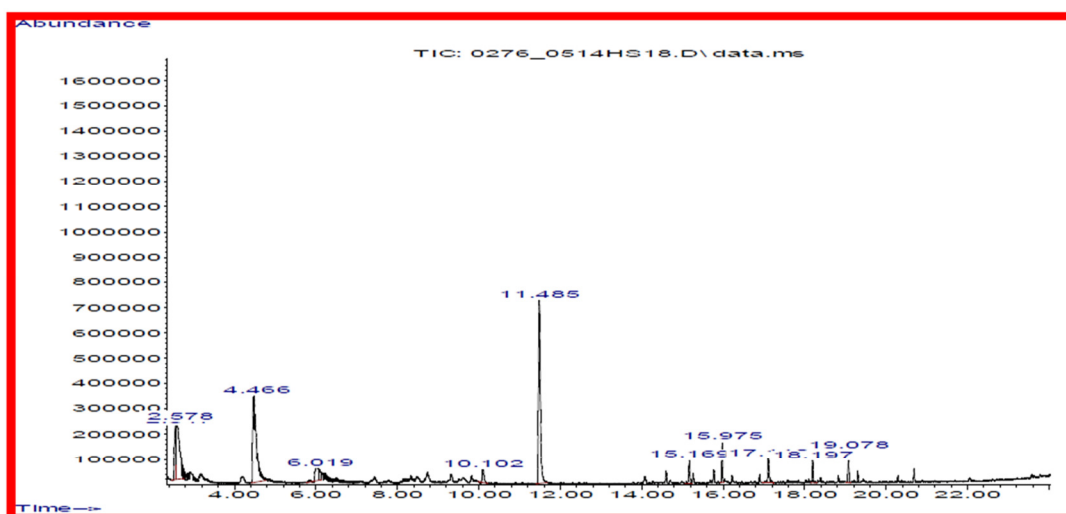
Table 8.23 - Sample 8: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5
31.88	antioxidant (m/z = 147,441,646)(Irgafos 168)	-	36

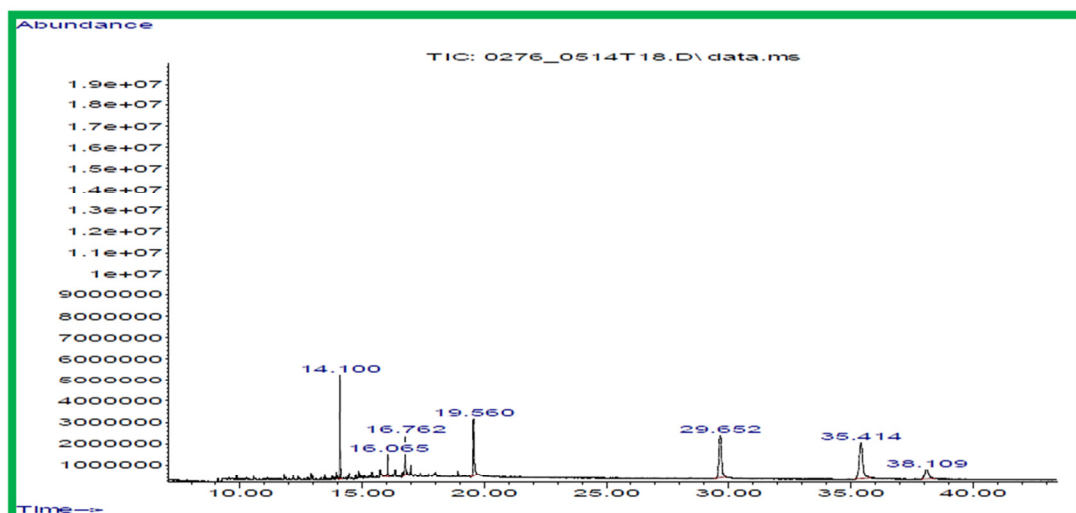
Table 8.24 - Sample 8: Internal surface

SAMPLE 9: PET/PE-EVOH-PE



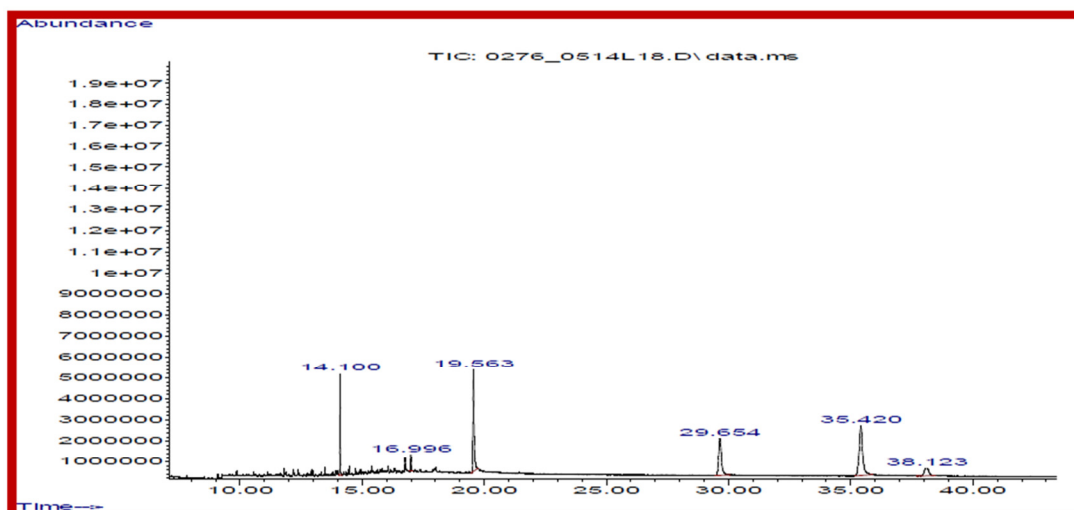
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.58	ethanol	80	2,2
4.47	ethylacetate	83	2,5
6.02	methoxypropanol	86	0,5
10.10	1-octene	95	0,2
11.49	Benzene, chloro (internal standard)	94	2,8
15.17	aliphatic hydrocarbon	-	0,2
15.98	aliphatic hydrocarbon	-	0,3
17.11	siloxane	-	0,3
18.20	aliphatic hydrocarbon	-	0,2
19.08	Siloxane *	-	0,2

Table 8.25 - Sample 9: Head space



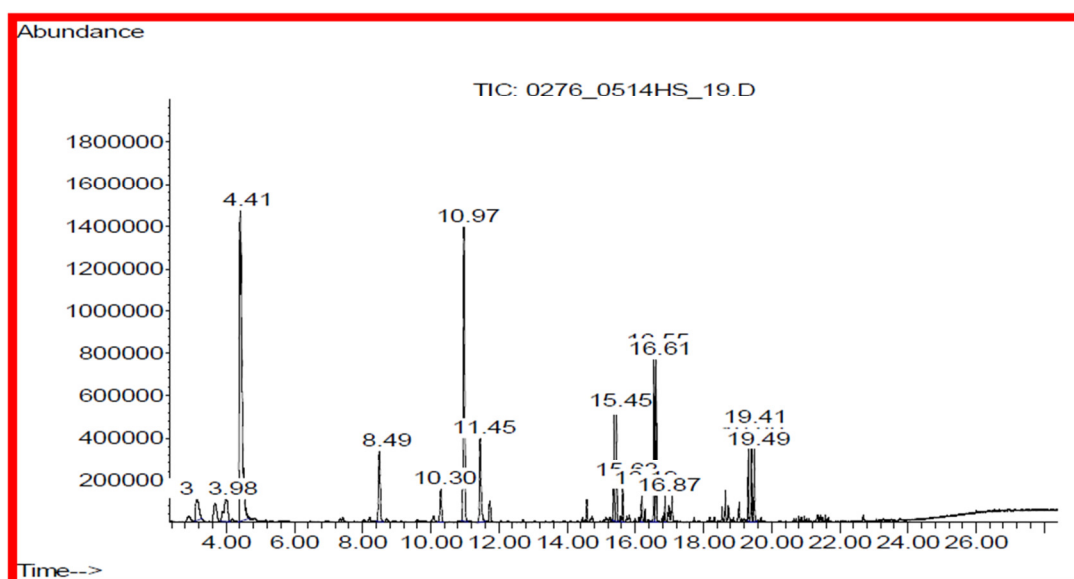
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.10	Dipropyl phthalate (internal standard)	98	25
16.07	acetyl tributyl citrate	80	7,7
16.76	oleamide	91	14
19.56	erucamide	87	32
29.65	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	56
35.41	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	67
38.11	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	22

Table 8.26 - Sample 9: Total extract



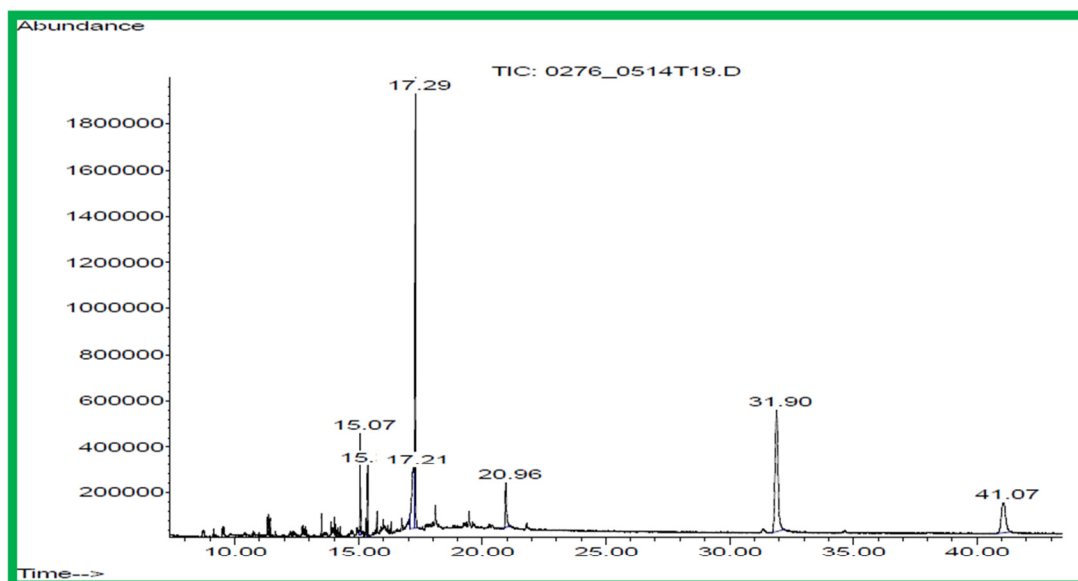
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
14.10	Dipropyl phthalate (internal standard)	98	12,5
17.00	aliphatic hydrocarbon	-	2,9
19.56	erucamide	87	26
29.65	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	27
35.42	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	45
38.12	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	9,2

Table 8.27 - Sample 9: Internal surface

SAMPLE 10: PET/PE-EVOH-PE

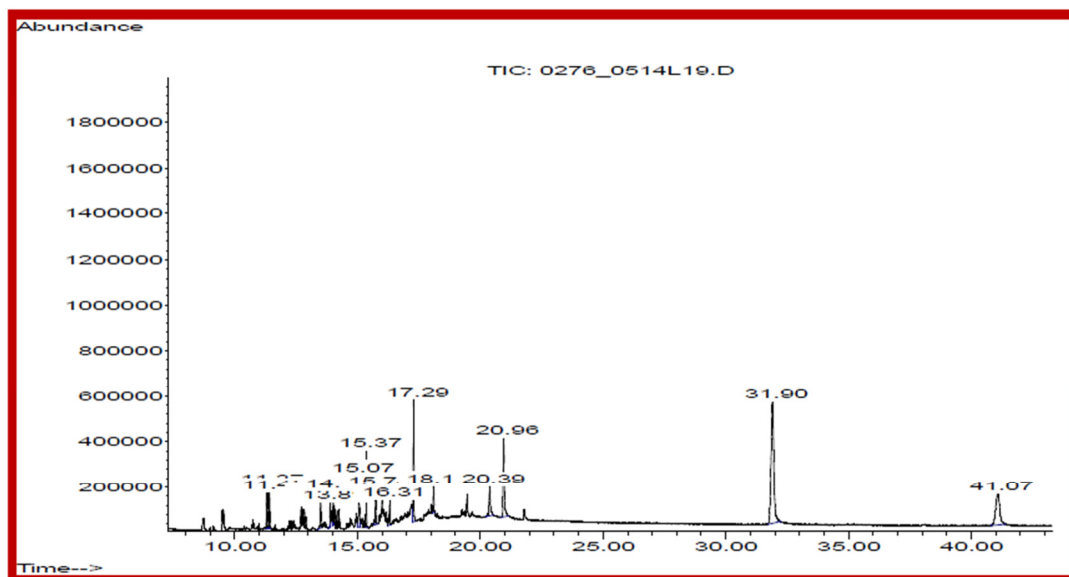
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
3.98	cyclohexane	86	1,8
4.41	ethyl acetate	83	37
8.49	heptane, 4-methyl-	91	2,5
10.30	heptane, 2,4-dimethyl-	87	1,0
10.97	2,4-dimethyl-1-heptene	87	8,6
11.45	Benzene, chloro (internal standard)	97	2,8
from 15.45 to 19.49	aliphatic hydrocarbon	-	14

Table 8.28 - Sample 10: Head space



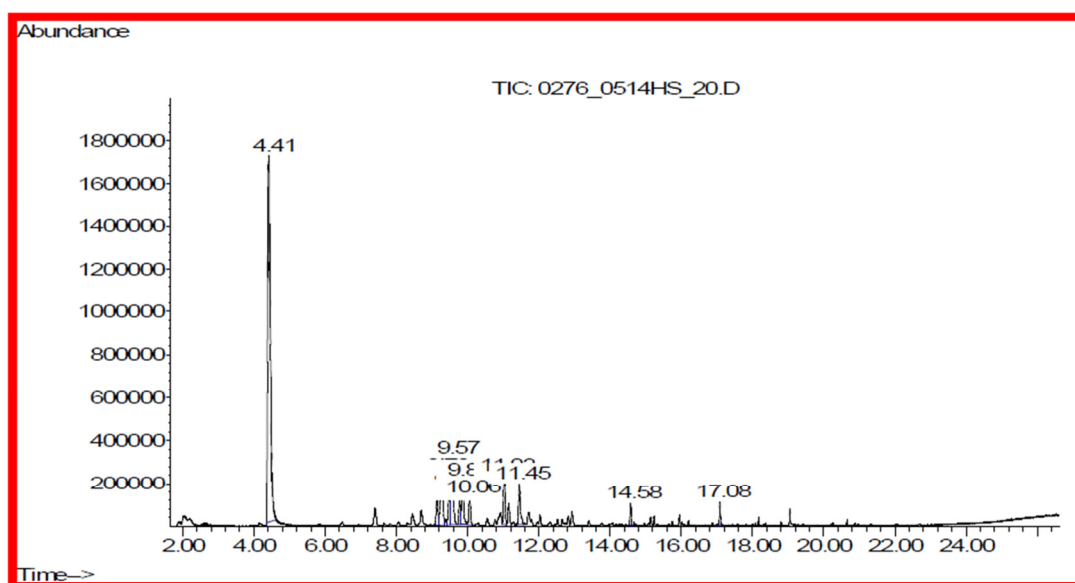
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.07	not identified (m/z =99,111,173)	-	47
15.37	Dipropyl phthalate (internal standard)	98	25
17.29	acetyl tributyl citrate	80	218
20.96	erucamide	81	39
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	249
41.07	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	92

Table 8.29 - Sample 10: Total extract



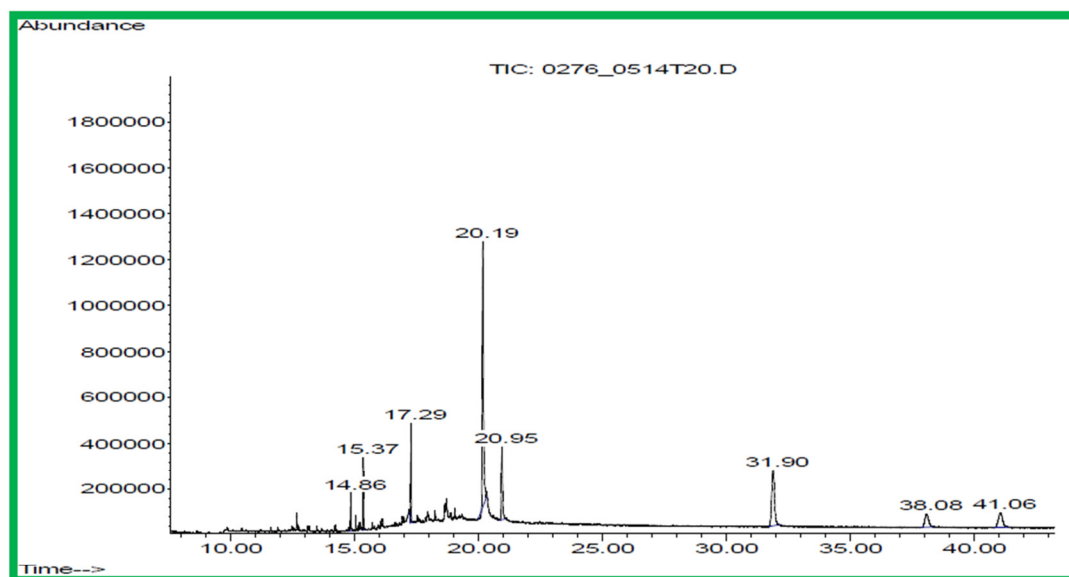
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
from 11.31 to 14.02	aliphatic hydrocarbon	-	36
15.07	not identified (m/z = 84,99,111,173)	-	14
15.37	Dipropyl phthalate (internal standard)	98	12,5
15.74	aliphatic hydrocarbon	-	7,6
17.29	acetyl tributyl citrate	80	25
18.10	Analytical system contaminant	-	-
20.39	Analytical system contaminant	-	-
20.96	erucamide	81	29
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	110
41.07	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	41

Table 8.30 - Sample 10: Internal surface

SAMPLE 11: PETpvdc/PE

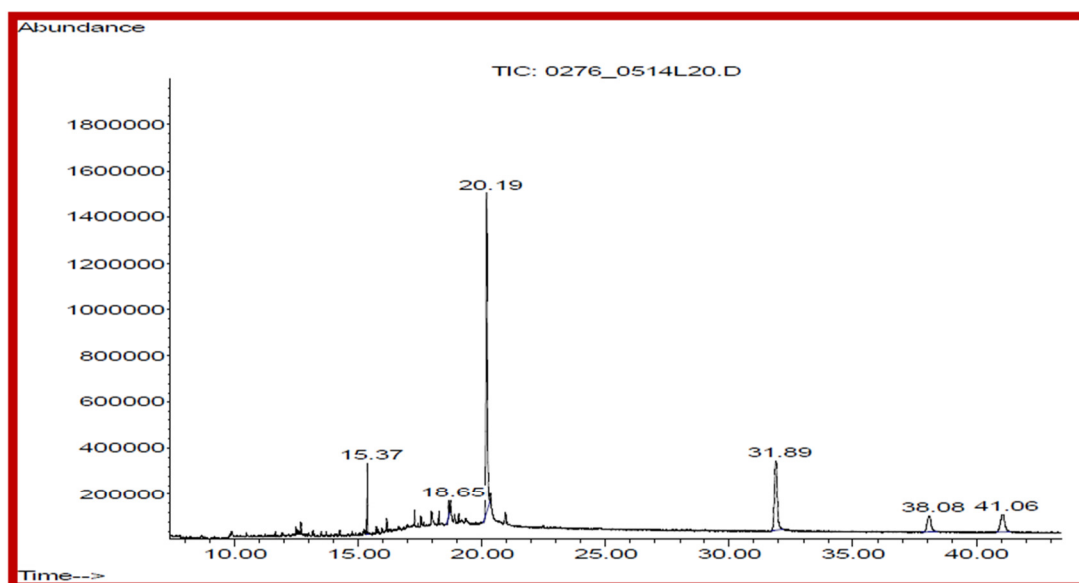
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.41	ethyl acetate	83	46
from 9.14 to 11.03	aliphatic hydrocarbon	-	24
11.45	Benzene, chloro (internal standard)	97	2,8
14.58	Siloxane *	-	-
17.08	Siloxane *	-	-

Table 8.31 - Sample 11: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.86	not identified (m/z = 102,141)	-	15
15.37	Dipropyl phthalate (internal standard)	98	25
17.29	acetyl tributyl citrate	80	45
20.19	oleic acid, 3-hydroxypropyl ester	91	219
20.95	erucamide	81	55
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	110
38.08	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	80	33
41.06	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	43

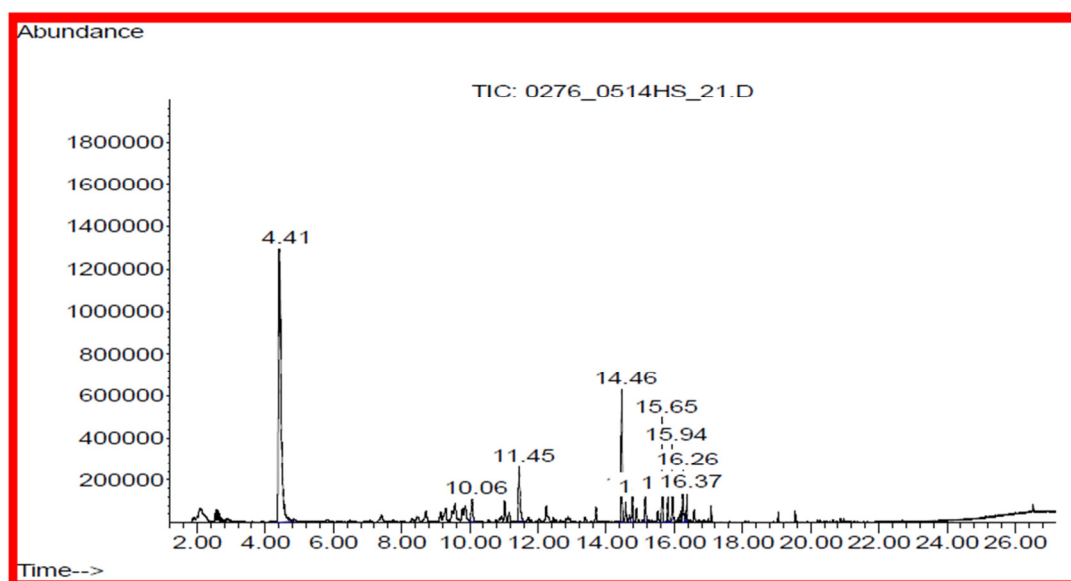
Table 8.32 - Sample 11: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5
18.65	Hexadecanoic acid, ester	-	3,1
20.19	oleic acid, 3-hydroxypropyl ester	91	137
31.89	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	71
38.08	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	80	22
41.06	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	27

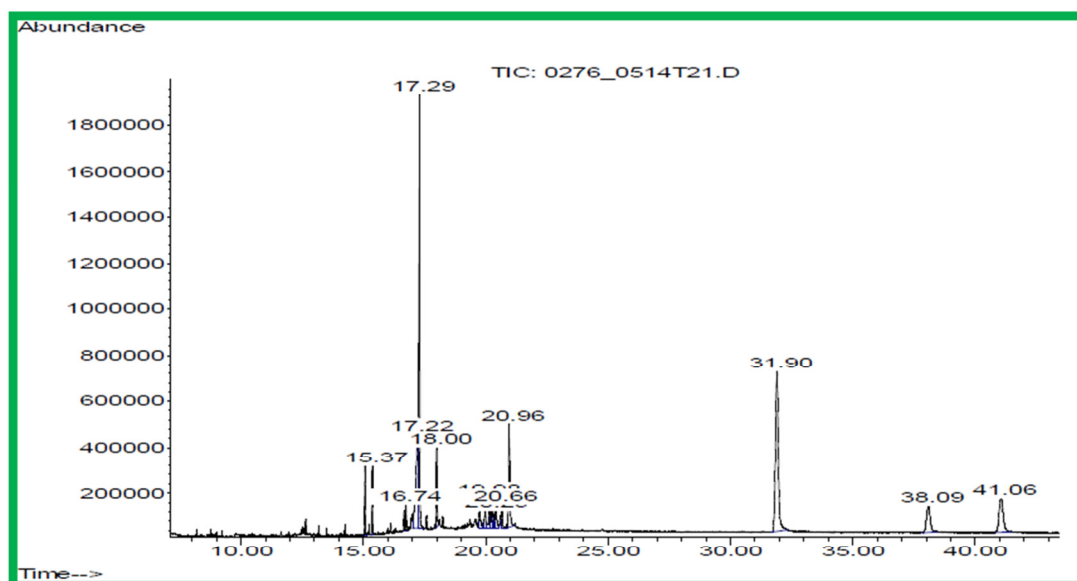
Table 8.33 - Sample 11: Internal surface

SAMPLE 12: PETmet/PE



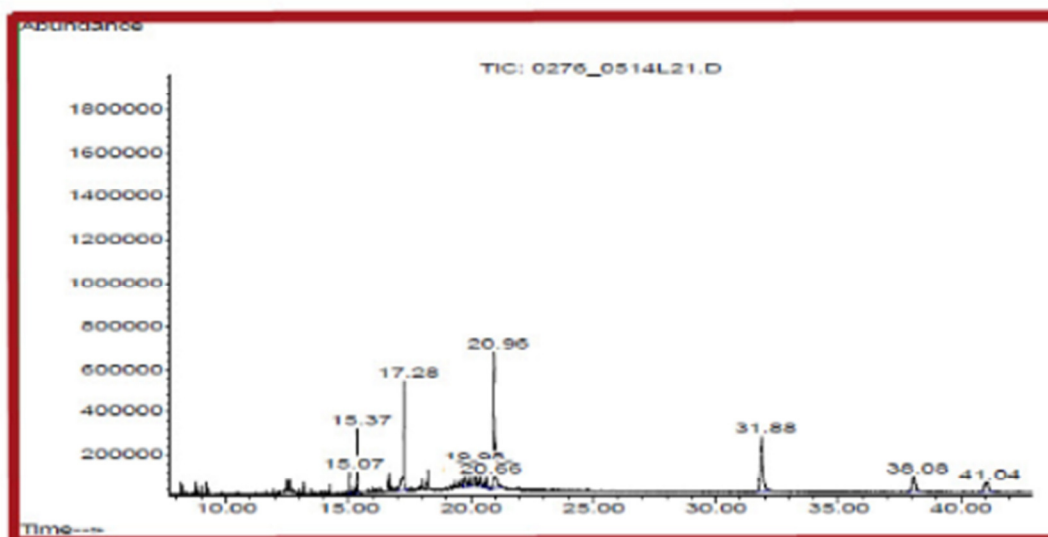
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.41	ethyl acetate	83	32
10.06	1-octene	87	1,2
11.45	Benzene, chloro (internal standard)	94	2,8
14.46	aliphatic hydrocarbon	-	3,8
14.77	aliphatic hydrocarbon	-	1,0
15.15	aliphatic hydrocarbon	-	1,1
15.65	aliphatic hydrocarbon	-	2,7
15.81	aliphatic hydrocarbon	-	0,7
15.94	aliphatic hydrocarbon	-	1,9
16.26	aliphatic hydrocarbon	-	1,4
16.37	aliphatic hydrocarbon	-	0,7

Table 8.34 - Sample 12: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
15.07	not identified (m/z =99,111,173)	-	29
15.37	Dipropyl phthalate (internal standard)	98	25
16.74	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	9
17.29	acetyl tributyl citrate	80	320
18.00	oleamide	87	40
from 19.75 to 20.66	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	130
20.96	Erucamide	97	87
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	325
38.09	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	94	70
41.06	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	101

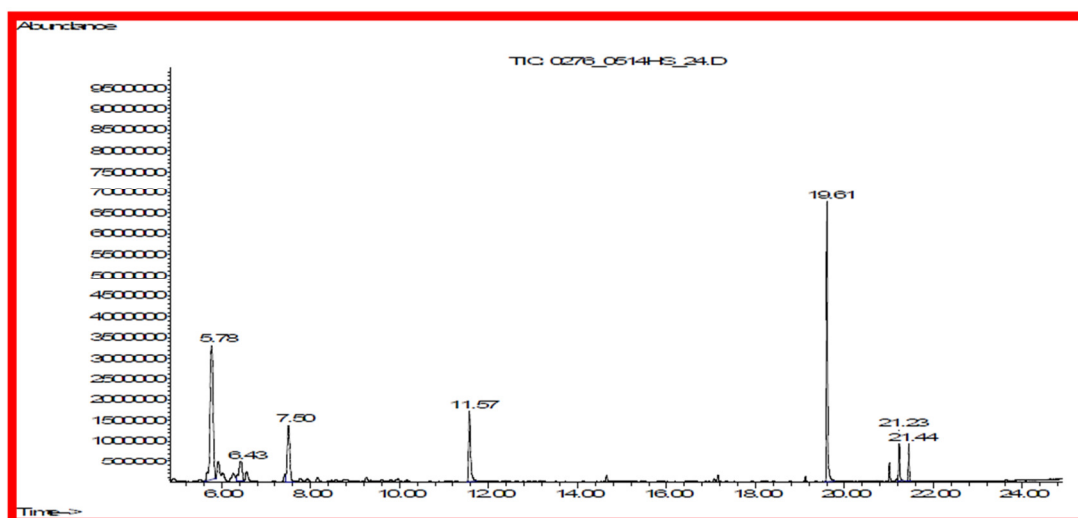
Table 8.35 - Sample 12: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.07	not identified (m/z =84,99,111,173)	-	4,9
15.37	Dipropyl phthalate (internal standard)	98	12,5
17.29	acetyl tributyl citrate	80	38
from 19.75 to 20.66	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	26
20.96	Erucamide	90	62
31.88	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	59
38.08	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	94	21
41.04	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	18

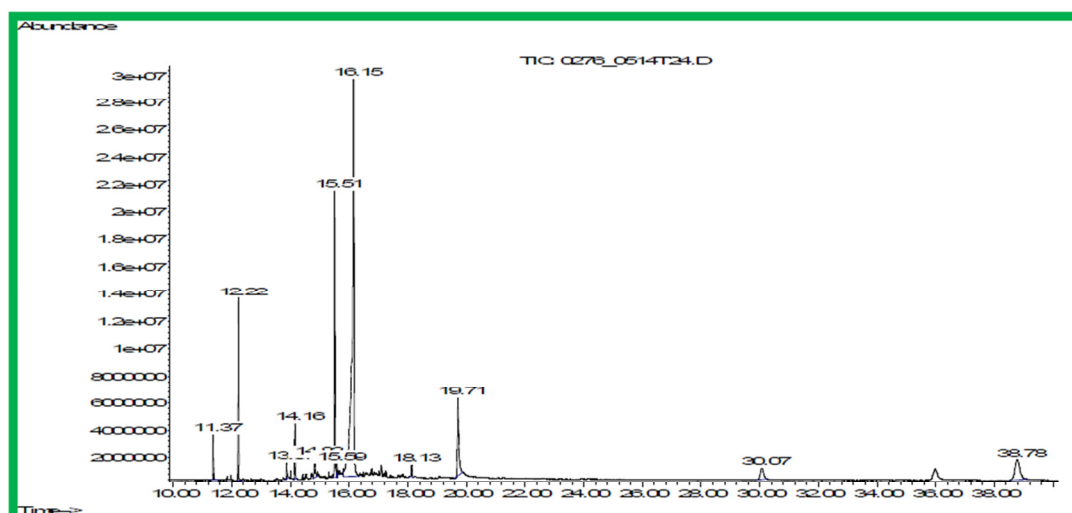
Table 8.36 - Sample 12: Internal surface

SAMPLE 13: OPPcoex



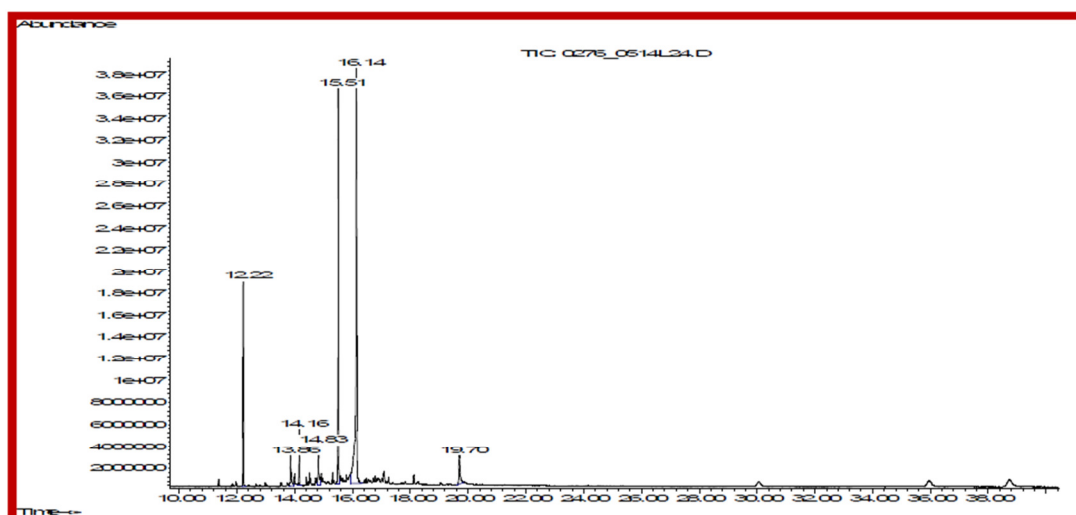
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
5.78	Cyclohexane	91	8,3
7.50	Cyclohexane, methyl	94	2,9
11.57	Benzene, chloro (internal standard)	94	2,8
19.61	Triacetin	83	5,4
21.23	2,5-CYCLOHEXADIEN-1-ONE, 2,6-BIS(1,1-DIMETHYLETHYL)-4-METHYLENE-	99	1,0
21.44	BHT	98	0,7

Table 8.37 - Sample 13: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.37	Triacetin	83	24
12.22	BHT	98	78
13.87	Cyclohexadecane	91	11
14.16	Di propyl phthalate (internal standard)	94	25
14.83	7,9-Di-tert-butyl-1-oxaspiro(4,5) deca-6,9-diene-2,8-dione	98	19
15.51	Sebacic acid, dibutyl ester	91	129
16.15	Tributyl acetylcitrate	91	805
18.13	Analytical system contaminant	-	-
19.71	Erucamide	87	83
30.07	Antioxidant (m/z = 308,441,646)(Irgafos 168)	-	30
38.78	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	83

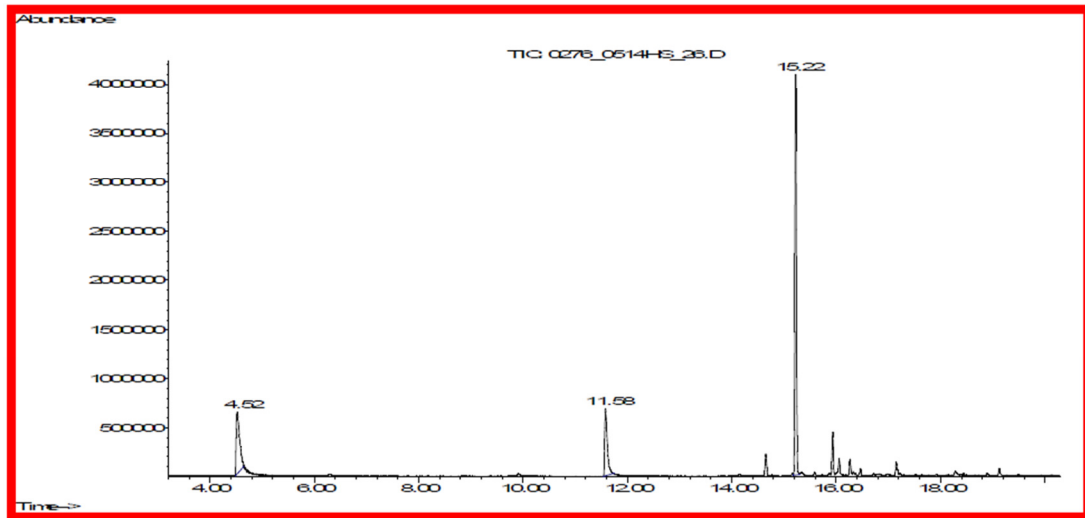
Table 8.38 - Sample 13: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
12.22	BHT	98	45
13.86	Cyclohexadecane	91	11
14.16	Di propyl phthalate (internal standard)	94	12,5
14.83	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	98	13
15.51	Sebacic acid, dibutyl ester	91	84
16.14	Tributyl acetyl citrate	91	145
19.70	Erucamide	87	15

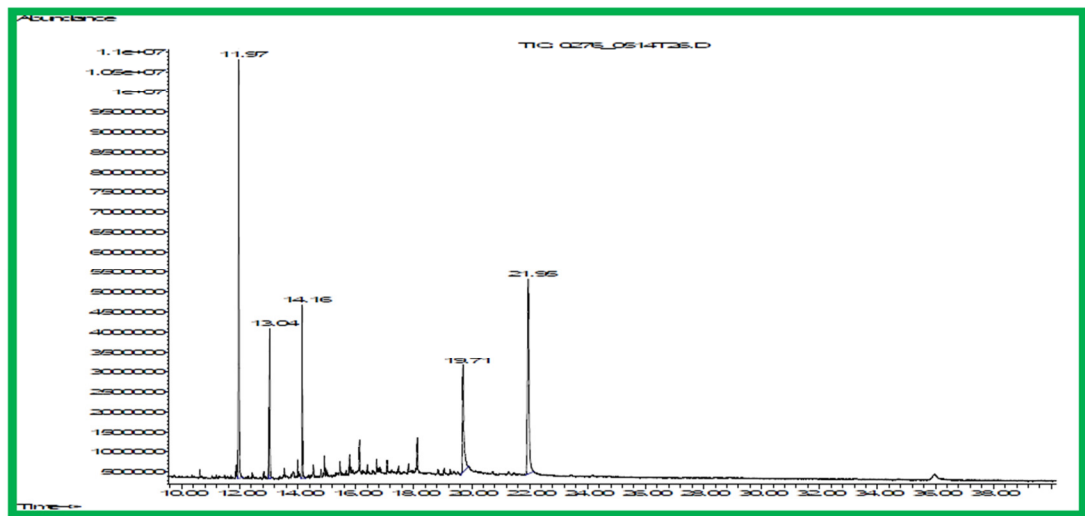
Table 8.39 - Sample 13: Internal surface

SAMPLE 14: PET/Aluminum/PE



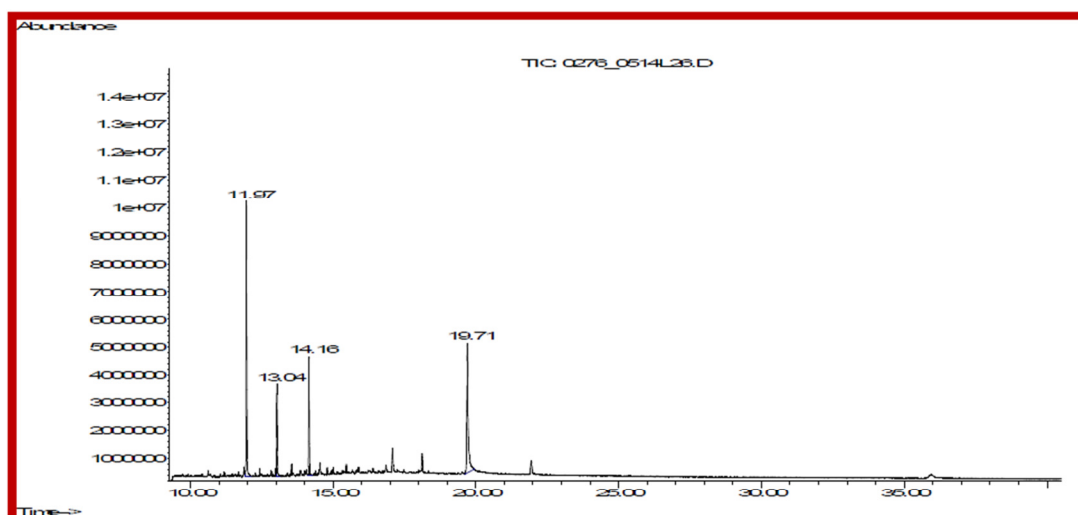
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.52	Ethyl acetate	84	4,1
11.58	Benzene, chloro (internal standard)	94	2,8
15.22	Pentamethyl, eptane	94	9,0

Table 8.40 - Sample 14: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.97	Silane,trimethoxy[3-(oxiranylmethoxy)propyl]	91	63
13.04	Not identified (m/z=101,111,129)	-	23
14.16	Di propyl phthalate (internal standard)	94	25
19.71	Erucamide	87	39
21.95	Not identified (m/z=111,129,215,343)	-	77

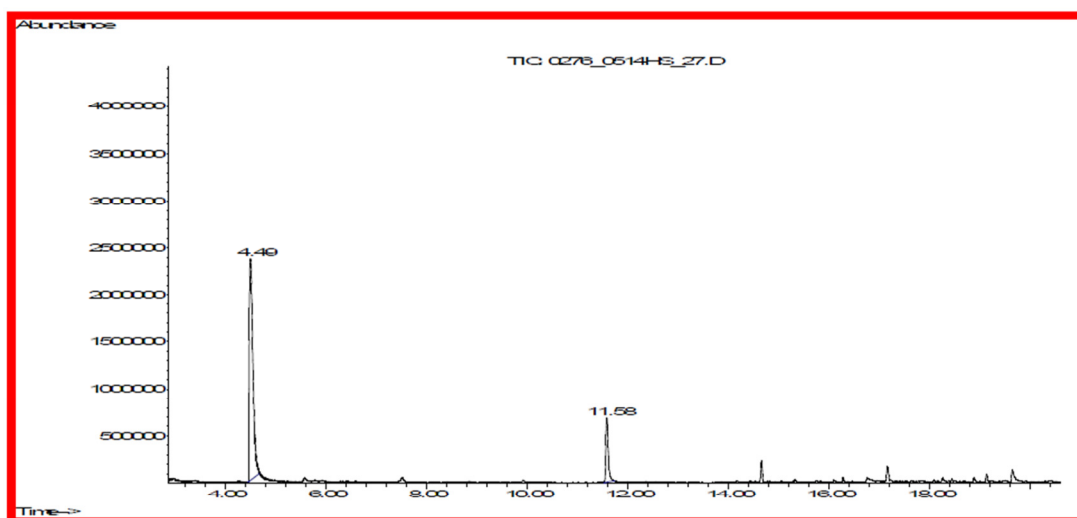
Table 8.41 - Sample 14: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.37	Silane,trimethoxy[3-(oxiranylmethoxy)propyl]	91	29
13.04	Not identified (m/z=101,111,129)	-	10
14.16	Di propyl phthalate (internal standard)	94	12,5
19.71	Erucamide	87	32

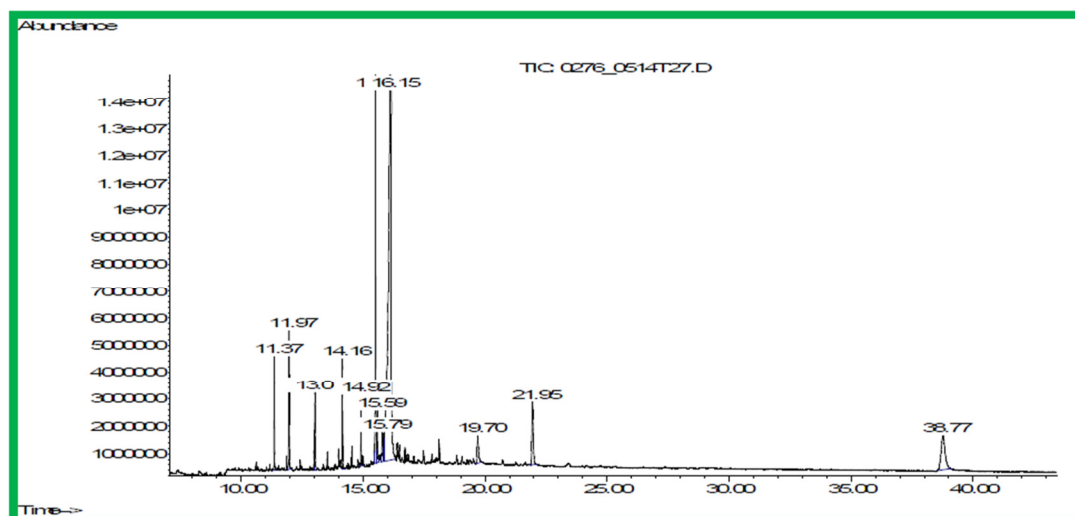
Table 8.42 - Sample 14: Internal surface

SAMPLE 15: PETmet/PE



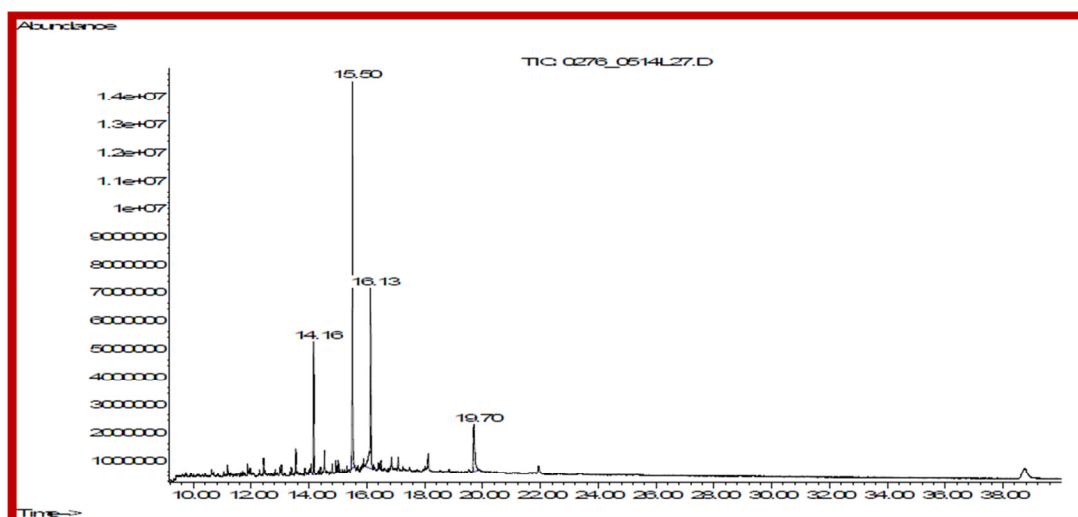
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.49	Ethyl acetate	84	23
11.58	Benzene, chloro (internal standard)	94	2,8

Table 8.43 - Sample 15: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.37	BHT		25
11.97	Silane,trimethoxy[3-(oxiranylmethoxy)propyl]	91	33
13.04	Not identified (m/z=101,111,129)	-	20
14.16	Di propyl phthalate (internal standard)	94	25
14.92	Docosane	90	14
15.51	Sebacic acid, butyl ester	91	200
16.15	Tributyl acetyl citrate	89	1028
19.70	Erucamide	87	39
21.95	Not identified (m/z=111,129,215,343)	-	38
38.77	Antioxidant (m/z=308,441,646) (Irgafos 168)	-	64

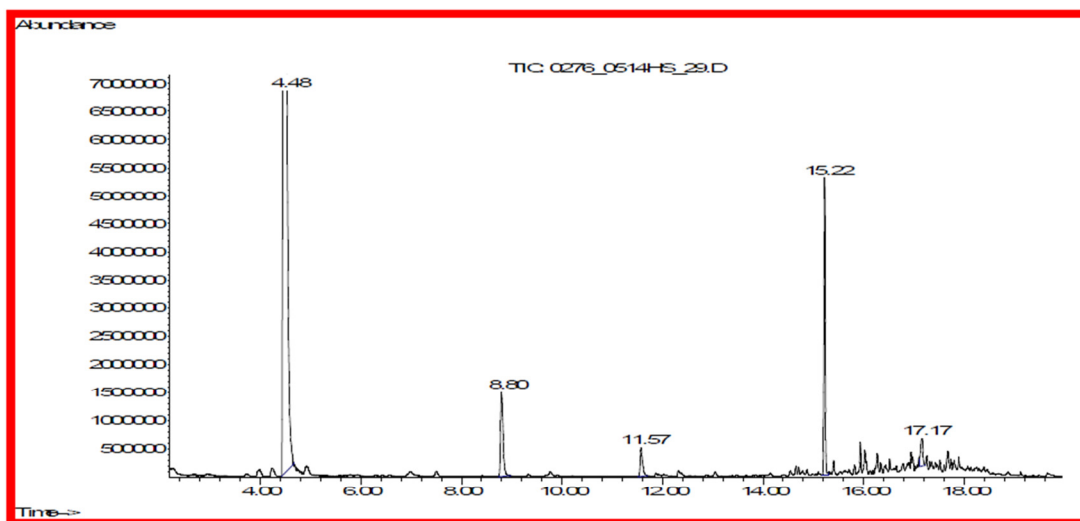
Table 8.44 - Sample 15: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Di propyl phthalate (internal standard)	94	12,5
15.50	Sebacic acid, butyl ester	91	41
16.13	Tributyl acetylacrylate	89	25
19.70	Erucamide	87	12

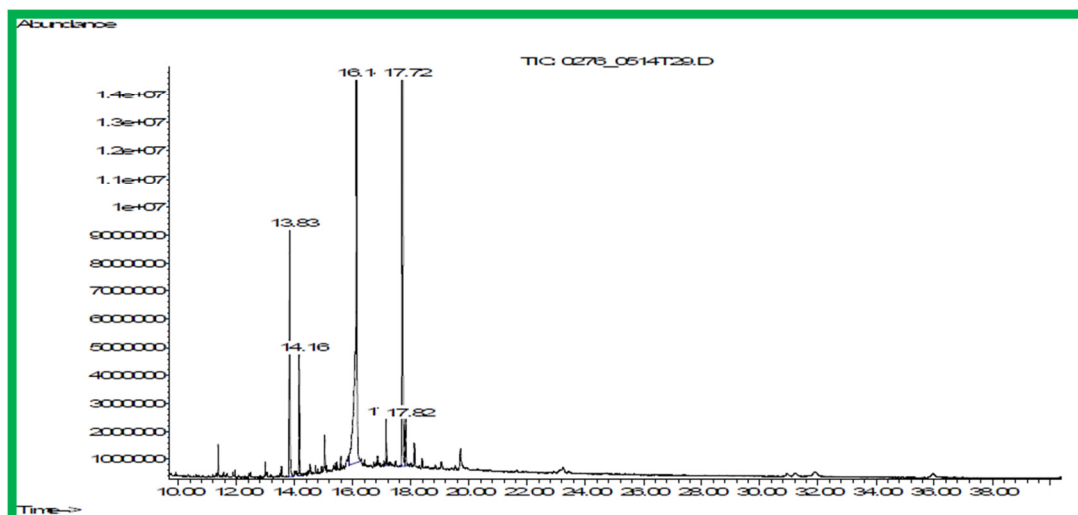
Table 8.45 - Sample 15: Internal surface

SAMPLE 16: PAPER/Aluminum/PE



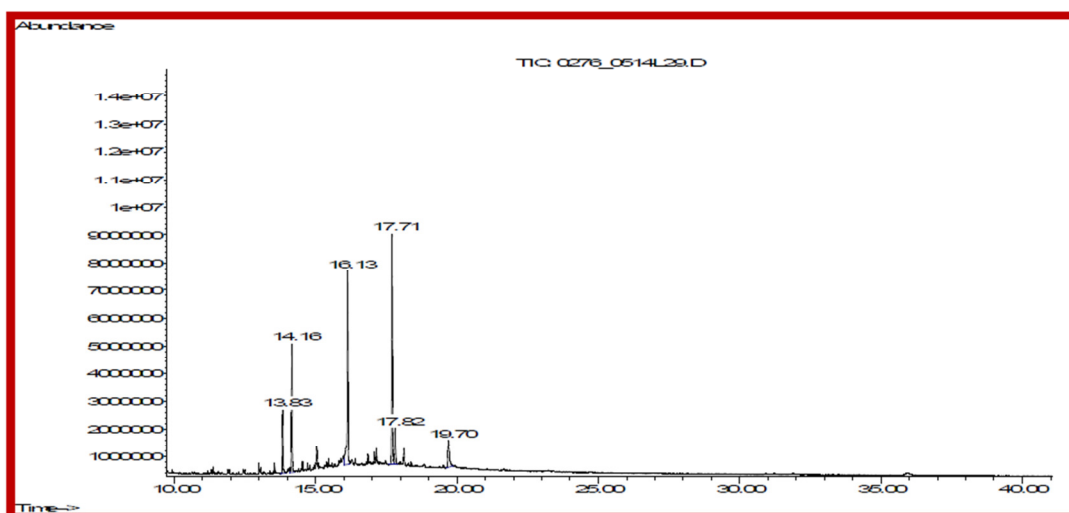
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.48	Ethyl acetate	84	190
8.80	Toluene	94	8,8
11.58	Benzene, chloro (internal standard)	94	2,8
15.22	Heptane, pentamethyl	83	16
17.17	Aliphatic hydrocarbon	-	2,9

Table 8.46 - Sample 16: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.83	Not identified (m/z=84,99,111,173)	-	53
14.16	Di propyl phthalate (internal standard)	94	25
16.13	Tributyl acetyl citrate	89	350
17.71	2-Ethylhexyl diphenyl phosphate	95	209
17.82	Di 2-ethylhexil phthalate	90	14
19.70	Erucamide	91	12

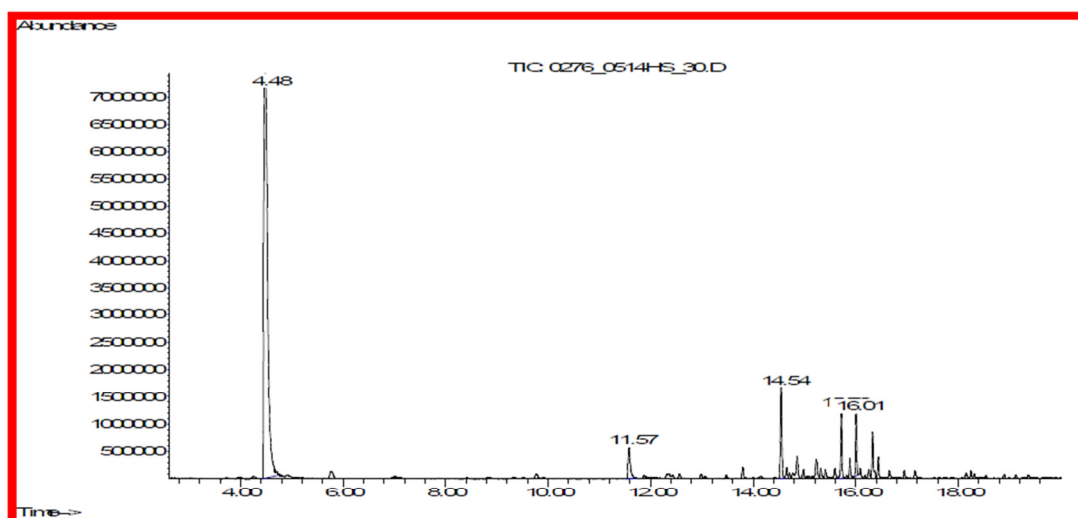
Table 8.47 - Sample 16: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.83	Not identified (m/z=84,99,111,173)	-	7,0
14.16	Di propyl phthalate (internal standard)	94	12,5
16.13	Tributyl acetylcitrate	89	25
17.71	2-Ethylhexyl diphenyl phosphate	95	30
17.82	Di 2-ethylhexil phthalate	90	5,0
19.70	Erucamide	91	7,5

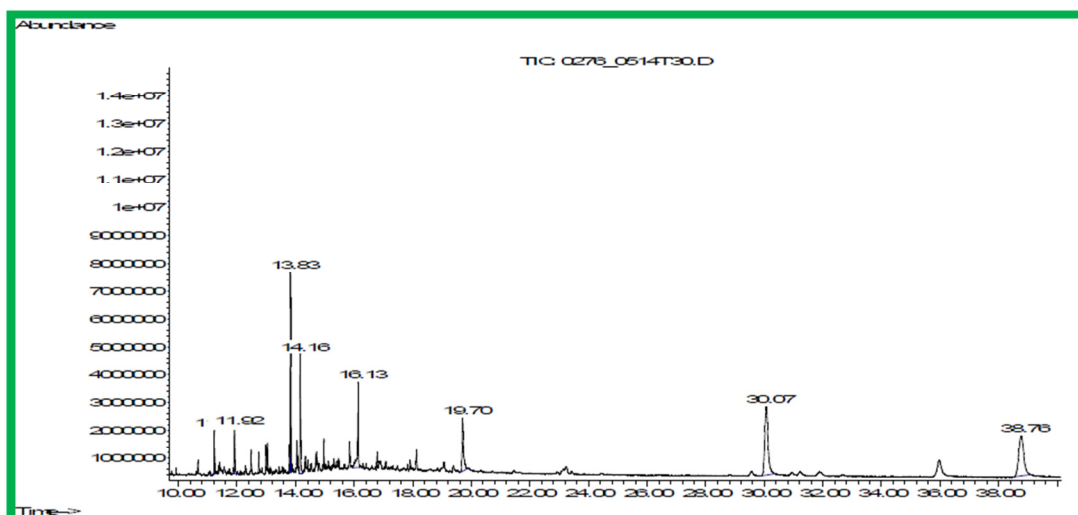
Table 8.48 - Sample 16: Internal surface

SAMPLE 17: OPA/PE



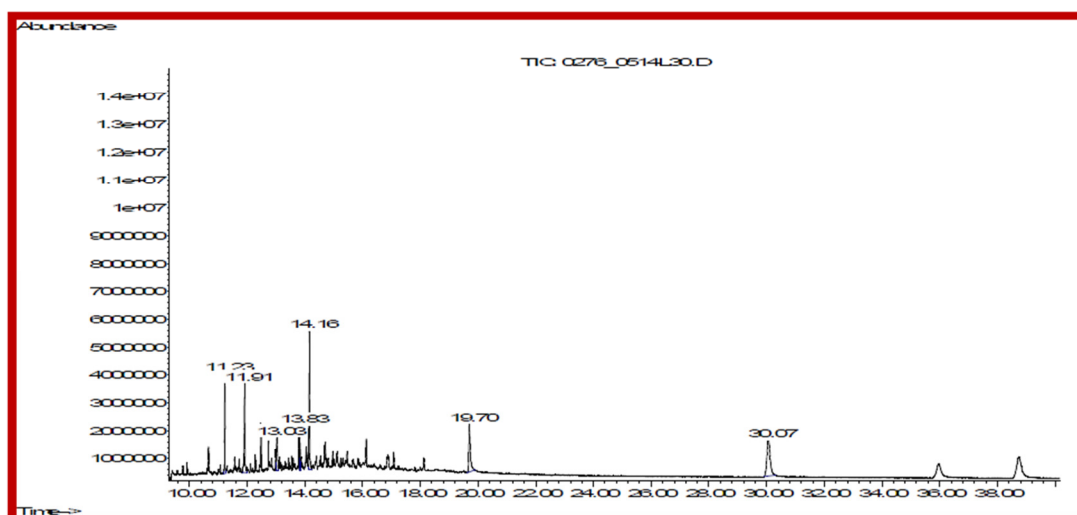
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.48	Ethyl acetate	84	80
11.57	Benzene, chloro (internal standard)	94	2,8
15.22	Heptane, pentamethyl	83	16
From 14.54 to 16.01	Aliphatic saturated hydrocarbons	>80	11 sum

Table 8.49 - Sample 17: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.23	Cyclohexane, octyl	96	8,5
11.92	1-hexadecene	96	11
13.83	Not identified (m/z=84,99,111,173)	-	44
14.16	Di propyl phthalate (internal standard)	94	25
16.13	Tributyl acetylcitrate	89	26
19.70	Erucamide	91	28
30.07	Antioxidant (m/z=308,441,646) (Irgafos 168)	-	72
38.76	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	71

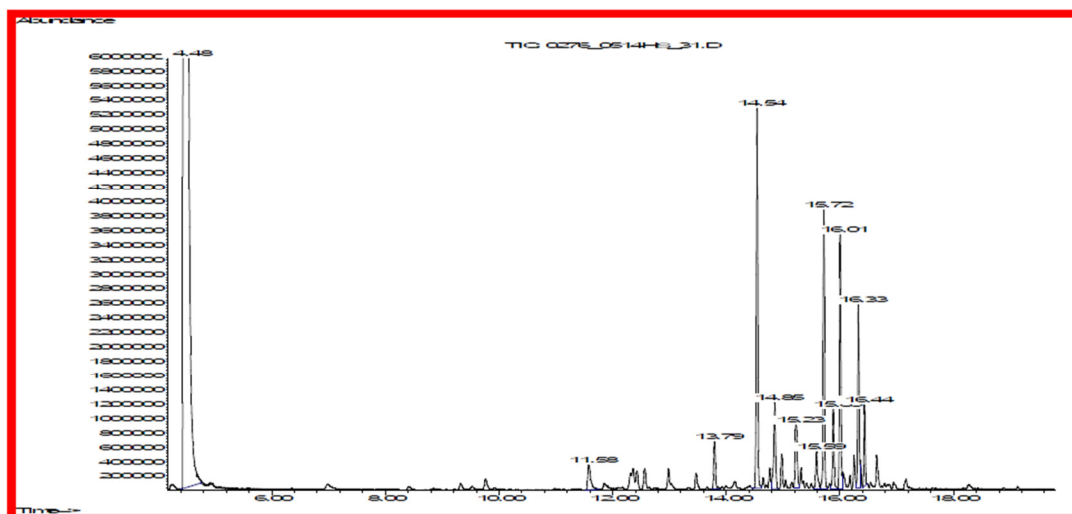
Table 8.50 - Sample 17: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.23	Cyclohexane, octyl	96	7,0
11.91	1-hexadecene	96	9,4
13.83	Not identified (m/z=84,99,111,173)	-	4,4
14.16	Di propyl phthalate (internal standard)	94	12,5
19.70	Erucamide	91	11
30.07	Antioxidant (m/z=308,441,646) (Irgafos 168)	-	17

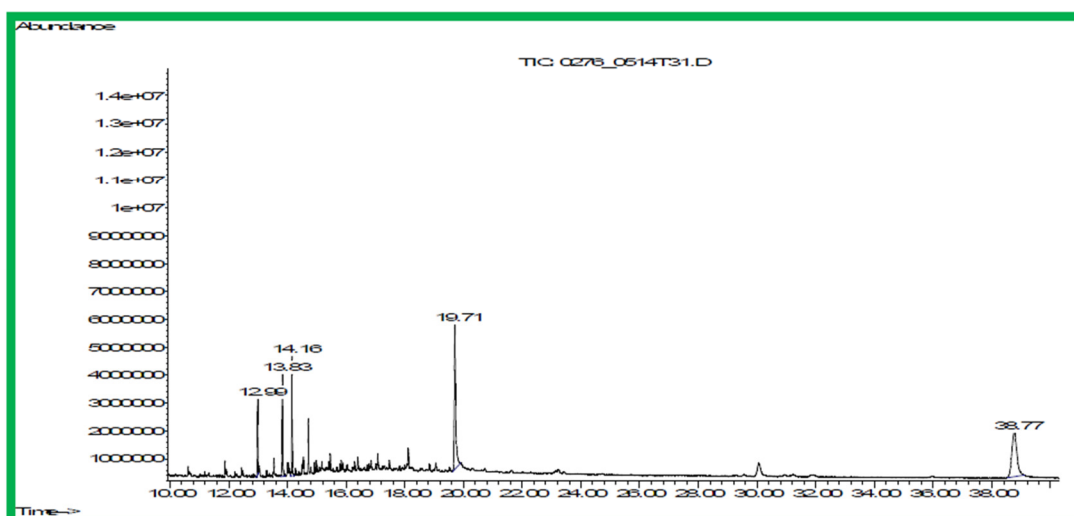
Table 8.51 - Sample 17: Internal surface

SAMPLE 18: PET/Aluminum/PE



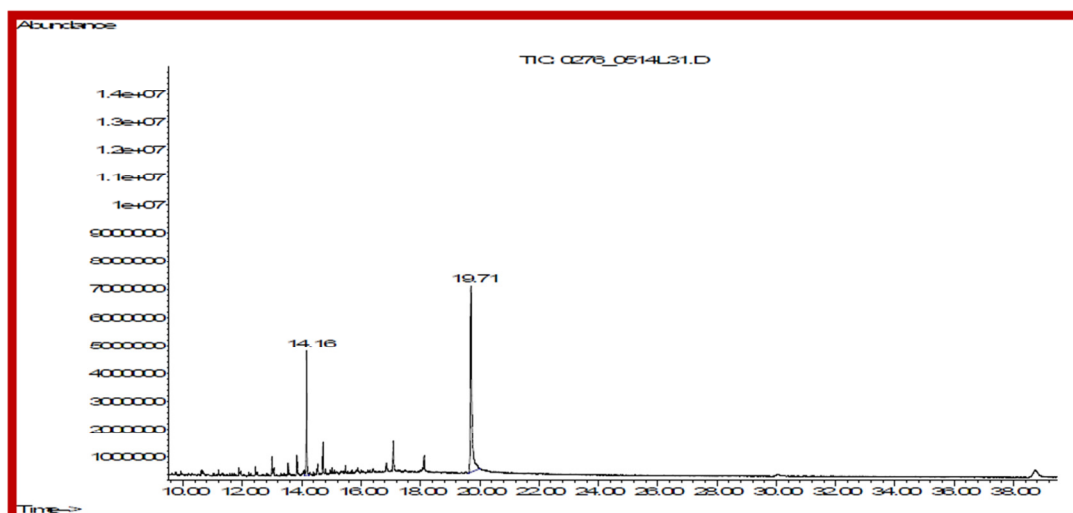
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.48	Ethyl acetate	84	210
11.57	Benzene, chloro (internal standard)	94	2,8
From 13.78 to 16.44	Aliphatic saturated hydrocarbons	>80	84 sum

Table 8.52 - Sample 18: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
12.99	Octadecane	96	12
13.83	Not identified (m/z=84,99,111,173)	-	24
14.16	Di propyl phthalate (internal standard)	94	25
19.71	Erucamide	91	70
38.77	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	77

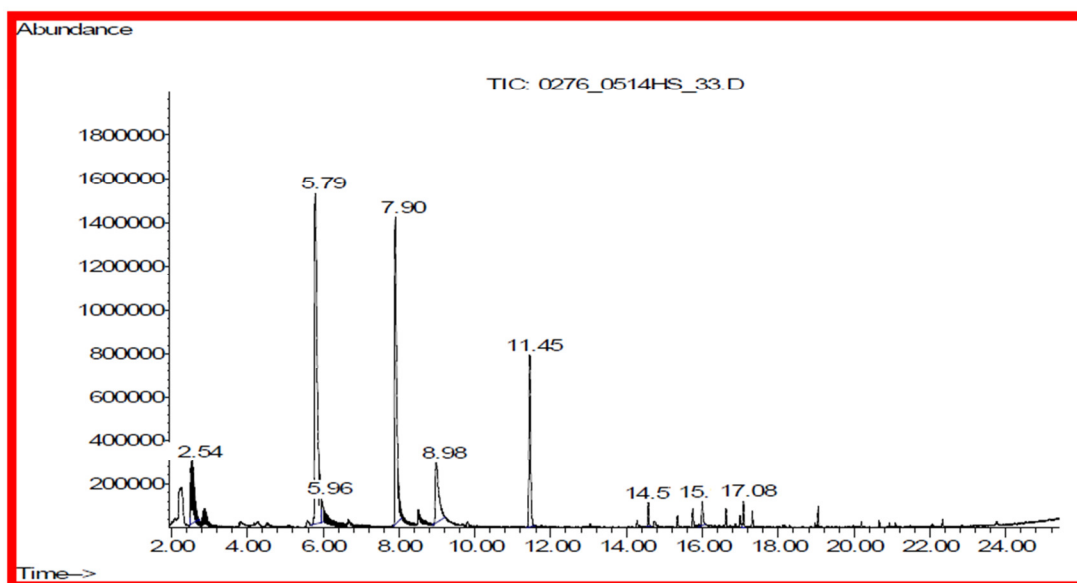
Table 8.53 - Sample 18: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Di propyl phthalate (internal standard)	94	12,5
19.71	Erucamide	91	45

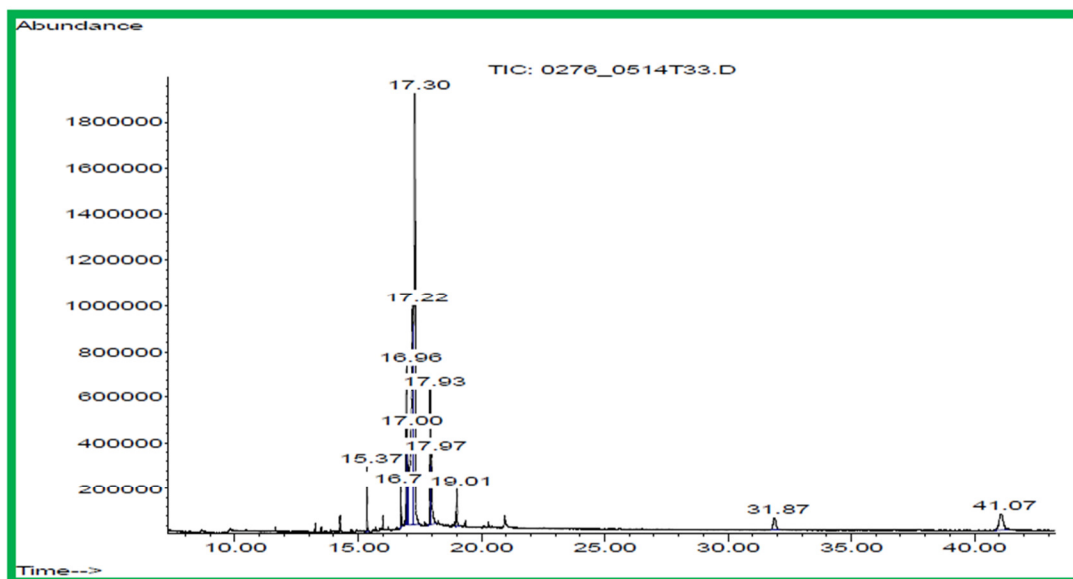
Table 8.54 - Sample 18: Internal surface

SAMPLE 19: OPPcoex



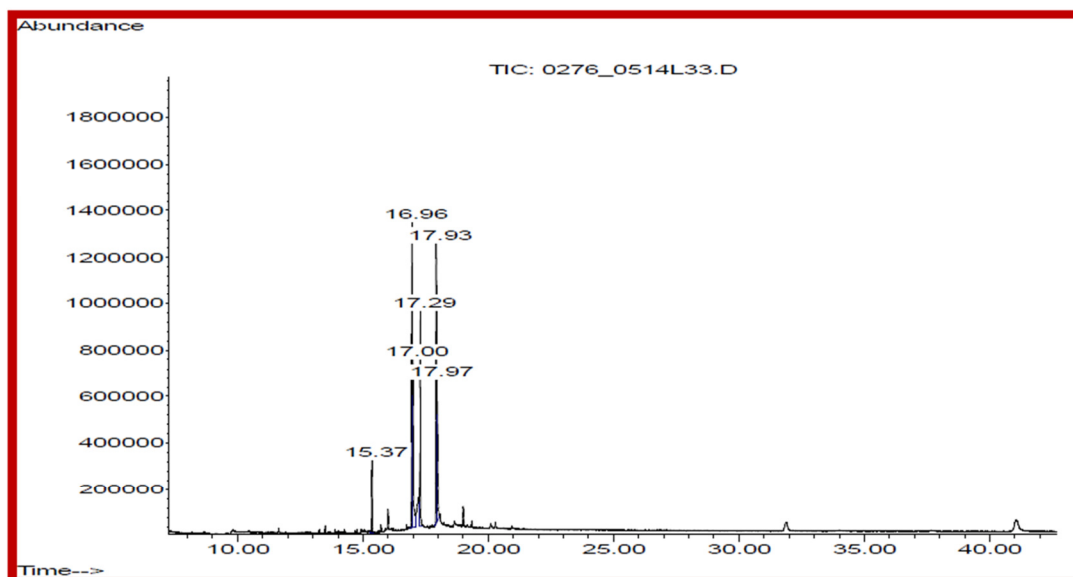
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.54	Ethanol	80	1,8
5.79	2-Propanol, 1-methoxy-	86	8,4
7.90	2-Propanol, 1-ethoxy-	83	6,1
8.98	acetyl acetone	80	2,0
11.45	Benzene, chloro (internal standard)	94	2,8
14.58	Siloxane *	-	0,2
16.00	benzyl alcohol	93	0,3
17.08	Siloxane *	-	0,2

Table 8.55 - Sample 19: Head space



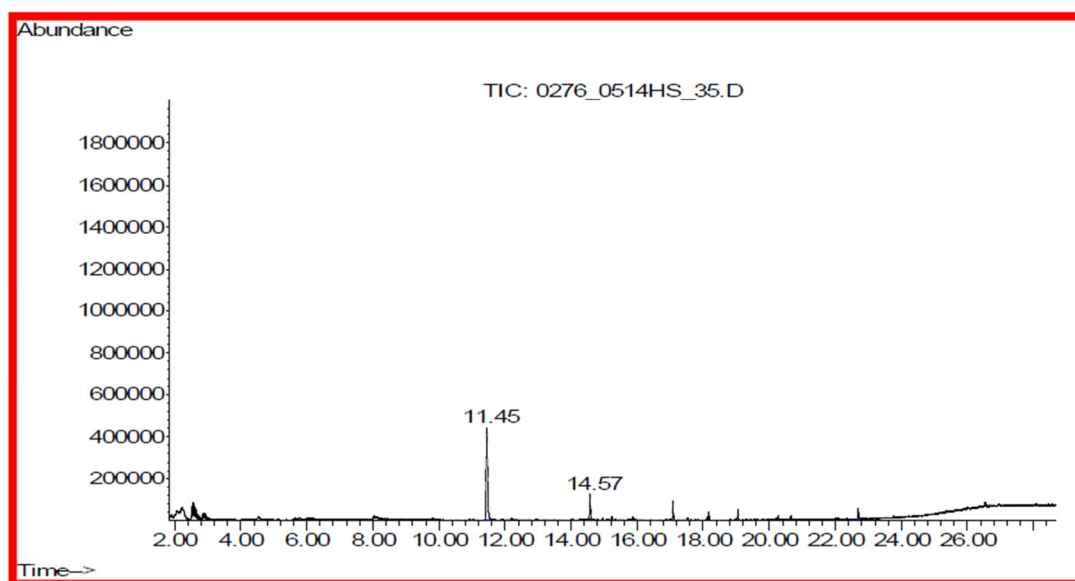
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
15.37	Dipropyl phthalate (internal standard)	98	25
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	16
16.96	not identified (m/z = 118,239,270)	-	78
17.00	not identified (m/z = 118,239,270)	-	60
17.30	acetyl tributyl citrate	80	770
17.93	not identified (m/z = 118,267,298)	-	72
17.97	not identified (m/z = 118,267,298)	-	56
19.01	Di-(2-ethylhexyl) phthalate	80	22
31.87	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	26
41.07	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	53

Table 8.56 - Sample 19: Total extract



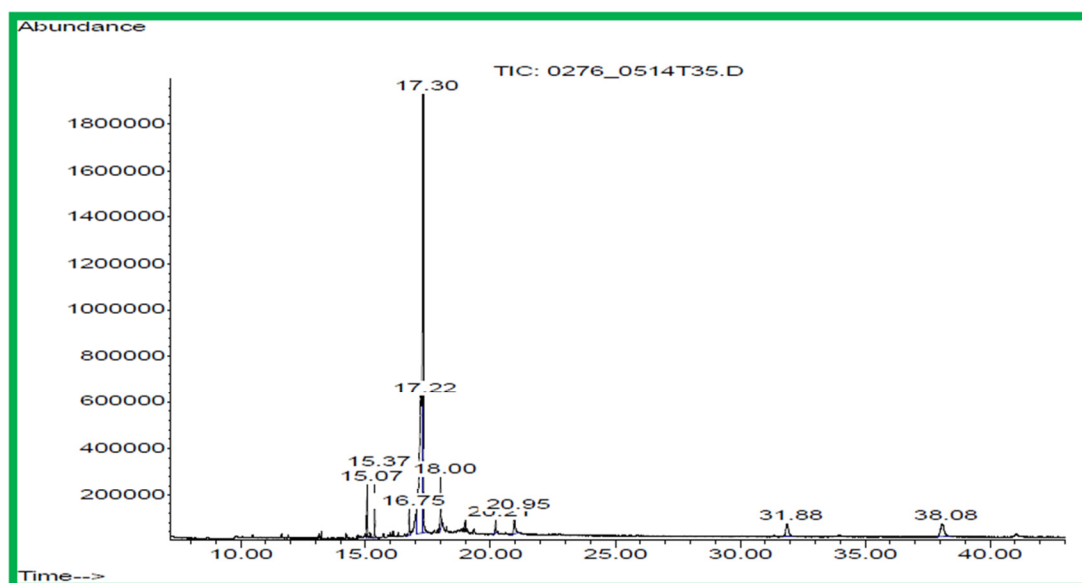
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
15.37	Dipropyl phthalate (internal standard)	98	12,5
16.96	not identified (m/z = 118,239,270)	-	62
17.00	not identified (m/z = 118,239,270)	-	45
17.29	acetyl tributyl citrate	78	44
17.93	not identified (m/z = 118,267,298)	-	65
17.97	not identified (m/z = 118,267,298)	-	39

Table 8.57 - Sample 19: Internal surface

SAMPLE 20: PET/PE

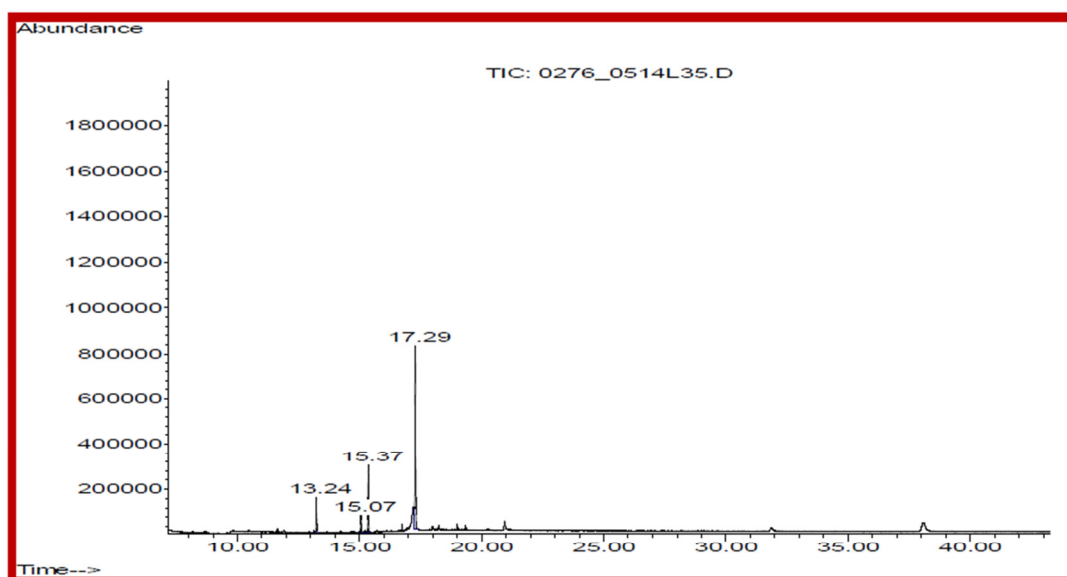
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.45	Benzene, chloro (internal standard)	94	2,8
14.57	siloxane	-	0,5

Table 8.58 - Sample 20: Head space



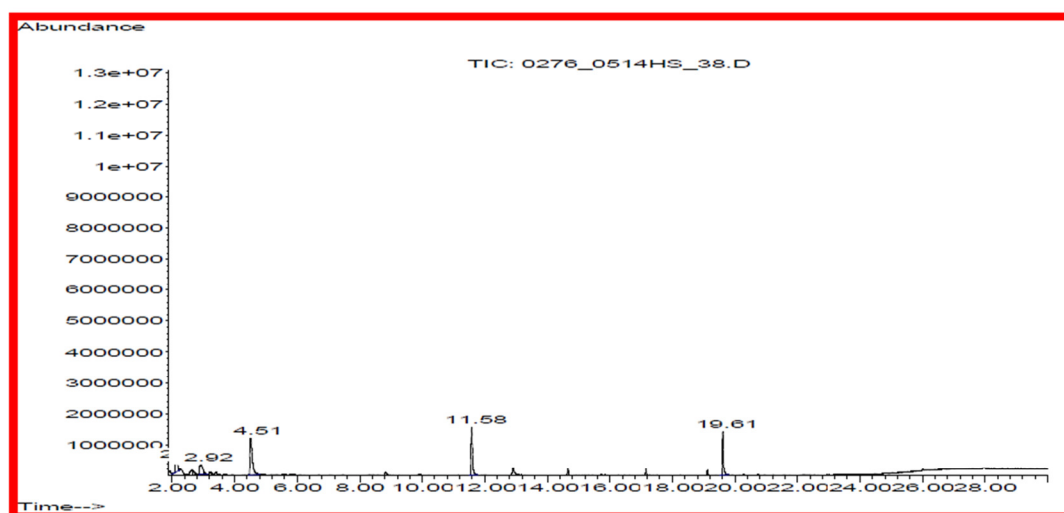
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.07	not identified (m/z = 84,99,111,173)	-	24
15.37	Dipropyl phthalate (internal standard)	98	25.0
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	11
17.30	acetyl tributyl citrate	80	472
18.01	oleamide	95	26
20.21	phenol,2,4-bis (1-methyl-1-phenylethyl)-	93	6,8
20.95	erucamide	90	21
31.88	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	27
38.09	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	35

Table 8.59 - Sample 20: Total extract



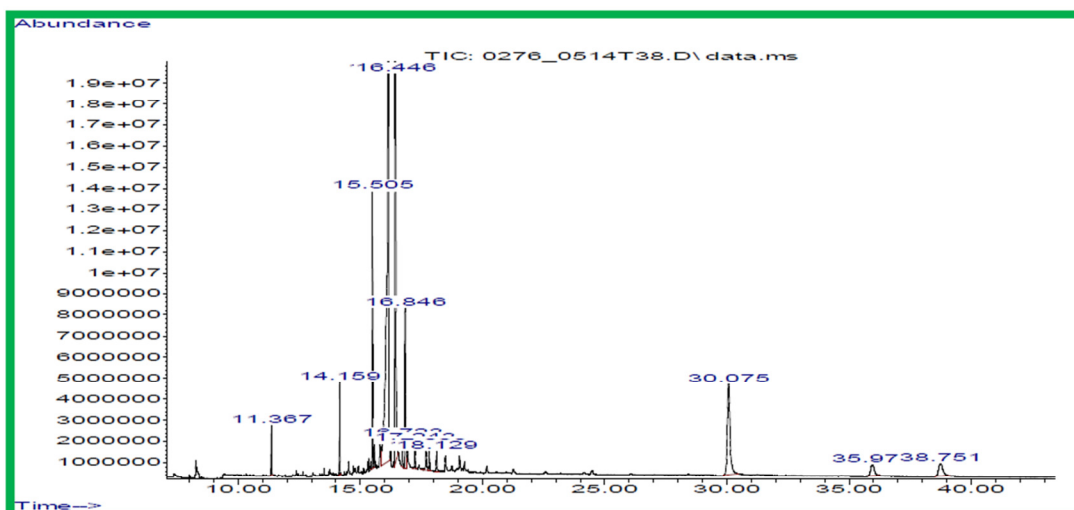
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.24	siloxane	-	6,5
15.07	not identified (m/z = 84,99,111,173)	-	4,2
15.37	Dipropyl phthalate (internal standard)	98	12,5
17.30	acetyl tributyl citrate	80	42

Table 8.60 - Sample 20: Internal surface

SAMPLE 21: OPPpvc/acr

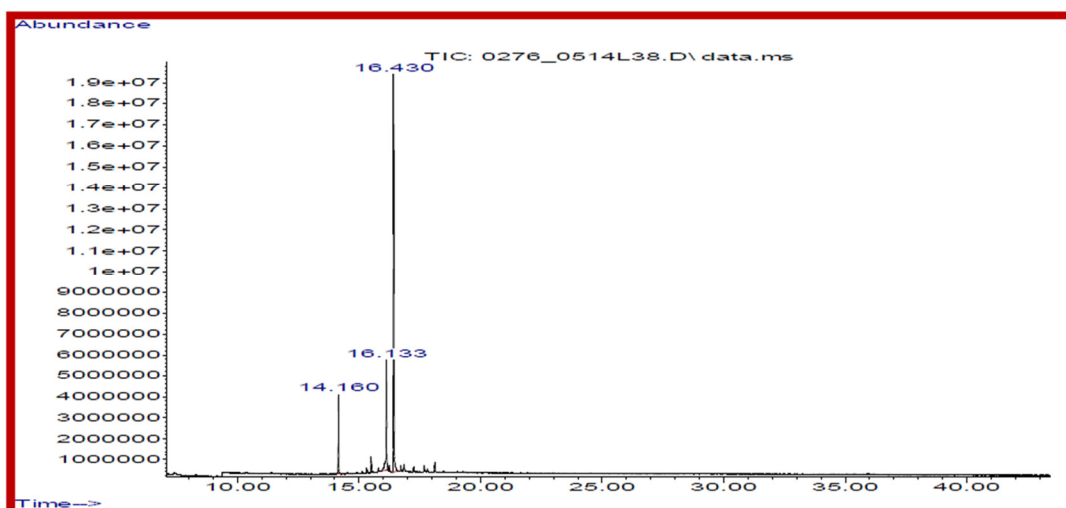
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.92	iso-propanol	74	1,4
4.51	ethylacetate	83	3,7
11.58	Benzene, chloro (internal standard)	94	2,8
19.62	Triacetin	83	1,6

Table 8.61 - Sample 21: Head space



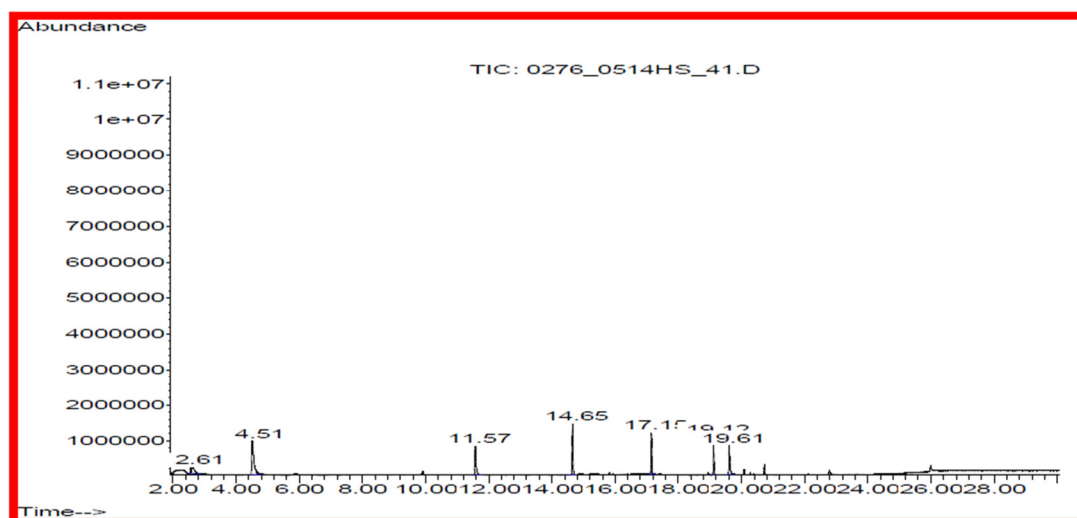
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
11.37	Triacetin	83	15
14.16	Dipropyl phthalate (internal standard)	98	25
15.51	Decanedioic acid, di butylester	91	75
16.15	acetyl tributyl citrate	80	781
16.45	di-2-ethylhexyl adipate	90	794
16.72	aliphatic hydrocarbon	-	9
16.85	Oleamide	80	69
17.24	aliphatic hydrocarbon	-	10
17.69	2-ethylhexyl diphenyl phosphate	91	16
17.83	aliphatic hydrocarbon	-	8
18.13	not identified (m/z = 91,117,207)	-	10
30.08	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	153
35.97	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	27
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	35

Table 8.62 - Sample 21: Total extract



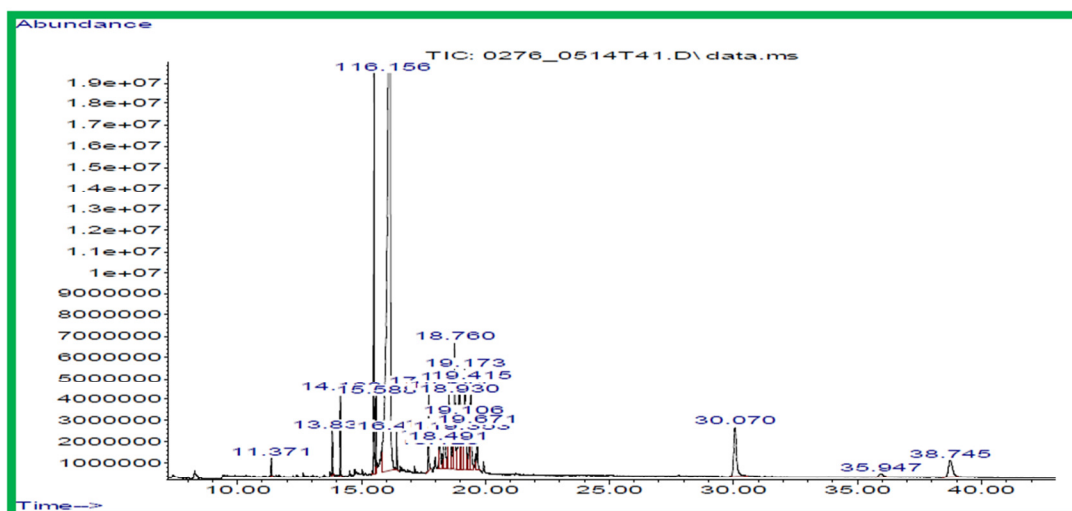
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION µg/dm ²
14.16	Dipropyl phthalate (internal standard)	98	12,5
16.13	acetyl tributyl citrate	80	22
16.43	di-2-ethylhexyl adipate	90	74

Table 8.63 - Sample 21: Internal surface

SAMPLE 22: PAPER/OPP coex

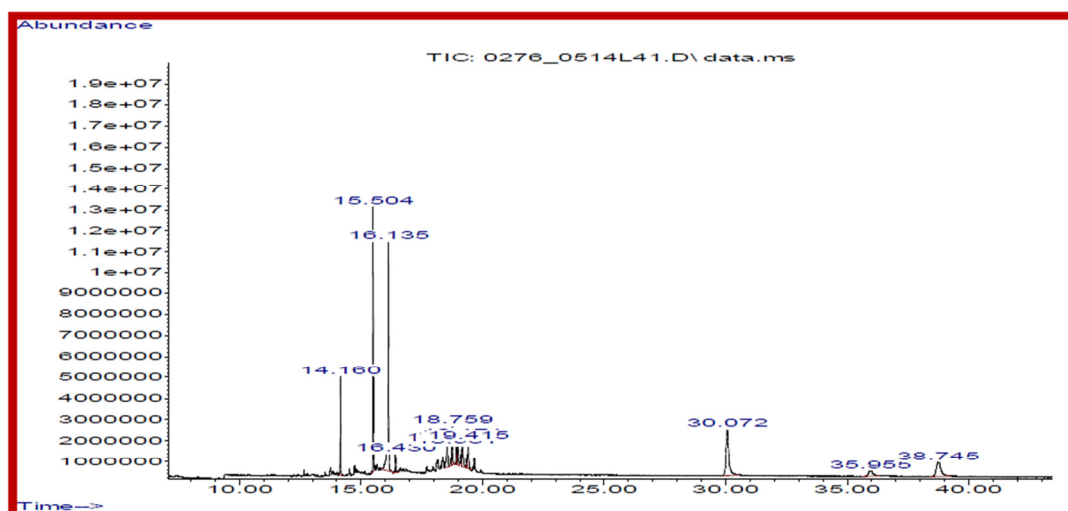
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.61	ethanol	80	1,6
4.51	ethylacetate	83	5,3
11.57	Benzene, chloro (internal standard)	94	2,8
14.65	Siloxane *	-	-
17.15	Siloxane *	-	-
19.12	Siloxane *	-	-
19.61	Triacetin	83	1,8

Table 8.64 - Sample 22: Head space



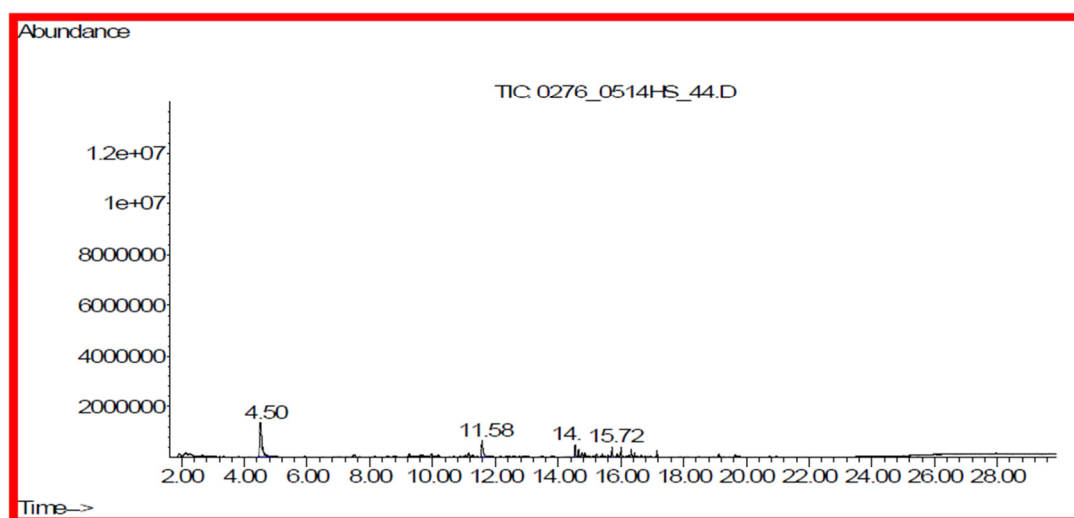
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
11.37	Triacetin	83	6.1
13.83	not identified (m/z = 84,99,111,173)	-	14
14.16	Dipropyl phthalate (internal standard)	98	25
15.51	Decanedioic acid, di butylester	91	122
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	24
16.16	acetyl tributyl citrate	80	1637
16.43	di-2-ethylhexyl adipate	90	12
17.71	2-ethylhexyl diphenyl phosphate	91	34
from 18.13 to 19.67	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	605
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	88
35.95	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	11
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	44

Table 8.65 - Sample 22: Total extract



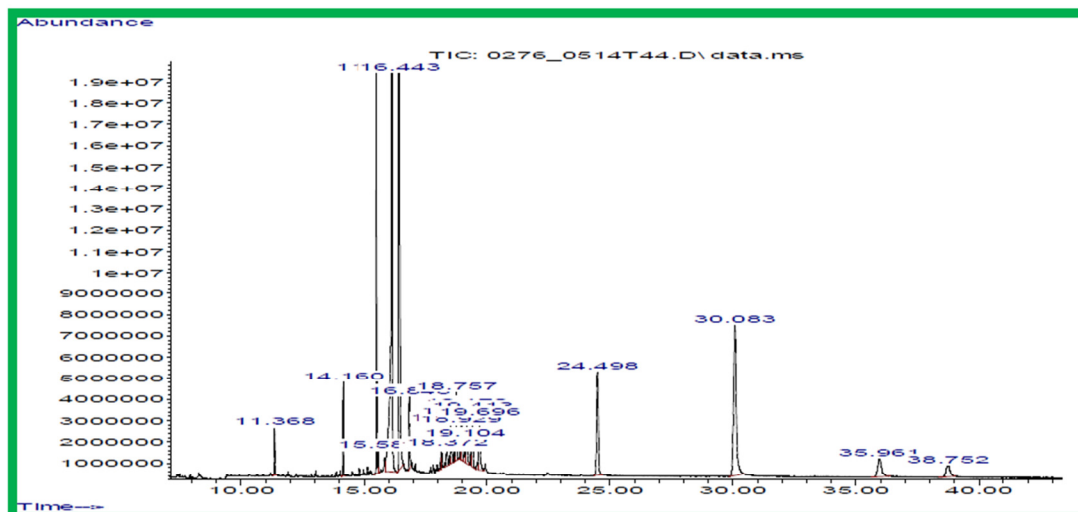
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Dipropyl phthalate (internal standard)	98	12,5
15.50	Decanedioic acid, di butylester	91	30
16.14	acetyl tributyl citrate	80	43
16.43	di-2-ethylhexyl adipate	90	3,2
from 18.54 to 19.42	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	45
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	35
35.96	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	6,6
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	19

Table 8.66 - Sample 22: Internal surface

SAMPLE 23: PETmet/oppCOEX

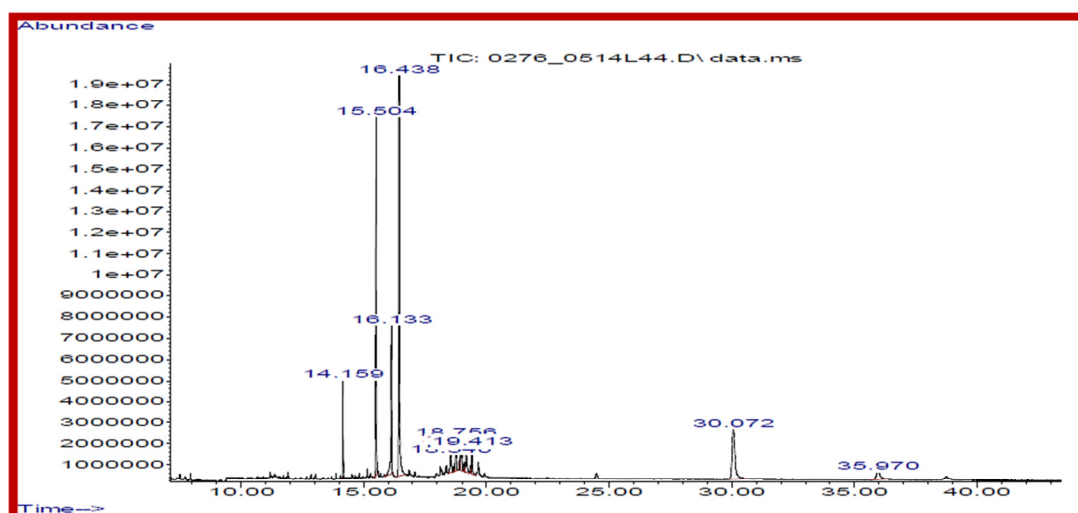
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.50	ethylacetate	83	9,1
11.58	Benzene, chloro (internal standard)	94	2,8
14.55	aliphatic hydrocarbon	-	1,2
15.72	aliphatic hydrocarbon	-	0,9

Table 8.67 - Sample 23: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.37	Triacetin	80	15
14.16	Dipropyl phthalate (internal standard)	98	25
15.51	Decanedioic acid, di butylester	91	141
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	6,8
16.14	acetyl tributyl citrate	80	532
16.44	di-2-ethylhexyl adipate	90	746
16.84	Oleamide	94	28
from 18.13 to 19.70	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	250
24.50	Bisphenol A diglycidyl ether	97	95
30.08	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	237
35.96	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	44
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	28

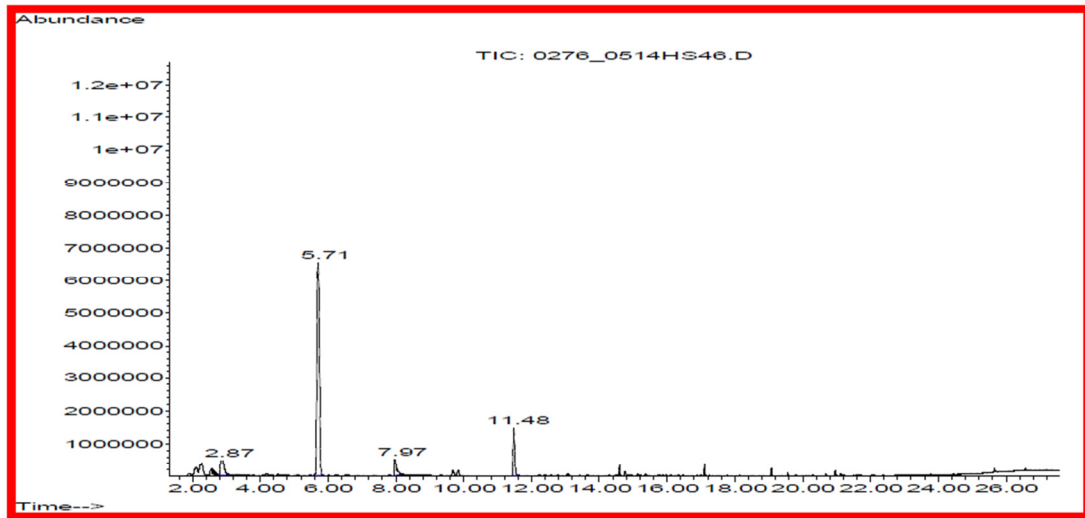
Table 8.68 - Sample 23: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
14.16	Dipropyl phthalate (internal standard)	98	12,5
15.50	Decanedioic acid, di butylester	91	42
16.13	acetyl tributyl citrate	80	26
16.44	di-2-ethylhexyl adipate	90	245
from 18.54 to 19.41	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	37
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	40
35.97	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	8,5

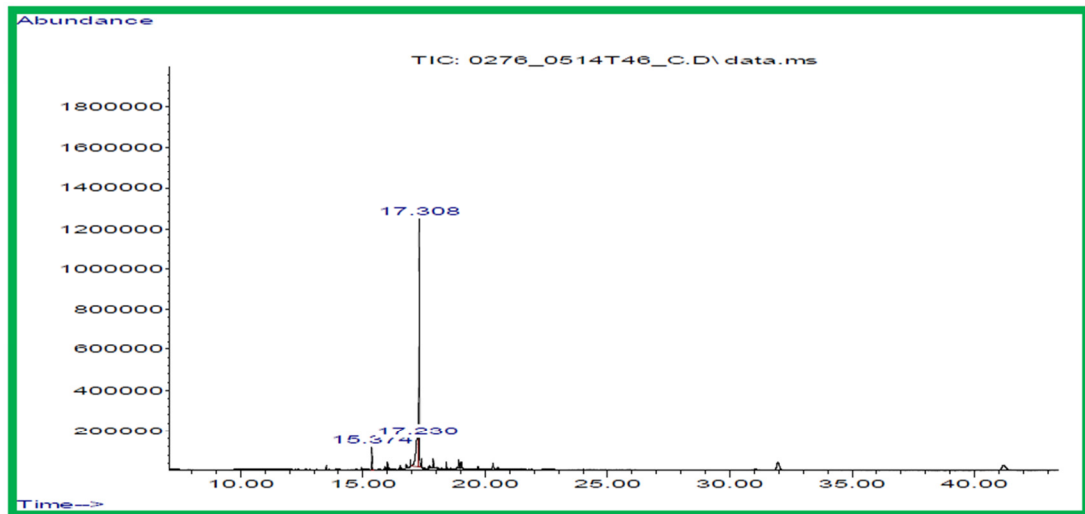
Table 8.69 - Sample 23: Internal surface

SAMPLE 24: OPPcoex



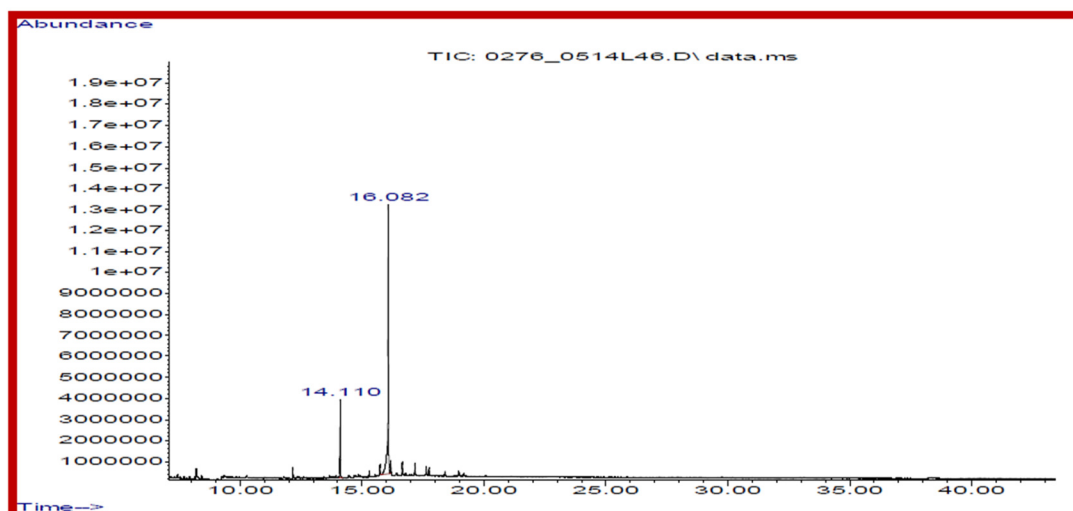
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2,87	iso-propanol	80	2,2
5.71	cyclohexane	83	20
7.97	ethoxypropanol	80	1,5
11.48	Benzene, chloro (internal standard)	94	2,8

Table 8.70 - Sample 24: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	25
17.31	acetyl tributyl citrate	80	332

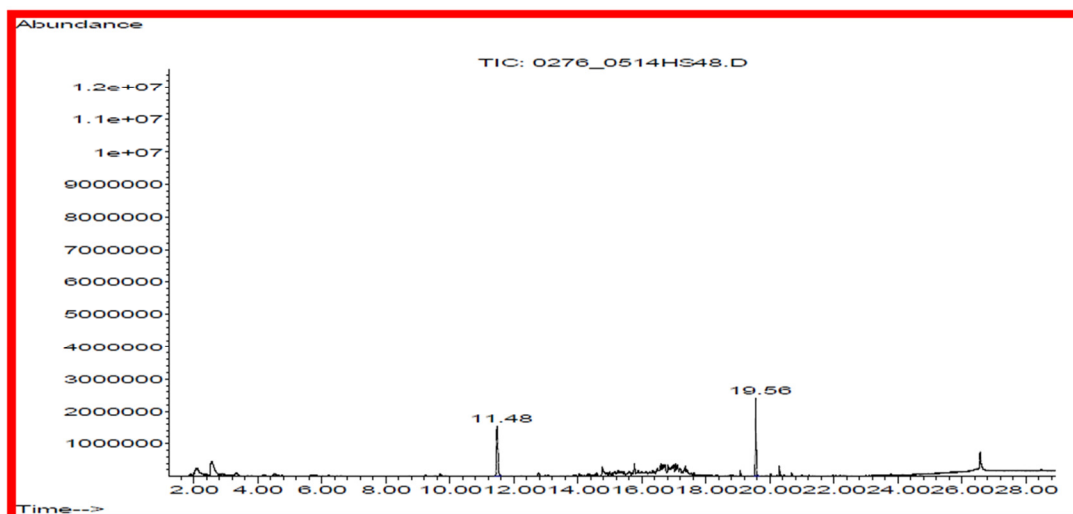
Table 8.71 - Sample 24: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.11	Dipropyl phthalate (internal standard)	98	50
16.08	acetyl tributyl citrate	80	237

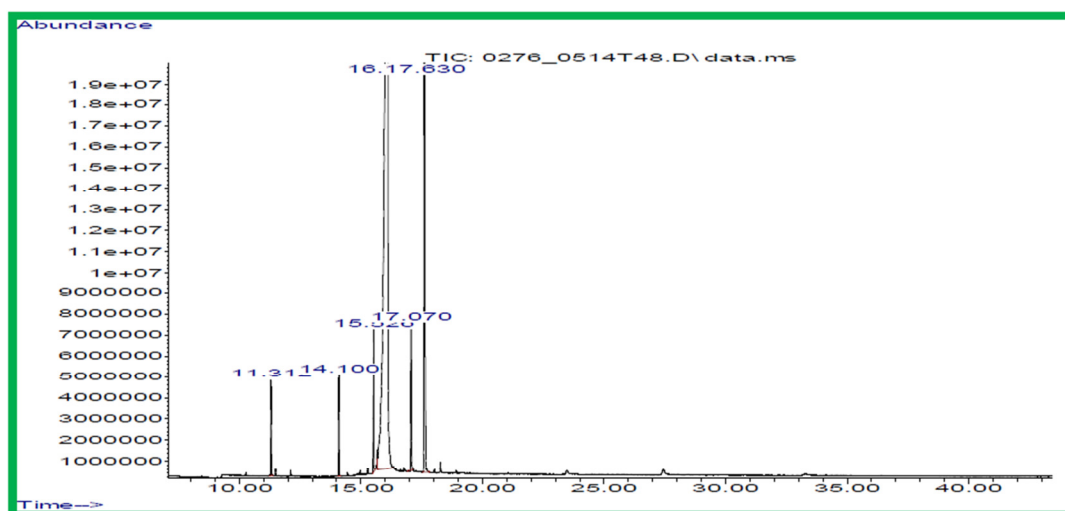
Table 8.72 - Sample 24: Internal surface

SAMPLE 25: Aluminum/Paper



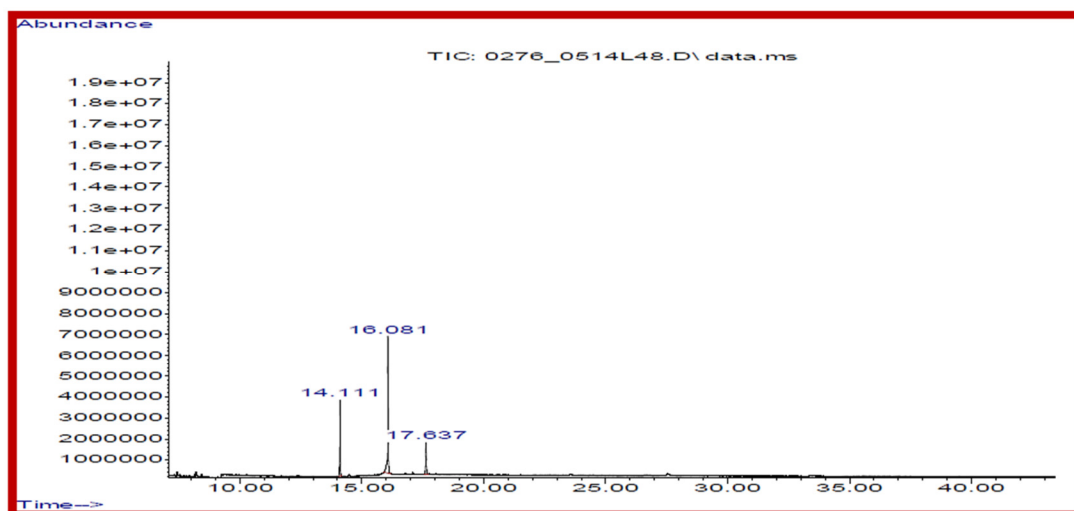
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.48	Benzene, chloro (internal standard)	94	2,8
19.56	Triacetin	83	1,8

Table 8.73 - Sample 25: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.31	Triacetin	83	25
14.10	Dipropyl phthalate (internal standard)	98	25
15.53	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	33
16.09	acetyl tributyl citrate	80	2.088
17.07	not identified (m/z = 94,175)	-	45
17.63	2-ethylhexyl diphenyl phosphate	91	533

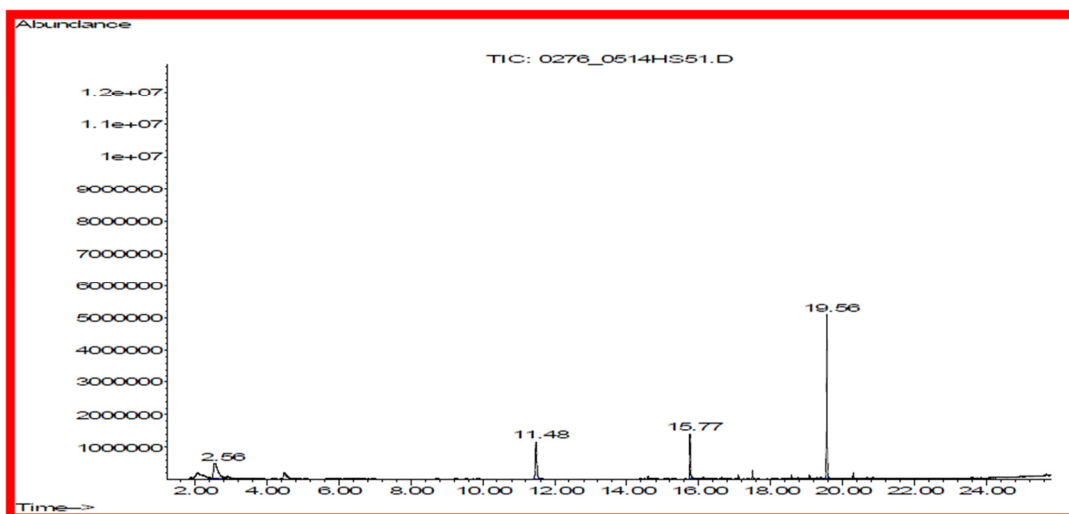
Table 8.74 - Sample 25: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.11	Dipropyl phthalate (internal standard)	98	50
16.08	acetyl tributyl citrate	80	119
17.64	2-ethylhexyl diphenyl phosphate	91	31

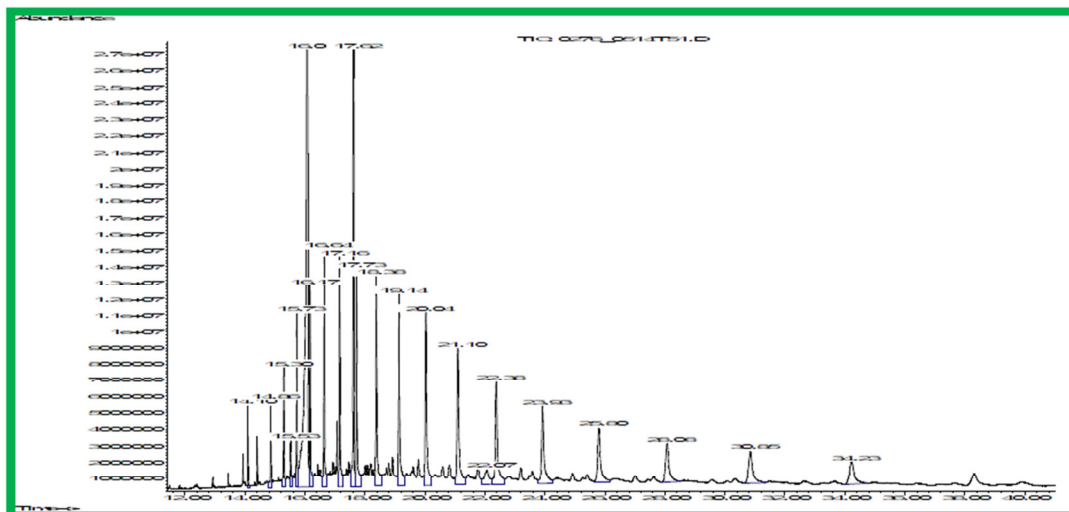
Table 8.75 - Sample 25: Internal surface

SAMPLE 26: Paper/Aluminum



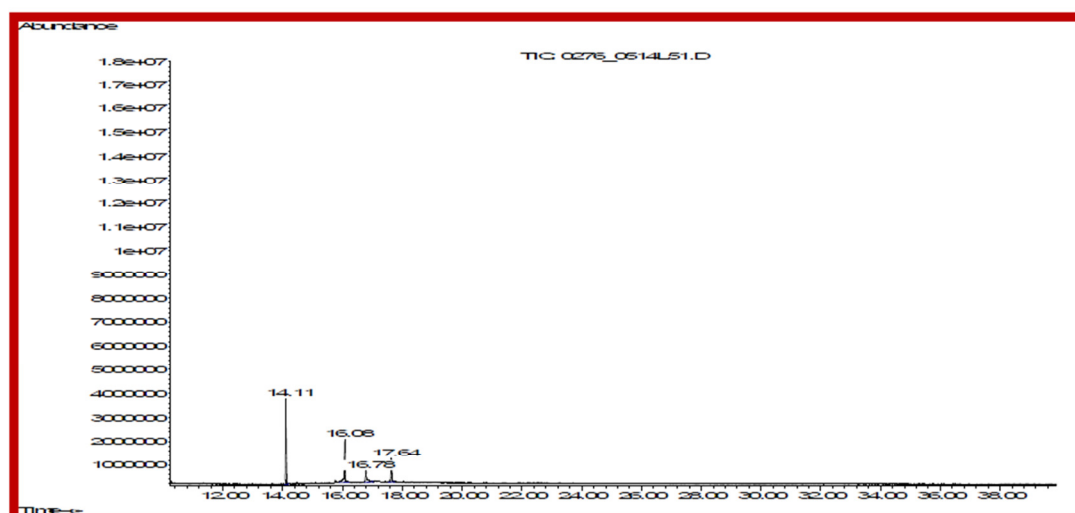
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2,56	ethanol		-
11,48	Chloro, benzene (internal standard)	96	2,8
15,77	2-ethyl 1-hexanol	89	1,8
19,56	triacetine	92	5,1

Table 8.76 - Sample 26: Head space



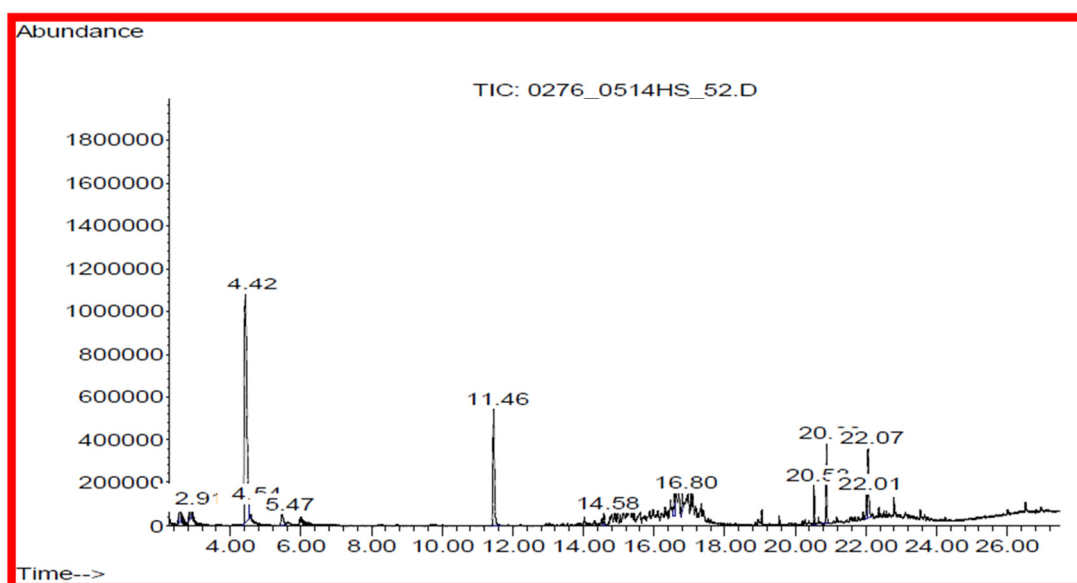
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.31	Triacetin	83	25
14.10	Dipropyl phthalate (internal standard)	98	25
From 14.86 to 34.22	Aliphatic saturated hydrocarbons	>80	1.510 sum
15.52	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	21
16.08	acetyl tributyl citrate	80	693
17.62	2-ethylhexyl diphenyl phosphate	91	275

Table 8.77 - Sample 26: total extract



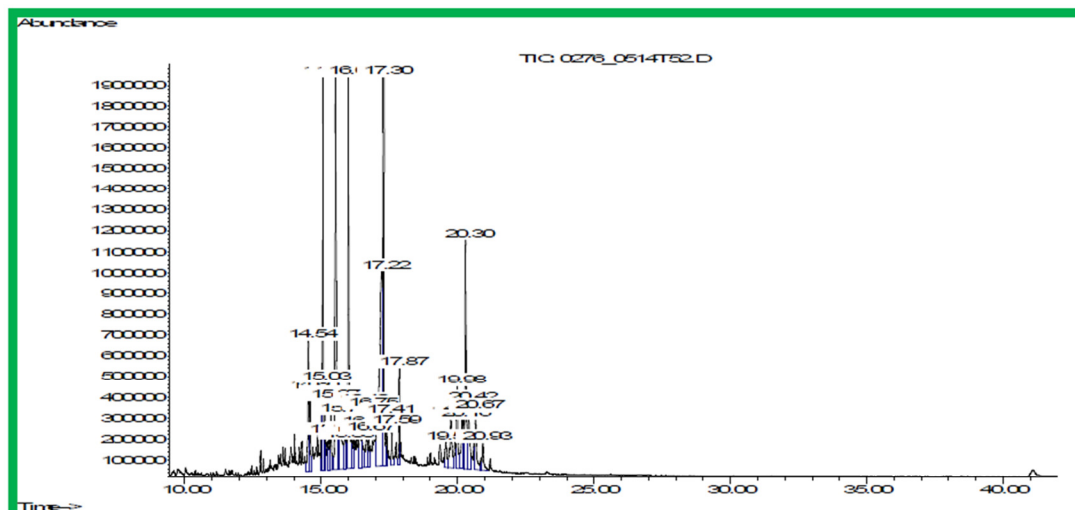
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.11	Dipropyl phthalate (internal standard)	98	50
16.08	acetyl tributyl citrate	80	36
17.64	2-ethylhexyl diphenyl phosphate	91	20

Table 8.78 - Sample 26: Internal surface

SAMPLE 27: Paper/OPP

TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.58	ethanol	80	0,4
2,87	iso-propanol	80	0,4
4.42	ethylacetate	86	8,9
5.47	iso-propyl acetate	83	0,4
11.46	Benzene, chloro (internal standard)	97	2,8
from 14.58 to 16.80	aliphatic hydrocarbon	-	1,0
20.53	longicyclene	99	0,4
20.89	junipene	99	1,0
22.01	aliphatic hydrocarbon	-	0,3
22.07	diethyl phthalate	96	1,2

Table 8.79 - Sample 27: Head space

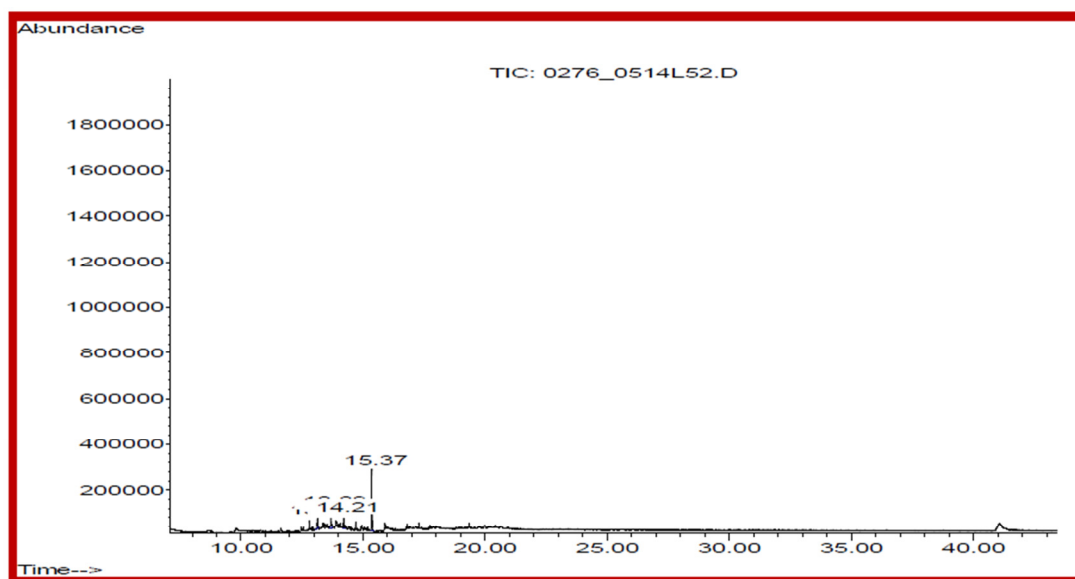


TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.54	tetradecanoic acid	99	76
14.60	n-propyl p-hydroxybenzoate	94	38
15.06	Aliphatic unsaturated hydrocarbon	-	239
15.14	n-butyl p-hydroxybenzoate *	96	30
15.37	Dipropyl phthalate (internal standard)	98	25
15.53	n-hexadecanoic acid	94	339
16.01	aliphatic unsaturated hydrocarbon	-	271
16.43	Oleic acid	96	33
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	91	17
17.30	acetyl tributyl citrate	80	680
17.87	2-propenoic acid, 3(4-methoxyphenyl)-, 2 ethylexyl ester **	98	36
from 19.76 to 20.93	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	656

(*) butyl paraben (CAS N. 94-26-8): antimicrobial – antifungal.

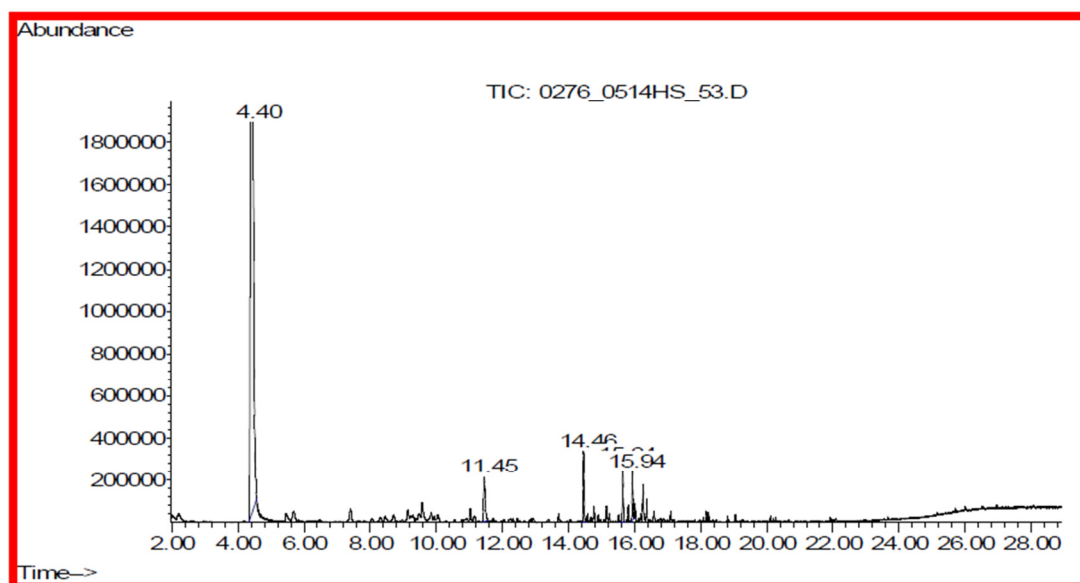
(**) octil methoxy cinnamate (CAS N. 5466-77-3) anti UV.

Table 8.80 - Sample 27: Total extract



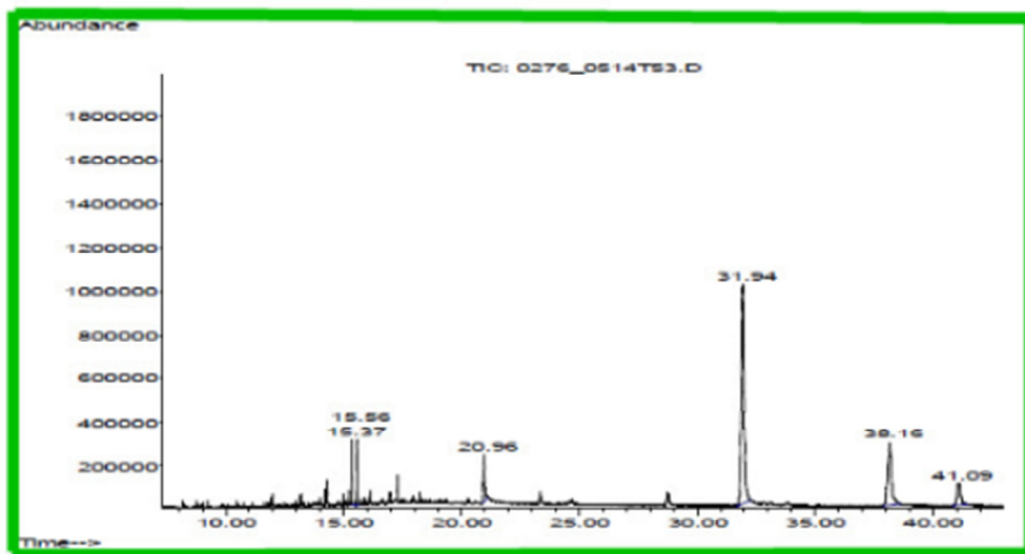
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
from 13.14 to 14.21	aliphatic hydrocarbon	-	11
15.37	Dipropyl phthalate (internal standard)	91	12,5

Table 8.81 - Sample 27: Internal surface

SAMPLE 28: PET/Aluminum/PE

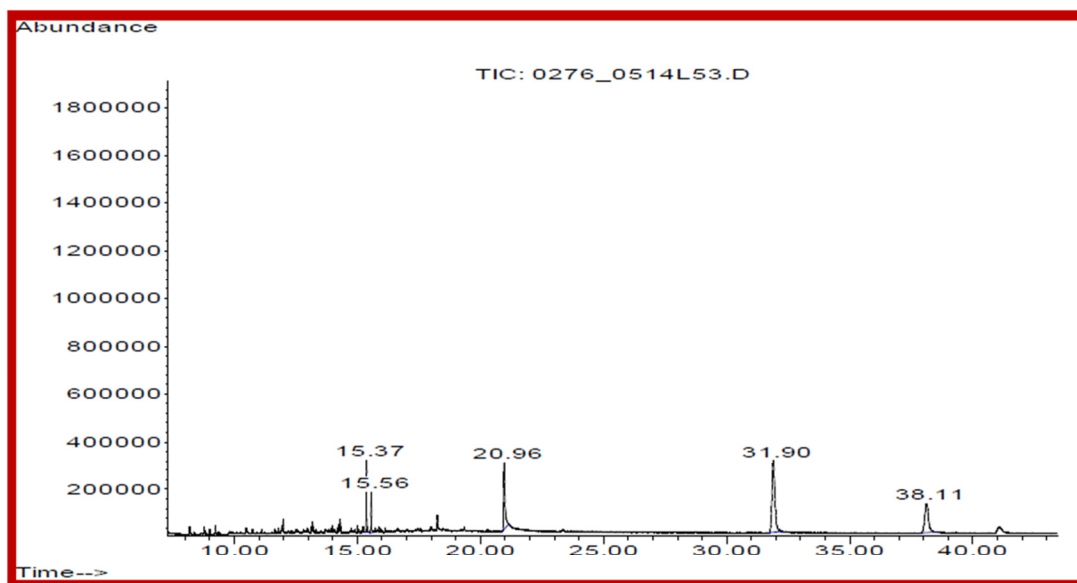
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.41	ethylacetate	90	116
11.45	Benzene, chloro (internal standard)	94	2,8
14.46	aliphatic hydrocarbon	-	2,5
15.65	aliphatic hydrocarbon	-	1,9
15.94	aliphatic hydrocarbon	-	1,7

Table 8.82 - Sample 28: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	25
15.56	not identified (m/z = 55,82,111,129)	-	36
20.96	erucamide	80	48
31.94	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	488
38.16	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	190
41.09	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	74

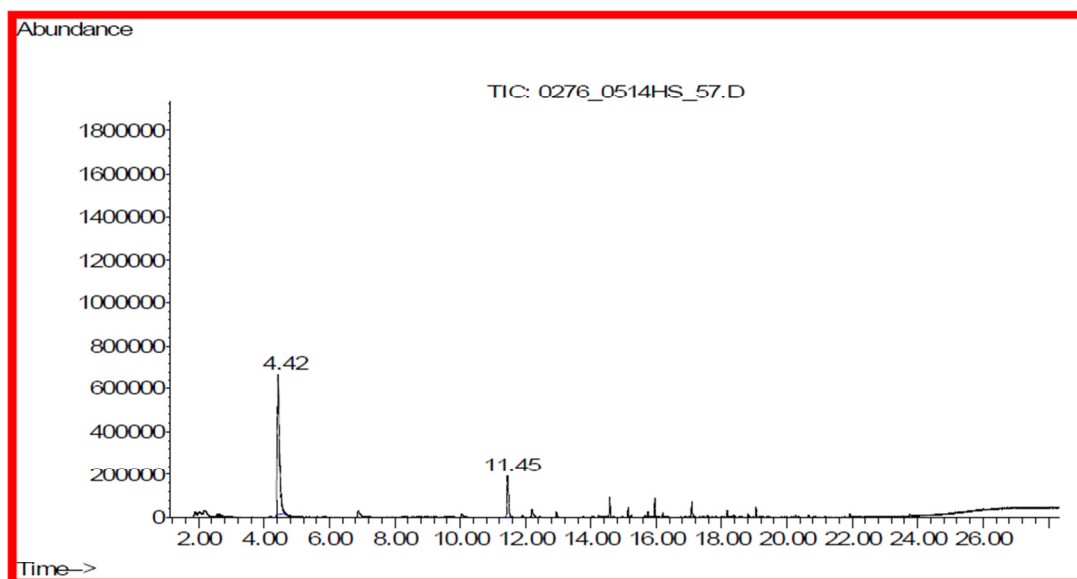
Table 8.83 - Sample 28: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5
15.56	not identified (m/z = 55,82,111,129)	-	8,2
20.96	erucamide	87	32
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	73
38.11	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	90	39

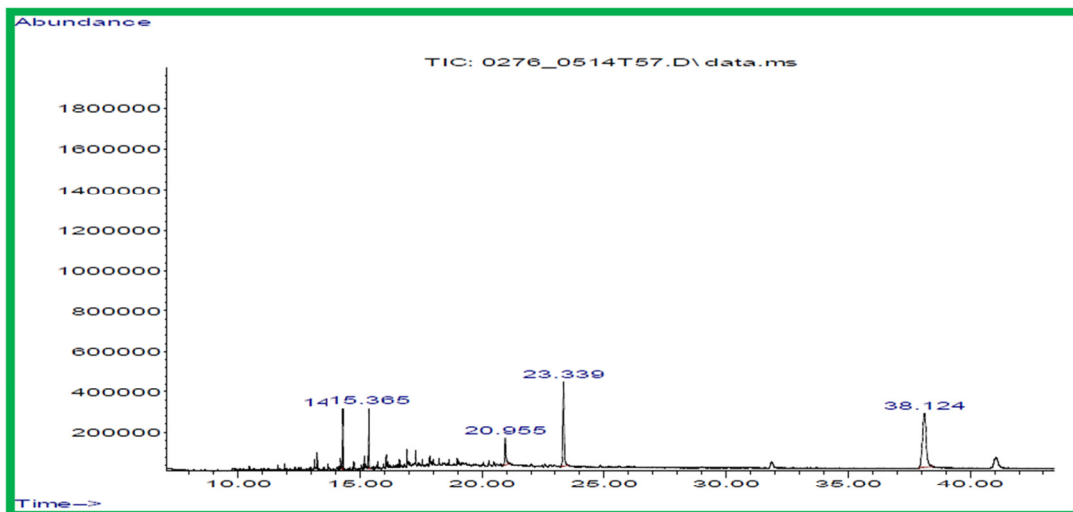
Table 8.84 - Sample 28: Internal surface

SAMPLE 29: PET/Aluminum/PE



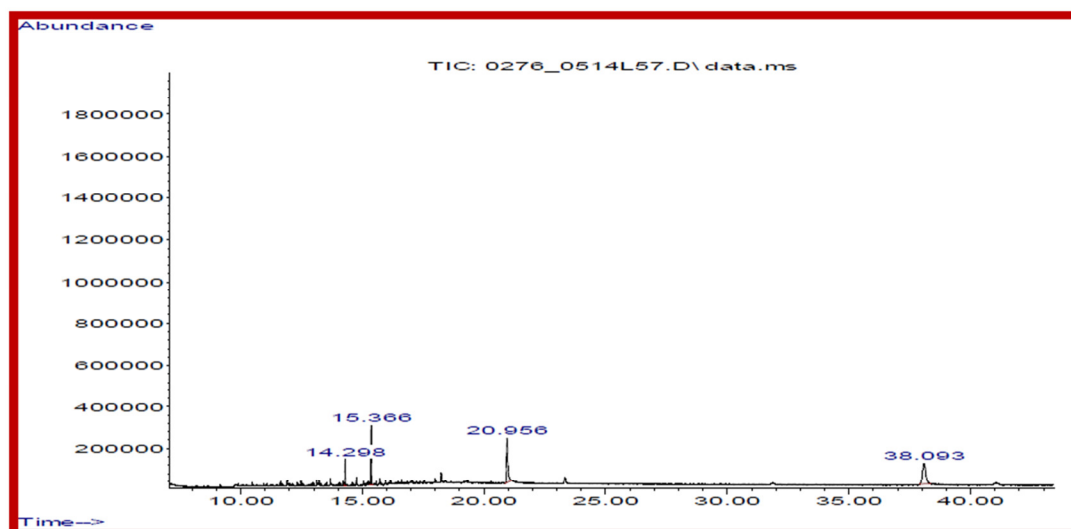
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.42	ethyl acetate	83	13,2
11.45	Benzene, chloro (internal standard)	97	2,8

Table 8.85 - Sample 29: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.30	not identified (m/z = 111,129)	-	28
15.36	Dipropyl phthalate (internal standard)	91	25
20.96	Erucamide	96	28
23.34	not identified (m/z = 129,215)	-	93
38.12	Irganox 1076	-	161

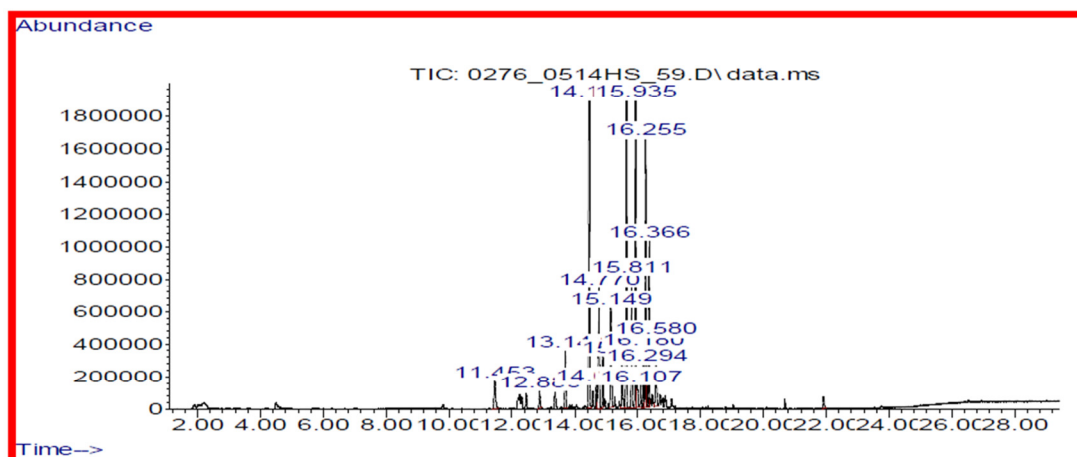
Table 8.86 - Sample 29: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.30	not identified (m/z = 111,129)	-	7,0
15.37	Dipropyl phthalate (internal standard)	98	12,5
20.96	Erucamide	96	27
38.09	Irganox 1076	-	35

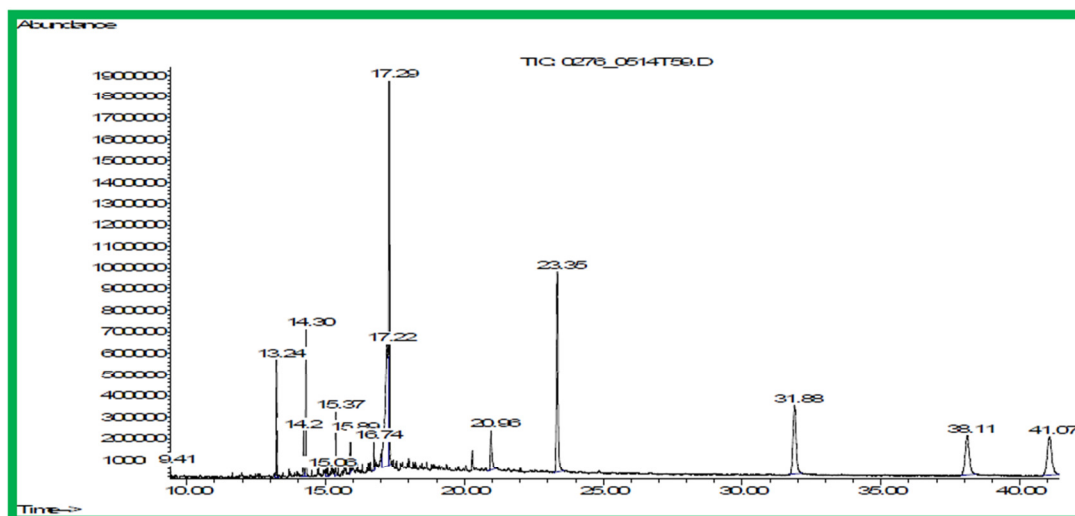
Table 8.87 - Sample 29: Internal surface

SAMPLE 30: OPPcoex/Aluminum/PE



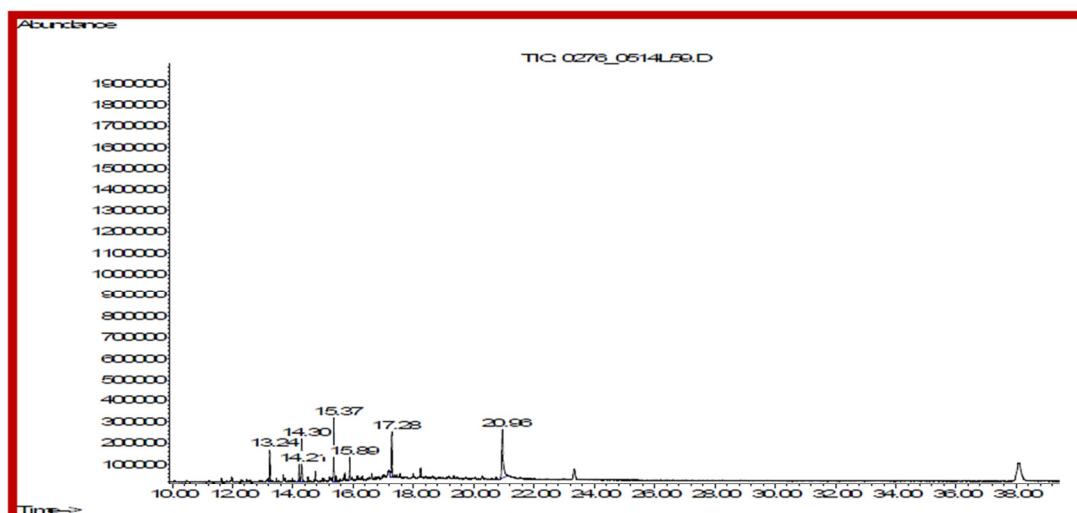
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.45	Benzene, chloro (internal standard)	94	2,8
from 13.7 to 16.6	aliphatic hydrocarbon	-	138

Table 8.88 - Sample 30: Head space



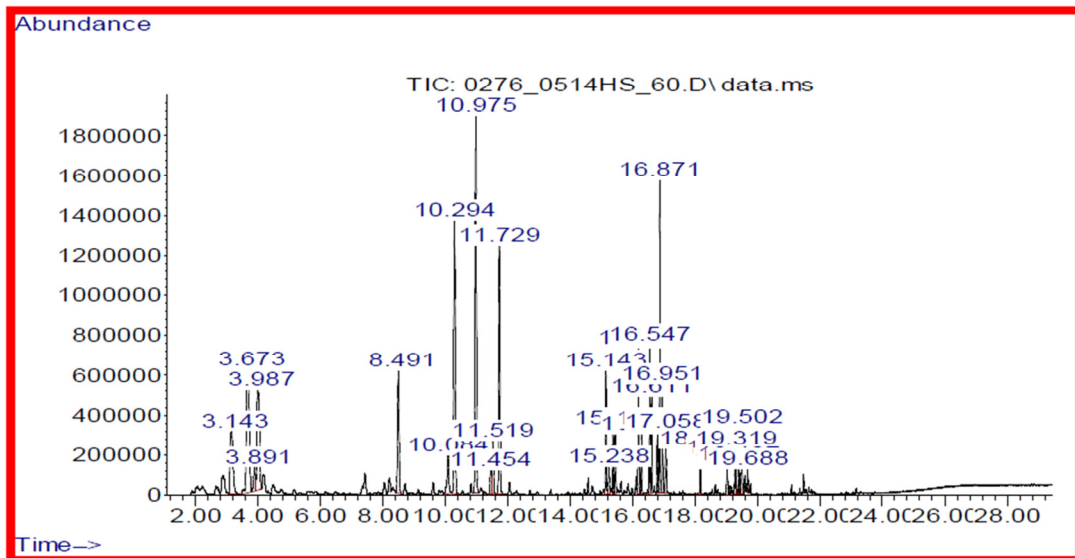
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.23	not identified (m/z = 91,121,147)	-	44
14.21	aliphatic hydrocarbon	-	16
14.30	not identified (m/z = 101, 111,129)	-	64
15.36	Di propyl phthalate (internal standard)	98	25
15.89	not identified (m/z = 126,155,173)	-	17
16.74	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	16
17.29	acetyl tributyl citrate	80	435
20.96	erucamide	93	42
23.35	not identified (m/z = 111,129, 215,428)	-	210
31.88	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	145
38.10	Irganox 1076	83	112
41.07	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	124

Table 8.89 - Sample 30: Total extract



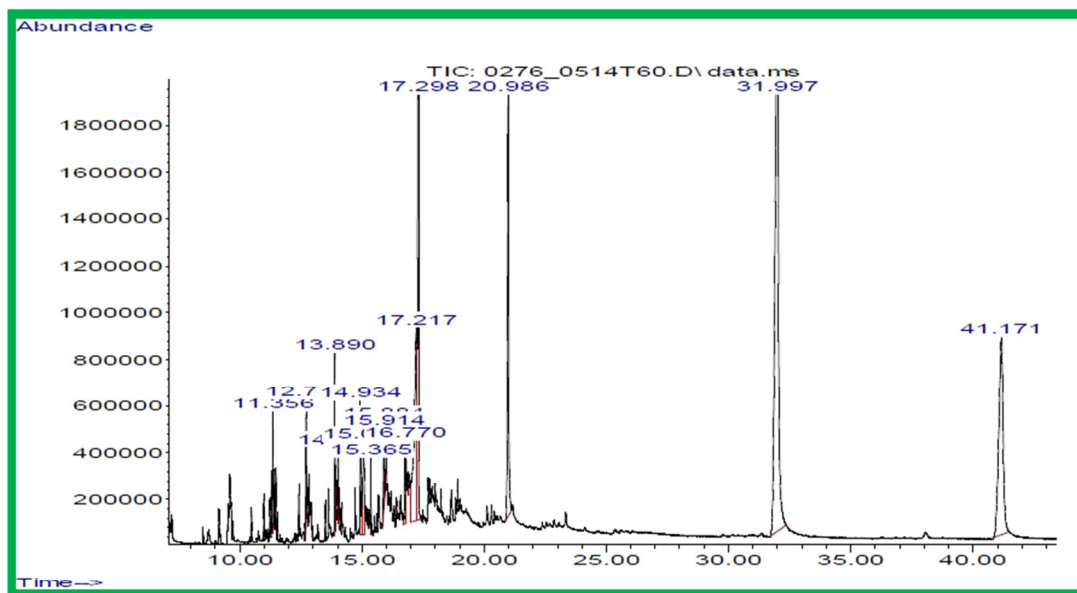
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
from 8.1 to 8.5	aliphatic hydrocarbon	-	57
13.23	not identified (m/z = 91,121,147)	-	8
14.30	not identified (m/z = 111,129, 184)	-	10
15.36	Dipropyl phthalate (internal standard)	98	12,5
15.89	not identified (m/z = 126,155,173)	-	4
17.29	acetyl tributyl citrate	80	11
20.96	erucamide	93	24

Table 8.90 - Sample 30: Internal surface

SAMPLE 31: CASTPP/PP-EVOH-PP

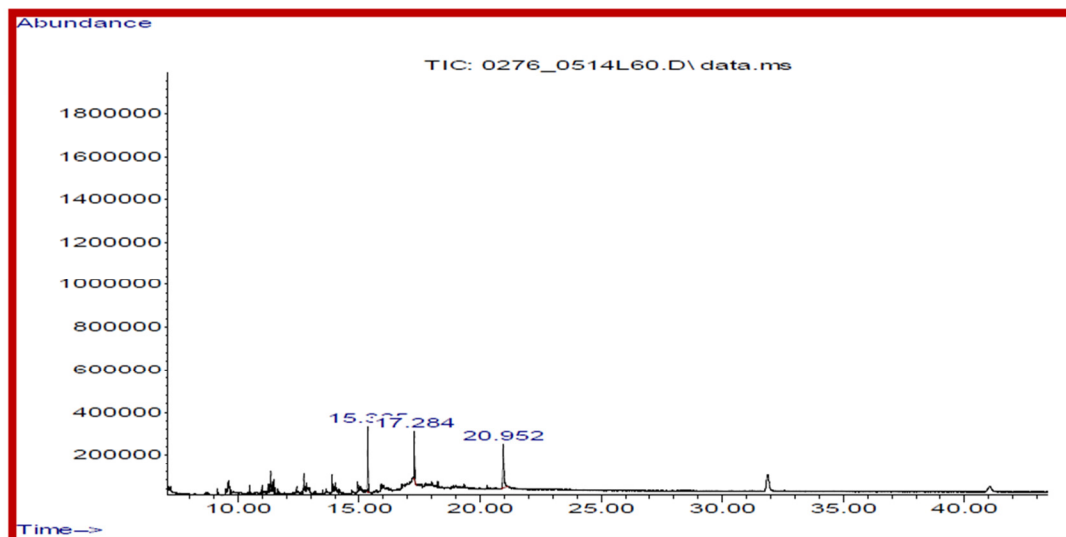
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION µg/dm ²
3.67	2-methyl pentane	80	33
3.99	1-pentene,2-methyl	86	25
8.49	heptane, 4-methyl	91	17
10.08	aliphatic hydrocarbon	-	6,2
10.29	heptane, 2,4-dimethyl	91	34
10.98	1-heptene, 2,4-dimethyl	90	51
11.45	Benzene, chloro (internal standard)	90	2,8
11.52	1-heptene, 2,3-dimethyl	90	6,6
11.73	octane, 4-methyl	91	29
from 15.14 to 19.69	aliphatic hydrocarbons	>80	106

Table 8.91 - Sample 31: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
from 11.36 to 16.77	aliphatic hydrocarbons	>80	410
15.37	Dipropyl phthalate (internal standard)	98	25
17.30	acetyl tributyl citrate	80	542
20.99	erucamide	95	335
32.00	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	1.260
41.17	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	539

Table 8.92 - Sample 31: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	12,5
17.28	acetyl tributyl citrate	87	9,5
20.95	erucamide	97	20

Table 8.93 - Sample 31: Internal surface

SAMPLE 32: PA/PP/PE

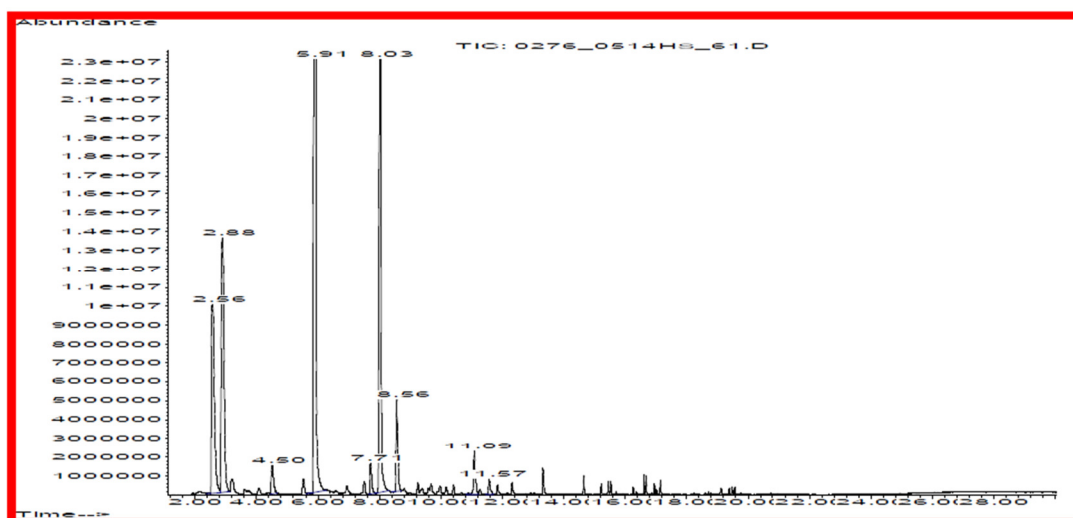
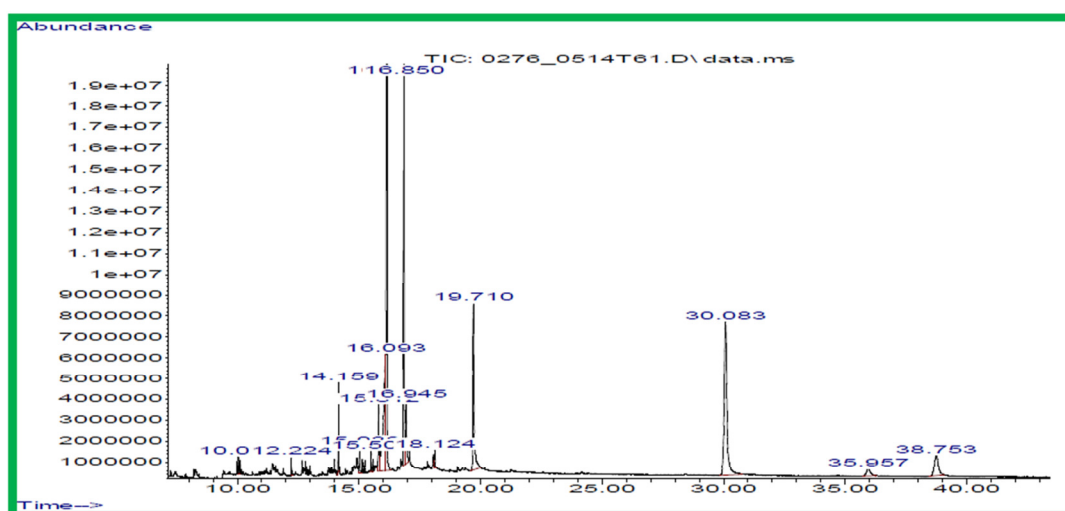
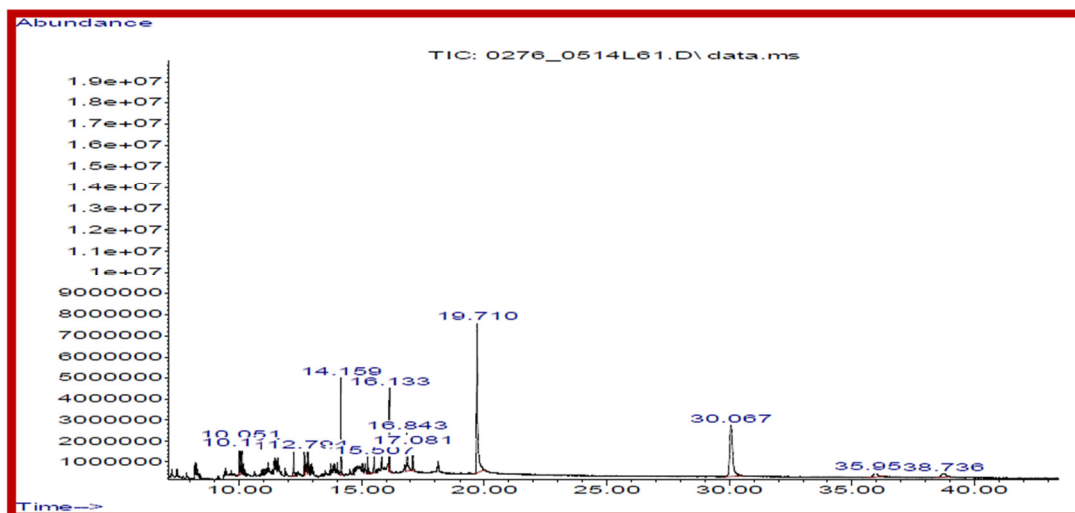


Table 8.94 - Sample 32: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION µg/dm ²
10.05	aliphatic hydrocarbon	-	6,4
12.22	Butylated hydroxy toluene (BHT)	98	7,2
14.16	Dipropyl phthalate (internal standard)	98	25
15.81	Hexadecanamide	93	40
16.14	acetyl tributyl citrate	80	397
16.85	Oleamide	94	231
19.71	Erucamide	91	128
30.08	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	281
35.96	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	19
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	55

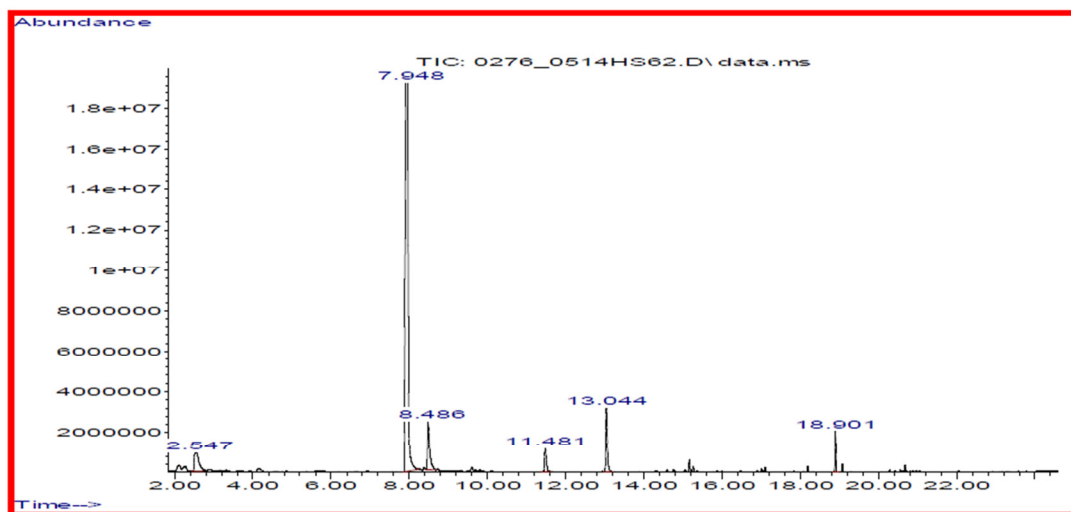
Table 8.95 - Sample 32: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION µg/dm ²
10.05	aliphatic hydrocarbon	-	5,2
12.22	Butylated hydroxy toluene (BHT)	98	3,6
14.16	Dipropyl phthalate (internal standard)	98	12,5
16.13	acetyl tributyl citrate	80	12
16.84	Oleamide	94	9,6
19.71	Erucamide	91	47
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	40
35.95	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	5,1
38.74	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	5,0

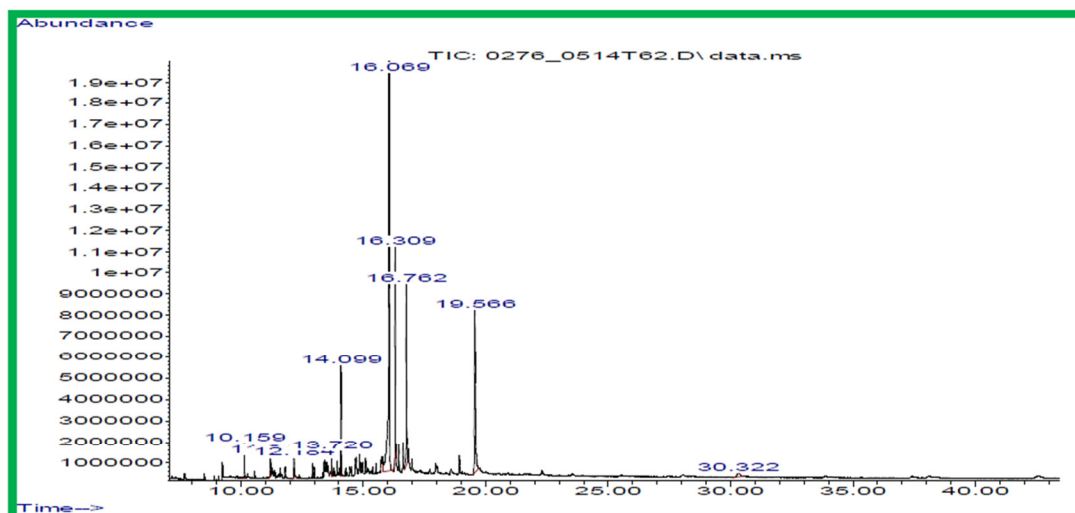
Table 8.96 - Sample 32: Internal surface

SAMPLE 33: PE/PA-EVOH/PE



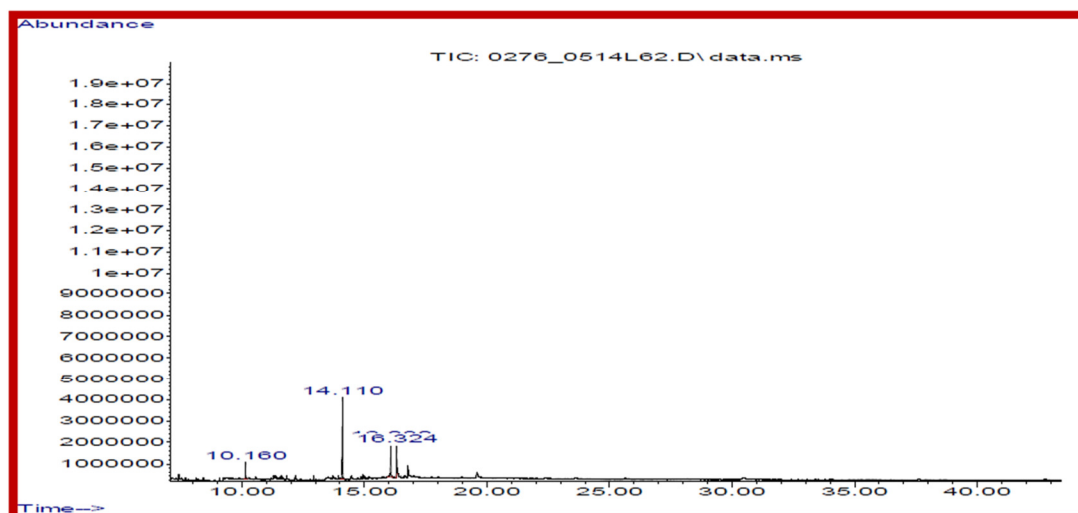
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.55	ethanol	80	5,7
7.95	ethoxypropanol	83	88
8.49	not identified (m/z = 73.1, 45)	-	6,8
11.48	Benzene, chloro (internal standard)	94	2,8
13.04	Cyclohexanone	83	6,2
18.90	benzene, 1,3-bis(1,1-dimethylethyl)-	90	2,2

Table 8.97 - Sample 33: Head space



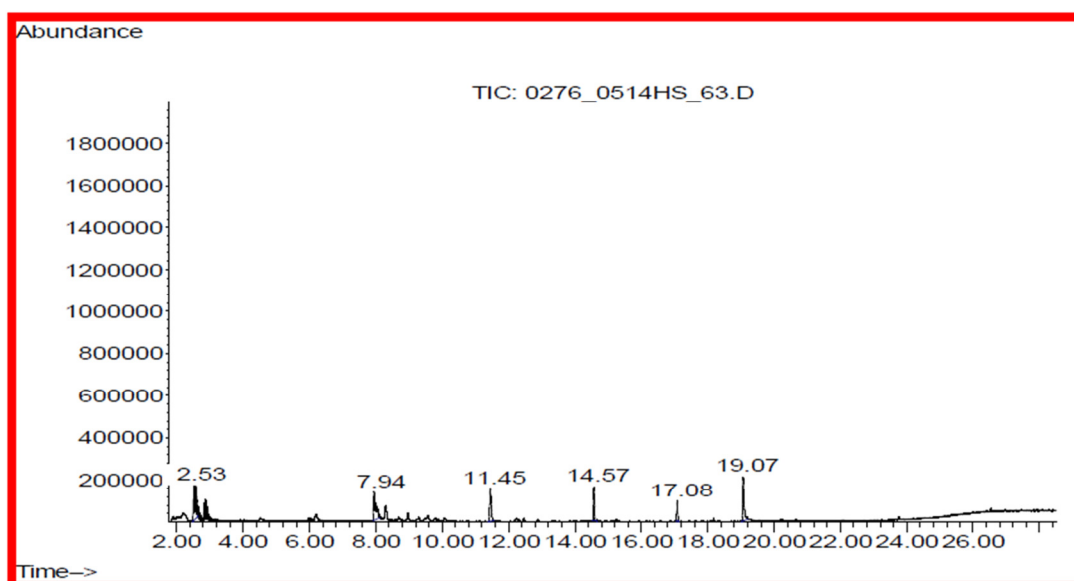
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
10.16	benzene, 1,3-bis(1,1-dimethylethyl)-	94	8,2
11.22	2,4-diisoyanato, toluene	98	6,0
12.18	2,4-ditert-butylphenol	97	5,7
13.72	nonylphenol (isomers)	92	8,2
14.10	Dipropyl phthalate (internal standard)	98	25
16.07	acetyl tributyl citrate	80	203
16.31	octadecadienoic acid, methyl ester	99	45
16.76	oleamide	90	58
19.57	erucamide	87	80

Table 8.98 - Sample 33: Total extract



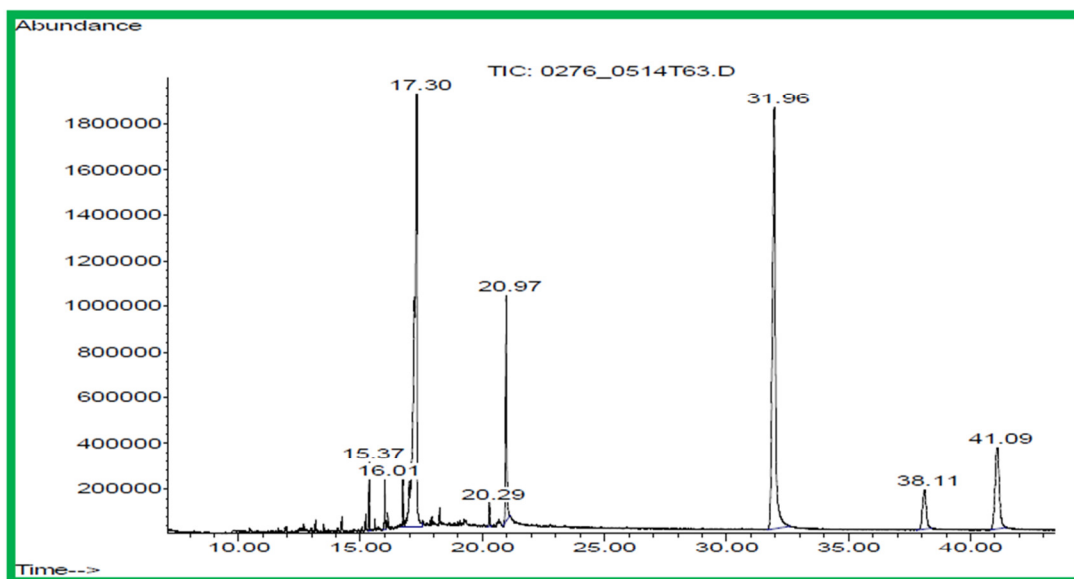
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
10.16	benzene, 1,3-bis(1,1-dimethylethyl)-	94	2,8
14.11	Dipropyl phthalate (internal standard)	98	12,5
16.08	acetyl tributyl citrate	80	7,1
16.32	octadecadienoic acid, methyl ester	99	4,8

Table 8.99 - Sample 33: Internal surface

SAMPLE 34: PE/EVA/PE-EVOH-PE/IONOMER

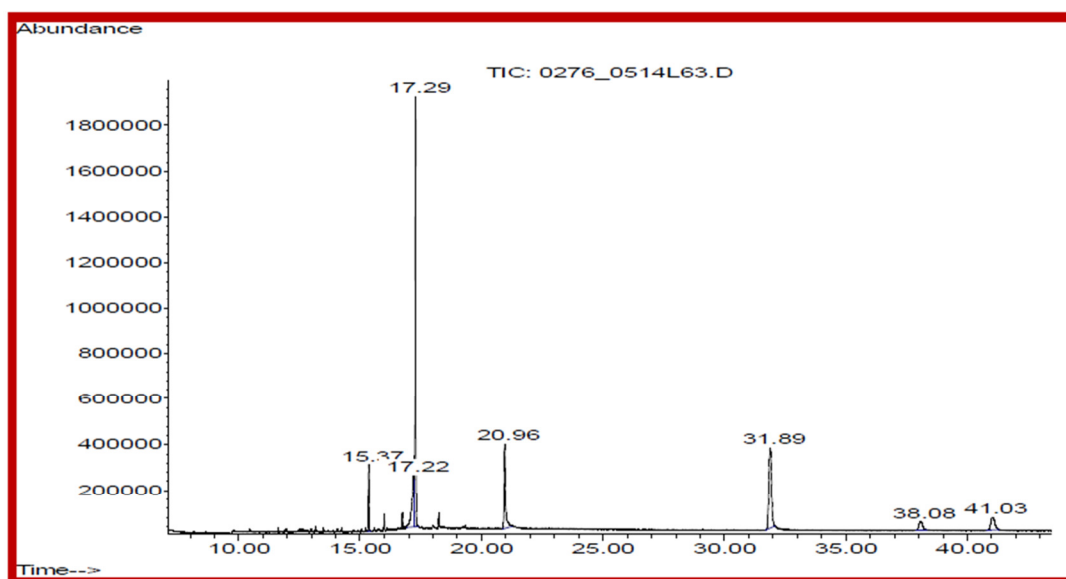
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.53	Ethanol	80	3,9
7.94	1-ethoxy, 2-propanol	78	3,4
11.45	Benzene, chloro (internal standard)	90	2,8
14.58	Siloxane *	-	-
17.08	Siloxane *	-	-
19.07	caprolactam	94	3,2

Table 8.100 - Sample 34: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	98	25.0
16.01	7,9-diterbutyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	99	21
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	93	20
17.30	acetyl tributyl citrate	80	1229
20.97	erucamide	95	168
31.96	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	925
38.11	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	105
41.09	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	248

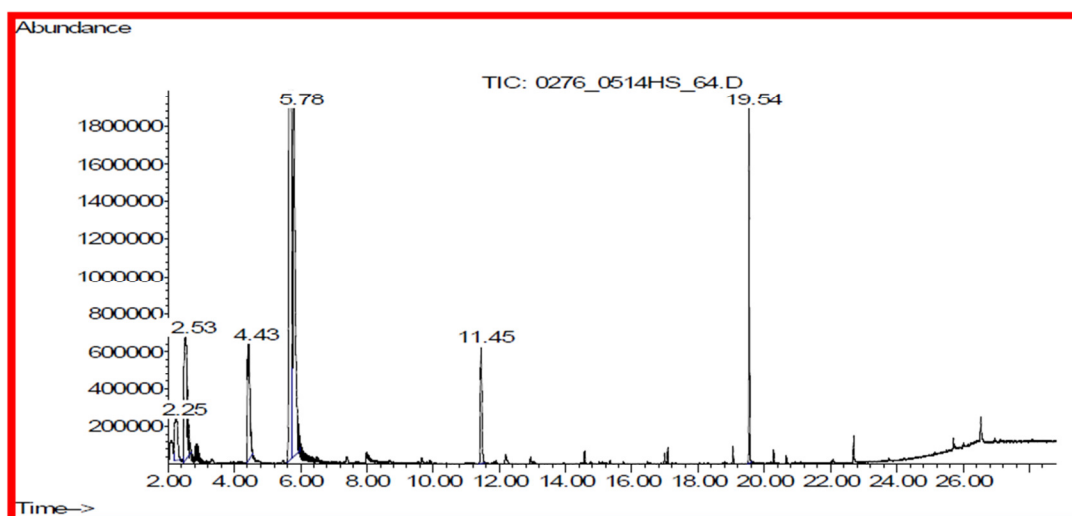
Table 8.101 - Sample 34: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
15.37	Dipropyl phthalate (internal standard)	98	12,5
17.29	acetyl tributyl citrate	80	96
20.96	erucamide	95	41
31.89	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	80
38.08	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	12
41.03	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	20

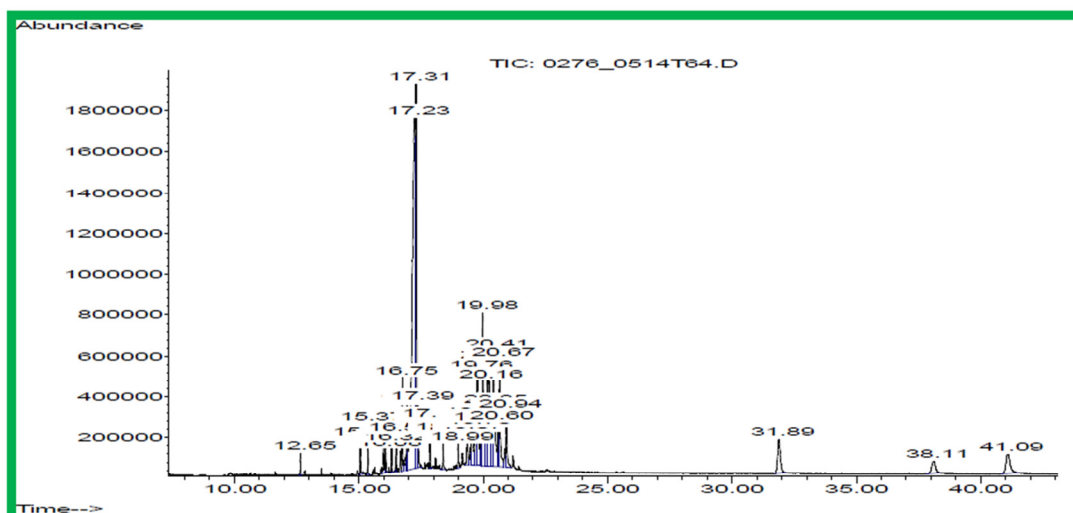
Table 8.102 - Sample 34: Internal surface

SAMPLE 35: OPPmet /OPPcoex



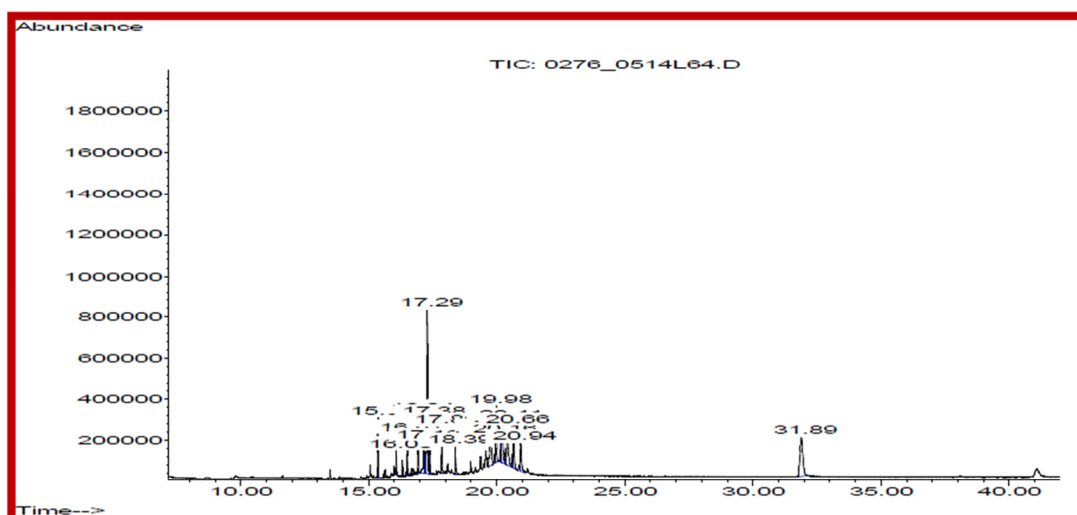
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2.25	1-propene, 2-methyl-	70	2,3
2.56	ethanol	80	6,2
4.43	ethyl acetate	83	4,2
5.58	cyclohexane	80	36
5.78	2-propanol,1-methoxy	70	18
11.45	Benzene, chloro (internal standard)	94	2,8
19.54	triacetin	83	3,8

Table 8.103 - Sample 35: Head space



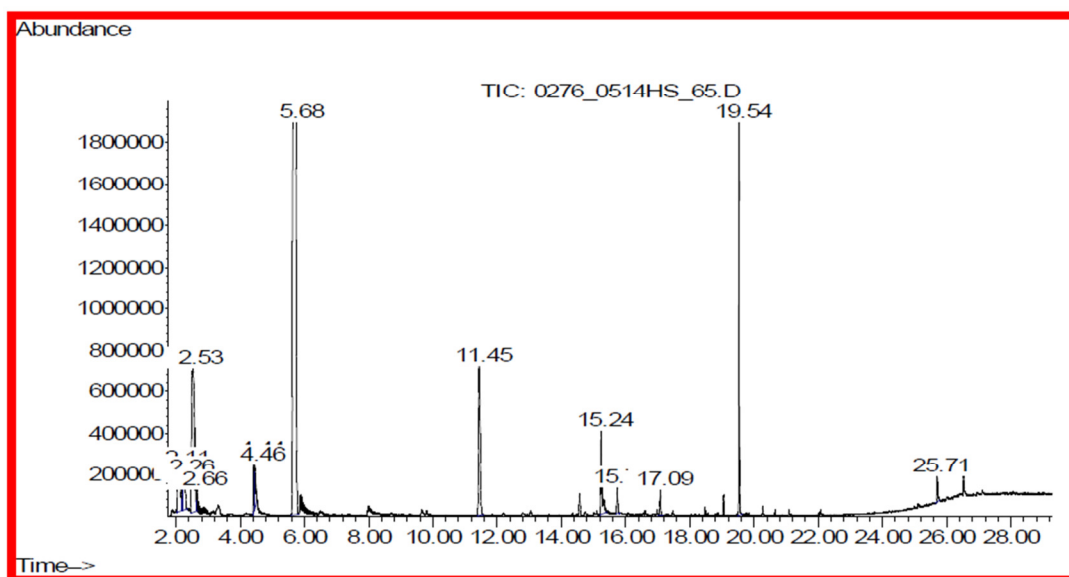
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
12.65	triacetin	80	11
15.06	not identified (m/z = 84,99,111,173)	-	24
15.36	Dipropyl phthalate (internal standard)	98	25
16.00	Aliphatic insature hydrocarbon	97	20
16.32	not identified (m/z = 100,127,185)	-	15
16.51	aliphatic hydrocarbon	-	17
16.74	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	50
16.94	aliphatic hydrocarbon	-	39
17.31	acetyl tributyl citrate	80	1.458
17.38	aliphatic hydrocarbon	-	43
17.87	aliphatic hydrocarbon	-	27
from 19.3 to 21.3	DINCH	80	1248
31.89	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	93
38.11	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	45
41.09	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	85

Table 8.104 - Sample 35: Total extract



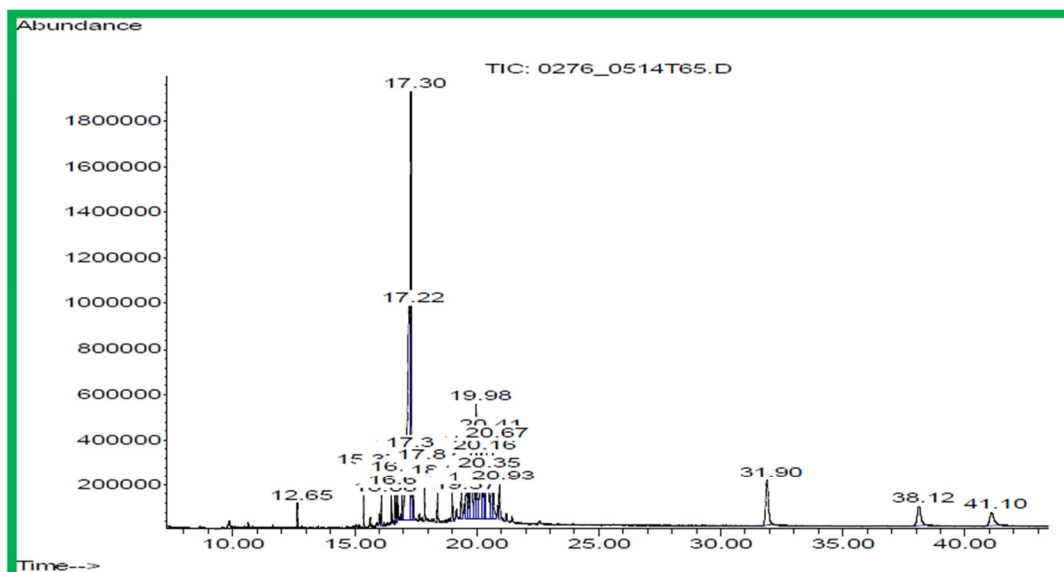
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.36	Dipropyl phthalate (internal standard)	98	12,5
16.08	aliphatic hydrocarbon	-	4
16.51	aliphatic hydrocarbon	-	8
16.94	aliphatic hydrocarbon	-	12
17.29	acetyl tributyl citrate	80	42
17.38	aliphatic hydrocarbon	-	13
17.80	aliphatic hydrocarbon	-	12
from 19.3 to 21.3	DINCH	80	129
31.89	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	45

Table 8.105 - Sample 35: Internal surface

SAMPLE 36: OPPmet white

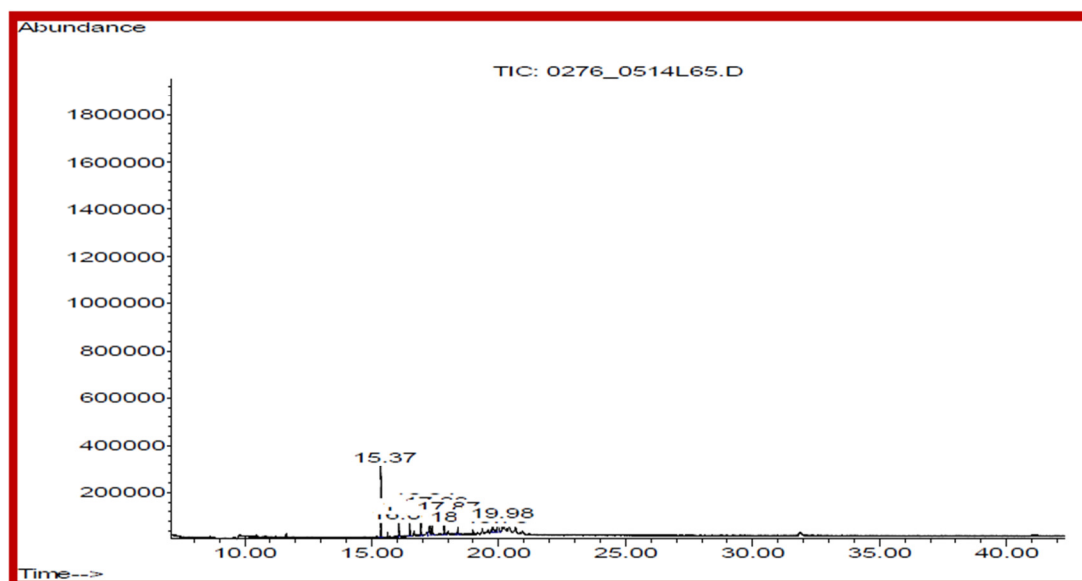
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
2.53	Ethanol	80	5,8
4.46	ethyl acetate	83	1,3
5.68	Cyclohexane	91	44
11.45	Benzene, chloro (internal standard)	97	2,8
15.24	ethanol-2-(2-ethoxyethoxy)	91	1,5
15.75	2-ethyl,1-hexanol	86	0,3
17.09	2-propenoic acid, 2-ethylhexyl ester	90	0,2
19.54	Triacetin	83	3,8

Table 8.106 - Sample 36: Head space



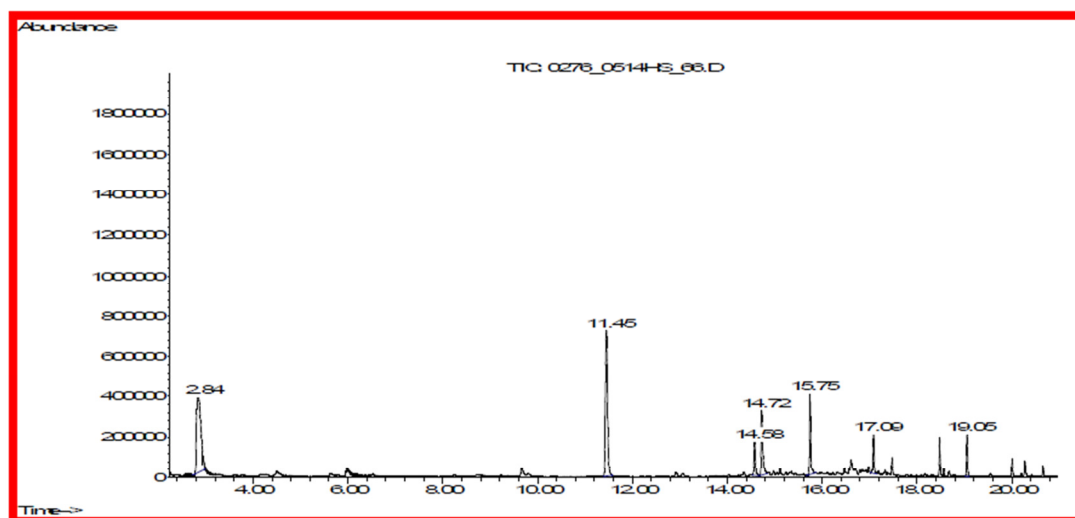
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
12.65	Triacetin	83	11
15.37	Dipropyl phthalate (internal standard)	90	25
16.08	aliphatic hydrocarbon	-	13
16.51	aliphatic hydrocarbon	-	18
16.67	Decanedioic acid, dibutyl ester	93	16
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	20
16.94	aliphatic hydrocarbon	-	32
17.30	acetyl tributyl citrate	80	797
17.39	aliphatic hydrocarbon	-	36
17.87	aliphatic hydrocarbon	-	28
18.40	aliphatic hydrocarbon	-	25
18.99	aliphatic hydrocarbon	-	21
From 19.37 to 20.93	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	830
31.90	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	101
38.13	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	60
41.10	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	48

Table 8.107 - Sample 36: Total extract



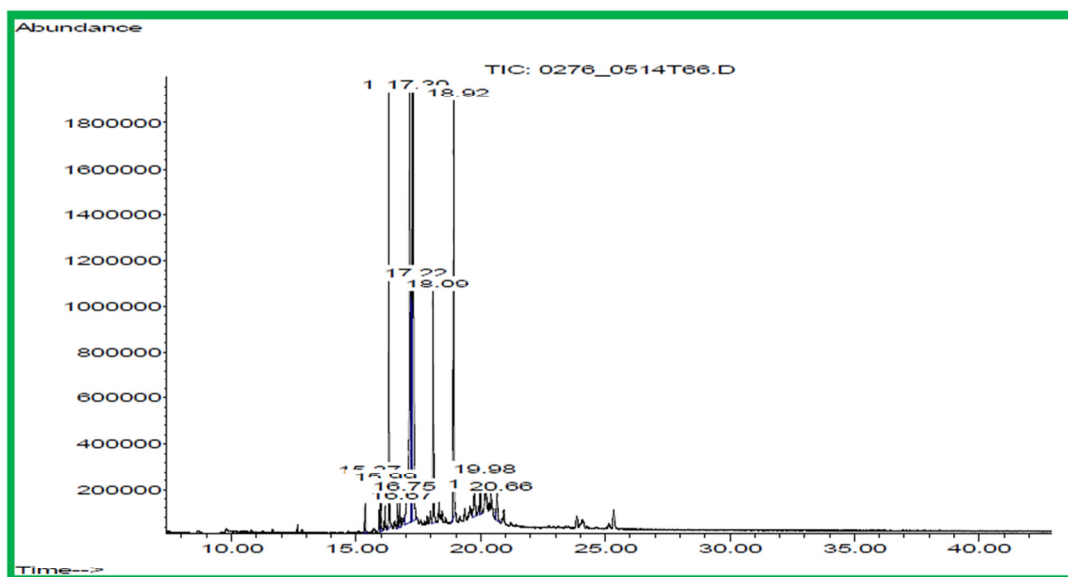
TR	peak identification	Qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.37	Dipropyl phthalate (internal standard)	90	50
16.08	aliphatic hydrocarbon	-	9
16.51	aliphatic hydrocarbon	-	15
16.94	aliphatic hydrocarbon	-	22
17.29	acetyl tributyl citrate	80	26
17.39	aliphatic hydrocarbon	-	20
17.87	aliphatic hydrocarbon	-	16
18.40	aliphatic hydrocarbon	-	9
From 19.37 to 20.93	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	40

Table 8.108- Sample 36: Internal surface

SAMPLE 37: PAPER/Aluminum

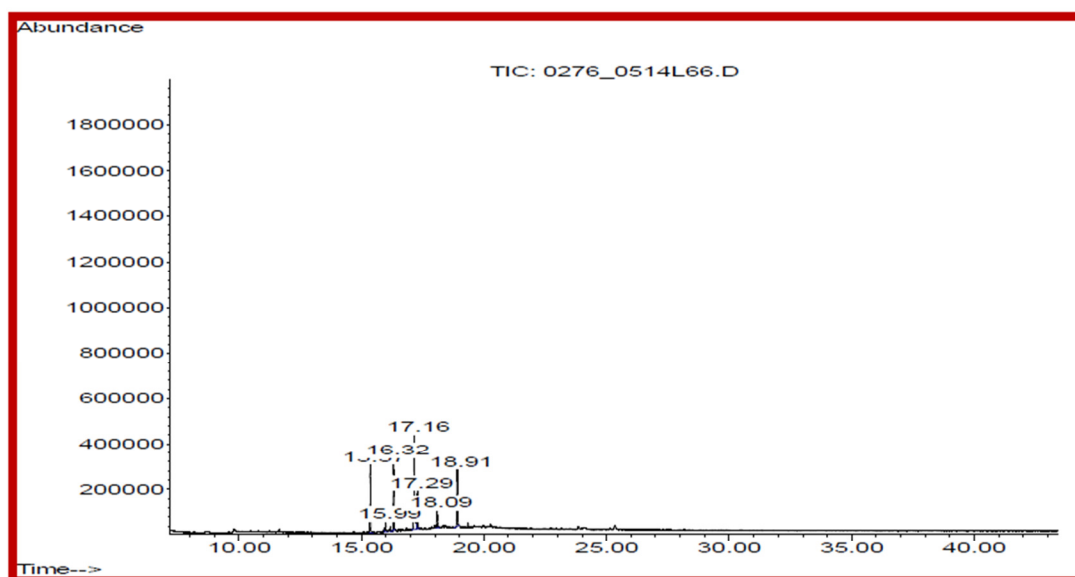
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
2,84	Iso-propanol	80	3,0
11.45	Benzene, chloro (internal standard)	94	2,8
14.58	Siloxane *	-	-
14.72	Benzaldehyde	97	1,0
15.75	1-hexanol,2-ethyl	90	0,9
17.09	Siloxane	-	-
19.05	Siloxane *	-	-

Table 8.109 - Sample 37: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.36	Dipropyl phthalate (internal standard)	98	25
15.99	Not identified (m/z = 243)	-	30
16.32	not identified (m/z = 100,127,185)	-	352
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	72	18
17.16	not identified (m/z = 127,155,185,213)	-	701
17.31	acetyl tributyl citrate	80	945
18.09	not identified (m/z = 155,213)	-	134
18.92	Phosphoric acid, 2-ethylhexyl diphenyl ester	93	249
from 19.3 to 21.3	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	94

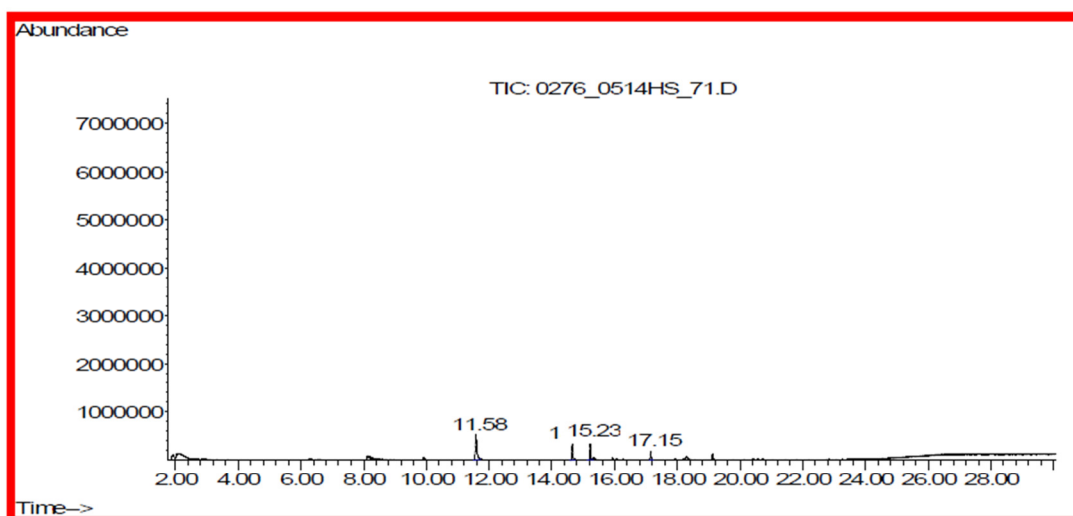
Table 8.110 - Sample 37: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
15.36	Dipropyl phthalate (internal standard)	98	25
15.99	Not identified (m/z = 243)	-	11
16.32	not identified (m/z = 100,127,185)	-	51
17.16	not identified (m/z = 127,155,185,213)	-	94
17.31	acetyl tributyl citrate	80	35
18.09	not identified (m/z = 155,213)	-	18
18.92	Phosphoric acid, 2-ethylhexyl diphenyl ester	93	60

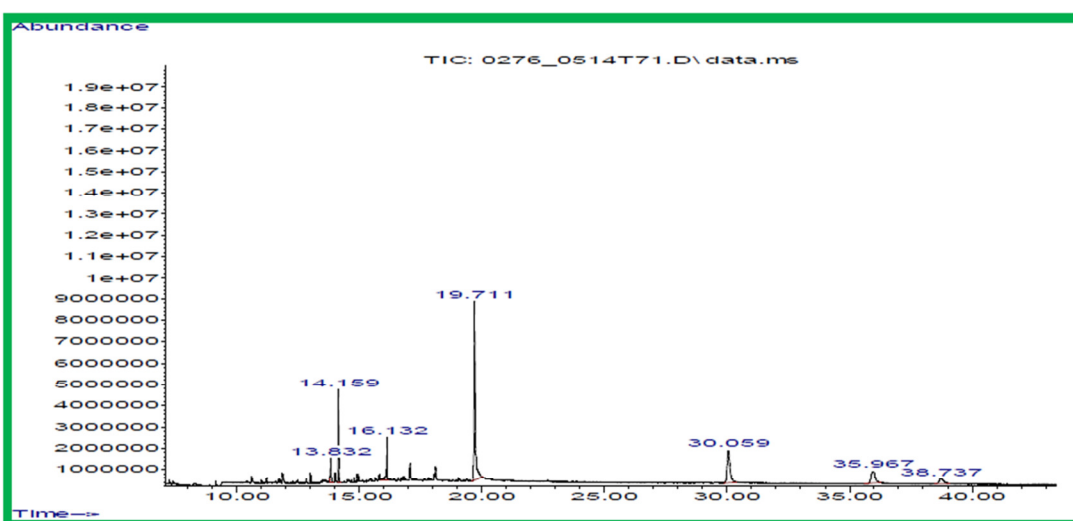
Table 8.111 - Sample 37: Internal surface

SAMPLE 38: OPA/PE



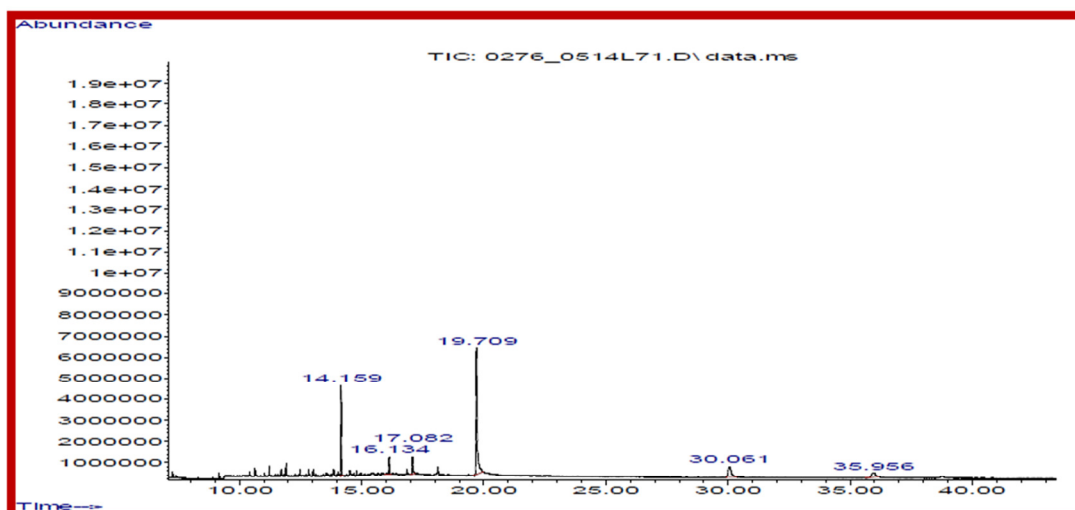
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.58	Benzene, chloro (internal standard)	94	2,8
14.65	siloxane	-	1,1
15.23	Heptane, 2,2,4,6,6-pentamethyl-	83	1,2
17.15	Siloxane *	-	-

Table 8.112 - Sample 38: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
13.83	not identified (m/z =99,111,173)	-	10
14.16	Dipropyl phthalate (internal standard)	98	25.0
16.13	acetyl tributyl citrate	80	18
19.71	Erucamide	90	122
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	55
35.97	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	28
38.74	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	15

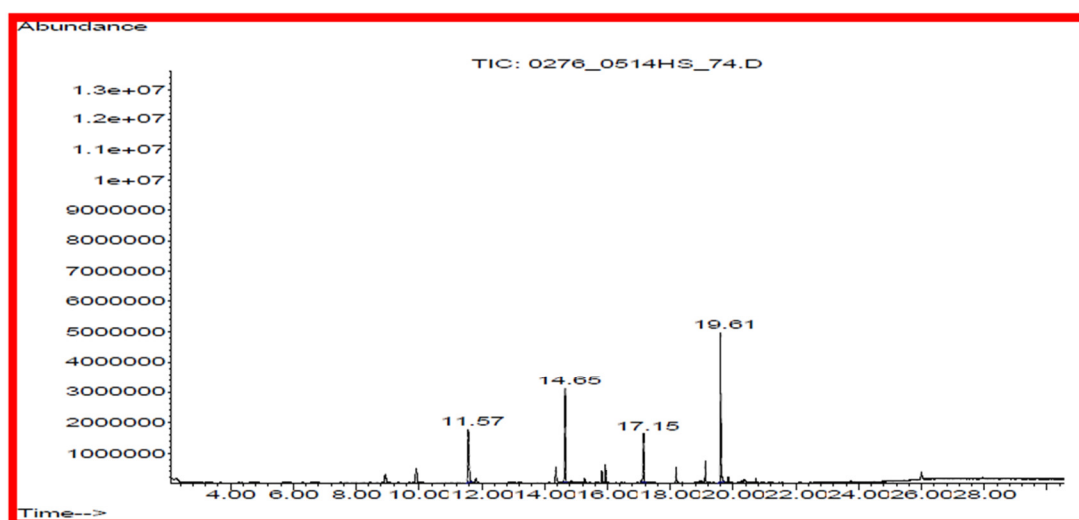
Table 8.113 - Sample 38: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Dipropyl phthalate (internal standard)	98	12,5
16.13	acetyl tributyl citrate	80	3,6
19.71	Erucamide	90	42
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	10
35.96	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	5,6

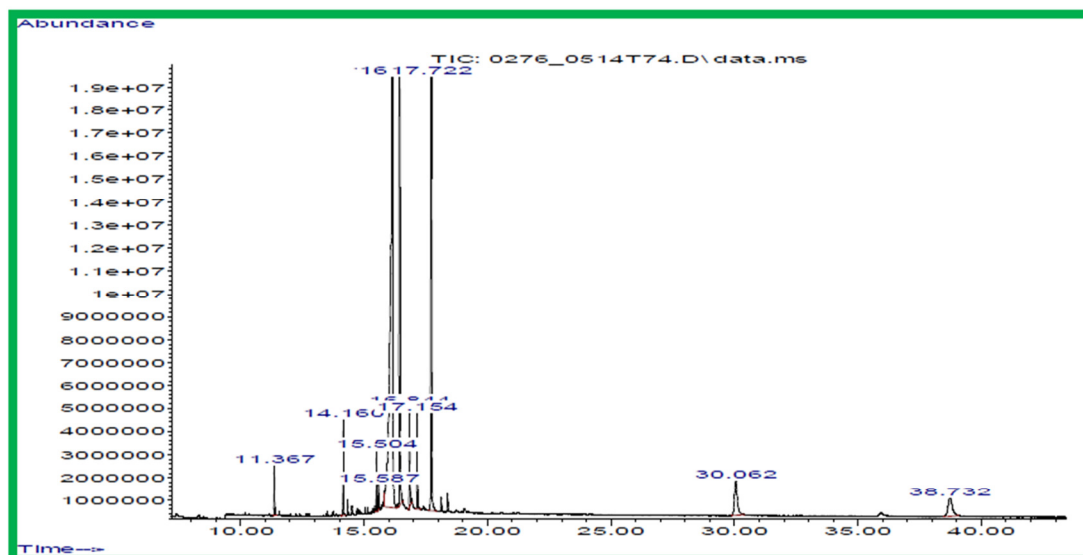
Table 8.114 - Sample 38: Internal surface

SAMPLE 39: OPP/met



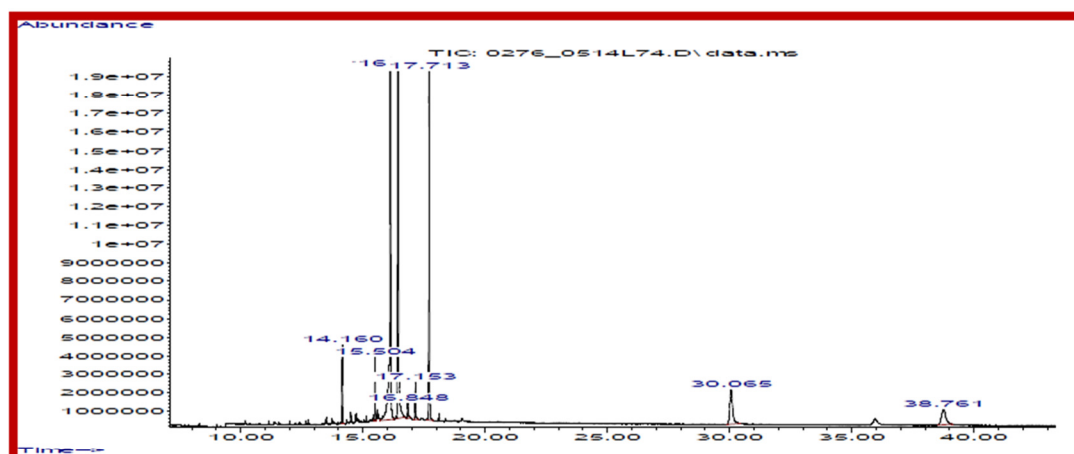
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.57	Benzene, chloro (internal standard)	94	2,8
14.65	Siloxane *	-	-
17.15	Siloxane *	-	-
19.61	Triacetin	83	3,7

Table 8.115 - Sample 39: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.37	Triacetin	90	15
14.16	Dipropyl phthalate (internal standard)	98	25
15.50	decanedioic acid, dibutyl ester	94	15
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	93	6,2
16.15	acetyl tributyl citrate	86	994
16.44	di-2-ethylhexyl adipate	90	431
16.84	oleamide	87	35
17.15	not identified (m/z = 175)	-	32
17.72	2-ethylhexyl diphenyl phosphate	91	473
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	54
38.73	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	43

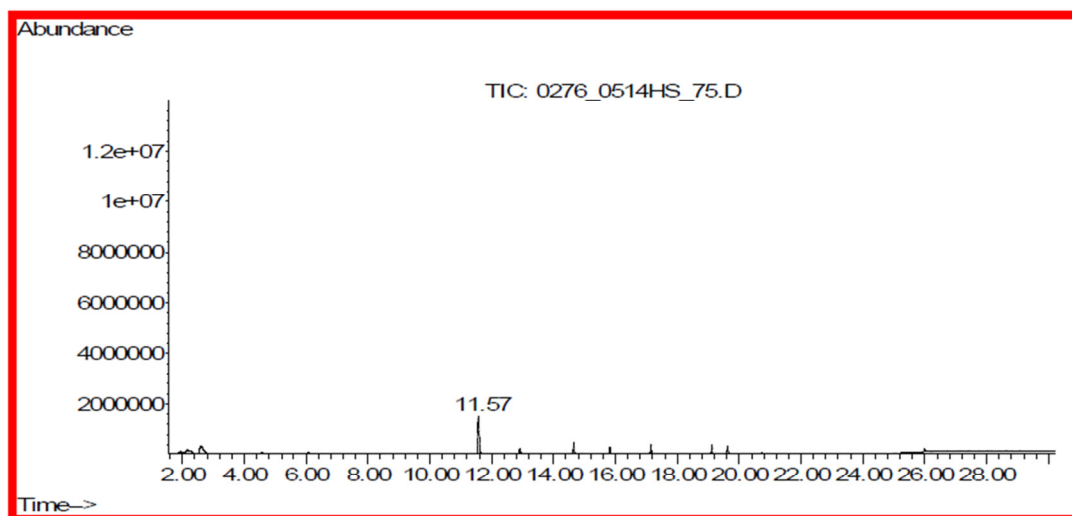
Table 8.116 - Sample 39: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Dipropyl phthalate (internal standard)	98	12,5
15.50	decanedioic acid, dibutyl ester	94	10
16.14	acetyl tributyl citrate	86	135
16.44	di-2-ethylhexyl adipate	90	321
16.85	oleamide	87	3,7
17.15	not identified (m/z = 175)	-	7,7
17.71	2-ethylhexyl diphenyl phosphate	91	72
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	32
38.76	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	22

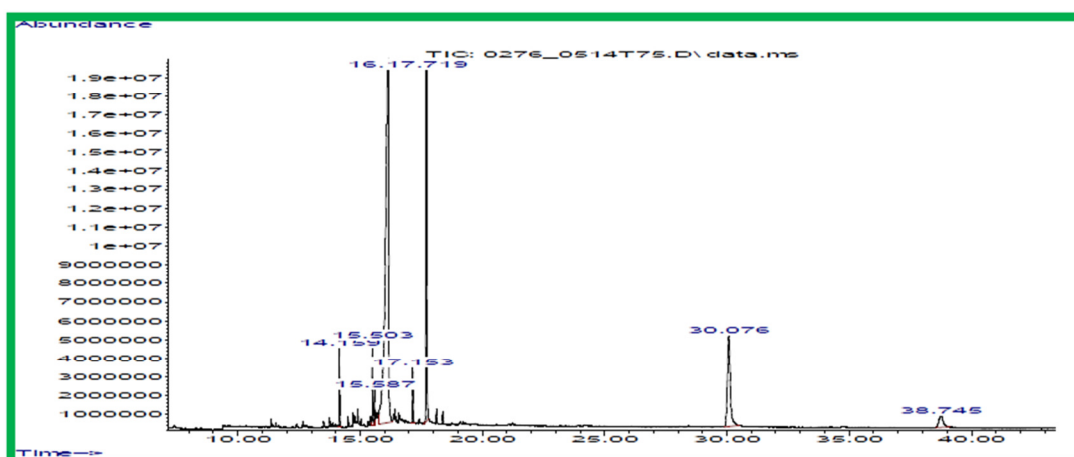
Table 8.117 - Sample 39: Internal surface

SAMPLE 40: OPP- Pvc/Its



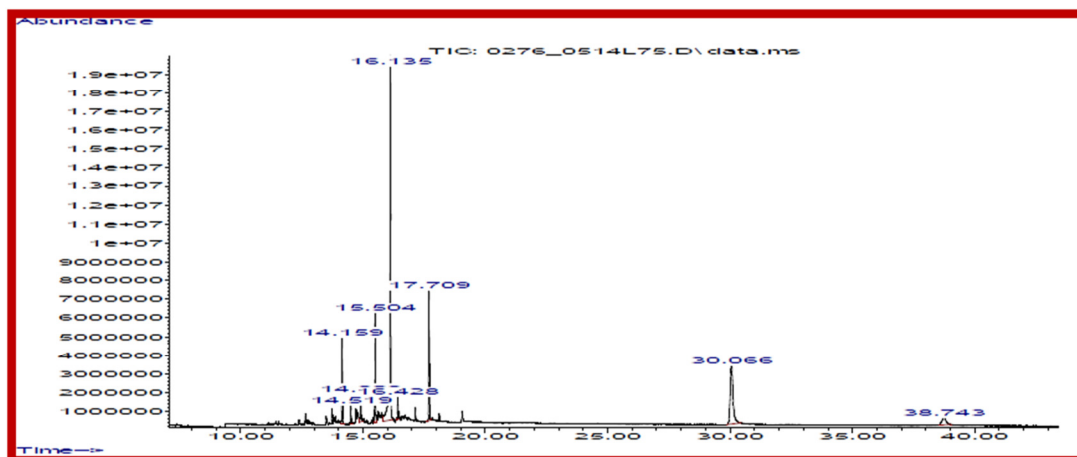
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
11.57	Benzene, chloro (internal standard)	94	2,8

Table 8.118 - Sample 40: Head space



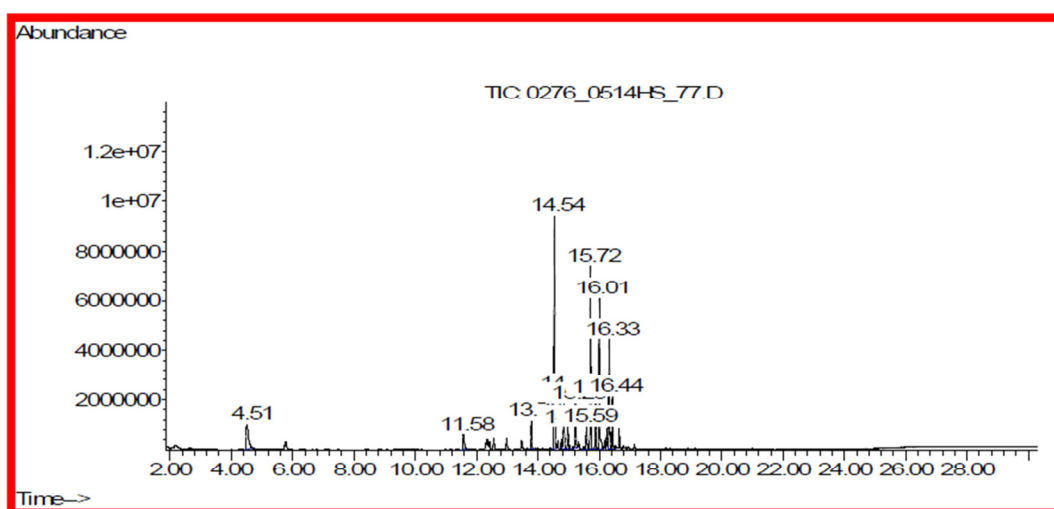
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
14.16	Dipropyl phthalate (internal standard)	98	25
15.50	decanedioic acid, dibutyl ester	94	27
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	98	12
16.15	acetyl tributyl citrate	86	1324
17.15	not identified (m/z = 175)	-	22
17.72	2-ethylhexyl diphenyl phosphate	91	371
30.08	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	174
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	34

Table 8.119 - Sample 40: Total extract



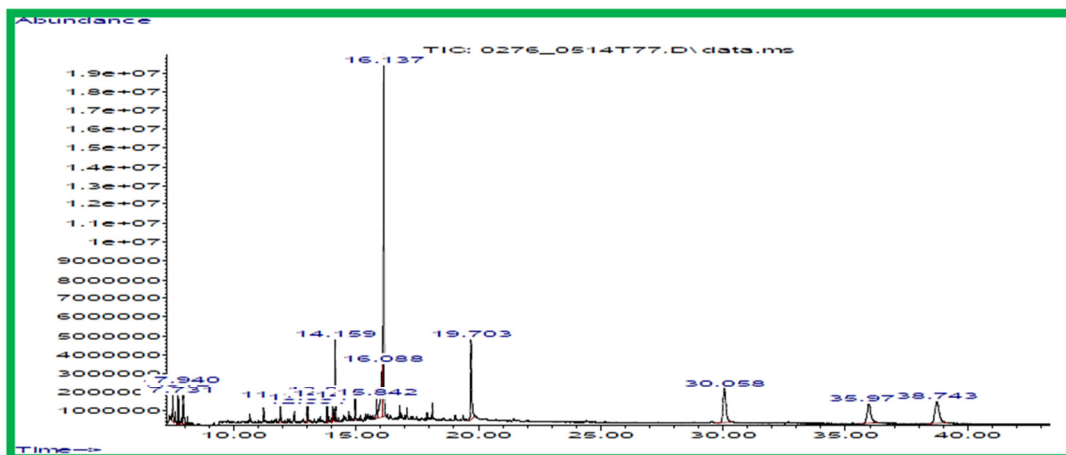
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
14.16	Dipropyl phthalate (internal standard)	98	12,5
14.52	diisobutyl phthalate	72	3,5
14.92	aliphatic hydrocarbon	-	5,1
15.50	decanedioic acid, dibutyl ester	94	16
16.14	acetyl tributyl citrate	86	87
16.43	not identified (m/z = 175)	-	3,6
17.71	2-ethylhexyl diphenyl phosphate	91	26
30.07	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	52
38.74	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	10

Table 8.120 - Sample 40: Internal surface

SAMPLE 41: PETpvc/PE

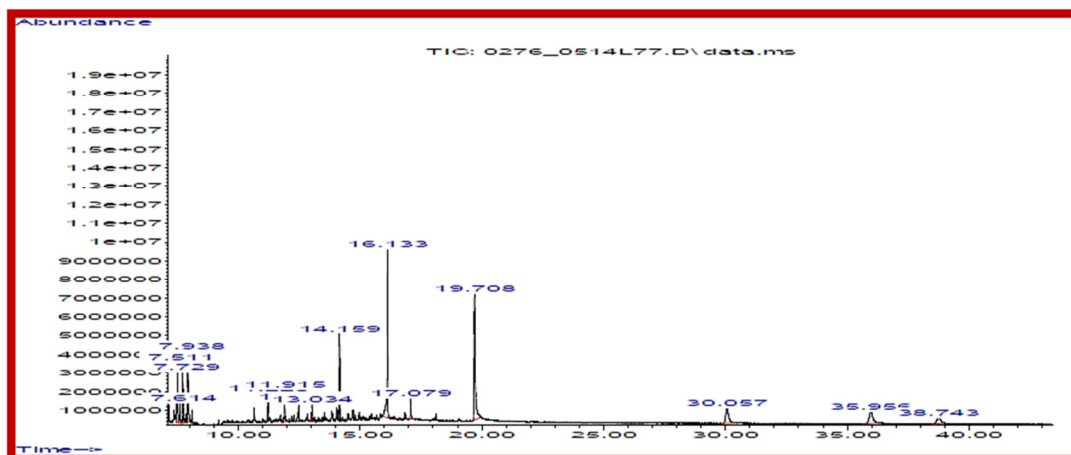
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.51	ethylacetate	90	7,5
11.58	Benzene, chloro (internal standard)	94	2,8
from 13.79 to 16.44	aliphatic hydrocarbons	-	101

Table 8.121 - Sample 41: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION µg/dm ²
7.51	aliphatic hydrocarbon	-	14
7.73	aliphatic hydrocarbon	-	14
7.94	aliphatic hydrocarbon	-	19
11.92	aliphatic hydrocarbon	-	9,0
12.99	aliphatic hydrocarbon	-	4,2
13.03	aliphatic hydrocarbon	-	6,9
13.83	not identified (m/z =84,99,111,173)	-	11
14.05	aliphatic hydrocarbon	-	6,7
14.16	Dipropyl phthalate (internal standard)	98	25
14.97	aliphatic hydrocarbon	-	5,5
15.84	aliphatic hydrocarbon	-	8,0
16.14	acetyl tributyl citrate	86	190
19.70	erucamide	93	58
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	62
35.98	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	46
38.74	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	57

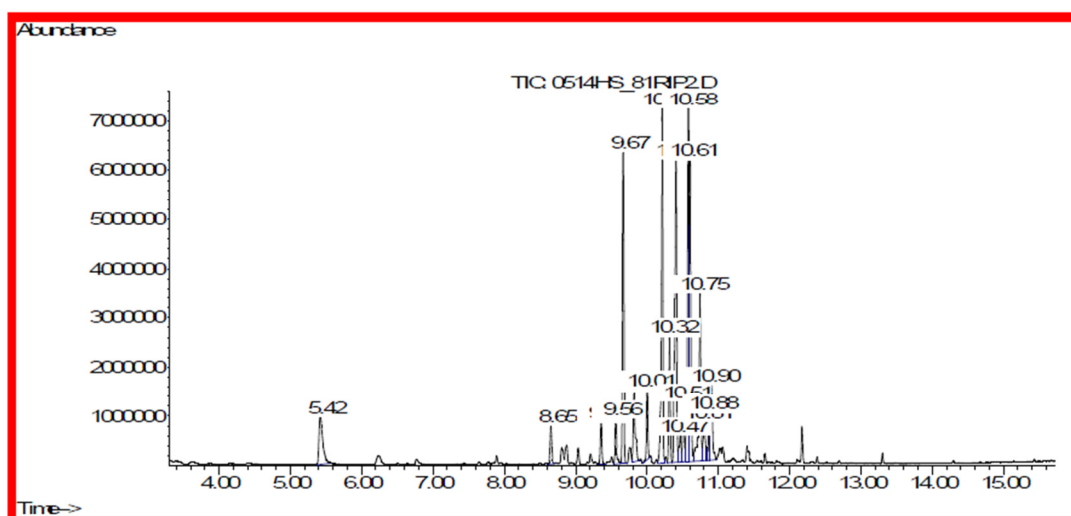
Table 8.122 - Sample 41: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
7.51	aliphatic hydrocarbon	-	13
7.61	aliphatic hydrocarbon	-	4.2
7.73	aliphatic hydrocarbon	-	13
7.94	aliphatic hydrocarbon	-	15
11.23	aliphatic hydrocarbon	-	3.8
11.92	aliphatic hydrocarbon	-	6.2
12.49	aliphatic hydrocarbon	-	4.5
13.03	aliphatic hydrocarbon	-	3.4
14.16	Dipropyl phthalate (internal standard)	98	12,5
16.13	acetyl tributyl citrate	86	33
17.08	aliphatic hydrocarbon	-	4.3
19.71	erucamide	93	45
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	14
35.96	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	13
38.74	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	7.5

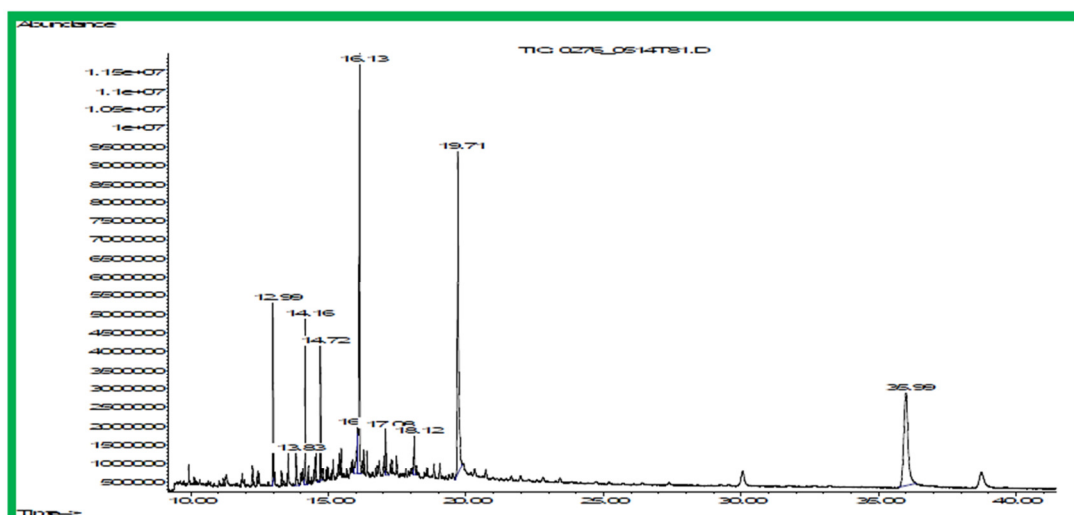
Table 8.123 - Sample 41: Internal surface

SAMPLE 42: PET /PE



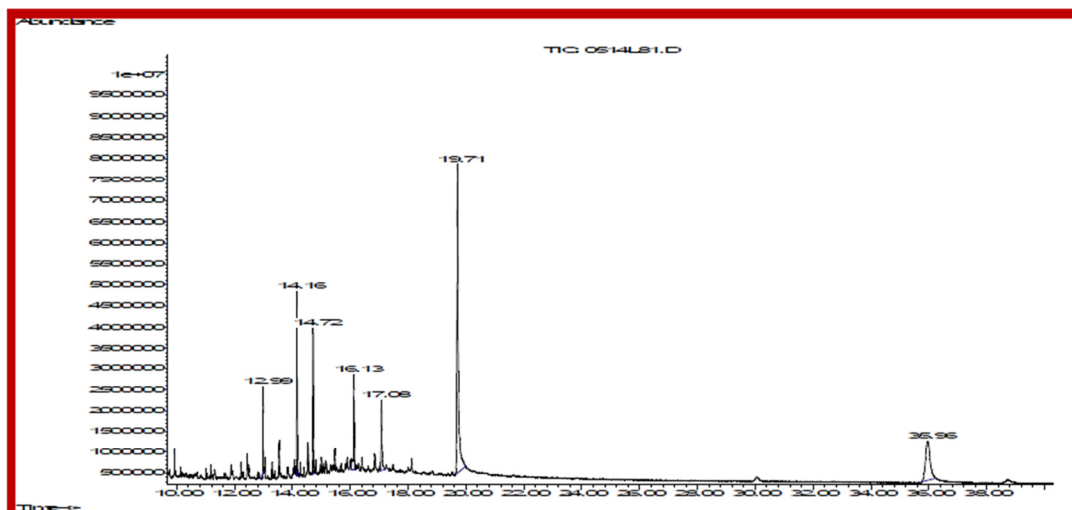
TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
5.42	Ethyl acetate	83	10
8.65	Benzene, chloro (internal standard)	94	2,8
9.36	aliphatic hydrocarbon	-	3,1
9.67	aliphatic hydrocarbon	-	21
9.82	aliphatic hydrocarbon	-	6,4
10.01	aliphatic hydrocarbon	-	4,8
10.21	aliphatic hydrocarbon	-	26
10.32	aliphatic hydrocarbon	-	7,7
10.41	aliphatic hydrocarbon	-	25
10.51	aliphatic hydrocarbon	-	4,5
10.58	aliphatic hydrocarbon	-	25
10.61	aliphatic hydrocarbon	-	19
10.75	aliphatic hydrocarbon	-	14
10.81	aliphatic hydrocarbon	-	3,5
10.88	aliphatic hydrocarbon	-	3,2
10.90	aliphatic hydrocarbon	-	4,4

Table 8.124 - Sample 42: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION ug/dm ²
12.99	aliphatic hydrocarbon	-	24
14.16	Dipropyl phthalate (internal standard)	98	25
14.72	not identified (m/z = 97,126,155,173)	-	19
15.84	aliphatic hydrocarbon	-	4.6
16.13	acetyl tributyl citrate	91	94
17.08-18.12	aliphatic hydrocarbons	-	25 sum
19.71	erucamide	90	94
35.99	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	90

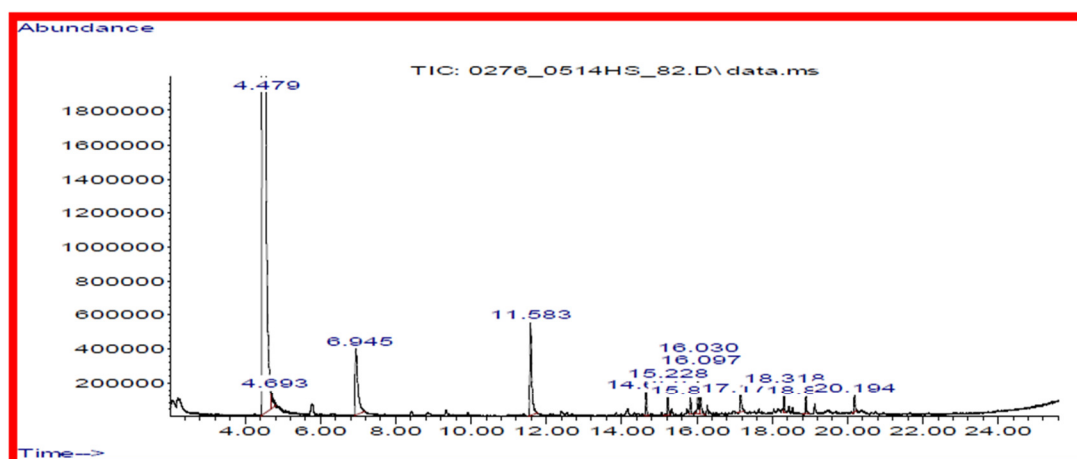
Table 8.125 - Sample 42: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
12.99	aliphatic hydrocarbon	-	6,4
14.16	Dipropyl phthalate (internal standard)	98	12,5
14.72	not identified (m/z = 97,126,155,173)	-	10
16.13	acetyl tributyl citrate	91	7,5
17.08	aliphatic hydrocarbon	-	8,3
19.71	erucamide	90	50
36.00	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	20

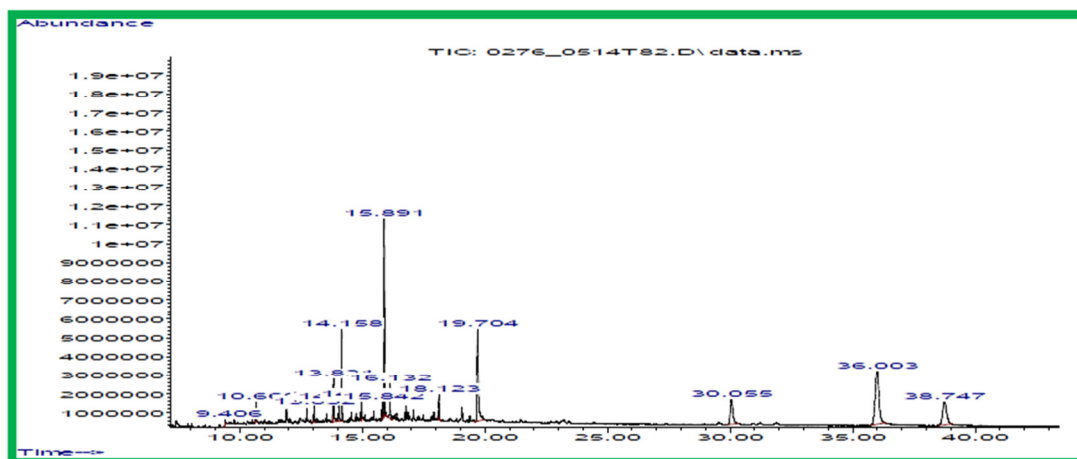
Table 8.126 - Sample 42: Internal surface

SAMPLE 43: PET /PET met/PE



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
4.48	Ethyl acetate	83	89
6.95	n-propyl acetate	83	2,7
11.58	Benzene, chloro (internal standard)	94	2,8
14.66	Siloxane *	-	-
15.23	heptane, 2,2,4,6,6-pentamethyl	83	0,6
16.03	not identified (m/z = 57,97,113)	-	0,9
16.10	cyclohexane, butyl	95	0,8

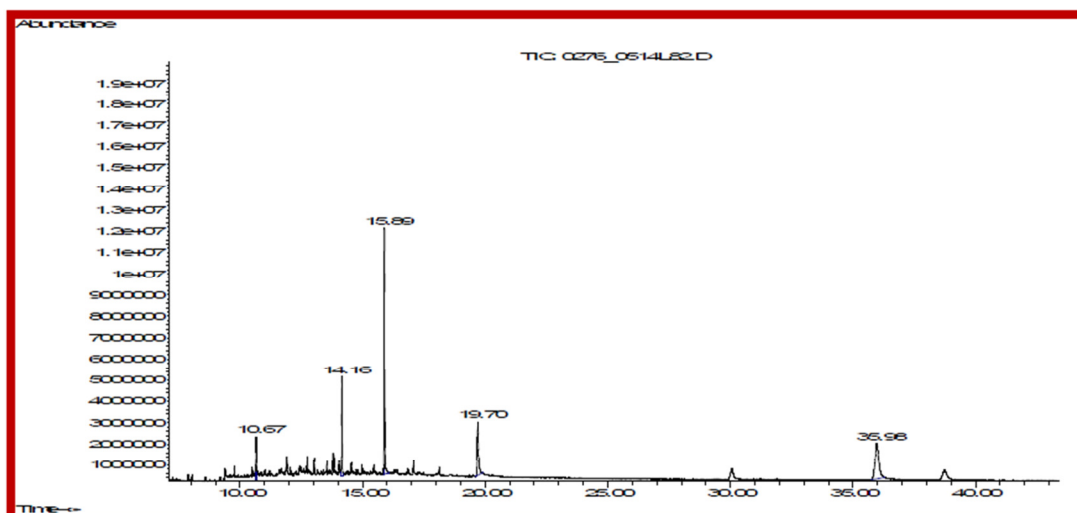
Table 8.127 - Sample 43: Head space



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
10.67	not identified (m/z = 57,83,97,111)	-	5,9
13.03	not identified (m/z = 57,83,97,111)	-	5,4
13.79	not identified (m/z = 57,71,127,155)	-	5,2
13.83	not identified (m/z = 173,99,111)	-	14
14.04	cyclooctacosane	93	6,1
14.16	Dipropyl phthalate (internal standard)	98	25
14.97	1-docosene	99	4,8
15.84	aliphatic hydrocarbon	-	4,6
15.89	oxybenzone (UV absorber) (*)	98	61
16.13	acetyl tributyl citrate	91	12
18.12	not identified (m/z = 91,117,207)	-	11
19.70	erucamide	90	64
30.06	antioxidant (m/z = 147,441,646) (Irgafos 168)	-	38
36.00	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	113
38.75	antioxidant (m/z = 316,647, 662) (Irgafos 168 mono-oxidated)	-	53

* UV ABSORBER - Listed on Reg. (EU) 10/2011

Table 8.128 - Sample 43: Total extract



TR	peak identification	qual	SEMIQUANTITATIVE EVALUATION $\mu\text{g}/\text{dm}^2$
10.67	not identified (m/z = 57,83,97,111)	-	4,9
14.16	Dipropyl phthalate (internal standard)	98	12,5
15.89	oxybenzone (UV absorber) (*)	98	40
19.70	erucamide	90	17
30.06	antioxidant (m/z = 147,441,646)	-	7,9
35.98	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	38
38.74	antioxidant (m/z = 647,316,662) (Irgafos 168)	-	10

* UV ABSORBER - Listed on Reg. (EU) 10/2011

Table 8.129 - Sample 43: Internal surface

8.2. Application of the MATRIX tool

In this paragraph we have been reported in details how the Matrix approach has been applied as tool to assess the potential risk of the substances extracted through GC-MS Analysis of 43 flexible packaging materials tested.

At the end of this exercise we obtained the following tables:

- 1-Calculation_Matrix_43_structures
- 2-Calculation_rows_columns_43_structures
- 3-Identification_specimens_table
- 4-Risk_assessment_table

As these tables are not printable because of their size, that make them difficult to be read, they will be loaded into a CD-ROM and made available as appropriate.

In this paragraph we describe each step and on how the above-mentioned tables has been built.

Picture 3 reported below shows the format used and explanation on how the data have been reported for the all the calculations: in column on the right it is showed the model packaging material chosen from the Matrix spreadsheet in Annex (*ALL AVG*) for each samples analyzed. This column also reports the average (*S AVG*) and maximum (*S Max*) surfaces, calculated as follows:

- summing up all surfaces in contact with each food item for the

considered model packaging material in each of the five Countries in the project (sum of the column corresponding to that model packaging material). This corresponds to calculating the total surface of the said model packaging material in contact with the whole diet for each Country;

- taking the average value of the above-mentioned five Countries, and the value in the Country corresponding to the maximum surface.

These values have eventually been used for the calculation of exposure by multiplying the concentration of a given substance, either volatile or non-volatile, by the corresponding surface as described above.

This giving maximum and average estimation of exposure.

In order to evaluate the total daily dietary concentration, we used the total surface in contact, i.e. the surface resulting by summing up all contributions of surfaces for each food item in contact with the model packaging chosen, and we multiply it by the concentration of the relevant substance for which exposure needs to be calculated:

Thus:

$$AVG \text{ exposure } (ZZ) \mu\text{g/person/dm}^2 = XX \text{ dm}^2/\text{person/day} * Conc \mu\text{g/dm}^2$$

$$MAX \text{ exposure } (WW) \mu\text{g/person/dm}^2 = YY \text{ dm}^2/\text{person/day} * Conc \mu\text{g/dm}^2$$

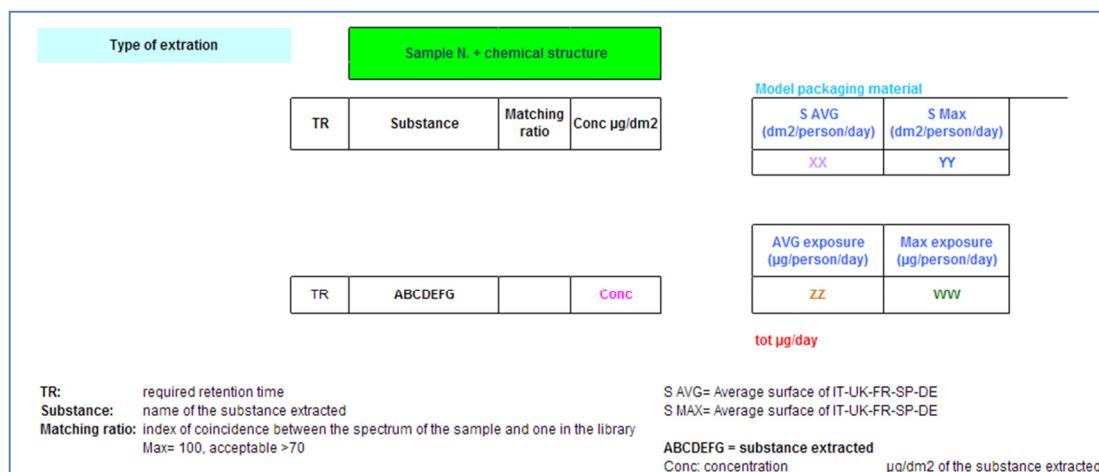


Figure 8.1 - format and explanation on how the data have been reported for the calculation

8.3. Calculations & results

In this paragraph we have reported all calculations and results obtained applying the matrix tool to assess the 43 flexible packaging materials analyzed by GC-MS.

The following tables show, highlighted in yellow, all extracted substances that after the calculation exceed the TEL:10 µg/dm², regardless whether they are or aren't listed into *Regulation(EU) 10/2011*. So, this tables at this stage includes both intentionally and not intentionally added substances, the screening will be done in a second step and it will be explained in details in the following pages.

HEAD SPACE				SAMPLE 1: PET/ALU/PE		PLASTIC/ALU/PE	
TR	Substance	Matching ratio	Conc: $\mu\text{g}/\text{dm}^2$	S AVG ($\text{dm}^2/\text{person}/\text{day}$)	S Max ($\text{dm}^2/\text{person}/\text{day}$)	AVG exposure ($\mu\text{g}/\text{person}/\text{day}$)	Max exposure ($\mu\text{g}/\text{person}/\text{day}$)
				0.22	0.64		
4.51	Ethyl Acetate	90	0			0.00	0.00
from 13.80 to 16.65	Aliphatic saturated hydrocarbons	>80	87			19	56
tot $\mu\text{g}/\text{day}$				19	56		

Figure 8.2 - Sample 1: calculation Head space

TOTAL SOLVENT				PLASTIC/ALU/PE		AVG exposure ($\mu\text{g}/\text{person}/\text{day}$)		Max exposure ($\mu\text{g}/\text{person}/\text{day}$)	
TR	Substance	Matching ratio	$\mu\text{g}/\text{dm}^2$	S AVG ($\text{dm}^2/\text{person}/\text{day}$)	S Max ($\text{dm}^2/\text{person}/\text{day}$)	AVG exposure ($\mu\text{g}/\text{person}/\text{day}$)	Max exposure ($\mu\text{g}/\text{person}/\text{day}$)		
				0.22	0.64				
11.28	Benzene, 2,4-diisocyanato-1-methyl	87	17			4	11		
12.99	Octadecane	97	8.2			2	5		
13.83	Not identified(m/z=84,99,111,173)		15			3	10		
14.72	Not identified(m/z=97,126,155,173)		5.2			1	3		
16.14	Tributyl acetylacrylate	87	42			9	27		
16.85	Oleamide	90	18			4	11		
18.13	Analytical system contaminant					0	0		
19.71	Erucamide	87	24			5	15		
36.03	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester (Irganox 1076)	78	108			23	69		
tot $\mu\text{g}/\text{day}$				52	151				

Figure 8.3 - Sample 1: calculation Total solvent

INTERNAL SURFACE				PLASTIC/ALU/PE		AVG exposure ($\mu\text{g}/\text{person}/\text{day}$)		Max exposure ($\mu\text{g}/\text{person}/\text{day}$)	
TR	Substance	Matching ratio	$\mu\text{g}/\text{dm}^2$	S AVG ($\text{dm}^2/\text{person}/\text{day}$)	S Max ($\text{dm}^2/\text{person}/\text{day}$)	AVG exposure ($\mu\text{g}/\text{person}/\text{day}$)	Max exposure ($\mu\text{g}/\text{person}/\text{day}$)		
				0.22	0.64				
13.84	Not identified(m/z=84,99,111,173)		2			0	1		
14.72	Not identified(m/z=97,126,155,173)		2.7			1	2		
16.13	Tributyl acetylacrylate	90	7			2	4		
19.7	Erucamide	87	14			3	9		
35.98	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester	78	26			6	17		
tot $\mu\text{g}/\text{day}$				11	33				

Figure 8.4 - Sample 1: calculation Internal surface

HEAD SPACE				SAMPLE 2: PET/AL/PET/PE		PLASTIC/ALU/PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.52	Ethyl Acetate	83	7.4	0.132	0.64	1	5
tot µg/day				1	5		

Figure 8.5 - Sample 2: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.132	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
13.83	Not identified (m/z=84,99,111,173)		17			2	11
18.13	Analytical system contaminant					0	0
19.71	Erucamide	87	68			9	43
36.03	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester (Irganox 1076)	78	137			18	87
tot µg/day				29	142		

Figure 8.6 - Sample 2: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.132	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
13.84	Not identified (m/z=84,99,111,173)		2.6			0.3	2
18.13	Analytical system contaminant					0.0	0.0
19.71	Erucamide	87	30			4	19
35.97	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester (Irganox 1076)	78	23			3	15
tot µg/day				7	35		

Figure 8.7 - Sample 2: calculation Internal surface

HEAD SPACE				SAMPLE 3: PAPER/AL/PE		CARTA/ALU/PLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.52	1.88		
2.56	Ethanol	80	1.7			1	3
4.41	ethyl acetate	83	31.2			16	59
6.84	n-propyl acetate	80	3.1			2	6
9.81	siloxane		1			1	2
14.58	siloxane		4.4			2	8
15.24	decane	94	1.1			1	2
16.87	undecane	91	3.6			2	7
18.17	dodecane	91	2.8			1	5
19.28	tridecane	94	1			1	2
tot µg/day				26	94		

Figure 8.8 - Sample 3: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.52	1.88	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
9.63	undecane	94	9			5	17
10.48	dodecane	94	11			6	21
11.23	tridecane	94	10			5	19
15.07	not identified (m/z=84,99,11,173)		39			20	73
17.29	acetyl tributyl citrate	80	258			135	485
20.34	not identified (m/z=99,171,127)		215			112	404
tot µg/day				283	1019		

Figure 8.9 - Sample 3: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.52	1.88	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
9.63	undecane	94	6			3	11
10.48	dodecane	94	9			5	17
11.23	tridecane	94	8			4	15
tot µg/day				12	43		

Figure 8.10 - Sample 3: calculation Internal surface

HEAD SPACE				SAMPLES 4: PAPER/AL/PE		PAPER/ALU/PLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2.85	iso-propanol	80	2.9	0.52	1.88	2	5
5.83	ethylacetate	83	5.4			3	10
14.72	benzaldehyde	95	3.4			2	6
15.23	aliphatic hydrocarbons		0.5			0	1
16.62	aliphatic hydrocarbons		1.4			1	3
16.79	aliphatic hydrocarbons		0.4			0	1
tot µg/day				7	26		

Figure 8.11 - Sample 4: calculation Head space

TOTAL SOLVENT				PAPER/ALU/PLASTIC		PAPER/ALU/PLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
17.29	acetyl tributyl citrate	91	277	0.52	1.88	145	521
tot µg/day						145	521

Figure 8.12 - Sample 4: calculation Total solvent

INTERNAL SURFACE				PAPER/ALU/PLASTIC		PAPER/ALU/PLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
	NO SUBSTANCES			0.52	1.88	0	0
	EXTRACTED						

Figure 8.13 - Sample 4: calculation Internal surface

HEAD SPACE				SAMPLE 5: PET/AL/OPA/PE		OTHER COMBINATION NON PLASTIC/PLASTIC	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2.53	ethanol	80	2.9	0.19	0.64	1	2
4.45	ethyl acetate	83	5.4			1	3
tot µg/day				2	5		

Figure 8.14 - Sample 5: calculation Head space

TOTAL SOLVENT				OTHER COMBINATION NON PLASTIC/PLASTIC		OTHER COMBINATION NON PLASTIC/PLASTIC	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.56	not identified(m/z=55,82,111,129)		44	0.19	0.64	8	28
20.95	erucamide	95	25			5	16
31.92	antioxidant(m/z=147,441,646) (irgafos 168)		473			90	303
38.12	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester (irganox 1076)	94	130			25	83
41.07	antioxidant (m/z= 316,647,662) (irgafos 168 mono-oxidated)		101			19	65
tot µg/day				147	495		

Figure 8.15 - Sample 5: calculation Total solvent

INTERNAL SURFACE				OTHER COMBINATION NON PLASTIC/PLASTIC		OTHER COMBINATION NON PLASTIC/PLASTIC	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.56	not identified(m/z=55,82,111,129)		8.2	0.19	0.64	2	5
20.95	erucamide	83	15			3	10
31.88	antioxidant(m/z=147,441,646) (irgafos 168)		57			11	36
38.09	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-,octadecyl ester (irganox 1076)	83	16			3	10
41.04	antioxidant (m/z= 316,647,662) (irgafos 168 mono-oxidated)		8.8			2	6
tot µg/day				20	67		

Figure 8.16 - Sample 5: calculation Internal surface

HEAD SPACE				SAMPLE 6: PET/PETsiox/CASTPP		OTHER PLASTIC/PP	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)		
2.55	ethanol	80	3.5	0.14	0.34	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.43	ethyl acetate	83	8.2			0.5	1.2
8.49	heptane, 4-methyl-	91	1.6			1.1	2.8
10.29	heptane,2,4-dimethyl	87	1.6			0.2	0.5
10.98	2,4 dimethyl-1-heptene	87	7			0.2	0.5
11.73	octane, 4-methyl	91	1.1			1.0	2.4
from 15.73 to 21.20	aliphatic hydrocarbon		20			0.1	0.4
tot µg/day				6	15		

Figure 8.17 - Sample 6: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PP			
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.14	0.34		
from 11.31 to 15.07	aliphatic hydrocarbon		85			12	29
31.93	Antioxidant (m/z= 147,441,646) (irgafos 168)		462			63	158
41.1	Antioxidant (m/z= 316,647,662) (irgafos 168 mono-oxidated)		105			14	36
tot µg/day				89	222		

Figure 8.18 - Sample 6: calculation Total solvent

INTERNAL SURFACE				OTHER PLASTIC/PP			
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.14	0.34		
from 11.31 to 13.19	aliphatic hydrocarbon		16			2	5
31.89	Antioxidant (m/z= 147,441,646) (irgafos 168)		71			10	24
tot µg/day				12	30		

Figure 8.19 - Sample 6: calculation Internal surface

HEAD SPACE				SAMPLE 7: OPPacr/acr	
TR	Substance	Matching ratio	µg/dm2	OPP	
				S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
2.27	2-methyl, 1-propene	70	1.6	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
5.81	methoxypropanol	80	12	2	4
7.96	ethoxypropanol	83	2.3	14	27
				3	5
tot µg/day				18	36

Figure 8.20 - Sample 7: calculation Head space

TOTAL SOLVENT					
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
15.44	Decanedioic acid, di butylester	91	127	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				147	286
15.53	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	10	12	23
16.08	acetyl tributyl citrate	80	653	757	1469
16.36	di-2-ethylhexyl adipate	90	227	263	511
16.76	oleamide	89	41	48	92
17.61	2-ethylhexyl diphenyl phospathe	91	10	12	23
29.66	antioxidant (m/z=147,441,646) (irgafos 168)		118	137	266
38.1	antioxidant (m/z=316,647,662) (irgafos 168 mono-oxidated)		17	20	38
tot µg/day				1395	2707

Figure 8.21 - Sample 7: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
13.68	aliphatic hydrocarbon		0.7	1	2
14.66	aliphatic hydrocarbon		1.7	2	4
14.69	aliphatic hydrocarbon		1.6	2	4
15.45	decanedioic acid, di butylester	91	81	94	182
15.56	aliphatic hydrocarbon		1.1	1	2
16.07	acetyl tributyl citrate	80	56	65	126
16.36	di-2-ethylhexyl adipate	90	167	194	376
16.76	oleamide	89	13	15	29
29.66	antioxidant (m/z= 147,441,646)(Irgafos 168)		38	44	86
38.1	antioxidant (m/z= 316,647,662)(Irgafos 168 mono-oxidated)		6.1	7	14
tot µg/day				425	824

Figure 8.22 - Sample 7: calculation Internal surface

HEAD SPACE				SAMPLE 8: OPA/castPP		OTHER PLASTIC/PP	
TR	Substance	Matchin ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.41	ethyl acetate	83	13.5	0.14	0.34	1.8	4.6
16.19	aliphatic hydrocarbon		0.7			0.1	0.2
17.72	siloxane		0.6			0.1	0.2
19.03	aliphatic hydrocarbon		0.6			0.1	0.2
22.69	not identified(m/z= 84,99,111,173)		0.3			0.0	0.1
tot µg/day				2	5		

Figure 8.23 - Sample 8: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PP		AVG exposure (µg/person/day)		Max exposure (µg/person/day)	
TR	Substance	Matchin ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)		
				0.14	0.34				
15.07	not identified (m/z=99,111,173)		108			15	37		
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester)	83	11			2	4		
17.29	acetyl tributyl citrate	80	513			72	174		
31.91	antioxidant (m/z=147,441,646) (Irgafos 168)		399			56	136		
41.05	antioxidant (m/z=316,647,662) (irgafos 168 mono-oxidated)		45			6	15		
tot µg/day				151	366				

Figure 8.24 - Sample 8: calculation Total solvent

INTERNAL SURFACE				OTHER PLASTIC/PP		AVG exposure (µg/person/day)		Max exposure (µg/person/day)	
TR	Substance	Matchin ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)		
				0.14	0.34				
31.88	antioxidant (m/z=147,441,646)(irgafos 168)		36			5	12		
tot µg/day				5	12.00				

Figure 8.25 - Sample 8: calculation Internal surface

HEAD SPACE				SAMPLE 9: PET/PE-EVOH-PE		OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2.58	Ethanol	80	2.2	0.28	0.73	0.6	1.6
4.47	ethylacetate	83	2.5			0.7	1.8
6.02	methoxypropanol	86	0.5			0.1	0.4
10.1	1-octene	95	0.2			0.1	0.1
15.17	aliphatic hydrocarbon		0.2			0.1	0.1
15.98	aliphatic hydrocarbon		0.3			0.1	0.2
17.11	siloxane		0.3			0.1	0.2
18.2	aliphatic hydrocarbon		0.2			0.1	0.1
19.08	siloxane*		0.2			0.1	0.1
tot µg/day						2	5

Figure 8.26 - Sample 9: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PE		AVG exposure (µg/person/day)	Max exposure (µg/person/day)
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)		
16.07	acetyl tributyl citrate	80	7.7	0.28	0.73	2	6
16.76	oleamide	91	14			4	10
19.56	erucamide	87	32			9	23
29.65	antioxidant (m/z=147,441,646) (Irgafos 168)		56			16	41
35.41	benzenepropanoic acid, 3,5-bis (1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	67			19	49
38.11	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		22			6	16
tot µg/day						56	145

Figure 8.27 - Sample 9: calculation Total solvent

INTERNAL SURFACE				S AVG (dm2/person/day)		S Max (dm2/person/day)	
TR	Substance	Matching ratio	µg/dm2	0.28	0.73		
17.00	aliphatic hydrocarbon		2.9	1	2		
19.56	erucamide	87	26	7	19		
29.65	antioxidant (m/z= 147,441,646)(irgafos 168)		27	8	20		
35.42	Benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-.octadecyl ester (irganox 1076)	83	45	13	33		
38.12	antioxidant (m/z= 316,647,662) (irgafos 168 mono-oxidated)		9.2	3	7		
tot µg/day				31	80		

Figure 8.28 - Sample 9: calculation Internal surface

HEAD SPACE				SAMPLE 10: PET/PE-EVOH-PE		OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.28	0.73		
3.98	cyclohexane	86	1.8			1	1
4.41	ethyl acetate	83	37			10	27
8.49	heptane, 4-methyl-	91	2.5			1	2
10.3	Heptane 2,4-dimethyl-1-heptene	87	1			0.3	1
10.97	2,4-dimethyl-1-heptene	87	8.6			2	6
from 15.45 to 19.49	Aliphatic hydrocarbon		14			4	10
tot µg/day				18	47		

Figure 8.29 - Sample 10: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.28	0.73	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.07	not identified (m/z=99,11,173)		47			13	34
17.29	acetyl tributyl citrate	80	218			61	159
20.96	erucamide	81	39			11	28
31.9	antioxidant(m/z=147, (irgafos 168)		249			70	182
41.07	antioxidant(m/z=316, (irgafos 168 monooxidated)		92			26	67
tot µg/day				181	471		

Figure 8.30 - Sample 10: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	0.28	0.73
from 11.31 to 14.02	aliphatic hydrocarbon not identified (m/z=84,99,111,173)		36	10	26
15.07	aliphatic hydrocarbon		14	4	10
15.74	aliphatic hydrocarbon		7.6	2	6
17.29	acetyl tributyl citrate	80	25	7	18
18.10	analytical system contaminant			0	0
20.39	analytical system contaminant			0	0
20.96	erucamide	81	29	8	21
31.90	antioxidant (m/z=147, 441,646)(irgafos 168)		110	31	80
41.07	antioxidant (m/z=316,647,662)(irgafos 168 monooxidated)		41	11	30
tot µg/day				74	192

Figure 8.31 - Sample 10: calculation Internal surface

HEAD SPACE				SAMPLE 11: PETpvc/PE		OTHER PLASTIC/PE	
TR	Substance	Matchin ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.41	ethyl acetate	83	46	0.28	0.73	13	34
from 9.14 to 11.03	aliphatic hydrocarbon		24			7	18
tot µg/day				20	51		

Figure 8.32 - Sample 11: calculation Head space

TOTAL SOLVENT				S AVG (dm2/person/day)		S Max (dm2/person/day)	
TR	Substance	Matchin ratio	µg/dm2	0.28	0.73	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
14.86	not identified (m/z= 102,141)		15			4	11
17.29	acetyl tributyl citrate	80	45			13	33
20.19	oleic acid, 3-hydroxypropyl ester	91	219			61	160
20.95	erucamide	81	55			15	40
31.9	antioxidant (m/z=147,441,646)(irgafos 168)		110			31	80
38.08	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	80	33			9	24
41.06	antioxidant (m/z=316,647,662)(irgafos 168 mono-oxidated)		43			12	31
tot µg/day				146	380		

Figure 8.33 - Sample 11: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matchin ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
18.65	Hexadecanoic acid ester		3.1	1	2
20.19	oleic acid, 3-hydroxypropyl ester	91	137	38	100
31.89	antioxidant (m/z=147,441,646)(irgafos 168)		71	20	52
38.08	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	80	22	6	16
41.06	antioxidant (m/z=316,647,662)(irgafos 168 mono-oxidated)		27	8	20
tot µg/day				73	190

Figure 8.34 - Sample 11: calculation Internal surface

HEAD SPACE				SAMPLE 12 : PETmet/PE			
TR	Substance	Matching ratio	µg/dm2	OTHERPLASTIC/PE			
				S AVG (dm2/person/day)	S Max (dm2/person/day)		
				0.28	0.73		
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)		
4.41	ethyl acetate	83	32	9.0	23.4		
10.06	1-octene	87	1.2	0.3	0.9		
14.46	aliphatic hydrocarbon		3.8	1.1	2.8		
14.77	aliphatic hydrocarbon		1	0.3	0.7		
15.15	aliphatic hydrocarbon		1.1	0.3	0.8		
15.65	aliphatic hydrocarbon		2.7	0.8	2.0		
15.81	aliphatic hydrocarbon		0.7	0.2	0.5		
15.94	aliphatic hydrocarbon		1.9	0.5	1.4		
16.26	aliphatic hydrocarbon		1.4	0.4	1.0		
16.37	aliphatic hydrocarbon		0.7	0.2	0.5		
tot µg/day				13	34		

Figure 8.35 - Sample 12: calculation Head space

TOTAL SOLVENT							
TR	Substance	Matching ratio	µg/dm2	OTHERPLASTIC/PE			
				S AVG (dm2/person/day)	S Max (dm2/person/day)		
				0.28	0.73		
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)		
15.07	not identified(m/z=99,111,173)		29	8	21		
16.74	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	9	3	7		
17.29	acetyl tributyl citrate	80	320	90	234		
18	oleamide	87	40	11	29		
from 19.75 to 20.66	1,2-cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	130	36	95		
20.96	erucamide	97	87	24	64		
31.9	antioxidant (m/z=147,441,646)(irgafos 168)		325	91	237		
38.09	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4- hydroxy-, octadecyl ester (irganox 1076)	94	70	20	51		
41.06	antioxidant (m/z=316,647,662)(irgafos 168 mono-oxitaded)		101	28	74		
tot µg/day				311	811		

Figure 8.36 - Sample 12: calculation Total solvent

INTERNAL SURFACE			
TR	Substance	Matching ratio	µg/dm ²
15.07	not identified(m/z=84,99,111,173)		4.9
17.29	acetyl tributyl citrate	80	38
from 19.75 to 20.66	1,2-Cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	26
20.96	erucamide	90	62
31.88	antioxidant (m/z=147,441,646)(Irgafos 168)		59
38.08	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4- hydroxy-, octadecyl ester (irganox 1076)	94	21
41.04	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		18
			tot µg/day

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.28	0.73

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
1	4
11	28
7	19
17	45
17	43
6	15
5	13
53	167

Figure 8.37 - Sample 12: calculation Internal surface

HEAD SPACE				SAMPLE 13: OPPcoex		OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.16	2.25		
5.78	cyclohexane	91	8.3			10	19
7.50	cyclohexane, methyl	94	2.9			3	7
19.61	triacetin	83	5.4			6	12
21.23	2,5-cyclohexadien-1-one, 2,6-bis (1,1-dimethylethyl)-4-methylene	99	1			1	2
21.44	BHT	98	0.7			1	2
tot µg/day				21	41		

Figure 8.38 - Sample 13: calculation Head space

TOTAL SOLVENT				OPP		AVG exposure (µg/person/day)		Max exposure (µg/person/day)	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)				
				1.16	2.25				
11.37	triacetin	83	24			28	54		
12.22	BHT	98	78			90	176		
13.87	cyclohexadecane	91	11			13	25		
14.83	7,9-di-tert-butyl-1-oxaspiro(4,5) deca-6,9-diene-2,8-dione	98	19			22	43		
15.51	sebacic acid, dibutyl ester	91	129			150	290		
16.15	tributyl acetyl citrate	91	805			934	1811		
18.13	analytical system contaminant					0	0		
19.71	erucamide	87	83			96	187		
30.07	antioxidant(m/z=308,441,646)(irgafos 168)		30			35	68		
38.78	antioxidant (m/z=316,647,662)(irgafos 168 mono-oxidated)		83			96	187		
tot µg/day				1464	2840				

Figure 8.39 - Sample 13: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
12.22	BHT	98	45	52	101
13.86	cyclohexadecane	91	11	13	25
14.83	7,9-di-tert-butyl-1-oxaspiro(4,5) deca-6,9-diene-2,8-dione	98	13	15	29
15.51	sebacic acid, dibutyl ester	91	84	97	189
16.14	tributyl acetylcitrate	91	145	168	326
19.70	erucamide	87	15	17	34
tot µg/day				363	704

Figure 8.40 - Sample 13: calculation Internal surface

HEAD SPACE				SAMPLE 14: PET/AL/PE		PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.52	ethyl acetate	84	4.1	0.22	0.64	1	3
15.22	pentamethyl, eptane	94	9			2	6
tot µg/day				3	8		

Figure 8.41 - Sample 14: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²			AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.97	silane, trimethoxy [3-(oxiranylmethoxy)propyl]	91	63	0.22	0.64	14	40
13.04	not identified (m/z=101,111,129)		23			5	15
19.71	erucamide	87	39			9	25
21.95	not identified (m/z=111,129,215,343)		77			17	49
tot µg/day				44	129		

Figure 8.42 - Sample 14: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²			AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.37	silane, trimethoxy[3-(oxiranylmethoxy)propyl]	91	29	0.22	0.64	6	19
13.04	not identified (m/z=101,111,129)		10			2	6
19.71	erucamide	87	32			7	20
tot µg/day				16	45		

Figure 8.43 - Sample 14: calculation Internal surface

HEAD SPACE				SAMPLE 15: PETmet/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
4.49	Ethyl acetate	84	23	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				6	17
tot µg/day				6	17

Figure 8.44 - Sample 15: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
11.37	BHT		25	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				7	18
11.97	silane, trimethoxy[3-(oxiranylmethoxy)propyl]trimethoxysilane	91	33		
				9	24
13.04	not identified (m/z=101,111,129)		20		
				6	15
14.92	docosane	90	14		
				4	10
15.51	sebacic acid, butyl ester	91	200		
				55	147
16.15	tributyl acetylcitrate	89	1028		
				284	755
19.7	erucamide	87	39		
				11	29
21.95	not identified (m/z=111,129,215,343)		38		
				10	28
38.77	antioxidant (m/z=308,441,646) (Irgafos 168)		64		
				18	47
tot µg/day				403	1072

Figure 8.45 - Sample 15: calculation Total solvent

INTERNAL SURFACE				OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
15.50	sebacic acid, butyl ester	91	41	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				11	30
16.13	tributyl acetylcitrate	89	25		
				7	18
19.70	erucamide	87	12		
				3	9
tot µg/day				22	57

Figure 8.46 - Sample 15: calculation Internal surface

HEAD SPACE				SAMPLE 16: PAPER/AL/PE	
TR	Substance	Matching ratio	µg/dm ²		
4.48	Ethyl acetate	84	190		
8.80	toluene	94	8.8		
15.22	Heptane, pentamethyl	83	16		
17.17	aliphatic hydrocarbon		2.9		
tot µg/day				114	409

PAPER/ALU/PE	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.52	1.88

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
99	357
5	17
8	30
2	5

Figure 8.47 - Sample 16: calculation Head space

TOTAL SOLVENT					
TR	Substance	Matching ratio	µg/dm ²		
13.83	not identified (m/z= 84,99,111,173)		53		
16.13	Tributyl acetylcitrate	89	350		
17.71	2-ethylhexyl diphenil phosphate	95	209		
17.82	di 2-ethylhexil phthalate	90	14		
19.7	erucamide	91	12		
tot µg/day				334	1198

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.52	1.88

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
28	99
183	657
109	392
7	26
6	23

Figure 8.48 - Sample 16: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.52	S Max (dm ² /person/day)
					1.88
13.83	not identified (m/z=84,99,11,17)		7	4	13
16.13	Tributyl acetylcitrate	89	25	13	47
17.71	2-ethylhexyl diphenyl phosphate	95	30	16	56
17.82	di 2-ethylhexil phthalate	90	5	3	9
19.70	erucamide	91	7.5	4	14
tot µg/day				39	140

Figure 8.49 - Sample 16: calculation Internal surface

HEAD SPACE				SAMPLE 17: OPA/PE	
TR	Substance	Matching ratio	µg/dm ²	OPA/PE	
				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.38	0.99
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.48	ethyl acetate	84	80	30	79
15.22	heptane, pentamethyl	83	16	6	16
from 14.54 to 16.01	aliphatic saturated hydrocarbons	>80	11	4	11
tot µg/day				41	106

Figure 8.50 - Sample 17: calculation Head space

TOTAL SOLVENT					
TR	Substance	Matching ratio	µg/dm ²		
				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.38	0.99
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.23	cyclohexane, octyl	96	8.5	3	8
11.92	1-hexadecane	96	11	4	11
13.83	not identified (m/z=84,99,111,173)		44	17	43
16.13	Tributyl acetilcitrate	89	26	10	26
19.7	erucamide	91	28	11	28
30.07	antioxidant (m/z=308,441,646) (irgafos 168)		72	27	71
38.76	antioxidant (m/z=316,647,662) (irgafos 168 mono-oxitated)		71	27	70
tot µg/day				99	257

Figure 8.51 - Sample 17: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.38	0.99		
11.23	cyclohexane, octyl	96	7	3	7		
11.91	1-hexadecene	96	9.4	4	9		
13.83	not identified (m/z=84,99,11,173)		4.4	2	4		
19.70	erucamide	91	11	4	11		
30.07	antioxydant (m/z=308,441,646) (irgafos 168)		17	6	17		
tot µg/day				18	48		

Figure 8.52 - Sample 17: calculation Internal surface

HEAD SPACE				SAMPLE 18: PET/AL/PE		PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4.48	ethyl acetate	84	210	0.22	0.64	46	134
from 13.78 to 16.44	Aliphatic saturated hydrocarbons	>80	84			18	54
tot µg/day				64	188		

Figure 8.53 - Sample 18: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.22	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
12.99	octadecane	96	12			3	8
13.83	not identified (m/z=84,99,111,173)		24			5	15
19.71	erucamide	91	70			15	45
38.77	antioxidant (m/z=316,647,663) (irgafos 168 mono-oxidated)		77			17	49
tot µg/day				40	117		

Figure 8.54 - Sample 18: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.22	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
19.71	Erucamide	91	45			10	29
tot µg/day				10.00	29.00		

Figure 8.55 - Sample 18: calculation Internal surface

HEAD SPACE				SAMPLE 19: OPPcoex	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
2.54	ethanol	80	1.8	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
5.79	2-propanol, 1-methoxy-	86	8.4	2	4
7.90	2-propanol, 1-ethoxy-	83	6.1	10	19
8.98	acetyl acetone	80	2	7	14
14.58	Siloxane		0.2	2	5
16.00	benzyl alcohol	93	0.3	0	0
17.08	Siloxane		0.2	0	1
tot µg/day				22	43

Figure 8.56 - Sample 19: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	1.16	2.25
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	16	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.96	not identified (m/z=118,239,270)		78	19	36
17	not identified (m/z=118,239,270)		60	90	175
17.3	acetyl tributyl citrate	80	770	70	135
17.93	not identified (m/z=118,267,298)		72	893	1730
17.97	not identified (m/z=118,267,298)		56	84	162
19.01	di-(2-ethylhexyl)phthalate	80	22	65	126
31.87	antioxidant (m/z=147,441,646) (Irgafos 168)		26	26	49
41.07	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		53	30	58
tot µg/day				1337	2591

Figure 8.57 - Sample 19: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	1.16	2.25
16.96	not identified (m/z=118,239,270)		62	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
17.00	not identified (m/z=118,239,270)		45	72	140
17.29	acetyl tributyl citrate	78	44	52	101
17.93	not identified (m/z=118,267,298)		65	51	99
17.97	not identified (m/z=118,267,298)		39	75	146
tot µg/day				296	574

Figure 8.58 - Sample 19: calculation internal surface

HEAD SPACE				SAMPLE 20: PET/PE		OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)		
				0.28	0.73		
						AVG exposure (µg/person/day)	Max exposure (µg/person/day)
14.57	siloxane		0.5			0.14	0.37
tot µg/day						0.14	0.37

Figure 8.59 - Sample 20: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PE			
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)		
				0.28	0.73		
						AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.07	not identified (m/z=84,99,111,173)		24			7	18
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	11			3	8
17.3	acetyl tributyl citrate	80	472			130	346
18.01	oleamide	95	26			7	19
20.21	phenol,2,4-bis(1-methyl-1-phenylethyl)-	93	6.8			2	5
20.95	erucamide	90	21			6	15
31.88	antioxidant (m/z=147,441,646) (irgafos 168)		27			7	20
38.09	benzenepropanoic acid, 3,5-bis (1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	35			10	26
tot µg/day						172	457

Figure 8.60 - Sample 20: calculation Total solvent

INTERNAL SURFACE				OTHER PLASTIC/PE			
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)		
				0.28	0.73		
						AVG exposure (µg/person/day)	Max exposure (µg/person/day)
13.24	siloxane		6.5			2	5
15.07	not identified (m/z=84,99,111,173)		4.2			1	3
17.30	acetyl tributyl citrate	80	42			12	31
tot µg/day						15	39

Figure 8.61 - Sample 20: calculation Internal surface

HEAD SPACE				SAMPLE 21: OPPpvc/acr	
TR	Substance	Matching ratio	µg/dm ²	OPP	
				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2.92	iso-propanol	74	1.4	2	3
4.51	ethylacetate	83	3.7	4	8
19.62	Triacetin	83	1.6	2	4
tot µg/day				8	15

Figure 8.62 - Sample 21: calculation Head space

TOTAL SOLVENT				OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.37	triacetin	83	15	17	34
15.51	Decanedioic acid, di butylester	91	75	87	169
16.15	acetyl tributyl citrate	80	781	908	1757
16.45	di-2-ethylhexyl adipate	90	794	921	1787
16.72	aliphatic hydrocarbon		9	10	20
16.85	oleamide	80	69	80	155
17.24	aliphatic hydrocarbon		10	12	23
17.69	2-ethylhexyl diphenyl phosphate	91	16	19	36
17.83	aliphatic hydrocarbon		8	9	18
18.13	not identified (m/z= 91,117,207)		10	12	23
30.08	antioxidant (m/z=147,441,646) (irgafos 168)		163	177	344
35.97	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	27	31	61
38.75	antioxidant (m/z= 316,64,662) (irgafos 168)		35	41	79
tot µg/day				2322	4505

Figure 8.63 - Sample 21: calculation Total solvent

INTERNAL SURFACE				OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.13	acetyl tributyl citrate	80	22	26	50
16.43	di-2-ethylhexyl adipate	90	74	86	167
tot µg/day				111	216

Figure 8.64 - Sample 21: calculation Internal surface

HEAD SPACE		SAMPLE 22:Paper/OPPcoex		PAPER/PLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.409	5.408
2.61	ethanol	80	1.6	2	9
4.51	ethylacetate	83	5.3	7	29
14.65	siloxane			0	0
17.15	siloxane			0	0
19.12	siloxane			0	0
19.61	triacetin	83	1.8	3	10
tot µg/day				12	47

Figure 8.65 - Sample 22: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	1.409	5.408	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.37	triacetin	83	6.1			9	33
13.83	not identified (m/z=84,99,11,173)		14			20	76
15.51	decanedioic acid, di butylester	91	122			172	660
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	24			34	130
16.16	acetyl tributyl citrate	80	1637			2307	8853
16.43	di-2-ethylhexyl adipate	90	12			17	65
17.71	2-ethylhexyl diphenil phosphate	91	34			48	184
from 18.13 to 19.67	1,2-cyclohexane dicarboxylic acid diisononylester (DINCH)	80	605			852	3272
30.07	antioxidant (m/z=147,441,646)(irgafos 168)		88			124	476
35.95	benzenepropanoic acid, 3,5-bis (1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	11			15	59
38.75	antioxidant (m/z= 316,647,662)(irgafos 168 mono-oxidated)		44			62	238
tot µg/day				3659	14045		

Figure 8.66 - Sample 22: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	1.409	5.408	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.50	decanedioic acid, di butylester	91	30			42	162
16.14	acetyl tributyl citrate	80	43			61	233
16.43	di-2-ethylhexyl adipate	90	3.2			5	17
from 18.54 to 19.42	1,2-cyclohexane dicarboxylic acid diisononylester (DINCH)	80	45			63	243
30.07	antioxydant (m/z= 147,441,646) (irgafos 168)		35			49	189
35.98	benzenepropanoic acid, 3,5-bis (1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	6.6			9	36
38.75	antioxydant (m/z= 316,647,662)(irgafos 168 mono-oxidated)		19			27	103
tot µg/day				256	983		

Figure 8.67 - Sample 22: calculation Internal surface

HEAD SPACE				SAMPLE 23:PETmet/OPPcoex		PLASTIC/OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.024	0.092		
4.5	ethylacetate	83	9.1			0.2	0.8
14.55	aliphatic hydrocarbon		1.2			0.0	0.1
15.72	aliphatic hydrocarbon		0.9			0.0	0.1
tot µg/day				0.3	1.0		

Figure 8.68 - Sample 23: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.024	0.092	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
11.37	triacetin	80	15			0	1
15.51	decanedioic acid, di butylester	91	141			3	13
15.59	1-propene-1,2,3-tricarboxylic acid trybutyl	83	6.8			0	1
16.14	acetyl tributyl citrate	80	532			13	49
16.44	di-2-ethylhexyl adipate	90	746			18	69
16.84	oleamide	94	28			1	3
from 18.13 to 19.70	1,2-cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	250			6	23
24.5	bisphenol A diglycidyl ether	97	95			2	9
30.08	antioxidant (m/z=147,441,646) (irgafos 168)		237			6	22
35.96	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	44			1	4
38.75	antioxidant (m/z=316,647,662) (irgafos 168 mono-oxidated)		28			1	3
tot µg/day				51	195		

Figure 8.69 - Sample 23: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.024	0.092	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.50	decanedioic acid, di butylester	91	42			1	4
16.13	acetyl tributyl citrate	80	26			1	2
16.44	di-2-ethylhexyl adipate	90	245			6	23
from 18.54 to 19.41	1,2-cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	37			1	3
30.07	Antioxidant (m/z= 147,441,646) (irgafos 168)		40			1	4
35.97	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	8.5			0.2	1
tot µg/day				10	37		

Figure 8.70 - Sample 23: calculation Internal surface

HEAD SPACE				SAMPLE 24:OPPcoex		OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.16	2.25		
2.87	iso-propanol	80	2.2			3	5
5.71	cyclohexane	83	20			23	45
7.97	ethoxypropanol	80	1.5			2	3
tot µg/day				27	53		

Figure 8.71 - Sample 24: calculation Head space

TOTAL SOLVENT				OPP		OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.16	2.25		
17.31	acetyl tributyl citrate	80	332			385	747
tot µg/day				385	747		

Figure 8.72 - Sample 24: calculation Total solvent

INTERNAL SURFACE				OPP		OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.16	2.25		
16.08	acetyl tributyl citrate	80	237			275	533
tot µg/day				275	533		

Figure 8.73 - Sample 24: calculation Internal surface

HEAD SPACE				SAMPLE 25: ALU/Paper	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.409	1.877
19.56	triacetin	83	1.8	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.7	3.4
tot µg/day				0.7	3.4

Figure 8.74 - Sample 25: calculation Head space

TOTAL SOLVENT				ALU/PAPER	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.409	1.877
11.31	triacetin	83	25	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				10	47
15.53	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	33		62
16.09	acetyl tributyl citrate	80	2.088	1	4
17.07	not identified (m/z=94,175)		45	18	84
17.63	2-ethylhexyl diphenyl phosphate	91	533	218	1000
tot µg/day				261	1198

Figure 8.75 - Sample 25: calculation Total solvent

INTERNAL SURFACE				ALU/PAPER	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.409	1.877
16.08	acetyl tributyl citrate	80	119	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				49	223
17.64	2-ethylhexyl diphenyl phosphate	91	31	13	58
tot µg/day				61	282

Figure 8.76 - Sample 25: calculation Internal surface

HEAD SPACE				SAMPLE 26: Paper/ALU	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
2.56	ethanol			1.083	5.408
15.77	2-ethyl 1-hexanol	89	1.8		
19.56	triacetine	92	5.1		
tot µg/day				7	37

PAPER/AL	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
1.083	5.408
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
0	0
2	10
6	28
7	37

Figure 8.77 - Sample 26: calculation Head space

TOTAL SOLVENT				PAPER/AL	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
11.31	triacetin	83	25	1.083	5.408
from 14.86 to 34.22	aliphatic saturated hydrocarbons	>80	1.510		
15.52	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	21		
16.08	acetyl tributyl citrate	80	693		
17.62	2-ethylhexyl diphenyl phosphate	91	275		
tot µg/day				1100	5492

PAPER/AL	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
1.083	5.408
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
27	135
2	8
23	114
751	3748
298	1487
1100	5492

Figure 8.78 - Sample 26: calculation Total solvent

INTERNAL SURFACE				PAPER/AL	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
16.08	acetyl tributyl citrate	80	36	1.083	5.408
17.64	2-ethylhexyl diphenyl phosphate	91	20		
tot µg/day				61	303

PAPER/AL	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
1.083	5.408
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
39	195
22	108
61	303

Figure 8.79 - Sample 26: calculation Internal surface

HEAD SPACE				SAMPLE 27: Paper/OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.409	5.408
2.58	ethanol	80	0.4	1	2
2.87	iso-propanol	80	0.4	1	2
4.42	ethylacetate	86	8.9	13	48
5.47	iso-propyl acetate	83	0.4	1	2
from 14.58 to 16.80	aliphatic hydrocarbon		1	1	5
20.53	longicyclene	99	0.4	1	2
20.89	junipene	99	1	1	5
22.01	aliphatic hydrocarbon		0.3	0	2
22.07	diethyl phthalate	96	1.2	2	6
tot µg/day				20	76

Figure 8.80 - Sample 27: calculation Head space

TOTAL SOLVENT				SAMPLE 27: Paper/OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.409	5.408
14.54	tetradecanoic acid	99	76	107	411
14.60	n-propyl p-hydroxybenzoate	94	38	54	206
15.06	aliphatic unsaturated hydrocarbon		239	337	1293
15.14	n-butyl p-hydroxybenzoate	96	30	42	162
15.53	n-hexadecanoic acid	94	339	478	1833
16.01	aliphatic unsaturated hydrocarbon		271	382	1466
16.43	oleic acid	96	33	46	178
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	91	17	24	92
17.3	acetyl tributyl citrate	80	680	958	3677
17.87	2-propenoic acid, 3(4-methoxyphenyl)-,2 ethylexyl ester	98	36	51	195
from 19.76 to 20.93	1,2-cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	656	924	3548
tot µg/day				3403	13060

Figure 8.81 - Sample 27: calculation Total solvent

INTERNAL SURFACE				SAMPLE 27: Paper/OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.409	5.408
from 13.14 to 14.21	aliphatic hydrocarbon		11	15	59
tot µg/day				15	59

Figure 8.82 - Sample 27 calculation Internal surface

HEAD SPACE				PLASTIC/ALU/PE	
SAMPLE 28:PET/AL/PE				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	0.22	0.64
4.41	ethylacetate	90	116	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
14.46	aliphatic hydrocarbon		2.5	26	74
15.65	aliphatic hydrocarbon		1.9	0.6	1.6
15.94	aliphatic hydrocarbon		1.7	0.4	1.2
				0.4	1.1
tot µg/day				27	78

Figure 8.83 - Sample 28: calculation Head space

TOTAL SOLVENT				PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
15.56	not identified (m/z= 55,82,111,129)		36	0.22	0.64
20.96	erucamide	80	48	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
31.94	antioxidant (m/z= 147,441,646) (Irgafos 168)		488	8	23
38.16	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	190	11	31
41.09	antioxidant (m/z= 316,647,662) (Irgafos 168 mono-oxidated)		74	107	312
				42	122
tot µg/day				16	47
				184	535

Figure 8.84 - Sample 28: calculation Total solvent

INTERNAL SURFACE				PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
15.56	not identified (m/z= 55,82,111,129)		8.2	0.22	0.64
20.96	erucamide	87	32	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
31.90	antioxidant (m/z= 147,441,646) (Irgafos 168)		73	2	5
38.11	benzenepropanoic acid, 3,5-bis (1,1- dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	90	39	7	20
				16	47
tot µg/day				9	25
				33	97

Figure 8.85 - Sample 28: calculation Internal surface

HEAD SPACE				SAMPLE 29:PETchim/ALU/PE		PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.22	0.64		
4.42	ethyl acetate	83	13.2			3	8
tot µg/day						3	8

Figure 8.86 - Sample 29: calculation Head space

TOTAL SOLVENT				S AVG (dm2/person/day)		S Max (dm2/person/day)	
TR	Substance	Matching ratio	µg/dm2	0.22	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
14.3	not identified (m/z=111,129)		28			6	18
20.96	erucamide	96	28			6	18
23.34	not identified (m/z=129,215)		93			20	60
38.12	irganox 1076		161			35	103
tot µg/day						68	198

Figure 8.87 - Sample 29: calculation Head space

INTERNAL SURFACE				S AVG (dm2/person/day)		S Max (dm2/person/day)	
TR	Substance	Matching ratio	µg/dm2	0.22	0.64	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
14.3	not identified (m/z=111,129)		7			2	4
20.96	erucamide	96	27			6	17
38.09	irganox 1076		35			8	22
tot µg/day						15	44

Figure 8.88 - Sample 29: calculation Internal surface

HEAD SPACE		SAMPLE 30:OPPcoex/ALU/PE		PLASTIC/ALU/PE	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				0.22	0.64
from 13.7 to 16.6	aliphatic hydrocarbon		138	AVG exposure (µg/person/day) 30	Max exposure (µg/person/day) 88
tot µg/day				30	88

Figure 8.89 - Sample 30: calculation Head space

TOTAL SOLVENT					
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				0.22	0.64
13.23	not identified (m/z=91,121,147)		44	AVG exposure (µg/person/day) 10	Max exposure (µg/person/day) 28
14.21	aliphatic hydrocarbon		16	4	10
14.30	not identified (m/z=101,111,129)		64	14	41
15.89	not identified (m/z=126,155,173)		17	4	11
16.74	1-propene-1,2,3-tricarboxylic acid tributyl ester	83	16	4	10
17.29	acetyl tributyl citrate	80	435	96	278
20.96	erucamide	93	42	9	27
23.35	not identified (m/z=111,129,215,428)		210	46	134
31.88	antioxidant (m/z=147,441,646) (irgafos 168)		145	32	93
38.1	irganox 1076	83	112	25	72
41.07	antioxidant (m/z=316,647,662) (irgafos 168 mono-oxidated)		124	27	79
tot µg/day				270	784

Figure 8.90 - Sample 30: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				0.22	0.64
from 8.1 to 8.5	aliphatic hydrocarbon		57	AVG exposure (µg/person/day) 13	Max exposure (µg/person/day) 36
13.23	not identified (m/z=91,121,147)		8	2	5
14.30	not identified (m/z=111,129,184)		10	2	6
15.89	not identified (m/z=126,155,173)		4	1	3
17.29	acetyl tributyl citrate	80	11	2	7
20.96	erucamide	93	24	5	15
tot µg/day				25	73

Figure 8.91 - Sample 30: calculation Internal surface

HEAD SPACE				SAMPLE 31:CASTPP/PP-EVOH-PP		OTHER PLASTIC/PP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.136	0.341		
3.67	2-methyl pentane	80	33			4	11
3.99	1-pentene,2-methyl	86	25			3	9
8.49	heptane,4-methyl	91	17			2	6
10.08	aliphatic hydrocarbon		6.2			1	2
10.29	heptane,2,4-dimethyl	91	34			5	12
10.98	1-heptene,2,4-dimethyl	90	51			7	17
11.52	1-heptene,2,3-dimethyl	90	6.6			1	2
11.73	octane,4-methyl	91	29			4	10
from 15.14 to 19.69	aliphatic hydrocarbon	>80	106			14	36
tot µg/day				42	105		

Figure 8.92 - Sample 31: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.136	0.341	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
from 11.36 to 16.77	aliphatic hydrocarbons	>80	410			56	140
17.30	acetyl tributyl citrate	80	542			74	185
20.99	erucamide	95	335			46	114
32.00	antioxidant (m/z=147,441,646)(Irgafos 168)		1.26			0	0
41.17	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		539			73	184
tot µg/day				249	623		

Figure 8.93 - Sample 31: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.136	0.341	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
17.28	acetyl tributyl citrate	87	9.5			1	3
20.95	erucamide	97	20			3	7
tot µg/day				4	10		

Figure 8.94 - Sample 31: calculation Internal surface

HEAD SPACE				SAMPLE 32: PA/PP/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
2.56	ethanol	80	65	18	47
2.88	iso-propanol	80	79	22	58
4.50	ethylacetate	83	7.4	2	5
5.91	2-propanol,1-methoxy	82	158	44	115
7.71	1-butanol,2-methyl	78	5.9	2	4
8.03	2-propanol,1-ethoxy	83	123	34	90
8.56	1-pentanol	70	16	4	12
11.09	2,4-dimethyl-1-heptene	90	8.4	2	6
tot µg/day				130	338

Figure 8.95 - Sample 32: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.28	0.73
10.05	aliphatic hydrocarbon		6.4	2	5
12.22	butylated hydroxy toluene (BHT)	98	7.2	2	5
15.81	hexadecanamide	93	40	11	29
16.14	acetyl tributyl citrate	80	397	111	290
16.85	oleamide	94	231	65	169
19.71	erucamide	91	128	36	93
30.08	antioxidant (m/z=147,441,646) (Irgafos 168)		281	79	205
35.96	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	19	5	14
38.75	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		55	15	40
tot µg/day				326	850

Figure 8.96 - Sample 32: calculation Total solvent

INTERNAL SURFACE			
TR	Substance	Matching ratio	µg/dm ²
10.05	aliphatic hydrocarbon		5.2
12.22	butylated hydroxy toluene (BHT)	98	3.6
16.13	acetyl tributyl citrate	80	12
16.84	oleamide	94	9.6
19.71	erucamide	91	47
30.07	antioxidant (m/z= 147,441,646) (Irgafos 168)		40
35.95	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	5.1
38.74	antioxidant (m/z= 316,647,662) (irgafos 168 mono-oxidated)		5
tot µg/day			

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.28	0.73

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
1	4
1	3
3	9
3	7
13	34
11	29
1	4
1	4
36	93

Figure 8.97 - Sample 32: calculation Internal surface

HEAD SPACE				SAMPLE 33: PE/PA-EVOH-PE	
TR	Substance	Matching ratio	µg/dm ²		
2.55	ethanol	80	5.7		
7.95	ethoxypropanol	83	88		
8.49	not identified (m/z=73.1, 45)		6.8		
13.04	cyclohexanone	83	6.2		
18.90	benzene,1,3-bis(1,1-dimethylethyl)	90	2.2		
				tot µg/day	11

PLASTIC/PA/PE	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.104	0.444

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
1	3
9	39
1	3
1	3
0	1

Figure 8.98 - Sample 33: calculation Head space

TOTAL SOLVENT					
TR	Substance	Matching ratio	µg/dm ²		
10.16	benzene,1,3-bis(1,1-dimethylethyl)-	94	8.2		
11.22	2,4-diisoyanato, toluene	98	6		
12.18	2,4-ditert-butylphenol	97	5.7		
13.72	nonyphenol(isomers)	92	8.2		
16.07	acetyl tributyl citrate	80	203		
16.31	octadecadienoic acid,methyl ester	99	45		
16.76	oleamide	90	58		
19.57	erucamide	87	80		
				tot µg/day	43

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.104	0.444

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
1	4
1	3
1	3
1	4
21	90
5	20
6	26
8	36

Figure 8.99 - Sample 33: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm ²		
10.16	benzene,1,3-bis(1,1-dimethylethyl)	94	2.8		
16.08	acetyl tributyl citrate	80	7.1		
16.32	octadecadienoic acid, methyl ester	99	4.8		
				tot µg/day	2

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.104	0.444

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
0.3	1
0.7	3
0.5	2

Figure 8.100 - Sample 33: calculation Internal surface

HEAD SPACE				OTHER PLASTIC/OTHERPLASTIC	
SAMPLE 34: PE/EVA/PE-EVOH-PE/IONOMERO				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	0.02	0.075
2.53	Ethanol	80	3.9	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
7.94	1-ethoxy,2 propanol	78	3.4	0.1	0.3
14.58	siloxane			0.1	0.3
17.08	siloxane			0.0	0.0
19.07	caprolactam	94	3.2	0.0	0.0
tot µg/day				0.1	0.2
				0.2	0.8

Figure 8.101 - Sample 34: calculation Head space

TOTAL SOLVENT				OTHER PLASTIC/OTHERPLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.02	0.075
16.01	7,9-diterbutyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	99	21	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.75	1-propene-1,2,3-tricarboxylic acid trybutyl ester	93	20	0	2
17.30	acetyl tributyl citrate	80	1229	0	2
20.97	erucamide	95	168	25	92
31.96	antioxidant(m/z= 147,441,646) (Irgafos 168)		925	3	13
38.11	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	105	19	69
41.09	antioxidant(m/z= 316,647,662) (Irgafos 168 mono-oxidated)		248	2	8
tot µg/day				5	19
				54	204

Figure 8.102 - Sample 34: calculation Total solvent

INTERNAL SURFACE				OTHER PLASTIC/OTHERPLASTIC	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.02	0.075
17.29	acetyl tributyl citrate	80	96	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
20.96	erucamide	95	41	1.9	7.2
31.89	antioxidant (m/z=147,441,646) (Irgafos 168)		80	0.8	3.1
38.08	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	12	1.6	6.0
41.03	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		20	0.2	0.9
tot µg/day				0.4	1.5
				5	19

Figure 8.103 - Sample 34: calculation Internal surface

HEAD SPACE				SAMPLE 35: OPPmet/OPPcoex	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.387	0.561
2.25	1-propene,2-methyl	70	2.3	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2.56	ethanol	80	6.2	1	1
4.43	ethyl acetate	83	4.2	2	3
5.58	cyclohexane	80	36	2	2
5.78	2-propanol,1-methoxy	70	18	14	20
19.54	triacetin	83	3.8	7	10
tot µg/day				27	40

Figure 8.104 - Sample 35: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	0.387	0.561
12.65	triacetin	80	11	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.06	not identified (m/z=84,99,111,173)		24	4	6
16.00	aliphatic insaturated hydrocarbon	97	20	9	13
16.32	not identified (m/z=100,127,185)		15	8	11
16.51	aliphatic hydrocarbon		17	6	8
16.74	1-propene 1,2,3-tricarboxylic acid tributyl ester	83	50	7	10
16.94	aliphatic hydrocarbon		39	19	28
17.31	acetyl tributyl citrate	80	1.458	15	22
17.38	aliphatic hydrocarbon		43	1	1
17.87	aliphatic hydrocarbon		27	17	24
from 19.3 to 21.3	DINCH	80	1248	10	15
31.89	antioxidant (m/z=147,441,646) (Irgafos168)		93	483	700
38.11	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	45	36	52
41.09	antioxidant (m/z=316,647,662) (Irgafos168 mono-oxidated)		85	17	25
tot µg/day				665	964

Figure 8.105 - Sample 35: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)	S Max (dm ² /person/day)
TR	Substance	Matching ratio	µg/dm ²	0.387	0.561
16.08	aliphatic hydrocarbon		4	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.51	aliphatic hydrocarbon		8	2	2
16.94	aliphatic hydrocarbon		12	3	4
17.29	acetyl tributyl citrate	80	42	5	7
17.38	aliphatic hydrocarbon		13	16	24
17.80	aliphatic hydrocarbon		12	5	7
from 19.3 to 21.3	DINCH	80	129	5	7
31.89	antioxidant (m/z=147,441,646)(Irgafos 168)		45	50	72
tot µg/day				103	149

Figure 8.106 - Sample 35: calculation Internal surface

HEAD SPACE				SAMPLE 36: OPPmet-bianco	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
2.53	ethanol	80	5.8	1.16	2.25
4.46	Ethyl acetate	83	1.3		
5.68	cyclohexane	91	44		
15.24	ethanol-2-(2-ethoxyethoxy)	91	1.5		
15.75	2-ethyl,1-hexanol	86	0.3		
17.09	2-propenoic acid,2-ethylhexyl ester	90	0.2		
19.54	triacetin	83	3.8		
tot µg/day				66	128

OPP	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
1.16	2.25
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
7	13
2	3
51	99
2	3
0.3	1
0	0
4	9

Figure 8.107 - Sample 36: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	1.16	2.25	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
12.65	triacetin	83	11			13	25
16.08	aliphatic hydrocarbon		13			15	29
16.51	aliphatic hydrocarbon		18			21	41
16.67	dedecanoic acid, dibutyl ester	93	16			19	36
16.75	1-propene-1,2,3-tricarboxyl acid tributyl ester	83	20			23	45
16.94	aliphatic hydrocarbon		32			37	72
17.30	acetyl tributyl citrate	80	797			925	1793
17.39	aliphatic hydrocarbon		36			42	81
17.87	aliphatic hydrocarbon		28			32	63
18.4	aliphatic hydrocarbon		25			29	56
18.99	aliphatic hydrocarbon		21			24	47
from 19.37 to 20.93	1,2-cyclohexane dicarboxylic acid diisononyl ester(DINCH)	80	830			963	1868
31.9	antioxidant (m/z=147,441,646) (Irgafos168 mono-oxidated)		101			117	227
38.13	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	60			70	135
41.1	antioxidant (m/z=316,647,662) (Irgafos168 mono-oxidated)		48			56	108
tot µg/day				2384.96	4626.00		

Figure 8.108 - Sample 36: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	1.16	2.25	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.08	aliphatic hydrocarbon		9			10	20
16.51	aliphatic hydrocarbon		15			17	34
16.94	aliphatic hydrocarbon		22			26	50
17.29	acetyl tributyl citrate	80	26			30	59
17.39	aliphatic hydrocarbon		20			23	45
17.87	aliphatic hydrocarbon		16			19	36
18.40	aliphatic hydrocarbon		9			10	20
from 19.37 to 20.93	1,2-cyclohexane dicarboxyl acid diisononyl ester (DINCH)		45			52	101
tot µg/day				188	365		

Figure 8.109 - Sample 36: calculation Internal surface

HEAD SPACE				SAMPLE 37 :PAPER/AL		PAPER/ALU	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.083	5.408	3	16
2.84	iso-propanol	80	3			0	0
14.58	siloxane					1	5
14.72	benzaldehyde	97	1			1	5
15.75	1-hexanol, 2-ethyl	90	0.9			0	0
17.09	siloxane					0	0
19.05	siloxane					0	0
tot µg/day				5	26		

Figure 8.110 - Sample 37: calculation Head space

TOTAL SOLVENT				PAPER/ALU		PAPER/ALU	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				1.083	5.408	32	162
15.99	not identified (m/z=243)		30			381	1904
16.32	not identified (m/z=100,127,185)		352			19	97
16.75	1-propene-1,2,3-tricarboxylic acid tributyl ester	72	18			759	3791
17.16	not identified (m/z=127,155,185,213)		701			1023	5111
17.31	acetyl tributyl citrate	80	945			145	725
18.09	not identified (m/z=155,213)		134			270	1347
18.92	phosphoric acid,2-ethylhexyl diphenyl ester	93	249			102	508
from 19.3 to 21.3	1,2-cyclohexane dicarboxylic acid diisononyl ester (DINCH)	80	94				
tot µg/day				2732	13644		

Figure 8.111 - Sample 37: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.083	5.408
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.99	not identified (m/z= 243)		11	12	59
16.32	not identified (m/z=100,127,185)		51	55	276
17.16	not identified (m/z=127,155,185,213)		94	102	508
17.31	acetyl tributyl citrate	80	35	38	189
18.09	not identified (m/z=155,213)		18	19	97
18.92	phosporic acid, 2-ethylhexyl diphenyl ester	93	60	65	324
tot µg/day				291	1455

Figure 8.112 - Sample 37: calculation Internal surface

HEAD SPACE				SAMPLE 38: OPA/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.379	0.988
14.65	siloxane		1.1	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.23	heptane,2,2,4,6,6-pentamethyl	83	1.2	0.4	1
17.15	siloxane			0.5	1
				0.0	0.0
tot µg/day				1	2

Figure 8.113 - Sample 38: calculation Head space

TOTAL SOLVENT				OPA/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.379	0.988
13.83	not identified (m/z=99,111,173)		10	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
16.13	acetyl tributyl citrate	80	18	4	10
19.71	erucamide	90	122	7	18
30.06	antioxidant (m/z=147,441,646) (Irgafos 168)		55	46	121
35.97	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	28	21	54
38.74	antioxidant (m/z=316,647,662) (Irgafos 168 mono-oxidated)		15	11	28
				6	15
tot µg/day				94	245

Figure 8.114 - Sample 38: calculation Total solvent

INTERNAL SURFACE				OPA/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.379	0.988
16.13	acetyl tributyl citrate	80	3.6	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
19.71	erucamide	90	42	1	4
30.06	antioxidant(m/z=147,441,646) (Irgafos 168)		10	16	41
35.96	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	5.6	4	10
				2	6
tot µg/day				23	60

Figure 8.115 - Sample 38: calculation Internal surface

HEAD SPACE		SAMPLE 39: OPPmet		OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
14.65	siloxane			0	0
17.15	siloxane			0	0
19.61	triacetin	83	3.7	4	8
tot µg/day				4	8

Figure 8.116 - Sample 39: calculation Head space

TOTAL SOLVENT				OPP	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				1.16	2.25
11.37	triacetin	90	15	17	34
15.50	decanedioic acid, dibutyl ester	94	15	17	34
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	93	6.2	7	14
16.15	acetyl tributyl citrate	86	994	1153	2237
16.44	di-2-ethylhexyl adipate	90	431	500	970
16.84	oleamide	87	35	41	79
17.15	not identified (m/z=175)		32	37	72
17.72	2-ethylhexyl diphenyl phosphate	91	473	549	1064
30.06	antioxidant (m/z=147,441,646)(Irgafos 168)		54	63	122
38.73	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		43	50	97
tot µg/day				2434	4721

Figure 8.117 - Sample 39: calculation total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	1.16	S Max (dm ² /person/day)
					2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
15.50	decanedioic acid, dibutyl ester	94	10	12	23
16.14	acetyl tributyl citrate	86	135	157	304
16.44	di-2-ethylhexyl adipate	90	321	372	722
16.85	oleamide	87	3.7	4	8
17.15	not identified(m/z=175)		7.7	9	17
17.71	2-ethylhexyl diphenyl phosphate	91	72	84	162
30.07	antioxidant (m/z=147,441,646)(Irgafos 168)		32	37	72
38.76	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		22	26	50
tot µg/day				700	1358

Figure 8.118 - Sample 39: calculation Total solvent

HEAD SPACE				SAMPLE 40: OPPpvc-Its	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
	NOT SUBSTANCES EXTRACTED			AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				0.00	0.00
				tot µg/day	
				0.00	0.00

Figure 8.119 - Sample 40: calculation Head space

TOTAL SOLVENT				OPP	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				31	61
15.50	decanedioic acid, dibutyl ester	94	27	14	27
15.59	1-propene-1,2,3-tricarboxylic acid tributyl ester	98	12	1536	2979
16.15	acetyl tributyl citrate	86	1324	26	50
17.15	not identified (m/z=175)		22	430	835
17.72	2-ethylhexyl diphenyl phosphate	91	371	202	392
30.08	antioxidant (m/z=147,441,646)(Irgafos 168)		174	39	77
38.75	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		34		
				tot µg/day	
				2278	4419

Figure 8.120 - Sample 40: calculation Total solvent

INTERNAL SURFACE				OPP	
TR	Substance	Matching ratio	µg/dm2	S AVG (dm2/person/day)	S Max (dm2/person/day)
				1.16	2.25
				AVG exposure (µg/person/day)	Max exposure (µg/person/day)
				4	8
14.52	diisobutyl phthalate	72	3.5	6	11
14.92	aliphatic hydrocarbon		5.1	19	36
15.50	decanedioic acid, dibutyl ester	94	16	101	196
16.14	acetyl tributyl citrate	86	87	4	8
16.43	not identified(m/z=175)		3.6	30	59
17.71	2-ethylhexyl diphenyl phosphate	91	26	60	117
30.07	antioxidant (m/z=147,441,646)(Irgafos 168)		52	12	23
38.74	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		10		
				tot µg/day	
				236	457

Figure 8.121 - Sample 40: calculation Internal surface

HEAD SPACE		SAMPLE 41: PETpvc/PE		OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.276	0.734
4.51	ethylacetate	90	7.5	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
from 13.79 to 16.44	aliphatic hydrocarbons		101	2	6
				28	74
			tot µg/day	30	80

Figure 8.122 - Sample 41: calculation Head space

TOTAL SOLVENT		SAMPLE 41: PETpvc/PE		OTHER PLASTIC/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.276	0.734
7.51	aliphatic hydrocarbon		14	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
7.73	aliphatic hydrocarbon		14	4	10
7.94	aliphatic hydrocarbon		19	4	10
11.92	aliphatic hydrocarbon		9	5	14
12.99	aliphatic hydrocarbon		4.2	2	7
13.03	aliphatic hydrocarbon		6.9	1	3
				2	5
13.83	not identified (m/z= 84,99,111,173)		11	3	8
14.05	aliphatic hydrocarbon		6.7	2	5
14.97	aliphatic hydrocarbon		5.5	2	4
15.84	aliphatic hydrocarbon		8	2	6
16.14	acetyl tributyl citrate	88	190	52	139
19.70	erucamide	93	58	16	43
30.06	antioxidant (m/z=147,441,646)(Irgafos 168)		62	17	46
35.98	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	46	13	34
38.74	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		57	16	42
			tot µg/day	141	375

Figure 8.123 - Sample 41: calculation Total solvent

INTERNAL SURFACE			
TR	Substance	Matching ratio	µg/dm2
7.51	aliphatic hydrocarbon		13
7.61	aliphatic hydrocarbon		4.2
7.73	aliphatic hydrocarbon		13
7.94	aliphatic hydrocarbon		15
11.23	aliphatic hydrocarbon		3.8
11.92	aliphatic hydrocarbon		6.2
12.49	aliphatic hydrocarbon		4.5
13.03	aliphatic hydrocarbon		3.4
16.13	acetyl tributyl citrate	86	33
17.08	aliphatic hydrocarbon		4.3
19.71	erucamide	93	45
30.06	antioxidant (m/z=147,441,646)(Irgafos 168)		14
35.96	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	13
38.74	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		7.5

S AVG (dm2/person/day)	S Max (dm2/person/day)
0.278	0.734

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
4	10
1	3
4	10
4	11
1	3
2	5
1	3
1	2
9	24
1	3
12	33
4	10
4	10
2	6

tot µg/day	50	132
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Figure 8.124 - Sample 41: calculation Internal surface

HEAD SPACE				SAMPLE 42: PET/PE	
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.276	0.734
5.42	ethyl acetate	83	10		
9.36	aliphatic hydrocarbon		3.1		
9.67	aliphatic hydrocarbon		21		
9.82	aliphatic hydrocarbon		6.4		
10.01	aliphatic hydrocarbon		4.8		
10.21	aliphatic hydrocarbon		26		
10.32	aliphatic hydrocarbon		7.7		
10.41	aliphatic hydrocarbon		25		
10.51	aliphatic hydrocarbon		4.5		
10.58	aliphatic hydrocarbon		25		
10.61	aliphatic hydrocarbon		19		
10.75	aliphatic hydrocarbon		14		
10.81	aliphatic hydrocarbon		3.5		
10.88	aliphatic hydrocarbon		3.2		
10.9	aliphatic hydrocarbon		4.4		

OTHER PLASTIC/PE	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.276	0.734

AVG exposure (µg/person/day)	Max exposure (µg/person/day)
3	7
1	2
6	15
2	5
1	4
7	19
2	6
7	18
1	3
7	18
5	14
4	10
1	3
1	2
1	3

Figure 8.125 - Sample 42: calculation Head space

TOTAL SOLVENT				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.276	0.734	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
						7	18
12.99	aliphatic hydrocarbon		24			5	14
14.72	not identified (m/z=97,126,155,173)		19			1	3
15.84	aliphatic hydrocarbon		4.6			26	69
16.13	acetyl tributyl citrate	91	94			7	18
17.08-18.12	aliphatic hydrocarbons		25			26	69
19.71	erucamide	90	94				
35.99	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	90			25	66
tot µg/day						97	257

Figure 8.126 - Sample 42: calculation Total solvent

INTERNAL SURFACE				S AVG (dm ² /person/day)		S Max (dm ² /person/day)	
TR	Substance	Matching ratio	µg/dm ²	0.276	0.734	AVG exposure (µg/person/day)	Max exposure (µg/person/day)
						2	5
12.99	aliphatic hydrocarbon		6.4			3	7
14.72	not identified (m/z=97,126,155,173)		10			2	6
16.13	acetyl tributyl citrate	91	7.5			2	6
17.08	aliphatic hydrocarbon		8.3			14	37
19.71	erucamide	90	50				
36	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (irganox 1076)	83	20			6	15
tot µg/day						28	75

Figure 8.127 - Sample 42: calculation Internal surface

HEAD SPACE		SAMPLE 43: PET/PETmet/PE	
TR	Substance	Matching ratio	µg/dm ²
4.48	Ethyl acetate	83	89
6.95	n-propyl acetate	83	2.7
14.66	siloxane		
15.23	heptane,2,2,4,6,6-pentamethyl	83	0.6
16.03	not identified (m/z=57,97,113)		0.9
16.10	cyclohexane, butyl	95	0.8
			tot µg/day

OTHER PLASTIC/PE	
S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.276	0.734
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
25	65
1	2
0.0	0.0
0.2	0.4
0.2	1
0.2	1
tot µg/day	
26	69

Figure 8.128 - Sample 43: calculation Head space

TOTAL SOLVENT			
TR	Substance	Matching ratio	µg/dm ²
10.67	not identified (m/z=57,83,97,111)		5.9
13.03	not identified (m/z=57,83,97,111)		5.4
13.79	not identified (m/z=57,71,127,155)		5.2
13.83	not identified (m/z=173,99,111)		14
14.04	cyclooctacosane	93	6.1
14.97	1-docosene	99	4.8
15.84	aliphatic hydrocarbon		4.6
15.89	oxybenzone (UV absorber)	98	61
16.13	acetyl tributyl citrate	91	12
18.12	not identified (m/z=91,117,207)		11
19.70	erucamide	90	64
30.06	antioxidant (m/z=147,441,646)(Irgafos 168)		38
36.00	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	113
38.75	antioxidant (m/z=316,647,662)(Irgafos 168 mono-oxidated)		53
			tot µg/day

S AVG (dm ² /person/day)	S Max (dm ² /person/day)
0.276	0.734
AVG exposure (µg/person/day)	Max exposure (µg/person/day)
2	4
1	4
1	4
4	10
2	4
1	4
1	3
17	45
3	9
3	8
18	47
10	28
31	83
15	39
tot µg/day	
109.85	292.13

Figure 8.129 - Sample 43: calculation Total solvent

INTERNAL SURFACE					
TR	Substance	Matching ratio	µg/dm ²	S AVG (dm ² /person/day)	S Max (dm ² /person/day)
				0.276	0.734
10.67	not identified (m/z=57,83,97,111)		4.9	1	4
15.89	oxybenzone (UV absorber) (*)	98	40	11	29
19.7	erucamide	90	17	5	12
30.06	antioxidant (m/z=147,441,646)		7.9	2	6
35.98	benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	83	38	10	28
38.74	antioxidant (m/z=647, 316, 662)(Irgafos 168)		10	3	7
tot µg/day				32.52	86.49

Figure 8.130 - Sample 43: calculation Internal surface

8.4. Screening of substances assessed

As derived from the calculations shown in this report, a new Table was prepared (2- *Calculation_rows_columns_43_structures*), which includes all substances extracted in function of the model packaging materials from where they are originated. This Table allows us to identify the model packaging materials that gives the highest contribution to the exposure of a detected substance, as well as to identify whether combinations of concentrations may be operated for evaluating the exposure to a given substance or class of substances. As a typical example, long chain hydrocarbons can be associated to other substances identified as “mineral oils”, giving rise to a more comprehensive category that may result in similar potential toxicological effects.

The same table has been done for each kind of extraction done: *head space*, *total solvent* as well as *internal washing*.

See the samples reported below:

Type of extraction	Sample1	Sample2	Sample3	Sample4	Sample5	SampleX	Tot Row µg/day	MAX Row µg/day
SUBSTANCES (µg/day)	PET/AL/PE	PET/AL/PET/PE	PAPER/AL/PE	PAPER/AL/PE	PET/AL/OPA/PE	AA/BB/CC		
Benzene, 2,4-diisocyanato-1-methyl	11						xx	xx
benzene, 1,3-bis(1,1-dimethylethyl)-								
benzenepropanoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, octadecyl ester (Irganox 1076)	09	87			83		xx	xx
BHT								
bisphenol A diglycidyl ether								
cyclohexadecane								
cyclohexane, octyl								
cyclooctacosane								
Decanedioic acid, di butylester							xx	xx
di 2-ethylhexyl phthalate								
di-2-ethylhexyl adipate								
docosane								
dodecane			21				xx	xx
Erucamide	15	43			10		xx	xx
hexadecanamide								
n-butyl p-hydroxybenzoate								
2-propenoic acid, 2-ethylhexyl ester								
acetyl acetone				5				
aliphatic hydrocarbons							xx	xx
Etc...								
Tot column µg/day							ZZ	WW

Table 8.131 : excerpt of “rows x columns” table

At this stage a new table has been derived (*3-identification specimens table*) where all substances were grouped in different classes by using the following filters:

- all substances listed on the *Regulation (EU) 10/2011* (on which the risk assessment is not done as they are addressed by the regulation itself);
- all the non-listed substances -NIAS & NLS- (have to be assessed in order to understand the potential risk) -8.4.1 paragraph-;
- all the not identified substances (with the aim to link properly all mass spectra and chemicals not recognized by the reference library, a closer cooperation with the supplier of raw material was made to identify, quantify and assess all the unknown compounds) see -8.4.2. paragraph-;

- aliphatic hydrocarbons (the assessment of which can be made based on the *EFSA opinion* *_EFSA Journal 2010; 8(5):1334.*) see 8.4.3. paragraph.

At the end of this exercise we obtained two “ *identification specimens tables*”:

1. Total extract identification specimens table

2. Internal washing identification specimens table

Note: as semi-volatile and non-volatile extractions are more aggressive through the materials and we can assume that volatile substances evaporate before the product gets in contact with food, this study was simplified and results obtained from head-space extraction were not tested. Any subsequent treatment should take in consideration also the exposure of the volatile substances themselves.

INTERNAL WASHING IDENTIFICATION SPECIMENS TABLE					
SUBSTANCES	IUPAC NAME	CAS NUM	SMILES	Cramer class	InChi
1,2-cyclohexane dicarboxyl acid diisononyl ester (DINCH)		166412-78-8			LISTED
1-hexadecene		544-76-3	CCCCCCCCCCCCCCC	I	1S/C16H34/c1-3-5-7-9-11-13-15-16-14-12-10-8-6-4-2/h3-16H2,1-2H3
2-ethylhexyl diphenyl phosphate		1241-94-7			LISTED as phosphoric acid, diphenyl 2-ethylhexyl ester
di 2-ethylhexyl phthalate	phthalic acid, bis(2-ethylhexyl) ester	117-81-7			LISTED
di-2-ethylhexyl adipate		103-23-1			LISTED
7,9-diferbutyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione		82304-66-3	CC(C)(C)C1=CC2(CCC(=O)O2)C=C(C1=O)C(C)	III	
acetyl tributyl citrate		77-90-7			LISTED as tri-n-butyl acetyl citrate
aliphatic hydrocarbons					
antioxidant (m/z=316,647,662 (Irgafos 168 mono-oxidated) antioxidant (m/z= 316,647,662) (Irgafos 168 mono-oxidated) Antioxidant (m/z= 147,441,646) (Irgafos 168) antioxidant (m/z=308,441,646) (Irgafos 168)		31570-04-4			LISTED as phosphorous acid, tris(2,4-di-tert-butylphenyl)ester

Table 8.132 excerpt of “ Identification specimens table” internal washing

8.4.1. Risk assessment of Non-listed substances

Concerning Non-Listed substances (NIAS & NLS), we have proceeded to study in depth each structure extracted. A hazard analysis was carried out as a first step, the analysis begun by gathering the substances into families and attributing (i) Iupac name (ii) CAS number where possible, (iii) SMILES or INCHI encryption codes by using the following websites:

<http://cactus.nci.nih.gov/translate>

<http://pubchem.ncbi.nlm.nih.gov/edit2/index.html>

Encrypted structures were then used in a QSAR system called *Toxtree* 2.5.0 in order to identify their Cramer class, this corresponds to hazard analysis.

QSAR system : Quantitative Structure Activity Relationships (QSARs) are mathematical models that are used to predict measures of toxicity from the molecular structure of chemicals under examination (known as molecular descriptors); in particular Toxtree Toxic Hazard Estimation by decision tree approach is a full-featured and flexible user-friendly open source application, which is able to estimate toxic hazard by applying a decision tree approach.

ToxTree allows to classify NIAS based on the toxicity class to which they belong. More in particular, the Cramer classification has been used.

In the application of the Threshold of Toxicological Concern (TTC) concept to non-cancer endpoints, the decision tree proposed by Cramer, Ford and Hall in 1978, commonly referred to as the Cramer scheme, is probably the most widely used approach for classifying and ranking chemicals according to their expected level of oral systemic toxicity. The decision tree categorizes chemicals, mainly on the basis of chemical structure and reactivity, into three classes indicating a high (Class III), medium (Class II) or low (Class I) level of concern. Each Cramer class is associated with a specified human exposure level, below which chemicals are considered to present a negligible risk to human health. In the absence of experimental hazard data, these exposure threshold (TTC) values have formed the basis of priority setting in the risk assessment process.

To facilitate the application of the TTC approach, the original Cramer scheme, and an extended version, have been implemented in Toxtree, a freely available software tool for predicting toxicological effects and mechanisms of action.

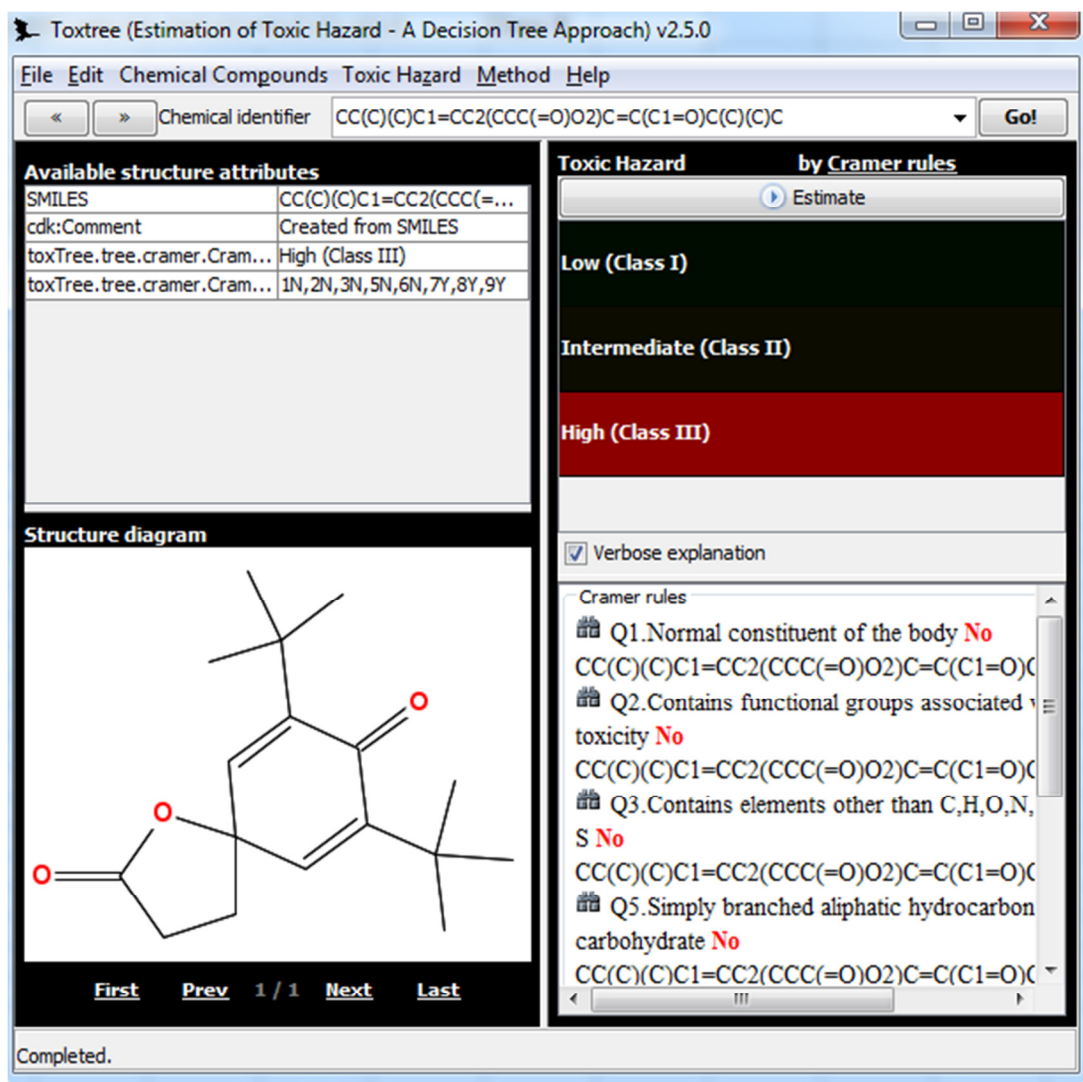


Figure 8.1 : Example Identification of Cramer class

A further elaboration of the two tables mentioned before (Total extract identification specimens table and Internal washing identification specimens table) lead to the following:

1. Total extract risk assessment table
2. Internal washing risk assessment table

(both of them are in table number 4 *Risk_Assessment_Table*)

where we reported:

- ✓ Samples names,

- ✓ Relevant Cramer class
- ✓ Max $\mu\text{g/day}$ and the Total $\mu\text{g/day}$ of 43 structures collected from the rows * columns table
- ✓ as well as :
- ✓ the Exposure figure
- ✓ the Risk ranking

In the absence of recognized methods for the evaluation of Exposure and the Risk, the following criteria were adopted: A risk assessment spreadsheet has been adopted, as reported in picture 8.2 below. In such spreadsheet, “*risk characterization*” -Y axis - corresponds to the evaluation of the intrinsic toxicological properties of the substances involved, while the “*risk identification*” -X axis- can be associated with the dietary exposure to the same substances. Both parameters i.e. potential toxicity and exposure, have been evaluated during the course of this study, and a combination can be made through the above mentioned spreadsheet in order to assess the risk associated to each substance. Missing step is the identification of the allocation criteria for the different classes of risk characterization (Y axis) and identification (X axis).

Here below are reported the criteria that were used for the allocation of each substance to any such class. These criteria may be arbitrary and may be modified or refined in the future; they have been used, as

previously outlined, in absence of other ranking criteria.

Y-axis: characterization/toxicity

Three categories were assigned :

- I. First class: Cramer 1, substances with *no or slightly harmful* presumption of toxicity
- II. Second class: Cramer 2-3, *harmful*. Here are classified all substances for which any possible presumption of toxicity can be anticipated, with the exception of endpoints that are attributed to very toxic substances
- III. Third class: substances that may be classified as highly toxicity (Carcinogen, Mutagenic or Reprotoxic substances, Endocrine Disrupting Chemicals, neurotoxic as carbamates and organophosphates, other substances showing toxicological alerts for the above mentioned endpoints etc.), *very harmful*

X-axis: exposure classification

- I. First group: *Low exposure* <10 µg/day. Such threshold has been assumed based on the 10 mg/kg detection limit set in *Reg. EU 10/2011* for the substances that may be used behind a Functional Barrier. If one assumes that 1 kg of food is consumed daily, this will transform in 10 µg/day.

II. Second group: *Medium exposure* $10 < M < 90 \mu\text{g/day}$. The threshold of $90 \mu\text{g/day}$ has been set as the Threshold of Toxicological Concern for substances in Cramer Class III, i.e. with higher presumption of toxicity.

III. Third group: *High exposure* $> 90 \mu\text{g/day}$

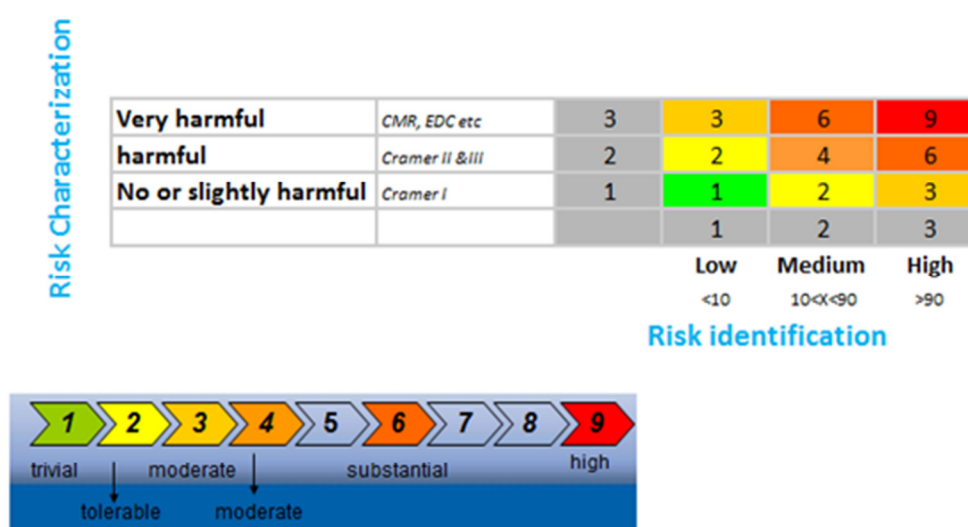


Figure 8.2: Risk assessment spreadsheet adopted for the evaluation of Exposure and Risk

At this stage, once known the Cramer class and the Exposure of each substance, a risk assessment calculation and relevant ranking may be done using the table built before.

i.e. consider *1-hexadecene*, it has a Cramer class = 1, and max quantity extracted = $9 \mu\text{g/day}$, thus it will be:

- risk characterization = 1 that is First class: Cramer 1, *no or slightly harmful*
- risk identification = 1 that is *Low exposure* $< 10 \mu\text{g/day}$

so 1-hexadecene will be show an Exposure low and a risk = 1 as reported

on the first line into the table below.

The same approach has been used to calculate the Exposure and the risk for each substance assessed, both internal washing and total extract, here below an excerpt of the risk assessment tables is reported (picture 8.133 and picture 8.134).

INTERNAL WASHING RISK TABLE -NIAS & NLS-					
SUBSTANCES	Cramer Class	MAX µg/day	TOT µg/day 43 Structures	exposure	RISK
1-hexadecene	I	9	9	L	1
7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	III	29	29	M	4
benzene, 1,3-bis(1,1-dimethylethyl)-	I	1	1	L	1
cyclohexadecane	I	25	25	M	2
dodecane	I	17	17	M	2
Hexadecanoic acid ester	I	2	2	L	1
octadecadienoic acid, methyl ester	I	2	2	L	1
oleic acid, 3-hydroxypropyl ester	I	100	100	H	3
silane, trimethoxy[3-(oxiranylmethoxy)propyl]	III	19	19	M	4
tridecane	I	15	15	M	2
undecane	I	11	11	M	2

I = LOW CLASS
 II= INTERMEDIATE CLASS
 II= HIGH CLASS

Table 8.133: excerpt of “Internal Washing Risk Table” obtained after the determination of Risk and Exposure

TOTAL EXTRACT RISK TABLE RISK TABLE -NIAS & NLS-					
SUBSTANCES	CRAMER class	MAX µg/day	TOT µg/day 43 Structures	exposure	RISK
1-docosene	I	4	4	L	1
1-hexadecene	I	11	11	M	2
1-propene-1,2,3-tricarboxylic acid tributyl ester	I	130	700	H	3
2,4-ditert-butylphenol	I	3	3	L	1
2-propenoic acid, 3(4-methoxyphenyl)-,2 ethylhexyl ester	I	195	195	H	3
7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	III	43	45	M	4
benzene,1,3-bis(1,1-dimethylethyl)-	I	4	4	L	1
cyclohexadecane	I	25	25	M	2
cyclohexane, octyl	II	8	8	M	2
cyclooctacosane	I	4	4	L	1
Decanedioic acid, dibutylester	I	660	1259	H	3
docosane	I	10	10	L	1
dodecane	I	21	21	M	2
hexadecanamide	III	29	31	H	4
n-butyl p-hydroxybenzoate	I	162	162	H	3
n-hexadecanoic acid	I	1833	1833	H	3
nonyphenol (isomers)	III	4	4	L	2
octadecadienoic acid,methyl ester	I	20	20	M	2
Octadecane	I	8	13	M	2
oleic acid, 3-hydroxypropyl ester	I	160	160	H	3
phenol,2,4-bis(1-methyl-1-phenylethyl)-	III	5	5	M	2
silane, trimethoxy[3-(oxiranylmethoxy)propyl]	III	40	64	M	4
triacetin	I	135	332	H	3
tridecane	I	19	19	M	2
undecane	I	17	17	M	2

Table 8.134: excerpt of “Total extract Risk Table” obtained after the determination of Risk and Exposure

From these tables all substances that showed a Medium and an High level of exposure and a Risk >3 were selected and reported below as they are the NIAS and NLS that are to be further assessed.

	SUBSTANCES	Cramer Class	RISK	exposure
A	7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	III	4	M
B	silane, trimethoxy[3-(oxiranylmethoxy)propyl]	III	4	M
C	hexadecanamide	III	4	H
D	1-propene-1,2,3-tricarboxylic acid tributyl ester	I	3	H
E	2-propenoic acid, 3(4-methoxyphenyl)-,2 ethylhexyl ester	I	3	H
F	oleic acid, 3-hydroxypropyl ester	I	3	H
G	Decanedioic acid, dibutylester	I	3	H
H	n-butyl p-hydroxybenzoate	I	3	H
I	n-hexadecanoic acid	I	3	H
L	triacetin	I	3	H

Table 8.135: NIAS/NLS substances table identified

8.4.1.1. Examination of NIAS/NLS substances with Cramer class 3 risk 4

Based on the combination of Risk , exposure and Cramer class the first three substances reported into the above table : substance A, B, C have been more carefully examined finding information in literature as reported below. Basically it was found that they are degradation products of antioxidants that are commonly used for the plastics materials.

About the remaining substances, from D to L, even if the exposure is high, the corresponding Cramer class is equal to 1, thus these substances have been not examined further.

Substance A

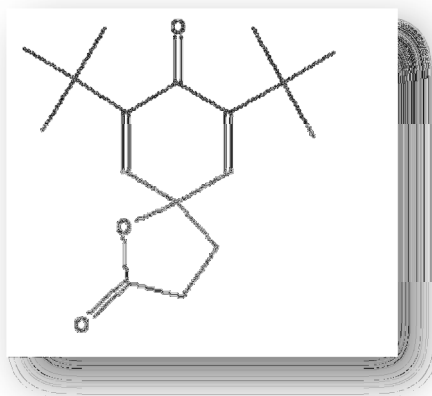
7,9-di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione)

CAS Number: 82304-66-3

Molecular Formula: C₁₇H₂₄O

Molecular weight: 276.3707

Structural Formula:



It is a decomposition product of IRGANOX 1076.

IRGANOX 1076 is a phenolic antioxidant, stabilizer for organic substrates such as plastics, synthetic fibers, elastomers, adhesives, waxes, oils and fats. [25]

Substance B

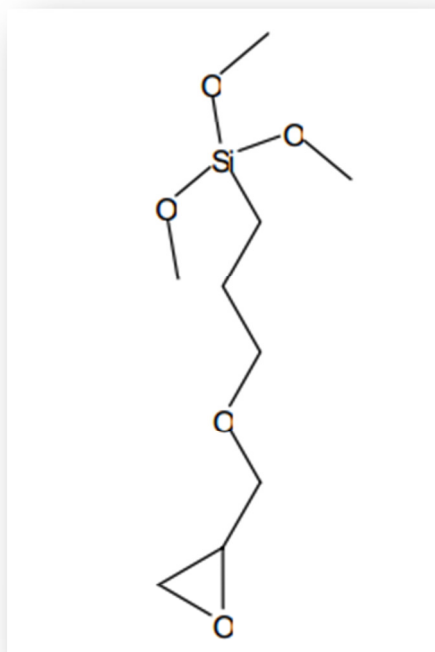
Silane, trimethoxy [3-(oxiranylmethoxy)propyl] (TMSPGE)

CAS Number: 2530-83-8

Molecular Formula: C₉H₂₀O₅Si

Molecular Weight: 236

Structural Formula:



TMSPGE is used as an active sealants, adhesion promoter, coupling agent, or cross-linker in adhesives, sealants, and encapsulants. [26]

Substance C

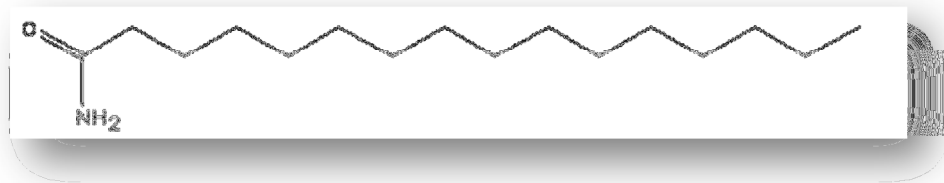
Hexadecanamide

CAS Number: 629-54-9

Molecular Formula: $C_{16}H_{33}NO$

Molecular Weight: 255.4393

Structural Formula:



It is also known as Palmitamide and is a fatty amide of palmitic acid.[27]

8.4.2. Risk assessment of not identified substances

A chromatographic peak is defined as “not identified” when the related mass spectrum is not comparable to anyone between the ones available into the mass spectra libraries.

The risk assessment, in that case, should be completed with information given from raw materials suppliers in order to have the identification of these compounds, or at least the origin of them.

If enough information given from the suppliers is available, it would be easy to get some hypothesis like the following:

- they could be “listed compounds” without using limitation: not significant risk;
- they could be “listed compounds” with specific migration limit: to verify if the limit is respected;
- they could be “not listed compounds”, with or without presumption of toxicity, in this case a risk assessment as the one showed in the previous paragraph can be done.

It may be accepted that full identification of all peaks will be hardly

possible, and some non-identified substances will remain so. In these cases it would be necessary to identify the raw material or the process step from which those compounds are generated, and verify whether possible reactions or degradation are likely to lead to the formation of substances with any presumption of toxicity.

Thanks to the information given from the raw material suppliers and IrcPack Lab we have been able to identify most of the “*not identified substances*” ; these are reported in the tables below. As outlined above, the peaks that remained not identified cannot be attributed to any substance.

Internal washing	Probable identification
not identified (m/z= 243)	colophony (paper)
not identified (m/z= 55,82,111,129)	ester of acid adipic with neopentil glycol
not identified (m/z= 84,99,111,173)	cyclic ester with 2 molecules of acid adipic (Adhesive)
not identified (m/z=100,127,185)	not identified
not identified (m/z=101,111,129)	ester of acid adipic with neopentil glycol (Adhesive)
not identified (m/z=111,129)	ester of acid adipic with neopentil glycol (Adhesive)
not identified (m/z=111,129,184)	ester of acid adipic with neopentil glycol (Adhesive)
not identified (m/z=118,239,270)	not identified
not identified (m/z=118,267,298)	not identified
not identified (m/z=126,155,173)	ester of acid adipic with 1,4 butanediol
not identified (m/z=127,155,185,213)	cyclic ester of acid adipic
not identified (m/z=155,213)	not identified
not identified (m/z=57,83,97,111)	not identified
not identified (m/z=91,121,147)	glycidoxypropyl silane
not identified (m/z=97,126,155,173)	ester of acid adipic with 1,4 butanediol
not identified (m/z=175)	not identified

Table 8.136: Not identified probable identification table- internal washing-

Total extract	Probable identification
not identified (m/z=243)	colophony (paper)
not identified (m/z= 55,82,111,129)	ester of acid adipic with neopentil glycol (Adhesive)
not identified (m/z=84,99,111,173)	Estere ciclico con 2 mol. acido adipico (ADESIVO)
not identified (m/z=100,127,185)	not identified
Not identified (m/z=101,111,129)	ester of acid adipic with neopentil glycol (adhesive)
not identified (m/z=111,129)	ester of acid adipic with neopentil glycol (adhesive)
not identified (m/z= 118,239,270)	not identified
not identified (m/z= 118,267,298)	not identified
not identified (m/z=126,155,173)	ester of acid adipic with 1,4 butanediol (adhesive)
not identified (m/z= 127,155,185,213)	ciclic ester of acid adipic
not identified (m/z=155,213)	not identified
not identified (m/z=57,83,97,111)	not identified
not identified (m/z=91,121,147)	glycidoxypropyl silane
not identified (m/z=97,126,155,173)	ester of acid adipic with 1,4 butanediol
not identified (m/z=175)	not identified
not identified (m/z= 102,141)	not identified
not identified (m/z= 129,215)	ciclic ester of acid adipic
not identified (m/z= 91,117,207)	silane
not identified (m/z=111,129,215,343)	ciclic ester of acid adipic
not identified (m/z=173,99,111)	ciclic ester with 2 molecules of acid adipic (Adhesive)
not identified (m/z=57,71,127,155)	not identified
not identified (m/z=94,175)	not identified
not identified (m/z=99,111,173)	ciclic ester with 2 molecules of acid adipic (Adhesive)
not identified (m/z=99,171,127)	not identified

Table 8.137: Not identified probable identification table - total extract--

8.4.3. Risk assessment of Aliphatic Hydrocarbons

Hydrocarbons are a heterogeneous group of organic substances that are primarily composed of carbon and hydrogen molecules. Hydrocarbons can be classified as being aliphatic, in which the carbon moieties are arranged in a linear or branched chain, or aromatic, in which the carbon moieties are arranged in a mono or poly condensed benzene, naphthalene or highest rings.

As reported below we detected a relatively high quantity of Aliphatic hydrocarbons (saturated + unsaturated). We can't assess them as we have done for the other substances, as the incidence of aromatic (although presumably low or negligible) cannot be made through this study, therefore no class of risk can be attributed. An evaluation by

reference can be done by consulting the EFSA *opinion on Mineral Oils: EFSA Journal 2010; 8(5):1334*. A more detailed treatment of this subject is not addressed in this study.

INTERNAL WASHING RISK TABLE **Aliphatic Hydrocarbon**					
SUBSTANCES	Cramer class	MAX µg/day	TOT µg/day 43 Structures	exposure	RISK
aliphatic hydrocarbon		263	511		

Table 8.138: Aliphatic Hydrocarbons - internal washing-

TOTAL EXTRACT RISK TABLE **Aliphatic Hydrocarbons**					
SUBSTANCES	CRAMER class	MAX µg/day	TOT µg/day 43 Structures	exposure	RISK
Aliphatic hydrocarbons (sum)		2759	3590		

Table 8.139 Aliphatic Hydrocarbons - total extract-

9. CONCLUSION

The production of food packaging involves the use of different kind of raw materials i.e: plastics, inks, adhesives, paper, cardboard, aluminum sheets etc.

The *Regulation 10/2011*, through its Article 19, has introduced the obligation to carry out Risk Assessment for a number of substances not listed in the said Regulation, including NIAS and NLS. Therefore other kinds of screenings in addition to the already known migration tests become now necessary.

These methods have to be developed through this study, thus they could be a valid instrument for the evaluation and the risk assessment of food packaging.

As resulted from this study, performed for the risk assessment of 43 commercial flexible food packaging, the Matrix approach can be considered a valid method to carry out the risk assessment of NIAS and NLS. With this method we are able first to calculate the exposure of each substance extracted and second also to perform the risk assessment for the substances not listed into the *Regulation 10/2011*.

Some main points can be outlined:

1. The largest majority of the substances found during the study have

been identified, only a limited number of GC peaks remained non-identified.

2. No substances of particular concern have been detected. The only case that might be examined more in detail is the one associated to Hydrocarbons, but the potential concern is only associated to the quantity detected rather than structural alerts.

ACRONYMS

ADI: Acceptable Daily Intakes

AP's: aids to polymerization

BADGE: Bysphenol A Diglycidyl Ether

BFDGE: Bisphenol F Diglycidyl Ether

CAC: Codex Alimentarius Commision

CeficFCA: General assembly conference organized by the food contact additives sector group of the European chemical industry council

CMR: Carcinogen, Mutagen or toxic to Reproduction

EEA: Ethylene Ethyl Acrylate Copolymers

EFSA: European Food and Safety Authority

EuPC: European Plastics Converters

EUPIA: European Printing Ink Association

EVA: Ethylene Vinyl Acetate Copolymer

FACET: Flavoring Additives (food) Contact materials, Exposure Task

FAO/WHO: Food and Agriculture Organization of the United Nations and the World Health Organization

FCM: Food Contact Material

FDA: Food and Drug Authority

FEICA: European Sealant and Adhesives Industry

FPE: Flexible Packaging Europe

GC: Gas Chromatography

GC-MS: Gas Chromatography/Mass Spectroscopy

GMPs: Good Manufacturing Practice

HPLC: High Performance Liquid Chromatography

IPPC: International Plant Protection Convention

IR: Infrared Spectroscopy

IS: Internal Standard

MS/MS: Mass Spectroscopy

NIAS: non-intentionally-added-substances

NLS: non-listed-substances

NMR: Nuclear Magnetic Resonance Spectroscopy

NOEL: No Observed Effect Level

NOGE: Novolac Glycidyl Ether

OIE: World Organization for Animal Health

OML: Overall Migration Limit

PAA's: Polymer production aids

PIM: Plastics Implementing Measure

QM: Maximum Contents

SBS: Styrene-Butadiene-Styrene Copolymers

SIS: Styrene-Isoprene-Styrene Copolymers

SML: Specific Migration Limit

SPS: Sanitary and Phytosanitary Measures

TEL: Tolerable Exposure Level

TR: Peak Retention Time

TTC: Threshold of Toxicological Concern

VOC: Volatile Organic Compound

WTO: World Trade Organization

BIBLIOGRAFY

- [1] *Risk assessment of non-listed substances (NLS) and not-intentionally added substances (NIAS) under article 19* , Plastic Europe
- [2] *Migration from Food Contact Materials* edited by L.L. Katan, Leonard L. Katan
- [3] *Chemical migration and food contact materials, chapter 1: Chemical migration into food: an overview* L.Castle, Defra Central Science Laboratory, UK
- [4] *Chemical migration and food contact materials, chapter 13:Food packaging inks and varnishes and chemical migration into food*, B.Aurela, KLC Finland and L.Söderhjelm, Finland
- [5] <http://www.foodpackagingforum.org/Food-Packaging-Health/Food-Packaging-Materials/Printing-Inks>
- [6] *EuPIA Guideline on Printing Inks applied to the non-food contact surface of food packaging materials and articles* November 2011 - corrigendum July 2012 -
- [7] <http://www.foodproductiondaily.com/Packaging/EuPIA-issues-new-guidelines-on-printing-inks-in-food-packaging>
- [8] AURELA B, '*Safety of fibre-based food packaging – role of printing ink*', *Food packaging:Ensuring the safety, quality and*

- traceability of foods*, Barcelona, arranged by ILSI. Europe, 2004 (poster).
- [9] K.Bentayeb, L.K. Ackerman, T.Lord & T.H. Begley *Non-visible print set-off of photoinitiators in food packaging: detection by ambient ionisation mass spectrometry*.
- [10] BRADLEY E L et al., '*Test method for measuring non-visible set-off from inks and lacquers on the food-contact surface of printed packaging materials*', Food Addit. Contam., 2005
- [11] *Chemical migration and food contact materials* (chapter 14)
- [12] McMinn, Beth W, Snow, W. Scott, and Bowman, Dan T., "*Solvent-Based to Waterbased Adhesive-Coated Substrate Retrofit, Vol. 1: Comparative Analysis*", National Risk Management Research Laboratory, Research Triangle Park, EPA-600/R-95-011a, April 1996.
- [13] <http://pffc-online.com/mag/4038-cold-seal-adhesives-0106>
- [14] December 31, 2005, David J. Bentley Jr., *Contributing Editor*
- [15] http://www.foodbase.org.uk/ /admintools/reportdocuments/12_28_Adhesives_final_report_290306.pdf.
- [16] (BONNELL, A. and LAWSON, G. (1997) *Chemical composition and migration level of packaging adhesives*. Summary report 3. MAFF Project No. IC074.)
- [17] <http://www.foodpackagingforum.org/News/How-adhesives->

manufacturers-comply-with-EU-regulation

- [18] Schaefer, A., *EU legislation*, in *Global legislation for Food Packaging Materials*, R.V. Rinus Rijk, Editor. 2010, Wiley-VCH: Weinheim. p. 1-25
- [19] Baughan, J.S. and D. Attwood, *Food Packaging Law in the United States*, in *Global Legislation for Food Packaging Materials*, R.V. Rinus Rijk, Editor. 2010, Wiley-VCH: Weinheim. p. 223-239
- [20] <http://www.foodpackagingforum.org/Food-Packaging-Health/Regulation-on-Food-Packaging/Food-Packaging-Regulation-in-Europe> autor: charlotte wagner
- [21] http://www.plasticseurope.org/documents/document/20111208094327-foodcontact_pim_explanatory_document_7_december_2011.pdf
- [22] *Scientific Opinion on Risk Assessment Terminology* EFSA Scientific Committee², ³ European Food Safety Authority (EFSA), Parma, Italy (EFSA Journal 2012;10(5):2664)
- [23] *Matrix project guidance* document edition 26.01.2011
- [24] http://ihcp.jrc.ec.europa.eu/our_labs/predictive_toxicology/doc/EUR_24898_EN.pdf
- [25] http://www.telko.com/files/images/telko/ru/basf/termostabilizator/irganox_1076_tds.pdf
- [26] <http://www.inchem.org/documents/sids/sids/2530838.pdf>

[27] [http://webbook.nist.gov/cgi/cbook.cgi?ID=C629549&Units=SI
&Mask=3FFF](http://webbook.nist.gov/cgi/cbook.cgi?ID=C629549&Units=SI&Mask=3FFF)

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