

HANDBOOK

FOR THE CHEMICAL ANALYSIS OF PLASTIC AND POLYMER ADDITIVES

Michael Bolgar
Jack Hubball
Joe Groeger
Susan Meronek



CRC Press
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PREFACE

Importance of Polymers

Polymers touch virtually all aspects of our lives, from everyday packaging to unseen applications such as gas pipelines under our streets. Polymers can include simple thermoplastics like polyethylene, a huge range of rubber compounds, adhesives, coatings, sealants, and many others. We wear polymers, we walk over them, we are fed with them, we coat our metals with protective polymers, and we even use polymers in the preparation of materials such as ceramics. Polymers, however, are seldom used in pure form. To make them more useful, easy to work with, or even more attractive, additives are added at many different times during the manufacturing process. The vast majority of commercial polymers are compounded with chemicals and/or other polymers to improve their usability or durability. These additives can be used to tune a polymer to a specific application, imparting high temperature oxidation resistance, improved flexibility, color retention, anti-static performance, or adding impact resistance to name a few examples. Compounding can also be done for technical reasons, where by a polymer is developed for a specific range of applications, using carefully selected additives. Other polymers are compounded for economic reasons, where a costly base polymer may be extended by addition of lower cost additives such as clays, reground polymer, other polymers, or a blowing agent that reduces density.

Formulation

Compounding is typically proprietary, with types and concentrations of ingredients carefully protected as intellectual property. Formulation information provided through Material Safety Data Sheet (MSDS) disclosure is typically incomplete or non-specific regarding the identity of all of the ingredients. Therefore, the end user may be left with little option but direct chemical analysis where composition information is imperative. Identifying the materials in the final plastic by analysis is extremely challenging. And although many reference handbooks currently exist that address the selection and application of performance-enhancing additives for polymers, there really is no good reference for the identification of these materials in finished goods. This handbook aims to fill this void by providing a comprehensive reference library for chemists, and to provide the information needed to extract, identify, and quantify additives used in polymers and plastic additives by common, readily available laboratory techniques such as gas chromatography/mass spectrometry (GC/MS).

Need for Analysis

The analysis of these materials is even more critical with recent increased interest in their environmental impact on ecological systems and human health. A number of frequently used additives, such as adipate plasticizers, have been identified as environmental pollutants, and the fate of these chemicals is the subject of on-going studies. Concern over the total composition of plastics has increased the focus on the total life cycle of polymeric materials. Government attention to toxic substances has increased over the years through the US Toxic Substances Control Act (TSCA) and the REACH initiative in the EU. These regulations may prohibit or otherwise impact the exportability of the plastic goods or other products that come in contact with the plastics. This, coupled with increased consumer attention and disclosures of 'chemicals' in consumer products, has increased the attention and need for a more complete analysis of polymeric materials. Combustion of rubber and plastic materials for energy production has also increased the awareness of organic and inorganic additives and the analysis of these products. Unintended combustion in fires, for example, has led to a significant increase in sensitivity to desorbed organic compounds and

decomposition products in closed environments. This has significantly affected the formulation of polymeric materials used in aircraft furnishings and building wiring, for example.

Additives as Possible Hazards

Increased attention has also been directed to some of the higher volume organic additives in polymer compounds, such as plasticizers, flame-retardants, and antioxidants. Some of these are recognized endocrine disruptors, or suspected carcinogens. Ingredients that have been used for many years are now being increasingly detected during analysis when they may have been overlooked in the past for lack of reference information and/or suitable reference compounds. More and more consumer items are sold as 'phthalate free.' Some states such as California are taking additional steps to regulate these chemicals in consumer goods, for example, the recently proposed ban on bisphenol-A in children's items. Some of these compounds are regulated through government agencies such as the US Food and Drug Administration (FDA), and guidelines are available through the US Code of Federal Regulations (CFR) for use in consumer applications. Compared to regulations for other items, plastics and polymers are surprisingly unregulated for most uses. Consumers also need to know what is in the plastic that interacts with or holds their product. Everyone from toy manufacturers, to food packaging, pharmaceutical packaging and even wire and cable manufacturers, will be held accountable for the materials they use.

Analytical Protocols, Historical

Comprehensive protocols for the analysis of plastics/polymers need to be developed. In the past analytical protocols included extractions performed with a polar and a non-polar solvent which were used to extract organic compounds from a polymer for subsequent analysis by GC using a flame ionization detector (FID). But FID alone may not be a definitive test, since the identity is based on column retention time, which is not a unique characteristic for many of these complex organic compounds.

Purpose

This handbook's primary aim is to provide the tools to help a bench chemist to obtain a more complete listing of additives present in a particular matrix. The techniques that we have been using successfully are described in this book to help the analyst to correctly identify the complex nature of the materials that have been added to the plastic. We provide information on analyzing polymers through thermal desorption, and the use of GC with a mass selective detector (MSD). Many compounds break apart either during extraction or analysis, so identification by key fragments, and typical moieties for the final compound is critical. The use of the GC/MS system allows the analyst to characterize a compound based on the utilization of these fragments or moieties.

To add even more complexity to an already daunting challenge, many additives are disclosed by trade name, not chemical name or CAS number. This handbook aims to address all of these items by providing a listing that can be cross referenced by trade name, chemical name, CAS number, and even key mass unit ions from the GC/MS run. This handbook serves as a library of additives that can be used to identify individual compounds commonly found in plastics.

The primary function of this handbook is to serve as a reference for the chemist who is monitoring a plastic for regulatory or internal compliance. However, through many years of analysis of polymers for a wide range of applications, we have seen other applications where analysis could be used to troubleshoot or develop better compounding practices suited for specific applications, or for process improvement.

Polymers have undoubtedly changed the world and have provided countless products that directly improve our quality of life. As more regulations are promulgated, and with the continued oversight of possible health hazards presented by the multitude of additives incorporated into these plastics, it becomes imperative that the monitoring of these compounds can be supported by high-quality reference materials and dependable analytical techniques.

HOW TO USE THIS HANDBOOK

The information in this text was formatted in a consistent manner to make a usable bench handbook for a chemist performing real-world analyses. Compounds were chosen trying to obtain a representative sampling of all the primary classes of additives.

For each material or compound listed the following data is presented:

The data section:

- *Chemical Information.* Such information as the unique structure (if available), CAS and RTECs number (if available), common abbreviations, the formula and the molecular weight of the product can be found in this section.
- *Brand Names and Manufacturers.* Many of these products are produced under a variety of trade names. This section lists other companies that may produce this same compound as a different brand name. These other names are all cross-referenced in the subject index.
- *Physical Properties.* This section contains the general physical properties of the compound. For the solubilities the following abbreviations are used: U – Unknown, E – Emulsifiable.
- *Application, Regulatory and Environmental Information.* Information regarding the uses and regulations governing the compound are contained in this section. Laws and regulations, as well as our understanding of the toxicity and nature of chemicals change on an almost a daily basis. Please, use this text as a reference, but be sure to verify the current status of any regulations prior to proceeding with any project.

The Mass Spectral Information

This is the actual analytical run of the compound. It may contain from one to three pages, depending on the nature of the material. Tabulated for each spectrum is the mass-to-charge ratio of the five most abundant ions in the spectrum, as well as the molecular weight of the material.

Indexed in the back of the book are:

Appendix A

Chromatograms for all the compounds and their analytical conditions.

Appendix B

A list of definitions and abbreviations used in the text.

Subject Index

In addition to key words and terms, this index contains all the synonyms listed in text cross referenced to their corresponding pages.

Five Peak Index

This index can be used to identify an unknown compound from your own analytical data. It contains the following data, tabulated by the 100 percent abundance ion from each spectrum:

- The first five columns are the mass to charge ratios of the five most abundant ions in the spectrum - with the most abundant bolded.
- The MW column has the molecular weight of the parent compound as reported in the text.

- The relative intensities of the five most abundant ions (integral values, proportional to 100 for the most abundant ion).
- The compound name and page number of the compound of interest.

Molecular Weight Index

CAS Number Index

RTECs Number Index

The authors will be grateful to the readers of this handbook who make suggestions for future improvements, as well as calling our attention to any errors that may be discovered.

We look forward to adding additional materials in the future, and expanding the library of materials to cover an even greater sampling of the additives commonly found in consumer goods and the environment.

Overview of Polymers, Additives, and Processing

Introduction

Polymers are available in a wide range of formulations and properties achieved through selection of the base polymer and additives. Two types of chemical reactions produce polymers:

1) Condensation between polyfunctional molecules (monomers) that react with each other. This reaction is heat driven, sometimes with the aid of a catalyst. The longer the exposure to heat, the longer the polymer chain becomes. A common example of this is nylon, a reaction of a diamine with a dicarboxylic acid producing a polyamide.

2) Reaction of a molecule that is activated with an initiator to form a free radical. This free radical, when reacting with a “normal” molecule creates a new free radical, causing a full fledged chain reaction. This process creates, from a monomer, a long chain polymer instantaneously. No intermediate chain length polymers are present. This process is also called vinyl polymerization.

Both reactions are controlled by stoppers (telomers), which in the first process caps the ends, and in the second process captures the free radicals.

Most polymers are identified on the basis of their common name. Examples are polyethylene, polyvinyl chloride, butyl rubber, acrylonitrile-butadiene, styrene (co-polymer ABS). However, few polymers are used in pure form since they often require chemical modification to achieve optimum properties, and promote non-inherent performance. Some of these include improved resistance to oxidation, high temperatures, flammability, impact loads, surfactants, ultraviolet radiation, as well as modification of a wide range of other properties. The process of adding essential ingredients to polymers to achieve these results is termed *compounding*. However, it is generally not practical to precisely match the inherent properties of a base polymer to a specific application. While some polymers such as polyethylene are available with a wide range of properties based on a range of molecular weights, molecular weight distributions, and tacticity, other polymers have a finite range of properties for which compounding provides a practical method for adjustment of general or specific properties. For example, polyvinyl chloride is the most commonly used thermoplastic. In the raw form, this is a rigid, transparent polymer, however in the most familiar applications, this “vinyl” polymer is flexible and colored as in black electrical tape or a yellow rain coat.

As stated above, the modification to achieve these results is usually achieved by mixing a polymer with other polymers, both organic and inorganic materials including additives, metal powders, glass fibers, and other materials to match the end-use application.

This chapter addresses three basic classes of polymers and the approaches for processing them into compounds. These classes include thermoplastic polymers, and two types of elastomers - crosslinked elastomers, and thermoplastic elastomers. Compounds prepared from each class have a range of achievable properties, and each category of compounds may have overlapping properties. Each category is prepared by different technical approaches with varying controls, energy requirements, and limitations. A brief definition of each class follows. Also included, later in the chapter, is a detailed description of how additives influence the production process.

Overview of Polymeric Compounds

In the form of raw materials, polymers exhibit a wide range of compositions and properties. These properties can be enhanced or tuned to specific applications through the preparation of compounds. This section addresses three basic classes of polymers and the approaches for the preparation of compounds.

Thermoplastic Polymers

Thermoplastics are polymers that can be melted, made into a desired form, and then re-melted. Thermoplastics can be processed into a desired shape through many processes, the most common of which are injection molding and extrusion. Blow molding, transfer molding, calendaring, casting, and other forming operations are all possible with thermoplastics.

Elastomers

The properties that define polymers as an elastomer are that they must be amorphous when unstretched and must be above their glass transition temperature to be elastic. This can be compared to thermoplastics that must be crystalline or must be used below this temperature to preserve dimensional stability.

Crosslinked elastomers are polymers that are first prepared by compounding a base elastomeric polymer with property-modifying additives and a reactive crosslinking agent. Polymers of this type can be formed into a desired shape through many different operations, however the final operation requires that the shaped article be heated to a temperature at which the crosslinking agent decomposes to produce free radicals. These radicals react with the base polymer to form chemical crosslinks transforming the linear “two dimensional chain” into a “three dimensional object”. Retaining elastomeric properties with the shape “frozen” by virtue of the chemical crosslinks. This class of material cannot be melted and reformed. Alternate crosslinking methods are used for special applications including the use of ionizing (gamma) radiation, ultraviolet radiation, and water-initiated (silanol) cure systems.

Thermoplastic elastomers are a more recently developed class of polymer in which the neat polymer has inherently elastomeric properties, yet it behaves thermoplastically. With some limitations, these materials can be formed by essentially the same operations as thermoplastics, but the final object has elastomeric behavior. Objects molded with thermoplastic elastomers can be melted and re-shaped. Since these are not crosslinked, their creep resistance and extended high temperature use are limited.

Compounding Objectives

Compounds must behave as a *system*, consisting of the base polymer and additives, selected to achieve a set of final properties. During compounding, mixing must occur at two fundamental levels; dispersive mixing and distributive mixing. *Dispersive mixing* relies on shear action to blend the additives into the polymer. Dispersive mixing must overcome differences in viscosity, surface energy, chemical compatibility, melting temperature, and others. Improperly dispersed polymer compounds will typically contain domains where ingredients have not been blended properly, as shown in Figure 1-1. Dispersive mixing focuses on short-range blending of the compound, while distributive mixing addresses the overall homogeneity of a batch. *Distributive mixing* places different requirements on the mixing process, depending on the type of equipment that is being used. This will be further addressed in the “Compounding Supplement” at the end of the chapter.

During the compounding process, it is essential that all ingredients added to a polymer remain in the compound in a manner that assures functionality. Thermal degradation and excessive shear action may selectively degrade different additives. It is imperative that processes are developed and validated by functional testing of the final compound. Mixing processes must be very carefully controlled to assure consistent quality. Variations in compound quality can have an adverse and varying impact on components prepared from the compound.

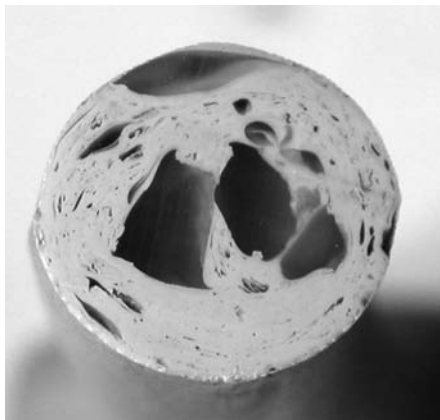


Figure 1-1 Example of Poorly Mixed Polymer Compound

Thermoplastic Compounding

Thermoplastic compounds are typically prepared by mixing organic and/or inorganic compounds with a single base polymer, copolymers, or blends. The base polymer may consist of a chemically bonded blend such as the block copolymer acrylonitrile-butadiene styrene (ABS) or a second base polymer may be used to enhance the overall end properties of the compound.

A base polymer, such as an ethylene-propylene (EP) copolymer, can be acquired in a range of compositions, molecular weights, various ethylene-to-propylene ratios, various molecular weight distributions, and a range of densities. Each of these variations results in a base polymer that has specific practical properties such as flexibility, elastic recovery, tensile strength and thermal limit to name a few. As a base polymer, ethylene-propylene polymers and most other non-crosslinked elastomers have no significant commercial application, since they are essentially a liquid with very high viscosity.

Organic Additives

Antioxidants

Thermoplastics may contain a wide range of organic additives that are incorporated into the additives to improve selected properties. In virtually all cases, an antioxidant must be added to allow the compound to be blended with other ingredients, to be pelletized or chopped into intermediate form, and to survive thermal stresses associated with the final forming process. In some cases, the base polymer is blended with an antioxidant at the time of preparation of the base resin. This type of antioxidant is intended to add thermal stability for processing considerations. External antioxidants can also be added to improve shelf life of the product and/or to improve its high temperature stability, while adding a stability margin during thermal processing.

Internal Lubricants

These may be added to the polymer to reduce the shear rate during processing, especially when an inorganic material is being added. If the shear level gets too high, thermal damage and polymer chain scission can result. The lubricant must be selected properly to avoid having it decompose or affect the polymer compound in some adverse manner. Common lubricants include fatty alcohols (C14-C18), fatty acid esters (C14-C18), dicarboxylic acid esters (C14-C18), fatty acid amides (C16-C18), and esters (C26-C32), for example.

Release Agents

They are often blended into compounds that are developed for injection molding applications. Where such an additive is absent, molded components tend to stick to mold surfaces. To prevent this, mold surfaces must be treated between every cycle, or they can be coated with a range of semi-permanent mold release treatments. Inclusion of an internal release agent prevents mold surface build-up, surface charring, and simplifies production. Internal mold release agents may include hydrocarbons, alcohols, carboxylic acids, halogenated compounds, ketones, carboxylic acid esters, amides, metal salts, and silicone compounds.

Plasticizers

Plasticizers are added to thermoplastic compounds to improve flexibility, increase the acceptance level for inorganic additives, and to aid in processing, such as melt flow reduction. Synergistic effects can also be obtained such as reduction of shear during mixing and improved impact resistance. Plasticizer compounds typically include phthalates, adipates, esters, and fatty acid esters (oleates, palmitates, stearates).

Impact Modifiers

These are often added to otherwise brittle thermoplastics to improve impact resistance. In some cases, the addition of inorganic materials renders plastics hard and brittle, thus requiring the addition of an impact modifier. Impact resistance can be improved through addition of polymers with increased flexibility and/or elastomeric characteristics. Acrylics and butadiene are common impact modifiers. Styrene is commonly impact-modified through graft polymerization with acrylonitrile and/or polybutadiene (hence ABS [acrylonitrile-butadiene-styrene]), or it can be grafted to an ethylene propylene diene elastomer. Polypropylene can be made impact resistant through various blending methods to incorporate ethylene-propylene monomer.

Electrostatic Control Agents

They are required for thermoplastics applications. There are a number of compounds available for this function and these can be divided into two general categories; bulk and surface-modifying. Bulk additives may be simple, such as carbon black, which, when added in sufficient concentration, provides a semiconducting matrix, thus controlling the accumulation of localized charge. Metal salts can also be used for this purpose in some polymers. Cationic compounds can impart bulk conductive properties and these include compounds with a bulky cation such as quaternary ammonium, sulphonium salts, or imidazoline compounds. Anionic compounds are also used and these include, for example, alkylsulphonates. Nonionic compounds can also be used for controlling charge distribution through interfacial activity. Compounds in this category include ethoxylated fatty amines, ethanolamides, and polyethylene glycol esters, for example. Some organic compounds are also useful for controlling surface charge. These function by having limited solubility in the host polymer. Compounds of this type migrate to the surface of the polymer where their nominally low concentration increases locally at the surface, and thus provide a conductive surface bridge.

Dyes and Organic Pigments

Dyes are chemical compounds that impart color to plastic compounds. These dissolve in the host polymer and are therefore not present as discrete particles. Dyes are typically azo or anthraquinone compounds.

Pigments are discrete particulate materials of very small particle size, which are blended into a thermoplastic compound to impart color. Organic pigments are typically of an azo or cyanine structure. Most organic pigments also have good thermal stability across the thermoplastic processing range. Due to their insolubility in the polymer, these also serve as nucleating agents, though often less effective since some would be above their melting temperature as a polymer is being processed in the molten state.

Polymer Blending

For some applications, polymers are blended to provide a balance of properties. Some polymers blend well due to mutual solubility, but if the solubility parameter of the candidate polymers is different by more than about 3 SI units, the polymers must be blended with an intermediate material to improve compatibility. Typically, this involves an intermediate polymer with a low molecular weight. In the melt, this serves to reduce the surface tension between two incompatible polymers, thus improving dispersion. Low molecular weight polyethylene is an example of a polymer blending aid. In other cases, metal stearates or salts can be used to aid dispersion. Examples include zinc stearate and calcium stearate.

Inorganic Additives

Fillers and Reinforcers

Thermoplastics often have physical properties that are inherently well suited to a particular application. In such a case, there is little need for addition of inorganic materials. Inorganic additives are very useful for improving the physical strength and deformation resistance of thermoplastics. They function by forming a network of pinning points in the polymer wherein the slippage of polymer chains under mechanical stress is impeded. Inorganic reinforcements are of many types, ranging from natural minerals to synthetic minerals to specialized materials with directional physical properties. Clays in common use for higher quality plastics include kaolin and other natural silicates, calcium silicates, and others. Synthetic and high purity reinforcements include titanium dioxide, calcium carbonate, silica, and many others.

Inorganic additives are also useful for controlling the onset temperature, extent, and dimensions of the crystalline phase in semi crystalline polymers. The inorganic component acts as a site for heterogeneous nucleation of polymer crystallites. By initiating nucleation at many closely spaced sites, the polymer solidifies with a network of small uniformly distributed crystalline sites. By balancing the comparative strengths, flexibility, and creep resistance of crystalline and amorphous phases of a polymer, a balance can be achieved for engineering applications. Heterogeneous nucleation is also helpful for controlling the structure of polymers with a slow rate of recrystallization. During injection molding, for example, as the molded part cools, heat transfer to the chilled mold causes the polymer in the outer surface of the part to nucleate first, followed by the core of the component. Heterogeneous nucleation occurs at the mold interface, but homogeneous nucleation may occur in the core of the sample. This would proceed slowly due to the ratio of heat capacity of the polymer to poor thermal conductivity. Addition of a matrix of fine inorganic particles speeds forming process time and improves the bulk properties of the polymer. Titanium dioxide and silica are typical additives in this category. Titanium dioxide has a dual purpose in

many cases in that it is a very efficient whitener. Nucleating agents can also have the form of dispersed polymers with a higher melting point.

Pigments

Wide ranges of compositions are used to impart color to thermoplastic compounds. Pigments are discrete particulate materials, of very small particle size, that are blended into a thermoplastic compound to impart color. These may be organic or inorganic. Inorganic pigments are commonly found in the form of metallic compounds. Oxides of iron, chromium, molybdenum, cadmium, nickel, antimony, and titanium produce a wide range of vivid colors. Variations in oxygen stoichiometry have a pronounced effect on the color of many of these metal oxides. Carbon black is also a very effective colorant. Inorganic pigments are very stable in a polymer and generally exhibit high color retention. These often have a synergistic effect on the recrystallization performance of polymers during thermal processing, due to their role as heterogeneous nucleators.

Crosslinked Elastomer Compounding

Organic Additives

Antioxidants

Raw elastomeric polymers typically contain an antioxidant that is added at the time of manufacture to provide thermal stability for compounding, milling, and subsequent operations to produce beads, bales, or other forms where the polymer is first heated, then cooled into an intermediate form. The as-provided antioxidant may provide sufficient stability to protect an elastomeric compound through final forming and curing.

External antioxidants are often added to provide additional protection for elastomer compounds, especially during mixing and curing operations where temperatures will be highest. Antioxidants are available in many forms and they vary in functionality, according to their composition and structure. Typical antioxidants for elastomers include a range of phenolics, amines, and bisphenol derivatives.

Crosslinking Agents (Peroxides)

Elastomers must be crosslinked to hold their final form. The crosslinking reaction takes place through generation of free radicals that promote bonding at sites of unsaturation. The most common crosslinking agents for this include reactive peroxides, such as dicumyl peroxide, diacetyl peroxide, di-tert butyl peroxide, and others. Since each has a different temperature at which thermal decomposition initiates, curing conditions vary with the peroxide type.

Curing Agents

For some products, elemental sulfur is added to the compound as a curing agent. Sulfur reacts to form C-S-C bonds. This is an inexpensive reaction scheme and it is useful for production of rubber compounds across a very wide hardness range. Residual sulfur compounds lead to odors and acid products that are not well suited to applications where clean materials are desired.

Accelerators

The crosslinking reaction rate may be too slow for some commercial processes and the reaction may exceed the oxidation resistance time for the elastomer compound. In such cases, curing accelerators are used with the sulfur-curing process. Zinc oxide is a commonly used accelerator, however thioureas, hexamethylenetetramine, and others are effective. For organic peroxides, the cure rate can be greatly increased with an increase in applied temperature, though oxides of zinc,

magnesium, or calcium can be used to limited effect. The rate of crosslinking reaction can be slowed for those cases when the rate exceeds the formation process for some components. Cure retarders include compounds such as nitrosodiphenylamine, benzoic acid, and phthalic anhydride. Use of a cure retarder increases the burden on an antioxidant to protect the polymer against thermal degradation.

Lubricants and Related Compounds

During the compounding operation, shear stresses in an elastomer compound are very high. To reduce shear and to promote more efficient wetting of inorganic ingredients, processing aids can be used. Zinc and calcium soap compounds are very efficient for reducing shear viscosity during mixing. Fatty acid compounds and fatty acid esters are also useful and examples include stearic acid and palmitic acid.

Coupling Agents

Elastomer compounds are typically blended with an inorganic reinforcement. Bonding between these is typically mechanical rather than chemical in nature. Due to the high flexibility of elastomers in normal applications, shear stresses at the interface between the inorganic and polymer can cause a failure of the mechanical bond. For high performance compounds a coupling agent is used to form a chemical bond between the host polymer and an inorganic, such as kaolin clay. Typically, siloxane compounds are used as coupling agents.

Strength Modifiers (Carbon Black)

Carbon black is a very effective strength modifier for a wide range of elastomeric compounds. Since carbon black contains reactive surface groups, it bonds and interacts efficiently with the base polymer. Carbon black can be blended from a concentration of a few phr (parts per hundred rubber by weight) to as much as 40 phr to achieve a wide range of physical properties. Due to the chemical bonding between carbon black and rubber, it is very effective at increasing hardness without a corresponding major reduction in tensile strength, tear resistance or elongation limit. Carbon black addition reduces the free volume in rubber compounds, thus improving solvent tolerance, oil tolerance, and gas impermeability. Carbon black improves oxidative stability and protects the polymer against UV damage. Carbon blacks are available from a range of sources and all are produced from an incomplete combustion process. Sources include oils, tars, and reclaimed hydrocarbon materials. In other cases, carbon blacks of high purity can be derived from acetylene gas, low molecular weight polymers, and other clean sources.

Release Agents

Organic release agents and anti-blocking agents are occasionally used for elastomer compounds. Generally, these compounds have limited solubility in the elastomer compound, so they migrate and concentrate at the surface, where they can be effective to prevent cohesion and/or adhesion. Waxes and high molecular weight adipic acid esters are examples of compounds in this category.

Liquid polymers are occasionally used for softer grades of rubber compounds, where a base polymer will not provide the required balance between strength and flexibility. Liquid rubbers are of low molecular weight and would be fairly useless unless blended with other materials. In some cases, an external diene is added through a liquid base polymer. Liquid rubber is typically added during the milling operation.

Plasticizers

Elastomer compounds can be plasticized by addition of organic compounds. Elastomer compounds are inherently flexible and selection of a base polymer on the basis of molecular weight characteristics, chemical composition, and degree of crystallinity serves as the basis for the properties of the compound from which an elastomer is made. Oils are the most common plasticizer for elastomers. Oils of paraffinic structure or aromatic structure can be used with elastomers in which they are compatible. Paraffin wax would also be included in this category. Other plasticizers include phthalic acid esters and adipic acid esters. Fatty acids can be used as plasticizers but these contribute to an increase in surface tack of elastomer compounds. Examples include stearic and palmitic acid. Plasticizer addition has the added benefit of aiding with incorporation of inorganic materials.

Pigments and Dyes

Crosslinked rubbers follow the same description presented for thermoplastic compounds. A major problem with the use of organic pigments and dyes is that many decompose when high temperature curing agents are used. For these compounds, inorganic pigments are typically the only option.

Inorganic Additives

Fillers and Reinforcement Agents

Many commercial elastomer compounds are mechanically reinforced through the addition of inorganic compounds. These physically and/or chemically bond to the polymer to provide a more rigid matrix. Reinforcement agents include talc, various clays, silica, titanium dioxide, and many others. In some cases, fillers with high aspect ratios are used to impart directional reinforcement. A balance between particle size, surface structure, and dispersion efficiency is necessary for obtaining the best and most uniform performance of an elastomer compound. Many inorganic additives are first dried at high temperature (calcining) to split off water of hydration. This prevents moisture release during compounding and crosslinking. Moisture produces voids and often inhibits proper curing.

Inorganic additives for rubber compounds also include materials that enhance performance under various accelerated stress conditions. Zinc oxide is an effective heat stabilizer for some types of elastomers. Iron oxide, lead compounds, barium salts, and specially treated clays, such as kaolinite, add performance margin in wet aging conditions.

Thermoplastic Elastomer Compounding

Compounded polymers prepared with thermoplastic elastomers (TPE) are prepared in much the same manner as thermoplastics, with some exceptions. Thermoplastic elastomers generally combine the flexibility and frictional behavior of rubber compounds with the practical forming considerations of thermoplastic materials. These are commonly encountered in automotive and appliance applications where non-slip surfaces are desirable. Since compounds in this class have elastomeric physical characteristics, this often requires that a twin-screw mixer makes use of screws with a profile that is different than for thermoplastic compounding. Differences include the use of tapered screws, an increased frequency of barriers along the screw length to increase localized shear, separate zones of high and low shear action, and others. TPE compounds use mixers with high length-to-diameter (L/D) ratios (see Compounding Supplement at the end of the chapter).

Thermoplastic elastomers are most commonly formulated from elastomeric polyurethane or block copolymers of polystyrene-elastomer, polyamide-elastomer, or polyether-elastomer bases. Thermoplastic elastomers are provided as a raw material in pelletized form for subsequent compounding. The internal domain structure that is required for thermoplastic-elastomeric performance has been established by specific considerations of blending and structural-chemical interactions. In compounding operations, specific temperature ranges are required to assure that phase separation does not occur in the TPE base polymer.

Organic and inorganic compounds for modification of thermoplastic elastomers follow the previous descriptions for thermoplastics. Addition of inorganic materials requires a screw type mixer with sufficient cooling to remove the heat developed due to high shear viscosity. The mixer must also include some areas with very high shear to assure proper dispersive mixing. Antioxidants for thermoplastic elastomer protection during compounding must have good longevity at elevated temperature and they must have good solubility in the compound to prevent separation.

COMPOUNDING SUPPLEMENT

Introduction

This compounding supplement is intended to provide the reader with an overview of compounding methods and equipment.

Since possible contamination and subsequent failure of an end product can be associated with a compounding process, the authors believe that a brief introduction into the engineering aspect of compounding is relevant, and may provide a better understanding of the process as a whole.

Methods of Compounding: Thermoplastic Polymers

Thermoplastic polymer compounds are typically prepared by use of a single- or twin-screw mixer. This consists of parallel, threaded cylinders (screws) that are enclosed within a heated barrel. Heating is applied and separately controlled in zones along the barrel. The screws are caused to rotate with a gear reduction electric drive at one end. The barrel is a high strength enclosure, designed to sustain very high pressure, temperature, and shear conditions. The screws counter-rotate and the rate is variable. At the driven end of the mixer, polymer is added through a hopper into the throat of the mixer. Pre-weighed and mixed additives are also incorporated or metering hoppers may add proportioned quantities of polymer and additives that will form the compound. Due to the threaded nature of the screws and their proximity in an enclosed heated barrel, the ingredients are subjected to high shear as they melt. The thread pitch causes the compound to travel down the barrel, where mixing time increases and viscosity drops as the compound heats. Mixers for thermoplastics typically have long barrels and a length-to-diameter ratio of at least 20. At the end of the mixer is a screen pack, followed by a die for extruding the compound into of tapes, strands, or other forms. A rotary cutter may be mounted over a strand die to produce the "pellet" form in which the bulk of thermoplastics are supplied. The screen pack is used to remove any non-dispersed materials and to capture large particles or contaminants that would otherwise be detrimental to the finished compound. The screen pack also contributes to effective mixing by providing back pressure.

Figure 1-2 presents an illustration of several types of mixing screws. These show variations in thread pitch as different profiles or offsets in the diameter of the screws between the threaded lands. Screw profiles vary for the type of compound being mixed. In some cases, very high shear is required to assure proper dispersion of ingredients. For other compounds, aggressive shear will

damage the base polymer, so reduced shear and longer mixing times are targeted. Screw profiles vary in thread land, length, and distribution of thread pitch along the screw length. Some screws contain radial pins, staggered knives, or other features for specialized applications. Some mixers include three or more nested screws.

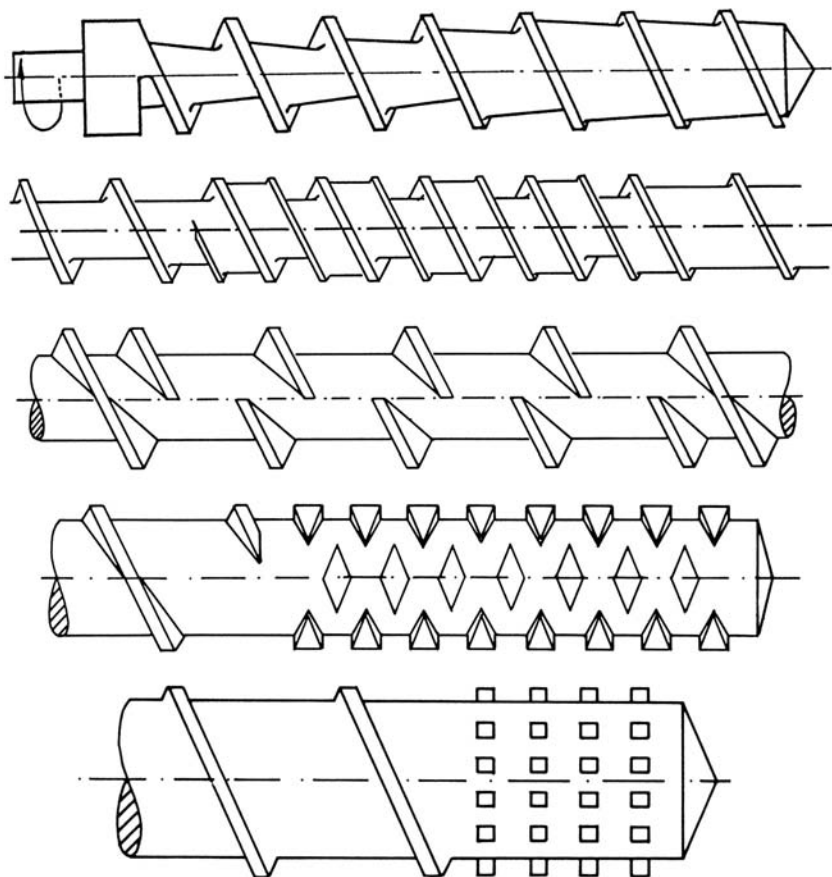


Figure 1-2 Several Types of Thermoplastic Mixing Screws

Some thermoplastic compounds require multi-step mixing. This is required where a high degree of homogeneity is essential and ingredients may require sequential addition to avoid segregation or chemical interactions. For compounds of this type, the intermediate compound is typically extruded into pellets or chopped strips for re-introduction into the mixer and further addition of compounding ingredients.

A Buss mixer is a variation of the screw mixer design in which a long barrel can be configured to allow high shear mixing of ingredients at one end, with separate feed ports for sensitive additives into a less aggressive mixing zone. This design also allows liquid additives to be directly added during compounding. With a traditional screw type mixer, liquids are often added in the form of a mixture with inorganic materials. Figure 1-3 shows a view of a Buss mixer and Figure 1-4 illustrates the internal and external configuration. Polymer compounding with a Buss mixer is a continuous process. Batches are typically defined in context of a campaign wherein a batch of raw materials is used to completion or a particular production target compound weight is met. Precise metering of the raw materials is a key consideration for assuring consistent quality of the thermoplastic compound.

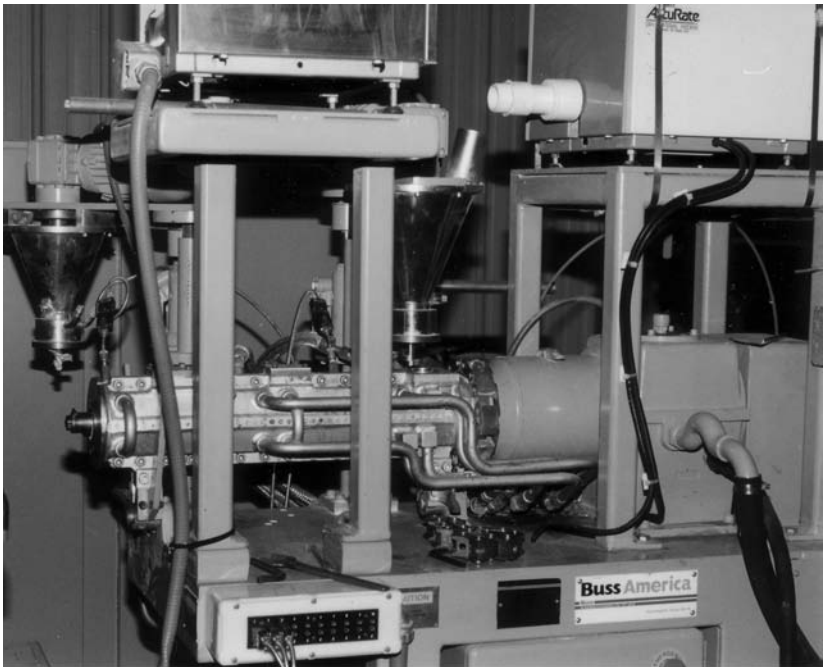


Figure 1-3 Buss Mixer

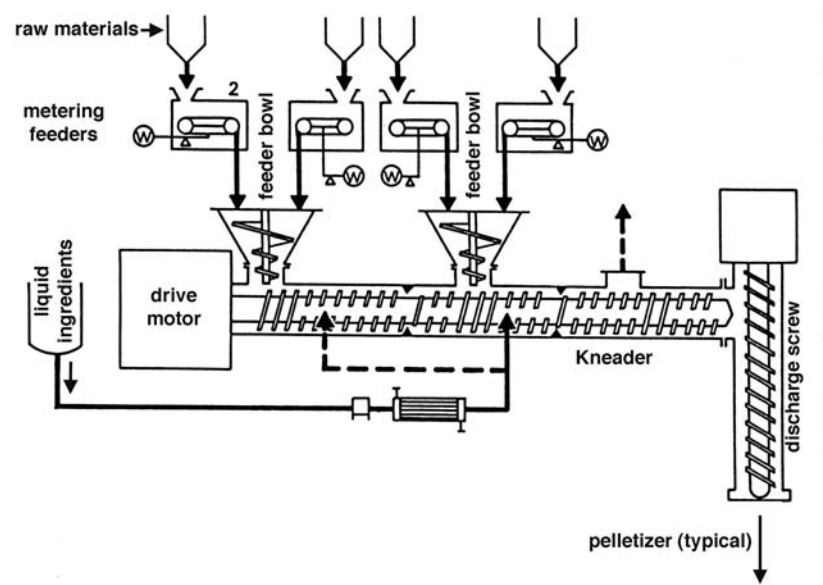


Figure 1-4 Illustration of a Buss Mixer

It is rare to use a Buss mixer for multi-stage compounding operations. In Figure 1-4, the output of the Buss mixer is directly fed into a feed screw machine where high pressure forces the compound through a die or into a pelletizer head.

Multistage Mixing

In some cases, polymers may be compounded from simpler starting compounds formed with two or more of the raw materials. These are identified as master batches and are often prepared when bulk addition to a single stage process would cause them to separate or to alter the bulk polymer properties during mixing to the point where mixing would be inefficient.

Proper dispersive mixing, which focuses on short-range blending of the compound, is achieved through careful selection of the proper mixing screw, mixing temperature, screw rotational speed, back-pressure, sequence of addition, and proper preparation of the raw materials to avoid caking. Distributive mixing, which addresses the overall homogeneity of the batch, is controlled in a single compounding operation by careful and absolutely consistent metering of raw materials. Without a second mixing step, distributive mixing is limited to the volume of compound contained within the mixer barrel. Improved distributive mixing can be achieved where the compound is prepared in two stages.

Mixer Cleaning

Cleaning of the mixer is required between runs and when changing to a different compound. In some cases, the extruder is torn down and the barrel and screws are mechanically cleaned. An alternate method is to run a high-shear cleaning compound through the mixer, followed by a purge period with the new compound before production of the new compound begins. Some types of compounds with sensitive end-use considerations are isolated to particular machines to protect against carryover risk.

Final Form

Thermoplastic compounds are most commonly supplied in the form of pellets. These are formed by extrusion of the polymer through a strand-forming die plate with a pattern of round holes. This is run under water, in a water-spray environment, or in a chilled airstream. As the hot polymer is extruded, a continuously rotating blade cuts the polymer strands into short segments, thus forming the pellet geometry. With water-cooled pelletizing, the quality of the quench water must be controlled to prevent contamination.

Methods of Compounding: Crosslinked Elastomers

Elastomeric compounds are typically prepared in a two-stage process. The base polymer enjoys a certain level of fluidity, so it typically does not require much heat addition for processing. Since the viscosity is very high and does not lower significantly with temperature, mixing requires very high shear of the ingredients. Mixers contain two intermeshing counter-driven rotors, Figure 1-5, each of which has a complementary lobed or convoluted profile. These profiles serve to shear the compound in the gaps, while also circulating the ingredients. The profiles vary and are recognized typically by the mixer manufacturer, such as Farrell (Figure 1-6), Banbury, Francis Shaw, Werner & Pfleiderer, and others. The rotors are enclosed in a heavy casing since the internal pressure and shear energy are very high. Mixers are water-jacketed so that the frictional heat developed during mixing can be removed through a heat exchanger. With the completely enclosed internal mixer, compounds are prepared in one batch. In other words, all ingredients get introduced and co-mixed in a closed mixing cycle. A variation of this technology will be described later in this chapter.



Figure 1-5 Intermeshing Rotors from Internal Mixer

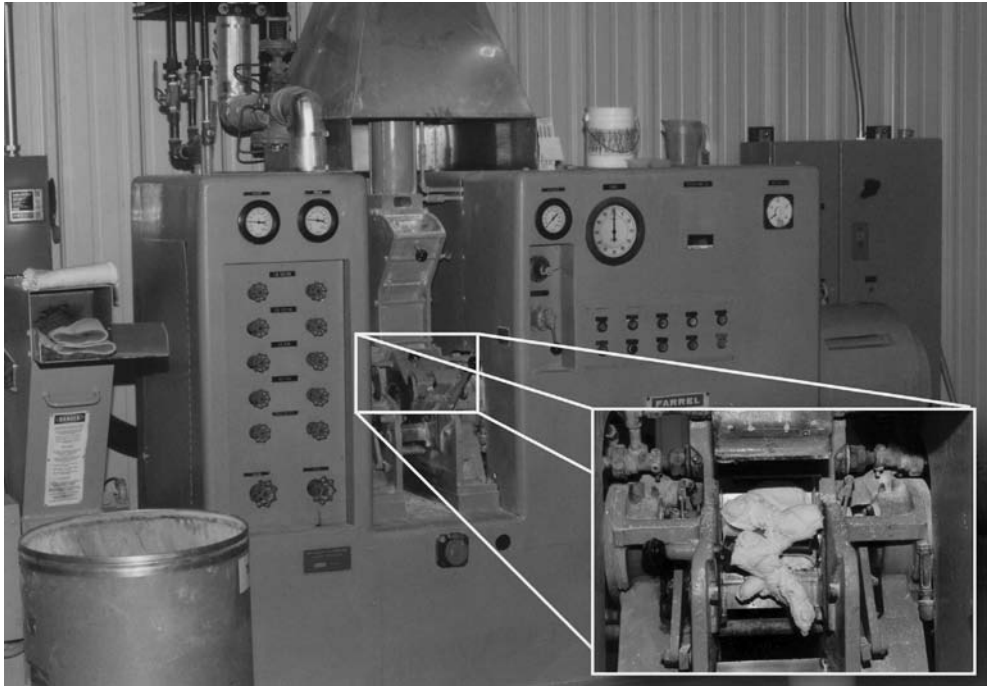


Figure 1-6 Photograph and Close Up of Farrell Internal Mixer

Batch Mixing

Mixing occurs in stages, beginning with the base polymer. This is pressure-fed into the mixer by injection of a bale, strips, or pellets, using a hydraulic or pneumatic ram. The polymer heats and its viscosity reduces, then the inorganic ingredients are added. Processing aids such as carboxylic acids may be added to help reduce shear and to improve wetting of the inorganic compound. If an external antioxidant is needed, this would be added with or before introduction of the reinforcement to protect the polymer against oxidation. Liquid processing aids and coupling agents may be added first to the inorganic so that they are not lost during processing. Due to the extremely fine particle size and low density of carbon black, this is normally added in the form of a high concentration of carbon black in the base polymer or other polymer, separately prepared into a master batch by twin-screw mixing.

In other stages of mixing, additional polymers, waxes, extender oils, and internal lubricants might be added. Addition sequence is driven by melting temperature, viscosity and thermal stability of the ingredient. Internal mixers are sealed against leaks of high viscosity, cohesive elastomer compounds, however ingredients in liquid form will not be retained in the mix unless added in master batch form or blended with inorganic ingredients.

In a final mixing step, the crosslinking agent is added. Internal heat generation in the mix must be low enough to prevent the peroxide from decomposing and initiating a crosslinking reaction within the mixer.

Internal mixers must be run in a full or nearly full condition, so a batch recipe is calculated to provide an appropriate volume. If not filled, the ingredients will not be properly sheared and heat transfer will be compromised. Typical commercial mixers have a batch size of at least 100 pounds of compound. A mixer of this size will have a drive motor of no less than 75 horsepower. Proper dispersive mixing is a balance between proper shear, sequence of addition of ingredients, and thermal stability. Mixers have extensive monitoring instrumentation that provides continuous feedback about thermal conditions, rotor torque, and rotor speed. Once a mixing process has been developed, a standard protocol is followed for preparation of the compound.

An internal mixer provides the shear necessary to mix a raw elastomer with its compounding ingredients. It is imperative that the compound is homogeneous throughout the batch so that its properties are uniform. For distributive mixing, a second stage of mixing is used. In many cases, an internal mixer is mounted above a two-roll mill, Figure 1-7, and when mixing is completed a bottom hatch is opened, allowing the compound to fall onto the two-roll mill. In other cases, the compound will be transported to the mill.

Processing

A two-roll mill consists of two large diameter counter-rotating cylinders, with a variable gap between them. The rolls are maintained at a fixed temperature through internal fluid heating and an external heat exchanger. The elastomer compound forms a sheet on the roll surface. This is continuously cut into wide strips by the operator, folded over, and placed back on the rolls. This process is repeated for perhaps 15 minutes to assure that the compound is fully homogenized.

In some cases, the curing agent is added during the milling operation, generally in the form of a master batch. This practice is used for peroxides that decompose at a lower temperature, to reduce the risk of accidental curing in the internal mixer, when localized temperature can be very high.

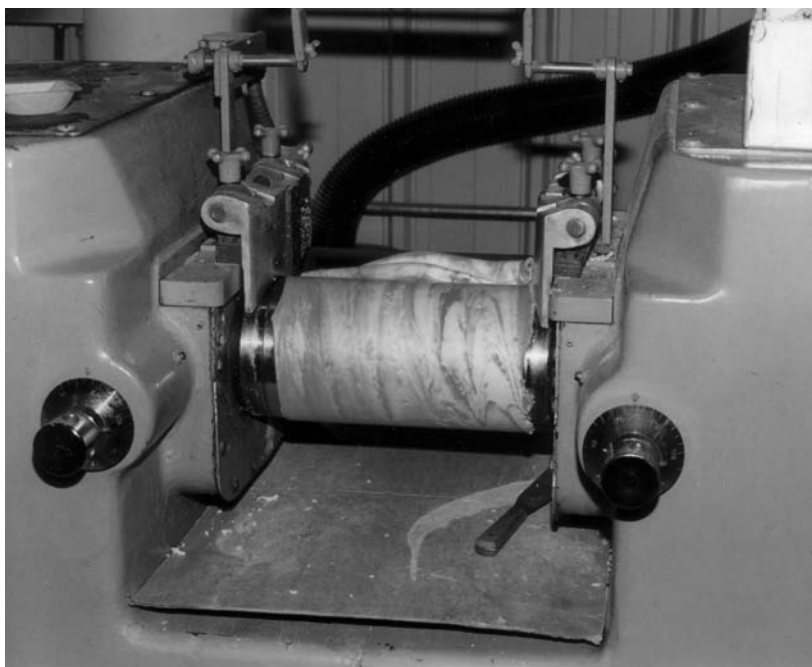


Figure 1-7 Laboratory Scale Two-Roll Mill

With a closed mixer, control of distributive mixing is inherently good, since all materials are added in a single batch and mixing occurs in two stages. Failure to add an ingredient or to improperly treat raw materials may lead to dispersion and homogeneity problems.

Continuous Mixing

A second type of elastomer compounding makes use of a continuous mixer. This type of machine is most often used where a high volume of rubber compound is required to feed large production lines for applications that include tires, sheet rubber products, cable insulation, hoses, belts, and others. Figure 1-8 is an illustration that shows the internal configuration of a continuous mixer. This is a hybrid design that features a feed screw, similar to a screw type mixer that feeds raw materials into a heated high shear rotor type mixer. As shown in this figure, raw materials are fed continuously and mixed compound is continuously discharged. Control of dispersive mixing is achieved by designing a process that optimizes residence time in the mixer, rotor speed, temperature, and rotor profile. Continuously blended rubber compound is typically transferred directly to a two-roll or calendaring mill for distributive mixing.

Since internal mixers can be opened for material feed and compound removal, these are generally simpler to clean when compared to screw-type mixers. It is a common practice to run natural rubber or special high-tack, cohesive compounds through a mixer as a final stage of cleaning. Further, the first batch of compound is typically sacrificed or saved for experimental work following clean-out.

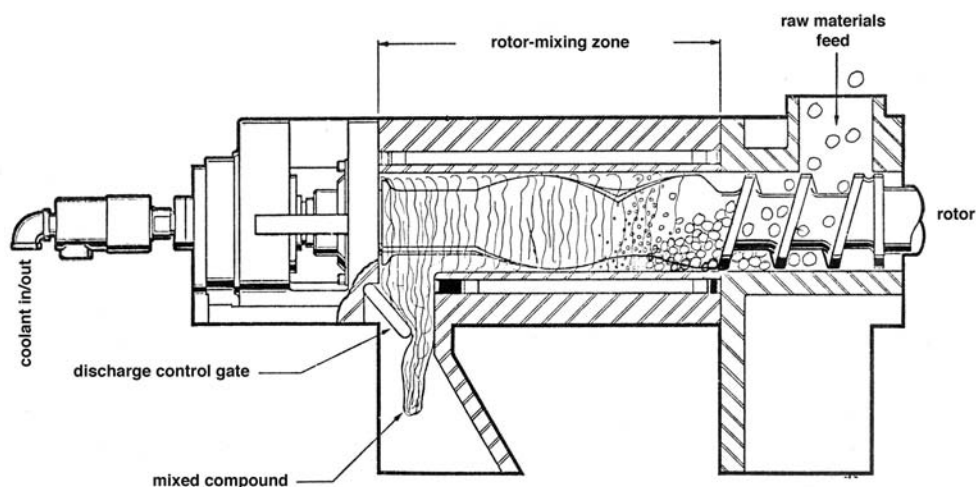


Figure 1-8 Continuous Mixer for Elastomer Compounding

Mixer Cleaning

Cleaning of the two-roll mill is a simple operation since the compound only contacts the exposed external surface of the rolls. Typically a natural rubber compound may be used for surface cleaning and/or the first batch of polymer compound might be used for this purpose.

Intermediate Forms of Compounds

Strips of elastomer compound can be manually or automatically cut directly from the milling operation and placed into release packaging. In other cases, the warm compound might be placed directly into an extruder where it is pressed through a cylindrical or rectangular die and cut into short sections or coiled for subsequent use. In all cases, non-crosslinked rubber compounds cohere strongly, therefore a release agent (anti-blocking compound) or physical method is required to maintain a manageable form of the compound. Surface treatment options are significant. These may include water baths with talc, direct application of talc, treatment with the same inorganic in the compound, surface wetting with silicones, and others. Physical treatments include release films, physical separation of pre-forms onto release layers, or packaging into trays that prevent contact between pre-forms.

The more amorphous grades of elastomer compounds tend to have high surface tack before crosslinking, so the elastomer in the form of pellets tends to form an inseparable bond between pellets. Blocking can be reduced by the addition of an inorganic anti-blocking ingredient, such as talc. This is generally added in a water slurry, so that the talc coats the exterior surface of the compound with a very thin layer. Surfactants are often used to enhance talc coating of the surface. In some cases, organic anti-blocking agents are used.

Prior to crosslinking, softer grades of elastomer compounds flow slowly, so these cannot be produced in a form that is unconstrained. A common intermediate form of such compounds is long, continuous ribbons that are dusted with a release agent and coiled. Sheets or other forms can also be hot-pressed, dusted, and shipped with release packaging that helps to separate the layers for subsequent processing. In still other cases, the elastomer compound is wrapped into polyethylene

sheet to hold its shape and to protect against contamination. In this approach, the elastomer bonds to the packaging material and both are blended in the final extrusion operation.

Final Form

Crystalline forms of elastomer compounds can be produced into pellet form in some cases. These are typically pressed in a compression molding operation or in a continuous molding press, resulting in pellets that are about 0.5 inch diameter. If a compound has a high density, it may retain its shape sufficiently to allow it to be packaged into gaylords in pellet form. Contracted forms are often supplied from compounders to molders. The latter might specify compounds in the form of molded disks which can then be fed directly into molding machines where the final forms are produced and crosslinked.

Extraction and Analysis

Introduction

As discussed throughout this work, the identification, classification and suitability of additives directly affects the cost and/or profit of end-use products. Included in this area are product quality, production control and product aging/weathering. A particular additive may contain several components, but only list the major one in the description. Therefore it is important also to know the composition and purity of the additives themselves. This is best achieved by developing and/or acquiring an inventory of well-defined standards. The authors have seen numerous examples of additive-associated problems which have been traced to poorly characterized materials employed at the front end of the production cycle. The use of such materials can result in serious legal and/or financial problems for the end-use manufacturer. Additionally, the use of plastics additives is becoming a target for scrutiny by regulatory (FDA) and environmental (EPA) agencies (e.g. food-related materials).

Extraction Methods

The above factors have proven to be justification for the development and implementation of a variety of extraction methods which have been reviewed periodically (1-5).

Table 1 lists methods commonly used to extract additives from various types of plastics/polymers.

As seen in Table 1, extraction methods are divided into two basic groups - liquid/solid and thermal desorption. Both groupings may employ sample preparation techniques such as grinding or cutting to increase surface area and improve extraction efficiency.

Table 1 Extraction methods for additives

Method	Comments	References
Preparation: Grinding and Cutting of Plastics	Increase the surface area via ball mills/cutting mills - ambient or cryogenic temperature. Suitable for liquid/solid and thermal desorption methods.	(2)
Dissolution/Reprecipitation	Dissolution of plastic in suitable solvent or solvent system. Direct analysis or precipitation of polymer with non-solvent.	(2), (6)
Sonication	Use of ultrasound energy to agitate the plastic, releasing additives.	(7)
Soxhlet Extraction - Traditional and Improved (i.e. Randale)	Solvent extraction of solids - choice of solvent or solvent system.	(5), (8)
Focused Microwave assisted Soxhlet Extraction (FMASE)	Water is used as the extractant in the application of focused microwaves to enhance the extraction.	(9)

Table 1 Extraction methods for additives

Method	Comments	References
Accelerated Soxhlet Extraction	Sample is extracted with a suitable solvent at elevated temperature and pressure.	(10)
Supercritical Fluid Extraction	Use of supercritical fluid CO ₂ to solubilize and extract additives	(11)
Pyrolysis GC/MS	Pyrolysis of polymers and additives identified by interpretation of MS programs.	(12)
Thermal Desorption (indirect)	Thermally desorb additives into traps or directly onto chromatography column.	(13)
Thermal Desorption (direct)	Vacuum/thermal desorption/extraction via direct MS direct insertion probe - no separation.	(5)
Thermal Desorption (direct)	Direct thermal desorption from sample located within the injection port liner (see discussion below).	

Efficient extraction of the additive(s) is important for accurate compound identification; and essential in attempts to quantify them. Realistically, however, factors attributed to both the plastic matrix (non-homogeneous mixing of the additives) as well as the extraction methods employed (insolubility, decomposition, rearrangement and/or loss during the extraction) make accurate quantitative analysis a difficult goal to achieve.

While the inherent thermal decomposition of some additives such as light stabilizers has initiated the development of less destructive techniques like supercritical fluid extraction (SFE), it does not preclude the use of thermal desorption methods. Actually, the thermal decomposition products of the additives can be used to assign an identity to a particular compound.

The authors have developed a thermal desorption technique based on the heat of a gas chromatograph (GC) injection port. In this technique, a plastic/polymeric sample is placed into the injection port liner (Figure 2-1). In our Agilent GC/MS system, we utilize a split liner with an inside cup (Agilent part number 18740-80190) for ease of handling, and to improve the efficiency of the technique, we have installed the agilent flip top inlet sealing system to the 6890 GC of our Agilent GC/MS system. For lower molecular weight plastic samples, we insert a loose-fitting plug of aluminum foil into the liner ahead of the sample to prevent melted plastic from flowing into the cup portion of the liner. In addition to prolonging the use of a liner, it prevents any melted material from fouling the injection port and/or the GC column during the analytical run. Although we prefer this liner, there are a number of configurations offered by suppliers which would satisfy the requirements of this technique.

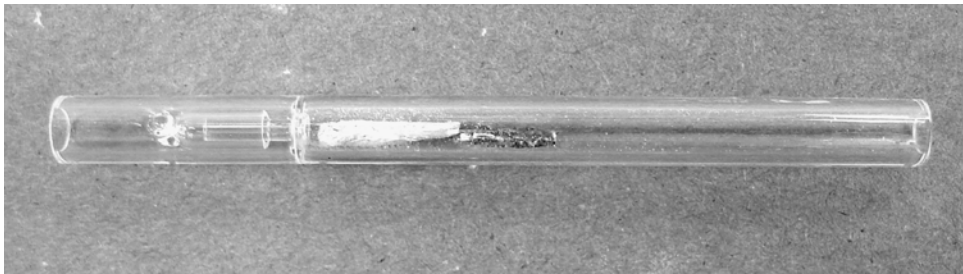


Figure 2-1 Plastic in Injection Port Liner

The heat from the injection port liner combined with the GC column flow causes the volatiles contained in the sample to be thermally desorbed directly onto the GC column. This reduces or eliminates interfering components of the sample matrix. An example of this “additive specific” extraction is shown in Figure 2-2. This technique also can be used to obtain the purity and identity of neat additive standards which are not readily soluble. By altering the injection port temperature, an analyst can extract various types of additives without thermally degrading the sample matrix. There are no limitations on the additive/polymer combinations which can be analyzed. Another advantage of this technique is that it requires only a few milligrams of sample; typically 2-5 milligrams per analysis.

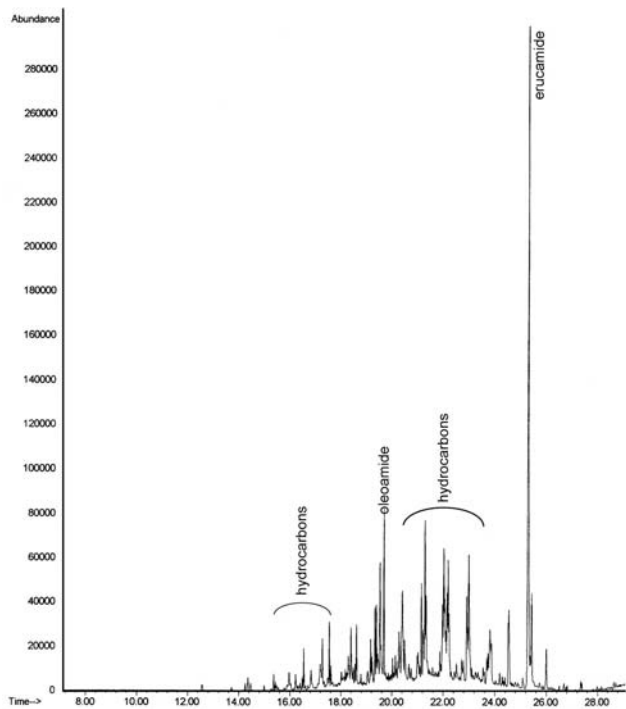


Figure 2-2 Additive Specific Extraction of a Polyethylene Plastic Bag

In addition to being an efficient and reliable extraction technique for the qualitative analysis of additives from a variety of plastic/polymeric matrices, there are additional applications where this technique can be used to provide information on the sample matrix. Sequentially increasing the

extraction temperature (injection port temperature) can provide insight into the efficiency of the polymer cross-linking process without resorting to the destruction (pyrolysis) of the sample. Also, the thermal stability of the polymer/additive interaction can be monitored. This can result in an approximation of thermal aging and thermal decomposition of the plastic/polymer matrix. The authors have used this approach when studying underground cable failures.

Analytical Methods

The emphasis of this work is on the analysis of plastic additives through gas chromatography/mass spectrometry (GC/MS). GC/MS systems are a common analytical tool in quality control and analytical service laboratories; and electron impact (EI) mass spectra are recognized as reliable data for the identification of organic compounds. Traditional methods have employed a flame ionization detector (FID) with identifications based solely on GC retention time data. These methods lack the specificity necessary to distinguish between components attributable to the sample matrix or the additive(s).

Of course, there are additives which may require an inorganic analysis technique. An example is shown in Figure 2-3 which depicts the energy dispersive spectroscopy (EDS) spectrum of Akro fax A, elemental sulfur. However most additives are based on organic compounds and are suitable for GC/MS analysis. The main weakness of this technique is the maximum molecular weight limit since a number of additives possess molecular weights in excess of 1000 daltons. This shortcoming has been addressed by recent advances in both quadrupole and time of flight GC/MS instruments which have extended upper ranges above 1000 daltons.

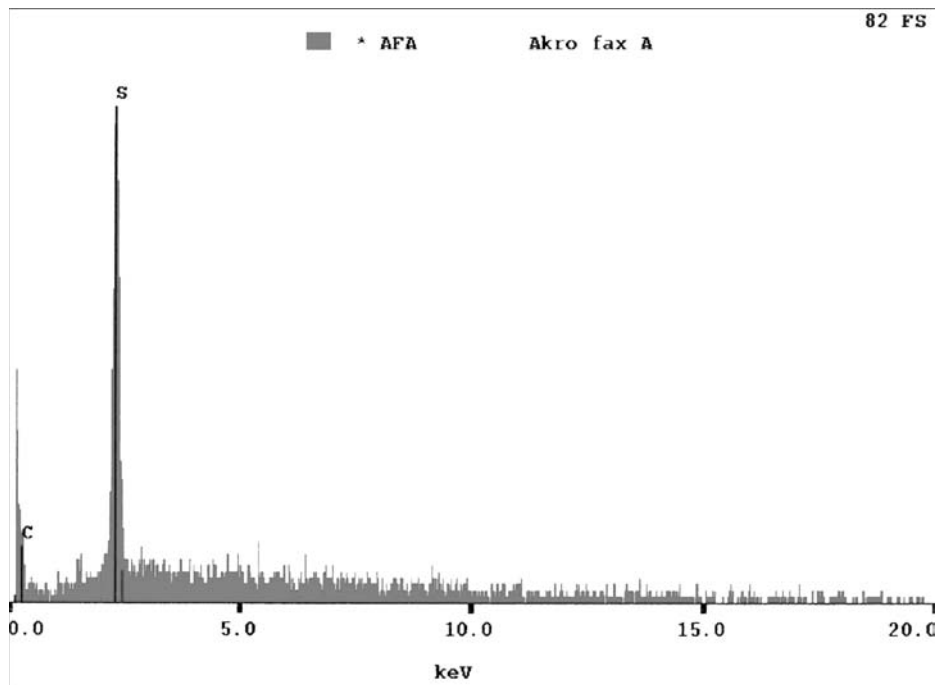


Figure 2-3 Energy Dispersive Spectrum - Elemental Sulfur

Despite the fact that a molecular ion cannot be attained for some additives, the characteristic ion fragmentation pattern can be used to classify the type of additive used. An example of this is illustrated in Figure 2-4, which depicts a (di-tert-butyl-4-hydroxyphenyl)propionate moiety of

Ethanox 310. Several antioxidant additives are based on this type of structure. Without identifying the molecular ion of the molecule, an analyst can establish the fact that a substituted propionate type of antioxidant is present in the material. It is this premise which is the basis for the value of the MS data.

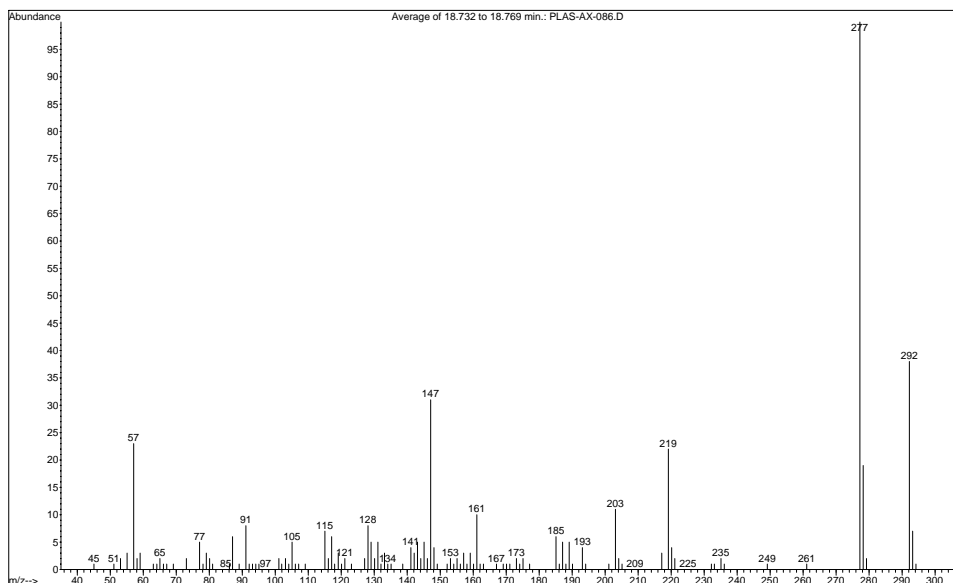


Figure 2-4 Ethanox 310 Propionate Moiety

Instrumental Conditions

All standards and “real-world” samples were chromatographed using a 30 meter, 0.25 mm i.d., 0.25 micron film MS-5 column (QuadRex Corporation, Bethany, CT).

The additive standards for the MS library were dissolved in a suitable solvent and a sample was injected into the GC/MS system, or a sample was transferred into an injection port liner as is done for “real world” samples. Additive standards were run at temperature program rates of 10 °C or 15 °C due to the lack of the necessity for multi-component separation. The actual temperature program used is listed on each Total Ion Chromatogram (TIC).

GC conditions for all standards:

- Injection port: 220 °C
- Temperature programs: 50-330 or 340 °C
- Temp. program rates: 10 or 15 °C

MS parameters:

- MS transfer line: 310 °C
- MS source temp: 230 °C
- Threshold: 500
- MS mass range: 45-800 daltons

Determining the instrumental conditions for “real world” samples involves some trial-and-error. As was discussed earlier in this chapter, the injection port temperature is critical for the success of this extraction technique. The authors have achieved good success for most samples with injection

port temperatures in the 180-220 °C range. In our experience a starting oven temperature of 50 °C is adequate to reveal any lower boiling range compounds; and a temperature program of 8-10 °C/minute provides sufficient chromatographic resolution for all but the most degraded samples.

Sample Size of “Real-world” Samples

A sample size of 2-5 milligrams produces enough data to obtain a good chromatographic and MS profile of any additives. In cases where a large amount of the plastic/polymer is analyzed, multiple samples should be done to ensure the homogeneity of the sample matrix.

System Maintenance

Gas Chromatograph

Although good laboratory practices dictate a comprehensive scheduled maintenance program, plastic/polymer and additives samples present a unique problem. They include a broad range of materials and chemicals which have a variety of physical properties; and obtaining accurate analytical results require diligent instrument maintenance and an adequate consumables budget. Compounds which are easily soluble in an organic solvent can foul both injection port liners and GC syringes when injections are made. Cleaning syringes immediately after use ensures that the syringe barrel and/or needle will not become plugged. Some plastic/polymer samples could melt into the retainer cup of the liner which renders it unfit for further use. Consequently, we like to keep 8-10 clean and silanized liners ready for sampling. Liners should be cleaned on a regular basis. After each analysis, we use organic solvents in an ultrasonic bath to remove any sample/additives residue. This is followed by heating to 300 °C for 30 minutes. All liners are silanized after several cleanings to ensure that there is minimal interaction between the sample and the glass surface. Depending upon the type of GC used, it also may be necessary to change the injector seal and washer as they come in contact with the volatiles from the sample. Split vent lines should be cleaned periodically to prevent carry-over and the presence of “ghost” peaks from one sample to another. We routinely cut 2-3 inches from the injector end of the GC capillary column. Since resolution is a function of the square root of the theoretical plates, loss of column resolution is minimal. However, retention data windows, if utilized, must be changed at regular intervals. We also rinse the GC column periodically to remove insoluble components. We use an alternate column during this process to decrease instrument downtime.

Mass Spectrometer

The physical properties of plastic/polymer matrices and additives samples combined with the high GC column temperatures result in the mass spectrometer ion source becoming dirty more quickly than with typical usage.

To limit instrument downtime, and if financially feasible, it is a good idea to have an extra ion source which can be exchanged after venting the instrument. This encourages more frequent source maintenance and provides more consistent analytical results.

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CHAPTER 3

Accelerators

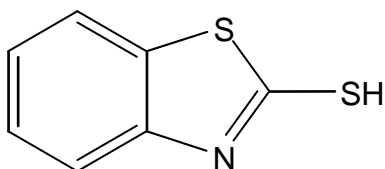
Rubber, in its natural state, is not durable, is very sticky, and will begin to deteriorate in a matter of days. Vulcanization (curing) of rubber is a chemical process whereby polymer molecules are linked to other polymer molecules by atomic bridges. In general, the process is brought about by heating rubber in the presence of sulfur. The end result is that the springy rubber molecules become cross-linked. This makes the final product harder, much more durable and also more resistant to chemical attack.

An accelerator is a substance that speeds up the vulcanization of rubber or allows it to happen at a lower temperature. Accelerators may also enhance tensile properties and improve age resistance of the final product.

Most accelerators are organic substances that contain either nitrogen or sulfur, or both. They can be classed as either primary or secondary accelerators and are often used in combinations, depending on the desired final outcome.

Accelerator MBT, MBT/MG

Akrochem Corporation

**CAS Number** 149-30-4**RTECS Number** DL6475000**Abbreviation** 2-MBT**Formula** C₇H₅S₂N**Molecular Weight** 167.25**IUPAC Name**

2-mercaptobenzothiazole

Synonyms

2-benzothiazolethiol; 2-benzothiazolylmercaptan; 2(3H)-benzothiazolethione

Brand Names & Manufacturers

Captax/Rotax (purified form)

R.T. Vanderbilt Company

Perkacit[®] MBT

Akzo Nobel Chemicals B.V.

Thiotax

Solutia, Inc.

Physical Properties**Appearance** Off-white to yellow powder**Melting Point** 180-182 °C**Boiling Point** 260 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	2.0	10.0	U	U

Application Application, Regulatory & Environmental Information

Used as a vulcanization accelerator for rubber mixes based on natural and synthetic rubbers and in the production of plastics and lacquers.

Regulatory Information

FDA approved 1998 for the following materials to be used in contact with food: adhesive preservatives, 21CFR175.105; a rubber accelerator (up to 1.5% of weight of rubber), 21CFR177.2600; in the synthesis of slimicides for use in paper/paper-board, 21CFR176.300; an adjuvant in the manufacture of foamed plastics, 21CFR178.3010. Listed in 40CFR136.1 and USEPA Method 640: The Determination of Mercaptobenzothiazole in Municipal and Industrial Wastewaters.

Environmental Impact

Does not biodegrade in river water in 8 weeks. Slightly susceptible to indirect photolysis. Medium to low mobility in soil, and marginal to no mobility in sediment. This substance may be hazardous to the environment; special attention should be given to fish. Log Pow value of 2.41 indicates a low potential to bioaccumulate.

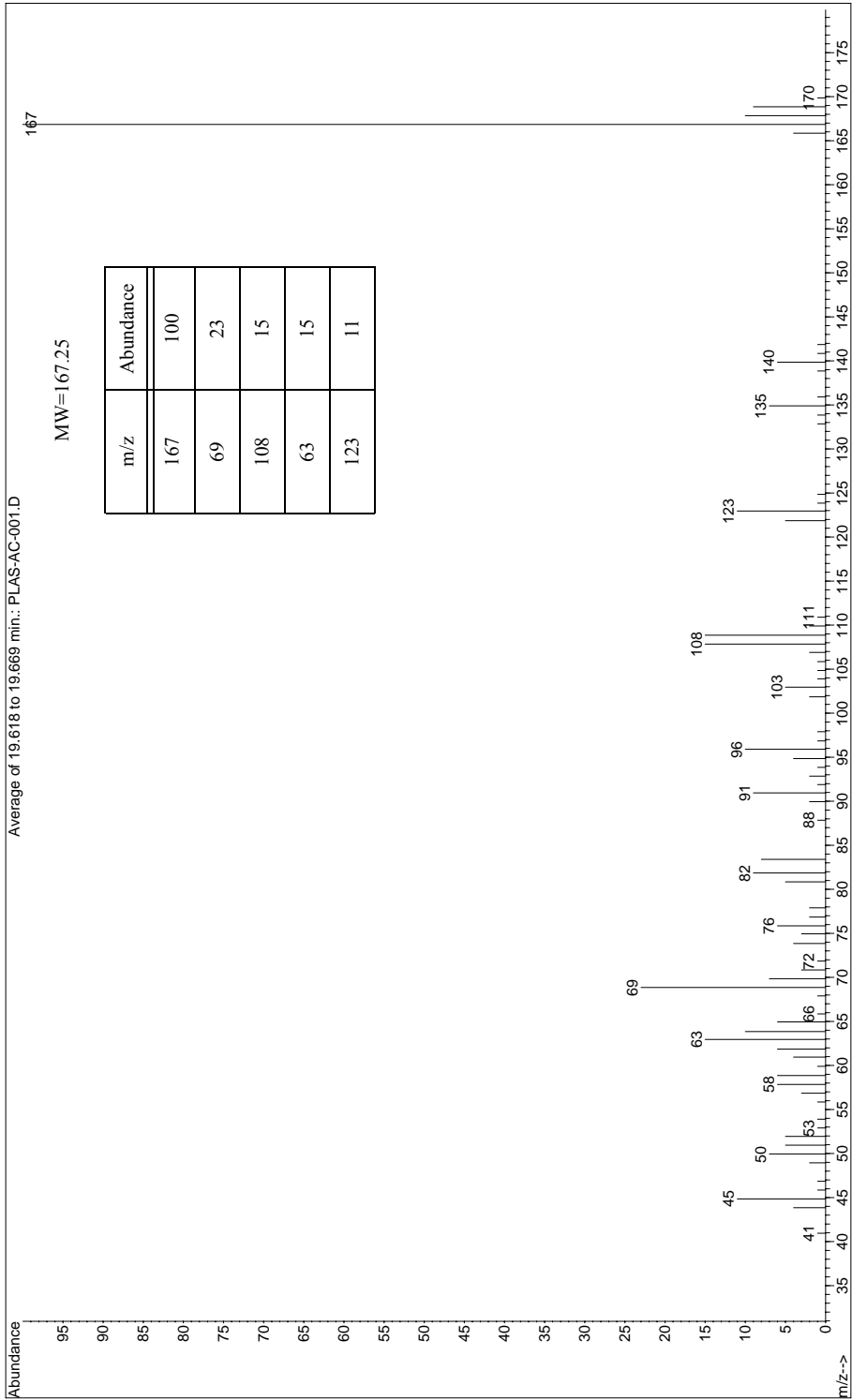
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

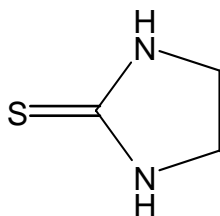
A 2-year NTP study on rats indicates evidence of carcinogenic activity in rats gavaged with 750 mg/kg BW (male) and 375 mg/kg BW (female). No carcinogenic effect on bacteria and yeast cells.

Mass Spectrum for Accelerator MBT, MBT/MG - PLAS-AC-001



Accelerator ETU-22 PM

Akrochem Corporation

**CAS Number** 96-45-7**RTECS Number** NI9625000**Abbreviation** ETU**Formula** C₃H₆N₂S**Molecular Weight** 102.11**IUPAC Name**

ethylene thiourea

Synonyms

2-imidazolidinethione; 2-imidazoline-2-thiol; 2-mercaptoimidazoline

Brand Names & Manufacturers

Pennac® CRA

Pennwalt Corp.

Nocceler® 22

Ohuchi Shinko Co., Ltd.

Soxinol® 22

Sumitomo Chemical Co., Ltd.

Vulkacit® NPV/C

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** White powder**Melting Point** 203 °C**Boiling Point** 347.18 °C**Stability** Stable under normal conditions of use.**Solubility**
(g/100mL 20°C)**Water**
~2**MeOH**
10-40**EtOH**
10-40**Acetone**
<0.1**CH₂Cl₂**
U**Hexane**
U**Application Application, Regulatory & Environmental Information**

ETU is used as an accelerator in the vulcanization of polychloroprene (Neoprene) and other elastomers; for coated fabrics, for epichlorohydrin and for chlorosulfonated polyethylene rubbers. It is also an intermediate for antioxidants, insecticides, fungicides, dyes, pharmaceuticals, and synthetic resins.

Regulatory Information

FDA: Use of ETU as a food additive is prohibited. EPA (1995): Health Advisory for long-term exposure is 0.4 mg/L. Can be monitored in water by EPA Method 509 - Determination of Ethylene Thiourea (ETU) in Water Using Gas Chromatography with a Nitrogen-Phosphorus Detector. FAO/WHO (1993): ADI: 0.004 mg/kg BW.

Environmental Impact

ETU is a trace contaminant and metabolic degradation product of a widely used class of ethylene bisdithiocarbamate fungicides such as Maneb and Zineb. Half-life in H₂O is 7-13 days. Octanol/water partition coefficient as log Pow: -0.66 (calculated).

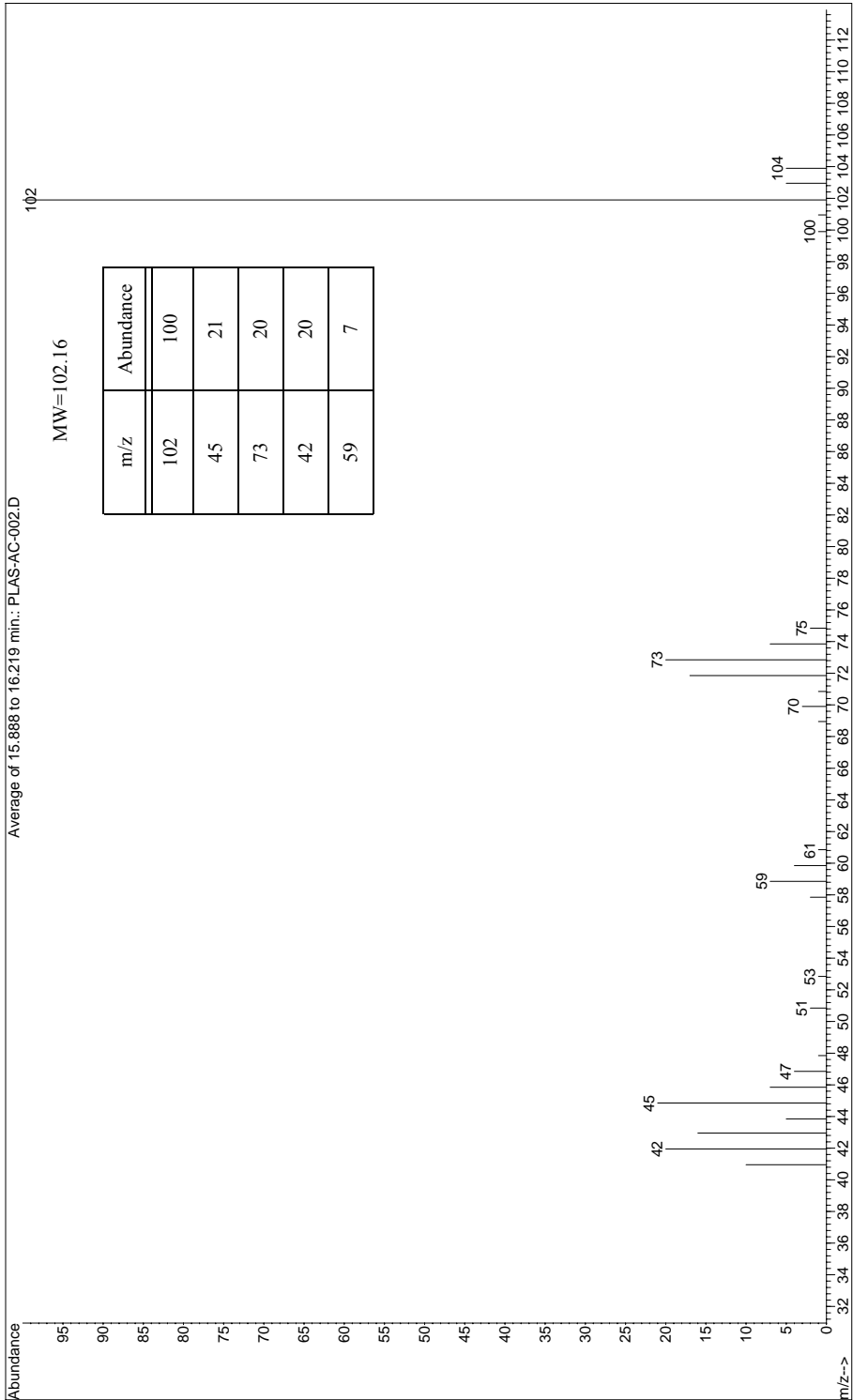
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

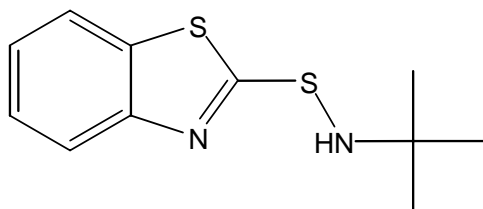
Ethylene thiourea is toxic and known to produce thyroid neoplasms (thyroid hyperplasia) in rats and liver neoplasms in mice following long-term administration; NIOSH: potential occupational carcinogen; NTP: Suspect carcinogen; OSHA: Possible suspect carcinogen. Acute oral toxicity (LD₅₀): 1832 mg/kg [Rat].

Mass Spectrum for Accelerator ETU-22 PM - PLAS-AC-002



Accelerator BBTS

Akrochem Corporation

**CAS Number** 95-31-8**RTECS Number** DL6200000**Abbreviation** TBBS/BBS**Formula** C₁₁H₁₄N₂S₂**Molecular Weight** 238.38**IUPAC Name**

N-(1,1-dimethylethyl)-2-benzothiazolesulfenamide

Synonyms

N-(1,1-dimethylethyl)benzothiazolesulfenamide; benzothiazolyl-2-tert-butylsulfenamide; benzothiazyl-2-tert-butylsulfenamide

Brand Names & Manufacturers

Delac® NS	Uniroyal Chemical Co.
Pennac® TBBS	Pennwalt Corp.
Perkacit® TBBS	Akzo Nobel Chemicals B
Santocure® NS	Solutia Inc.

Physical Properties

Appearance	Cream to buff powder or pellets					
Melting Point	105 °C			Boiling Point	Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water 0.345	MeOH U	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application TBBS is used as a vulcanization accelerator in NR, SBR, BR and rubber blends. Normally used alone or with small quantities of ultra accelerators in tire compounds or other industrial rubber products.

Regulatory Information

FDA approved 1998 for use as an accelerator in the manufacture of rubber material intended for use in all stages of production, processing, packaging and transport of food: 21CFR177.2600.

Environmental Impact

TBBS does not ionize at environmental pHs, is not readily biodegradable, but hydrolyzes in less than 1 day at pH 9 or less. The identified hydrolysis products: mercaptobenzothiazole, di(benzothiazoyl)disulfide, t-butylamine, and benzothiazole are non-volatile, with a low potential for bioaccumulation, and are not readily biodegradable. Indirect photo-oxidation by hydroxy radicals is predicted with a half-life estimated at 2.8 hours. Log Pow of 3.9 at room temperature.

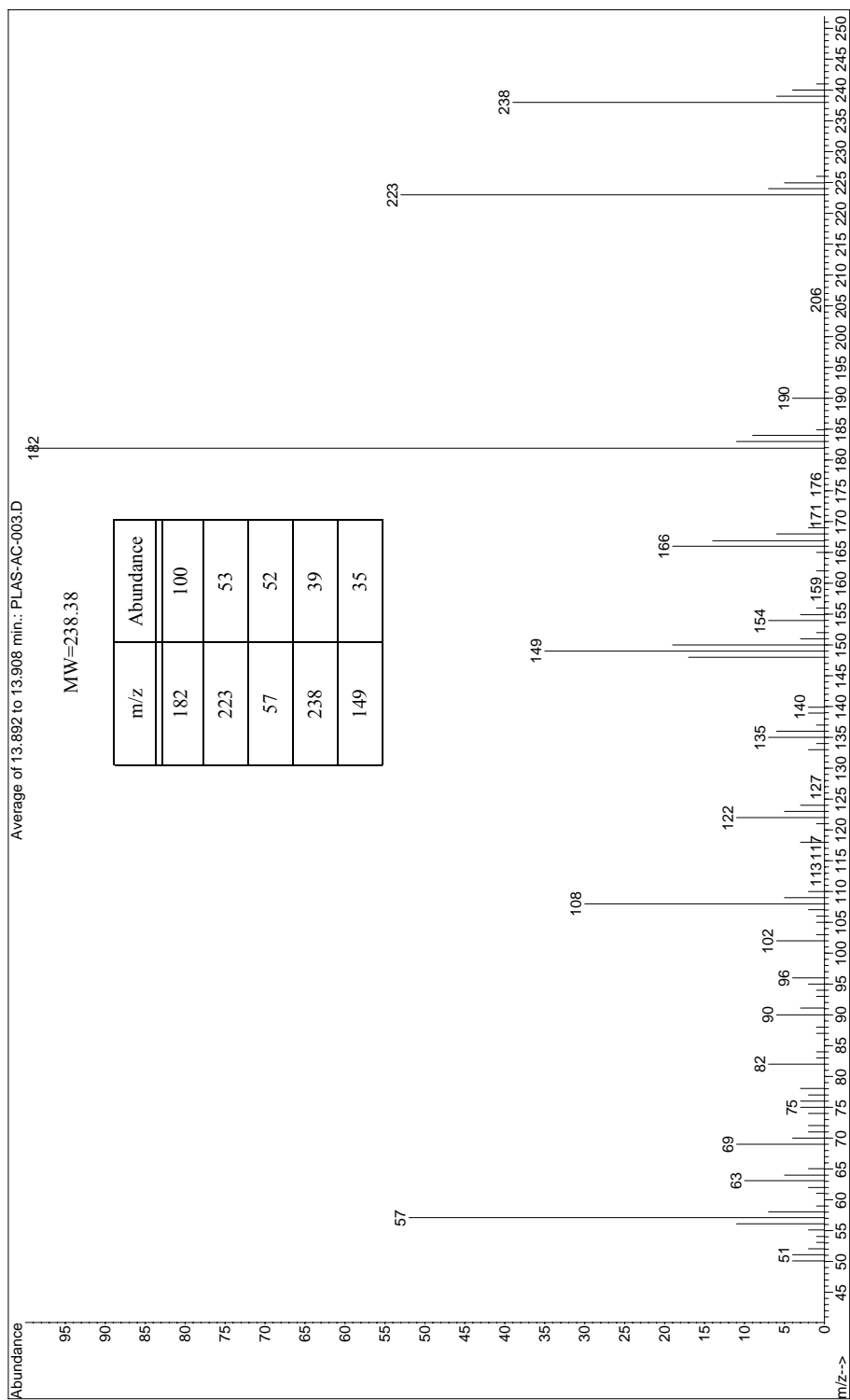
Point of Release

Due to the vulcanization process, finished rubber products contain only small amounts of TBBS or synthesis by-products (benzothiazole, 2-mercaptobenzothiazole and 2-mercaptobenzothiazole disulfide). Release to the environment of these chemicals may occur during the use of rubber products. Fugacity model (Mackay level III) data suggest that it would mostly distribute to soil (if released to the air or soil compartments) and to water (if released to the water compartment).

Toxicological Data

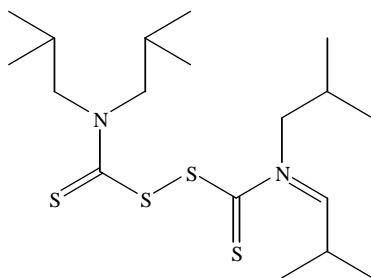
TBBS may be absorbed by the gastro-intestinal route, undergoing hydrolysis in vivo. Studies suggest that the hydrolysis products are toxic primarily to the liver and kidney. It was not found to be mutagenic in bacteria or in vitro mammalian gene mutation assays. It was not genotoxic in an in vivo mouse micronucleus assay. (LD50): >7940 mg/kg dermal [Rabbit]. It did induce chromosomal aberrations in mouse lymphoma cells in vitro with metabolic activation. Carcinogenicity not known.

Mass Spectrum for Accelerator BBTS - PLAS-AC-003



Cure-Rite® IBT

Noveon, Inc.

**CAS Number** 3064-73-1**RTECS Number** Not available**Abbreviation** TIBTD**Formula** C₁₈H₃₆N₂S₄**Molecular Weight** 408.76**IUPAC Name**

tetraisobutylthiuram disulfide

Synonyms

tetra(isobutyl)thioperoxydicarbamic acid

Brand Names & Manufacturers

React-Rite® TIBTD

Resource Innovations, Inc.

Westco TIBTD

Western Reserve Chemical Corp.

Physical Properties**Appearance** Pale yellow to white powder**Melting Point** 70-73 °C**Boiling Point** Not available**Stability** Stable under normal conditions

Solubility (g/100mL 20°C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Used as an accelerator and vulcanizing agent in rubber (EPDM, SBR, Nitrile, and Natural). Especially useful when the formation of nitrosoamines is a concern.

Regulatory Information

FDA approved for use with rubber food-contact materials per 21CFR178.2010 and 178.3860.

Environmental Impact

Due to its low solubility in water and therefore the non-availability to species, this product is not expected to be toxic to aquatic organisms. Estimated log Kow value of 3.4 indicates a low to moderate potential to bioaccumulate.

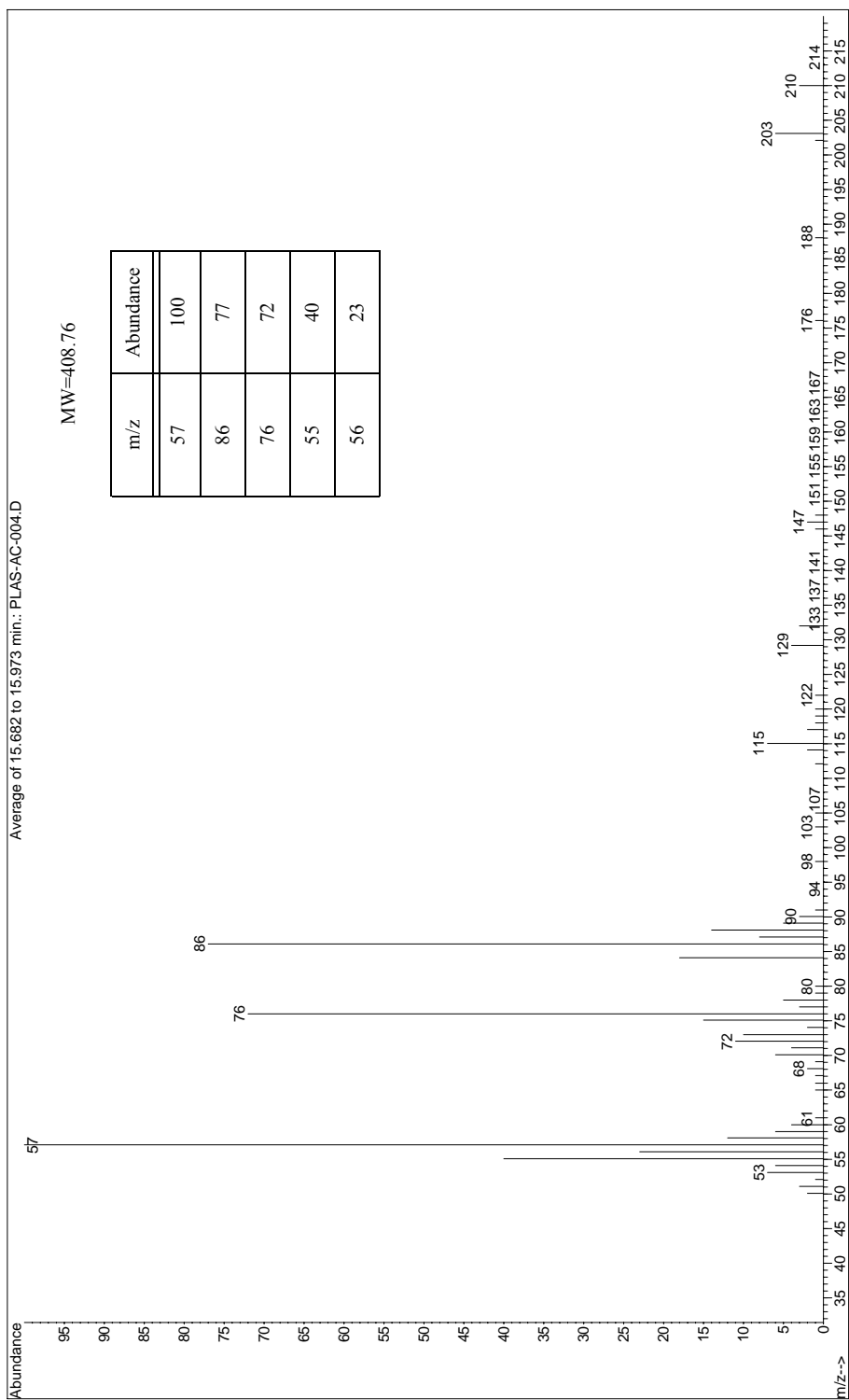
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

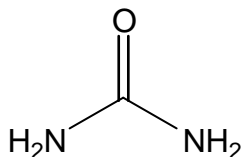
Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Cure-Rite® IBT - PLAS-AC-004



Activator OT Urea

Akrochem Corporation

**CAS Number** 57-13-6**RTECS Number** YR6250000**Abbreviation****Formula** CH₄N₂O**Molecular Weight** 60.07**IUPAC Name**

urea

Synonyms

carbonyl diamide; carbamide; isourea

Brand Names & Manufacturers

Supercel 3000

Varioform II

Physical Properties**Appearance** White solid**Melting Point** 133-135 °C**Boiling Point** Decomposes 135 °C**Stability** Decomposes at 135 °C (MP)

Solubility (g/100mL 20 °C)	Water >80	MeOH ~16	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Urea is used in the manufacture of urea-formaldehyde plastics, adhesives, polymers, synthetic fibers, dyes etc.

Regulatory Information

FDA approved 1998 for the following applications: in the manufacture of resin and polymer-based coatings in contact with food, 21CFR175.300; in the manufacture of cellophane for packaging food, 21CFR177.1200. EU (1990) determined Urea acceptable for use in plastic materials in contact with foodstuffs. In 1993 a joint FAO/WHO Committee on food additives determined 3% urea in chewing gum is not toxic.

Environmental Impact

Although urea has generally low ecotoxicity to organisms, its well documented indirect and long-term effects to the ecosystems, e.g. eutrophication, groundwater pollution, soil acidification and ammonia emissions to air should be considered. When released to soil, this material will hydrolyze into ammonium in a matter of days to several weeks. This material is not anticipated to bioaccumulate - it has a BCF <100.

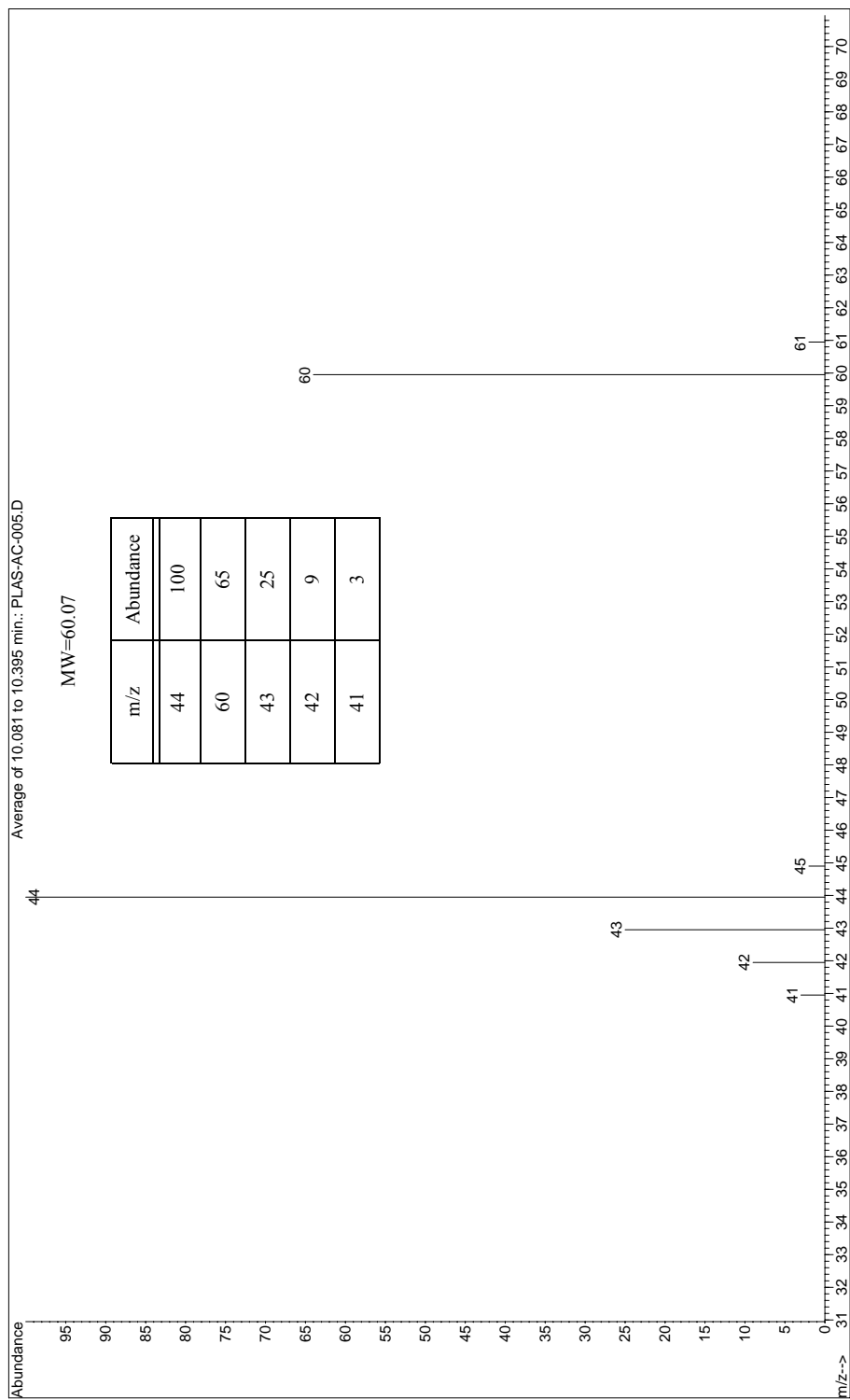
Point of Release

Occupational and environmental exposure during production is possible due to accidental process breakdown and disorders in reactor operations, pumping cycles, evaporation and crystallization processes; in maintenance, loading and unloading operations. Potential occupational exposure occurs via inhalation of aerosols from urea melt and hot saturated solutions, splashed to skin or eyes or inhalation of dust.

Toxicological Data

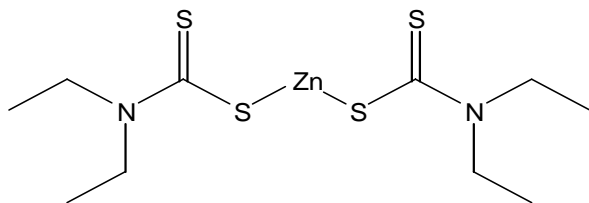
No documented toxic effects at low doses. Chronic exposure is carcinogenic and mutagenic: 821 g/kg [Rat] and 394 g/kg [Mouse] for one year results in Lymphomas and Hodgkin's disease. Long term toxicity: High doses affect cholinergic and bioenergetic processes and modify CNS structure. Acute oral toxicity (LD50): 14.3 g/kg BW [Rat], 11 g/kg [Mouse].

Mass Spectrum for Activator OT Urea - PLAS-AC-005



Accelerator EZ & EZ-SP

Akrochem Corporation

**CAS Number** 14324-55-1**RTECS Number** ZH0350000**Abbreviation** DEDTZ/ZDEC**Formula** C₁₀H₂₀N₂S₄ • Zn**Molecular Weight** 361.93**IUPAC Name**

zinc diethyldithiocarbamate

Synonyms

bis(diethyldithiocarbamato)zinc; diethyldithiocarbamic acid, zinc salt; ethyl zimate

Brand Names & Manufacturers

Ethasan

Solutia, Inc.

Perkacit[®] ZDEC

Akzo Nobel Chemicals B.V.

Soxinol[®] EZ

Sumitomo Chemical Co., Ltd.

Vulcacure

Alco Oil and Chemical Corp.

Physical Properties**Appearance** White powder**Melting Point** 178-181 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	S	S	U

Application, Regulatory & Environmental Information**Application**

ZDEC is used in the following applications: as a fast primary or secondary vulcanization accelerator in NR, SBR, IIR, EPDM and for natural and synthetic latex; a stabilizer in butyl, butadiene, and urethane rubbers; an antioxidant in rubber-based adhesive systems; a stabilizer in cement; a heat stabilizer for polyethylene.

Regulatory Information

FDA approved 1998 for use as an accelerator in the manufacture of rubber material (up to 1.5% of weight of rubber) intended for use in all stages of production, processing, packaging and transport of food: 21CFR177.2600. Regulated for use under 21CFR175.105 for components of adhesives.

Environmental Impact

Ecological impact not determined. Similar compounds show low to moderate biodegradability, but rapid hydrolysis under acidic conditions. Similar compounds are also determined to have low bioaccumulation potential and environmental persistence: 96 Hour LC50 0.23 mg/L [Rainbow Trout], 0.40 mg/L [Bluegill Sunfish], 0.26 mg/L [Fathead Minnow], 48 Hr EC50 0.44 mg/L [Daphnia Magna].

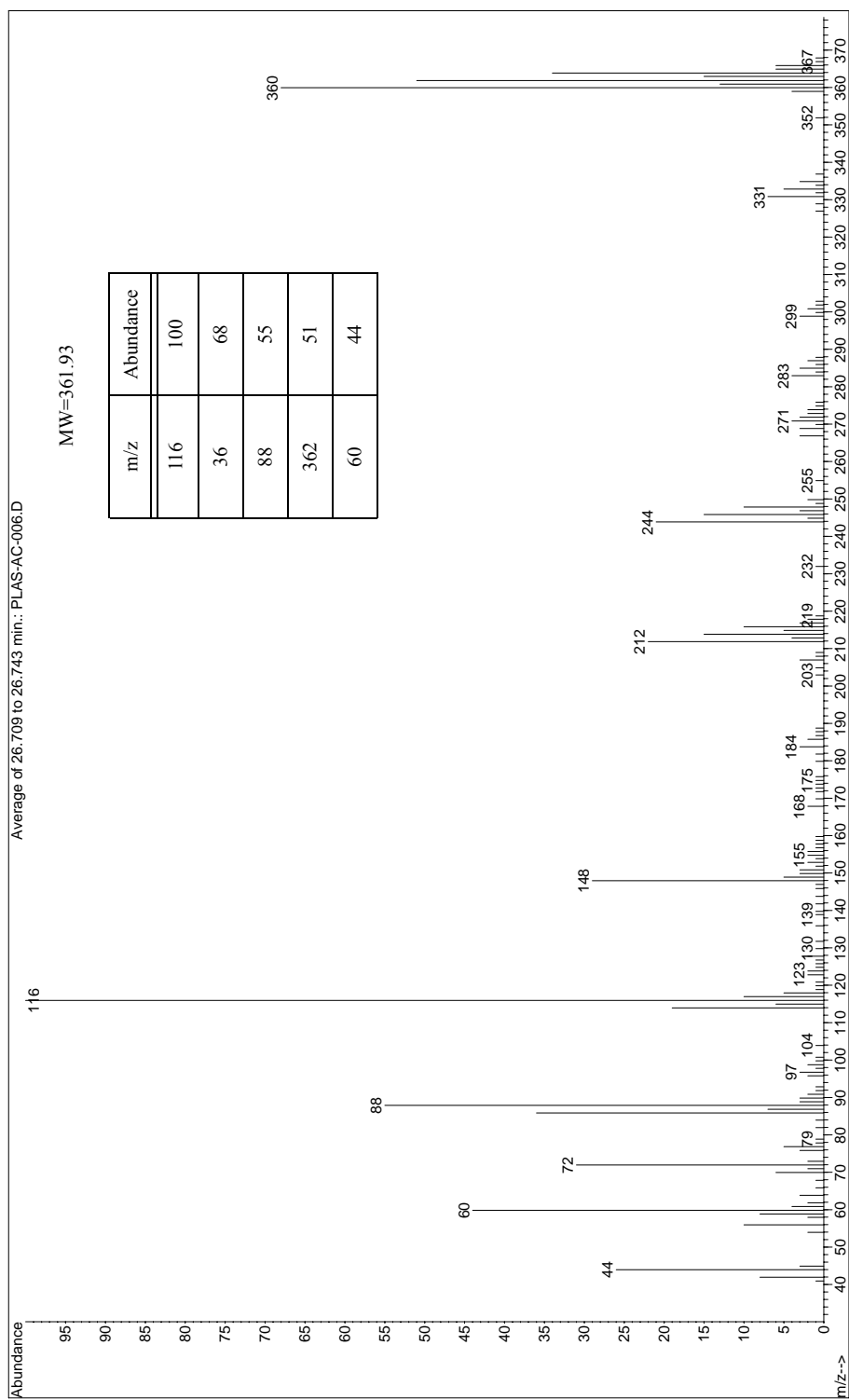
Point of Release

Migration of ZDEC into water after 3 days exposure at 20 °C is 0.6 mg/L.

Toxicological Data

Not listed as a suspected carcinogen by NTP, IARC, or OSHA. Reactions with nitrosylating agents during vulcanization may yield suspected carcinogens such as nitrosamines. Studies of rats and mice gavaged with ZDEC yields no genotoxic, or teratogenic effects. Long-term exposure to large doses may have neurodegenerative effects in addition to altering hydrolytic enzymes in the human brain. Acute Oral (LD50): 3530 mg/kg [Rat]. Acute Dermal (LD50): >3160 mg/kg [Rabbit].

Mass Spectrum for Accelerator EZ & EZ-SP - PLAS-AC-006



CHAPTER 4

Antidegradants

Antidegradant is a generic term for an additive that stops the degradation of the finished plastic product. There are several types of antidegradants. The largest class, by far, is antioxidants, and these are included in their own chapter. The following classes are addressed in this chapter.

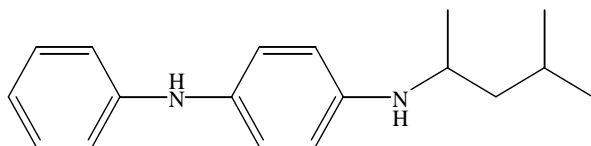
Antiozonants

These materials are added to plastics to slow the deterioration of the finished product that occurs from exposure to ozone. They typically work by migrating to the surface of the product and then create an ozone-impermeable barrier or skin on the surface. More expensive antiozonants work by initiating a reaction with the ozone that prevents their damaging effects.

UV Stabilizers

Ultraviolet radiation from the sun can be very destructive to polymers used in vinyl siding, windows, doors and outdoor furniture. UV Stabilizers help prevent discoloration, cracking, embrittlement and loss of physical properties in these products that may occur upon exposure to sunlight.

The most common UV absorbers used commercially are hindered amine light stabilizers, which can also function as heat stabilizers in some plastics. Other UV absorbers include benzotriazoles and benzophenones, salicylate esters, cyanoacrylates, malonates and benzilidenes. Factors such as the nature of the resin, type and level of pigments being used, and the presence of crosslinkers and catalysts govern the selection of UV absorber to be used.

Santoflex® 6PPD**Flexsys****CAS Number** 793-24-6**RTECS Number** Not available**Abbreviation****Formula** C₁₈H₂₄N₂**Molecular Weight** 268.40**Chemical Name**

N-(1,3-dimethylbutyl)-N'-phenyl-p-phenylenediamine

Synonyms

Brand Names & Manufacturers

Physical Properties**Appearance** Off-white to dark-brown pastilles**Melting Point** 46-51 °C**Boiling Point** 227 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Provides antiozonant and antioxidant properties with high temperature, fatigue and flex resistance to rubber compounds. Used in pneumatic tire components, solid tires, belts, hoses, cables, automotive mounts, bushings and general mechanical products that are exposed to continuous and intermittent dynamic operating conditions that require protection from ozonation.

Regulatory Information

Santoflex 6PPD is not approved for use in FDA food contact applications.

Environmental Impact

Octanol/Water Coefficient: 59000 ± 34000 (Calculated). Log P = 4.68. Chemical Fate Information: Bioconcentration Factor = 490 (calculated). Other Information: Aerobic Biodegradation: 50% after 2.9 hours. Rapid degradation via hydrolysis: 93% after 24 hours at pH 7.0 and 25°C. Tests indicate this material will not bioaccumulate or persist in the environment.

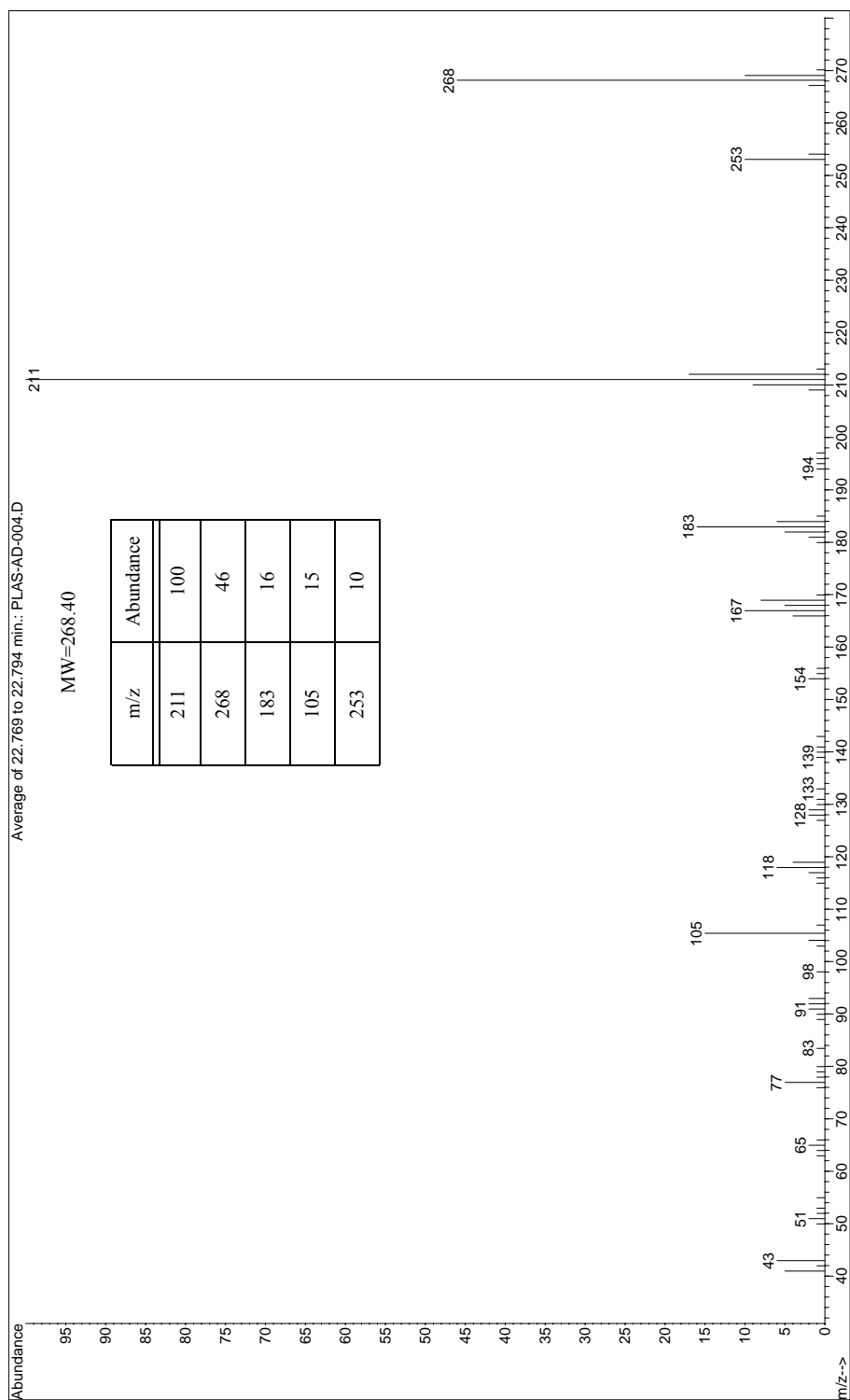
Point of Release

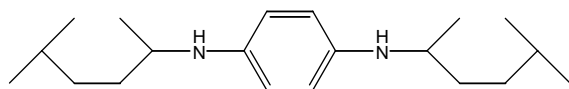
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute Oral (LD50): 3580 mg/kg [Rat]; Acute Dermal (LD50): >7940 mg/kg [Rabbit]. Not listed as a carcinogen or a suspected carcinogen by NTP, IARC or OSHA.

Mass Spectrum for Santoflex® 6PPD - PLAS-AD-004



Santoflex® 77PD**Solutia Inc.****CAS Number** 3081-14-9**RTECS Number** SS8400000**Abbreviation****Formula** C₂₀H₃₀N₂**Molecular Weight** 304.58**Chemical Name**

N,N'-bis(1,4-dimethylpentyl)-p-phenylenediamine

Synonyms

N,N'-di(1,4-dimethylpentyl)-p-phenylenediamine

Brand Names & Manufacturers

Physical Properties

<i>Physical Properties</i>						
Appearance	Dark-red oily liquid					
Melting Point	-36 °C			Boiling Point 183 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ U	Hexane U

Application **Application, Regulatory & Environmental Information**

Santoflex 77PD is used as an antiozonant in natural and synthetic elastomer compounds that can tolerate discoloration (it will discolor compounds and cause severe contact and migration staining). It also protects against catalytic degradation by copper and other heavy metals.

Regulatory Information

Santoflex 77PD is regulated for use in articles in contact with food as specified under BgVV XXI, Category 4 (Germany). Santoflex 77PD is not regulated for use in FDA food contact applications.

Environmental Impact

Acute Fish Toxicity: (LC50 96 Hr): 32 mg/L [Rainbow Trout], 182 mg/L [Bluegill Sunfish], 0.28 mg/L [Fathead Minnow]. Bioaccumulation, potential, 5.34 log Pow. This product rapidly degrades via hydrolysis up to 97% after 24 hours at pH 7.0 @ 25°C. Tests indicate this material will not bioaccumulate or persist in the environment.

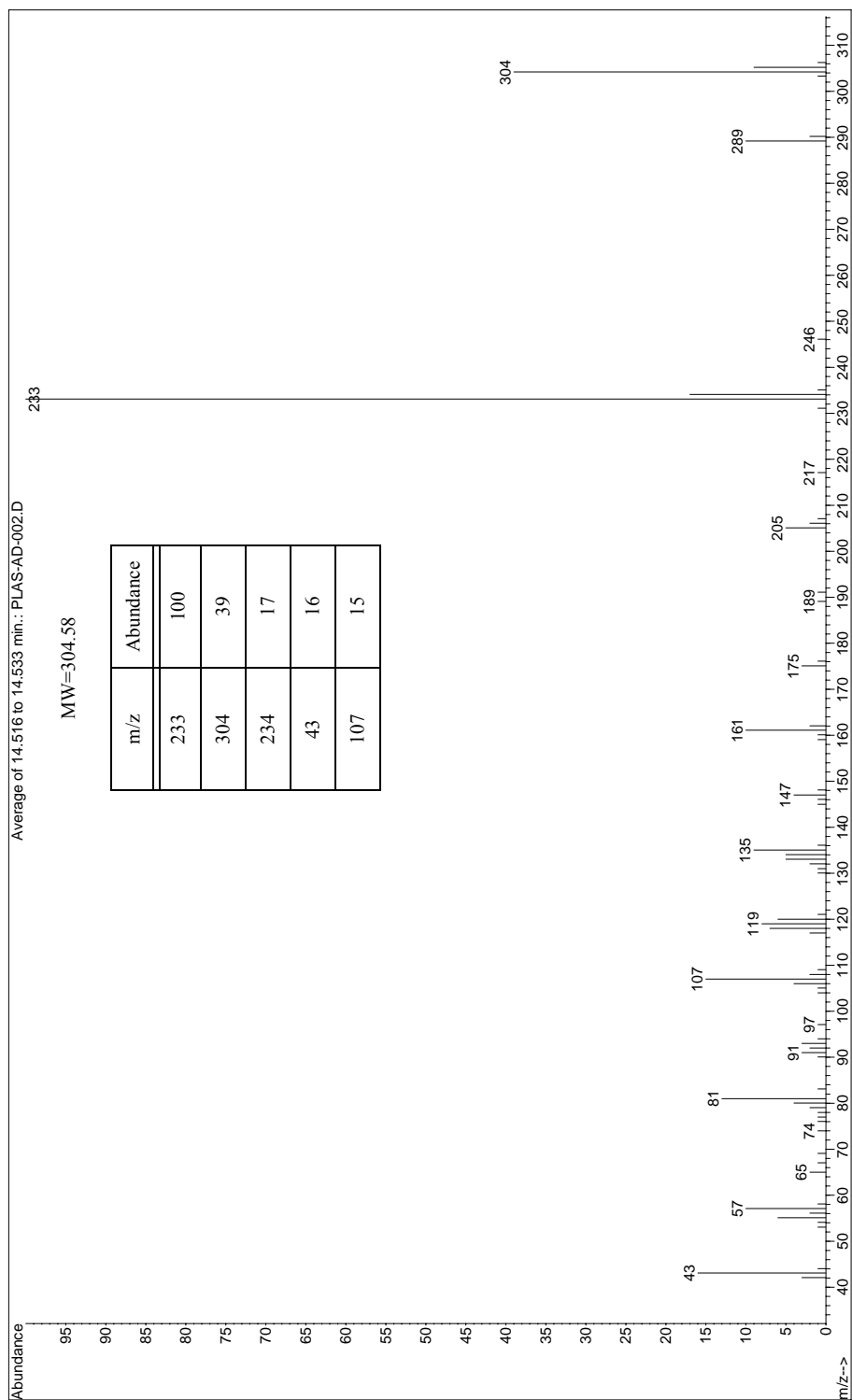
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

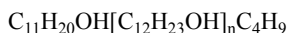
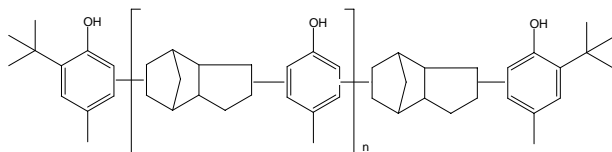
(LD50): 750 mg/kg-1.6 g/kg BW [Rat], 0.8 g/kg BW [Mouse]. This material or its emissions may cause an allergic or sensitization reaction and thereby aggravate systemic disease such as liver disorders. This compound is not listed as a carcinogen or suspected carcinogen by NTP, IARC, or OSHA.

Mass Spectrum for Santoflex® 77PD - PLAS-AD-002



Lowinox® CPL

Chemtura Corporation

**CAS Number** 68610-51-5**RTECS Number** Not available**Abbreviation****Formula** See Below Structure**Molecular Weight** 600-700**Chemical Name**

butylated reaction product of p-cresol and dicyclopentadiene

Synonyms

poly (dicyclopentadiene-co-p-cresol); polymeric sterically hindered phenol

Brand Names & Manufacturers

Antioxidant 12

Akrochem Corporation

WingStay® L

Eliokem

Vanox® L

R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** Yellow-brown powder or pellets**Melting Point** >105 °C**Boiling Point** Not available**Stability** Stable under normal conditions.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	10-40	10-40	5-40	U	<0.1

Application, Regulatory & Environmental Information**Application**

Applications include in-process stabilization of polymers as well as use in manufactured goods such as elastic thread, carpet backing, foam rubber mattresses, household and surgical gloves, medical products, baby bottle teats, bath mats, hot water bottles, automotive components, household appliances (gaskets, liners, parts, housing, etc.), electronic appliance housings, and paper coatings.

Regulatory Information

This product is approved for use by the FDA in a number of food-contact applications as an Indirect Food Additive, including 21CFR175.105 (Components of Adhesives); 21CFR175.125 (Pressure-Sensitive Adhesives); 21CFR177.2600 (Rubber Articles - Antioxidants); and 21CFR178.2010 (Antioxidants and/or Stabilizers for Polymers).

Environmental Impact

This product is not biodegradable and has a high potential to bioaccumulate based on an estimated Log Kow value greater than 9. It is not expected to be toxic to fish due to its low water solubility.

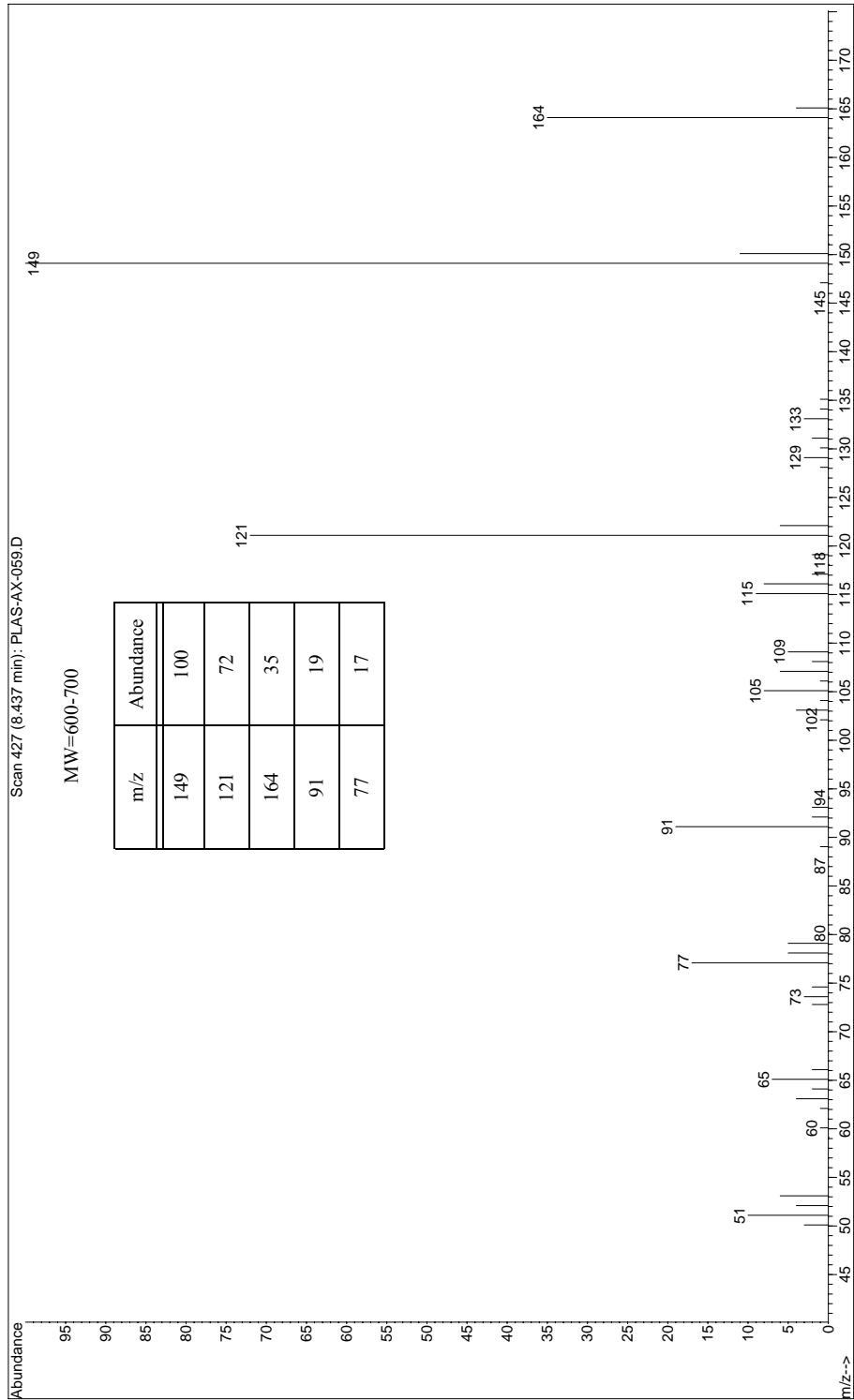
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

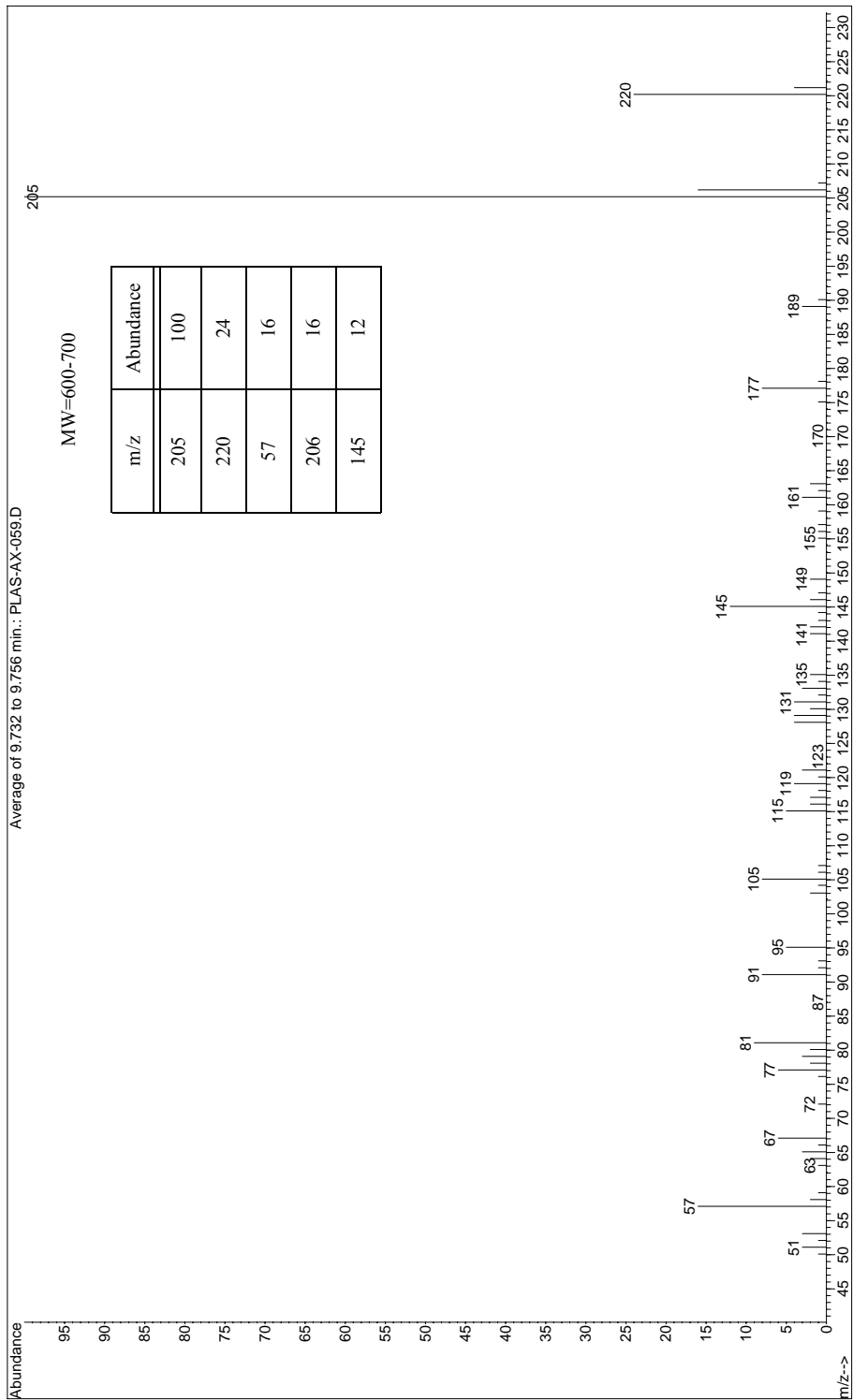
Toxicological Data

Acute oral toxicity (LD50): >4000 mg/kg [Rat], Acute dermal toxicity (LD50): >5010 mg/kg [Rabbit], Acute inhalation (LC50) >165 mg/kg [Rat], Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

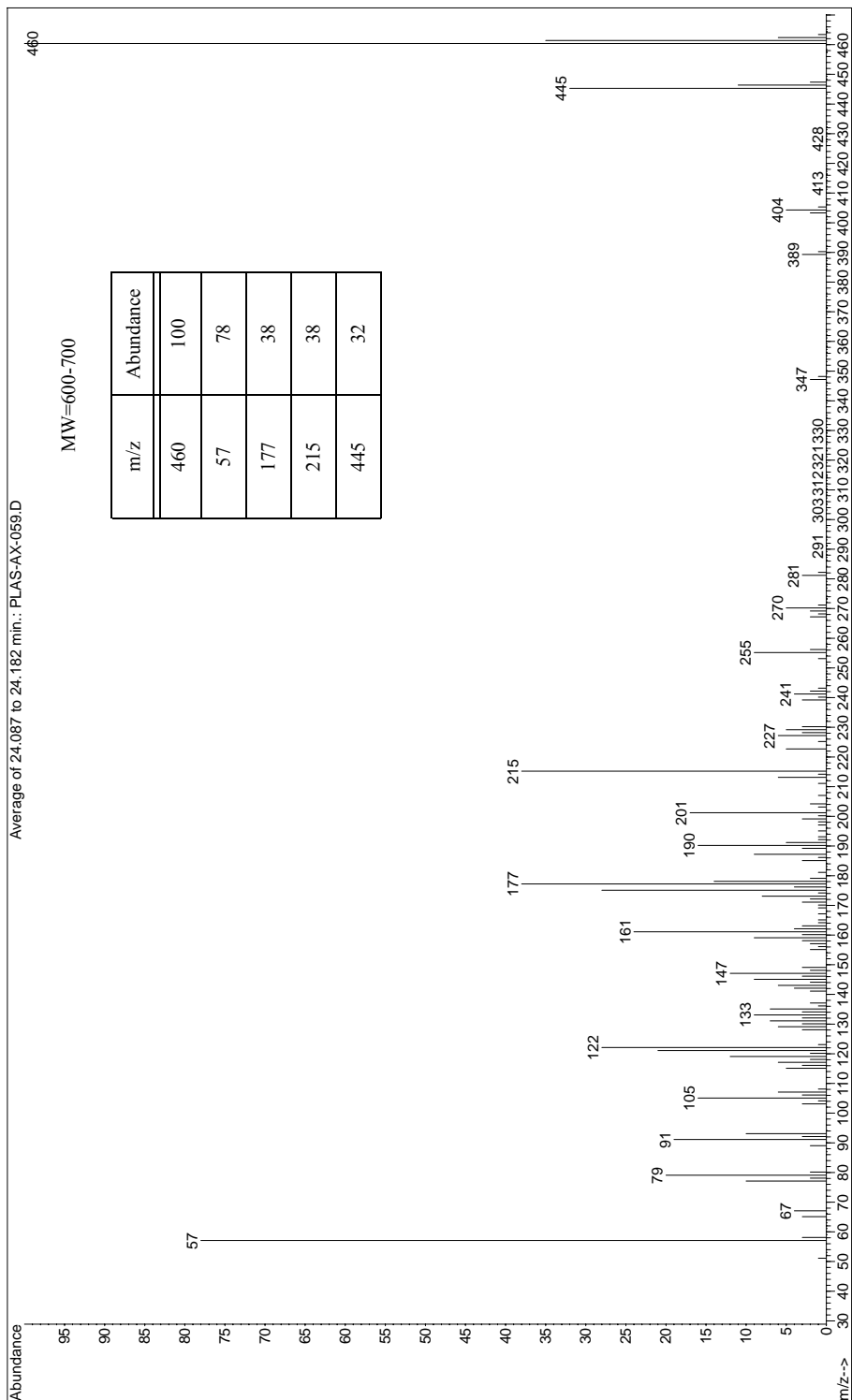
Mass Spectrum for Lowinox® CPL - PLAS-AX-059



Mass Spectrum for Lowinox® CPL - PLAS-AX-059

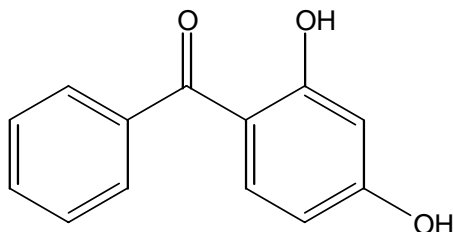


Mass Spectrum for Lowinox® CPL - PLAS-AX-059



Uvinul® 3000

BASF Corporation



CAS Number 131-56-6

RTECS Number DJ0700000

Abbreviation

Formula C₁₃H₁₀O₃

Molecular Weight 214.22

Chemical Name

2,4-dihydroxybenzophenone

Synonyms

(2,4-dihydroxyphenyl)phenylmethanone; benzophenone-1

Brand Names & Manufacturers

Dansorb® 240

Dannier

Lowilite® 24

Chemtura Corporation

Magnolol

Atkin Chemicals

Physical Properties**Appearance** Off-white powder**Melting Point** 144 °C**Boiling Point** 194 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	34	40	70.9	U	1.0

Application Application, Regulatory & Environmental Information

This product is an ultraviolet light absorber for use in polystyrene, unsaturated polyesters, coatings, varnishes, lacquers, and coatings based on epoxy or phenolic alkyds. It is also used in pressure sensitive adhesives, polymethylacrylate (film or sheeting), thermoplastic rubbers, polyisoprene latex and alcohol based cosmetics.

Regulatory Information

This product is not approved by the FDA for food contact applications.

Environmental Impact

Readily biodegradable and is not expected to bioaccumulate based on a log Pow value of 2.96 and its insolubility in water.

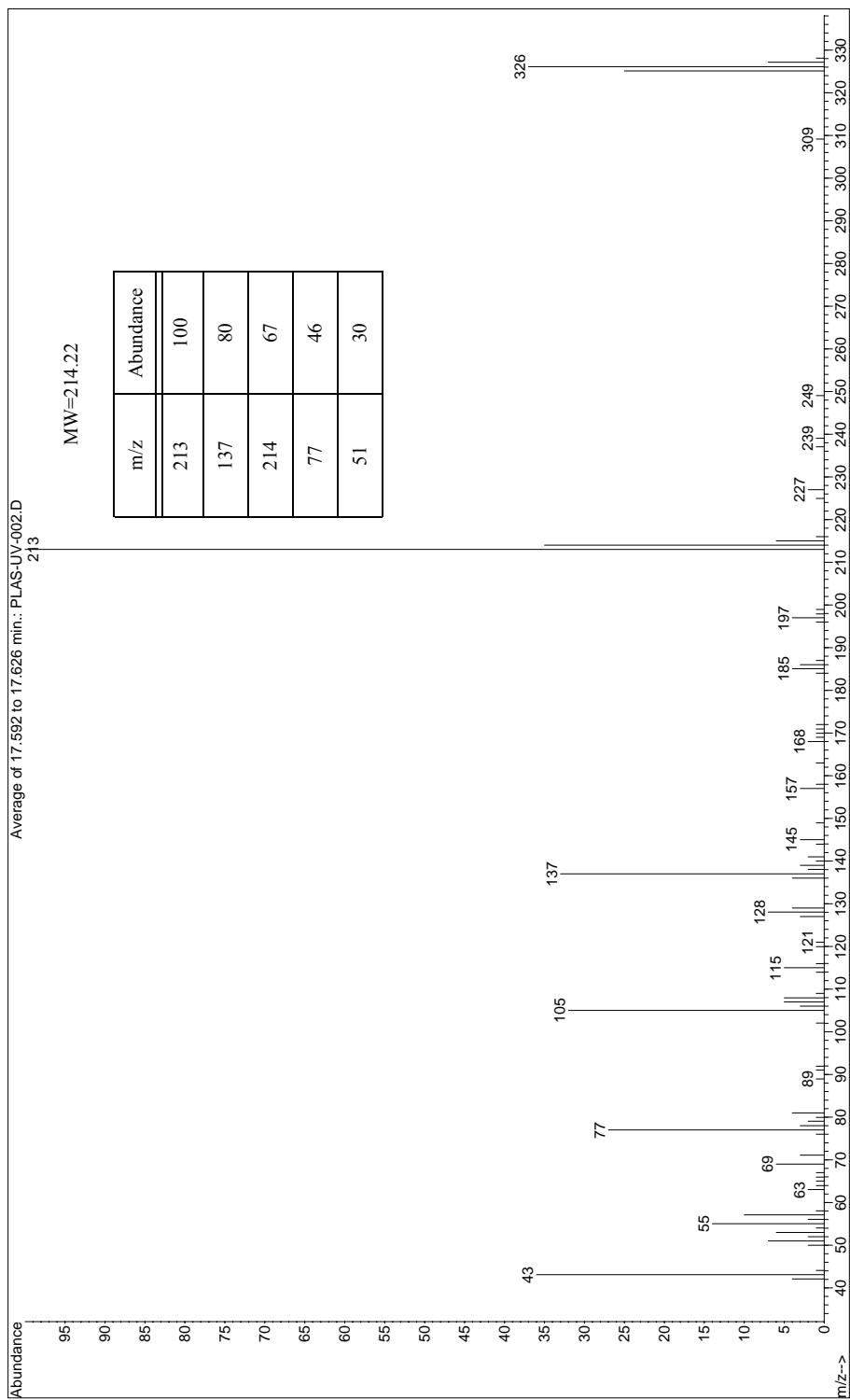
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

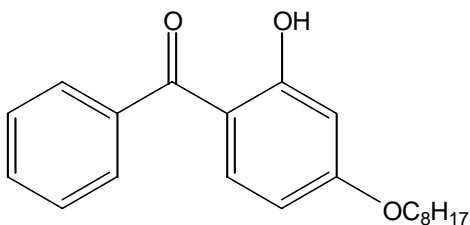
May cause chronic liver, kidney and blood effects based on animal data. Acute oral (LD50): >2000 mg/kg [Rat], 2500 mg/kg [Mouse]. Carcinogenicity: Not listed by ACGIH, IARC, NIOSH, NTP, or OSHA.

Mass Spectrum for Uvinul® 3000 - PLAS-UV-001



Uvinul® 3008

BASF Corporation



CAS Number 1843-05-6

RTECS Number DJ1595000

Abbreviation

Formula $C_{21}H_{26}O_3$

Molecular Weight 326.43

Chemical Name

2-hydroxy-4-octyloxybenzophenone

Synonyms

octabenzone; (2-hydroxy-4-(octyloxy)phenyl)phenylmethanone

Brand Names & Manufacturers

Chimassorb® 81

Ciba Specialty Chemicals

Cyasorb® 531

Cytek

Lowilite® 22

Chemtura Corporation

Physical Properties**Appearance** Yellowish powder**Melting Point** 48-49 °C**Boiling Point** >300 °C Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	2	2	70	67	25

Application Application, Regulatory & Environmental Information

2-Hydroxy-4-n-octyloxybenzophenone is an effective photostabilizer for a variety of plastic systems. It may be used in food packaging materials as an antioxidant and stabilizer and in addition may be used as a stabilizer in petroleum wax. When used in packaging materials, it prevents UV-radiation from reaching the stored product and increases the stability of the container.

Regulatory Information

Approved by the FDA under the 21CFR178.2010 for use in aqueous foods, dairy products (water-in-oil emulsions), bakery products without oil and dry foods without oil at a maximum concentration of 0.5%.

Environmental Impact

This product is toxic to aquatic organisms and should not be released into the environment. It is not readily biodegradable and has a medium potential to bioaccumulate based on the estimated Log Kow value of >6.0.

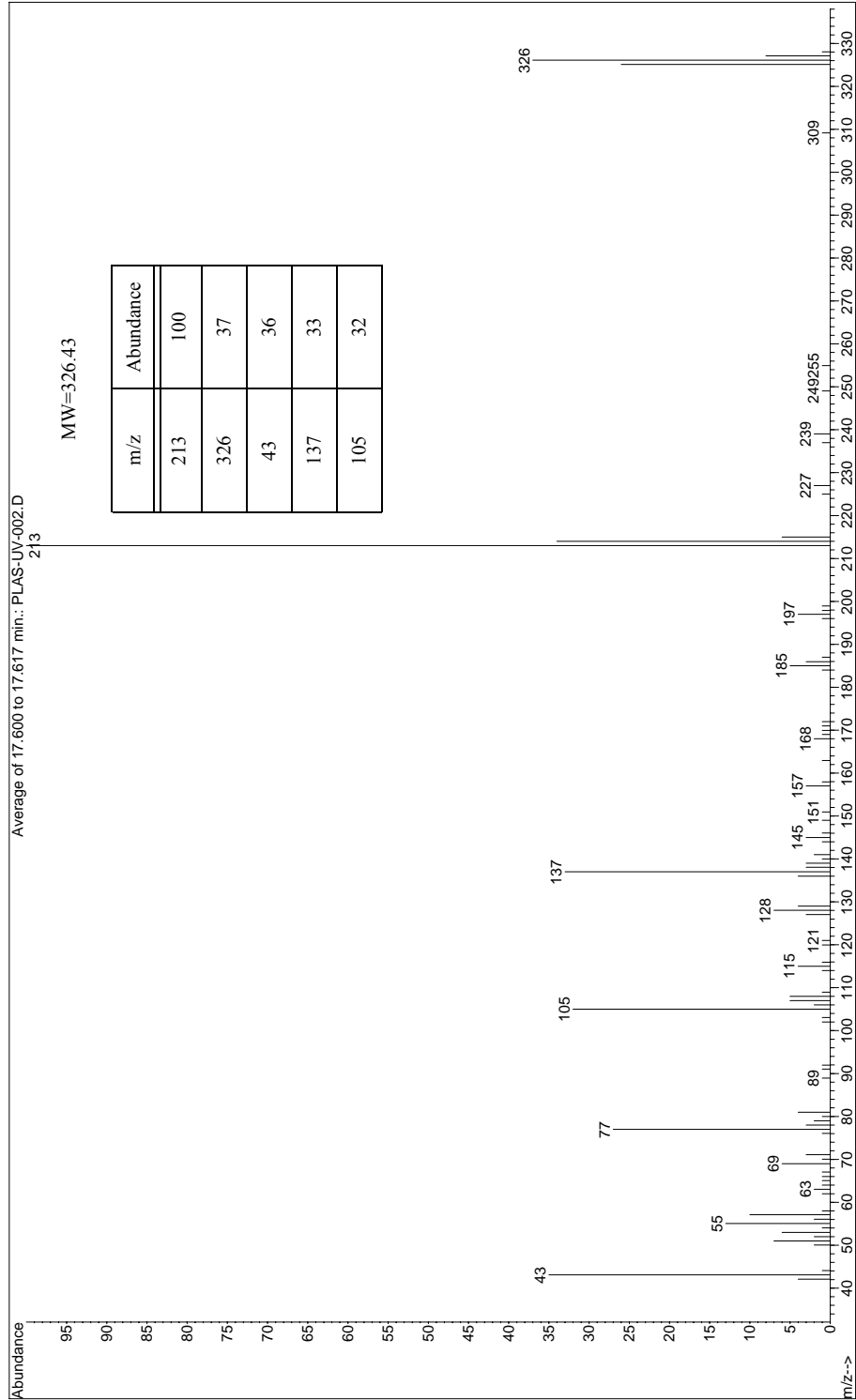
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

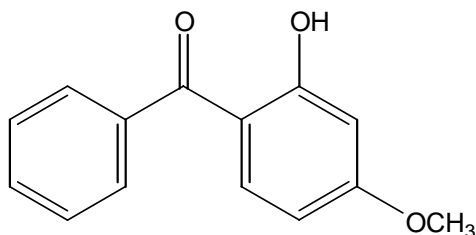
Acute oral (LD50): >10 g/kg [Rat]; Acute dermal (LD50): >10 g/kg [Rabbit]. There are no IARC, OSHA, NTP or ACGIH exposure guidelines available for this product.

Mass Spectrum for Uvinul® 3008 - PLAS-UV-002



Uvinul® 3040

BASF Corporation



CAS Number 131-57-7

RTECS Number DJ1575000

Abbreviation

Formula $C_{14}H_{12}O_3$

Molecular Weight 228.26

Chemical Name

2-hydroxy-4-methoxybenzophenone

Synonyms

benzophenone compound; oxybenzone; (2-hydroxy-4-methoxyphenyl)phenylmethanone

Brand Names & Manufacturers

Lowilite® 20

Chemtura Corporation

Physical Properties**Appearance** Pale-yellow powder**Melting Point** 62 °C**Boiling Point** 150-160 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 5	EtOH 5	Acetone 50	CH₂Cl₂ 20	Hexane U
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Application Application, Regulatory & Environmental Information

Uvinul® 3040 is readily compatible with many plastics. It is a particularly effective UV absorber in PVC, acrylic resins, alkyd resins, cellulose nitrate, phenolic resins, and oil colors.

Regulatory Information

Approved by the FDA under 21CFRPart 177 (Indirect Food Additives: Polymers) Subpart B (Substances for Use as Basic Components of Single and Repeated Use Food Contact Surfaces), and Section 177.1010 (Acrylic and modified acrylic plastics, semirigid and rigid).

Environmental Impact

Readily biodegradable, but may be inherently toxic to aquatic organisms.

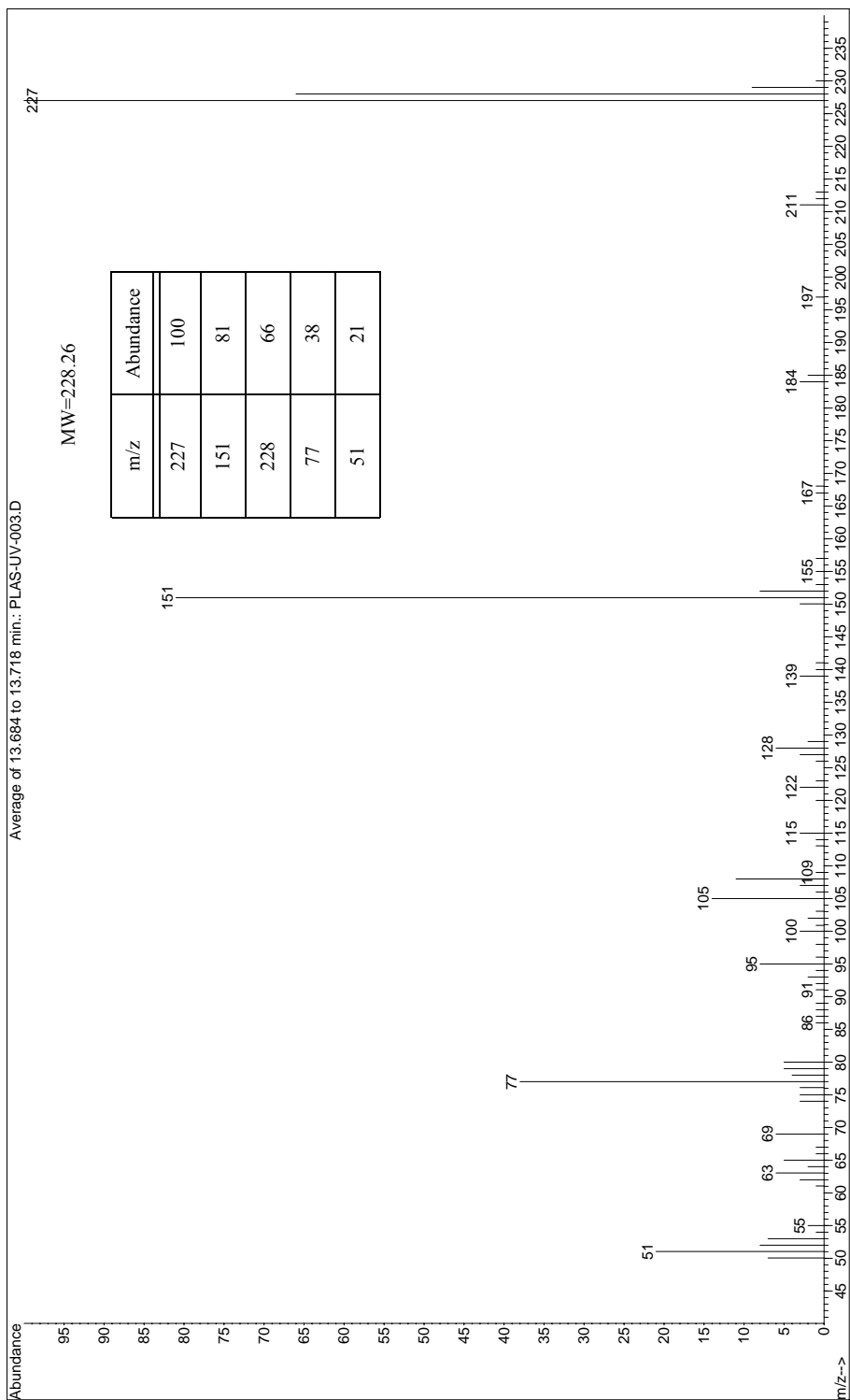
Point of Release

May be absorbed through the skin from cosmetic use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

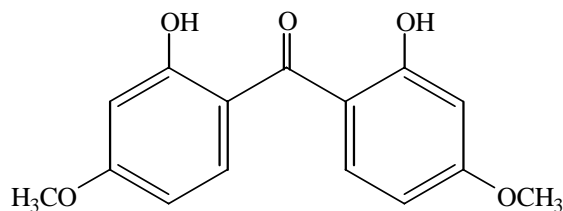
May cause adverse reproductive effects and may affect genetic material (mutagenic). Lowest Published Toxic Dermal Dose (TDLo): 6500 mg/kg/13W-I [Rat].

Mass Spectrum for Uvinul® 3040 - PLAS-UV-003



Uvinul® 3049

BASF Corporation



CAS Number 131-54-4

RTECS Number DJ0900000

Abbreviation

Formula C₁₅H₁₄O₅

Molecular Weight 274.29

Chemical Name

2,2-dihydroxy-4,4-dimethoxybenzophenone

Synonyms

benzophenone compound; bis(2-hydroxy-4-methoxyphenyl)methanone; benzophenone-6

Brand Names & Manufacturers

Helisorb® 11

Norquay

Maxgard® 300

Lycus Ltd.

Unisorb® BP6

UniProma

Physical Properties**Appearance** Pale yellow powder**Melting Point** 131-136 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<1	<1	U	U	U

Application Application, Regulatory & Environmental Information

Primarily used as a UV absorber for polyester film. Can also be used in carbonate lenses, SBR rubbers, polyurethane, PET/PETG, PVC, acrylic resins, alkyd resins, epoxy resins, cellulose nitrate, and phenolic resins.

Regulatory Information

This product has FDA approval for food contact applications.

Environmental Impact

This chemical is not considered to be a persistent toxin and has a low potential to bioaccumulate. It is, however, considered to be inherently toxic to aquatic organisms.

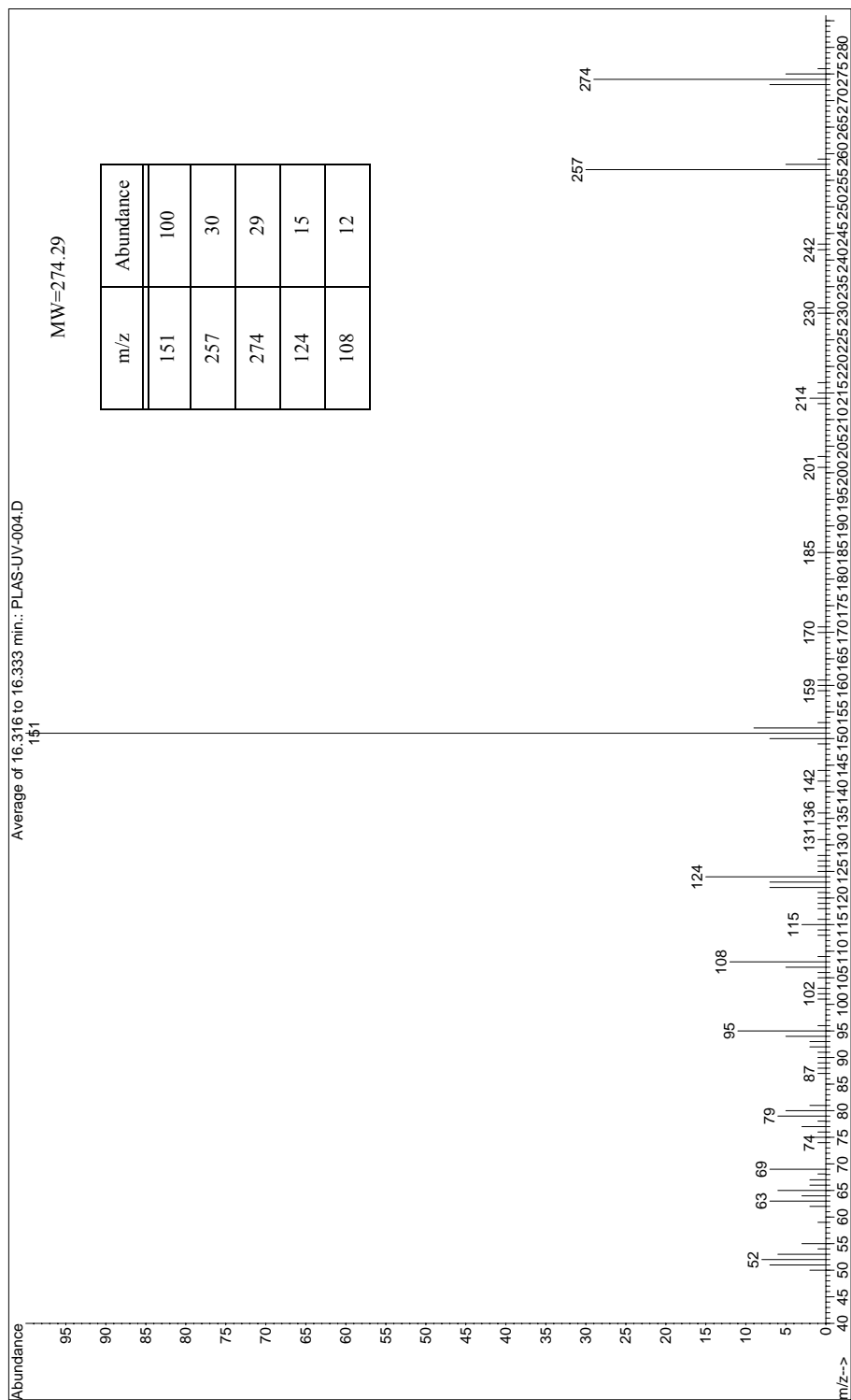
Point of Release

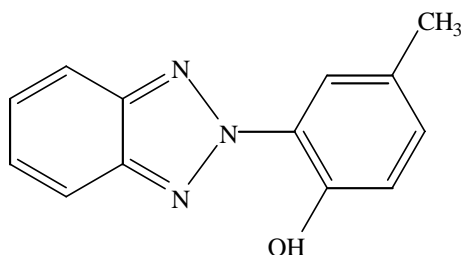
May be absorbed through the skin from cosmetic use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Classified as an endocrine disruptor and may cause adverse health effects in humans.

Mass Spectrum for Uvinul® 3049 - PLAS-UV-004



Tinuvin® PED**CAS Number** 2440-22-4**RTECS Number** GO6860000**Abbreviation****Formula** C₁₃H₁₁N₃O**Molecular Weight** 225.27**Chemical Name**

2-benzotriazol-2-yl-4-methyl-phenol

Synonyms

2-(2-hydroxy-5-methylphenyl)benzotriazole; 2-(2'-hydroxy-5'-methylphenyl)benzotriazole; drometrizole

Brand Names & Manufacturers**Physical Properties****Appearance** Yellow crystalline powder**Melting Point** 128-133 °C**Boiling Point** 225 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	0.2	10	3	16	0.8

Application, Regulatory & Environmental Information**Application**

UV stabilizer particularly effective in styrenic polymers, PVC, unsaturated polyesters, polyurethanes, acrylic polymers and polycarbonates.

Regulatory Information

Tinuvin® PED has FDA approval for use in a wide variety of food contact applications.

Environmental Impact

This material is not readily biodegradable. If released into the environment, it is expected to partition mainly into the soil due to its insolubility in water. It is considered to be nontoxic to aquatic organisms and its potential to bioaccumulate is low.

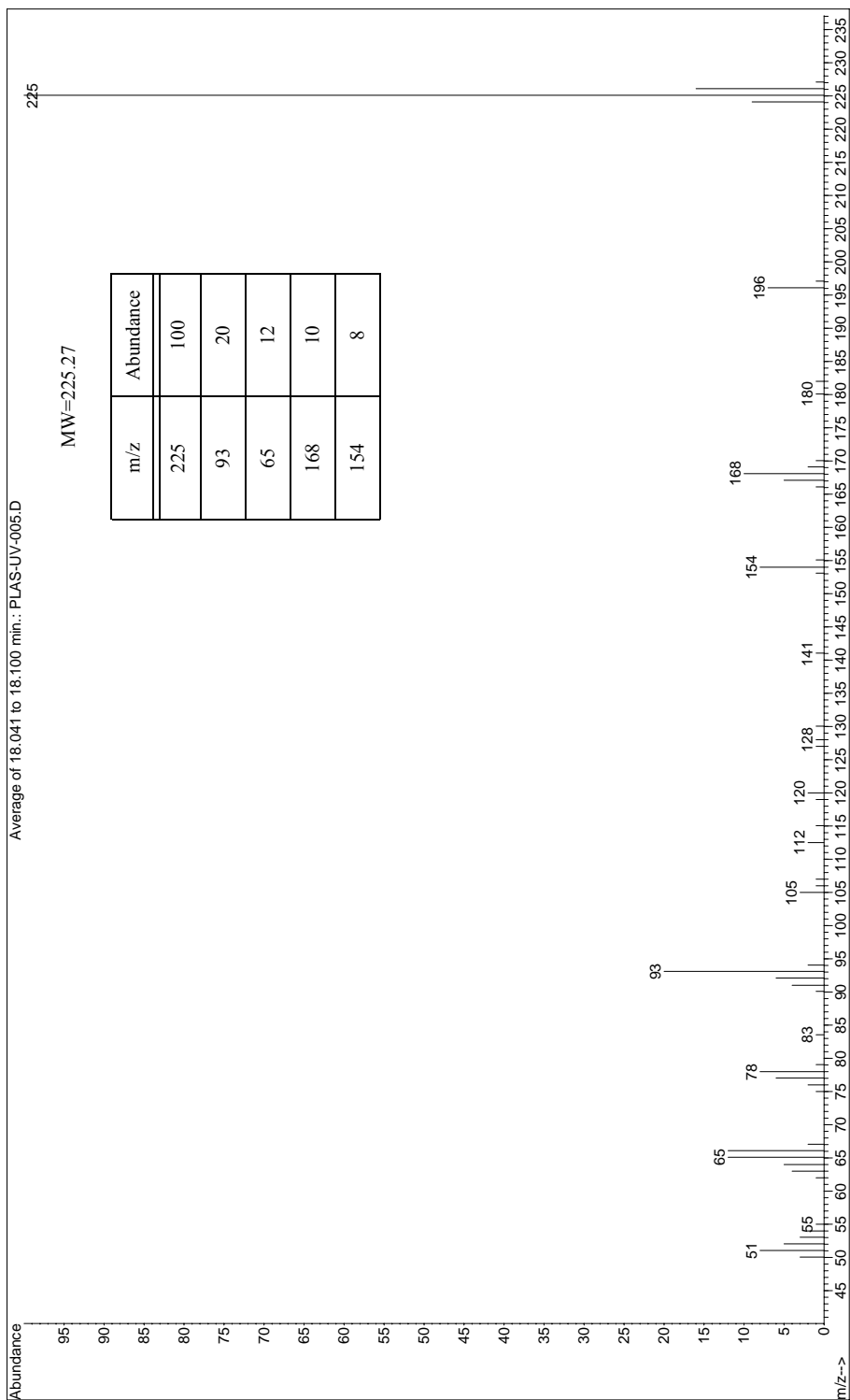
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Primary Irritant. Acute Oral Toxicity (LD50): 6500 mg/kg [Mouse]. Lowest Published Toxic Oral Dose (TDLo): 270 gm/kg/90D-C [Rat]. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Tinuvin® PED - PLAS-UV-005



CHAPTER 5

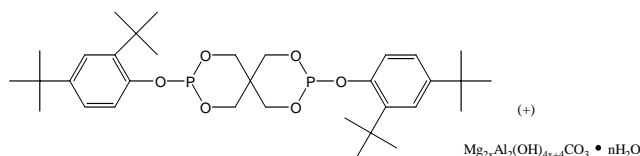
Antioxidants

Exposure of polymers to heat, light or atmospheric oxygen can result in some degradation of the polymer properties during processing, storage and end use. In hydrocarbon polymers, the presence of tertiary hydrogen atoms makes the polymer prone to free radical formation, ultimately resulting in chain scission or crosslinking that degrades performance. Antioxidants are used to terminate these chain reactions by removing radical intermediates. Antioxidants are used in most hydrocarbon polymers including polyethylene, polypropylene, polystyrene, and ABS.

Several factors are typically considered when selecting an antioxidant, including required concentration, compatibility with the substrate, stability, toxicity, ease of use and cost. Organophosphites are the most commonly used antioxidants. They are used to protect the color and molecular weight of the polymer during processing and have been shown to decompose peroxides, as well as chelate and react with metals. Other antioxidant groups include sterically-hindered phenols (BHT), thioesters and amines.

Alkanox® P27

Chemtura Corporation

**CAS Number** 26741-53-7**RTECS Number****Abbreviation****Formula** $\text{C}_{33}\text{H}_{50}\text{O}_6\text{P}_2$ **Molecular Weight** 604**Chemical Name**

bis(2,4-di-tert-butylphenyl)pentaerythritol diphosphate & magnesium aluminum hydroxy carbonate hydrate

Synonyms

23:2 Mixture of Alkanox® P24 (26741-53-7):magnesium aluminum hydroxy carbonate hydrate (11097-59-9)

Brand Names & Manufacturers**Physical Properties****Appearance** White powder or granules**Melting Point** 160-175 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water <0.01	MeOH ~2	EtOH U	Acetone ~11	CH₂Cl₂ ~34	Hexane ~7
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Application, Regulatory & Environmental Information

Data above for CAS, Formula, and Molecular Weight are for the primary organic molecule - Alkanox® P24.

Decomposes peroxides during processing and reduces activity of catalyst residues which reduces peroxide formation. Suitable for polyolefins as well as other plastics, elastomers, and adhesives.

Regulatory Information

Listed as having broad approval for indirect food contact in many countries including USA, Canada, Europe, and Japan.

Environmental Impact

Hydrolysis may produce hindered phenols which are irritating to the eyes, skin, and mucous tract.

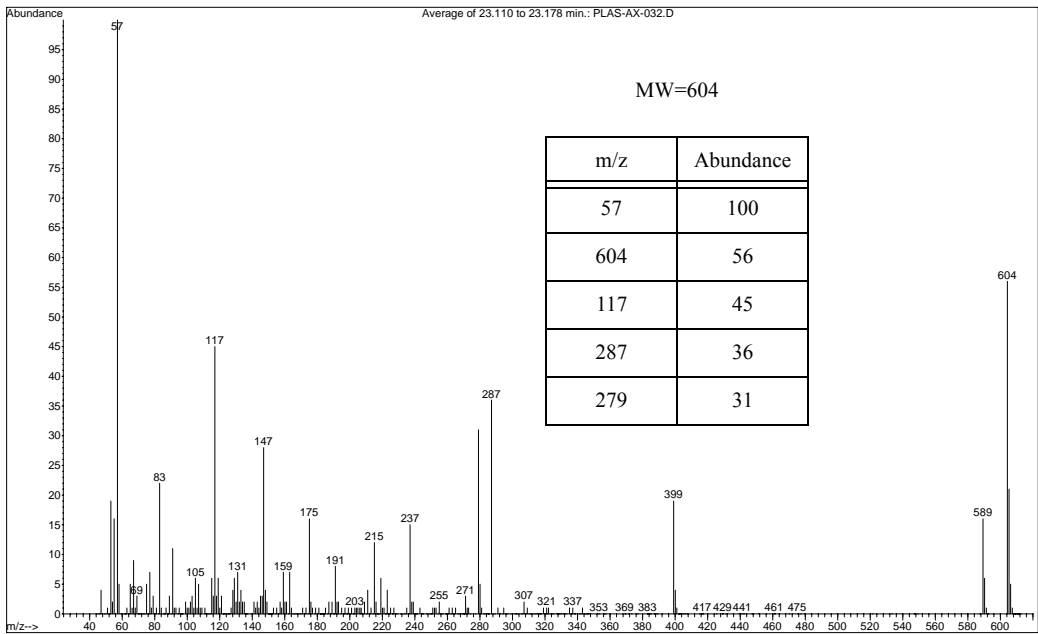
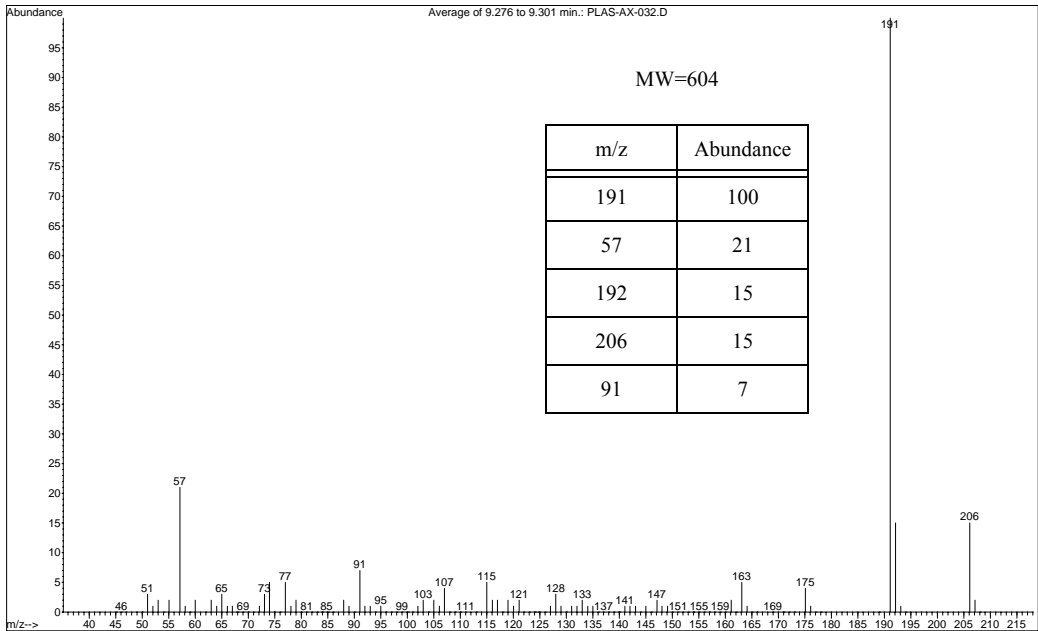
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

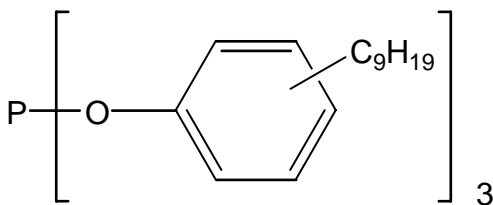
Alkanox® P24 - This material has been evaluated as a probable neurotoxin. In a 90 day feeding study with rats dosed at 100, 300, and 1,000 ppm levels, no effects were seen with the exception of very slight to slight extramedullary hematopoiesis in liver and spleen of animals fed the highest dose. In a two year feeding study in rats at 100 and 500 ppm in the diet, no effects were observed. The material is reportedly not a carcinogen, mutagen or teratogen.

Mass Spectra for Alkanox® P27 - PLAS-AX-032



Alkanox® TNPP

Chemtura Corporation

**CAS Number** 26523-78-4**RTECS Number** Not available**Abbreviation** TNPP**Formula** C₄₅H₆₉O₃P**Molecular Weight** 689.00**Chemical Name**

tris(mono-nonylphenyl) phosphite with up to 1% triisopropanol amine

Synonyms

Tris nonylphenyl phosphite; tris(mono-nonylphenyl) phosphite; nonylphenyl phosphite (3:1)

Brand Names & ManufacturersNaugard® P
Mark® 1178Chemtura Corporation
Crompton-Witco**Physical Properties****Appearance** Clear yellow liquid**Melting Point** Not available**Boiling Point** Decomposes @185 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	<2.3	U	>80	U	>80

Application, Regulatory & Environmental Information

Application TNPP is used as a phosphite antioxidant and a stabilizer for elastomers such as SBR, NBR, and SIS. Used as a stabilizer and a chelator/complexing agent in PC, PE, PP, PVC, copolymers such as ABS (Acrylonitrile-Styrenic based), SBR, and EVA (Ethylene-vinyl acetate) and in polymer latex and other aqueous systems. TNPP also prevents gel formation during polymerization finishing, storage, and factory processing.

Regulatory Information

FDA approved for a variety of food contact applications.

Environmental Impact

(EC50 48hr): 0.42 mg/mL [Daphnia magna], (LC50 96hr) < 10 mg/mL [Zebra fish]. (EBC50): > 100 mg/mL [Green Algae], (LC50): > 100 mg/mL [Aerobic bacteria].

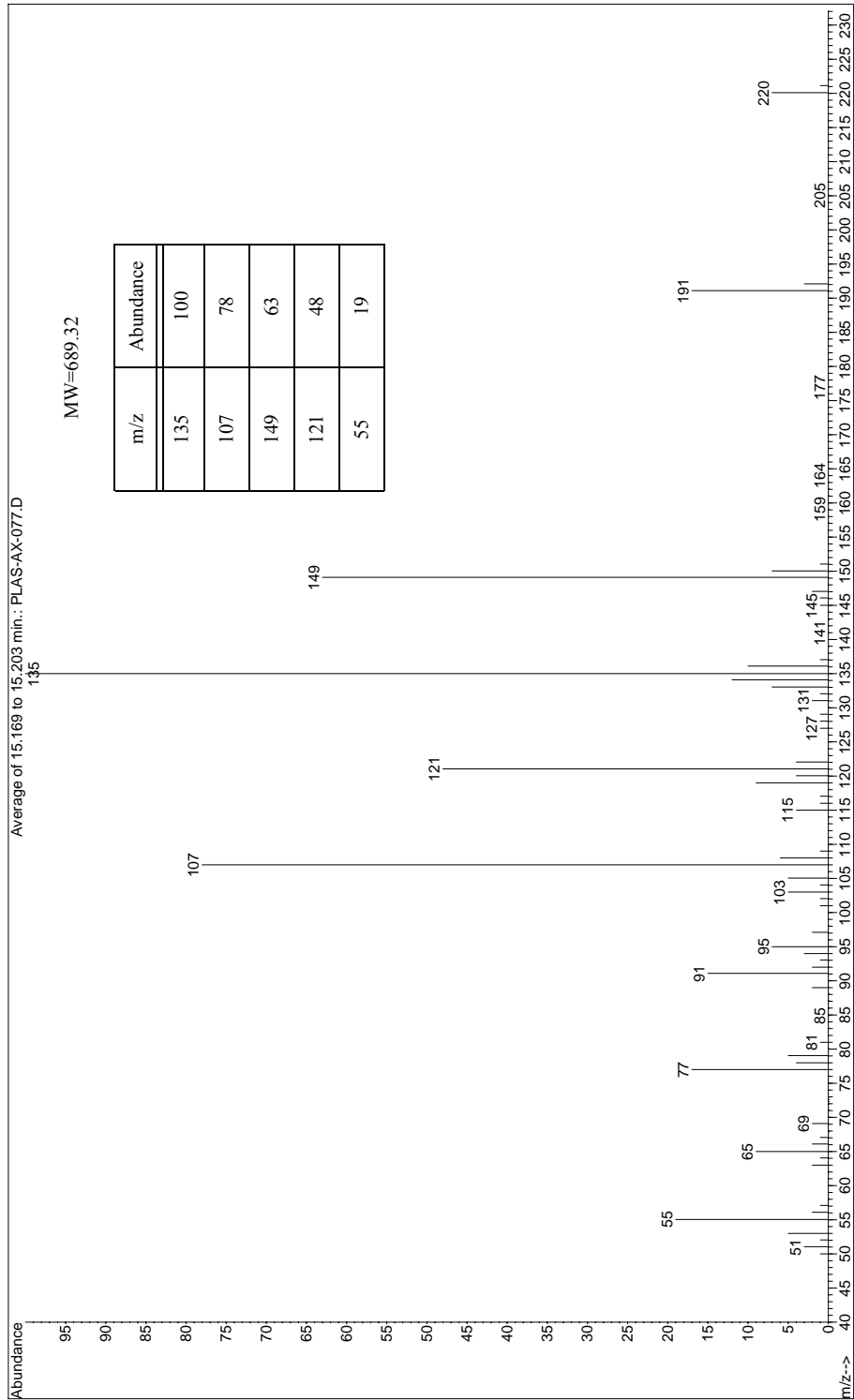
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

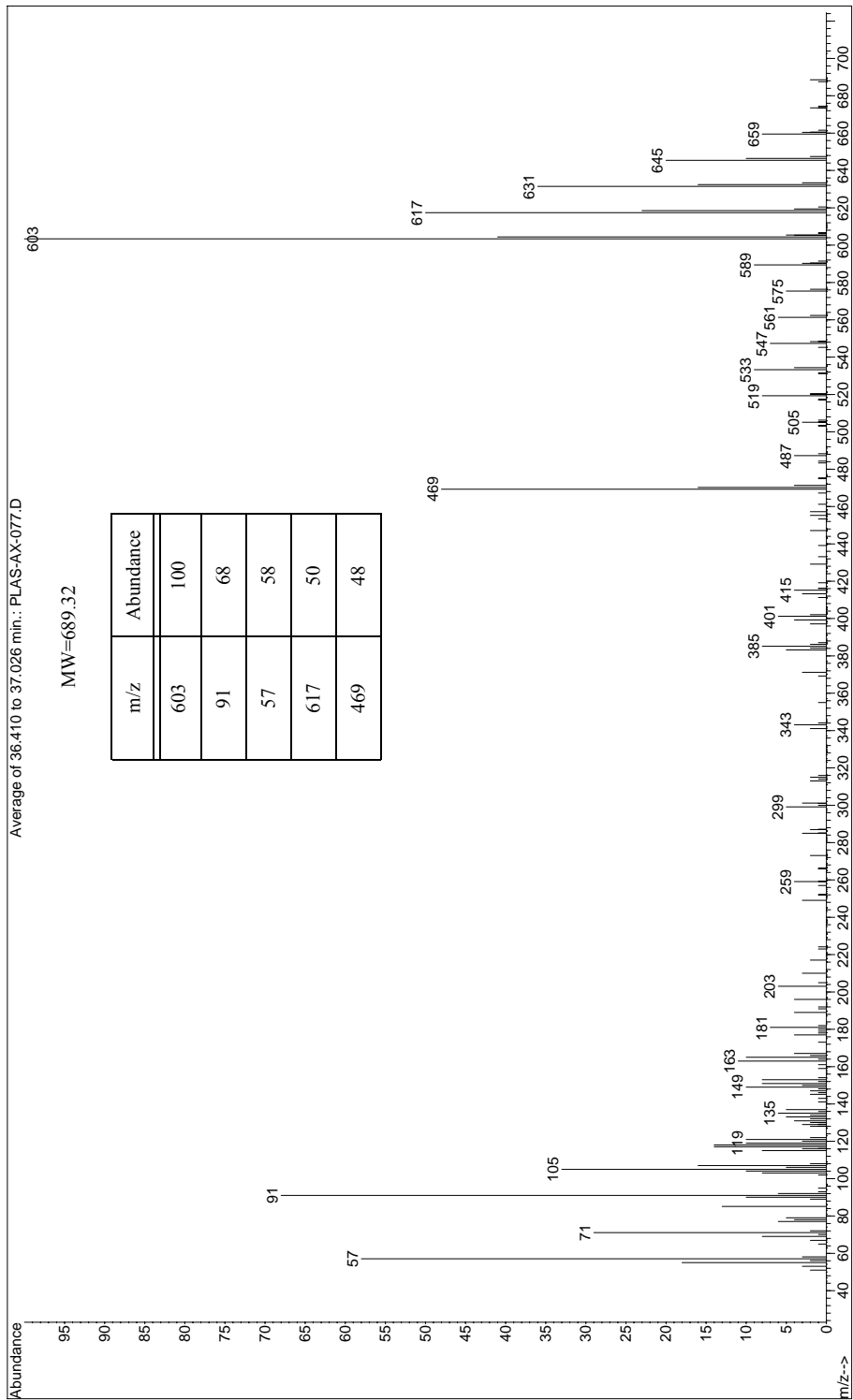
Toxicological Data

May be toxic to kidney based on laboratory animal testing. Irritating to the gastrointestinal system and upper respiratory tract if overexposed. Not reported as carcinogenic.

Mass Spectrum for Alkanox® TNPP - PLAS-AX-077

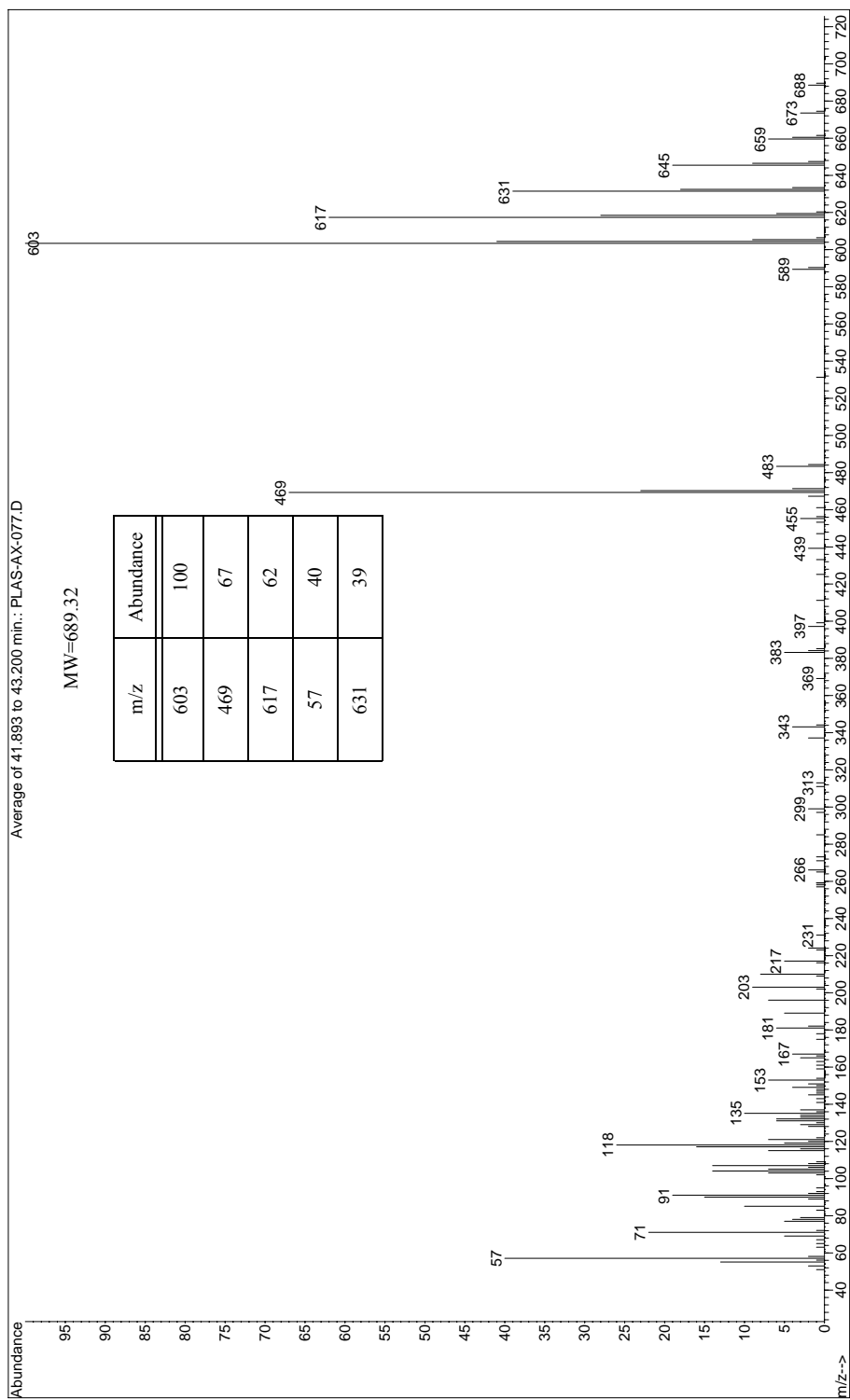


Mass Spectrum for Alkanox[®] TNPP - PLAS-AX-077



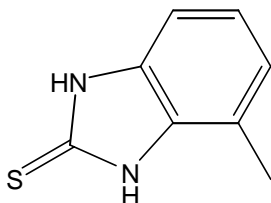
For Chromatogram See Appendix A - PLAS-AX-077 - page 351

Mass Spectrum for Alkanox® TNPP - PLAS-AX-077



Antioxidant 60

Akrochem Corporation

**CAS Number** 53988-10-6**RTECS Number** DE1176050**Abbreviation** MMBI**Formula** C₈H₈N₂S**Molecular Weight** 164.23**Chemical Name**

2H-benzimidazole-2-thione, 1,3-di-hydro-4(or 5)-methyl

Synonyms

1,3-dihydro-4(or 5)-methyl-2H-benzimidazole-2-thione; 2-mercaptopotoluidazole; 2-mercapto-4(5)-methyl-benzimidazole

Brand Names & ManufacturersVanox[®] MTI

R.T. Vanderbilt Company, Inc.

Nocrac[™] MMB

Ohuchi Shinko Co., Ltd.

Vulkanox[®] MB-2

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** White to off-white powder**Melting Point** > 250 °C**Boiling Point** Decomposes**Stability** Stable under ordinary conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	10-40	10-40	10-40	U	U

Application, Regulatory & Environmental Information**Application**

MMBI is a rubber antioxidant that, in synergy with amine or phenolic antioxidants, protects against oxygen, heat, and metals (especially in thiuram and dithiocarbamate vulcanizates) at the cost of a retarding effect in the vulcanization process and the reduction of modulus. It also confers steam resistance to rubber compounds and has a brightening effect on transparent materials. It is non-staining/coloring and does not bloom.

Regulatory Information

Not approved by the FDA for use in food contact applications.

Environmental Impact

Possibly hazardous short-term degradation products are not likely. However, long-term degradation products may arise. Expected to readily biodegrade. Fish Toxicity: (LC50 96hr): 22 mg/L [Brachydanio rerio]; (LC100 96 Hr): 63 mg/L [Brachydanio rerio].

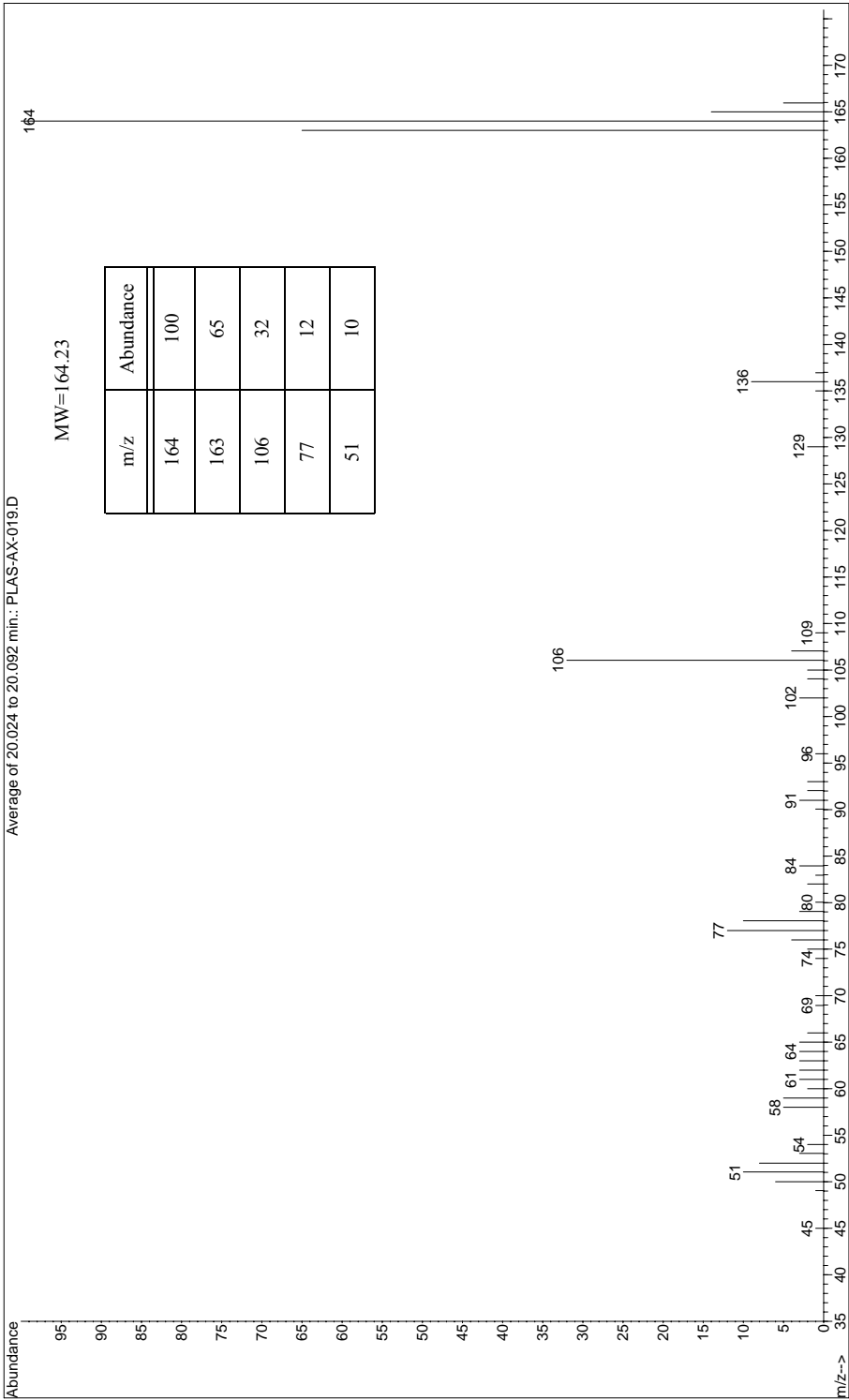
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

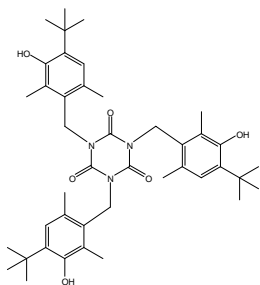
MMBI is markedly less toxic than its demethylated compound (MBI or Mercaptobenzoimidazoles). A decrease of thyroid toxicity by methyl substitution of MBI is caused mainly by a decrease in systemic exposure to the compounds and partly by a decrease in inhibition of thyroid hormone synthesis. Oral (LD50): 340 mg/kg [Rat].

Mass Spectrum for Antioxidant 60 - PLAS-AX-019



Cyanox® 1790

Cytex Technology Corporation

**CAS Number** 4061-76-1**RTECS Number** Not available**Abbreviation****Formula** C₄₂H₅₇N₃O₆**Molecular Weight** 699.92**Chemical Name**

1,3,5-tris(4-tert-butyl-3-hydroxy-2,6-dimethylbenzyl)-1,3,5-triazine-2,4,6-(1h, 3h,5h)-trione

Synonyms**Brand Names & Manufacturers**

Lowinox® 1790

Chemtura Corporation

Physical Properties**Appearance** White powder**Melting Point** 159-162 °C**Boiling Point** >300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1.4	U	U	U	U

Application, Regulatory & Environmental Information

Application Used for polyurethane, polypropylene, polyester and polyamide fibers where it provides gas fading resistance at low load levels. In addition, the molecular structure and the relatively high molecular weight results in a high extraction resistance in demanding applications like hot water conducting polypropylene pipes.

Regulatory Information

Cyanox® 1790 is approved as an antioxidant at levels not to exceed 0.1% in olefin polymers used in the manufacture of articles that contact food, subject to the provisions of 21CFR178.2010(b) of the Food Additives Regulations, and is approved for use in polystyrene and rubber-modified polystyrene under 21CFR177.1640.

Environmental Impact

This substance is not readily biodegradable and has a log Kow value of 15.281, which would indicate a potential to bioaccumulate. This substance is not expected to be hazardous to aquatic substances due to its limited solubility in water.

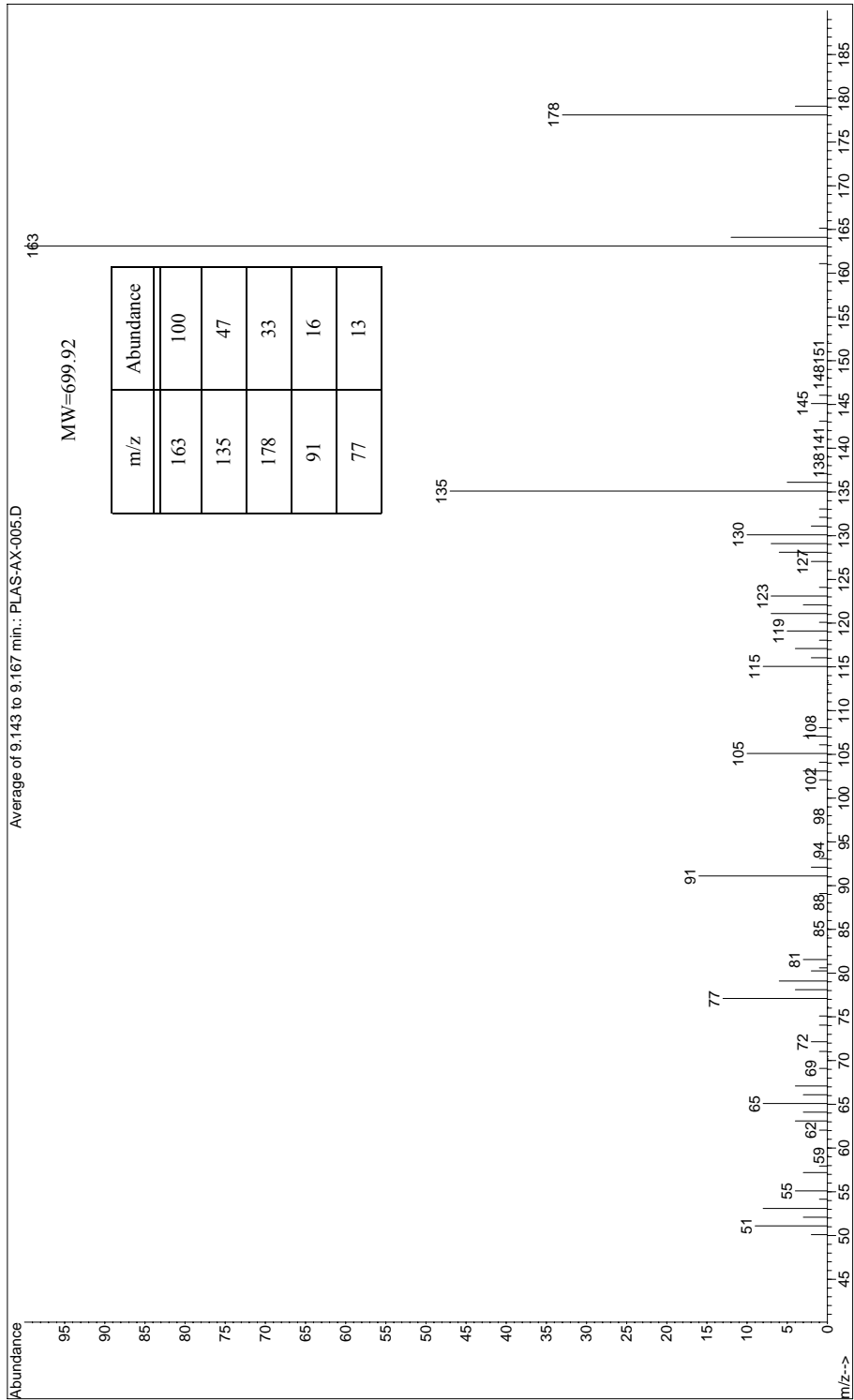
Point of Release

Capable of transferring constituents of the additive into food substances.

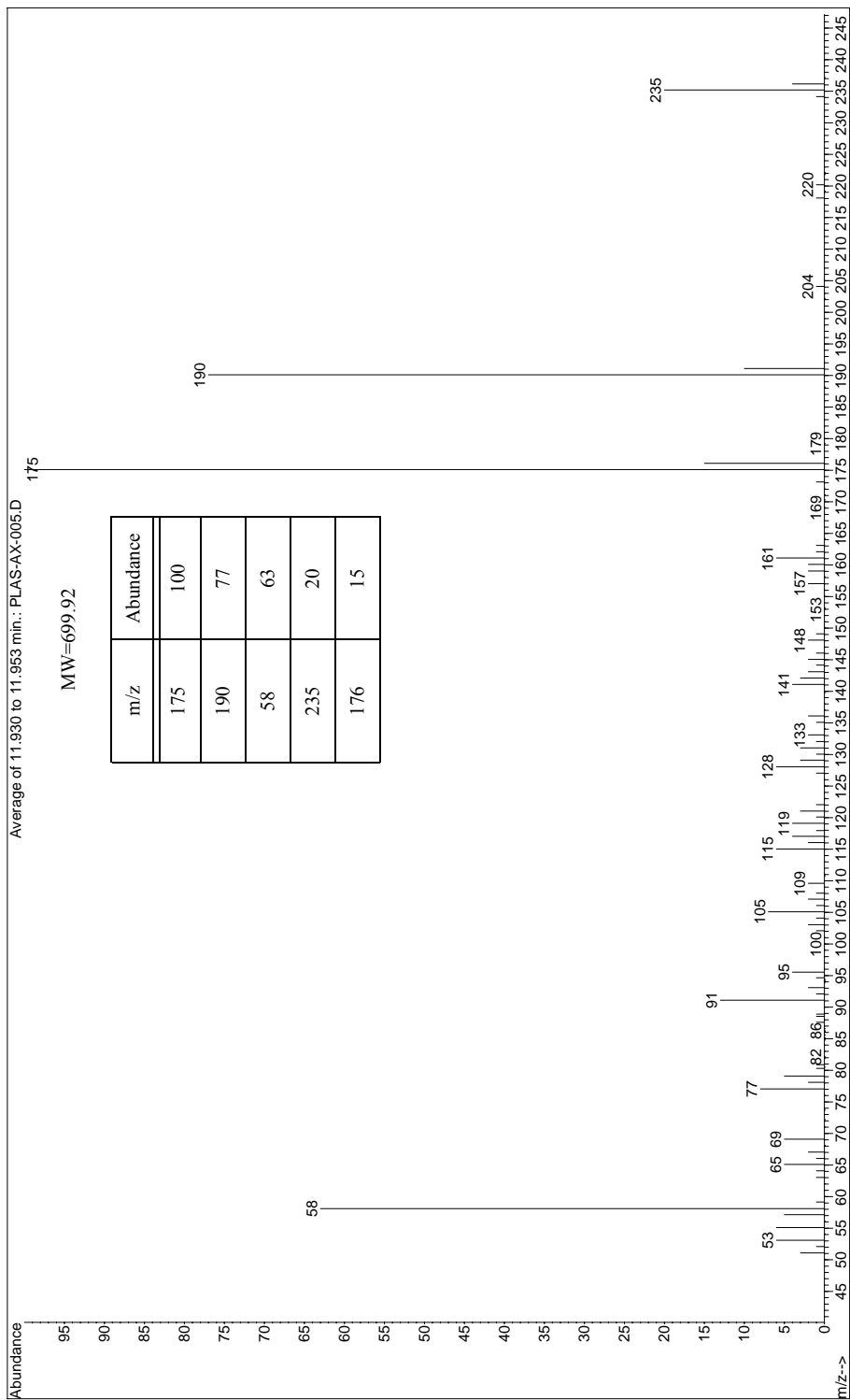
Toxicological Data

Acute oral (LD50): >10,000 mg/kg [Rat], >5000 mg/kg [Rabbit].

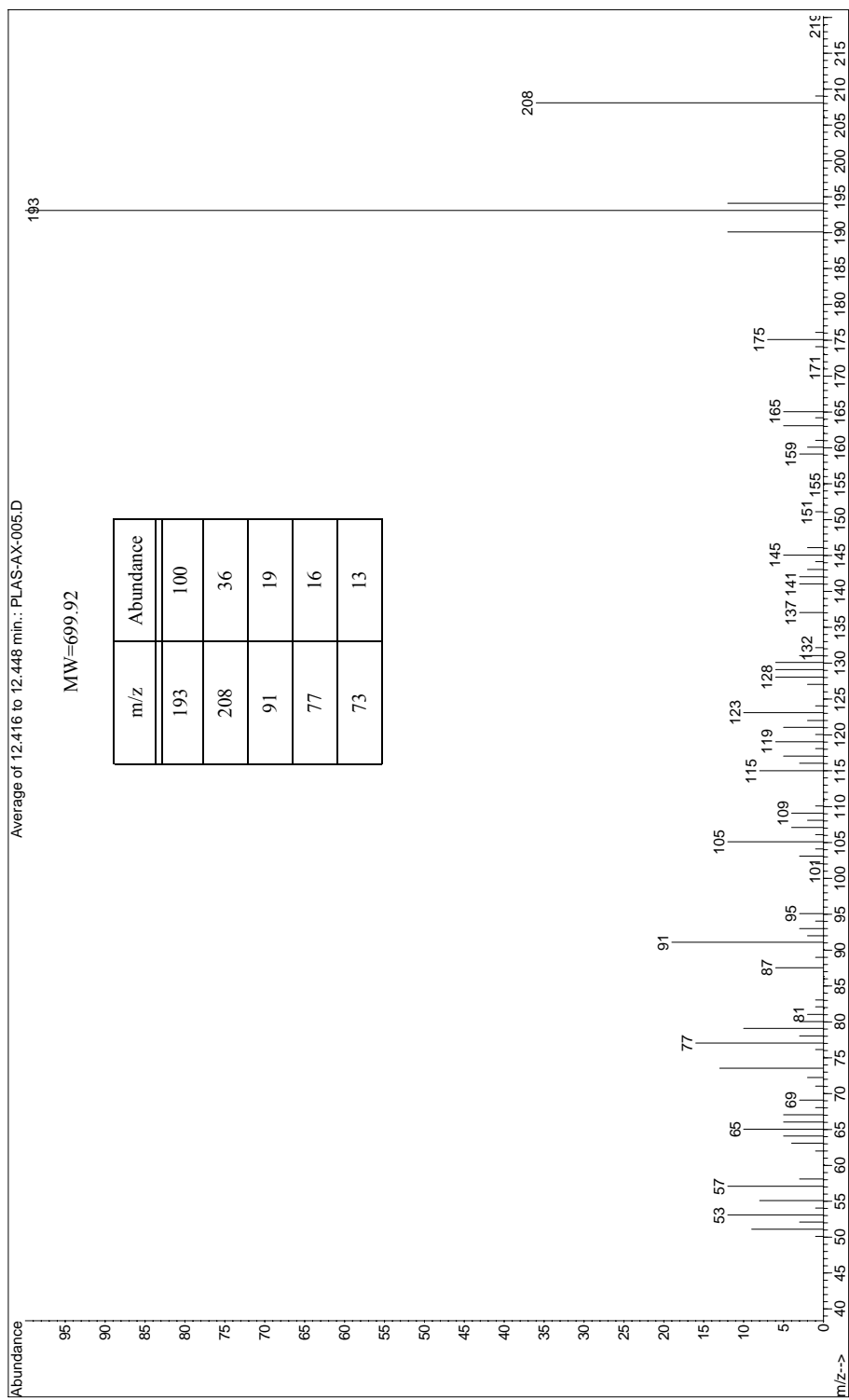
Mass Spectrum for Cyanox® 1790 - PLAS-AX-005



Mass Spectrum for Cyanox® 1790 - PLAS-AX-005

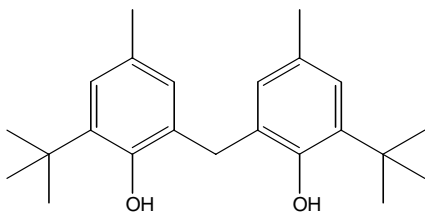


Mass Spectrum for Cyanox® 1790 - PLAS-AX-005



Cyanox® 2246

Cytec Technology Corporation



CAS Number 119-47-1

RTECS Number PA3500000

Abbreviation

Formula $C_{23}H_{32}O_2$

Molecular Weight 340.55

Chemical Name

2,2'-methylene-bis(4-methyl-6-tert-butyl-phenol)

Synonyms

bis(2-hydroxy-3-tert-butyl-5-methylphenyl)methane; 2,2'-methylenebis(6-tert-butyl-4-methylphenol); 2,2'-methylenebis(6-tert-butyl-p-cresol)

Brand Names & Manufacturers

Advastab®

Rohm and Haas Chemicals LLC

Lowinox® 22M46

Chemtura Corporation

Antioxidant 235

Akrochem Corporation

Plastanox® 2246

American Cyanamid Corp

Physical Properties**Appearance** White crystalline powder, faint phenolic odor**Melting Point** 127-129 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	154	175	U	U

Application, Regulatory & Environmental Information**Application**

Used as a thermo/light-stabilizing phenolic antioxidant in the manufacture (compounding and end use) of white, light-colored, and transparent vulcanizates based on natural or synthetic rubber, PS, polyolefins, and pentaplast. Also used in POM and ABS thermoplastics because of its low volatility and migration properties.

Regulatory Information

FDA Approved 1998: olefin polymer material in contact with food, not to exceed 0.1% w/w, POM copolymers, not to exceed 1.0% w/w, POM homopolymers, not to exceed 0.5% w/w. 21 CFR allows for the use in all stages of production, processing and packaging of food for the following applications: 21CFR175.105 use in adhesives 21CFR177.2600 manufacturing rubber material and 21CFR178.2010 manufacturing antioxidants/stabilizers.

Environmental Impact

(LC50): > 100 mg/L [Leuciscus idus], (LC50 96hr): > 50 mg/L [Fish], (EC50 3hr): >10 g/L [Bacteria]. No effects observed in tests on Pseudomonas putida and e-coli.

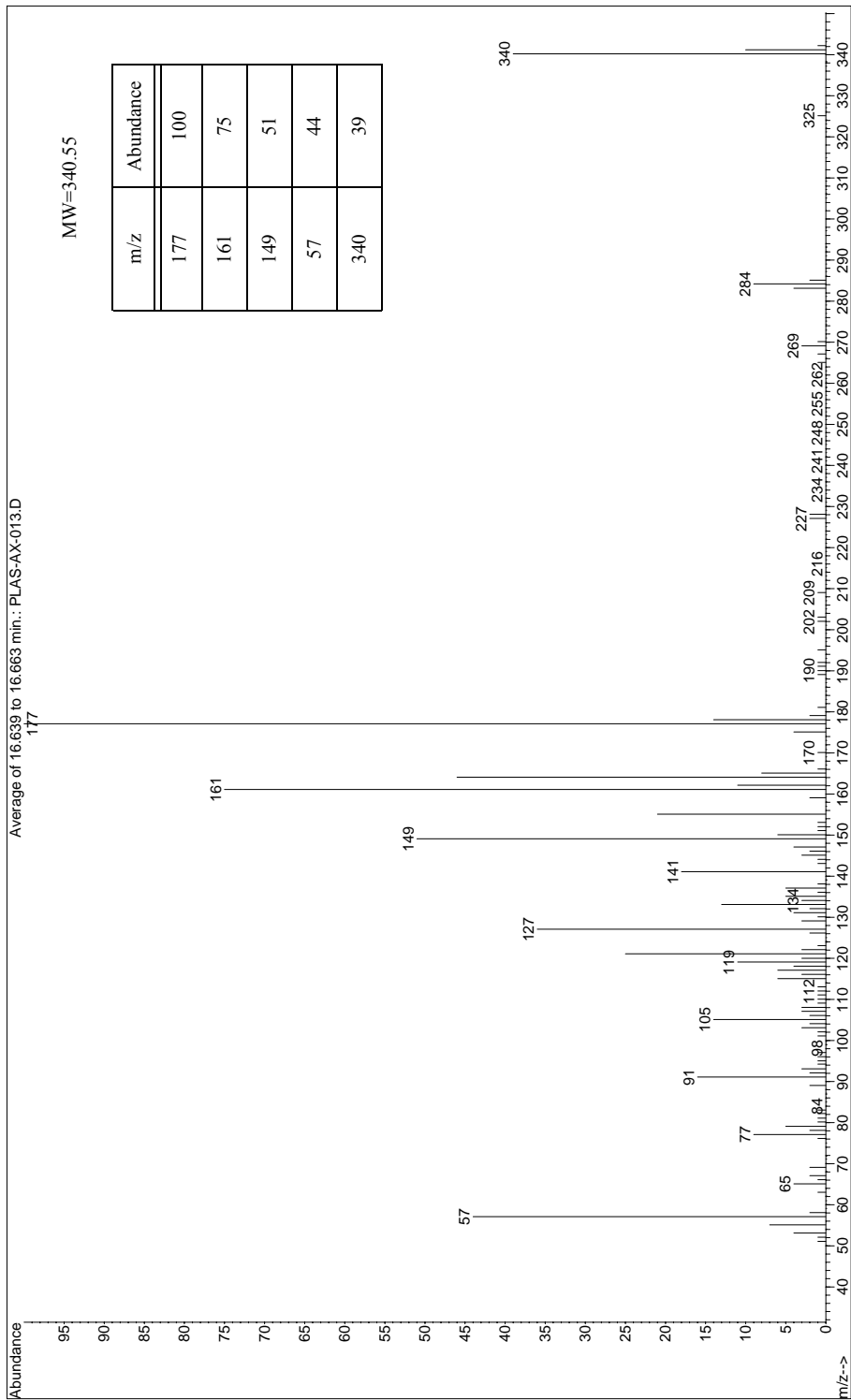
Point of Release

The compound possesses low volatility and migration.

Toxicological Data

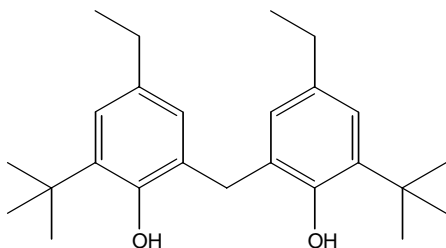
The toxicological properties of this material have not been thoroughly investigated. Not listed (ACGIH, IARC, NTP, OSHA) as a cancer causing agent. Acute oral (LD50): >10 g/kg [Rat]; Acute dermal (LD50): >10 g/kg [Rabbit].

Mass Spectrum for Cyanox® 2246 - PLAS-AX-013



Cyanox® 425

Cytac Technology Corporation



CAS Number 88-24-4

RTECS Number SL9800000

Abbreviation

Formula $C_{25}H_{36}O_2$

Molecular Weight 368.55

Chemical Name

2,2'-methylenebis(4-ethyl-6-tert-butylphenol)

Synonyms

2,2'-Methylenebis(6-tert-butyl-4-ethylphenol)

Brand Names & Manufacturers

Physical Properties

Appearance	Cream-colored free-flowing powder					
Melting Point	117-129 °C			Boiling Point	Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U

Application **Application, Regulatory & Environmental Information**

Cyanox® 425 is a bisphenol compound recommended for use in rubber modified plastics and is effective in the stabilization of ABS.

Regulatory Information

FDA approved under 21CFR178.2010 for use in acrylonitrile-butadiene-styrene copolymers at levels not to exceed 0.6% by weight of the copolymer. Section 177.1010 for use in semi-rigid and rigid acrylics at levels not to exceed 0.1% by weight of the plastic, and Section 175.105 as a component of food packaging adhesives. Also, approved by the FDA as an antioxidant in the preparation of rubber articles at a level not to exceed 5% by 21CFR177.2600.

Environmental Impact

Due to extreme low solubility in water, and therefore the non-availability to species, this product is regarded as not hazardous to aquatic organisms. The product is also not readily biodegradable, and potential bio-accumulation could occur, based on the molecular structure and the calculated log Pow.

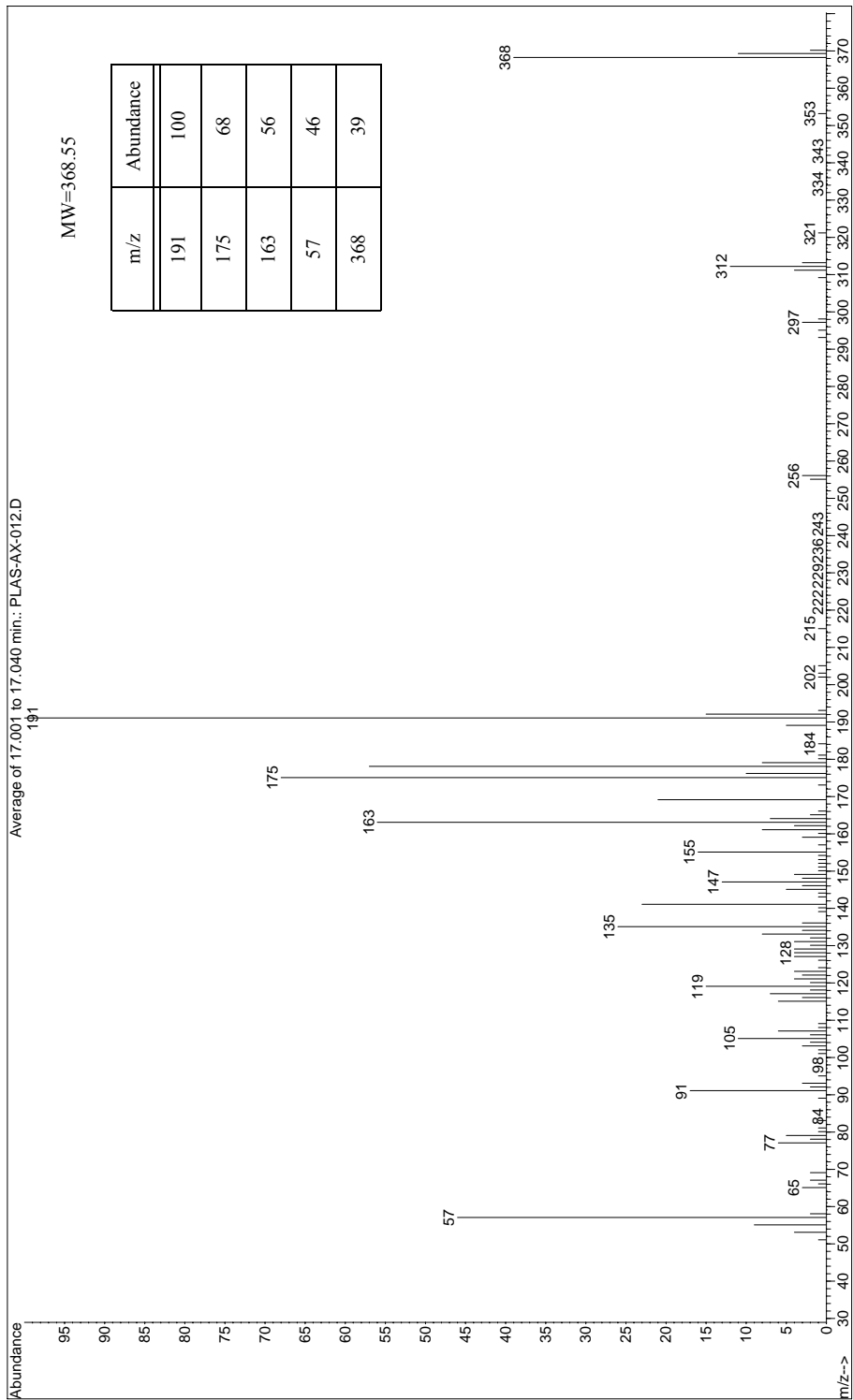
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

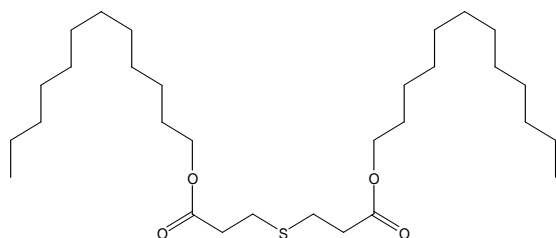
RTECS CLASS OF COMPOUND: Reproductive Effector. Acute Oral Toxicity (LD50): >10 gm/kg [Rat], Lowest Published Toxic Oral Dose (TDLo): 80 gm/kg/12W-C [Rat].

Mass Spectrum for Cyanox® 425 - PLAS-AX-012



Cyanox® LTDP

Cytec Technology Corporation

**CAS Number** 123-28-4**RTECS Number** UF8000000**Abbreviation** LTDP**Formula** C₃₀H₅₈O₄S**Molecular Weight** 514.85**Chemical Name**

dilaurylthiopropionate

Synonyms

di-lauryl-3,3'-thiodipropionate; 3,3'-thiodipropionic acid, didodecyl ester; didodecyl-3,3'-thiopropionate

Brand Names & Manufacturers

Advastab® 800

Rohm and Haas Chemicals LLC

Lowinox® DLTDP

Chemtura Corporation

Naugard® DLTDP

Chemtura Corporation

Physical Properties**Appearance** White crystalline powder, characteristic sweet odor**Melting Point** 38-41 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	<0.01	U	U	U

Application, Regulatory & Environmental Information**Application**

LTDP is a thiosynergist antioxidant additive to thermo/light-stabilizers (used in combination with phenolic antioxidants) with plasticizing properties used to decompose and neutralize hydroperoxides, formed by the auto-oxidation of polymers, primarily in PE, PP, ABS, polyester, and polyamide.

Regulatory Information

FDA approved 1998 for the manufacture of resinous/polymeric coatings in safe contact with food for articles for use in all stages of production, processing, packaging and transport of food, 21CFR175.300. Joint FAO/WHO committee on Food Additives recommended an ADI of 3.0 mg/kg BW. Inventories: AICS (Australia); DSL (Canada); ECL (Korea); EINECS (Europe); ENCS (Japan); List I (China); PICCS (Philippines); TSCA (USA).

Environmental Impact

(LC50 96hr): 71 mg/L [Fish], (EC50 24hr): 10 mg/L [Daphnia], (EbC 72hr): 33.9 mg/L [Algae].

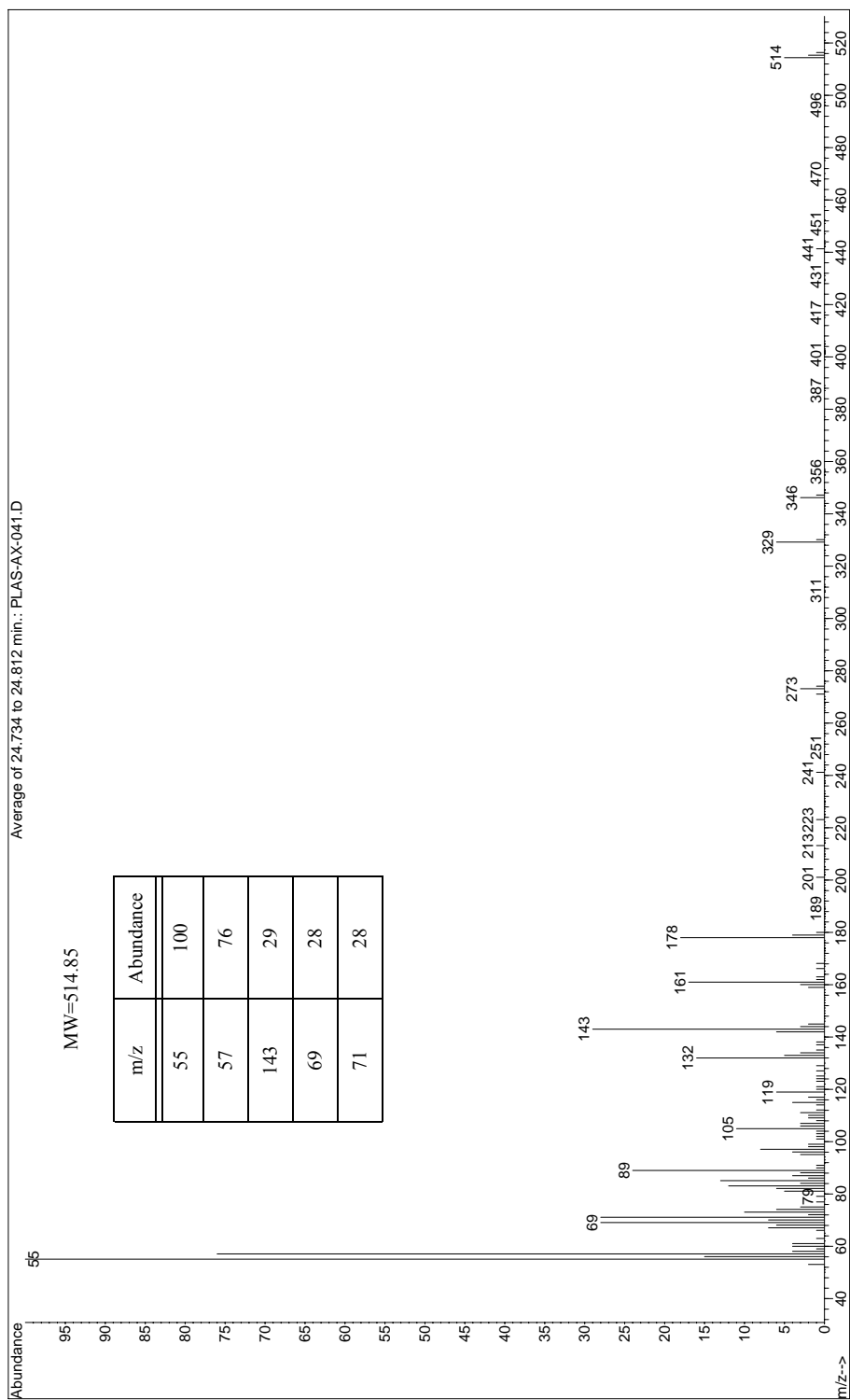
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

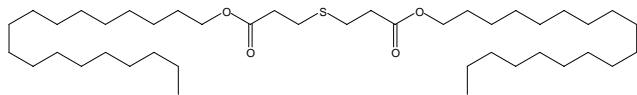
Not listed by ACGIH, IARC, NTP, or OSHA as a cancer causing agent. The toxicological properties of this material have not been thoroughly investigated. Acute inhalation (4h) (LC50): >3000 ppm [Rat], Acute intraperitoneal (LD50) >2 g/kg [Mouse], Acute oral (LD50): >2 g/kg [Mouse], >25 g/kg [Rat], Acute dermal (LD50): >10 g/kg [Rabbit]. Long-term toxicological effect of growth-retardation in rats fed 1 and 3 % LTDP over 2 years, no changes in visceral organs reported.

Mass Spectrum for Cyanox® LTDP - PLAS-AX-041



Cyanox® STDP

Cytex Technology Corporation



CAS Number 693-36-7

RTECS Number UF8010000

Abbreviation DSTDP

Formula C₄₂H₈₂O₄S

Molecular Weight 683.30

Chemical Name

distearylthiopropionate

Synonyms

distearyl-3,3'-thiodipropionate; thiodipropionic acid, dioctodecyl ester; distearyl beta-thiodipropionate

Brand Names & Manufacturers

Advastab® 802

Rohm and Haas Chemicals, LLC

Lowinox® DSTDP

Chemtura Corporation

Naugard® DSTDP

Chemtura Corporation

Physical Properties**Appearance** White crystalline powder**Melting Point** 63-67 °C**Boiling Point** ~658 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.01	<0.01	U	S	S

Application, Regulatory & Environmental Information**Application**

STDP is a thiosynergist antioxidant additive to thermo/light-stabilizers (used in combination with phenolic antioxidants) with plasticizing properties used to decompose and neutralize hydroperoxides, formed by the auto-oxidation of polymers, primarily in PE, PP, ABS, polyester, and polyamide.

Regulatory Information

FDA: Approved (1998) use of STDP in the manufacture of resinous/polymeric coatings in safe contact with food for articles for use in all stages of production, processing, packaging and transport of food, 21CFR175.300.

Environmental Impact

Inherently biodegradable OECD 302C: 60%. Log Kow 17.68 (estimated). Hydrolysis >2 years. Toxicity to aquatic biota: (LC50 96 Hr): >100 mg/L [Fish]; (EC50 24 Hr): 780 mg/L [Daphnia]; EbC50 (72 Hr): 60 mg/L [Algae].

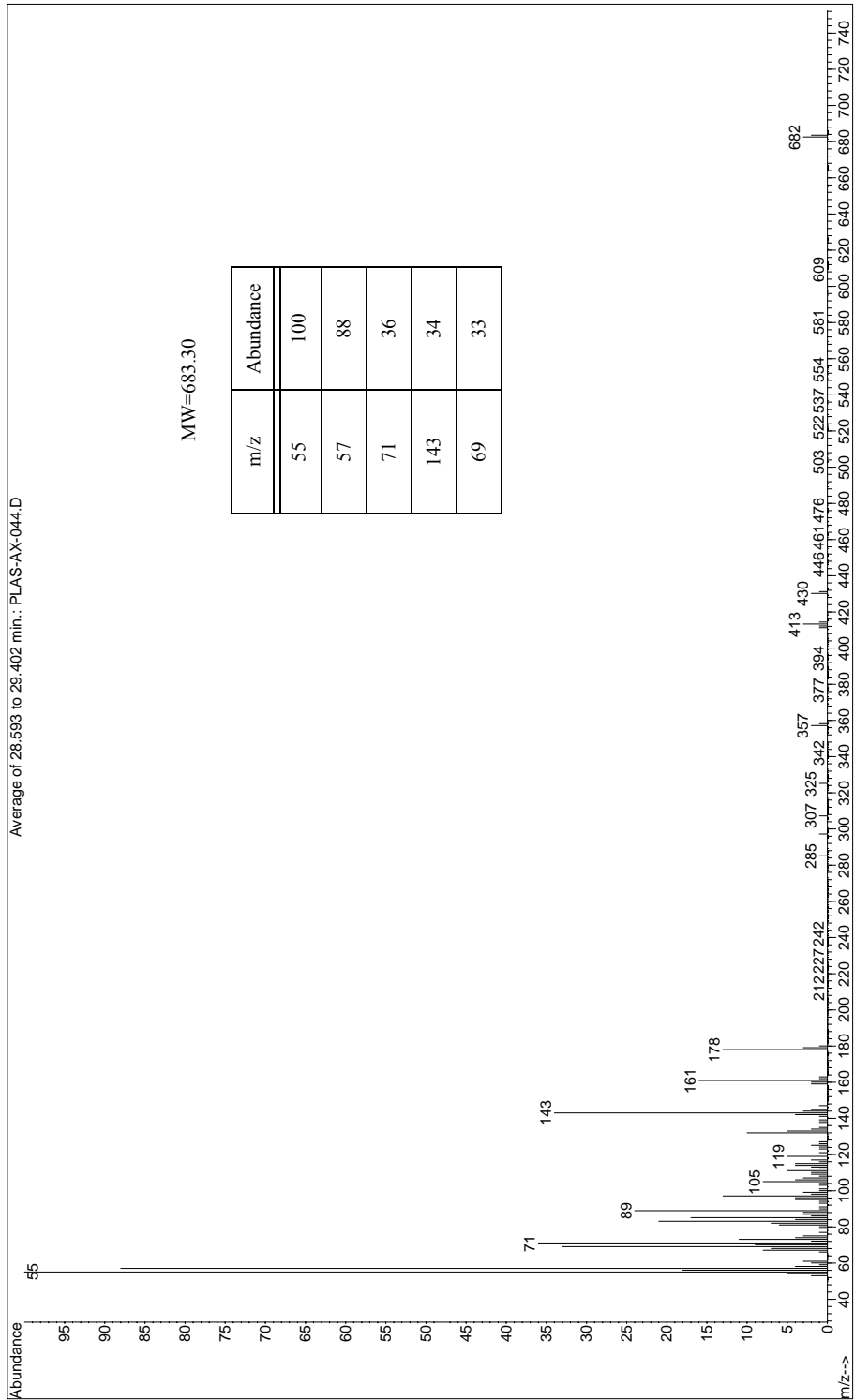
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

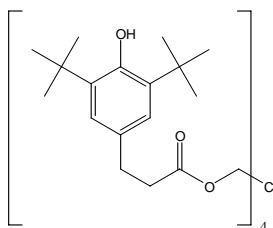
Long-term toxicological effect of BW growth-retardation in rats fed 3% LTDP in their diet over 2 years - no changes in visceral organs reported. Not determined to be carcinogenic (NTP, IARC, OSHA, ACGIH). Acute oral LD50: > 5 g/kg [Rat]. Acute dermal LD50: > 2 g/kg [Rabbit].

Mass Spectrum for Cyanox® STDP - PLAS-AX-044



Ethanox[®] 310

Albemarle Corporation

**CAS Number** 6683-19-8**RTECS Number** DA8340000**Abbreviation** PE**Formula** C₇₃H₁₀₈O₁₇**Molecular Weight** 1177.65**Chemical Name**

pentaerythritol tetrakis (3-(3,5-di-t-butyl-4-hydroxyphenyl)propionate)

Synonyms

2,2-bis{3-[3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl]-1-oxopropoxy}-1,3-propanediyl ester

Brand Names & Manufacturers

Anox [®] 20	Chemtura Corporation
Ultranox [®] 210	Chemtura Corporation
Irganox [®] 1010	Ciba Specialty Chemicals
Cyanox [®] 2110 (EF)	Cytec Technology Corp.

Physical Properties

Appearance	White crystalline powder					
Melting Point	110-125 °C			Boiling Point	Not available	
Stability	Stable at normal conditions of use.					
Solubility (g/100mL 20°C)	Water <0.01	MeOH 0.9	EtOH 1.5	Acetone 47	CH₂Cl₂ 63	Hexane 0.3

Application Application, Regulatory & Environmental Information

Used as an antioxidant and thermosabilizer for polypropylene, polyethylene, impact resistant polystyrene, poly-4-methyl-pentene. Can be used as a stabilizer for natural and synthetic rubber, polyvinyl chloride. A copolymer of acrylonitrile with butadiene and styrene, polyacetals, alkyde resins, polyamides and polyesters.

Regulatory Information

FDA - Approved for use in indirect food contact applications.

British Standard - Listed as an antioxidant for polyethylene and polypropylene compositions used in contact with foodstuffs or water intended for human consumption (max permitted in final compound 0.5%).

Environmental Impact

Experimental data shows that this category of chemicals are not readily biodegradable. This class of compounds photodegrade rapidly. In the environment, occurrence would be partitioned primarily to soil and sediments rather than air or water.

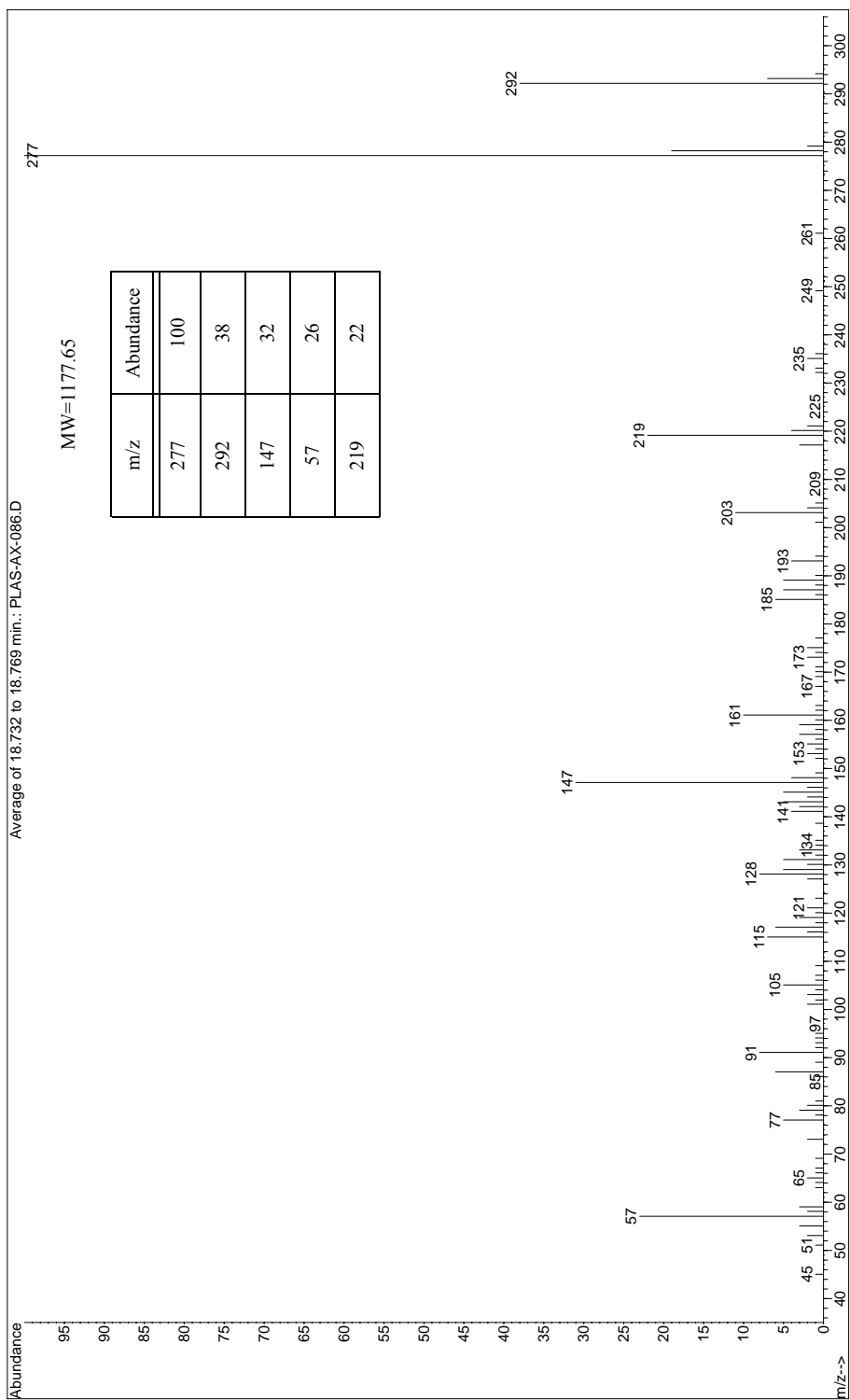
Point of Release

Migration is greater from polypropylene than from high-density polyethylene. Little migration is found to aqueous media. Migration is highest into n-heptane, ethanol and corn oil.

Toxicological Data

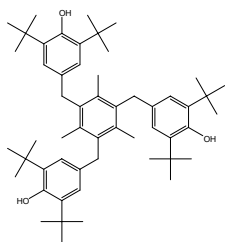
Toxicity of this compound is considered low. LD50 was not quantitated, rats tolerated administration of 5.0 g/kg body-weight and mice tolerated up to 10 mg/kg bodyweight.

Mass Spectrum for *Ethanox*[®] 310 - PLAS-AX-086



Ethanox® 330

Albemarle Corporation

**CAS Number** 1709-70-2**RTECS Number** DC3750000**Abbreviation****Formula** C₅₄H₇₈O₃**Molecular Weight** 775.32**Chemical Name**

1,3,5-trimethyl-2,4,6-tris(3,5-di-tert-butyl-4-hydroxybenzyl) benzene

Synonyms

4,4',4''-((2,4,6-trimethyl-1,3,5-benzenetriyl)tris(methylene))tris(2,6-bis(1,1-dimethylethyl)phenol); methylene bis ethyl butyl phenol; 2,4,6-Tri-(3',5'-di-tert-butyl-4'-hydroxybenzyl)mestitylene

Brand Names & Manufacturers

Anox® 330

Chemtura Corporation

Antioxidant 330

Akrochem Corporation

Ionox® 330

Shell Oil Company

Irganox® 330

Ciba Specialty Chemicals Corpora-

Physical Properties**Appearance** White crystalline powder**Melting Point** 240-245 °C**Boiling Point** 822 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.2	U	23.0	47.0	1.7

Application Application, Regulatory & Environmental Information

Ethanox® 330 is a phenolic stabilizer for manufacturing synthetic rubber, mineral oils, and oils in some food products; providing protection from light and heat aging, and for light and colored rubbers. May also be used as a thermo stabilizer for polyethylene and polypropylene fiber. High molecular weight phenolic antioxidants are commonly used in wide variety of applications, including elastomers, hot melt adhesives, tackifiers and engineering blends.

Regulatory Information

Ethanox® 330 is allowed by the FDA in all polymers for food contact applications subject to the limitations provided in 21CFR178.2010.

Environmental Impact

This compound has a calculated partition coefficient (log Pow) of > 6. Based on this and its other physical-chemical properties, the substance in the environment is likely to bind to the soil and sediment where it is expected to be immobile and have limited bioavailability. The material is not readily biodegradable.

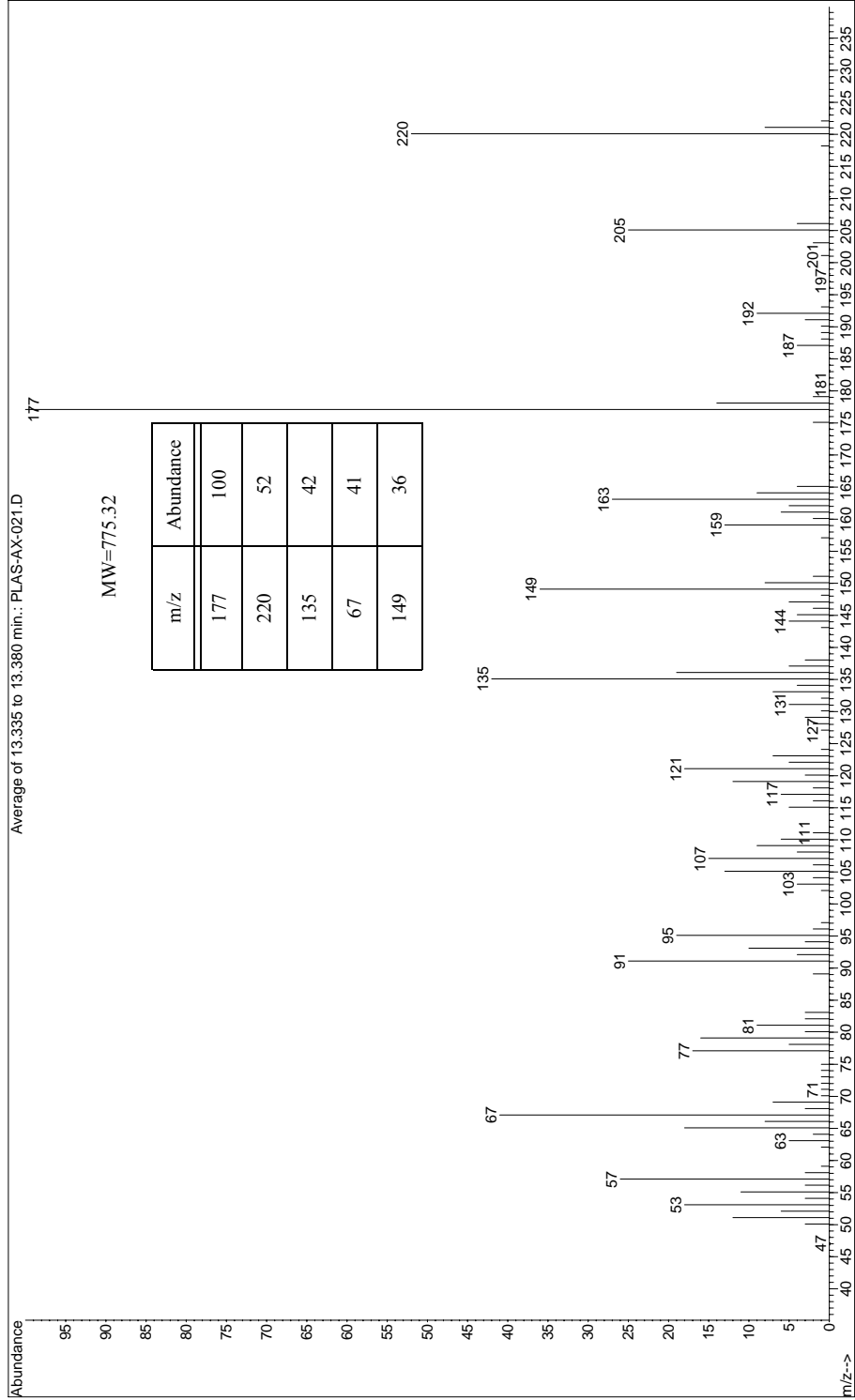
Point of Release

When Ethanox® 330 is incorporated in the polymer matrix it is relatively immobile and release-exposure to humans or the environment is considered minimal.

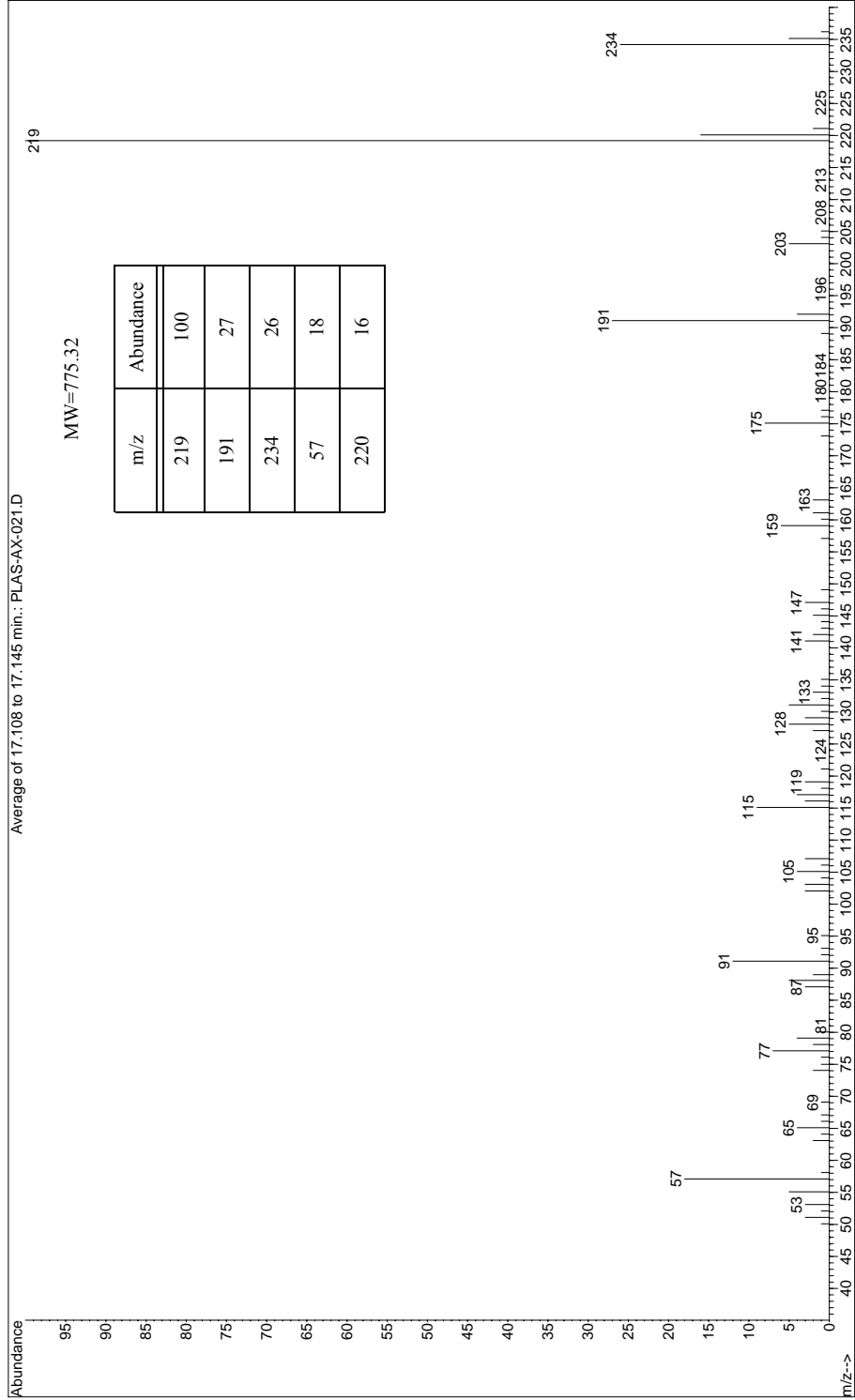
Toxicological Data

RTECS CLASS OF COMPOUND: Reproductive Effector. Acute Oral Toxicity (LD50): 1100 mg/kg [Rat]. Lowest Published Toxic Oral Dose (TDLo): 5000 mg/kg [Rat].

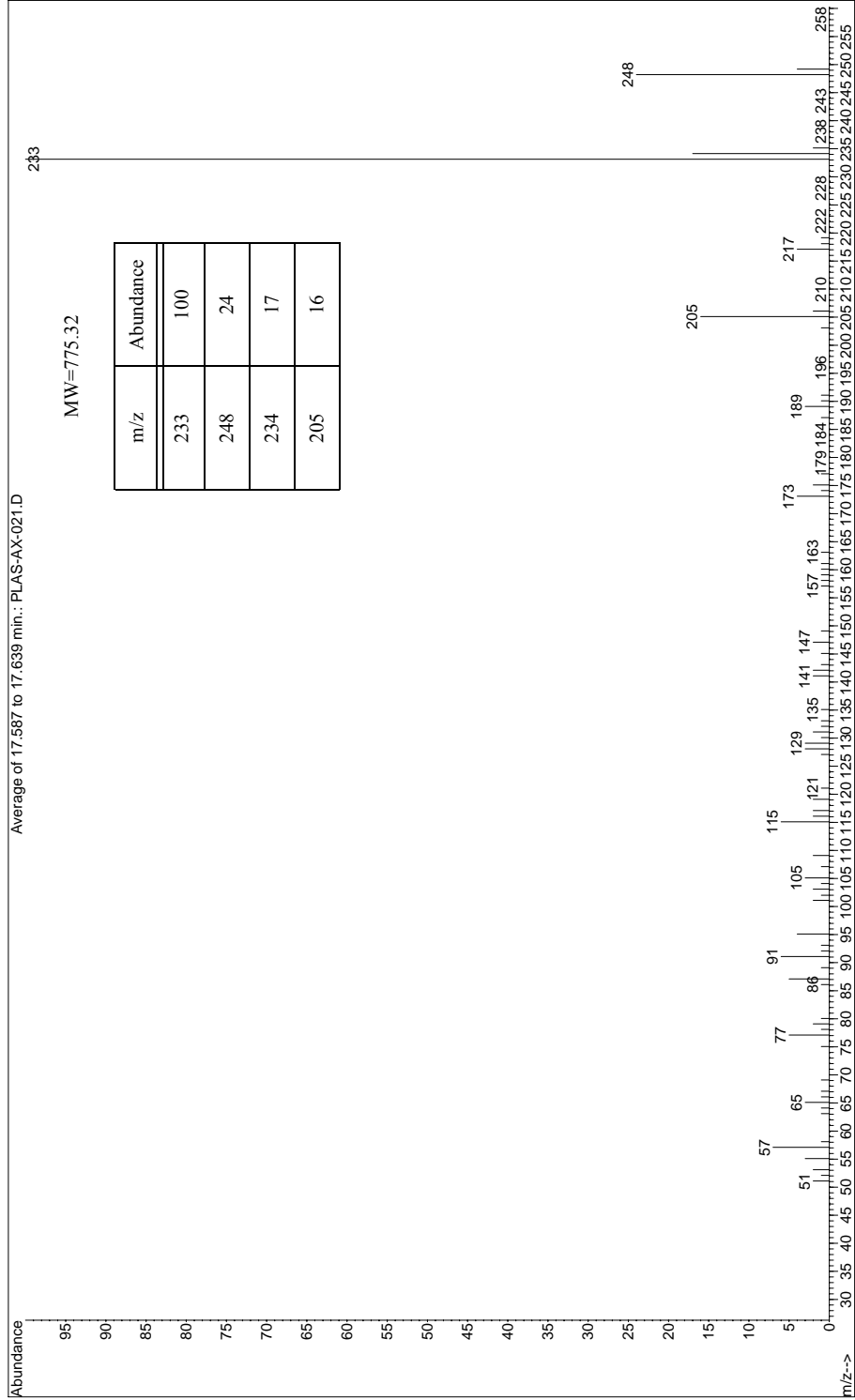
Mass Spectrum for *Ethanox[®] 330 - PLAS-AX-021*



Mass Spectrum for *Ethanox*[®] 330 - PLAS-AX-021

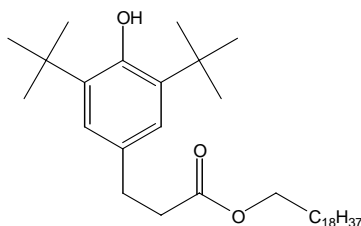


Mass Spectrum for *Ethanox[®] 330 - PLAS-AX-021*



Ethanox® 376

Albemarle Corporation

**CAS Number** 2082-79-3**RTECS Number** Not available**Abbreviation****Formula** C₃₅H₆₂O₃**Molecular Weight** 530.87**Chemical Name**

3,5-di-tert-butyl-4-hydroxyhydrocinnamic acid, octadecyl ester

Synonyms

octadecyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate; stearyl 3-(4-hydroxy-3,5-di-tert-butyl-4-hydroxyphenyl)propionate; 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid

Brand Names & Manufacturers

Anox® PP 18

Chemtura Corporation

Antioxidant 1076

Akrochem Corporation

Irganox® 1076

Ciba Specialty Chemicals

Naugard® 76

Chemtura Corporation

Physical Properties**Appearance** White or yellowish crystalline powder**Melting Point** 50-55 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.6	1.5	19	U	32

Application Application, Regulatory & Environmental Information

Ethanox® 376 is a stabilizer that provides heat stability by preventing thermo-oxidative degradation during processing and service life. It provides compatibility with resins and extraction resistance. It can be applied in polyolefins, such as polyethylene, polypropylene, polybutene-1 and other polymers such as engineering plastics, styrenes, polyurethanes, saturated and unsaturated elastomers, styrenics, rubber modified styrenics, segmented block copolymers, and PVC.

Regulatory Information

FDA approved for use in indirect food contact applications.

Environmental Impact

This product is of low toxicity to aquatic organisms

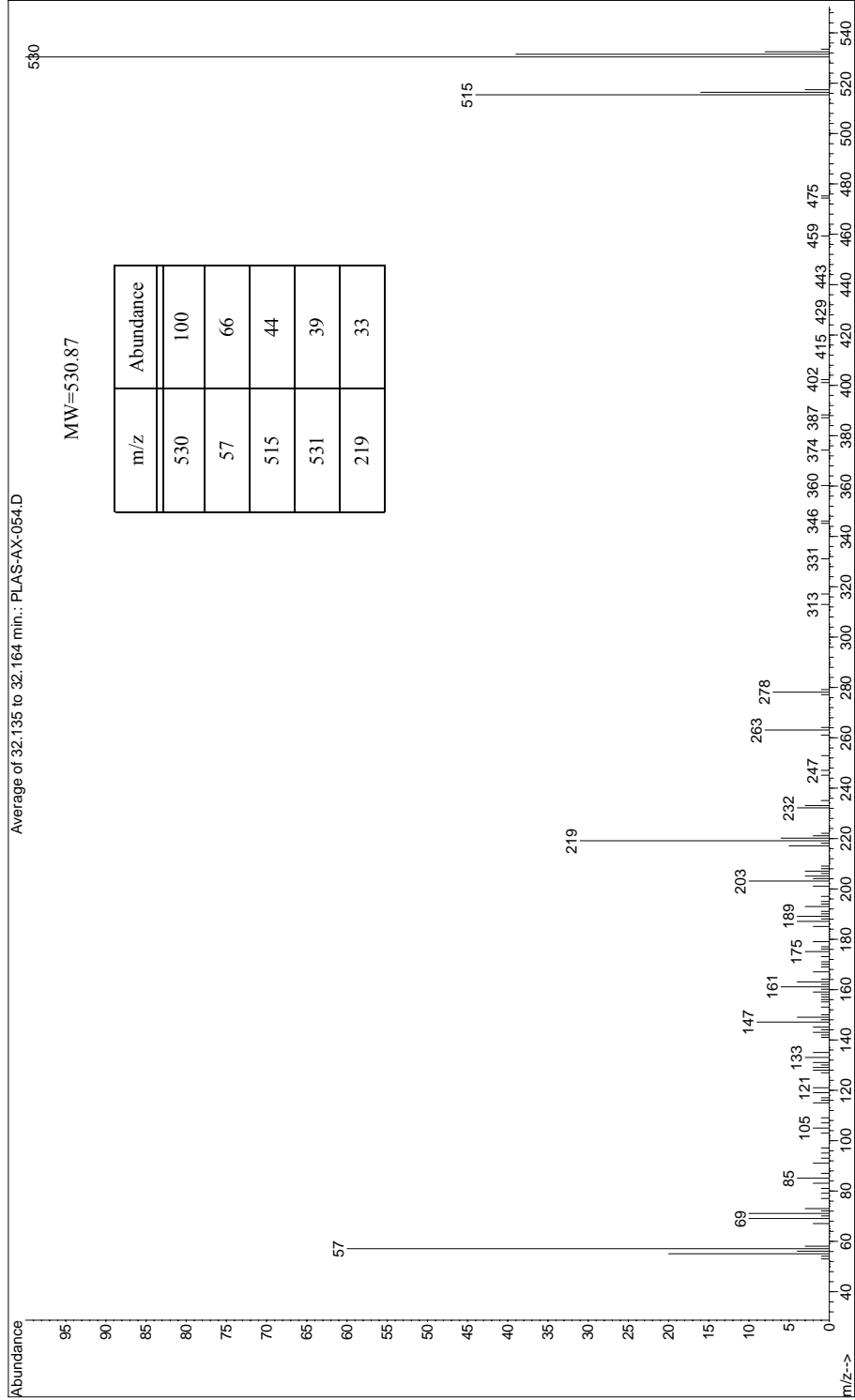
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

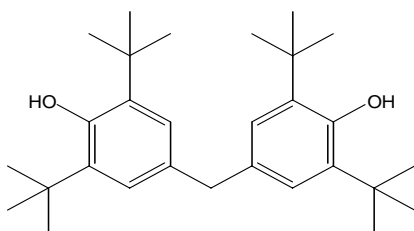
This product presents little or no immediate hazard to people if spilled or released. Acute Oral Toxicity (LD50) > 6,000 mg/kg [Hamster], >10,000 mg/kg [Rat]; Acute Dermal Toxicity (LD50): [Rabbit] >2,000 mg/kg; Acute Inhalation Toxicity: (LC50) > 1.8 mg/l [Rat] air for a 4-hour dust exposure with approximately 90% of particles > 7 microns diameter. There were no mortalities at this concentration.

Mass Spectrum for *Ethanox*[®] 376 - PLAS-AX-054



Ethanox® 702

Albemarle Corporation

**CAS Number** 118-82-1**RTECS Number** SL9650000**Abbreviation** TBMD**Formula** C₂₉H₄₄O₂**Molecular Weight** 424.66**Chemical Name**

4,4'-methylenabis(2,6-di-tert-butylphenol)

Synonyms

di(4-hydroxy-3,5-di-tert-butylphenyl)methane

Brand Names & Manufacturers

Ionol® 220

Degussa

Physical Properties**Appearance** Light-yellow fine crystals**Melting Point** 155 °C**Boiling Point** 289 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	U	U	1-10

Application Application, Regulatory & Environmental Information

This material may be used in natural and synthetic elastomers, polyolefin plastics, resins, adhesives, petroleum oil and waxes.

Regulatory Information

This material is approved by the FDA, as specified 21CFR in the following applications: adhesives and polymers in food contact in the following polymers: petroleum hydrocarbon resins, polyethylene, and polybutadiene.

Environmental Impact

Products of degradation may produce persistent bioaccumulative toxins.

96H (LC50): ~ 1000 mg/L [Fathead minnow], 48H (LC50): ~ 1000 mg/L [Daphnia Magna].

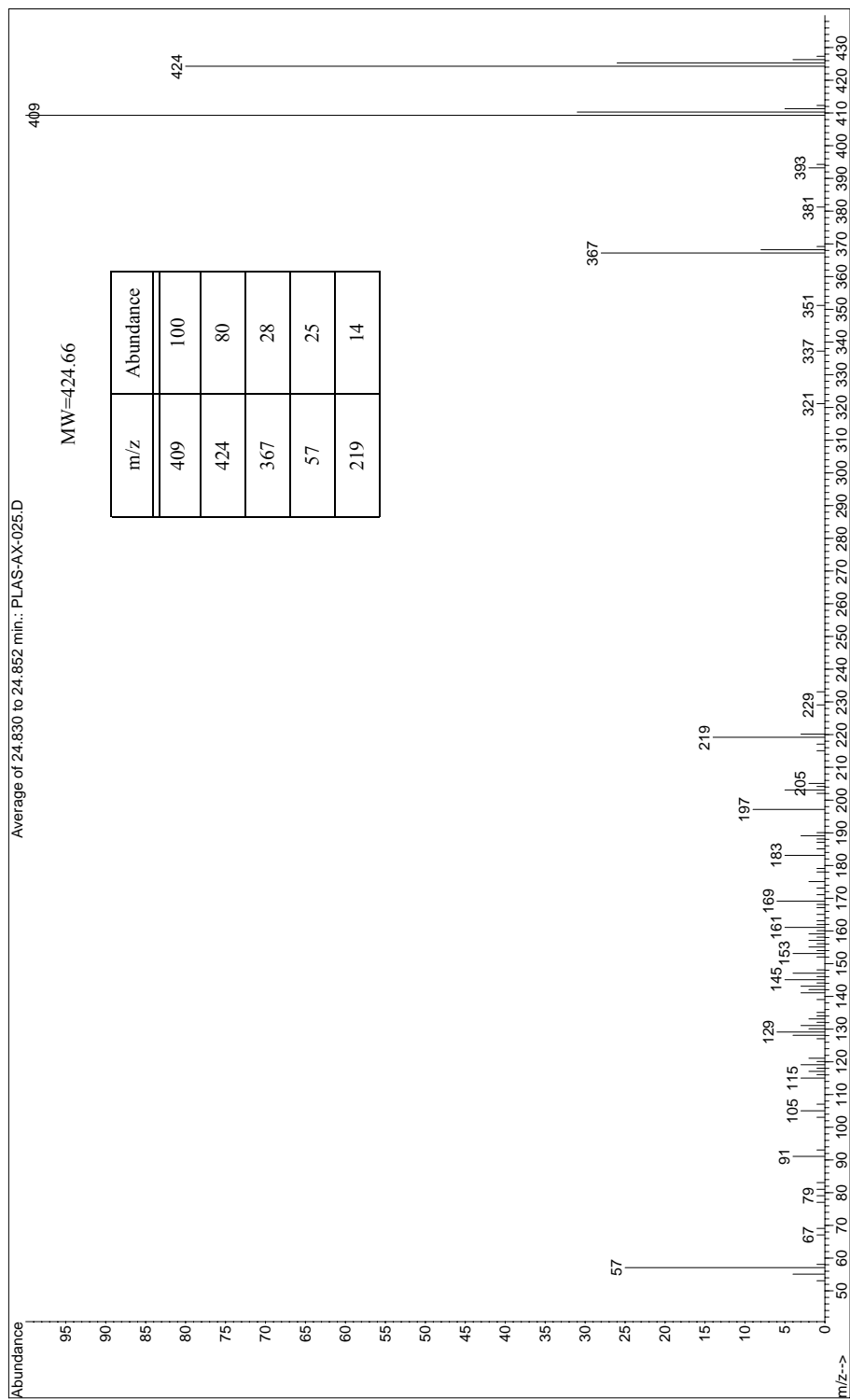
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

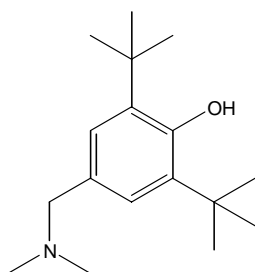
Acute oral toxicity (LD50): >24000 mg/kg [Rat]; acute dermal toxicity (LD50): >2000 mg/kg [Rat].

Mass Spectrum for *Ethanox*[®] 702 - PLAS-AX-025



Ethanox[®] 703

Albemarle Corporation

**CAS Number** 88-27-7**RTECS Number** GO7887000**Abbreviation****Formula** C₁₇H₂₉NO**Molecular Weight** 263.42**Chemical Name**

2,6-di-tert-butyl-N,N-dimethylamino-p-cresol

Synonyms

4-((dimethylamino)methyl)-2,6-bis(1,1-dimethylethyl)phenol

Brand Names & Manufacturers

Physical Properties

Appearance Light-yellow powder**Melting Point** 93-94 °C**Boiling Point** 172 °C (30 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 1-10	EtOH 10-40	Acetone U	CH₂Cl₂ U	Hexane U
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Application **Application, Regulatory & Environmental Information**

Ethanox[®] 703 antioxidant is used as an oxidation inhibitor in natural and synthetic elastomers, polyolefin plastics, resins, adhesives, petroleum oil and waxes. Applications include steam turbine oils, hydraulic fluids, transformer oils, industrial gear oils and greases.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

This material is not biodegradable, but low log Kow value indicates that it will not bioaccumulate. Degradation byproducts may produce persistent bioaccumulative toxins.

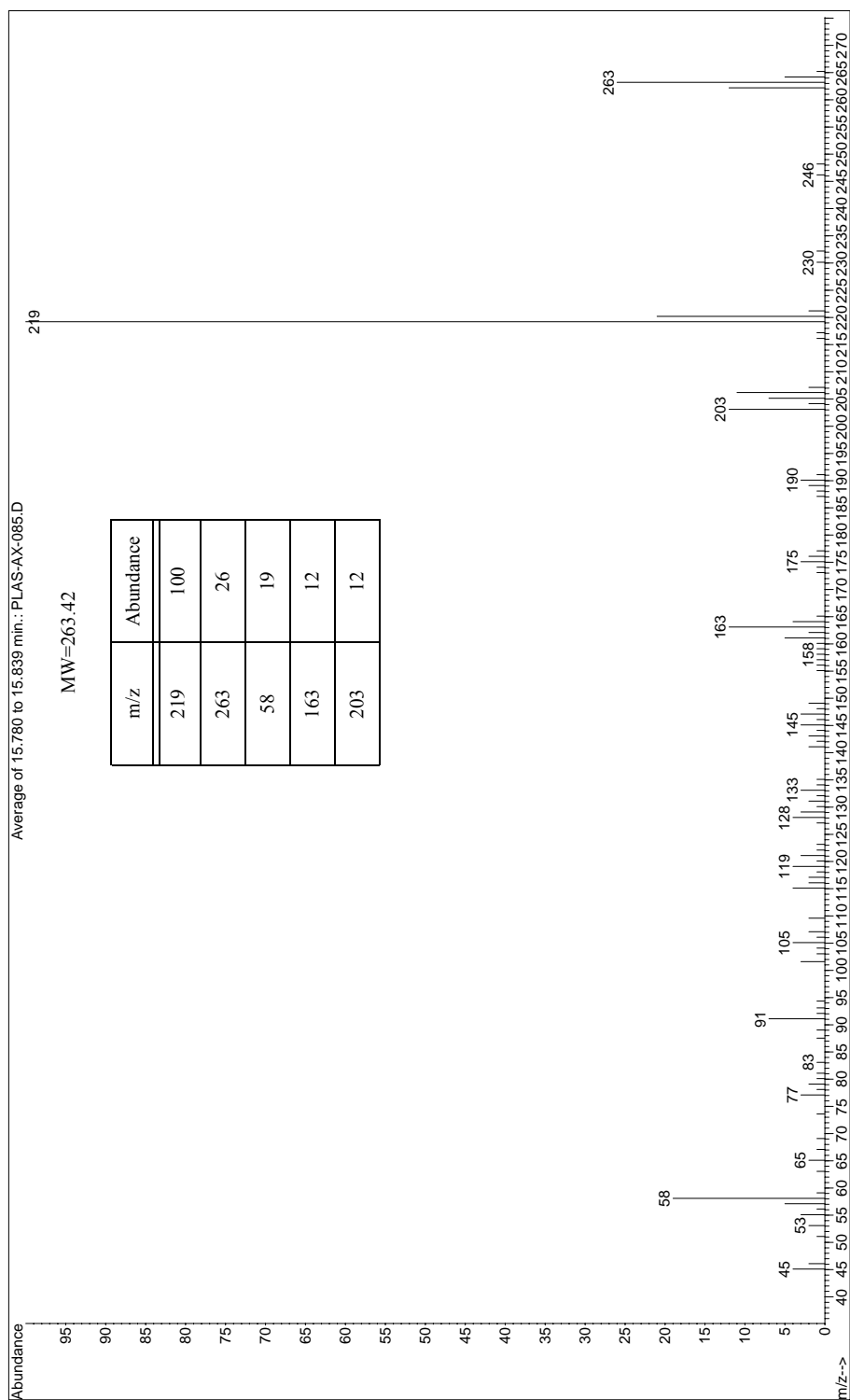
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

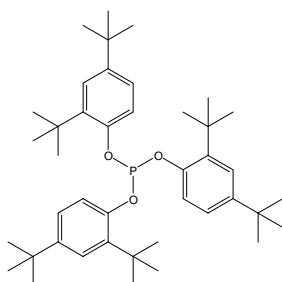
Acute oral toxicity (LD50): 1030 mg/kg [Rat]; dermal (LD50): 4000 mg/kg [Rabbit]. This material is a severe, but reversible eye irritant.

Mass Spectrum for Ethanox® 703 - PLAS-AX-085



Ethaphos® 368

Albemarle Corporation

**CAS Number** 31570-04-4**RTECS Number** Not available**Abbreviation****Formula** C₄₂H₆₃O₃P**Molecular Weight** 646.92**Chemical Name**

tris(2,4-di-tert-butylphenyl) phosphite

Synonyms

2,4-bis(1,1-dimethylethyl)phenol, phosphite (3:1)

Brand Names & Manufacturers

Alkanox® 240

Chemtura Corporation

Irgafos® 168

Ciba Specialty Chemicals

Naugard® 524

Chemtura Corporation

Ultranox® 668

Chemtura Corporation

Physical Properties**Appearance** White crystalline powder**Melting Point** 183-187 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	<0.01	0.1	1	36	11

Application, Regulatory & Environmental Information**Application**

Phosphite processing stabilizer for polypropylene, polyethylene, and adhesives.

Regulatory Information

FDA approved for indirect food contact applications.

Environmental Impact

Potential for slight bioaccumulation, not readily biodegradable log Pow >6 (calculated). (LC50 96 hours): > 100 mg/L [Fish], no effects at the highest tested concentration. The tested concentration is well above its water solubility. (EC50 24 hours): 510 mg/L [Daphnia].

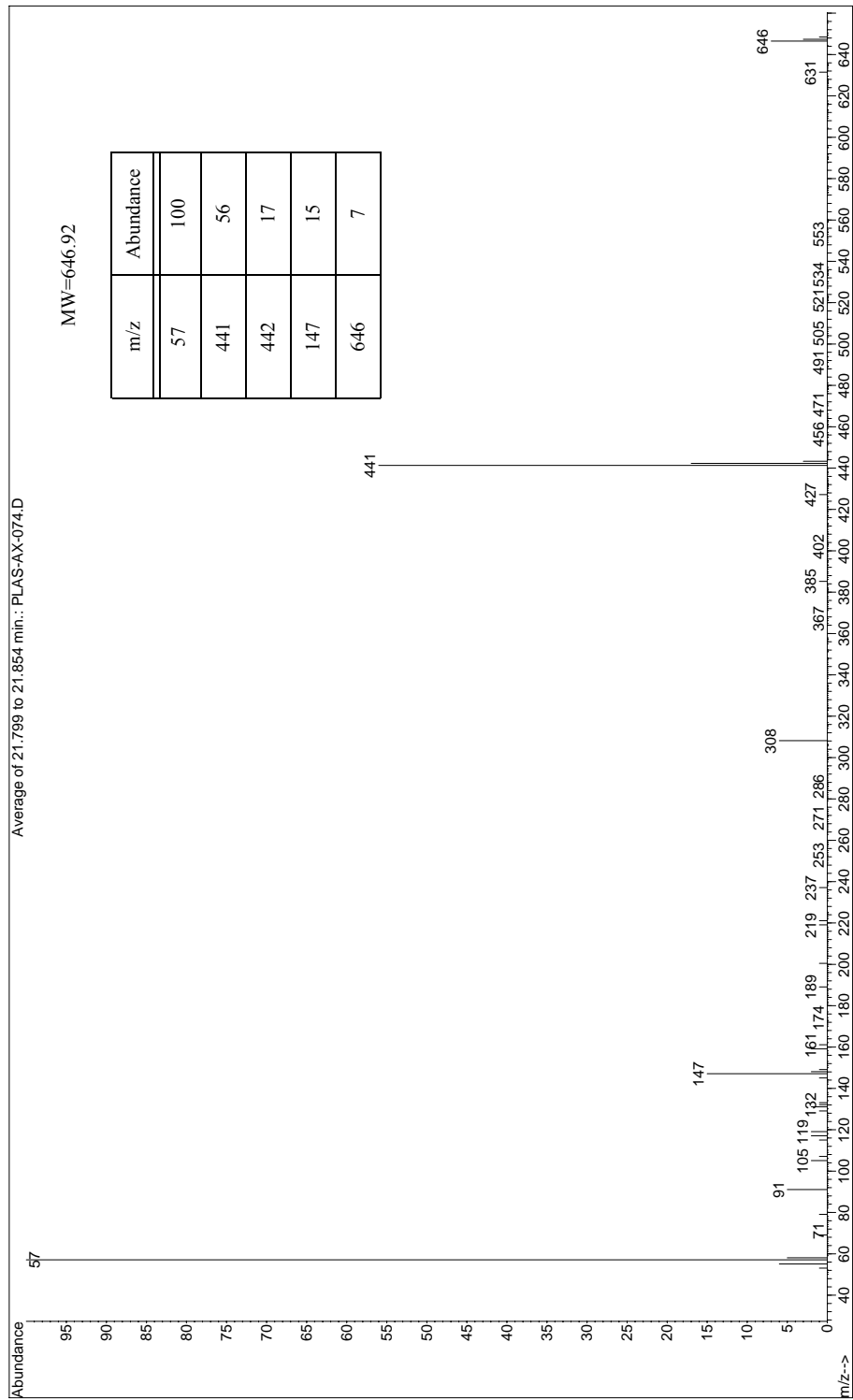
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

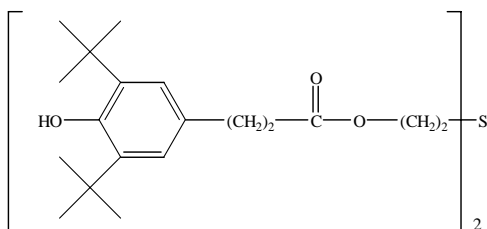
Not regarded as a health or environmental hazard under current legislation. Acute oral toxicity (LD50): > 2000 mg/kg [Rat]; Acute skin toxicity (LD50): > 2000 mg/kg [Rat].

Mass Spectrum for Ethaphos® 368 - PLAS-AX-074



Irganox® 1035

Ciba Specialty Chemicals

**CAS Number** 41484-35-9**RTECS Number** DA8342500**Abbreviation****Formula** C₃₈H₅₈O₆S**Molecular Weight** 642.93**Chemical Name**

thiodiethylene bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate)

Synonyms

3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid thiodi-2,1-ethanediyl ester; 2,2'-thio-bis{ethyl-B-(3,5-ditertbutyl-4-hydroxyphenyl)}-propionate

Brand Names & Manufacturers

Anox® 70

Naugard® EL-50

BNX® 1035

Chemtura Corporation

Chemtura Corporation

Mayzo, Inc.

Physical Properties**Appearance** White to off-white crystalline powder**Melting Point** 63-78 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	5	U	56	U	5

Application, Regulatory & Environmental Information**Application**

Non-discoloring, sulfur containing phenolic antioxidant and stabilizer that provides long-term heat stability by preventing thermo-oxidative degradation. Used for the process stabilization of polyethylene wire and cable resins; for polyethylene during extruder compounding. Can also be applied in styrenic polymers, polypropylene, elastomers such as EPDM and SBR and for carboxylated SBR latex, polybutadiene rubber and polyisopropene rubber.

Regulatory Information

This compound has been approved by the FDA as an indirect food additive for use "in polymers, resins or adhesives intended for food contact applications."

Environmental Impact

Irganox® 1035 does not readily degrade in the environment. Toxicity to aquatic organisms is observed only at doses that exceed the solubility of this compound in water. Further, this material appears to be nontoxic to mammals and nonmutagenic. This compound does have the potential to migrate from food-contact materials into fatty foods such as olive oil.

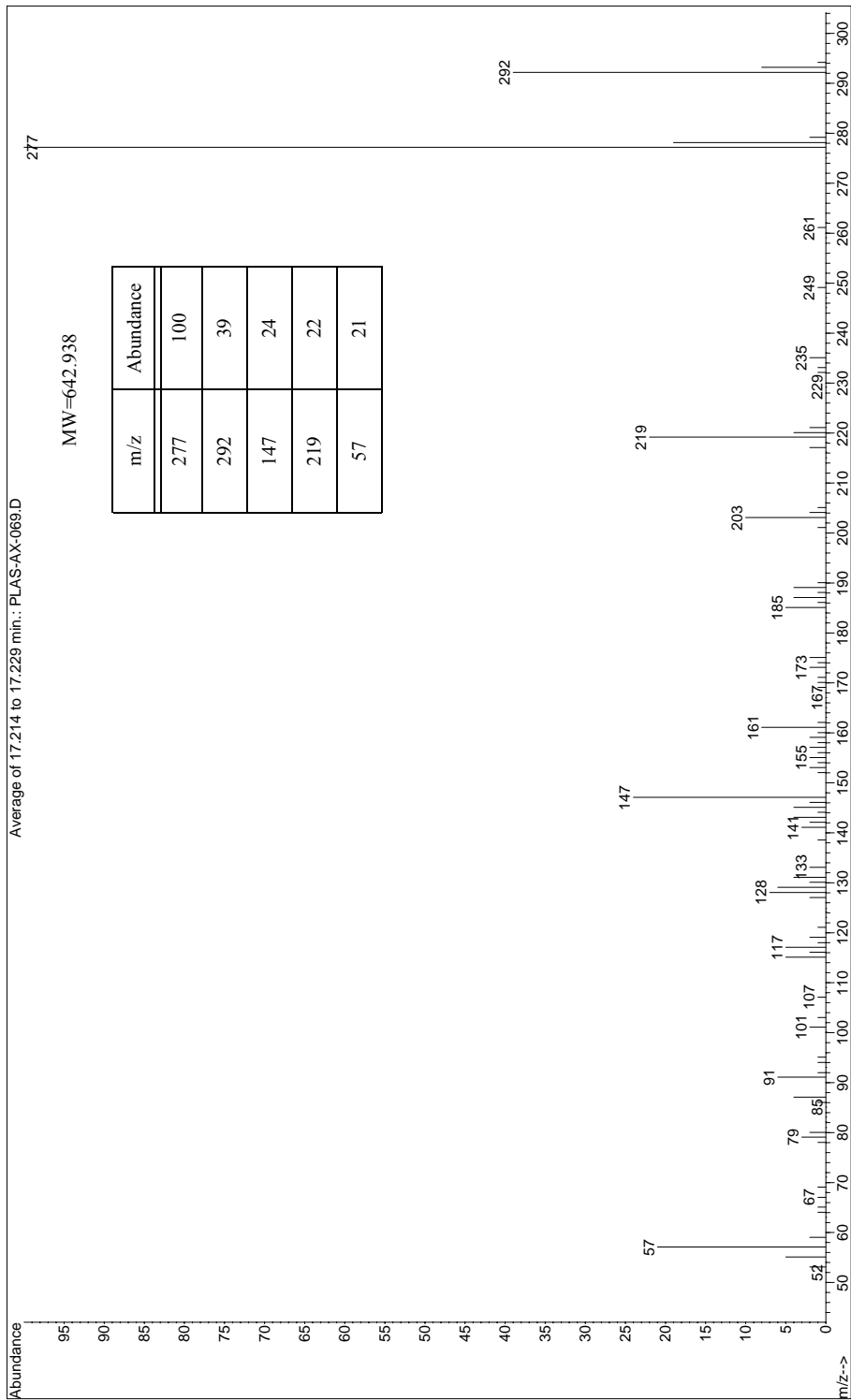
Point of Release

Major human exposure occurs only in the workplace, with consumer exposure being extraordinarily low.

Toxicological Data

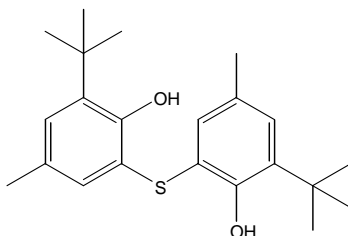
Irganox® 1035 appears to be non-toxic through multiple routes (oral, dermal, and inhalation), with an oral LD50 greater than 5 g/kg [rat], and an acute dermal LD50 greater than 3 g/kg [rabbit], and an acute inhalation LD50 over 6.3 g/m³ [rat]. Subchronic further supports its non-toxic characteristics; NOELs have been calculated from 60 to 10,000 ppm in rats and dogs. These studies included a histological examination of all internal organs that showed no significant toxic effects.

Mass Spectrum for Irganox® 1035 - PLAS-AX-069



Irganox® 1081

Ciba Specialty Chemicals



CAS Number 90-66-4

RTECS Number Not available

Abbreviation

Formula $C_{22}H_{30}O_2S$

Molecular Weight 358.54

Chemical Name

6,6'-di-tert-butyl-2,2'-thiodi-p-cresol

Synonyms

2,2'-thiobis[6-(1,1-dimethylethyl)-4-methylphenol]; 2,2'-dihydroxy-3,3'-di-tert-butyl-5,5'-dimethyldiphenyl-sulfide; bis(5-methyl-3-tert-butyl-2-hydroxyphenyl) monosulfide

Brand Names & Manufacturers

Rionox 2246S

Rionlon Chemical Co.

Physical Properties**Appearance** White to light-yellow crystalline powder**Melting Point** 81-86 °C**Boiling Point** Decomposes**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	35	U	>50	>50	28

Application Application, Regulatory & Environmental Information

Sulfur containing, high performance primary (phenolic) antioxidant and heat stabilizer used for the base stabilization of polyethylene wire and cable resins.

Regulatory Information

FDA approved for use in food contact applications.

Environmental Impact

Estimated Log Pow >6 would indicate the potential for this chemical to bioaccumulate. It is not readily biodegradable and is considered to be toxic to aquatic organisms.

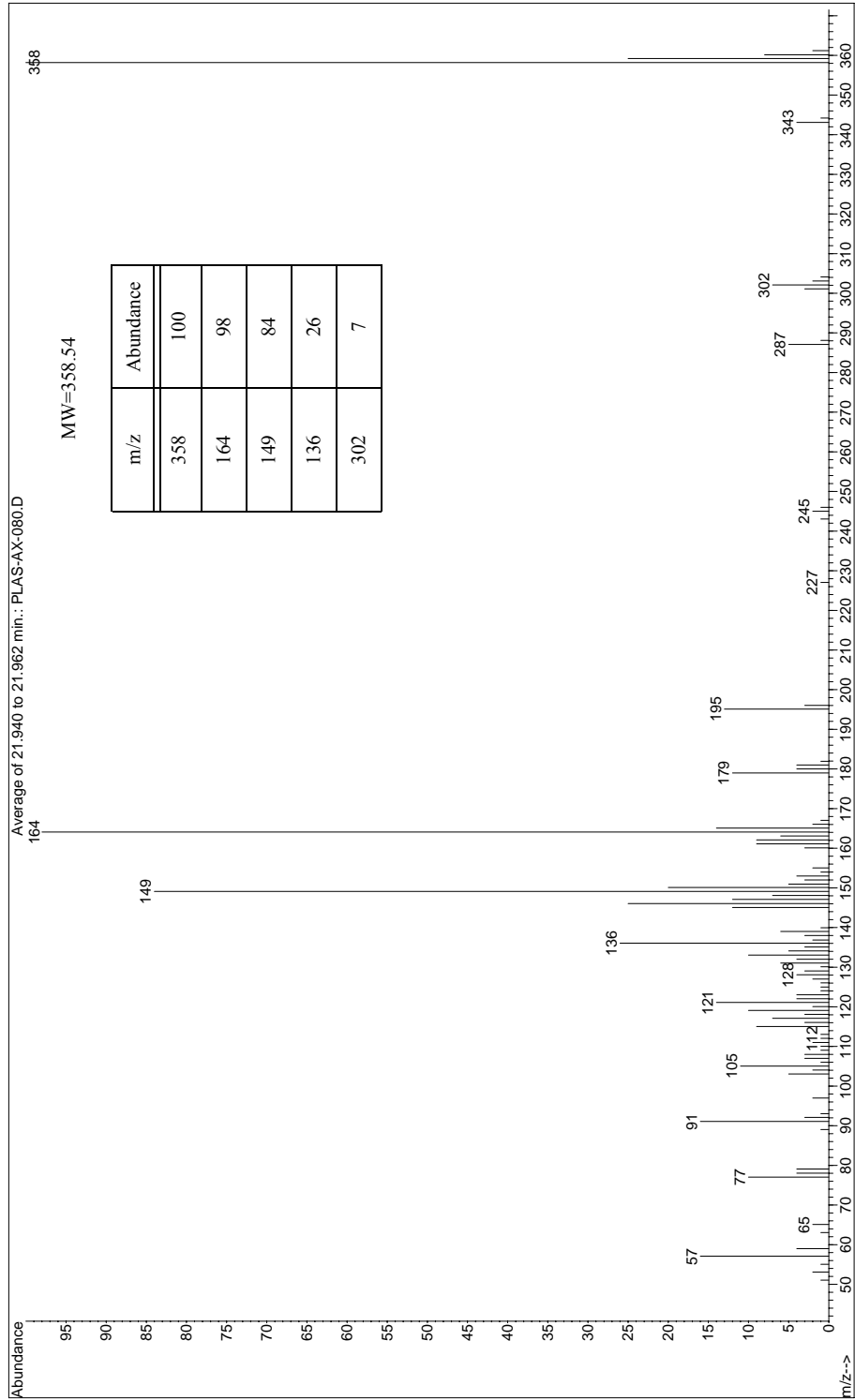
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

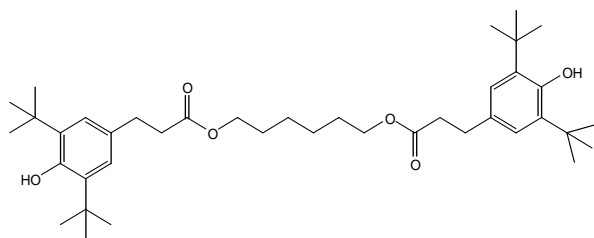
The toxicological properties of this material have not been fully determined.

Mass Spectrum for Irganox® 1081 - PLAS-AX-080



Irganox® 259

Ciba Specialty Chemicals

**CAS Number** 35074-77-2**RTECS Number** DA8342450**Abbreviation****Formula** C₄₀H₆₂O₆**Molecular Weight** 638.92**Chemical Name**

hexamethylene bis(3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate)

Synonyms

hexamethylene bis(3,5-di-tert-butyl-4-hydroxyhydrocinnamate); 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, 1,6-hexanediyl ester

Brand Names & Manufacturers**Physical Properties****Appearance** White to off-white crystalline powder**Melting Point** 104-108 °C**Boiling Point** 654.4 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	1.7	U	36	U	1.5

Application Application, Regulatory & Environmental Information

Irganox® 259 is a stabilizer for organic substrates such as plastics, synthetic fibers, and elastomers.

Regulatory Information

FDA approved for the following applications: polymers, resins or adhesives intended for food contact applications under 21CFR178.2010 and lubricants with incidental food contact.

Environmental Impact

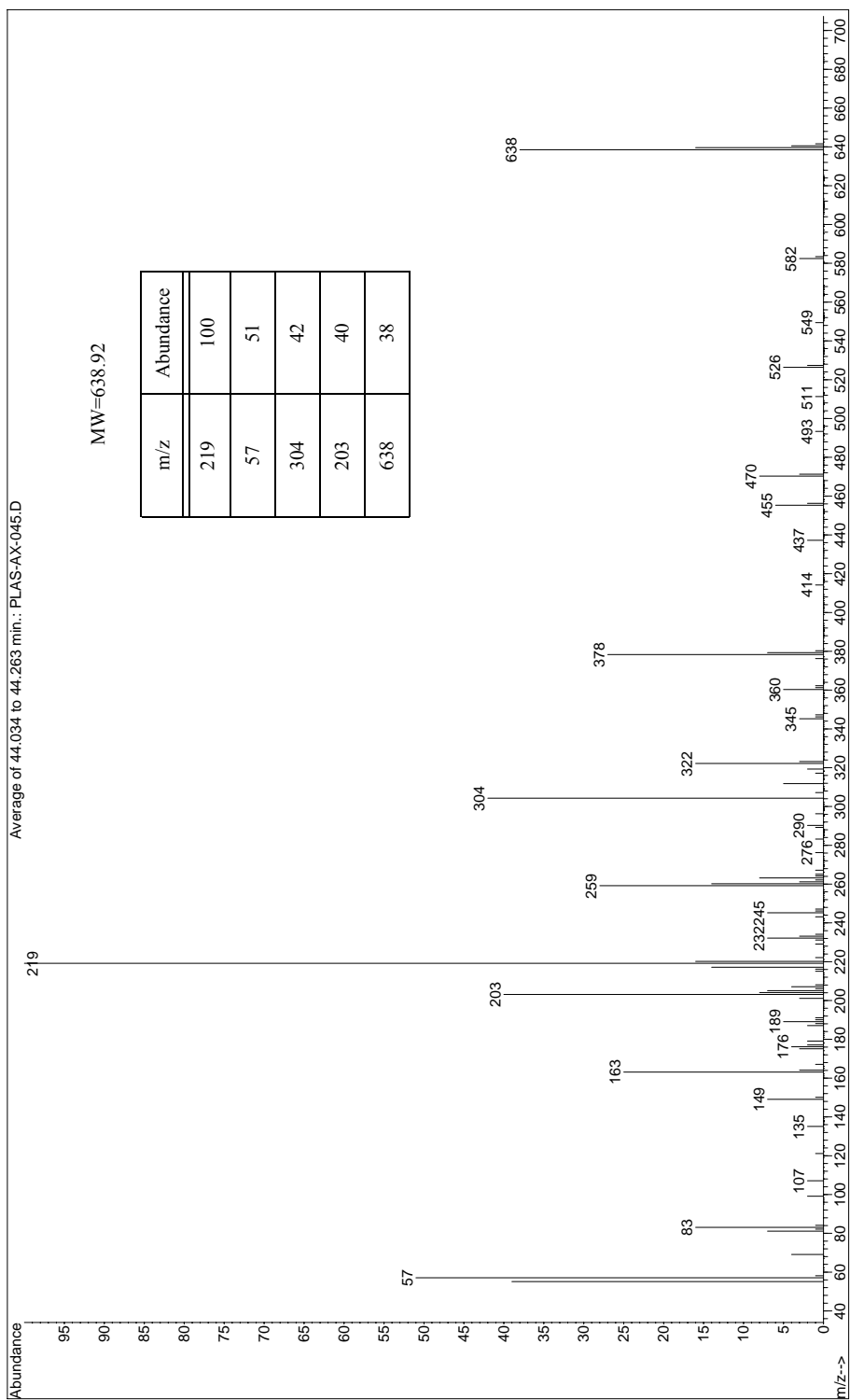
The low water solubility of the material makes it unlikely that hydrolysis would be a significant route of environmental degradation. Environmental accumulation is likely to occur in sediment and not in water.

Point of Release

Release can occur during manufacturing and shipping. Release may also occur from leaching from finished products especially in the presence of fatty esters.

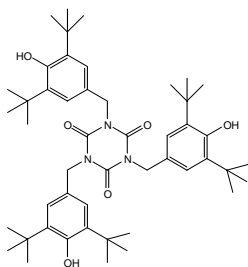
Toxicological DataLowest Published Toxic Oral Dose (TDLo): 45500 mg/kg/13W-I [rat]; (LC50 96 h): > 100 mg/L [Fish]; (EC50 0-72 h): > 100 mg/L [Aquatic Plants]; (EC50 24 h) > 100 mg/L [Aquatic Invertebrates]; Oral (LD50): > 7,750 mg/kg [Mouse], > 10,000 mg/kg [Rabbit]; Inhalation (LD50) > 1700 mg/m³ [Rat].

Mass Spectrum for Irganox® 259 - PLAS-AX-045



Irganox® 3114 FF

Ciba Specialty Chemicals

**CAS Number** 27676-62-6**RTECS Number** Not available**Abbreviation****Formula** C₄₈H₆₉N₃O₆**Molecular Weight** 784.08**Chemical Name**

1,3,5-tris(3,5-di-tert-butyl-4-hydroxybenzyl)-1,3,5-triazine-2,4,6-(1H,3H,5H)-trione

Synonyms1,3,5-tris((3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl)methyl)-1,3,5-triazine-2,4,6(1H,3H,5H)-trione;
Tris(3,5-di-tert-butyl-4-hydroxybenzyl) isocyanurate**Brand Names & Manufacturers**

Cyanox® 1741

Cytec Technology Corp.

Ethanox® 314

Albemarle Corporation

Vanox® GT

R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** White crystalline powder.**Melting Point** 218-220 °C**Boiling Point** 961 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	0.5	1.5	29	U	0.6

Application, Regulatory & Environmental Information**Application**

High molecular weight hindered phenolic antioxidant with photo- and thermo-stability. Provides low volatility and resistance to extraction from polymer compounds. Suitable for PP, PE, polystyrene, ABS, PVC, nylon, and polyurethane. Also used as a radical scavenger providing stabilization for polyolefins.

Regulatory Information

FDA approved for use in various polymers and adhesives intended for food contact applications as defined in 21CFR178.2010 and 175.105.

Environmental Impact

Ecotoxicology data indicates that there is low concern for acute toxicity to fish, aquatic plants and aquatic invertebrates. The data indicate that the material is not readily biodegradable, however, due to the low water solubility, environmental exposures are expected to be low. There is a low potential for bioaccumulation.

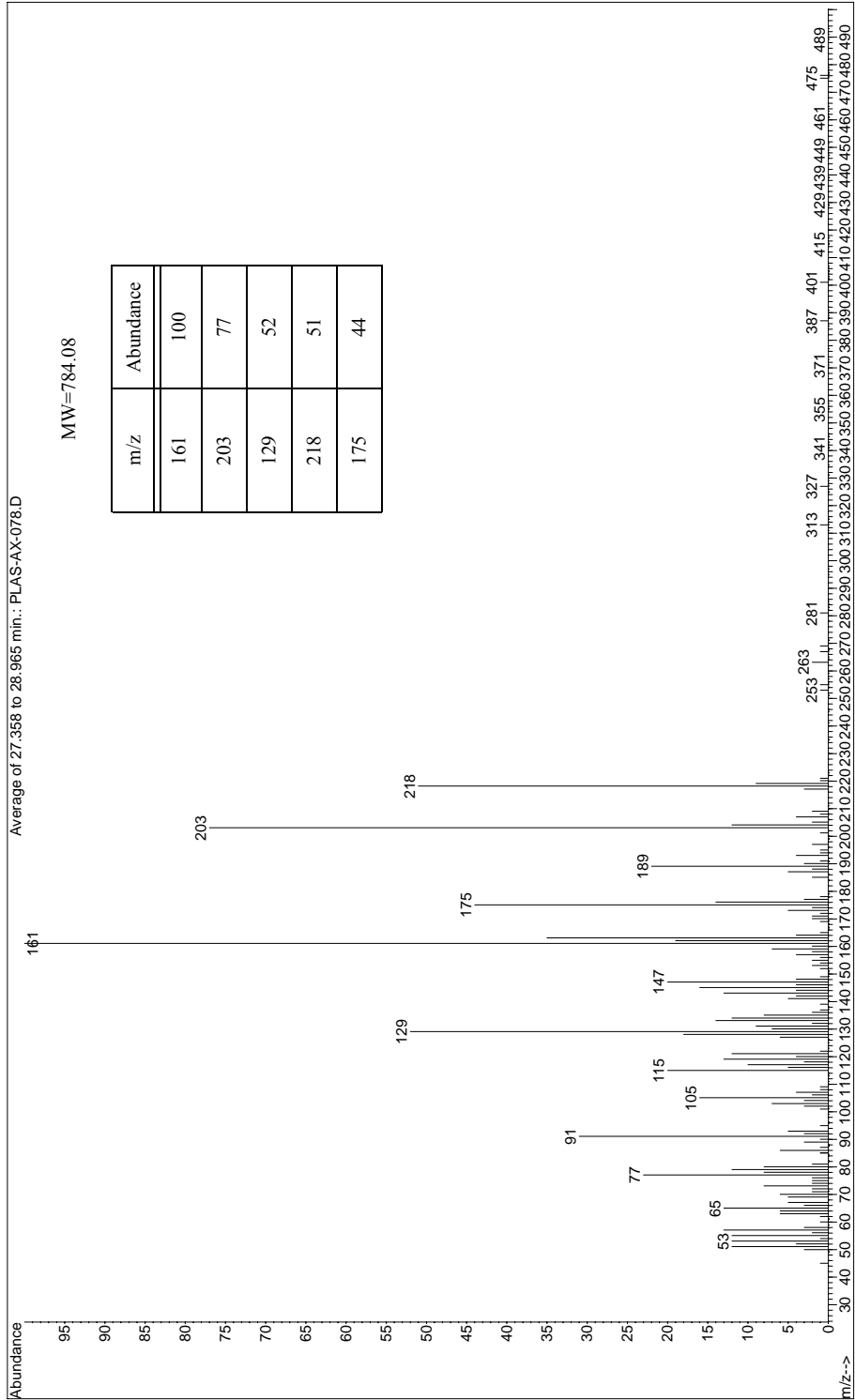
Point of Release

Can be released as point source pollution during manufacture, shipping and use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

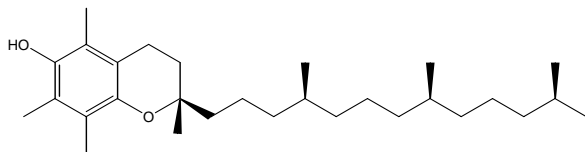
This substance was found to be neither carcinogenic nor a reproductive toxicant. Acute oral toxicity (LD50): >5000 mg/kg [Rat], Acute dermal toxicity (LD50): >2000 mg/kg [Rat], Acute toxicity of the dust (LC50): 270000 mg/m³ 4 hour(s) [Rat].

Mass Spectrum for Irganox® 3114 FF - PLAS-AX-078



Irganox® E 201

Ciba Specialty Chemicals

**CAS Number** 10191-41-0**RTECS Number** GA8746000**Abbreviation****Formula** C₂₉H₅₀O₂**Molecular Weight** 430.71**Chemical Name**

alpha-tocopherol

Synonyms

Vitamin E; ephanyl; 3,4-dihydro-2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-2H-1-benzopyran-6-ol;
2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)-6-chromanol

Brand Names & Manufacturers***Physical Properties***

Appearance	Brown to yellow viscous oil					
Melting Point	3 °C		Boiling Point 200-220 °C at 0.1 mmHg			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH >80	Acetone >80	CH₂Cl₂ >80	Hexane U

Application, Regulatory & Environmental Information**Application**

Can be used for the stabilization of polyethylene for food and medical packaging applications. Can aid in melt flow and color control during processing.

Regulatory Information

FDA classified as Generally Recognized as Safe (GRAS). Approved in many different countries for food applications.

Environmental Impact

This product and its degradation products are not expected to have any negative effects on the environment.

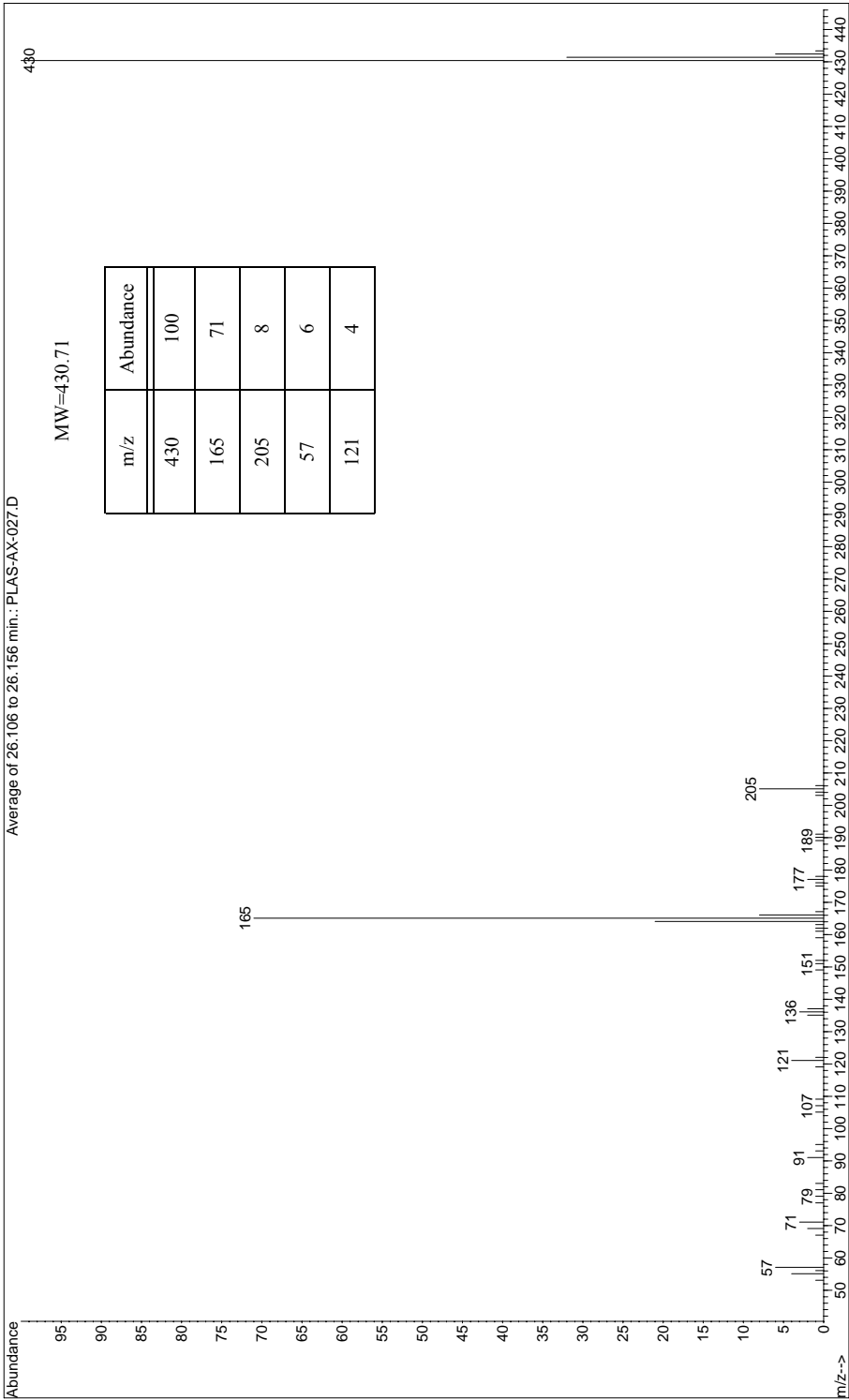
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

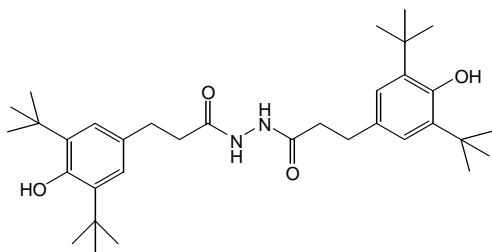
Vitamin E has not been associated with affecting genetic material or adverse reproductive effects in humans, however, when Vitamin E was given to mice in large doses, it was associated with growth retardation of the fetus and an increase in cleft palate. Furthermore, it did affect the genetic material of lab rats when doses of 2500 µg/kg were administered intraperitoneally. Acute oral toxicity (LD50): >4000 mg/kg [Mouse].

Mass Spectrum for Irganox® E 201 - PLAS-AX-027



Irganox® MD 1024

Ciba Specialty Chemicals

**CAS Number** 32687-78-8**RTECS Number** Not available**Abbreviation****Formula** C₃₄H₅₂N₂O₄**Molecular Weight** 552.79**Chemical Name**

1,2-bis(3,5-di-tert-butyl-4-hydroxyphenyl)hydrazide

Synonyms

2',3-bis((3-(3,5-Di-tert-butyl-4-hydroxyphenyl)propionyl))propionohydrazide

Brand Names & Manufacturers

Lowinox® MD24

Chemtura Corporation

Physical Properties**Appearance** White to slightly yellowish crystalline powder**Melting Point** 227-232 °C**Boiling Point** 742 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	4	U	4	U	<0.01

Application, Regulatory & Environmental Information**Application**

Metal deactivator that acts as a hindered phenolic antioxidant. Used in conjunction with phenolic antioxidants, phosphites/phosphonites, thio-synergists and other co-additives. Most suited for PA, PE, Rubbers and PP applications.

Regulatory Information

Irganox® MD 1024 is approved by the FDA for use in packaging polymers, resins and adhesives intended for food contact applications. It is approved in many countries for food contact applications.

Environmental Impact

After this material is incorporated in the polymer matrix it is relatively immobile and release/exposure to humans or the environment is considered minimal. Under environmental conditions the low solubility of the material should preclude the occurrence of acutely toxic exposures. The compound has very low volatility, and a calculated log Pow of >6. Based on its properties it is likely to bind to the soil and sediment where it is expected to be immobile and have limited bioavailability.

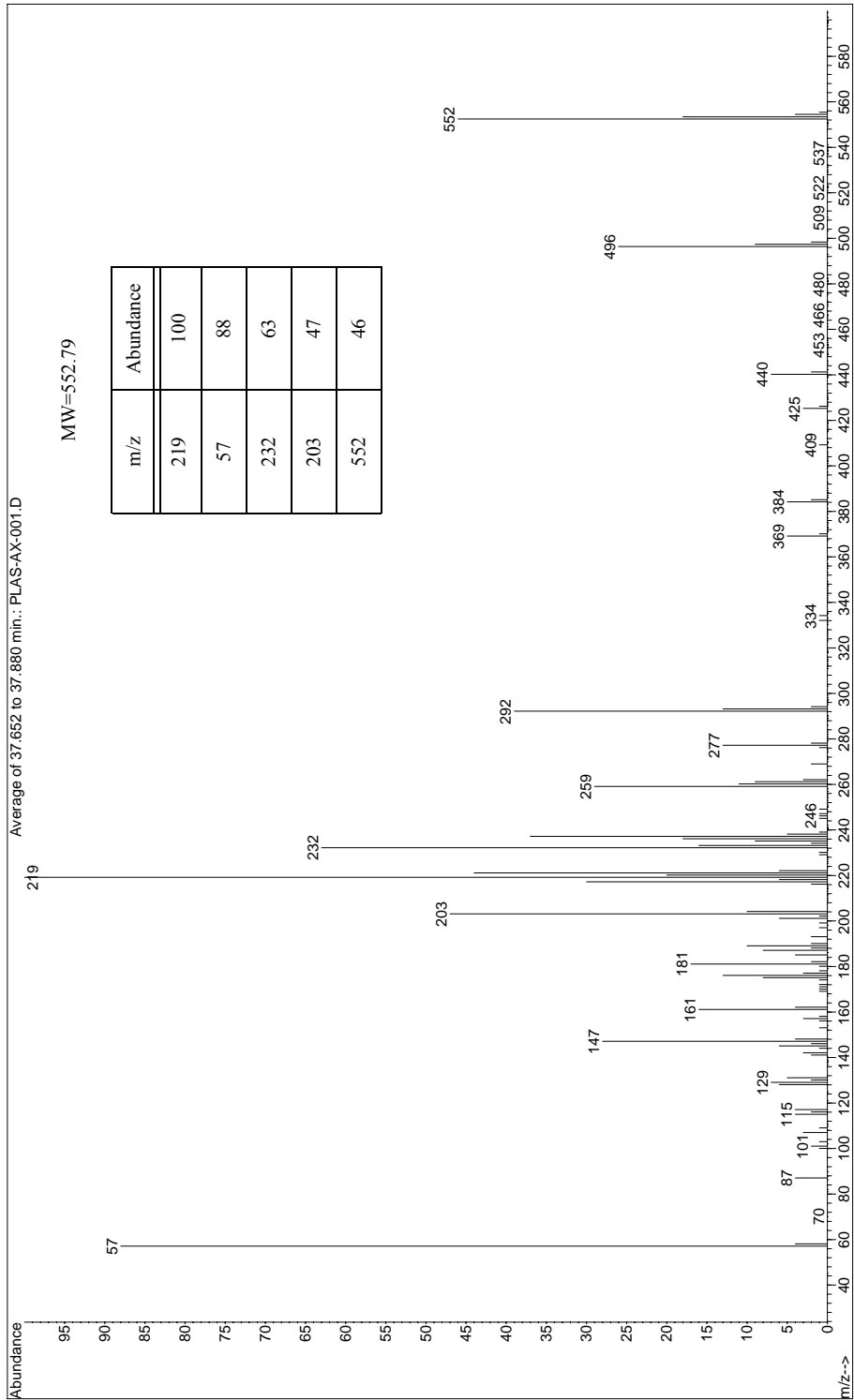
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

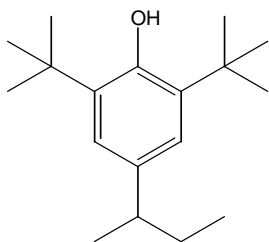
Available mammalian acute toxicity data indicates very low toxicity by oral, or inhalation exposure. It is neither teratogenic nor embryotoxic and it does not impact reproductive organs, even at relatively high exposure levels. Additionally, the compound is not mutagenic or clastogenic. In a subchronic 28 day toxicity study in the rat, there are no adverse effects up to 1000 mg/kg BW per day.

Mass Spectrum for Irganox® MD 1024 - PLAS-AX-001



Isonox[®] 132

SI Group Incorporated

**CAS Number** 17540-75-9**RTECS Number** Not available**Abbreviation****Formula** C₁₈H₃₀O**Molecular Weight** 262.43**Chemical Name**

2,6-di-tert-butyl-4-sec-butylphenol

Synonyms

4-sec-butyl-2,6-di-tert-butylphenol

Brand Names & Manufacturers**Physical Properties****Appearance** Clear liquid**Melting Point** ~25 °C**Boiling Point** 275 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Phenolic antioxidant for polyols, PVC, and adhesives.

Regulatory Information

FDA approved for food contact use in PVC not to exceed 0.06% by weight of the finished product.

Environmental Impact

Log Kow value of 6.43. Since it is relatively insoluble in water, primary accumulation anticipated in the sediment. This material is estimated to be aerobically degradable, with primary degradation occurring in weeks, and complete degradation in months. (LC50 96hr): 0.072 mg/L [Fish], (LC50 48hr): 0.22 mg/L [Daphnia].

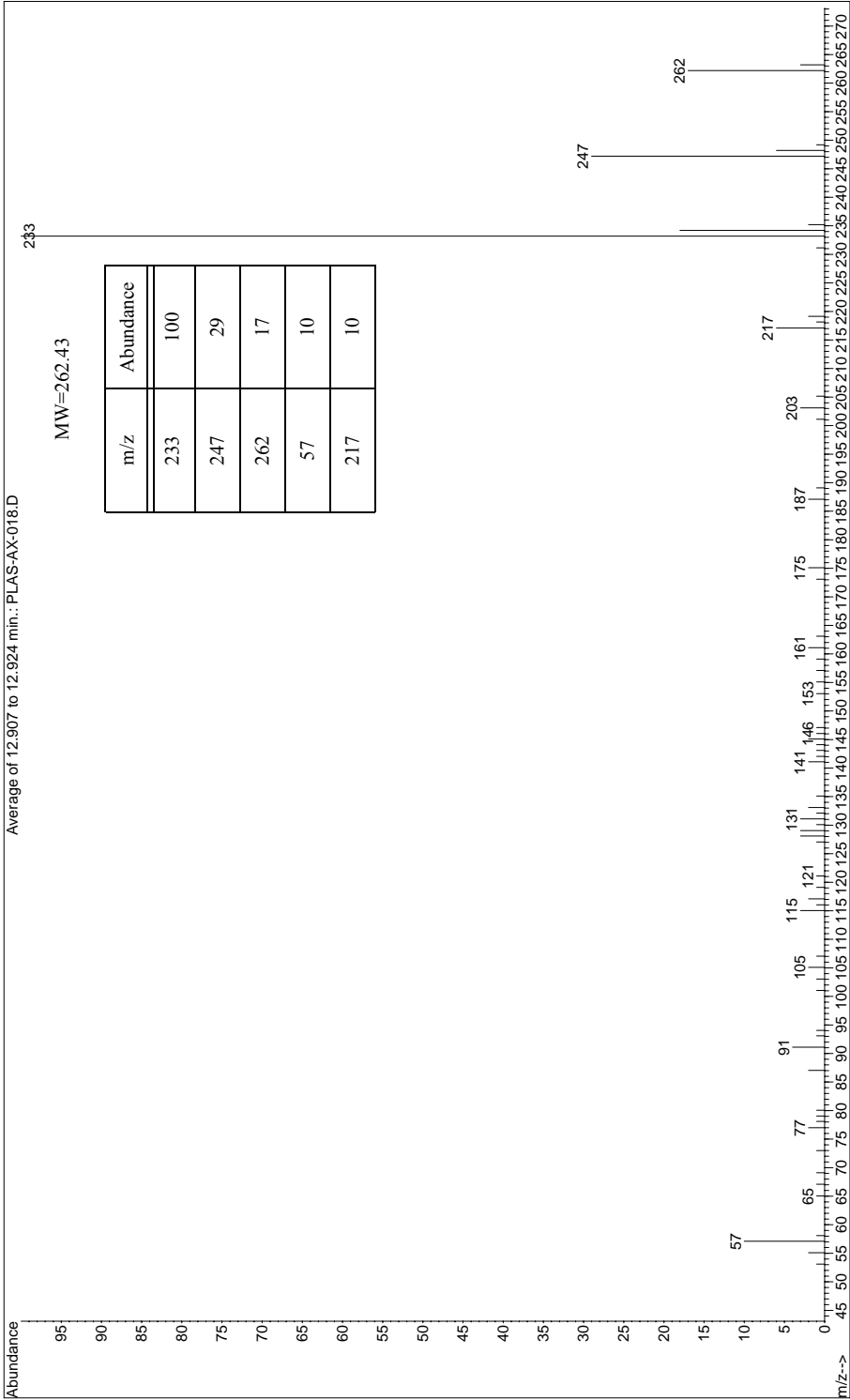
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

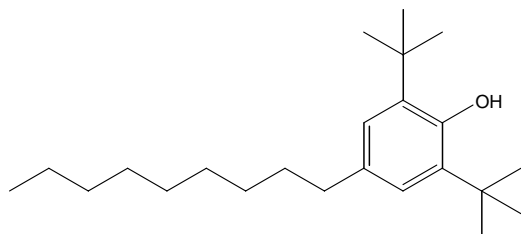
May cause respiratory or skin sensitization. Acute oral toxicity (LD50): 2000 mg/kg [Rat].

Mass Spectrum for Isonox® 132 - PLAS-AX-018



Isonox® 232

SI Group Incorporated

**CAS Number** 4306-88-1**RTECS Number** Not available**Abbreviation****Formula** C₂₃H₄₀O**Molecular Weight** 332.57**Chemical Name**

2,6-di-tert-butyl-4-nonylphenol

Synonyms

2,6-bis(1,1-dimethylethyl)-4-nonylphenol

Brand Names & Manufacturers

Ionol® 926

Degussa

Physical Properties**Appearance** Colorless to light-yellow liquid with a mild, aromatic odor**Melting Point** >5 °C**Boiling Point** 335-345 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Phenolic antioxidant for polyol and polyurethane foam. Also used as a lubricating oil additive.

Regulatory Information

No information available.

Environmental Impact

Aquatic toxicity: (LC50): >10 mg/L/96h [Rainbow trout]. Material can biodegrade (BOD28 ~30%).

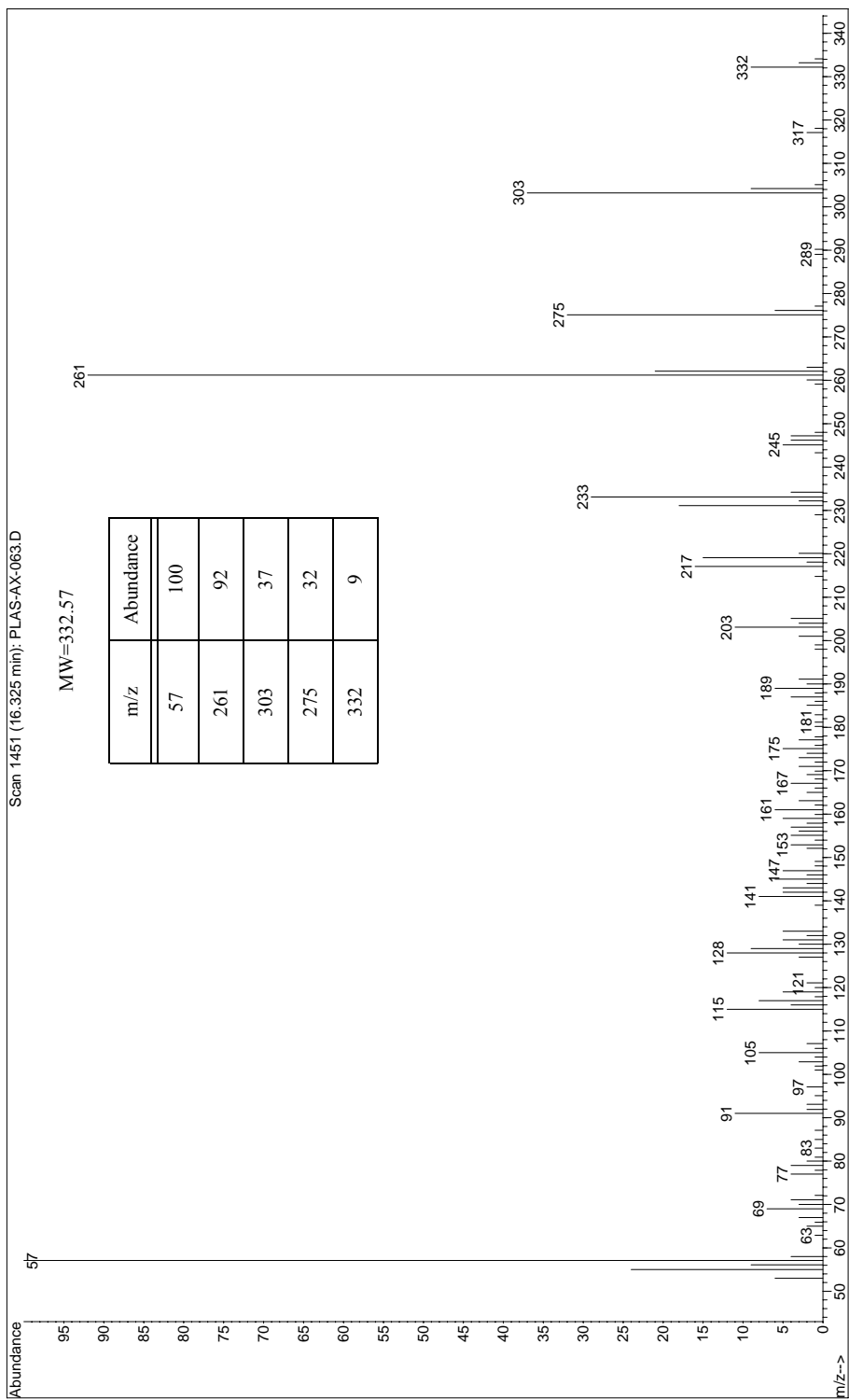
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

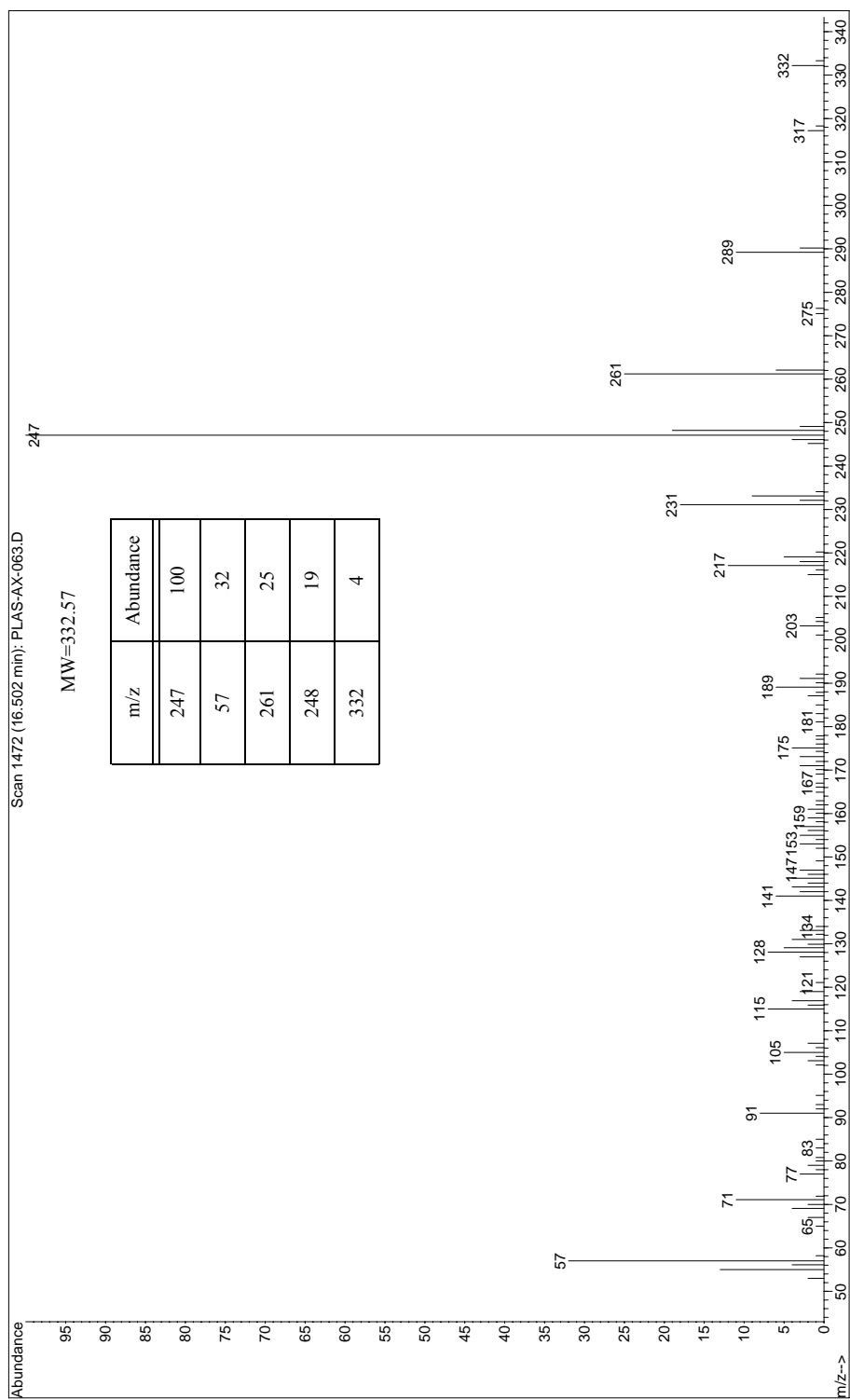
Toxicological Data

Acute oral toxicity (LD50): >2000 mg/kg [Rat].

Mass Spectrum for Isonox® 232 - PLAS-AX-063

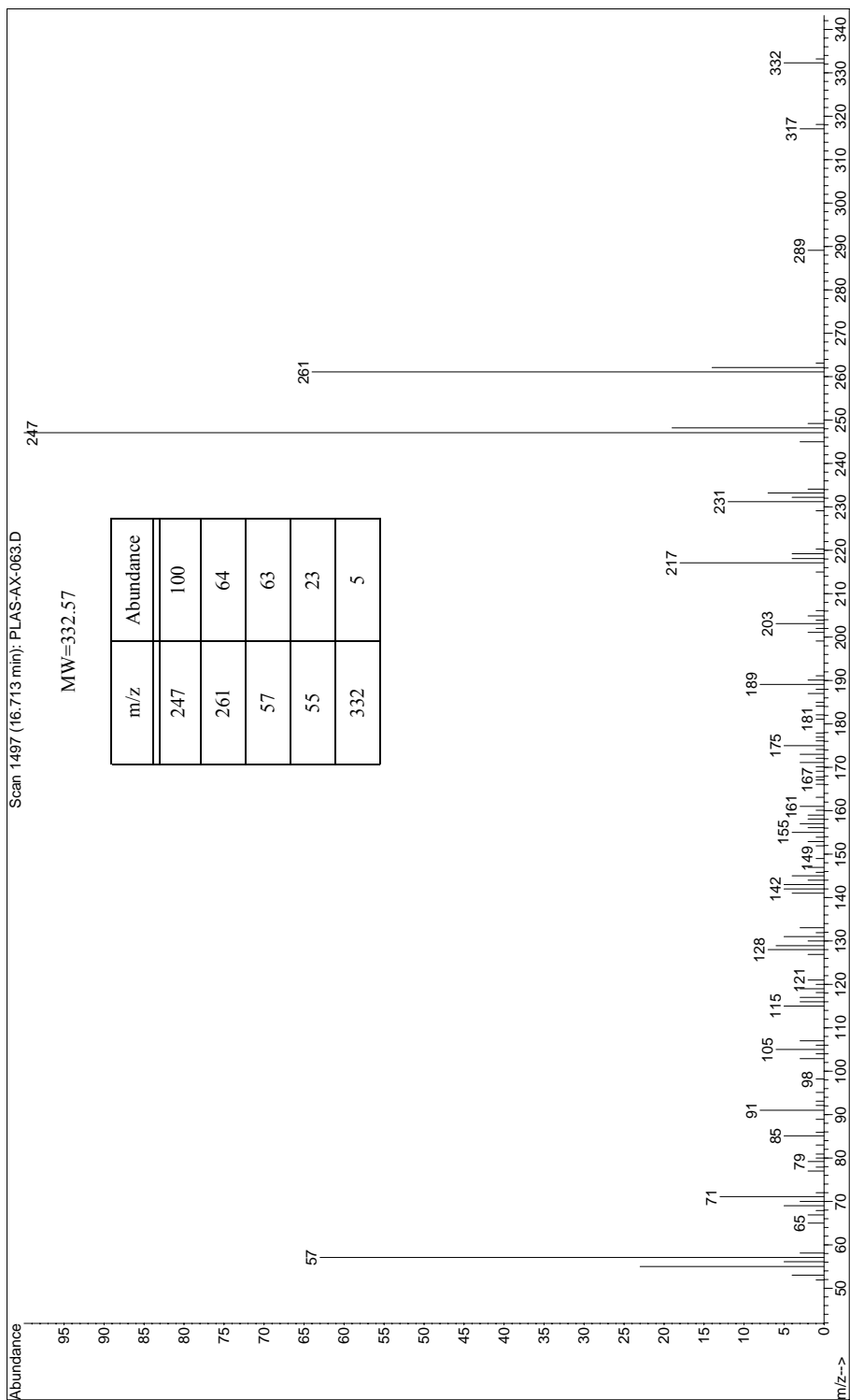


Mass Spectrum for Isonox[®] 232 - PLAS-AX-063



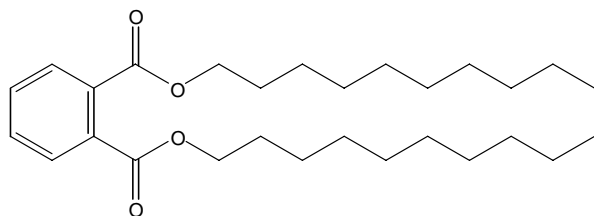
For Chromatogram See Appendix A - PLAS-AX-063 - page 371

Mass Spectrum for Isonox[®] 232 - PLAS-AX-063



Lowinox® AH25

Chemtura Corporation

**CAS Number** 79-74-3**RTECS Number** MX6300000**Abbreviation****Formula** C₁₆H₂₆O₂**Molecular Weight** 250.38**Chemical Name**

2,5-bis(1,1-dimethylpropyl)-1,4-benzenediol

Synonyms

2,5-di-tert-pentylhydroquinone; 2,5-bis(1,1-dimethylpropyl)hydroquinone; 2,5-di-tert-amylhydroquinone

Brand Names & Manufacturers

Antioxidant 250-SVA

Akrochem Corporation

Physical Properties**Appearance** White to cream powder or granules; odorless**Melting Point** 177-184 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	U	68	72	U	U

Application, Regulatory & Environmental Information**Application**

Lowinox® AH-25 is a phenolic antioxidant that reduces cold flow in unvulcanized rubber and protects against sun crack. Also slows the skinning (drying out) of paint resins and adhesive coating; extends tack in uncured adhesives, tapes, and hot-melt adhesives at up to a 0.5 to 4.0 phr level.

Regulatory Information

FDA: approved 1998 for the following applications: adhesives in safe contact with food in all stages of production, processing, and packaging; adhesives, 21CFR175.105; in the manufacture of rubber material intended for use in all stages of production, processing, packaging and transport of food, 21CFR177.2600.

Environmental Impact

Not readily biodegradable. Hazardous to the environment and toxic to aquatic organisms. (EC50 24hr): 0.91 mg/L [Daphnia]; (LC50 96hr): 0.067 mg/L [Trout], 34 µg/L [Bluegill], 0.12 mg/L [Fathead minnow]; (LC50 48hr): 35 µg/L [Bluegill]; (LC50 24hr): 42 µg/L [Rainbow trout], 49 µg/L [Bluegill]; (EC50 96hr): 1.7 ppm [Selenastrum capricornutum].

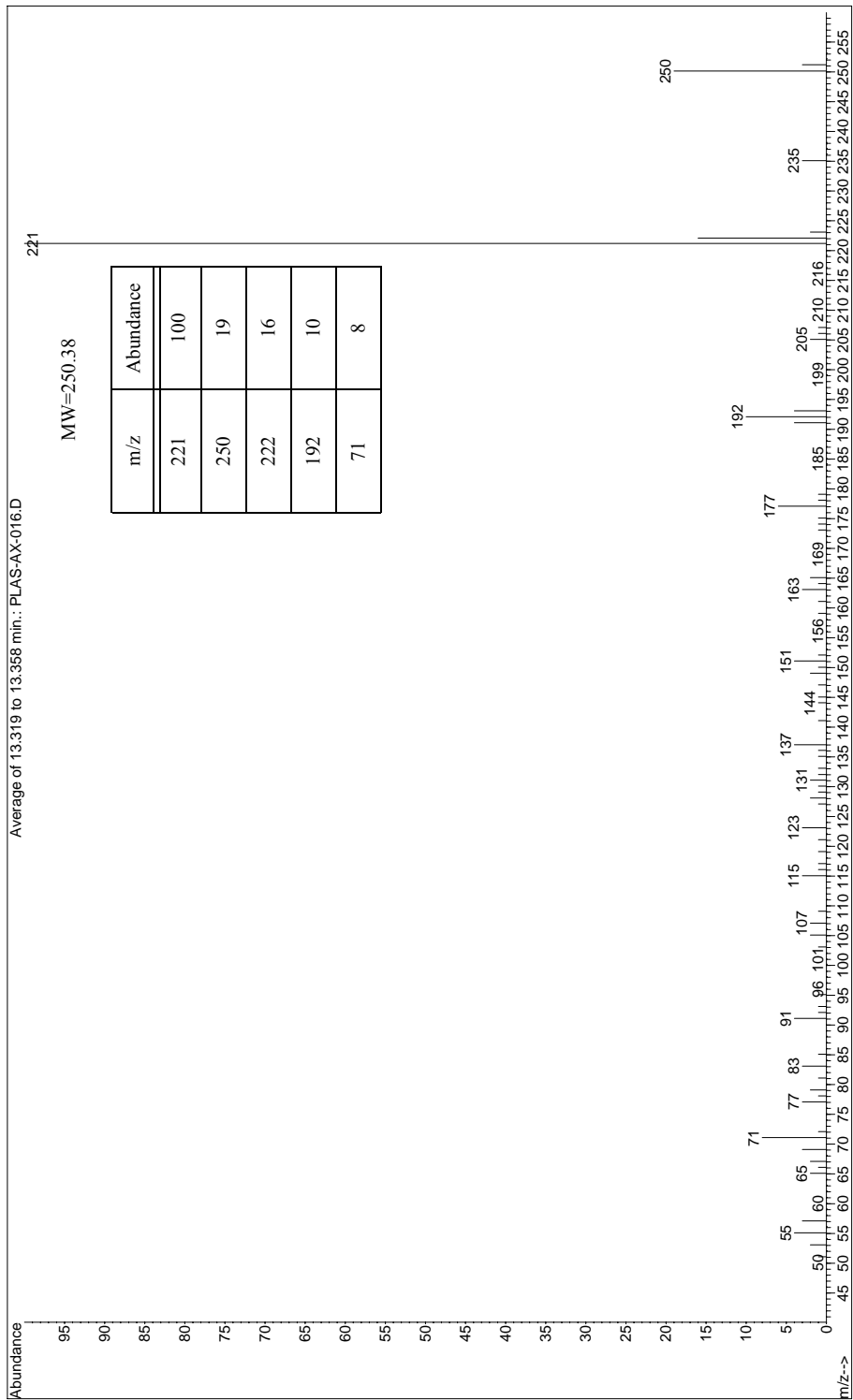
Point of Release

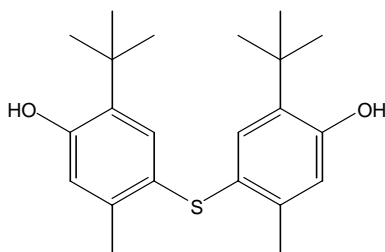
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

The toxicological properties of this material have not been thoroughly investigated. Not listed (ACGIH, IARC, NTP, OSHA) as a cancer causing agent. Acute intraperitoneal (LD50): 200 mg/kg [Mouse]; Acute dermal (LD50): >3160 mg/kg [Rabbit]; Acute oral (LD50): 2 g/kg [Rabbit], 1900 mg/kg [Rat].

Mass Spectrum for Lowinox® AH25 - PLAS-AX-016



Lowinox® TBM-6

CAS Number 96-69-5

RTECS Number GP3150000

Abbreviation TBBC

Formula $C_{22}H_{30}O_2S$

Molecular Weight 358.54

Chemical Name

4,4'-thiobis(2-tert-butyl-5-methylphenol)

Synonyms

bis(3-tert-butyl-4-hydroxy-6-methylphenyl)sulfide; 4,4'-thiobis(6-tert-butyl-3-methylphenol); 1,1-thiobis(2-methyl-4-hydroxy-5-tert-butylbenzene)

Brand Names & Manufacturers

Cyanox® 1760

Cytec Technology Corp.

Santonox® TBMC

Flexsys America L.P.

Rhodianox TBM6 (P/T/TP)

Rhône-Poulenc Chimie Corp.

Physical Properties**Appearance** White to cream-colored crystalline powder; phenolic odor**Melting Point** 160-164 °C**Boiling Point** Decomposes at 300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.08	79	47	20	U	~0.75

Application, Regulatory & Environmental Information**Application**

TBBC is a hindered thiophenol antioxidant used in natural and synthetic rubbers with high thermo-oxidative degradation resistance properties. It is a polymerization and processing 'light-stabilizer' in PP, ABS, PVC, EPDM, polybutadienes and in HDPE / LDPE (for tubes, gas pipe connectors, high voltage cables, and films for food packaging applications). TBBC is also a heat stabilizer for lubricants, an anti-skinning agent for hot melt adhesives, and an anti-scorching agent for polyurethanes. Exhibits compatibility with peroxides and in tandem with carbon black.

Regulatory Information

FDA approved 1998 for the following applications: in the manufacture of antioxidants/stabilizers for polymers intended for use in all stages of production, processing, packaging and transport of food: 21CFR part178.2010. UK approved 1992 as an antioxidant for materials composed of PE and PP in contact with water or food intended for human consumption up to 0.25% of the final product composition.

Environmental Impact

Not readily biodegradable. TBBC lacks a hydrolyzable functional group, and therefore undergoes slow degradation. Toxic to aquatic organisms. (LC50 96hr): 0.24 mg/L [bluegill sunfish]; (EC50 24hr): 0.23 mg/L [Daphnia Magna].

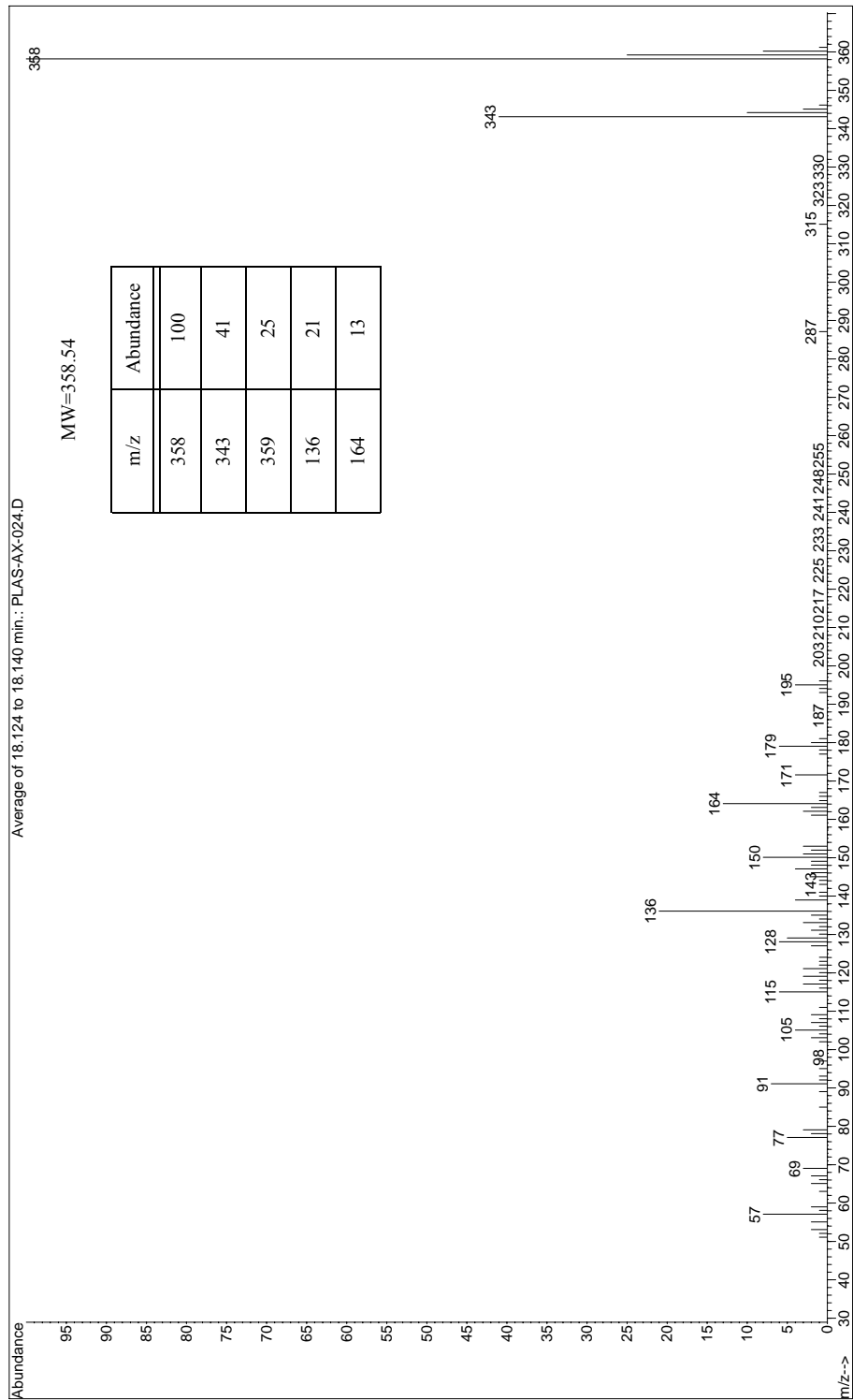
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

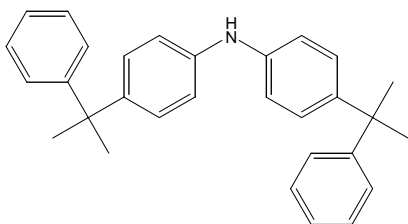
Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. TBBC is not mutagenic with or without metabolic activation. Acute intraperitoneal (LD50): 50 mg/kg [Mouse]; Acute oral (LD50) 2345 mg/kg [Rat], 4750 mg/kg [Mouse], 3200 mg/kg [Rabbit]; Acute dermal (LD50): >5010 mg/kg [Rabbit].

Mass Spectrum for Lowinox® TBM-6 - PLAS-AX-024



Naugard® 445

Chemtura Corporation



CAS Number 10081-67-1

RTECS Number Not available

Abbreviation

Formula $C_{30}H_{31}N$

Molecular Weight 405.57

Chemical Name

4,4'-bis(alpha,alpha-dimethylbenzyl)diphenylamine

Synonyms

4-(1-methyl-1-phenylethyl)-N-[4-(1-methyl-1-phenylethyl)phenyl]aniline; 4,4'-di-(alpha,alpha-dimethylbenzyl) diphenylamine

Brand Names & Manufacturers

Antioxidant 405

Akrochem Corporation

Physical Properties**Appearance** White powder or granules**Melting Point** 98-100 °C**Boiling Point** ~507 °C (estimated)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	0.7	U	40.8	U	0.7

Application, Regulatory & Environmental Information**Application**

Naugard® 445 is non-discoloring aromatic amine antioxidant that works synergistically with phosphites and phenolic antioxidants as a thermal stabilizer in polyolefins, styrenics, polyols, hot melt adhesives, lubricants, and polyamides.

Regulatory Information

FDA approved in food-contact surface of articles intended for use in the production, manufacturing, packing, processing, preparing, treating, packaging, transporting, or storage of food as defined in 21CFR175.300; as an antioxidant and/or stabilizer in polymers (not to exceed 0.3% weight of PP complying with 21CFR177.1520); and in PP (with non-fatty foods only) as defined in 21CFR178.2010.

Environmental Impact

Not readily biodegradable. Log Pow value = 8.51, indicates a high potential to bioaccumulate in aquatic organisms. Direct photolysis t(1/2) 0.6 hrs. Ecotoxicity: (LC50 96hr): 0.23 µg/L [Fish]; (EC50 48hr): 0.038 µg/L [Daphnia]; (EC50 96hr): 0.349 µg/L [Aquatic Plants].

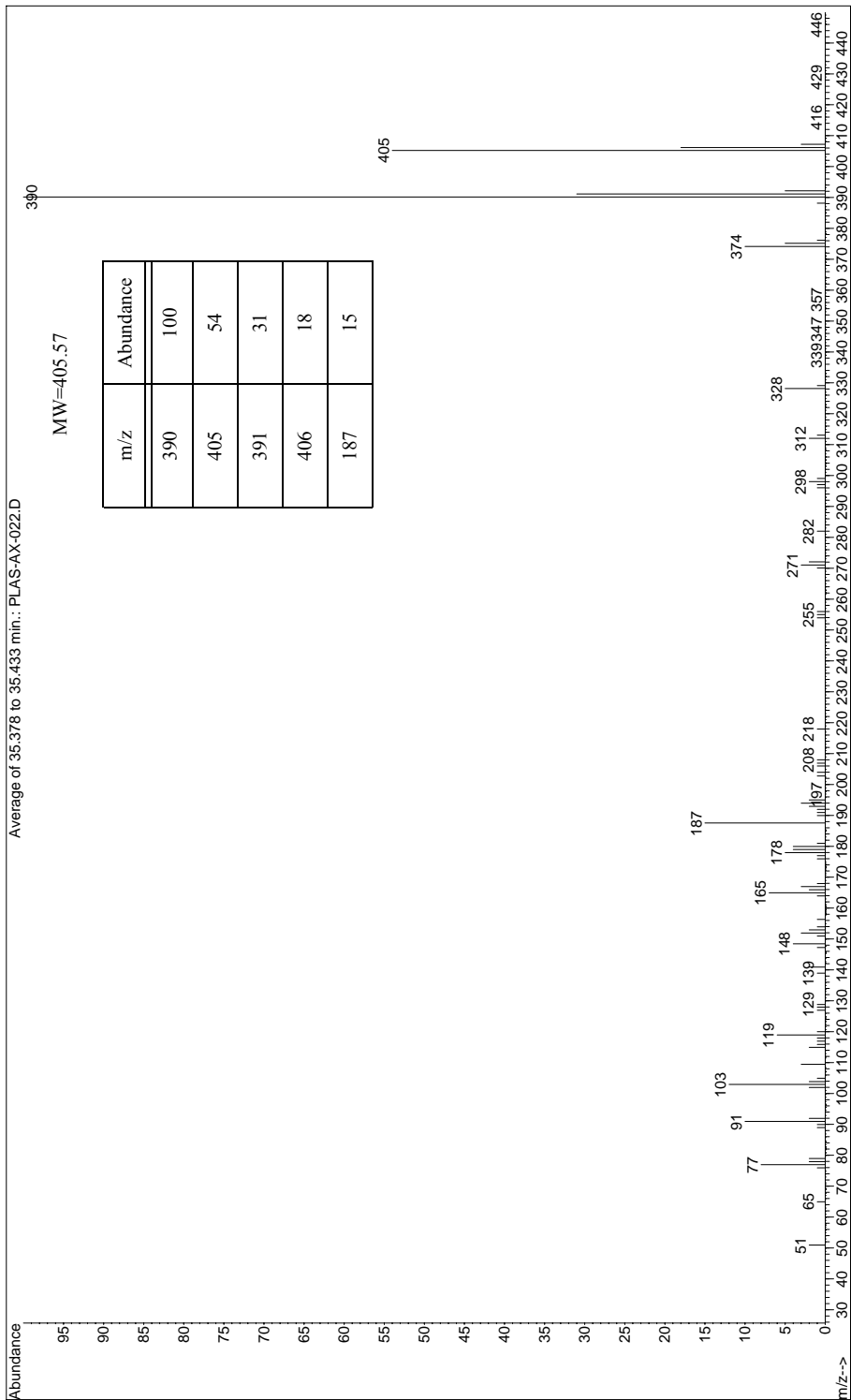
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

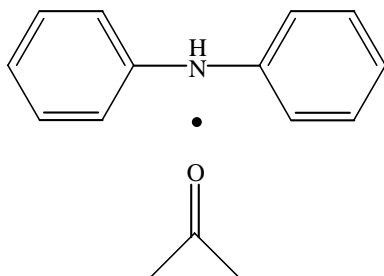
Not listed (ACGIH, IARC, NTP, OSHA) as a cancer-causing agent. Acute oral (LD50): >10 g/kg BW [Male Rat].

Mass Spectrum for Naugard® 445 - PLAS-AX-022



Naugard® A

Chemtura Corporation



CAS Number 68412-48-6

RTECS Number UC3810000

Abbreviation

Formula $C_{12}H_{11}N \cdot C_3H_6O$

Molecular Weight Not applicable

Chemical Name

acetone diphenylamine condensation products

Synonyms

2-propanone, reaction products with diphenylamine, ADPA

Brand Names & Manufacturers

AgeRite® Superflex®

RT Vanderbilt

Physical Properties**Appearance** Greenish-tan flake or powder**Melting Point** 85-95 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	40-80	U

Application Application, Regulatory & Environmental Information

Antioxidant for natural and synthetic rubber, tires, automotive and appliance molded goods, polyamides and carbon black filled olefin formulations for use in geomembranes, wire and cable jacketing, and irrigation piping.

Regulatory Information

Does not have FDA approval for use in food contact applications.

Environmental Impact

Classified as a persistent, bioaccumulative toxin and is inherently toxic to aquatic organisms.

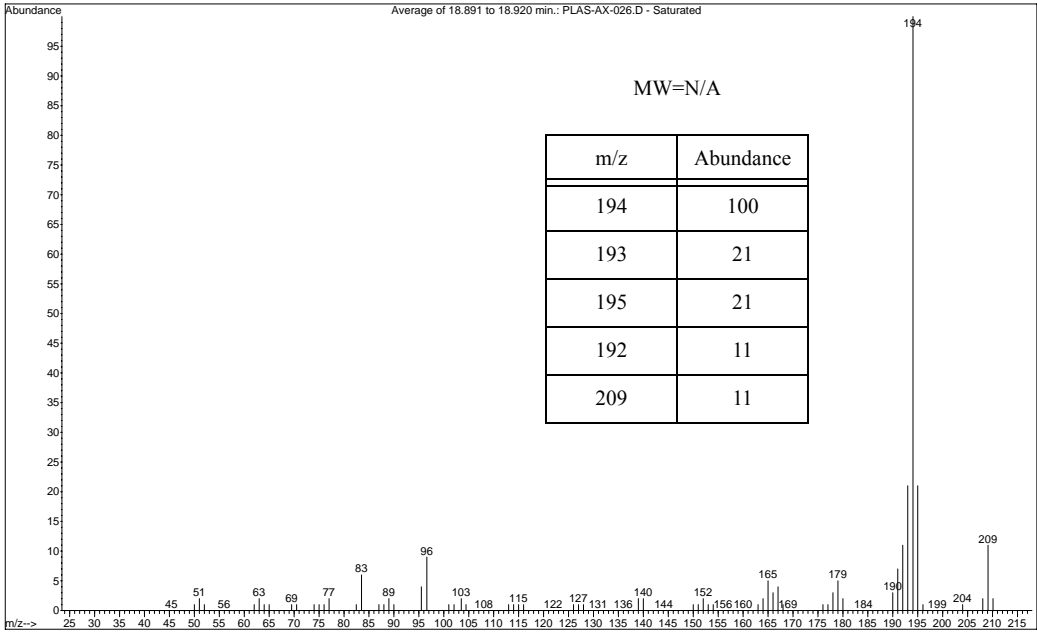
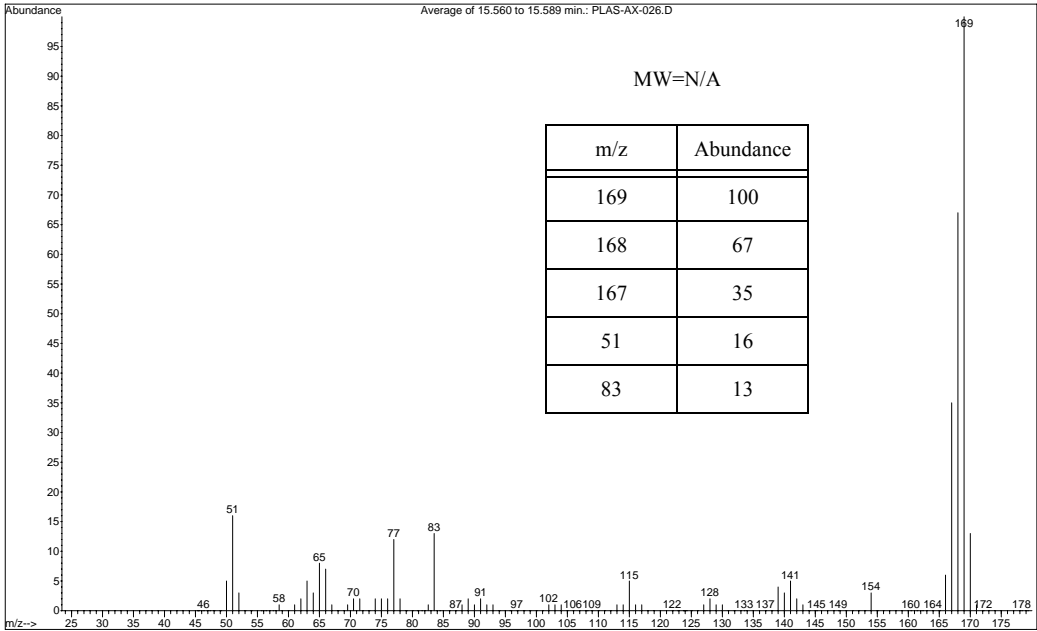
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

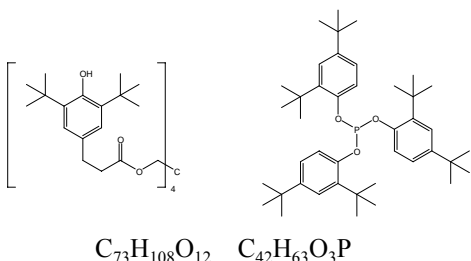
(LD50): > 10 g/kg oral, [Rat].

Mass Spectra for Naugard® A - PLAS-AX-026



Naugard® B-25

Chemtura Corporation

**CAS Number** See below**RTECS Number** Not available**Abbreviation****Formula** See below structure**Molecular Weight** 1177.65/ 646.92**Chemical Name**

1:1 blend of Naugard® 10 and Naugard® 524

Synonyms

tris(2,4-di-tert-butylphenyl)phosphite and tetrakis methylene(3,5-di-tert-butyl-4-hydroxyhydrocinnamate) methane (1:1 blend)

Brand Names & Manufacturers**Physical Properties****Appearance** White to off-white powder or granules**Melting Point** Not available**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water <0.1	MeOH <0.1	EtOH U	Acetone U	CH₂Cl₂ 55	Hexane <0.5
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Application, Regulatory & Environmental InformationApplication This compound is a blend of two compounds: CAS Numbers 6683-19-8 and 31570-04-4

Antioxidant used for wood or other natural fiber filled polyolefins, elastomers and hot melt adhesives when light exposure and maintenance of color is important.

Regulatory Information

FDA approved for various food contact applications.

Environmental Impact

Experimental data shows that this category of chemicals are not readily biodegradable. This class of compounds photodegrade rapidly. In the environment, occurrence would be partitioned primarily to soil and sediments rather than air or water.

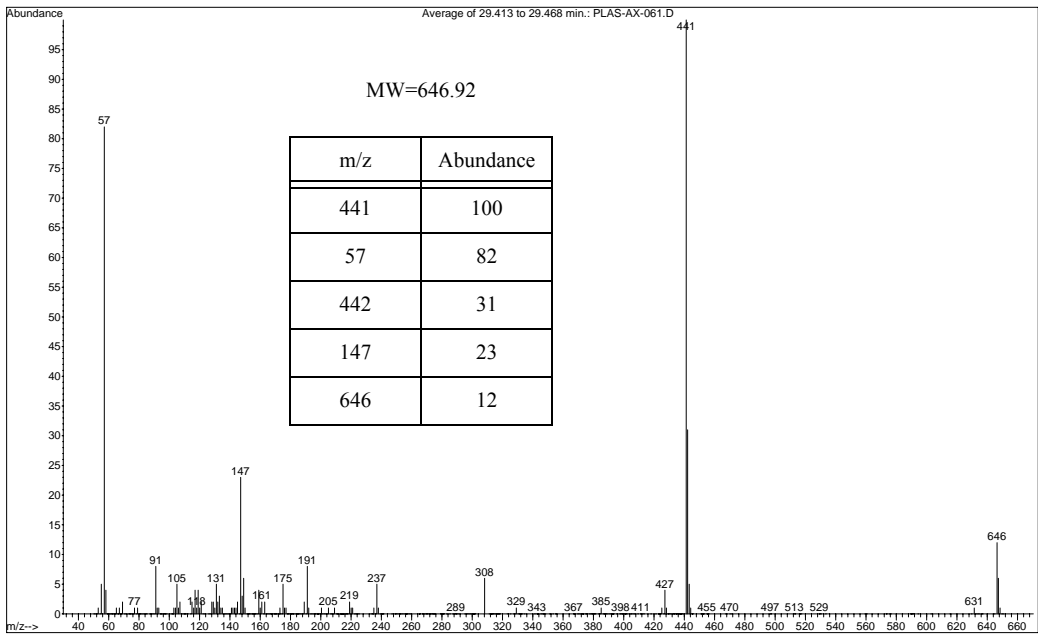
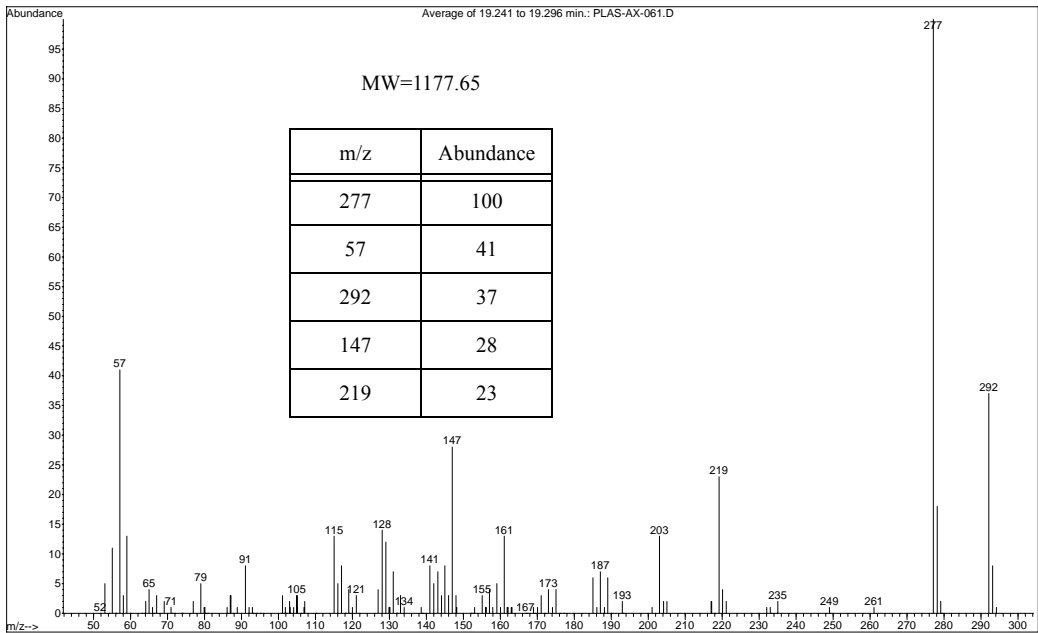
Point of Release

Migration is greater from polypropylene than from high-density polyethylene. Little migration is found to aqueous media. Migration is highest into n-heptane, ethanol and corn oil.

Toxicological Data

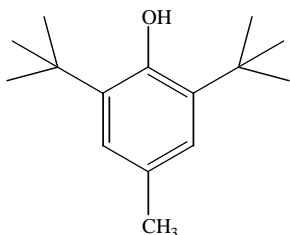
Toxicity of this compound is considered low. LD50 was not quantitated, rats tolerated administration of 5.0 g/kg body-weight and mice tolerated up to 10 mg/kg bodyweight. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectra for Naugard® B-25 - PLAS-AX-061



Naugard[®] BHT

Chemtura Corporation



CAS Number 128-37-0

RTECS Number GO7875000

Abbreviation BHT

Formula C₁₅H₂₄O

Molecular Weight 220.35

Chemical Name

2,6-di-tert-butyl-4-methylphenol

Synonyms

butylated hydroxytoluene; BHT; 2,6-di-tert-butyl-p-cresol

Brand Names & ManufacturersVulkanox[®] KB

Lanxess

Physical Properties**Appearance** White powder or granules**Melting Point** 69-71 °C**Boiling Point** 265 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 20-40	EtOH 26	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

General purpose phenolic antioxidant used for polyolefin applications such as petroleum, animal feed, and for food products and packaging.

Regulatory Information

FDA approved for food contact. Approved under 21CFR175.105 - adhesives (no limitations), 175.125 - pressure sensitive adhesives (0.1% max.) and 177.2600 - rubber articles intended for repeated use (5% max.).

Environmental Impact

The substance is harmful to aquatic organisms. Log Pow value of 5.1 indicates a medium to high potential for this substance to bioaccumulate. If released into the environment, the main target compartment would be air.

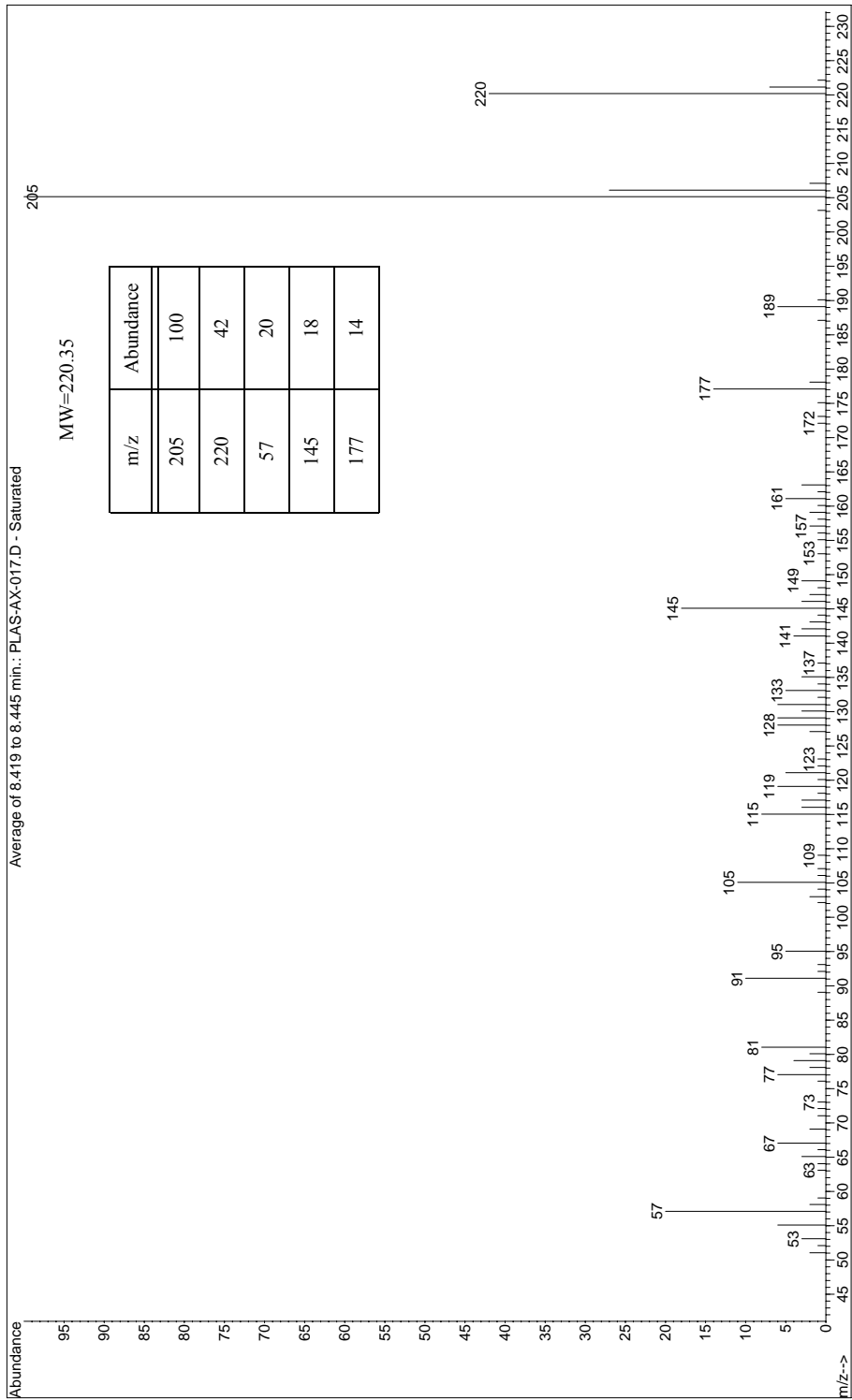
Point of Release

Releases into the environment may occur during production of BHT as well as during its use in different applications as stabilizer and during the use of the products that contain the substance. A significant release into the environment is expected from migration of BHT onto the surface of products containing the substance.

Toxicological Data

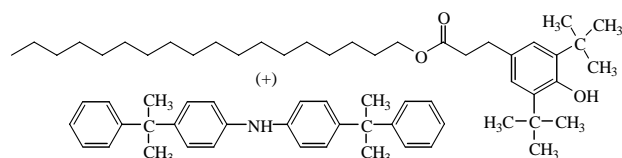
Oral (LD50): 890 mg/kg [Rat]. May have harmful effects on the liver.

Mass Spectrum for Naugard® BHT - PLAS-AX-017



Naugard® HM-22

Chemtura Corporation

**CAS Number****RTECS Number** Not available**Abbreviation****Formula** Not applicable**Molecular Weight** 531/406**Chemical Name**

blend of phenolic primary and diphenylamine secondary antioxidants (Naugards 76 and 445)

Synonyms

Brand Names & Manufacturers

Physical Properties

<i>Physical Properties</i>						
Appearance	White granules					
Melting Point	49 °C		Boiling Point		Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water <0.1	MeOH <1	EtOH U	Acetone 80	CH₂Cl₂ U	Hexane <2

Application, Regulatory & Environmental Information

Application Naugard® HM-22 is a 1:1 granular blend of Naugard® 76 and Naugard® 445. This phenolic/amine blend provides synergistic short and long term thermal protection against oxidation in polypropylene. It also exhibits color and viscosity stability, as well as gelation and skinning resistance in SIS, SBS, EVA, PE, and polyamide hot melt adhesives.

Regulatory Information

This material is not FDA approved for food contact.

Environmental Impact

This material is not readily biodegradable. Log Pow value of ~8 indicates a high potential to bioaccumulate.

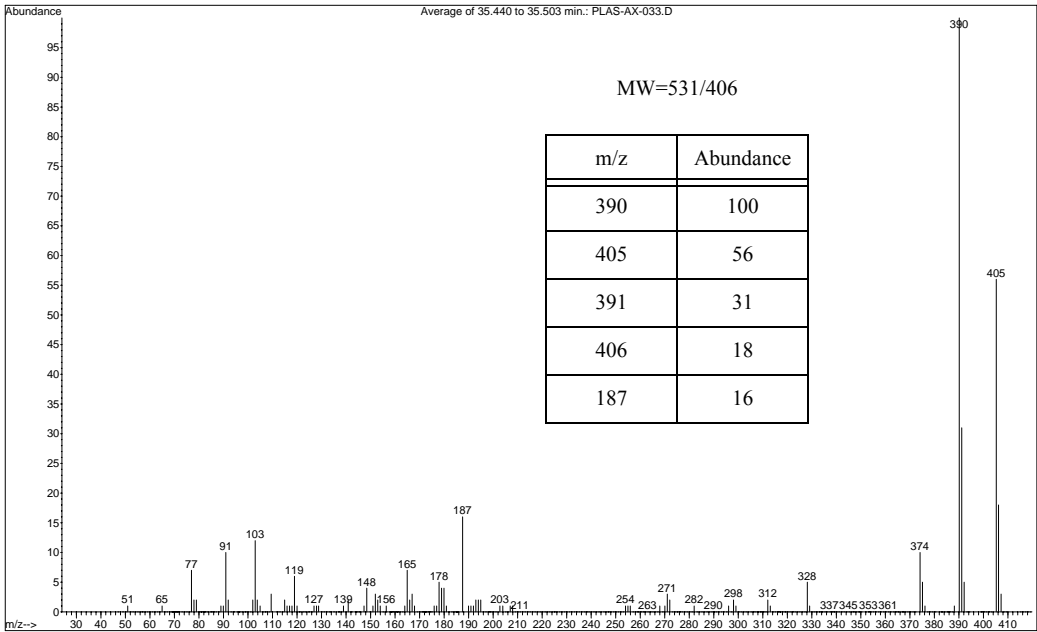
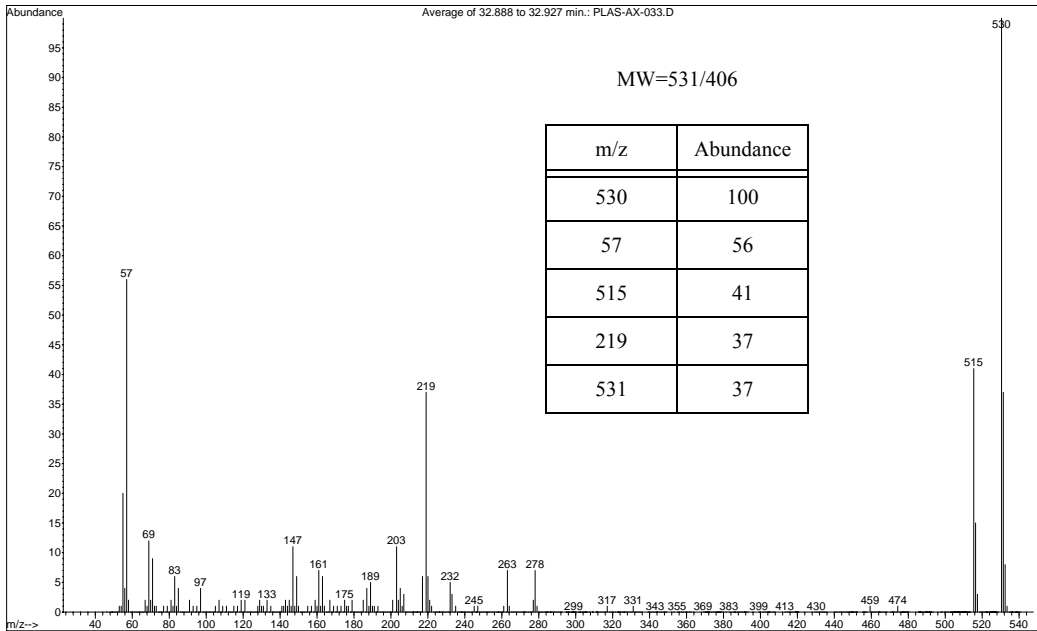
Point of Release

Can be released as a point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the longevity of the products and upon disposal of the products.

Toxicological Data

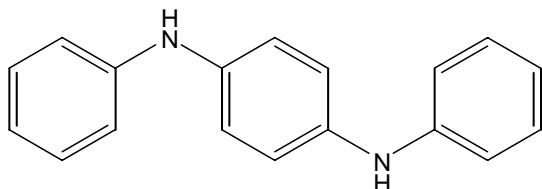
Acute toxicity: (LD50): >10000 mg/kg [Rat]. This material was not mutagenic in an Ames bacterial assay.

Mass Spectra for Naugard® HM-22 - PLAS-AX-033



Naugard® J

Chemtura Corporation



CAS Number 74-31-7

RTECS Number ST2275000

Abbreviation DPPD

Formula $C_{18}H_{16}N_2$

Molecular Weight 260.36

Chemical Name

N,N'-diphenyl-p-phenylenediamine

Synonyms

4-phenylaminodiphenylamine

Brand Names & Manufacturers

Agerite® DPPD

R.T. Vanderbilt

Physical Properties**Appearance** Light gray to brown powder**Melting Point** 144 °C**Boiling Point** 220-225 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application Application, Regulatory & Environmental Information

Amine antioxidant that offers protection against degradation due to copper and manganese. It also offers protection against outdoor flexing and static weather cracking in natural rubber and against thermal oxidation in polyethylene. Inhibits gum formation and degradation at elevated temperature in petroleum oils.

Regulatory Information

No information available.

Environmental Impact

Harmful to the environment. May cause long-term adverse effects.

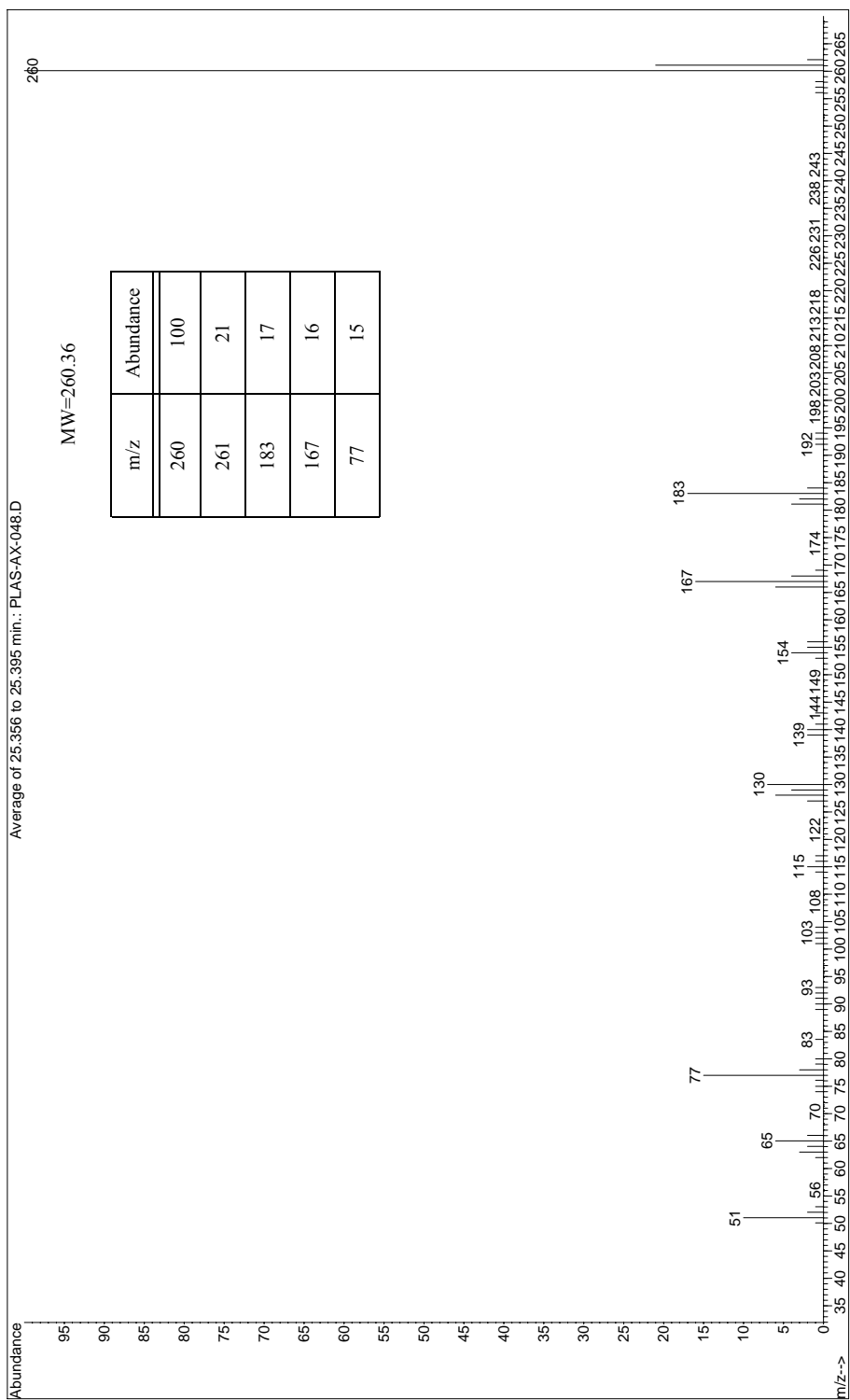
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

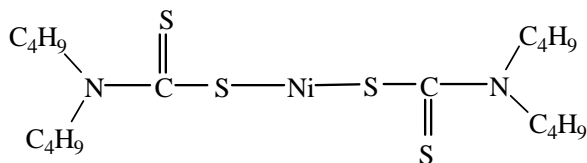
Oral (LD50): 2370 mg/kg, [Rat]. Suspected developmental toxin.

Mass Spectrum for Naugard® J - PLAS-AX-048



Naugard[®] NBC

Chemtura Corporation



CAS Number 13927-77-0

RTECS Number QR6140000

Abbreviation NBC

Formula $C_{18}H_{36}N_2NiS_4$

Molecular Weight 467.45

Chemical Name

nickel dibutyl dithiocarbamate

Synonyms

di-N-butyl dithiocarbamic acid, nickel salt; nickel N,N-di-n-dibutyl dithiocarbamate; nickel dibutyl dithiocarbamate

Brand Names & Manufacturers

Antiozonant NIBUD

Akrochem Corporation

Nocrac[™] NBC

Ohuchi Shinko Co., Ltd.

Perkacit[®] NDBC

Akzo Nobel Chemicals B.V.

Physical Properties**Appearance** Green powder**Melting Point** 85 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	40-80	40-80	U

Application Application, Regulatory & Environmental Information

Used as a secondary accelerator with antioxidant, antiozonant, and stabilizing function in synthetic rubber and high polymer materials in the plastics and rubber industries. Mainly used in styrene-butadiene rubber (SBR), chloroprene rubber (CR), epichlorohydrin, and chlorosulfonated polyethylene rubber. Promotes heat-resistance of chlorosulfonated polyethylene rubber, EPDM and CSM and sunshine resistance of CR.

Regulatory Information

This product is regulated for use in articles in contact with food as specified under BgVV XXI, Category 4 at 0.3-0.5%. It does not have FDA approval for food contact applications.

Environmental Impact

Ecological impact not determined. Similar compounds show low to moderate biodegradability, but rapid hydrolysis under acidic conditions. Similar compounds are also determined to have low bioaccumulation potential and environmental persistence. Bioconcentration factor (BCF) is 307.

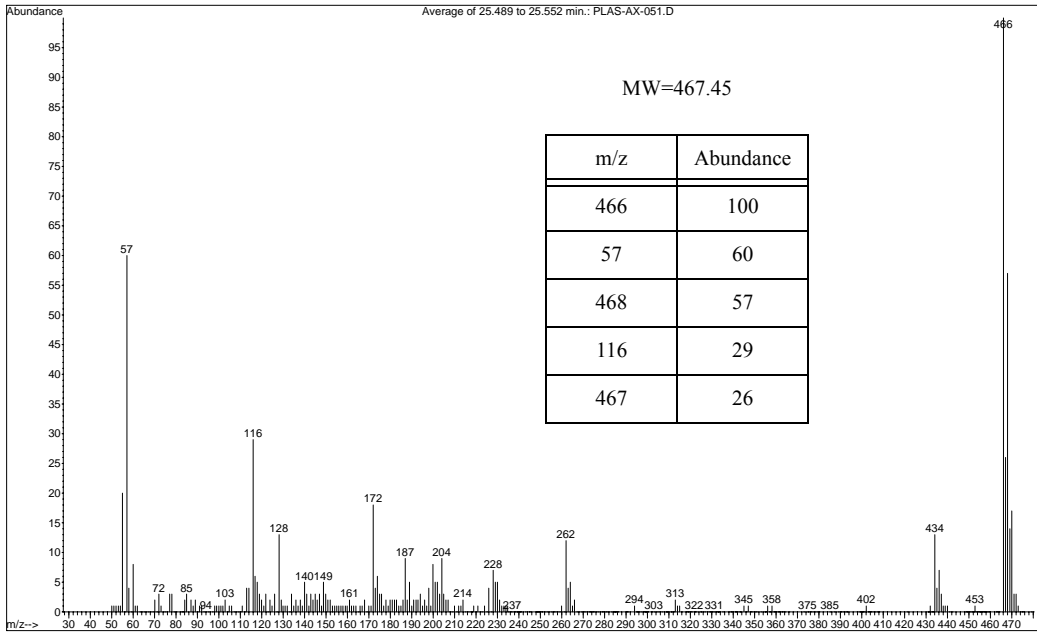
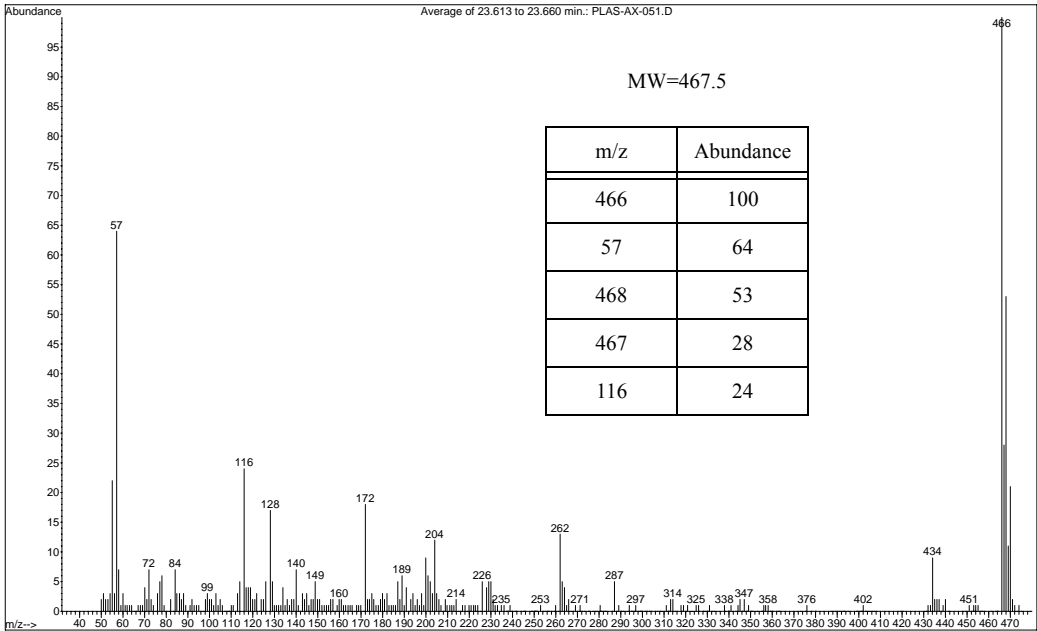
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

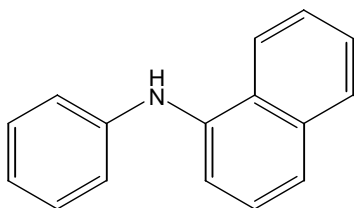
Classified as a confirmed carcinogen by RTECS and ACGIH, and a "anticipated human carcinogen" by the NTP. (LD50): 17 g/kg BW [Rat]. Induced lung cancer in mice after 1.5 years exposure.

Mass Spectrum for Naugard® NBC - PLAS-AX-051



Naugard® PANA

Chemtura Corporation



CAS Number 90-30-2

RTECS Number QM4500000

Abbreviation PNA-1

Formula C₁₆H₁₃N

Molecular Weight 219.28

Chemical Name

N-phenyl-1-naphthylamine

Synonyms

1-anilinonaphthalene; phenyl-alpha-naphthylamine

Brand Names & Manufacturers

Antioxidant PANA

Akrochem Corporation

Vulkanox® PAN

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** Light brown to violet crystalline powder**Melting Point** 55 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Used as a general purpose antioxidant for CR, NR and SBR. Can be used as a gel inhibitor.

Regulatory Information

FDA approved for food contact under 21CFR177.2600 - rubber articles intended for repeat uses, not to exceed 5% by weight of the total composition and 21CFR178.3570 - lubricants with incidental food contact not to exceed 1% by weight of the total composition.

Environmental Impact

This substance is very toxic to aquatic organisms. The reported log Pow value is 4.2, indicating a moderate potential to bioaccumulate.

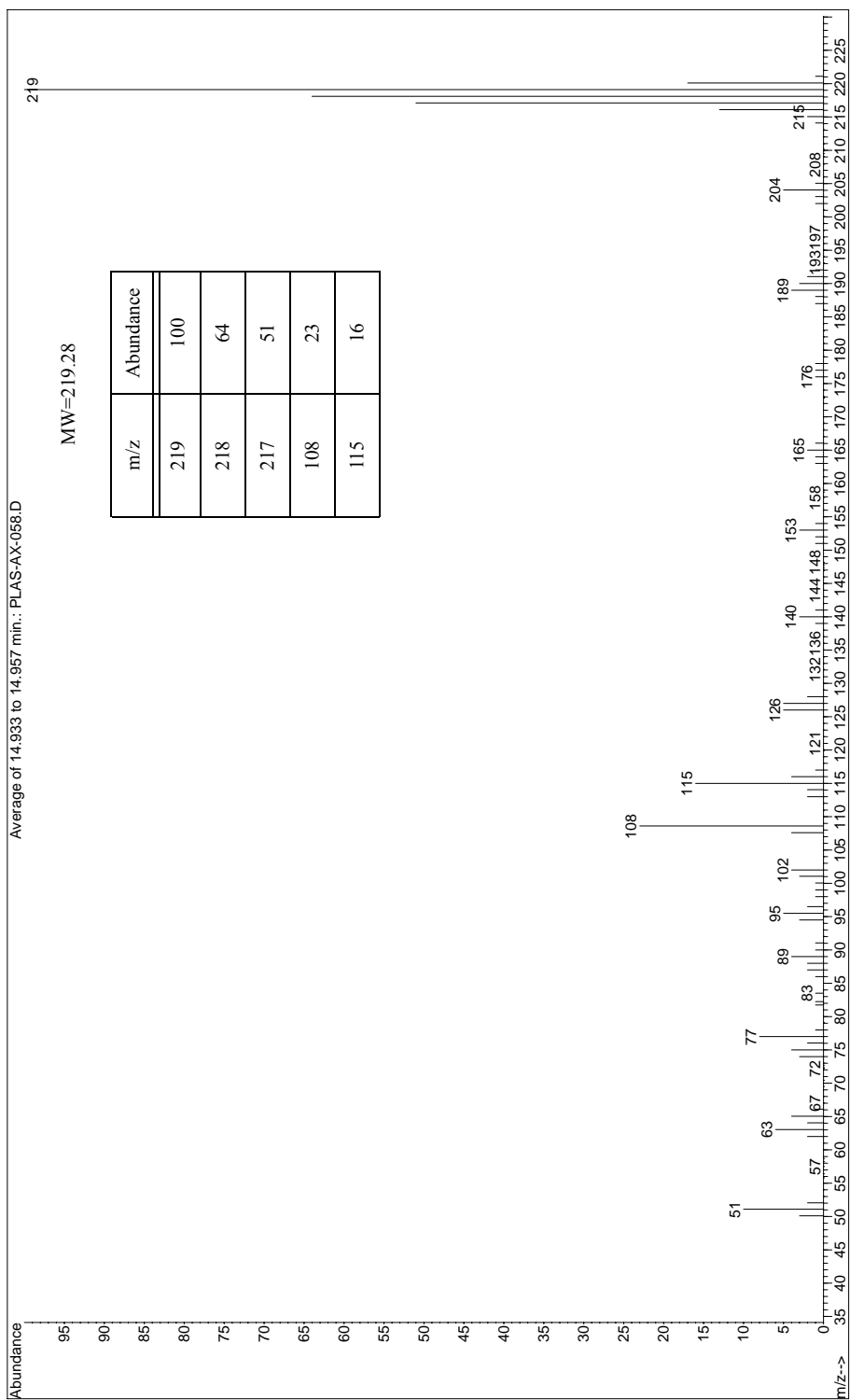
Point of Release

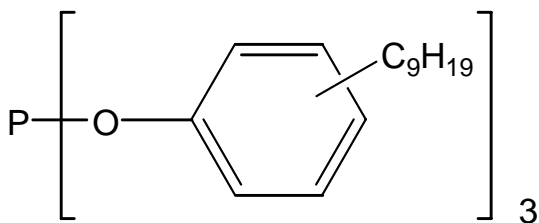
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): 1630 mg/kg [Rat]. Experimental evidence suggests carcinogenic potential.

Mass Spectrum for Naugard® PANA - PLAS-AX-058



Naugard® PHR

CAS Number 26523-78-4
RTECS Number Not available
Abbreviation TNPP

Formula C₄₅H₆₉O₃P
Molecular Weight 689.32

Chemical Name

tris(mono-nonylphenyl) phosphite with up to 1% triisopropanol amine

Synonyms

nonylphenyl phosphite (3:1); tris(mono-nonylphenyl) phosphite; Tris nonylphenyl phosphite; Tris(mono-nonylphenyl)phosphite, 2,2'-methylenebis(4-methyl-6-nonylphenol)

Brand Names & Manufacturers**Physical Properties**

Appearance	Light yellow viscous liquid					
Melting Point	Not available			Boiling Point >360 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH <2.3	EtOH U	Acetone 100	CH₂Cl₂ U	Hexane 100

Application, Regulatory & Environmental Information

Application
 Secondary liquid phosphite antioxidant that functions as a peroxide decomposer and as a processing stabilizer in a wide variety of polymers, including polyolefins and styrenics.

Regulatory Information

FDA approved under 21CFR175.125 - pressure sensitive adhesives; 175.300 - resinous and polymeric coatings; 175.390 - zinc-silicon dioxide matrix coatings, 177.1210 - closures with sealing gaskets for food containers; 177.2600 - rubber articles intended for repeated use and 178.2010 - antioxidants and/or stabilizers for polymers.

Environmental Impact

Classified as an environmentally hazardous substance and considered to be a marine pollutant.

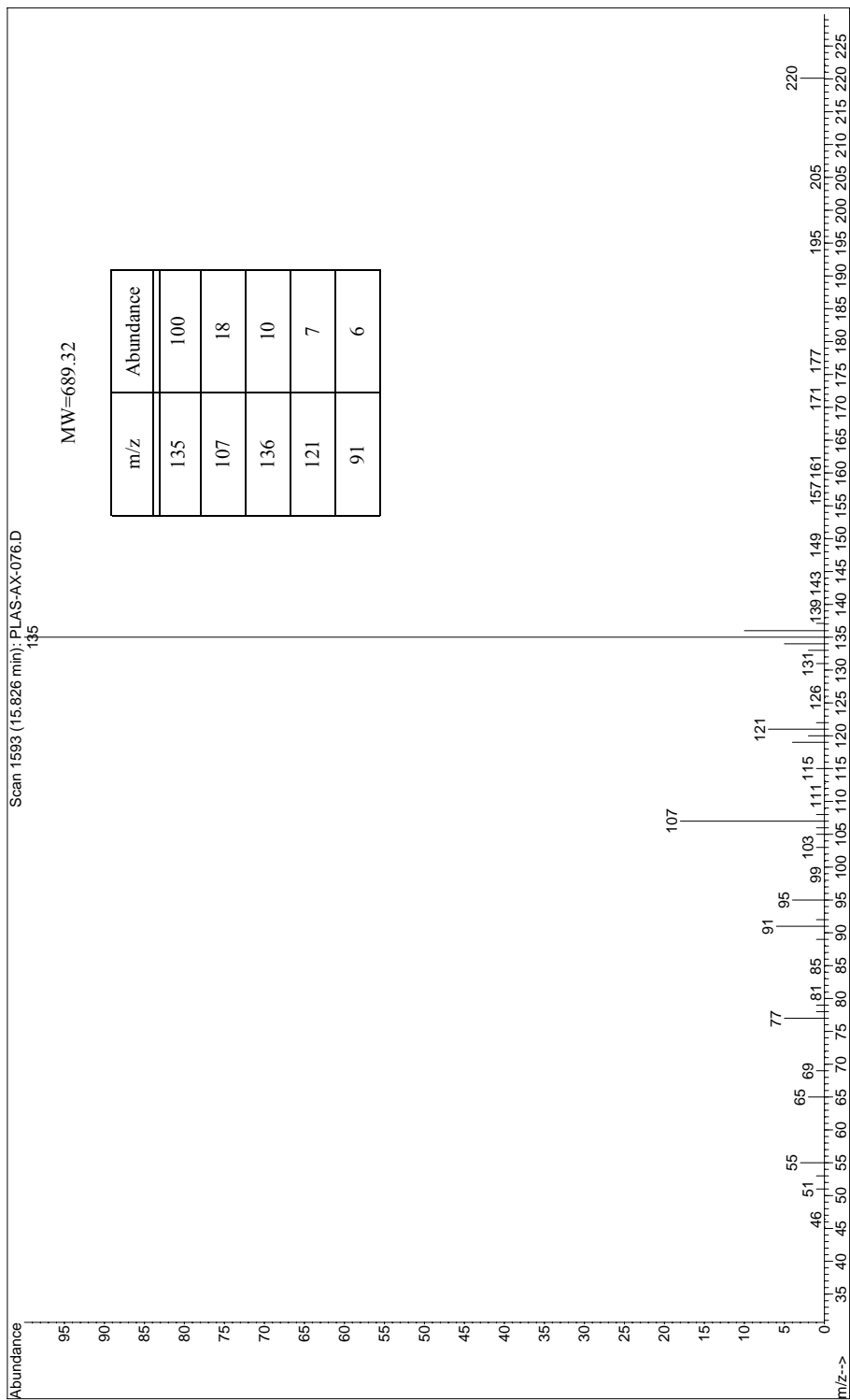
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

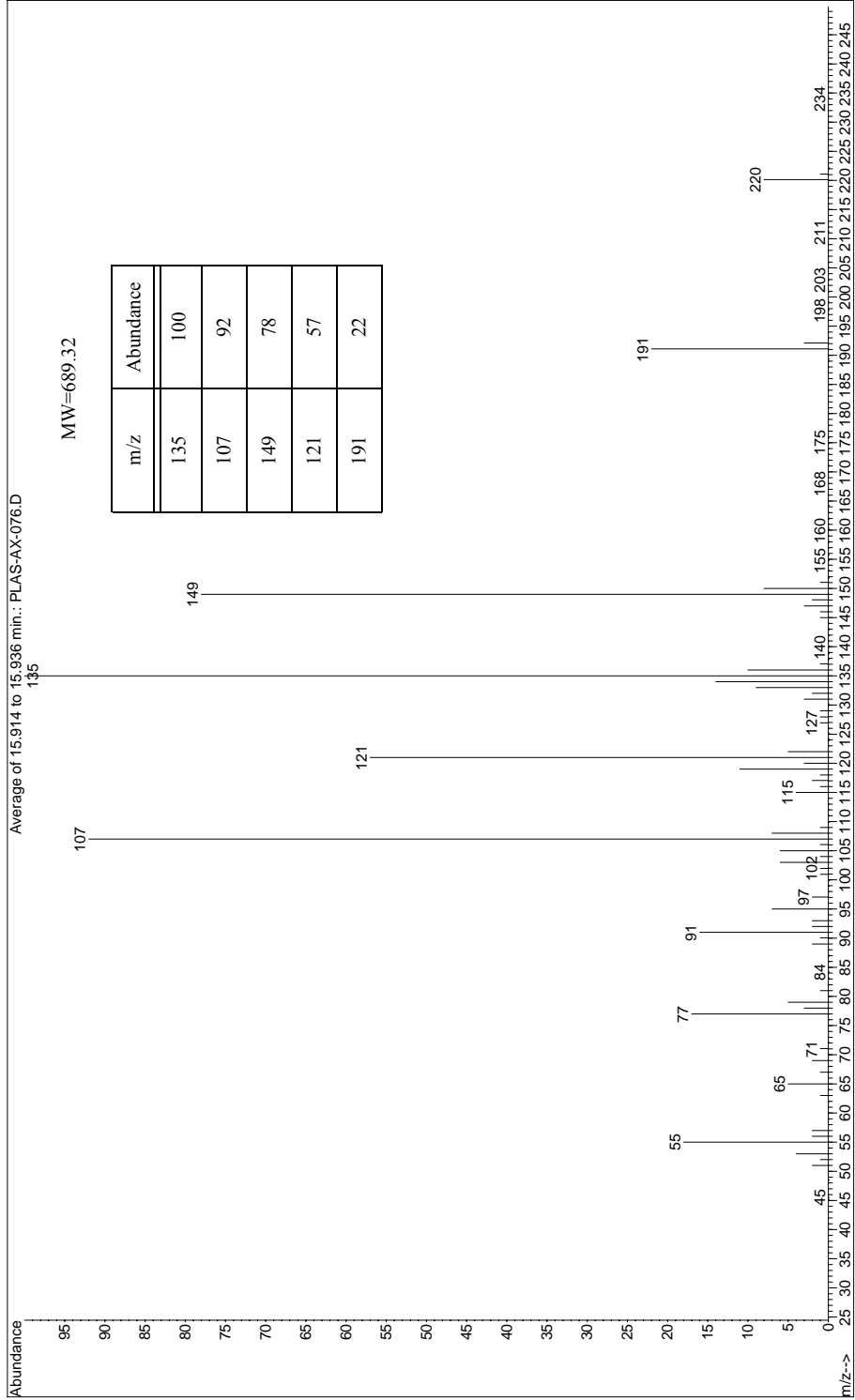
Toxicological Data

Oral (LD50): >2000mg/kg [Rat]; Skin (LD50): > 2000mg/kg [Rabbit]. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

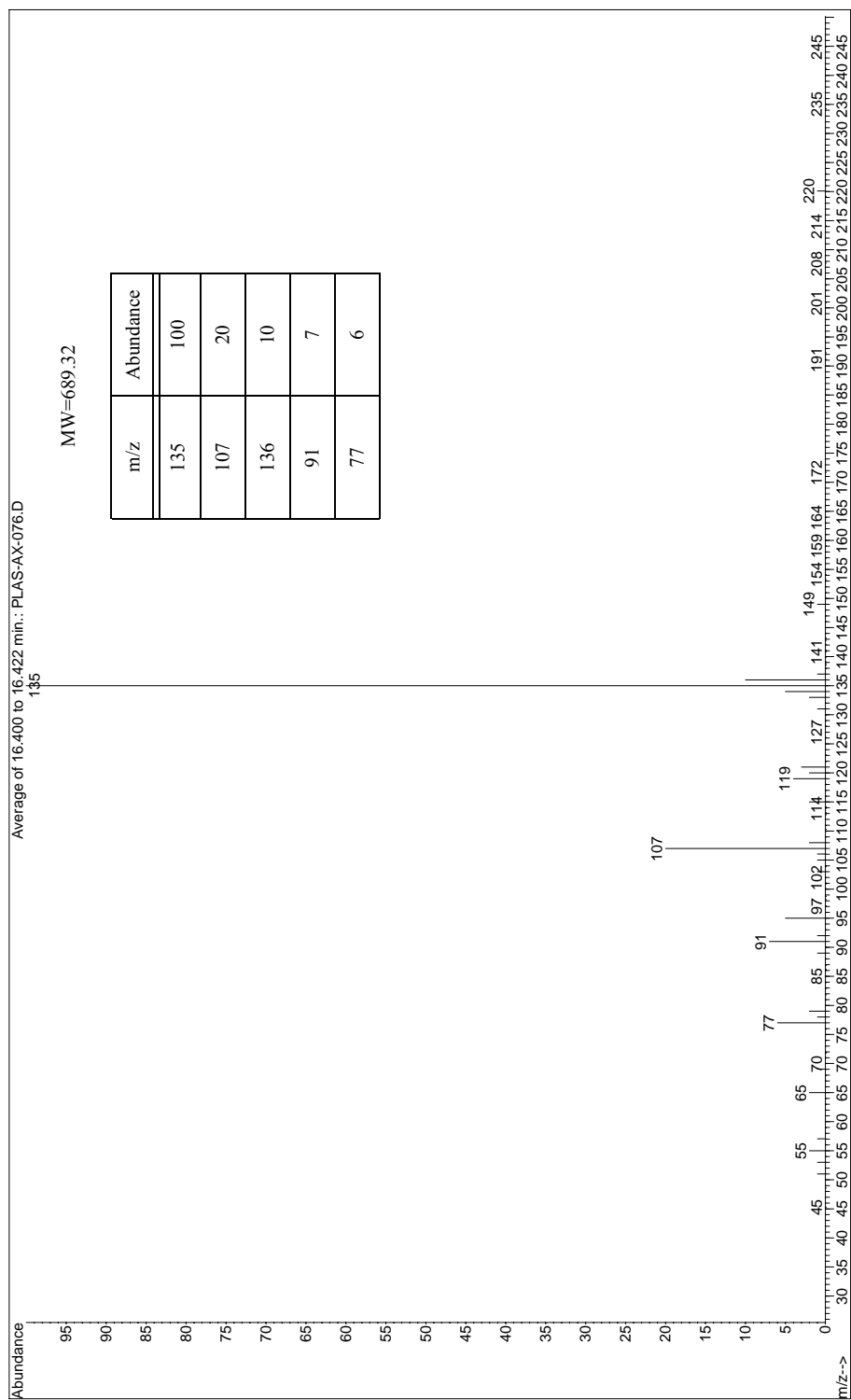
Mass Spectrum for Naugard® PHR - PLAS-AX-076



Mass Spectrum for Naugard® PHR - PLAS-AX-076

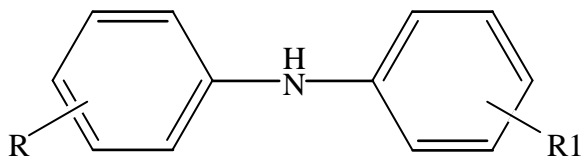


Mass Spectrum for Naugard® PHR - PLAS-AX-076



Naugard® PS-30

Chemtura Corporation



CAS Number 68411-46-1

RTECS Number Not available

Abbreviation

Formula $C_{12}H_{11}N \cdot C_8H_{16}$

Molecular Weight 281 (typical)

Chemical Name

Benzenamine, N-phenyl, reaction products with 2,4,4-trimethylpentene

Synonyms

diphenylamine, diisobutylene reaction product; N-phenylbenzenamine, 2,4,4-trimethyl-1-pentene, and 2,4,4-trimethyl-2-pentene reaction product; octylated diphenylamine

Brand Names & Manufacturers

Antioxidant S

Akrochem Corporation

Stangard® ODP

Harwick Chemical Corporation

Stalite® S

B.F. Goodrich Company

Vanox® 12

R.T. Vanderbilt Company, Inc.

Physical Properties**Appearance** Clear reddish to brown liquid**Melting Point** Not available**Boiling Point** >200°C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	10-40	10-40	10-40

Application, Regulatory & Environmental Information

Application Naugard® PS-30 is a liquid amine antioxidant typically used with phenolic antioxidants, phosphites, and synergists in poly-ether polyols to inhibit physical/color scorch associated with the production of flexible urethane foam.

Regulatory Information

FDA approved 2001 for use as an antioxidant with 2,4,4-trimethylpentene (at levels not to exceed 0.5 % weight of lubricant), in lubricants used in machinery (with incidental food contact) in production, manufacturing, packing, processing, preparing, treating, packaging, transporting, or storage applications, 21CFR 178.3570.

Environmental Impact

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

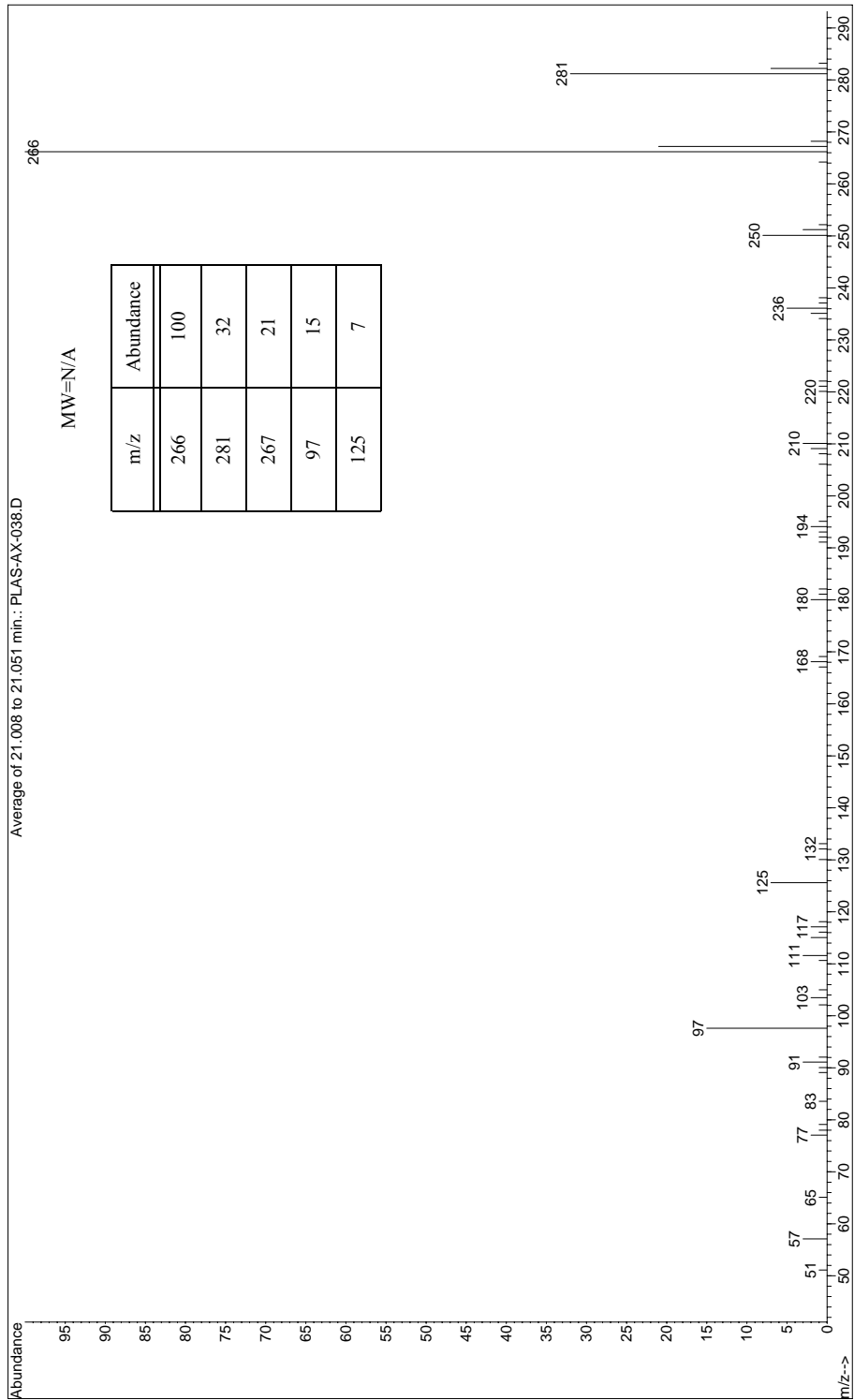
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

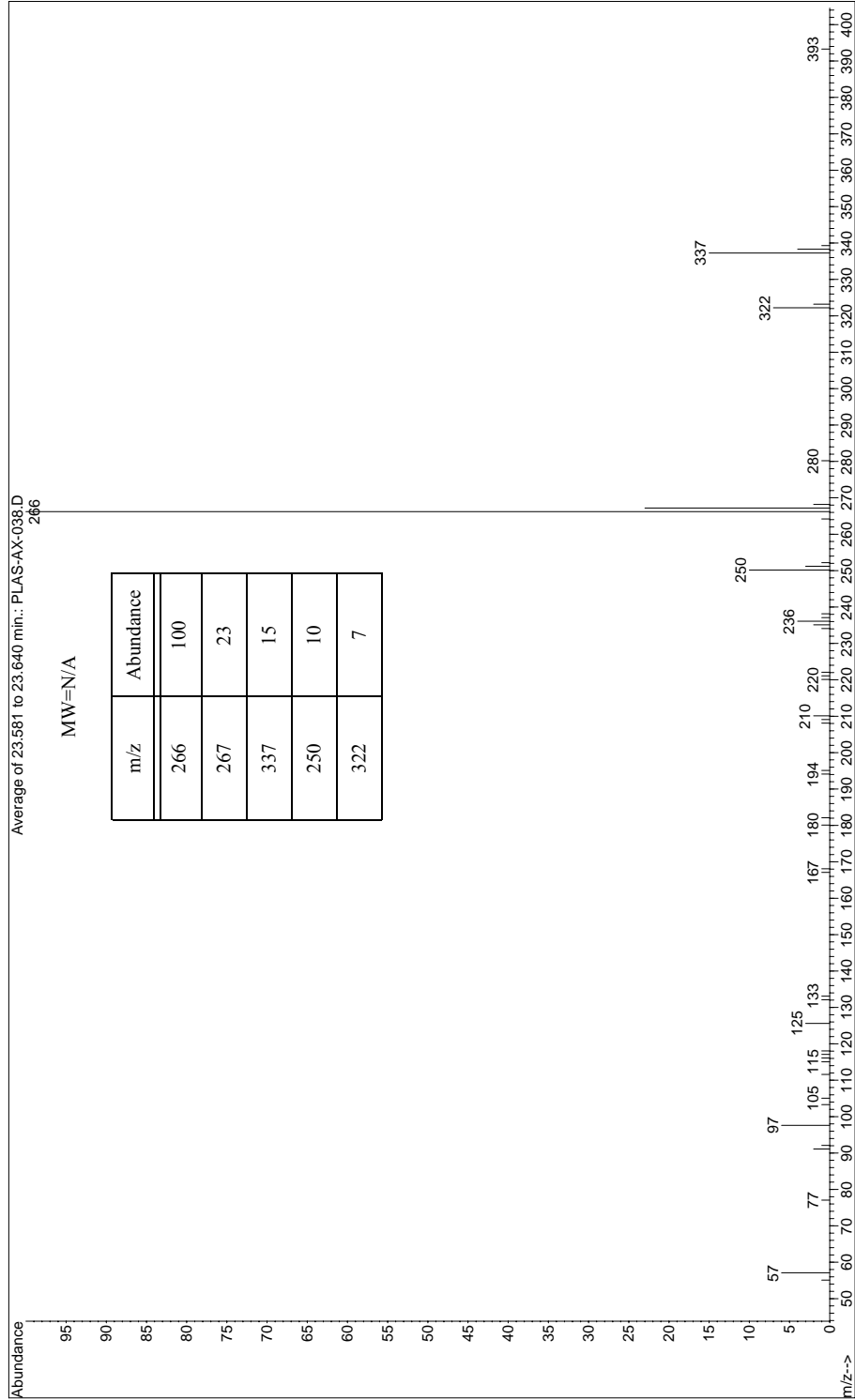
Toxicological Data

High levels of this material in the diet caused degenerative changes in the liver, kidney, adrenal medulla and thyroid of rats and a decrease blood prothrombin content in rats and dogs. Mutagenicity: This material was not mutagenic in an Ames bacterial assay. Acute oral toxicity (LD50): 7580 mg/kg [Rat].

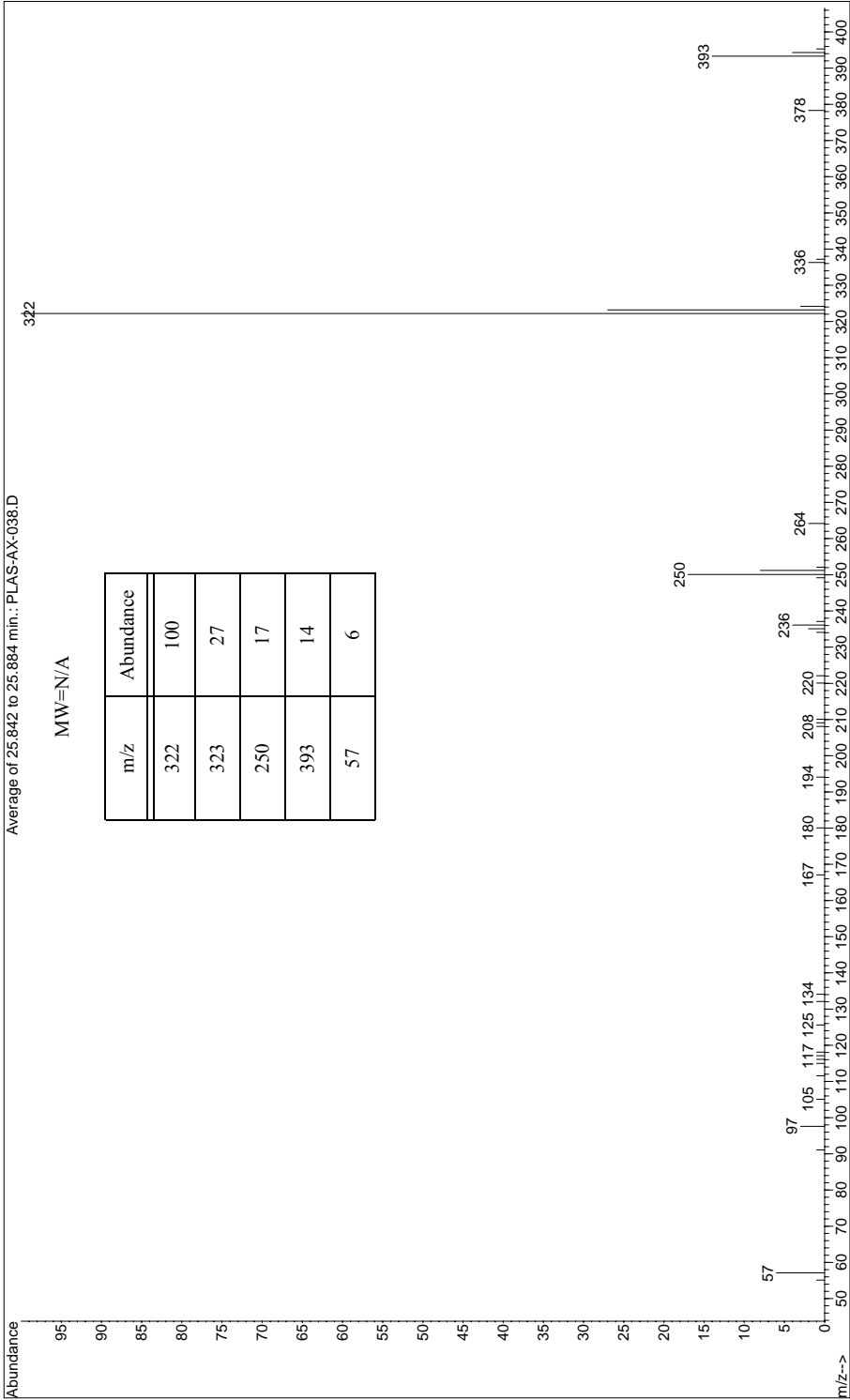
Mass Spectrum for Naugard® PS-30 - PLAS-AX-038



Mass Spectrum for Naugard® PS-30 - PLAS-AX-038



Mass Spectrum for Naugard® PS-30 - PLAS-AX-038



Naugard® PS-35

Chemtura Corporation

Unspecified
Structure

CAS Number Not available
RTECS Number Not available
Abbreviation

Formula Not available
Molecular Weight Not applicable

Chemical Name
Ternary blend of phenol, phosphites and amines

Synonyms

Brand Names & Manufacturers

Physical Properties

Appearance	Clear liquid					
Melting Point	Not available			Boiling Point 230 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH ₂ Cl ₂	Hexane
	<0.1	40-80	U	40-80	40-80	<0.1

Application Application, Regulatory & Environmental Information

An optimized blend of liquid phenolic antioxidant and liquid aromatic amine antioxidant with a small amount of a phosphite stabilizer. This blend was specifically developed for use as a heat and color stabilizer for polyols used for making flexible polyurethane foam.

Regulatory Information

No information available on FDA regulations regarding this specific blend, but several of the components are approved for indirect food contact per 21CFR175.105.

Environmental Impact

Based on data from the individual components of this blend, the log Kow value would be expected to be <4, indicating a low potential for bioaccumulation. Also, due to its insolubility in water, it is not likely to be toxic to aquatic wildlife.

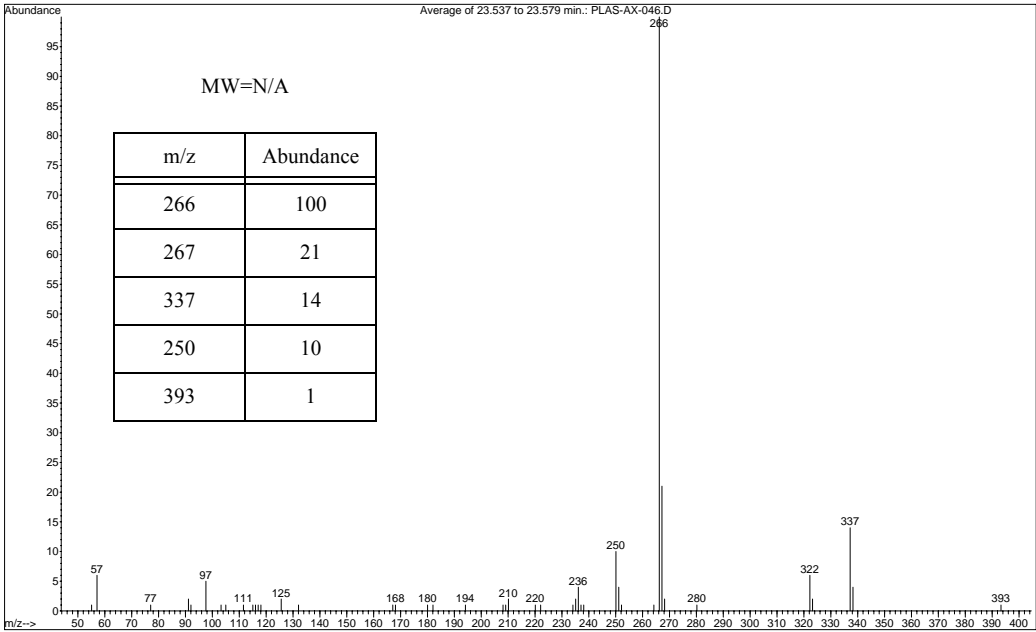
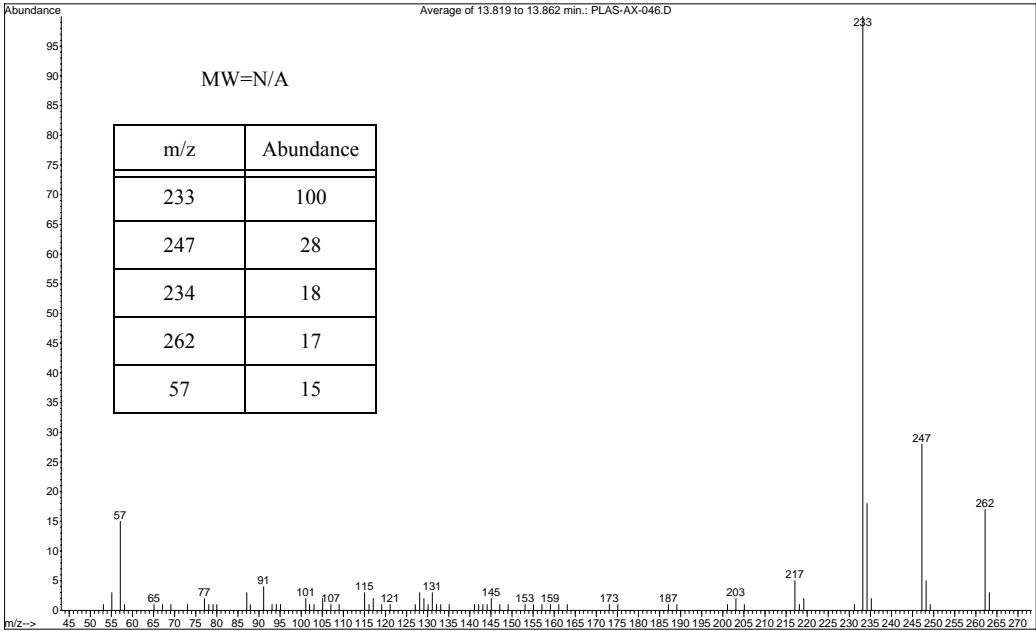
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

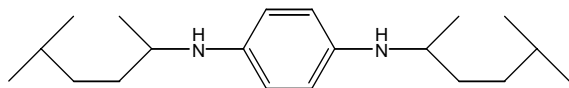
Acute Oral Toxicity (LD50): 1670 mg/kg [Rat]. Lowest Published Toxic Oral Dose (TDLo): 10914 mg/kg/3W-C [Rat].

Mass Spectra for Naugard® PS-35 - PLAS-AX-046



Naugard® Q Extra

Chemtura Corporation



CAS Number 26780-96-1

RTECS Number VB4900000

Abbreviation DTQ

Formula C₁₂H₁₅N

Molecular Weight 173.25

Chemical Name

1,2-dihydro-2,2,4-trimethylquinoline (polymerized)

Synonyms

2,2,4-trimethyl-1,2-dihydroquinone; Acetonanyl

Brand Names & Manufacturers

Agerite® resin D

R.T. Vanderbilt Company, Inc.

Flectol® A

Flexsys America L.P.

Vulkanox® HS/LG

Lanxess Deutschland GmbH Ltd.

Physical Properties**Appearance** Reddish-brown drops**Melting Point** 85-120 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	40-80	40-80	U	U

Application Application, Regulatory & Environmental Information

Protects against thermo-oxidative degradation in natural and synthetic rubbers as well as plastics. It is commonly used in applications such as tire carcasses, wire breaker retreads, apex, belts, hoses, seals, mechanical goods, footwear and wire.

Regulatory Information

Not FDA approved for food contact applications.

Environmental Impact

May be harmful to aquatic life and cause long-term adverse effects in the aquatic environment.

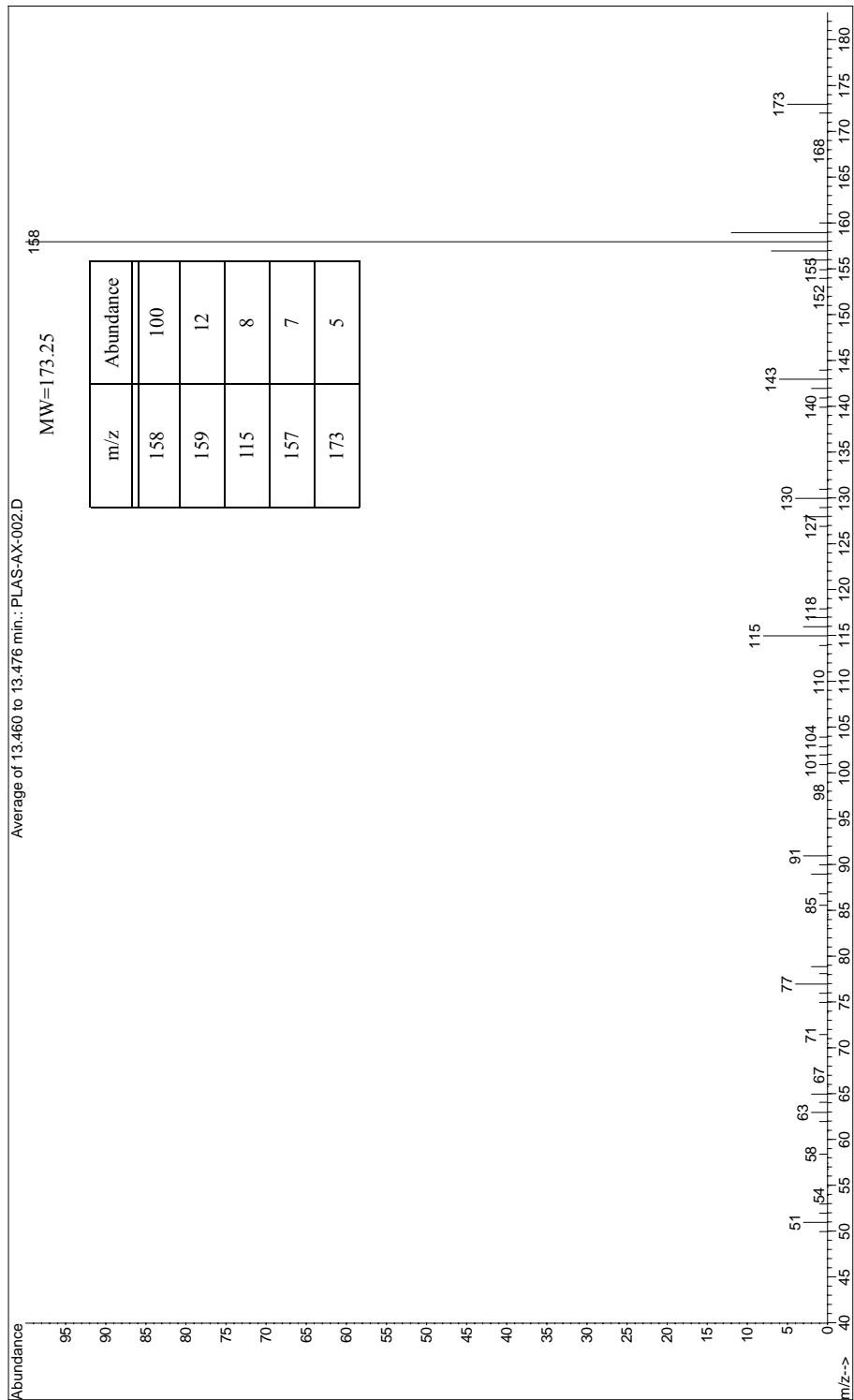
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

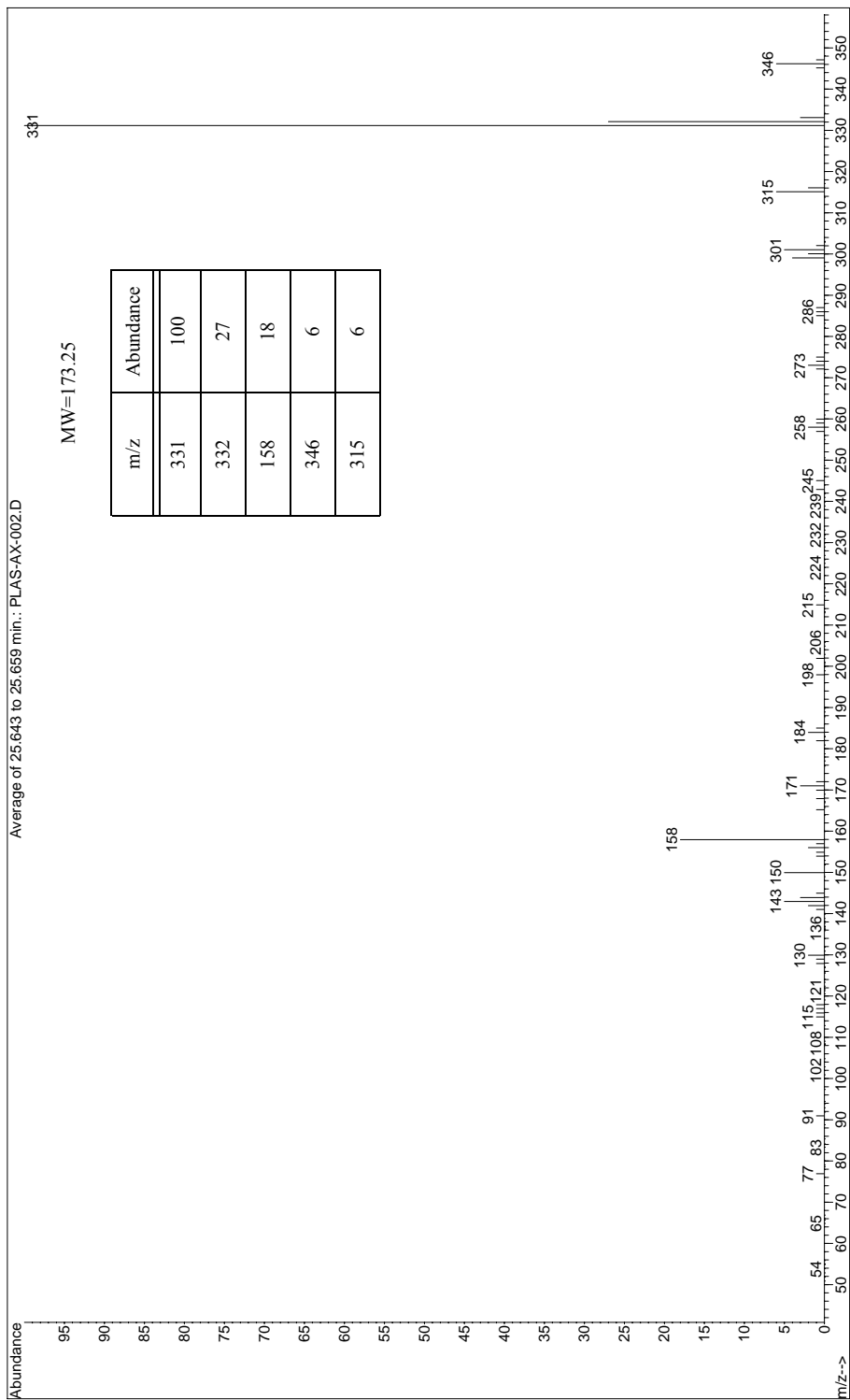
Toxicological Data

Poisonous doses target and inhibit CNS function; long-term toxicity also decreases BW gain, causes anemia, disrupts liver function in addition to CNS inhibition, decreases hemoglobin and erythrocytes. There is some evidence of carcinogenicity. Not determined to be mutagenic. (LD50): 2 g/kg BW oral, [Rats and Rabbits], (LD50): 1.45 g/kg BW oral [Mouse].

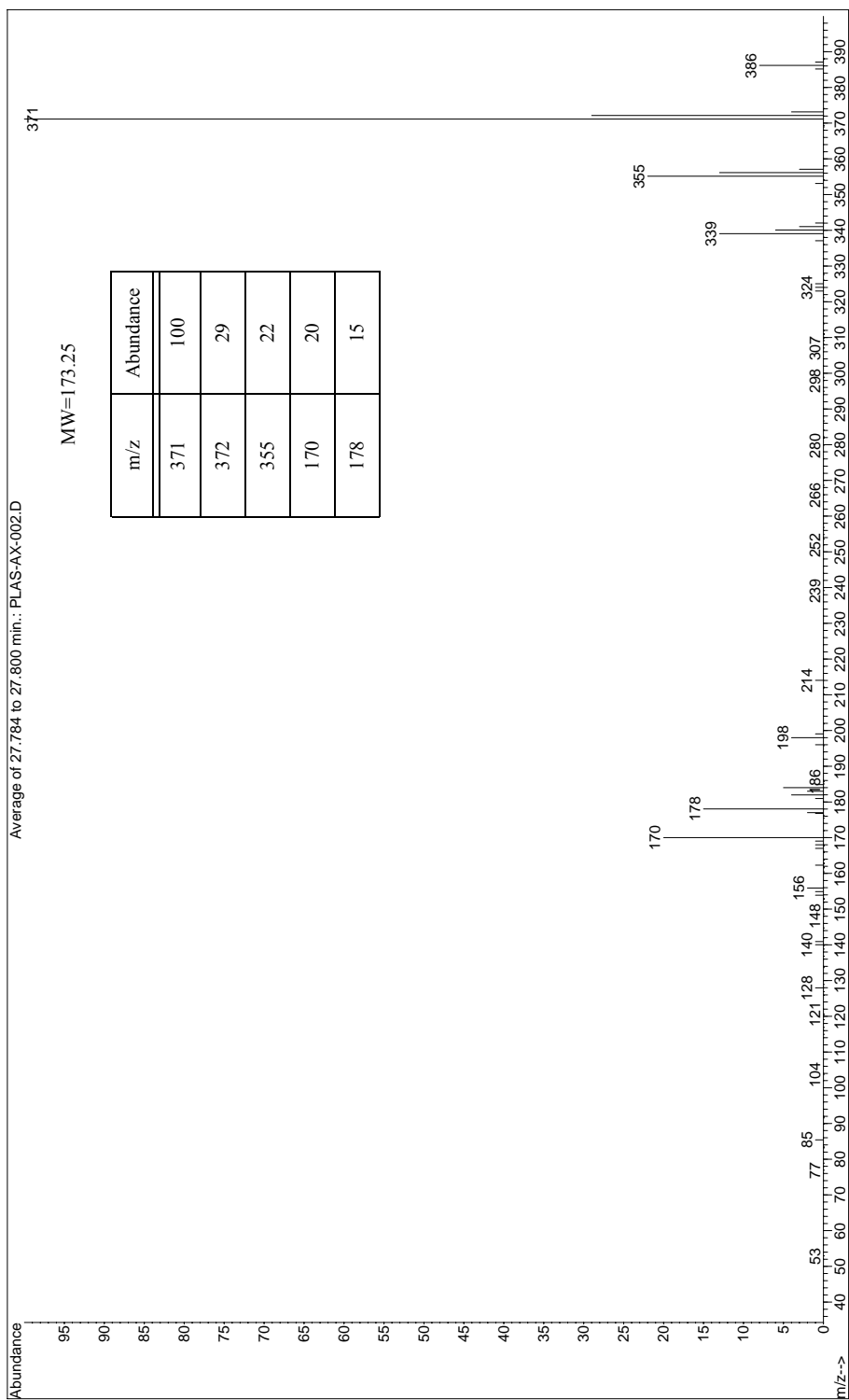
Mass Spectrum for Naugard® Q Extra - PLAS-AX-002



Mass Spectrum for Naugard® Q Extra - PLAS-AX-002

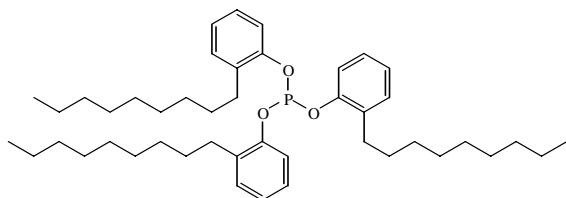


Mass Spectrum for Naugard® Q Extra - PLAS-AX-002



Naugard® RM-51

Chemtura Corporation



CAS Number 26523-78-4

RTECS Number Not available

Abbreviation

Formula $C_{45}H_{69}O_3P$

Molecular Weight 689.00

Chemical Name

blend of phenolic primary and phosphite secondary antioxidants

Synonyms

nonylphenyl phosphite (3:1); tris(mono-nonylphenyl) phosphite; Tris nonylphenyl phosphite; Tris(mono-nonylphenyl)phosphite, 2,2'-methylenabis(4-methyl-6-nonylphenol)

Brand Names & Manufacturers**Physical Properties****Appearance** Clear, gold to yellow viscous liquid**Melting Point** Not available**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application, Regulatory & Environmental Information**Application**

This material is an effective liquid antioxidant that is nonstaining and nondiscoloring. It is used in natural and synthetic rubbers for protection against oxygen, light and heat.

Regulatory Information

FDA approval under 21CFR177.2600 - Rubber Articles Intended for Repeated Use - Limitation - 5% Max.

Environmental Impact

(EC50 48hr): 0.42 mg/mL [Daphnia magna], (LC50 96hr): < 10 mg/mL [Zebra fish], (EBC50): > 100 mg/mL [Green algae], (LC50): > 100 mg/mL [Aerobic bacteria].

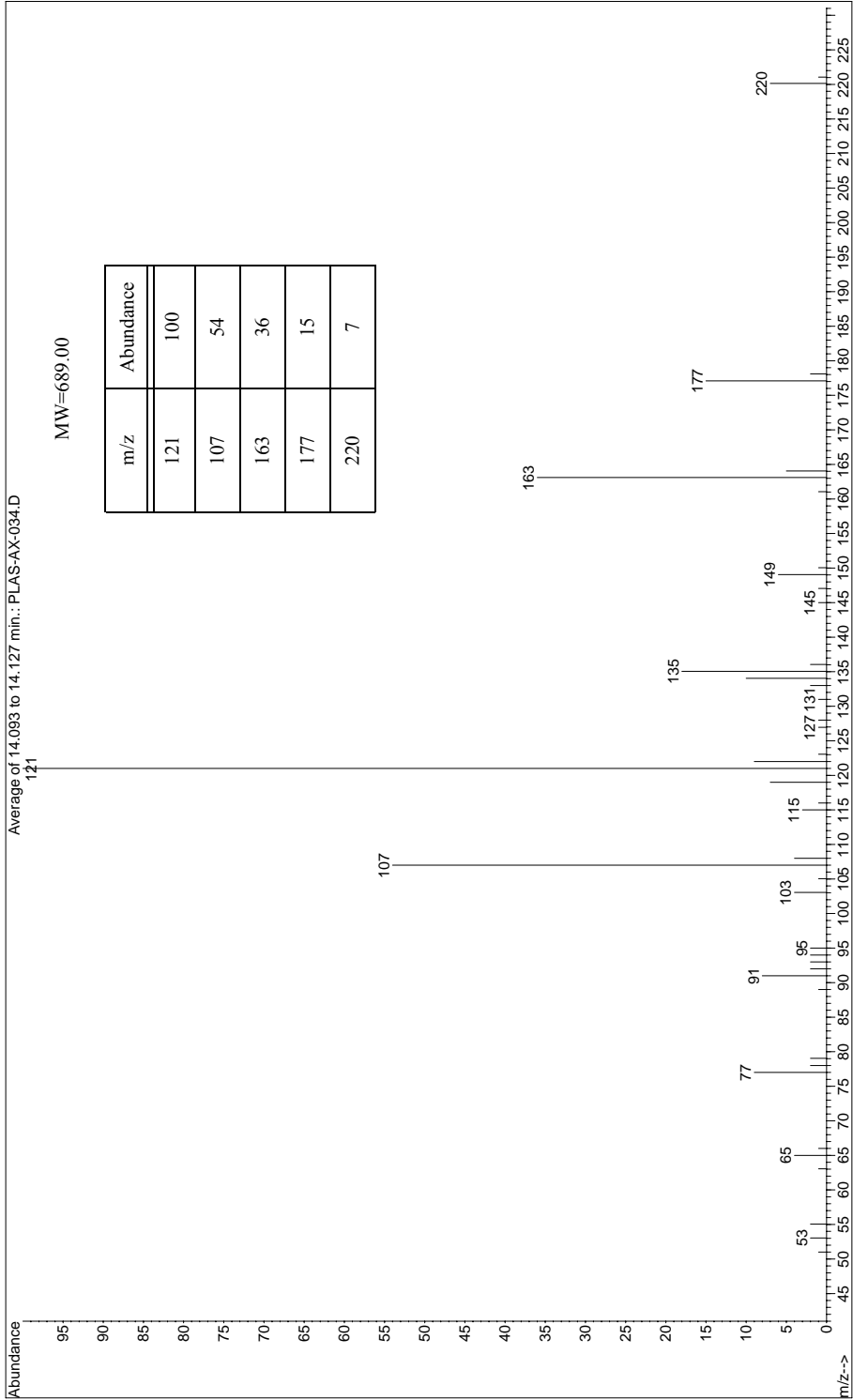
Point of Release

Can be released as point source pollution during manufacture, shipping and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

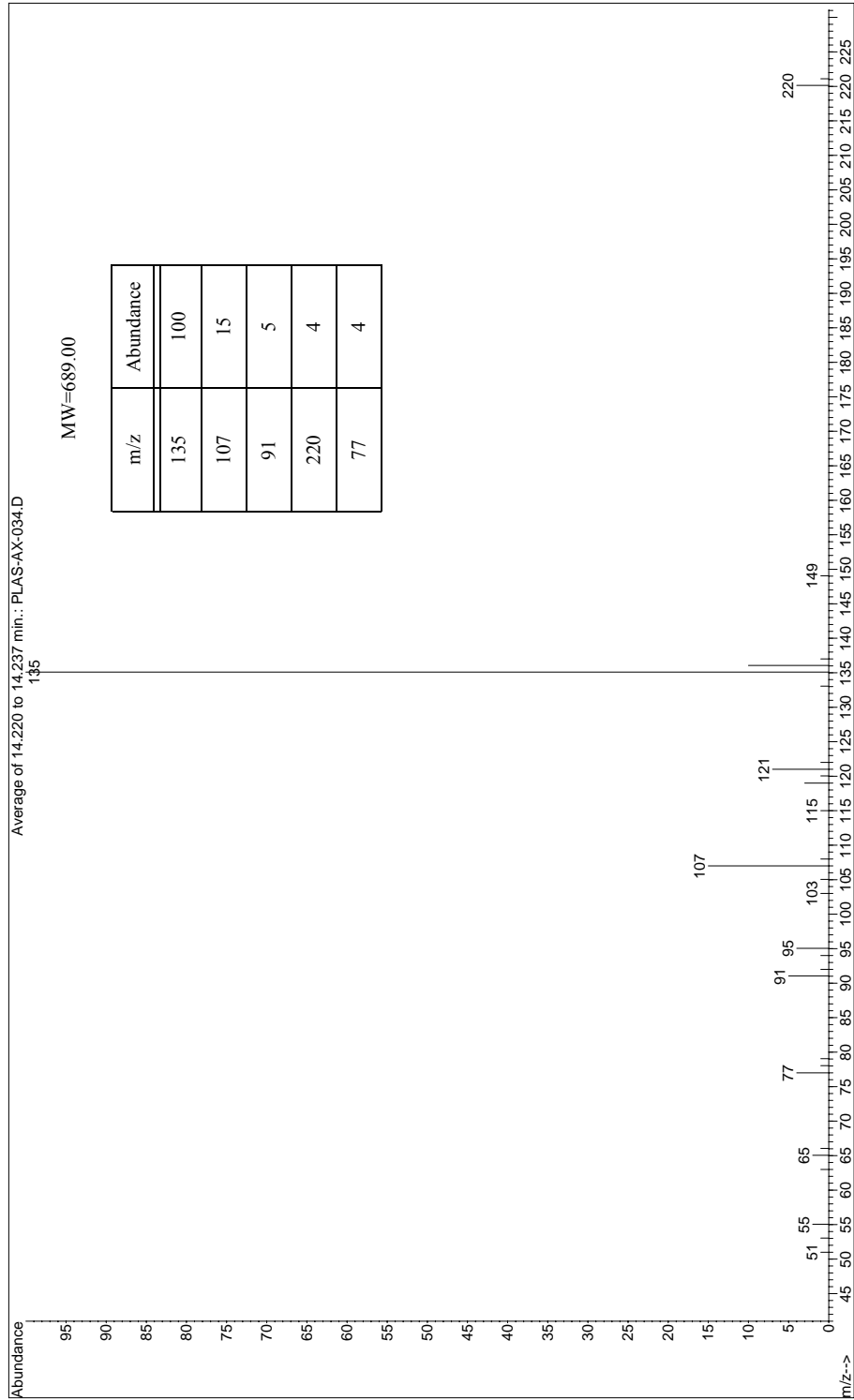
Toxicological Data

Acute toxicity: (LD50): >2000 mg/kg [Rat]. This material was not mutagenic in an Ames bacterial assay.

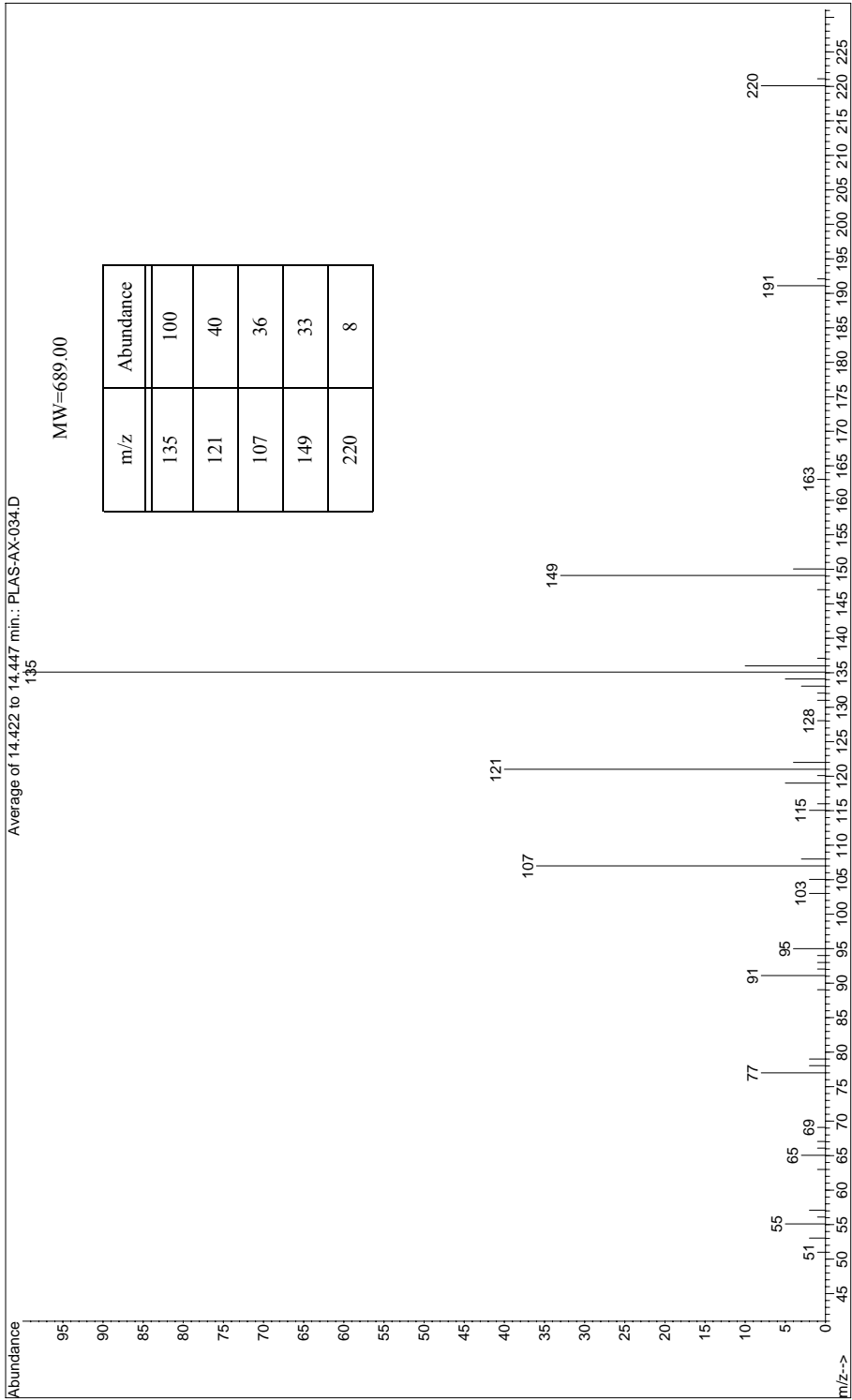
Mass Spectrum for Naugard® RM-51 - PLAS-AX-034



Mass Spectrum for Naugard® RM-51 - PLAS-AX-034

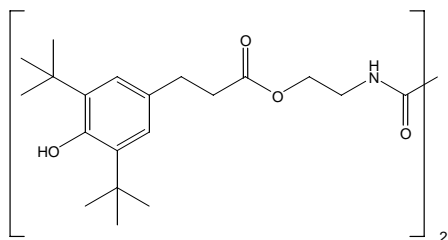


Mass Spectrum for Naugard® RM-51 - PLAS-AX-034



Naugard® XL-1

Chemtura Corporation

**CAS Number** 70331-94-1**RTECS Number** Not available**Abbreviation****Formula** C₄₀H₆₀N₂O₈**Molecular Weight** 697**Chemical Name**

2,2'-oxamidobis[ethyl-3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]

Synonyms

(1,2-dioxoethylene)bis(iminoethylene) bis[3-(3,5-di-tert-butyl-4-hydroxyphenyl)propionate]; 3,5-bis(1,1-dimethylethyl)-4-hydroxybenzenepropanoic acid, (1,2-dioxo-1,2-ethanediyl)bis(imino-2,1-ethanediyl) ester

Brand Names & Manufacturers

Rionox MD-697

Physical Properties

Appearance	White to off-white powder or granules					
Melting Point	170-180 °C			Boiling Point	Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 1.6	EtOH U	Acetone 10	CH₂Cl₂ U	Hexane <0.1

Application, Regulatory & Environmental Information**Application**

Non-discoloring, metal deactivator and antioxidant, acts as a hindered phenolic antioxidant. Typical end use applications include wire and cable insulation, film and sheet manufacture as well as automotive parts.

Regulatory Information

FDA approved per 21CFR175.105 in food packaging adhesives and 178.2010 for use in olefin polymers in food contact at usage levels not to exceed 0.1% by weight of finished product.

Environmental Impact

Based on test results of similar compounds, there is a high potential for this compound to bioaccumulate and be inherently toxic to aquatic wildlife.

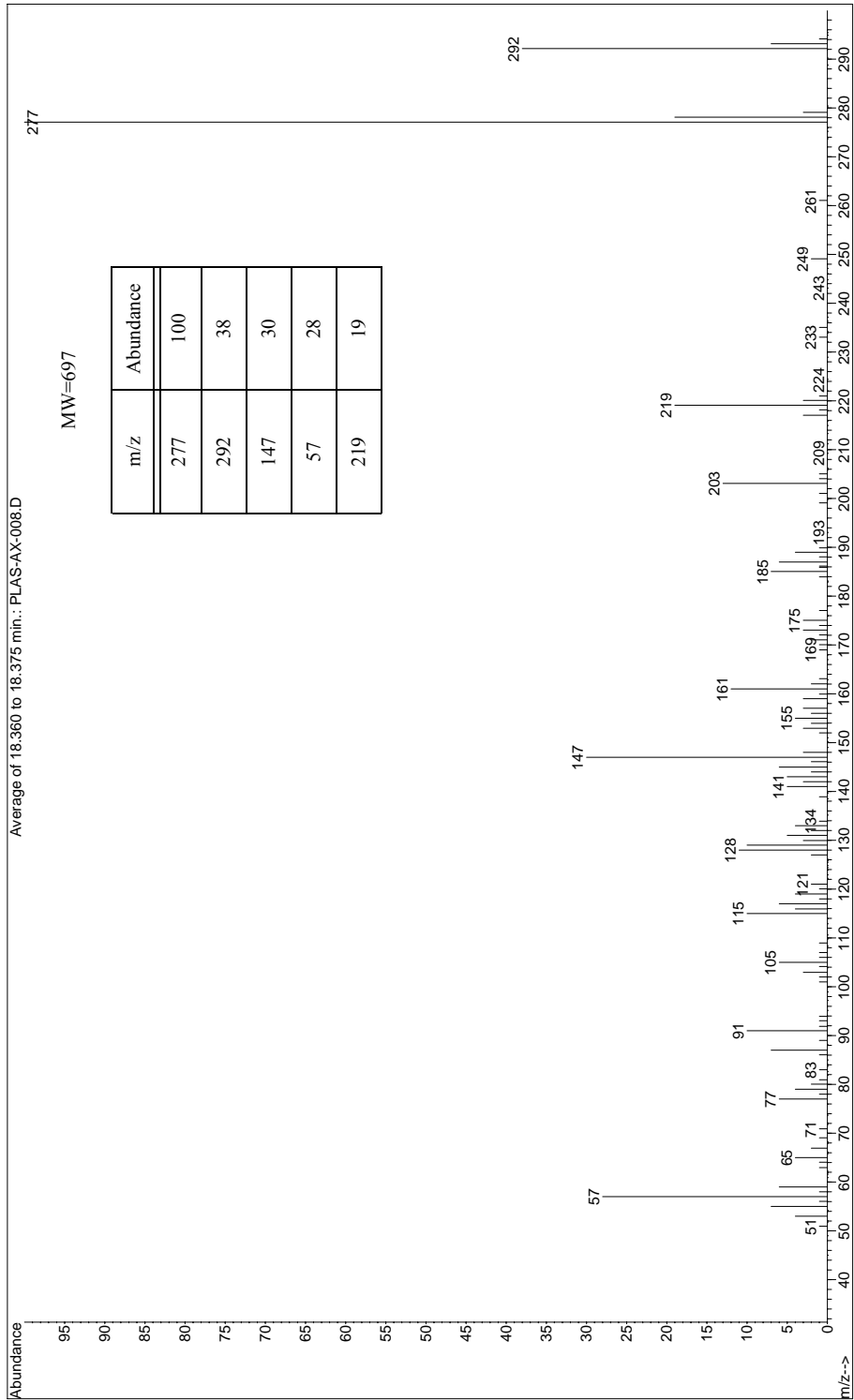
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

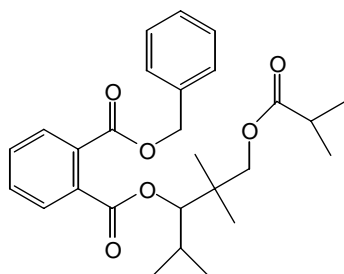
Acute oral (LD50): >10 g/kg [Rat].

Mass Spectrum for Naugard® XL-1 - PLAS-AX-008



Santicizer® 278

Solutia Inc.

**CAS Number** 16883-83-3**RTECS Number** Not available**Abbreviation****Formula** C₂₇H₃₄O₆**Molecular Weight** 454.56**Chemical Name**

benzyl 3-isobutyryloxy-1-isopropyl-2,2-dimethylpropyl phthalate

Synonyms

2,2-dimethyl-1-(1-methylethyl)-3-(2-methyl-1-oxopropoxy)propyl-1,2-benzenedicarboxylic acid phenylmethyl ester

Brand Names & Manufacturers**Physical Properties****Appearance** Clear, oily liquid**Melting Point** Not available**Boiling Point** 243 °C (10 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application
Santicizer 278 is used in PVC, acrylic coatings, polyurethanes, chlorinated rubber, butyl rubber, and polysulfides. It is a versatile plasticizer for use in many resin systems, from automobile sealants to water-blown methylene diisocyanate based polyurethane foams. Other applications include use as a yellowing inhibitor for thermoplastic polycarbonate resins exposed to gamma radiation and as a solvent for pressure-sensitive copying paper giving copies improved resistance to fading. It is also used for interlayers of sandwich glass for cars and buildings.

Regulatory Information

Not specifically listed in 21 CFR for use in food applications. When discarded, the compound is not a hazardous waste, as defined by the Resource, Conservation and Recovery Act (RCRA), and it is also not considered hazardous under the Department of Transportation (DOT) regulations. It is, however, listed in the Toxic Substances Control Act (TSCA) Inventory.

Environmental Impact

The EPA Registry classifies this compound as non-persistent, bioaccumulative, and inherently toxic to aquatic organisms.

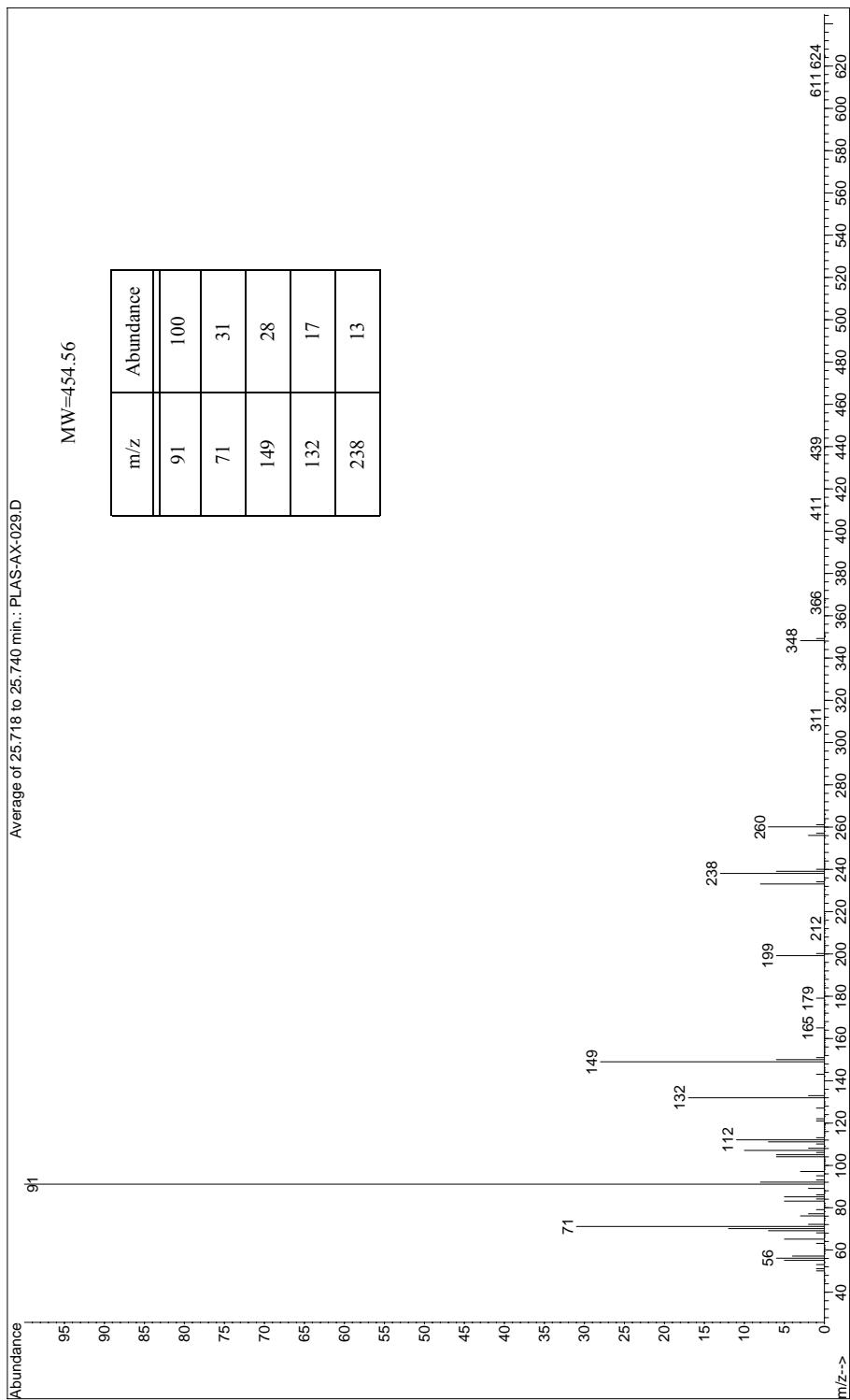
Point of Release

Phthalates are not chemically bound to the product and therefore may leach into the surrounding medium.

Toxicological Data

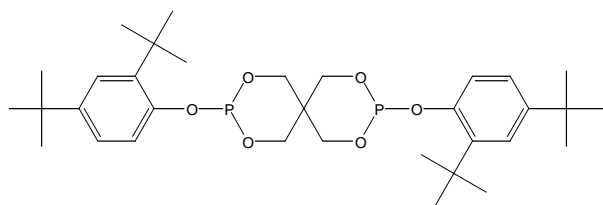
Acute Oral Toxicity (LD50): >15,800 mg/kg [Rat]; Acute Dermal Toxicity (LD50): >10,000 mg/kg [Rabbit]. When applied to the skin and eyes of six rabbits for a period of 24 hours, was reported to be practically non-irritating.

Mass Spectrum for Santicizer® 278 - PLAS-AX-029



Ultranox® 626

Chemtura Corporation

**CAS Number** 26741-53-7**RTECS Number** TG7400000**Abbreviation****Formula** C₃₃H₅₀O₆P₂**Molecular Weight** 604.69**Chemical Name**

bis(2,4-di-tert-butylphenyl)pentaerythritol diphosphite

Synonyms

Bis(2,4-di-tert-butylphenyl) pentaerythritol diphosphite; 3,9-Bis(2,4-di-tert-butylphenoxy)-2,4,8,10-tetraoxa-3,9-diphosphaspiro(5.5) undecane

Brand Names & Manufacturers

Alkanox® P24

Chemtura Corporation

Ethaphos® 326

Albemarle

Irgafos® XP 60

Ciba Specialty Chemicals

Physical Properties**Appearance** White powder or granule**Melting Point** 173-180 °C**Boiling Point** >311 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	2.1	U	11	34	7.3

Application, Regulatory & Environmental Information**Application**

Solid organophosphite antioxidant that provides color stability, reduces polymer degradation, and improves gas fading performance in many resins. It may be used in polyethylene, polypropylene, polystyrene, polyesters, elastomers, PVC and thermoplastics.

Regulatory Information

Approved by the FDA for food contact applications under 21CFR178.2010 covering antioxidants and/or stabilizers for polymers.

Environmental Impact

Log Pow of 10.6 indicates a high potential to bioaccumulate. This chemical is not estimated to be readily biodegradable.

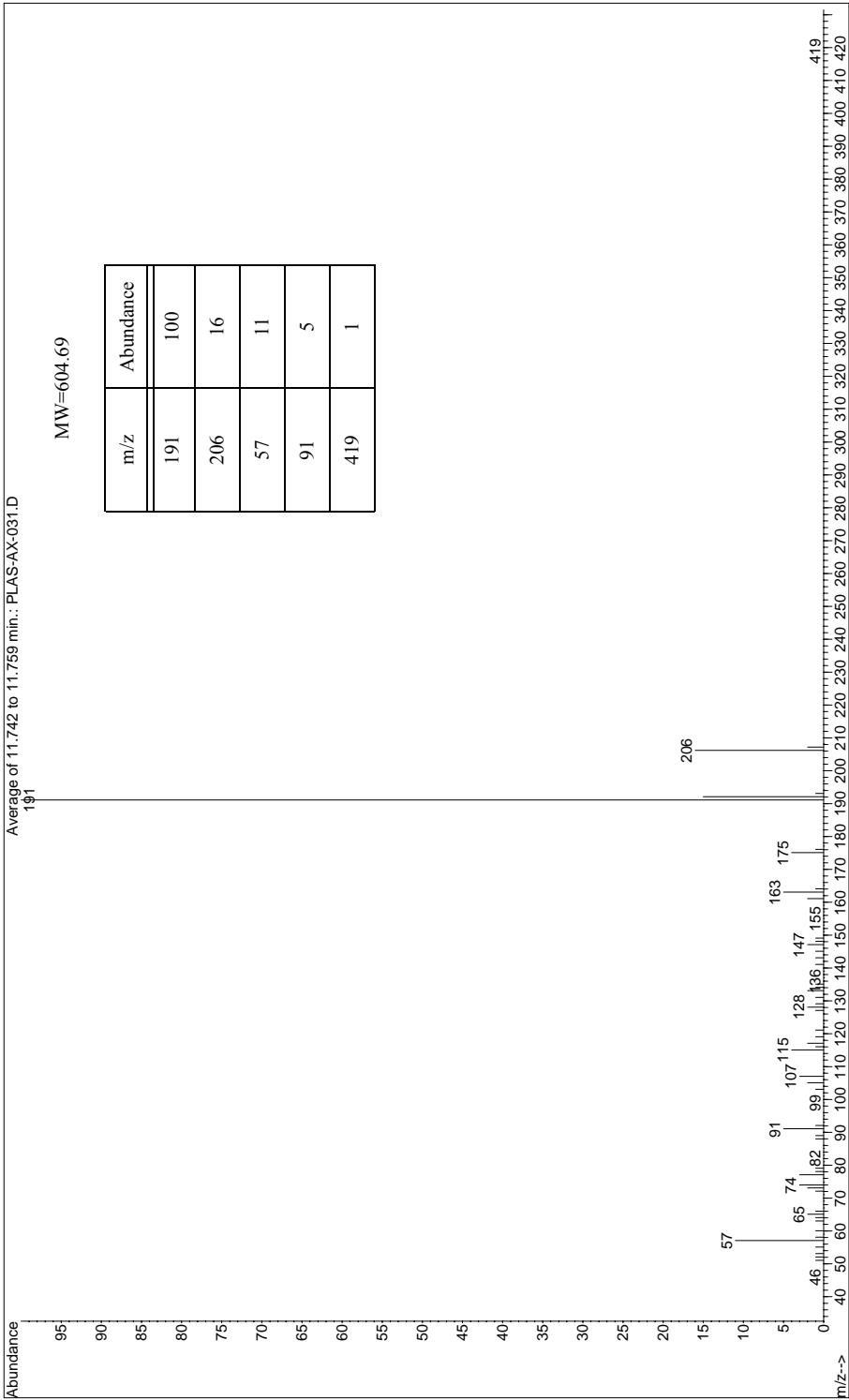
Point of Release

Can be released as a point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the longevity of the products and upon disposal of the products.

Toxicological Data

Acute Oral Toxicity (LD50): 5580 mg/kg [Rat], Acute Dermal Toxicity (LD50): >200 mg/kg [Rabbit].

Mass Spectrum for Ultrinox® 626 - PLAS-AX-031



CHAPTER 6

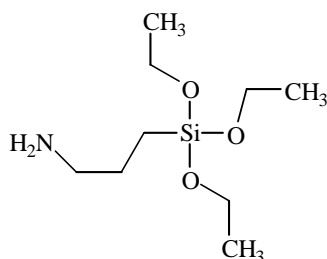
Coupling Agents

Coupling agents are substances that are capable of bonding organic polymer systems to inorganic substrates such as glass, mineral fillers, metals and metallic oxides. In composites, the stable bond formed via the coupling agent leads to significant property-enhancing effects. Coupling agents are used in filled polymer systems, including both thermosets and thermoplastics, such as glass fiber reinforced epoxy resins, phenolics, and rubber applications.

Organosilanes (compounds of silicon and hydrogen with a molecular formula of $\text{Si}_n\text{H}_{2n+2}$) are the most widely used coupling agents. The adhesion mechanism is due to two groups in the silane structure. The $\text{Si}(\text{OR})$ portion reacts with the inorganic reinforcement, while the organofunctional (vinyl-, amino-, epoxy-, etc.) group reacts with the resin.

Silquest® A-1100

General Electric Company

**CAS Number** 919-30-2**RTECS Number** TX2100000**Abbreviation** APTES**Formula** C₉H₂₃NO₃Si**Molecular Weight** 221.37**Chemical Name**

gamma-aminopropyltriethoxysilane

Synonyms

3-(triethoxysilyl)-1-propanamine; 3-(triethoxysilyl)propylamine; triethoxy(3-aminopropyl)silane

Brand Names & Manufacturers

Silquest® A-1102

General Electric Company

Physical Properties**Appearance** Clear liquid**Melting Point** <-70 °C**Boiling Point** 220 °C**Stability** Reacts rapidly with water/moisture

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information**Application**

This material is used in numerous applications including various applications as coupling agents and adhesion promoters in fiberglass, adhesives and sealants, foundry resins, and in pre-treatment for coatings.

Regulatory Information

This material is not FDA approved for food contact applications.

Environmental Impact

This product is biodegradable. The reactive nature of this material destroys the parent material in any moisture-containing environment, thus limiting environmental exposure to the silane. The parent material is hydrolyzed in a spill situation; the rapid hydrolysis means that the parent silane is unlikely to be found in the environment. Bioaccumulation is not anticipated.

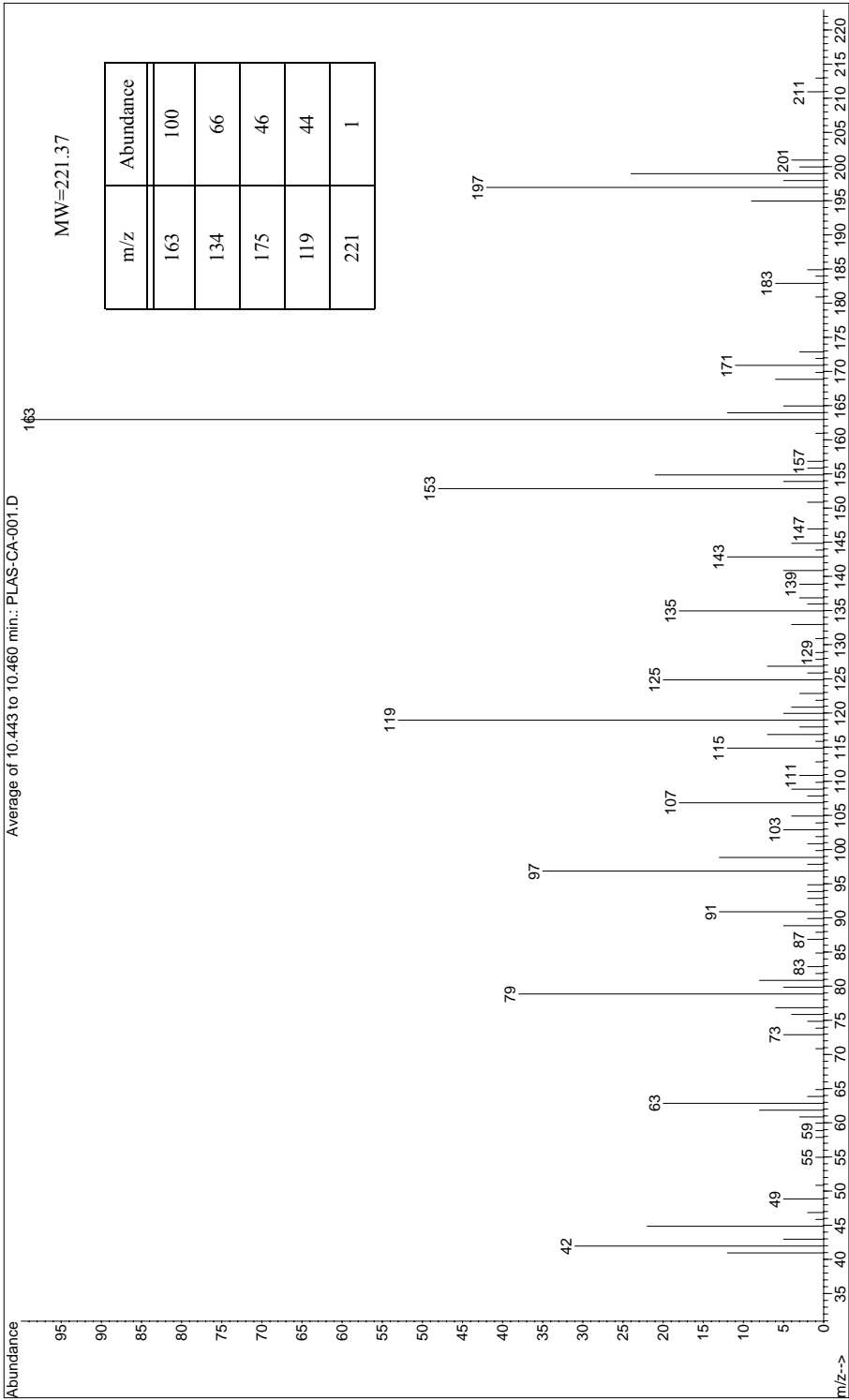
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Once APTES is added to a consumer or industrial product, the parent silane reacts with the components of the formulation and is generally present as the parent silane at 0.1-0.2% until after curing (use). After curing the parent silane is consumed into the polymer matrix and no longer exists and greatly reduces potential for consumer or worker exposure. APTES polymerizes during use.

Toxicological Data

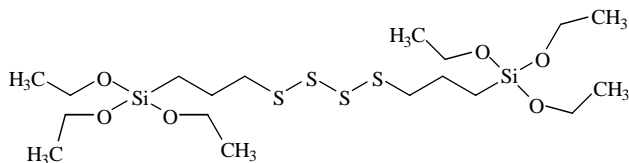
RTECS CLASS OF COMPOUND: Primary Irritant - toxic by ingestion. Acute oral toxicity (LD50): 1780 mg/kg [Rat]; acute dermal toxicity (LD50): 4 mL/kg [Rabbit]. Since APTES is sensitive to hydrolysis, which may occur during testing, observed toxicity is likely due to the hydrolysis products ethanol and trisilanols.

Mass Spectrum for Silquest® A-1100 - PLAS-CA-002



Silquest® A-1289

General Electric Company

**CAS Number** 40372-72-3**RTECS Number** Not available**Abbreviation****Formula** C₁₈H₄₂O₆S₄Si₂**Molecular Weight** 538.94**Chemical Name**

bis-(triethoxysilylpropyl)tetrasulfide

Synonyms

Brand Names & Manufacturers

Physical Properties**Appearance** Clear light yellow liquid**Melting Point** <-78 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application Used for sulfur-cure, mineral-filled rubber applications. Silica-filled tires with lower rolling resistance, longer lasting, heat resistant belts or hoses, and light weight shoe soles are some of the typical uses.

Regulatory Information

This material is not FDA approved for food contact applications.

Environmental Impact

Not readily biodegradable. Acute toxicity fish: (LC50): >100 mg/L. Acute toxicity to plants: > 100 mg/L. Acute toxicity to aquatic invertebrates: (EC50): >100 mg/L.

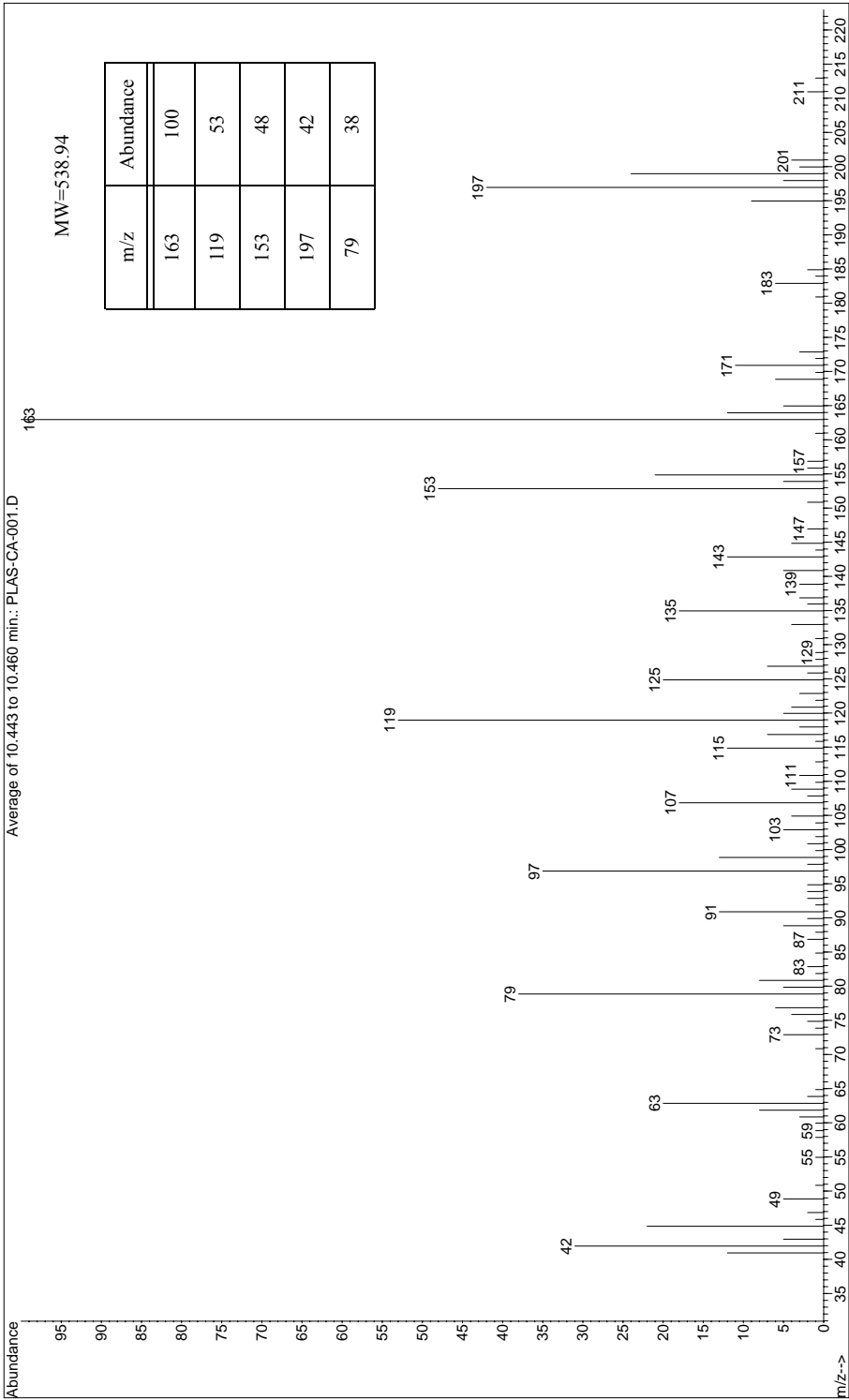
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

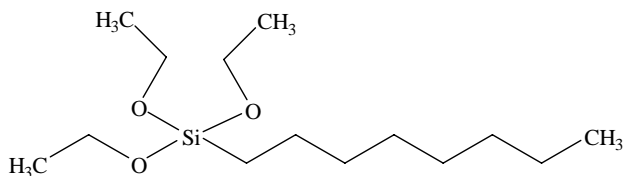
This product hydrolyzes in the stomach to form ethanol. Acute toxicity: Oral (LD50): >5000mg/kg [Rat]; Skin (LD50):>2000mg/kg [Rat].

Mass Spectrum for Silquest® A-1289 - PLAS-CA-001



Silquest® A-137

General Electric Company

**CAS Number** 2943-75-1**RTECS Number** VV6695500**Abbreviation****Formula** C₁₄H₃₂O₃Si**Molecular Weight** 276.55**Chemical Name**

octyltriethoxysilane

Synonyms

triethoxyoctylsilane

Brand Names & Manufacturers

Physical Properties

Appearance Clear, pale liquid**Melting Point** <-74 °C**Boiling Point** 250 °C**Stability** Reacts slowly with water.

Solubility (g/100mL 20 °C)	Water 40-80	MeOH 1-10	EtOH 1-10	Acetone 40-80	CH₂Cl₂ 40-80	Hexane U
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Application, Regulatory & Environmental Information

Application

Used as a water repellent for concrete and masonry.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

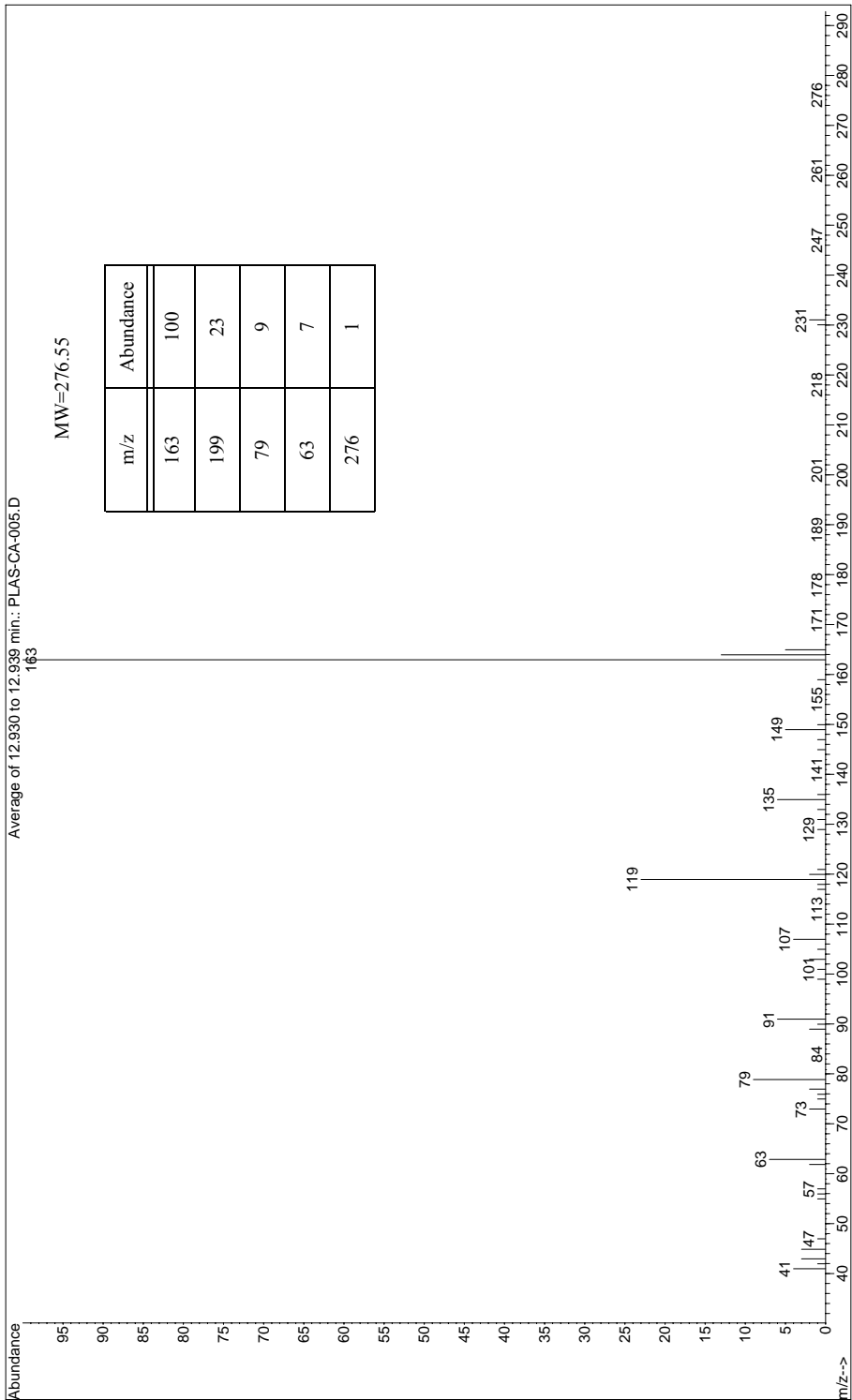
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

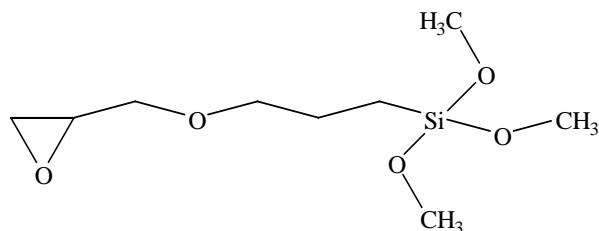
Acute Oral Toxicity (LD50): >2000 mg/kg [Rat]; acute dermal toxicity (LD50): >2000 mg/kg [Rat].

Mass Spectrum for Silquest® A-137 - PLAS-CA-005



Silquest® A-187

Chemtura Corporation

**CAS Number** 2530-83-8**RTECS Number** VV4025000**Abbreviation****Formula** C₉H₂₀O₅Si**Molecular Weight** 236.38**Chemical Name**

gamma-glycidoxypyriltrimethoxysilane

Synonyms

3-(2,3-epoxypropoxypropyl) trimethoxysilane

Brand Names & Manufacturers

Physical Properties

Appearance Clear pale liquid**Melting Point** <-70 °C**Boiling Point** 290 °C**Stability** Reacts with water/moisture.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application

Used as adhesion promoter in polysulfide, urethane, epoxy and acrylic caulks, coatings, sealants, and adhesives.

Regulatory Information

Not approved by the FDA for applications involving implantation within the body; direct or indirect contact with the blood pathway; contact with bone, tissue, tissue fluid, or blood; or prolonged contact with mucous membranes.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

Point of Release

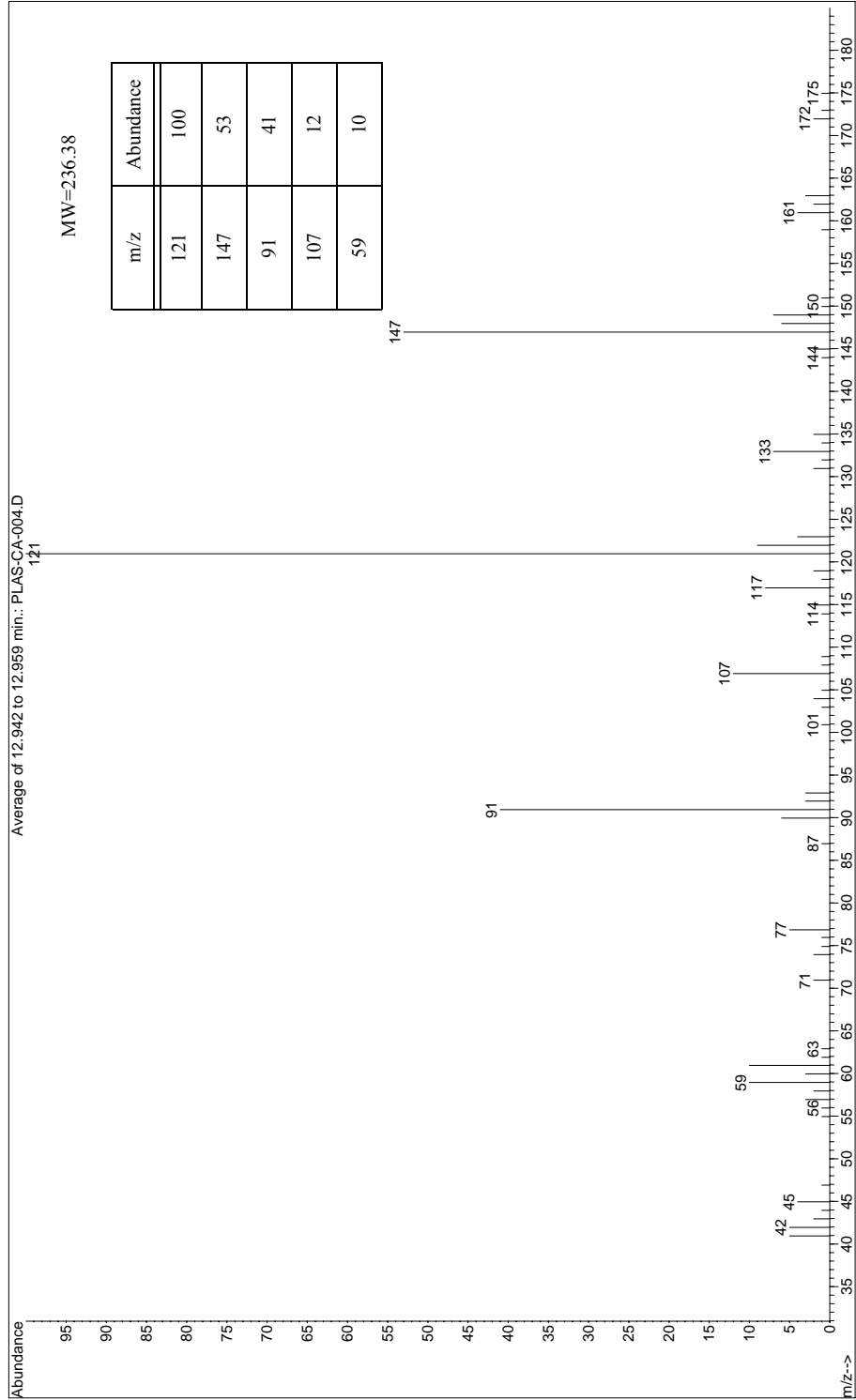
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Organometallic; Mutagen; Reproductive Effector; Primary Irritant.

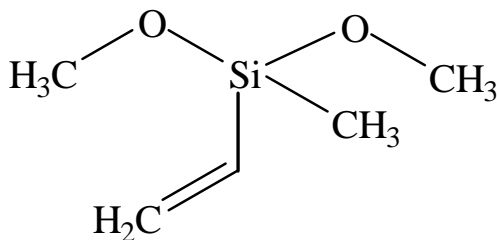
Acute Oral Toxicity (LD50): 22600 µL/kg [Rat]; acute dermal toxicity (LD50): 3970 µl/kg [Rabbit].

Mass Spectrum for Silquest® A-187 - PLAS-CA-004



Silquest® A-2171

General Electric Company



CAS Number 16753-62-1

RTECS Number Not available

Abbreviation

Formula $C_5H_{12}O_2Si$

Molecular Weight 132.24

Chemical Name

vinylmethyldimethoxysilane

Synonyms

dimethoxy methylvinyl silane

Brand Names & Manufacturers

Physical Properties

Appearance Clear pale yellow liquid**Melting Point** $<0^{\circ}C$ **Boiling Point** $106^{\circ}C$ **Stability** Stable; reacts slowly with water to form methanol.

Solubility (g/100mL $20^{\circ}C$)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	40-80	40-80	U

Application, Regulatory & Environmental Information

Application Silquest® A-2171 offers vinyl and silane functionality making it suitable for crosslinking of organic polymers. Similarly it is also useful as a crosslinker in systems where greater elongation is required. It is also recommended for chain extension of RTV Silicones or other silane or HO functional polymers. The resulting Si-O-Si crosslinked sites are resistant to exposure to moisture, chemicals and UV. Siloxane crosslinkers tend not to generate color and are resistant to environmental factors such as acid rain.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

Bioaccumulation is not expected to occur. Exotoxicity is expected to be low based on the reactivity with water. If spilled in the environment, the product would react with water and hydrolyze which results in highly cross-linked, high molecular weight polymers, further reducing the potential for exposure.

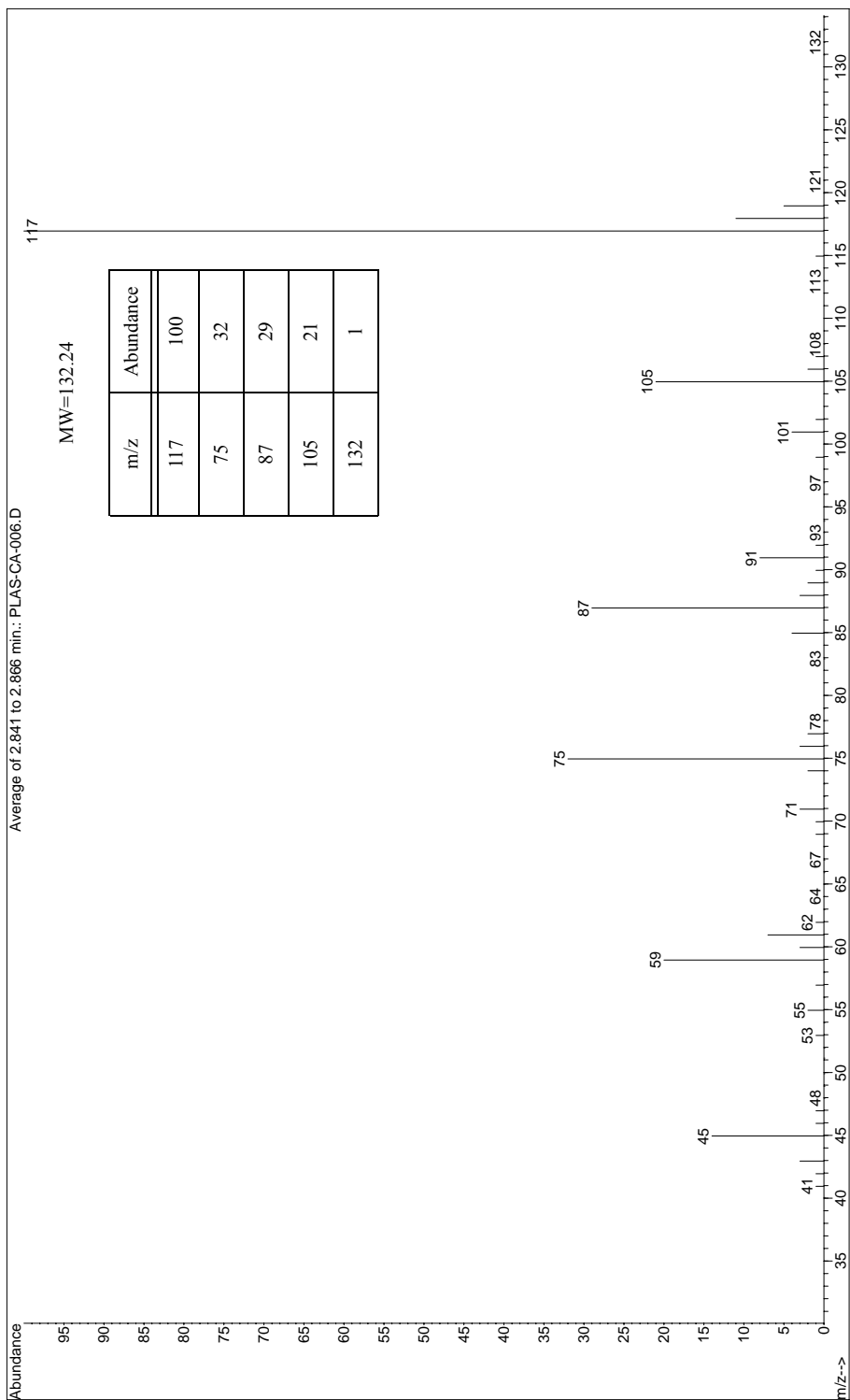
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

No adverse effects anticipated from available information. No evidence of embryotoxicity or teratogenicity. Material was not mutagenic in an Ames bacterial assay.

Mass Spectrum for Silquest® A-2171 - PLAS-CA-006



Flame Retardants

Flame retardants are added not to aid in processing, but rather to inhibit ignition or flammability of the end-use product. They are added so that the plastic is able to meet flammability standards established by either mandatory government regulations or voluntary specifications.

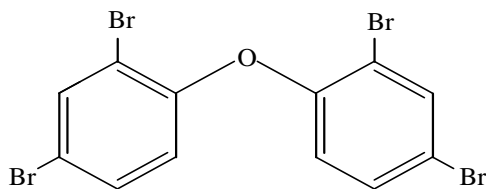
Common flame retardants are aluminum trihydrate, brominated compounds, phosphorous compounds, antimony oxide, chlorinated compounds, and boron compounds. Brominated flame retardants are preferred for thermoplastic resins such as polystyrene, polyesters, polyolefins and polyamides but are also used in epoxies, ABS and polycarbonates. Decabromodiphenyl oxide is the most common brominated flame retardant used.

Sometimes flame retardants can be found in polymers that were not added to the polymer during processing, giving evidence that these compounds can leach from other sources. For example, Aroclors can often be found in a plastic matrix that has merely been in contact with a fluid containing the Aroclors.

No matter the source, flame retardants, especially the poly brominated diphenyl ethers (PBDE's), are coming under scrutiny because they are persistent organic pollutants (POPs). They are appearing in human samples, most notably serum, adipose fat tissue and breast milk. PBDE's are also under investigation as potential endocrine mimickers or endocrine disruptors. As a result, PBDE's are the most highly regulated flame retardants. Their environmental fate will continue to be a topic of research for years to come.

Because many of these items are included as an individual congener or marker for the industrial additive and not as the additive, the format is slightly different from the rest of the book. Items such as environmental impact and point of release have been omitted.

Analysis of the Aroclors and Halowaxes is mainly by pattern recognition on the GC. The mass spectrum that is included is of the largest mass peak, because that is the most unique to that particular compound.

2,2',4,4'-Tetrabromodiphenyl ether

CAS Number 40088-47-9

RTECS Number DA6630000

Abbreviation

Formula $C_{12}H_6Br_4O$

Molecular Weight 485.82

Chemical Name

2,2',4,4'-tetrabromodiphenyl ether

Synonyms

BDE-47; tetrabromodiphenyl ether; PBDE-47

Usage

BDE-47 was a component of many commonly used flame retardants, including PeBDE, DE-71, Bromkal 70-SDE, and other popular mixtures. DE-71 was sold by Great Lakes Chemical Corporation as a flame retardant for unsaturated polyester, rigid and flexible polyurethane foams, epoxies, laminates, adhesives, and coatings. This material was phased out at the end of 2004. It typically contained somewhere between 20-50% BDE-47.

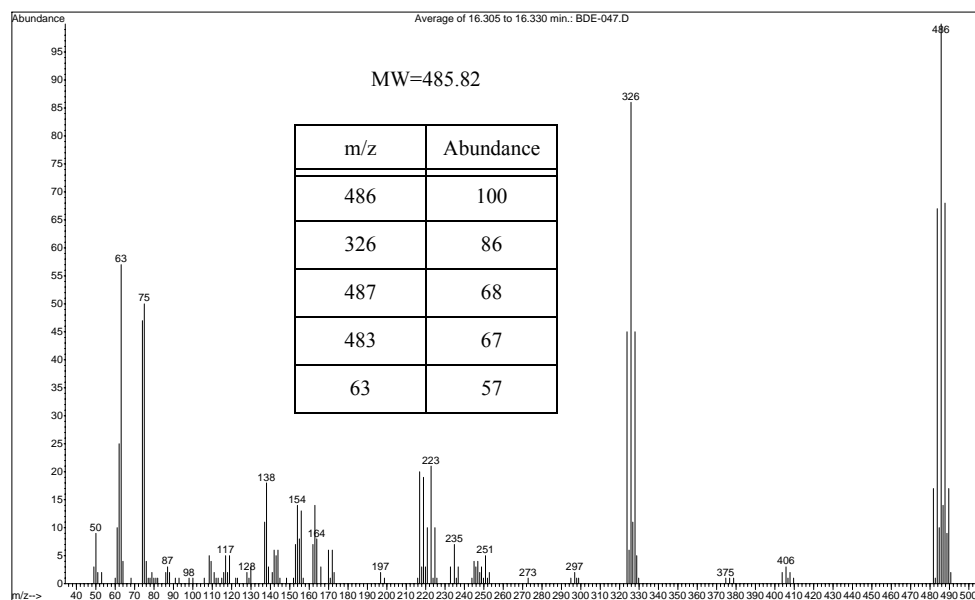
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-047 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

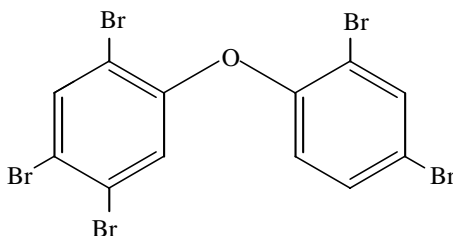
Toxicological and Environmental Data

BDE-47 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are on going.

Acute Oral Toxicity (LD50): >500 mg/kg [Rat].



For Chromatogram See Appendix A - BDE-047 - page 396

2,2',4,4',5-Pentabromodiphenyl ether

CAS Number 32534-81-9

RTECS Number DD6625350

Abbreviation

Formula C₁₂H₅Br₅O

Molecular Weight 564.72

Chemical Name

2,2',4,4',5-pentabromodiphenyl ether

Synonyms

BDE-99; pentabromodiphenyl ether; PBDE-99

Usage

BDE-99 was a component of many commonly used flame retardants, including DE-71, Bromkal G1, and other popular mixtures. DE-71 was sold by Great Lakes Chemical Corporation as a flame retardant for unsaturated polyester, rigid and flexible polyurethane foams, epoxies, laminates, adhesives, and coatings. This material was phased out at the end of 2004. It typically contained about 50% BDE-99.

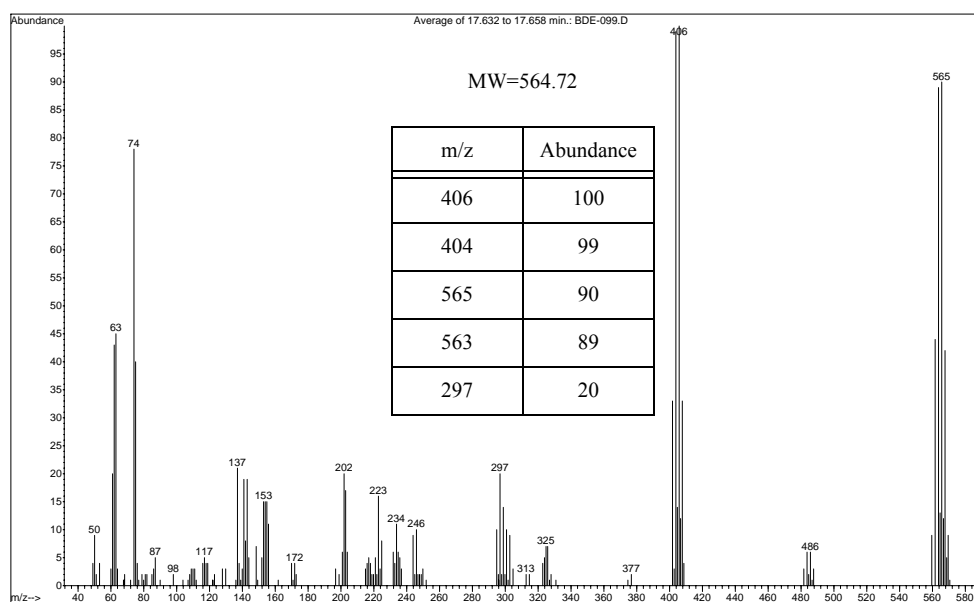
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-099 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

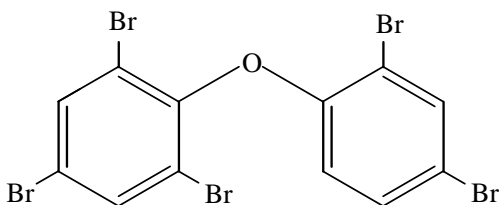
Toxicological and Environmental Data

Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment.

Acute Oral Toxicity (LD50): 5 gm/kg [Rat]; Acute Dermal Toxicity (LD50): 2 gm/kg/24H [Rabbit].



For Chromatogram See Appendix A - BDE-099 - page 397

2,2',4,4',6-Pentabromodiphenyl ether

CAS Number 189084-64-8

RTECS Number

Abbreviation

Formula $C_{12}H_5Br_5O$

Molecular Weight 564.69

Chemical Name

2,2',4,4',6-pentabromodiphenyl ether

Synonyms

BDE-100

Usage

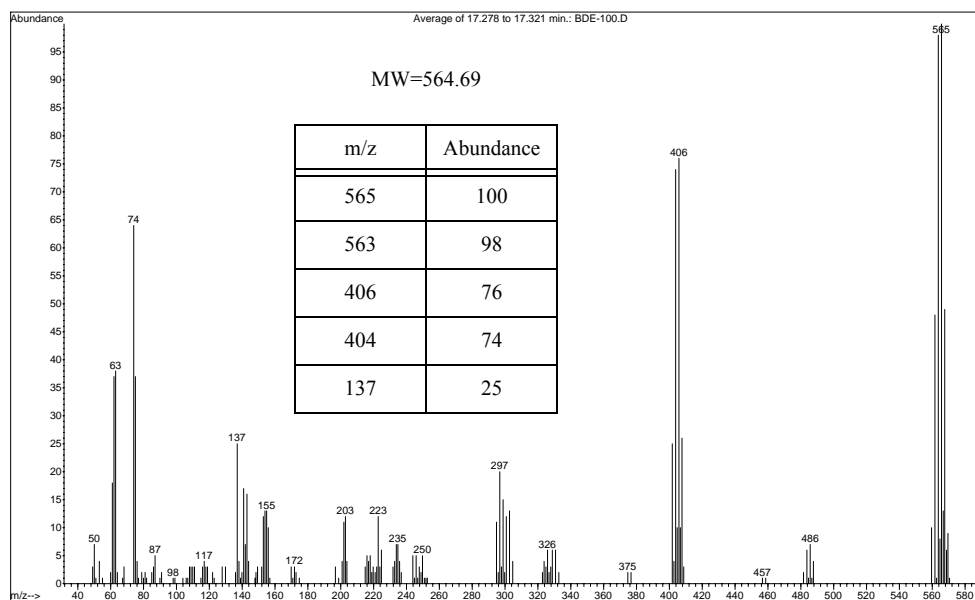
BDE-100 is a primary component of Penta-BDE which was mainly used as a flame retardant in polyurethane foam and textile applications. Penta-BDE is primarily used in North America. BDE-100 was also present in DE-71, at about 10%.

Regulatory Information

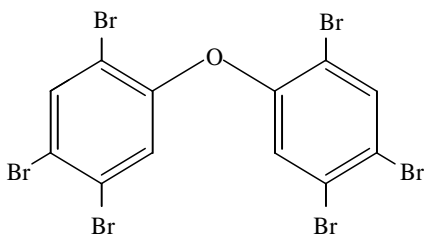
USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-100 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

Toxicological and Environmental Data

BDE-100 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are on going.



For Chromatogram See Appendix A - BDE-100 - page 398

2,2',4,4',5,5'-Hexabromodiphenyl ether

CAS Number 68631-49-2

RTECS Number DA6620000

Abbreviation

Formula $C_{12}H_4Br_6O$

Molecular Weight 643.62

Chemical Name

2,2',4,4',5,5'-hexabromodiphenyl ether

Synonyms

BDE-153

Usage

BDE-153 occurs primarily in the commercial Octa and Penta BDE mixtures. The Octa mix contains approximately 10-12% hexabrominated diphenyl ethers. Penta generally contained about 4-8% hexabrominated diphenyl ethers including BDE-153. Typical analysis shows that the Penta mix contains an equal distribution of BDE-153 and BDE-154. The commercial Penta mix was typically used in flexible polyurethane foam for furniture and cushions. It was also used in polyesters, and epoxy and phenolic resins. Octa is used primarily in rigid plastics for housing electronics.

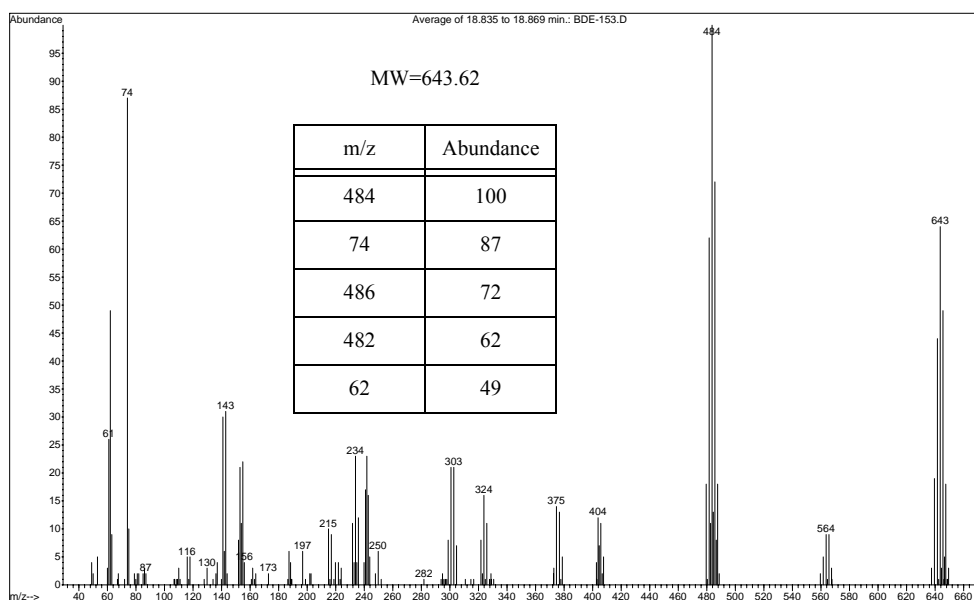
Regulatory Information

USEPA by the Unregulated Contaminant Monitoring Regulation (UCMR) Method 527 Determination of Selected Pesticides and Flame Retardants in Drinking Water by Solid Phase Extraction and Capillary Column GS/MS. USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. PentaBDE banned by EU Directive 793/93/EEC since 2004. BDE-153 Regulated RoHS/WEEE Regulations (2002/95/EC). PentaBDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

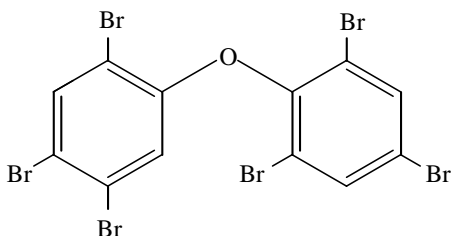
Toxicological and Environmental Data

BDE-153 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research. It is biologically persistent, and has a high bioaccumulation potential. It is under investigation as an endocrine disruptor and studies for human health concerns are on going.

Acute Oral Toxicity (LD50): >500 mg/kg [Rat].



For Chromatogram See Appendix A - BDE-153 - page 399

2,2',4,4',5,6'-Hexabromodiphenyl ether

CAS Number 207122-15-4

RTECS Number Not available

Abbreviation

Formula $C_{12}H_4Br_6O$

Molecular Weight 643.59

Chemical Name

2,2',4,4',5,6'-Hexabromodiphenyl ether

Synonyms

BDE-154

Usage

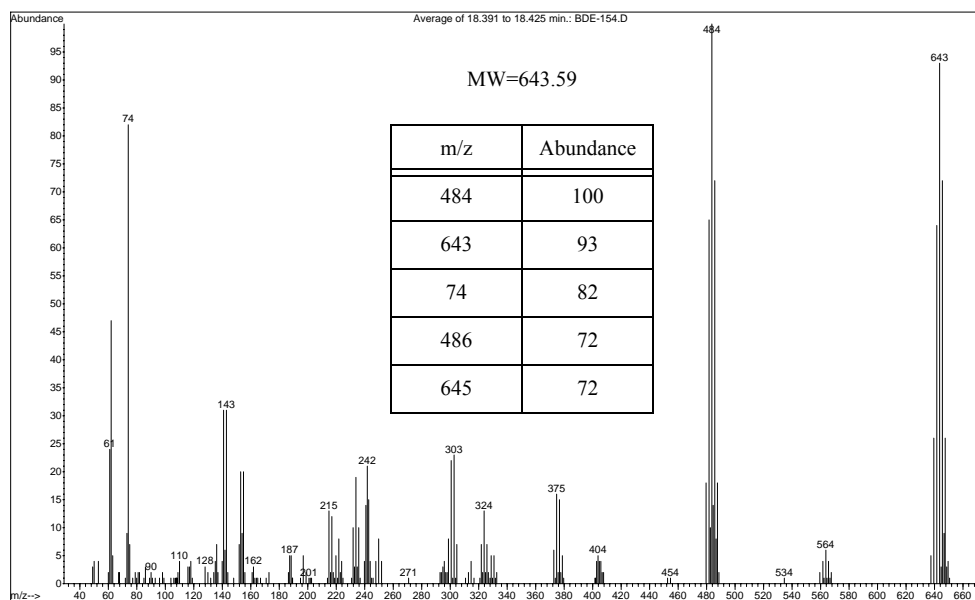
BDE-154 is a component of the commercially available octa-BDE, which is a complex mixture consisting typically of ~0.5% pentabromodiphenyl ether isomers, ~12% hexabromodiphenyl ether isomers, ~45% heptabromodiphenyl ether isomers, ~33% octaBDE isomers, ~10% nonabromodiphenyl ether isomers and ~0.7% decabromodiphenyl ether. It is used as a flame retardant in plastics for electrical and electronic equipment.

Regulatory Information

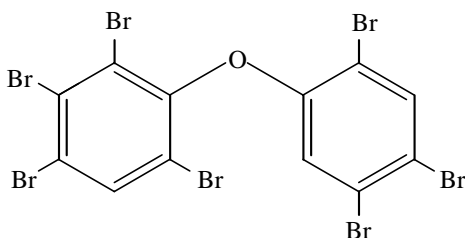
USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS and USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS.

Toxicological and Environmental Data

Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment. BDE-154 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research.



For Chromatogram See Appendix A - BDE-154 - page 400

2,2',3,4,4',5',6-Heptabromodiphenyl ether

CAS Number 207122-16-5

RTECS Number Not available

Abbreviation

Formula $C_{12}H_3Br_7O$

Molecular Weight 722.48

Chemical Name

2,2',3,4,4',5',6-heptabromodiphenyl ether

Synonyms

BDE-183

Usage

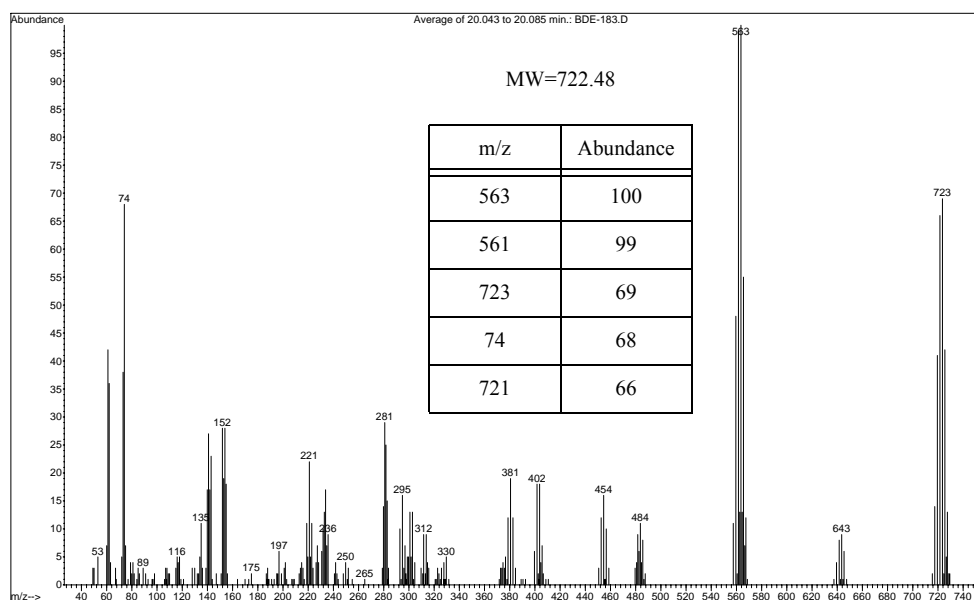
BDE-183 is a major component of the commercial octa-BDE, which is a complex mixture consisting typically of ~0.5% pentabromodiphenyl ether isomers, ~12% hexabromodiphenyl ether isomers, ~45% heptabromodiphenyl ether isomers, ~33% octaBDE isomers, ~10% nonabromodiphenyl ether isomers and ~0.7% decabromodiphenyl ether. It is used as a flame retardant in plastics for electrical and electronic equipment.

Regulatory Information

USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS, California Method 750-M and USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS.

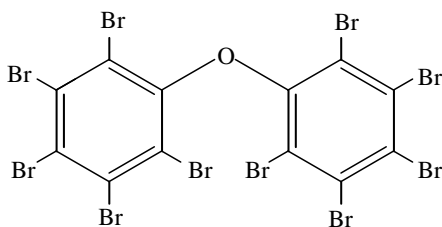
Toxicological and Environmental Data

Classified as a persistent organic pollutant, which can bioaccumulate through the food web, and pose a risk of causing adverse effects to human health and the environment. BDE-154 is one of the main PBDE congeners found in both environmental samples and human tissue, and is undergoing considerable research.



For Chromatogram See Appendix A - BDE-183 - page 401

Decabromodiphenyl ether



CAS Number 1163-19-5

RTECS Number KN3525000

Abbreviation

Formula $C_{12}Br_{10}O$

Molecular Weight 959.22

Chemical Name

decabromodiphenyl ether

Synonyms

BDE-209

Usage

Deca-BDE is the most common of all the commercial BDE flame retardants. The commercial Deca is generally 95% or more of the BDE-209 congener. It is primarily used as a flame retardant in the hard, dense plastics of consumer electronics products and in the latex back coating of flame retardant upholstery textiles. It can be found in many different polymers including polycarbonates, polyesters, polyolefins, ABS, Polyamides, PVC and rubbers.

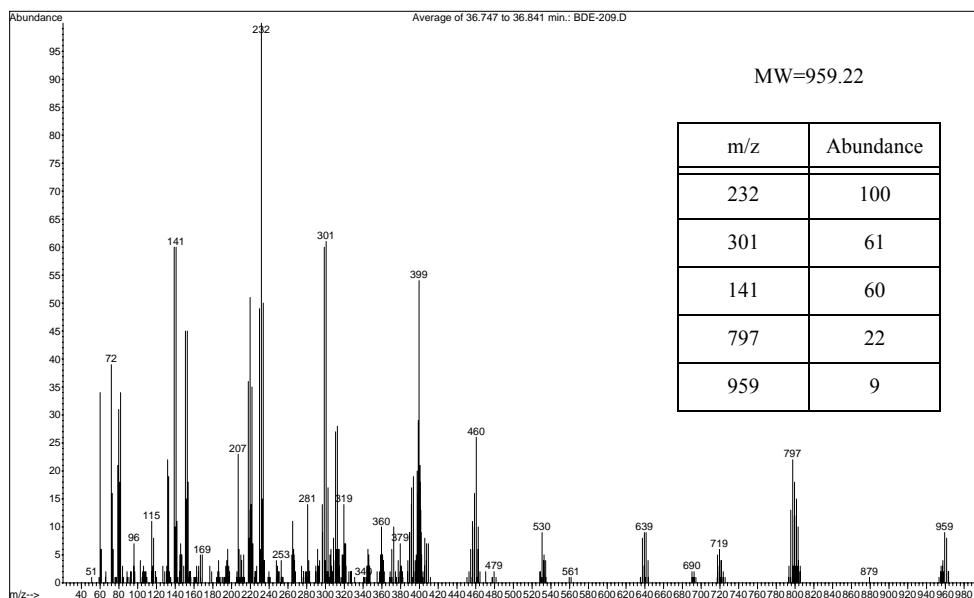
Regulatory Information

USEPA Method 1614 Brominated diphenyl ethers in water, soil, sediment, and tissue by HRGC/HRMS. BDE-209 Regulated RoHS/WEEE Regulations (2002/95/EC). Deca-BDE monitored under EU Directive 2000/60/EC as an endocrine disruptor. Included in ISO 22032:2006 Determination of selected polybrominated diphenyl ethers in sediment and sewage sludge using extraction and GC/MS.

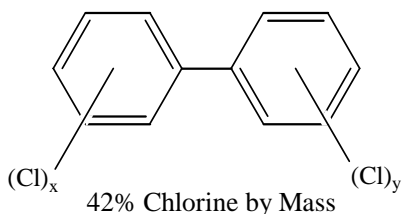
Toxicological and Environmental Data

RTECS CLASS OF COMPOUND: Tumorigen; Reproductive Effector; Primary Irritant.

Acute Oral Toxicity (LD50): 2 gm/kg [Rat], Acute Dermal Toxicity (LD50): 2 gm/kg/24H [Rabbit].



For Chromatogram See Appendix A - BDE-209 - page 402

Aroclor 1242**Monsanto****CAS Number** 53469-21-9**RTECS Number** TQ1356000**Abbreviation****Formula** Technical mixture**Molecular Weight** Not applicable**Chemical Name**

Not applicable

Synonyms

chlorodiphenyl (42% Cl)

Usage

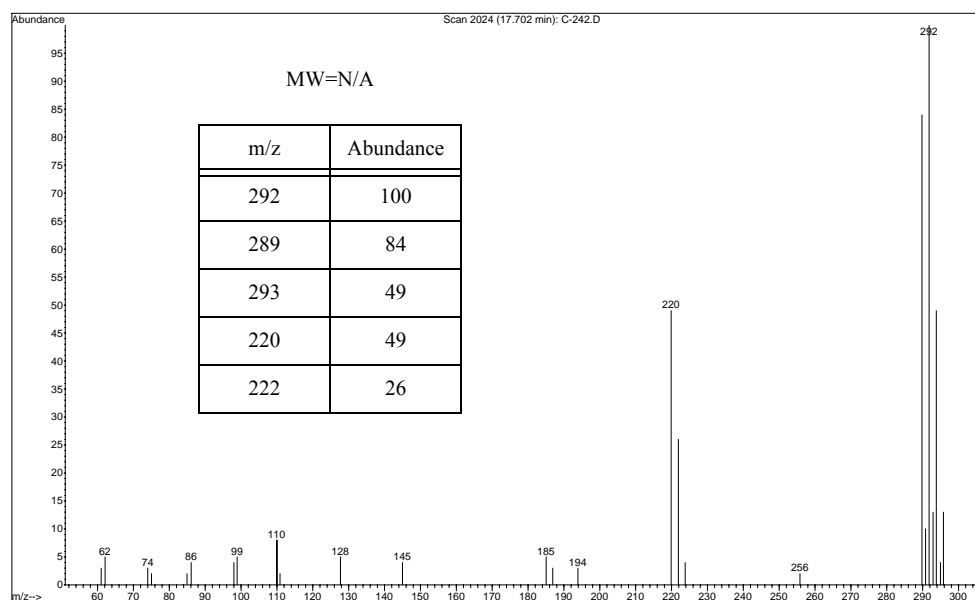
Used in electrical capacitors, electrical transformers, vacuum pumps, and gas-transmission turbines. Formerly used as heat transfer fluid, hydraulic fluids, rubber plasticizer, and in carbonless paper, adhesives and wax extenders. Although the production and sale was discontinued in late 1977, it is still present in transformers and capacitors now in use.

Regulatory Information

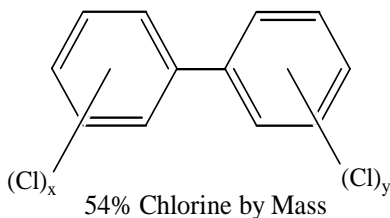
Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 milligrams of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills or accidental releases of 1 pound or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry and red meat contain no more than 0.2-3 parts of PCBs per million parts (0.2-3 ppm) of food.

Toxicological and Environmental Data

PCB's do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-242 - page 403

Aroclor 1254**Monsanto****CAS Number** 11097-69-1**RTECS Number** TQ1360000**Abbreviation****Formula** Technical mixture**Molecular Weight** Not applicable**Chemical Name**

Not applicable

Synonyms

chlorodiphenyl (54% Cl)

Usage

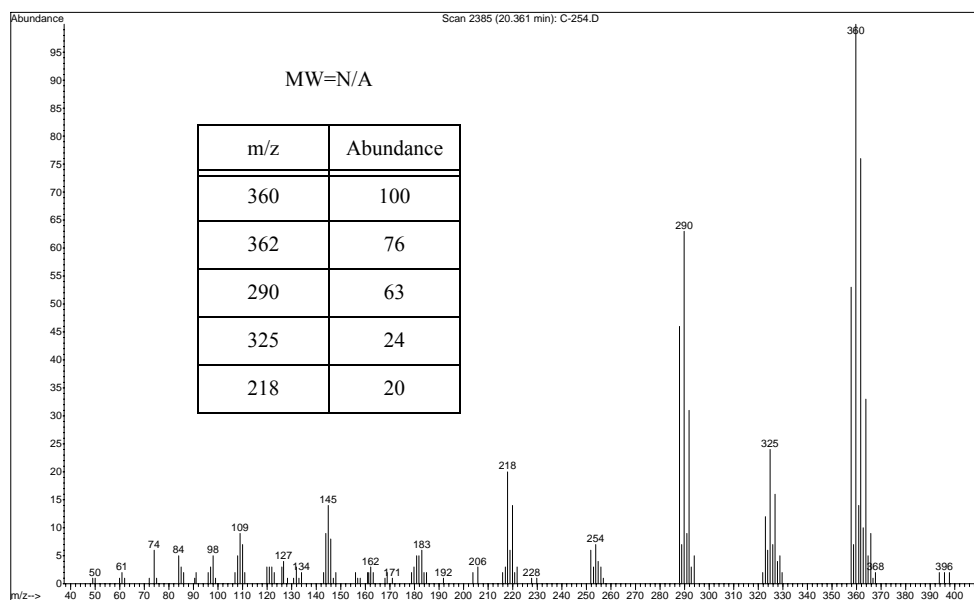
Formerly used in hydraulic fluid, rubber plasticizers, synthetic resin plasticizers, adhesives, wax extenders, dedusting agents, inks, cutting oils, pesticide extenders, sealants and caulking compounds. Although the production and sales was discontinued in late 1977, it is still present in transformers now in use, as well as in electrical capacitors, electrical transformers, vacuum pumps and gas-transmission turbines.

Regulatory Information

Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 milligrams of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills or accidental releases of 1 pound or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry and red meat contain no more than 0.2-3 parts of PCBs per million parts (0.2-3 ppm) of food.

Toxicological and Environmental Data

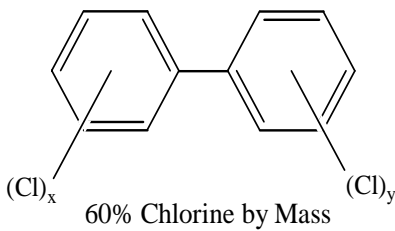
PCB's do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-254 - page 404

Aroclor 1260

Monsanto



CAS Number 53469-21-9
RTECS Number TQ1356000
Abbreviation

Formula Technical mixture
Molecular Weight Not applicable

Chemical Name
Not applicable

Synonyms
chlorodiphenyl (42% Cl)

Usage

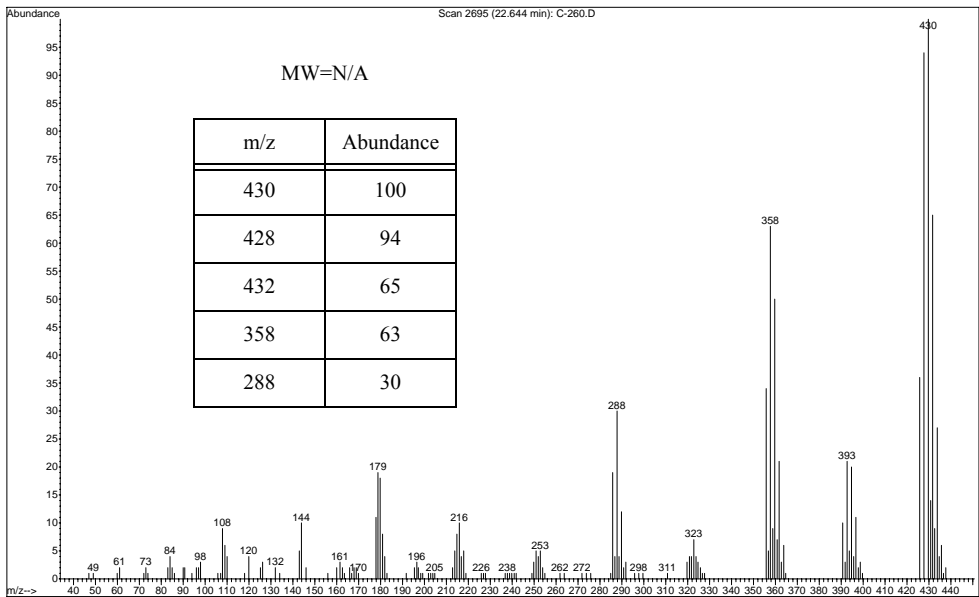
Used in electrical capacitors, electrical transformers, vacuum pumps, and gas-transmission turbines. Formerly used as heat transfer fluid, hydraulic fluids, rubber plasticizer, and in carbonless paper, adhesives and wax extenders. Although the production and sale was discontinued in late 1977, it is still present in transformers and capacitors now in use.

Regulatory Information

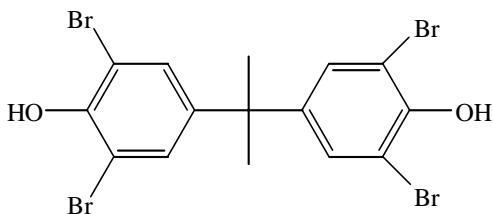
Section 6(e) of the Toxic Substances Control Act (TSCA) prohibits the manufacture, processing, and distribution in commerce of PCBs. In addition, the EPA has set a limit of 0.0005 milligrams of PCBs per liter of drinking water (0.0005 mg/L). Discharges, spills or accidental releases of 1 pound or more of PCBs into the environment must be reported to the EPA. The Food and Drug Administration (FDA) requires that infant foods, eggs, milk and other dairy products, fish and shellfish, poultry and red meat contain no more than 0.2-3 parts of PCBs per million parts (0.2-3 ppm) of food.

Toxicological and Environmental Data

PCB's do not readily break down in the environment and thus may remain there for very long periods of time. PCBs can travel long distances in the air and be deposited in areas far away from where they were released. In water, a small amount of PCBs may remain dissolved, but most stick to organic particles and bottom sediments. PCBs also bind strongly to soil. PCBs are taken up by small organisms and fish in water and accumulate up the food chain in fish and marine mammals.



For Chromatogram See Appendix A - C-260 - page 405

Firemaster BP4A**CAS Number** 79-94-7**RTECS Number** SM0894500**Abbreviation** TBBPA**Formula** C₁₅H₁₂Br₄O₂**Molecular Weight** 543.91**Chemical Name**

4,4'-(1-methylethylidene)bis(2,6-dibromophenol)

Synonyms

bromdian; Fireguard 2000; 2,2',6,6'-Tetrabromobisphenol A; 3,3',5,5'-Tetrabromobisphenol A; Tetrabromodiphenylpropane; Tetrabromodian

Usage

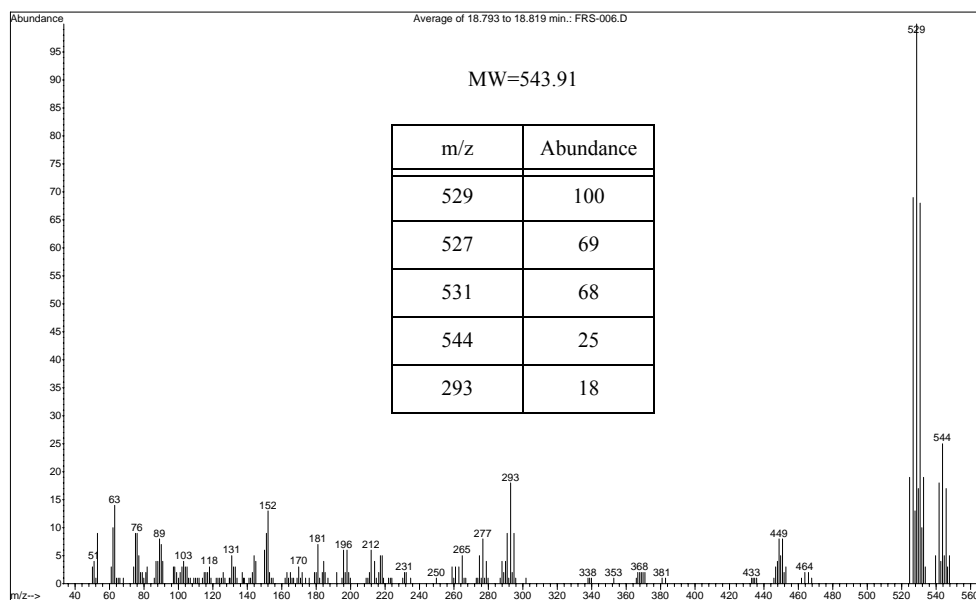
The primary use of TBBPA is as a flame retardant in epoxy resin circuit boards and in electronic enclosures made of polycarbonate-acrylonitrile-butadiene-styrene (PC-ABS). Other applications of TBBPA include its use as a flame retardant for plastics, paper, and textiles; as a plasticizer; in adhesives and coatings; and as a chemical intermediate for the synthesis of other flame retardants (e.g., TBBPA allyl ether). It is also been applied to carpeting and office furniture as a flame retardant.

Regulatory Information

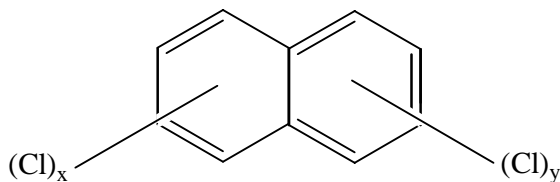
There are currently no legislative restrictions on the use of TBBPA.

Toxicological and Environmental Data

TBBPA enters waste streams from production of circuit boards and other applications and enters the environment via disposal of products containing TBBPA. RTECS CLASS OF COMPOUND: Reproductive Effector; Primary Irritant
Lowest Published Toxic Oral Dose (TDLo): 250 mg/kg (6-15D preg) [Rat].



For Chromatogram See Appendix A - FRS-006 - page 406

Halowax 1001**CAS Number** 58718-67-5**RTECS Number** Not available**Abbreviation****Formula** Technical mixture**Molecular Weight** ~255**Chemical Name**

polychlorinated naphthalene 1001

Synonyms**Usage**

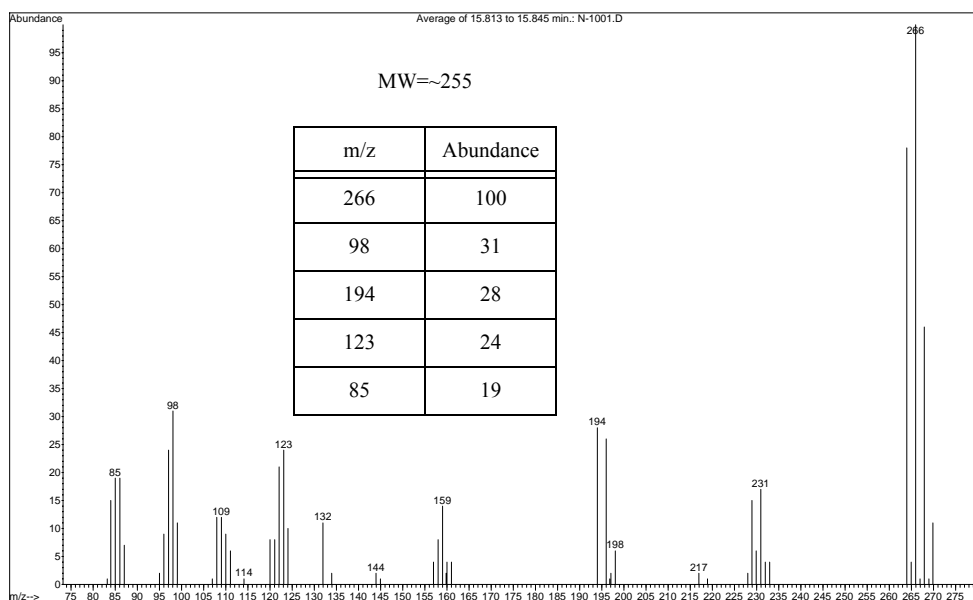
Used as paper impregnant in automobile capacitors (dielectrics). Electrical insulation and fire-resisting materials; impregnants; sealing compounds; crankcase additive; ingredient in penetrating oils; plasticizer; protective coatings.

Regulatory Information

Regulated by the EPA under the Clean Water Act (CWA), and the Clean Air Act.

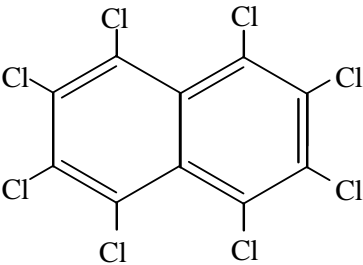
Toxicological and Environmental Data

Chlorinated naphthalenes (CN) are persistent environmental contaminants, which accumulate and biomagnify in human and wildlife food-chains. Many of the CN congeners show relatively high dioxin-like activity and have been identified as common food contaminants, especially in fish.



For Chromatogram See Appendix A - N-1001 - page 407

Halowax 1051



CAS Number 2234-13-1
RTECS Number QK0250000
Abbreviation

Formula Technical mixture
Molecular Weight 403.73

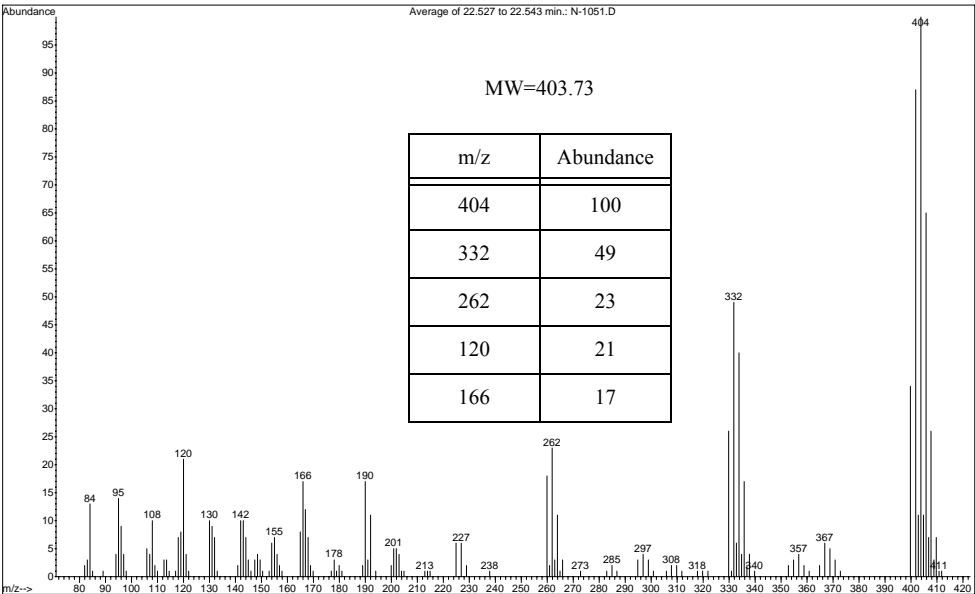
Chemical Name
octachloronaphthalene

Synonyms
octachloronaphthalene; perchloronaphthalene; 1,2,3,4,5,6,7,8-octachloronaphthalene

Usage
Insulating material in capacitors and cable manufacturing. Halowax 1051 is a technical mixture, the octachloronaphthalene is the primary and target component.

Regulatory Information
Regulated by the EPA under the Clean Water Act (CWA), CERCLA and the Clean Air Act.

Toxicological and Environmental Data
Chlorinated naphthalenes are persistent environmental contaminants, which accumulate and biomagnify in human and wild-life food-chains.



For Chromatogram See Appendix A - Halowax 1051 - page 408

CHAPTER 8

Plasticizers

Plasticizers are one of the most important classes of additives. These are the additives that give the plastics flexibility and durability. Most of these additives are used in PVC, which is in turn used in a wide variety of compounds ranging from plumbing and construction materials to plastic bottles. Unfortunately, since the additives are not reacted into the polymer, they can migrate to the surface of the finished plastic product and then evaporate or leach into the surrounding environment. This disadvantage for use is an advantage for analysis, because these plasticizers are easily desorbed from the base polymer.

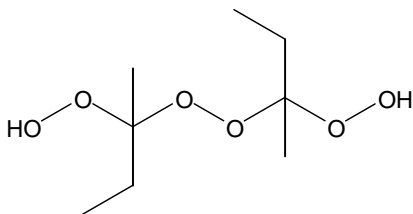
Just as there is a wide variety of plastics, there is also a wide variety of plasticizers used to achieve a desired result. The requirements of a plasticizer are: compatibility, low extractability by water and solvents, stability to heat and light, good low-temperature properties, ease of processing, and low odor, taste and toxicity. Since no single plasticizer meets all of these requirements, blending of multiple plasticizers is often necessary to achieve the desired result in the final product.

The most commonly used plasticizers are the phthalates. This includes dioctyl phthalate, (DEHP), diisodecyl phthalate, diisononyl phthalate and a number of other phthalate esters. Concerns about possible carcinogenetic effects have lead to a steady decrease in the use of phthalates.

Epoxidized oils such as soybean, linseed and tall oil fatty acids are also used as plasticizers. While they don't pose the same health risks as the phthalates, they have limited compatibility with PVC and cannot be used at high temperatures.

Other plasticizers include adipates, azelates, sebacates and various polymeric plasticizers made from glycols and aliphatic dicarboxylic acids.

Growing public concern about the environment and the potential health risks associated with plastics has prompted extensive research into developing new and more health and environmentally friendly plasticizers.

2-Butanone peroxide (in DMP)

CAS Number 1338-23-4

RTECS Number EL9450000

Abbreviation BP

Formula $C_8H_{18}O_6$

Molecular Weight 210.22

Chemical Name

di(1-methylethylketone)peroxide

Synonyms

methyl ethyl ketone peroxide; di(1-methylpropylidene)diperoxide

Brand Names & ManufacturersButanox[®] LPT

Akzo Nobel Chemicals B.V.

Hi-Point[®] 90

Chemtura Corporation

Lupersol[®]

Arkema, Inc.

Physical Properties**Appearance** Colorless, oily liquid with a pleasant mint-like odor**Melting Point** <-30 °C**Boiling Point** Decomposes 68 °C**Stability** Stable at or below 38 °C (100 °F).

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	S	U	U	U	U	S

Application, Regulatory & Environmental Information**Application**

BP is an organic peroxide commercially available as a 40-60% solution in dimethyl phthalate (DMP) for the manufacture of acrylic resins, as a polymerization initiator and curing agent for unsaturated polyester resins, and as a hardening agent for fiberglass reinforced plastics. The commercially available material is generally believed to be the MEK peroxide dimer (above), the monomer is $C_4H_{10}O_4$ mw 122.12.

Regulatory Information

FDA 1998 regulates BP as an indirect food additive. It is permitted as a catalyst not exceeding 2% of the finished resin, and as an optional adjuvant in the production of cross-linked polyester resins intended for repeated use in contact with food 21CFR177.2420. EPA Reportable Quantity 10lbs. For MEK Peroxide ACGIH TLV (ceiling) 0.2 ppm (1.5 mg/m³) and OSHA PEL (ceiling) of 0.7 ppm (5 mg/m³).

Environmental Impact

Has been identified by the EPA as a chemical likely to leach dangerous concentrations of toxic chemicals into ground water. Also classified as a toxic air contaminant.

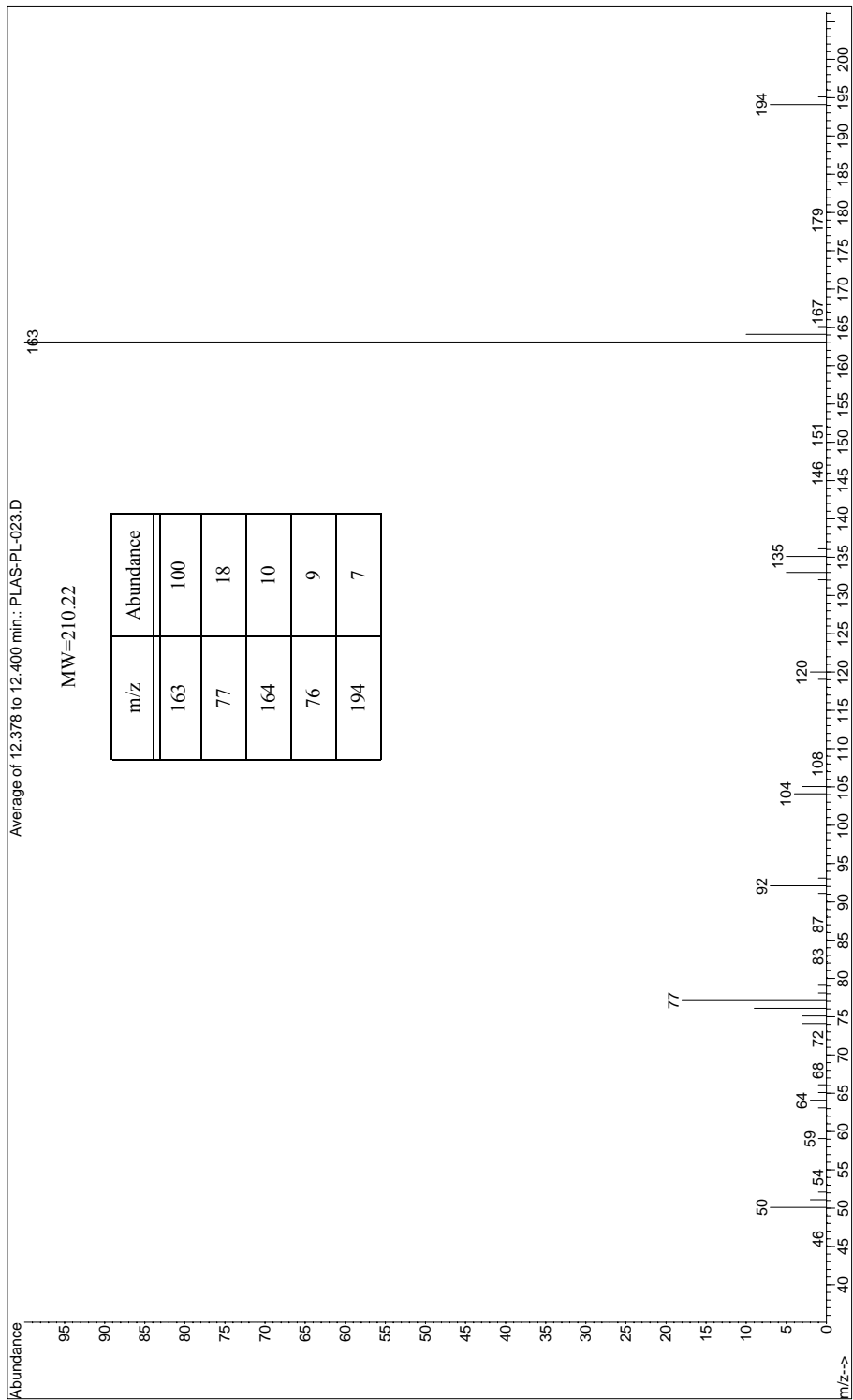
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

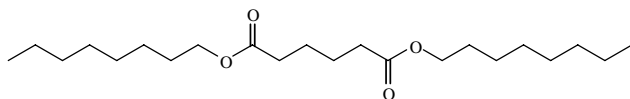
Human ingestion of 50 mL of 60% BP/40% cyclohexanone and DMP solution was fatal. LD50: 470-484 mg/kg BW [Rat], 260 mg/kg [Mouse], BP's toxicity is observed to be GI tract bleeding, abdominal burns, necrosis, perforation of stomach, stricture of esophagus, severe metabolic acidosis, hepatic failure, and respiratory insufficiency. Mice surviving a 7 mg dose of BP developed malignant tumors including subcutaneous sarcoma, malignant lymphomas, and pulmonary adenoma.

Mass Spectrum for 2-Butanone peroxide (in DMP) - PLAS-PL-023



Adimoll DO

Lanxess

**CAS Number** 123-79-5**RTECS Number** Not available**Abbreviation****Formula** C₂₂H₄₂O₄**Molecular Weight** 370.57**Chemical Name**

hexanedioic acid, dioctyl ester

Synonyms

di-N-octyl adipate; dioctyl hexanedioate; bis(2-ethylhexyl) hexanedioate; dicaprylyl adipate; adipic acid, dioctyl ester

Brand Names & Manufacturers

Jayflex® DOA

ExxonMobil

Kodaflex® DOA

Eastman Chemical

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** -70.0 °C**Boiling Point** 215 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application, Regulatory & Environmental Information

Application
Adimoll® DO is a low-temperature-resistant plasticizer suitable for a large number of polymers, e.g. polyvinyl chloride (PVC), acrylonitrile-butadiene rubber (NBR), styrenebutadiene rubber (SBR) and polyvinyl acetate (PVAC). Commonly used in plastic wraps for food storage.

Regulatory Information

Adimoll DO can be used when regulations and recommendations governing food contact applications need to be met. The FDA has approved this material to be used to make plastic packaging as indirect food additives (substances which may come in contact with food as part of packaging or processing equipment but are not intended to be added directly to food).

Environmental Impact

If released into the environment, this material is expected to partition into the soil and sediment. It has a high potential to bioaccumulate. Not considered to be a source of air pollution.

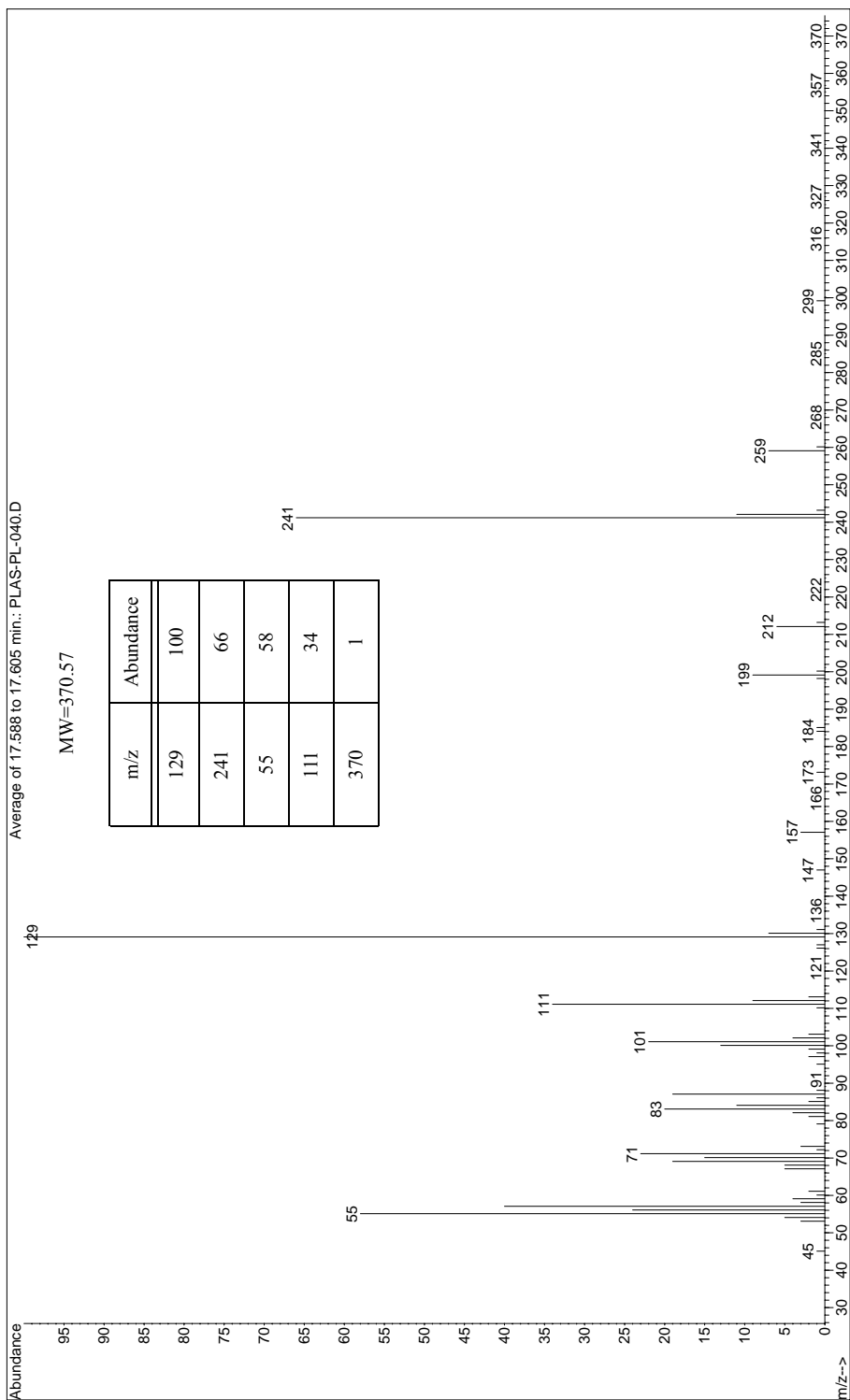
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products. Migrates into fatty foods with fat percentages >35%.

Toxicological Data

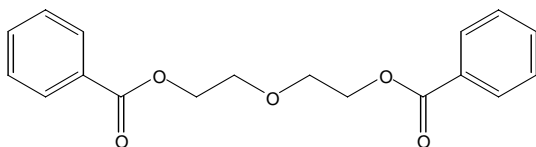
Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Adimoll DO - PLAS-PL-040



Benzoflex® 2-45

Velsicol Chemical Corporation

**CAS Number** 120-55-8**RTECS Number** ID6650000**Abbreviation** DEGDB**Formula** C₁₈H₁₈O₅**Molecular Weight** 314.33**Chemical Name**

diethylene glycol, dibenzoate

Synonyms

benzoic acid, diester with diethylene glycol; dibenzoyldiethyleneglycol ester; benzoyloxyethoxyethyl benzoate

Brand Names & Manufacturers

K-Flex® DE

Emerald Kalama Chemical, LLC

Physical Properties**Appearance** Liquid**Melting Point** 28 °C**Boiling Point** 236 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	1-10	1-10	1-10

Application, Regulatory & Environmental Information**Application**

Used as a plasticizing agent for cellulose acetate butyrate. Used in the production of food contact cellulose nitrate resins, ethyl cellulose resins, PMMA resins, and polyvinyl acetate.

Regulatory Information

FDA approved as a component of adhesives for use in contact with food, 21CFR175.105; a component of the uncoated or coated food surface of paper and paperboard intended for use in producing, manufacturing, packaging, processing, preparing, treating, packing, transporting, or holding dry, aqueous, and fatty foods, 21CFR176.170 and 21CFR176.180.

Environmental Impact

No Observed Effect Level: 1000 ppm, earthworm. (EC50): >10 mg/L, [Bacteria] (*Pseudomonas putida*); No inhibitory effect on the respiration rate of activated sludge at concentrations up to 100 mg/L. Considered ultimately biodegradable under anaerobic conditions in the biogas production test. European labeling: R52/53 - Harmful to aquatic organisms, may cause long-term adverse effects in the aquatic environment; S61 - Avoid release to the environment.

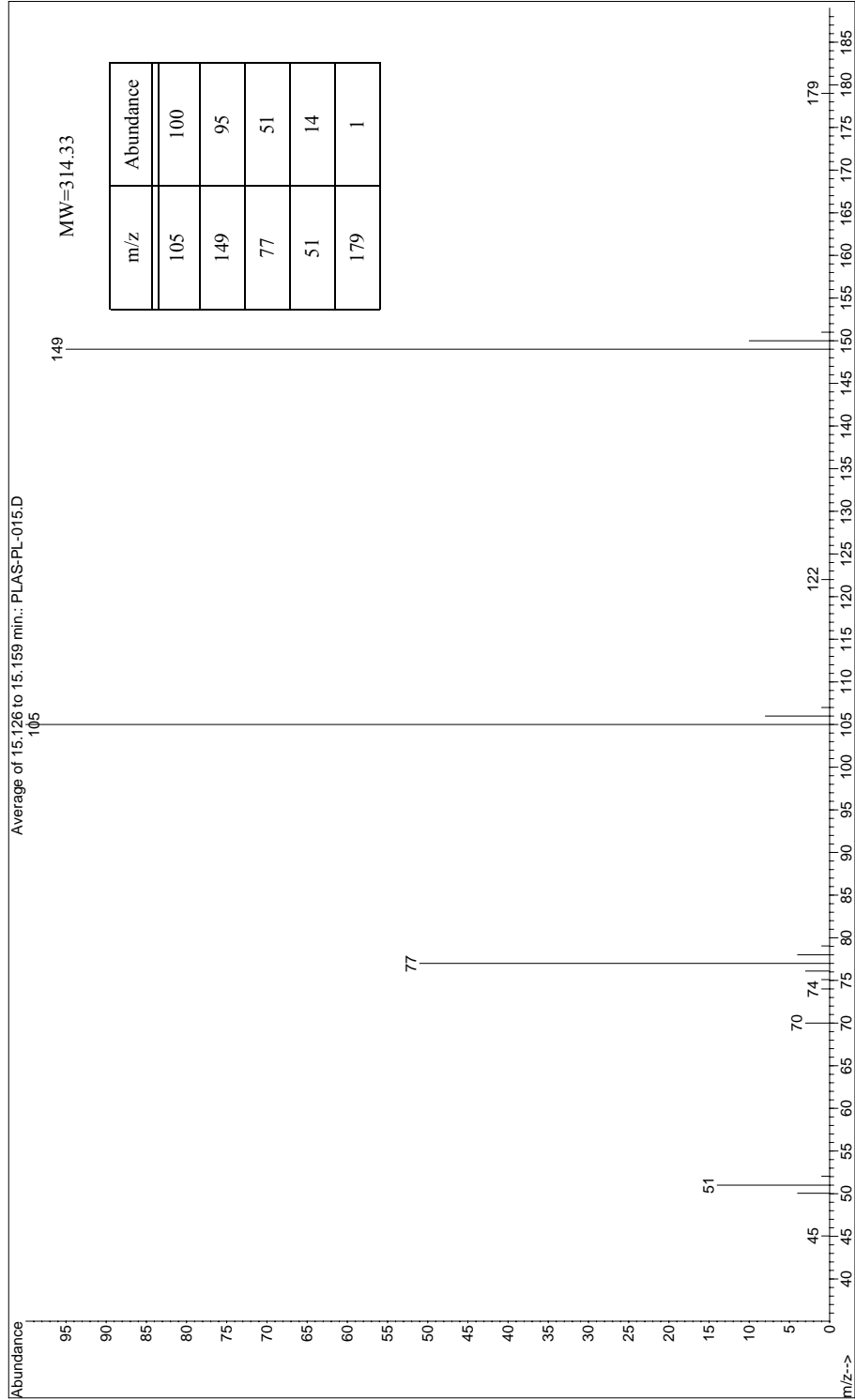
Point of Release

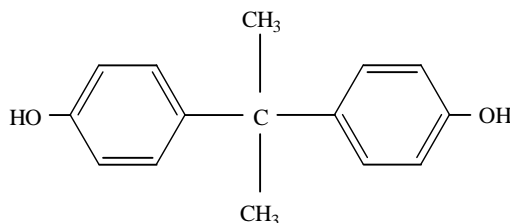
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Decreased body weight gain and blood, spleen and caecum effects were reported in rats given up to 2500 mg/kg/day DEGBD in their diet for 13 weeks. Acute dermal toxicity (LD50): 20 mL/kg [Rabbit]; Acute oral (LD50): 2,830-4,190 mg/kg [Rat]; Acute Dermal (LD50): > 2000 mg/kg [Rat].

Mass Spectrum for Benzoflex® 2-45 - PLAS-PL-015



Bisphenol A

CAS Number 80-05-7

RTECS Number SL6300000

Abbreviation BPA

Formula $C_{15}H_{16}O_2$

Molecular Weight 228.29

Chemical Name

4,4'-dihydroxy-2,2-diphenylpropane

Synonyms

4,4'-(propan-2-ylidene)diphenol; p,p'-isopropylidenebisphenol; 2,2-bis(4-hydroxyphenyl)propane

Brand Names & Manufacturers**Physical Properties**

Appearance	White to light brown flakes or powder					
Melting Point	157 °C			Boiling Point 220 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information**Application**

Originally synthesized in 1891 and was investigated in the 1930s as a possible synthetic estrogen. Currently, the primary use is in the manufacture of polycarbonate plastics and epoxy resins for coatings on metal cans to maintain the quality of canned food and beverages. Also used as a thermal stabilizer in PVC compounds and as a dental sealant.

Regulatory Information

FDA has approved the use of Bisphenol A as an component used to make polyarylate or 4,4'-Isopropylidenediphenol-epichlorohydrin resins to be used for single and repeated use food contact surfaces as outlined in 21CFR177, Parts 1440 and 1555. OSHA PEL in Shipyards ceiling concentration 0.5 ppm (2.8 mg/m³).

Environmental Impact

Real world monitoring studies show that BPA is rapidly biodegraded and extensively removed in wastewater treatment systems. Studies using real world surface water samples taken from various geographies demonstrate rapid degradation with a half-life in the range of 1 to 4 days. Bisphenol A does not accumulate in aquatic organisms to any appreciable extent and is not classified as bioaccumulative by the USEPA.

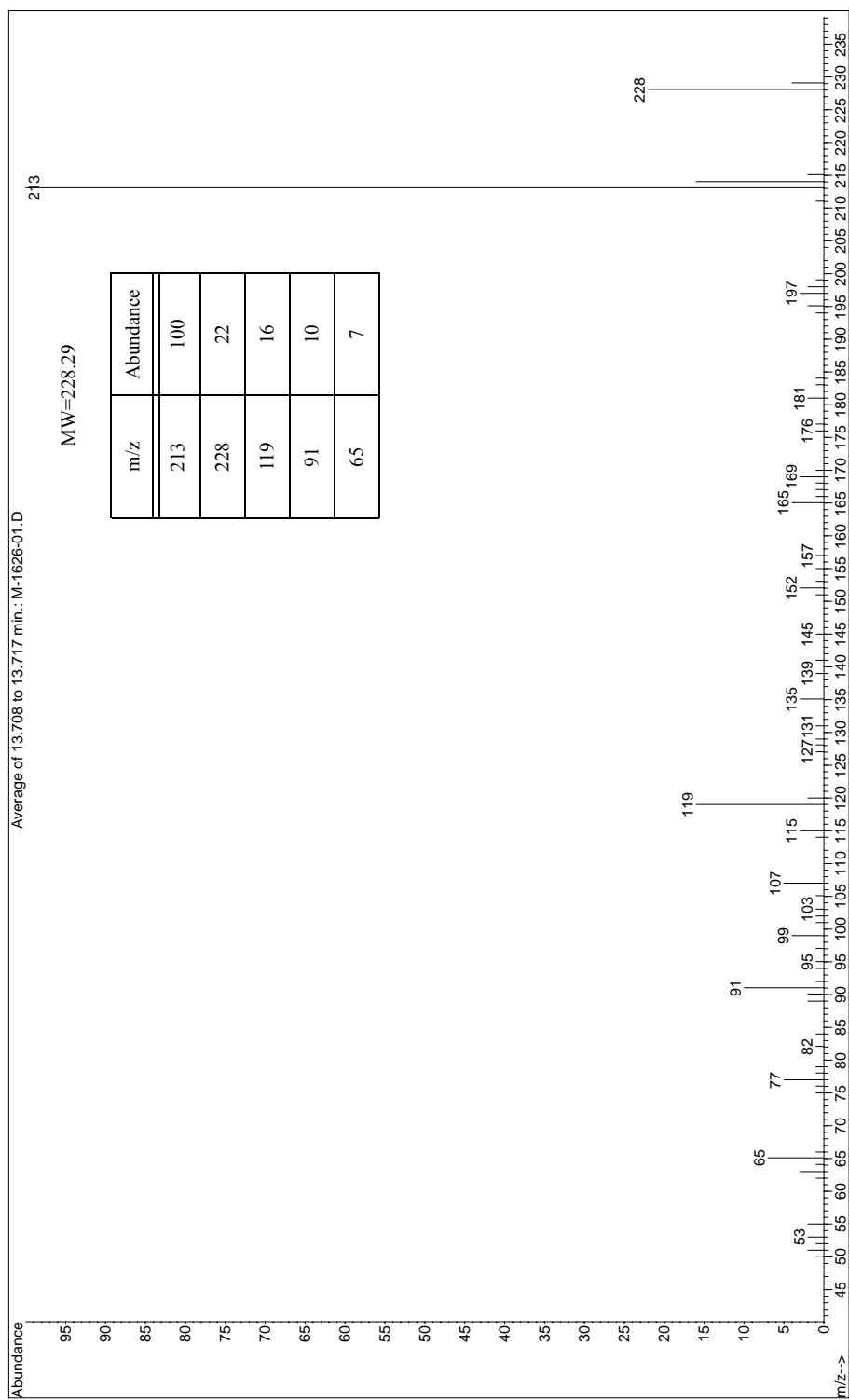
Point of Release

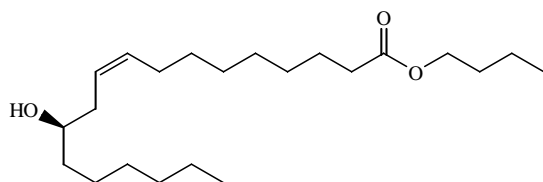
Low levels may be released to the environment in the effluent water from biological wastewater treatment plants. Scientists have known for many years that the polycarbonate bond created by BPA is unstable and that the chemical will eventually leach into food or beverages in contact with the plastic. The obvious concern today is that it may leach into food products, ranging from microwavable dinners to baby formula, that are packaged in polycarbonate plastic.

Toxicological Data

RTECS CLASS OF COMPOUND: Tumorigen; Hormone; Mutagen; Human Data; Primary Irritant; Reproductive Effector. Acute Oral Toxicity (LD50): 3250 mg/kg [Rat]; Acute Dermal Toxicity (LD50): 3 mL/kg [Rabbit]; Lowest Published Toxic Oral Dose (TDLo): 1000 mg/kg [Rat].

Mass Spectrum for Bisphenol A - M-1626-01



Butyl ricinoleate

CAS Number 151-13-3

RTECS Number Not available

Abbreviation

Formula $C_{22}H_{42}O_3$

Molecular Weight 354.57

Chemical Name

12-hydroxy-9-octadecenoic acid, butyl ester

Synonyms

butyl ricinoleate; ricinolic acid butyl ester

Brand Names & Manufacturers

Flexricin® P-3

G.R. O'Shea/Vertellus

Physical Properties**Appearance** Yellow to colorless liquid**Melting Point** -26 °C**Boiling Point** 275 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Butyl ricinoleate, is a plasticizer for polyvinyl butyral, rosin, vinsol resin, and cellulose acetate butyrate resins. Can also be used as a general purpose plasticizer for both nitrocellulose and ethylcellulose.

Regulatory Information

FDA approval under section 175.105 for use in adhesives with indirect food contact.

Environmental Impact

This chemical is expected to readily biodegrade. If released into the environment it is expected to partition to sediment.

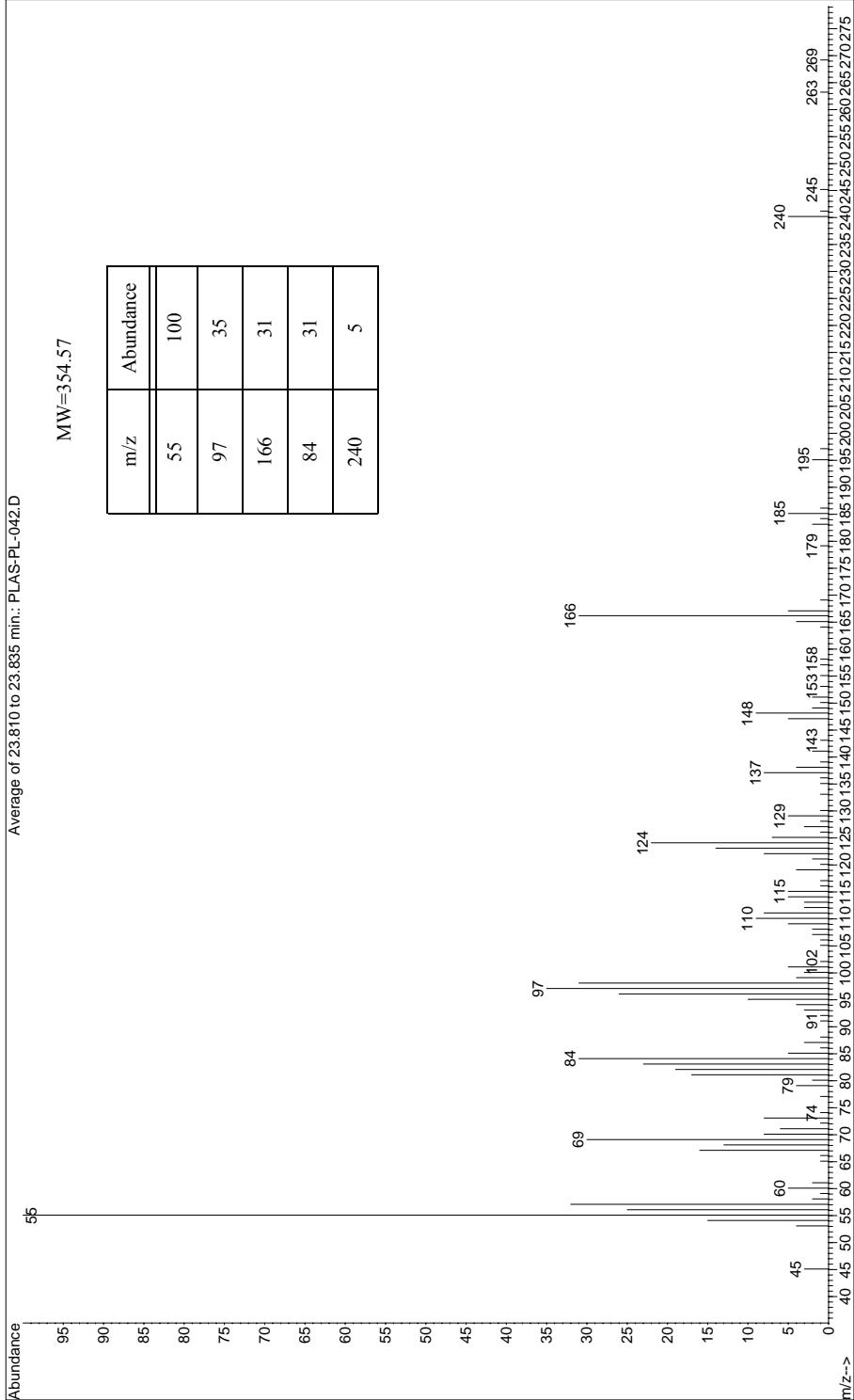
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

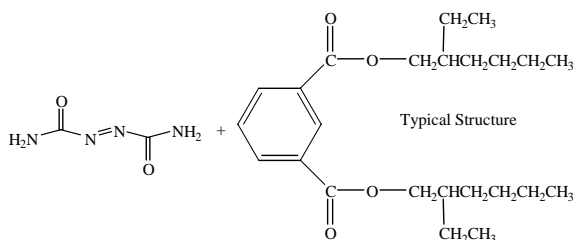
Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Butyl ricinoleate - PLAS-PL-042



Celogen® SD-125

Chemtura Corporation



CAS Number Not available

RTECS Number Not available

Abbreviation

Formula Not applicable

Molecular Weight Not applicable

Chemical Name

50% azodicarbonamide in a phthalate plasticizer

Synonyms

Brand Names & Manufacturers

Physical Properties

Appearance	Viscous, yellow liquid					
Melting Point	190-220°C		Boiling Point		Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water <0.1	MeOH <0.1	EtOH <0.1	Acetone <0.1	CH₂Cl₂ <0.1	Hexane <0.1

Application, Regulatory & Environmental Information**Application**

Celogen® SD dispersions eliminate dust, improve dispersability in PVC plastisols, and may be metered directly into the manufacturing process. May be found in sponge rubber and expanded plastics.

Regulatory Information

FDA approved under 21CFR175.300 - Resinous and Polymeric Coatings, limited to can end cement, 177.1210 - Closures with Sealing Gaskets for Food Containers (limitation - 2% Max.), and 177.2600 - Rubber Articles Intended for Repeated Use, (limitation - 5% Max.).

Environmental Impact

Degradation of azodicarbonamide by sewage sludge organisms has been investigated in three modified Sturm tests. The compound was "readily biodegradable" in two out of the three tests and was degraded by 21% over 30 days in the third test. According to Mackay Level I fugacity modelling, azodicarbonamide released to surface waters will partition to the hydrosphere with no significant sorption to particulates.

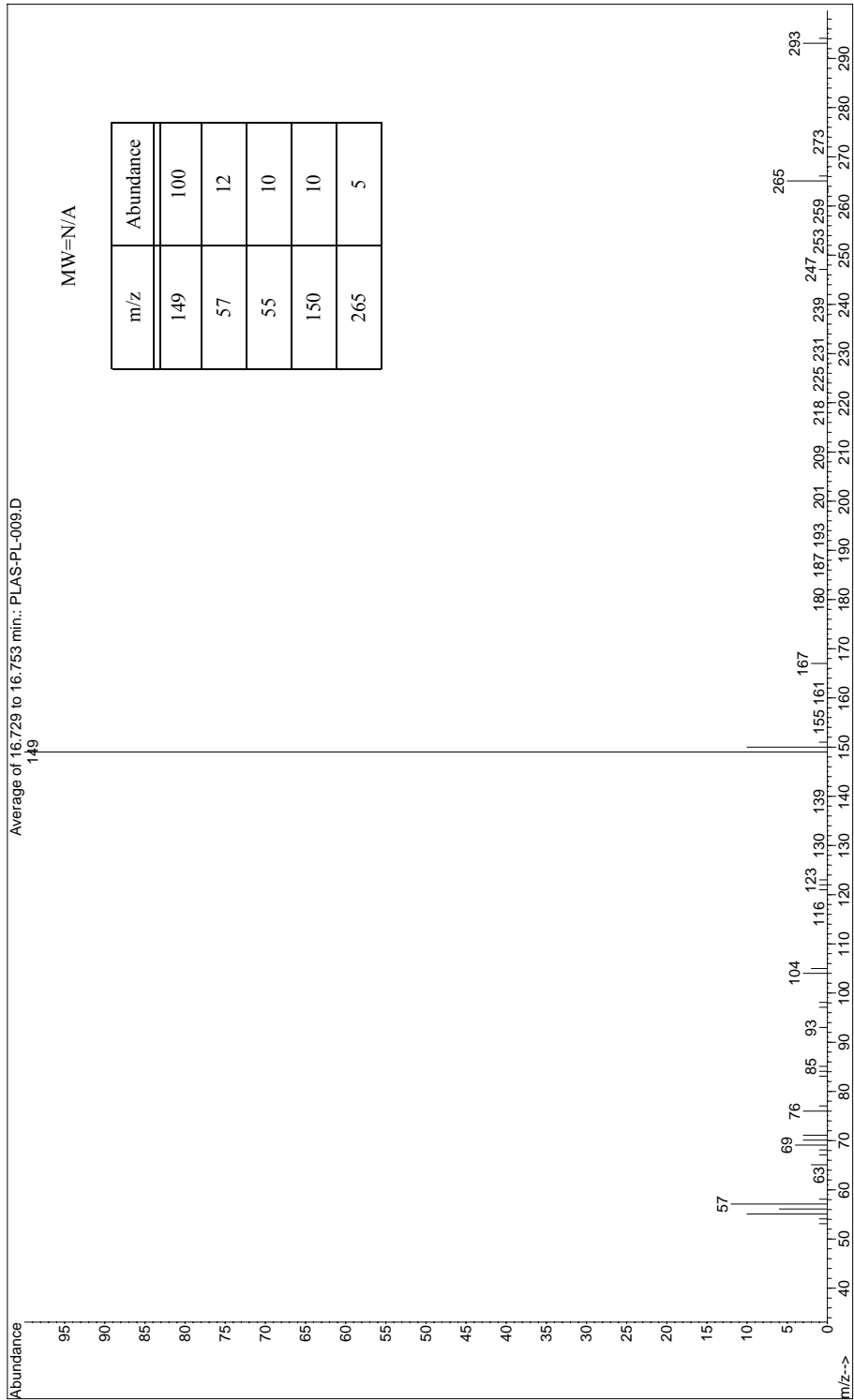
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

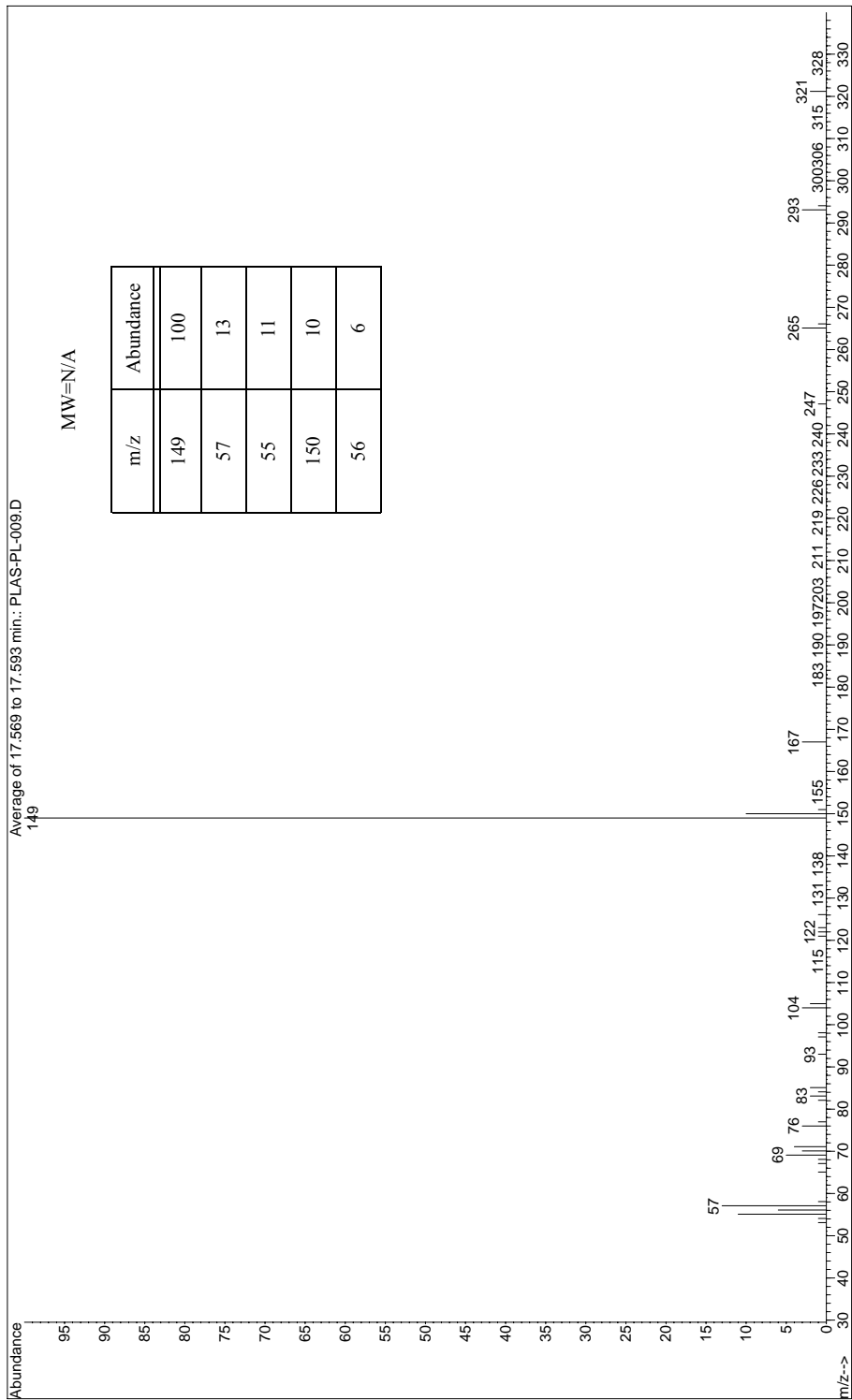
Toxicological Data

Studies in humans have concentrated solely on the ability of azodicarbonamide to induce asthma and skin sensitization. Evidence that azodicarbonamide can induce asthma in humans has been found from bronchial challenge studies with symptomatic individuals and from health evaluations of employees at workplaces where azodicarbonamide is manufactured or used. There are also indications that azodicarbonamide may induce skin sensitization.

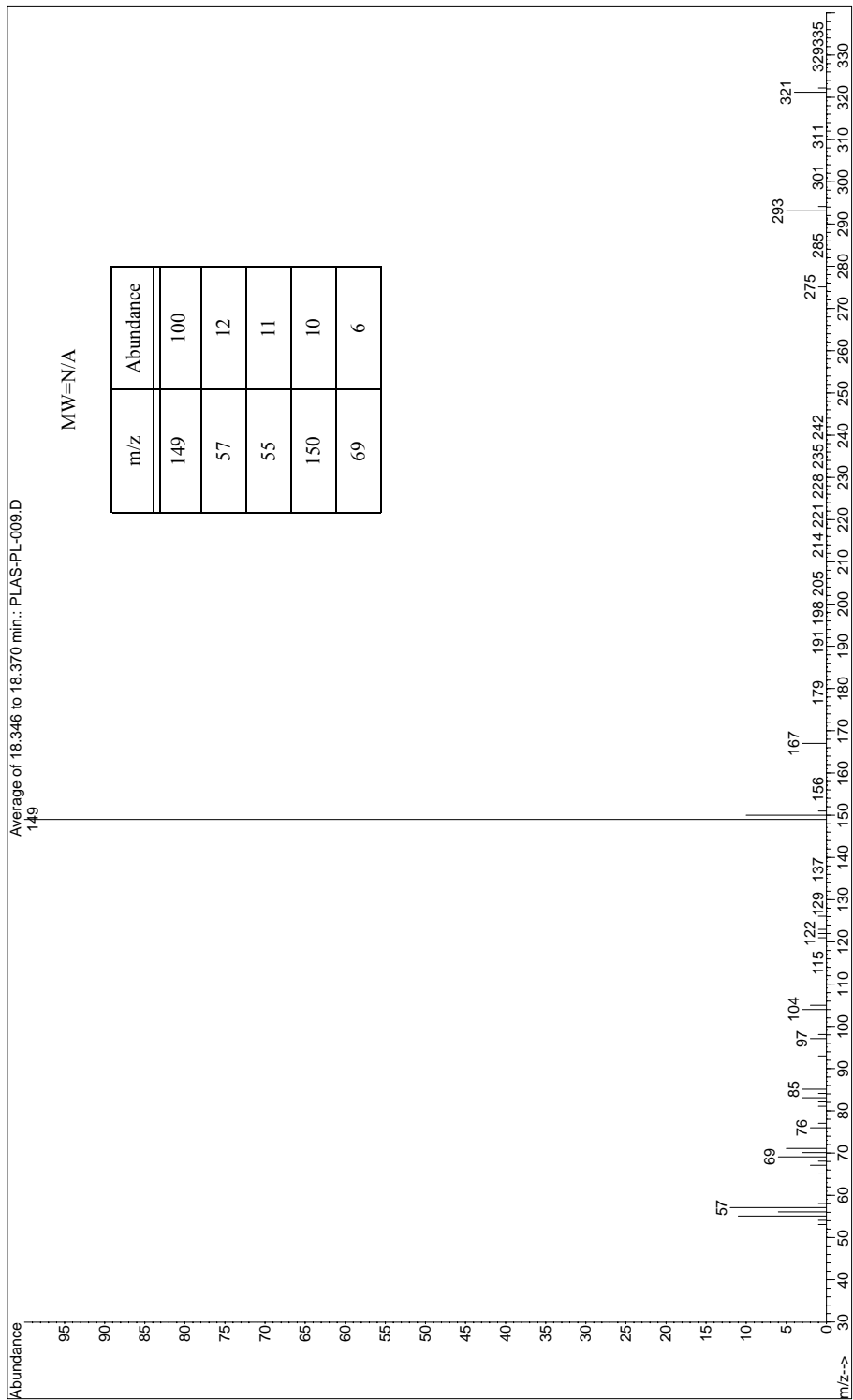
Mass Spectrum for Celogen® SD-125 - PLAS-PL-009



Mass Spectrum for Celogen® SD-125 - PLAS-PL-009

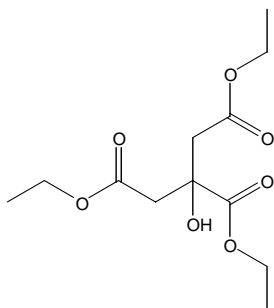


Mass Spectrum for Celogen® SD-125 - PLAS-PL-009



Citroflex® 2

Morflex, Inc.

**CAS Number** 77-93-0**RTECS Number** GE8050000**Abbreviation** TEC**Formula** C₁₂H₂₀O₇**Molecular Weight** 276.32**Chemical Name**

2-hydroxy-1,2,3-propanetricarboxylic acid, triethyl ester

Synonyms

Citric acid, triethyl ester; triethyl citrate

Brand Names & Manufacturers**Physical Properties**

Appearance	Colorless liquid					
Melting Point	-46.00 °C @ 760.00 mm			Boiling Point	127.00 °C @ 1.00 mm	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water 5.5	MeOH U	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information**Application**

TEC is used as a plasticizer that does not support fungal growth for cellulose derivatives (e.g. cellulose citrate), and polyvinyl acetate, as well as natural resins such as dammar and ester gums. It is also used as a fixing agent in perfumes and as a film strengthening agent in hair sprays, nail polish and as an active ingredient in deodorants.

Regulatory Information

FDA approved 1998 for manufacturing of resinous and polymeric coatings for food-contact surface articles 21CFR175.300 and as a plasticizer in resinous and polymeric coatings for polyolefin films used in food-contact surface articles 21CFR175.320 for producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food. EU approved 1995 as a food additive in dried egg whites. Joint FAO/WHO committee on Food Additives (1989) recommends ADI (Man): 10 mg/kg BW.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOC's), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

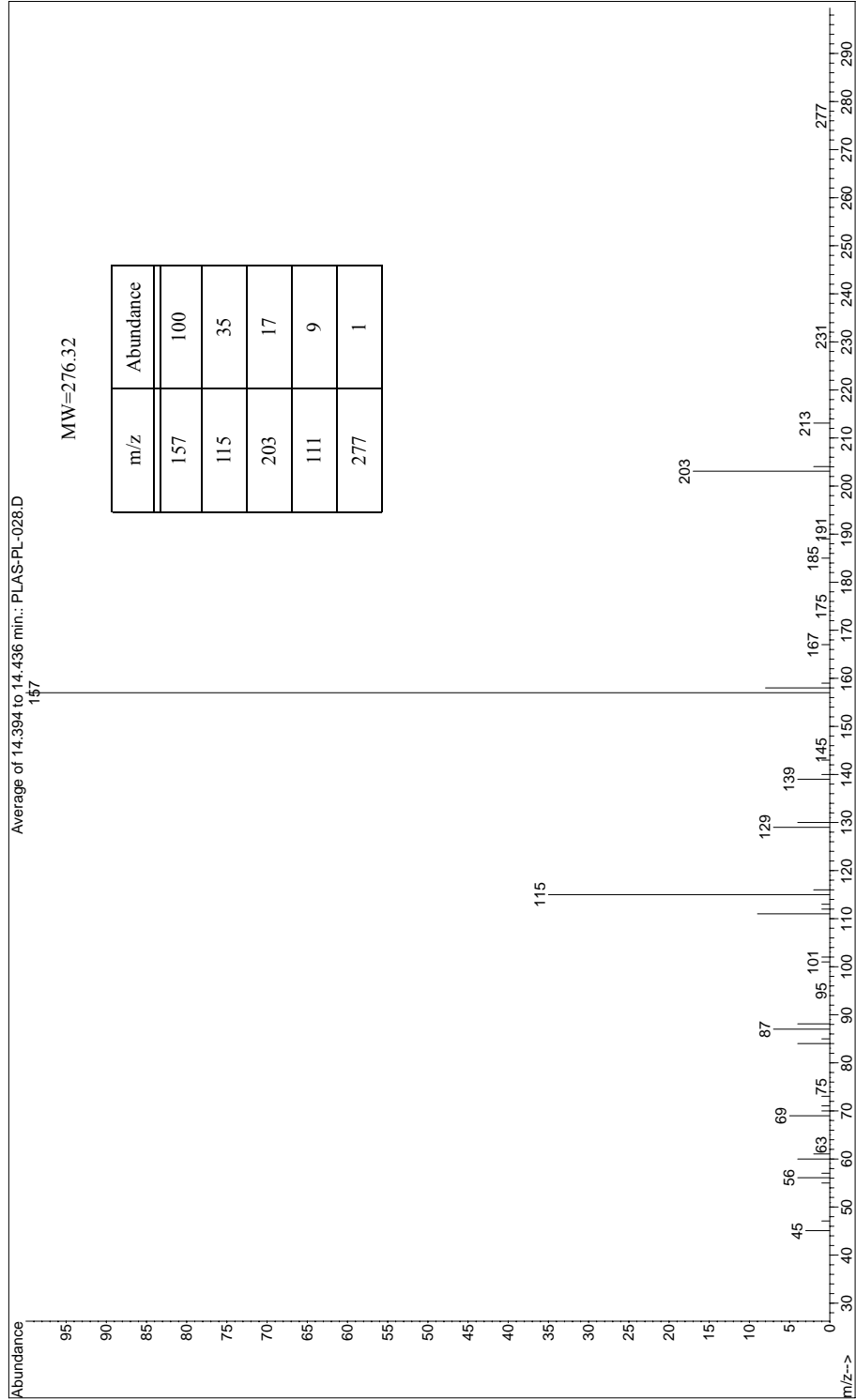
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

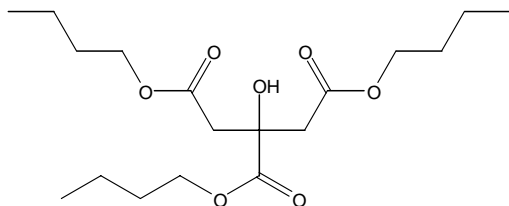
Toxic action of TEC may occur due to calcium binding in bodily fluids and a reduction of blood pressure. Acute oral toxicity (LD50): 5900 mg/kg [Rat], acute inhalation toxicity (LD50): 1300 ppm/6H [Rat], acute dermal toxicity (LD50): >5 g/kg [Rabbit].

Mass Spectrum for Citroflex® 2 - PLAS-PL-028



Citroflex[®] 4

Morflex, Inc.

**CAS Number** 77-94-1**RTECS Number** TZ8608000**Abbreviation** TBC**Formula** C₁₈H₃₂O₇**Molecular Weight** 360.45**Chemical Name**

2-Hydroxy-1,2,3-Propanetricarboxylic Acid, Tributyl Ester

Synonyms

butyl citrate; citric acid, tributyl ester; tributyl 2-hydroxy-1,2,3-propanetricarboxylate

Brand Names & Manufacturers

Physical Properties

Appearance	Clear, colorless, viscous liquid					
Melting Point	Not available		Boiling Point 322 °C			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane 40-80

Application Application, Regulatory & Environmental Information

TBC is used as a plasticizer that does not support fungal growth in cellulosic and vinyl resins (especially PVC), polyactic acid resins (as a biodegradable component), and furniture coatings. Also used as a solvent for nitrocellulose and lacquers intended for food contact applications. Additional applications include a defoaming agent in proteinaceous solutions.

Regulatory Information

FDA approved 1998 as a component of food contact adhesives to be used safely as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOC's), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

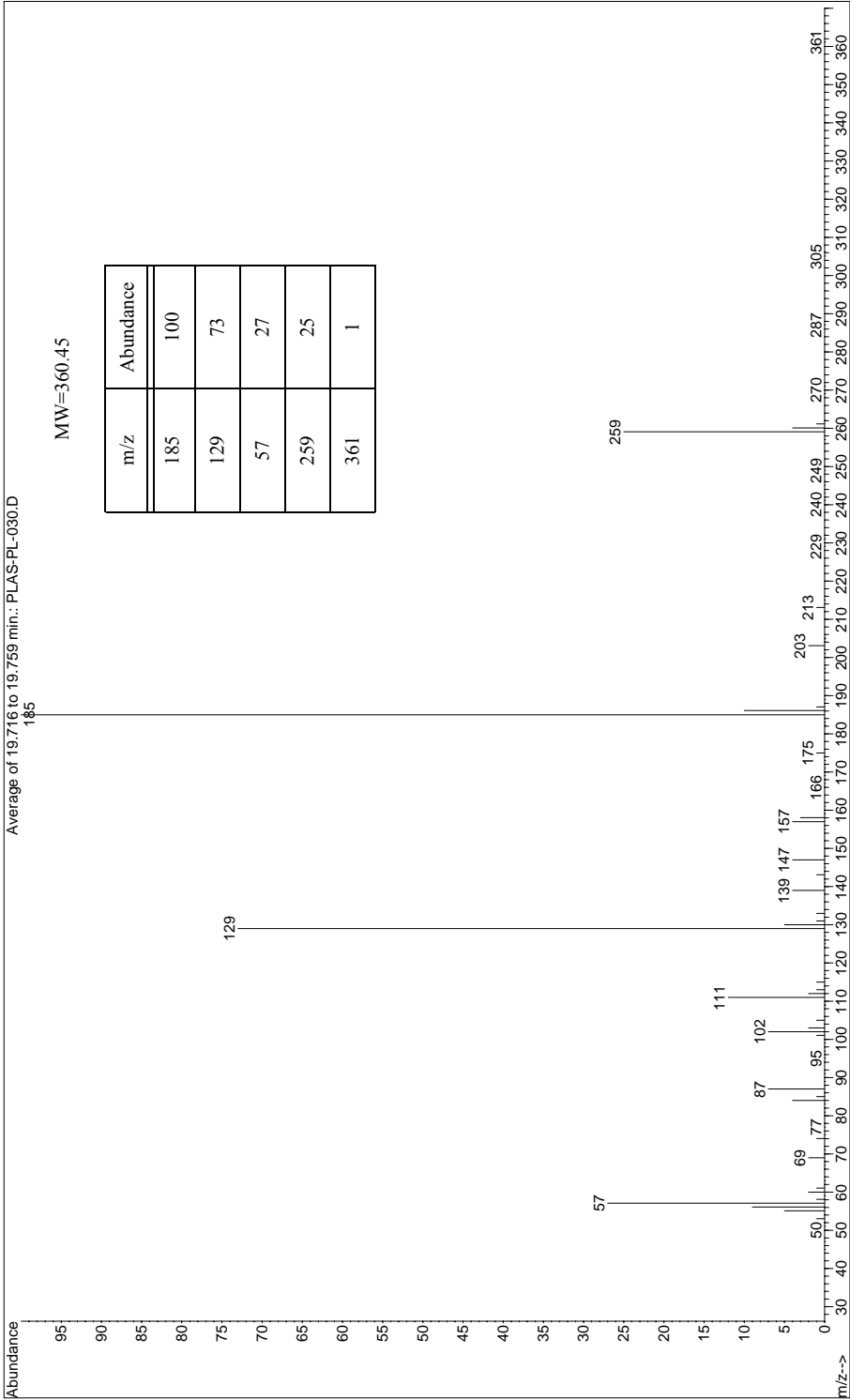
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

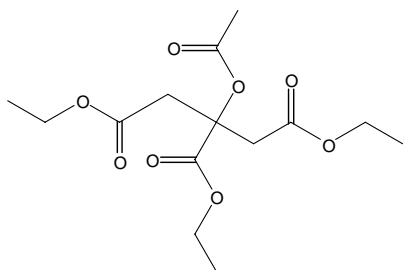
Insoluble in body fluids resulting in low toxicity. Single dose of 10-30 mL/kg BW does not result in intoxication.

Mass Spectrum for Citroflex® 4 - PLAS-PL-030



Citroflex[®] A-2

Morflex, Inc.

**CAS Number** 77-89-4**RTECS Number** GE8225000**Abbreviation** ATEC**Formula** C₁₄H₂₂O₈**Molecular Weight** 318.32**Chemical Name**

2-(acetyloxy)-1,2,3-propanetricarboxylic acid, triethyl ester

Synonyms

acetyltriethyl citrate; triethyl acetylcitrate

Brand Names & Manufacturers**Physical Properties**

Appearance	Clear liquid					
Melting Point	Not available			Boiling Point	228-229 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water 0.7	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane 40-80

Application Application, Regulatory & Environmental Information

Citroflex[®] A-2 is used as a plasticizer in food-packing materials. Additional applications include use as a fixative for perfumes, a film strengthening agent in hair sprays, nail polish and as a component in ink formulations.

Regulatory Information

FDA approved 1998 for the following applications: as a plasticizer in food-packaging materials, 21CFR178.3740; in adhesives as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105; in the manufacture of resinous or polymeric coatings for the food-contact surface of articles intended for use in producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food, 21CFR175.300; for use in the manufacture of resinous and polymeric coatings for polyolefin films, regulated under 21CFR175.320.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOC's), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

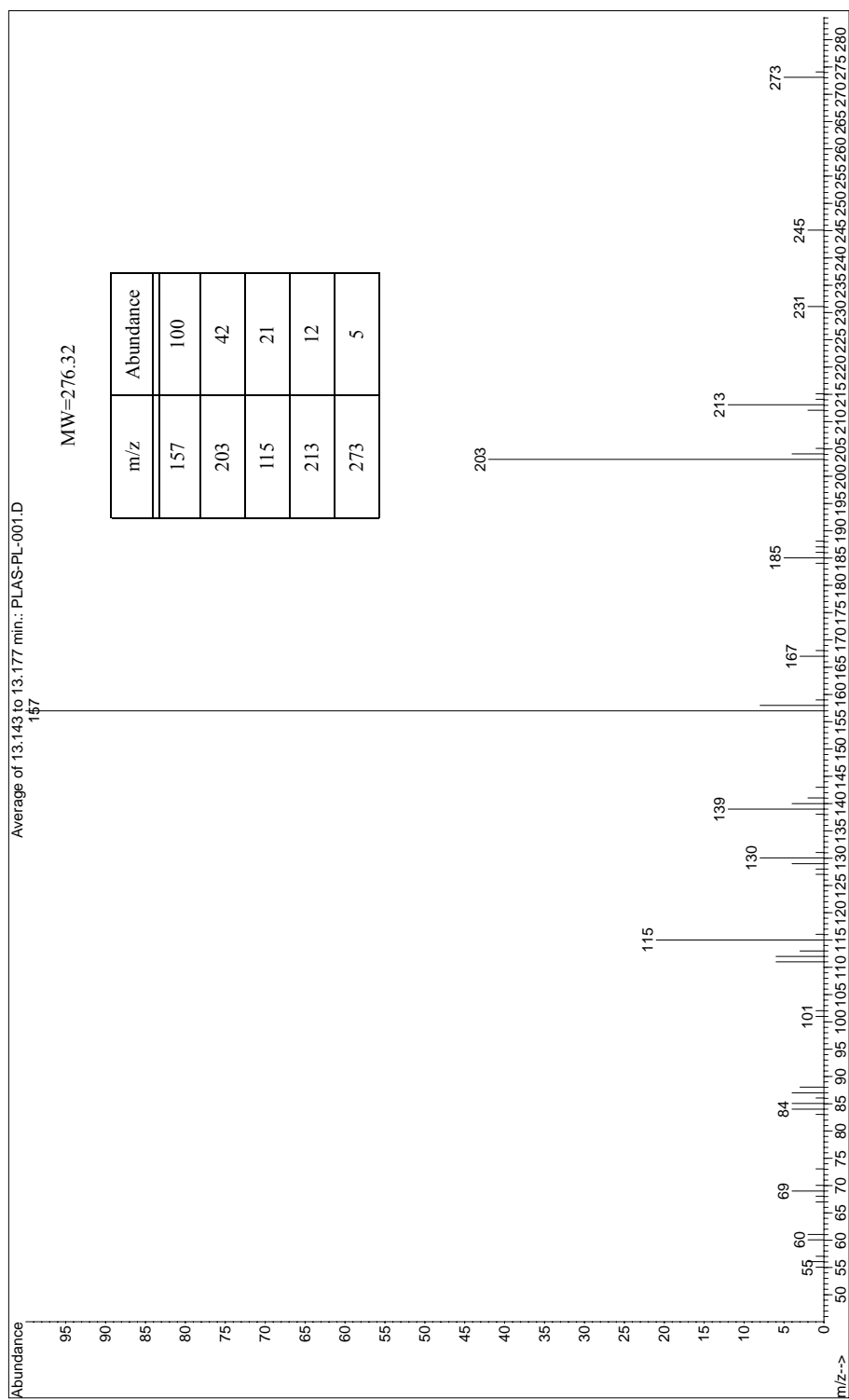
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

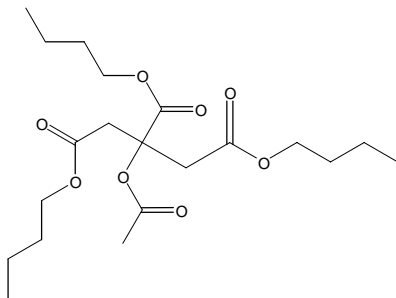
Acute toxicity: (LD50): 7.0 g/kg BW [Rat]

Mass Spectrum for Citroflex® A-2 - PLAS-PL-001



Citroflex® A-4

Morflex, Inc.

**CAS Number** 77-90-7**RTECS Number** TZ8330000**Abbreviation** ATBC**Formula** C₂₀H₃₄O₈**Molecular Weight** 402.54**Chemical Name**

2-Acetoxy-1,2,3-propanetricarboxylic acid, tributyl ester

Synonyms

acetyltri-n-butyl citrate; acetylcitric acid; acetyl tributyl citrate

Brand Names & Manufacturers**Physical Properties**

Appearance	Clear liquid					
Melting Point	Not available			Boiling Point	326 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane 40-80

Application Application, Regulatory & Environmental Information

ATBC is used as a plasticizer for flexible films made of vinylchloride-vinylidene chloride copolymer and cellulose. It is used as a plasticizer in food contact applications and in vinyl toys for children (low toxicity). ATBC provides adherence to metals, low volatility, and resistance to yellowing. Also used in: ink formulations, vinyl gloves, a non-VOC solvent in nitro-cellulose propellants, a plasticizer in nail polishes, adhesives and coatings, and for coating both paperboard and foil.

Regulatory Information

FDA: Approved 1998 as a plasticizer in food-packaging materials, 21CFR178.3740; in adhesives as a component of articles intended for use in packaging, transporting, or holding food, 21CFR175.105; in the manufacture of resinous and polymeric coatings for safe use as a food-contact surface of articles, 21 CFR175.300; in the manufacture of resinous or polymeric coatings in polyolefin films for the food-contact surface of articles intended for use in producing, manufacturing, packing, processing, preparing, treating, packaging, transporting, or holding food, 21CFR175.320.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOC's), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

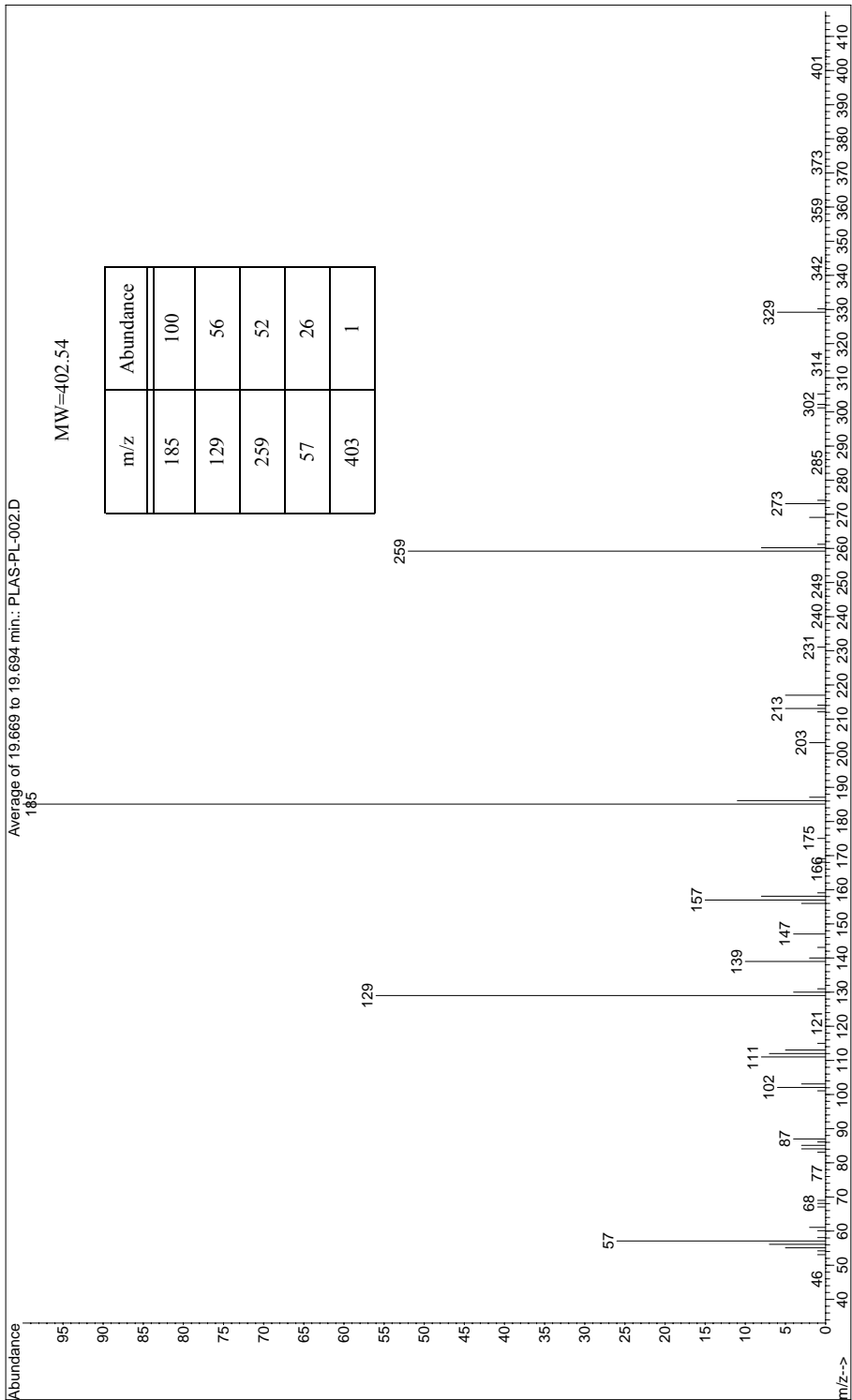
Point of Release

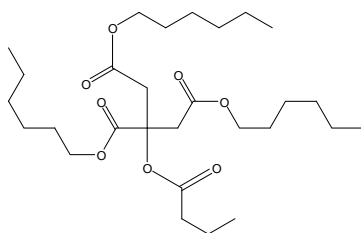
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 31400mg/kg [rat], Acute Intraperitoneal Toxicity (LD50): >4 gm/kg [mouse].

Mass Spectrum for Citroflex® A-4 - PLAS-PL-002



Citroflex[®] B-6**CAS Number** 82469-79-2**RTECS Number** Not available**Abbreviation** BTHC**Formula** C₂₈H₅₀O₈**Molecular Weight** 514.70**Chemical Name**

n-butyltri-n-hexyl citrate

Synonyms

2-(1-oxobutoxy)-1,2,3-propanetricarboxylic acid, trihexyl ester; butyrylcitric acid, tri-n-hexyl ester

Brand Names & Manufacturers***Physical Properties*****Appearance** Colorless to yellow, clear, oily liquid**Melting Point** -55 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Specifically designed for use in medical articles especially blood storage bags. Considered to be an effective replacement for DEHP (di-2-ethylhexyl) phthalate and DEHA (di-2-ethylhexyl) adipate.

Regulatory Information

Citroflex B-6 is a component of several FDA approved blood bag systems, has a Drug Master File and is manufactured under Current Good Manufacturing Practice (CGMP) guidelines.

Environmental Impact

Citrate plasticizers are free of volatile organic compounds (VOC's), have a low order of toxicity, low volatility, high flash-points, and are rapidly biodegradable.

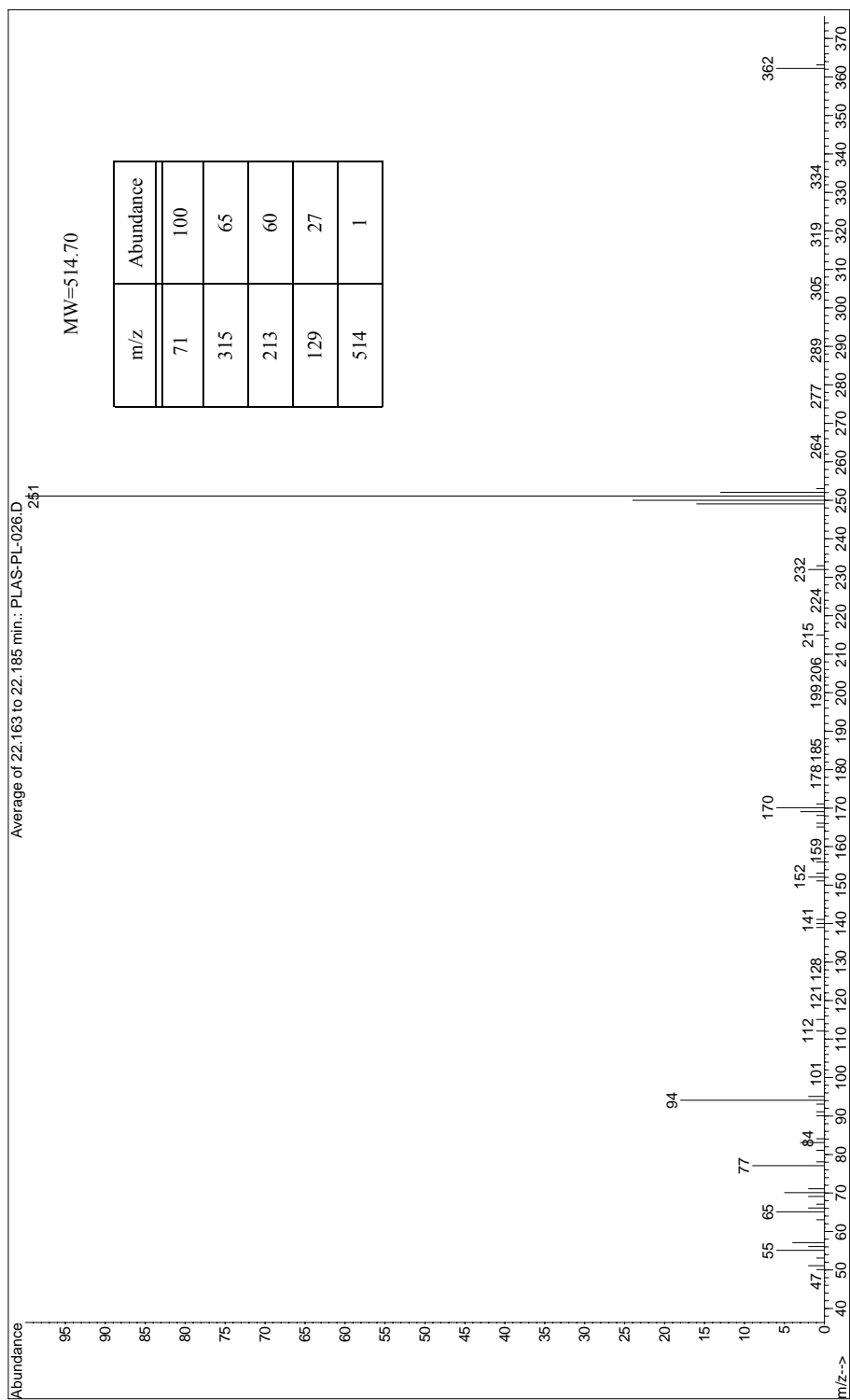
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

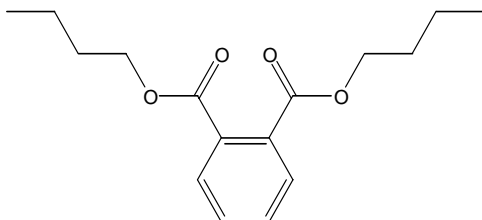
Acute oral toxicity (LD50): >20,000 mg/kg [Rat]. Rats fed this material showed no more abnormalities than those in the control group.

Mass Spectrum for Citroflex® B-6 - PLAS-PL-025



Dibutyl phthalate

Houghton Chemical

**CAS Number** 84-74-2**RTECS Number** TI0875000**Abbreviation** DBP**Formula** C₁₆H₂₂O₄**Molecular Weight** 278.34**Chemical Name**

dibutyl phthalate

Synonyms

1,2-benzenedicarboxylic acid, dibutyl ester; n-butyl phthalate

Brand Names & ManufacturersMorflex[®] 140
Polycizer[®] DBPMorflex, Inc.
Harwick Chemical Corporation**Physical Properties****Appearance** Colorless to yellow, viscous liquid**Melting Point** -35 °C**Boiling Point** 340 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	1	1	1	1	1

Application, Regulatory & Environmental Information**Application**

Plasticizer used in nitrocellulose lacquers, elastomers, explosives, nail polish and solid rocket propellants; solvent for perfume oils; perfume fixative; textile lubricating agent; safety glass; insecticides; printing inks; resin solvent; paper coatings; adhesives; insect repellent for textiles.

Regulatory Information

Regulated by the EPA under the Clean Water Act as a toxic pollutant. EU Directive 2005/84/EC (so called Phthalate Directive), restricts the use of DBP in toys and childcare articles.

Environmental Impact

This substance is toxic to aquatic organisms. The reported log Kow value is 4.77, which indicates a moderate potential to bioaccumulate. The chemical is biodegradable but tends to partition into sediment where it is relatively persistent.

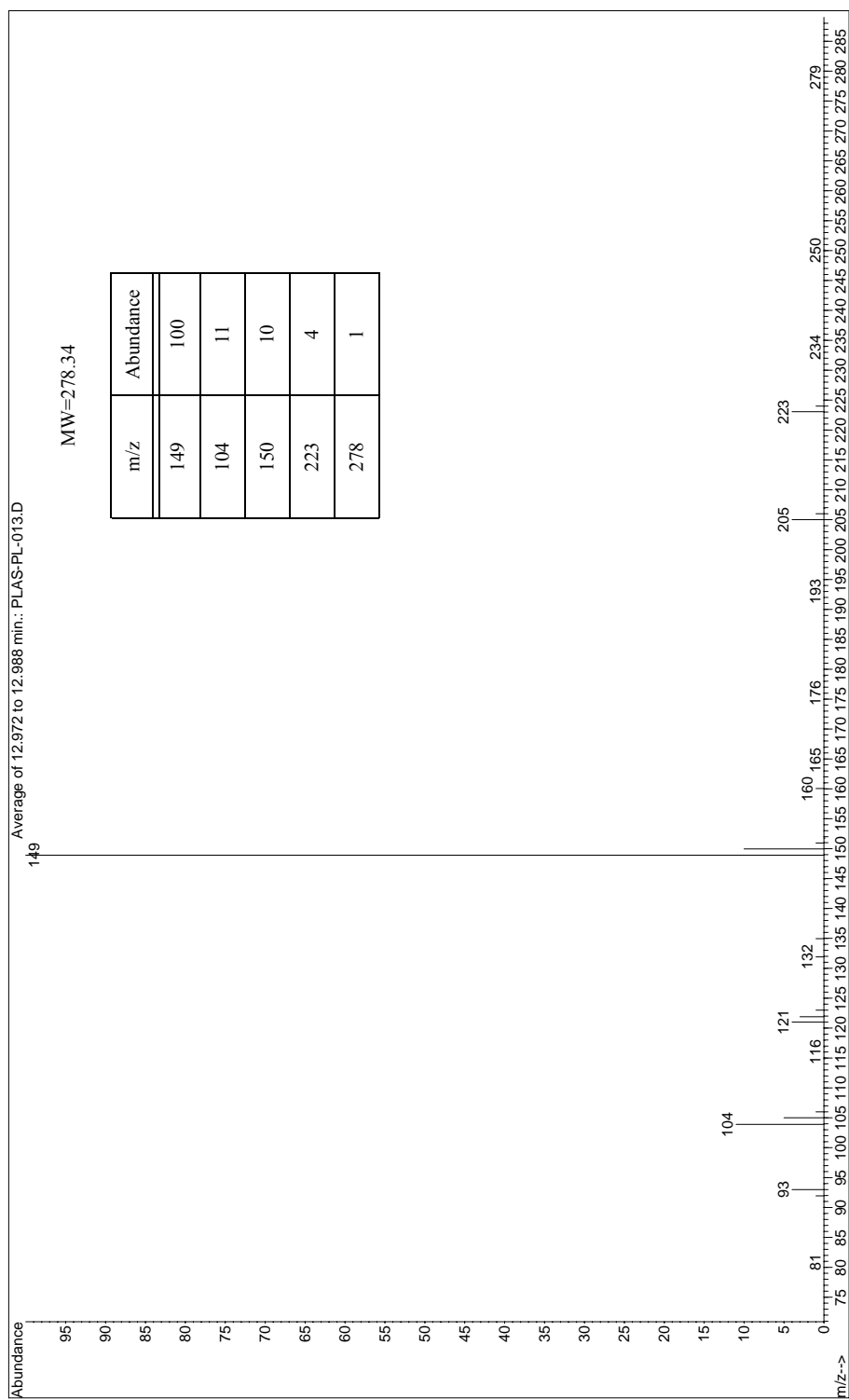
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

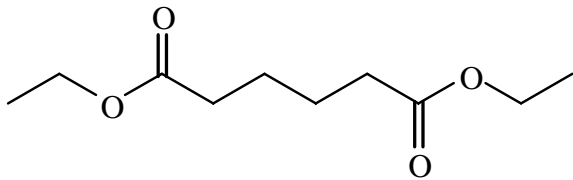
Toxicological Data

Acute oral toxicity (LD50): 7499 mg/kg [Rat]; Acute inhalation toxicity (LD50): 4250 mg/m³ [Rat]; Acute dermal toxicity (LD50): 6 g/kg [Rat]. Listed on CA Proposition 65 as a chemical known to have developmental toxicity.

Mass Spectrum for Dibutyl phthalate - PLAS-PL-013



Diethyl adipate



CAS Number 141-28-6
RTECS Number AV1100000
Abbreviation

Formula C₁₀H₁₈O₄
Molecular Weight 202.25

Chemical Name
hexanedioic acid, diethyl ester

Synonyms
1,6-diethyl hexanedioate; adipic acid, diethyl ester

Brand Names & Manufacturers

Physical Properties

Appearance	Colorless liquid					
Melting Point	-19.8 °C			Boiling Point	245 °C	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane 40-80

Application ***Application, Regulatory & Environmental Information***

Plasticizer for vinyl resins and solvent carriers or coupling agents for polyurethane and photographic films. Typically used in combination with phthalates.

Regulatory Information

Not approved by the FDA for food contact applications.

Environmental Impact

Listed by the EPA as a non-hazardous chemical. Diethyl adipate is readily biodegradable and has a low potential to bioaccumulate based on a measured log Kow value of 1.79.

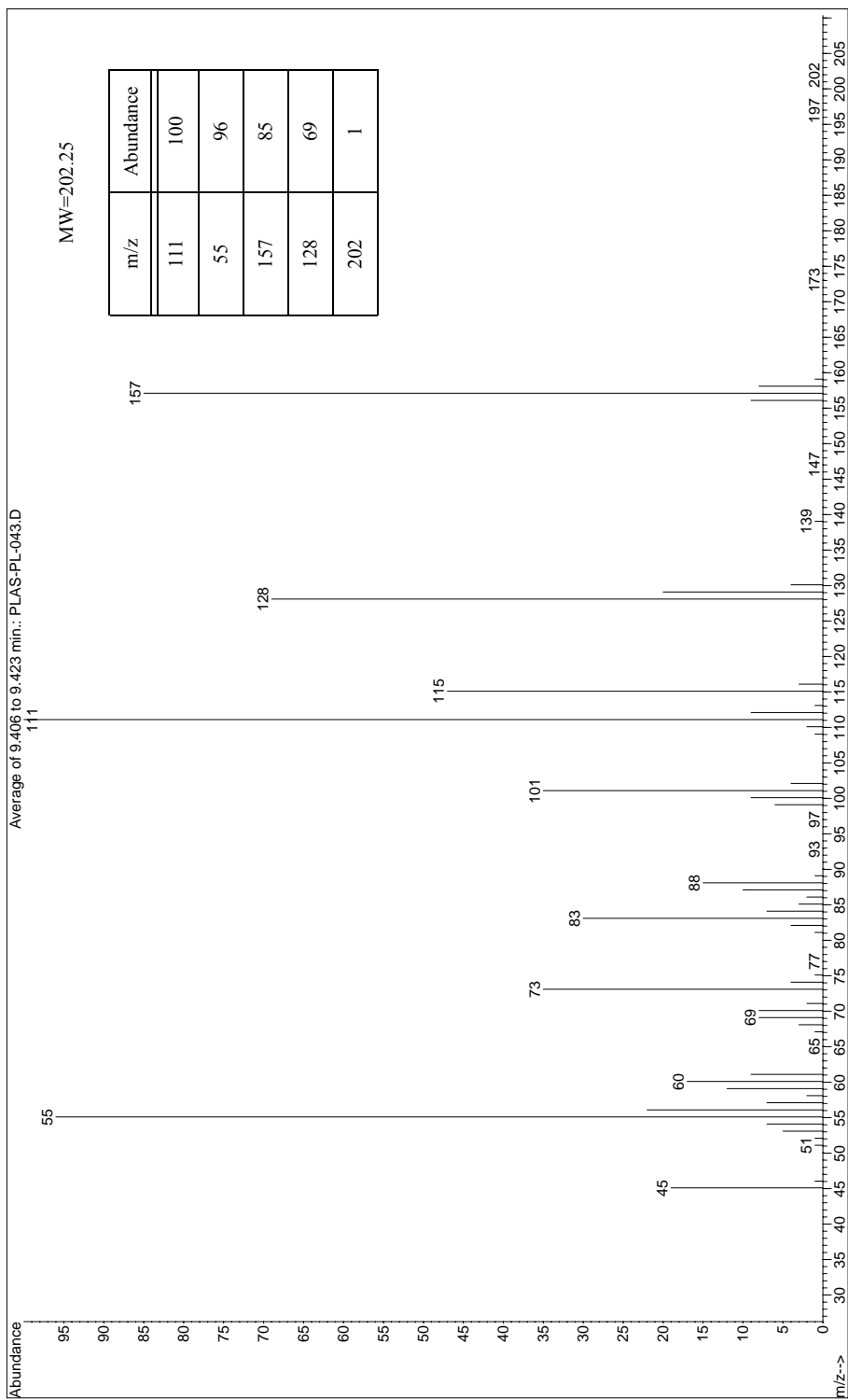
Point of Release

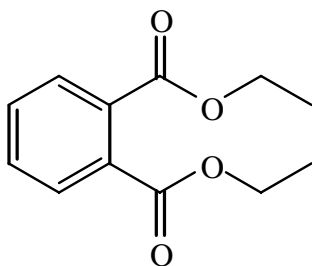
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral LD50; 8100 mg/kg [Mouse], Intraperitoneal LD50; 2190 mg/kg [Mouse]. Chronic Exposure - Teratogen: Dose: 837 mg/kg [Rat], Intraperitoneal exposure time: (5-15D PREG) resulted in developmental abnormalities and fetal death. Chronic Exposure - Mutagen: Dose: 1100 mg/kg [Mouse], Intraperitoneal Dose: 1100 mg/Kg Mutation test: Dominant lethal test.

Mass Spectrum for Diethyl adipate - PLAS-PL-043



Diethyl phthalate

CAS Number 84-66-2

RTECS Number TI1050000

Abbreviation DEP

Formula C₁₂H₁₄O₄

Molecular Weight 222.24

Chemical Name

1,2-benzenedicarboxylic acid, diethyl ester

Synonyms

diethyl phthalate; diethyl 1,2-benzenedicarboxylate; o-bis(ethoxycarbonyl)benzene; phthalic acid, diethyl ester

Brand Names & Manufacturers**Physical Properties****Appearance** Clear oily liquid**Melting Point** -40.5 °C**Boiling Point** 295 °C**Stability** Stable at normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	40-80

Application, Regulatory & Environmental Information**Application**

DEP is used as a plasticizer to make plastics more flexible. Commonly found in products such as toothbrushes, automobile parts, tools, toys, and food packaging. Also used as a plasticizer in solid rocket propellants and cellulose ester plastics such as photographic films and sheets, blister packaging, and tape applications.

Regulatory Information

SARA 313 reportable chemical. Classified as environmentally hazardous for shipping purposes. EPA regulated under the Clean Water Act.

Environmental Impact

Diethyl phthalate is designated a toxic pollutant under the Clean Water Act. This substance may be hazardous to the environment; special attention should be given to fish.

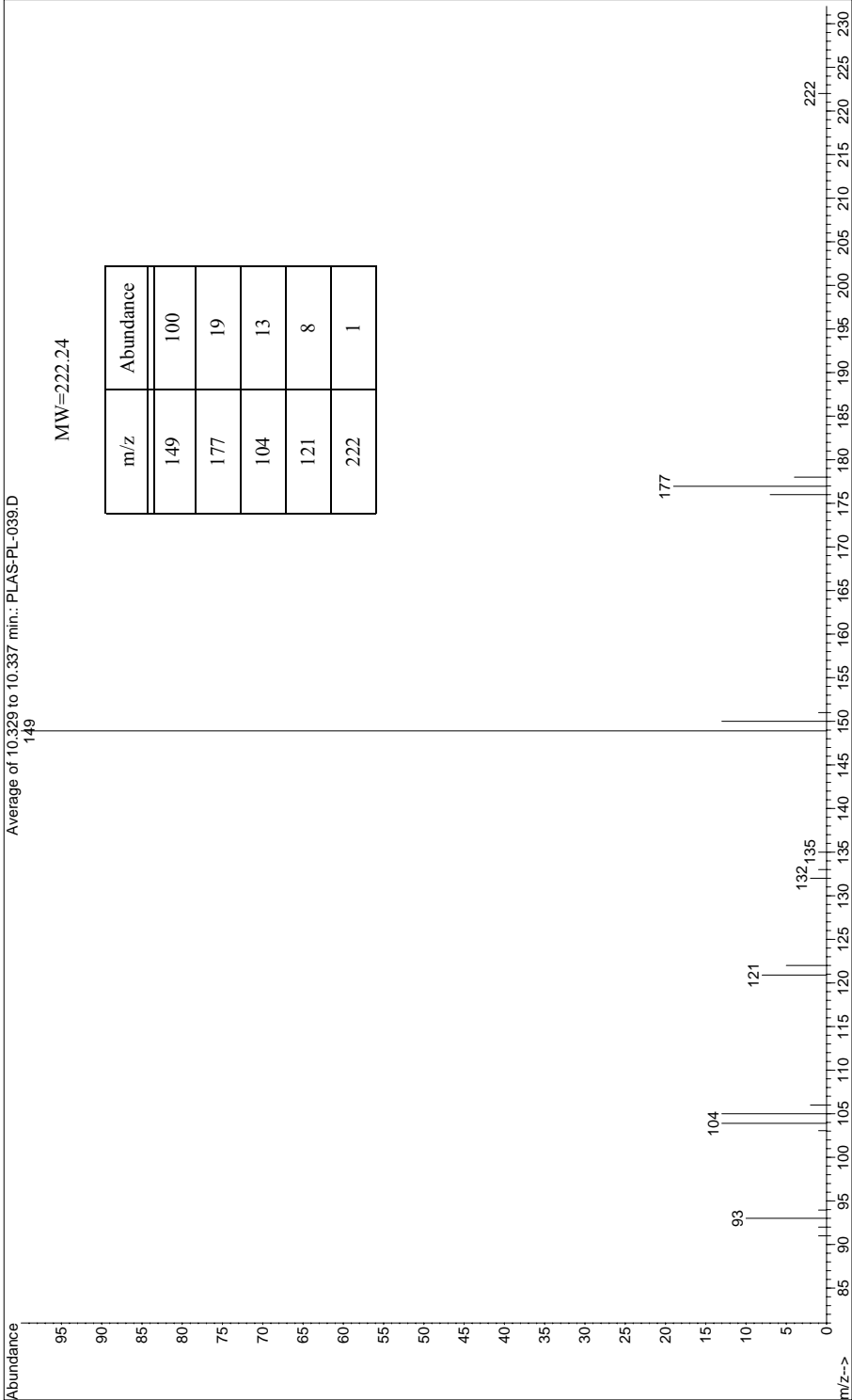
Point of Release

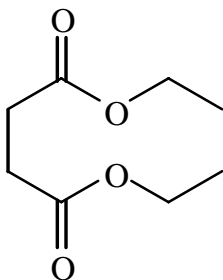
Because diethyl phthalate is not a part of the chain of chemicals, or polymers, which makes up the plastics, it can be released fairly easily from products in which it is used. Exposure may occur when you use plastics that contain it, and when you eat food from plastic containers made with it. This substance has been found in at least 248 of the 1,430 National Priorities List sites identified by the Environmental Protection Agency (EPA).

Toxicological Data

Oral (LD50): 9,000 mg/kg [Rat], 1,000 mg/kg [Rabbit]; Inhalation (LC50): > 4,640 mg/m³ [Rat]; Skin (LD50) > 20 mg/kg [Guinea pig].

Mass Spectrum for Diethyl phthalate - PLAS-PL-039



Diethyl succinate**CAS Number** 123-25-1**RTECS Number** WM7400000**Abbreviation****Formula** C₈H₁₄O₄**Molecular Weight** 174.19**Chemical Name**

butanedioic acid, diethyl ester

Synonyms

ethyl succinate; diethyl butanedioate; succinic acid, diethyl ester

Brand Names & Manufacturers

Physical Properties**Appearance** Colorless liquid**Melting Point** -21.0 °C**Boiling Point** 217.7 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.2	40-80	40-80	U	U	U

Application, Regulatory & Environmental Information**Application**

Plasticizer for PVC resins.

Regulatory Information

Diethyl succinate has FDA approval for use as a food additive. Also approved for use in a wide variety of food contact applications.

Environmental Impact

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise. The product itself and its products of degradation are not toxic to the environment.

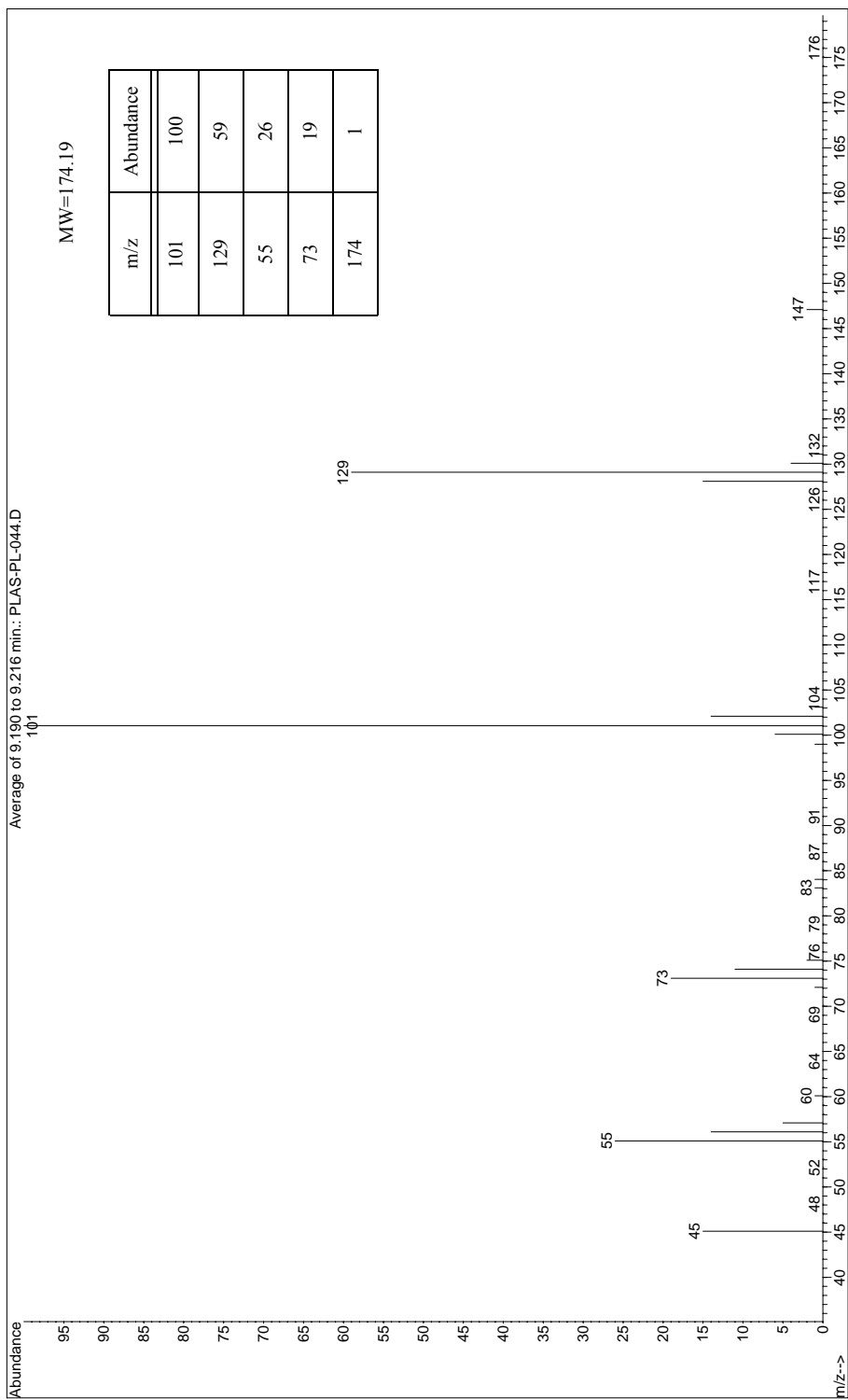
Point of Release

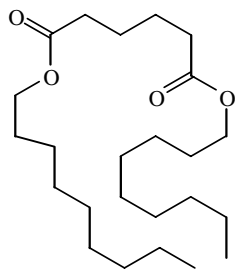
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): 8530 mg/kg [Rat]. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Diethyl succinate - PLAS-PL-044



Diisononyl adipate**CAS Number** 33703-08-1**RTECS Number** Not available**Abbreviation** DINA**Formula** C₂₄H₄₆O₄**Molecular Weight** 398.63**Chemical Name**

hexanedioic acid, diisononyl ester

Synonyms

bis(isononyl)adipate; diisononyl hexanedioate; adipic acid, diisononyl ester

Brand Names & Manufacturers

Jayflex® DINA

ExxonMobil

Plastomoll® DNA

BASF

Santicizer® DINA

Solutia Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** -65 °C**Boiling Point** 235 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application Application, Regulatory & Environmental Information

Diisononyl adipate is a highly efficient plasticizer that imparts low temperature flexibility and impact resistance to the base resin. Widely used in shrinkwrap, electrical wire jackets and films. Also used in sausage casings.

Regulatory Information

Approved by the FDA for use as a food additive and/or food contact material.

Environmental Impact

Adipates are sensitive to hydrolysis, recovering the acid and alcohols particularly under alkaline conditions. This contributes to their ability to degrade easily in the environment. Log Kow value of 9.24 indicates a potential to bioaccumulate. They are reported to have an acute toxicity to aquatic wildlife.

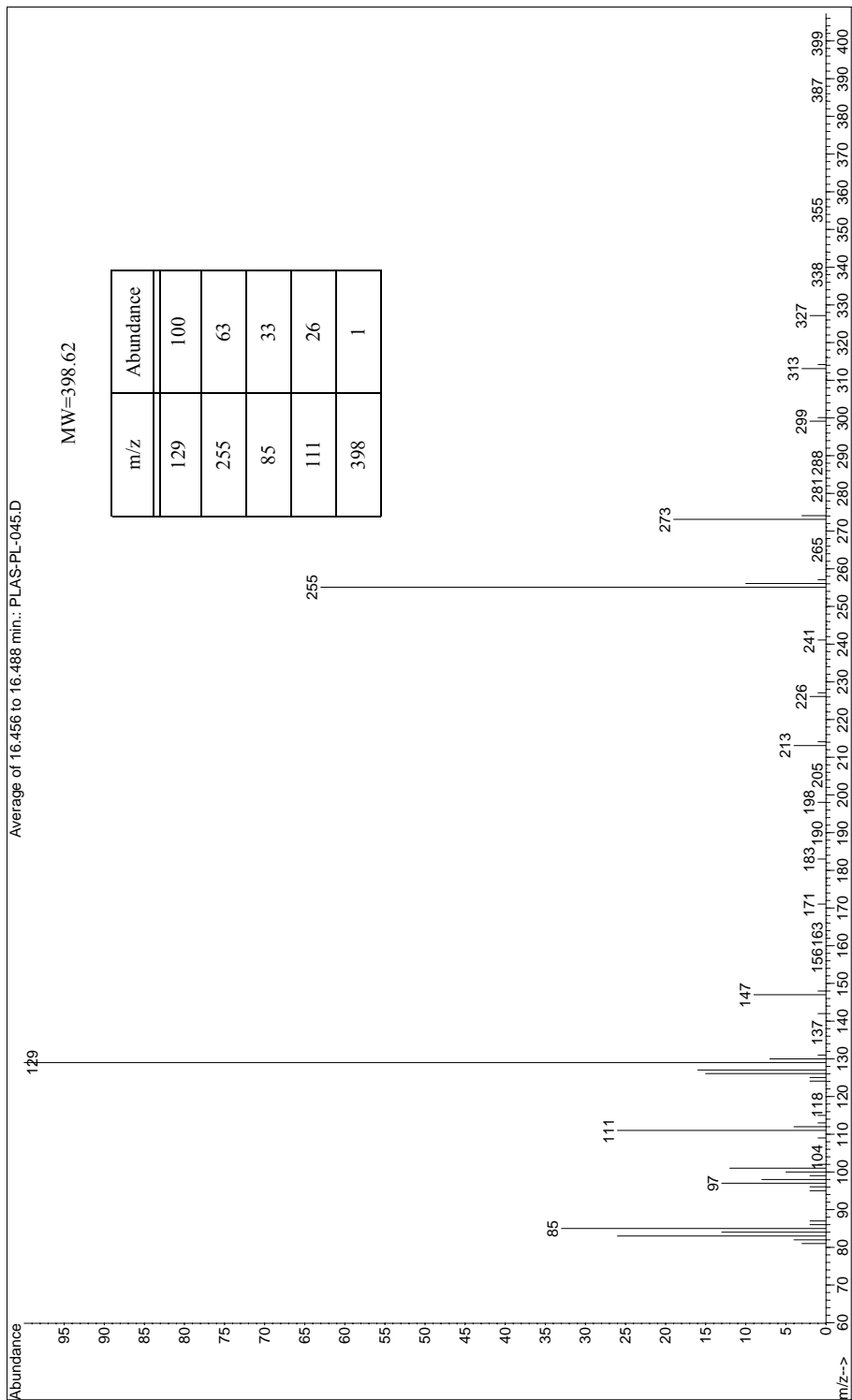
Point of Release

High-level contamination of DINA has been found in fish paste products and other packaged foods, presumably because of migration from plasticized wrapping film used for food packaging.

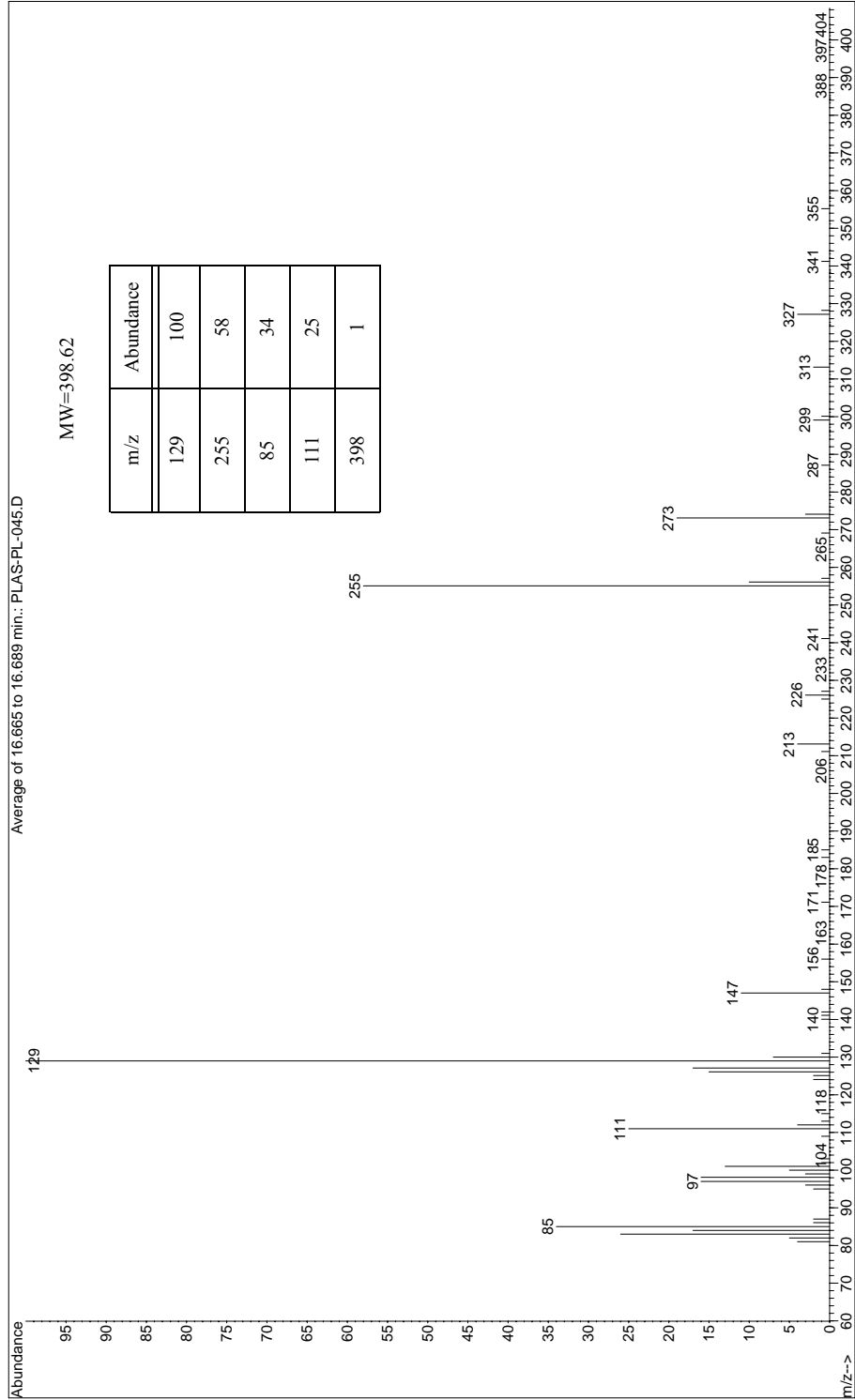
Toxicological Data

Concern over the mutagenic and carcinogenic potential of these materials was stimulated by the finding that one member of this class, di-(2-ethylhexyl) adipate (DEHA), induced liver tumors in female mice in a chronic feeding study. Accordingly, the genotoxic potential of DINA was evaluated in a battery of in vitro tests and did not exhibit any evidence of mutagenic or transforming potential in any of the assays utilized.

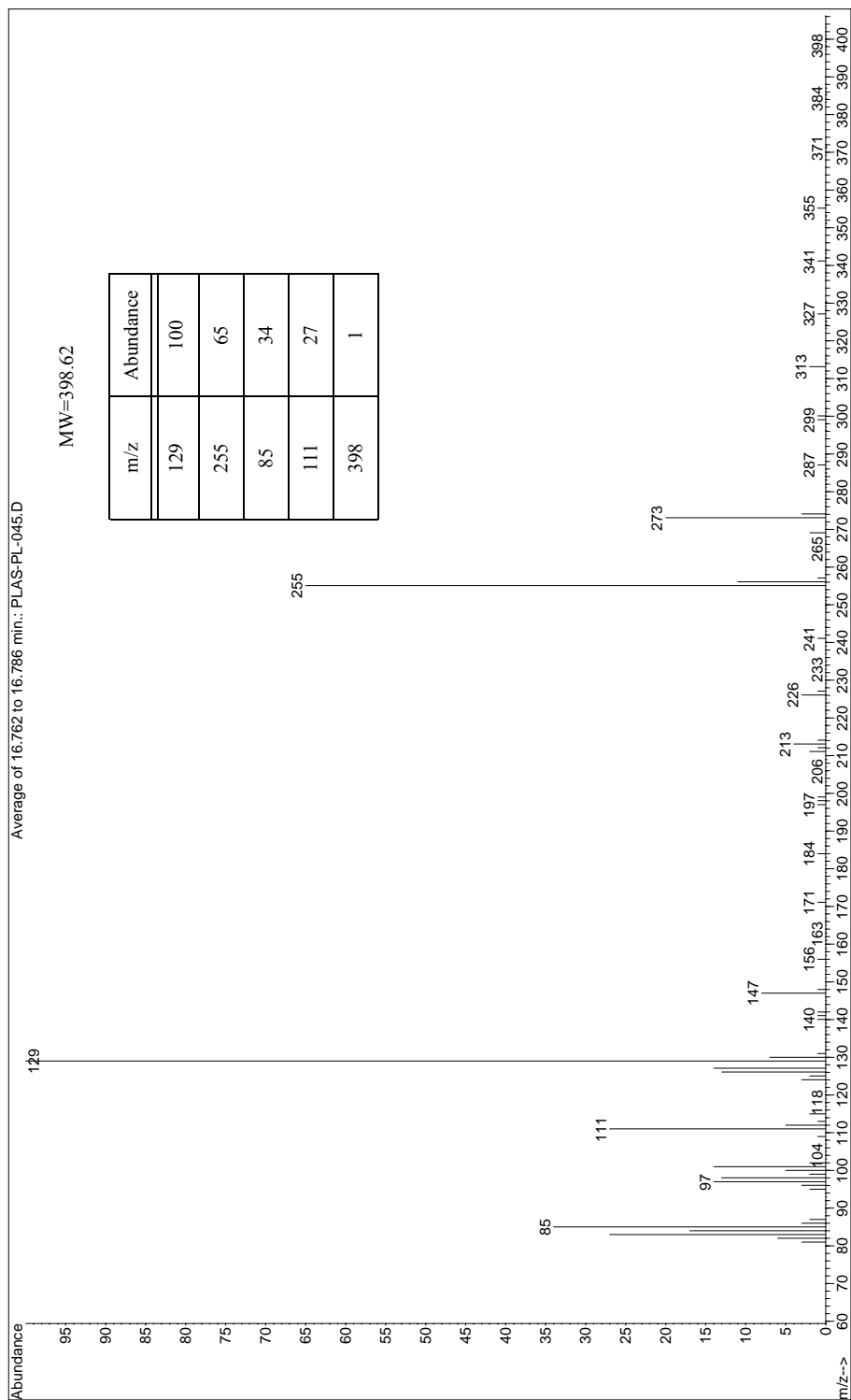
Mass Spectrum for Diisononyl adipate - PLAS-PL-045

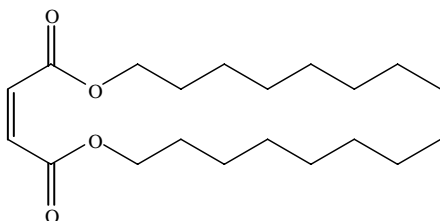


Mass Spectrum for Diisononyl adipate - PLAS-PL-045



Mass Spectrum for Diisononyl adipate - PLAS-PL-045



Diethyl maleate**CAS Number** 2915-53-9**RTECS Number** Not available**Abbreviation** DOM**Formula** C₂₀H₃₆O₄**Molecular Weight** 340.50**Chemical Name**

(2Z)-2-butenedioic acid

Synonyms

maleic acid, dioctyl ester

Brand Names & Manufacturers**Physical Properties****Appearance** Liquid**Melting Point** -40 °C**Boiling Point** 209 °C**Stability**

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane

Application, Regulatory & Environmental Information

Application Used as a plasticizer for vinyl resins and for applications involving co-polymerization with polyvinyl chloride and vinyl acetates in emulsion paints and adhesives. Provides elasticity and flexibility.

Regulatory Information

Diethyl maleate is FDA approved under 21CFR175.105 - Indirect Food Additives - Adhesives.

Environmental Impact

Readily biodegradable and has a low potential to bioaccumulate. Not expected to be toxic to the aquatic environment.

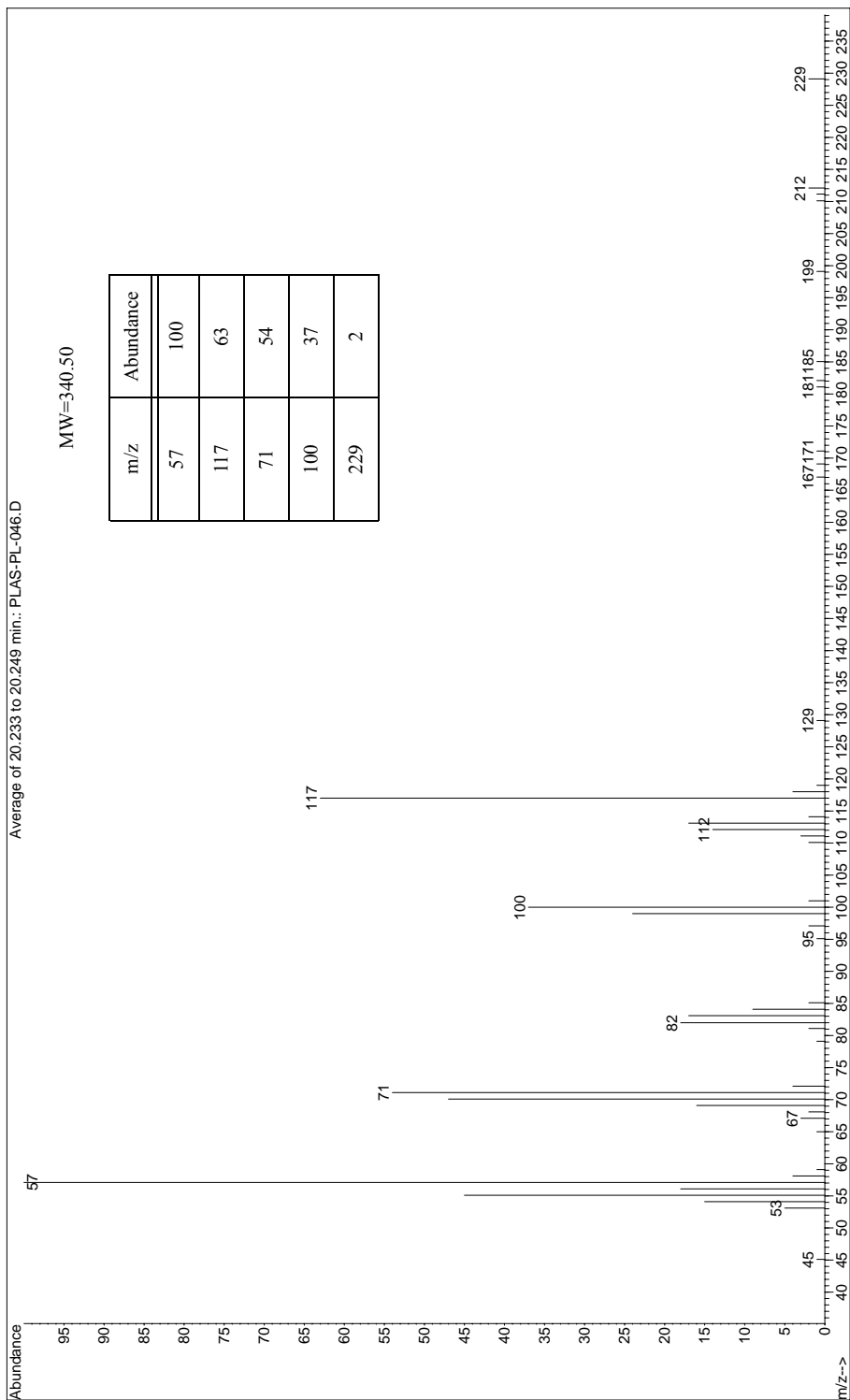
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

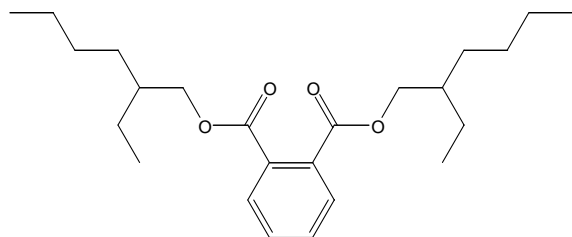
Oral (LD50): 2-5g/kg [Rat]; slightly toxic to animals. Dermal (LD50): 2.6 g/kg [Rabbits]; moderately to severely irritating to rabbit skin. Practically non-toxic to animals. Not a skin sensitizer. Inhalation (LC50): > 0.89 but < 5.3 mg/l [Rat] 4 hr; slightly toxic to animals.

Mass Spectrum for Dioctyl maleate - PLAS-PL-046



Diethyl phthalate (DOP)

Houghton Chemical

**CAS Number** 117-81-7**RTECS Number** TI0350000**Abbreviation** DOP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

dioctyl phthalate

Synonyms

DOP; bis(2-ethylhexyl)phthalate; di-2-ethylhexyl phthalate

Brand Names & Manufacturers

Plasthall® DOP

C. P. Hall Company

Polycizer® DOP

Harwick Chemical Corporation

Physical Properties**Appearance** Colorless, viscous liquid**Melting Point** -50 °C**Boiling Point** 385 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	40-80	40-80	40-80	1

Application, Regulatory & Environmental Information**Application**

Plasticizer for resins and elastomers which are used to manufacture many products, including teething rings, pacifiers, soft squeeze toys, balls, vinyl upholstery, tablecloths, shower curtains, raincoats, adhesives, polymeric coatings, components of paper and paperboard, defoaming agents, enclosures for food containers and vinyl gloves used for medical examinations and surgery.

Regulatory Information

EPA regulates DOP under the Clean Water Act (CWA), Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), Resource Conservation and Recovery Act (RCRA), Superfund Amendments and Reauthorization Act (SARA), and Toxic Substances Control Act (TSCA). Listed on CA Prop 65 as a known carcinogen.

Environmental Impact

This material is considered to be moderately toxic to aquatic organisms and will bioaccumulate, especially in fish. When released to soil, it attaches strongly to the soil and does not migrate away from where it was released. When released to water, it dissolves very slowly into underground water or surface waters. It takes many years for DOP in buried or discarded materials to disappear from the environment.

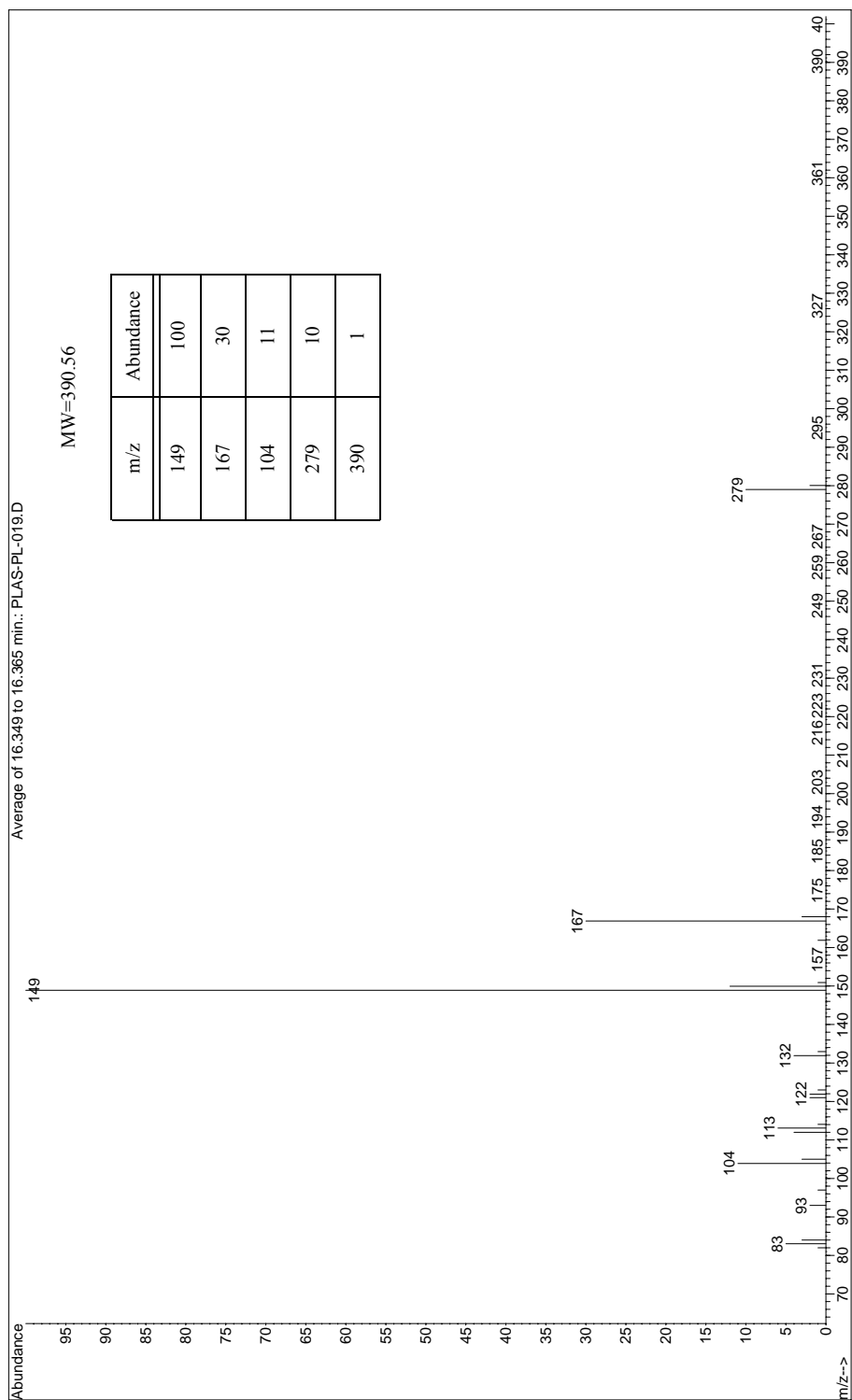
Point of Release

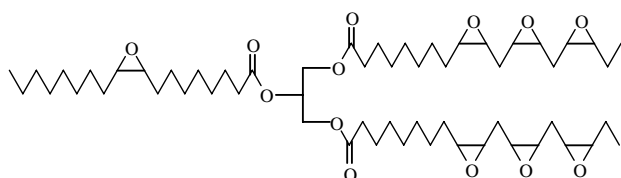
The primary routes of potential human exposure to DOP are air inhalation, ingestion, and dermal contact. For the general population, the most likely route of exposure is through contaminated food (i.e., food coming in contact with containers and wrappings containing this material). It has been detected in such foods as milk, cheese, fish, meat, margarine, eggs, and cereal products. Another potential source of exposure is the leaching of the chemical from plastic articles in landfills.

Toxicological Data

Acute oral toxicity (LD50): 30 g/kg [Rat], Acute dermal toxicity (LD50): 4 g/kg [Rat]. Listed by NTP as an anticipated human carcinogen and IARC as a possible human carcinogen. Also listed on CA Prop 65 as a known carcinogen.

Mass Spectrum for Dioctyl phthalate (DOP) - PLAS-PL-019



Epoxidized linseed oil

CAS Number 8016-11-3

RTECS Number Not available

Abbreviation

Formula $C_{57}H_{95}O_{13}$

Molecular Weight 1037.39

Chemical Name

linseed oil, epoxidized

Synonyms

epoxidized linseed oil

Brand Names & Manufacturers**Physical Properties**

Appearance	Liquid					
Melting Point	-2.2 °C			Boiling Point	Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water 0.09	MeOH U	EtOH 1-10	Acetone 1-10	CH₂Cl₂ U	Hexane 1-10

Application Application, Regulatory & Environmental Information

Used primarily to keep plastics and rubber soft and pliable in flooring, upholstery, food packaging, hoses, tubing, blood bags and other products. The epoxy functionality provides heat and light stability.

Regulatory Information

FDA approved for a wide variety of food contact applications.

Environmental Impact

Expected to be readily biodegradable. The estimated log Kow value is > 6.2, which indicates a high potential for bioaccumulation, however, their uptake into fish is expected to be hindered by their large molecular size. If taken up by fish, these carboxylate ester-containing substances are expected to be readily metabolized and excreted. Thus, the bioaccumulation potential is expected to be much lower than predicted from log Kow alone.

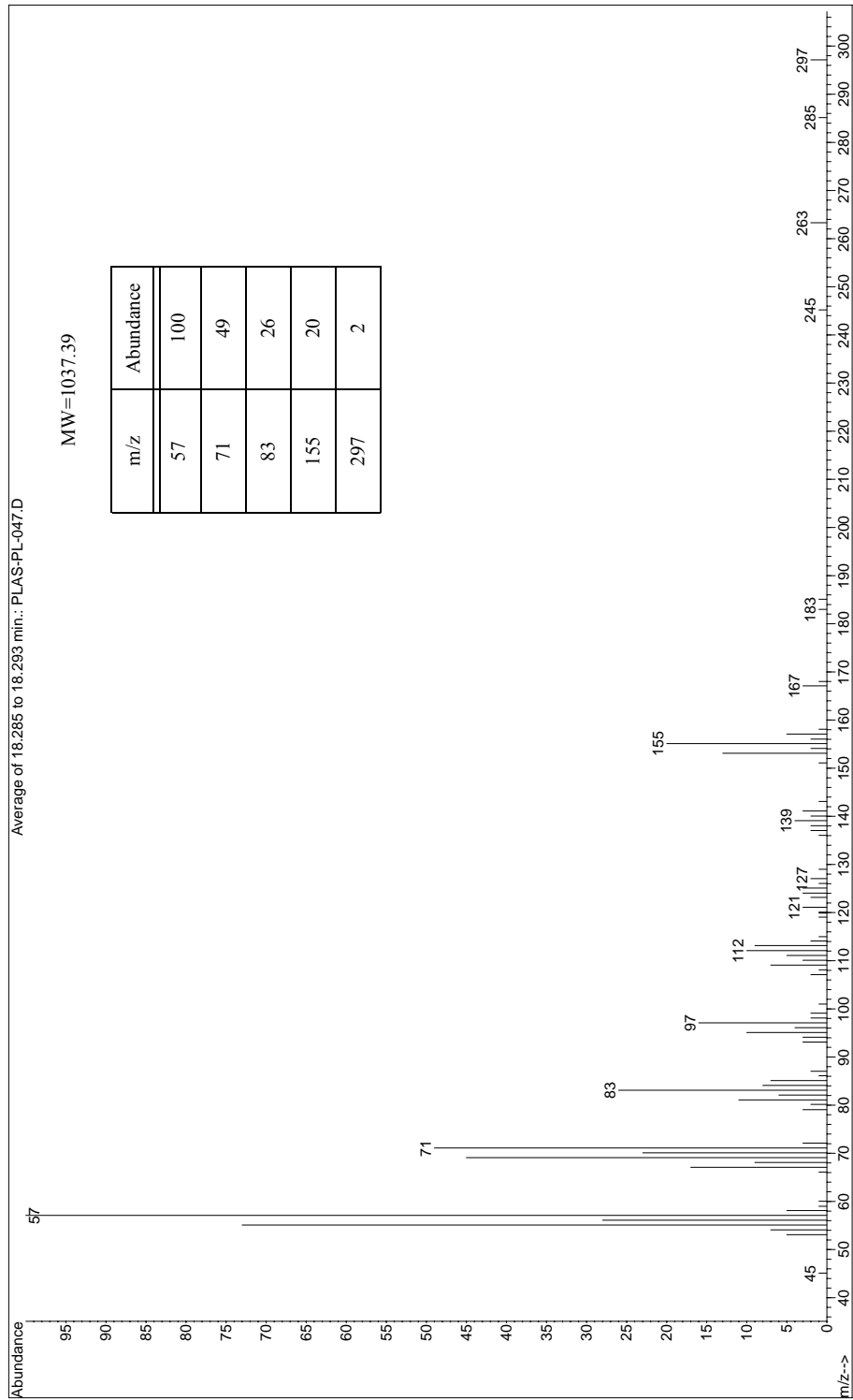
Point of Release

There may be low level losses in process waters, which are discharged to a waste water treatment system. Environmental release during transport is possible in the event of a spill or accident. The material has a very low vapor pressure, making airborne release very unlikely. Migration does occur from plastics during use and upon disposal.

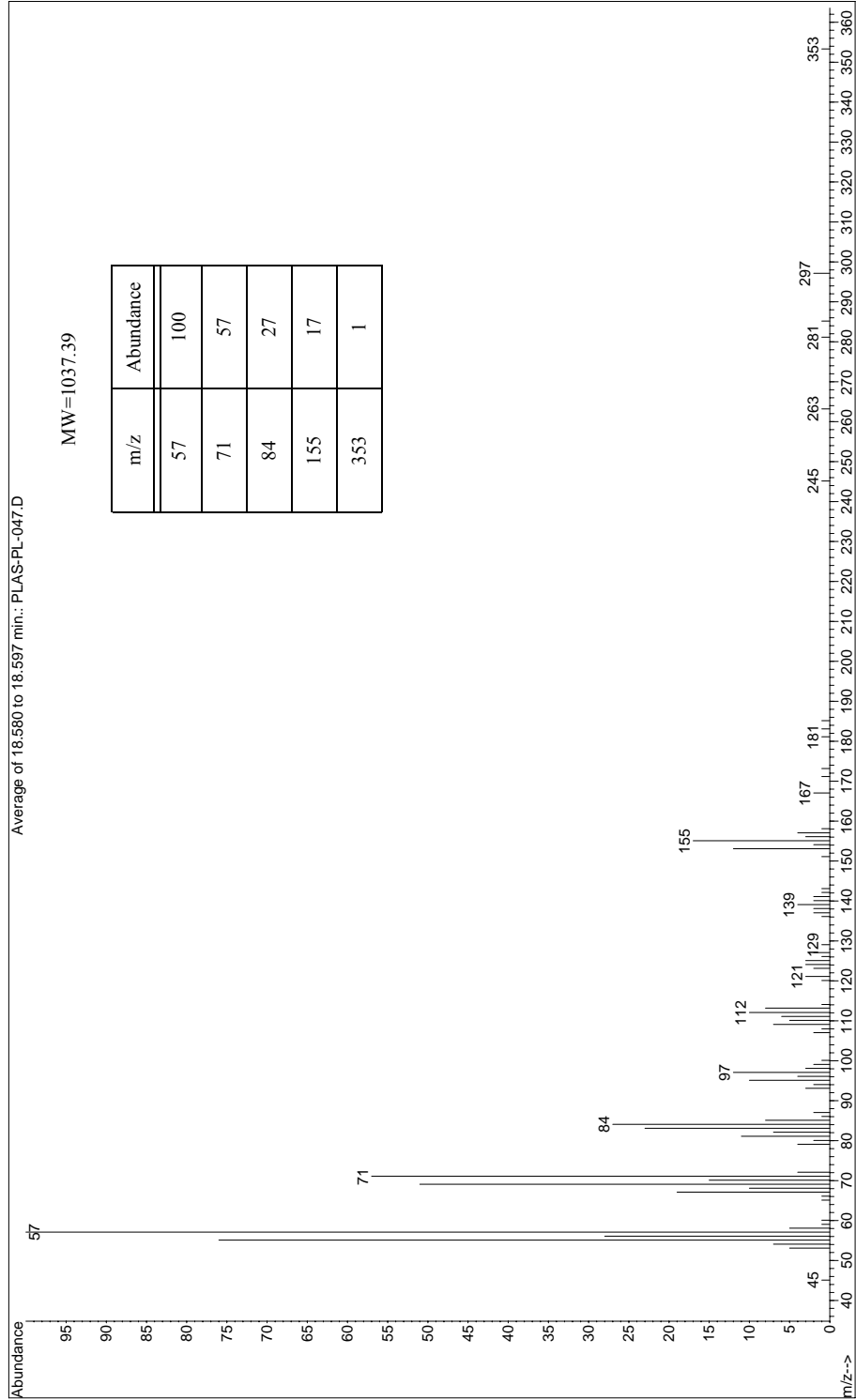
Toxicological Data

While there is no specific information on the metabolism of these materials, there is a large body of research on the metabolism and absorption of vegetable oils. Because of the similarity in physicochemical properties of these materials, it is assumed that they are absorbed and metabolized in a manner similar to vegetable oils, rather than simply excreted.

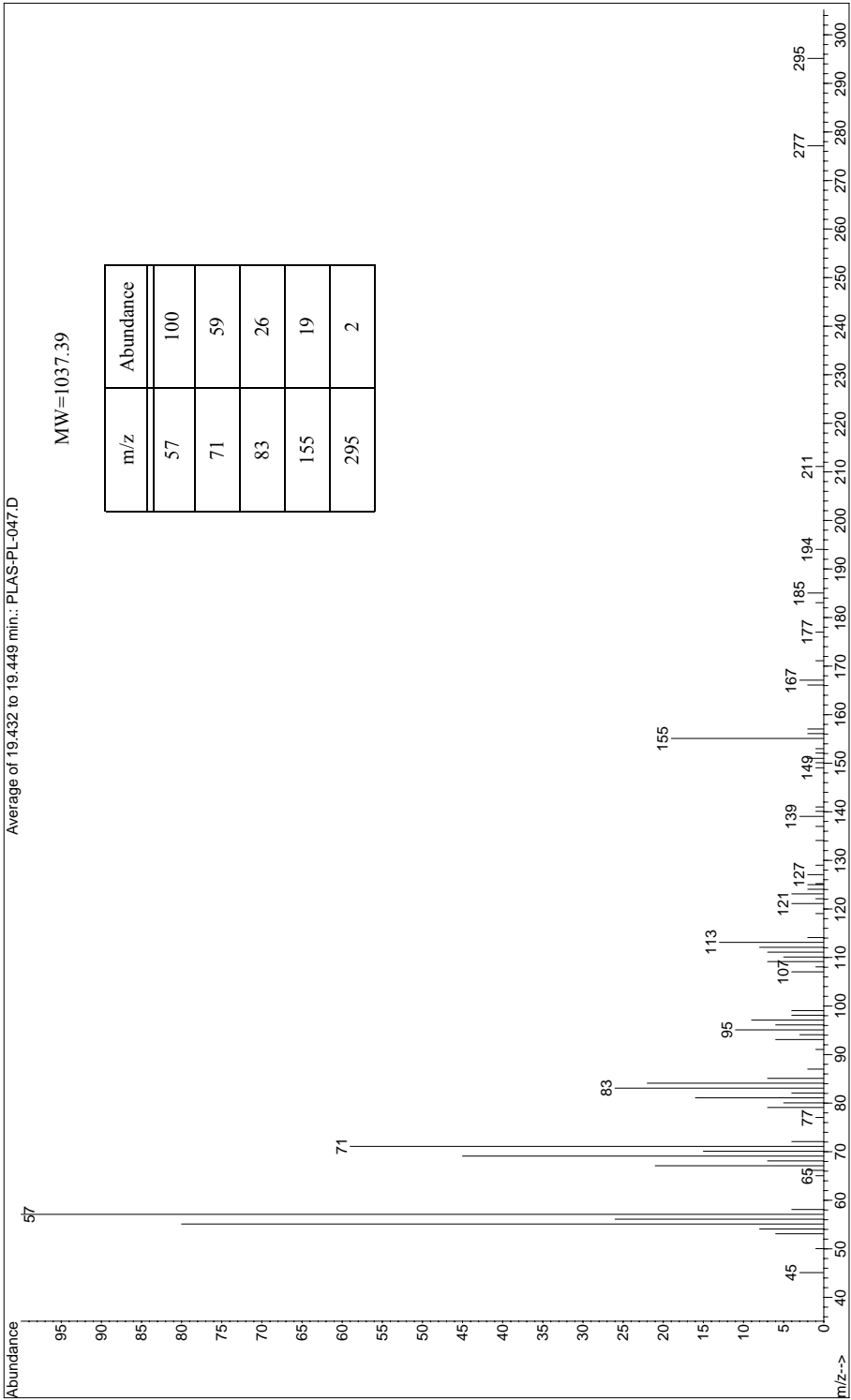
Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047



Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047

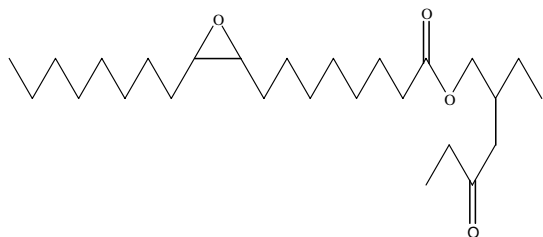


Mass Spectrum for Epoxidized linseed oil - PLAS-PL-047



Flexol® EP-8

Houghton Chemical Corporation

**CAS Number** 61789-01-3**RTECS Number** Not available**Abbreviation****Formula** C₂₆H₄₈O₄**Molecular Weight** 424.74**Chemical Name**

fatty acids, tall-oil, epoxidized, 2-ethylhexyl esters

Synonyms

2-ethylhexyl epoxy tallate; epoxidized 2-ethylhexyl ester of tall oil fatty acid; sec-octyl epoxytallate

Brand Names & Manufacturers**Physical Properties**

Appearance	Liquid					
Melting Point	-23.2 °C			Boiling Point	Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water 0.30	MeOH U	EtOH 1-10	Acetone 1-10	CH₂Cl₂ U	Hexane 1-10

Application Application, Regulatory & Environmental Information

Used primarily to keep plastics and rubber soft and pliable in flooring, upholstery, food packaging, hoses, tubing, blood bags and other products. The epoxy functionality provides heat and light stability.

Regulatory Information

FDA approved for a wide variety of food contact applications.

Environmental Impact

Expected to be readily biodegradable. The estimated log Kow value is > 6.2, which indicates a high potential for bioaccumulation, however, their uptake into fish is expected to be hindered by their large molecular size. If taken up by fish, these carboxylate ester-containing substances are expected to be readily metabolized and excreted. Thus, the bioaccumulation potential is expected to be much lower than predicted from log Kow alone.

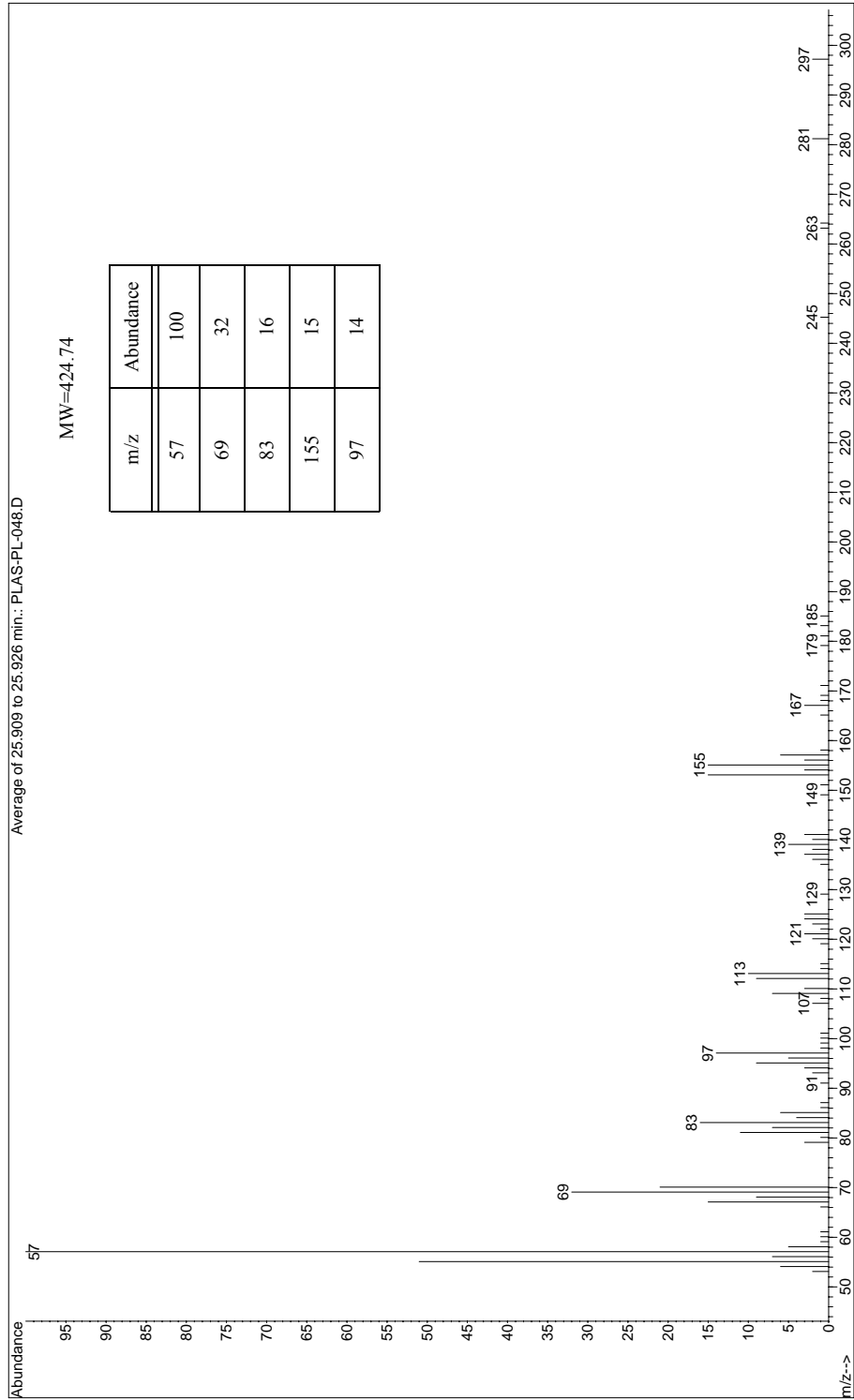
Point of Release

There may be low level losses in process waters, which are discharged to a waste water treatment system. Environmental release during transport is possible in the event of a spill or accident. The material has a very low vapor pressure, making airborne release very unlikely. Migration does occur from plastics during use and upon disposal.

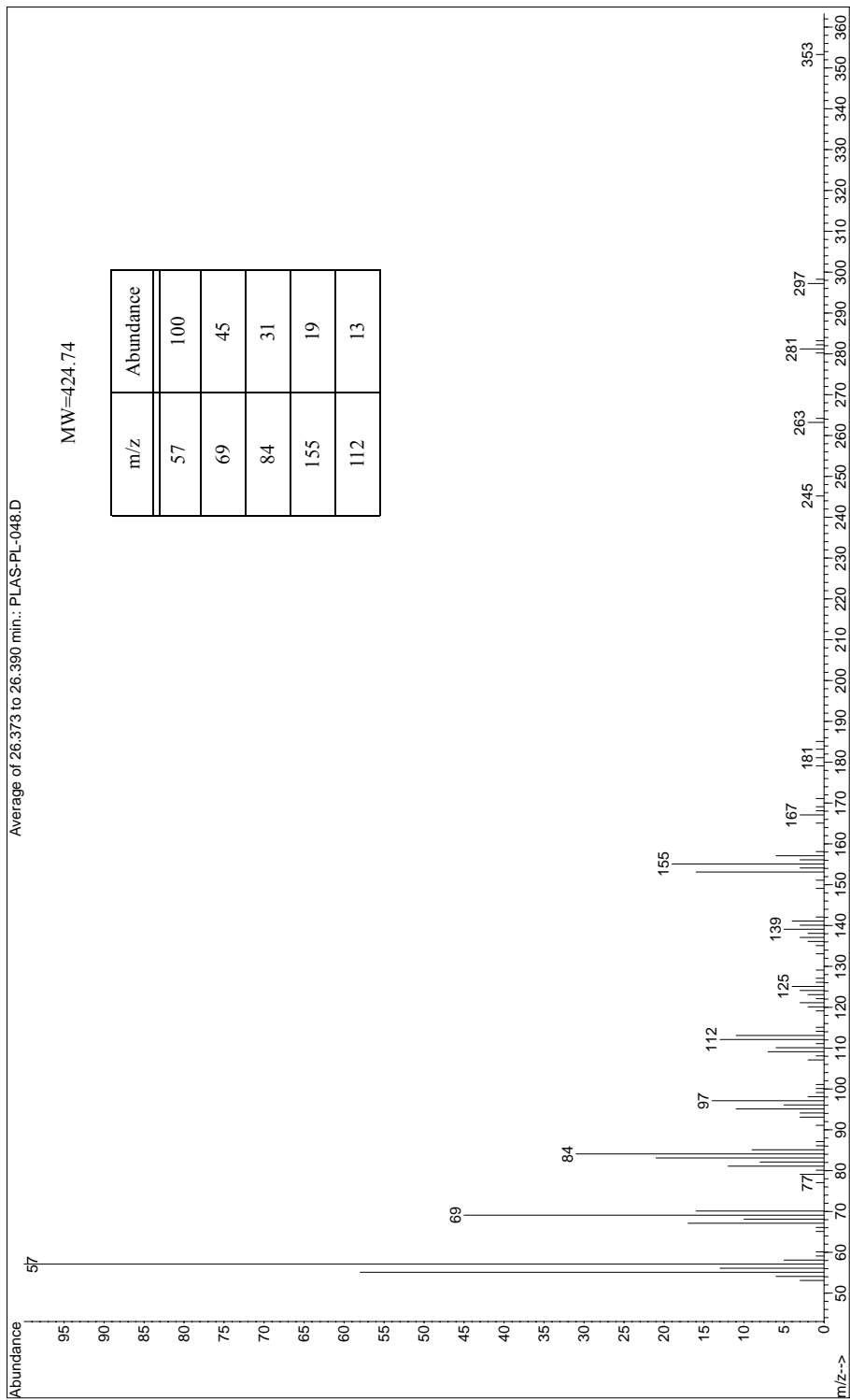
Toxicological Data

While there is no specific information on the metabolism of these materials, there is a large body of research on the metabolism and absorption of vegetable oils. Because of the similarity in physicochemical properties of these materials, it is assumed that they are absorbed and metabolized in a manner similar to vegetable oils, rather than simply excreted.

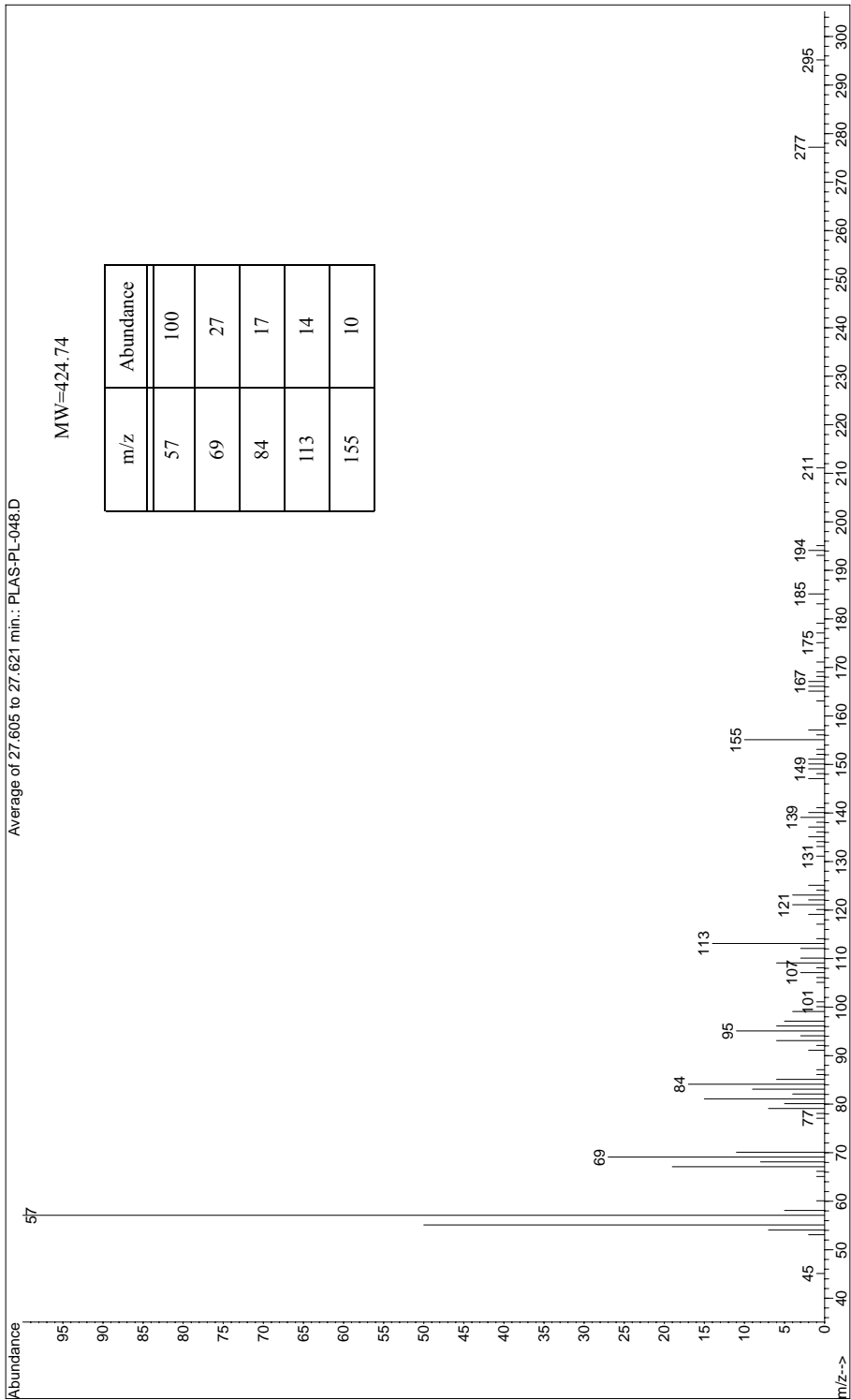
Mass Spectrum for Flexol® EP-8 - PLAS-PL-048



Mass Spectrum for Flexol® EP-8 - PLAS-PL-048

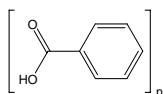
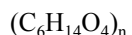
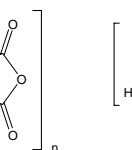
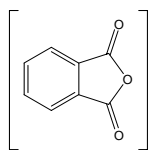
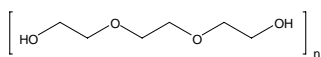


Mass Spectrum for Flexol® EP-8 - PLAS-PL-048



Hercoflex® 900

Hercules Incorporated

**CAS Number** 68186-30-1**RTECS Number** Not available**Abbreviation****Formula** See Below Structure**Molecular Weight** 420.41**Chemical Name**

1,3-isobenzofurandione, polymer with 2,2'-(1,2-ethanediylbis(oxy))bis(ethanol), benzoate

Synonyms**Brand Names & Manufacturers****Physical Properties****Appearance** Clear, viscous liquid**Melting Point** Not available**Boiling Point** 197 °C**Stability** Stable under recommended handling and storage conditions.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	40-80	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Plasticizer and adhesion promoter for polyvinyl acetate and other film-formers. Component in latex adhesives, paints, emulsion waxes, polishes, carpet backing, and variety of other formulations.

Regulatory Information

Approved by the FDA as a food contact additive by 21CFR175.105.

Environmental Impact

Listed as persistent, non-bioaccumulative and not inherently toxic to fish and aquatic organisms.

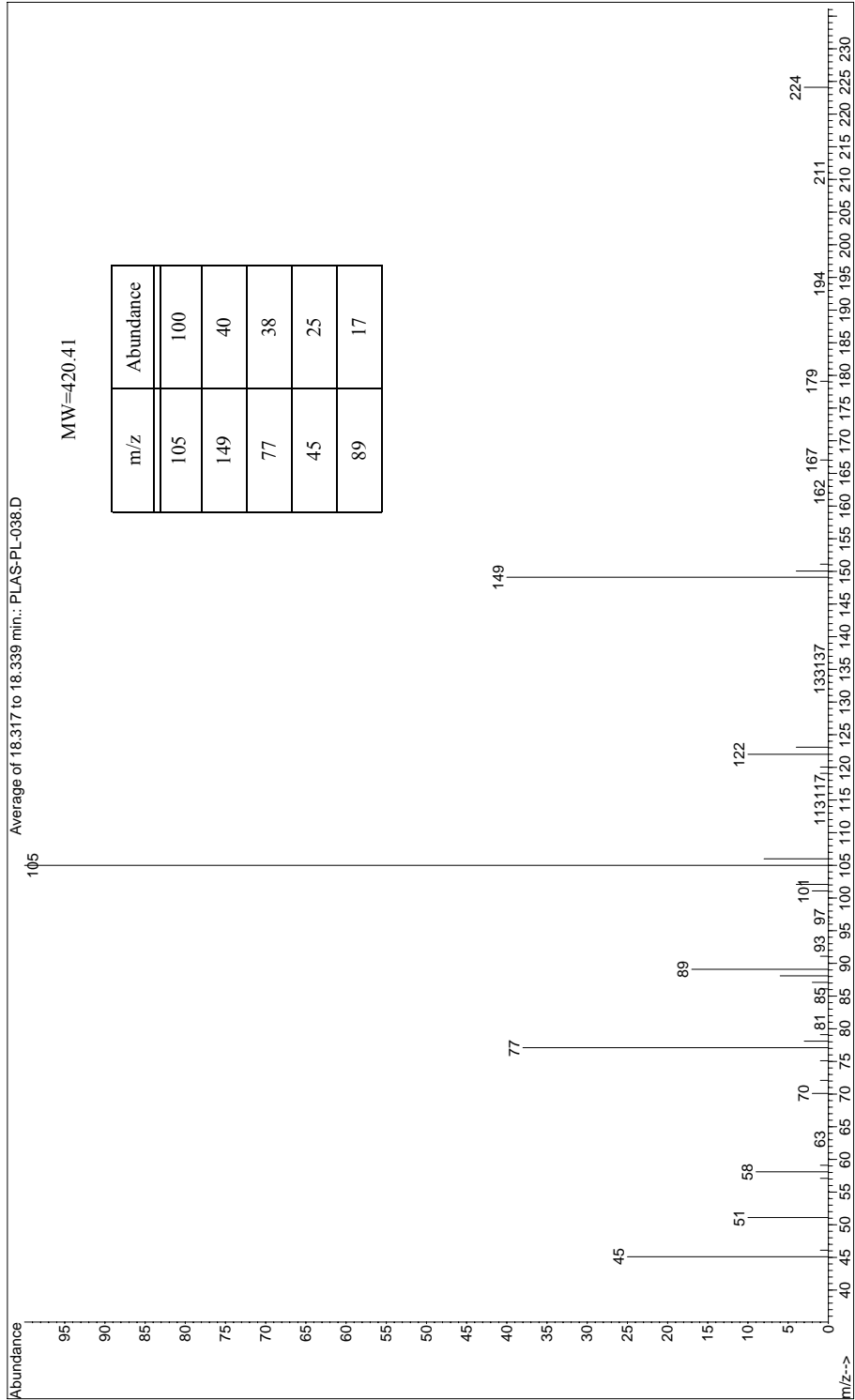
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

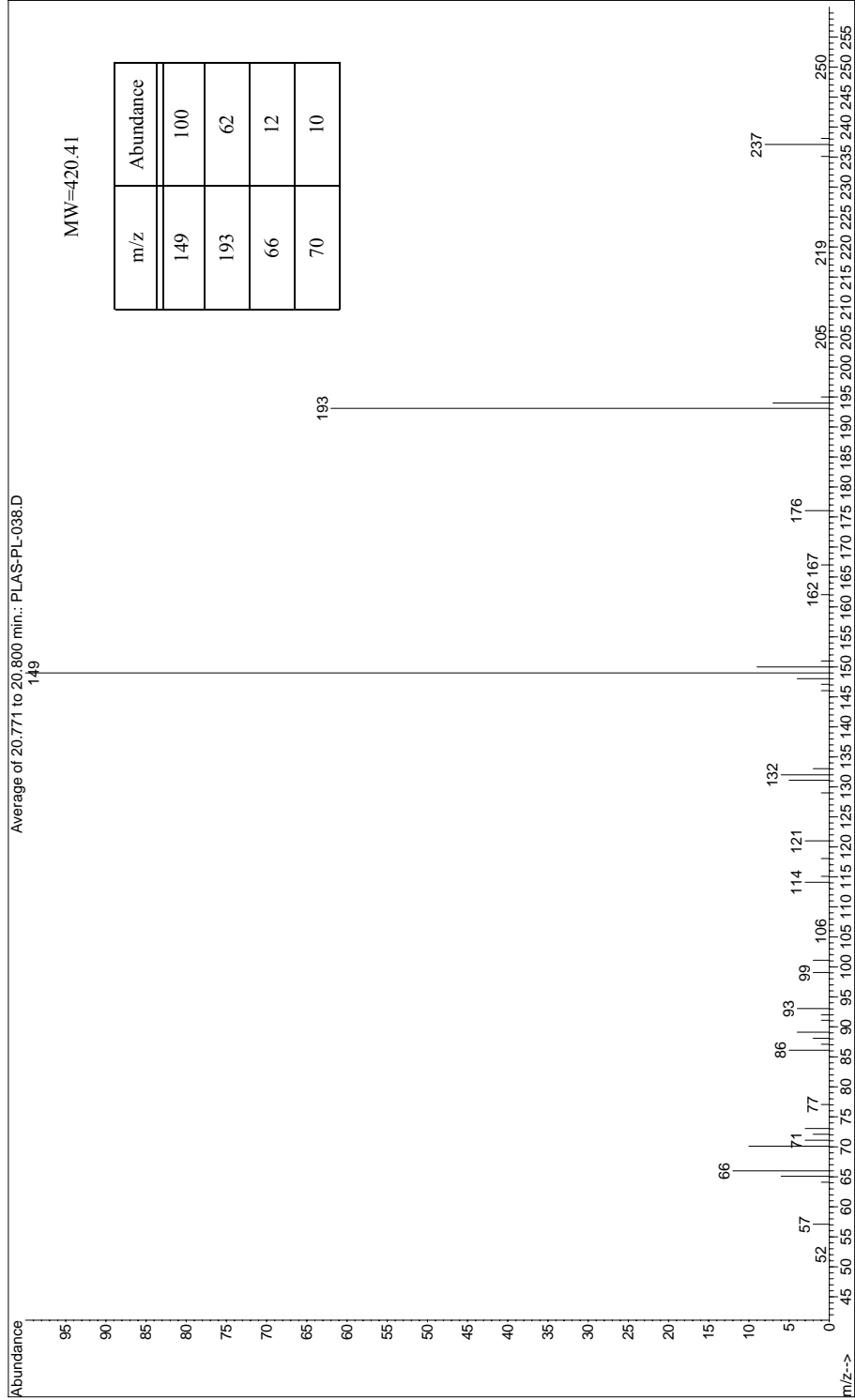
Toxicological Data

Acute oral (LD50): 7.9 g/kg [Rat].

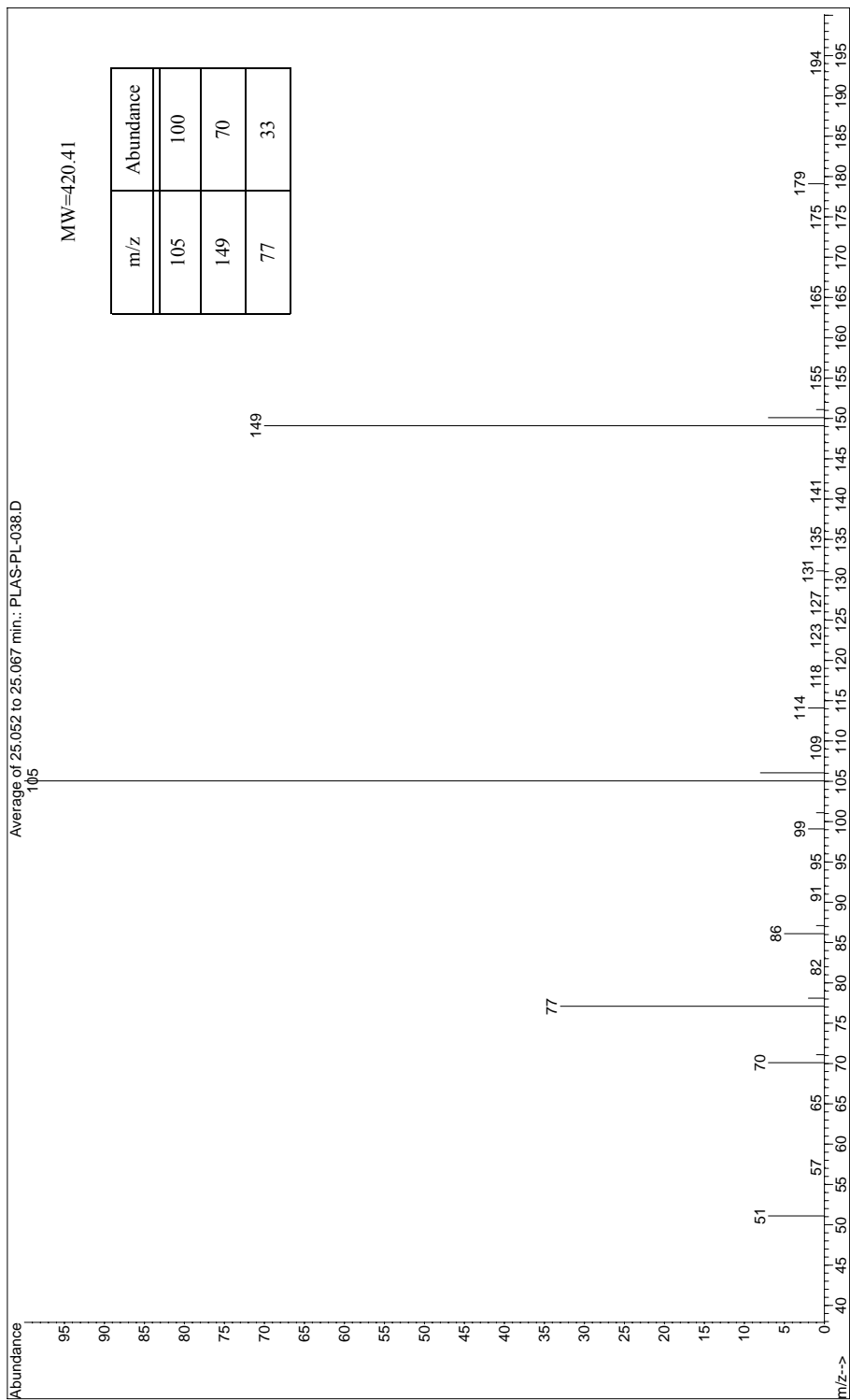
Mass Spectrum for Hercoflex® 900 - PLAS-PL-038



Mass Spectrum for Hercoflex® 900 - PLAS-PL-038



Mass Spectrum for Hercoflex® 900 - PLAS-PL-038



Hi-Point® PD-1

Chemtura Corporation

Unspecified
Structure**CAS Number** Not available**RTECS Number** Not available**Abbreviation****Formula** Not applicable**Molecular Weight** Not applicable**Chemical Name**

methyl ethyl ketone peroxide solution stabilized with dimethyl phthalate

Synonyms

Brand Names & Manufacturers

Physical Properties

Appearance	Clear liquid					
Melting Point	Not available			Boiling Point	Not available	
Stability	Stable if stored at or below 100°F.					
Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	10-40	10-40	10-40	10-40	10-40

Application Application, Regulatory & Environmental Information

Plasticizer solution containing ~20% methyl ethyl ketone peroxide, stabilized with dimethyl phthalate and a proprietary safety diluent, used principally in the curing of promoted unsaturated polyester resins where an extended catalyst is desired for improved concentration control.

Regulatory Information

EPA lists MEK peroxide as likely to leach dangerous concentrations of toxic chemicals into ground water and regulates it under TCLP. Dimethyl phthalate has been identified as a priority pollutant and is regulated under the Clean Water Act, the Clean Air Act, RCRA and the Superfund Amendment.

Environmental Impact

At least 50% of the components of this product are considered to be hazardous to the environment and toxic to aquatic organisms.

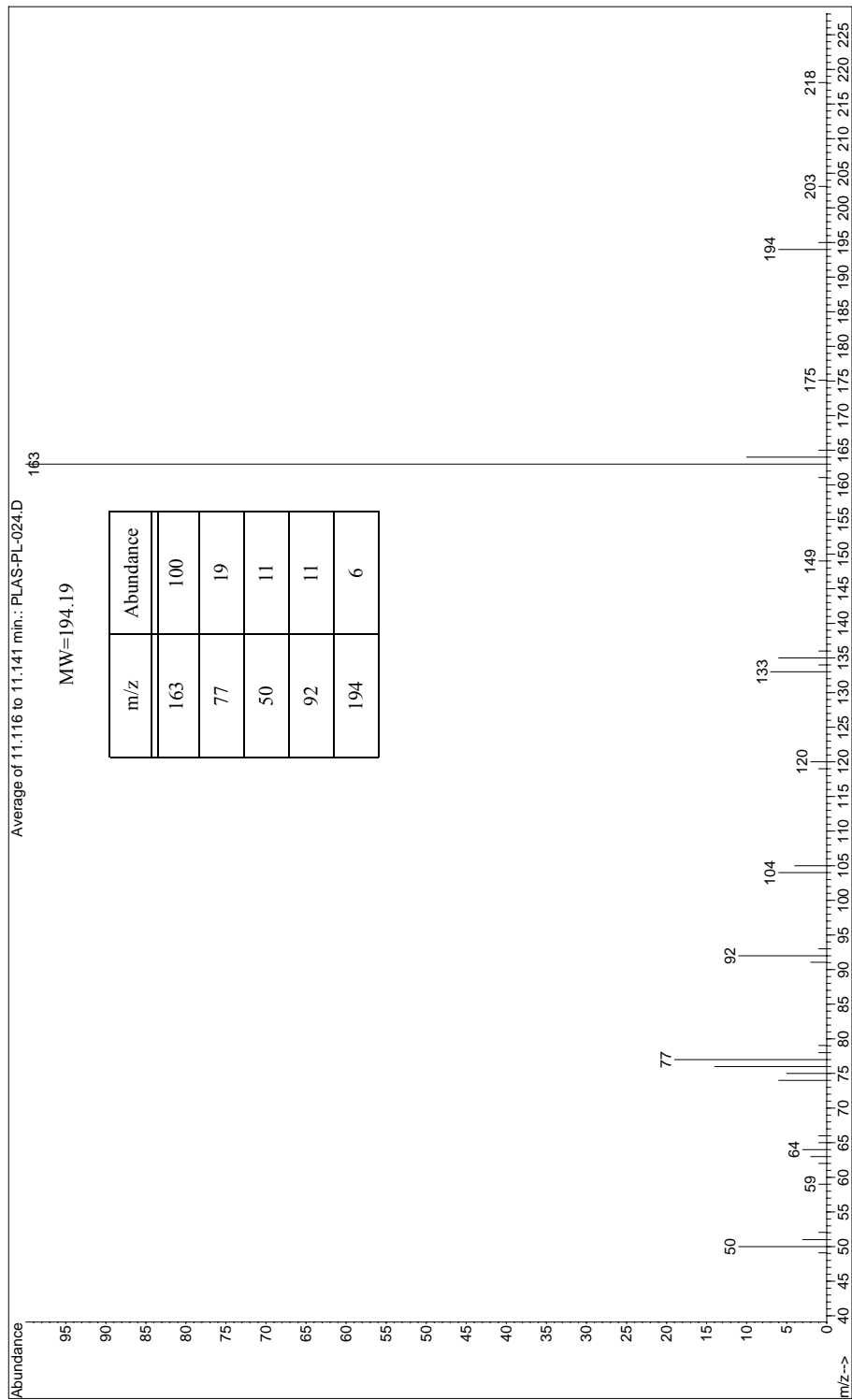
Point of Release

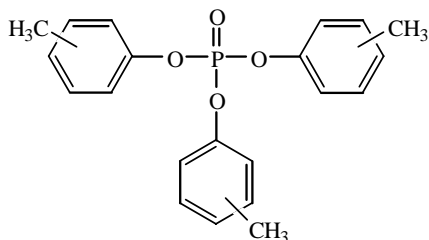
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute Toxicity oral (LD50): 017 mg/kg [Rat]; skin (LD50): 4000 mg/kg [Rabbit]; inhalation (LC50): 17 mg/L [Mouse].

Mass Spectrum for Hi-Point® PD-1 - PLAS-PL-024



Imol S-140**CAS Number** 1330-78-5**RTECS Number** TD0175000**Abbreviation** TCP**Formula** C₂₁H₂₁O₄P**Molecular Weight** 368.37**Chemical Name**

phosphoric acid, tris(methylphenyl) ester

Synonyms

tricesyl phosphate; tritolyl phosphate; phosphoric acid, tris(methylphenyl) ester

Brand Names & Manufacturers

Flexol Plasticizer TCP

Phosflex 179A

Physical Properties**Appearance** Clear, faintly yellow, viscous odorless liquid**Melting Point** -33 °C**Boiling Point** 420 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	U	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

TCP is used as a plasticizer in vinyl plastics, as a flame-retardant, and as an additive to extreme pressure lubricants. The main market for PVC-based products plasticized with organic phosphate esters is in the manufacture of automobile and other motor vehicle interiors in the USA.

Regulatory Information

This product is classified as a toxic material for shipping purposes. It is not approved by the FDA for food contact applications.

Environmental Impact

TCP's low water solubility and high adsorption to particulates causes adsorption onto river or lake sediment and soil. Biodegradation in river water is rapid, almost complete within 5 days. Abiotic degradation is slower with a half-life of 96 days. BCFs of 165-2768 were measured for several fish species in the laboratory using radiolabelled TCP. Radioactivity was lost rapidly on cessation of exposure, depuration half-lives ranged between 25.8 and 90 hours.

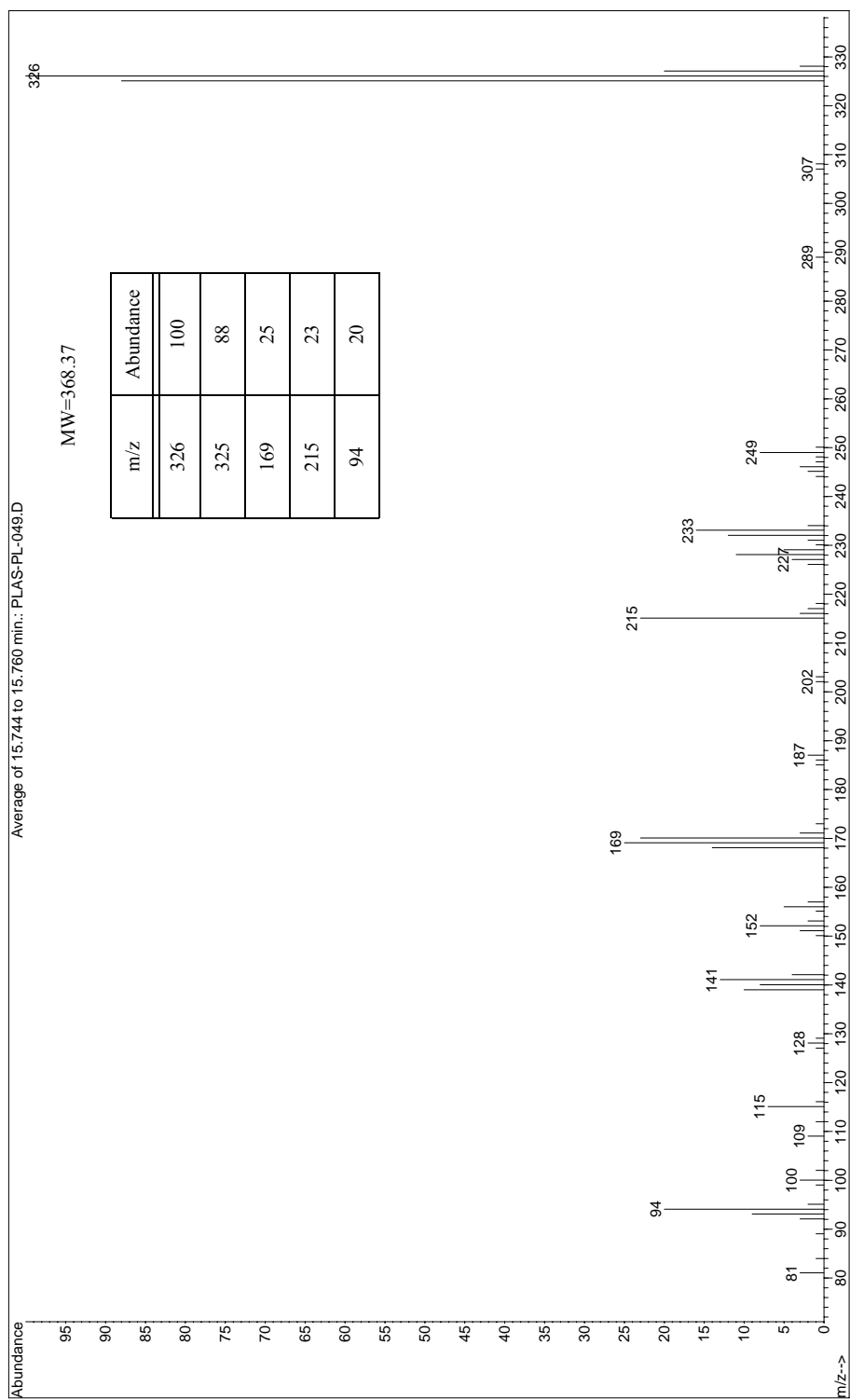
Point of Release

This product can be released into the atmosphere more rapidly in extreme temperatures. In addition, UV exposure from parking in the sun creates a favorable environment for chemical breakdown. The extreme conditions of heat and sunlight in the interior of an automobile can cause gasses to escape from the plasticizer.

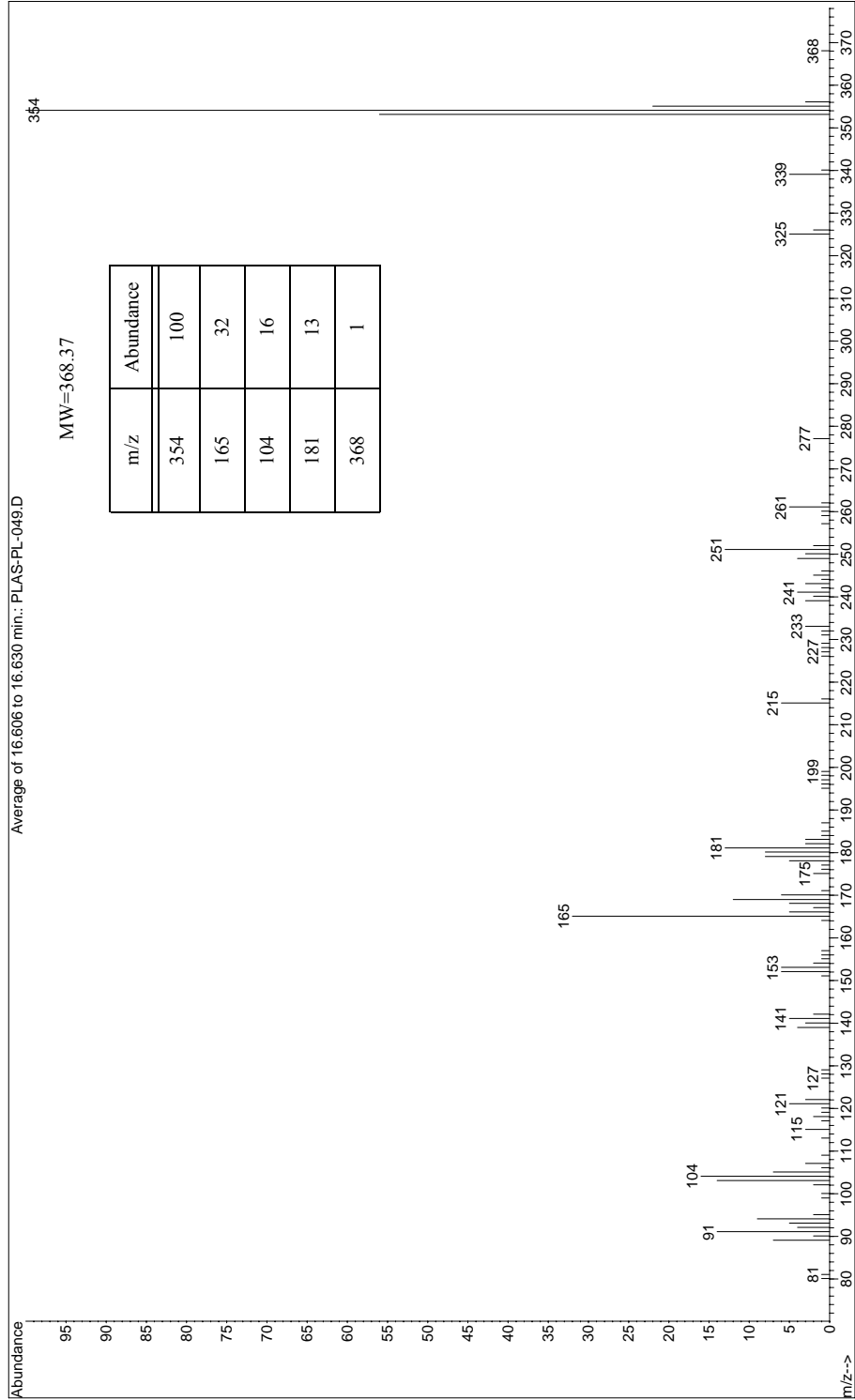
Toxicological Data

This substance is toxic to the central nervous system.

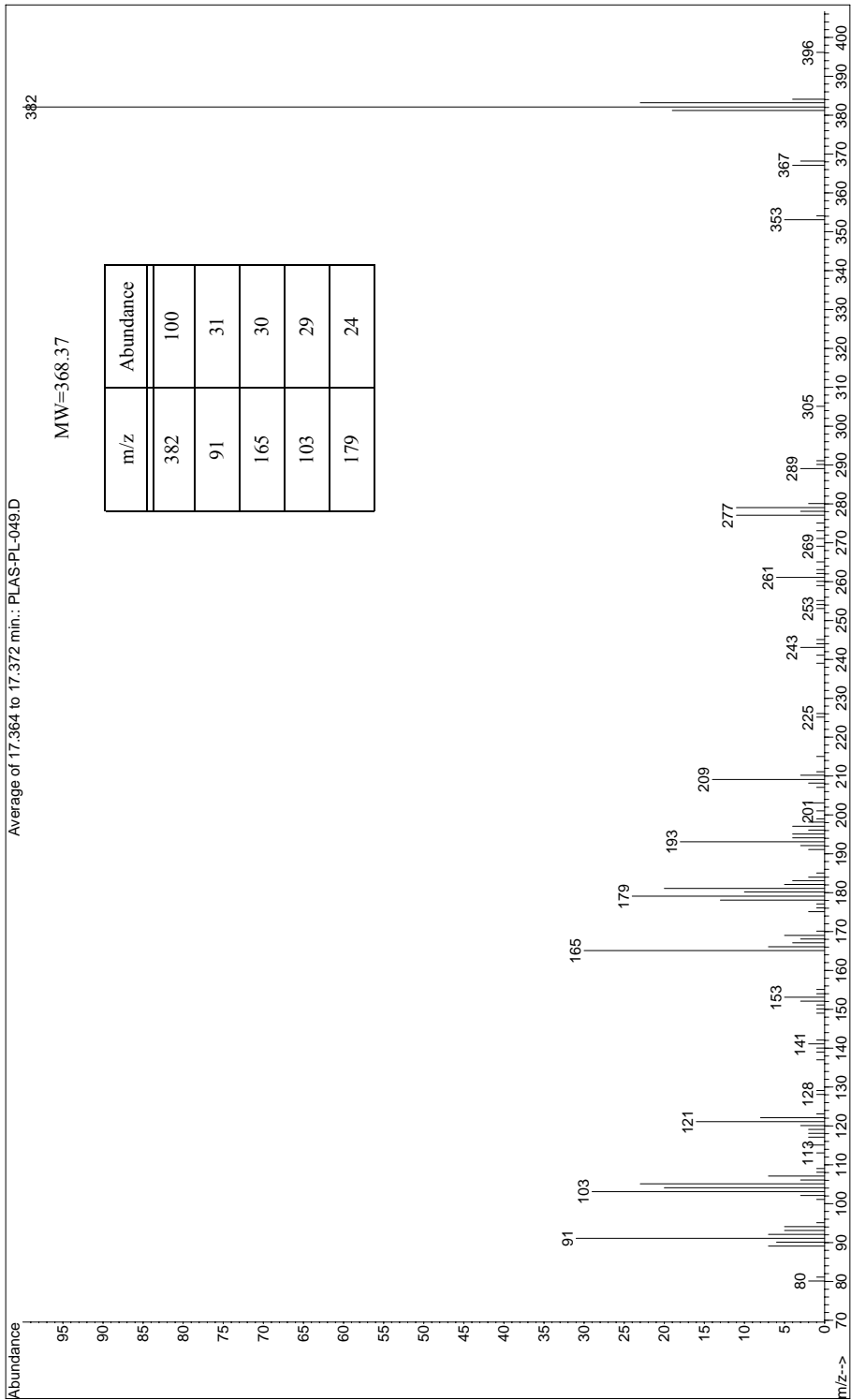
Mass Spectrum for Imol S-140 - PLAS-PL-049



Mass Spectrum for Imol S-140 - PLAS-PL-049

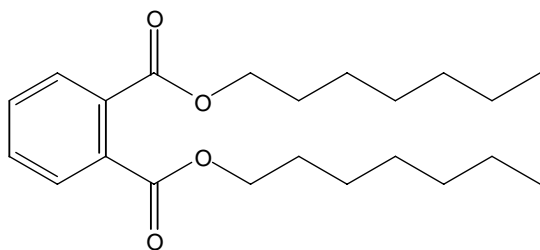


Mass Spectrum for Imol S-140 - PLAS-PL-049



Jayflex® 77

ExxonMobil Corporation

**CAS Number** 71888-89-6**RTECS Number** Not available**Abbreviation** DIHP**Formula****Molecular Weight****Chemical Name**
diisooheptyl phthalate**Synonyms**
1,2-benzenedicarboxylic acid

Brand Names & Manufacturers

Physical Properties

<i>Physical Properties</i>						
Appearance	Clear liquid, characteristic odor					
Melting Point	Not available			Boiling Point >300 °C		
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U

Application, Regulatory & Environmental Information

Application
Used as a plasticizer for molding and coating plastisols, vinyl flooring, tile, and carpet backing. May also be used as a partial replacement for higher molecular weight phthalate plasticizers (extrusion, injection molding, and calendaring applications).

Regulatory Information

This product does not have FDA approval for food contact applications.

Environmental Impact

Test data indicates no associated acute aquatic toxicity but may show chronic toxicity. It is reported to be readily biodegradable, but may pose a moderate bioaccumulative risk based on a log Kow value of 5.6.

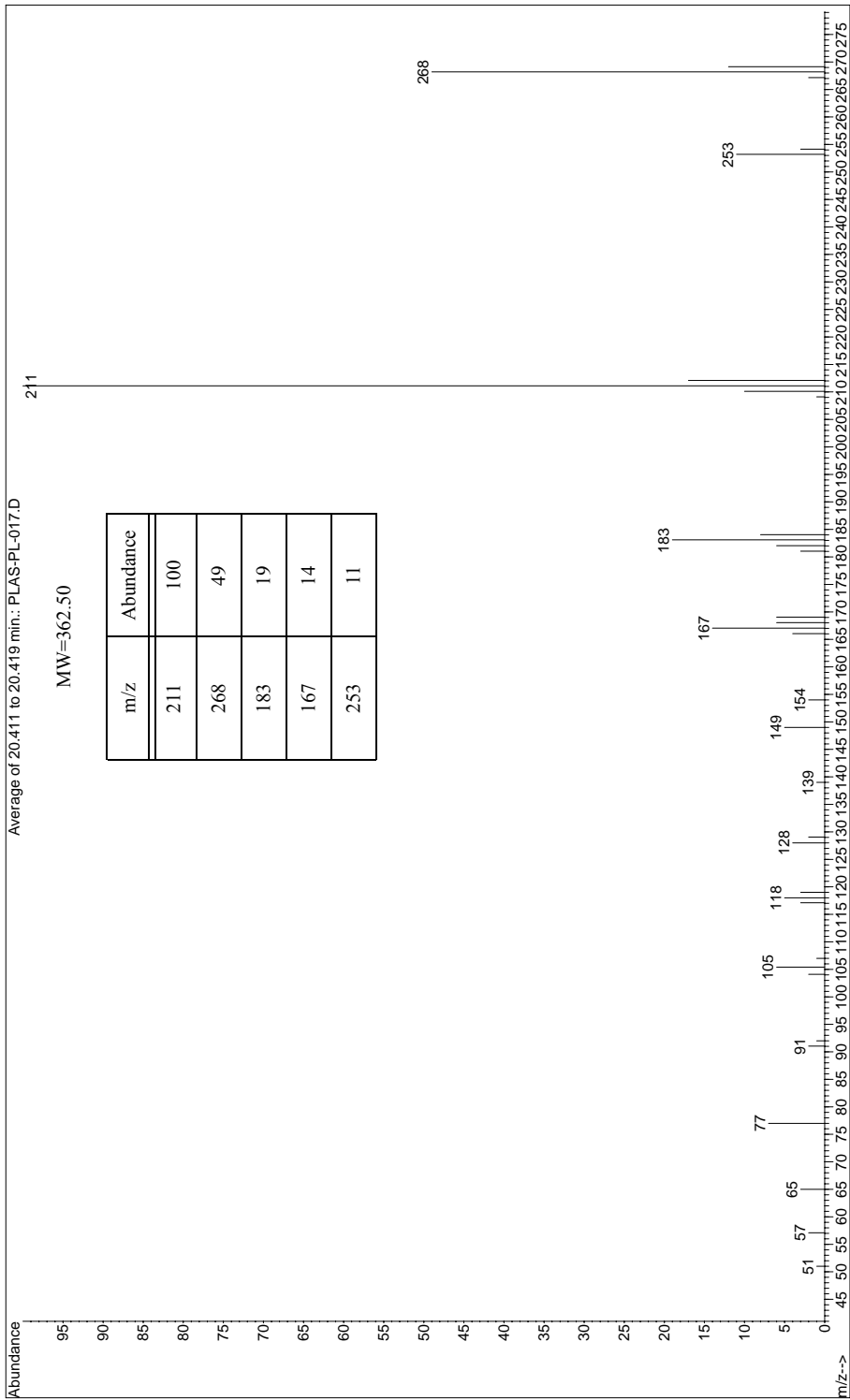
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

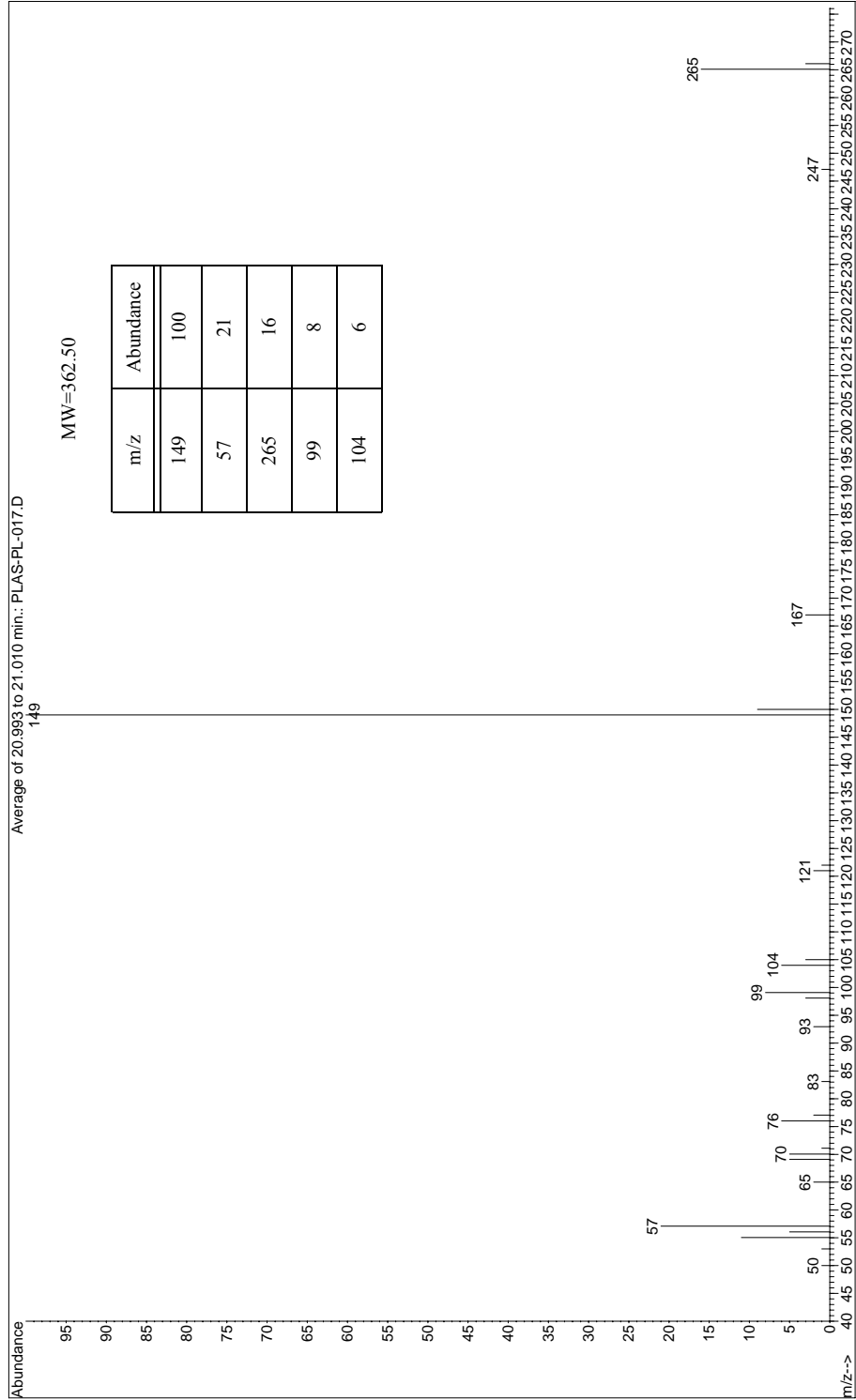
Toxicological Data

This compound is classified as a transitional phthalate, which has greater mammalian toxicity potential, particularly with regard to reproductive and developmental effects, compared to either the low or high molecular weight phthalate categories. It is not listed by ACGIH, IARC, NTP, OSHA as a cancer causing agent.

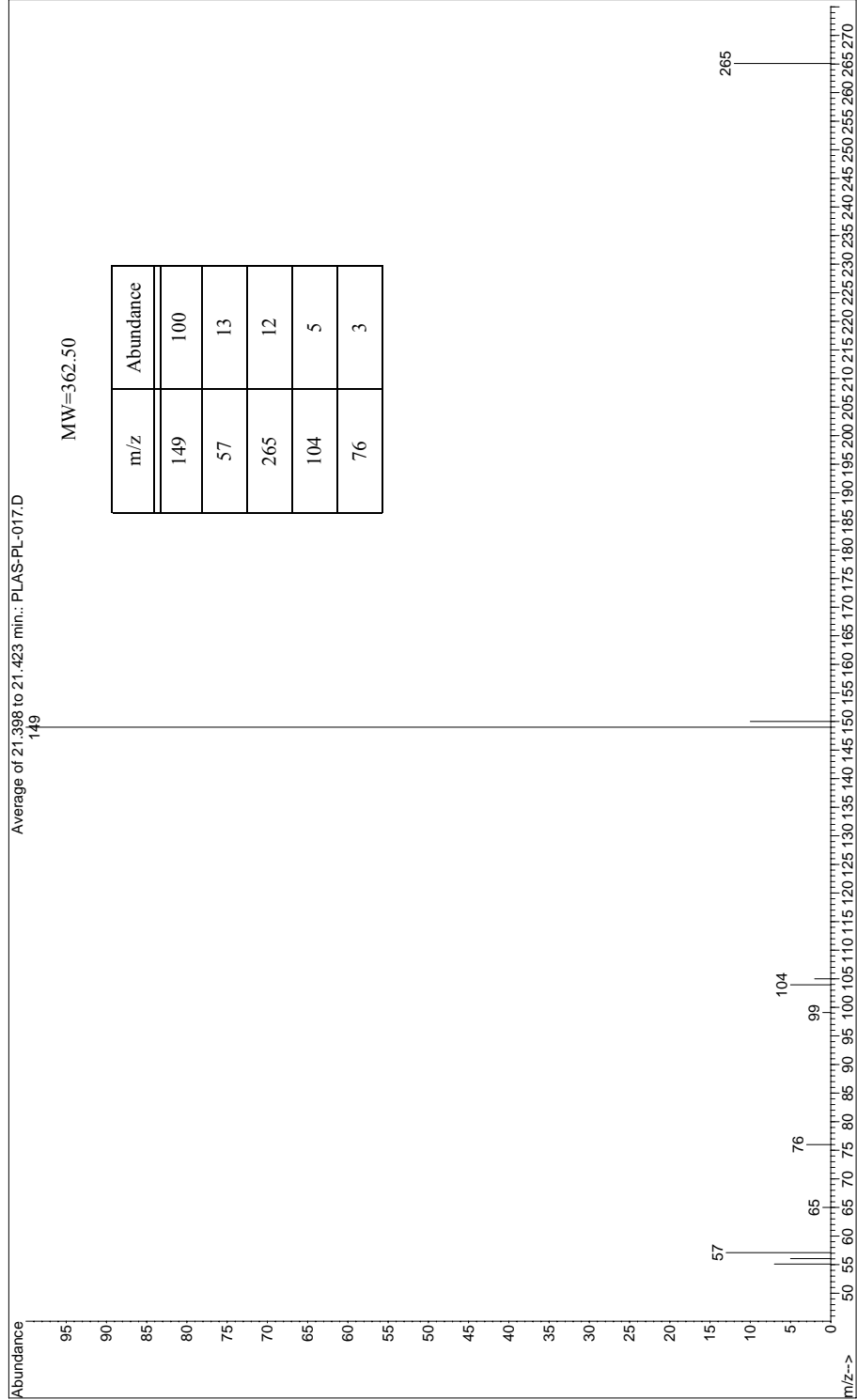
Mass Spectrum for Jayflex® 77 - PLAS-PL-017



Mass Spectrum for Jayflex® 77 - PLAS-PL-017

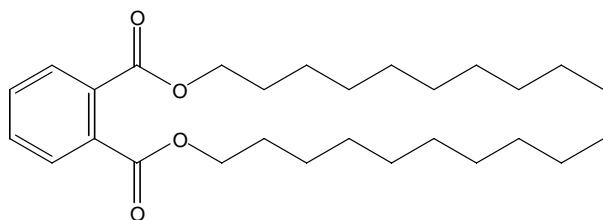


Mass Spectrum for Jayflex® 77 - PLAS-PL-017



Jayflex® DIDP

ExxonMobil Corporation

**CAS Number** 68515-49-1**RTECS Number** Not available**Abbreviation** DIDP**Formula** C₂₈H₄₆O₄**Molecular Weight** 446.66**Chemical Name**

diisodecyl phthalate

Synonyms

bis(8-methylnonyl) phthalate; 1,2-benzenedicarboxylic acid diisodecyl ester

Brand Names & Manufacturers

Palatinol® DIDP

BASF

Physical Properties**Appearance** Clear, oily liquid; mild odor**Melting Point** Not available**Boiling Point** 250-257 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

DIDP is a general purpose plasticizer with a broad range of applications used in flexible PVC. It is widely used in the toy, construction, automotive, and general consumer product markets. It has limited use in food packaging and is not used in medical applications.

Regulatory Information

Regulated by the State of California Safe Drinking Water Act of 1986.

Environmental Impact

This material is expected to be readily biodegradable and partition to sediment and wastewater solids if released to the environment, but is not expected to be harmful to aquatic organisms. Log Kow value of 8.8 indicates a high potential to bioaccumulate. It is also listed as a persistent bioaccumulative toxin in Europe.

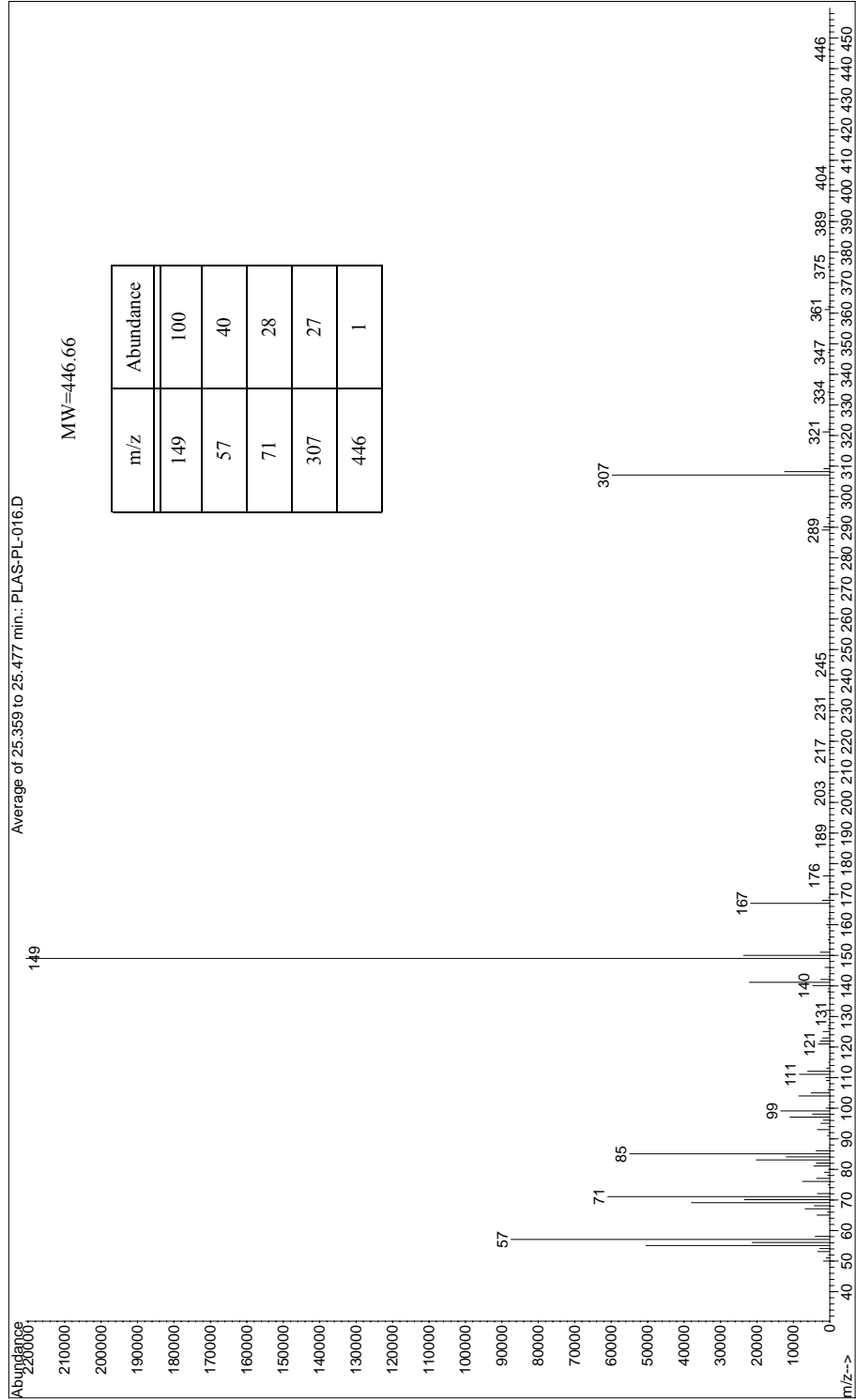
Point of Release

Humans may be exposed to DIDP by the oral, dermal, and inhalation routes of exposure. Occupational exposure occurs primarily through inhalation and dermal contact, while consumer exposure occurs primarily through oral and dermal routes. Exposure of children to DIDP through children's products is a public concern.

Toxicological Data

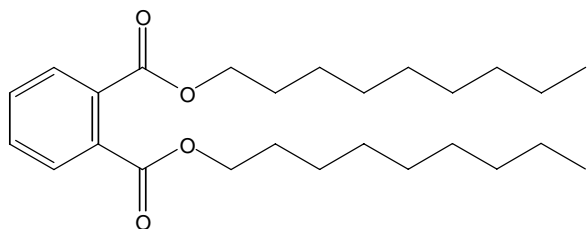
Not listed (ACGIH, IARC, NTP, OSHA) as a cancer causing agent although it has been shown to cause a small, but statistically significant increased early offspring mortality at high oral doses in a 2-generation reproductive study in laboratory animals. Is on CA Proposition 65 list as a chemical known to the State of California to cause developmental toxicity and reproductive toxicity for purposes of the Safe Drinking Water and Toxic Enforcement Act of 1986.

Mass Spectrum for Jayflex® DIDP - PLAS-PL-016



Jayflex® DINP

ExxonMobil Corporation

**CAS Number** 68515-48-0**RTECS Number** CZ3395000**Abbreviation** DINP**Formula** C₂₆H₂₂O₄**Molecular Weight** 418.61**Chemical Name**

diisononyl phthalate

Synonyms

1,2 benzenedicarboxylic acid, di-C9-11 branched alkyl ester

Brand Names & Manufacturers

Palatinol® DINP

BASF

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** Not available**Boiling Point** >250 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

General purpose branched phthalate plasticizer used in coated fabric, film and sheeting, flooring, injection molding and profile extrusion and plastisols.

Regulatory Information

Diisononyl phthalate is FDA approved at levels up to 43%.

Environmental Impact

Not expected to be harmful to aquatic organisms. Not expected to demonstrate chronic toxicity to aquatic organisms. Material is expected to partition to sediment and wastewater solids. Minimally volatile. Expected to be readily biodegradable and the potential to bioaccumulate is low.

Point of Release

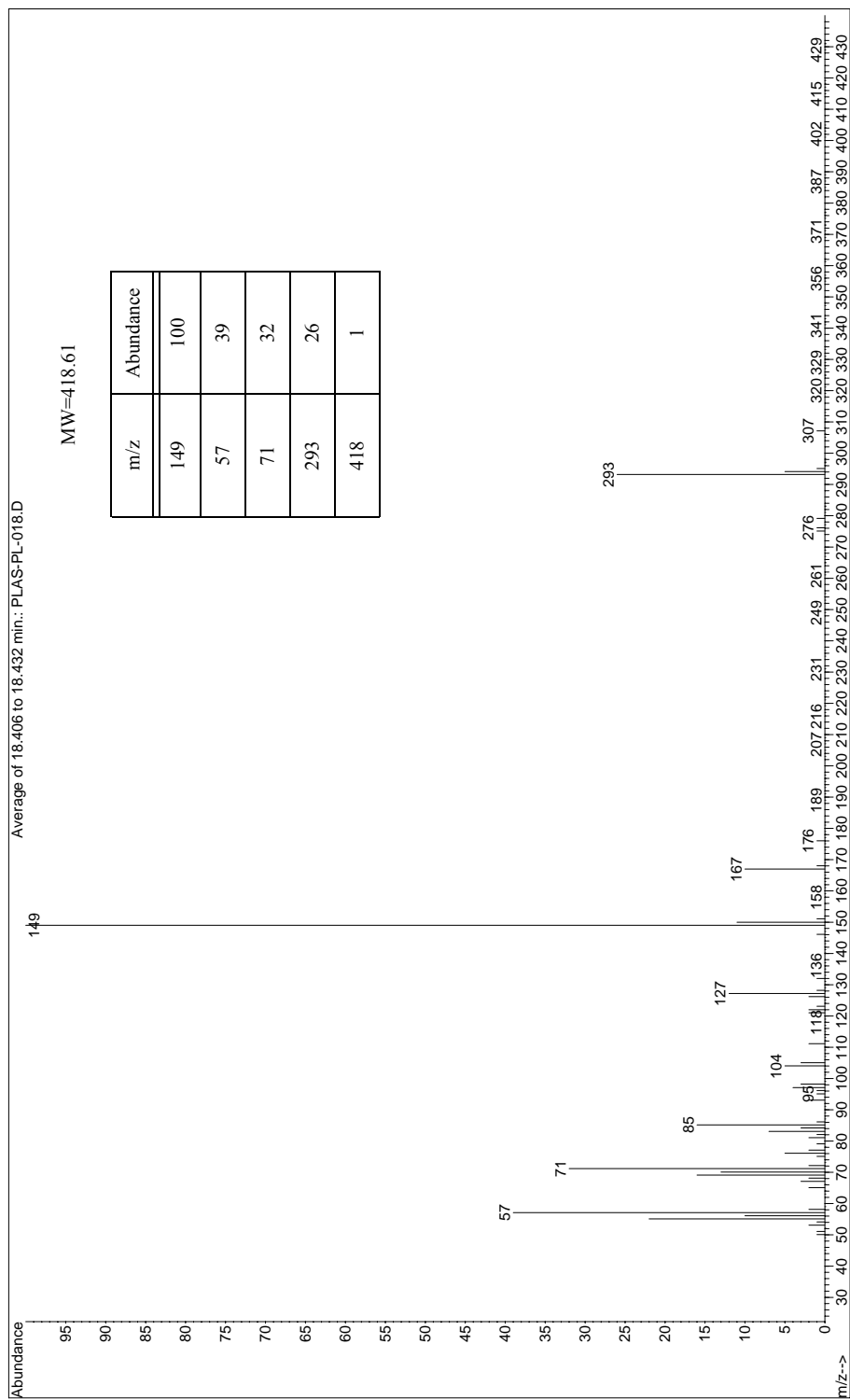
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

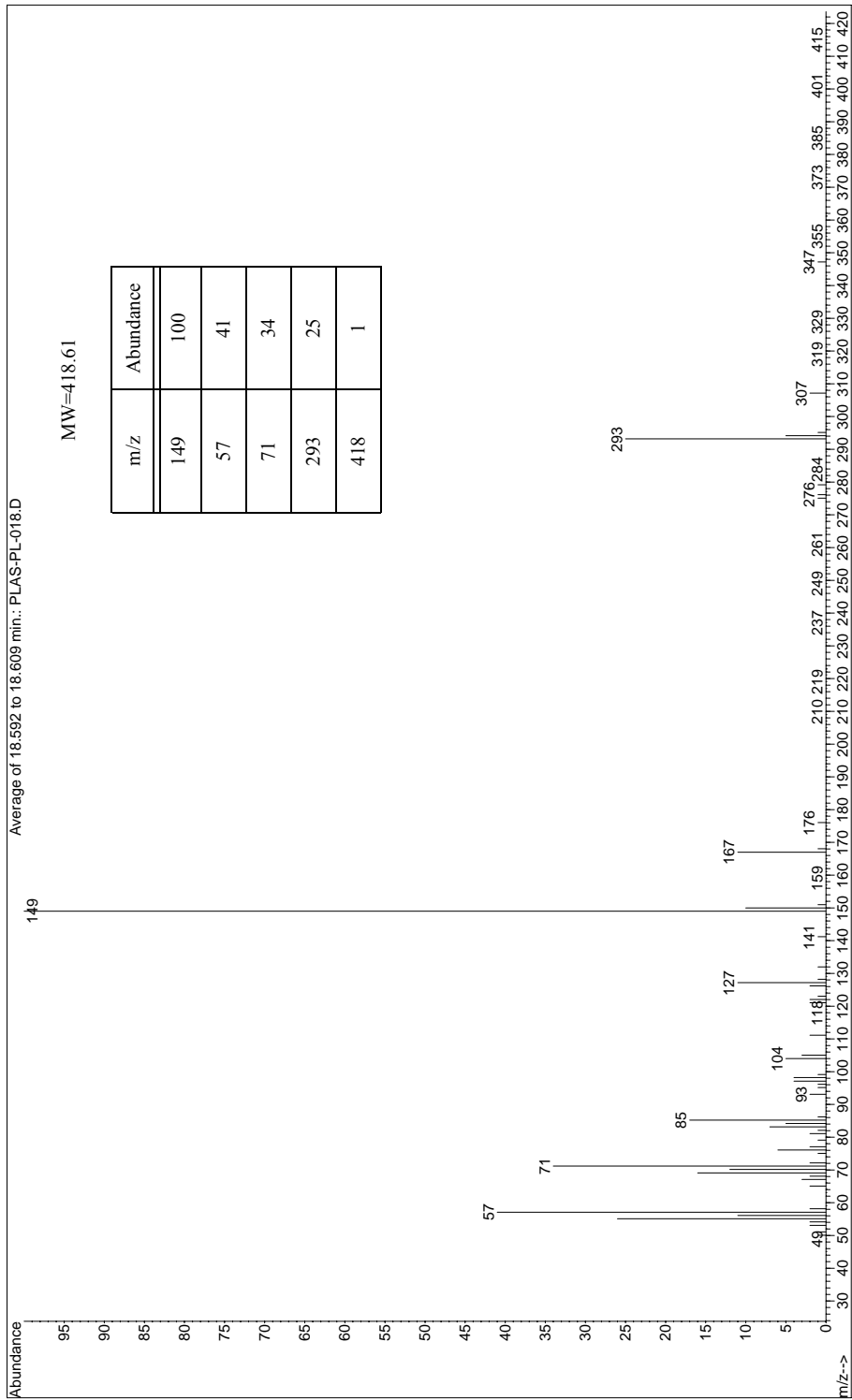
Lowest Published Toxic Oral Dose (TDLo): 32900 mg/kg/70D-C [Rat].

EPA lists as a suspected developmental toxin. Also produced kidney and liver effects when given to rodents in high oral doses.

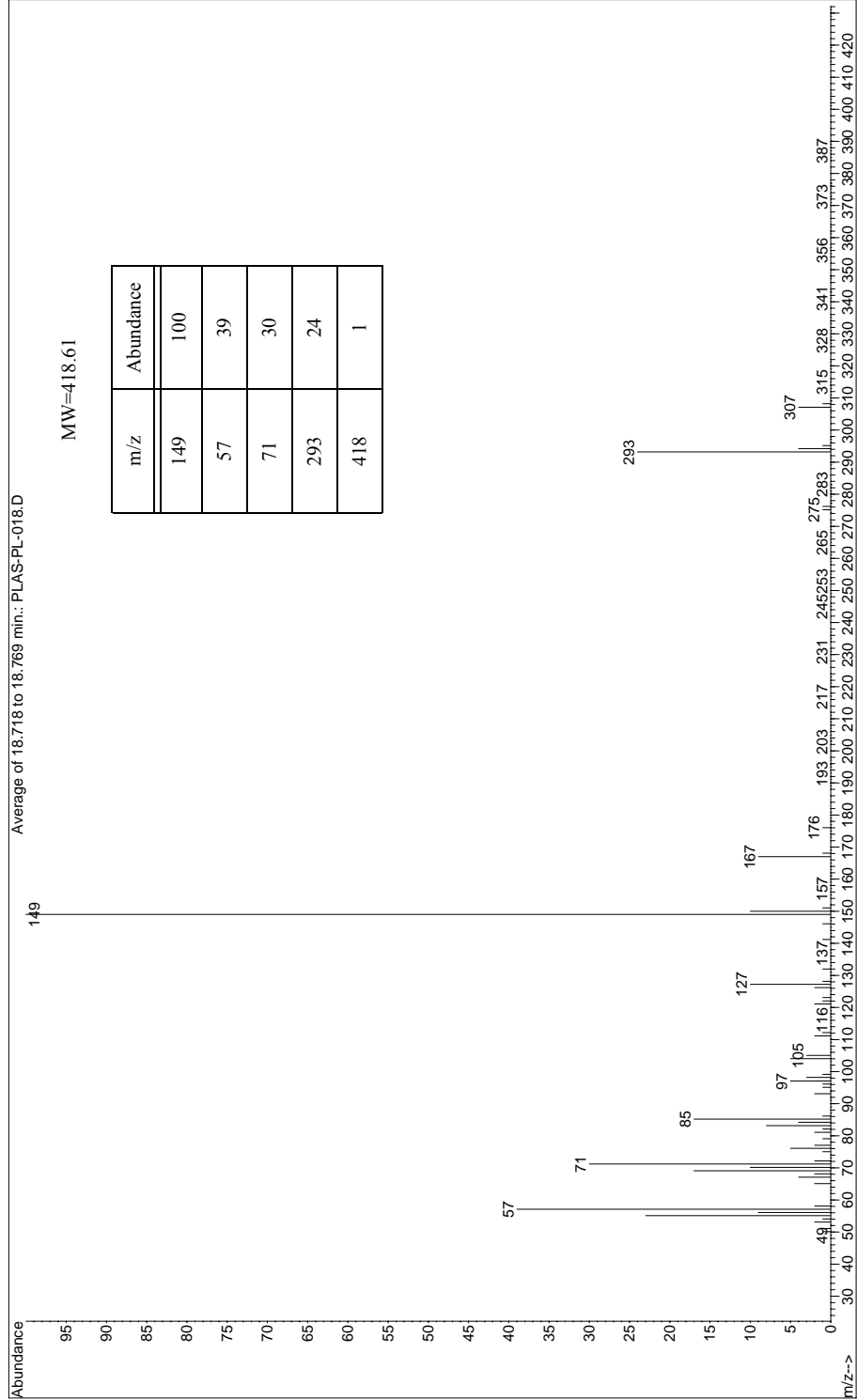
Mass Spectrum for Jayflex® DINP - PLAS-PL-018



Mass Spectrum for Jayflex® DINP - PLAS-PL-018

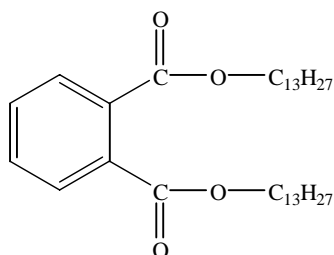


Mass Spectrum for Jayflex® DINP - PLAS-PL-018



Jayflex® DTDP

ExxonMobil Corporation

**CAS Number** 68515-47-9**RTECS Number** Not available**Abbreviation** DTDP**Formula** C₃₄H₅₈O₄**Molecular Weight** 530.92**Chemical Name**
ditridecyl phthalate**Synonyms**

1,2 benzenedicarboxylic acid, di-C11-14 branched alkyl ester

Brand Names & Manufacturers

Palatinol® 79P

BASF

Physical Properties**Appearance** Clear, colorless liquid**Melting Point** Not available**Boiling Point** > 250 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information**Application**

Highest molecular weight and most permanent monomeric phthalate plasticizer commercially available. Used for high temperature rated PVC insulation. Other end uses include traffic cones, automotive sealants, fabric coatings, fishing lures and shoe compounds.

Regulatory Information

Does not have FDA approval for food contact applications.

Environmental Impact

This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms. If released into the environment, it would be expected to partition to sediment and wastewater solids.

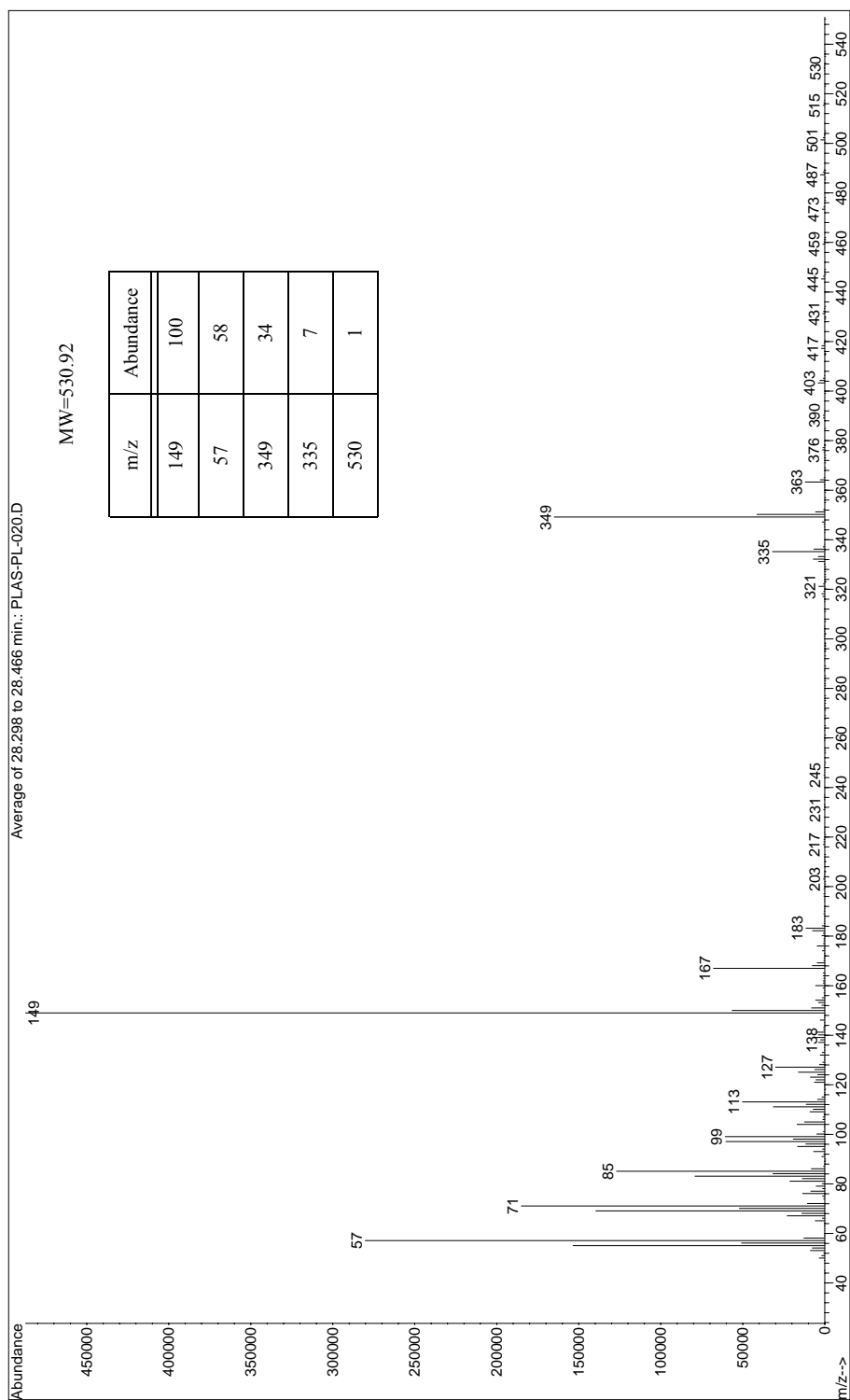
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

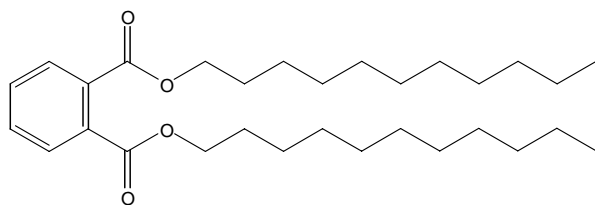
There are concerns regarding potential adverse health effects due to exposure to phthalates, particularly reproductive and developmental health effects.

Mass Spectrum for Jayflex® DTD[®] - PLAS-PL-020



Jayflex® L11P-E

ExxonMobil Corporation

**CAS Number** 3648-20-2**RTECS Number** TI1980000**Abbreviation** DUP**Formula** C₃₀H₅₀O₄**Molecular Weight** 474.72**Chemical Name**

diundecyl phthalate

Synonyms

DUP; 1,2-benzenedicarboxylic acid, diundecyl ester; phthalic acid, diundecyl ester

Brand Names & Manufacturers

Palatinol® 11P-I

BASF

Santicizer® 711

Solutia Inc.

Physical Properties**Appearance** Clear liquid with a characteristic odor**Melting Point** Not available**Boiling Point** 523 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	U	U	U	U	U

Application, Regulatory & Environmental Information**Application**

Highly permanent, low volatility, linear plasticizer used in wire and cable insulation for automotive and communications applications, low temp, high performance film and sheeting as well as low fogging automotive interiors.

Regulatory Information

Diundecyl phthalate is FDA approved for use as a component of poly (p-methylstyrene) and rubber-modified poly (p-methylstyrene) intended for use in contact with food, subject to 21CFR177.1635.

Environmental Impact

This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms. If released into the environment, it would be expected to partition to sediment and wastewater solids.

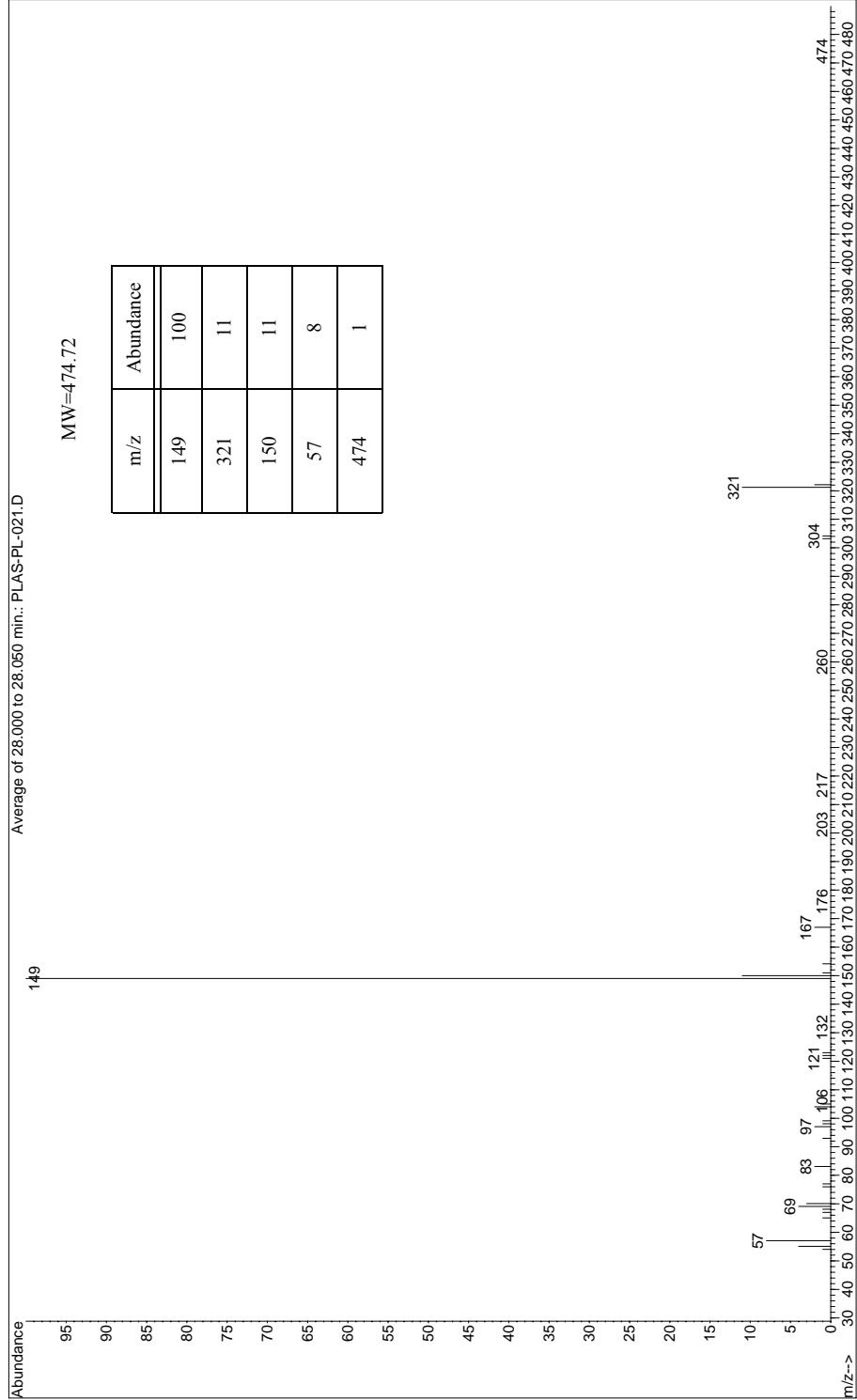
Point of Release

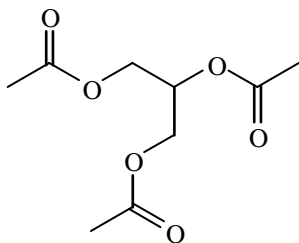
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed by ACGIH, IARC, NTP, or OSHA as a cancer causing agent. Acute intraperitoneal LD50 >15.8 g/kg [Mouse]; Acute dermal (LD50): >10 g/kg [Rabbit]; Acute oral (LD50): >20 g/kg [Rat]; Acute inhalation (LC50 6 hr) >6040 mg/m³ [Rat].

Mass Spectrum for Jayflex® L11P-E - PLAS-PL-021



Kesscoflex TRA

CAS Number 102-76-1

RTECS Number AK3675000

Abbreviation

Formula C₉H₁₄O₆

Molecular Weight 218.20

Chemical Name

1,2,3-propanetriol triacetate

Synonyms

triacetin; glycerol triacetate; glyceryl triacetate

Brand Names & Manufacturers

Kodaflex® triacetin

Eastman Chemical

Physical Properties**Appearance** Colorless, oily liquid**Melting Point** 3 °C**Boiling Point** 259 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	70	40-80	40-80	U	U	U

Application Application, Regulatory & Environmental Information

Plasticizer for cellulose nitrate (commonly used in cigarette filters). Also used as a solvent for basic dyes, fixative in perfumery, food additive, pharmaceuticals, and photographic films.

Regulatory Information

Triacetin is approved by the FDA for direct and indirect food contact applications.

Environmental Impact

Triacetin is readily biodegradable. The chemical is expected to have a low potential for bioaccumulation based on a low log Pow (0.21). Considered to be nontoxic to aquatic organisms and birds.

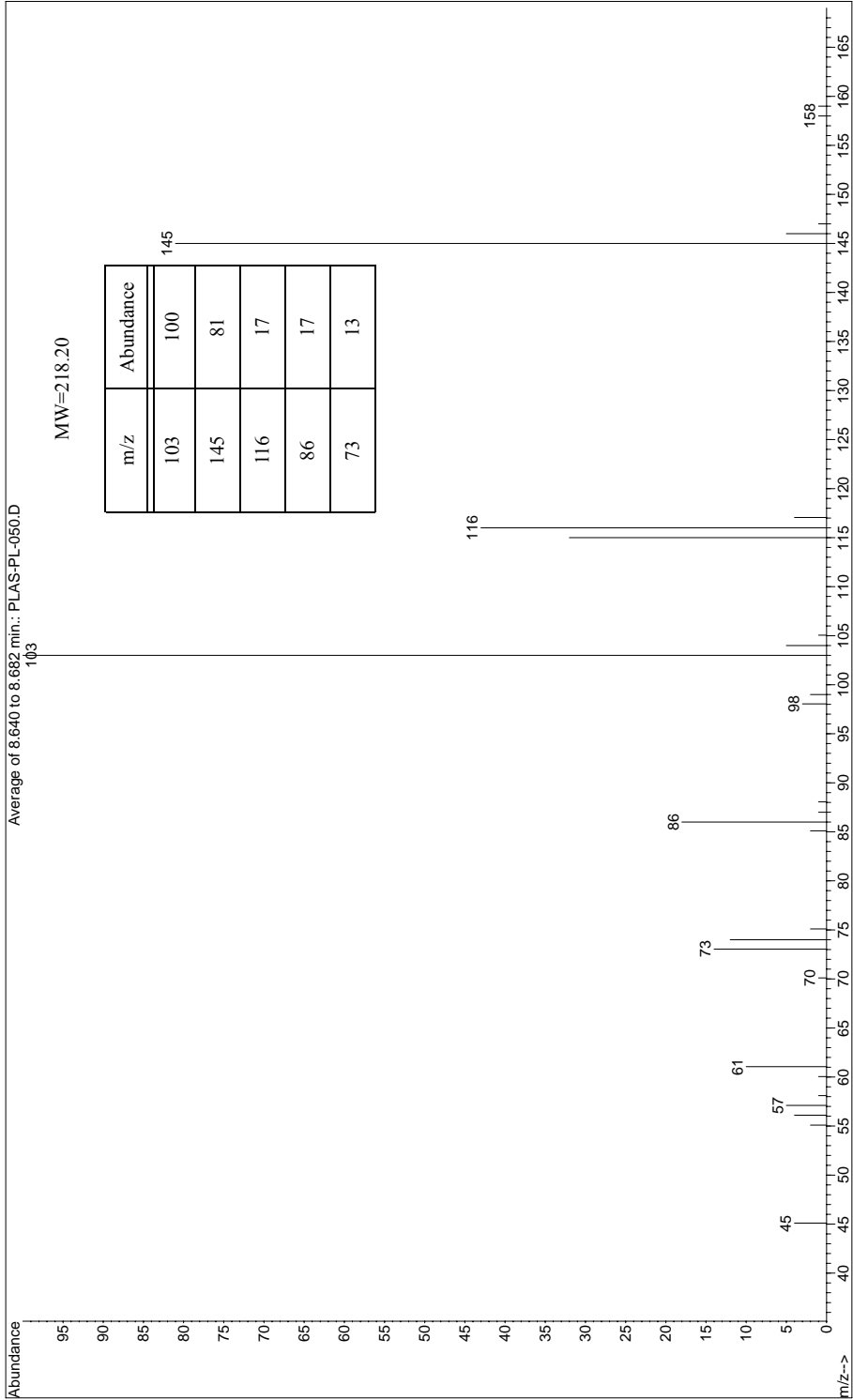
Point of Release

Environmental exposure may occur from emission to aquatic compartment from wastewater and evaporative emissions associated with its use in the perfume and cosmetic industries and its use as a solvent and CO₂ remover from natural gas, and disposal of consumer products containing triacetin.

Toxicological Data

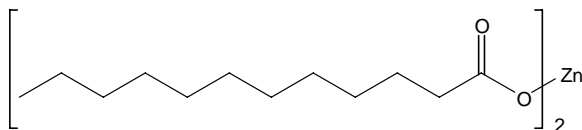
Based on the available data and anticipated daily intake (7.8 mg/day/adult), triacetin and a group of related triglycerides did not represent a hazard to human health.

Mass Spectrum for Kesscoflex TRA - PLAS-PL-050



Laurex®

Chemtura Corporation



CAS Number Not available

RTECS Number Not available

Abbreviation

Formula $C_{24}H_{46}O_4Zn$

Molecular Weight 464.01

Chemical Name

zinc salt of lauric and related fatty acids

Synonyms**Brand Names & Manufacturers****Physical Properties****Appearance** Tan, flaked solid**Melting Point** 107-118 °C**Boiling Point** Not available**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water <0.1	MeOH U	EtOH U	Acetone <0.1	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Activator and plasticizer for general use in natural and synthetic rubber products.

Regulatory Information

FDA approved by 21CFR175.105 - Adhesives - No Limitations and 177.2600 - Rubber Articles Intended for Repeated Use - 5% Max.

Environmental Impact

This compound is the zinc salt of a mixture of fatty acids, predominantly lauric acid, which is one of the three most widely distributed saturated fatty acids found in nature (coconut and palm oils). Consequently, no hazardous environmental impact is expected.

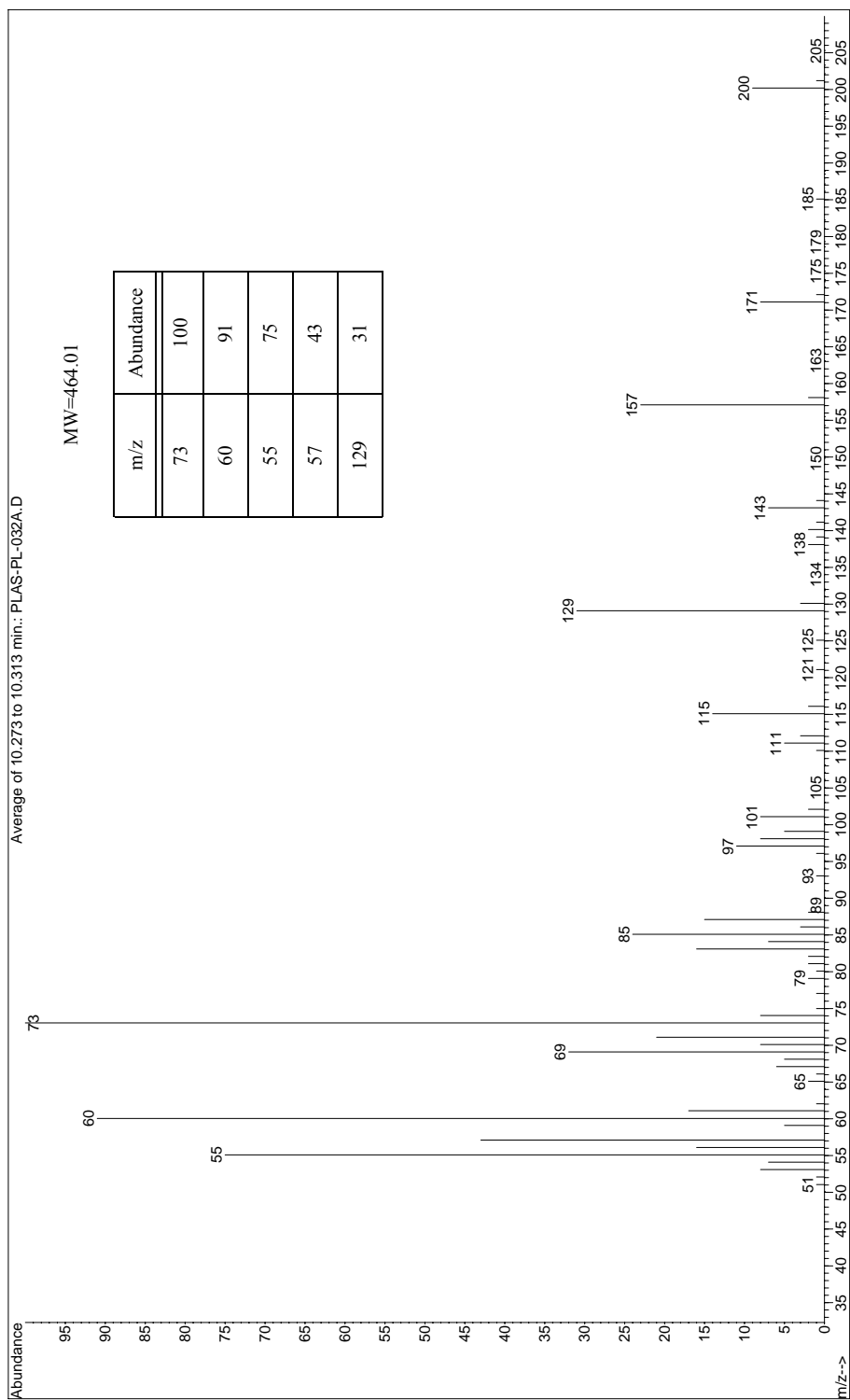
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

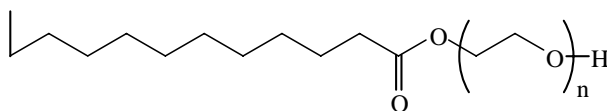
No health hazards have been identified.

Mass Spectrum for Laurex® - PLAS-PL-032



Markstat® 51

Chemtura Corporation



CAS Number 9004-81-3

RTECS Number TQ8701000

Abbreviation

Formula $(C_2H_4O)_n C_{12}H_{24}O_2$

Molecular Weight ~400

Chemical Name

poly(ethylene glycol) monolaurate

Synonyms

polyethylene glycol laurate; polyglycolester; polyoxyethylene monolaurate

Brand Names & Manufacturers**Physical Properties**

Appearance	Clear, yellowish, medium viscosity liquid					
Melting Point	Not available			Boiling Point 260 °C		
Stability	Stable, however discoloration may occur on exposure to air.					
Solubility (g/100mL 20 °C)	Water E	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane <0.1

Application, Regulatory & Environmental Information**Application**

Antistatic plasticizer used for PVC flooring, conveyor belts, hoses and plastic film.

Regulatory Information

Has FDA approval under Section 178.3910 to be used in surface lubricants for rolling of metallic foil or sheet stock provided that total residual lubricant remaining on the metallic article in the form in which it contacts food does not exceed 0.015 milligram per square inch of metallic food-contact surface.

Environmental Impact

This material is expected to be inherently biodegradable and has a low potential to bioaccumulate. It is not expected to be harmful to aquatic organisms.

Point of Release

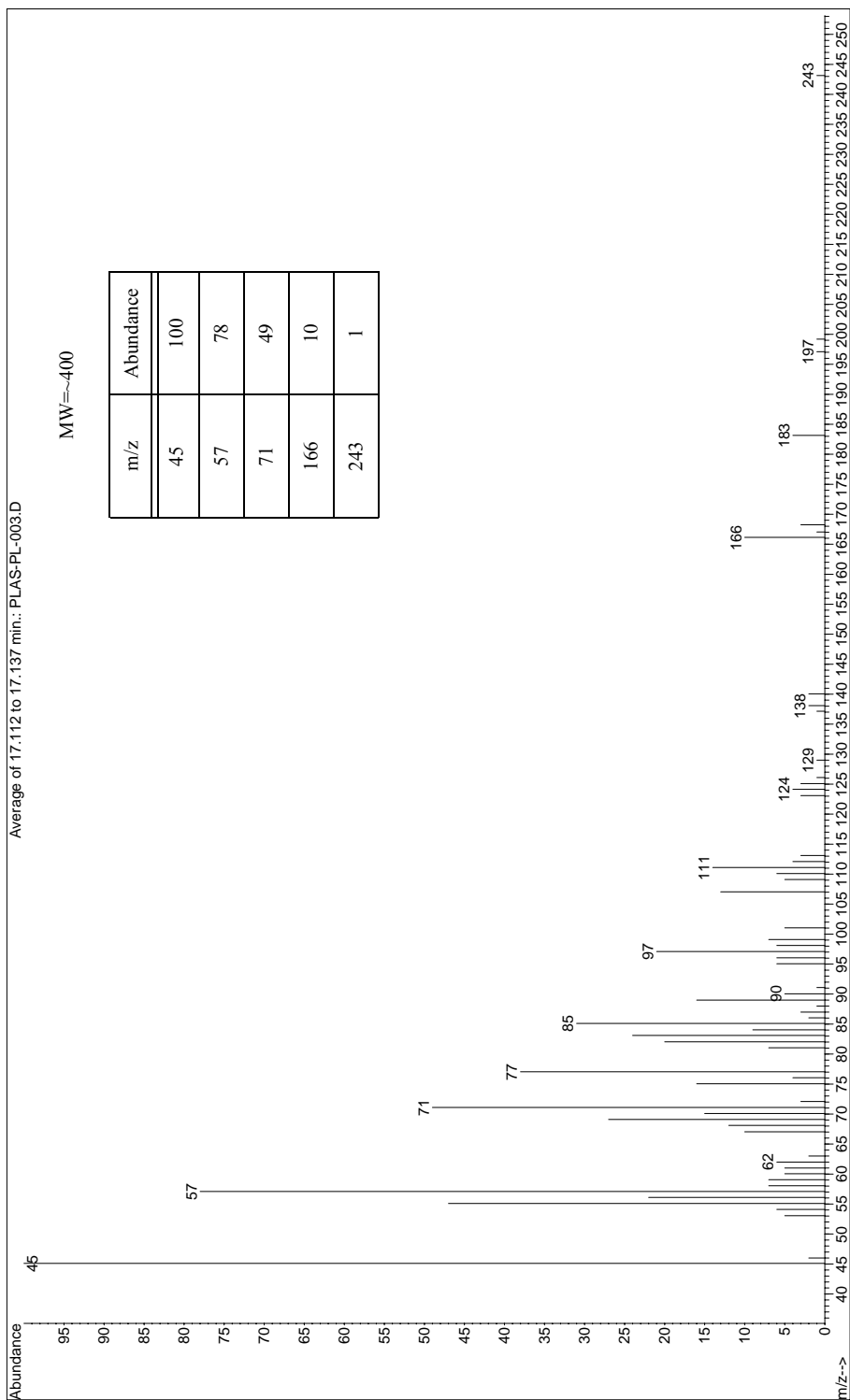
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

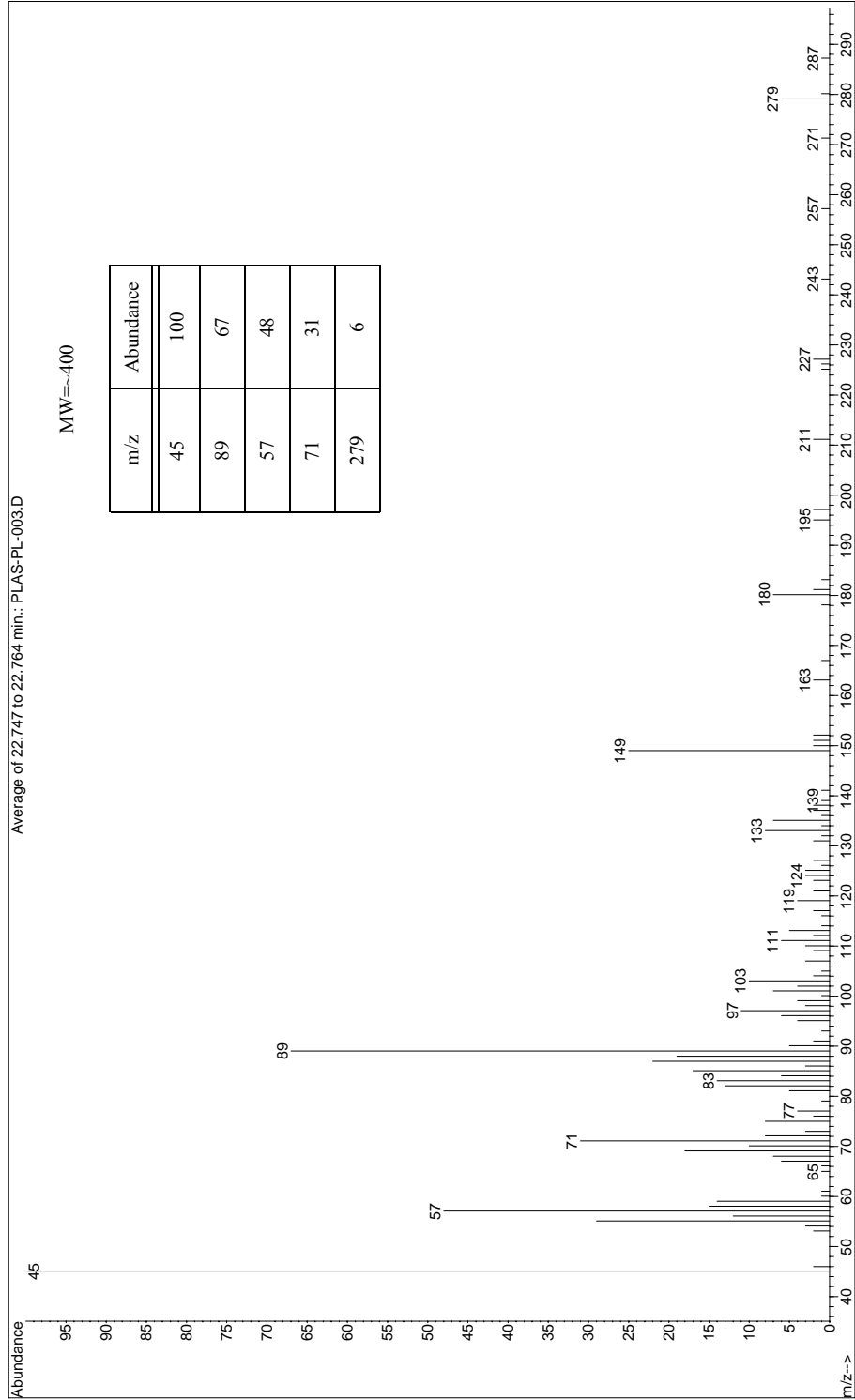
Acute oral toxicity (LD50): >2,500 mg/kg [Mouse]

Lowest Published Toxic Dose (TDLo): 889 gm/kg/70D-C [Rat].

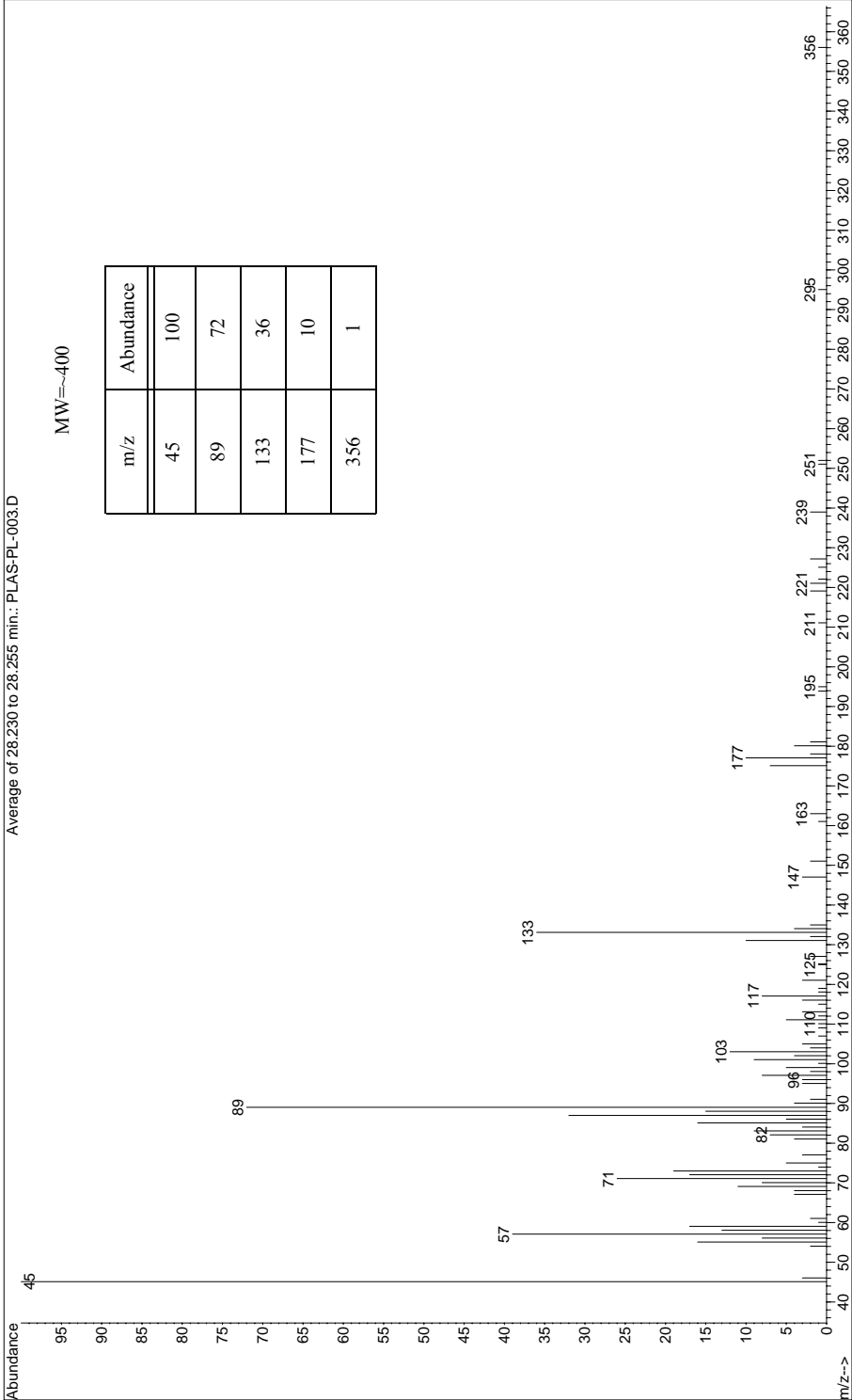
Mass Spectrum for Markstat® 51 - PLAS-PL-003



Mass Spectrum for Markstat® 51 - PLAS-PL-003

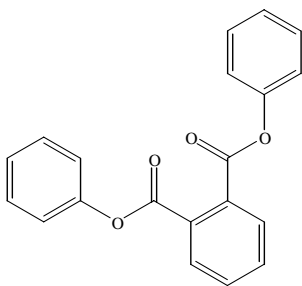


Mass Spectrum for Markstat® 51 - PLAS-PL-003



Morflex® 150

Morflex, Inc.

**CAS Number** 84-61-7**RTECS Number** TI0889000**Abbreviation** DCHP**Formula** C₂₀H₂₆O₄**Molecular Weight** 330.46**Chemical Name**
dicyclohexyl phthalate**Synonyms**

phthalic acid, dicyclohexyl ester; 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

Brand Names & Manufacturers

Unimoll® 66

Lanxess Corp

Physical Properties**Appearance** White powder**Melting Point** 63 °C**Boiling Point** 200-235 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	1-10	1-10	40-80	40-80	40-80

Application, Regulatory & Environmental Information**Application**

Used as a plasticizer in heat-sealable films, adhesives, coatings, under floor sealing compounds, and as a co-plasticizer in PVC.

Regulatory Information

This product does not have FDA approval for food contact applications.

Environmental Impact

Log Kow value of 5.6 indicates that this material is likely to bioaccumulate. It is not readily biodegradable and considered to be toxic to aquatic organisms.

Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

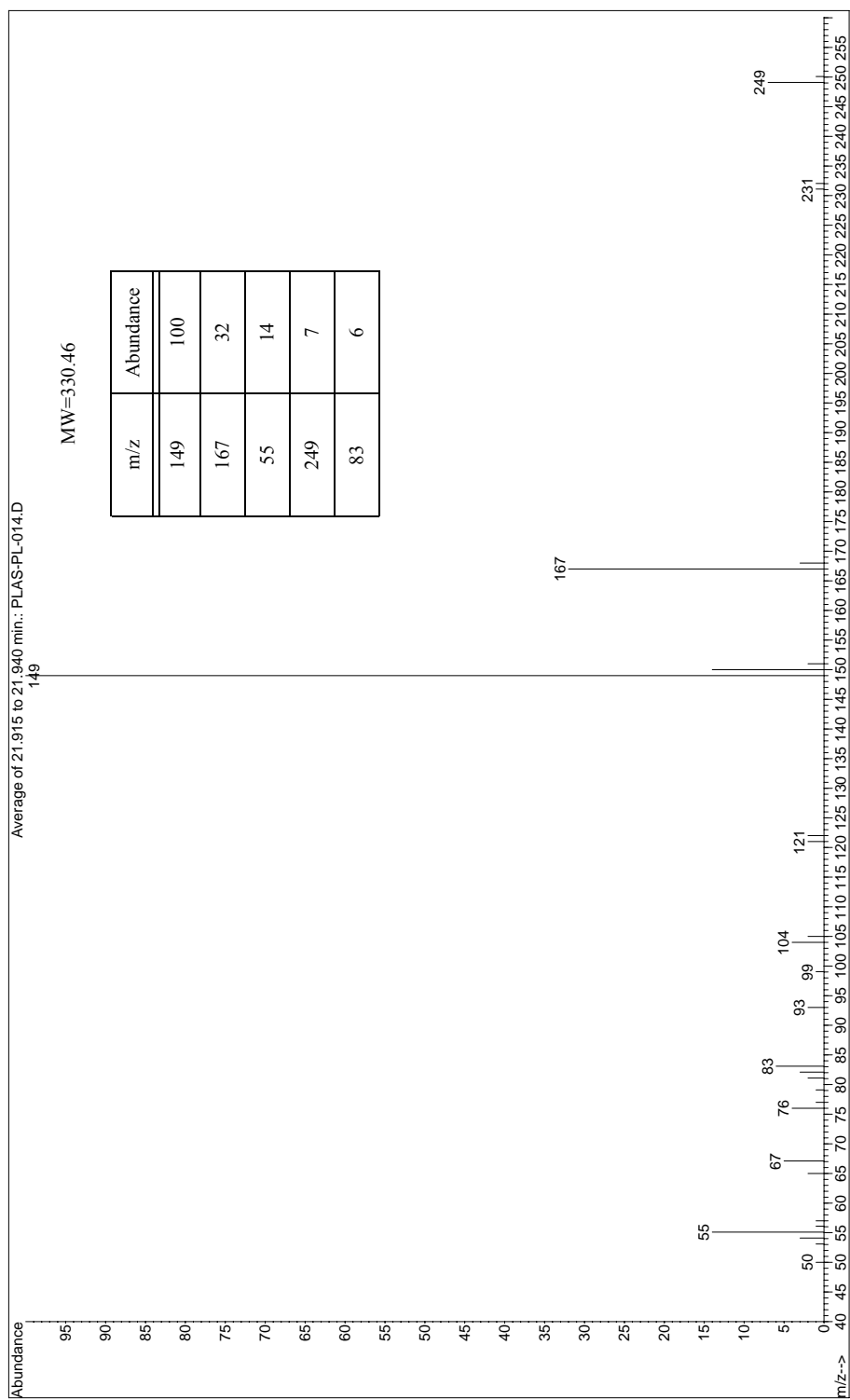
Toxicological Data

Acute Oral Toxicity (LD50): 30 mL/kg [Rat]

Lowest Published Toxic Oral Dose (TDLo): 10500 mg/kg/7D-C [Rat]

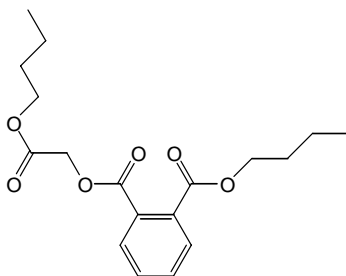
Suspected endocrine toxicant.

Mass Spectrum for Morflex® 150 - PLAS-PL-014



Morflex® 190

Morflex, Inc.

**CAS Number** 85-70-1**RTECS Number** TI 0535000**Abbreviation****Formula** C₁₈H₂₄O₆**Molecular Weight****Chemical Name**

butylphthalyl butyl glycolate (with <10% dibutyl phthalate)

Synonyms

dibutyl O-(o-carboxybenzoyl) glycolate; butyl carbobutoxymethyl phthalate; butyl glycolyl butyl phthalate

Brand Names & Manufacturers

Santicizer® B-16

Solutia Inc.

Physical Properties**Appearance** Clear liquid**Melting Point** <25 °C**Boiling Point** 220 °C (10 mmHg)**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application Application, Regulatory & Environmental Information

Used as a plasticizer in food-packaging material, PVC tubing and dental cushions.

Regulatory Information

Morflex® 190 is FDA approved for direct food contact. This product contains <10% Dibutyl phthalate which is a SARA 313 reportable compound.

Environmental Impact

The primary component, butylphthalyl butyl glycolate (BPBG), is expected to rapidly hydrolyze in environmental media under aerobic conditions. The dibutyl phthalate, (DBP) is also expected to hydrolyze in environmental media, however the DBP may be toxic to some aquatic organisms.

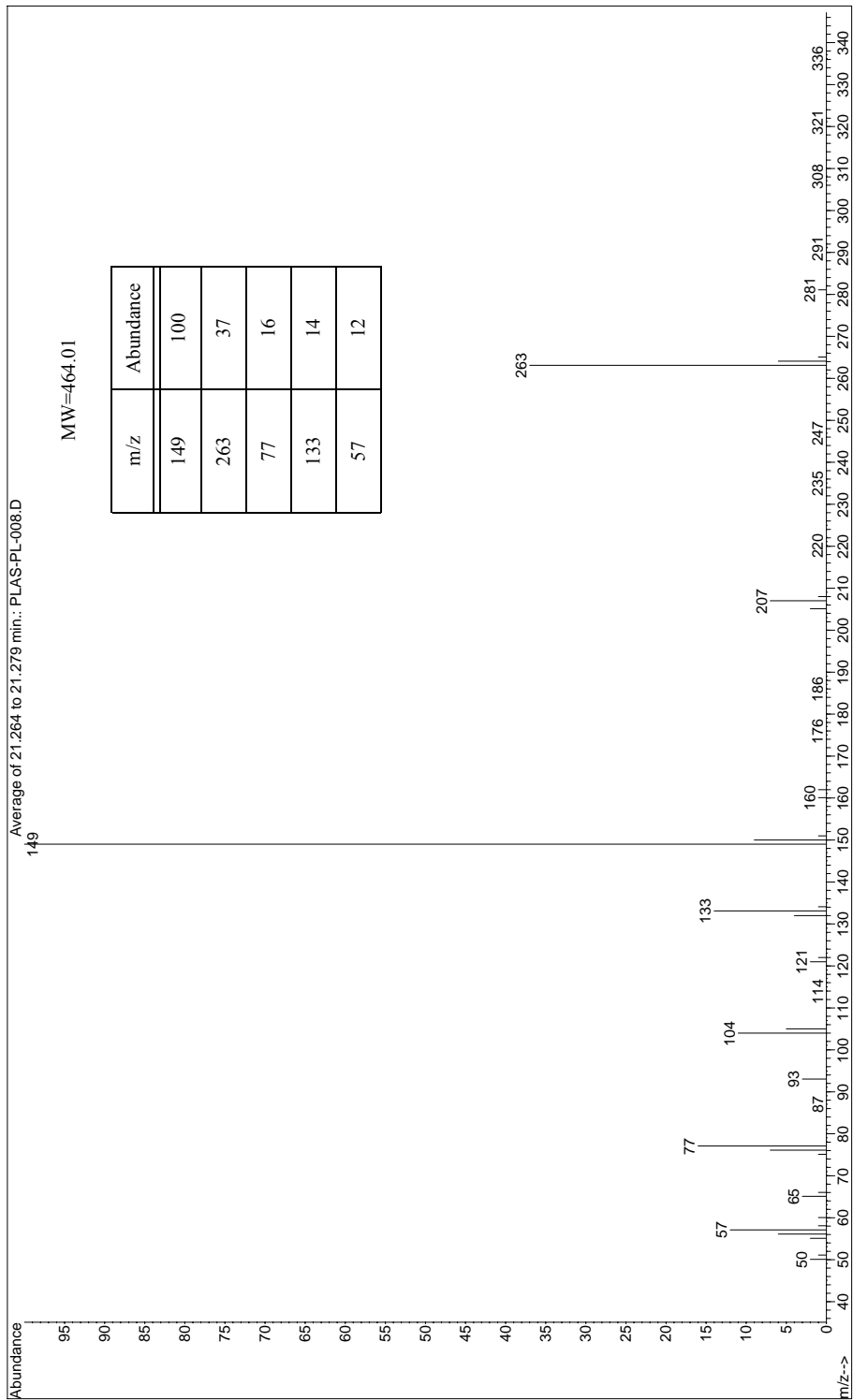
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

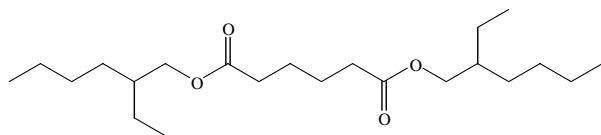
While neither component is classified as a carcinogen by IARC, NTP or OSHA, repeated or prolonged exposure to dibutyl phthalate may lead to adverse health effects.

Mass Spectrum for Morflex® 190 - PLAS-PL-008



Morflex® 310

Morflex, Inc.

**CAS Number** 103-23-1**RTECS Number** AU9700000**Abbreviation** DOA/DEHA**Formula** C₂₂H₄₂O₄**Molecular Weight** 370.57**Chemical Name**

hexanedioic acid, bis(2-ethylhexyl) ester; dioctyl adipate; di-(2-ethylhexyl) adipate; bis(2-ethylhexyl)hexanedioate

Synonyms**Brand Names & Manufacturers**Plasthall® DOA
Santicizer® DOAHallStar
Solutia Inc.**Physical Properties****Appearance** Colorless, oily liquid with an aromatic odor**Melting Point** -67.8 °C**Boiling Point** 417 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	40-80	U	40-80	U	U

Application, Regulatory & Environmental Information**Application**

DEHA is a plasticizer used primarily in food-contact wrapping, building materials and household furnishings.

Regulatory Information

Monitored under the federal Safe Drinking Water Act due to potential adverse health effects. It is approved by the FDA for food contact applications.

Environmental Impact

This substance is harmful to aquatic organisms and has a low bioaccumulation potential. It is readily degradable via abiotic (hydrolysis) and biotic processes.

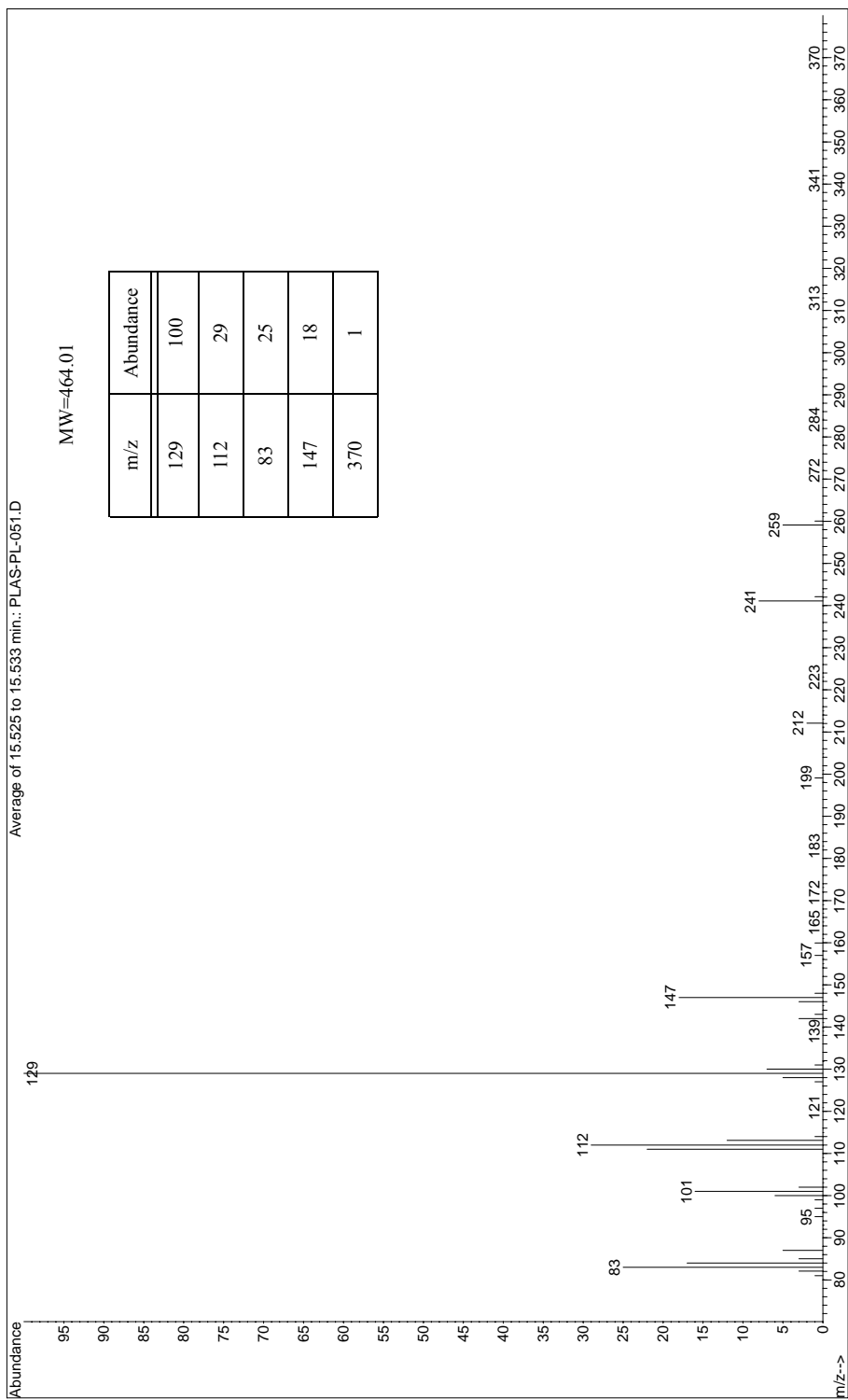
Point of Release

Occupational exposures are low based on production in a closed system and its low vapor pressure. The estimated exposure levels to the general population via consumer products, i.e. migration of DEHA from food wraps, is estimated at exposures of 117 µg/kg/d. The highest measured surface water concentration was 0.001 mg/L. Both of these results are considered to be low as well.

Toxicological Data

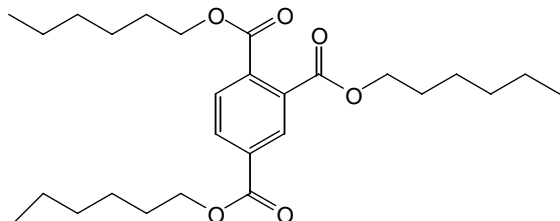
This product is a suspected carcinogen and endocrine toxicant. Classified as a possible development toxin. This substance is toxic to blood, the reproductive system, liver, upper respiratory tract.

Mass Spectrum for Morflex® 310 - PLAS-PL-051



Morflex® 560

Morflex, Inc.

**CAS Number** 1528-49-0**RTECS Number** Not available**Abbreviation****Formula** C₂₇H₄₂O₆**Molecular Weight** 462.62**Chemical Name**

tri-n-hexyl trimellitate

Synonyms

trihexyl benzene-1,2,4-tricarboxylate

Brand Names & Manufacturers

Physical Properties

Appearance	Oily liquid					
Melting Point	-45.5 °C			Boiling Point	260 - 262 °C (4 mmHg)	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ 40-80	Hexane 40-50

Application, Regulatory & Environmental Information
Application

Primarily used as a plasticizer for PVC and its copolymers. Vinyls plasticized with this ester find application in variety of markets including automotive and furniture upholstery, wire coatings and gasketing materials.

Regulatory Information

This product does not have FDA approval for direct or indirect food contact. It is not considered to be hazardous for shipping purposes.

Environmental Impact

The environmental fate of this product has not been thoroughly investigated.

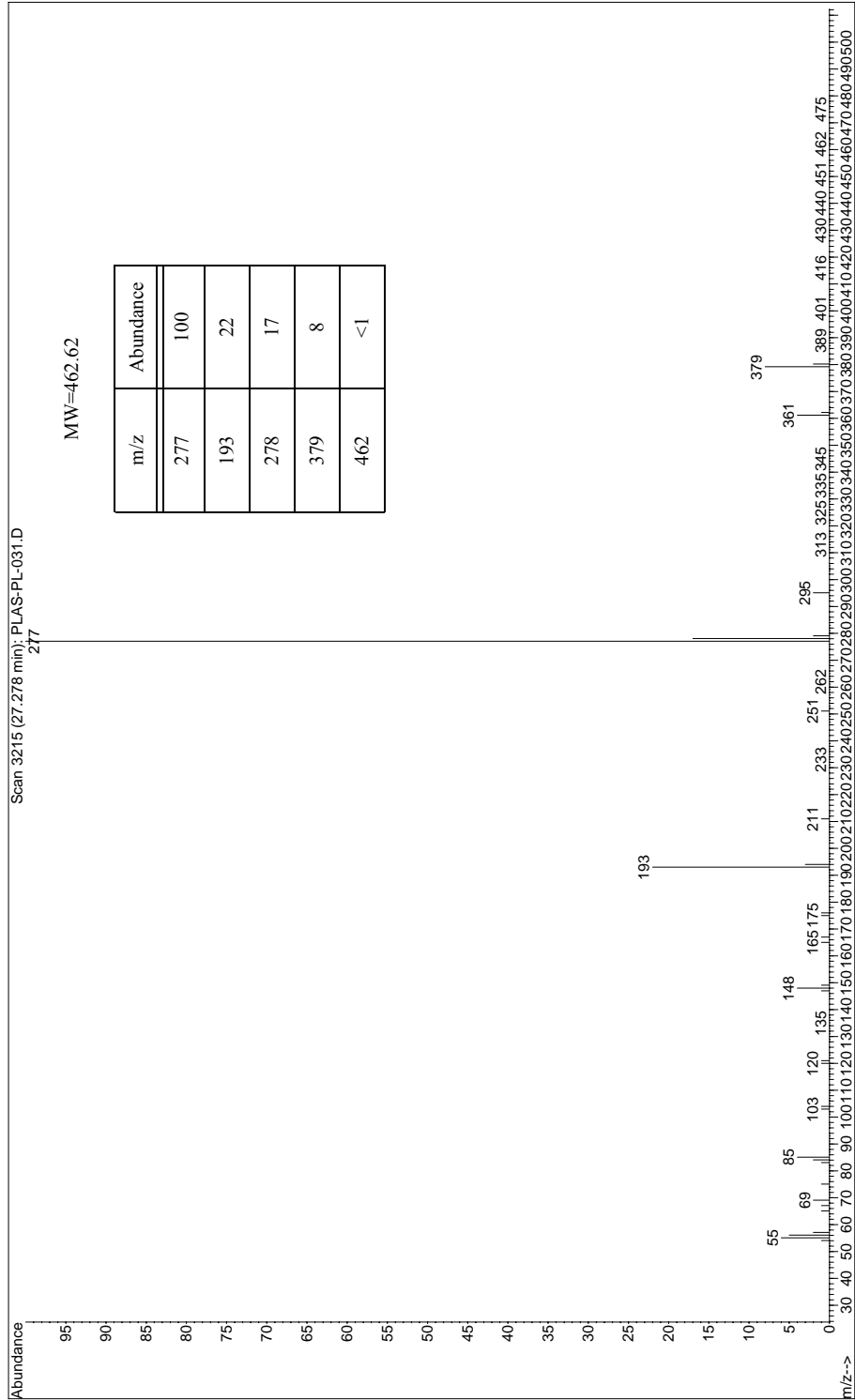
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

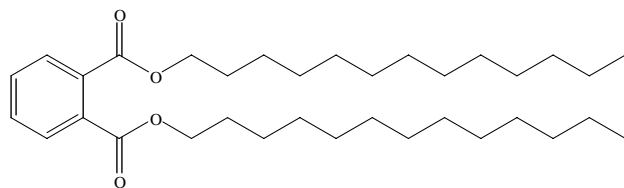
This product is not classified as a carcinogen by IARC, NTP or OSHA and the potential human health effects due to exposure are unknown.

Mass Spectrum for Morflex® 560 - PLAS-PL-031



Morflex® x-1125

Morflex, Inc.

**CAS Number** 119-06-2**RTECS Number** TI1950000**Abbreviation** DTDP**Formula** C₃₄H₅₈O₄**Molecular Weight** 530.93**Chemical Name**

1,2-benzenedicarboxylic acid, ditridecyl ester

Synonyms

di(tridecyl) phthalate; Phthalic acid, ditridecyl ester

Brand Names & Manufacturers

Jayflex® DTDP

Exxon Mobil Chemical

Physical Properties**Appearance** Clear, Viscous Liquid**Melting Point** Not available**Boiling Point** >285 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information**Application**

High temperature PVC insulation for wire and cable.

Regulatory Information

This material does not have FDA approval for food contact applications.

Environmental Impact

Phthalates are now being detected routinely in a range of environmental water samples including drinking water. They are widely dispersed in the environment. Due to the poor solubility of phthalates, sediments are the ultimate sink for phthalates released into the aquatic environment. Phthalates can accumulate in environments that are highly anaerobic and poorly colonized by microbes. Furthermore, cold environmental conditions slow their biodegradation.

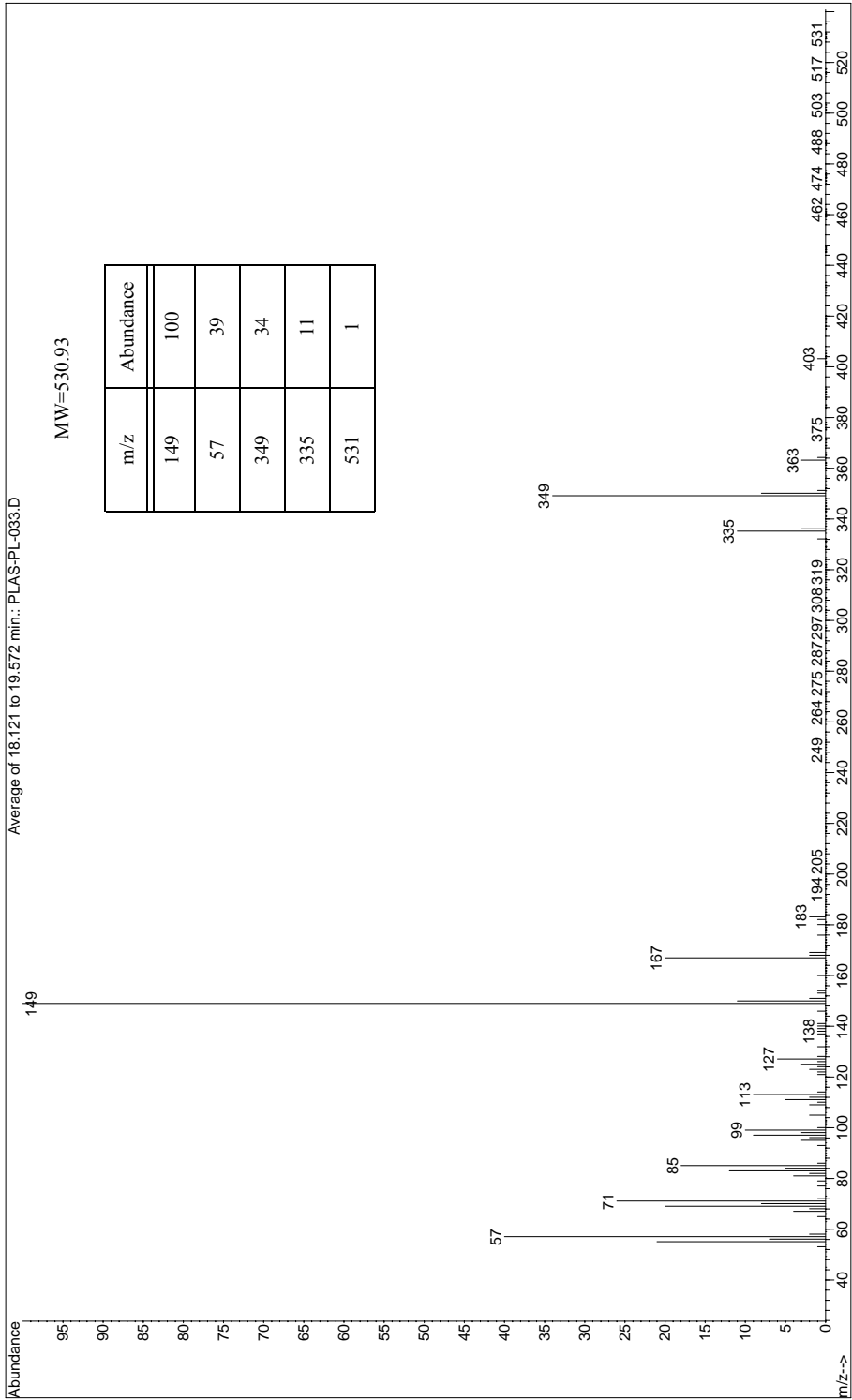
Point of Release

Can be released as point source pollution during production, distribution and incorporation into PVC resin. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Suspected endocrine toxin. (LD50): >2000 mg/kg [Rat].

Mass Spectrum for Morflex® x-1125 - PLAS-PL-033



Paraplex® G-30

HallStar

Unspecified
Structure

CAS Number Not available
RTECS Number Not available
Abbreviation

Formula Not available
Molecular Weight ~800

Chemical Name
proprietary dibasic acid polyester mixture

Synonyms

Brand Names & Manufacturers

Physical Properties

Appearance	Light yellow, viscous liquid; slight ester odor.					
Melting Point	Not available		Boiling Point		Not available	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH ₂ Cl ₂	Hexane
	<0.1	U	U	U	U	U

Application Application, Regulatory & Environmental Information

Low molecular weight polymeric plasticizer used in electrical wire insulation and coatings for wood, metal, fabrics and paper.

Regulatory Information

Does not have FDA approval for food contact and is not regulated as a hazardous waste by the EPA.

Environmental Impact

The 48-hour EC50 is 14 mg/L. The 48-hour NOEC is 5.2 mg/L.

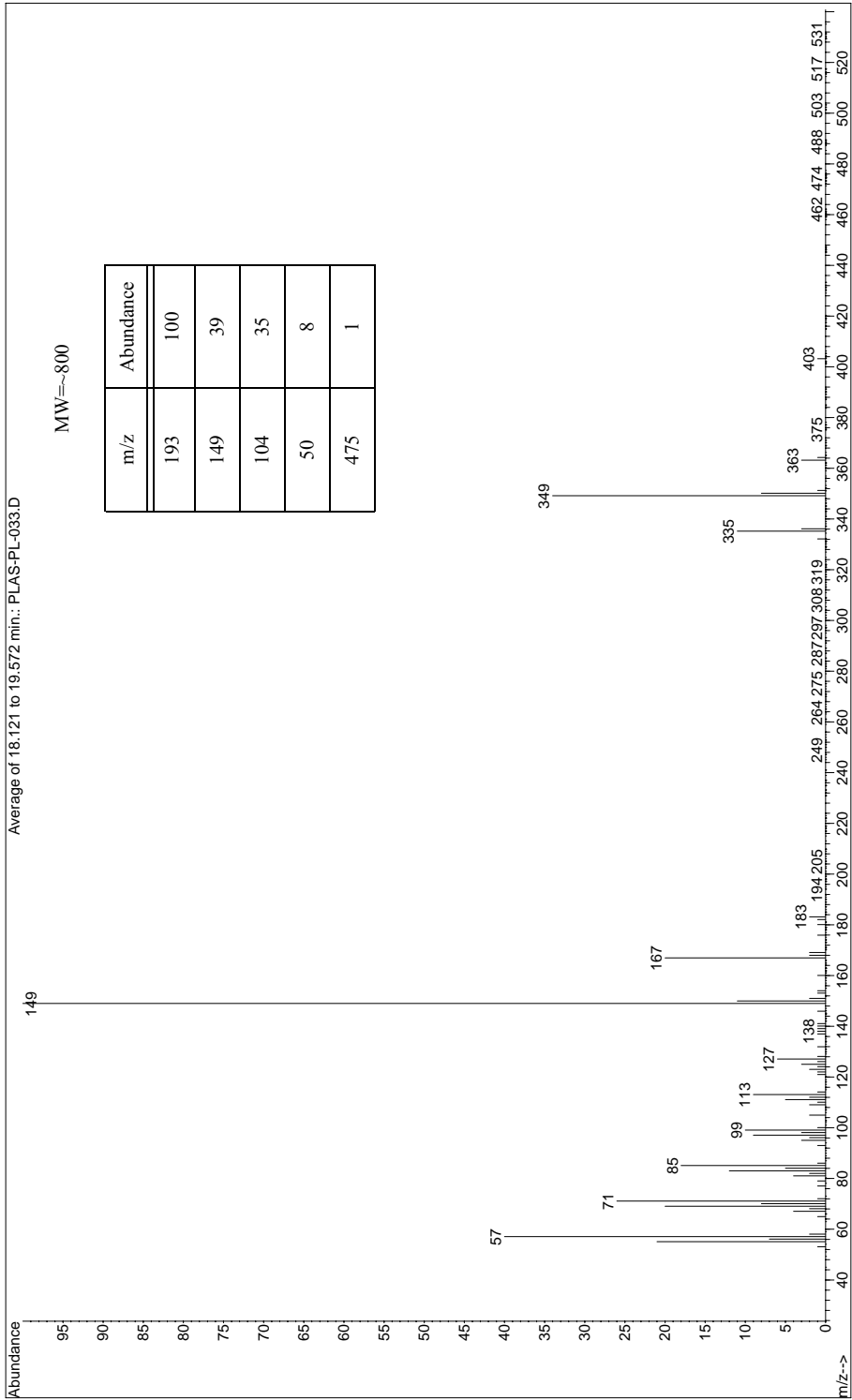
Point of Release

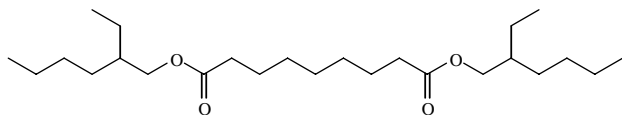
Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral (LD50): > 5.0 g/kg [Rat]. Primary Dermal Irritation: 1.0 (PII). No evidence of corrosion was noted. Not a primary irritant. Primary Ocular Irritation: No evidence of corrosion was noted.

Mass Spectrum for Paraplex® G-30 - PLAS-PL-033



Plasthall® DOZ**CAS Number** 2064-80-4**RTECS Number** CM2000000**Abbreviation** DOZ**Formula** C₂₅H₄₈O₄**Molecular Weight** 412.65**Chemical Name**

nonanedioic acid, dioctyl ester

Synonyms

dioctyl azelate; azelaic acid, dioctyl ester

Brand Names & Manufacturers

Kodaflex® DOZ

Eastman Chemical

Novaflex® DOZ

Cross Tech

Physical Properties**Appearance** Clear liquid**Melting Point** Not available**Boiling Point** 376 °C**Stability**

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	1-10	40-80	40-80	U	U	U

Application Application, Regulatory & Environmental Information

Used in conjunction with a monomeric plasticizer and a metal oxide to make an inherently hydrophobic material more hydrophilic. Commonly used in toys and medical equipment.

Regulatory Information

FDA approved in polymeric substances and as a component of adhesives intended for use in contact with food.

Environmental Impact

Listed as a moderate health priority based on persistence and bioaccumulative studies as of July 2006.

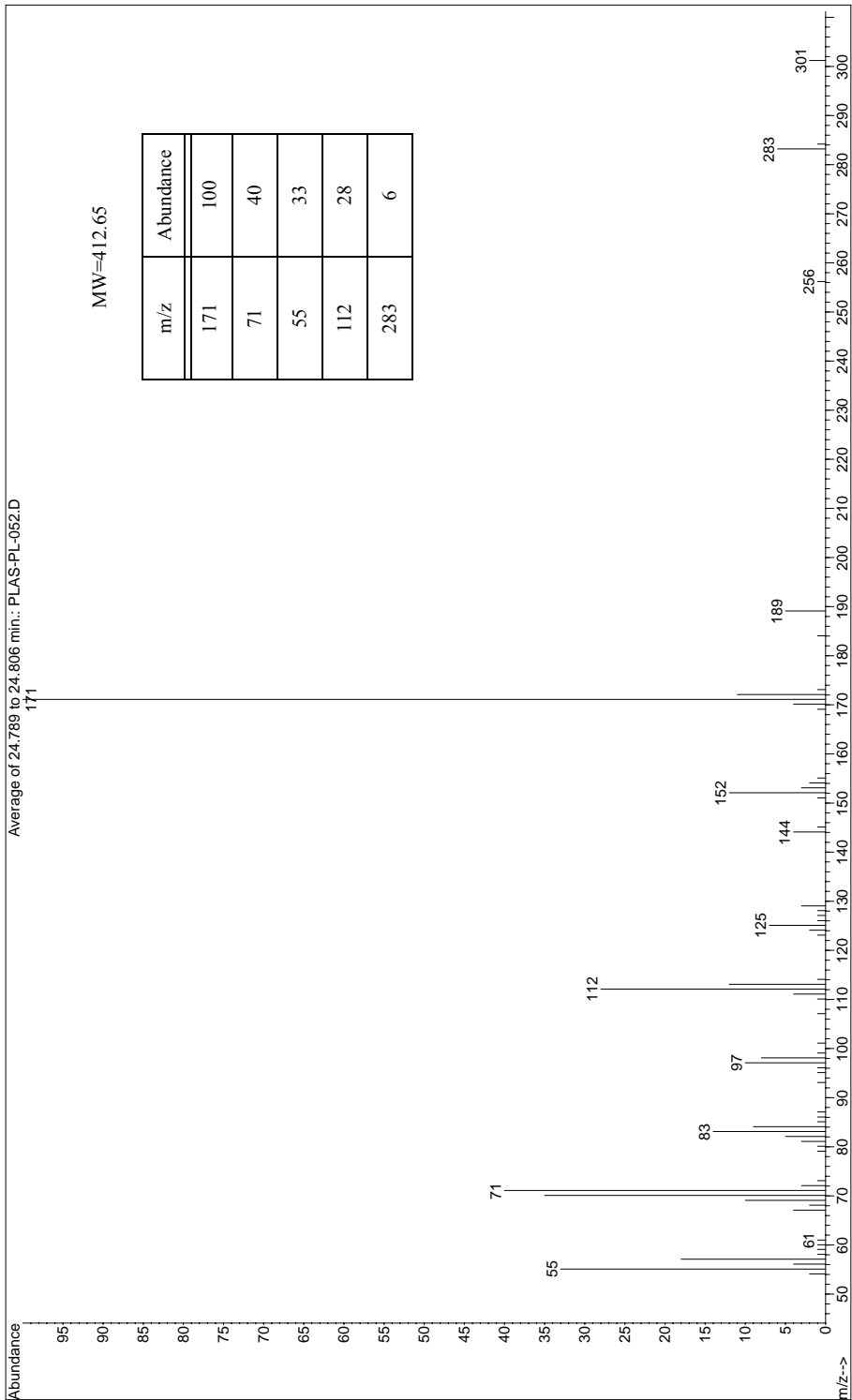
Point of Release

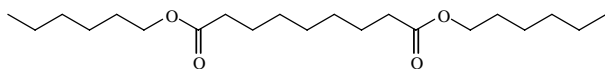
Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Plasthall® DOZ - PLAS-PL-052



Plastolein 9050

CAS Number 109-31-9

RTECS Number CM2100000

Abbreviation DnHA

Formula $C_{21}H_{40}O_4$

Molecular Weight 356.54

Chemical Name

nonanedioic acid, dihexyl ester

Synonyms

dihexyl azelate; azelaic acid, dihexyl ester

Brand Names & Manufacturers***Physical Properties*****Appearance** Colorless liquid**Melting Point** -80.0 °C**Boiling Point** 282 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.	MeOH 40-80	EtOH 40-80	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Used as a plasticizer in the production of polyvinyl chloride, polystyrene and other plastics used for food, drinks and for polypropylene food wrap.

Regulatory Information

FDA approved for use as a plasticizer at levels not exceeding 24% by weight of the permitted plastic substance used in contact with non-fatty foods and non-alcoholic beverages or fatty foods containing less than 30% fat or oil content.

Environmental Impact

Long-term environmental impact studies have not been completed.

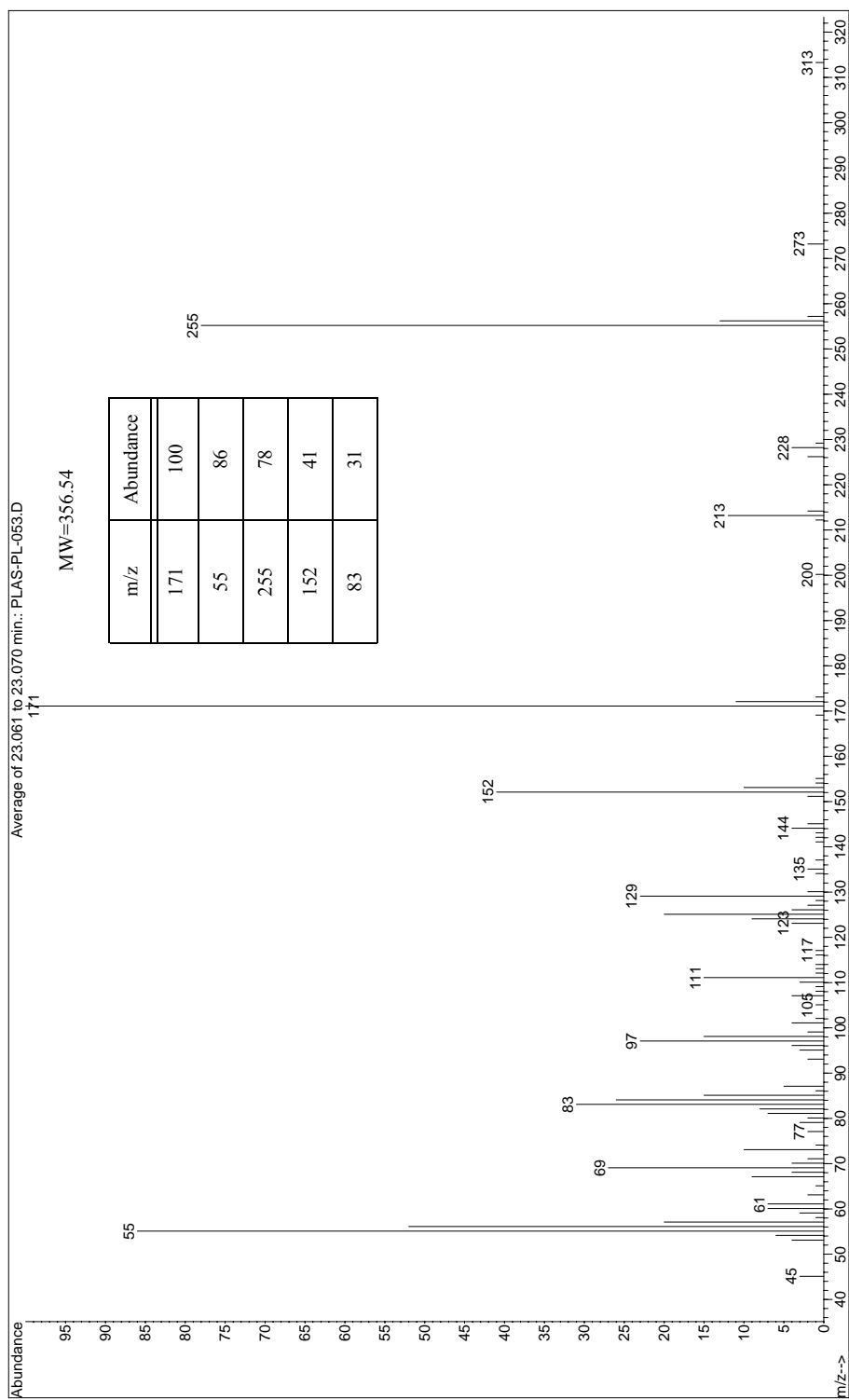
Point of Release

Can be released as point source pollution during manufacture, transportation and final product end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

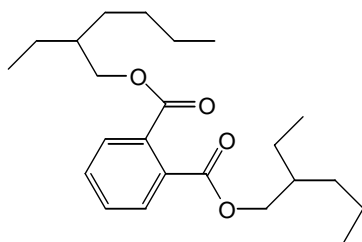
(LD50): 8.7-9.1 g/kg BW [Rat] and 11.5 g/kg BW [Mouse].

Mass Spectrum for Plastolein 9050 - PLAS-PL-053



Polycizer® 162

Harwick Chemical Corporation

**CAS Number** 117-84-0**RTECS Number** TI1925000**Abbreviation** DNOP**Formula** C₂₄H₃₈O₄**Molecular Weight** 390.56**Chemical Name**

1,2-benzenedicarboxylic acid, dioctyl ester

Synonyms

di-N-octyl phthalate; dioctyl phthalate; dioctyl o-benzenedicarboxylate; dicapryl phthalate

Brand Names & Manufacturers**Physical Properties**

Physical Properties						
Appearance	Clear, colorless, viscous liquid					
Melting Point	25 °C		Boiling Point 384 °C			
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 40-80	EtOH U	Acetone 40-80	CH₂Cl₂ 40-80	Hexane 1-10

Application Application, Regulatory & Environmental Information

Used to keep plastics soft and more flexible. This type of plastic can be used for medical tubing and blood storage bags, wire and cables, carpet back coating, floor tile, and adhesives. It is also used in cosmetics and pesticides.

Regulatory Information

This chemical is considered to be an environmental hazard and regulated by the EPA under the Clean Water Act. It does have FDA approval for food contact applications.

Environmental Impact

If di-n-octylphthalate is released into the air, it may be deposited on the ground or to surface water in rain or dust particles. Di-n-octylphthalate sticks tightly to soil, sediment, and dust particles. Small amounts of di-n-octylphthalate can build up in animals that live in water, such as fish and oysters.

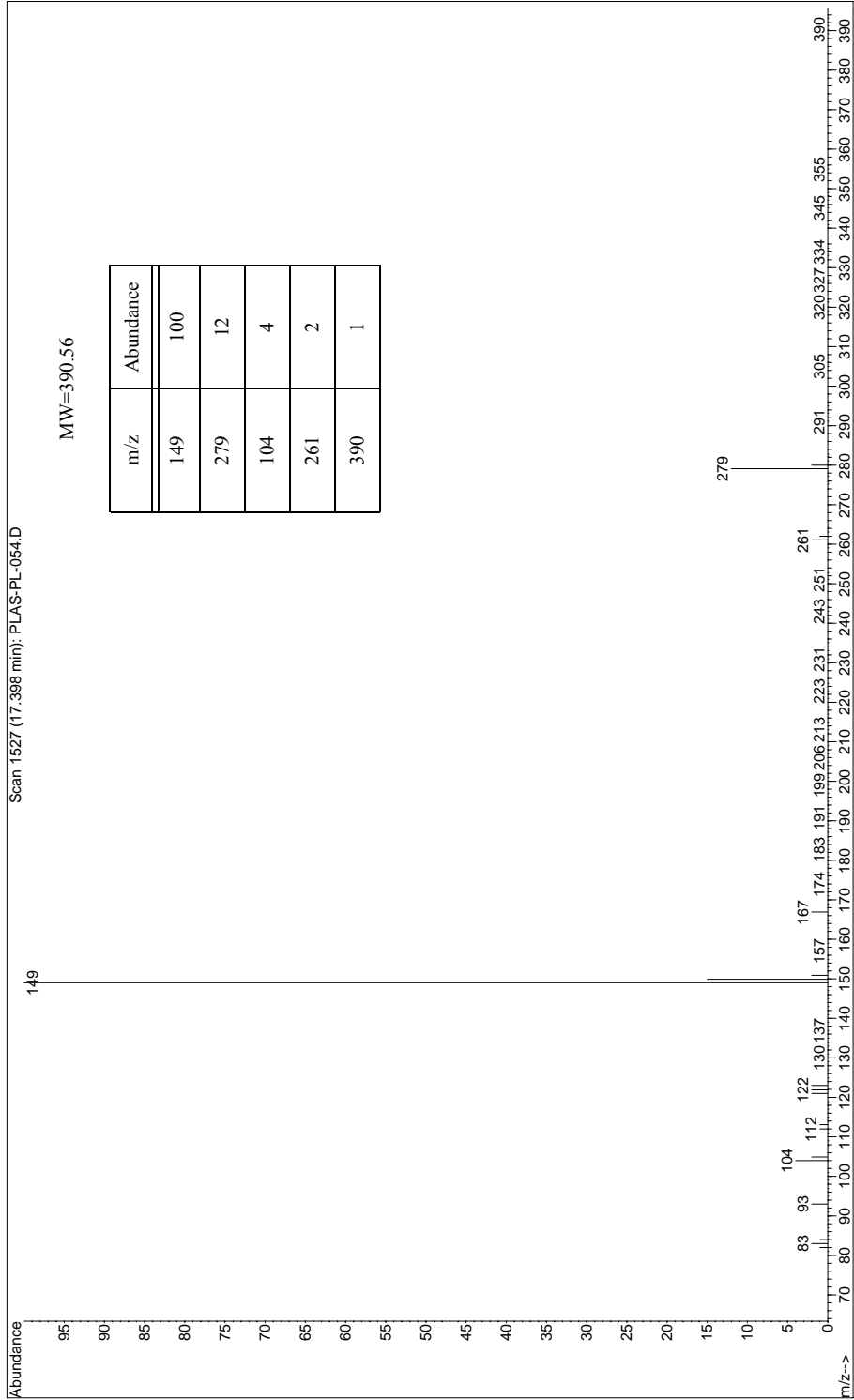
Point of Release

Exposure to di-n-octylphthalate occurs mainly from eating food or drinking water that is stored in plastic containers. This substance has been found in at least 300 of the 1,416 National Priorities List sites identified by the Environmental Protection Agency (EPA). Di-n-octylphthalate can be released to water or air during its manufacture, by leaking from plastics in landfills, or from the burning of plastic products.

Toxicological Data

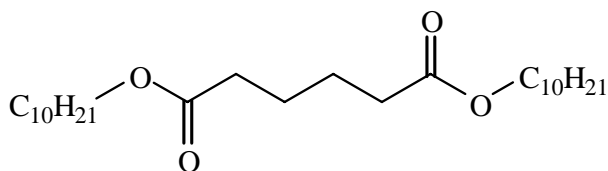
Di-n-octylphthalate has not been classified as to its carcinogenicity by the Department of Health and Human Services (DHHS) or the International Agency for Research on Cancer (IARC).

Mass Spectrum for Polycizer® 162 - PLAS-PL-054



Polycizer® 632

Harwick Chemical Corporation

**CAS Number** 105-97-5**RTECS Number** Not available**Abbreviation****Formula** C₂₆H₅₀O₄**Molecular Weight** 426.67**Chemical Name**

hexanedioic acid, didecyl ester

Synonyms

didecyl hexanedioate; didecyl adipate; adipic acid didecyl ester

Brand Names & Manufacturers

Physical Properties

Appearance Light-colored liquid**Melting Point** Not available**Boiling Point** 245 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information

Application

Plasticizer used in production of PVC, ethyl and nitrocellulose, polystyrene and synthetic rubber intended for contact with food and drink.

Regulatory Information

Didecyl adipate is FDA approved under 21CFR177.2600 - Rubber articles intended for repeated use.

Environmental Impact

Readily biodegradable and has a low potential to bioaccumulate. Not expected to be toxic to the aquatic environment.

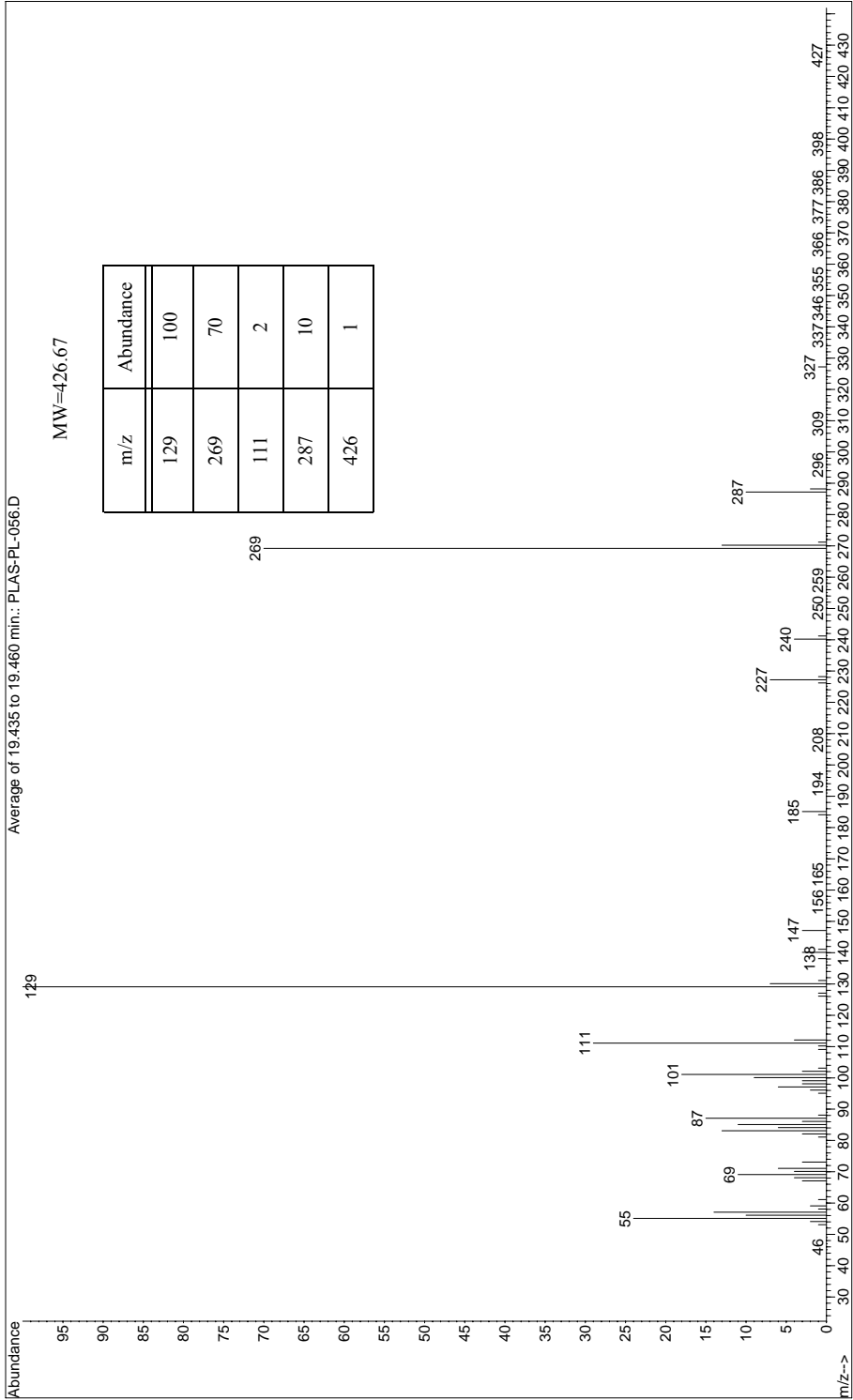
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

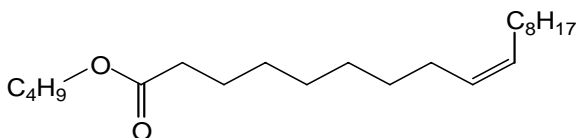
Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Polycizer® 632 - PLAS-PL-056



Polycizer[®] butyl oleate

Harwick Chemical Corporation

**CAS Number** 142-77-8**RTECS Number** RG3711000**Abbreviation****Formula** C₂₂H₄₂O₂**Molecular Weight** 338.57**Chemical Name**

butyl oleate

Synonyms

butyl cis-9-octadecenoate; oleic acid butyl ester

Brand Names & ManufacturersKessco[®] 554

Stepan Company

Vinicizer[®] 30

Kao Corporation

Witcizer 100

Physical Properties**Appearance** Off-white liquid**Melting Point** -26.4 °C**Boiling Point** 222.78°C @ 760 mm Hg**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	U	U	U

Application Application, Regulatory & Environmental Information

Plasticizer particularly for natural and synthetic rubber polymers. Used to impart a low temperature flexibility to neoprene formulations. Also used in cosmetics.

Regulatory Information

This product does not have FDA approval for direct or indirect food contact. It is not considered to be hazardous for shipping purposes, but is considered a primary irritant.

Environmental Impact

Possibly hazardous short term degradation products are not likely. However, long term degradation products may arise.

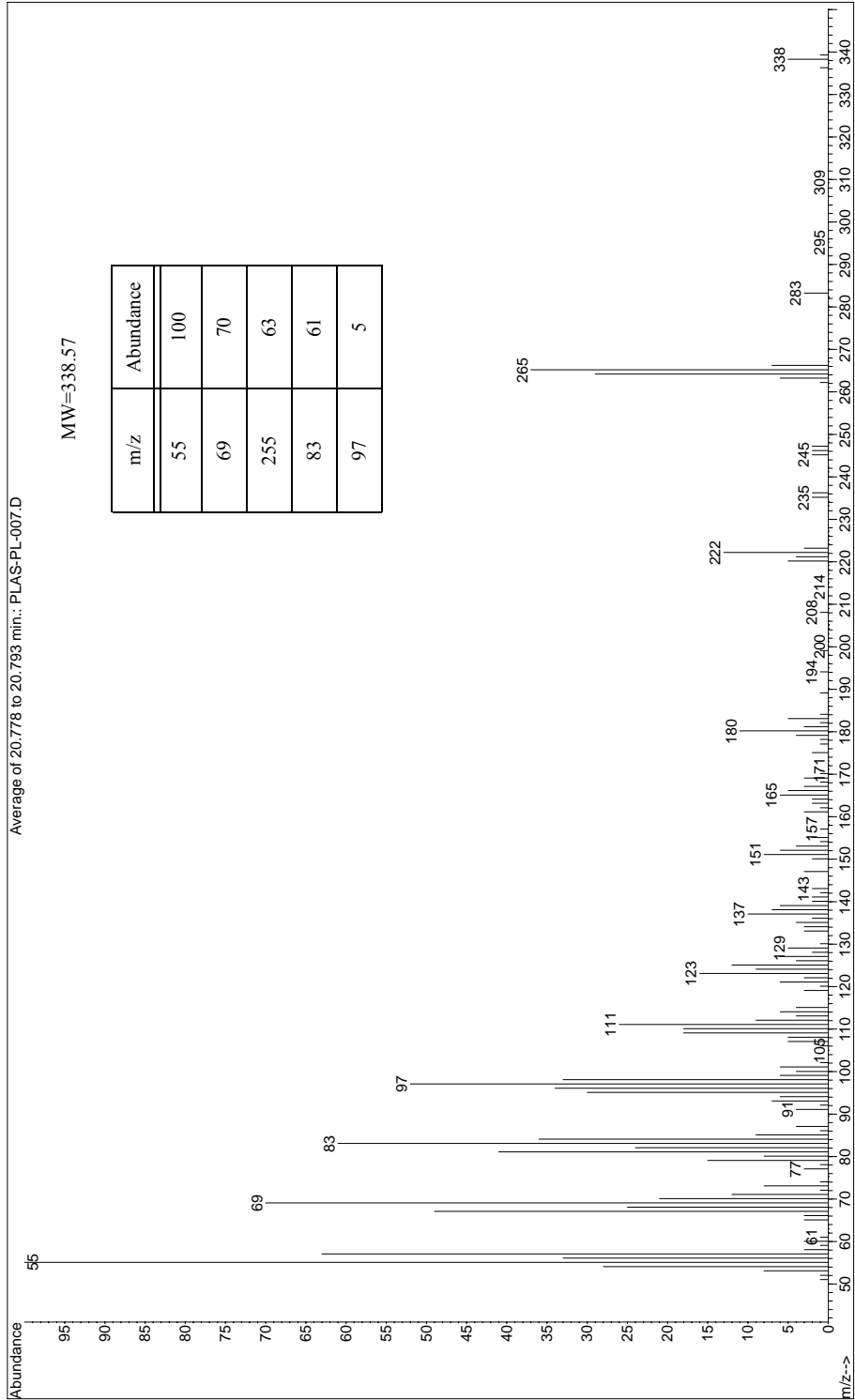
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

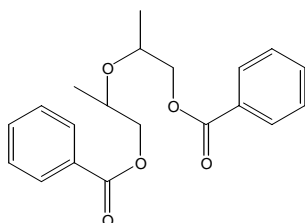
The product itself and its products of degradation are not toxic. It is considered to be hazardous in case of skin contact (irritant), of inhalation (lung irritant), and slightly hazardous in case of ingestion. It is not classified as a carcinogen by IARC, NTP or OSHA.

Mass Spectrum for Polycizer® butyl oleate - PLAS-PL-007



Polycizer® DP 500

Harwick Chemical Corporation

**CAS Number** 27138-31-4**RTECS Number** Not available**Abbreviation****Formula** C₂₀H₂₂O₅**Molecular Weight** 342.39**Chemical Name**

dipropylene glycol dibenzoate

Synonyms

PPG-2 dibenzoate; oxybispropanol dibenzoate

Brand Names & Manufacturers

Benzoflex® 9-88

Santicizer® 9100

Velsicol Chemical Corporation

Ferro

Physical Properties**Appearance** Colorless to straw-colored liquid**Melting Point** <16 °C**Boiling Point** 232 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	<0.1	U	U	40-80	40-80

Application Application, Regulatory & Environmental Information

Used in adhesives for the following applications: in the packaging industry for carton sealing/forming; for book binding and labeling; in textiles for both fibers and nonwoven fabrics; in construction to form decorative wall paneling, window frames, and other decorative construction products as well as producing mastics and caulking compounds. Also used in furniture, luggage, shoes and in cigarette tipping.

Regulatory Information

FDA approved for food contact under 21CFR175.105, 176.170 and 176.180. Regulated as an environmentally hazardous substance by DOT.

Environmental Impact

Toxic to aquatic organisms and may cause long-term adverse effects in the aquatic environment. Considered readily biodegradable.

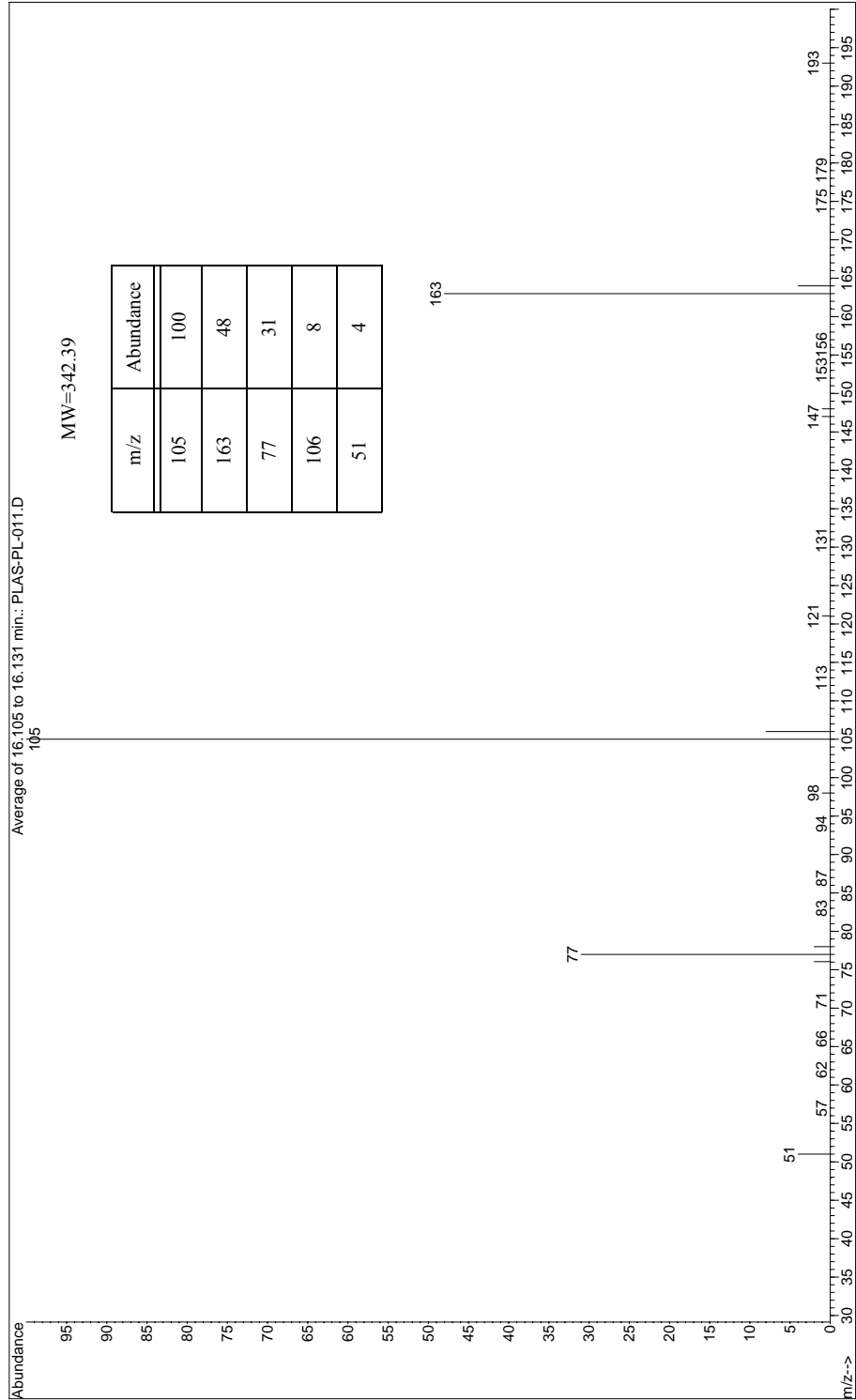
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

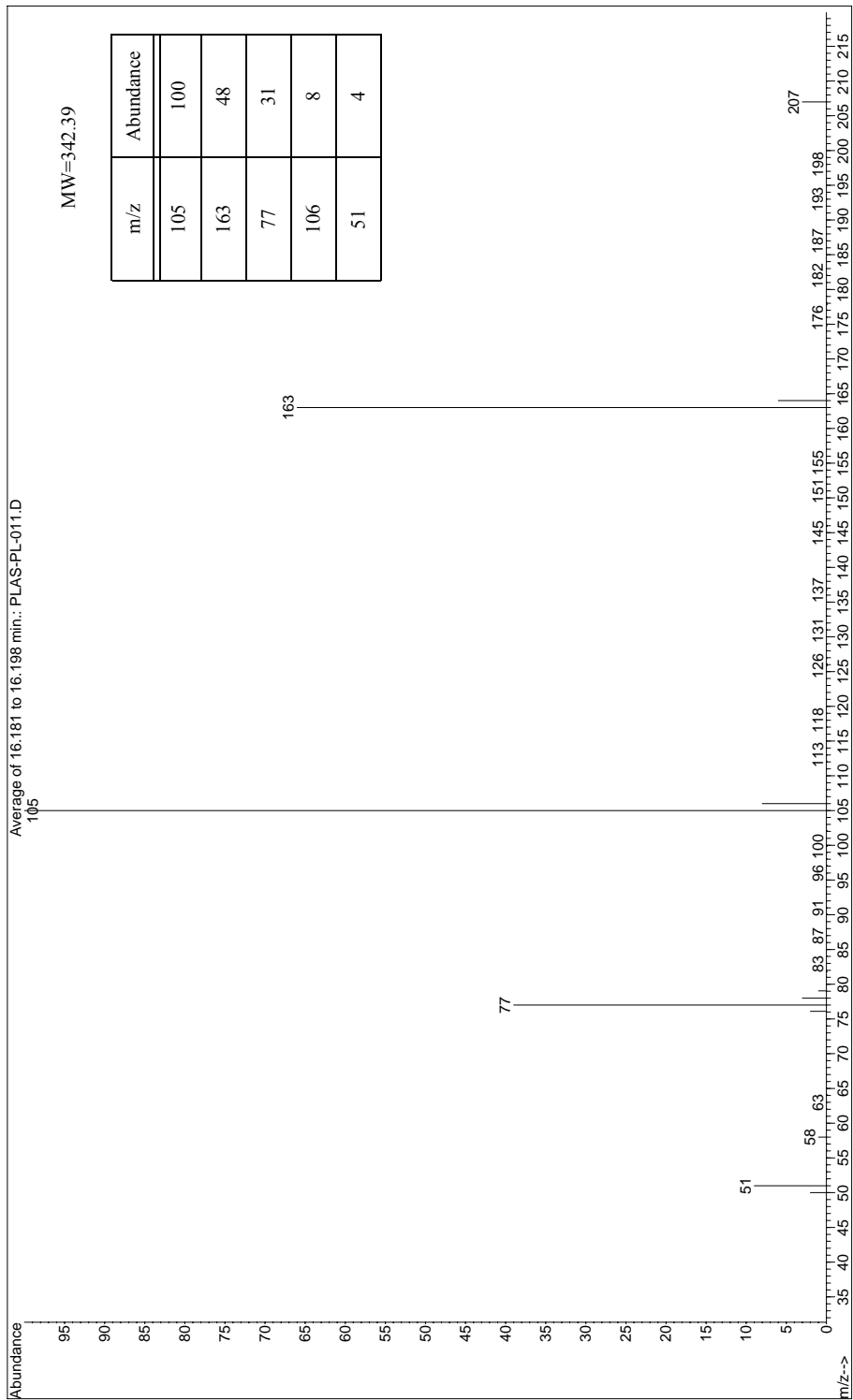
Toxicological Data

Acute oral toxicity (LD50): 9800 mg/kg [Rat].

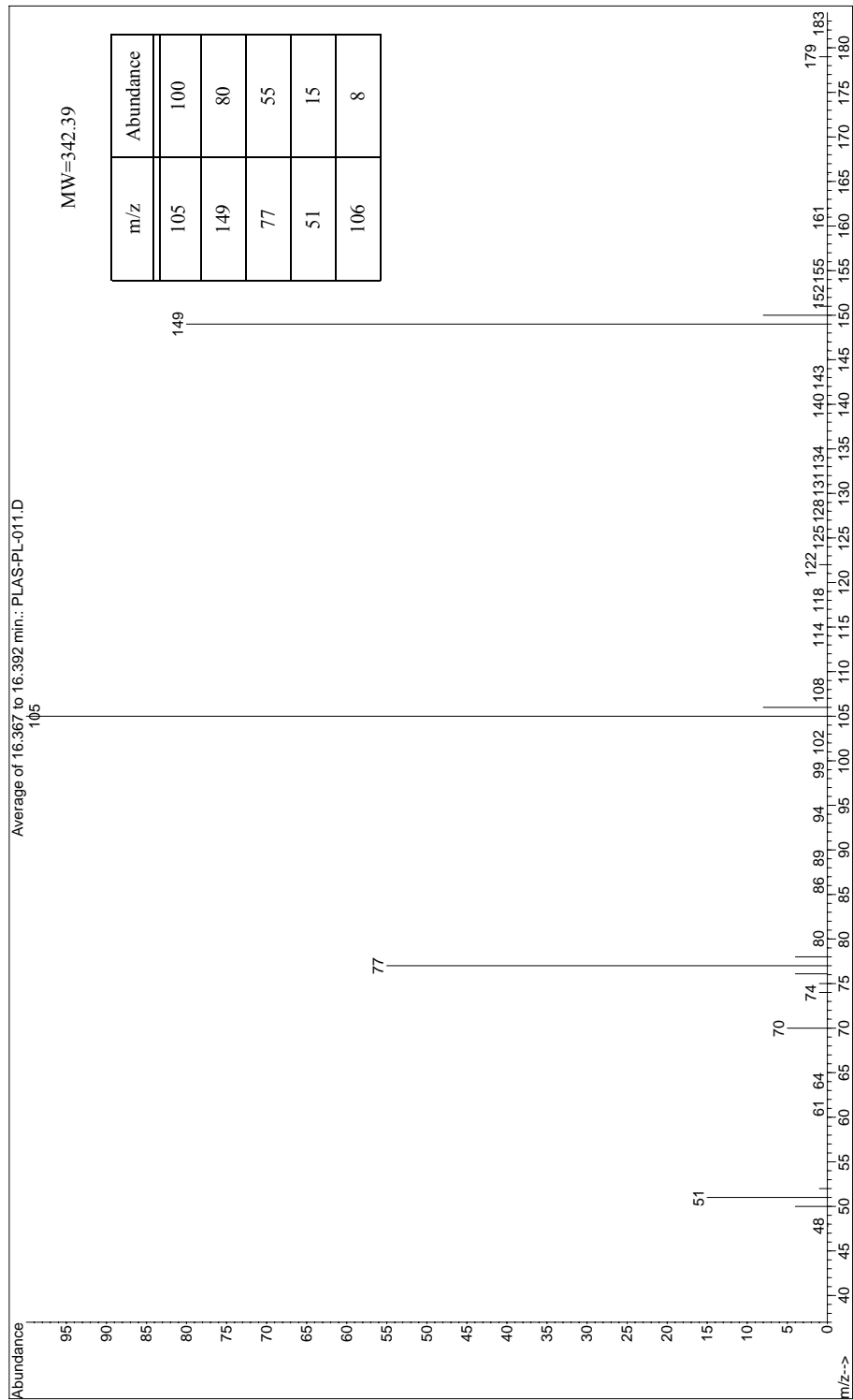
Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011

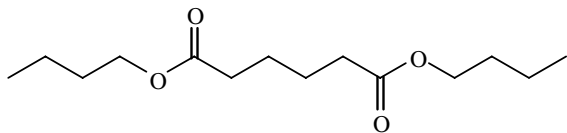


Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011



Mass Spectrum for Polycizer® DP 500 - PLAS-PL-011



Polycizer® W 260

CAS Number 105-99-7

RTECS Number AV0900000

Abbreviation

Formula C₁₄H₂₆O₄

Molecular Weight 258.35

Chemical Name

hexanedioic acid, dibutyl ester

Synonyms

dibutyl adipate; adipic acid, dibutyl ester

Brand Names & Manufacturers

Adimoll® DB

Bayer/Lanxess

Physical Properties**Appearance** Clear liquid**Melting Point** -32.4 °C**Boiling Point** 305 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	U	40-80	40-80	U

Application Application, Regulatory & Environmental Information

Used as low-temperature-resistant and low-viscosity plasticizer for PVC and its copolymers and cellulose esters, e.g., cellulose acetate butyrate, and cellulose propionates. May be found in eyeglass frames, safety goggles, animal collars, decorative trims and various types of film.

Regulatory Information

Dibutyl adipate is on the FDA GRAS (generally approved as safe) list.

Environmental Impact

Dibutyl adipate is readily biodegradable. Although it is considered to be moderately toxic to fish and daphnids and slightly toxic to algae, the environmental risk is considered to be low. Log Pow is 4.17 indicating that there is a moderate to low potential for bioaccumulation.

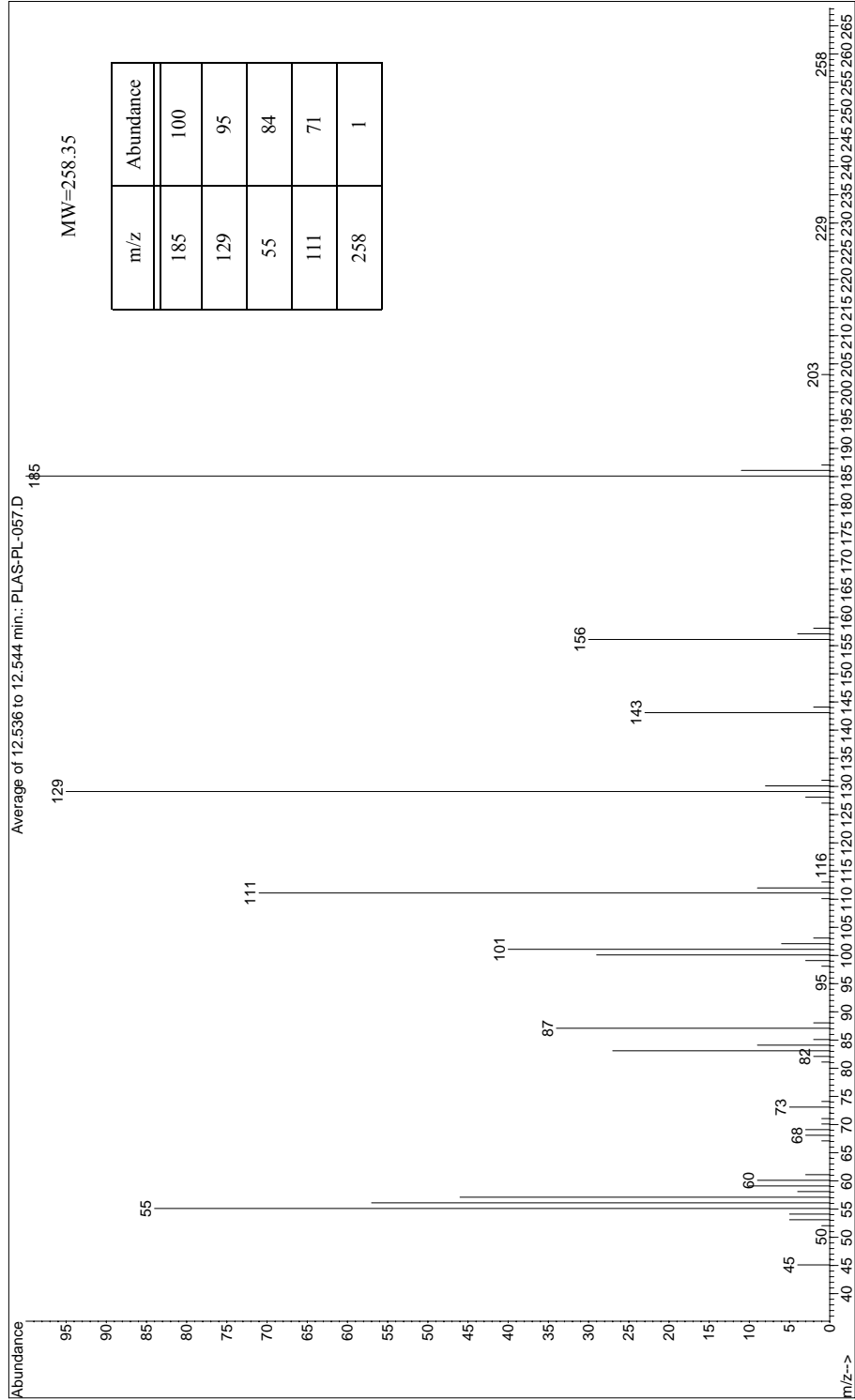
Point of Release

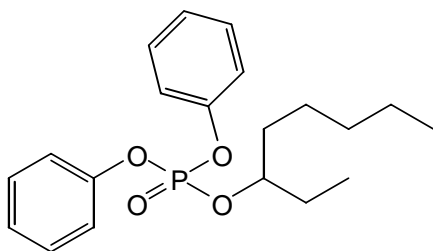
Primary exposure to dibutyl adipate is from skin contact with cosmetics and sunscreens containing this compound. It can also migrate from resins using this material as a plasticizer during the life cycle of the product and after disposal.

Toxicological Data

Dibutyl adipate is not toxic in acute oral or dermal animal toxicity tests.

Mass Spectrum for Polycizer® W 260 - PLAS-PL-057



Santicizer® 141**Solutia Inc.****CAS Number** 1241-94-7**RTECS Number** Not available**Abbreviation****Formula** C₂₀H₂₇O₄P**Molecular Weight** 362.40**Chemical Name**

2-ethylhexyldiphenyl phosphate

Synonyms

phosphoric acid, 2-ethylhexyl diphenyl ester; diphenyl-2-ethylhexyl phosphate

Brand Names & Manufacturers**Physical Properties****Appearance** Clear to yellow liquid**Melting Point** -80 °C**Boiling Point** 239 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.01	10-40	10-40	10-40	10-40	10-40

Application, Regulatory & Environmental Information

Application Flame retarding plasticizer used in cellulose, polyester and polyurethane. Mainly used in the manufacture of electrical (wire and cable) and automotive plastic parts. May also be used for the preparation of vinyl sheets, fabric coating, plastisols and organosols, adhesives, vinyl packing materials, and conveyor belts.

Regulatory Information

FDA approved for indirect food contact.

Environmental Impact

Highly toxic to fish and aquatic plants. Has the potential to bioaccumulate and is not readily biodegradable.

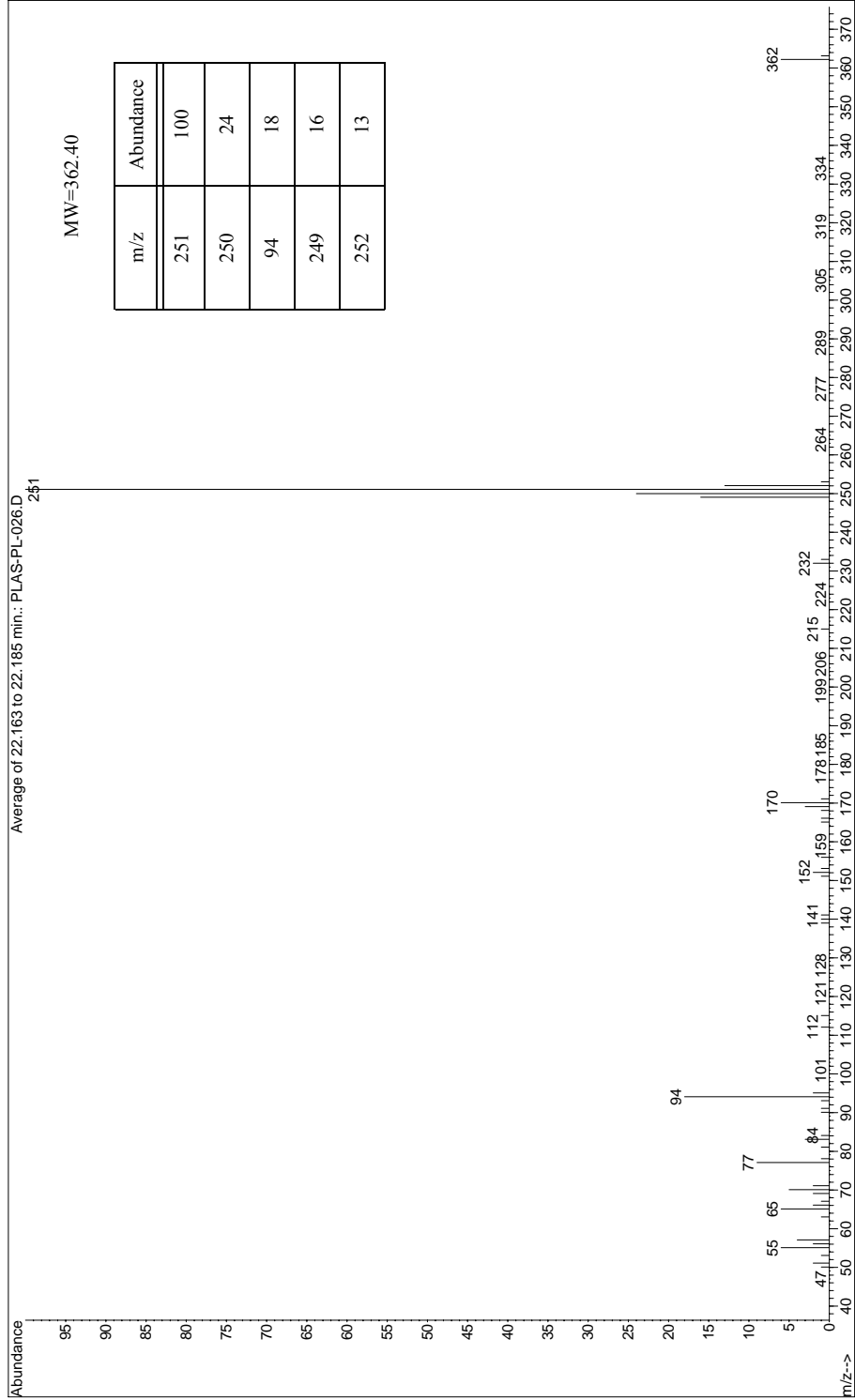
Point of Release

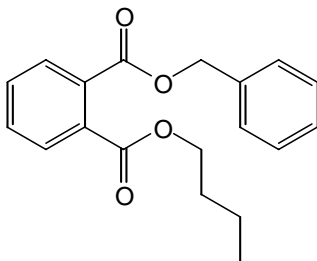
Organic phosphates are not chemically bonded to the polymer but can move in and out of the material. Evaporation of organic phosphates from car seats can result in a tacky coating on windows and other surfaces in the interior of the automobile, which can result in human exposure by skin contact and inhalation.

Toxicological Data

Acute oral (LD50): 218 mg/kg [Rabbit]; Acute dermal (LD50): >7900 mg/kg [Rabbit].

Mass Spectrum for Santicizer® 141 - PLAS-PL-026



Santicizer® 160**Solutia Inc.****CAS Number** 85-68-7**RTECS Number** TH9990000**Abbreviation****Formula** C₁₉H₂₀O₄**Molecular Weight** 312.37**Chemical Name**

benzyl butyl phthalate

Synonyms

1,2-benzenedicarboxylic acid, butyl phenylmethyl ester; butyl benzyl phthalate

Brand Names & Manufacturers

Palatinol® BB

BASF

Physical Properties**Appearance** Colorless, oily liquid**Melting Point** <-35 °C**Boiling Point** 370 °C**Stability** Stable under recommended storage and handling conditions.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH U	EtOH U	Acetone U	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Butyl benzyl phthalate is a plasticizer added to polymers to give flexibility and softness. It is used extensively in polyvinyl chloride and in cellulose plastics, polyvinyl acetate, polysulfides, and polyurethane. Also used in flexographic inks for food packaging applications and acrylic coatings, profile extrusions, slush moulding, film and sheeting, coated fabrics, floor and wall coverings, vinyl foams and plastisols for car sealants.

Regulatory Information

Considered a priority pollutant and is regulated by the federal Clean Water Act, RCRA and Superfund. FDA approved under 21CFR175.105 - Adhesives; 175.300 - Resinous and Polymeric Coatings; 176.170 - Components of Paper & Paperboard in Contact with Fatty or Aqueous Food; 175.180 - Components of Paper & Paperboard in Contact with Dry Food; 177.2420 - Cross-linked Polyester Resins (as solvent); and 178.3740 - Polymeric Substances (Extraction limitations).

Environmental Impact

This substance is very toxic to aquatic organisms. Bioaccumulation of this chemical may occur in fish.

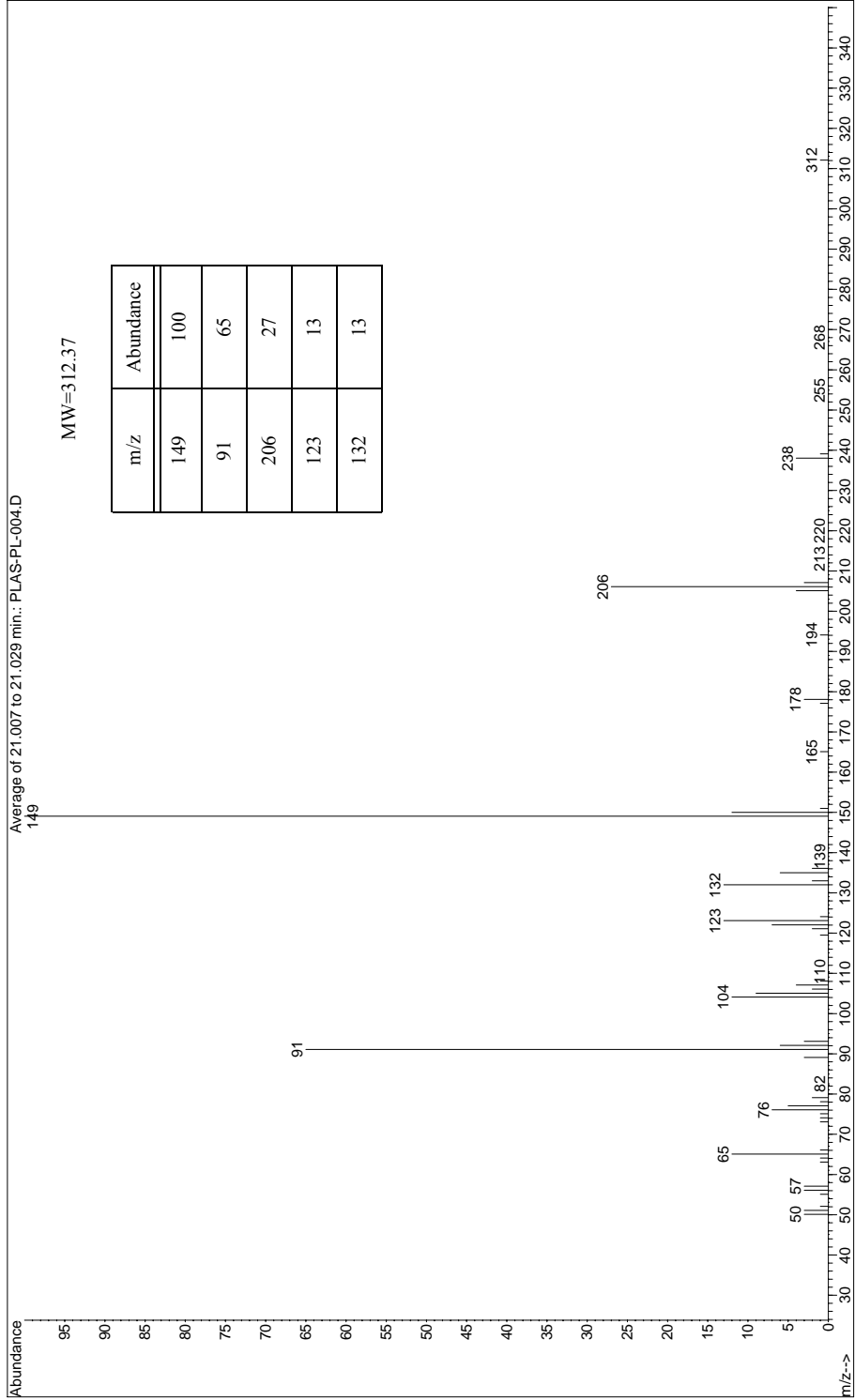
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

RTECS CLASS OF COMPOUND: Tumorigen; Mutagen; Reproductive Effector. Acute Oral Toxicity (LD50): 2330 mg/kg [Rat]. Acute Dermal Toxicity (LD50): 6700 mg/kg [Rat]. Lowest Published Toxic Oral Dose (TDLo): 68250 mg/kg/91D-C [Rat]. State of California (Proposition 65) as known to cause reproductive toxicity.

Mass Spectrum for Santicizer® 160 - PLAS-PL-004



Vinsol[®] resin

Unspecified
Structure

CAS Number 8050-09-7

RTECS Number VL0480000

Abbreviation

Formula Unspecified

Molecular Weight Not applicable

Chemical Name

gum rosin

Synonyms

disproportionated rosin; polymerized rosin; colophony

Brand Names & Manufacturers

Physical Properties

Appearance	Dark reddish-brown solid					
Melting Point	75-81 °C			Boiling Point >572 °C		
Stability	Stable under recommended storage and handling conditions.					
Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH ₂ Cl ₂	Hexane
	<0.1	40-80	40-80	40-80	U	<0.1

Application, Regulatory & Environmental Information

Application
Used as an air entraining agent in cements, mortars, and concrete to improve strength, workability, and freeze/thaw resistance. Also used as an asphalt emulsifier for anionic, slow setting emulsions for paving, surfacing, and sealing applications. Other uses include adhesives, sealants, inks, coatings, binder in paperboard and composition board, foundry molds and core washes.

Regulatory Information

FDA approved for a wide range of applications ranging from direct food additives such as chewing gum base to indirect food additives in adhesives, paper and paperboard, and polymers as per 21CFR175, 176, 177, and 178.

Environmental Impact

Based upon data from this or similar materials, this product cannot be regarded as readily biodegradable; however, it may be slowly biodegradable. Acute 96-hour (LL50): > 1000 mg/L [Fathead Minnow]. Acute 48-hour (EL50): 911 mg/L. [Daphnia magna], Algae growth inhibition test 72-hour (EL50): > 1000 mg/L.

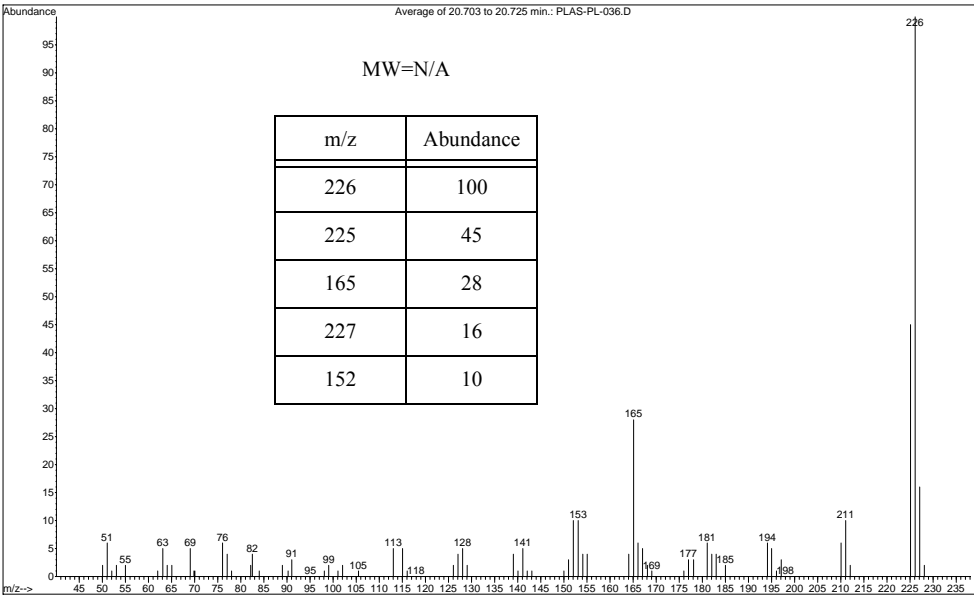
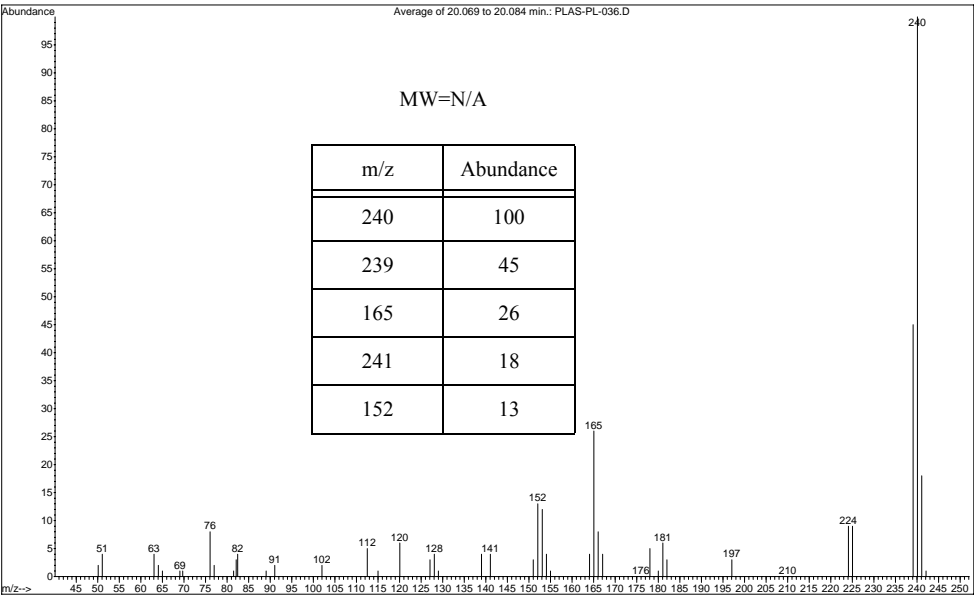
Point of Release

Can be released as point source pollution during manufacture. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Not considered a carcinogen by OSHA, IARC or NTP. Acute inhalation toxicity (LD50): 110 mg/m3 [Rat]. Acute oral toxicity (LD50): 2.2 mg/kg [Mouse], 3.0 mg/kg [Rat].

Mass Spectra for Vinsol[®] resin - PLAS-PL-036

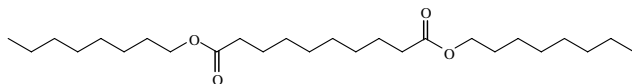


Witamol 500

CAS Number 2432-87-3

RTECS Number Not available

Abbreviation DOS

Formula $C_{26}H_{50}O_4$

Molecular Weight 426.67

Chemical Name

decanedioic acid, dioctyl ester

Synonyms

dioctyl sebacate; di-n-octyl sebacate; sebacic acid, dioctyl ester; dioctyl decanedioate

Brand Names & Manufacturers***Physical Properties*****Appearance** Colorless liquid**Melting Point** -67 °C**Boiling Point** 300 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water <0.1	MeOH 40-80	EtOH 40-80	Acetone 40-80	CH₂Cl₂ U	Hexane U
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Application, Regulatory & Environmental Information**Application**

Plasticizer for PVC, and its copolymers, nitrocelluloses, styrene resins and synthetic rubbers where low temperature performance is required. The end applications include anti-frosting cable and PVC linoleum.

Regulatory Information

Di-n-octyl sebacate has FDA approval under 21CFR178.3910 - Surface Lubricants Used in the Manufacture of Metallic Articles.

Environmental Impact

Based on studies of isomers, this material is expected to be readily biodegradable. If released into the environment, it would be expected to partition into the soil and sediment. Bioaccumulation potential is low.

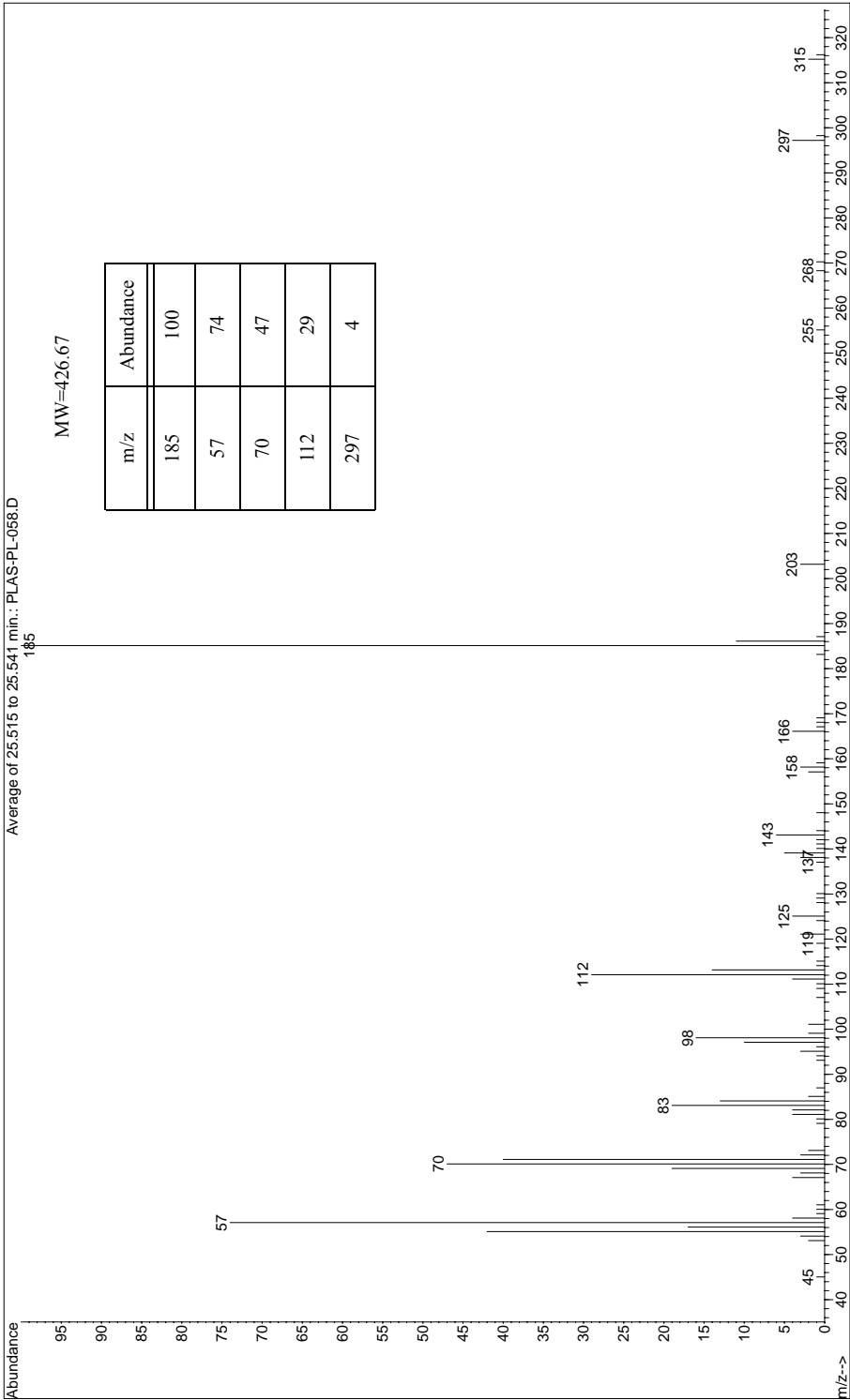
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Oral Toxicity (LD50): 9500 mg/kg [Mouse]. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Witamol 500 - PLAS-PL-058



Other Compounds of Interest

This chapter contains information on additives such as crosslinking agents, processing aids, retarders and stearates. While these compounds may not be as widely used as plasticizers or antioxidants, they play an important role in plastic and rubber processing.

Crosslinking agents

Crosslinking agents are used to form chemical links between molecular chains and create a three-dimensional network of connected molecules. The vulcanization process used in rubber is an example of how crosslinking is used to convert raw rubber from a weak plastic to a highly resilient elastomer. This strategy is also used to control and enhance the properties of polymer systems in thermosets and coatings. The degree of crosslinking can have a profound impact on the swelling characteristics of the crosslinked system.

Processing aids

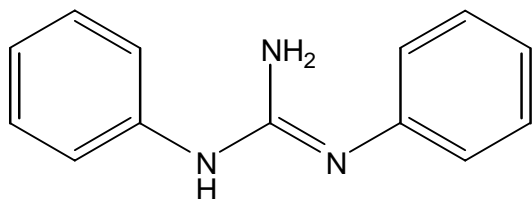
This group includes compounds that lower the viscosity without increasing the plasticizer level (viscosity depressants), parting agents applied to the surface of a mold to provide a release coating and prevent molded articles from sticking to the mold (mold-release agents), compounds added to provide additional stability by increasing internal adhesion in heterogeneous systems or emulsions (emulsifier/surfactants), modifiers used to provide lubrication during processing (slip agents) and preservatives added to prevent attack from fungi, bacteria and yeast (antimicrobials) to name a few.

Retarders

Retarders are chemical reagents used to slow down the reaction process. They are used to control how long the polymer matrix can remain viscous and moldable before setting into a rigid plastic.

Stearates

This group includes salts and esters of stearic acid, which is a saturated fatty acid. Often termed as “metallic stearates,” these compounds are used as release agents in processing polyolefins, polystyrenes, polyesters and rubbers.

Perkacit® DPG

CAS Number 102-06-7

RTECS Number MF0875000

Abbreviation DPG

Formula C₁₃H₁₃N₃

Molecular Weight 211.27

Chemical Name

N,N'-diphenylguanidine

Synonyms

1,3-Diphenylguanidine; Diphenylguanidine; DPG; Melaniline; Sym-diphenylguanidine

Brand Names & Manufacturers

Vanax® DPG

R.T. Vanderbilt Company, Inc.

Vulkacit® D

Lanxess

Soxinol® D

Sumitomo Chemical Co., Ltd.

Physical Properties**Appearance** White to pale-yellow powder**Melting Point** 150 °C**Boiling Point** Decomposes 170 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20°C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	0.08	U	40-80	U	40-80	U

Application Application, Regulatory & Environmental Information

Used as a secondary accelerator with thiazoles and sulfenamides in NR and SBR compounds. Exhibits better storage stability compared to thiuram and dithiocarbamates but is not as active. Perkacit® DPG can be used in latex as a foam stabilizer in the silico-fluoride foam process.

Regulatory Information

FDA approved for use as an accelerator in the manufacture of rubber material (up to 1.5% of weight of rubber) intended for use in all stages of production, processing, packaging and transport of food under 21CFR177.2600.

Environmental Impact

Does not bioaccumulate or persist in environment: Biodegradability: > 90% in <2 weeks. Considered to be toxic to aquatic organisms.

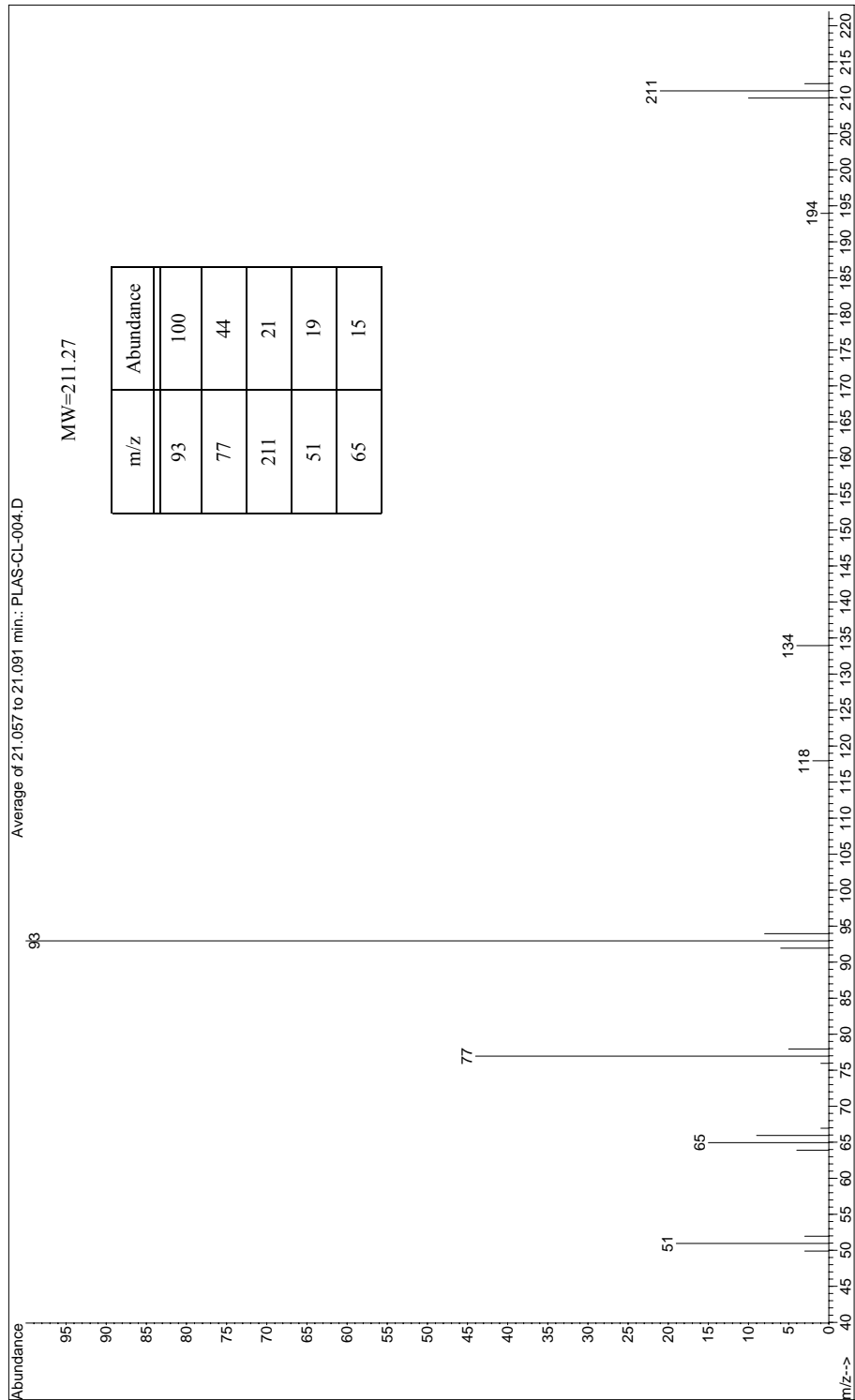
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

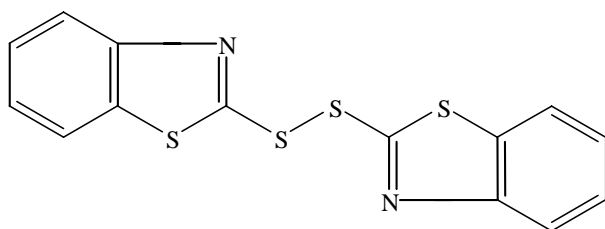
Toxicity of this compound is considered low. Not carcinogenic, with negative to weak results in genotoxicity tests, but does cause reproductive/blood effects. Acute oral (LD50): 350-507 mg/kg [Rat], Acute Dermal (LD50): >2000 mg/kg [Rabbit].

Mass Spectrum for Perkacir® DPG - PLAS-CL-004



Perkacit® MBTS

Akzo Nobel Chemicals B.V.

**CAS Number** 120-78-5**RTECS Number** DL4550000**Abbreviation** DTBT**Formula** C₁₄H₈N₂S₄**Molecular Weight** 332.48**Chemical Name**

2,2'-dithiobis(benzothiazole)

Synonyms

benzothiazole disulfide; di-2-benzothiazolyl disulfide; dibenzoyl disulfide; 2,2'-dithiobisbenzothiazole; 2-mercaptopbenzothiazole disulfide

Brand Names & Manufacturers

Altax® (MBTS)

R.T. Vanderbilt Company, Inc.

Naugex®

Chemtura Corporation

Thiofide

Solutia Inc.

Physical Properties**Appearance** Off-white powder**Melting Point** 177-180 °C**Boiling Point** 260 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Used as a medium-fast vulcanization accelerator for butyl, isoprene, and diene (natural and synthetic) rubbers. Also used as a retarder in neoprene. Commonly found in industrial rubber products such as footwear, hose, roofing and automotive components.

Regulatory Information

FDA approved for use in articles in contact with food as specified under 21CFR177.2600 and 175.105.

Environmental Impact

Undergoes sunlight photolysis with T(1/2) of 3 hours, slightly susceptible to indirect photolysis. Product is considered harmful to aquatic organisms and has a low to moderate potential to bioaccumulate based on an estimated log Pow value of 4.2.

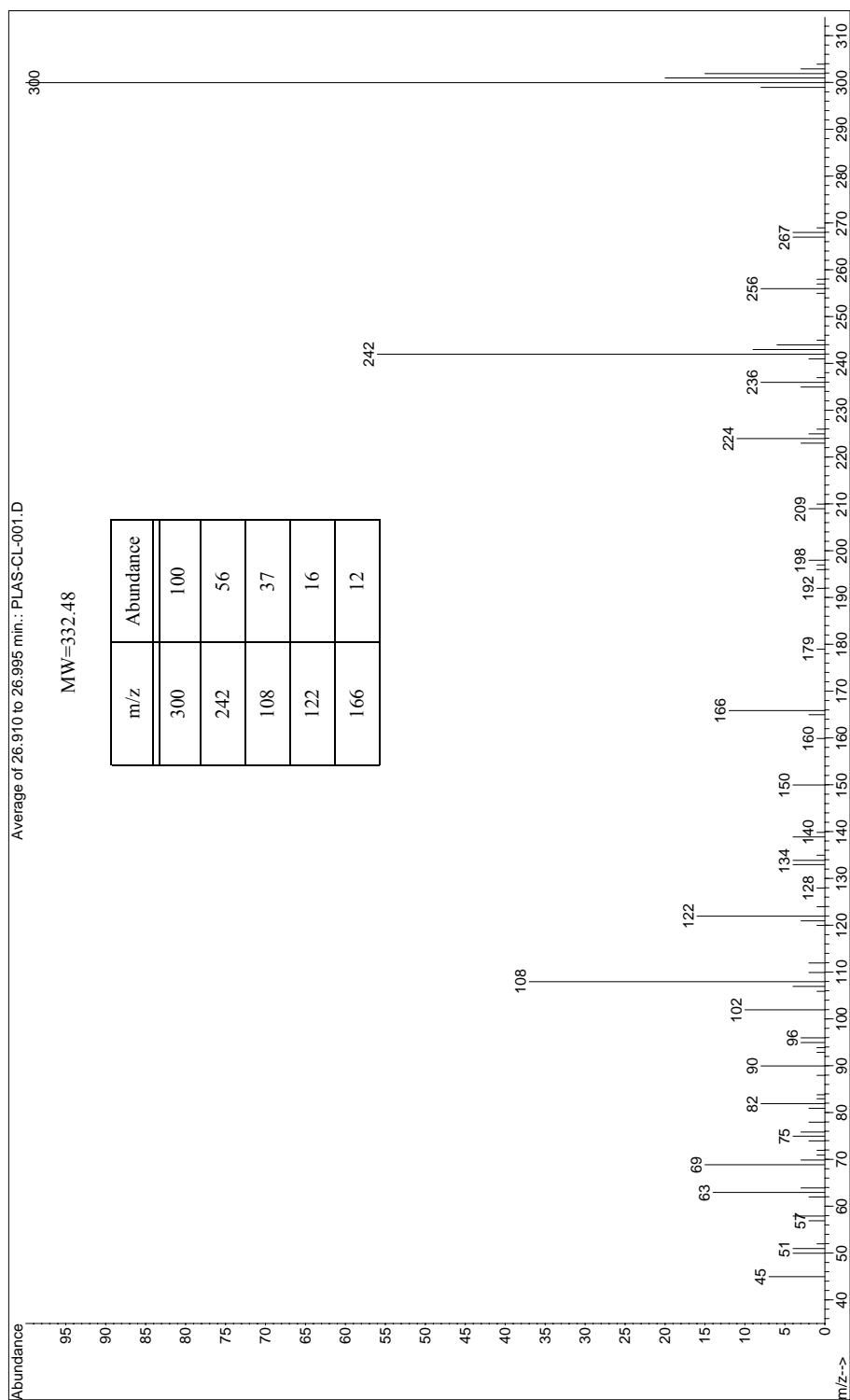
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

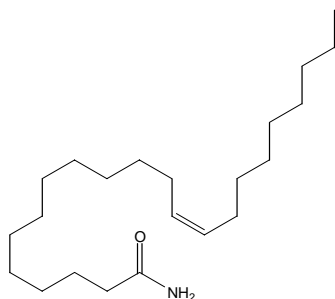
Toxicity of DTBT is low. No evidence of carcinogenicity or gonadotoxicity. Only a minor dust hazard. Acute oral (LD50): >7940 mg/kg [Rat]; Acute Dermal (LD50): >7940 mg/kg [Rabbit].

Mass Spectrum for Perkacir® MBTS - PLAS-CL-001



Kemamide® E ultra

Chemtura Corporation

**CAS Number** 112-84-5**RTECS Number** Not available**Abbreviation****Formula** C₂₂H₄₃NO**Molecular Weight** 337.58**Chemical Name**
erucamide**Synonyms**

erucyl amide; 13-docosenamide; (Z)-docos-13-enamide

Brand Names & Manufacturers**Physical Properties**

Appearance	Powder					
Melting Point	80-85 °C			Boiling Point	Decomposes	
Stability	Stable under normal conditions of use.					
Solubility (g/100mL 20 °C)	Water <0.01	MeOH 10	EtOH 10	Acetone 10	CH₂Cl₂ U	Hexane U

Application Application, Regulatory & Environmental Information

Additive used for thermoplastic applications requiring lubrication, slip and anti-blocking properties. Commonly used in polyethylene and polypropylene films, as a lubricant in polyvinyl chloride, mold release agent, dyestuff dispersant for printing inks and surface coatings, and a blending agent for polyamide resins.

Regulatory Information

FDA approved for use with rubber food-contact materials per 21CFR178.2010 or 178.3860.

Environmental Impact

Not expected to be an immediate hazard to the environment. Long term effects have not been thoroughly investigated.

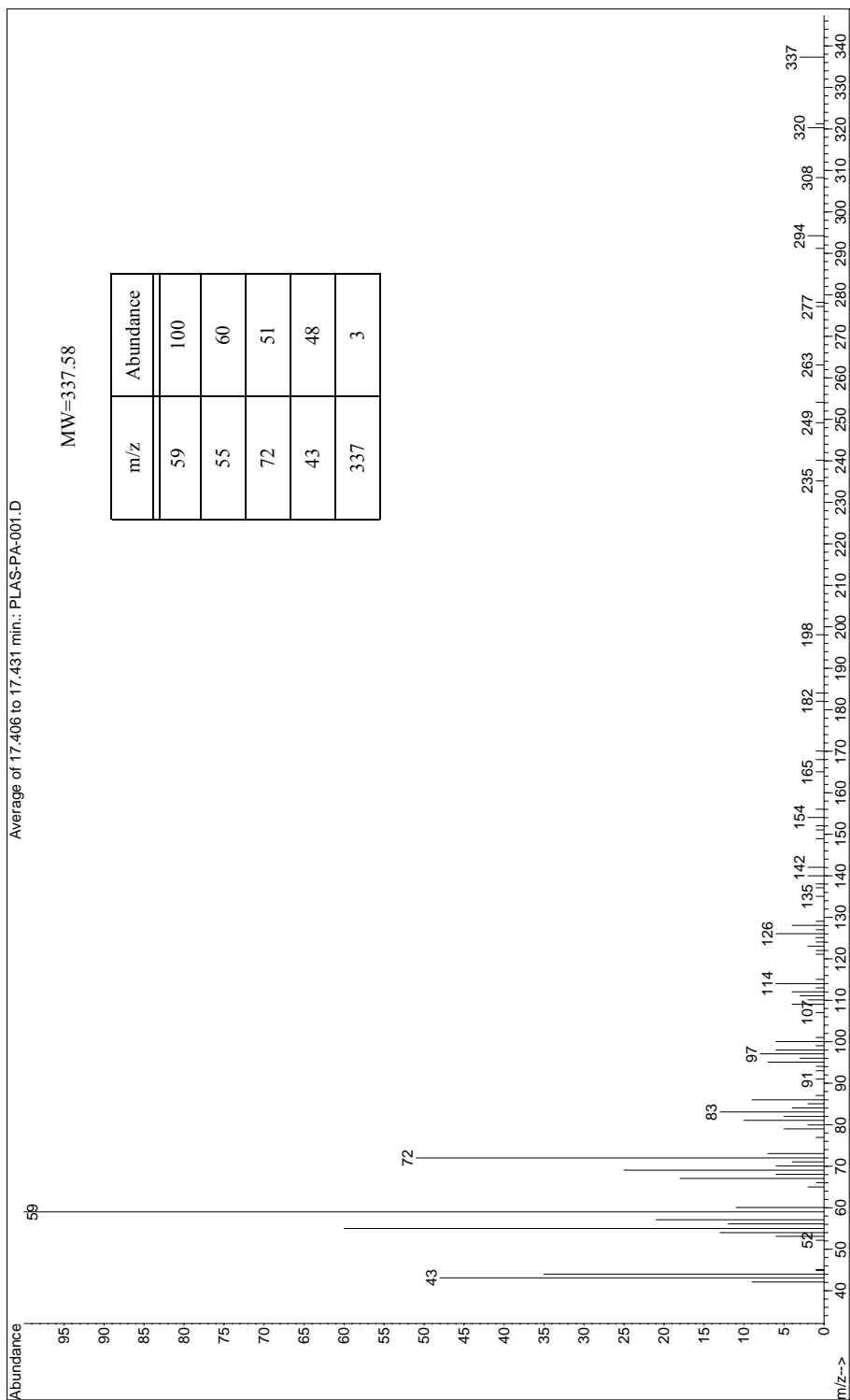
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

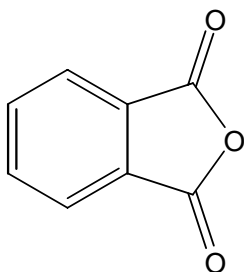
Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA. Also not listed on California Proposition 65.

Mass Spectrum for Kemamide® E ultra - PLAS-PA-001



Retarder AK

Akrochem Corporation

**CAS Number** 85-44-9**RTECS Number** TI3150000**Abbreviation****Formula** C₈H₄O₃**Molecular Weight** 148.12**Chemical Name**
phthalic anhydride**Synonyms**

1,3-isobenzofurandione; phthalic acid anhydride; 1,2-benzenedicarboxylic acid anhydride

Brand Names & Manufacturers**Physical Properties****Appearance** White powder**Melting Point** 123-132 °C**Boiling Point** 284 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	1-10	40-80	40-80	40-80	U	U

Application, Regulatory & Environmental Information**Application**

Retarding agent for most types of rubber. Also used as an intermediate in the production of pigments and dyes, agricultural, pharmaceutical, and several other chemical products. Phthalic anhydride containing materials are used in coatings applications for home appliances, automobiles, medical devices and furniture.

Regulatory Information

Regulated by the EPA under the Clean Air Act as a hazardous air pollutant and the Clean Water Act as a hazardous water pollutant. Phthalic anhydride is approved by the FDA for a variety of food contact applications.

Environmental Impact

When released to moist soil or water, this material is expected to hydrolyze. When released into water, this material is not expected to evaporate significantly, and it will have a half-life of less than 1 day. This material has an estimated bioconcentration factor (BCF) of less than 100. This material is not expected to significantly bioaccumulate. When released into the air, this material is expected to have a half-life of greater than 30 days.

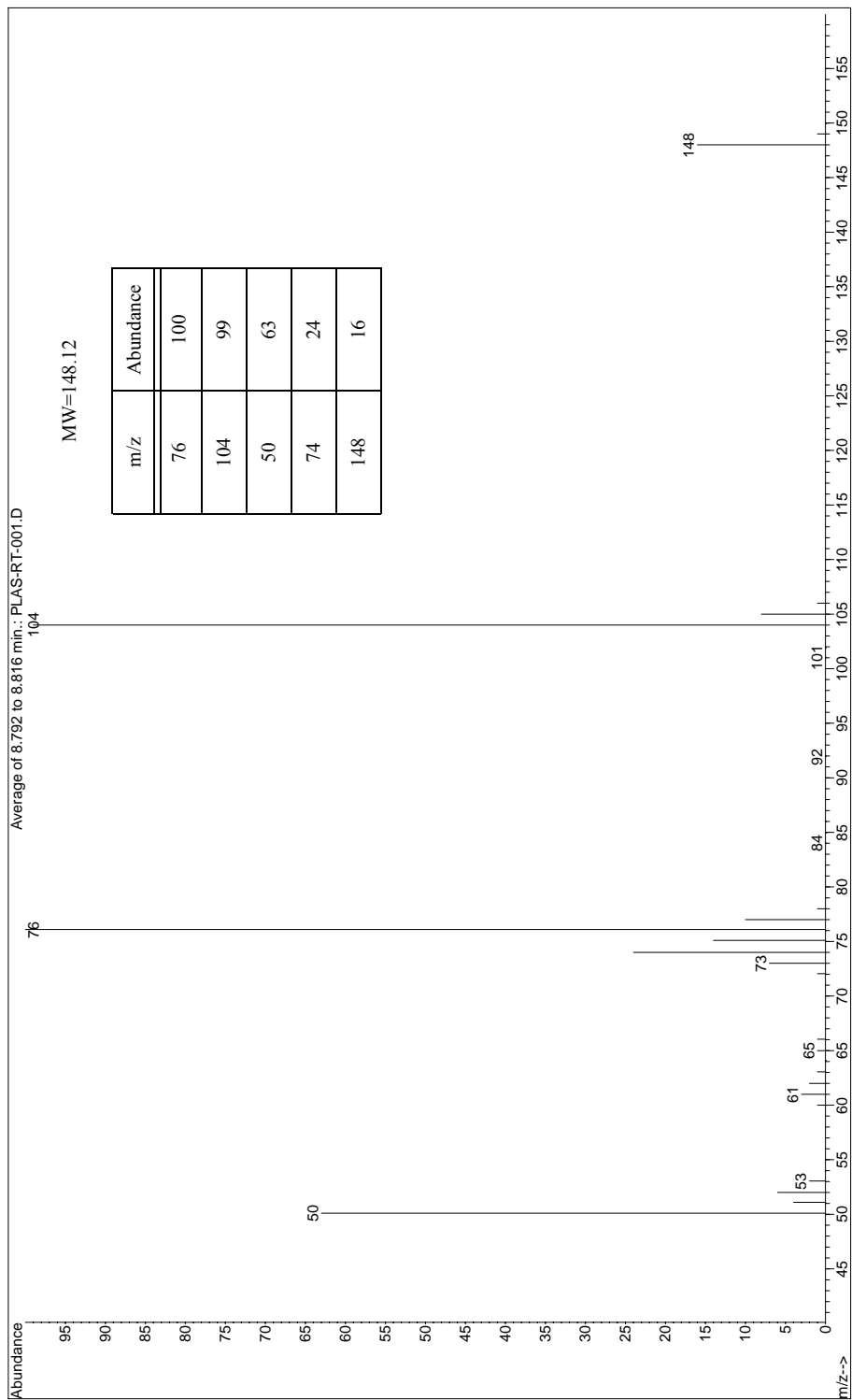
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, consumers may be exposed to phthalic anhydride from the use of plastics, furniture, glues, coatings and home products from which phthalic anhydride may leach, and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): 1530 mg/kg [Rat], Acute dermal (LD50): >10 gm/kg [Rabbit]. Acute inhalation (1h) (LC50): >210 mg/m³ [Rat]. Has shown teratogenic effects in laboratory animals. Not listed as a carcinogen by IARC, NTP, ACGIH or OSHA.

Mass Spectrum for Retarder AK - PLAS-RT-001



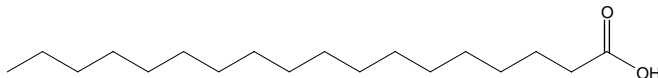
Stearic Acid RG (rubber grade)

Akrochem Corporation

CAS Number 57-11-4

RTECS Number W12800000

Abbreviation

Formula $C_{18}H_{36}O_2$

Molecular Weight 284.48

Chemical Name

stearic acid

Synonyms

octadecanoic acid; cetylacetic acid; 1-heptadecanecarboxylic acid

Brand Names & Manufacturers

Glycon® DP

Glycon Corporation

Physical Properties**Appearance** Colorless, waxy solid**Melting Point** 67-72 °C**Boiling Point** 361 °C**Stability** Stable under normal conditions of use.

Solubility (g/100mL 20 °C)	Water	MeOH	EtOH	Acetone	CH₂Cl₂	Hexane
	<0.1	40-80	40-80	U	40-80	U

Application Application, Regulatory & Environmental Information

Dispersing agent and accelerator activator in rubber compounds. It aids dispersion of pigments and fillers and improves processing since it acts as a stock lubricant and can facilitate mold flow, improve extrusions and aid release.

Regulatory Information

FDA approval for food contact applications under 21CFR184-1090. On the FDA GRAS (generally approved as safe) list.

Environmental Impact

When released into soil or water, this material is expected to readily biodegrade.

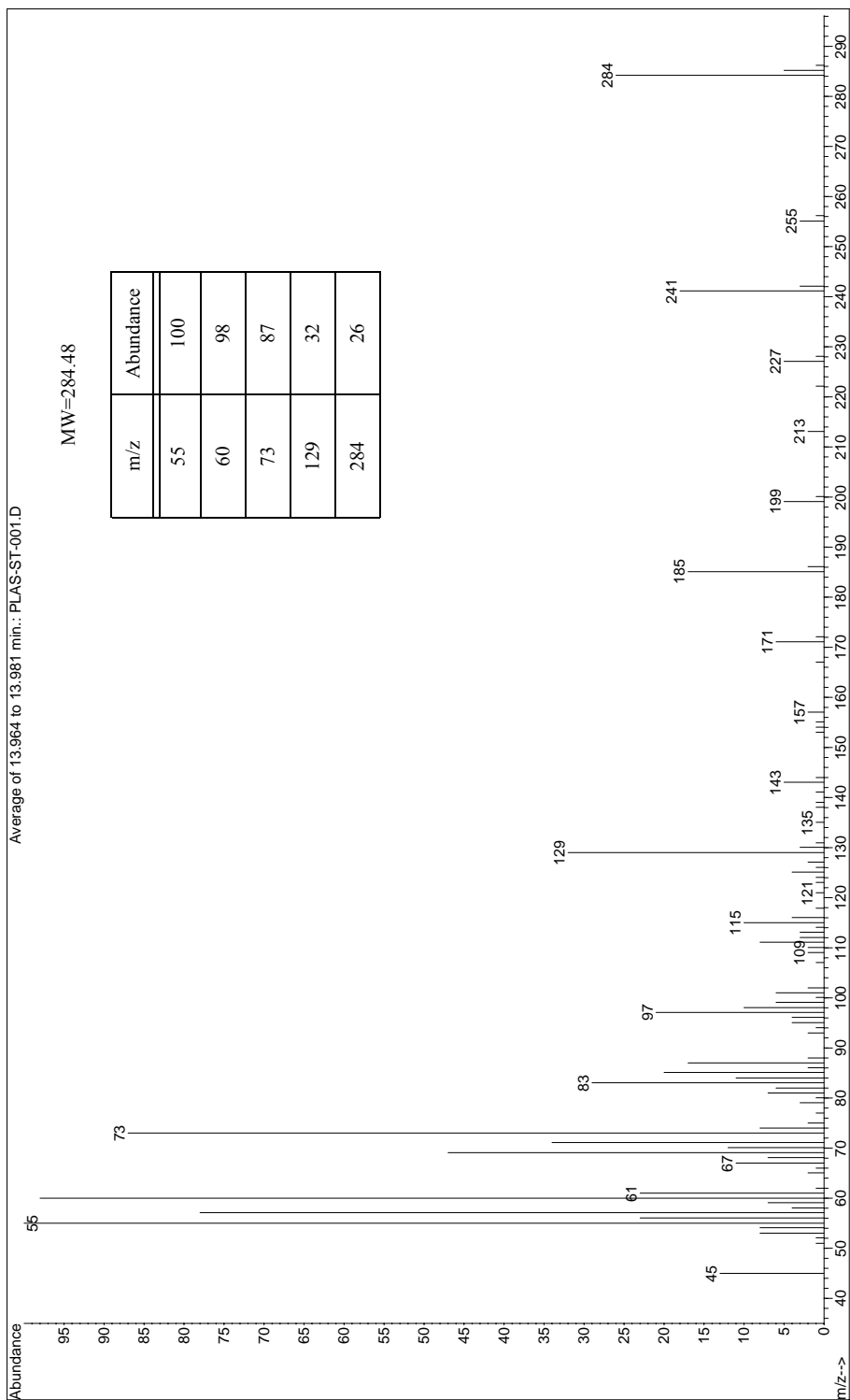
Point of Release

Can be released as point source pollution during manufacture, transportation and end use. Additionally, it may be released from manufactured products containing this material during the active life cycle of the products and/or upon disposal of the products.

Toxicological Data

Acute oral (LD50): >2000 mg/kg [Rat], Acute dermal (LD50): >5000 mg/kg [Rabbit].

Mass Spectrum for Stearic Acid RG (rubber grade) - PLAS-ST-001



Real World Problems Related to Additives

Introduction

Consultants are called in when problems show up in drug delivery devices containing plastic components. These problems are mostly caused by additives introduced during the manufacturing process.

From the files of one of the authors of this book are culled some of these interesting case studies. First we will present background on the issues involved.

CASE STUDIES: POLYMER ADDITIVES IN PHARMACEUTICAL PACKAGING

Background

Packaging for drugs ranges from simple tablet bottles and vials, to complex respiratory delivery devices that combine dry powder dispersion with a controlled air flow for asthma therapy. Other devices include point-of-delivery mixing of drug ingredients, pumps, diffusion membranes, and more. These may include polymer-coated metals, polymeric packaging with internal metal components, and combinations of thermoplastics, elastomers, and/or metals. Technical packaging components are engineered to achieve uniform drug stability, dose delivery rate, or both.

Although packaging suppliers may perform developmental work, many drug delivery systems are designed by pharmaceutical companies. This is especially true when a new device is required for which there is no precedent. Packaging suppliers also perform original development work. In some cases, existing devices are modified. For example, a coating for the interior surface of an aluminum metered dose inhaler (MDI) canister may be developed by a pharmaceutical manufacturer. Implementation of the design is then taken to a manufacturer for commercial production, during which time tooling is developed for the components or process. Engineers or technical persons typically select materials based on engineering properties. Impact resistant ABS (acrylonitrile-butadiene styrene) might be selected for a particular component. A critical omission may be that the details of the formulation are not investigated at the outset.

Additionally, subsequent analysis of the materials for compliance to various regulations is based on solvent extraction protocols followed by GC/FID (flame ionization detector) analysis. These protocols are generally based on specific target compounds that are regulated rather than analysis for all compounds present. From our experience we have documented many problems related to such an approach. The following case studies emphasize the need for thoroughly analyzing materials for suitability early on in the developmental process.

Case Study #1: Pre-Filled Syringe Vials

Injectable drug products are often pre-packed into vials that are inserted into syringe barrels for delivery into the patient. In some cases, the vials contain contaminants. In one instance, the drug in this vial was found to contain acetophenone, dibutyl phthalate, stearic acid, and myristic acid, none of which are components of the drug formulation. These substances each have negative health implications and are regulated for various applications.

Investigation into the vial manufacturing process was initiated at this point. The vials are most commonly glass, since this provides an inert contact surface and transparency for visual feedback. The vials must be sealed, and at one end a piston must be provided while at the opposite end a diaphragm is fitted to allow puncture by the needle inside the syringe barrel. The elastomeric

components of both are shown in Figure 10-1 and Figure 10-2. The diaphragm is surrounded by an aluminum ferrule that is crimped to form a seal after the vial is filled.



Figure 10-1 Crimped Diaphragm on Pre-Filled Syringe Vial



Figure 10-2 Piston on Pre-Filled Syringe Vial

The drug in this vial was subjected to GC/MS analysis at the end of its shelf life and the contaminants identified. GC/MS analysis of the vial piston and diaphragm were conducted. The GC/MS analysis of the vial piston shows a range of nitrile fragments, consistent with nitrile rubber. Silicone is typically present in this type of component to provide lubricity in the bore of the glass vial. Acetophenone was also found. It is a thermal decomposition product from the peroxide crosslinking agent in the rubber (dicumyl peroxide). Stearic and myristic fatty acids were present and are typically added in the manufacturing process during mixing to reduce shear viscosity. These materials dissolve into the drug compound over time. The result is that regulated, non-formulation organic compounds are injected in unknown amounts directly into the bloodstream of unsuspecting and often ill patients.

The root cause of this problem goes beyond determining and stopping the source of the contaminants. The root cause of the problem was that the designers of the vial did not consider contamination during the original design. The corrective action was to change the design approach so that possible contamination is part of the design criteria in addition to the engineering properties specified.

Case Study #2: Nasal Pump Delivery System

A wide range of over-the-counter and prescription pharmaceutical products use manually actuated pumps. A common example is the nasal spray container. When the design of these pumps allows contaminated products to be used, the patients and the manufacturer have a problem. This was the case, when palmitic, myristic, stearic, and oleic fatty acids (these are all non-formulation ingredients) were found in a nasal spray product.

The investigation was begun after complaints that the pumps became blocked over time. Pumps typically deliver a low pressure, fine droplet-sized mist at a controlled dose rate. Good control of the dose rate and spray pattern requires precision molding of the components and consistent performance of these components when they are in contact with the drug product for extended periods and over a wide range of ambient temperatures. These components are made of thermoplastic, elastomeric, and metallic materials. The pump actuator and its elastomeric check valve are vital components. Their relative position is shown in Figure 10-3.

The drug formulation contains an active ingredient, a thixotropic adjunct to promote drug retention on mucosal surfaces, water, stabilizers, a buffer, and alcohol.

In the course of the investigation into the blockage of the nasal spray actuators, devices that passed 100% spray-testing at the time of manufacture were found to become blocked after an extended period of non-use. Investigation into blockage revealed nothing unusual about the drug formulation. When a new actuator was placed on the pump, normal action resumed. Blockage within the actuator was removed and analyzed by GC/MS and was found to contain formulation ingredients plus fatty acids. These included palmitic, myristic, stearic, and oleic fatty acids. A gelled substance was present on the elastomeric check valve. This gelled substance is shown in Figure 10-3.

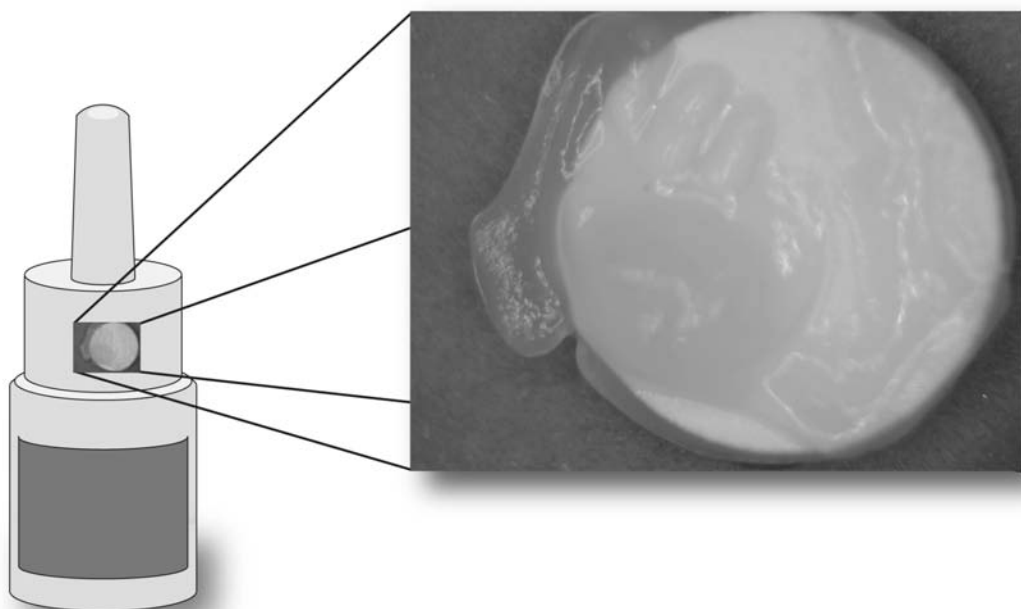


Figure 10-3 Gelled Nasal Formulation on Elastomeric Check Valve

The investigation turned to the identification of the gelled substance. It was found that fatty acids were included in the actuator's elastomeric gasket's rubber formulation. Laboratory experiments then replicated the formation of the gelled substance through interaction between the double bonds on the oleic acid and one of the formulation ingredients. The drug formulation is in stagnant contact with this elastomeric seal, and that caused the gelled material to form on the actuator surface. At some point the gelled material would break away. The high viscosity of the gel would not allow it to pass through the narrow internal passages in the actuator. Figure 10-4 shows the GC/MS analysis. The other compound found, the alkyl phenol, is an antioxidant. The specific identification of these compounds was made possible through comparison of mass spectra with reference materials.

The original problem had been identified as the clogged pump. However in the course of the investigation, it became apparent that contaminants had entered the drug formulation due to interaction between the drug and the container material, a potential health threat. Corrective actions were to replace the materials in the container and also to consider container material as possible contamination sources in the design stage.

Case Study #3: Dry Powder Inhalation Device

Dry powder inhalers have been in the market for approximately 20 years. Their use is increasing due to new forms of medications that can be micro-encapsulated in a manner that permits pulmonary delivery. As all products intended for human use must be considered for contaminants, it was surprising that in one recent case, dry powder inhalers were found to contain many compounds not found in the original formulation, including phthalates, alkanes, branched chain hydrocarbons, and alcohols. The investigation of the root cause demonstrates that the

understanding of contaminants needs to include not only the materials of the container, but also the processing of those materials.

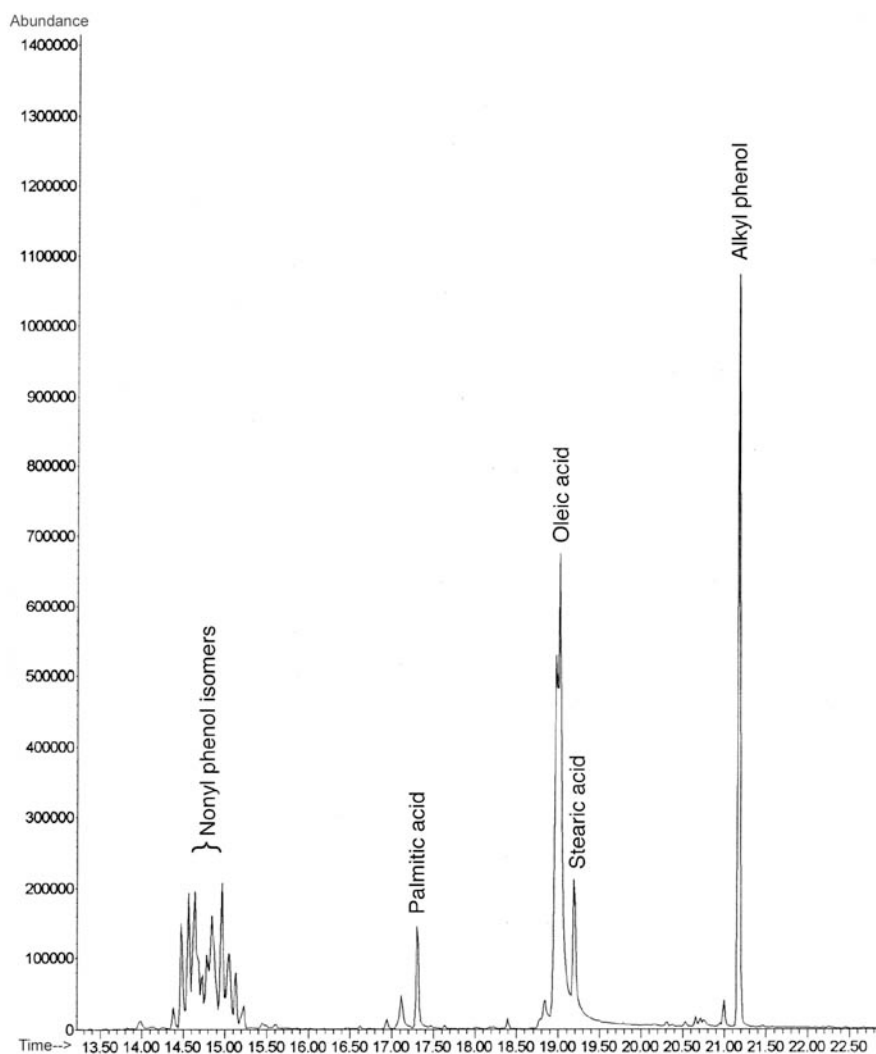


Figure 10-4 GC/MS Chromatogram of Ethanol Extract of Elastomeric Gasket

For one such device, polycarbonate was chosen from a particular supplier to form a high strength component that contacts the drug delivery stream. During chemical testing of devices from several Production Qualification (PQ) lots, anomalous analytical results were obtained with GC/MS sampling of the polycarbonate component. Figure 10-5 presents the analysis of the initial, qualified polycarbonate compound analyzed by thermal desorption GC/MS. This analysis contains traces of thermal decomposition products of the polycarbonate, an antioxidant, and a trace of bis-phenol A (BPA), one of the starting materials for polymerization of polycarbonate. A commercial compounder prepared this polycarbonate with a specific non-staining antioxidant that is safe for drug contact. While bis-phenol A would not be desirable for patient contact, this compound was

accepted, as it was believed that this trace concentration could not reach the patient through normal use of this device.

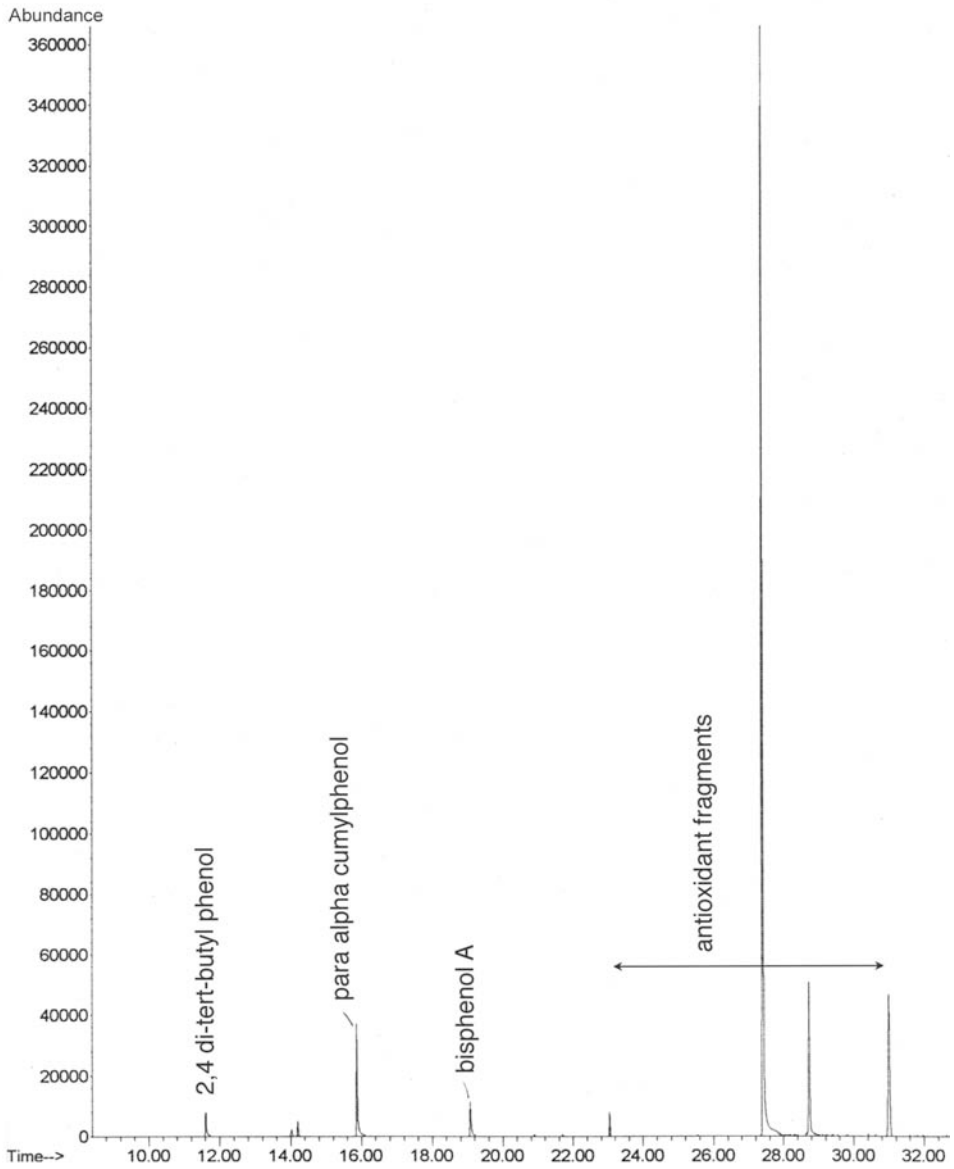


Figure 10-5 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler

While subjecting two other PQ lots of these components to GC/MS analysis, the polycarbonate formulations were found to be very different from the original. Figure 10-6 shows a second PQ run and Figure 10-7 shows a third PQ run. The second and third PQ lots were found to contain many compounds not found in the original, including phthalates, alkanes, branched chain hydrocarbons, and alcohols. The third run also contained fatty acids. This level of inconsistency led to a production hold on this device and subsequent investigation.

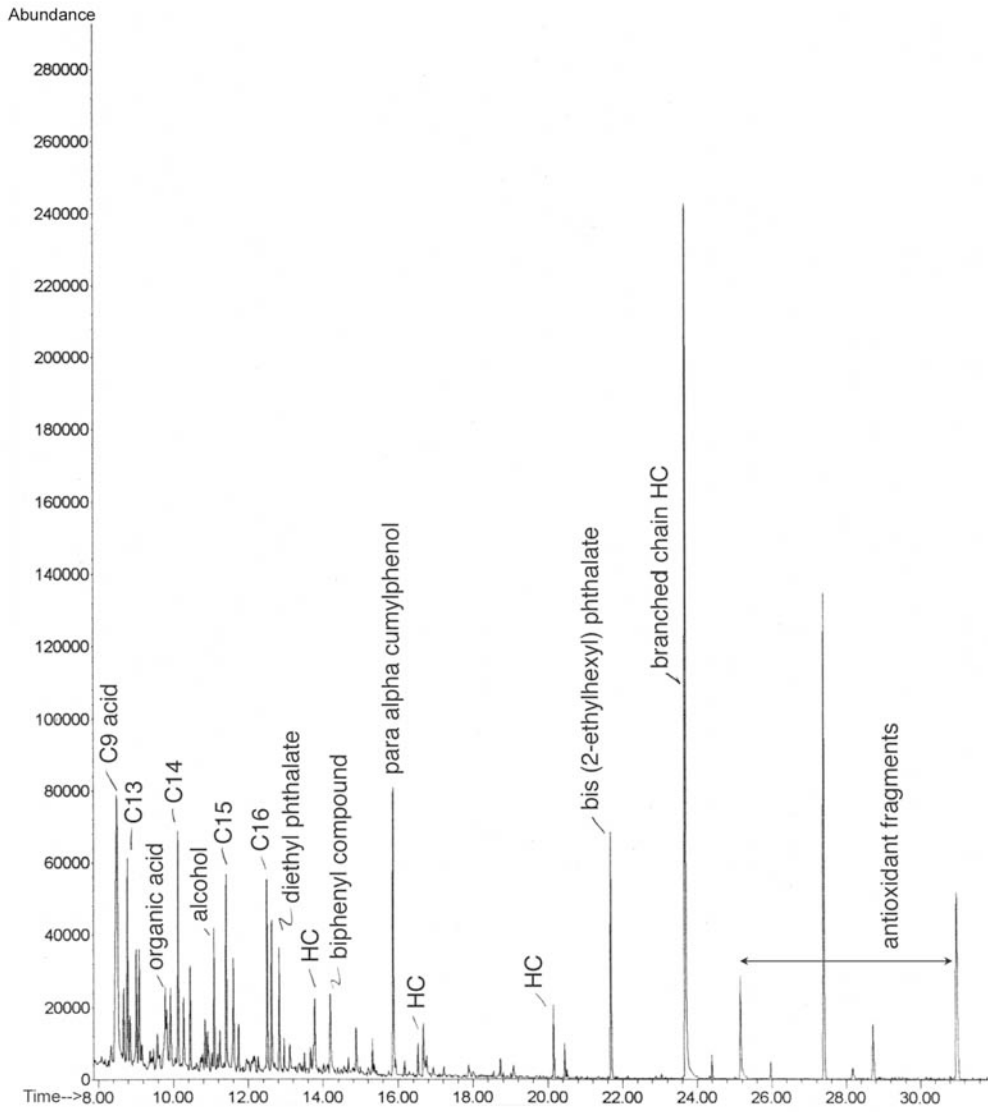


Figure 10-6 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler, Second Lot

The supplier of the base polycarbonate resin provided all production details and controls and site visits confirmed that it was highly unlikely that the base resins could vary in this manner. The commercial compounding site was visited and production runs of this and other resins were witnessed and reviewed. It was discovered that the mixing equipment was being shared and was used for mixing other polymers from other customers. Adequate purging protocols were not in place to ensure that the material from previous runs was fully purged from the mixing system before the next run was started. Corrective actions included amending the processing work instructions and training to include more complete purging methods. The manufacturer of the Dry Powder Inhalation Device also amended its own formulation specifications to include review of the purging methods.

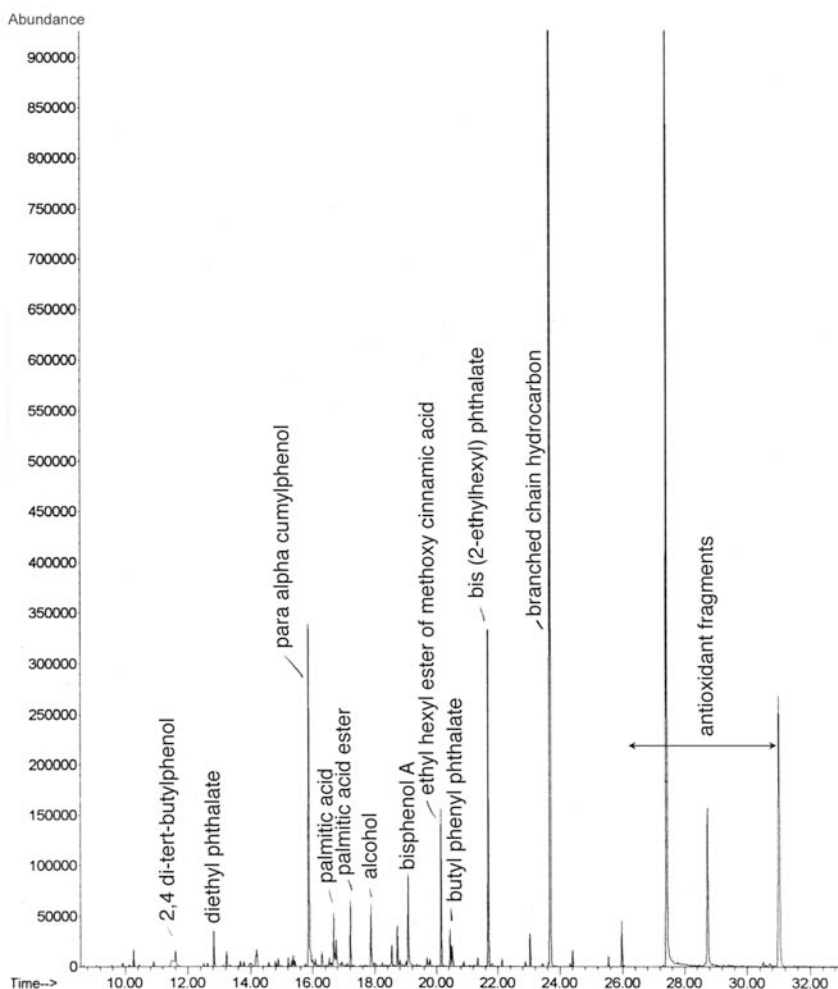


Figure 10-7 GC/MS Chromatogram of Polycarbonate Part of Dry Powder Inhaler, Third Lot

CASE STUDIES: CONTAMINATION FROM PACKAGING

Introduction

Polymeric packaging materials come into contact with both finished goods and raw materials. Governmental agencies such as the US FDA and agencies of the EU have regulations to monitor and control the presence and amount of these substances in food and drugs. Packaging for other applications are largely unregulated. The two case studies that follow are examples of unintended contaminants getting into packaging.

Uses of Additives

Packaging manufacturers and their suppliers develop materials that must meet a wide range of requirements including cost competitiveness. Most packaging materials are commodity products, sold to a general description, so the end product's components are not strictly controlled. Common types of plastic packaging include 'low density polyethylene' (LDPE), 'high density polyethylene' (HDPE), virgin polyethylene, polyethylene terephthalate (PETE), and many others. Typical

minimum functional requirements for packaging include the following: tear resistance, acceptable appearance (transparency, translucency, color, or opacity), anti-blocking performance (plastic bags must open freely without sticking), integrity (no pinholes or gaps in seams), gauge, and type of material. It is rarely practical to identify a packaging material that contains only the requested polymer (without additives).

Formulations from any given supplier can be expected to change periodically, since the packaging manufacturer may source from a number of different resin suppliers. This network is illustrated in Figure 10-8. As indicated, the packager has no direct relationship with the raw material suppliers; hence there is no direct control over the packaging material formulations. Information provided in Material Safety Data Sheets (MSDS) is insufficient for controlling packaging for critical applications. The formulation details disclosed in this documentation address principal ingredients that do not contain any detail about specific compounds or master batch ingredients.

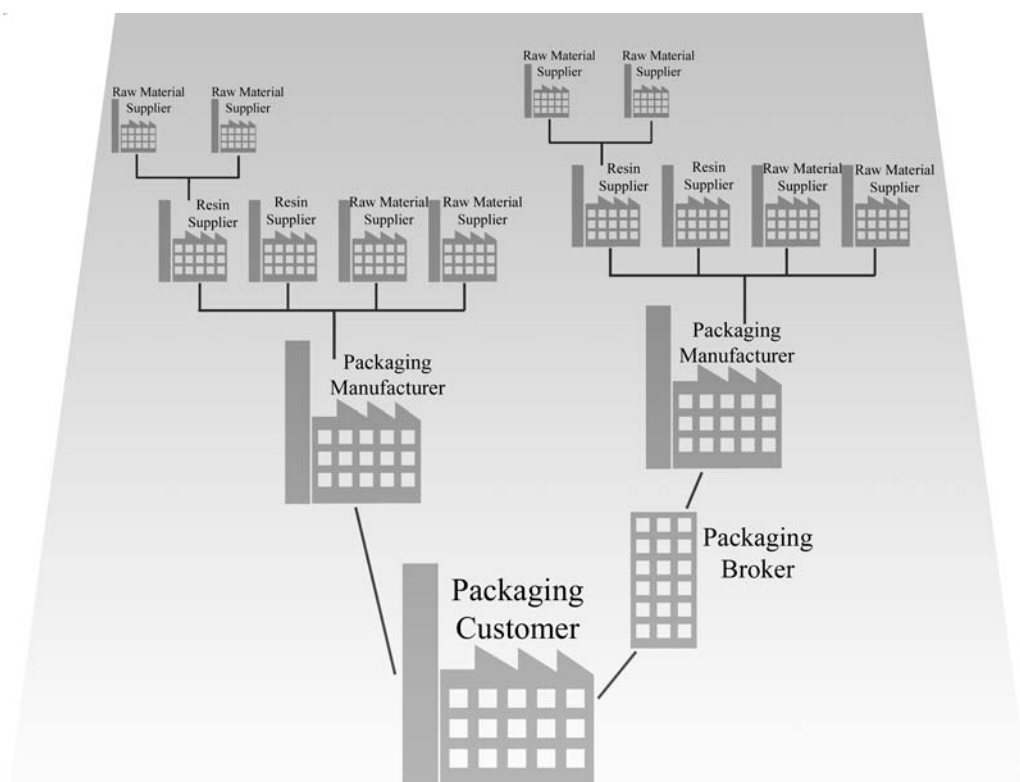


Figure 10-8 Packaging Supply Network

The type of process used also indicates the addition of polymer modifiers. Blow-molding requires that the polymer flows easily, while retaining good cohesive strength when molten, to avoid tears and voids. Melt flow modifiers are typically used for this purpose and include fatty acid esters, oleoamides, and adipates. Compounds of this type often also serve to prevent blocking (adhesion of one side of a bag to the other).

Typical minimum requirements for the packaging necessitate the addition of other polymer modifiers. Prevention of discoloration requires addition of an antioxidant. The resin supplier is

typically required to meet a general performance specification; however the final use of the packaging may not be stipulated or considered when an antioxidant is chosen. Ultraviolet resistance is required for some packaging where extended sunlight exposure is expected. A common additive is carbon black.

Case Study #1: Contaminants in Plastic Food Packaging

Routine chemical analysis of a frozen food product containing unsaturated vegetable oils showed sporadic contamination with phthalates and erucamide, a fatty acid amide. (Both substances are listed in the US FDA list of Indirect Food Additives as well as other regulations, and their presence in food is regulated.) This food product was packaged in a heat-sealed polyethylene bag. The packaging supplier attributed the presence of these organic compounds on the surface of the frozen food product to sources other than their packaging; however the packaging supplier stated that all of their film resin came from a single supplier. The specification for this resin stipulated a melt flow index, a whiteness index for the pigment, tensile strength, elongation limit, and low density polyethylene as the base resin. Figure 10-9 shows the composition of a typical package from this supplier. Thermal desorption GC/MS was applied and indicated hydrocarbons consistent with polyethylene plus butylated hydroxytoluene (BHT) as an antioxidant. BHT is approved as an antioxidant for food contact applications.

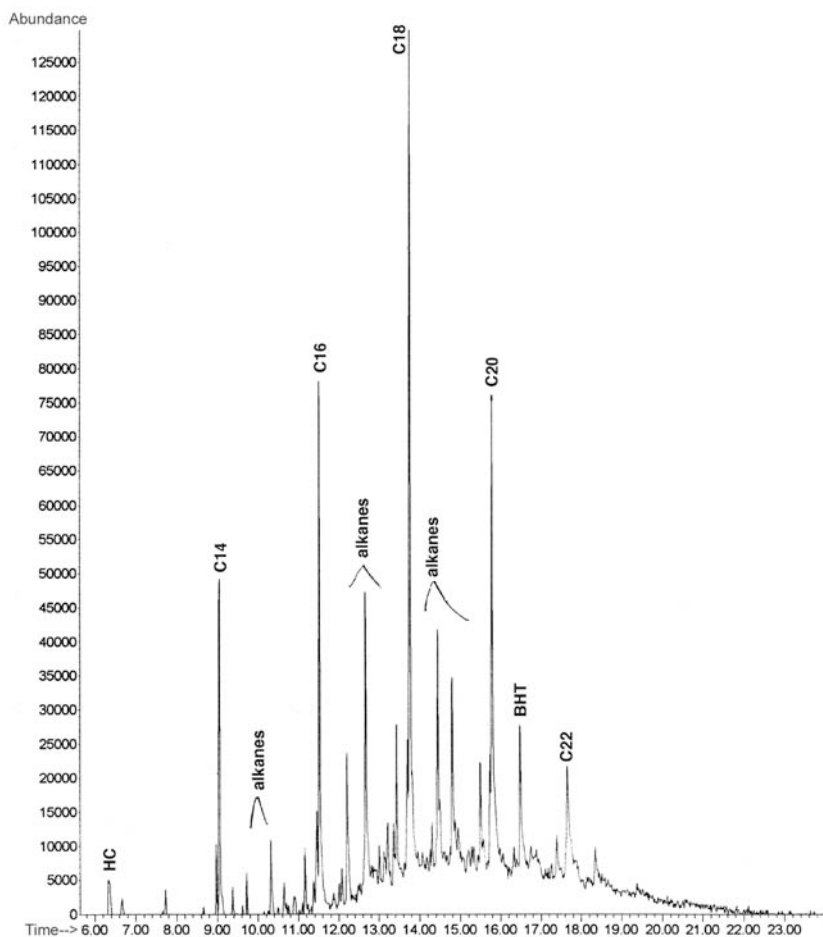


Figure 10-9 GC/MS Chromatogram of Typical Packaging Material

Investigation into the packaging film manufacturing processes was initiated. Packaging was screened at the food production warehouse. The screening was based on appearance and feel as an initial approach. Packaging film with a distinctly waxy surface was identified as abnormal and analyzed by thermal desorption GC/MS. Figure 10-10 shows the chromatogram of the analysis of one anomalous material sample indicating isobutyl phthalate, dioctyl phthalate and erucamide as ingredients in the polyethylene film. These substances are named in the US FDA list of Indirect Food Additives and their presence in food is regulated. This anomalous packing material was determined to be the cause of the food contamination.

Research into the source of these unexpected compounds determined that the packaging supplier had made a formulation change to offset the stiffness of a newer and less expensive source of polyethylene. The root cause goes beyond the source of the contaminants. It extends to why the formulation change was made without regard to the end use of the product. The corrective action was for the supplier to more tightly control processes and to verify component changes with the customer

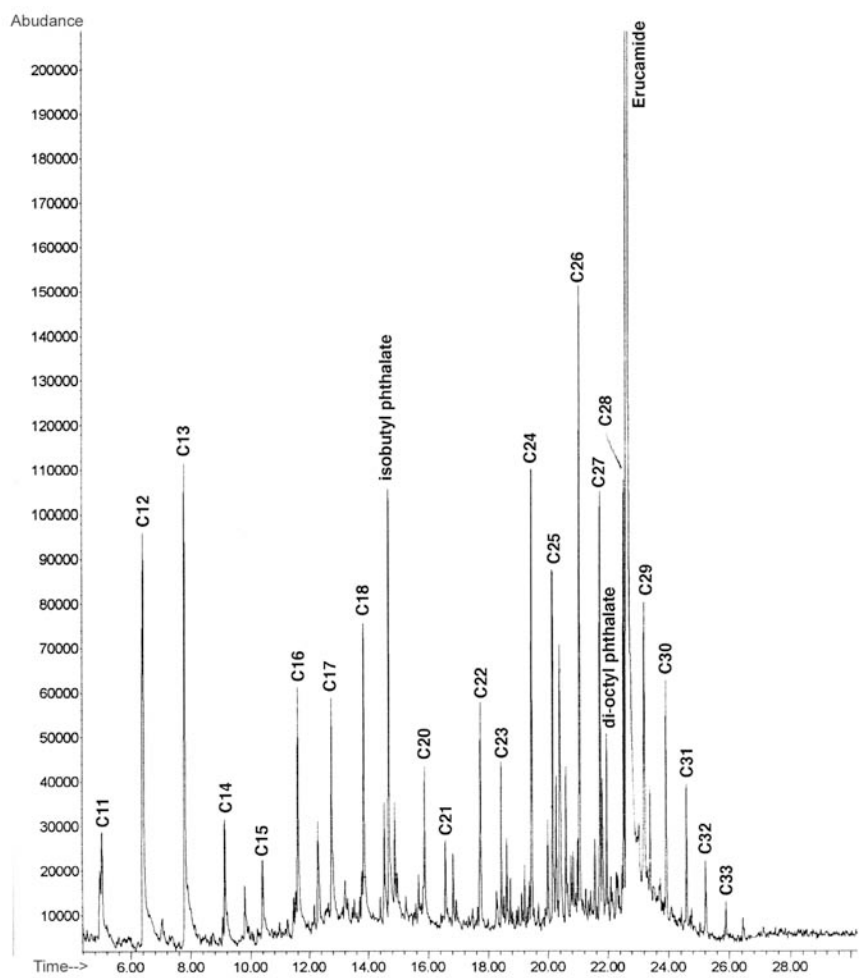


Figure 10-10 GC/MS Chromatogram of Anomalous Packing Material

Case Study #2: Peeling Labels

Adhesive labels are used on many products and need to remain on the product for many reasons including safety, identity and proper use of the product. In this case the adhesion failed and prevented the further use of the equipment in which the product was used.

Batteries are typically produced with deep drawn metal cans on which a pressure sensitive adhesive label is applied for product identification, branding and safety information. Customers began complaining of batteries becoming jammed in various types of equipment. Devices returned to the manufacturer showed that the pressure sensitive labels had peeled back, resulting in adhesion between the overturned label and the device. Further examination of batteries on store shelves for more than a year also indicated peeling labels in a low frequency of batteries. These labels consisted of laminates of paper and polyester. The labels are normally flat and stiff and when applied over a battery, the labels will return to the flat condition if the adhesive fails. This results in peel-back at the edges of the label.

Investigation into the battery processing was initiated. Comparative GC/MS analysis of peeling and non-peeling areas of the labels indicated that the peeling areas contained phthalates and palmitic acid. Both act as plasticizers in the pressure sensitive adhesive used for these labels. Since the labels are printed in a continuous process, it was unlikely that only specific areas would be affected. This was consistent with the observed low frequency of label peeling, and eliminated the deposition of adhesive as a potential root cause.

The cans used to produce the batteries are deep drawn with a water-based lubricant that does not contain the phthalates or the palmitic acid. The cans are then washed in a phosphate surfactant and then dried at high temperature. The cans are then bulk-packaged into cardboard gaylords, lined with plastic bags. In this case, the cans were dropped from the drying oven into the shipping container while still warm. Cans removed from the bag and randomly sampled by GC/MS showed no trace of phthalates or palmitic acid. However, upon further investigation, those cans that came into direct contact with the packaging did contain the phthalates and palmitic acid. Results of the GC/MS analysis of the corresponding bag is shown in Figure 10-11. This indicates that the bag contains diethyl phthalate, dibutyl phthalate and palmitic acid. The phthalates serve as plasticizers for the bag and palmitic acid is a lubricant that blooms to the surface and renders the bag easy to open. Both features are completely inconsistent with the requirement to maintain the battery cans in a clean, contaminant-free condition.

Again, the root cause of the non-conformance was that the environment (in this case the gaylords lined with the plastic bags) was not kept contaminant free. At a further level, there was a lack of awareness about what constitutes a contaminant on the part of the can manufacturer. The corrective action was to educate the manufacturer about possible contaminations, to review the manufacturer's processes and to promote dialog between the manufacturer and the customer on matters effecting contamination, process change and ingredient changes.

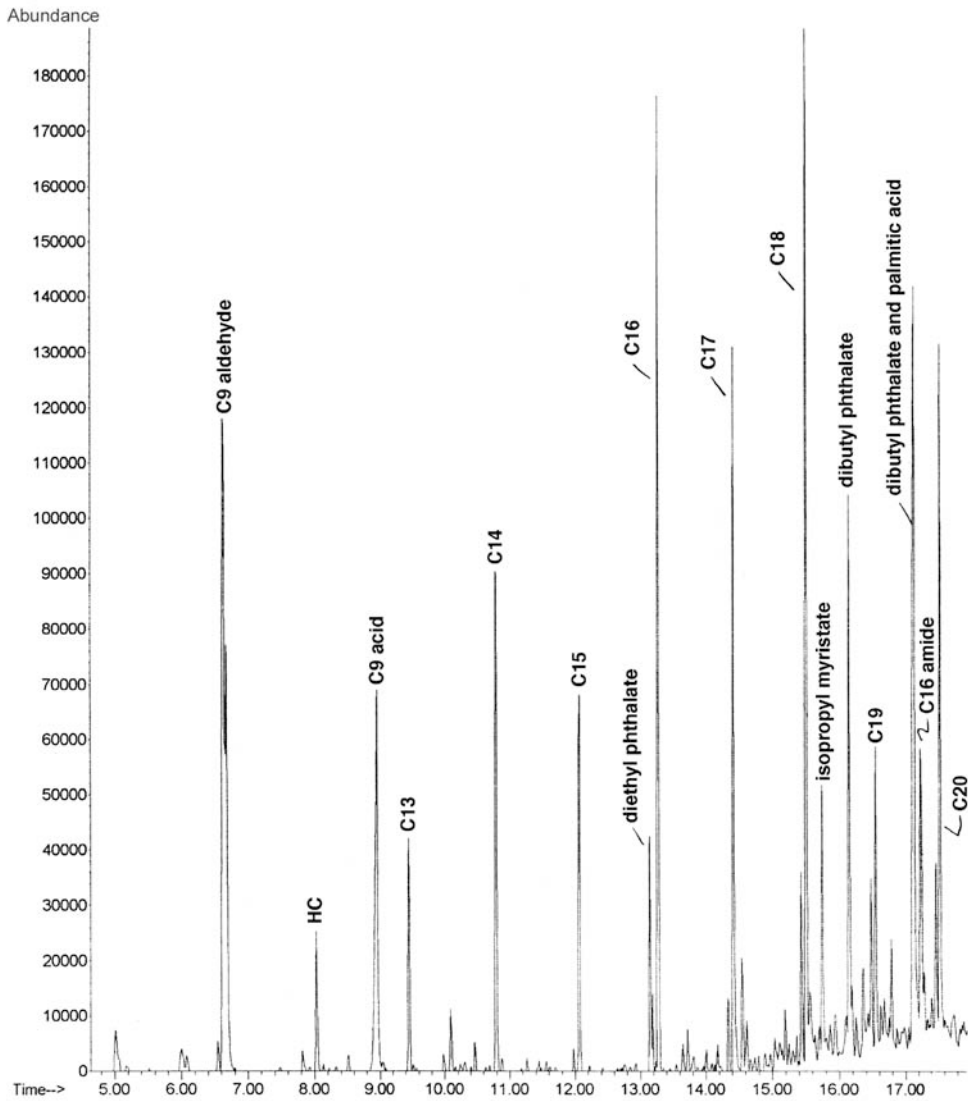


Figure 10-11 GC/MS Chromatogram of Gaylord Liner

CASE STUDIES: POLYMERS FOR ELECTRICAL EQUIPMENT APPLICATIONS

Introduction

Polymeric materials are widely used for electrical equipment applications. Use of these polymers is steadily increasing as traditional materials, such as porcelain and phenol formaldehyde resins are being replaced due to weight, cost, and technical considerations. Designs of electrical equipment are based on a combination of electrical and mechanical engineering principles. Equipment is typically qualified by standard industry and manufacturer-specific accelerated electrical stress testing in addition to mechanical testing for certain types of equipment. Polymeric materials often perform well under short-term conditions due to inherently favorable dielectric strength and low

dielectric losses, however significant experience from investigation of field-aged components shows a strong dependence on polymer formulation in achieving stable long-term performance.

Background

Polymeric materials cover a wide range of applications for electric power distribution and transmission equipment service. These may experience relatively benign aging conditions inside of electrical equipment. In other cases, direct exposure to a harsh combination of stresses is expected. For example, an outdoor polymeric insulator will be exposed to direct sunlight conditions, extremes of temperature, exposure to rain and ice, static and dynamic mechanical stresses, electrical stresses, and the insidious effects of corona. The latter is caused by ionization of the air due to highly localized electrical stresses. This leads to production of ozone, free radicals due to decomposition of contaminants, and ion bombardment. The combined effects lead to favorable hydrolysis conditions for many polymers, accelerated by heating from high energy equipment.

Other electrical equipment is either directly buried or installed in underground conduit systems. In this type of environment, the extremes of temperature are less often experienced; however localized and transient heating is experienced when power loads are high or when equipment runs near steam pipes for example. In underground installations, corrosive conditions are found based on road salts, lime extraction from concrete, and other minerals that become concentrated as water dries away. Exposure to microbes, oil run-off, decaying vegetation and other materials suggests that very stable polymers are required for this service.

The electric industry traditionally designs around and purchases equipment for a 40 year life expectation. Limited access to much of the overhead and underground equipment is unavoidable and the impracticality of temporarily removing equipment from service for inspection precludes significant opportunities for monitoring in-service performance.

Case Study #1: Electrical Insulators

Bis-phenol epoxy formulations are commonly used for outdoor high voltage insulators due to a favorable combination of good mechanical strength, excellent dielectric properties, and the ability to cast the resin around internal functional devices and electrical connections. Figure 10-12 shows two examples of outdoor high voltage insulators used for capacitor switching. A review of the formulation of these insulators was conducted to predict the most favorable long-term performance between several suppliers, based on fundamental polymer chemistry principles. Analysis by GC/MS was undertaken to investigate for UV stabilizers, residual polar curing agents and curing byproducts, and other organic compounds that may adversely influence long-term aging. Direct comparison based on long-term field-aging performance was not possible due to time constraints.

Chemical analysis of an insulator from one supplier indicated polymer fragments and curing byproducts, as shown in Figure 10-13. In contrast, an analysis of an insulator from another supplier indicated significant differences. In the second case, traces of polymer fragments were found in addition to thorough crosslinking of the epoxy compound.



Figure 10-12 Comparison of Outdoor High Voltage Insulators

No traces of curing agents were found, further indicating a complete curing reaction. Triphenyl phosphate flame retardant was also found in this analysis. Since devices of this type are predominantly mounted on wooden utility poles, a flame retardant formulation may provide a desirable operating margin in the event of an electrical failure. However, as shown in Figure 10-14, this same insulator was also found to contain polybrominated biphenyls (PBBs), which are banned from manufacture or use in most countries. The analysis of this material protected the electric utility company from potentially inadvertent deployment of a hazardous material.

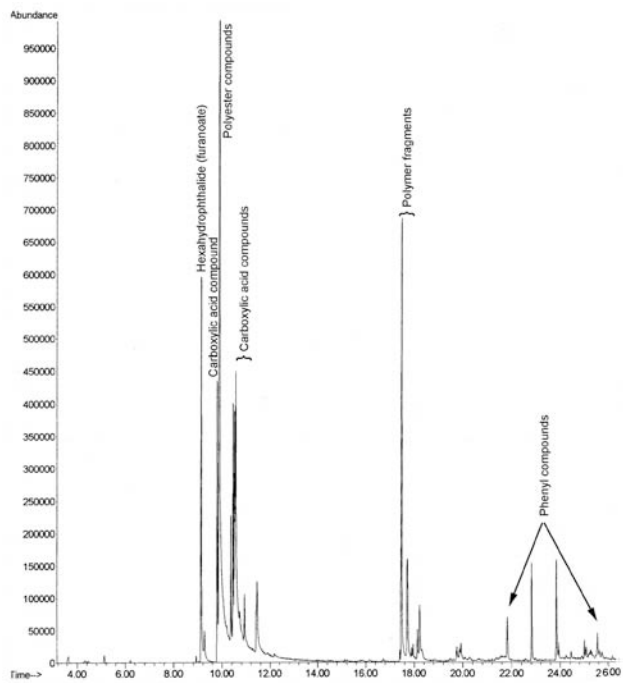


Figure 10-13 GC/MS Analysis of Insulator from Supplier A

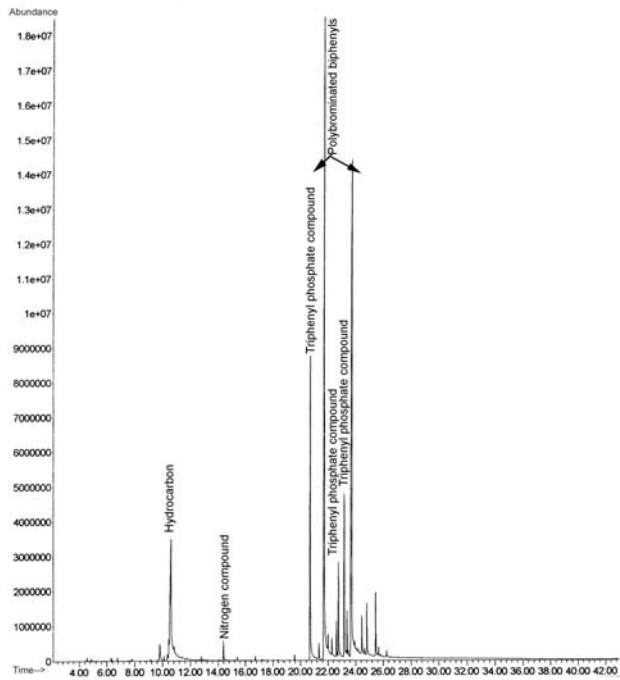


Figure 10-14 Analysis of Insulator Containing Banned PBB Material

Case Study #2: Review of Field-Aged Elastomeric Materials

Elastomer compounds are used as insulators for many electrical components. These are typically applied over fiberglass rods where load support is needed. Review of rubber formulations that have suffered significant aging damage is useful as a basis for considering alternate formulations. In Figure 10-15, a severely degraded rubber insulator is shown. This device had been in service for approximately 30 years, with direct sunlight exposure. Figure 10-16 compares another example of the same formulation where there was no direct or prolonged sunlight exposure. Based on this difference, UV degradation of the rubber compound is clearly a significant factor in reducing the useful life of this component.



Figure 10-15 Example of Severely Degraded Elastomeric Insulator



Figure 10-16 Same Insulator without Sunlight Exposure

Analysis of the degraded elastomer insulator shown in Figure 10-15 by GC/MS is presented in Figure 10-17. This indicates a hydrocarbon rubber, based on the homologous series of hydrocarbon peaks, plus myristic, palmitic, and stearic fatty acids. This sample was obtained from the core of the device, where significant weathering had not damaged the material. Hydrocarbon rubber is very susceptible to UV-induced chain scission and protection is required to extend useful service life. In this example, the grey color is imparted by silicate clay. This adds strength to the rubber; however it is inefficient as a UV absorber. Further, GC/MS analysis indicates that no coupling agent was used to promote chemical bonding between the rubber and clay. Fatty acids were added as a processing aid for mixing of the rubber compound. These are easily hydrolyzed by water in combination with UV radiation. As the fatty acids are removed, the free volume of the elastomer increases, thus increasing the specific surface area available for UV interaction. The absence of a clay/coupling agent system also leads to increased free volume as the elastomer degrades.

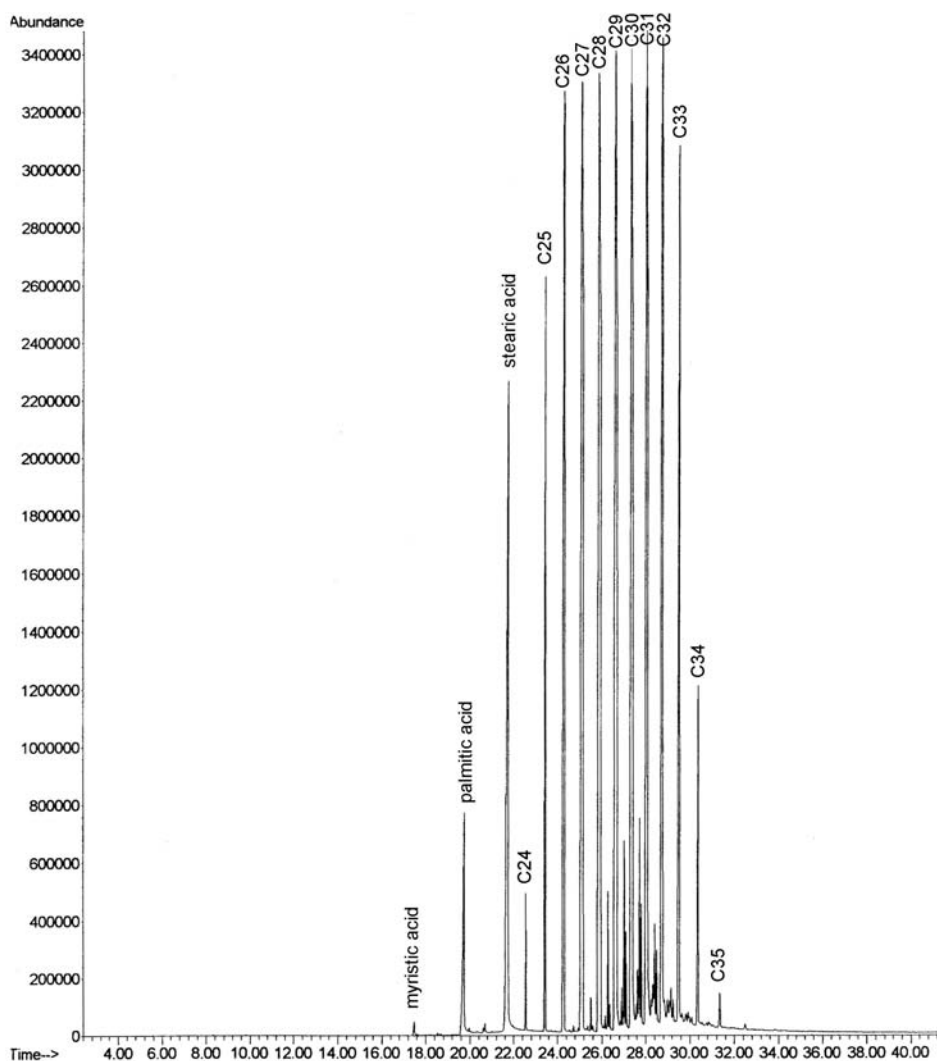


Figure 10-17 GC/MS Analysis of Poor Performing Rubber Compound

Figure 10-18 presents the GC/MS analysis of a rubber formulation for an elastomeric insulator for devices to replace those that had been characterized after field-aging. In this example, a high quality silicone rubber was selected for inherent resistance to oxidation and UV damage, plus favorable dielectric properties. Figure 10-18 presents the GC/MS analysis of this elastomer, confirming pure silicone rubber and Tinuvin P, a UV absorbing polymer stabilizer. To reduce cost, many suppliers provide 'silicone rubber' components that are often combined with butyl or nitrile rubber to reduce cost.

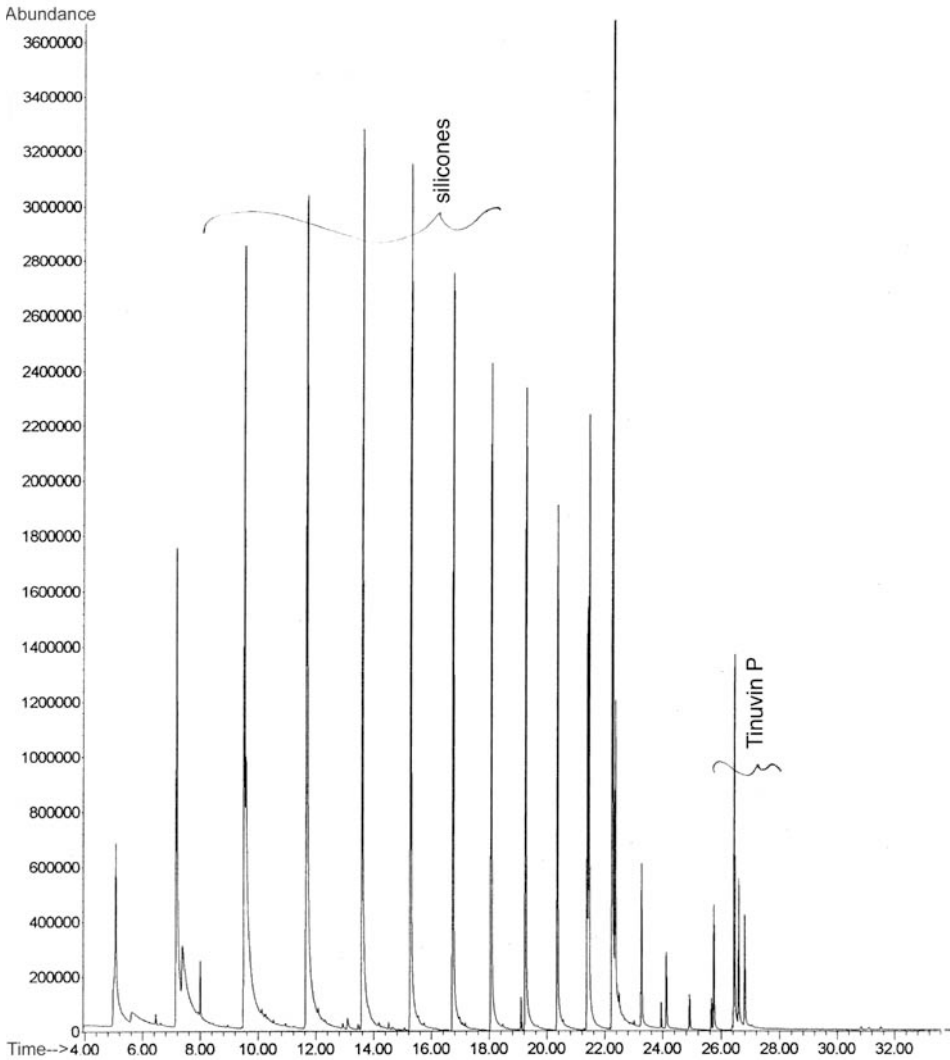


Figure 10-18 Composition of Preferred Silicone Rubber Formulation with UV Stabilizer

Case Study #3: Performance of Polymeric Seals

Polymeric seals are used for many electrical applications including oil retention, nitrogen or sulfur hexafluoride gas pressure barrier, moisture exclusion, and lubricant retention. Mechanical seals and O-rings are typically specified based on polymer type (i.e., silicone, buna, Viton) and durometry. The latter is a measure of the elastic resilience of a seal. The base polymer is chosen on the basis of compatibility with the selected contact material. Catalogs from seal suppliers are

devoid of any significant technical details regarding formulation. For example, if a large cover that is sealed with an O-ring must be opened periodically for inspection, adhesion of the O-ring cannot be tolerated. Figure 10-19 presents the GC/MS analysis of an O-ring from such an example, where a cover of 1.5 m diameter, weighing more than 200 kg must be opened for periodic inspection of internal components of an electrical circuit breaker.

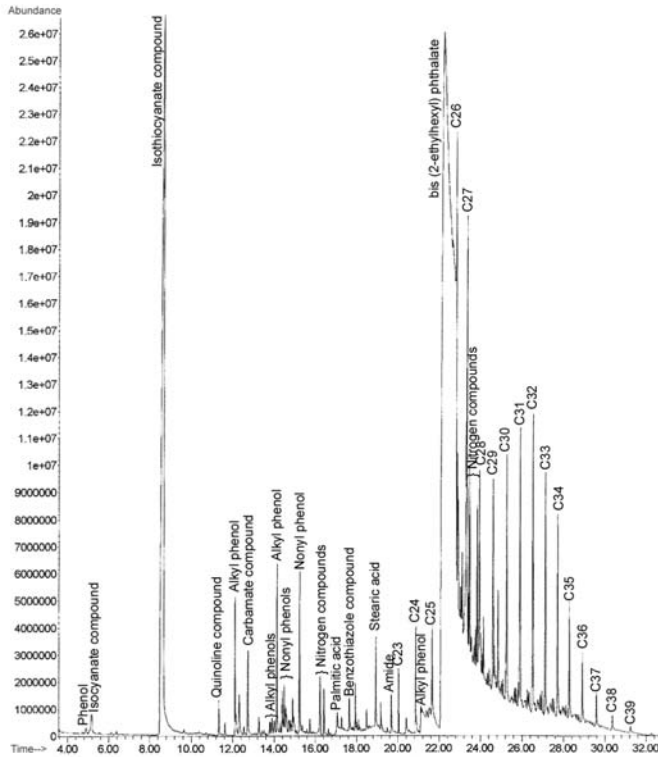


Figure 10-19 Sticky O-Ring Analysis by GC/MS

The rubber formulation is complex and includes residual thiocyanate curing compounds, alkyl phenols as antioxidants, bis (2-ethylehexyl) phthalate plasticizer, and hydrocarbon fragments from the butyl rubber base polymer. Phthalate plasticizers are added to improve the flexibility and reduce hardness in rubber compounds; however these have limited solubility in most polymers. A plasticizer of this type migrates to the free surface where it becomes trapped against the metal sealing surface. Hyper-plasticization of the O-ring surface results, leading to a very tacky surface that adheres well to metals. The O-ring chosen is not suitable for this application. A material requiring less plasticizer would be a better choice to correct this issue.

APPENDIX A

Chromatograms

This appendix includes the chromatograms from which the mass spectral data was obtained.

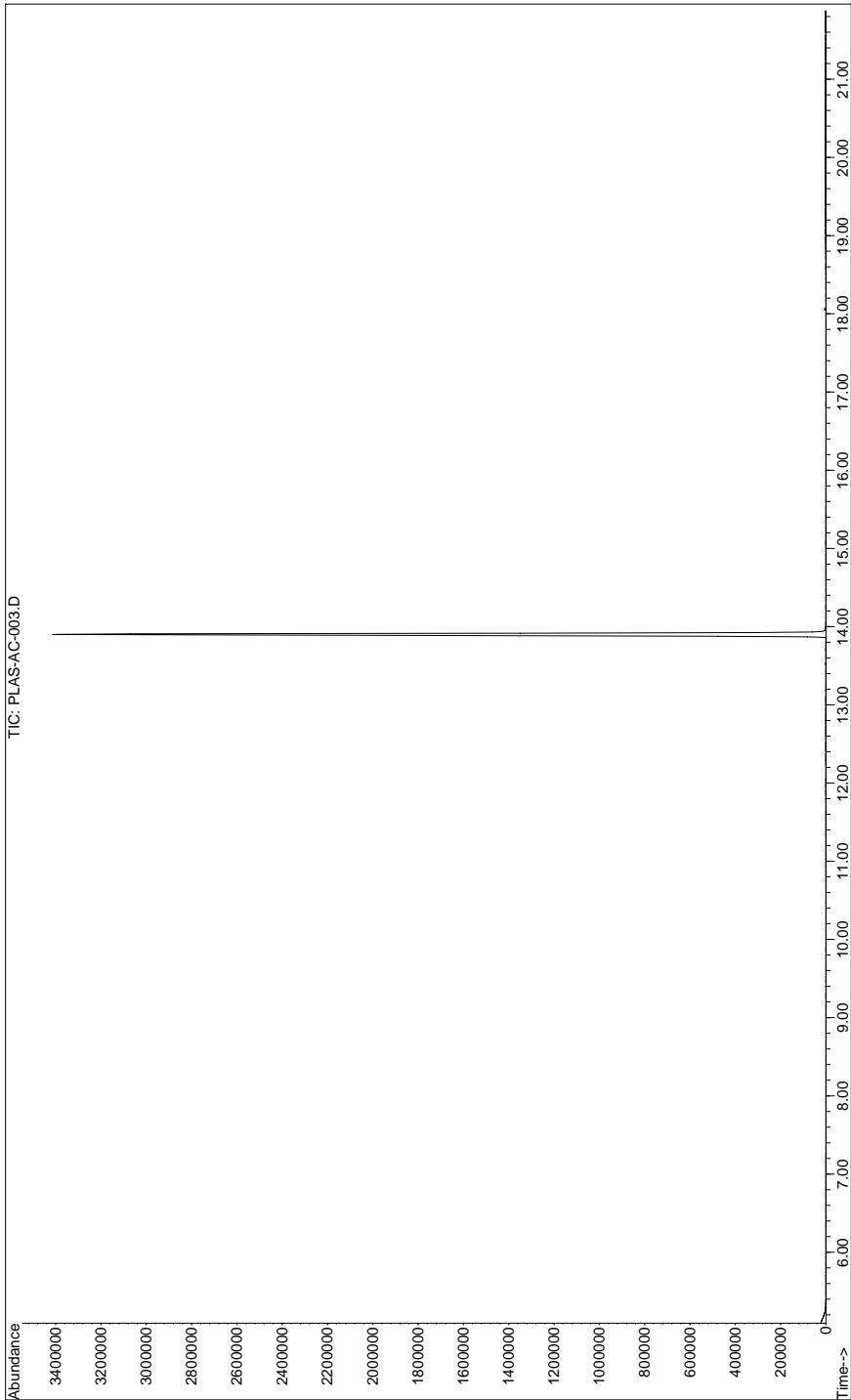
For some compounds, such as the aroclors, the pattern recognition of the chromatogram can be much more informative than the mass spectral information.

As much as possible, each chromatogram was run under the same conditions to allow comparison between the different compounds.

Analytical Information

Chromatogram for Accelerator BBTS - PLAS-AC-003

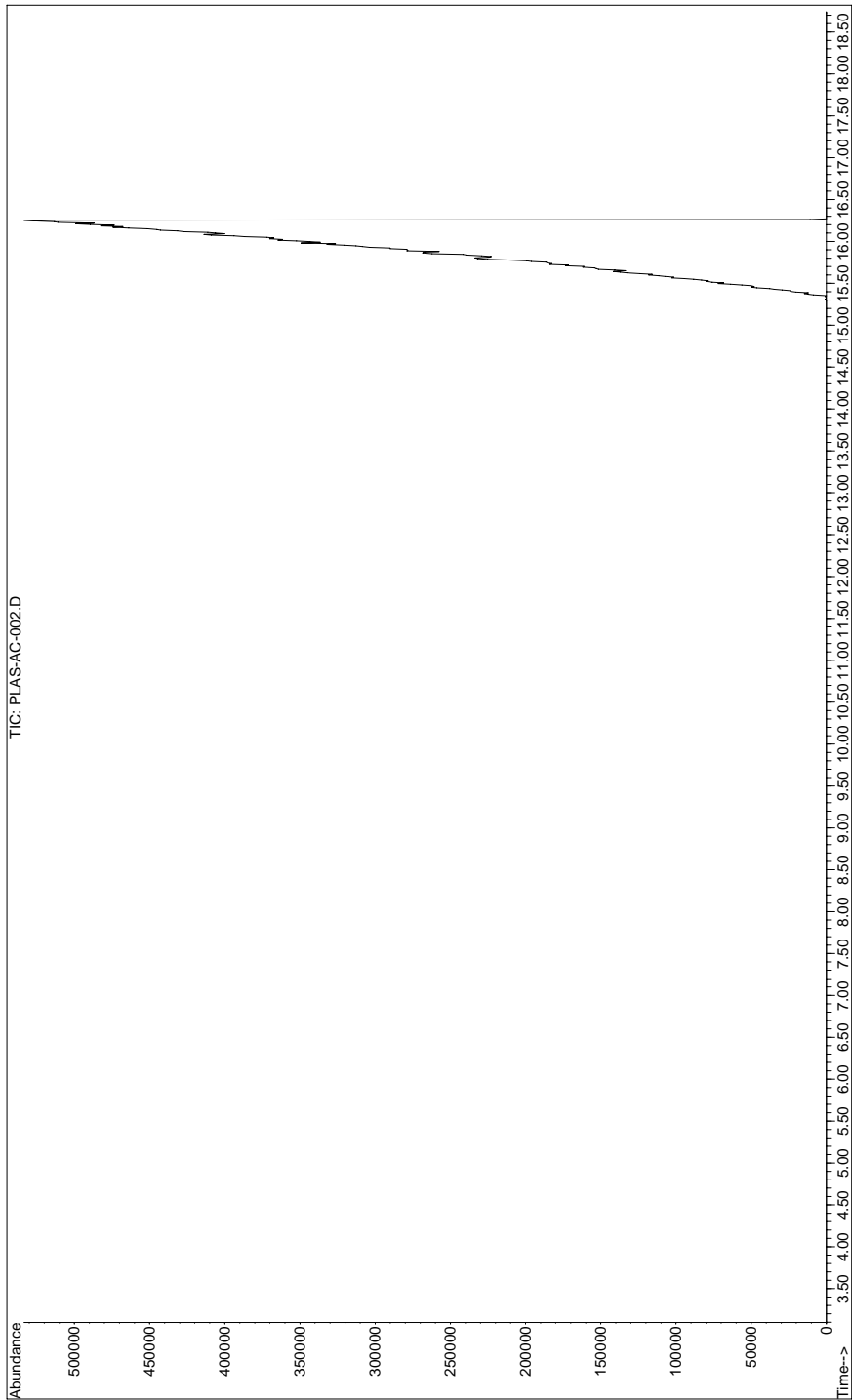
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Analytical Information

Chromatogram for Accelerator ETU-22 PM - PLAS-AC-002

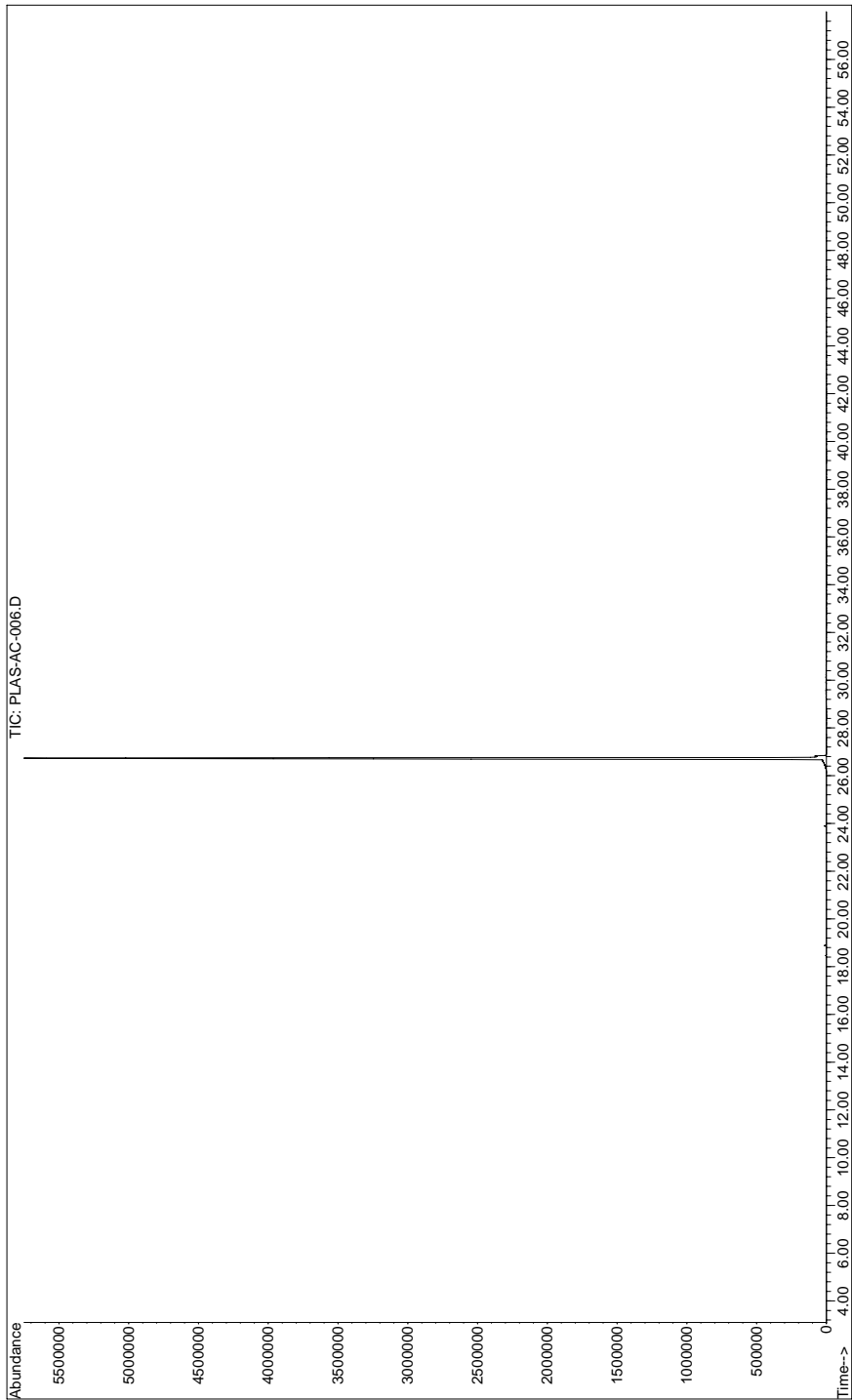
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Accelerator EZ and EZ-SP - PLAS-AC-006

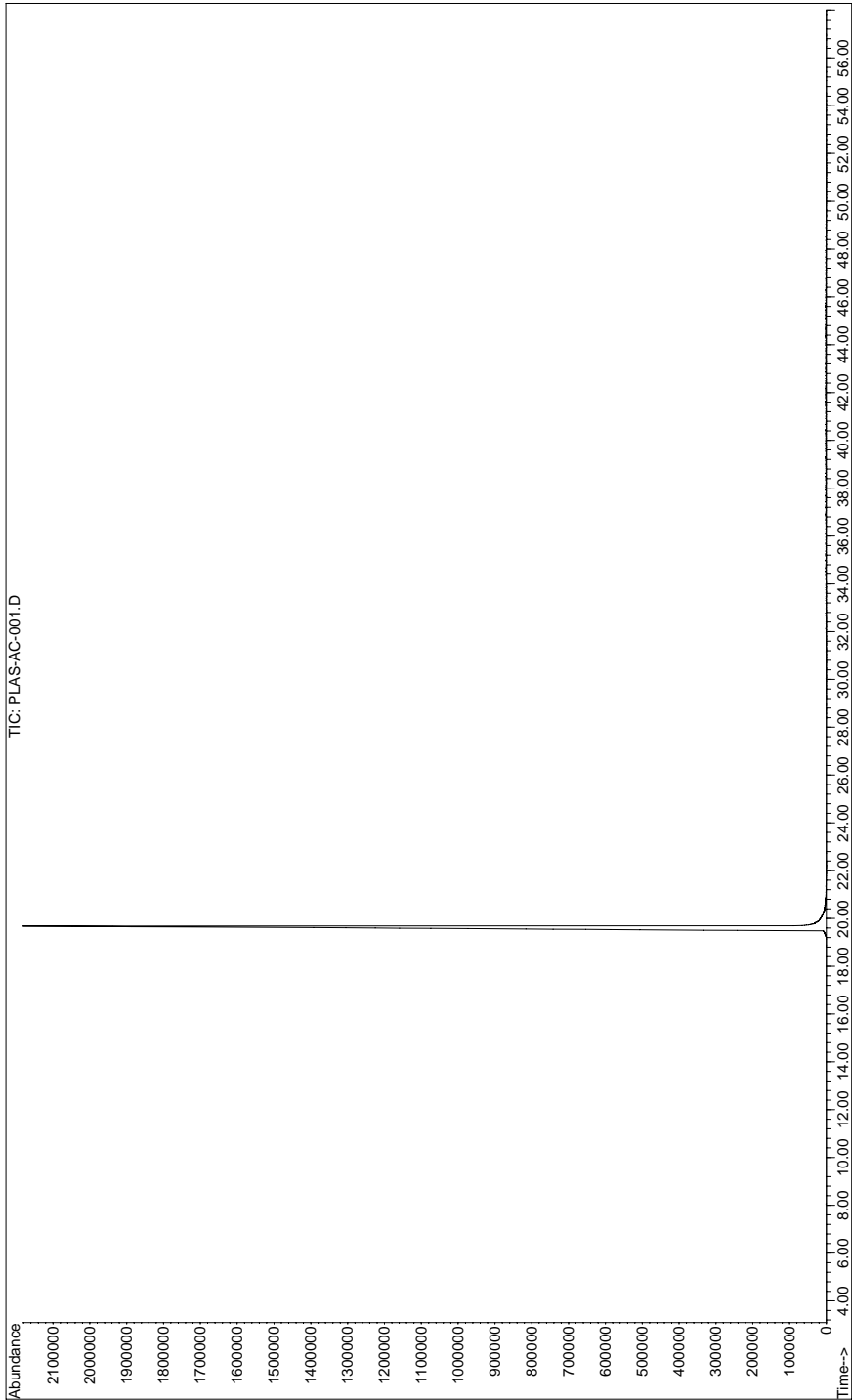
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Accelerator MBT, MBT/MG - PLAS-AC-001

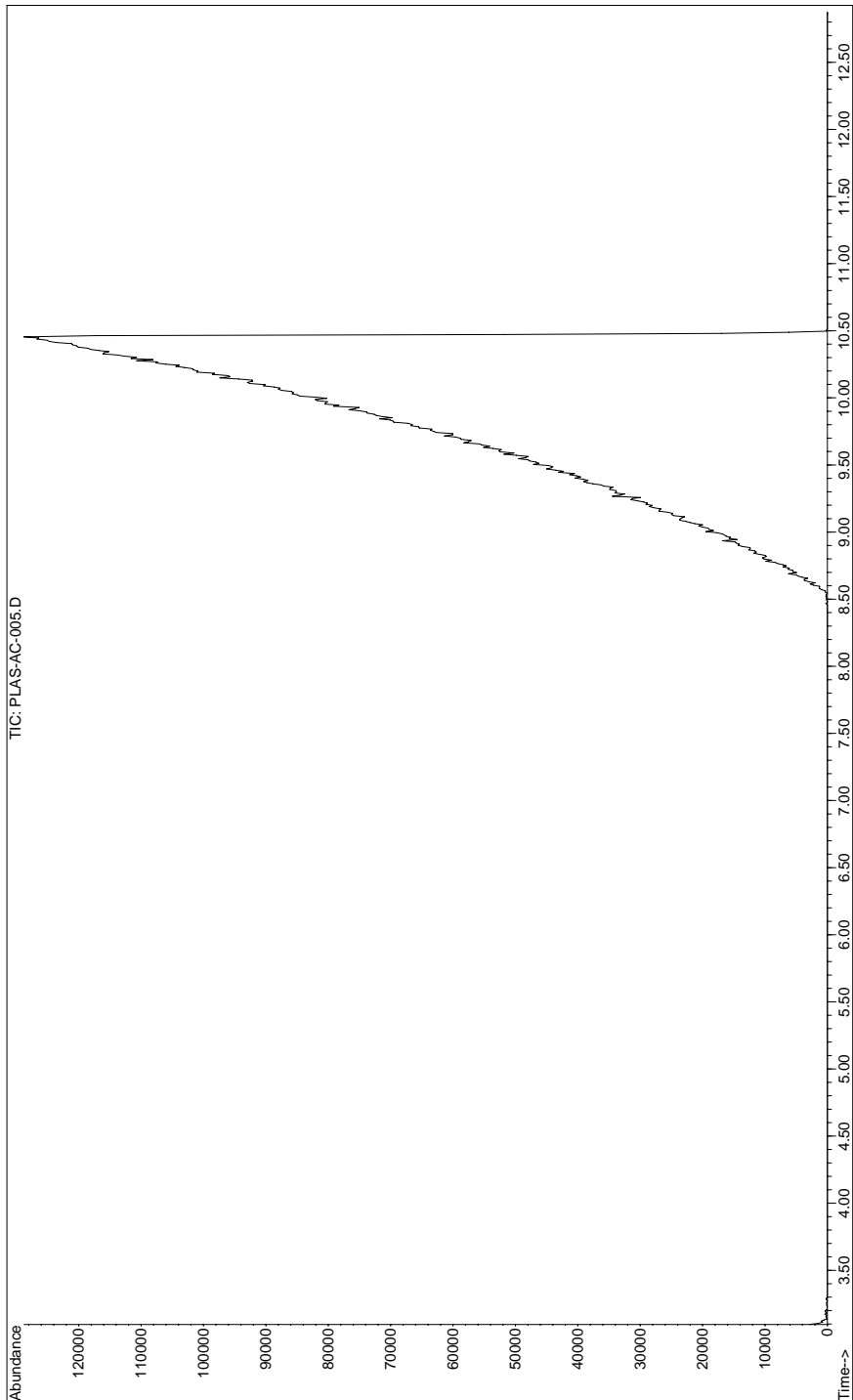
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Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Activator OT Urea - PLAS-AC-005

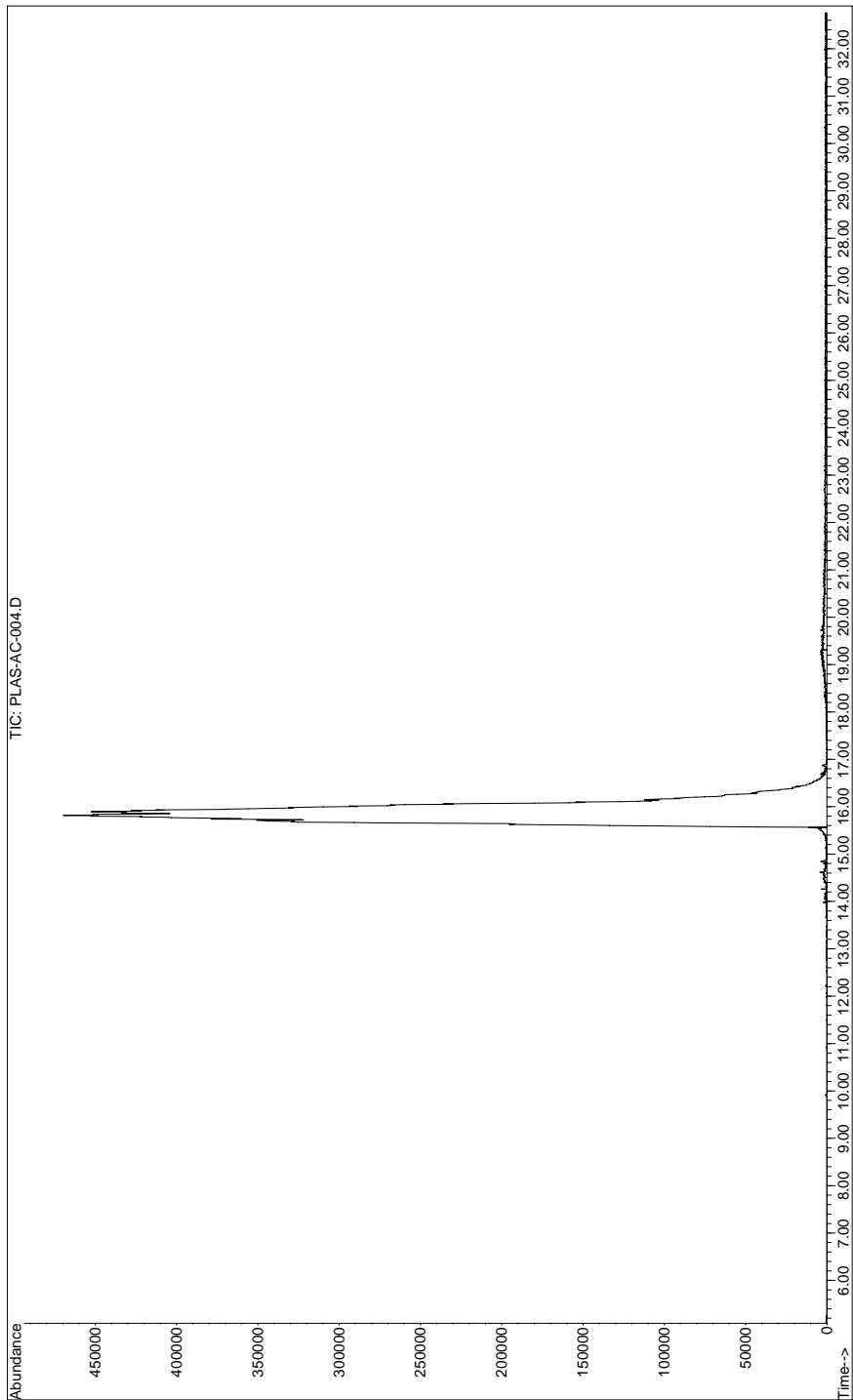
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Cure-Rite®* IBT - PLAS-AC-004

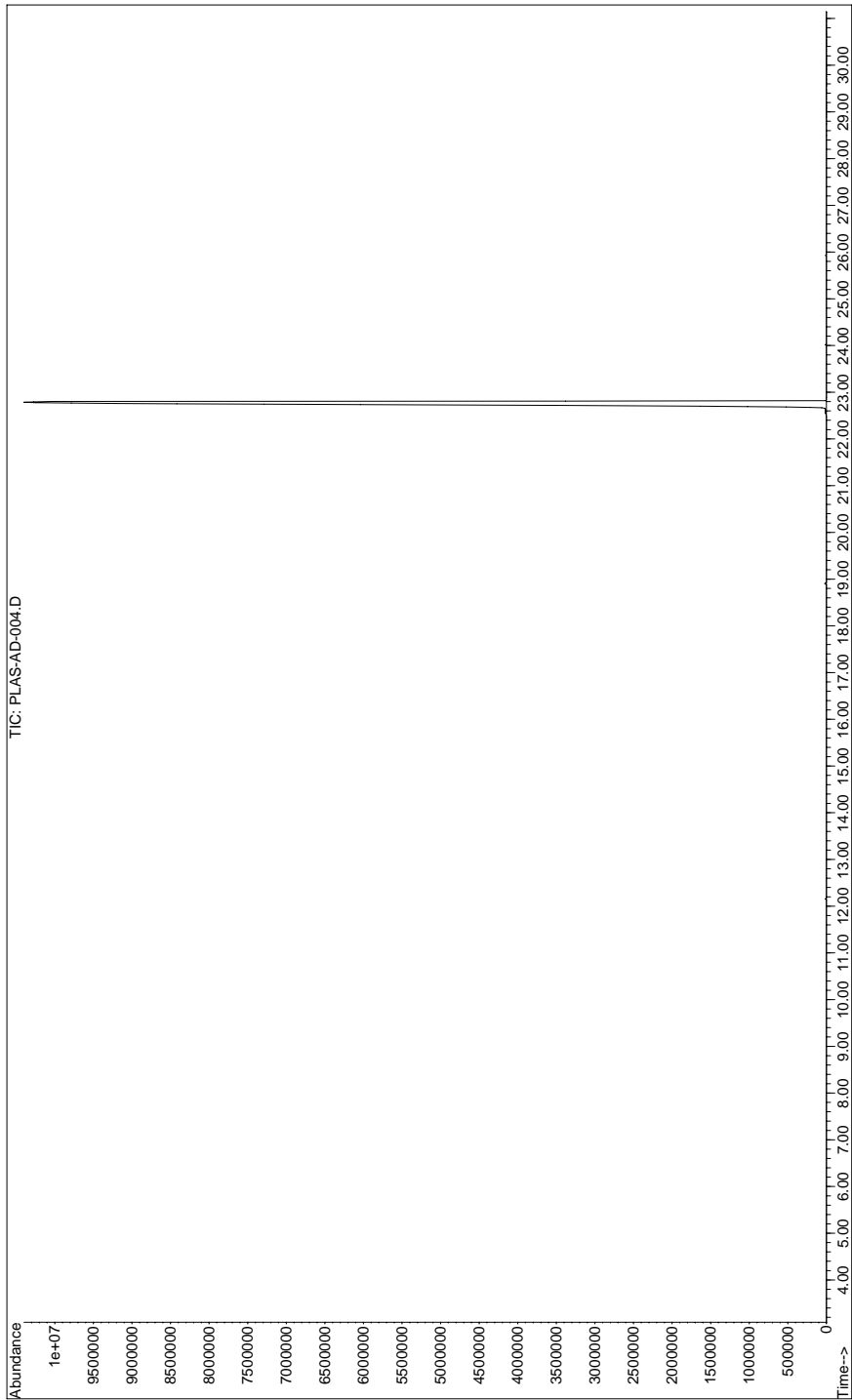
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Santoflex*[®] 6PPD - PLAS-AD-004

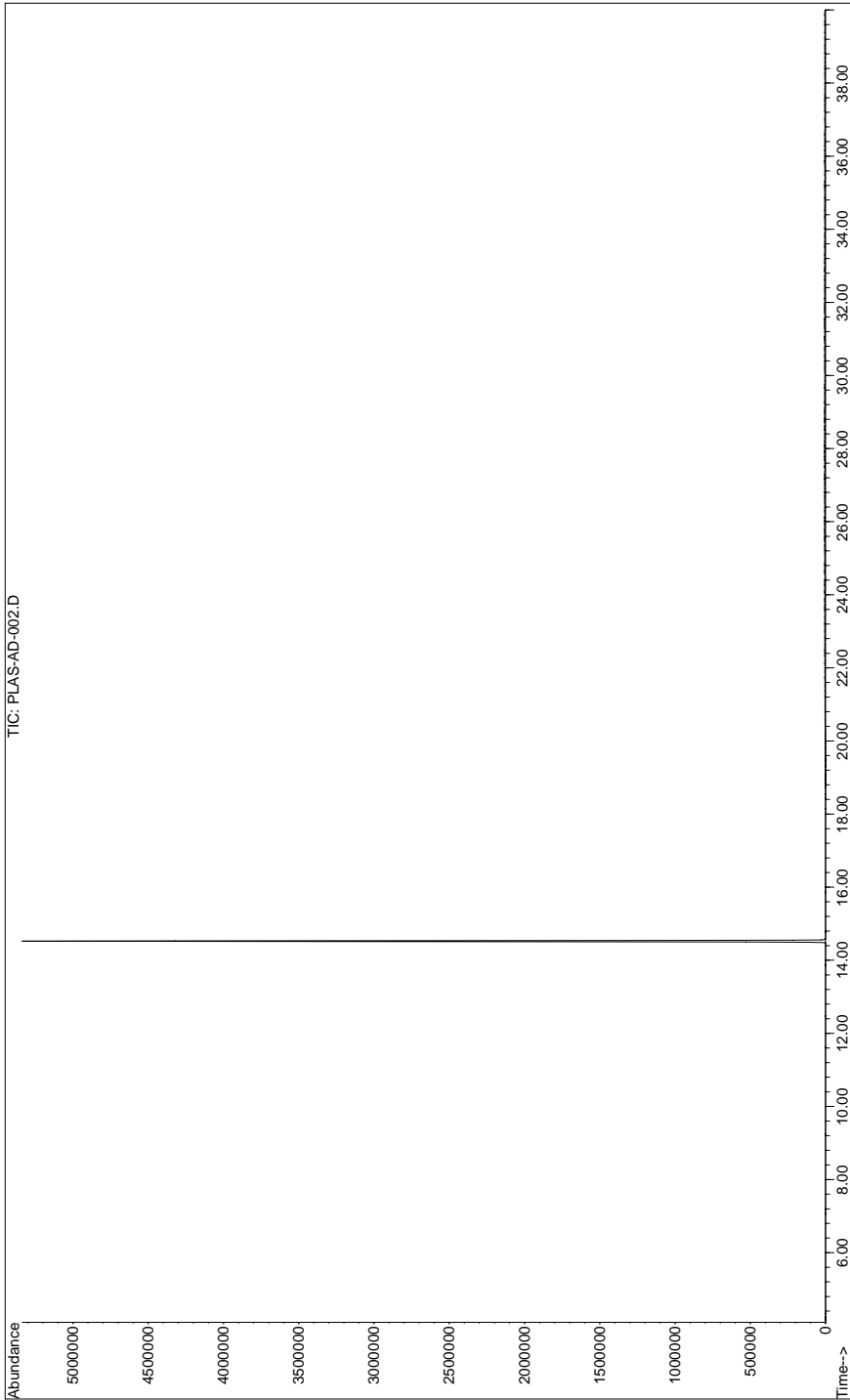
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Santoflex*[®] 77PD - PLAS-AD-002

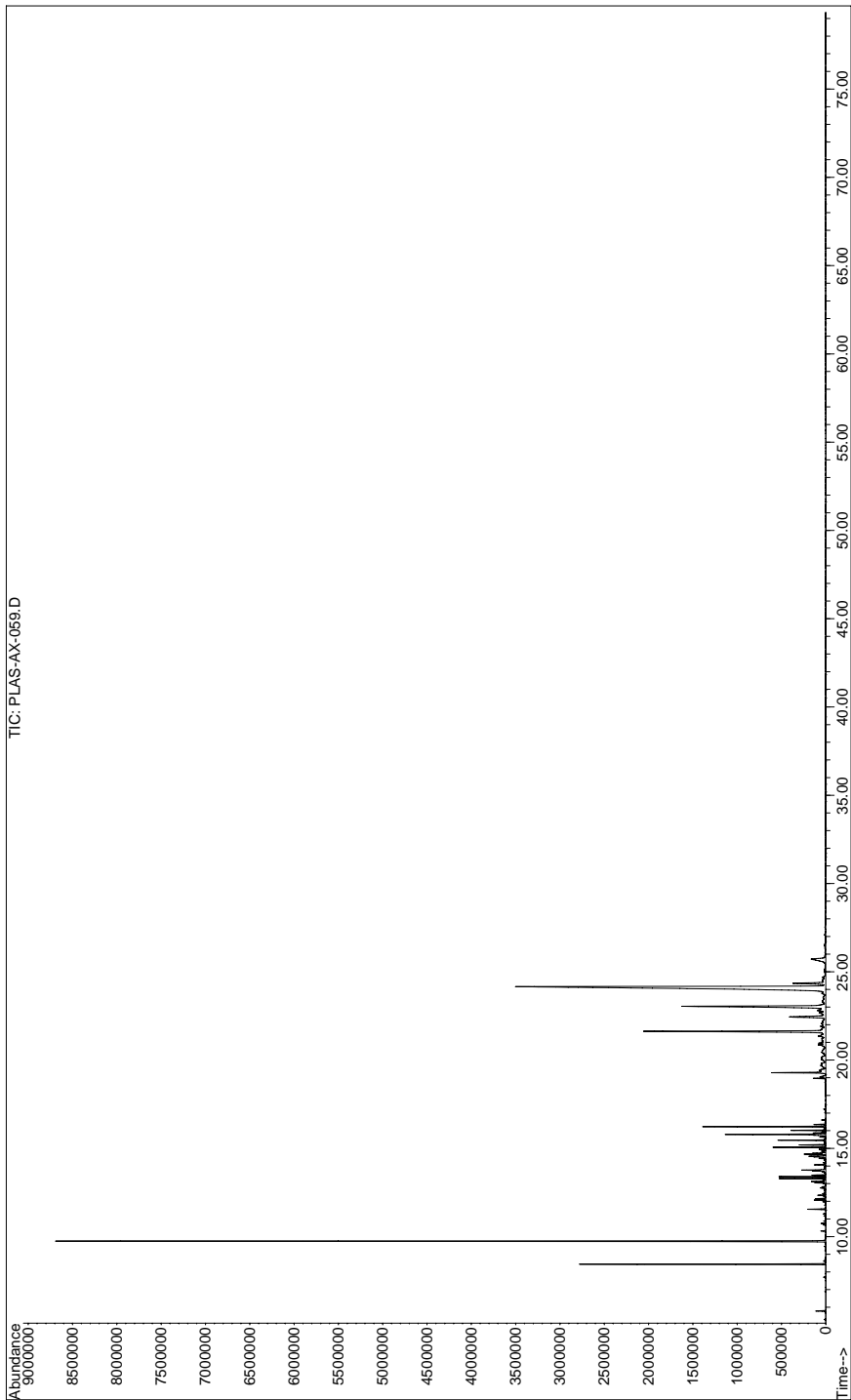
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Analytical Information

Chromatogram for *Lowinox® CPL - PLAS-AX-059*

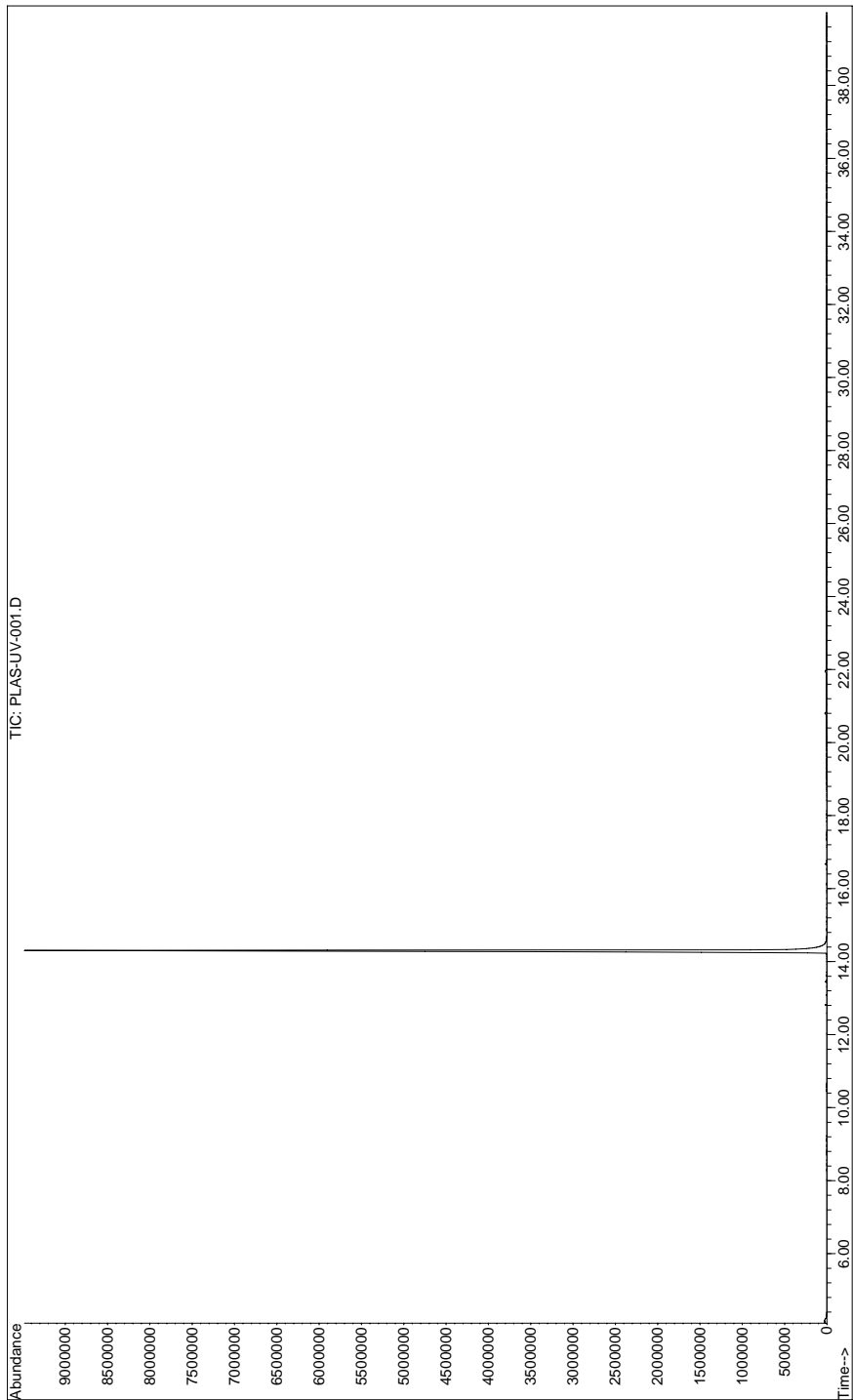
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Analytical Information

Chromatogram for Uvinul® 3000 - PLAS-UV-001

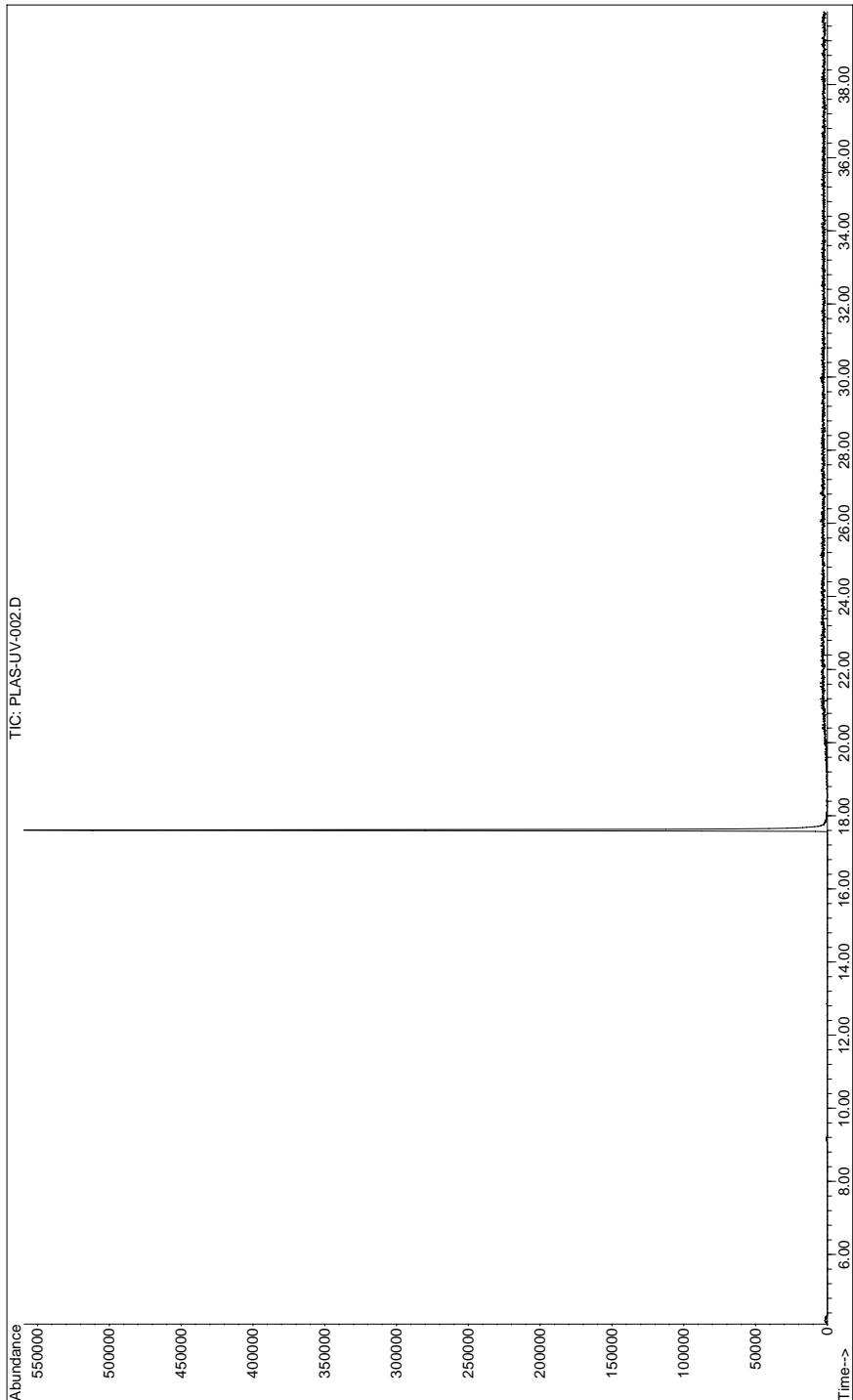
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Uvinul® 3008 - PLAS-UV-002

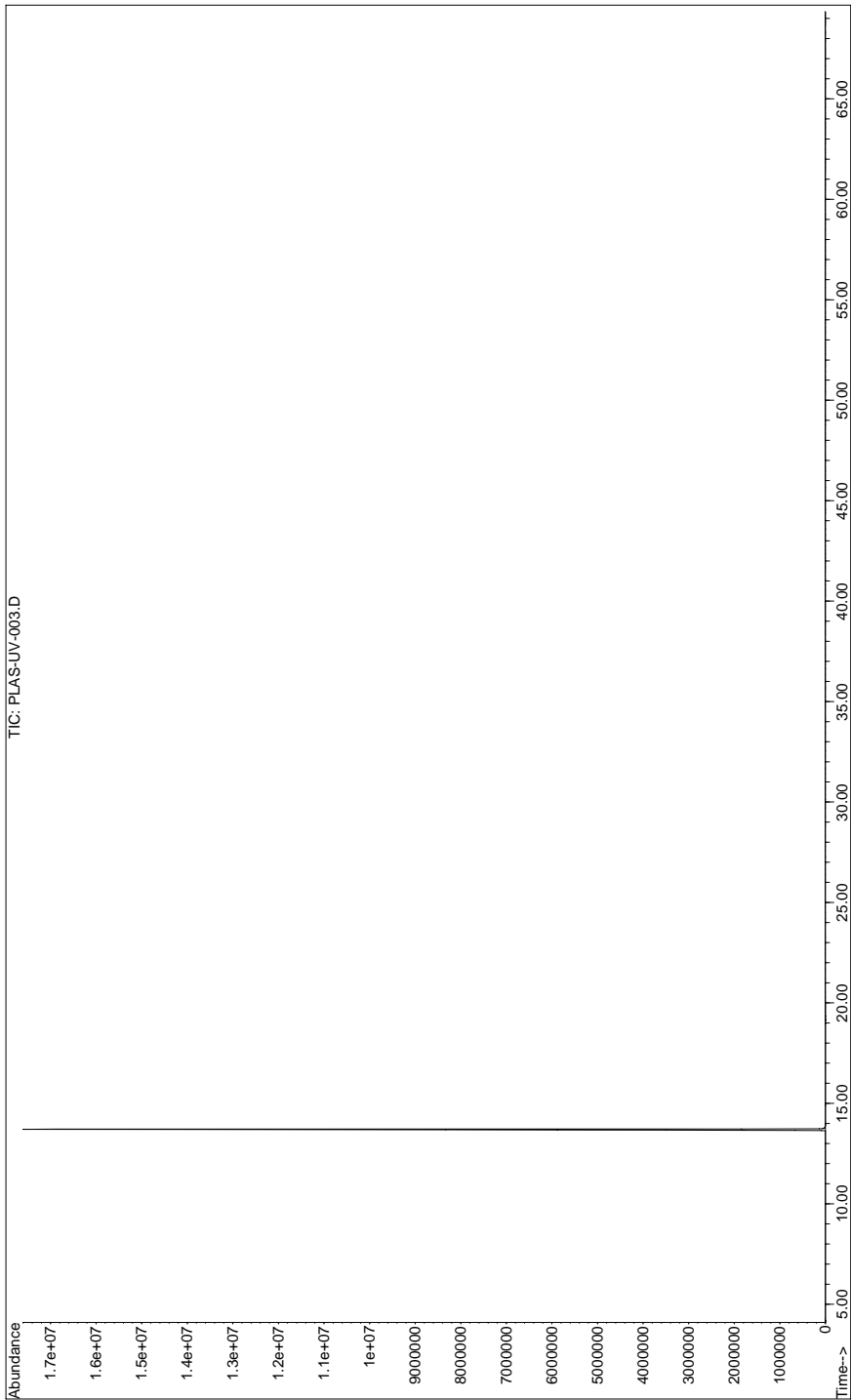
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Analytical Information

Chromatogram for Uvinul® 3040 - PLAS-UV-003

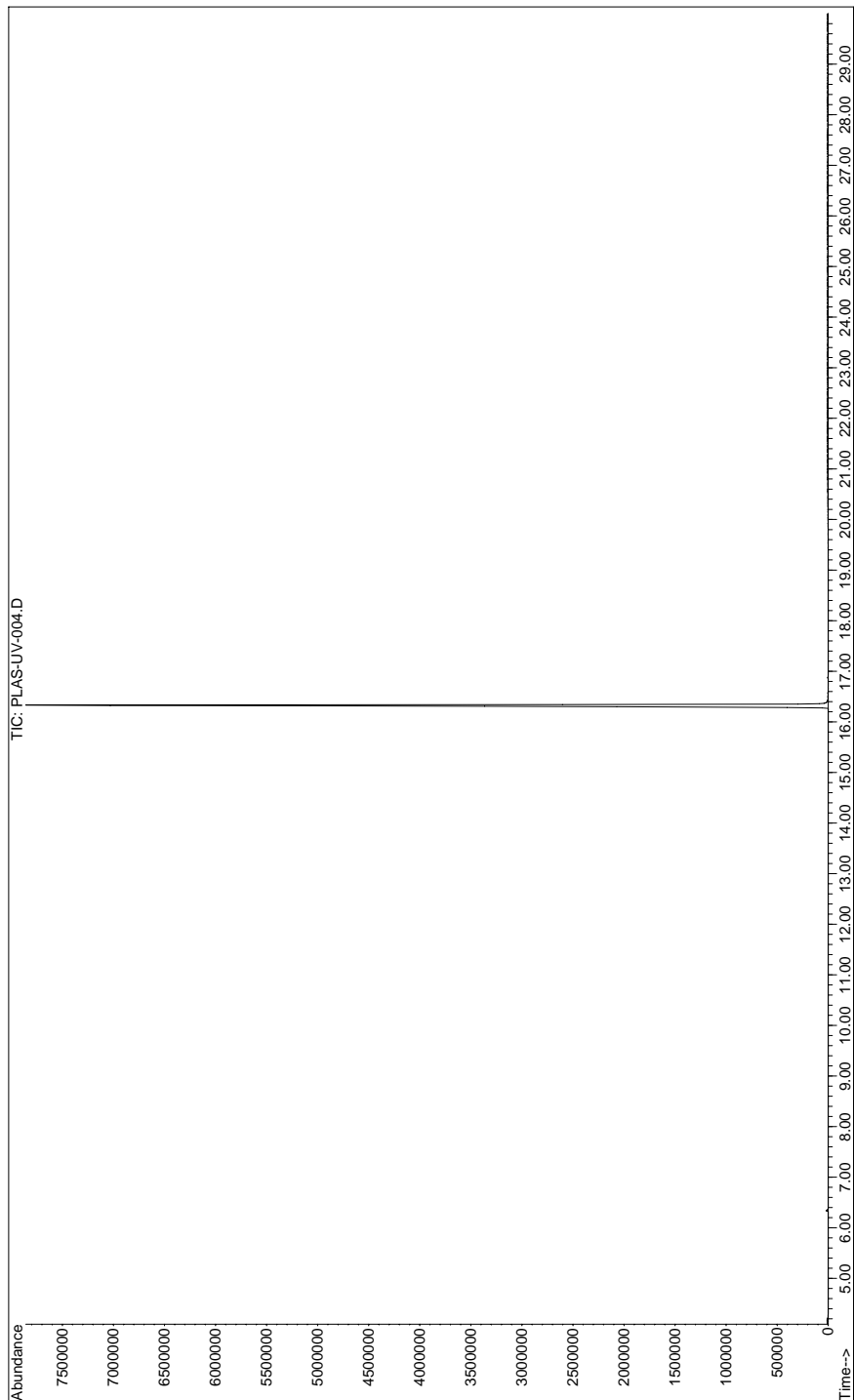
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Analytical Information

Chromatogram for Uvinul® 3049 - PLAS-UV-004

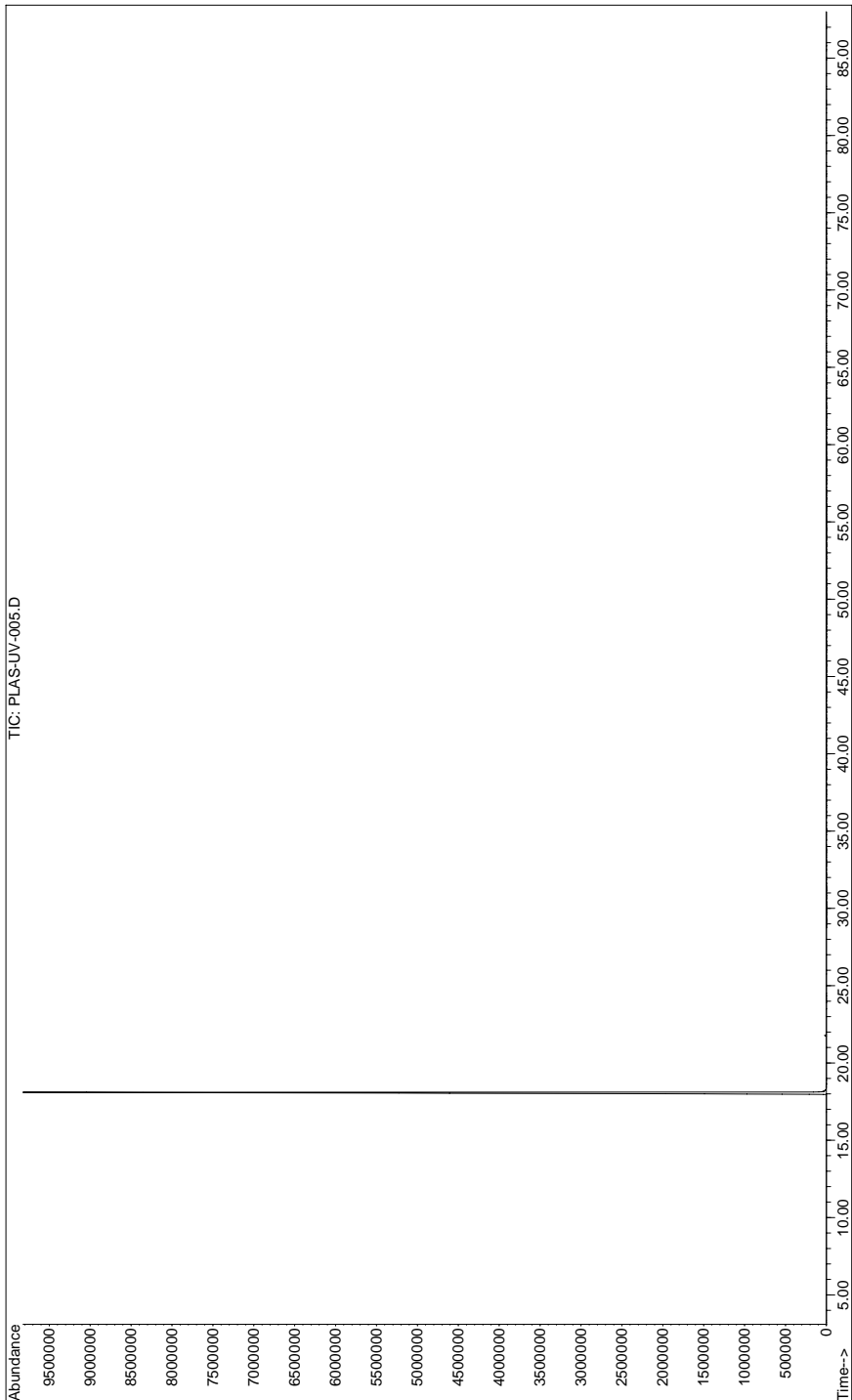
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Tinuvin*[®] PED - PLAS-UV-005

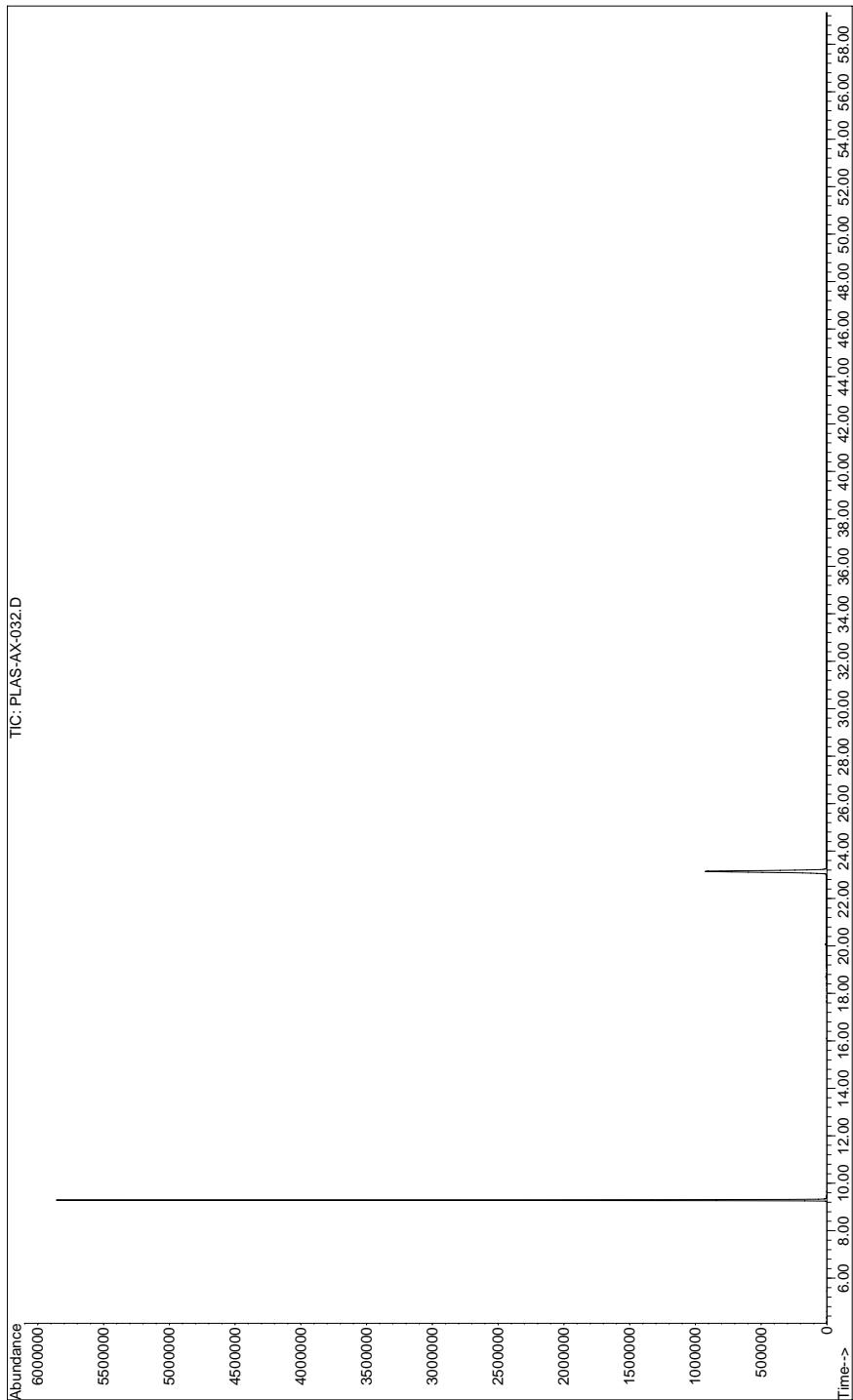
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Alkanox*[®] P27 - PLAS-AX-032

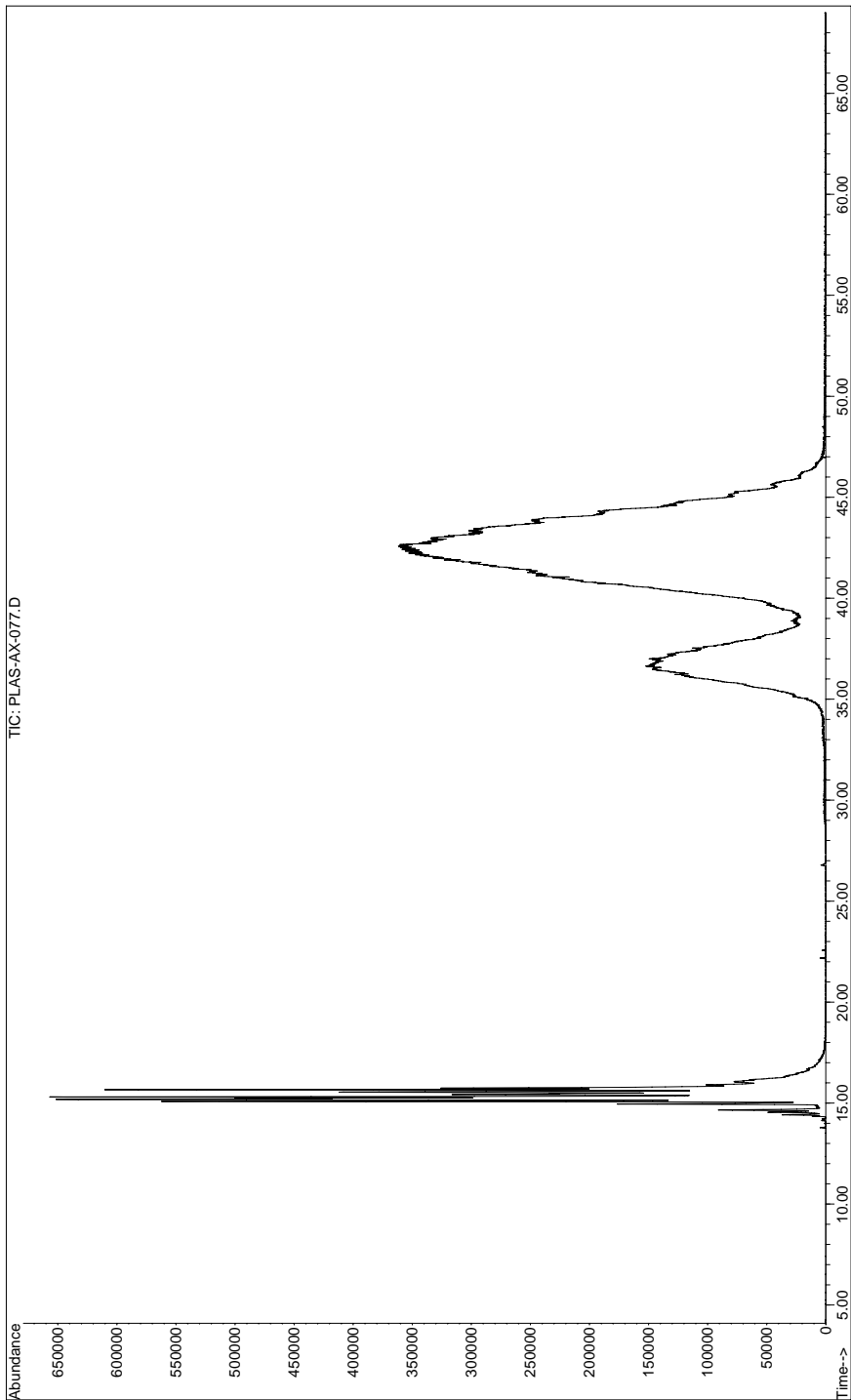
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Alkanox*[®] TNPP - PLAS-AX-077

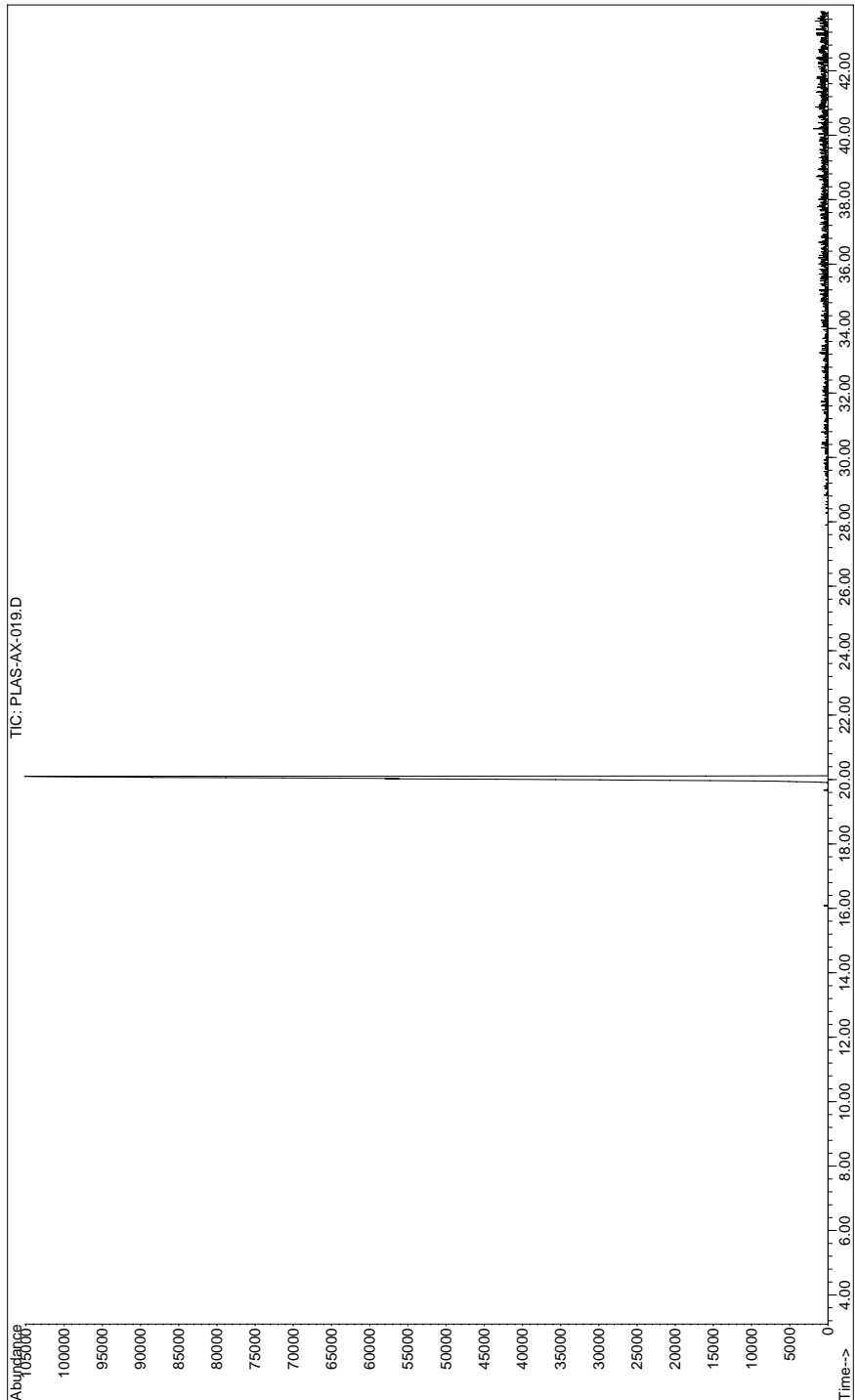
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Antioxidant 60 - PLAS-AX-019

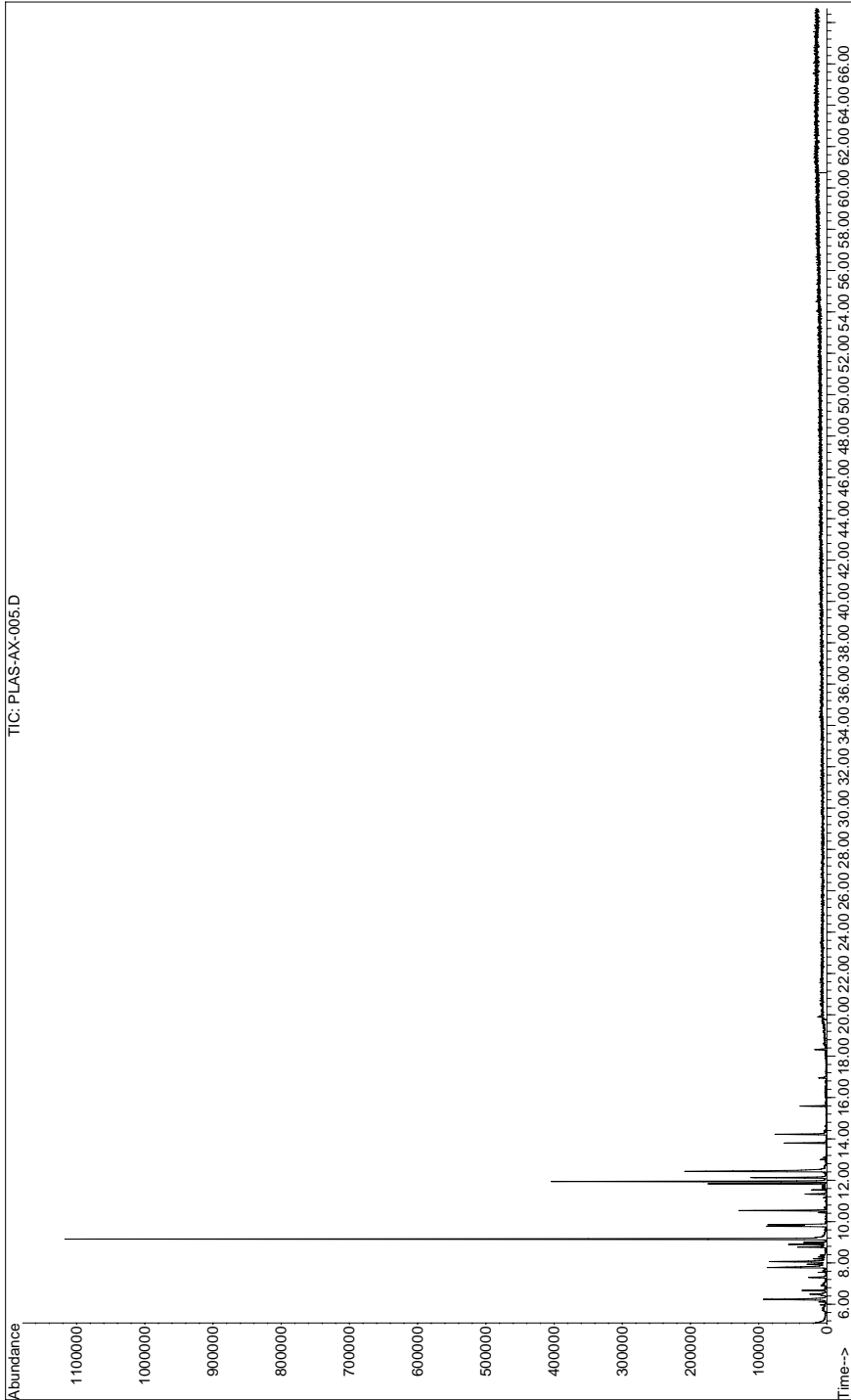
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Cyanox*[®] 1790 - PLAS-AX-005

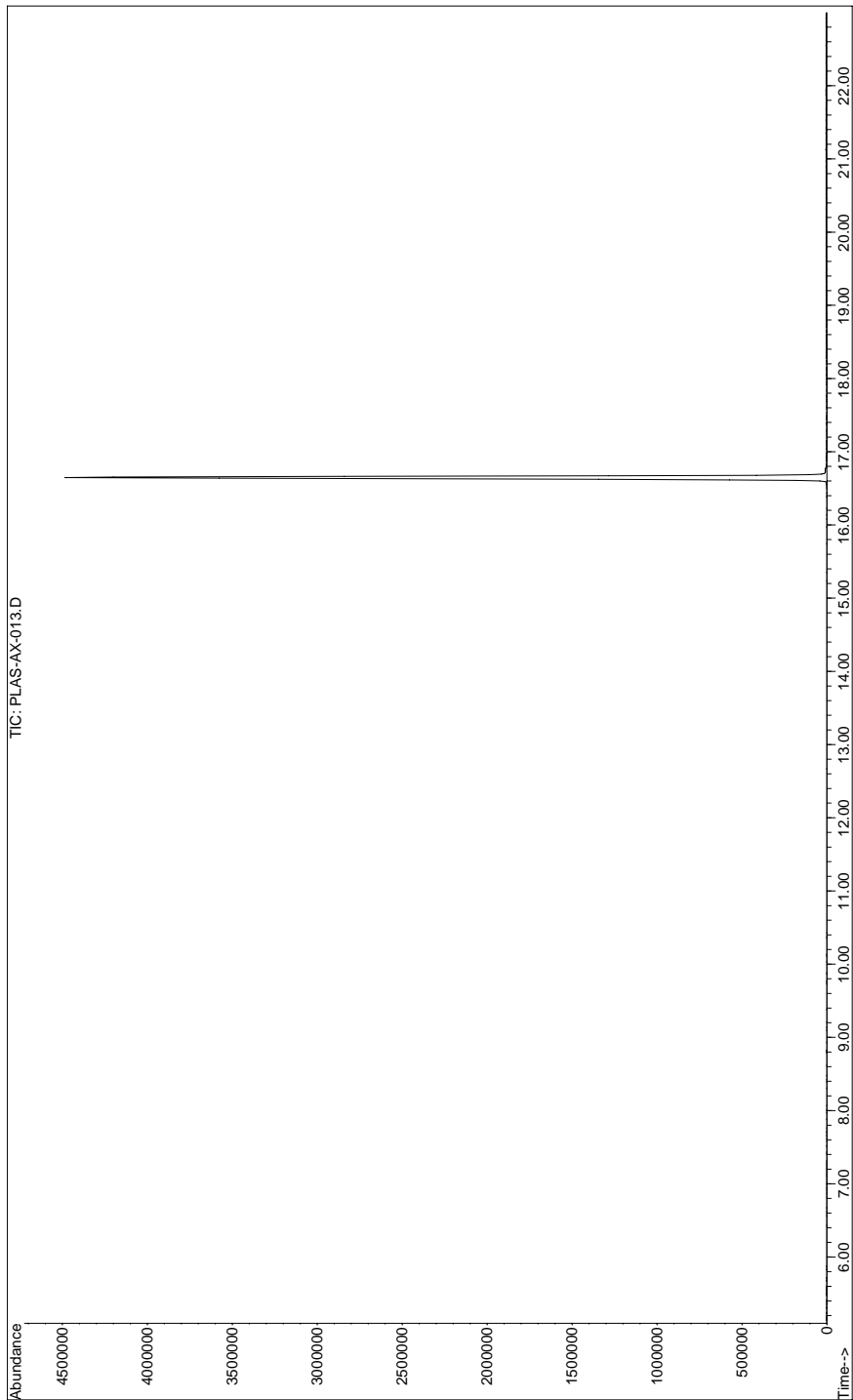
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Cyanox*[®] 2246 - PLAS-AX-013

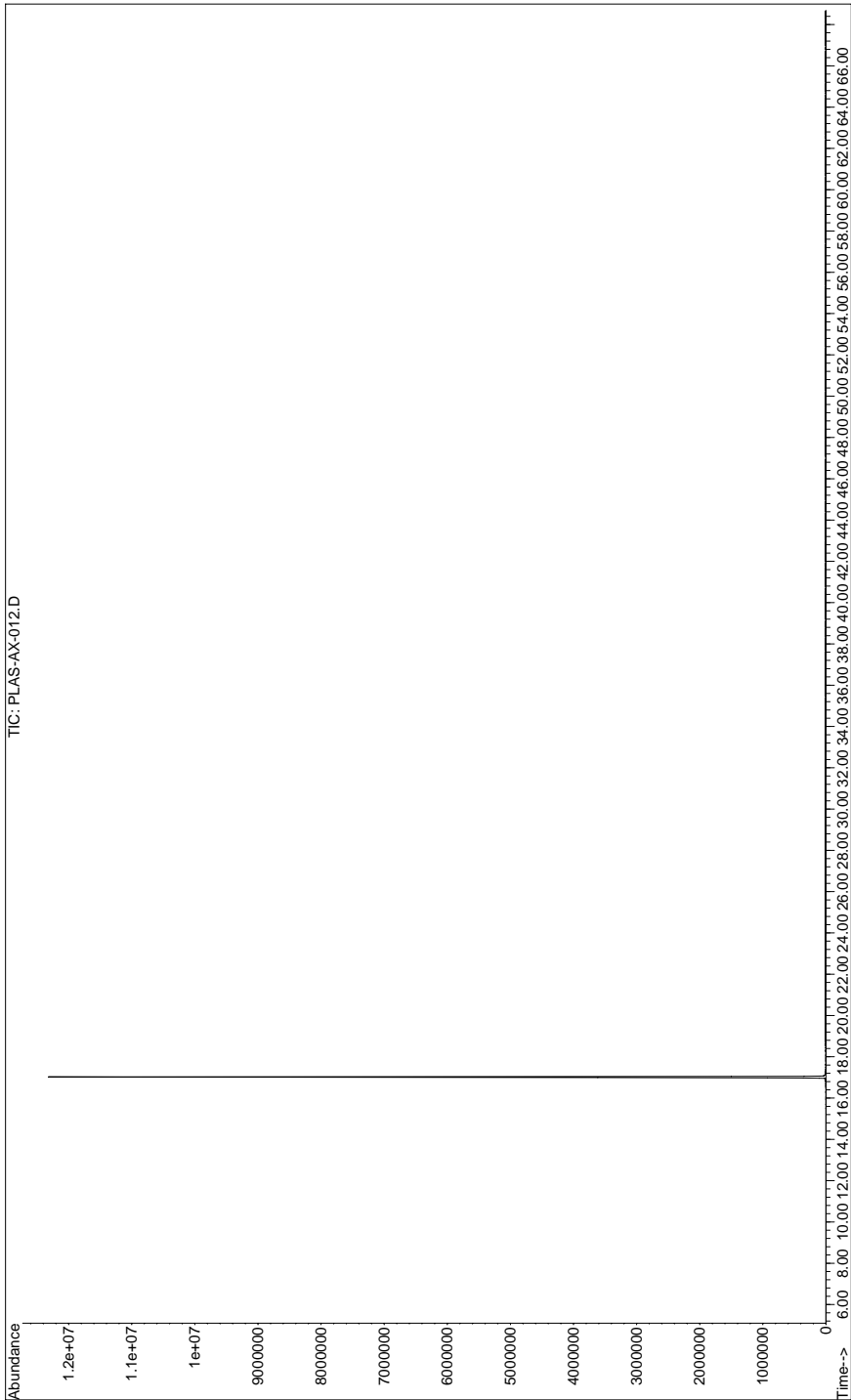
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Cyanox*[®] 425 - PLAS-AX-012

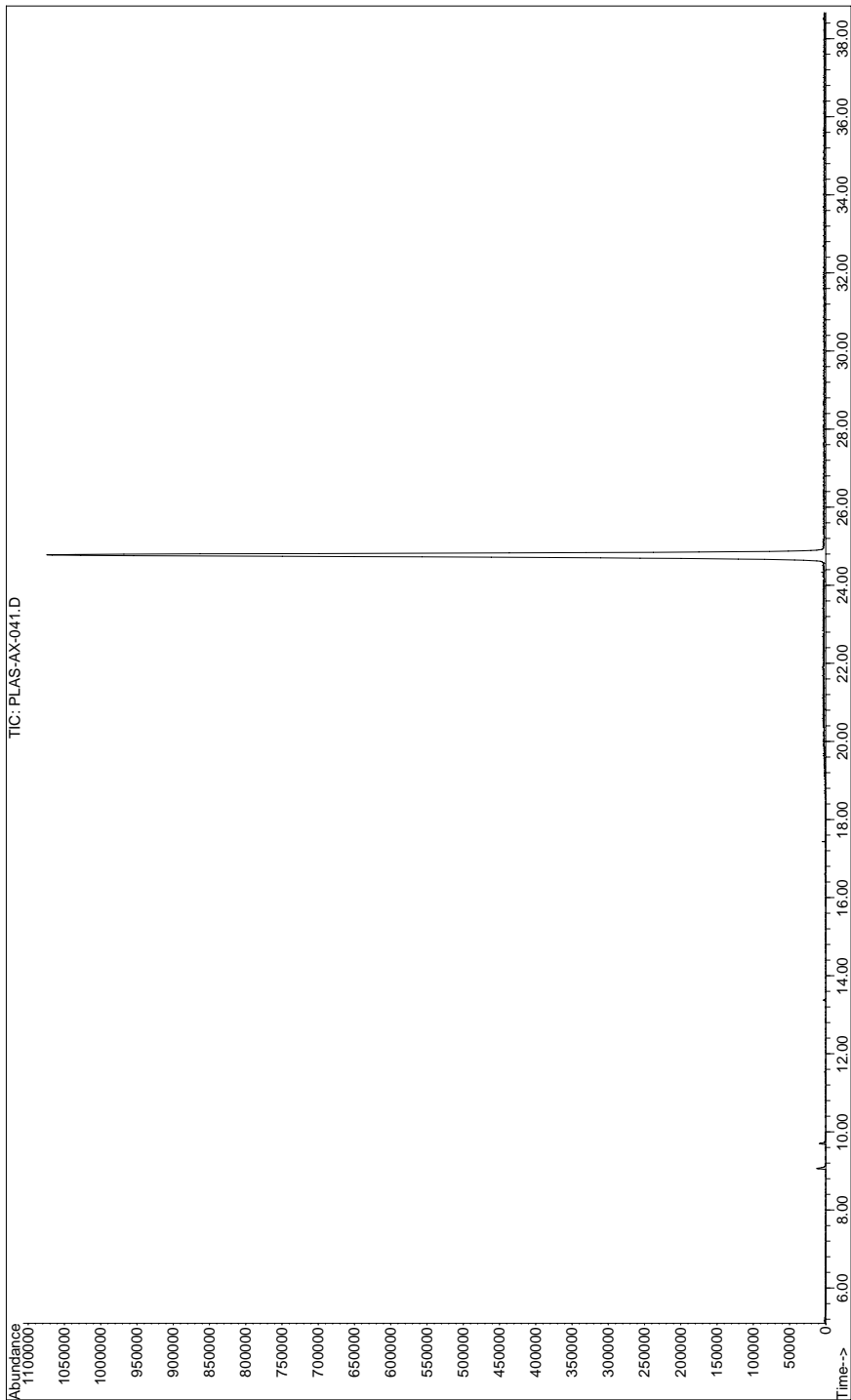
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Cyanox*[®] LTDP - PLAS-AX-041

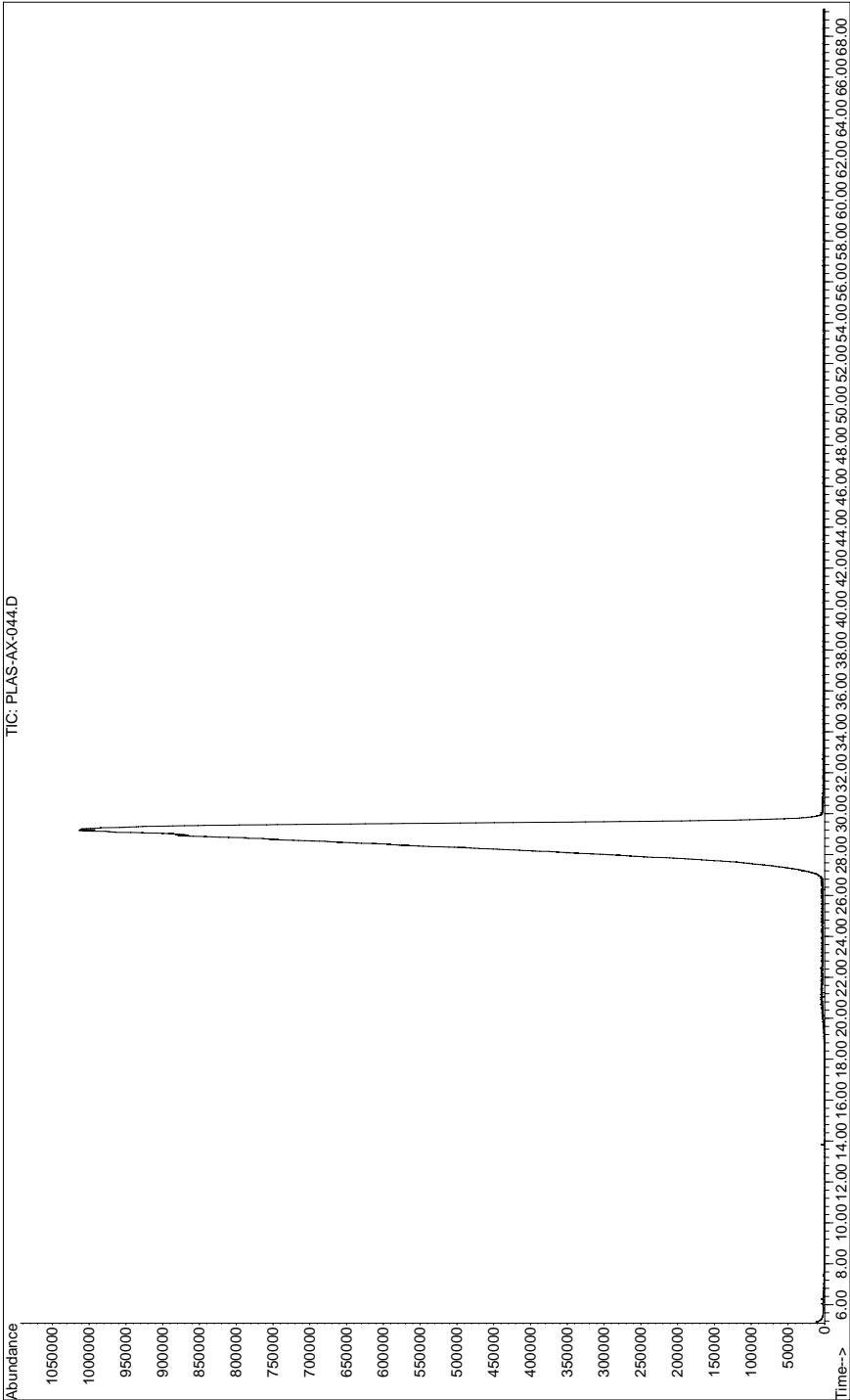
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Cyanox*[®] STDP - PLAS-AX-044

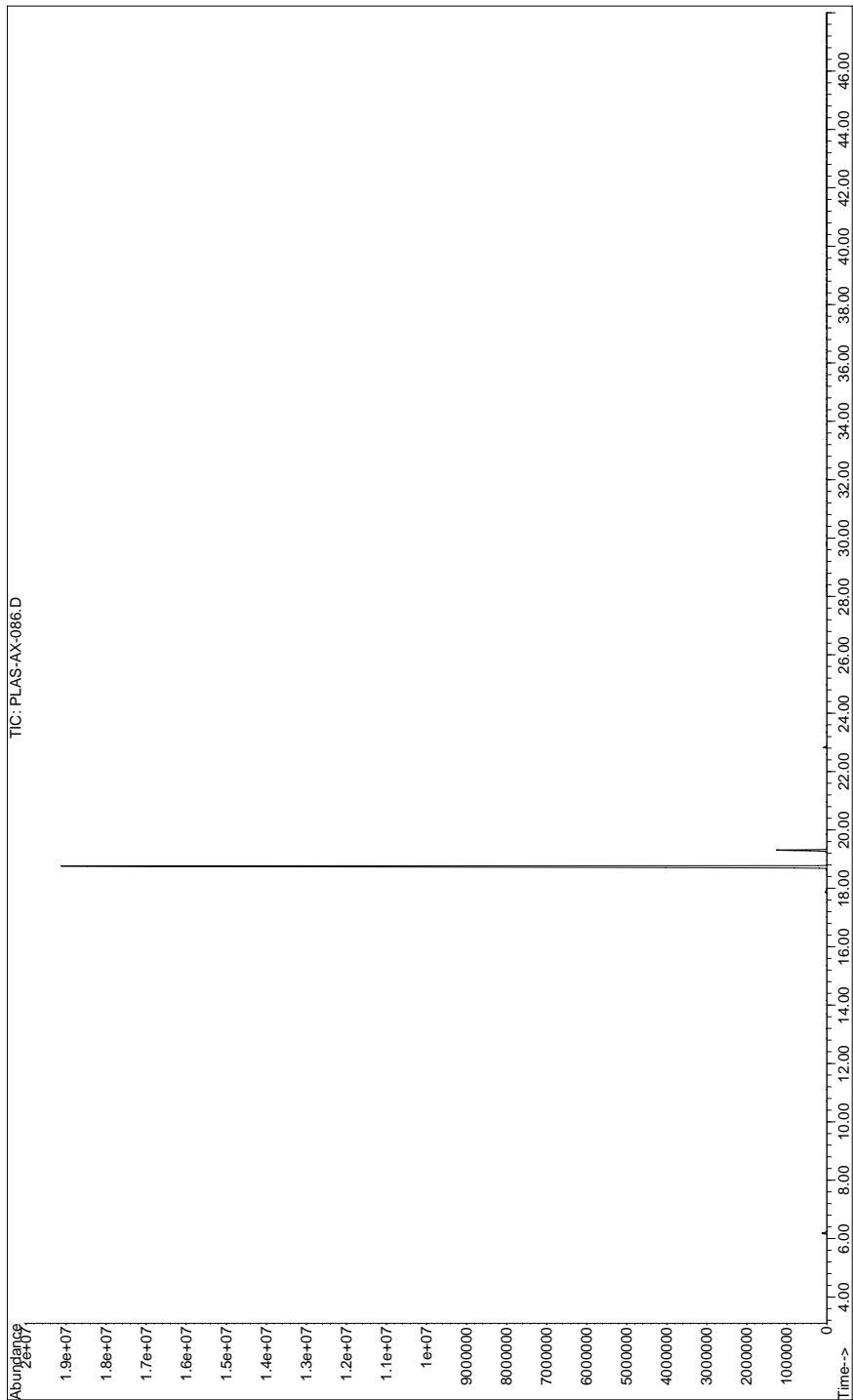
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Ethanox*[®] 310 - PLAS-AX-086

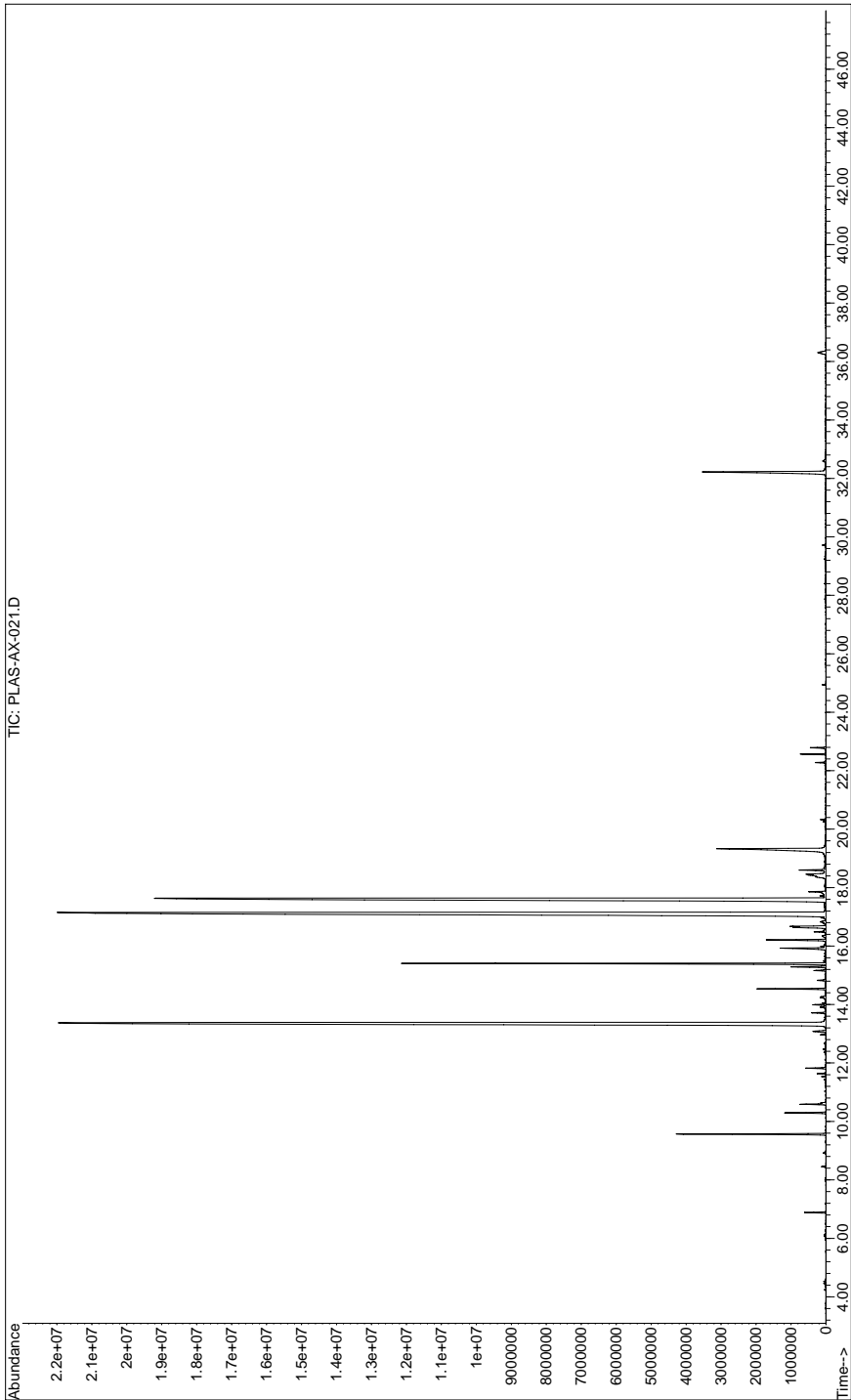
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Ethanox*[®] 330 - PLAS-AX-021

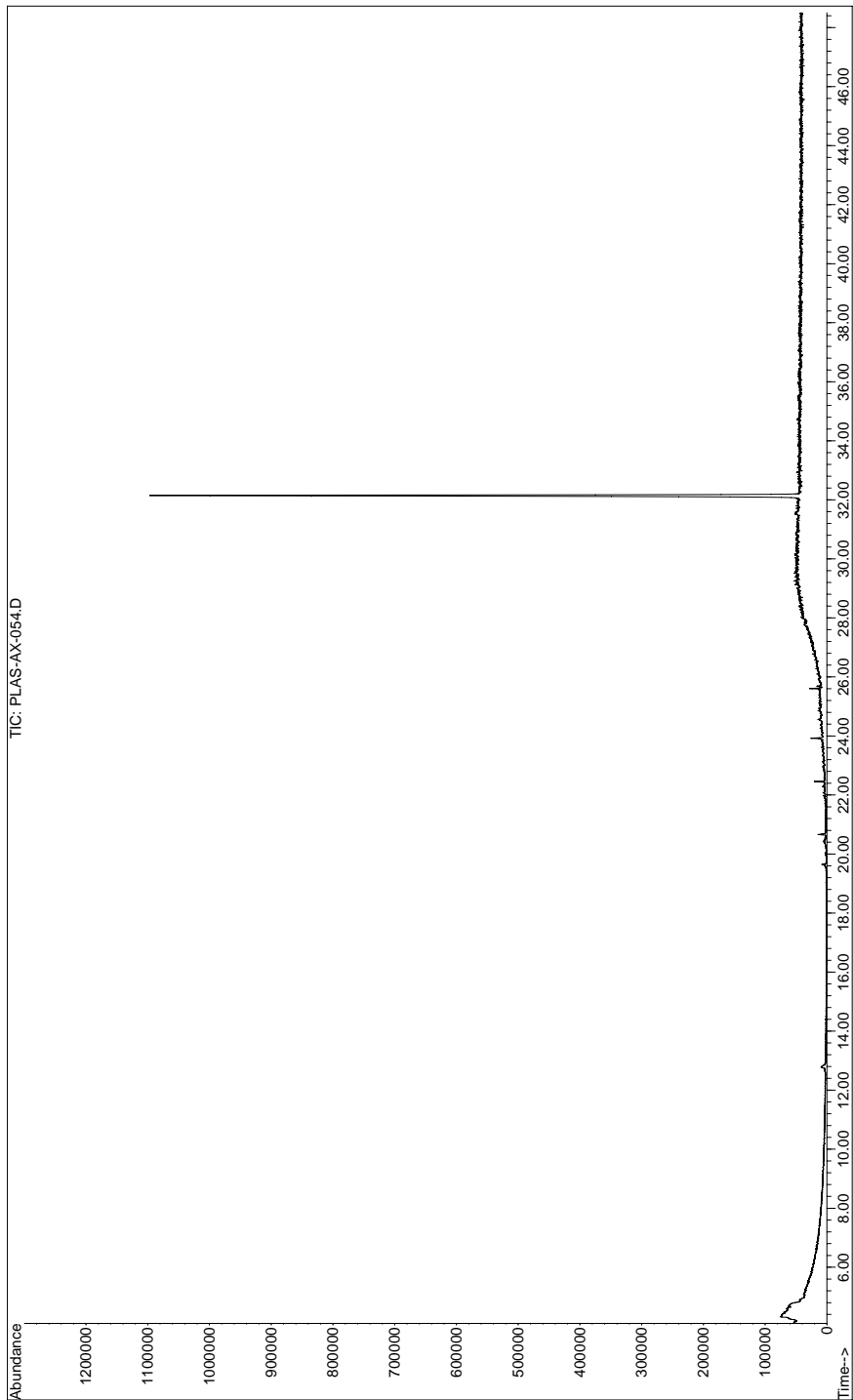
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Ethanox*[®] 376 - PLAS-AX-054

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Ethanox*[®] 702 - PLAS-AX-025

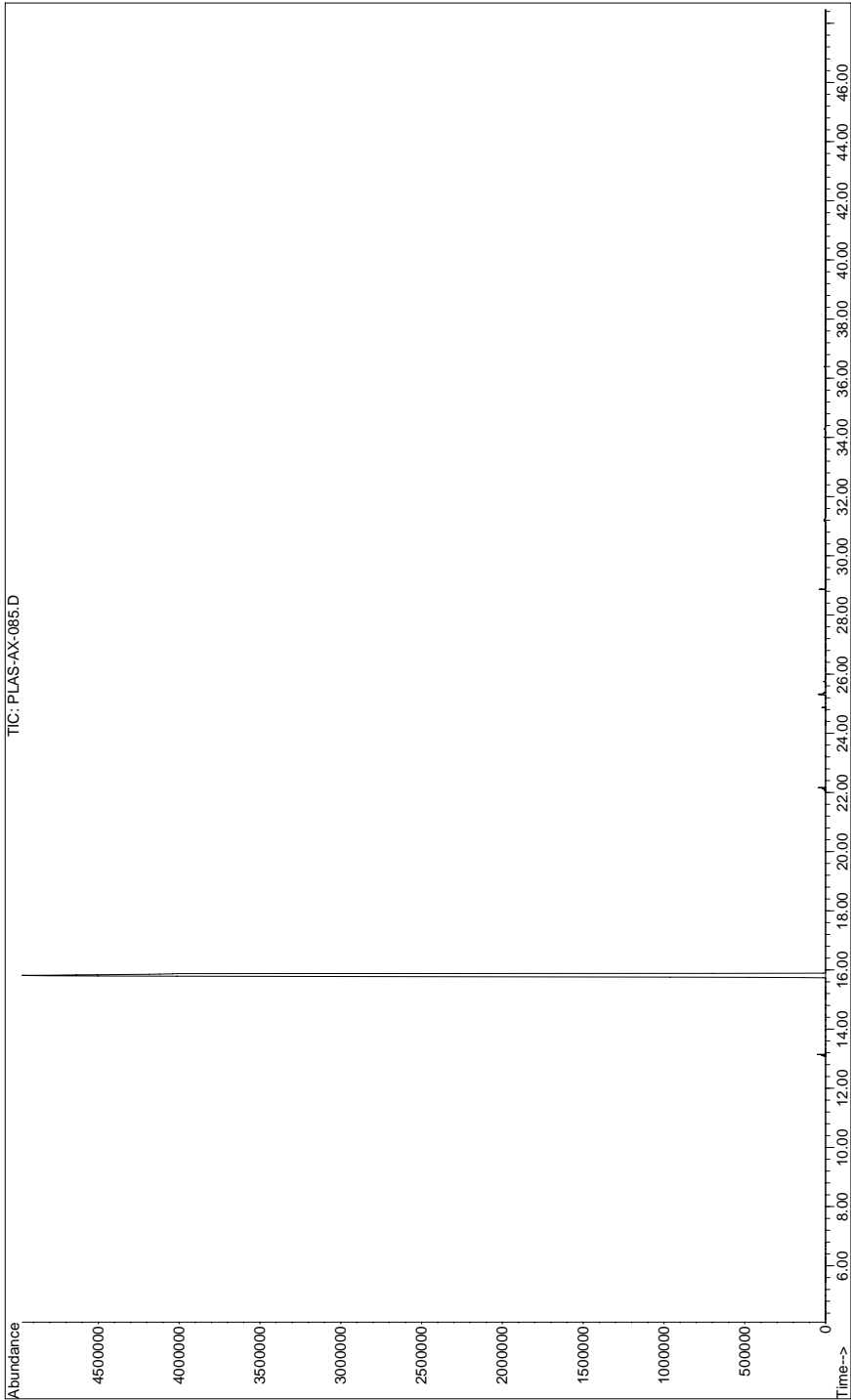
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Ethanox*[®] 703 - PLAS-AX-085

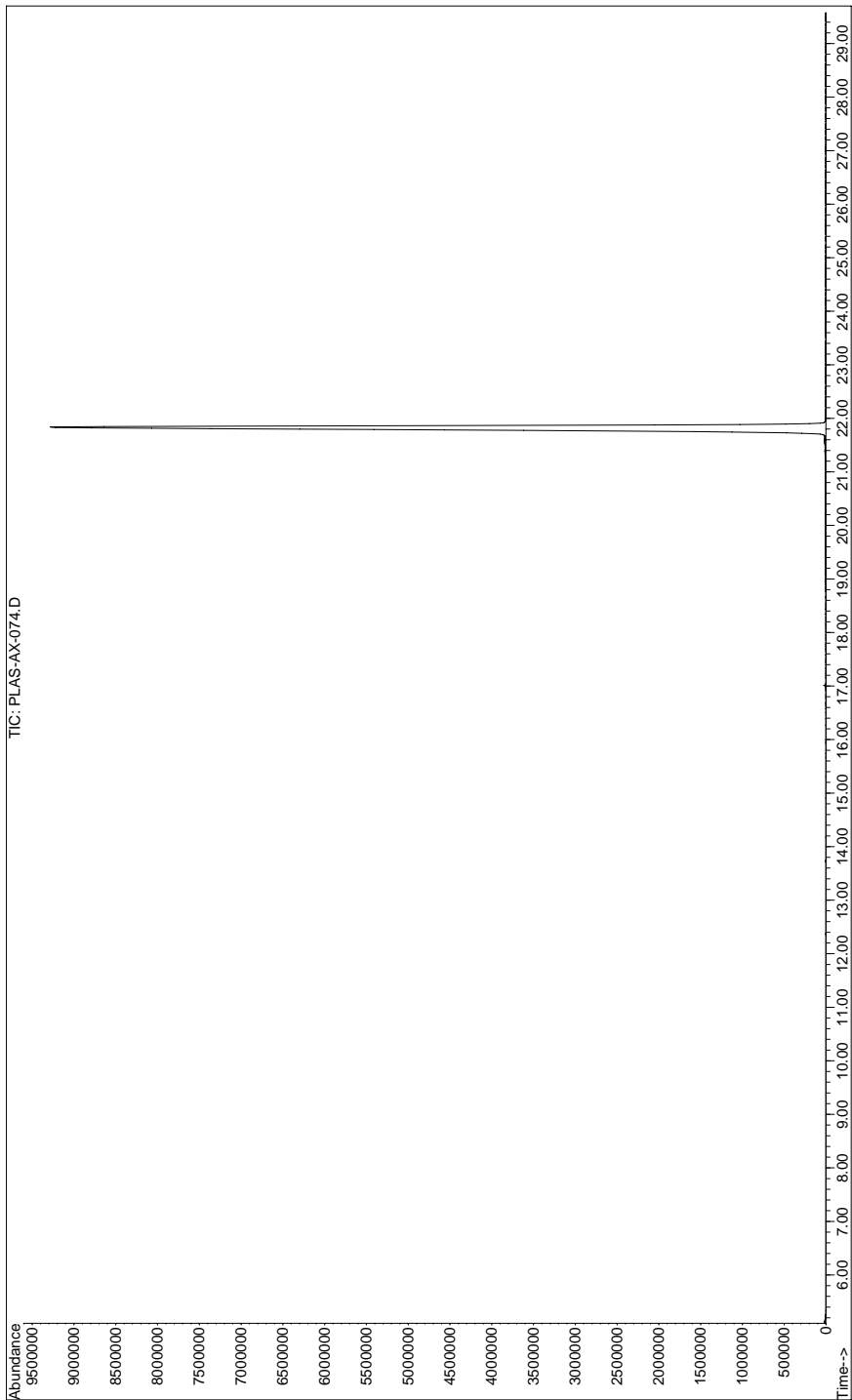
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Ethaphos*[®] 368 - PLAS-AX-074

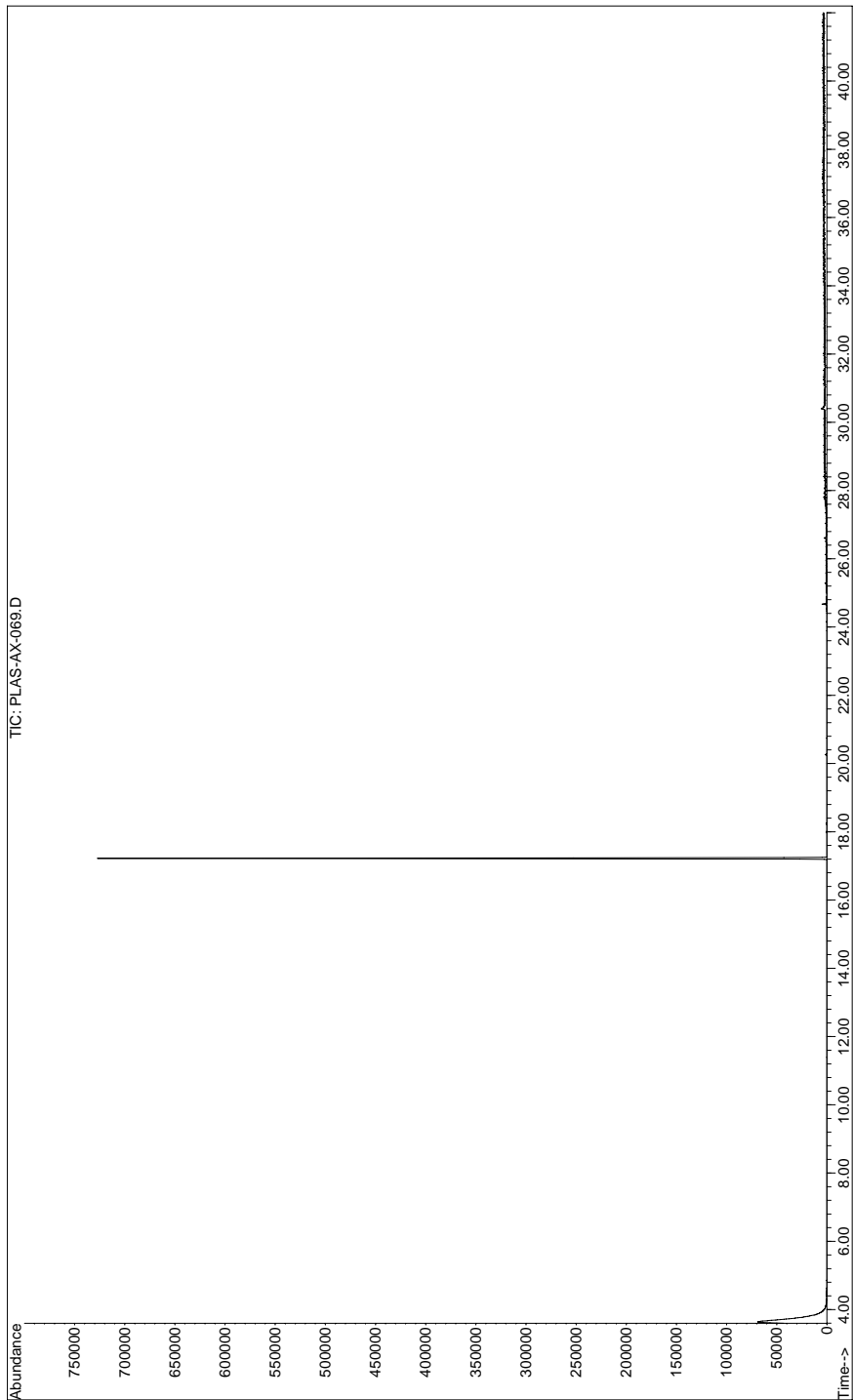
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Irganox® 1035 - PLAS-AX-069

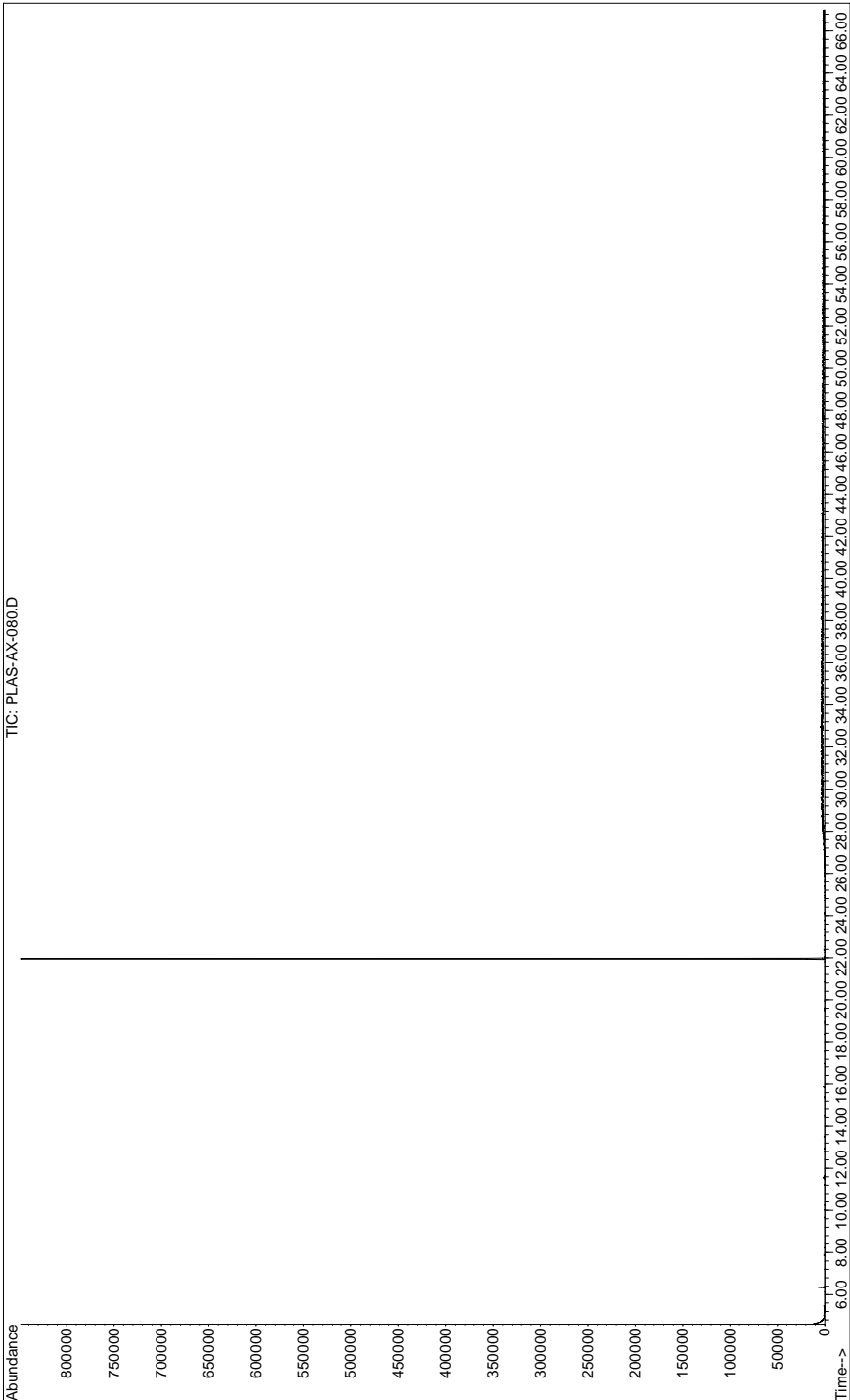
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Irganox® 1081 - PLAS-AX-080

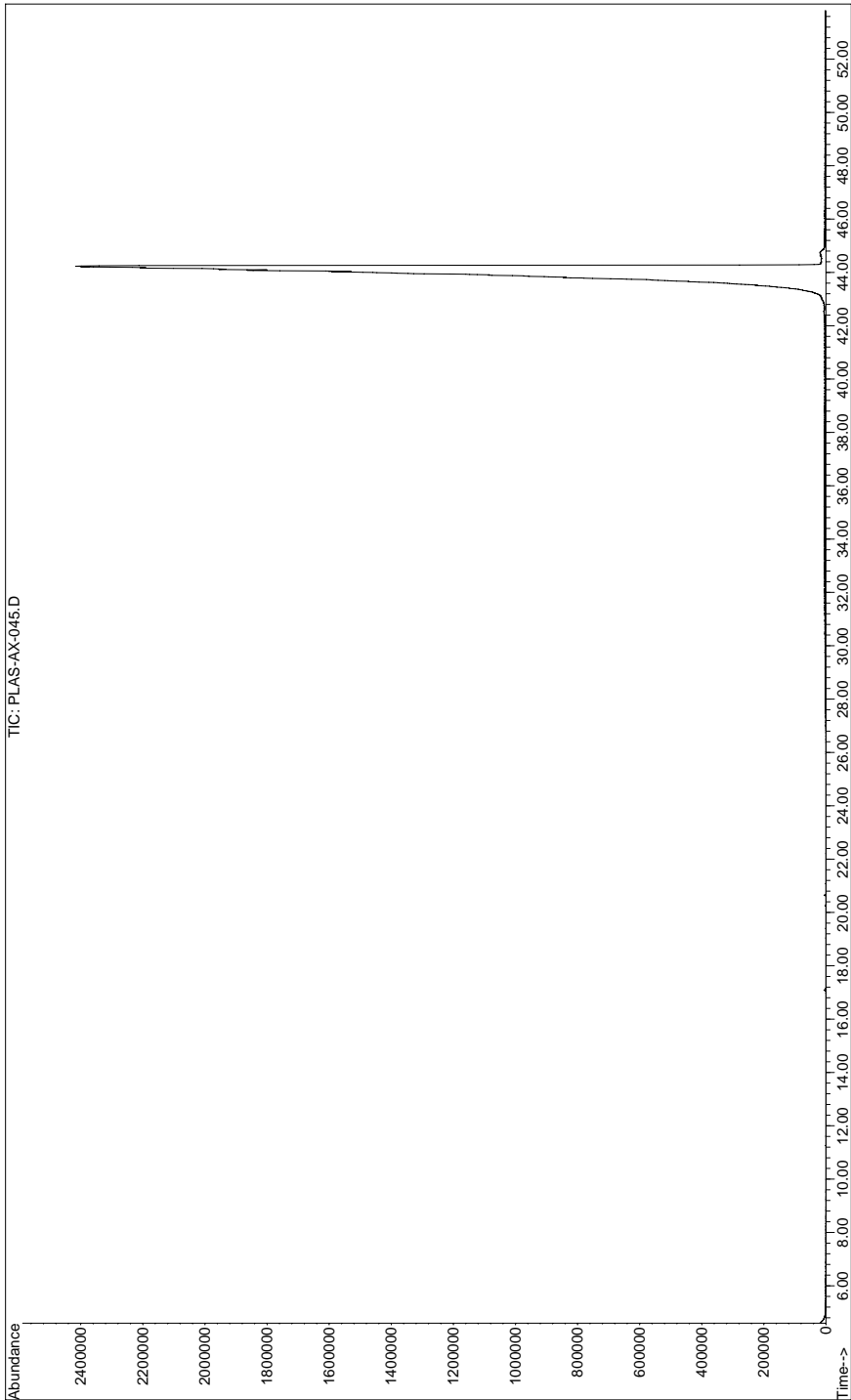
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Irganox® 259 - PLAS-AX-045

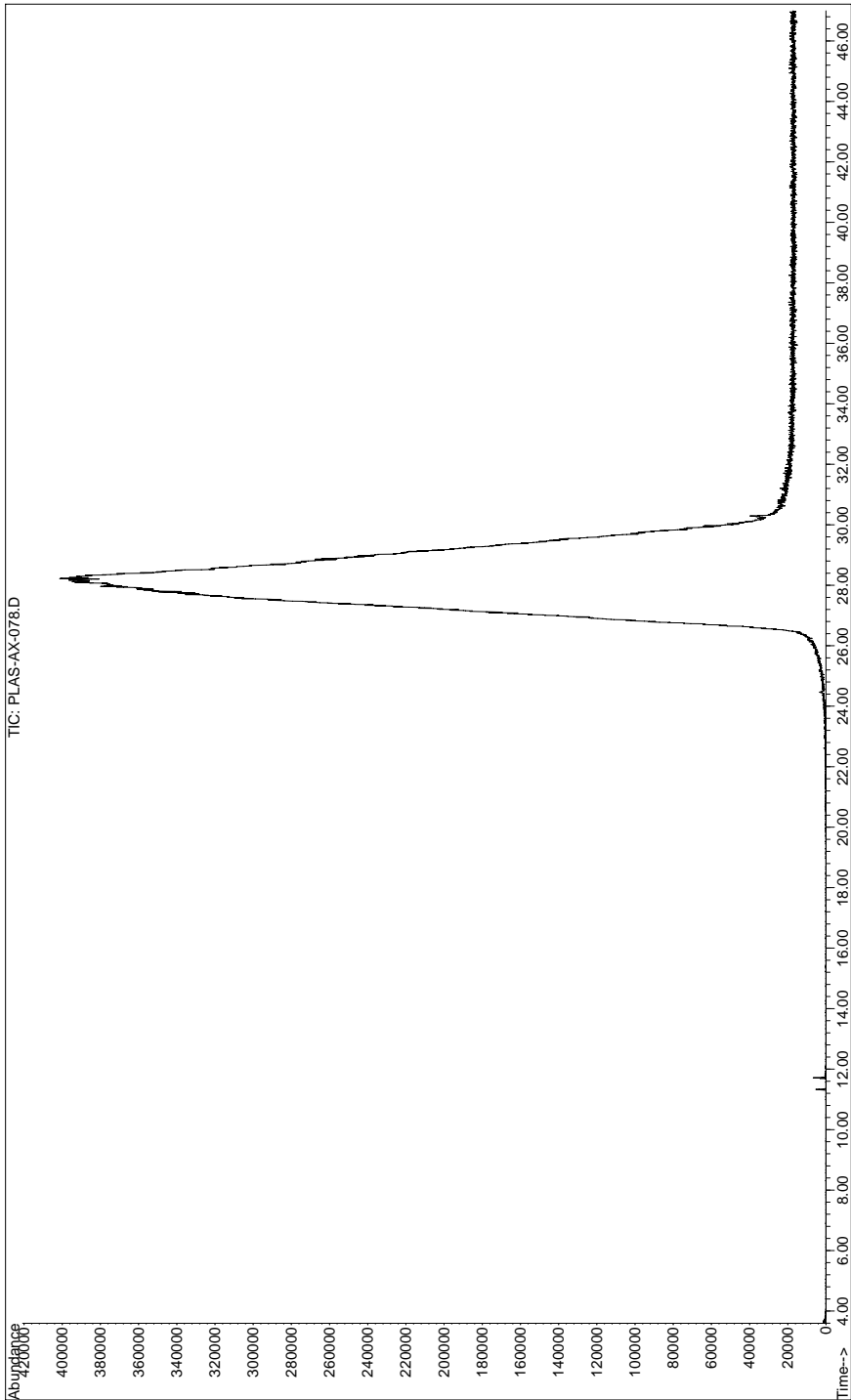
Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Irganox® 3114 FF - PLAS-AX-078

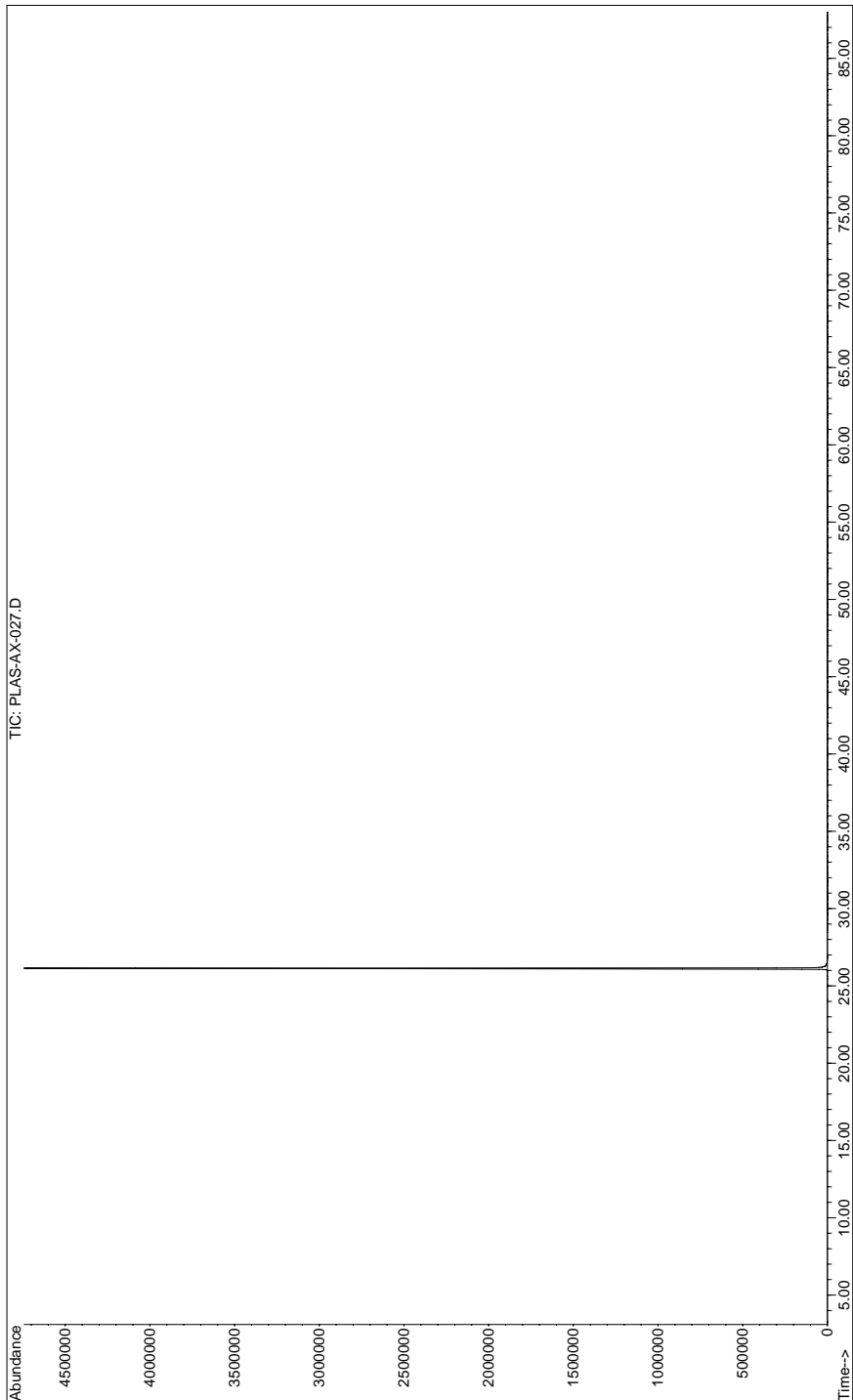
Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Irganox® E 201 - PLAS-AX-027

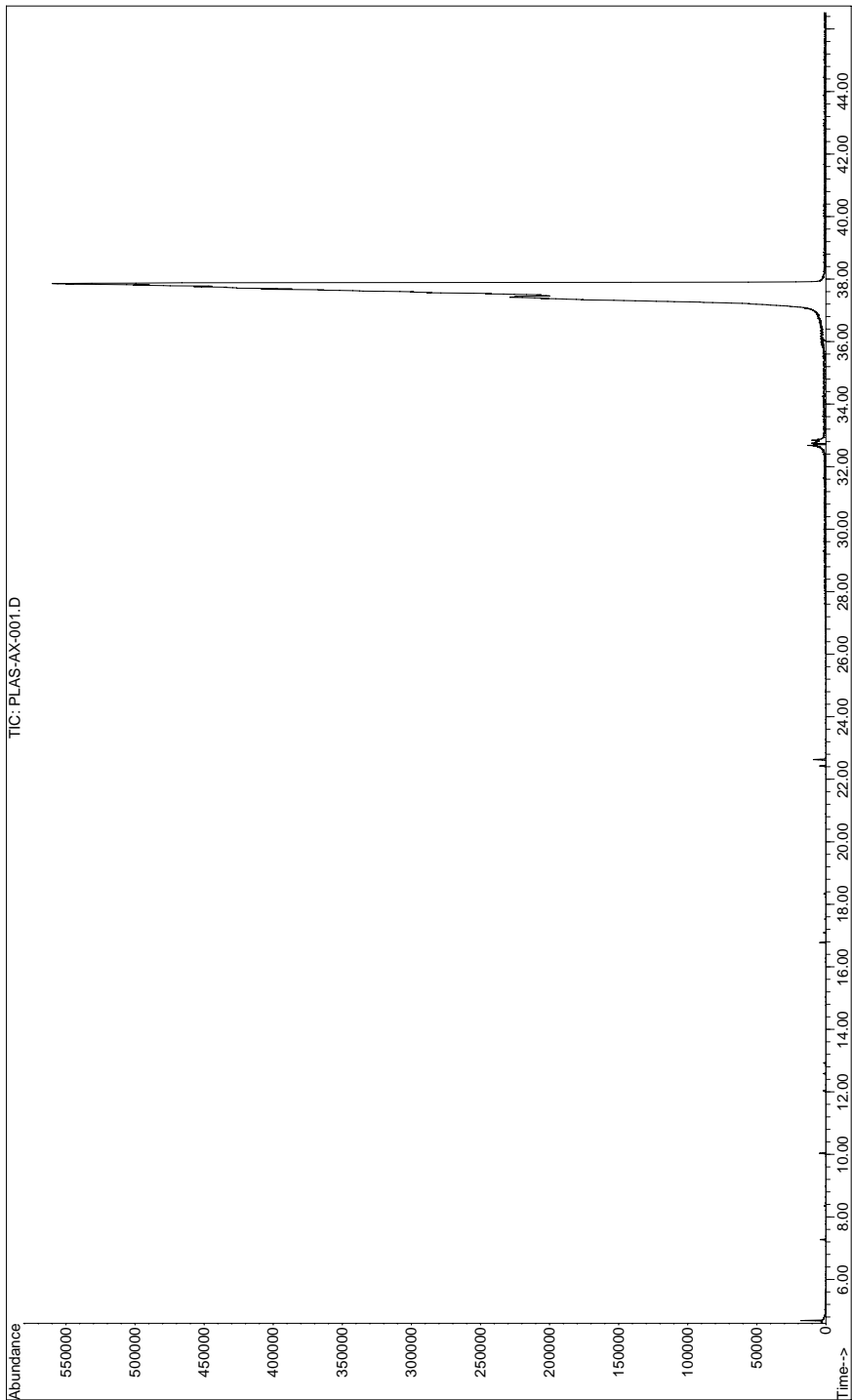
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Irganox® MD 1024 - PLAS-AX-001

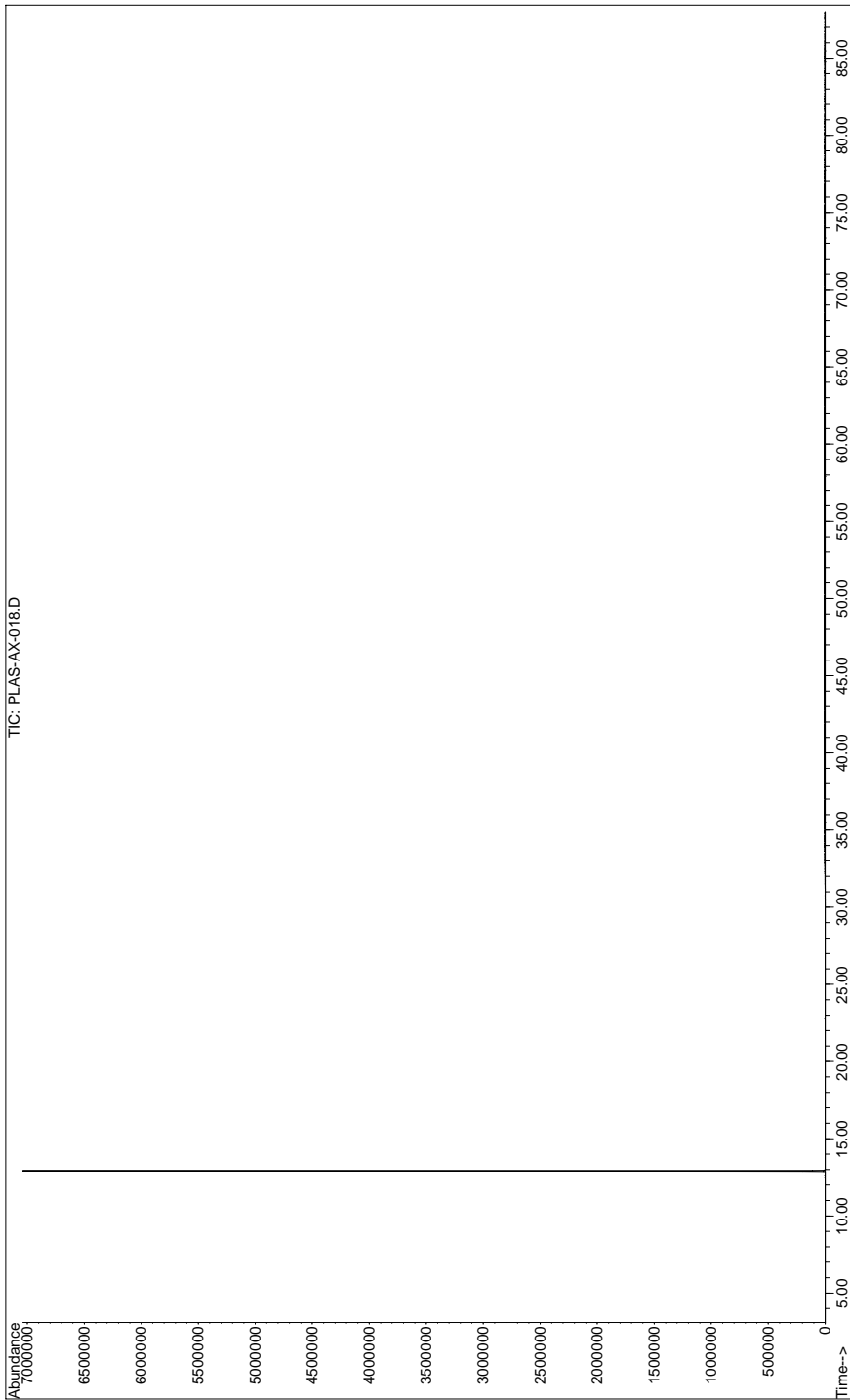
Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Isonox*[®] 132 - PLAS-AX-018

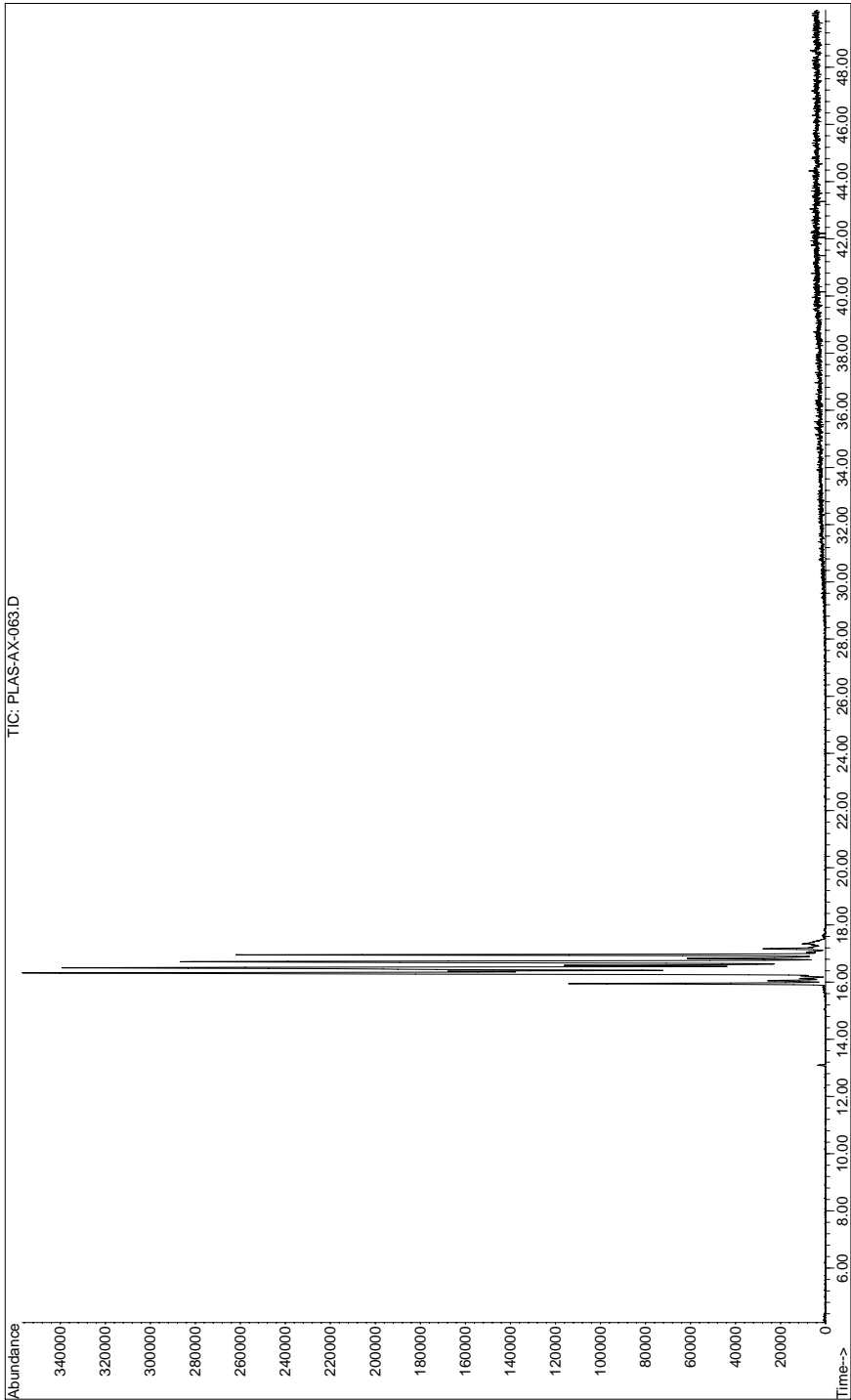
Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Isonox[®] 232 - PLAS-AX-063

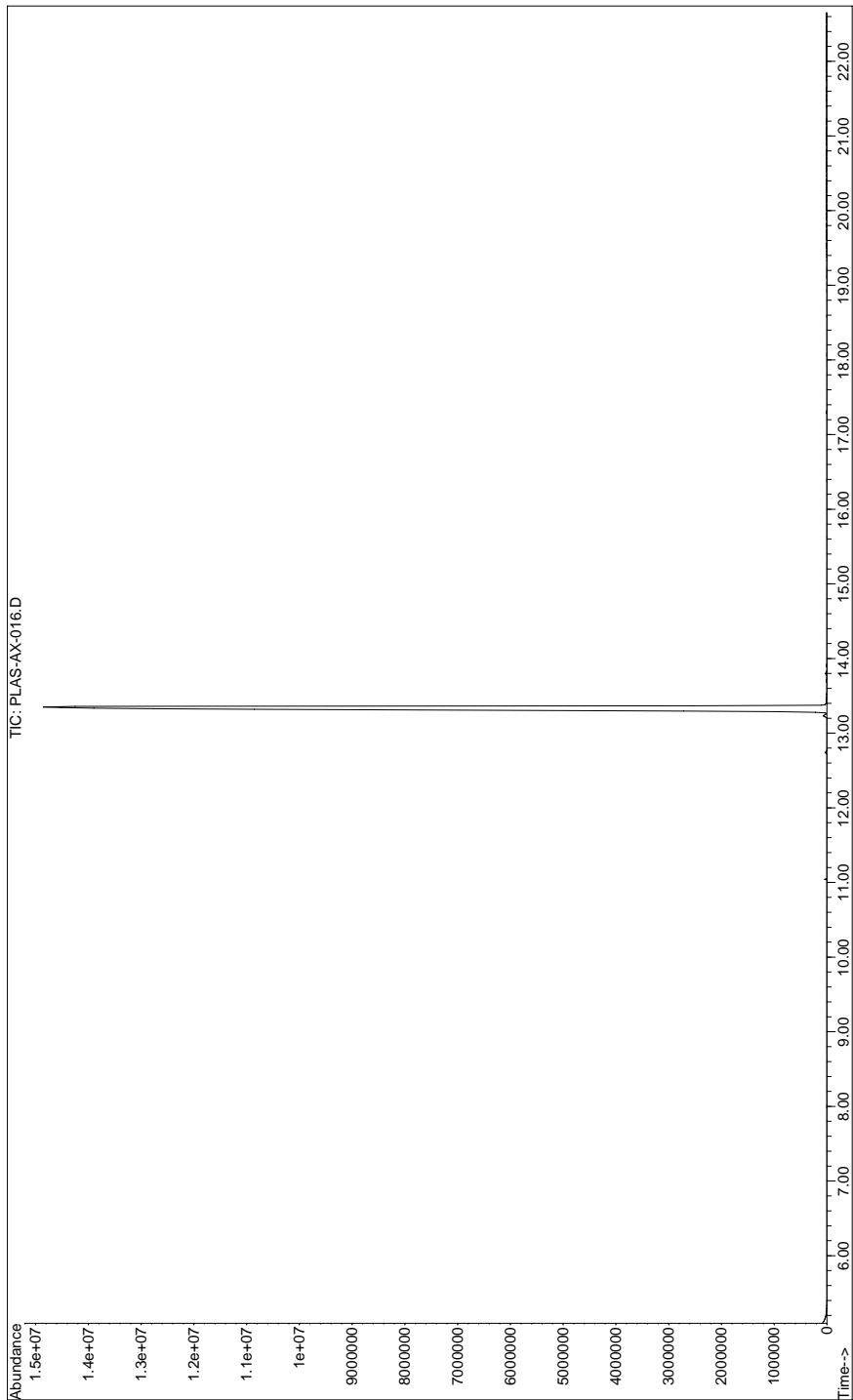
Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Lowinox*[®] AH25 - PLAS-AX-016

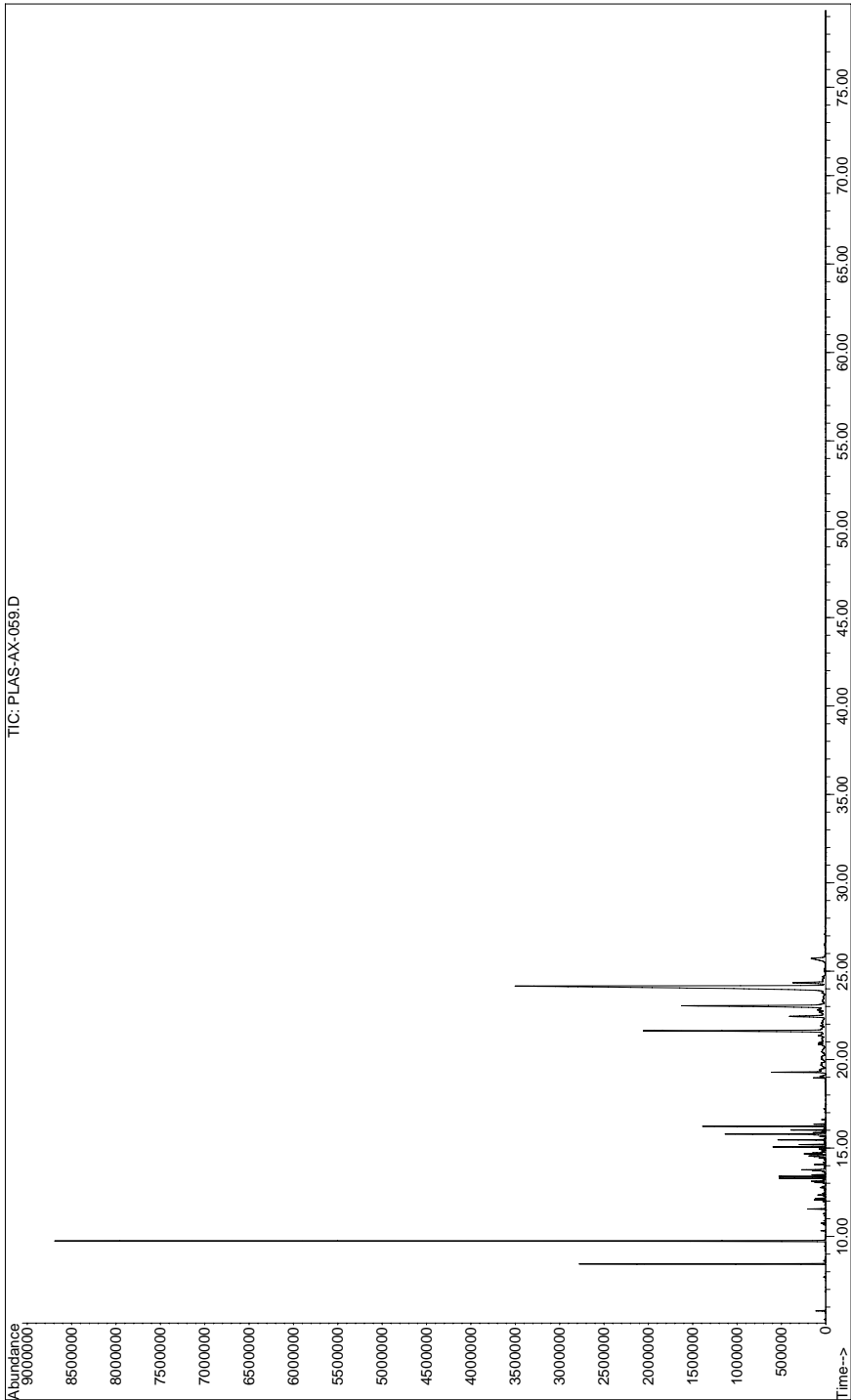
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Lowinox® CPL - PLAS-AX-059*

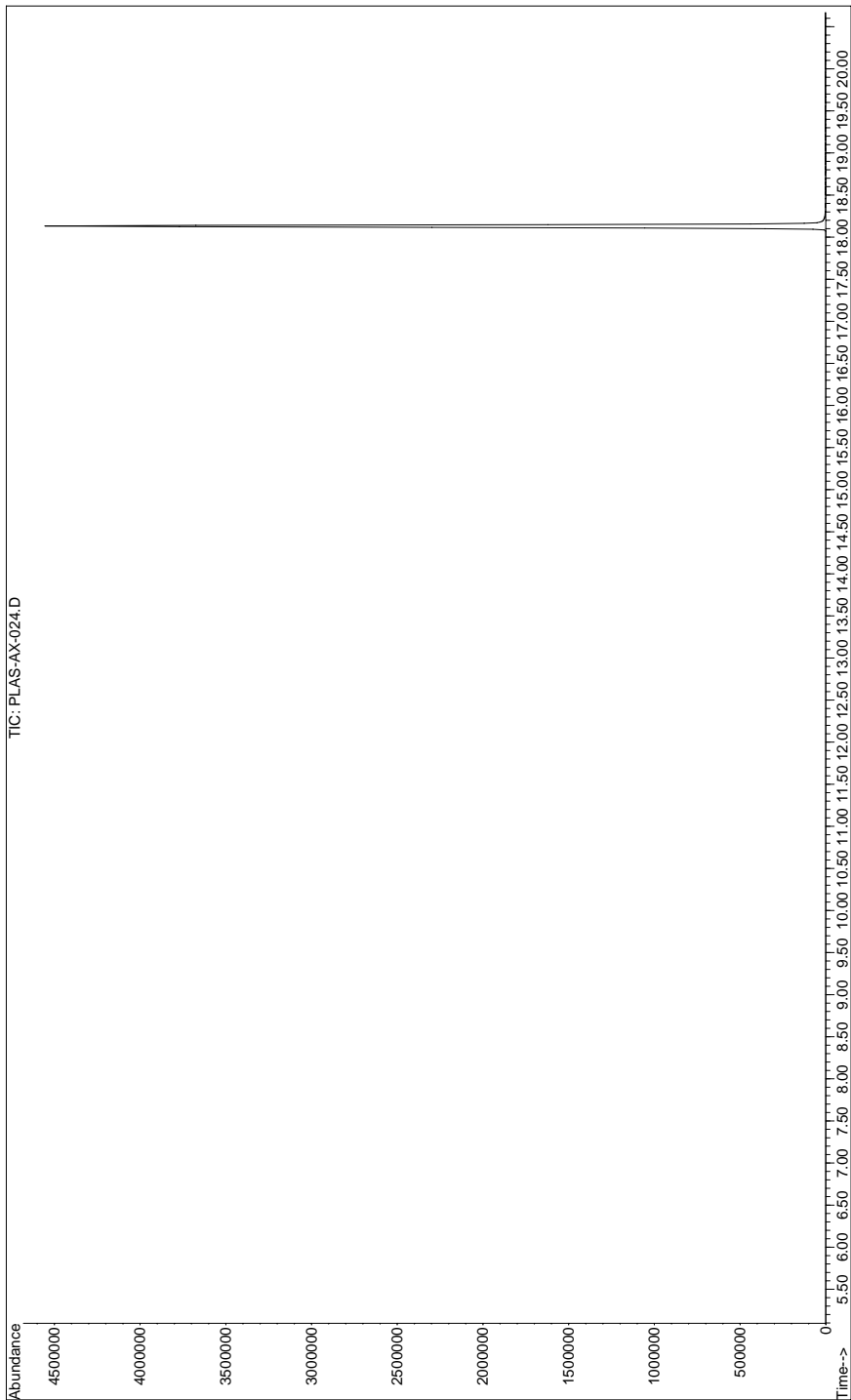
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Lowinox*[®] TBM-6 - PLAS-AX-024

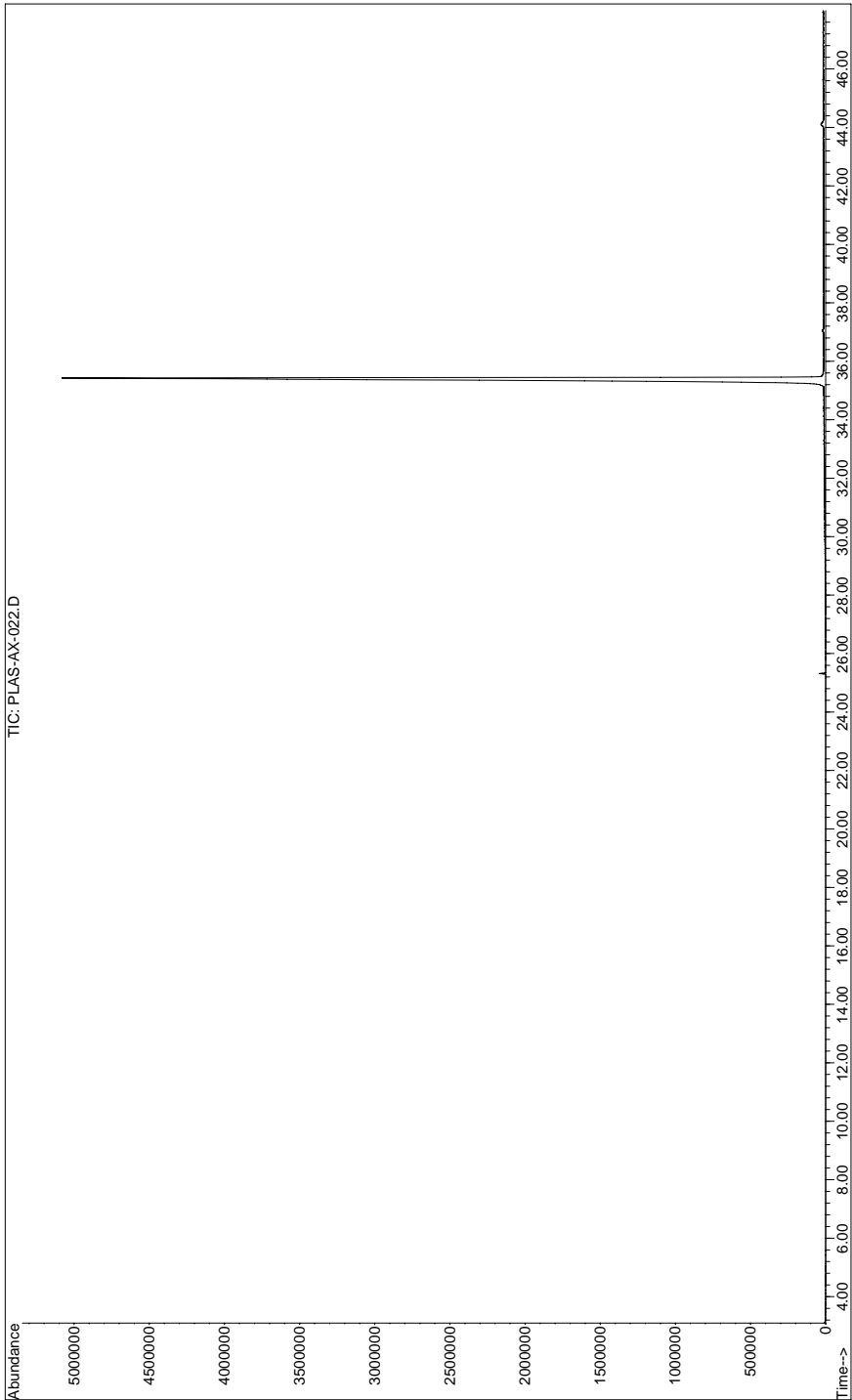
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Naugard® 445 - PLAS-AX-022

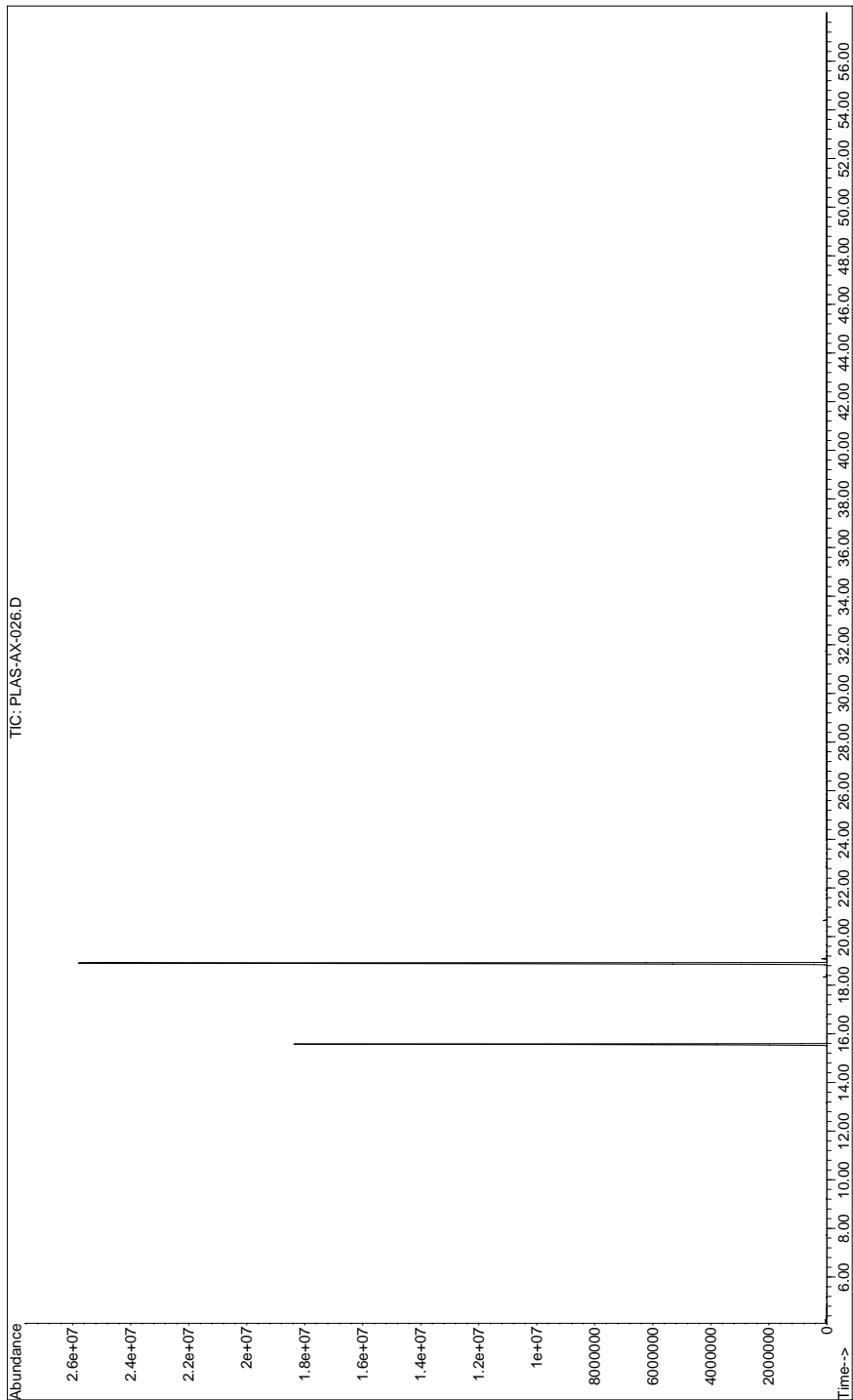
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® A - PLAS-AX-026

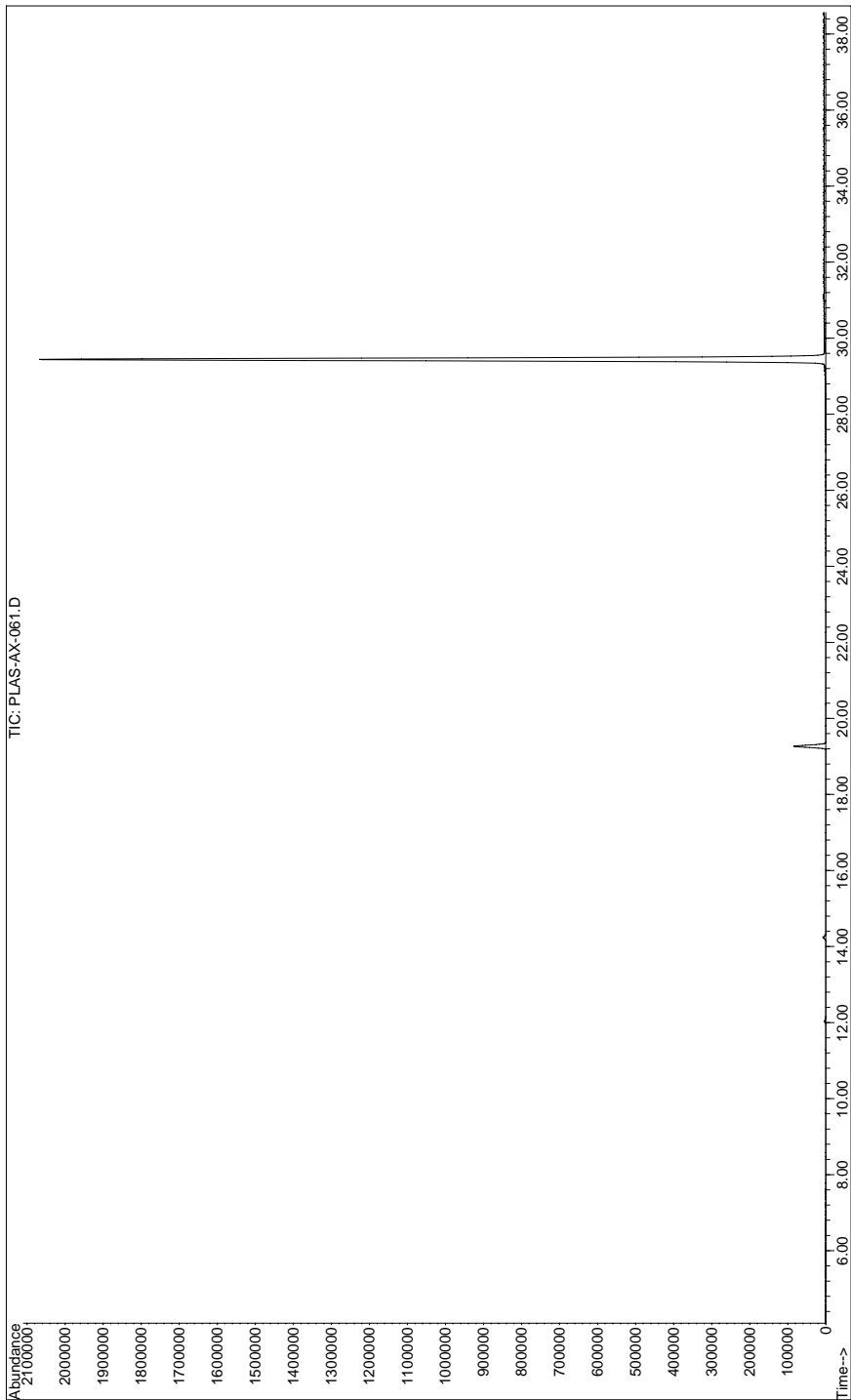
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® B-25 - PLAS-AX-061

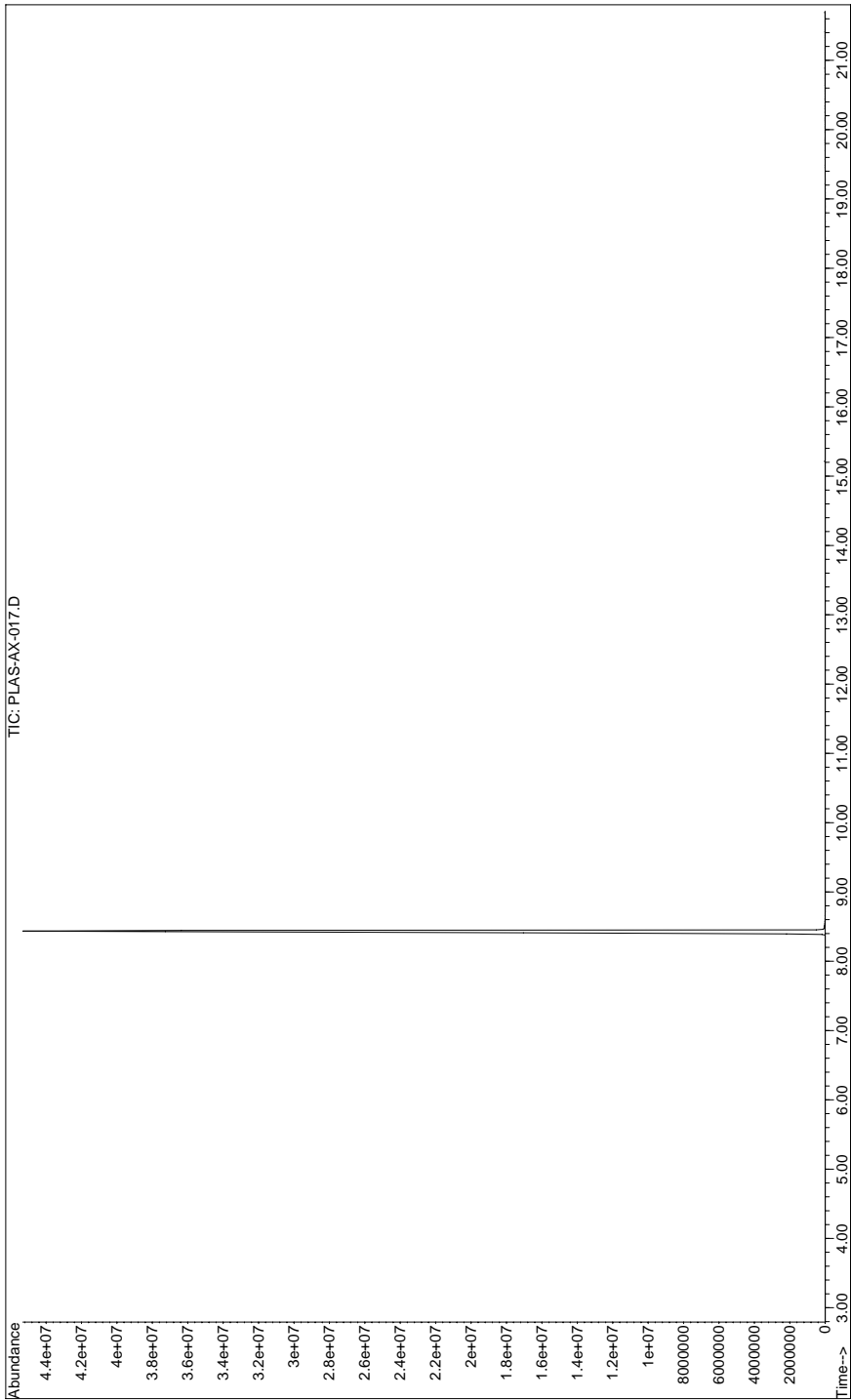
Analytical Conditions Summary 40 °C (0 min) to 320 °C (10 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Naugard® BHT - PLAS-AX-017

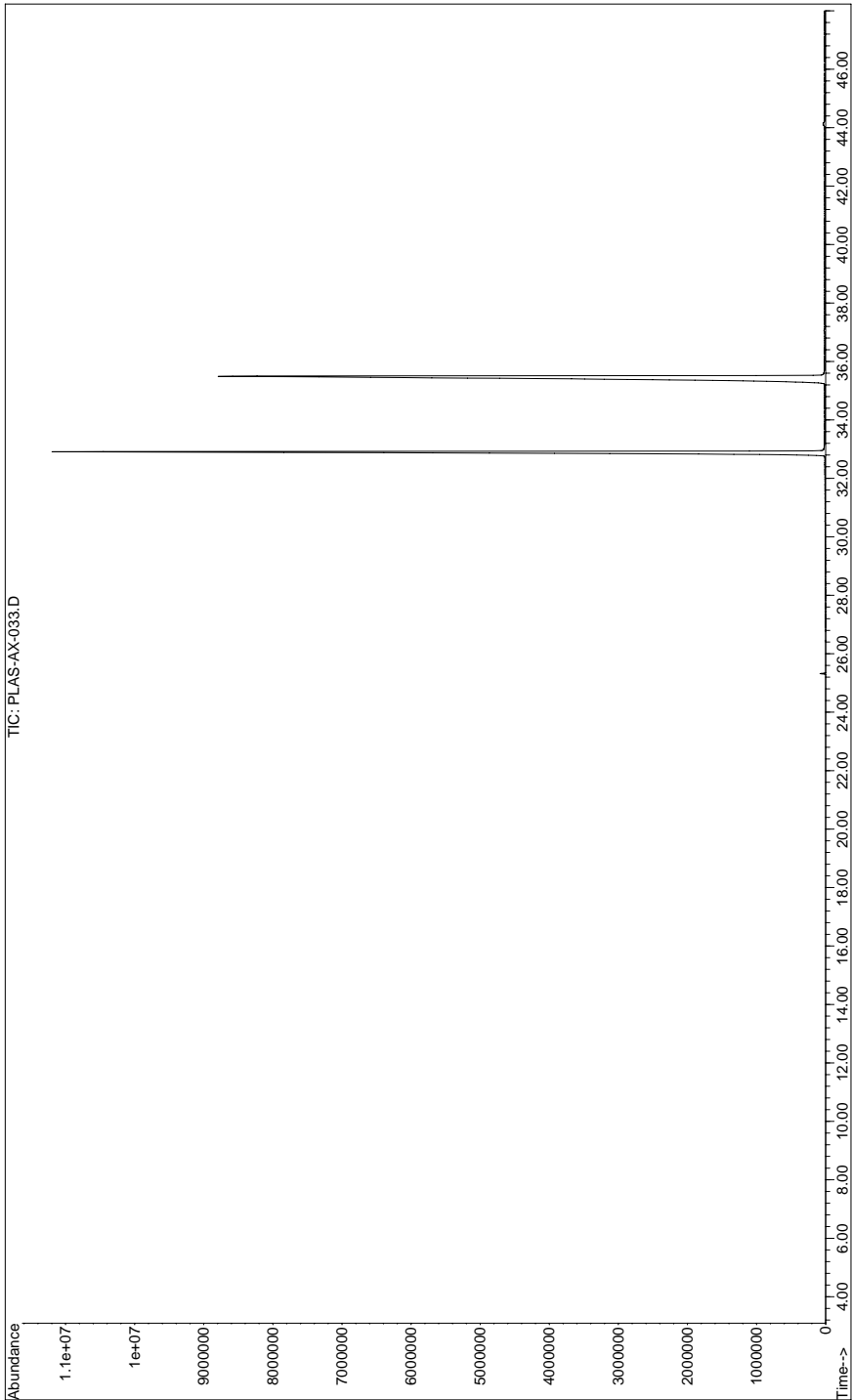
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Naugard® HM-22 - PLAS-AX-033

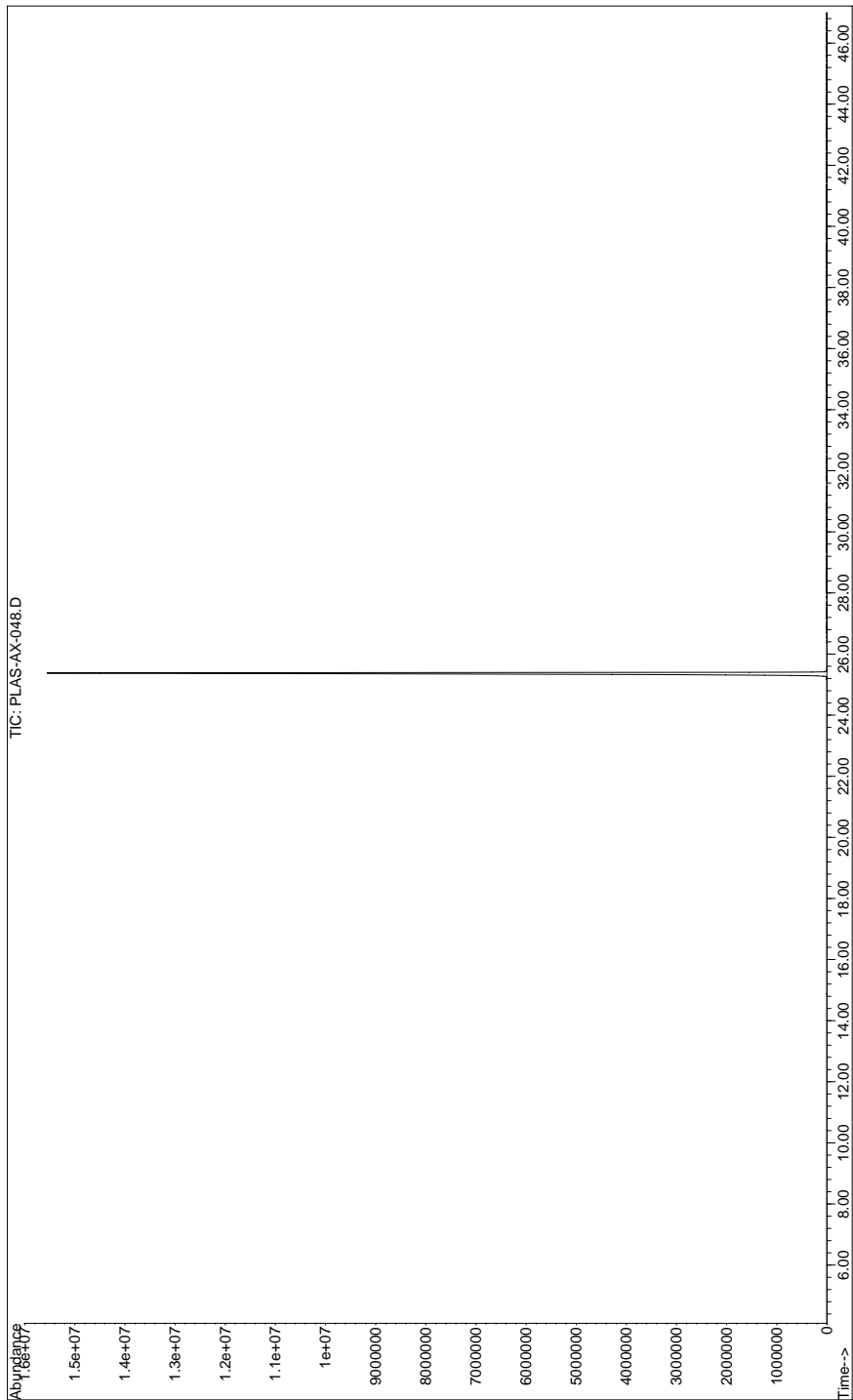
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® J - PLAS-AX-048

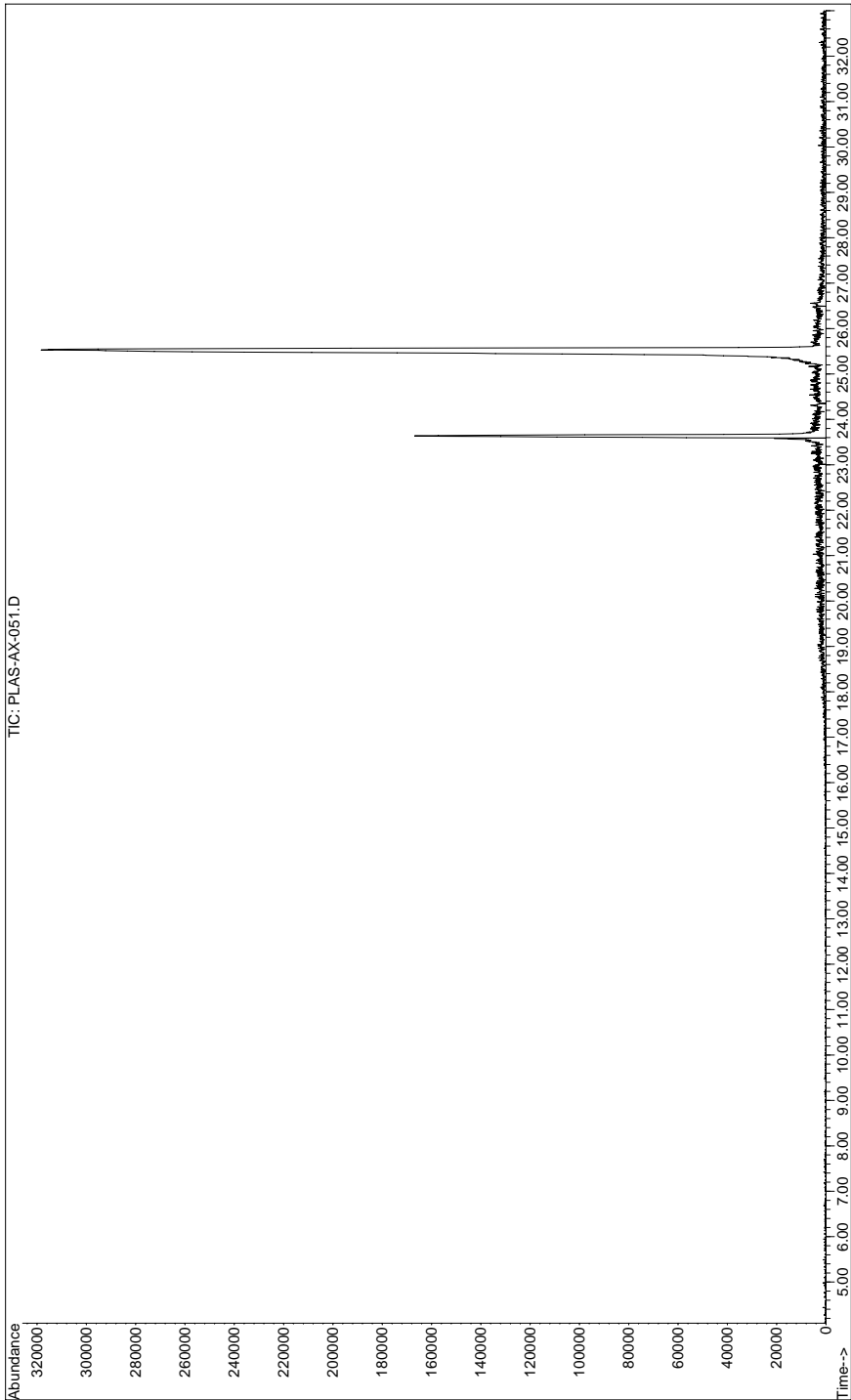
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® NBC - PLAS-AX-051

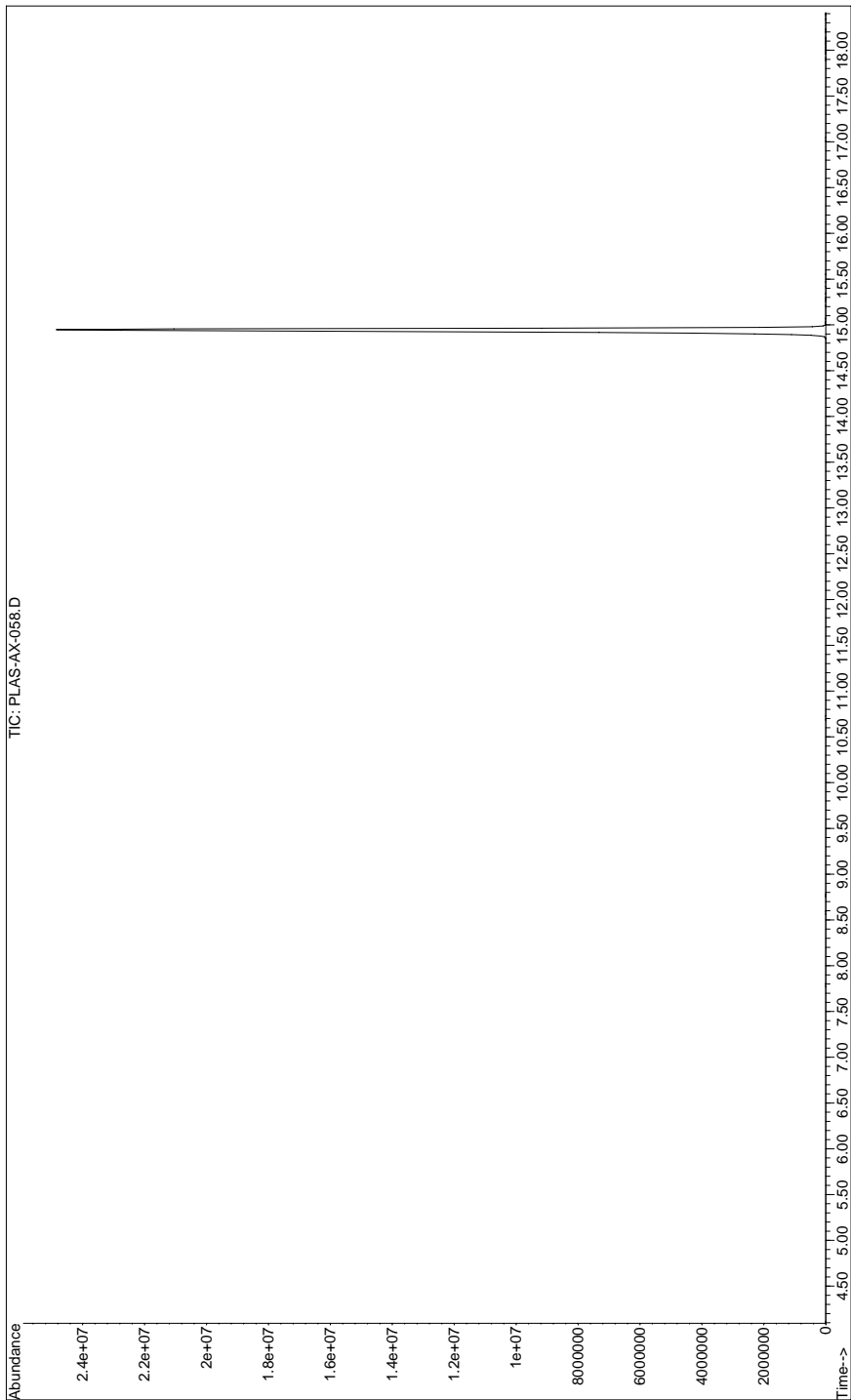
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Naugard® PANA - PLAS-AX-058

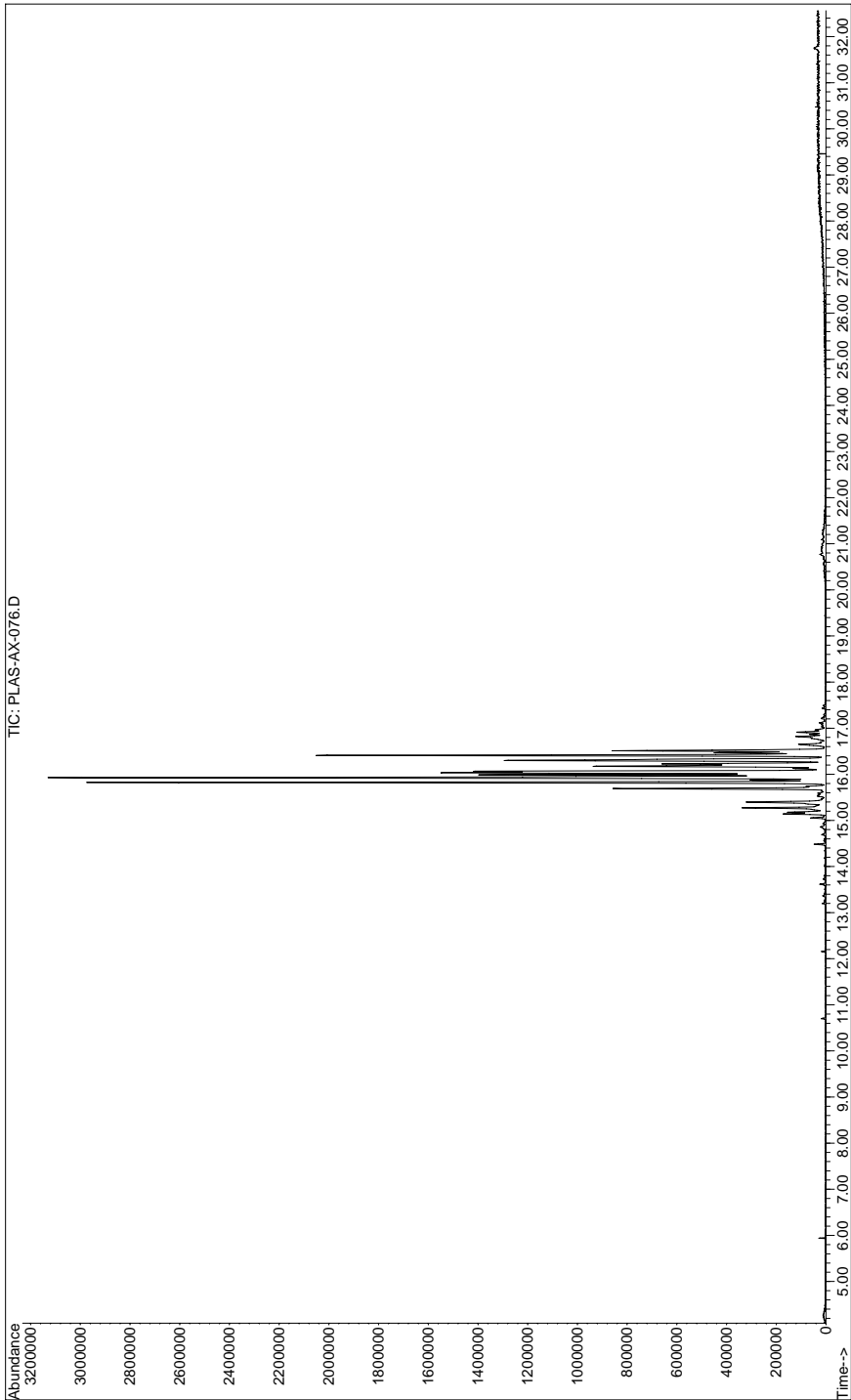
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Naugard® PHR - PLAS-AX-076

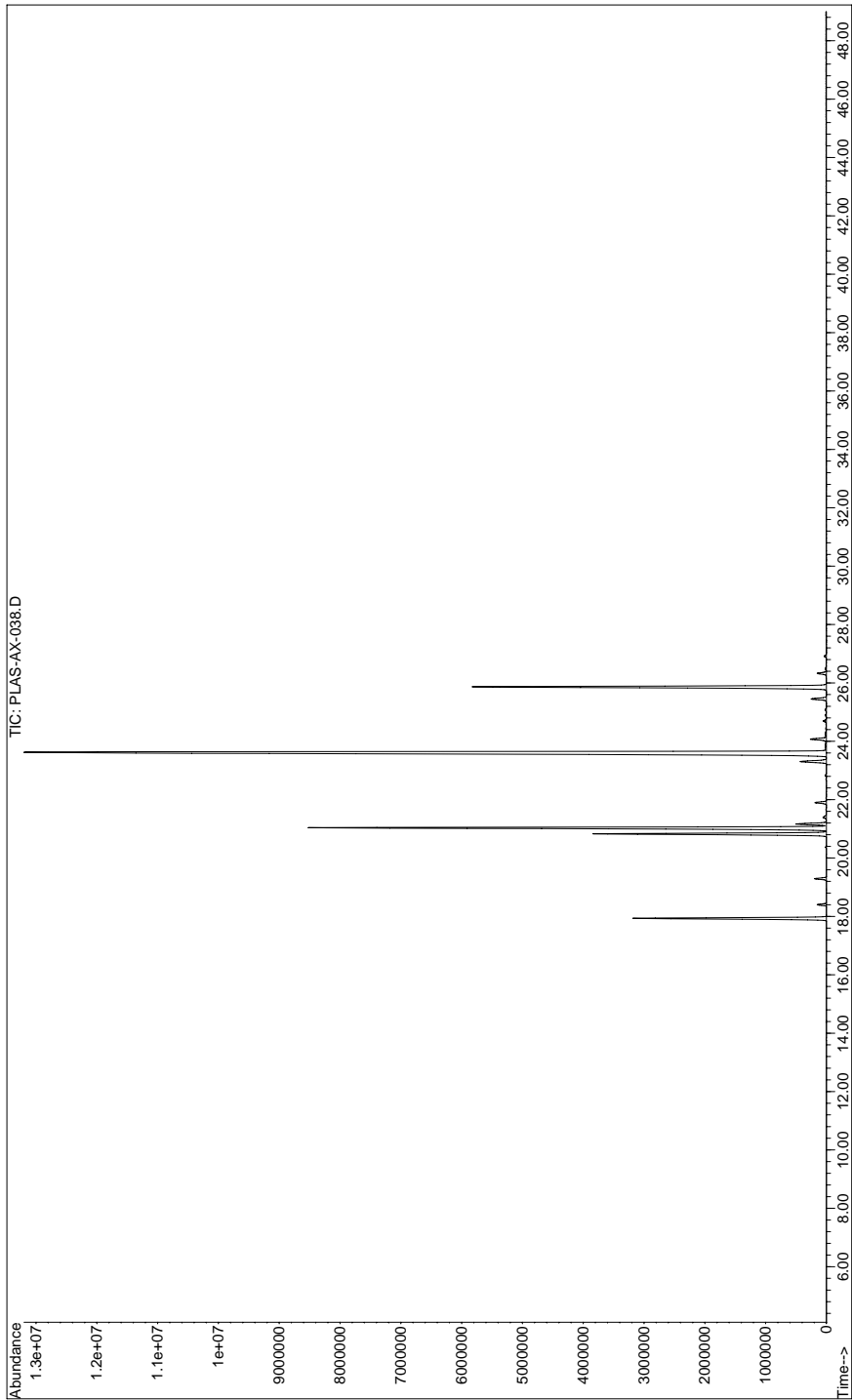
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® PS-30 - PLAS-AX-038

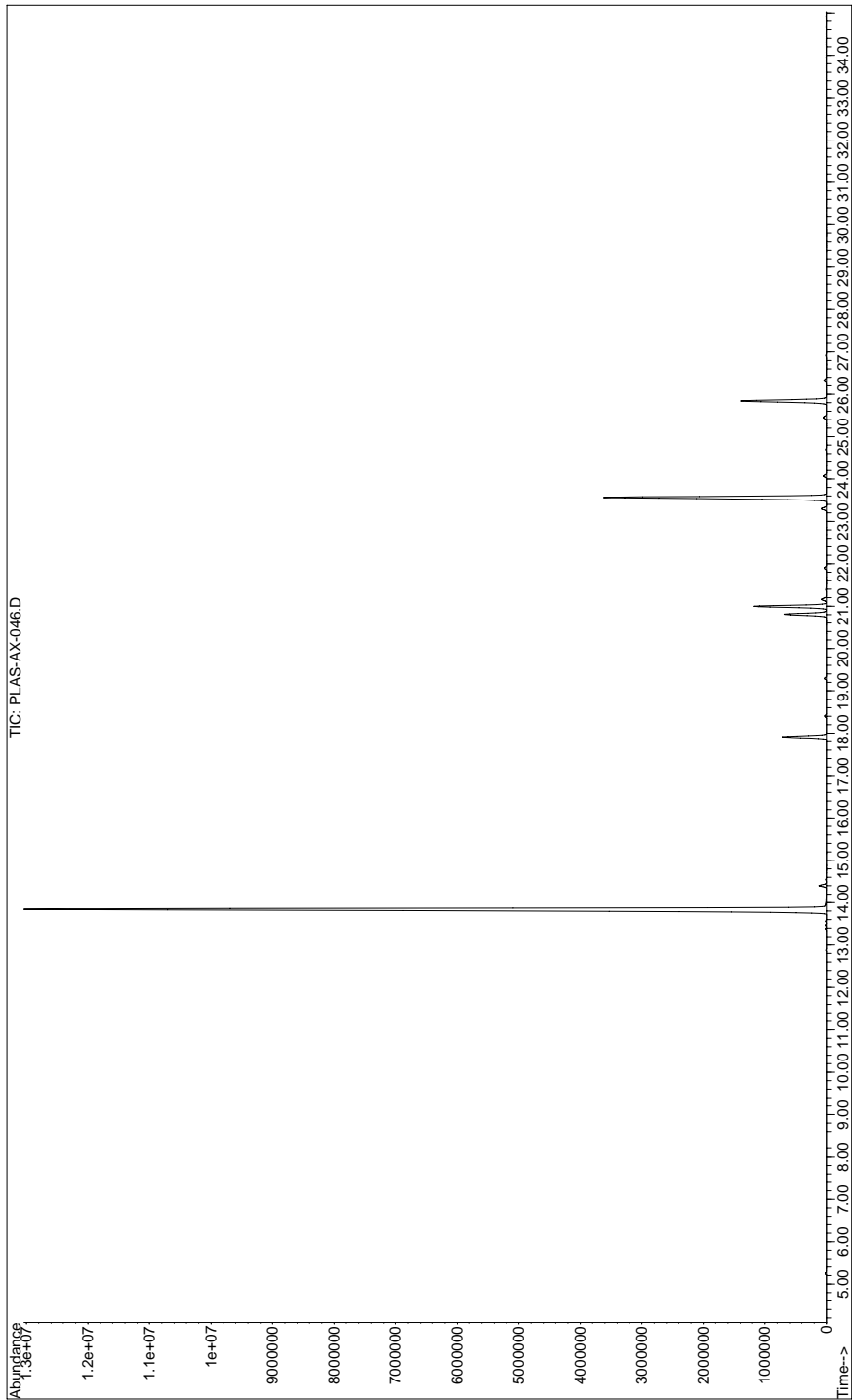
Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Naugard*[®] PS-35 - PLAS-AX-046

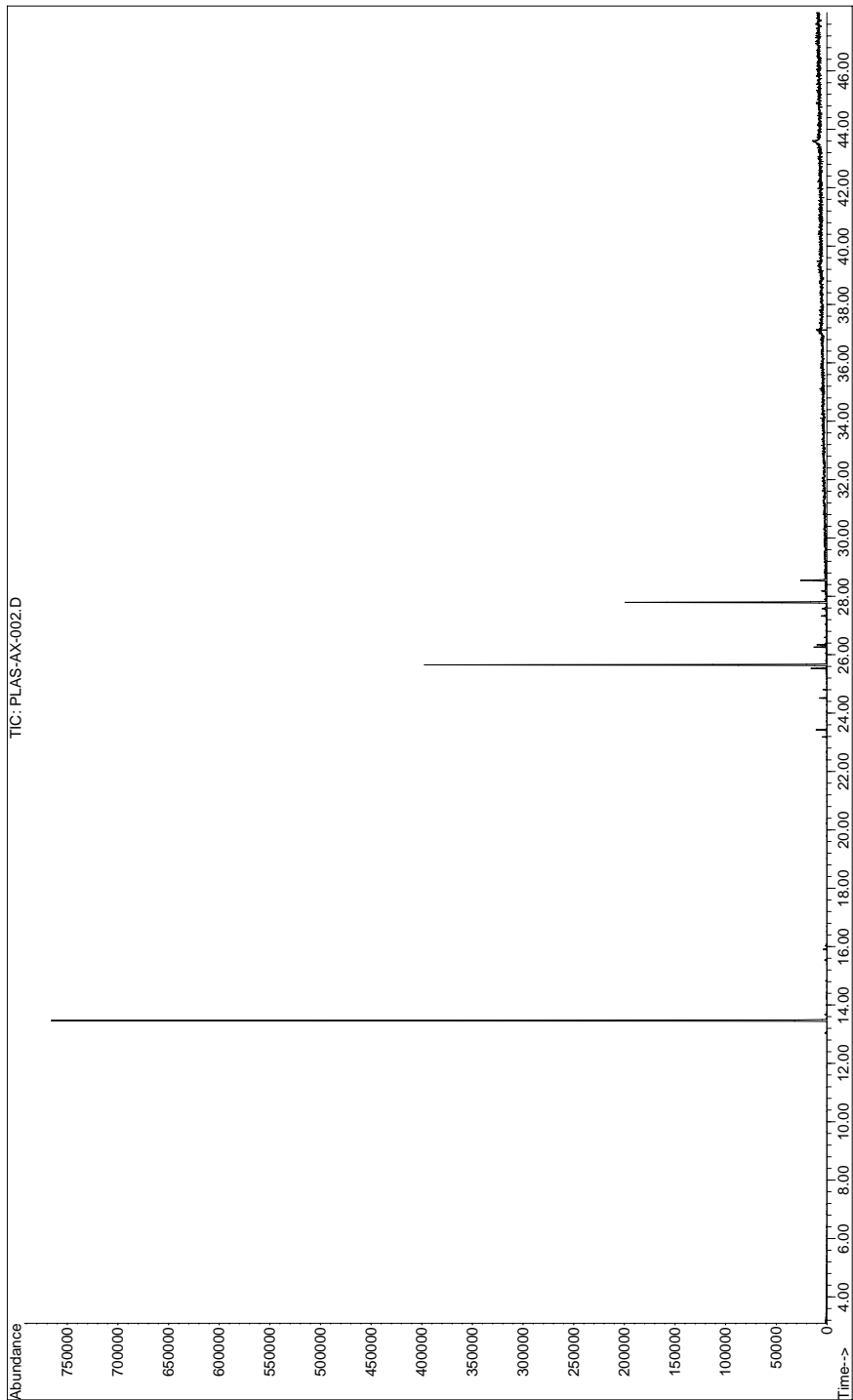
Analytical Conditions Summary 50 °C (0 min) to 350 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Naugard® Q Extra - PLAS-AX-002

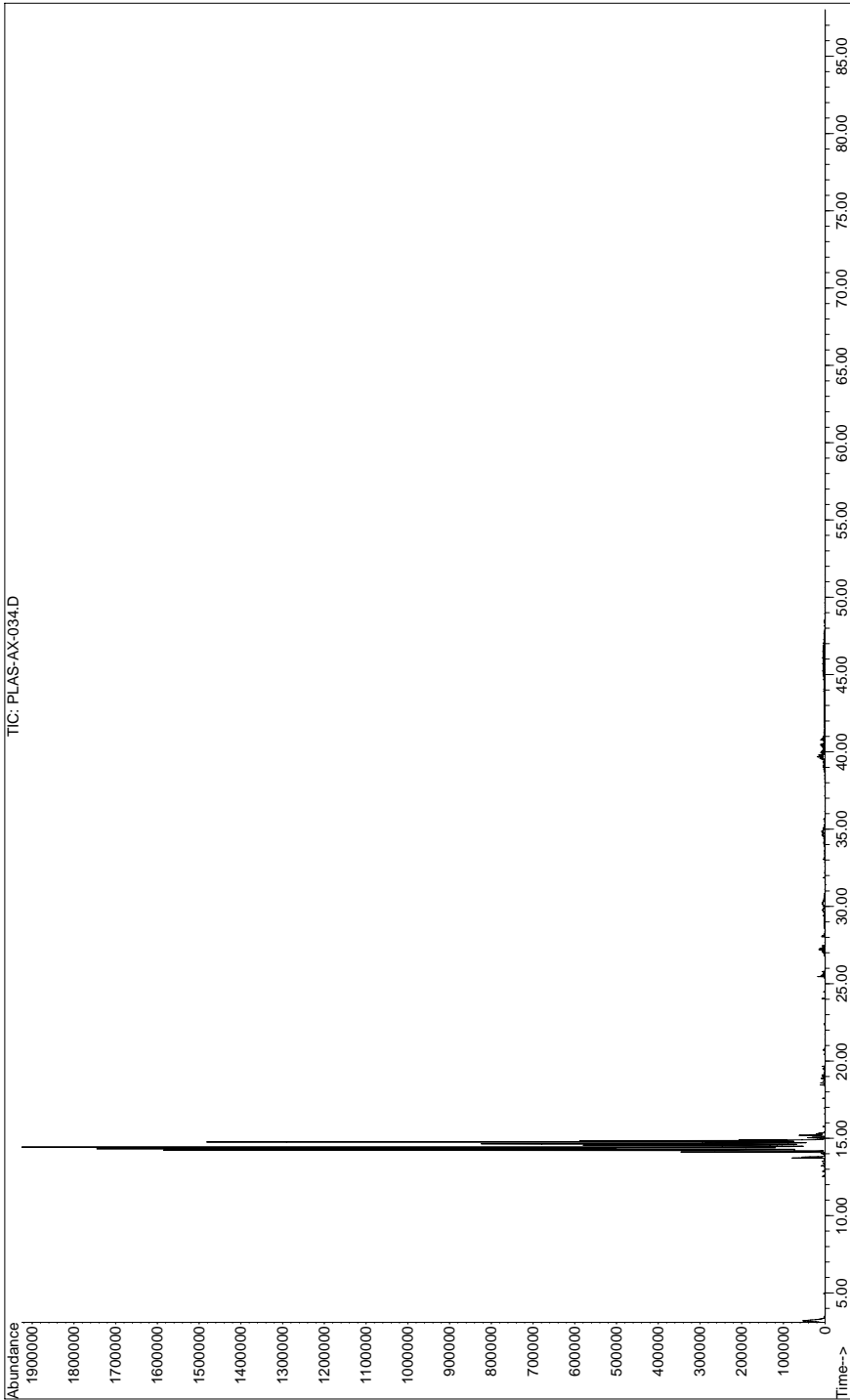
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® RM-51 - PLAS-AX-034

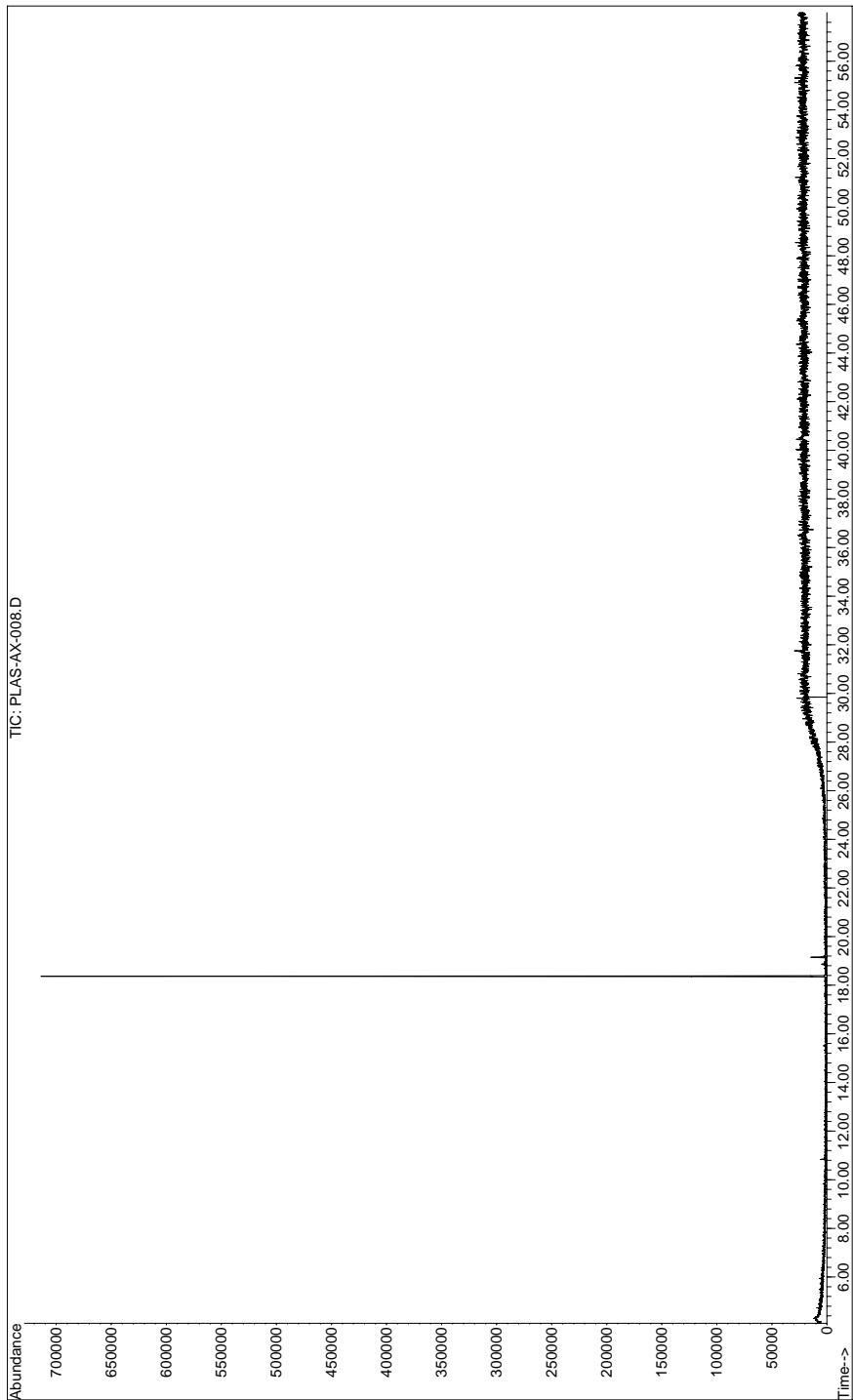
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Naugard® XL-1 - PLAS-AX-008

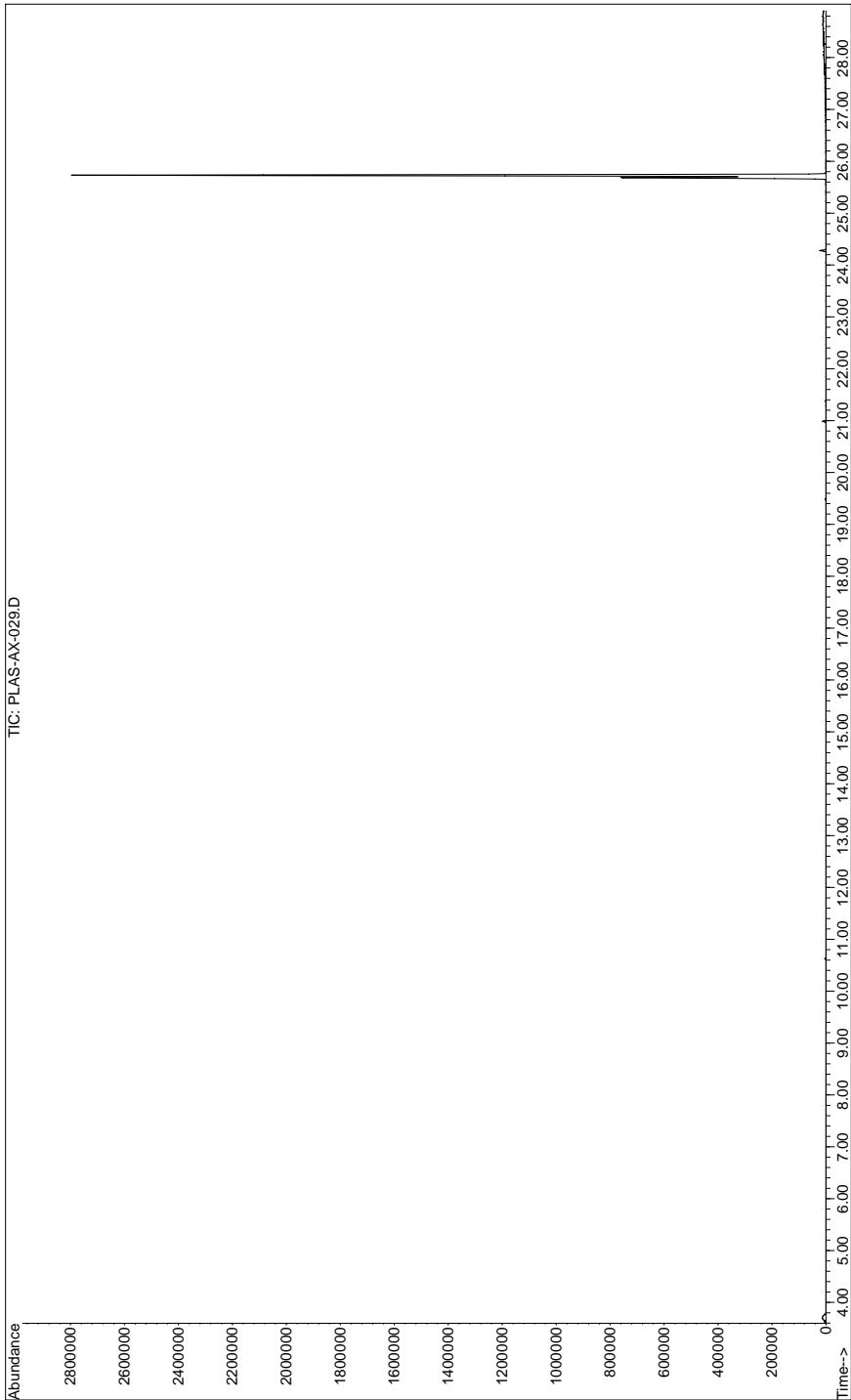
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Santicizer*[®] 278 - PLAS-AX-029

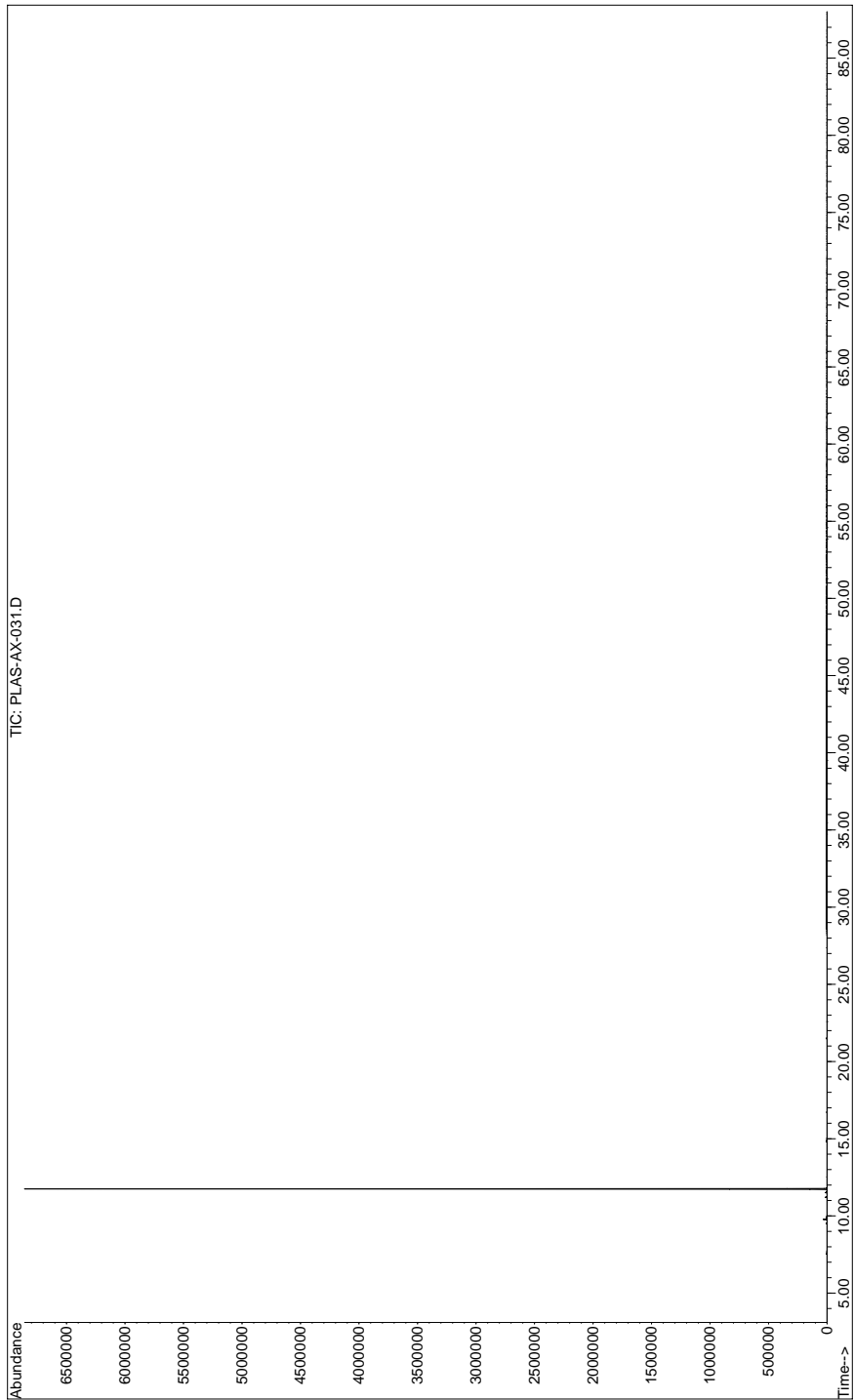
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Ultranox*[®] 626 - PLAS-AX-031

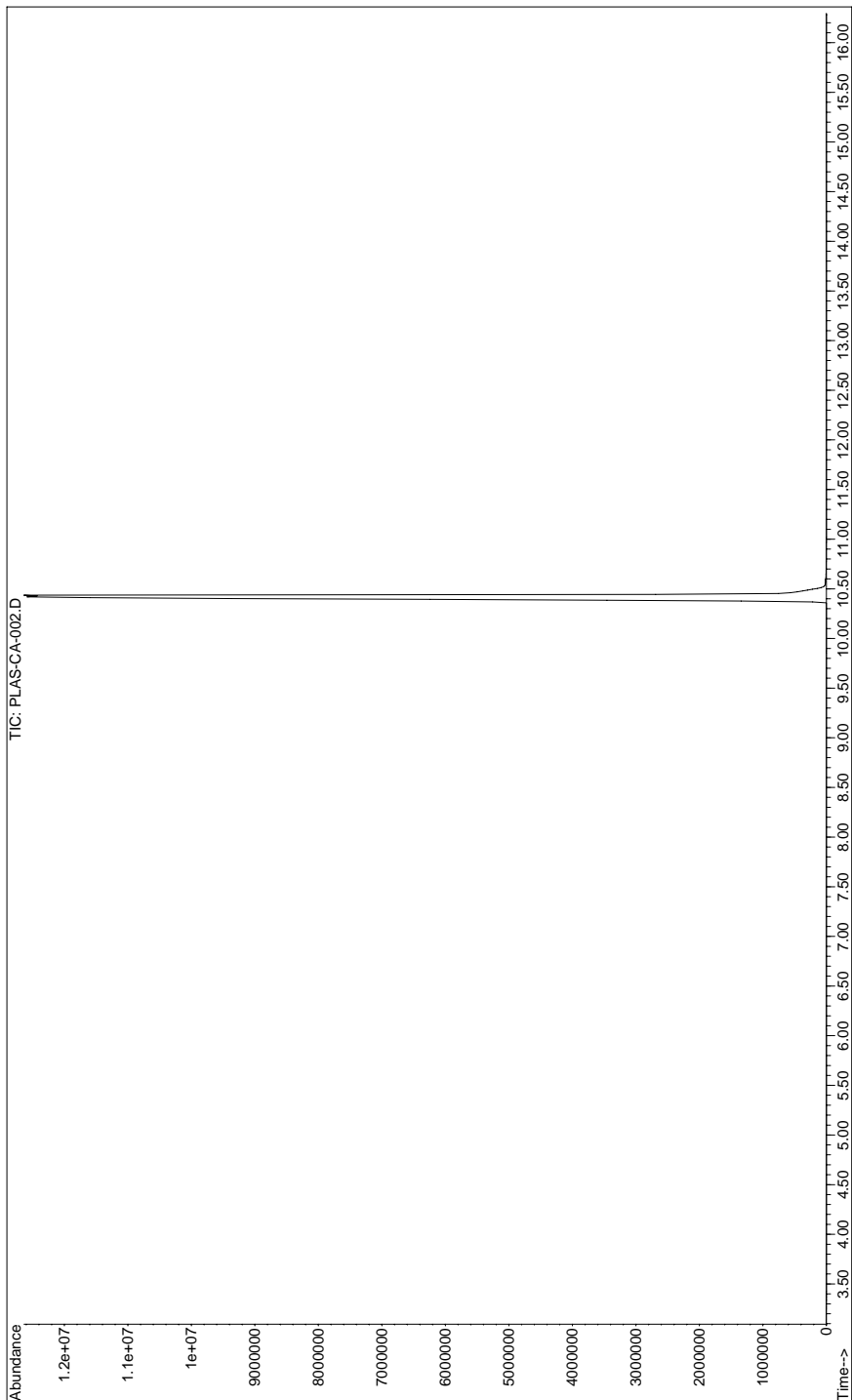
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Silquest® A-1100* - PLAS-CA-002

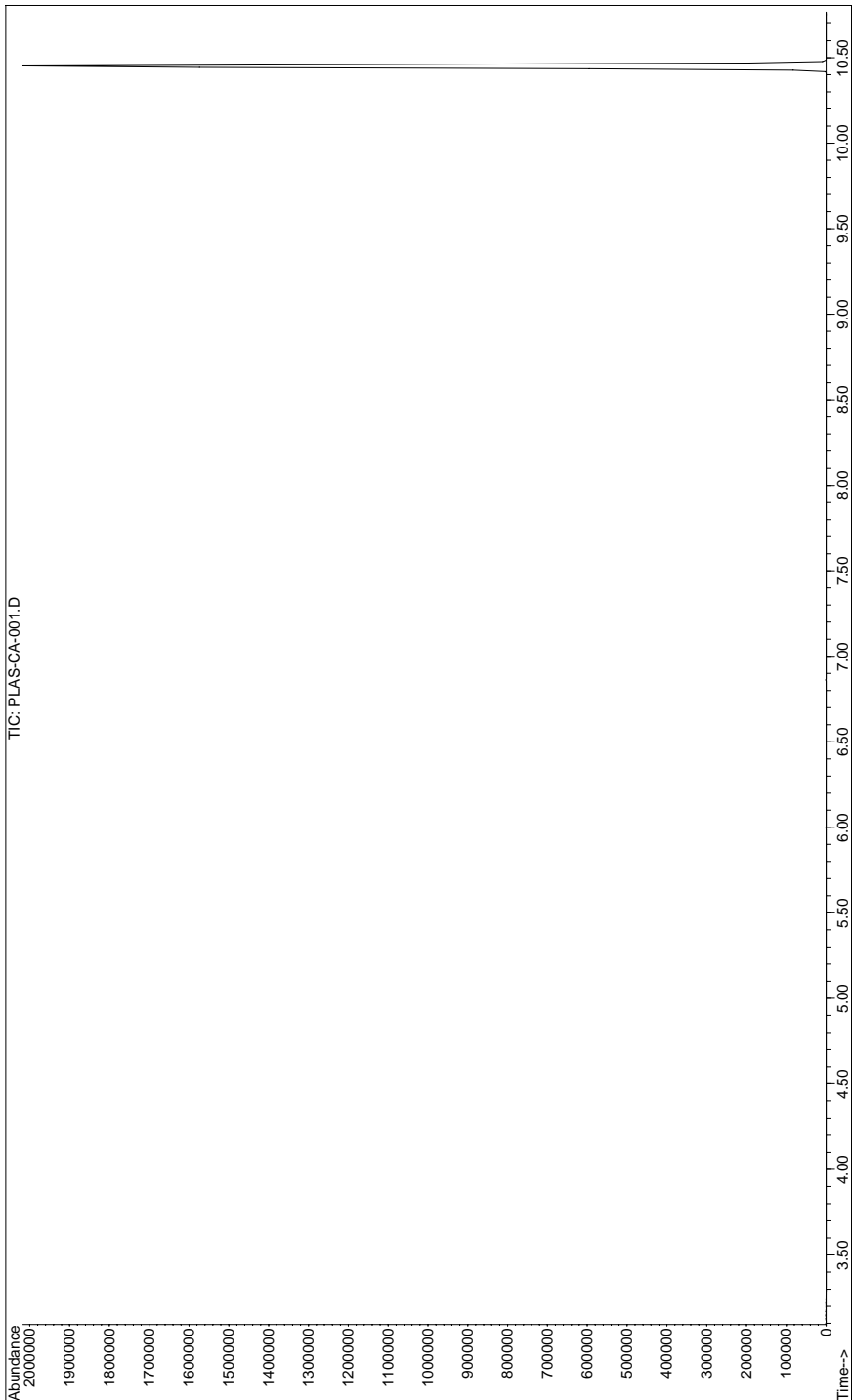
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Silquest® A-1289 - PLAS-CA-001*

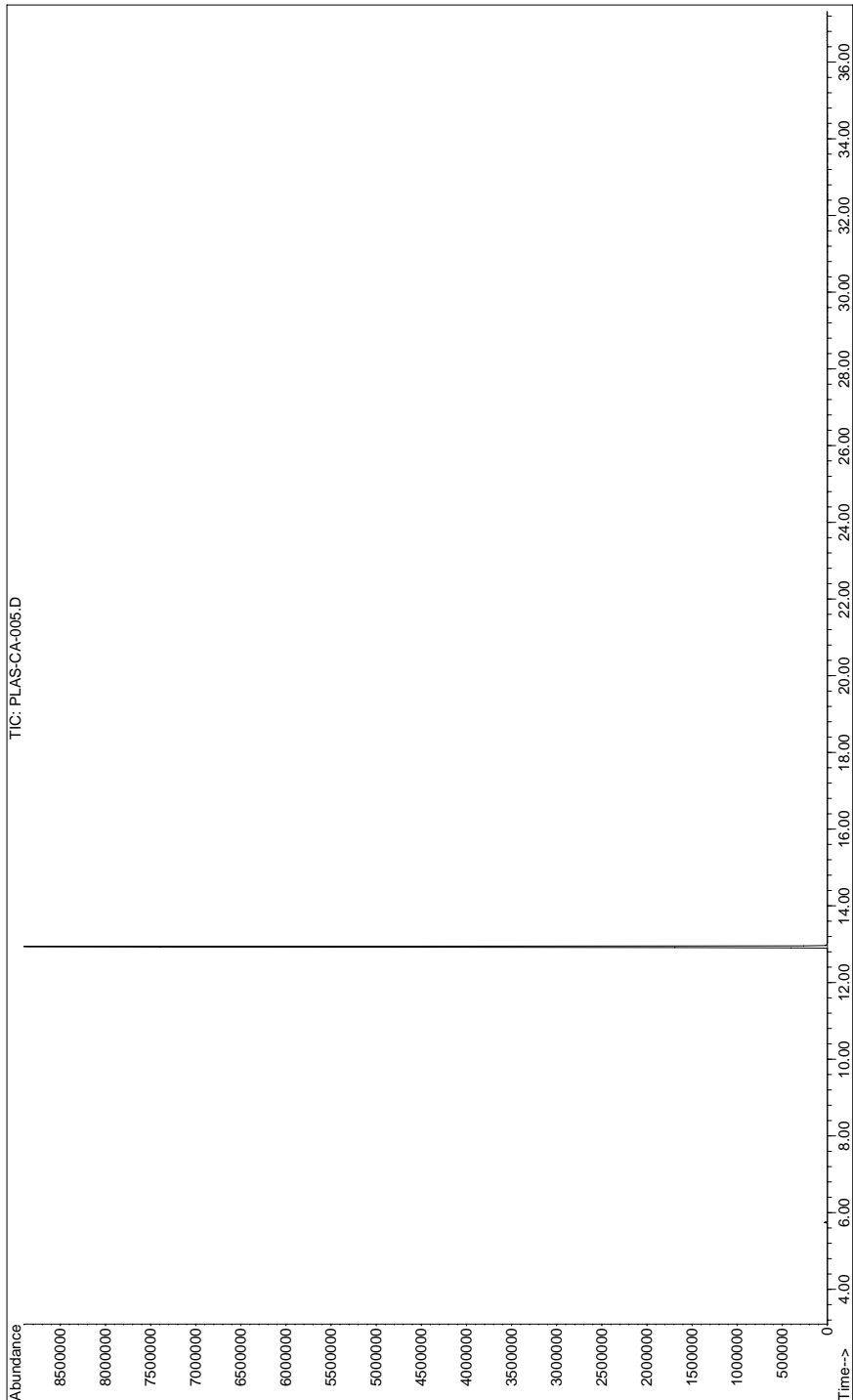
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Silquest® A-137 - PLAS-CA-005*

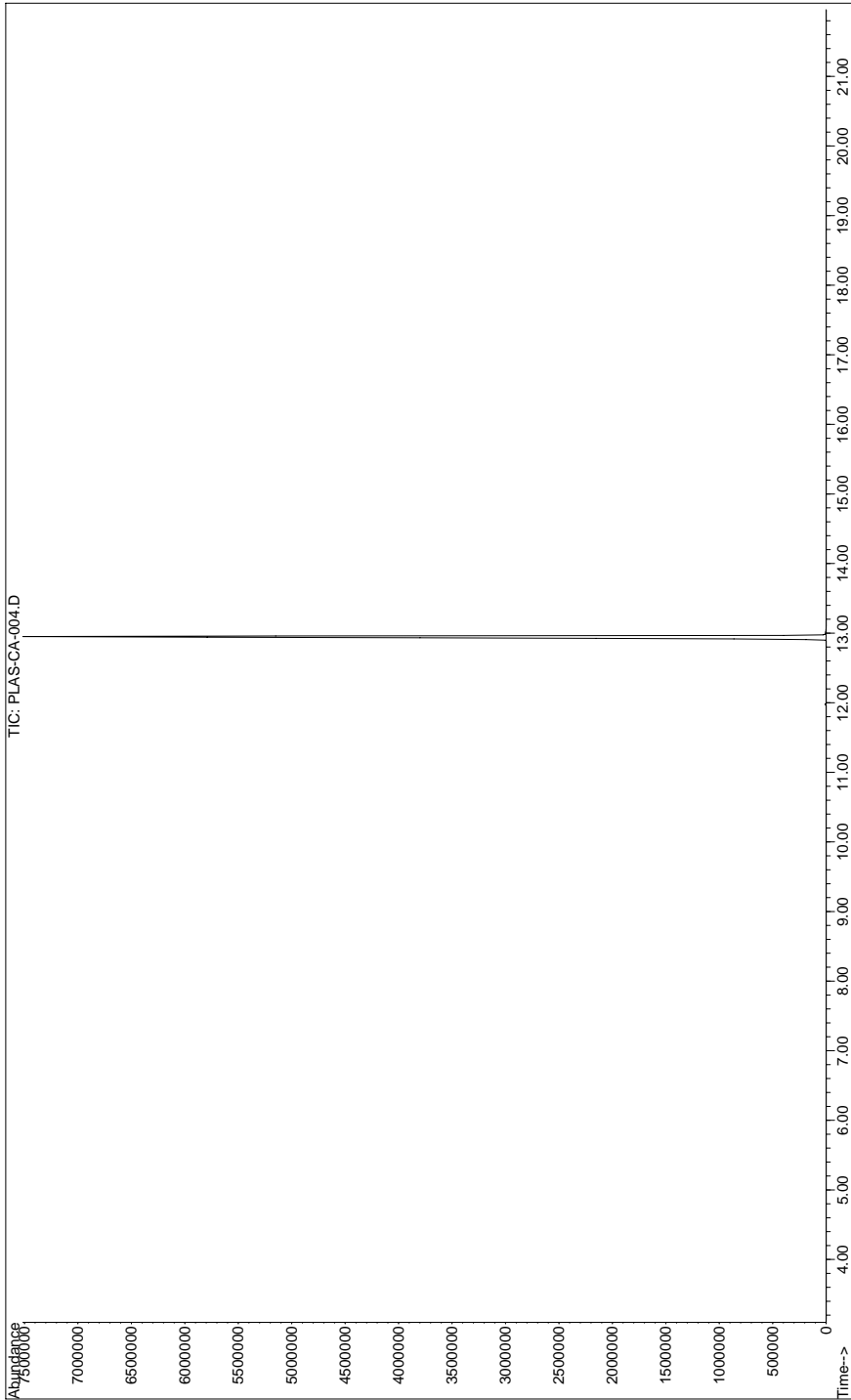
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Silquest® A-187 - PLAS-CA-004*

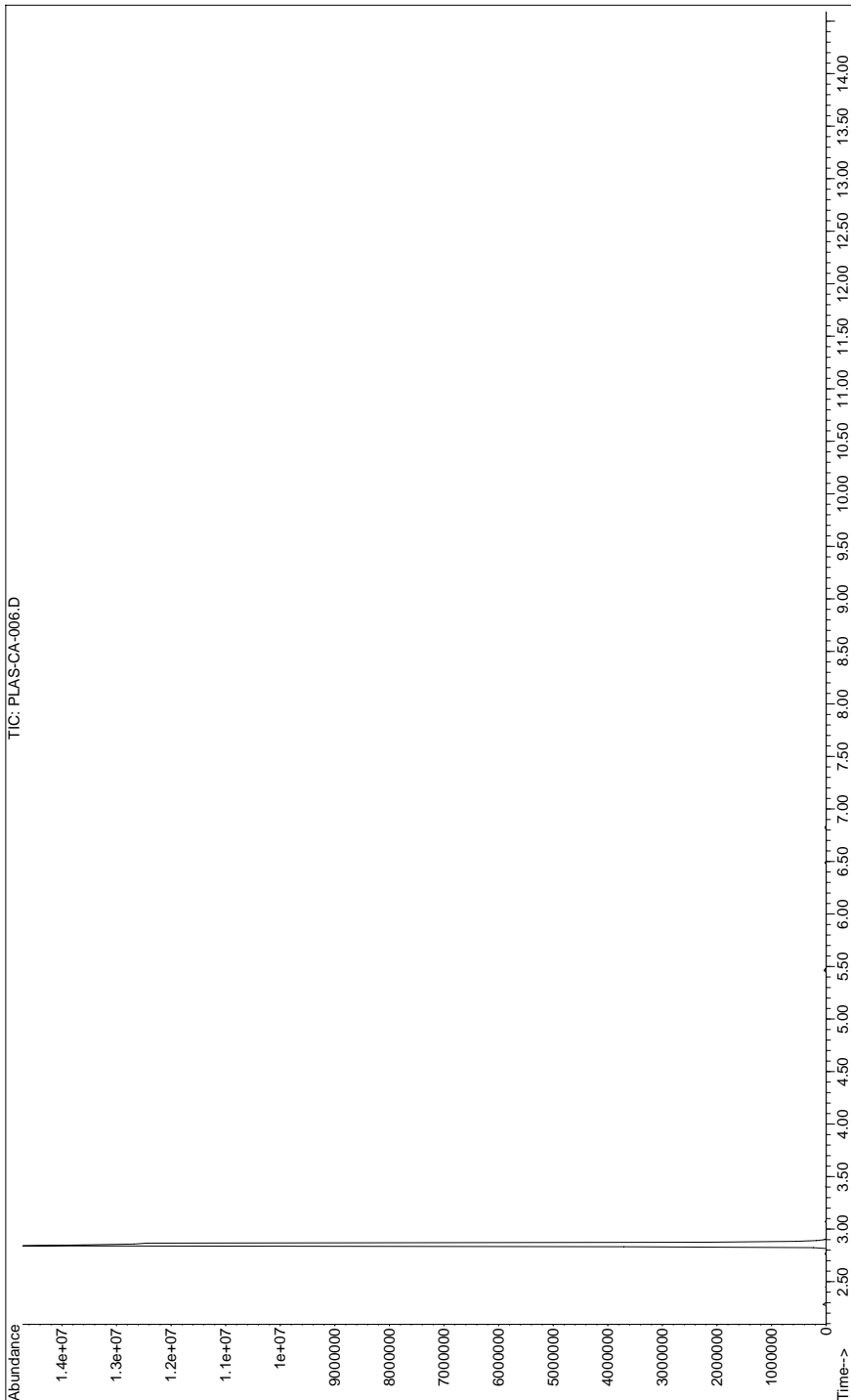
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Silquest® A-2171 - PLAS-CA-006*

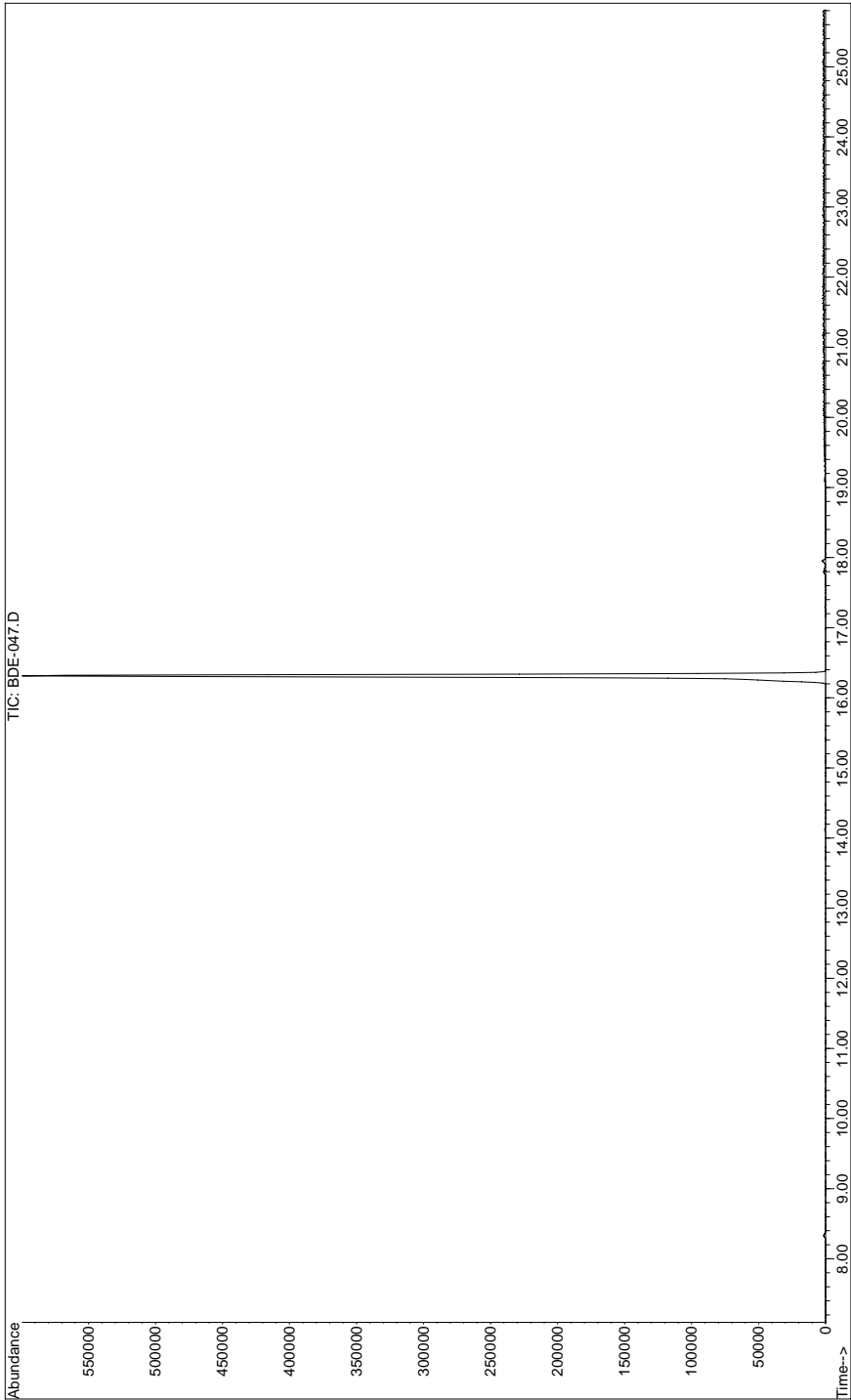
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for 2,2',4,4'-Tetrabromodiphenyl ether - BDE-047

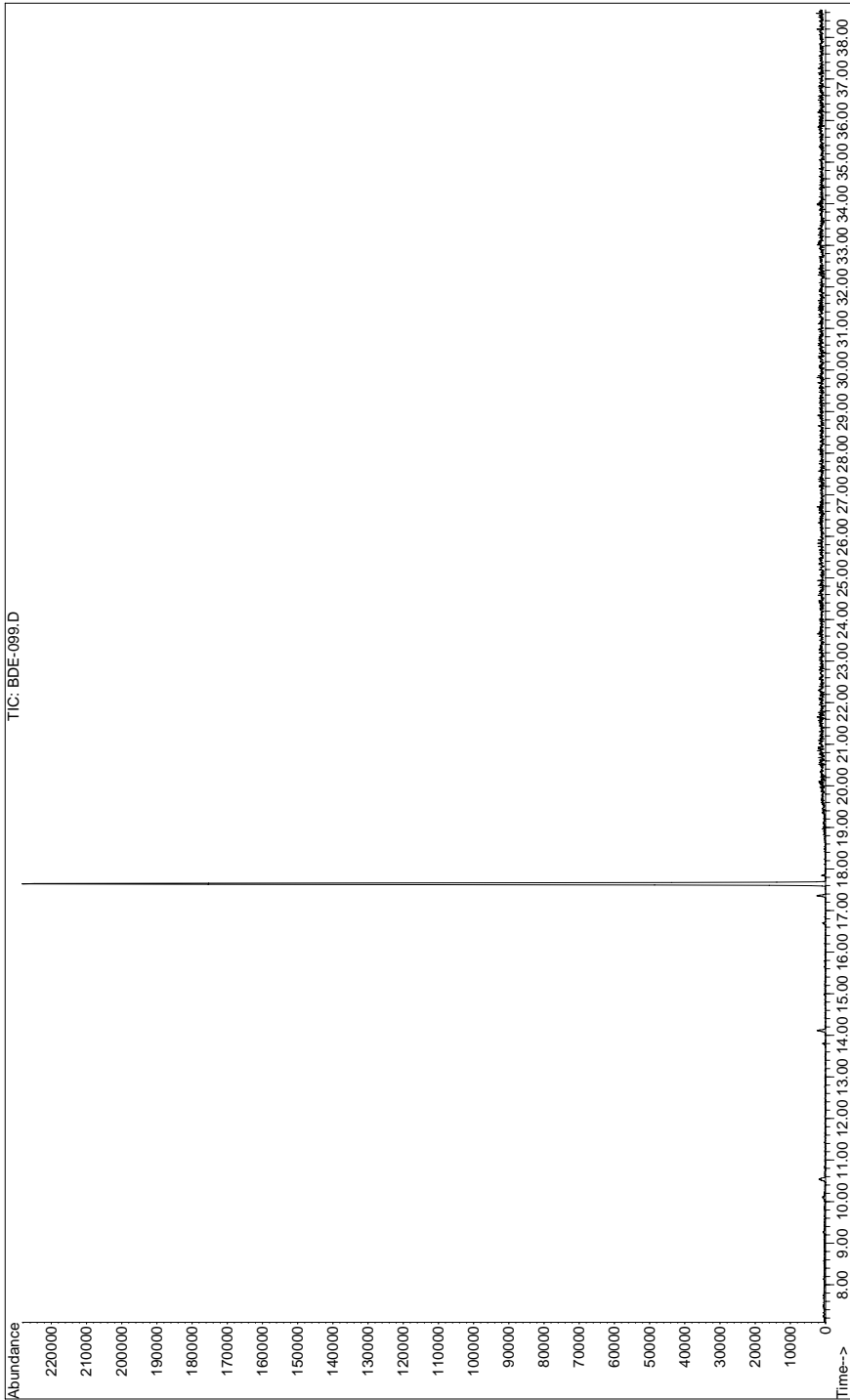
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for 2,2',4,4',5-Pentabromodiphenyl ether - BDE-099

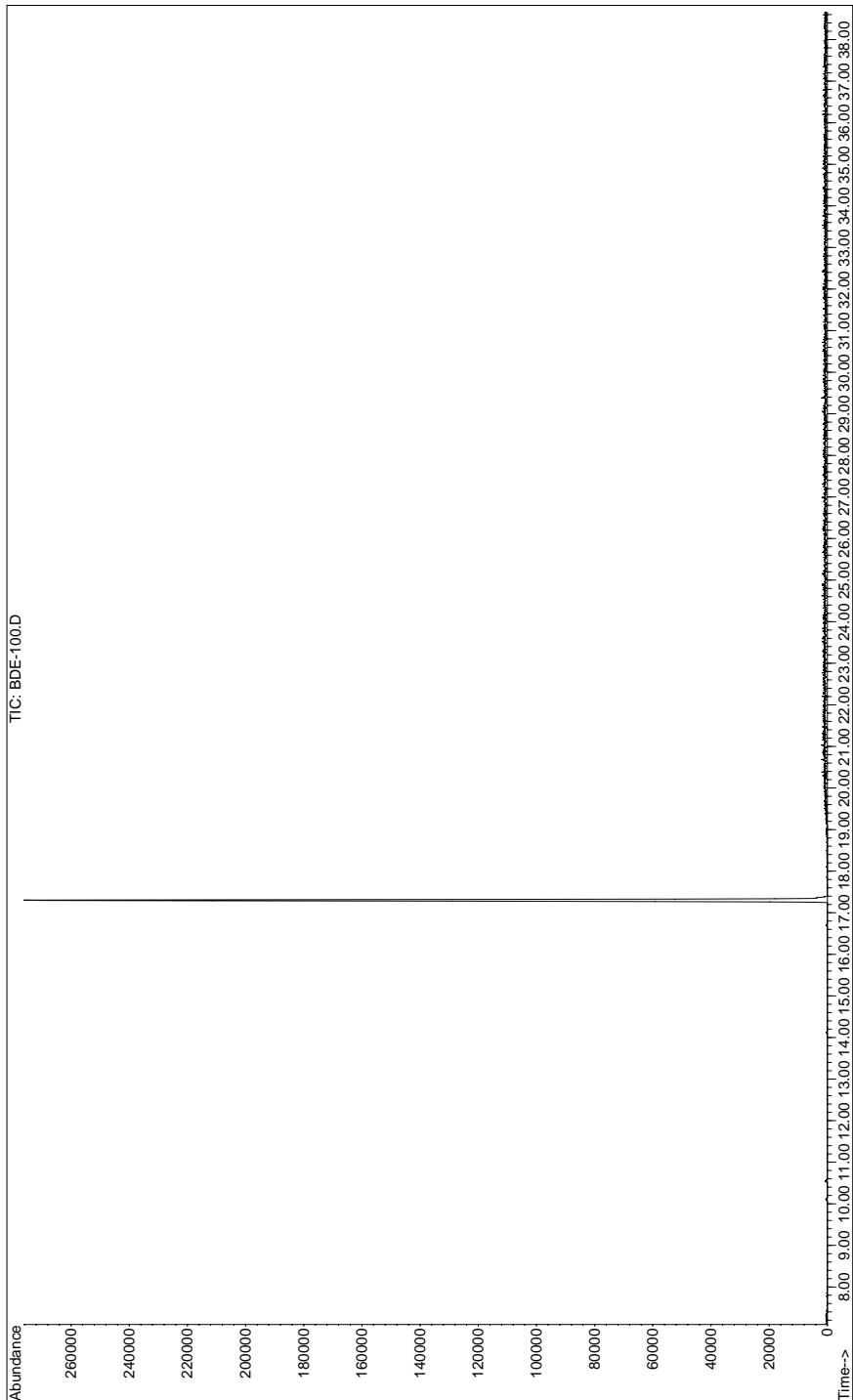
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for 2,2',4,4',6-Pentabromodiphenyl ether - BDE-100

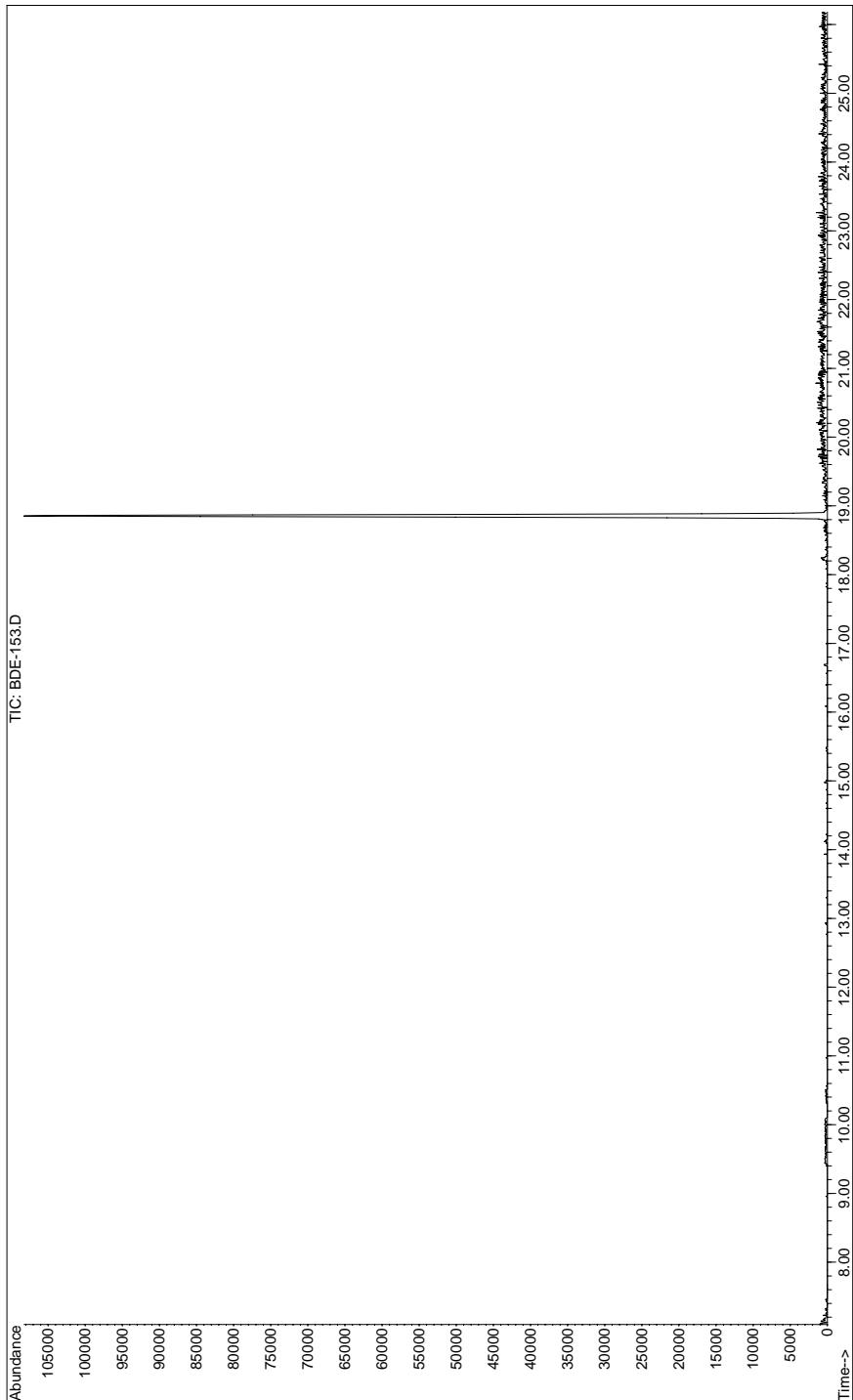
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for 2,2',4,4',5,5'-Hexabromodiphenyl ether - BDE-153

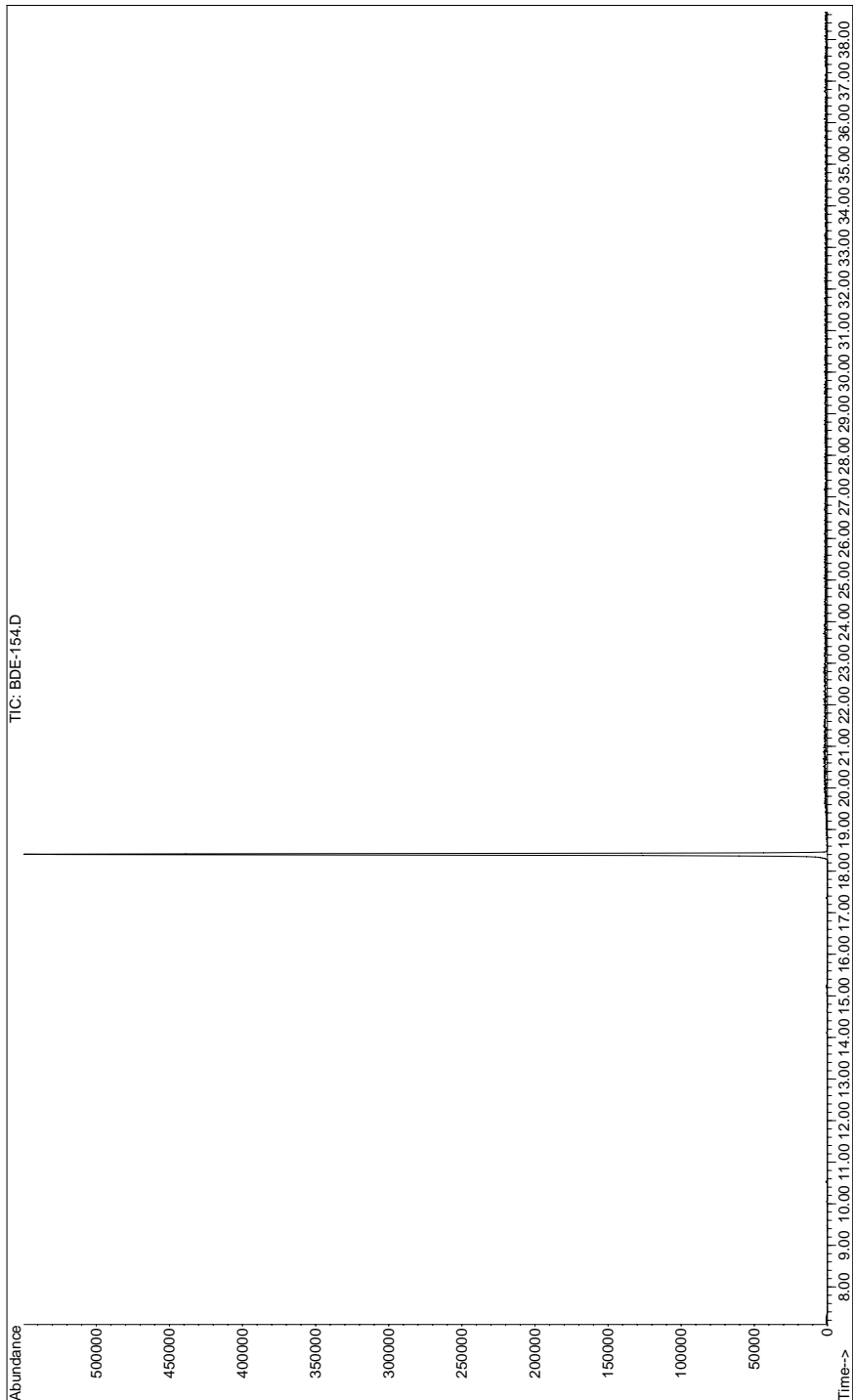
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for 2,2',4,4',5,6'-Hexabromodiphenyl ether - BDE-154

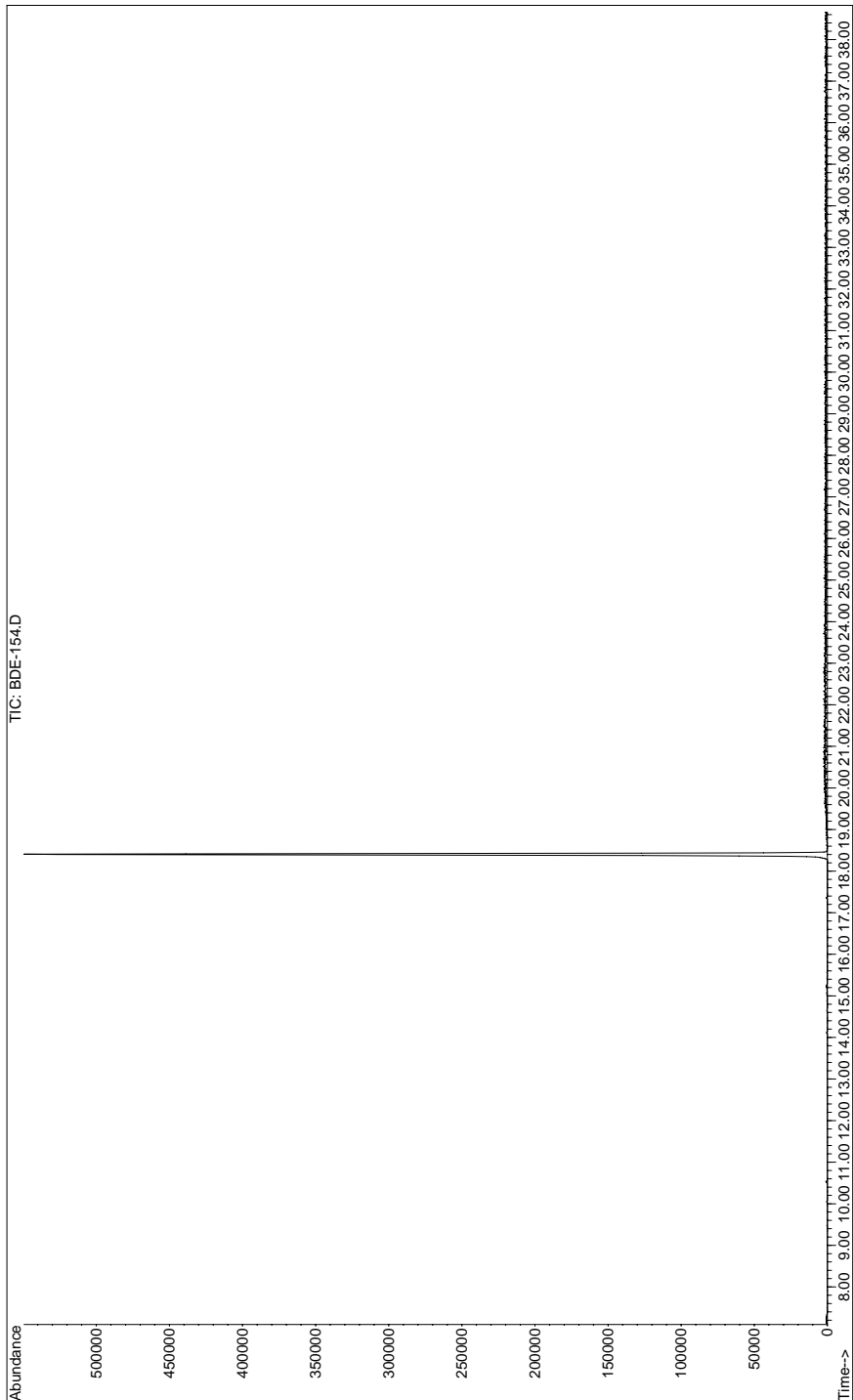
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for 2,2',3,4,4',5',6-Heptabromodiphenyl ether - BDE-183

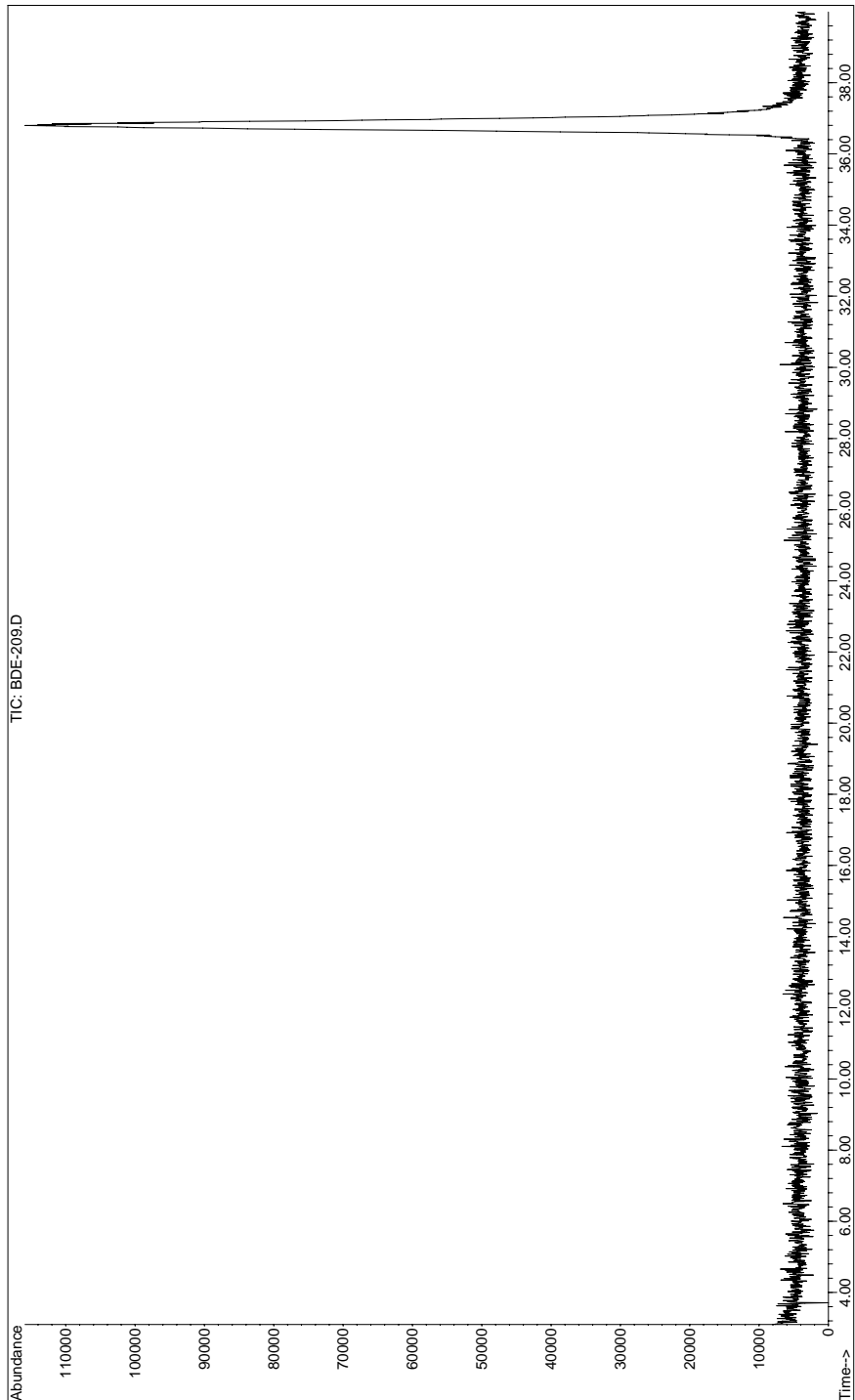
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Decabromodiphenyl ether - BDE-209

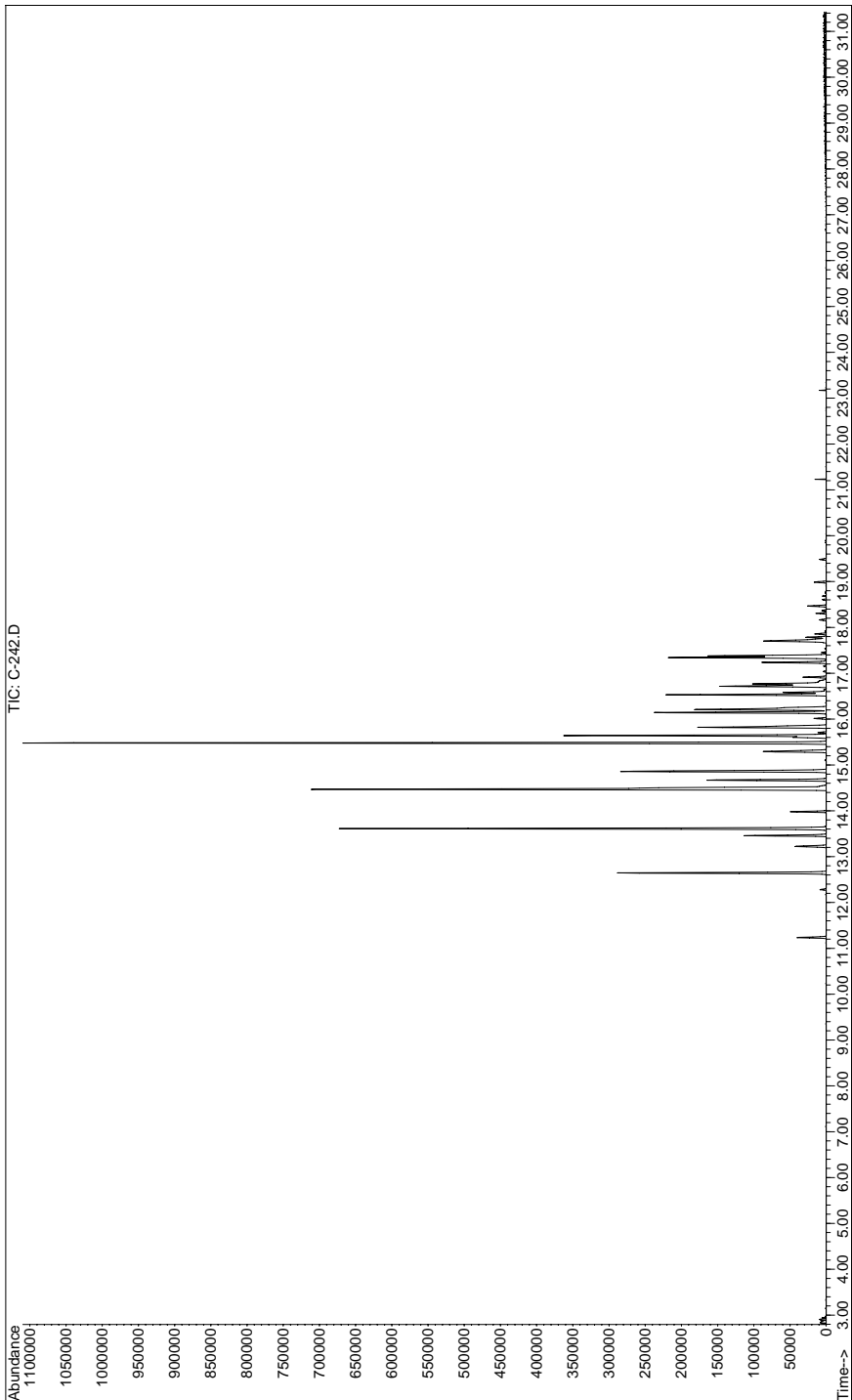
Analytical Conditions Summary 200°C (1min) to 340°C (10min) @ 40°C/min Det=MSD



Analytical Information

Chromatogram for Aroclor 1242 - C-242

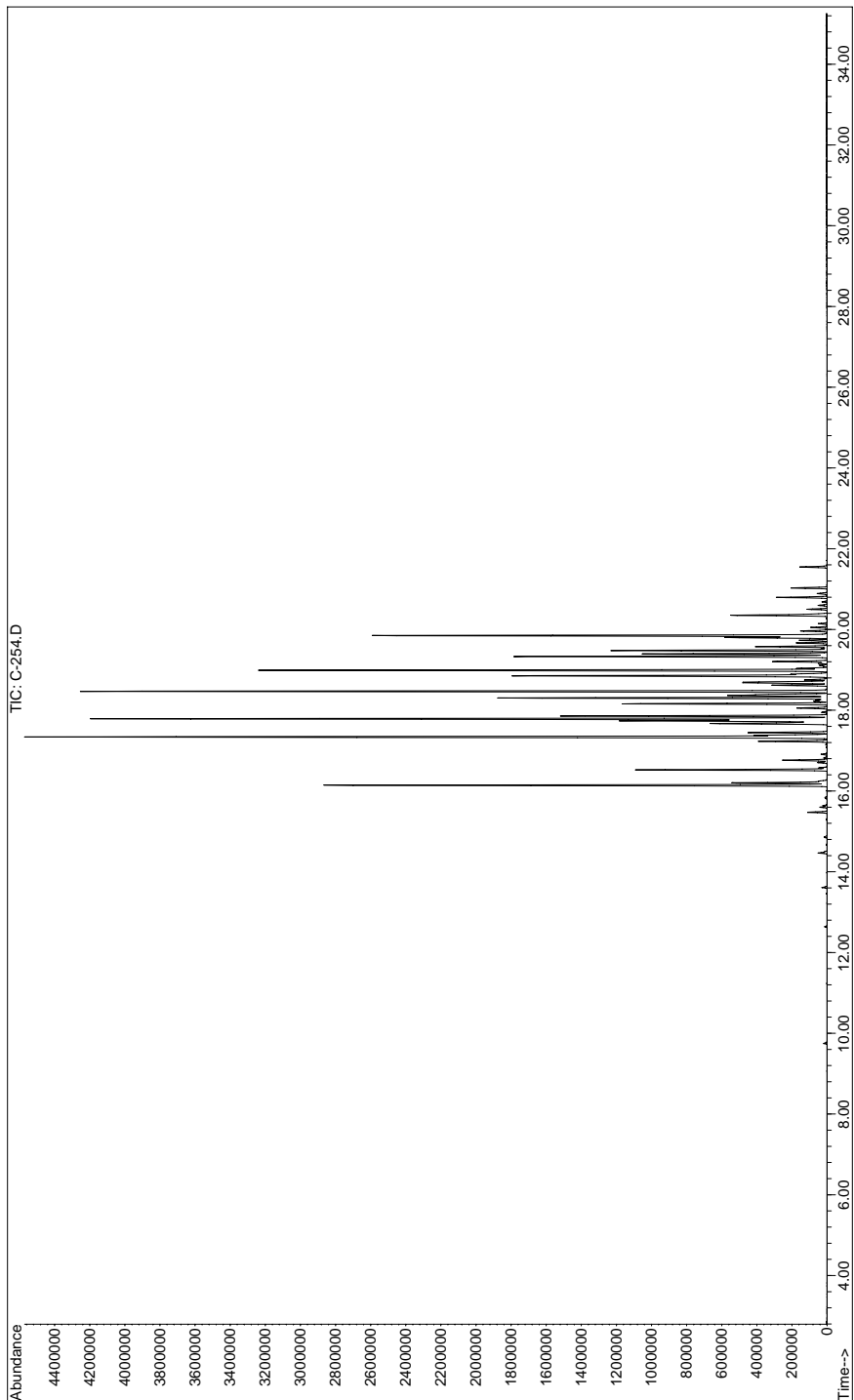
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Aroclor 1254 - C-254

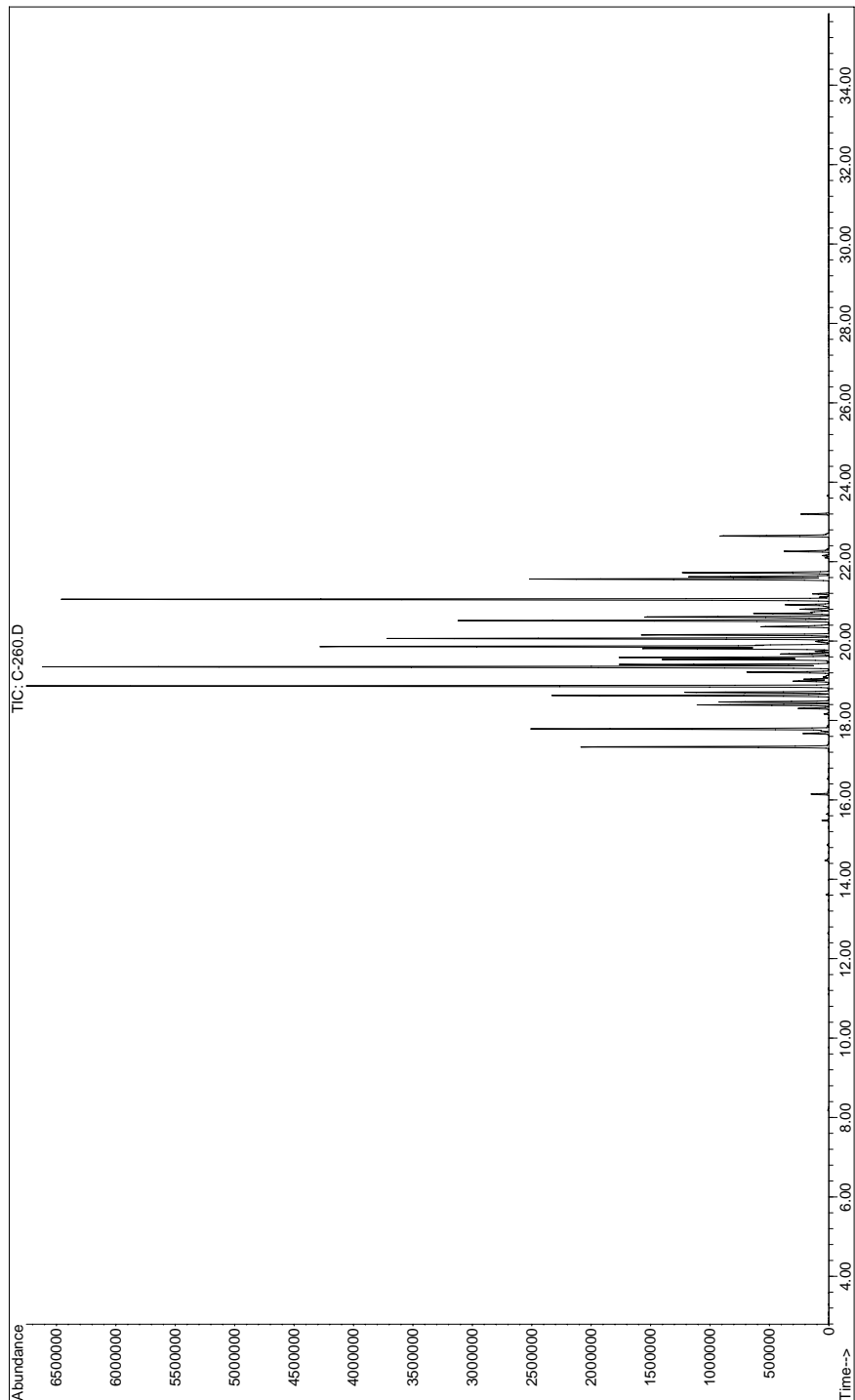
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Aroclor 1260 - C-260

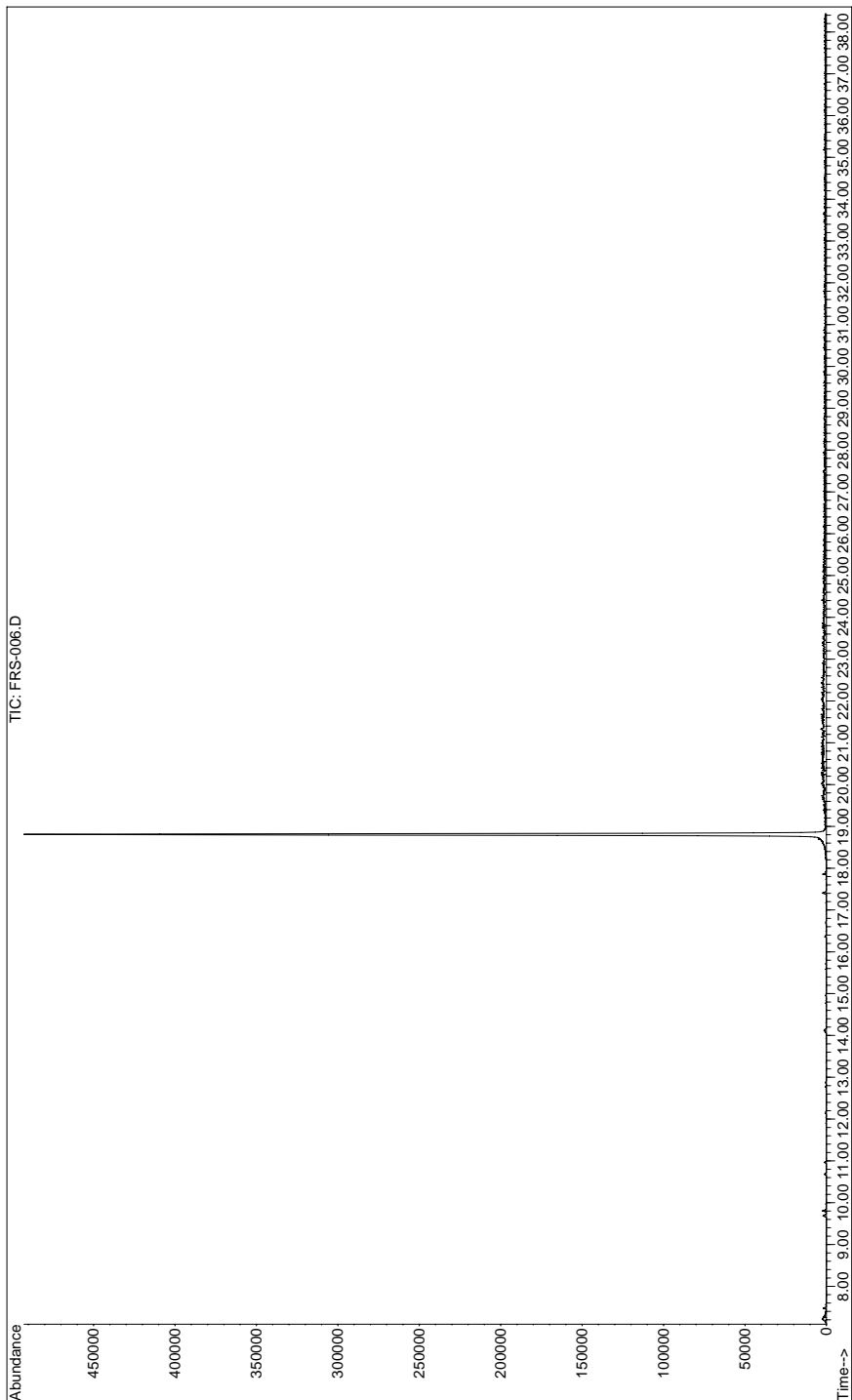
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Firemaster BP4A - FRS-006

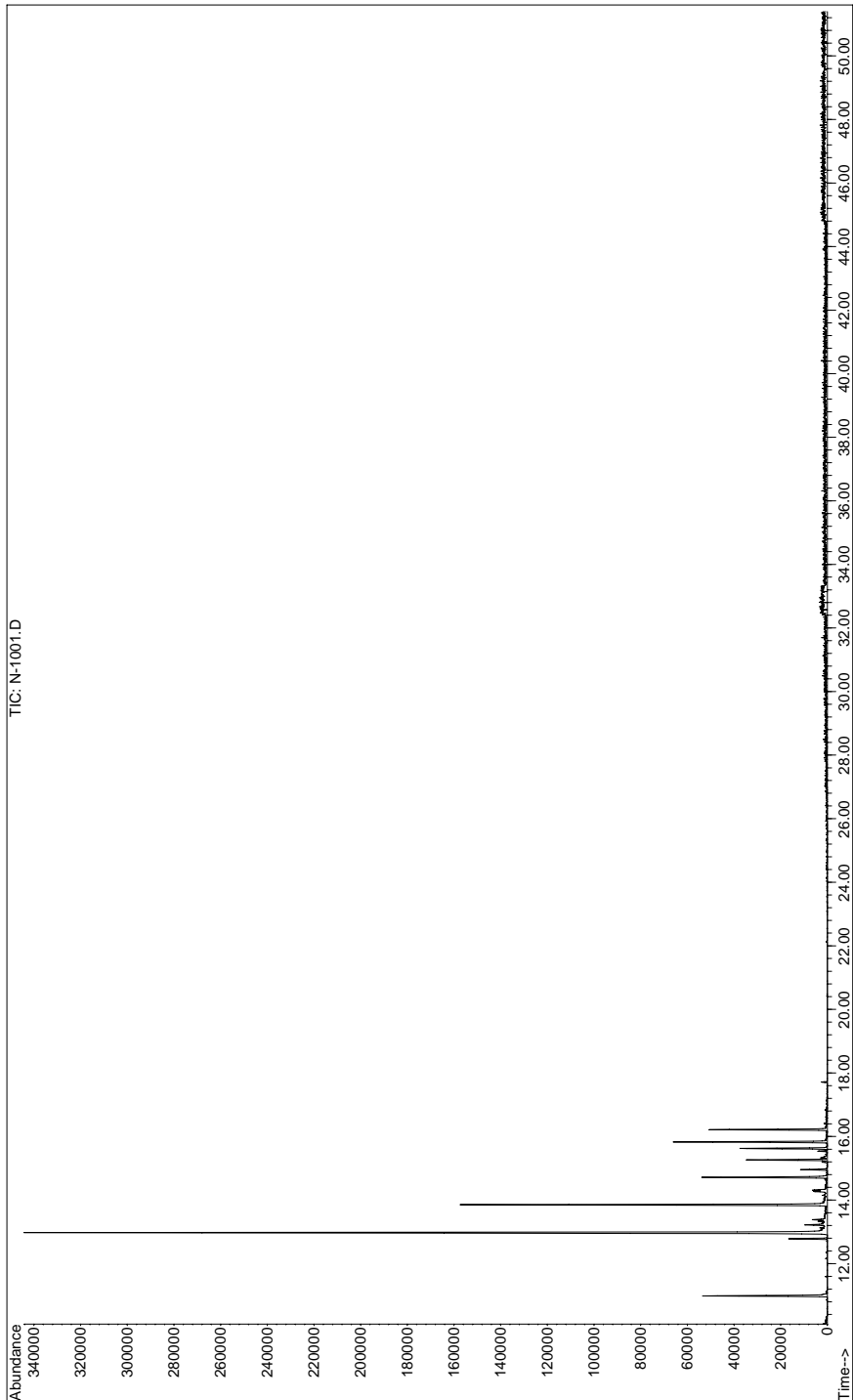
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Halowax 1001 - N-1001*

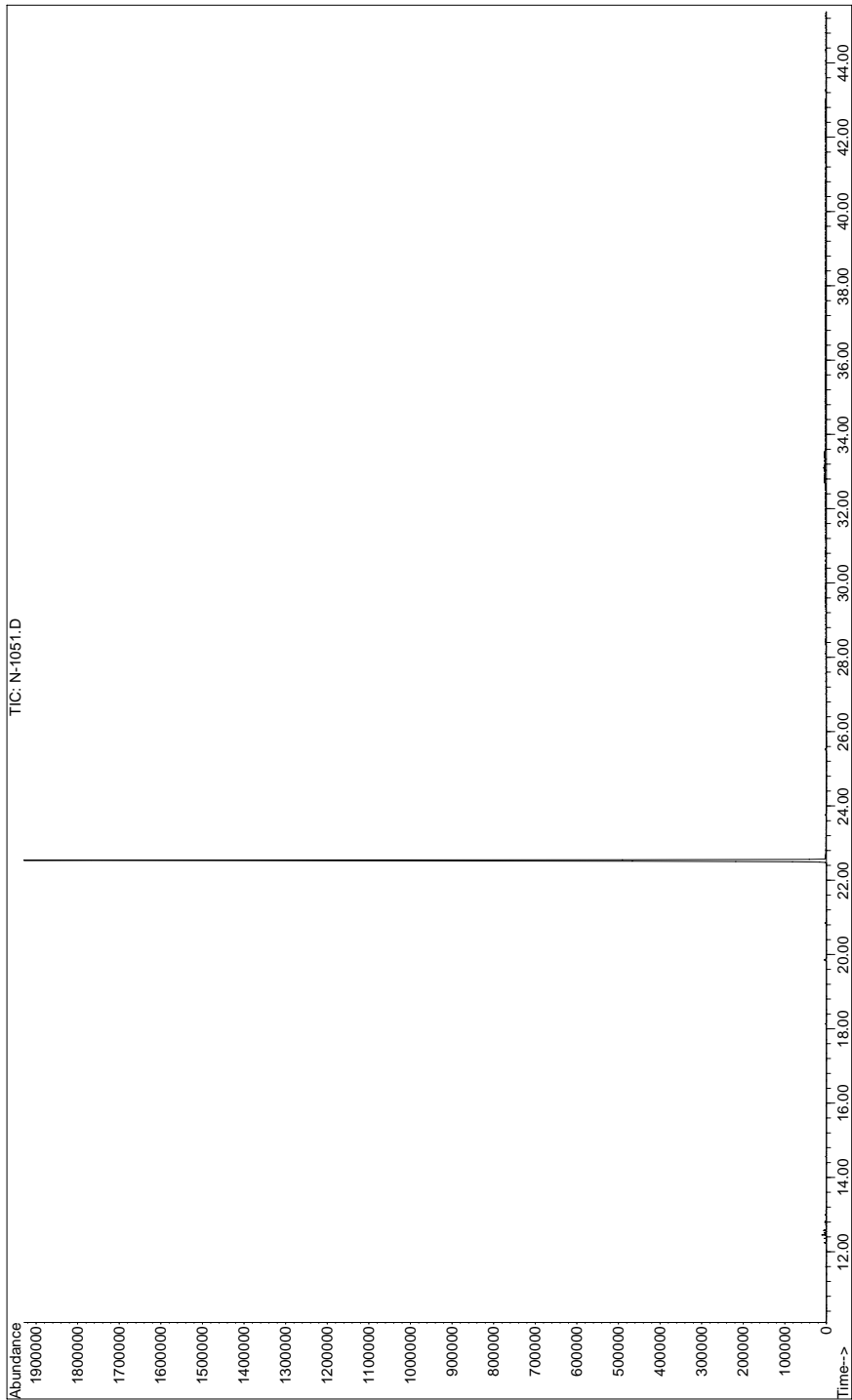
Analytical Conditions Summary 80 °C (0 min) to 340 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Halowax 1051 - N-1051*

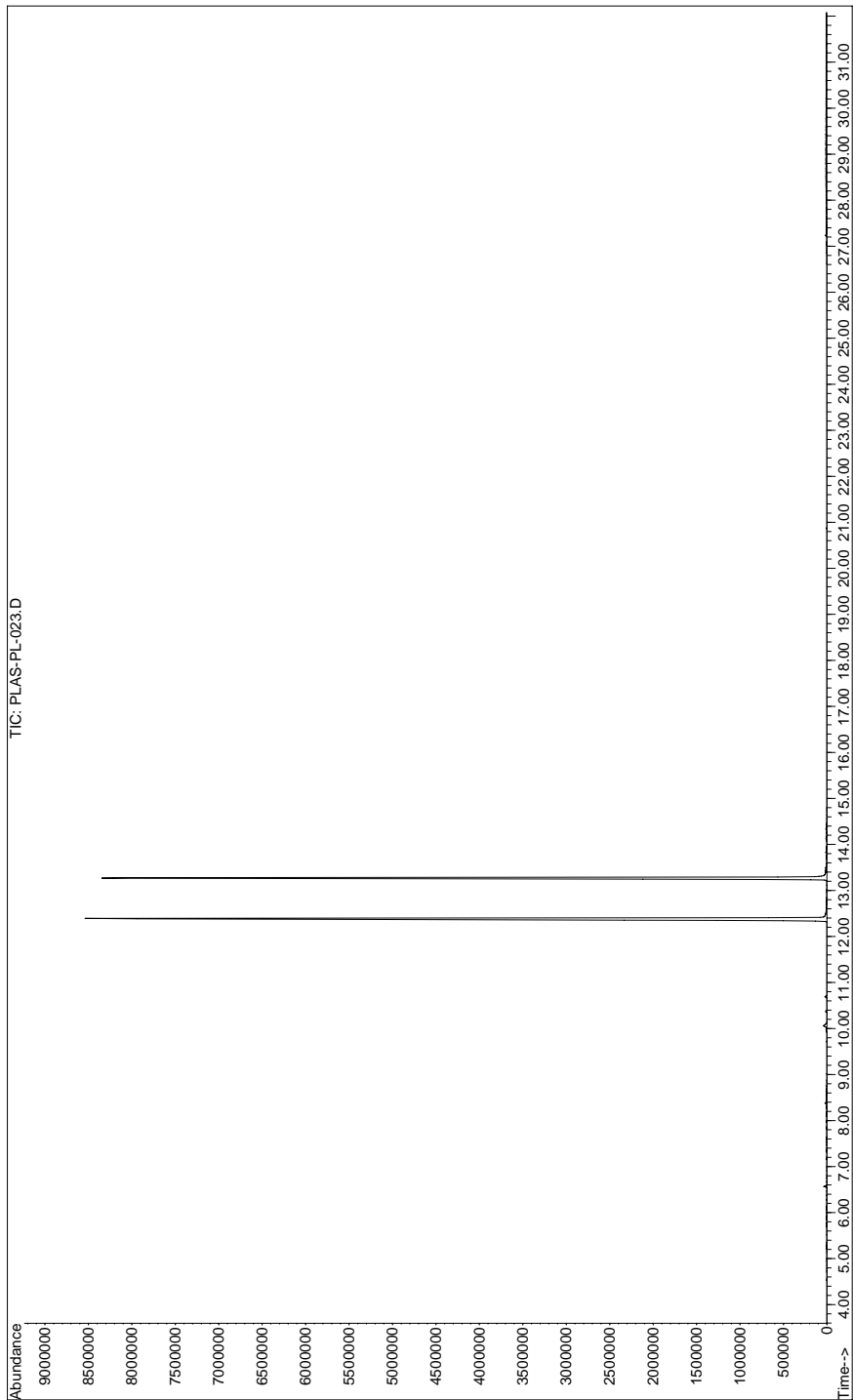
Analytical Conditions Summary 80 °C (0 min) to 340 °C (20 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for 2-Butanone peroxide (in DMP) - PLAS-PL-023

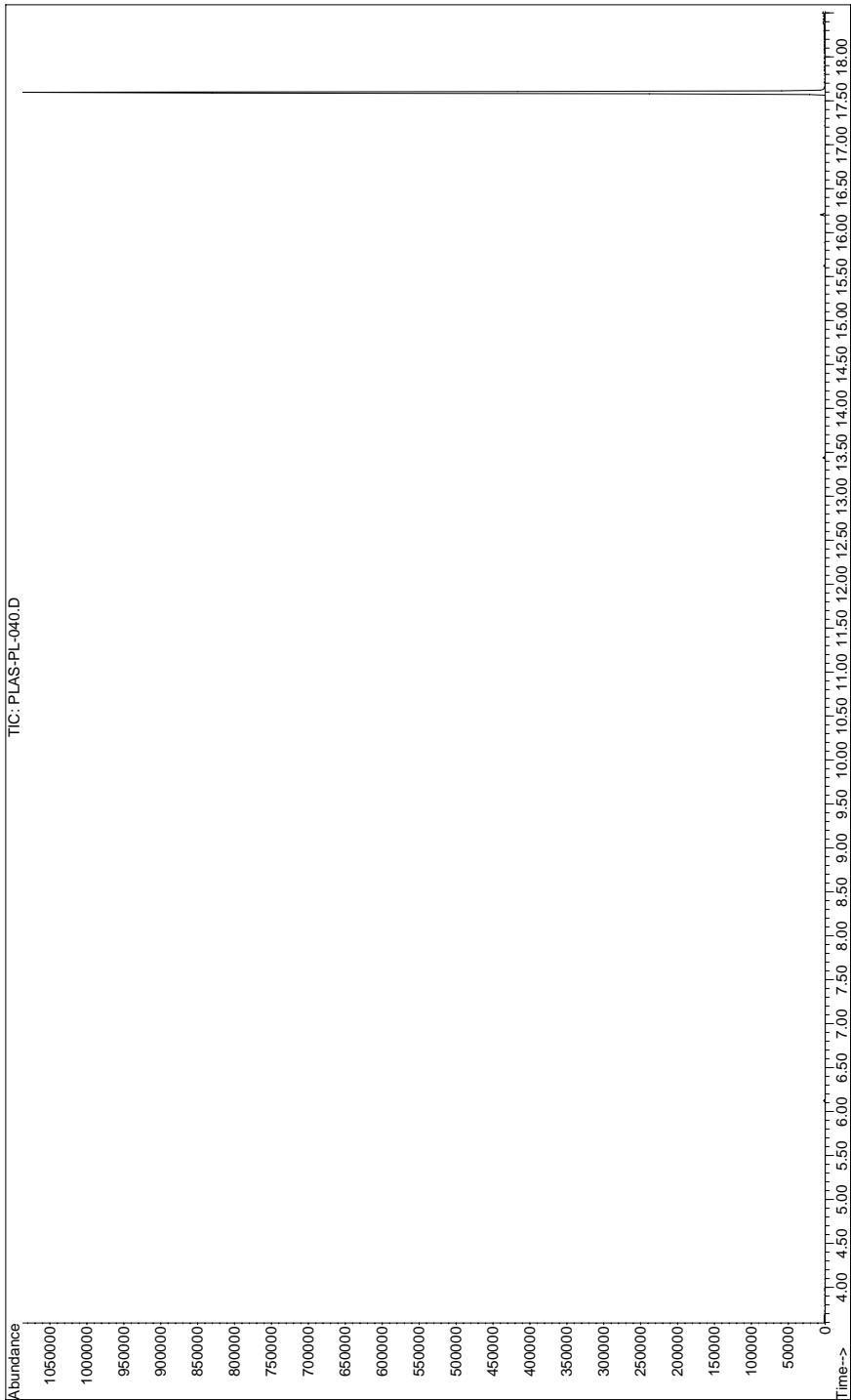
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Adimoll DO - PLAS-PL-040

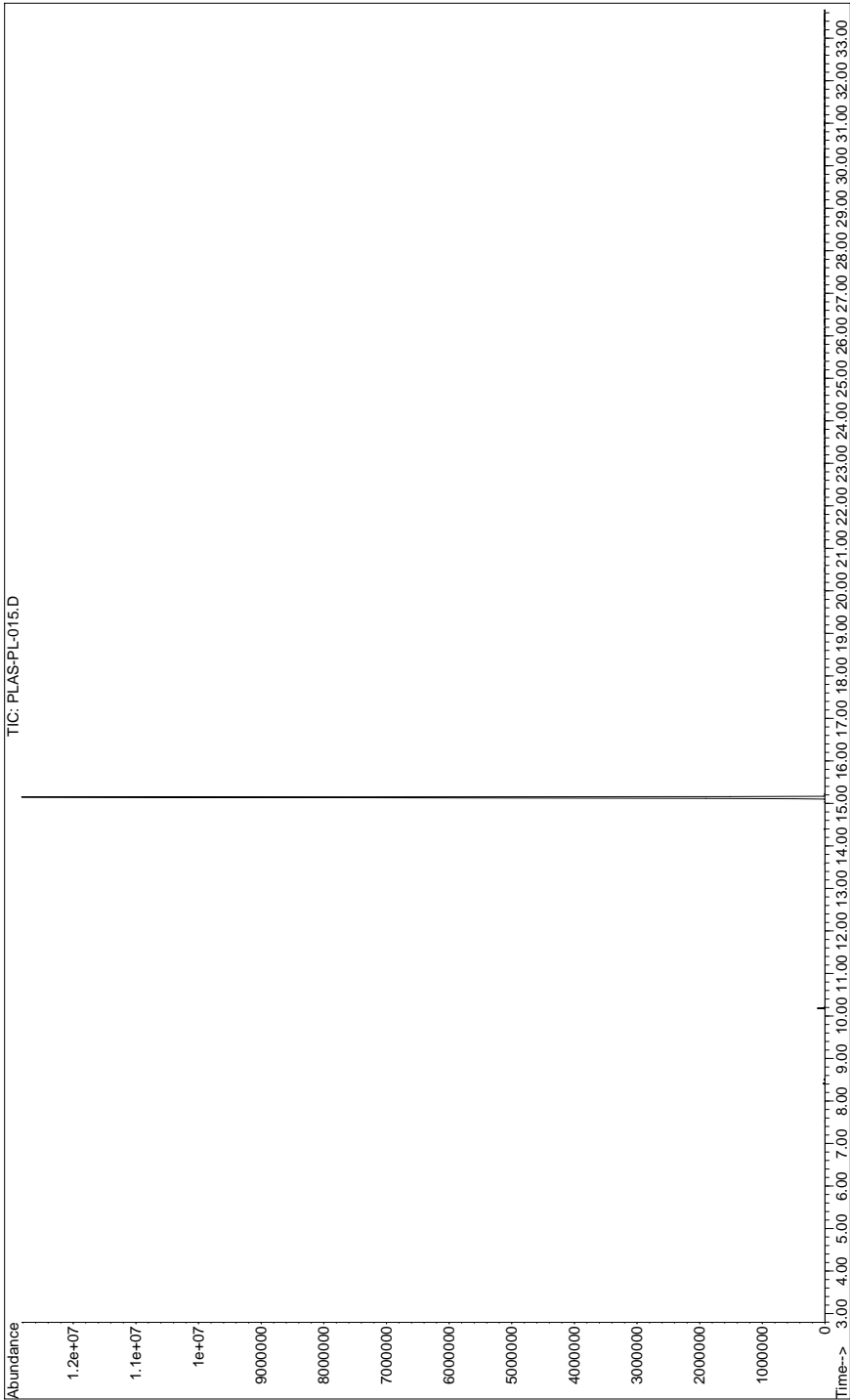
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Benzoflex® 2-45 - PLAS-PL-015

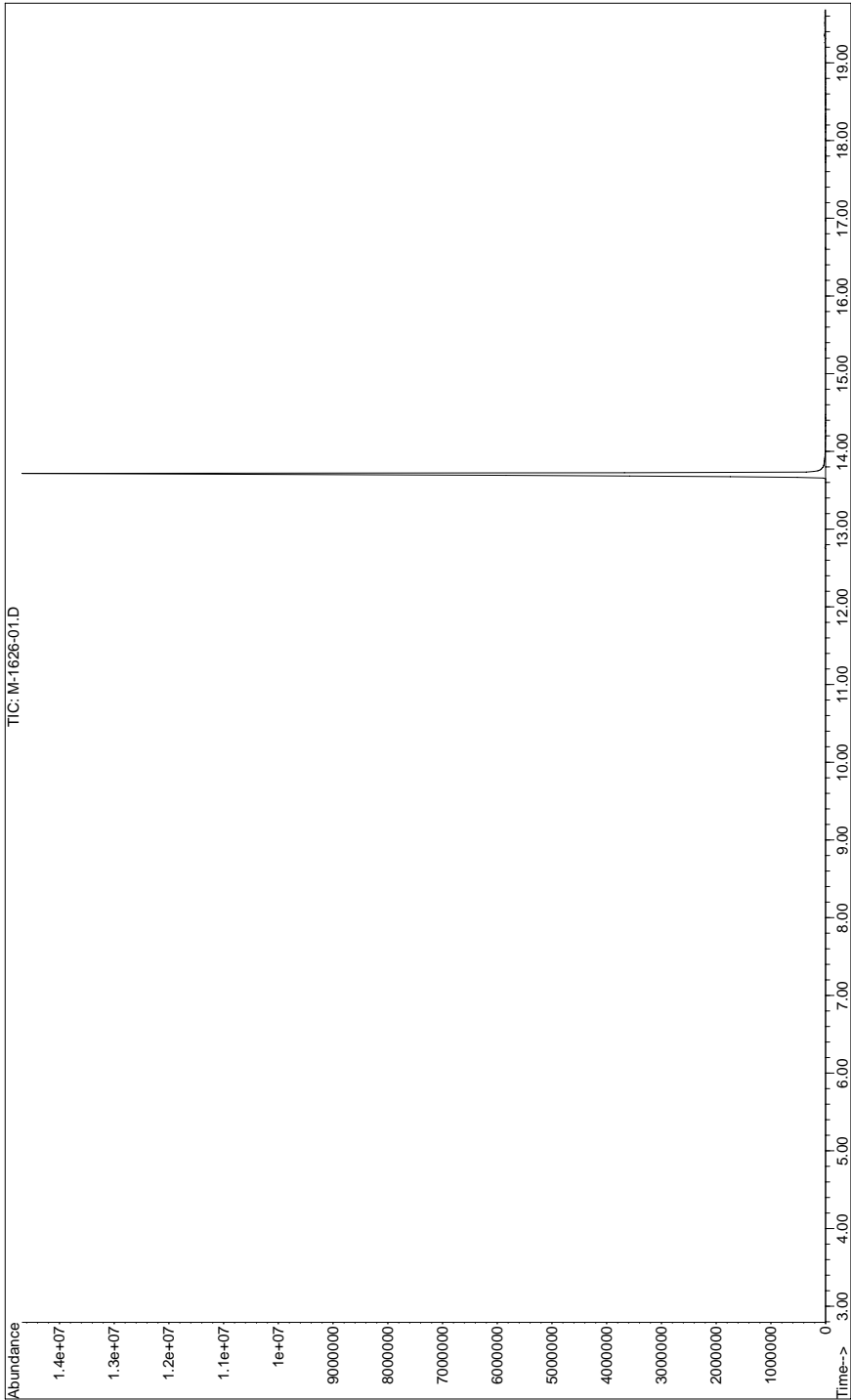
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Bisphenol A - M-1626-01

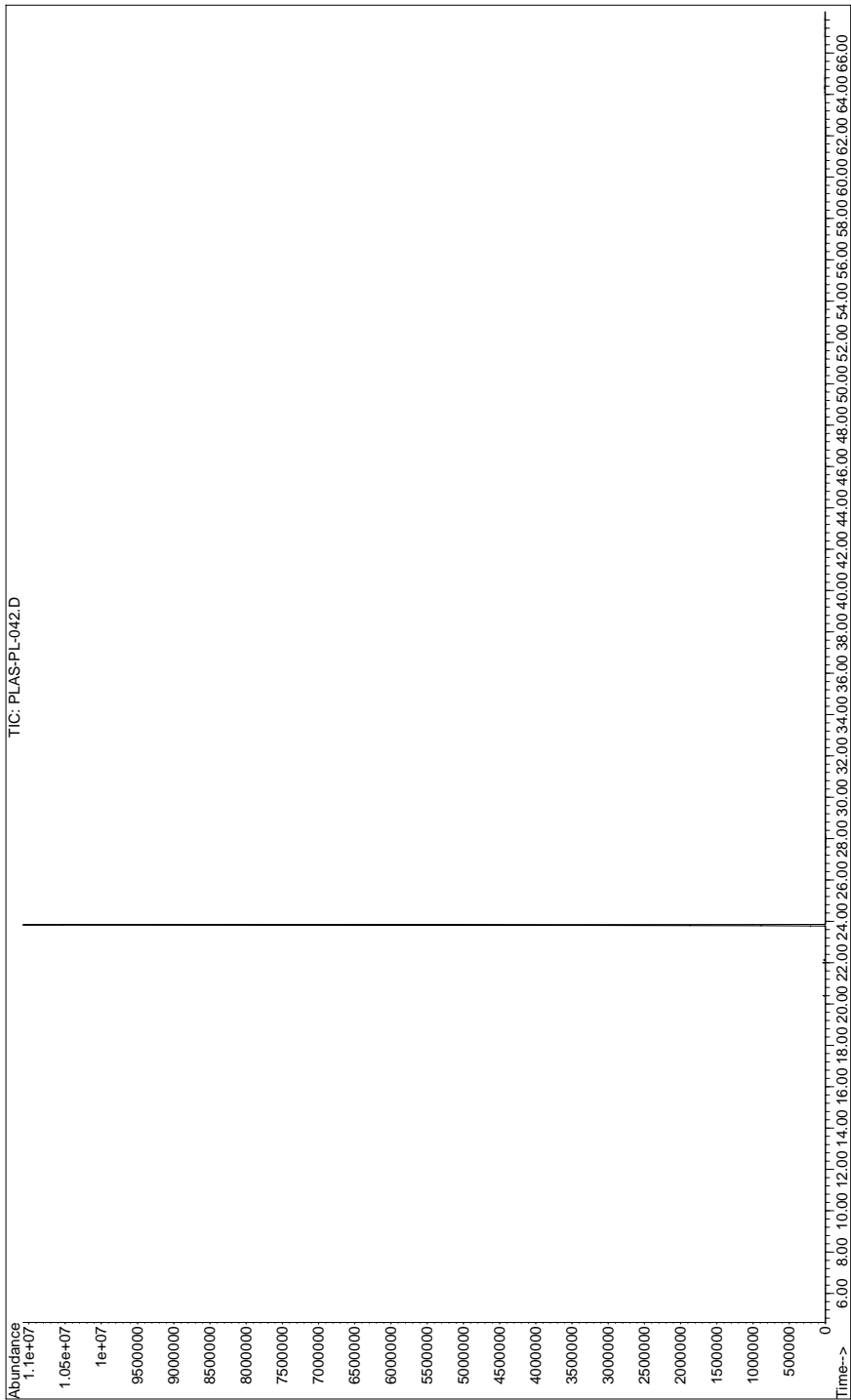
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Butyl ricinoleate - PLAS-PL-042

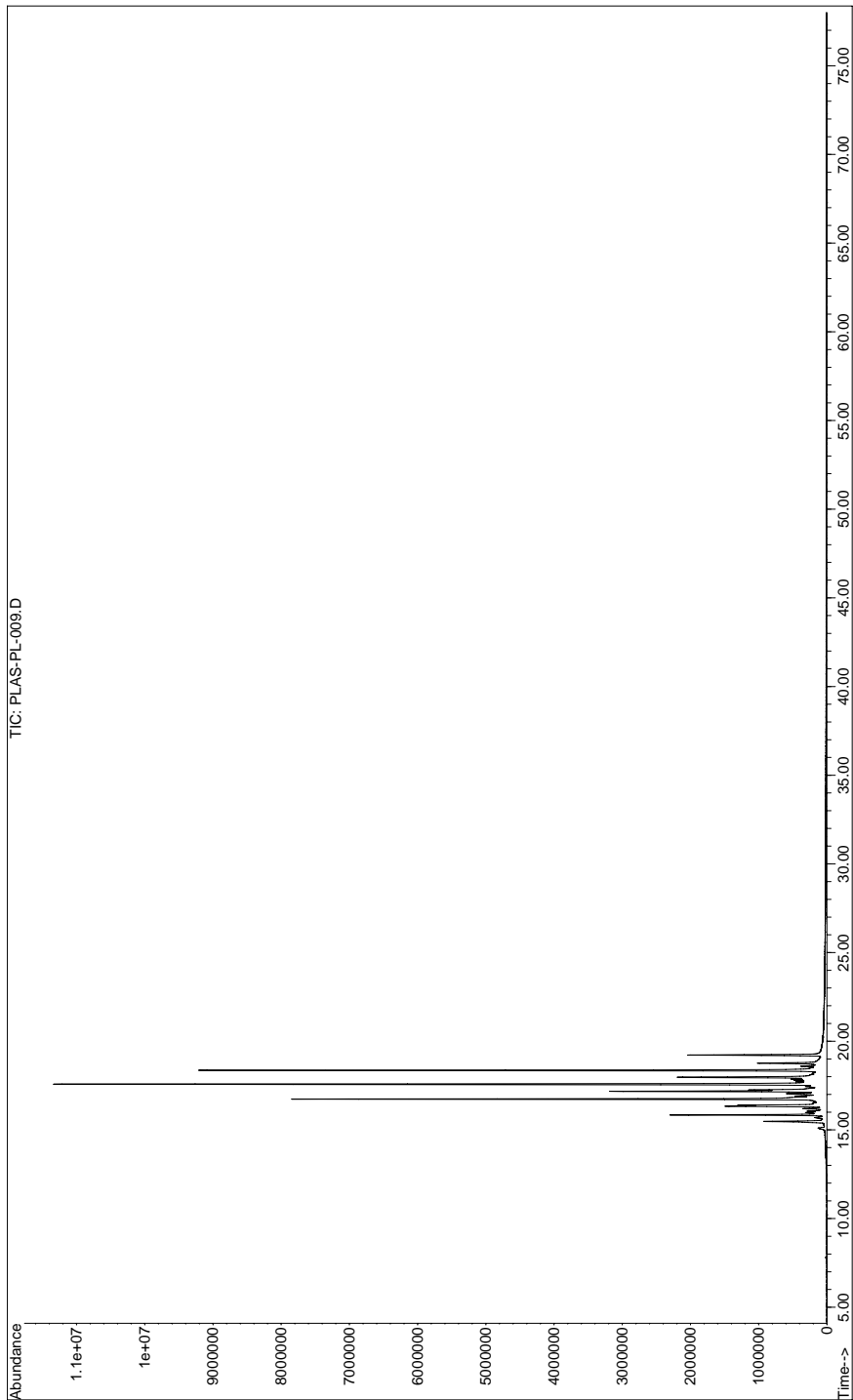
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Celogen® SD-125 - PLAS-PL-009

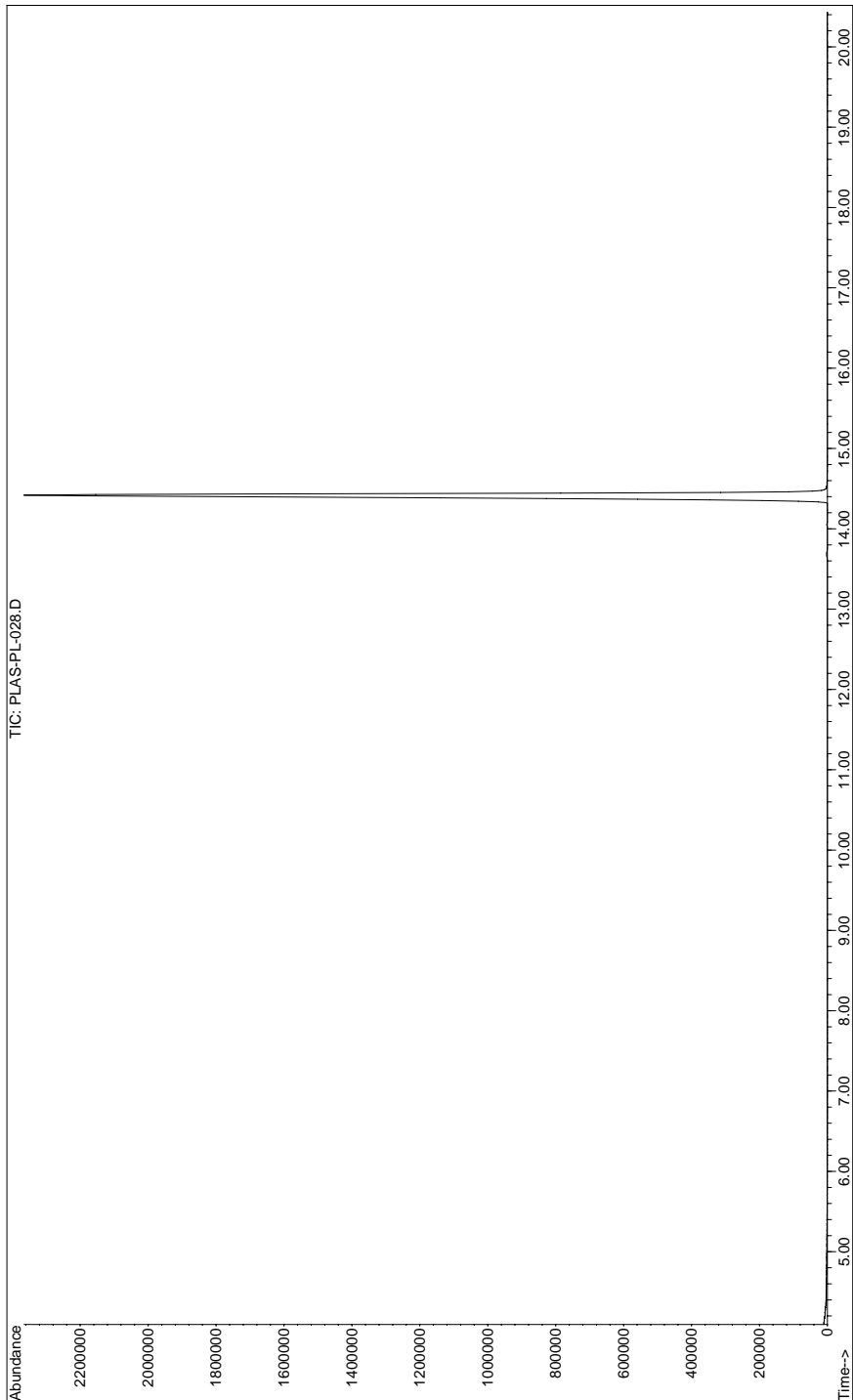
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Citroflex® 2 - PLAS-PL-028

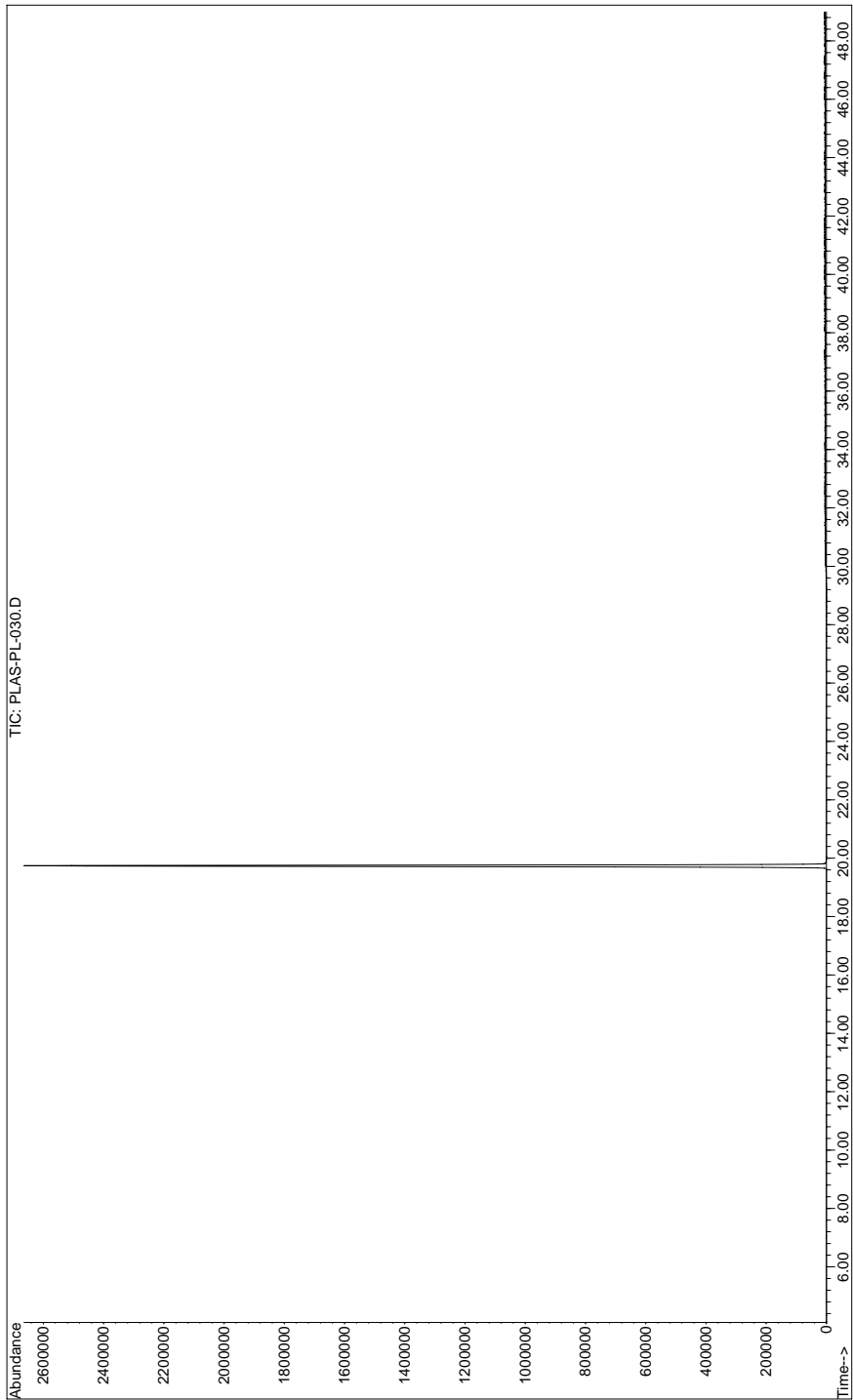
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/minDet=MSD



Analytical Information

Chromatogram for Citroflex® 4 - PLAS-PL-030

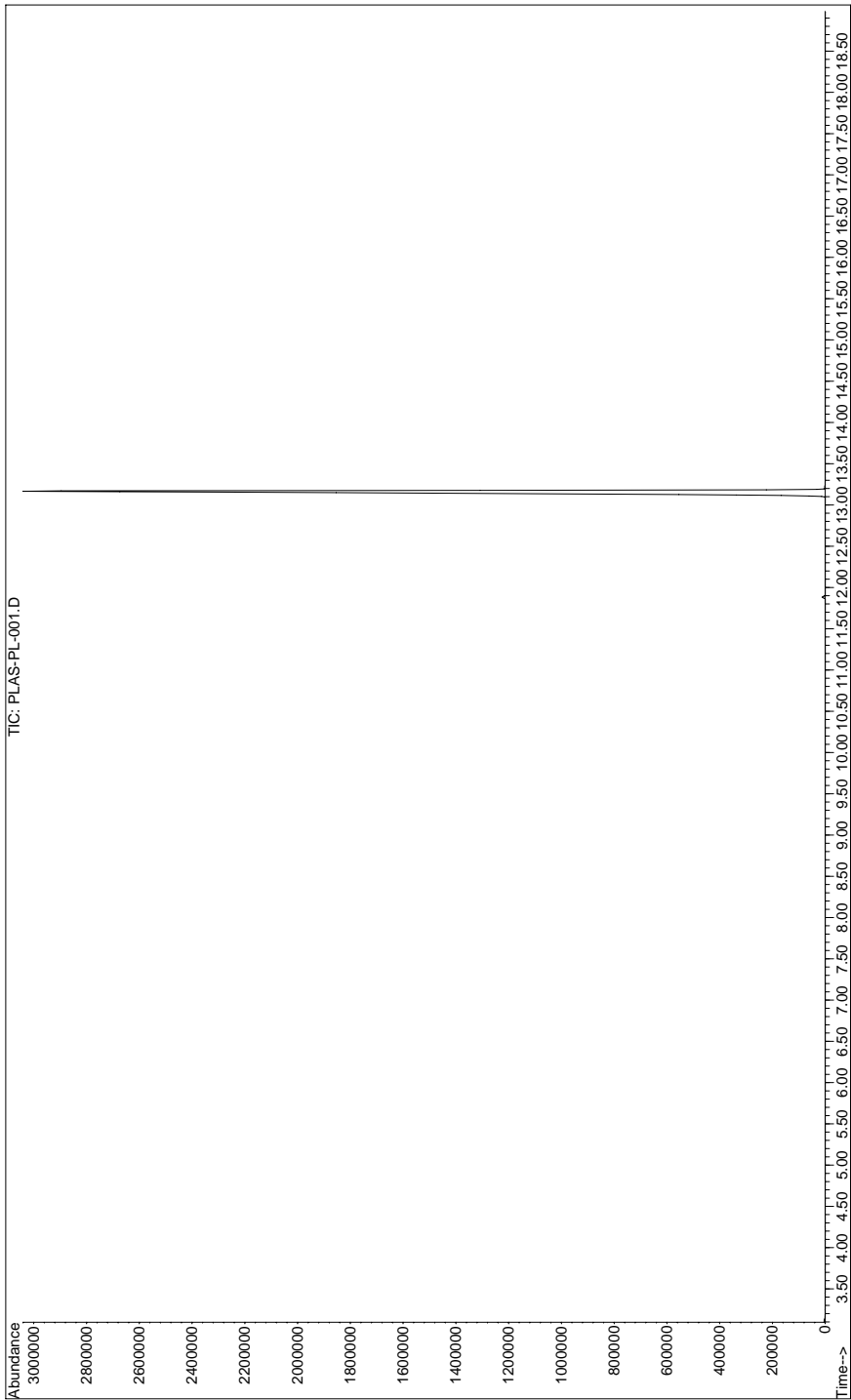
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Citroflex*[®] A-2 - PLAS-PL-001

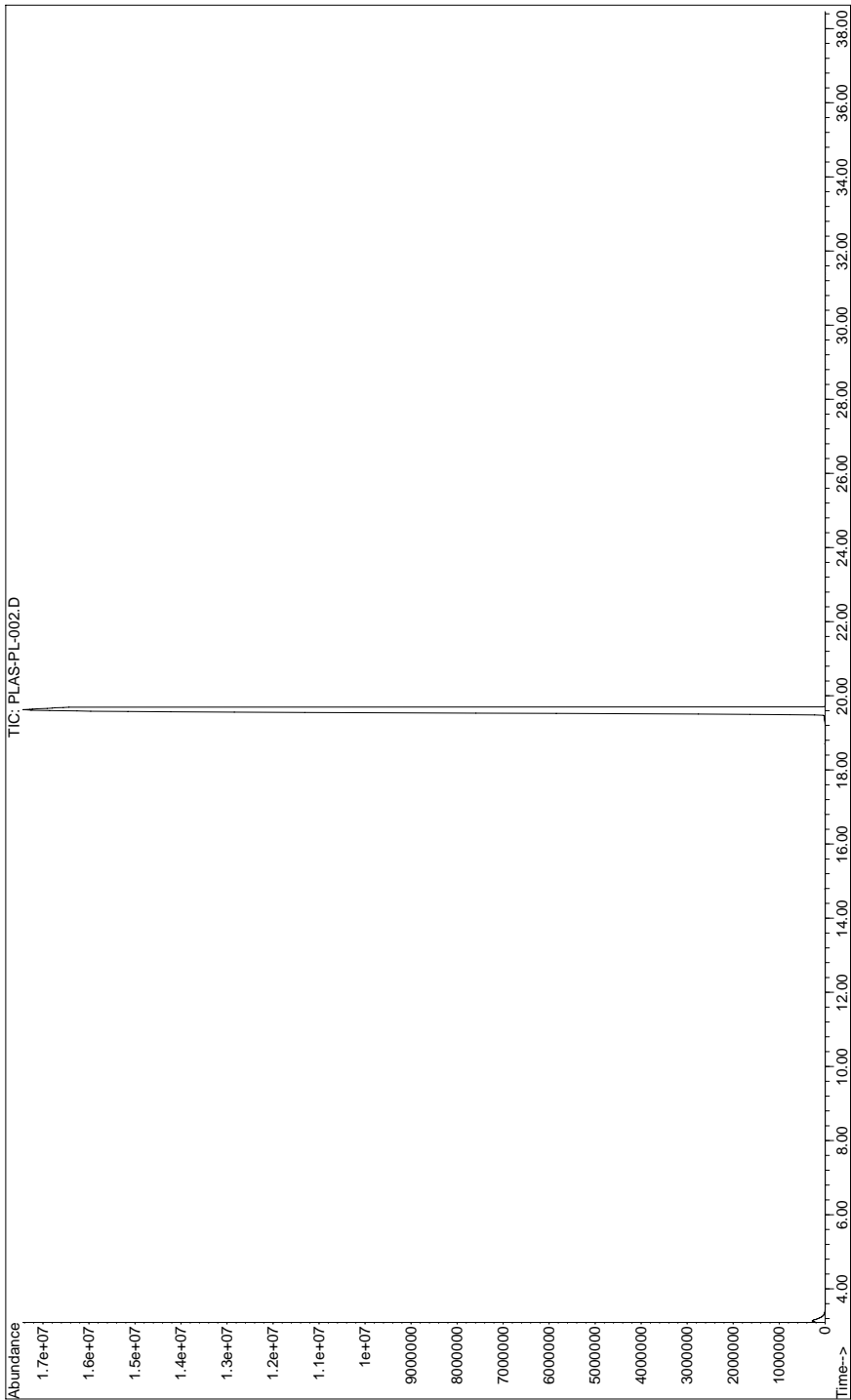
Analytical Conditions Summary 60 °C (0 min) to 300 °C (13 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Citroflex® A-4 - PLAS-PL-002

Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Citroflex® B-6 - PLAS-PL-025

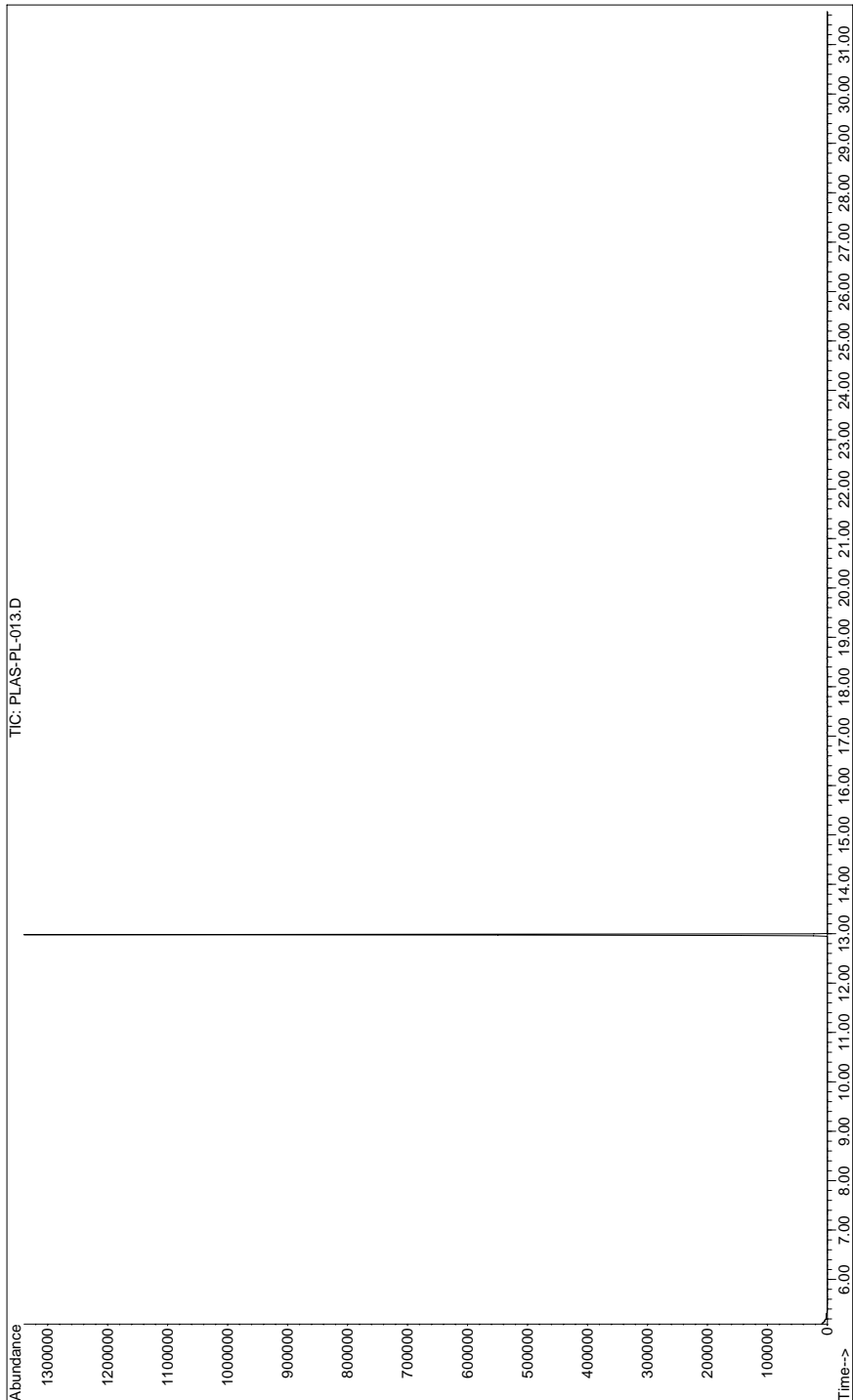
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Dibutyl Phthalate - PLAS-PL-013

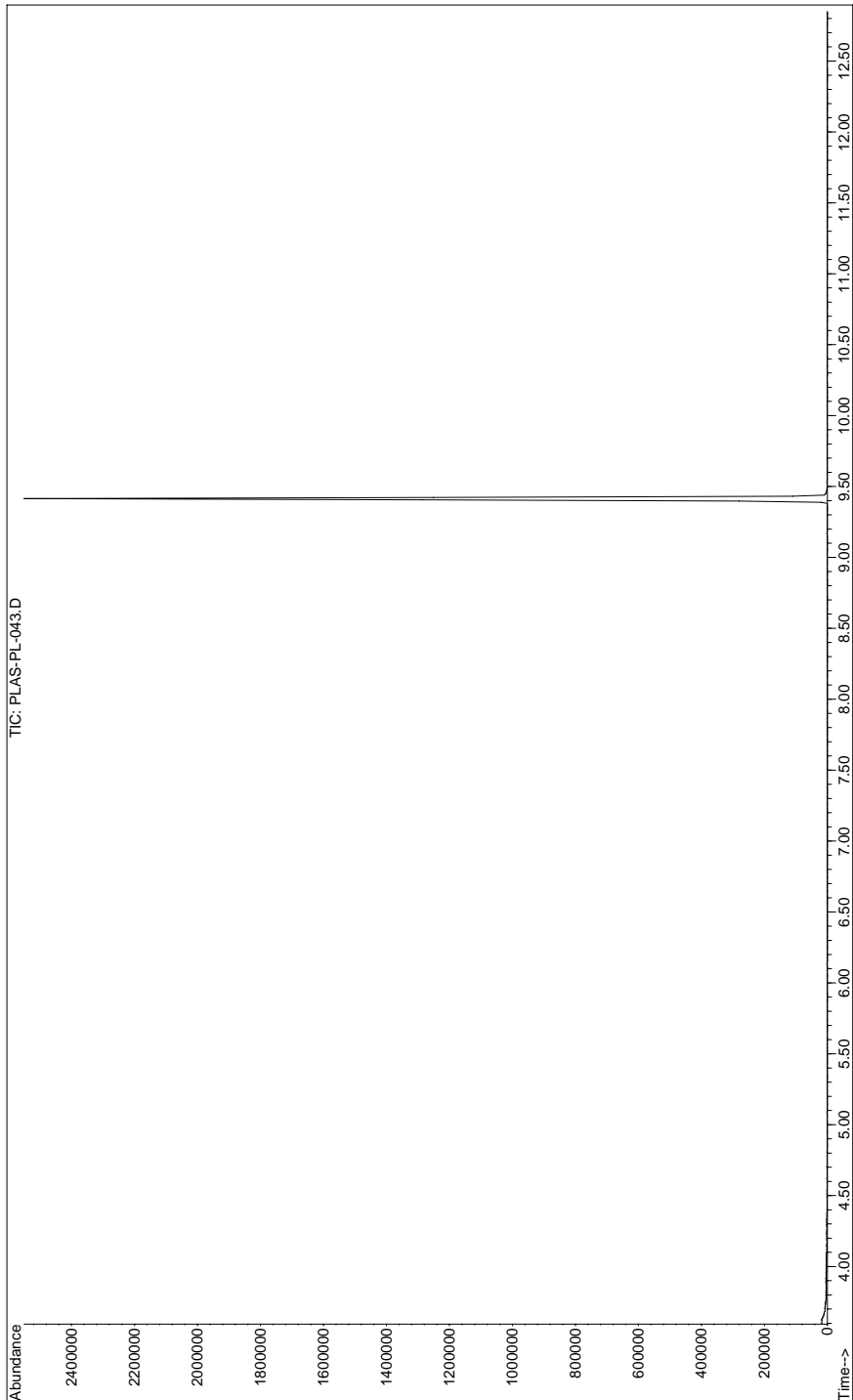
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Diethyl adipate* - PLAS-PL-043

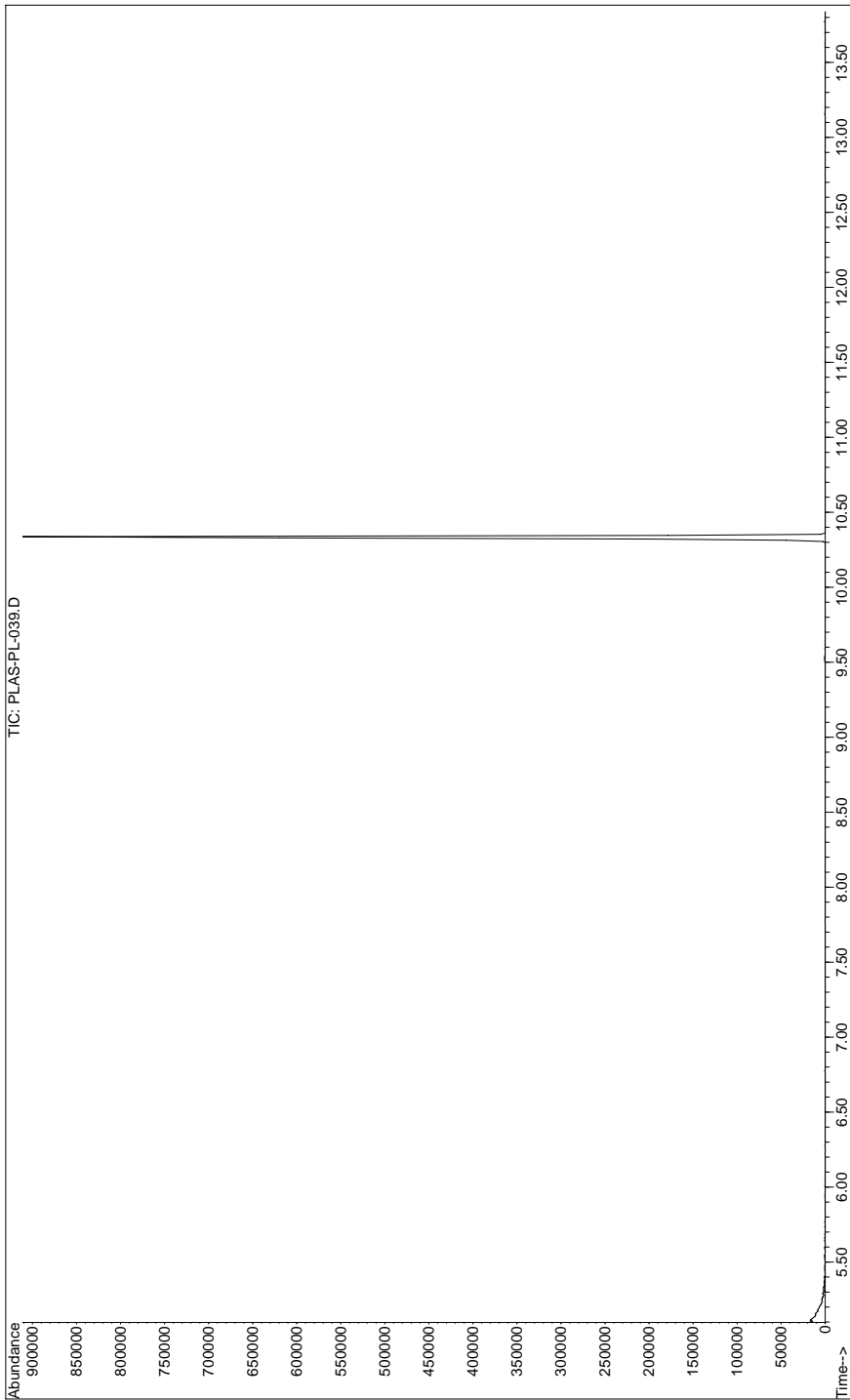
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Diethyl phthalate* - PLAS-PL-039

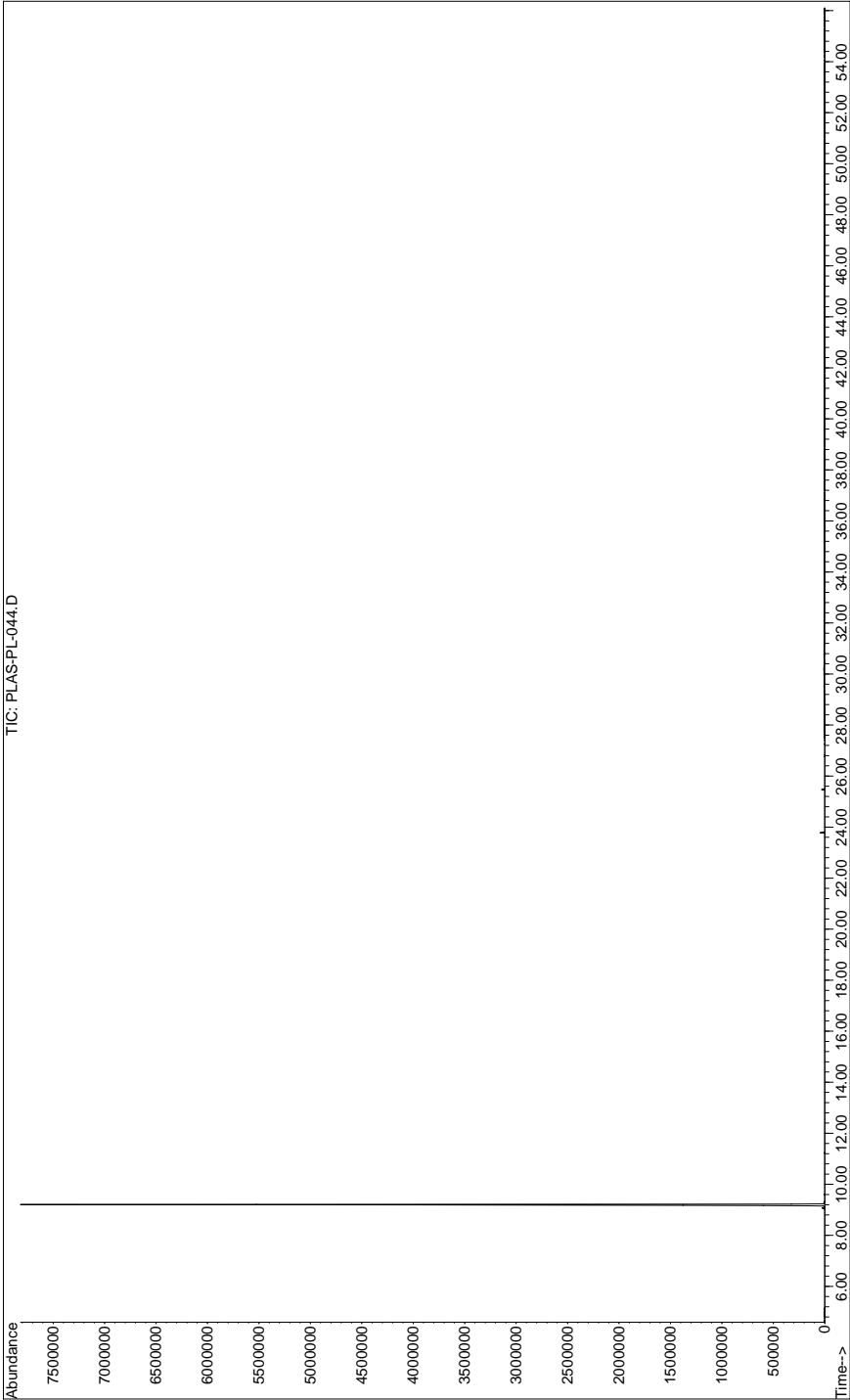
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Diethyl succinate* - PLAS-PL-044

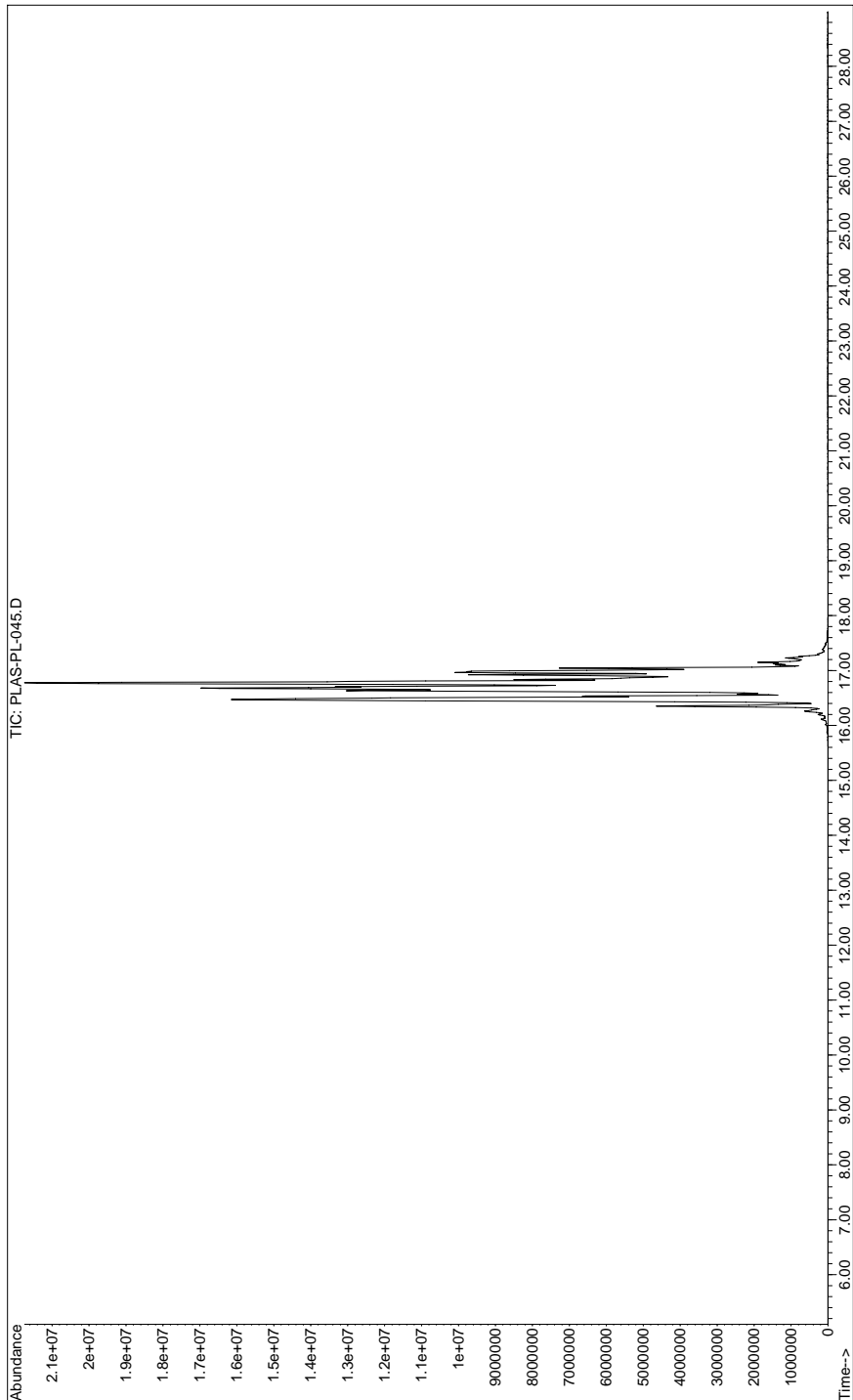
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Diisononyl adipate - PLAS-PL-045

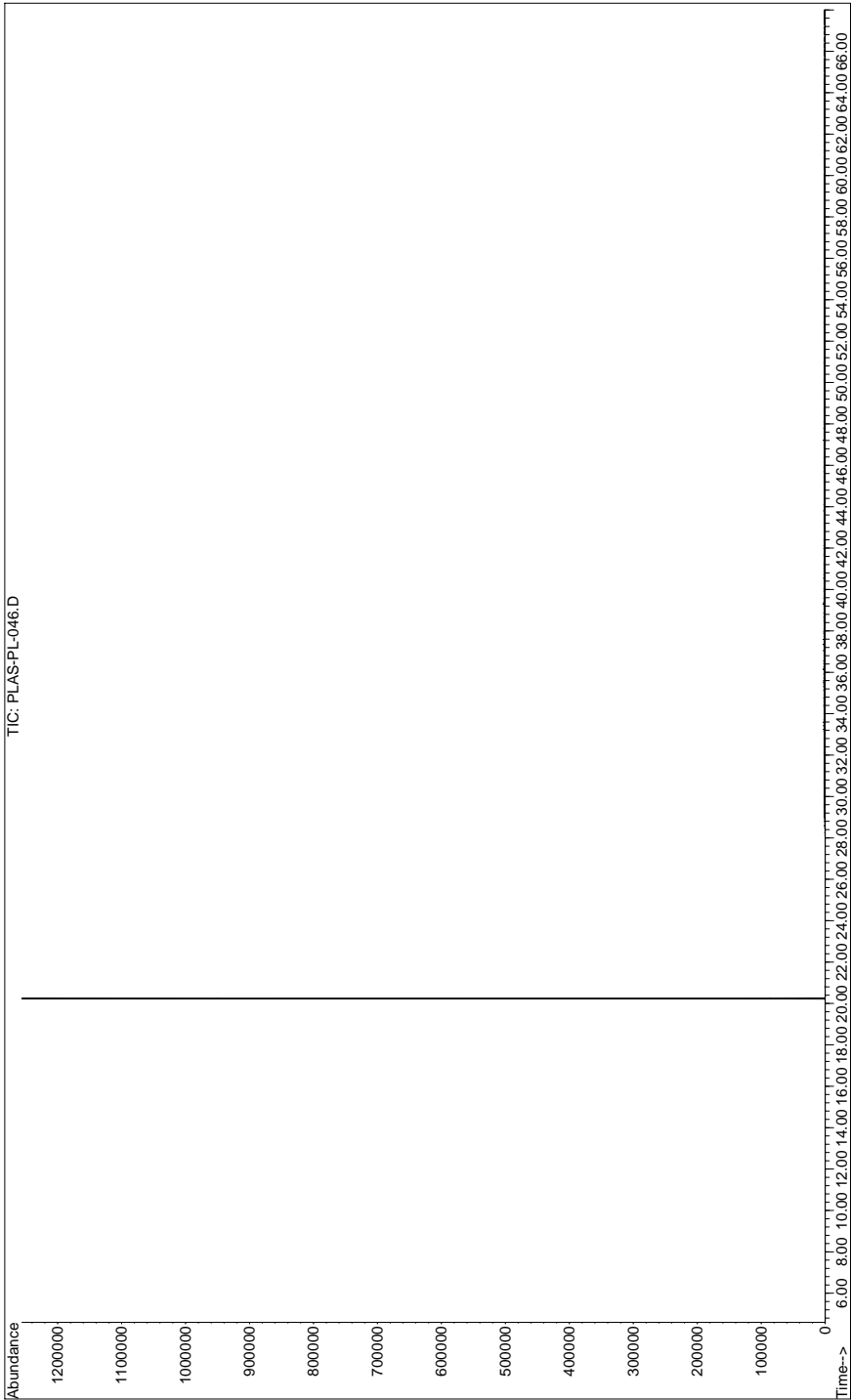
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Dioctyl maleate* - PLAS-PL-046

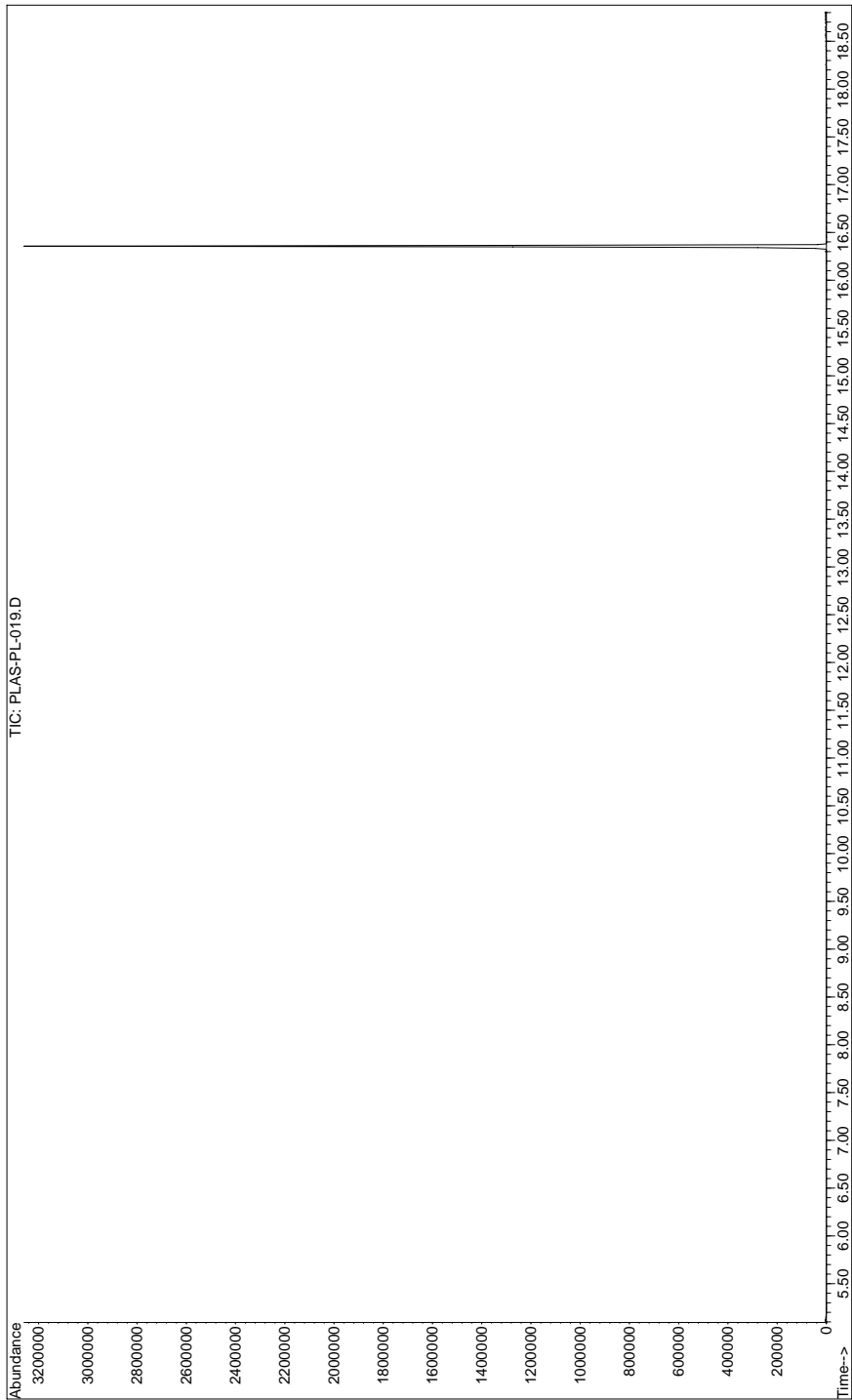
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Diocetyl phthalate (DOP) - PLAS-PL-019

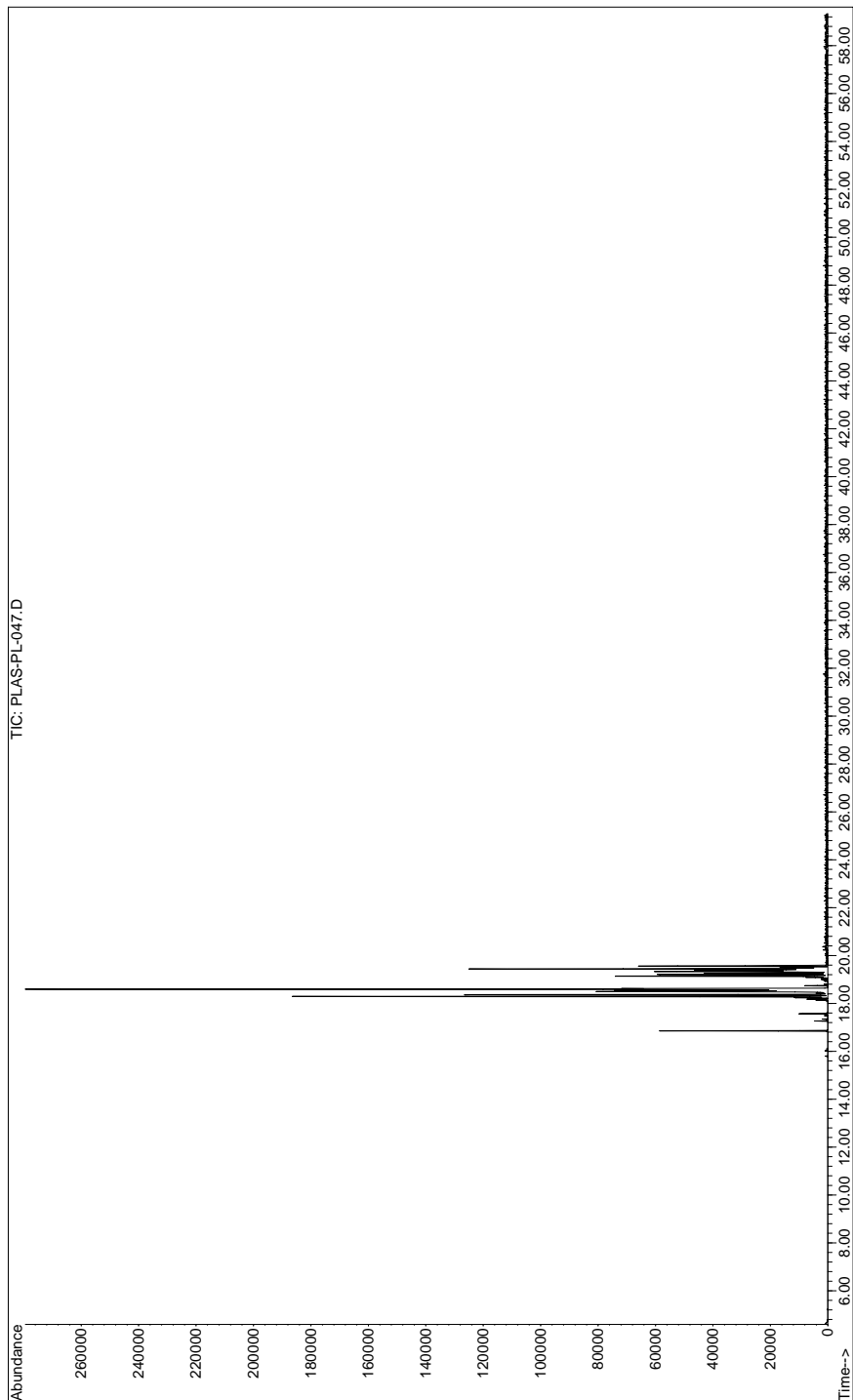
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for *Epoxidized linseed oil* - PLAS-PL-047

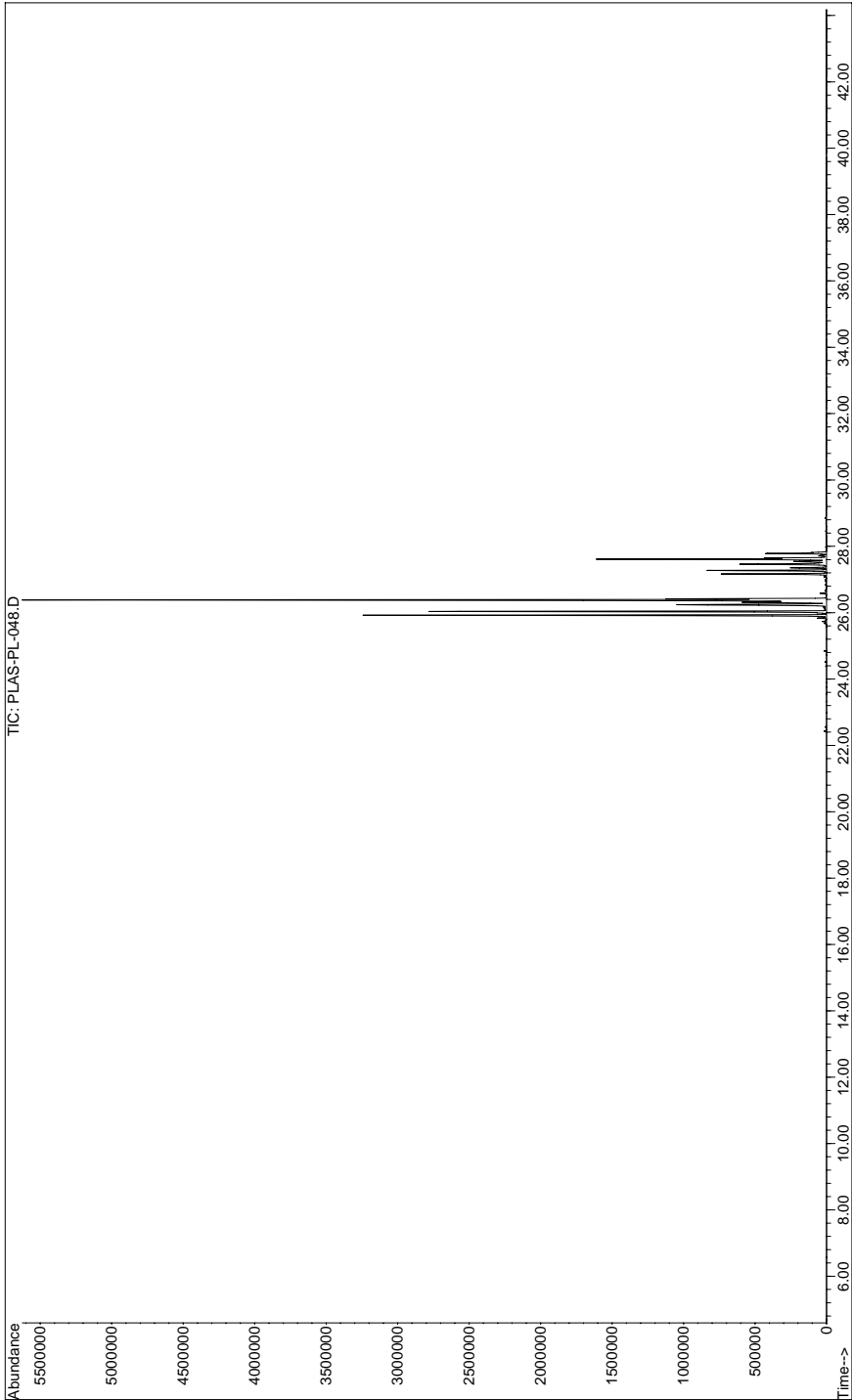
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Flexol EP-8 - PLAS-PL-048*

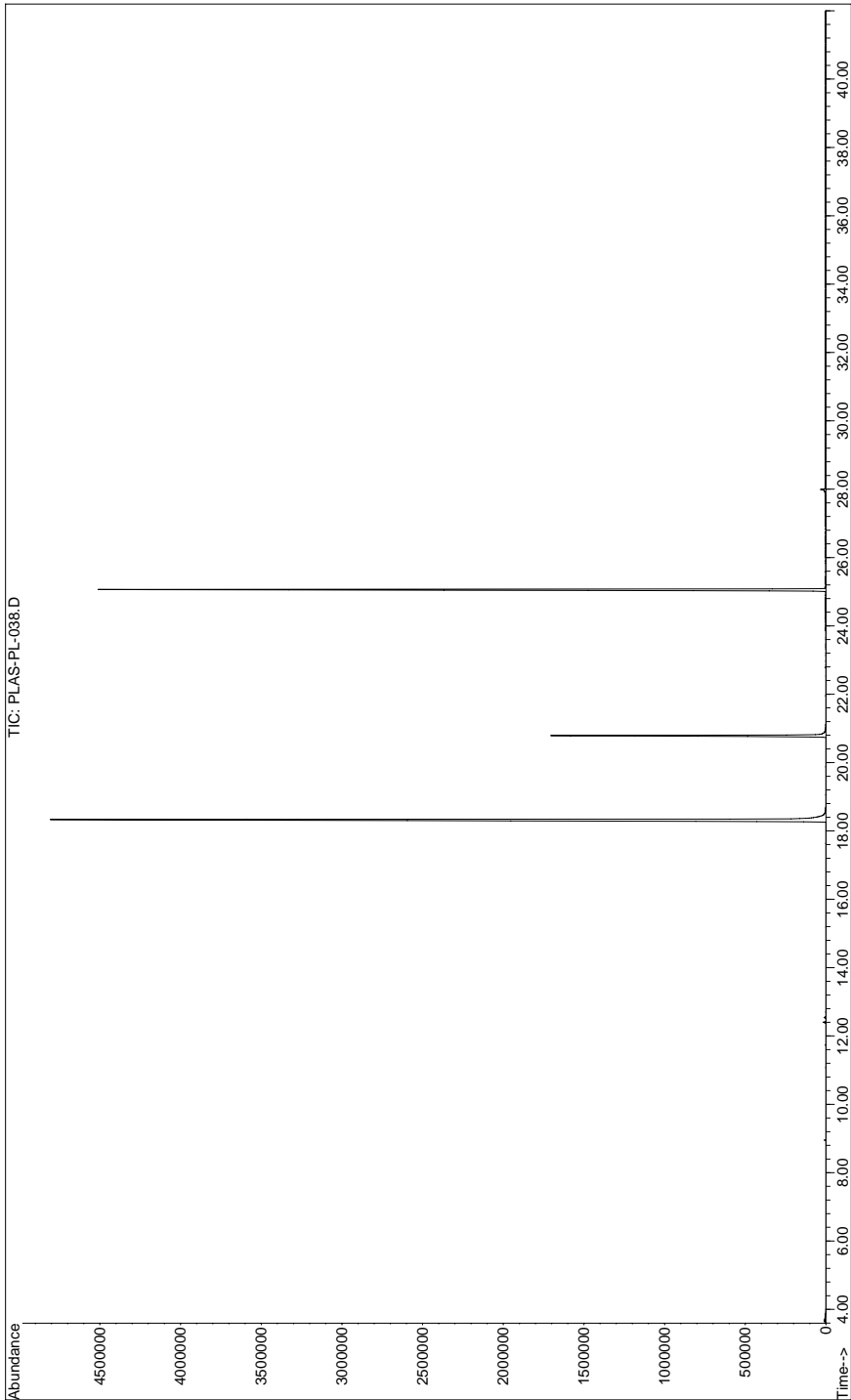
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Hercoflex*[®] 900 - PLAS-PL-038

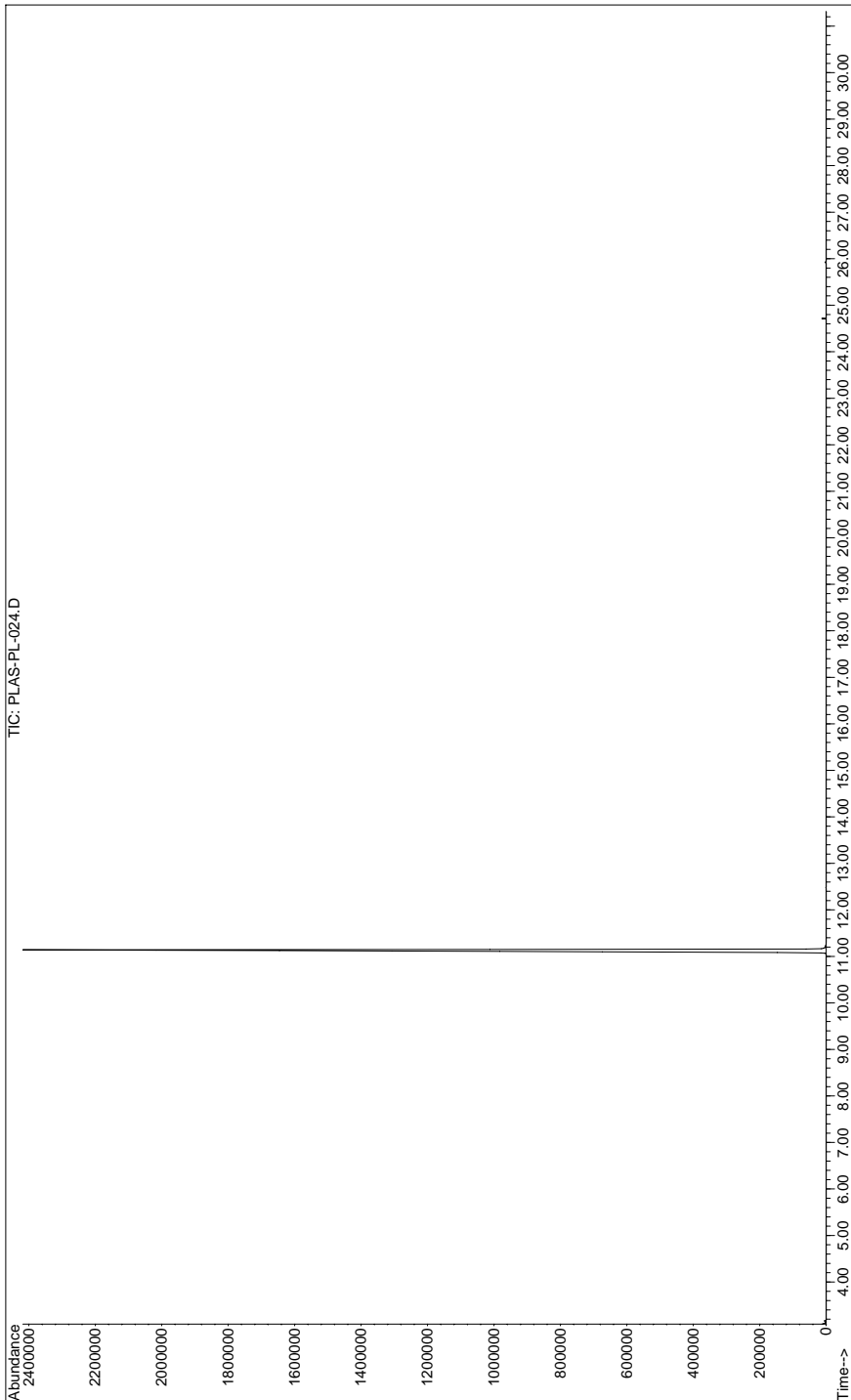
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Hi-Point*[®] PD-1 - PLAS-PL-024

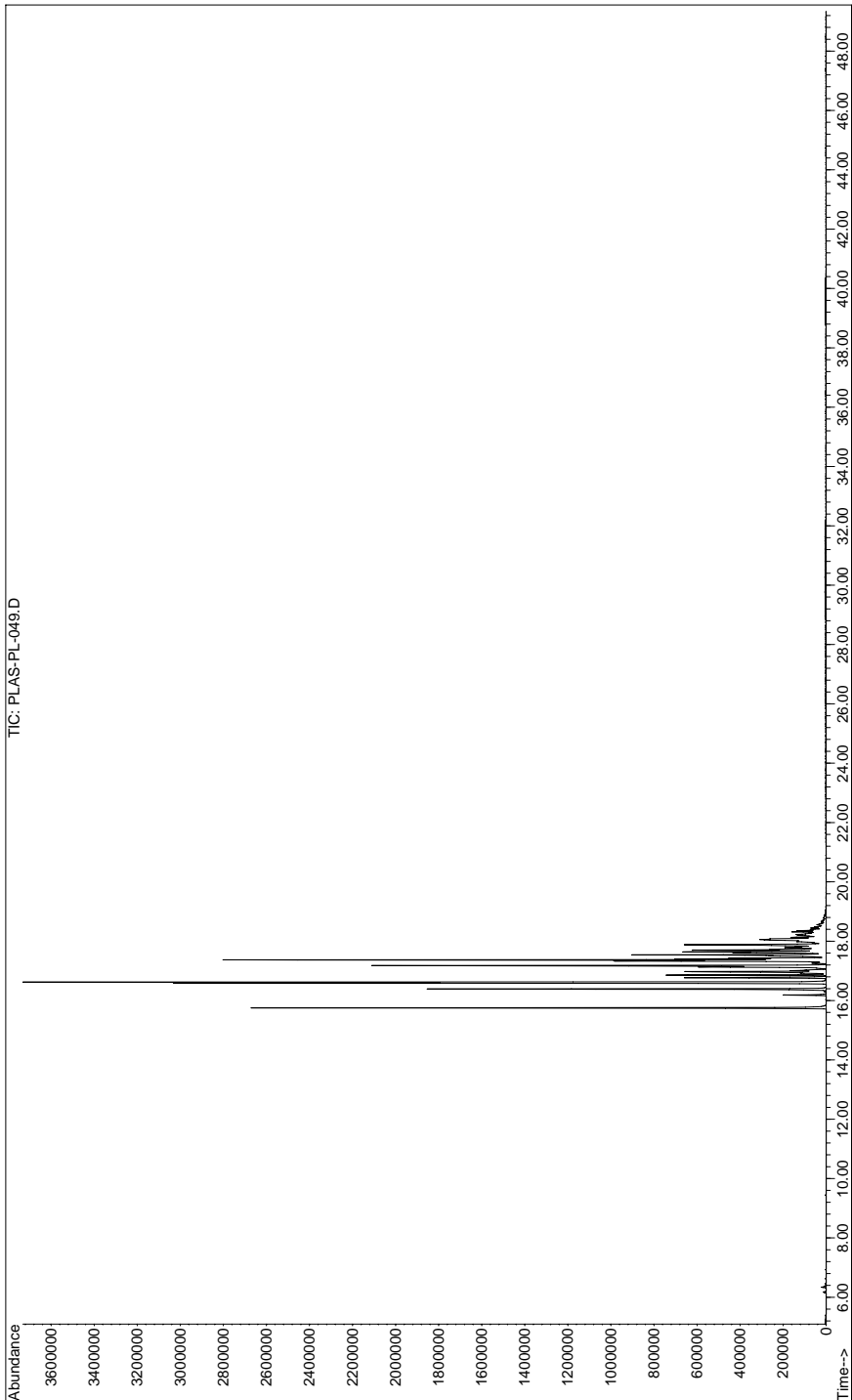
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Imol S-140 - PLAS-PL-049*

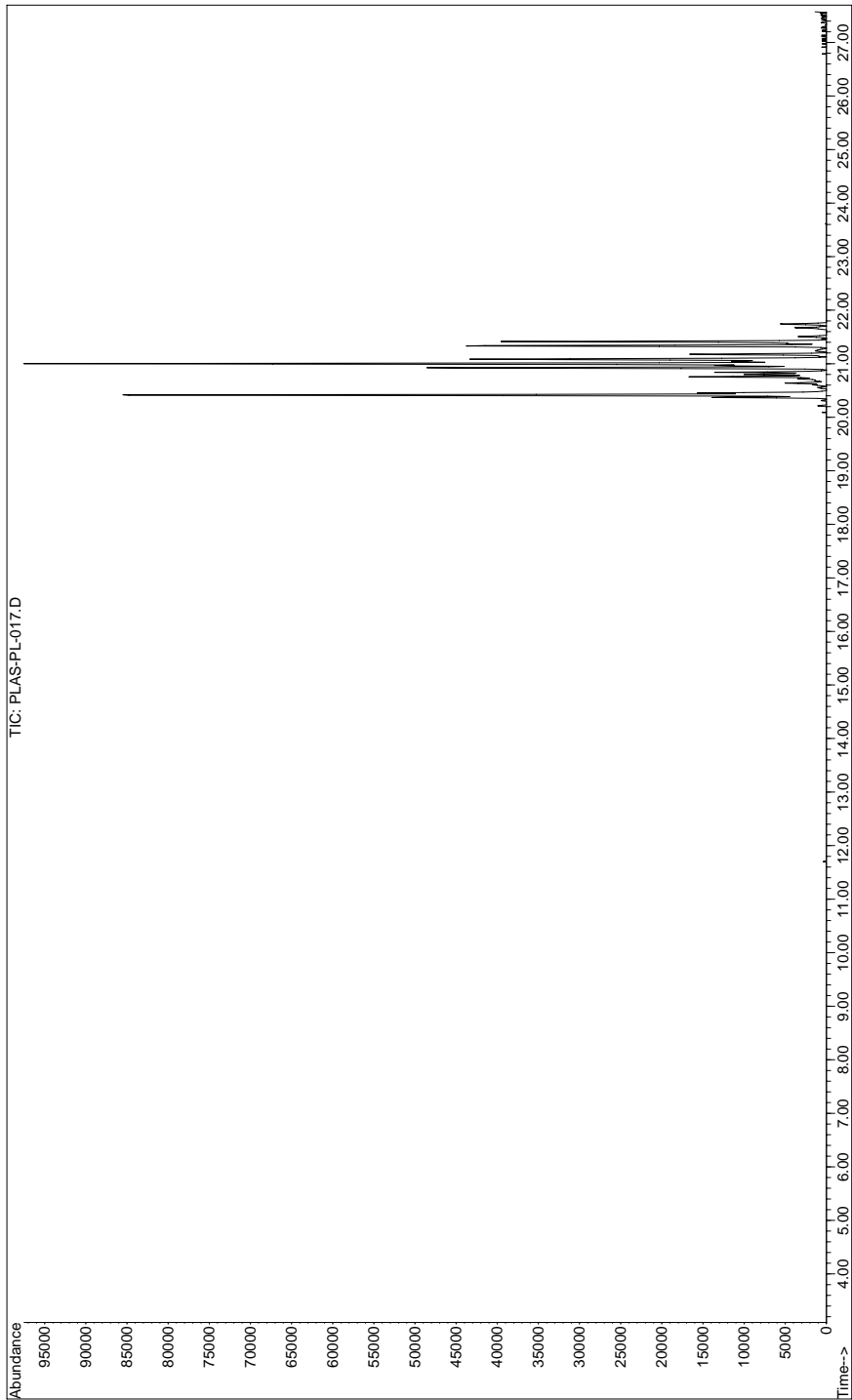
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Jayflex® 77 - PLAS-PL-017

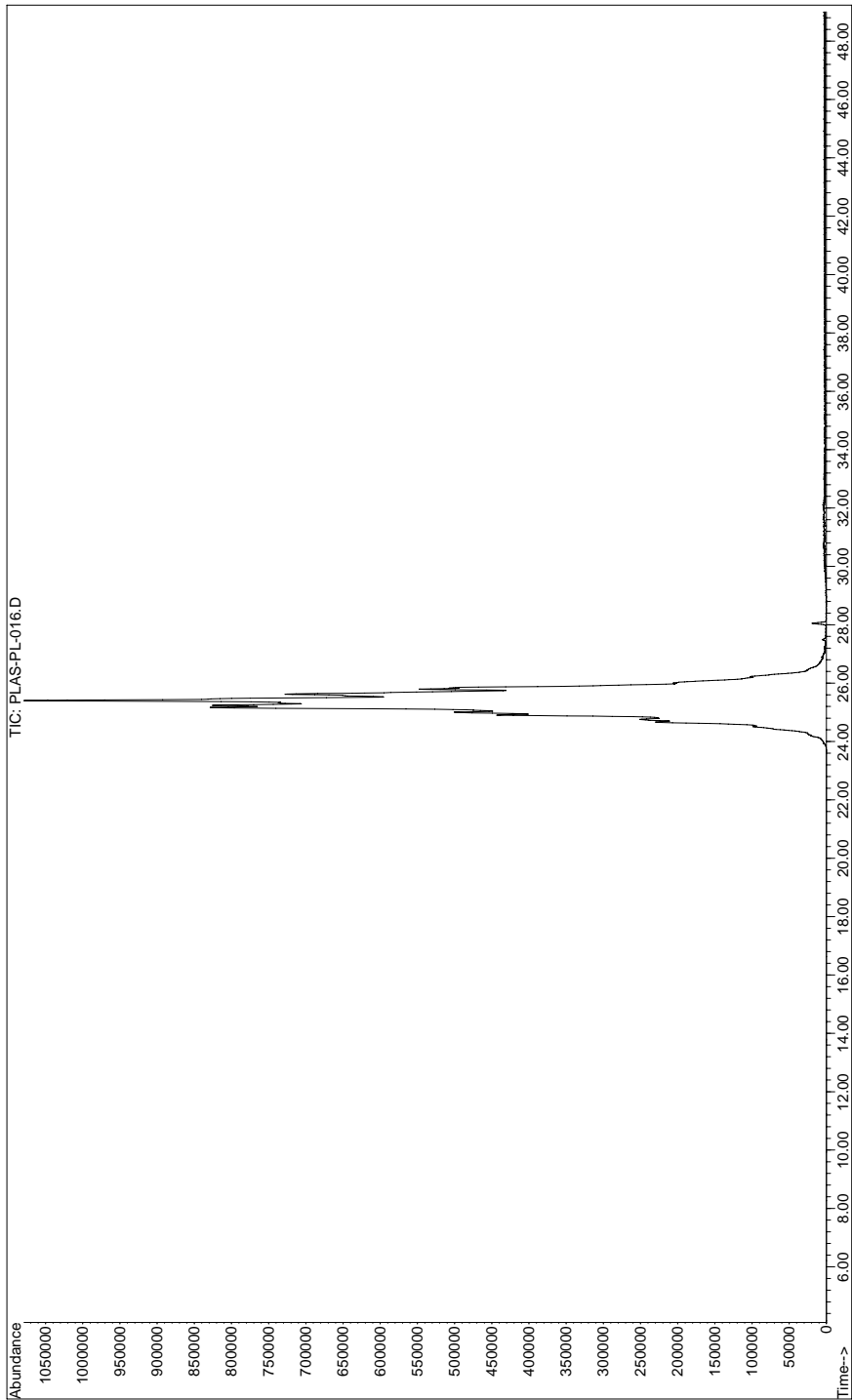
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Jayflex® DIDP - PLAS-PL-016

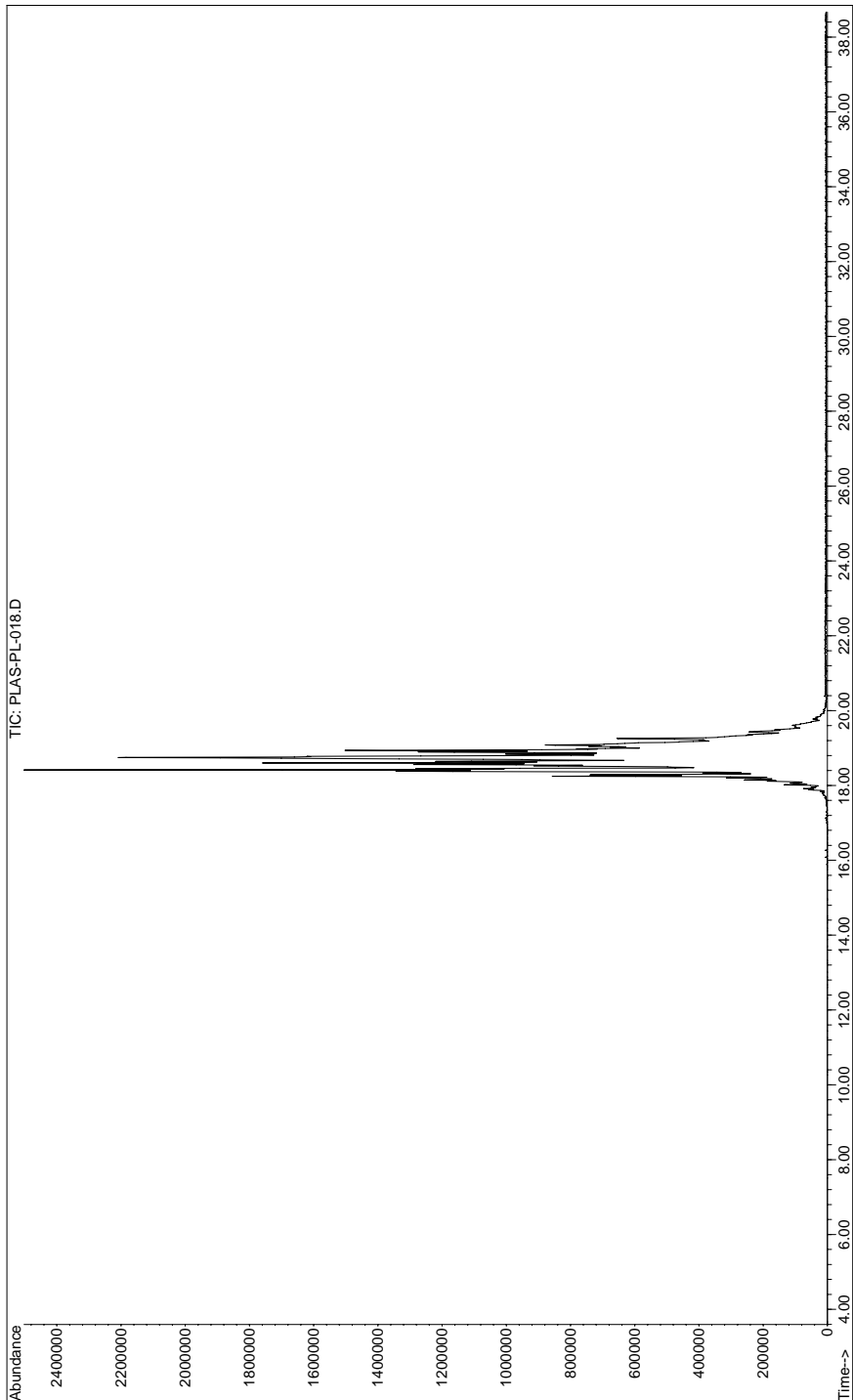
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Jayflex® DINP Plasticizer - PLAS-PL-018

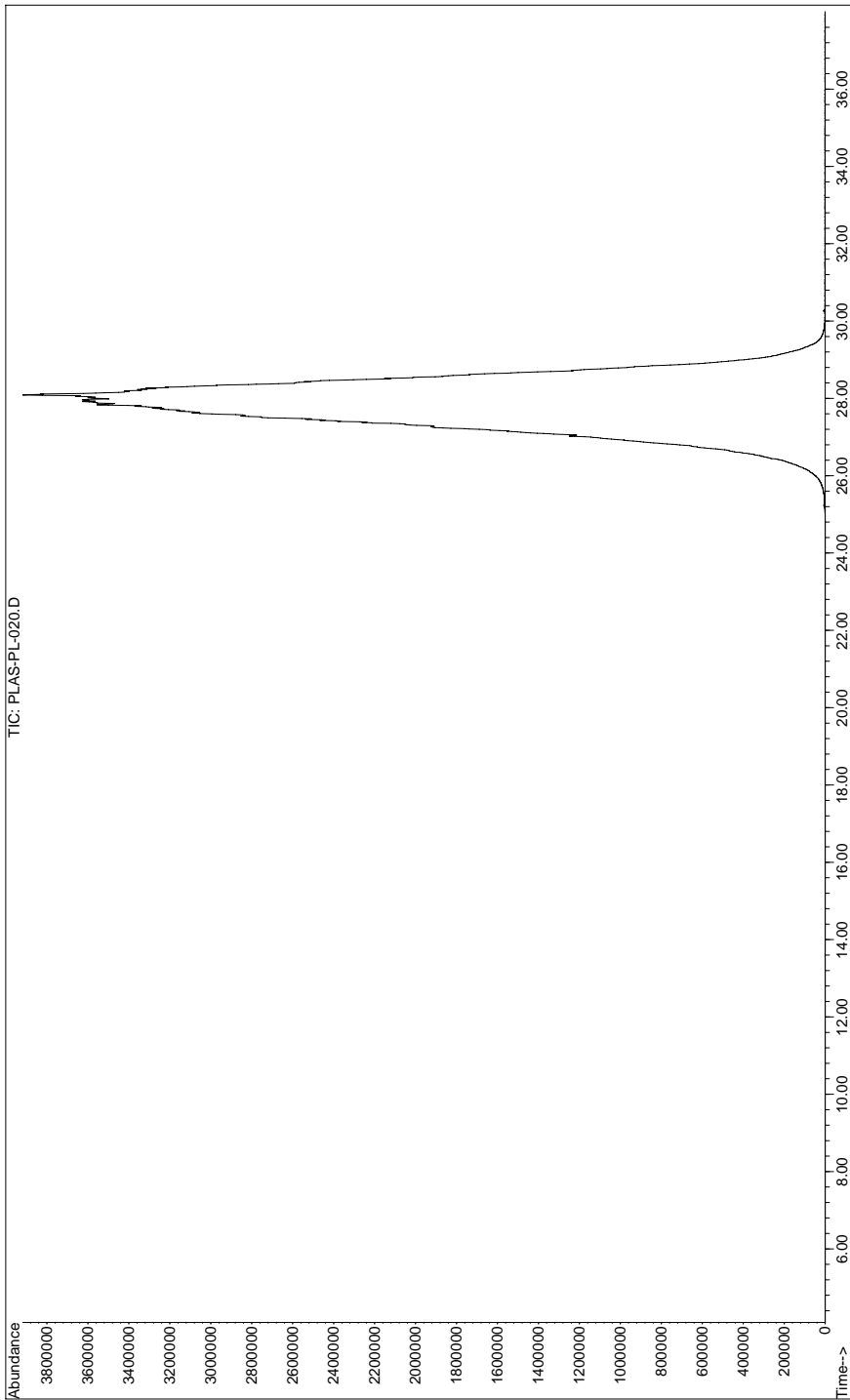
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Jayflex® DTDP plasticizer - PLAS-PL-020

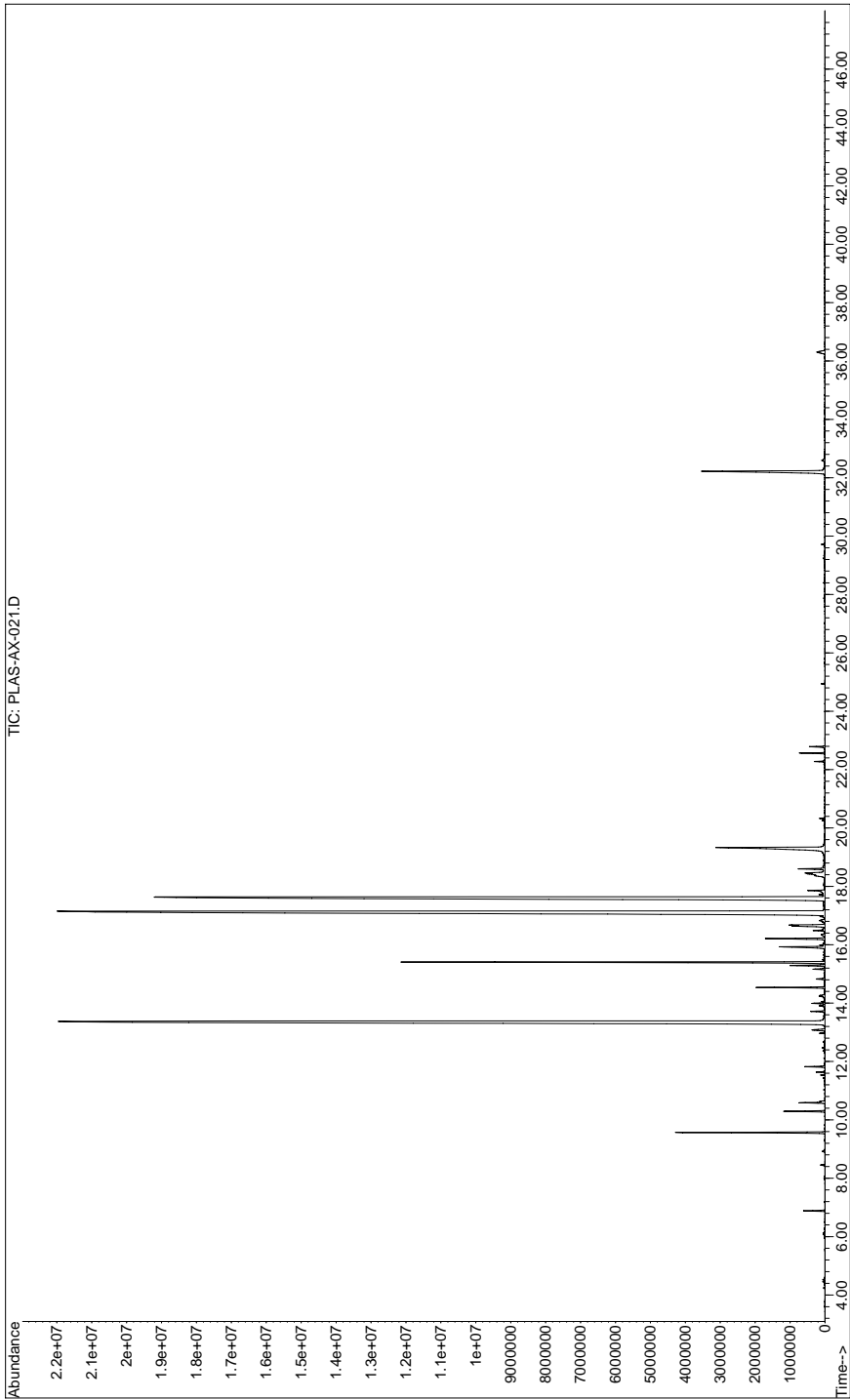
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Jayflex® L11P-E Plasticizer - PLAS-PL-021

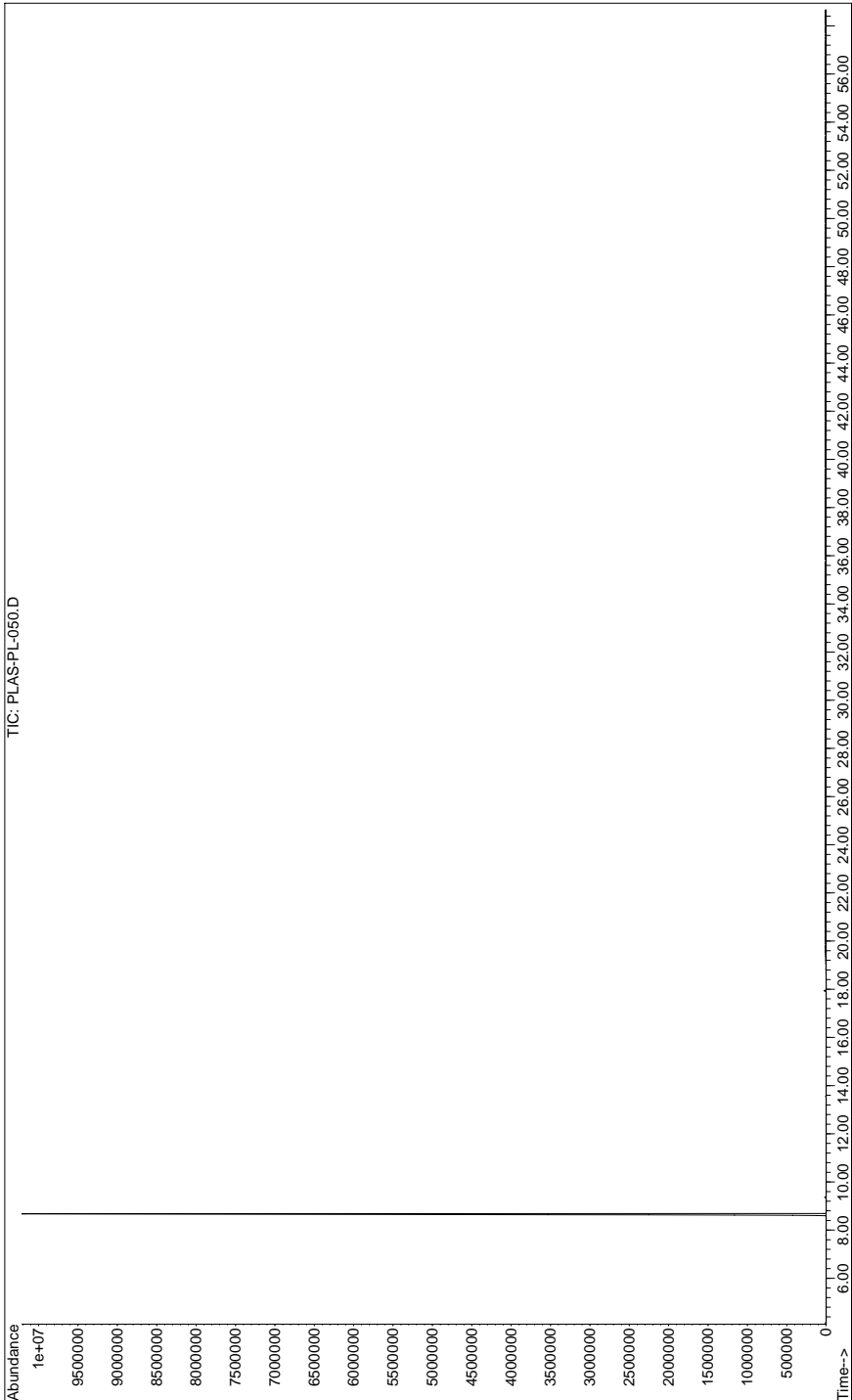
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 10 °C/min Det=MSD



Analytical Information

Chromatogram for Kesscoflex TRA - PLAS-PL-050

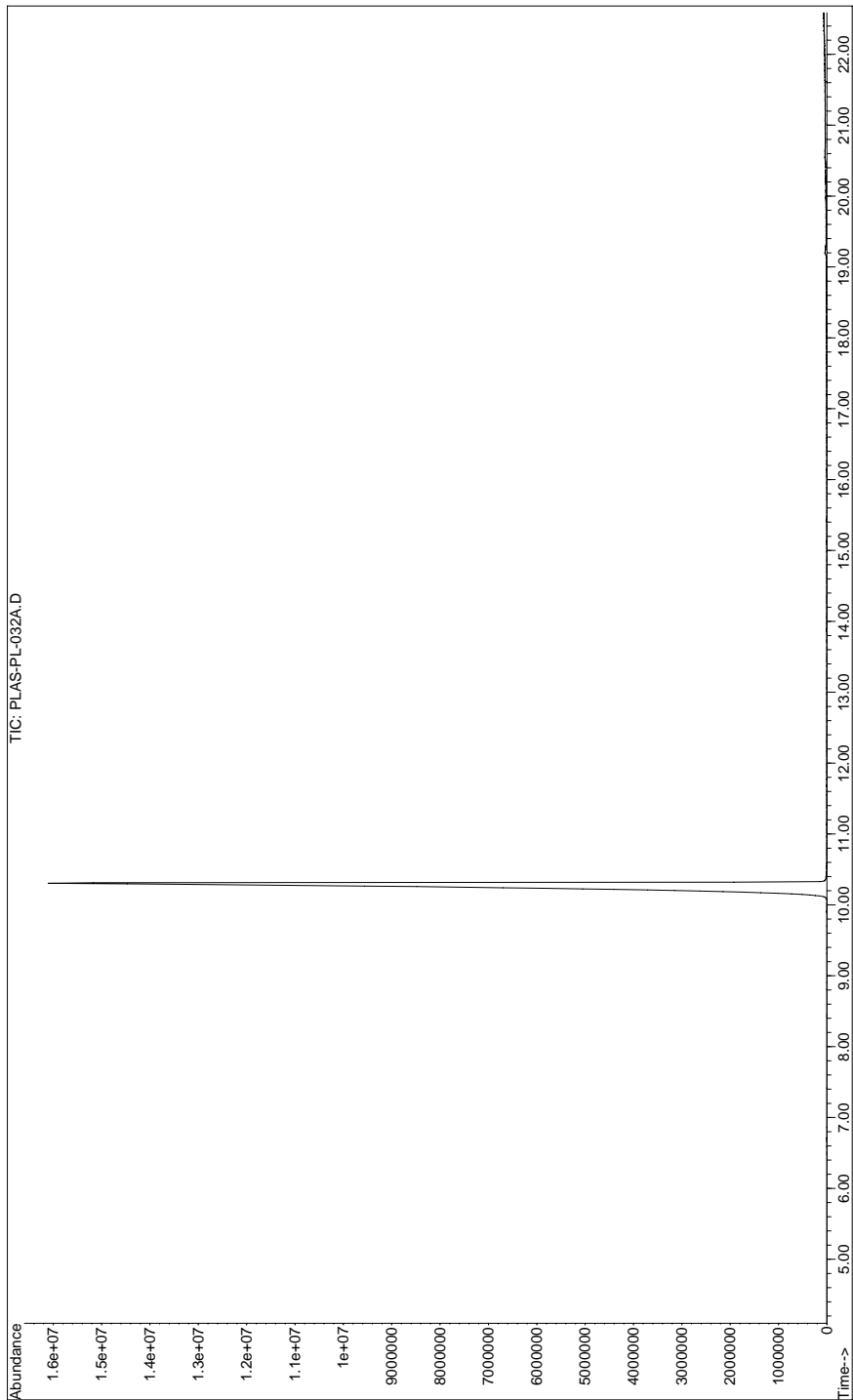
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Laurex*[®] - PLAS-PL-032

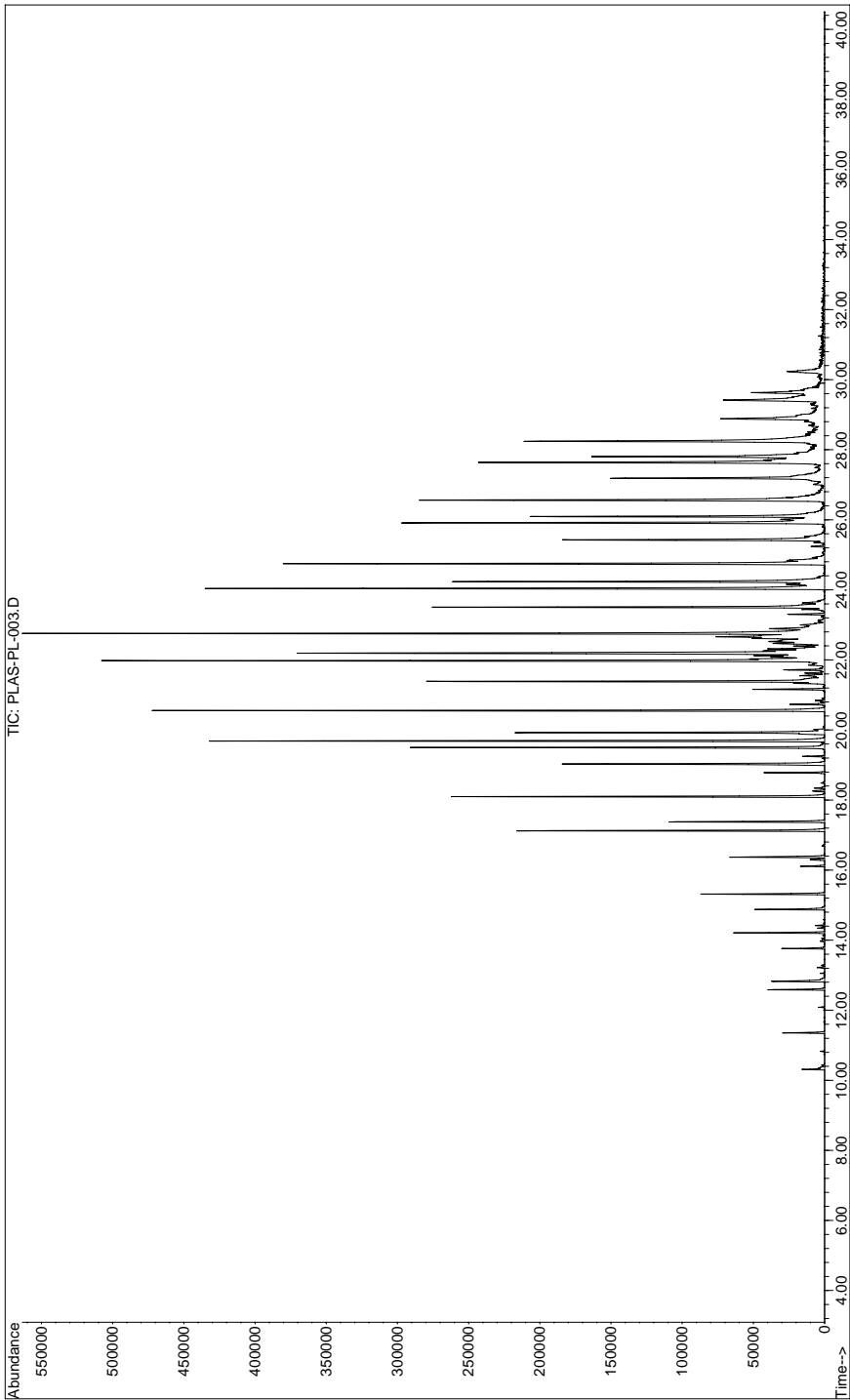
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Markstat*® 51 - PLAS-PL-003

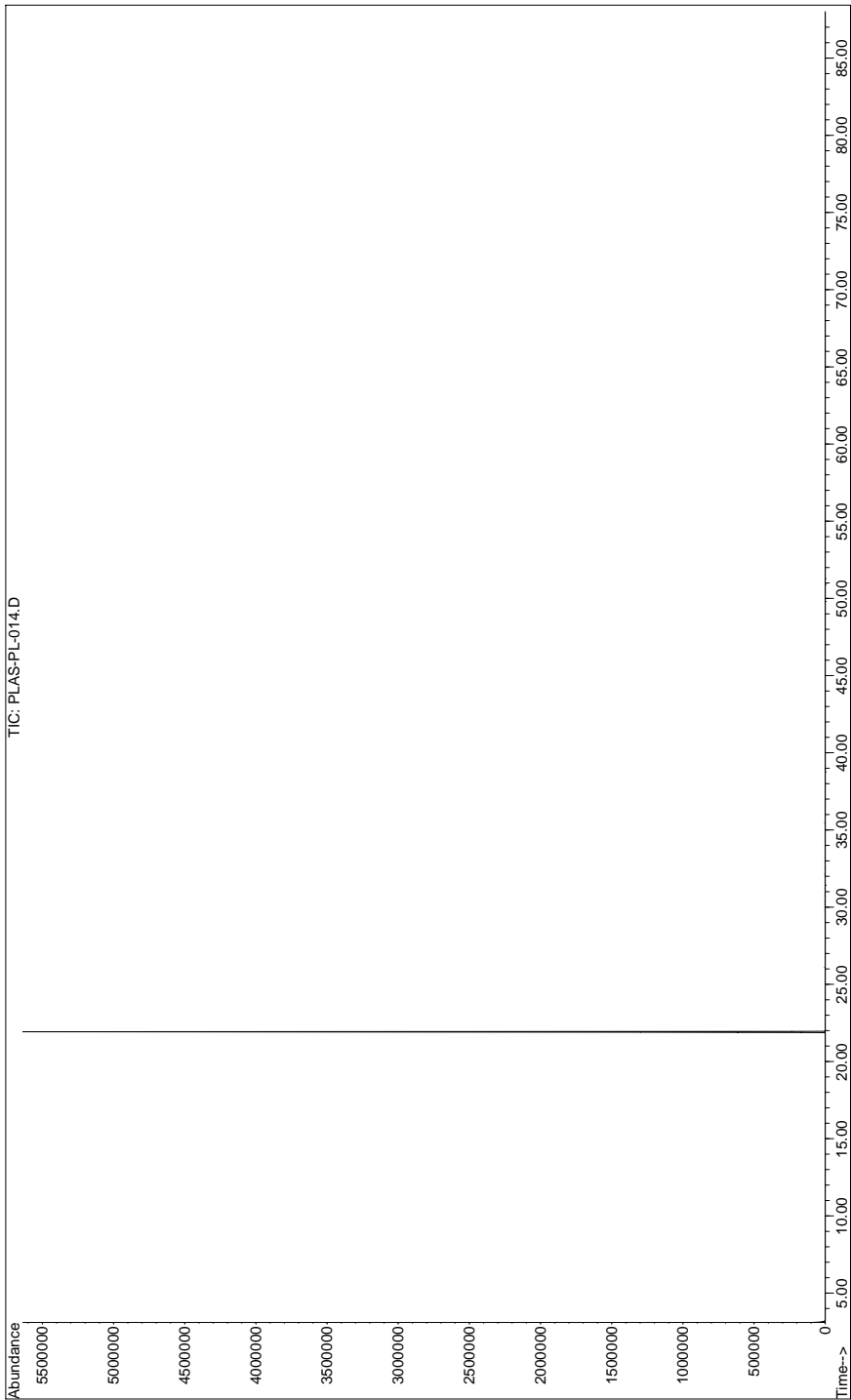
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Morflex[®] 150 - PLAS-PL-014

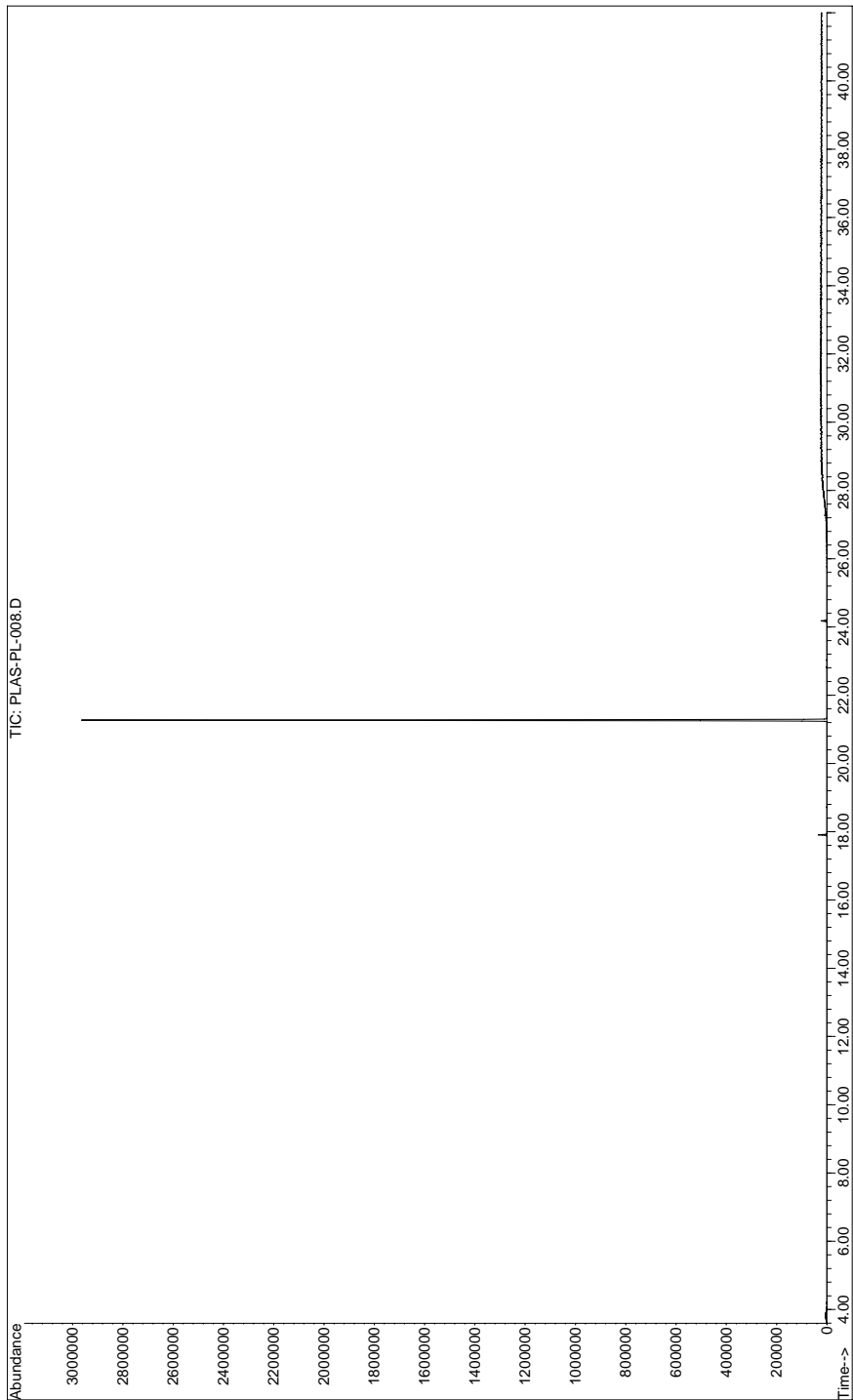
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Morflex[®] 190 - PLAS-PL-008

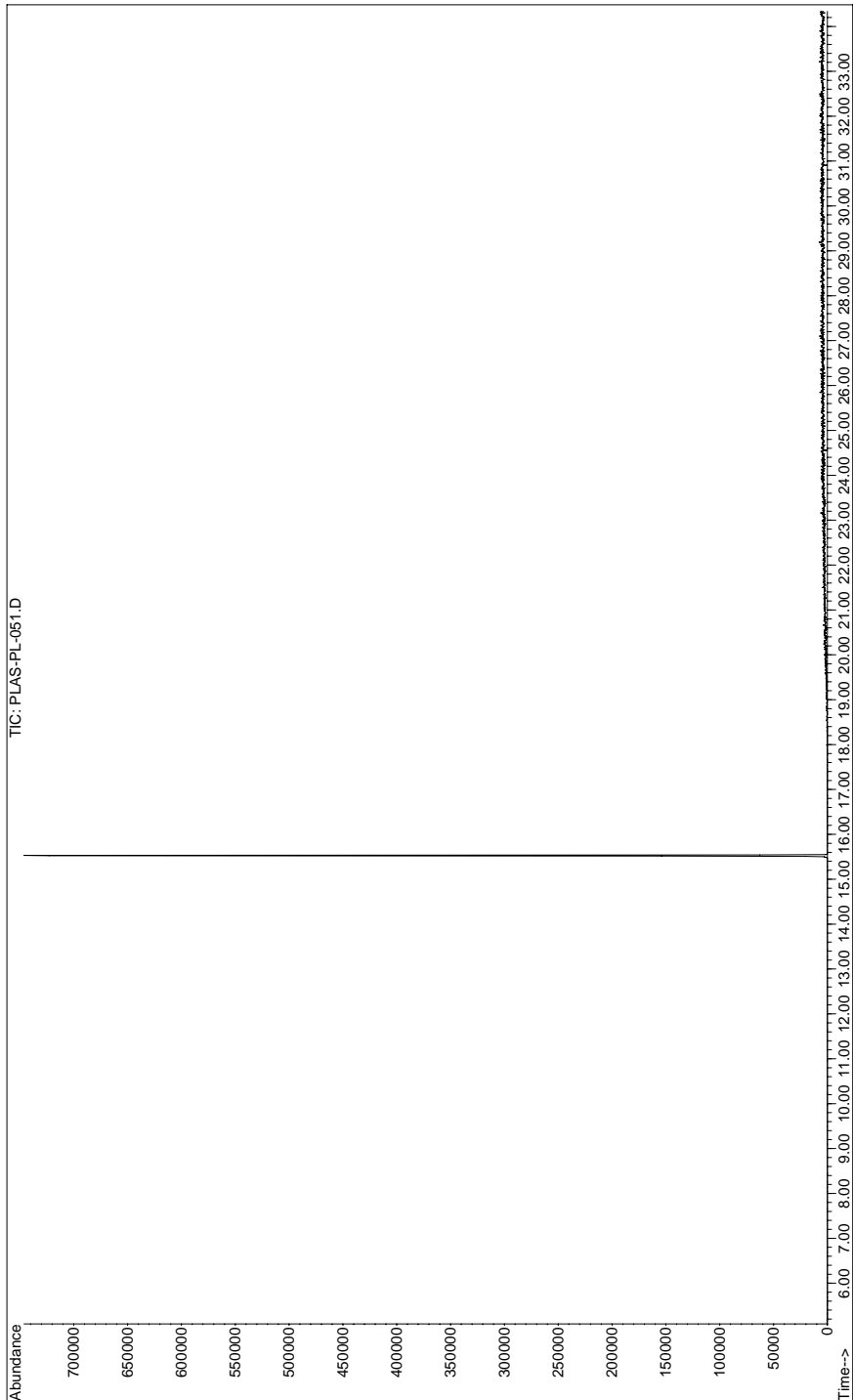
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Morflex® 310 - PLAS-PL-051

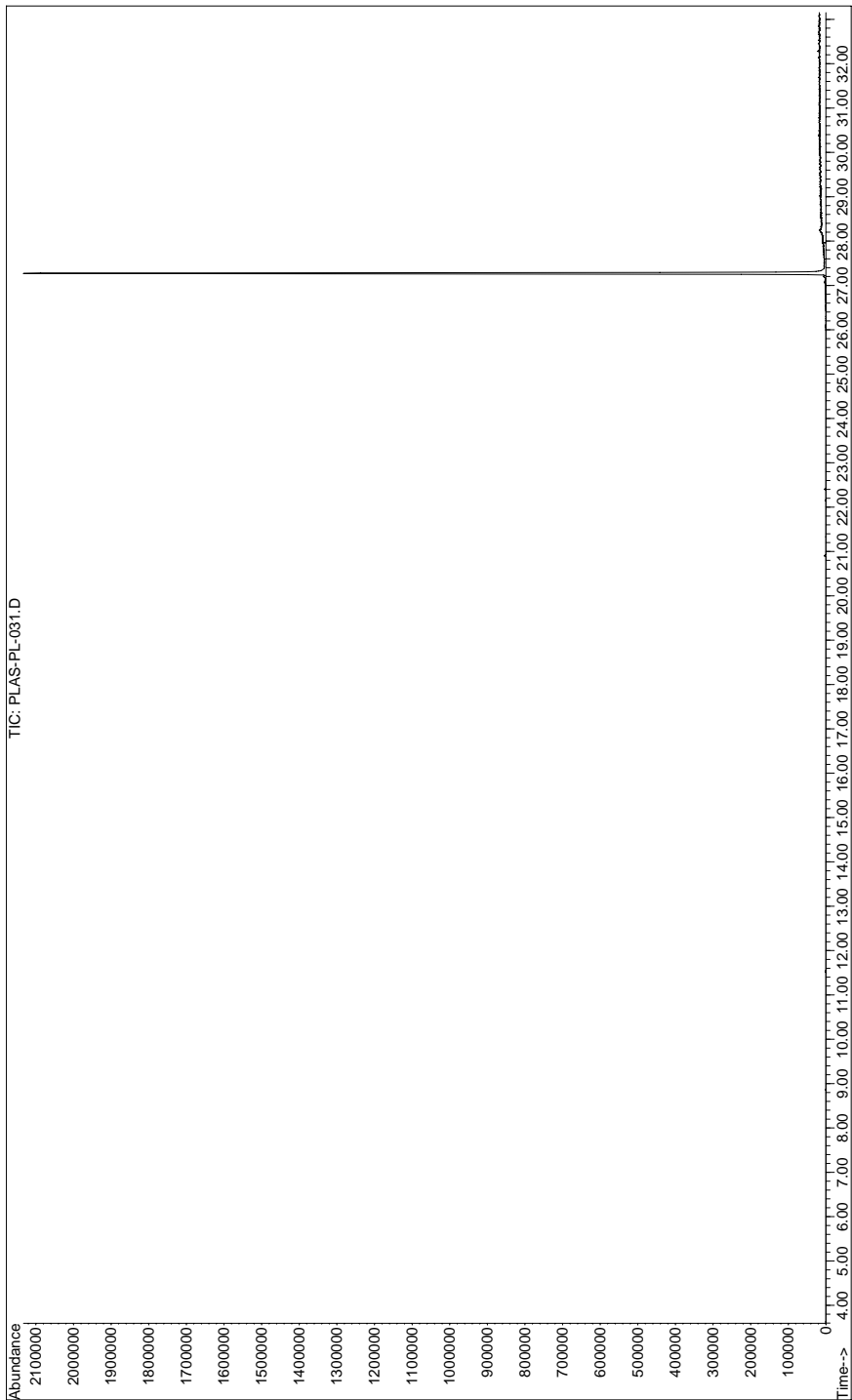
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Morflex® 560 - PLAS-PL-031

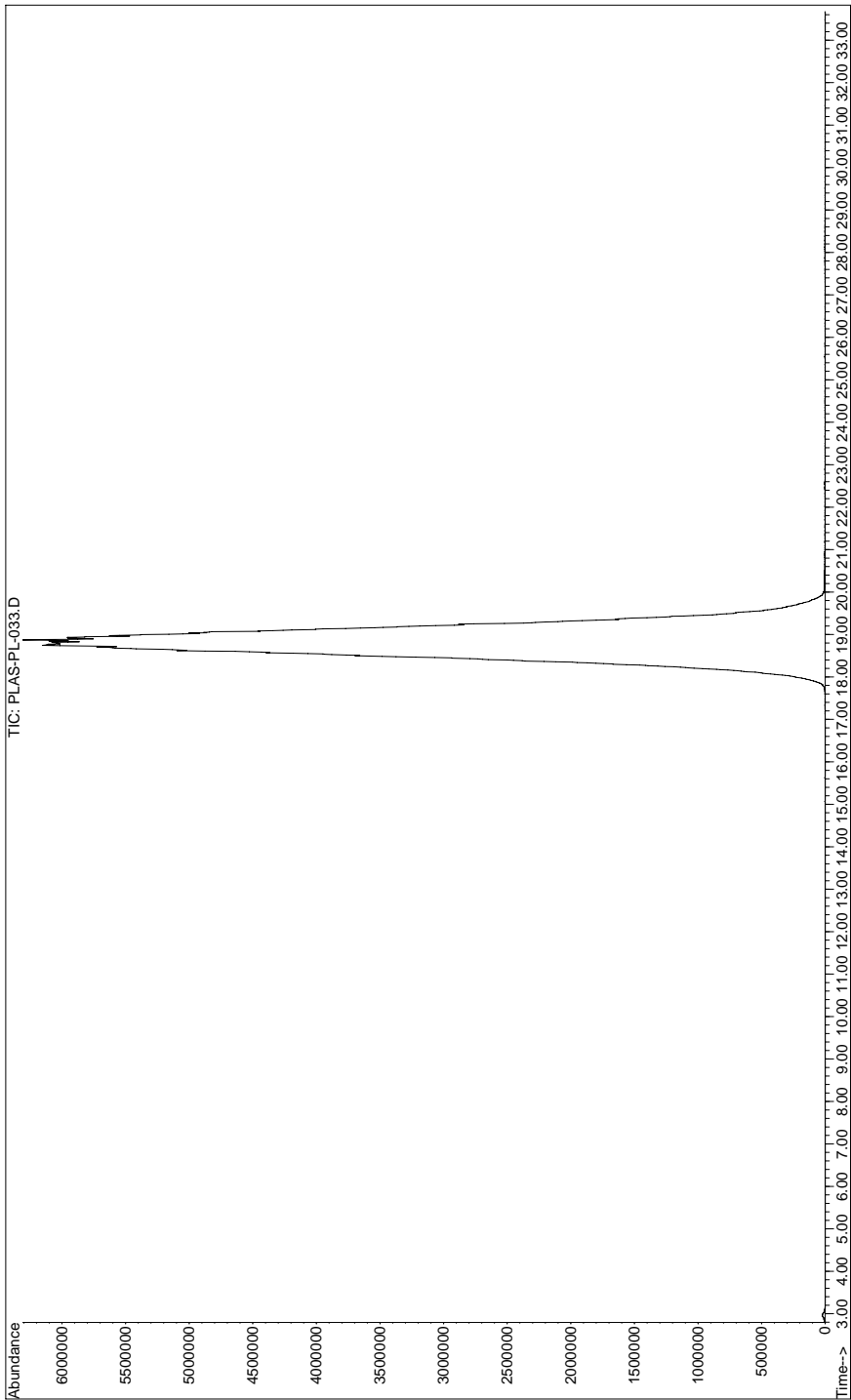
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Morflex[®] x-1125 - PLAS-PL-033

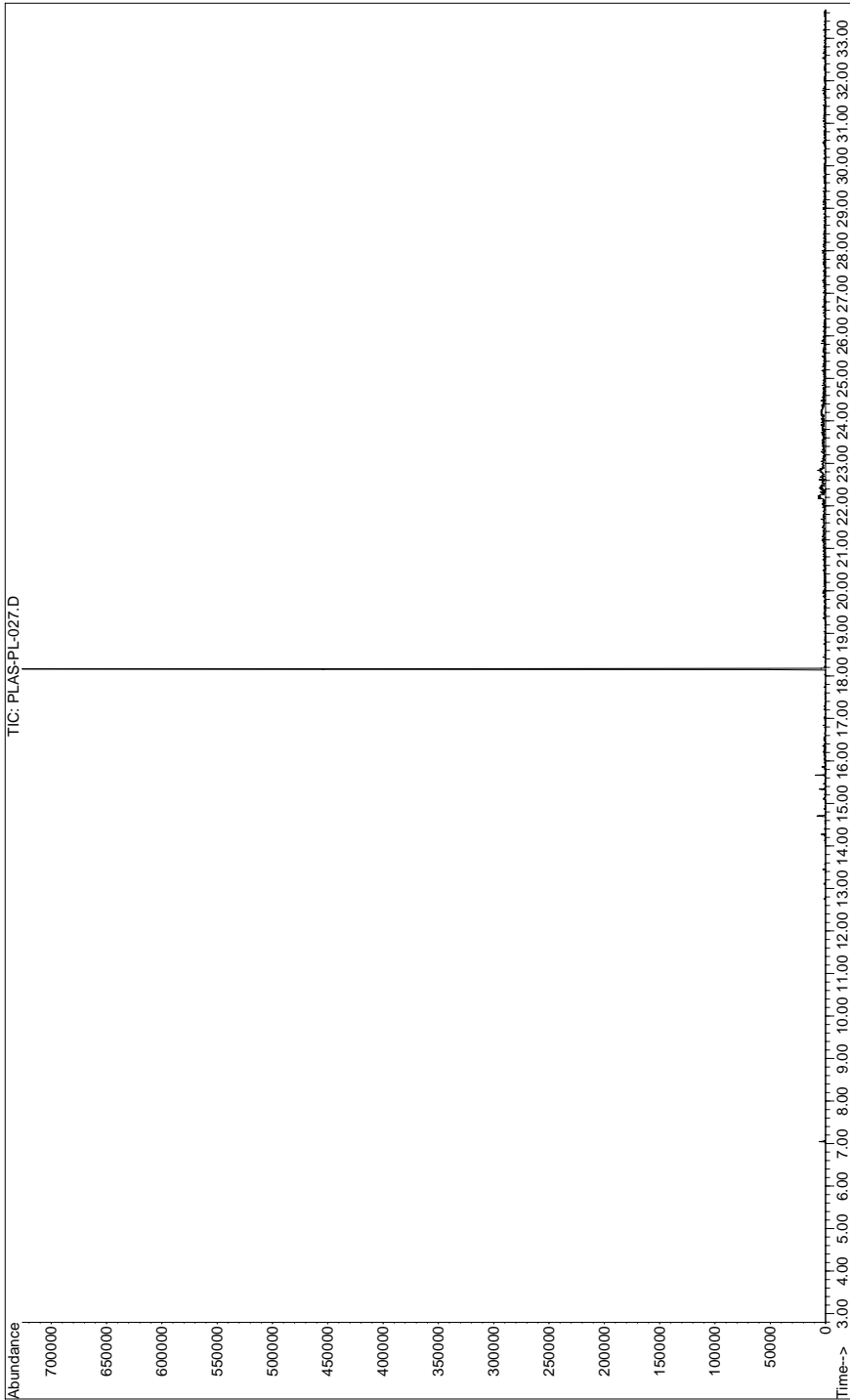
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Paraplex*® G-30 - PLAS-PL-033

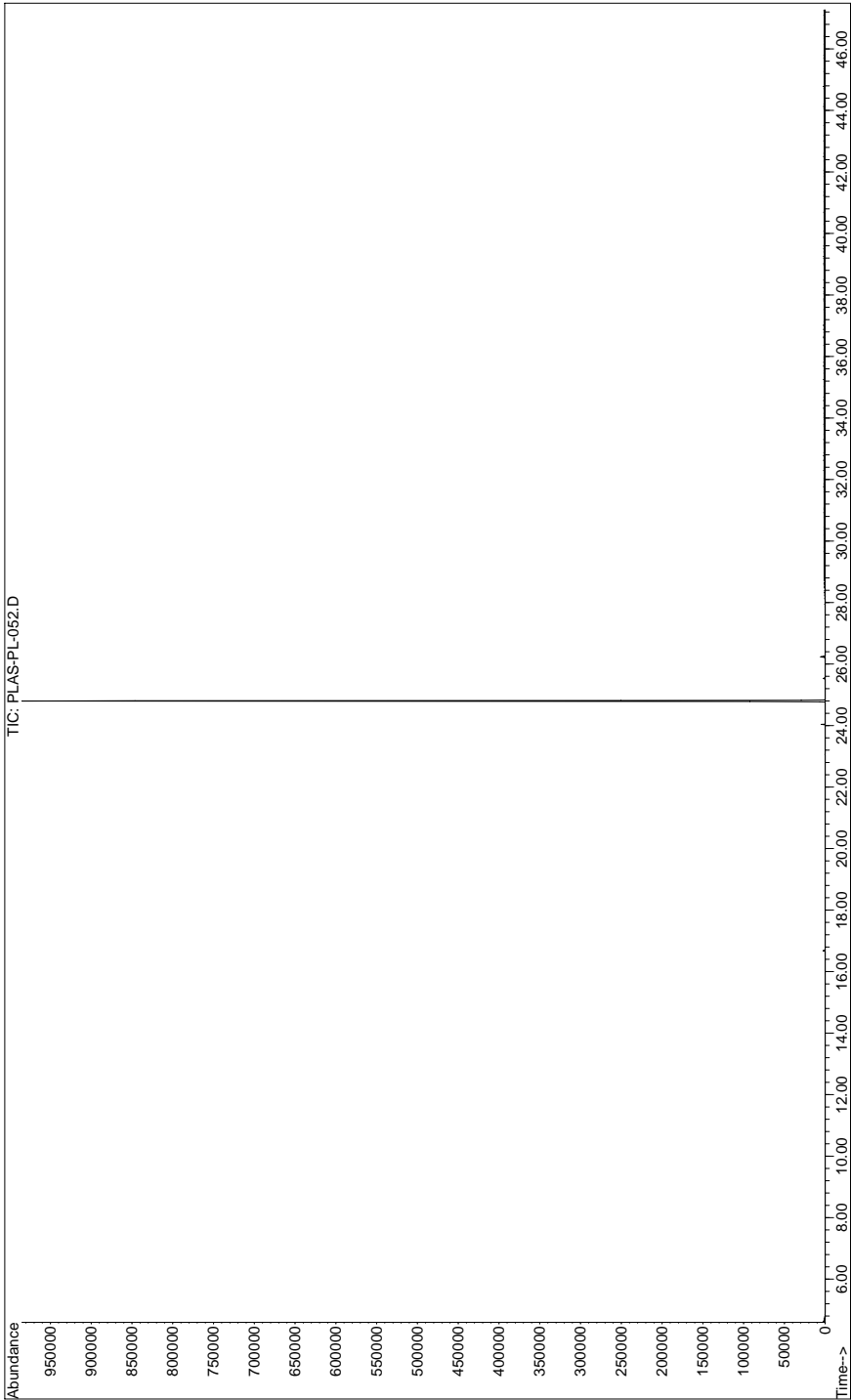
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Plasthall*[®] DOZ - PLAS-PL-052

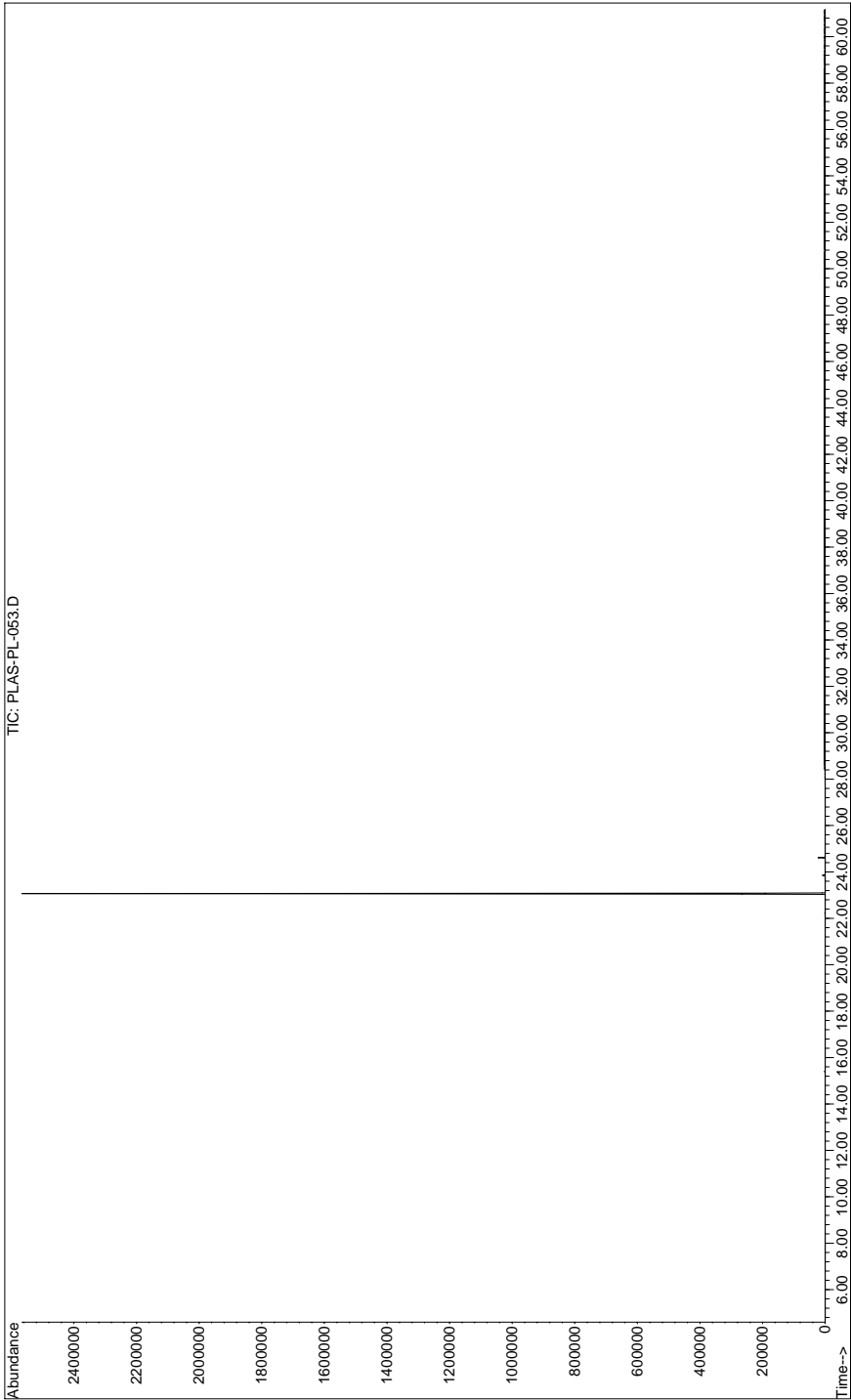
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Plastolein 9050* - *PLAS-PL-053*

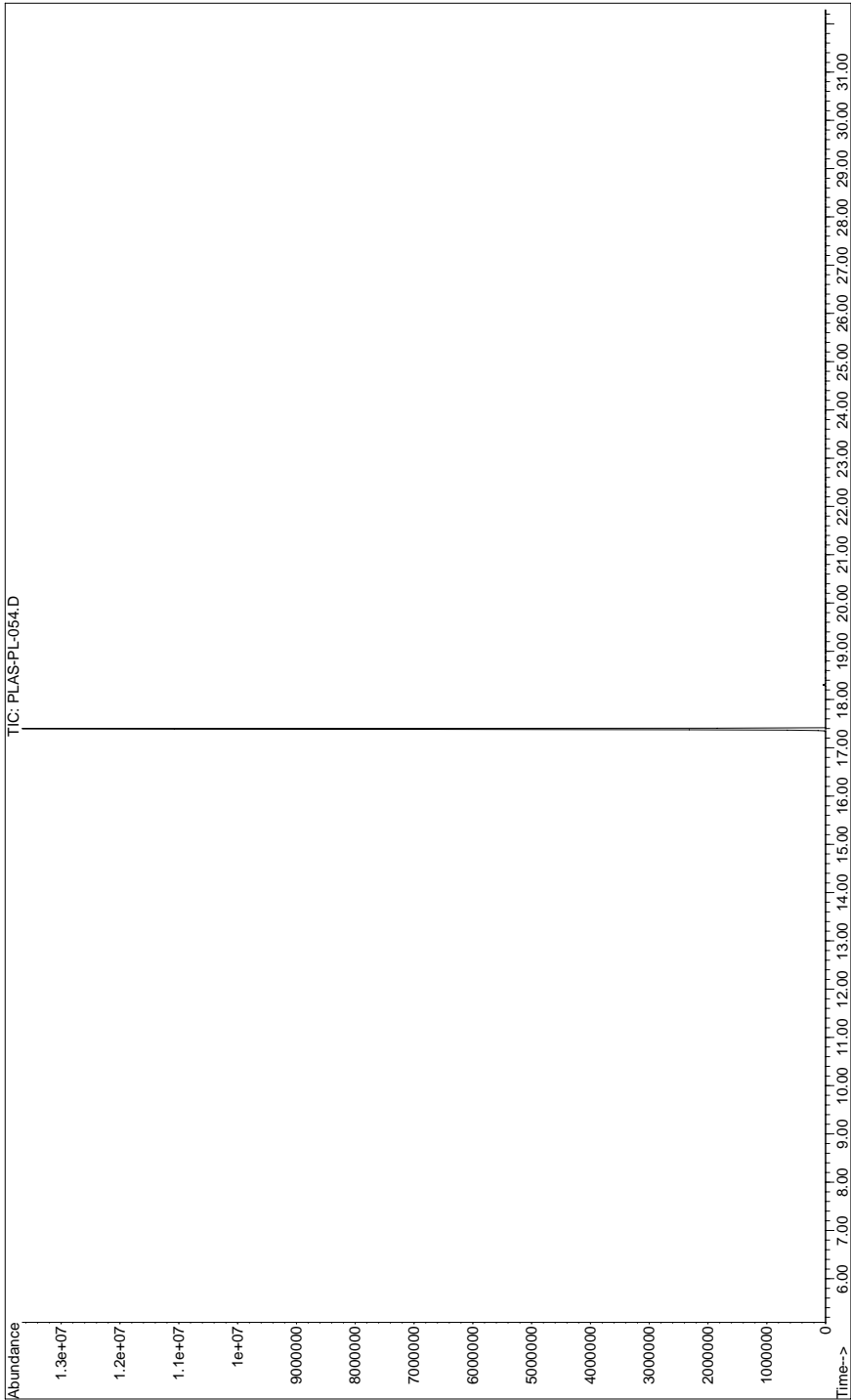
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Polycizer® 162 - PLAS-PL-054

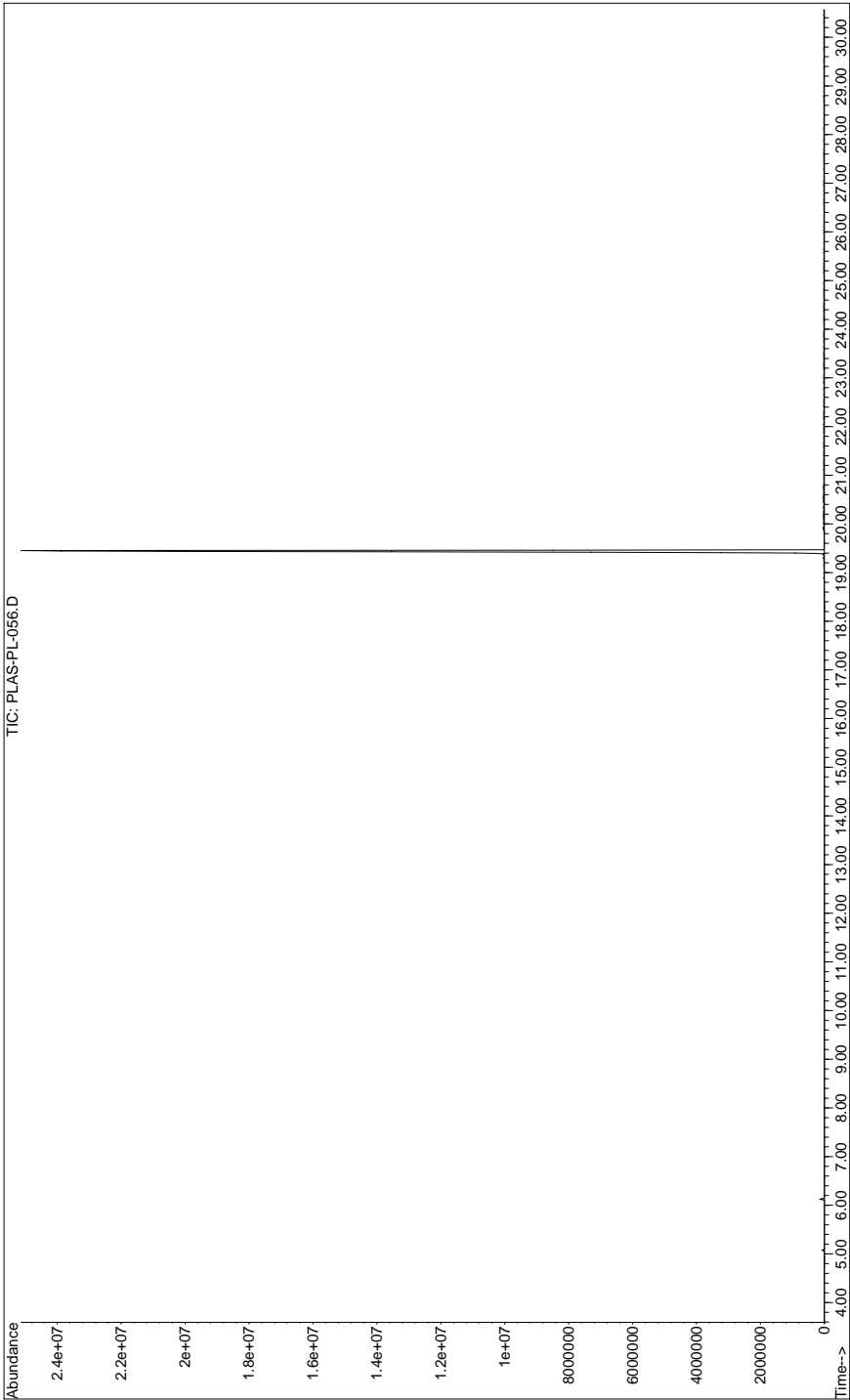
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for *Polycizer*[®] 632 - *PLAS-PL-056*

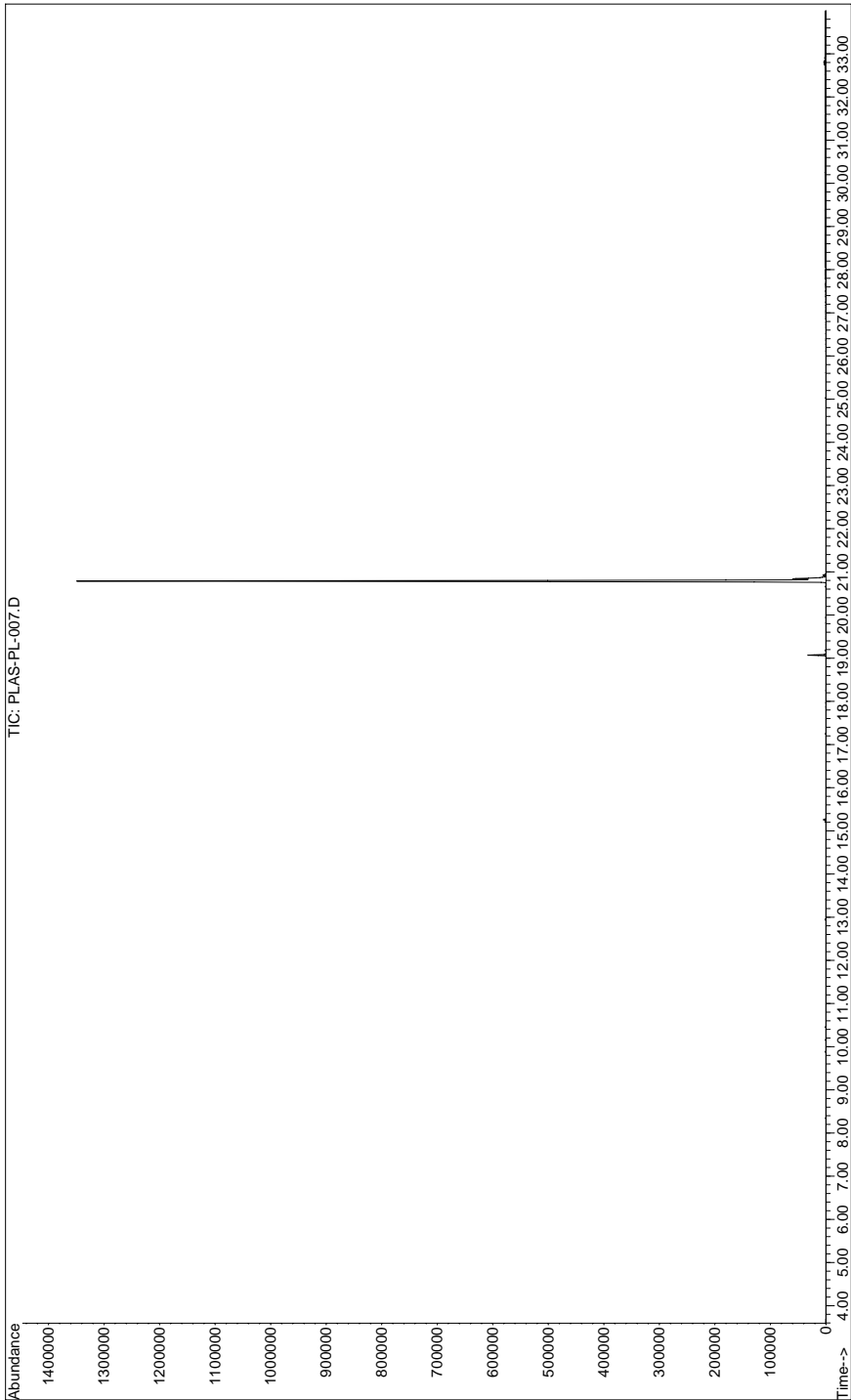
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for Polycizer® Butyl Oleate - PLAS-PL-007

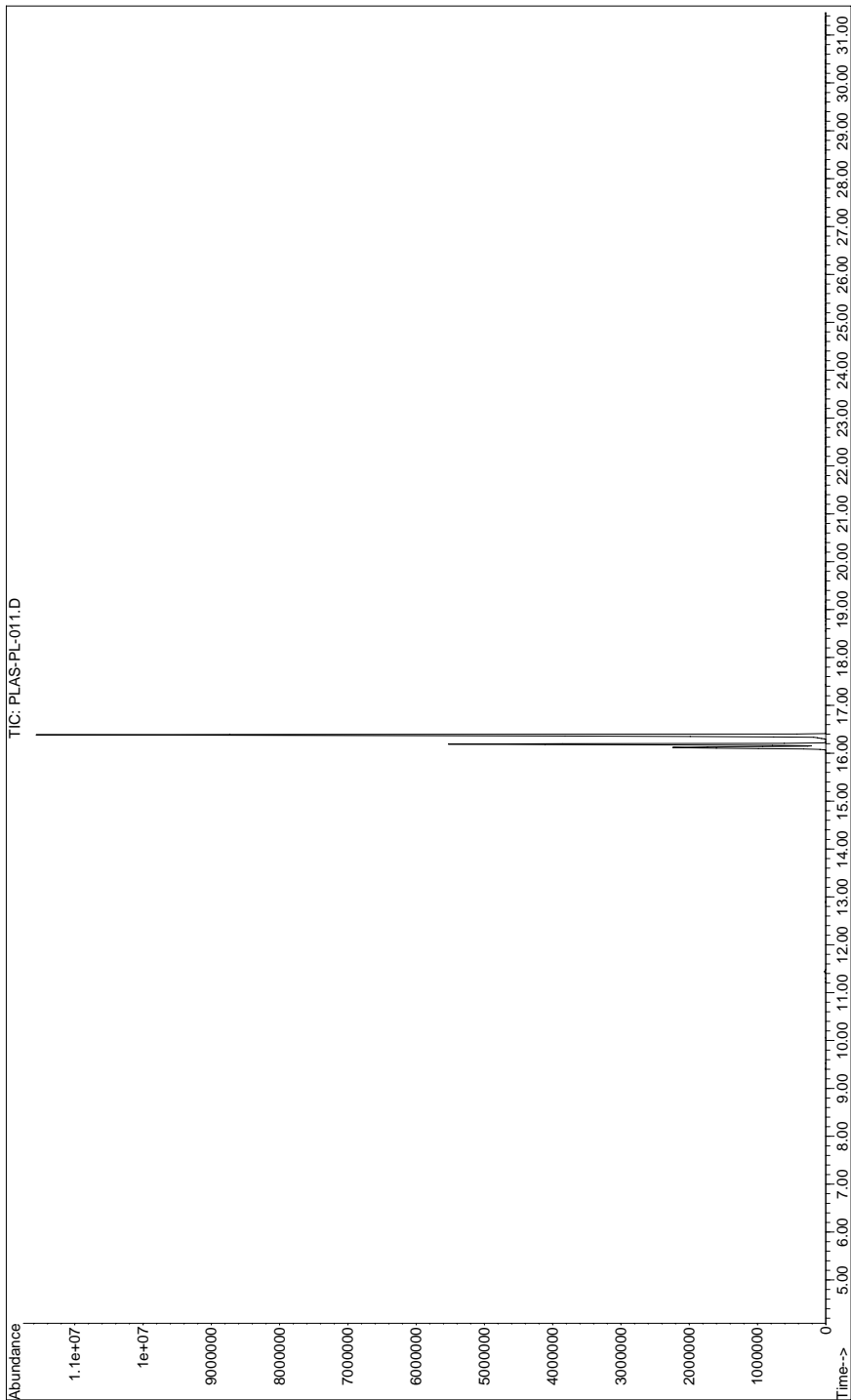
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for Polycizer® DP 500 - PLAS-PL-011

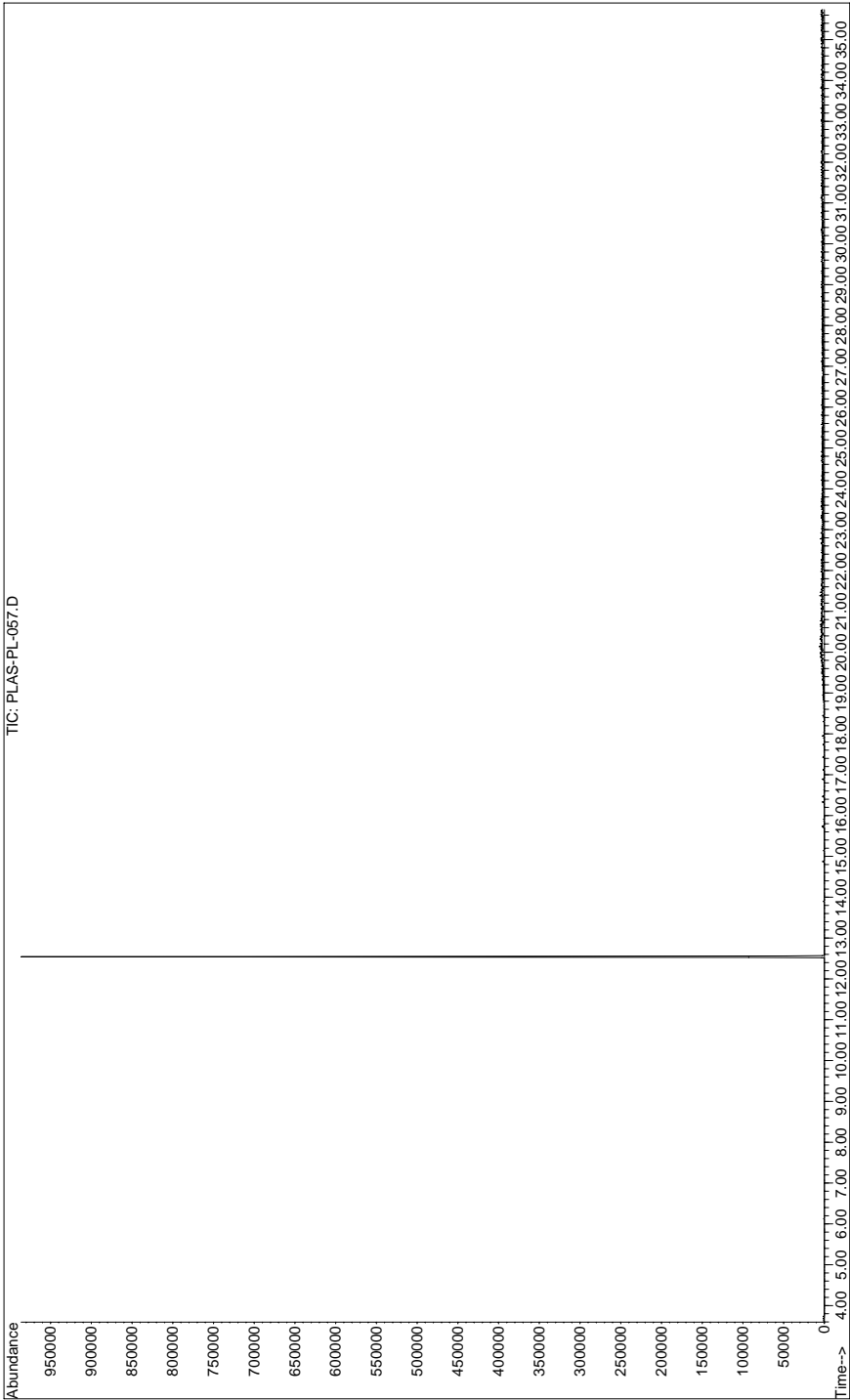
Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Polycizer® W 260 - PLAS-PL-057

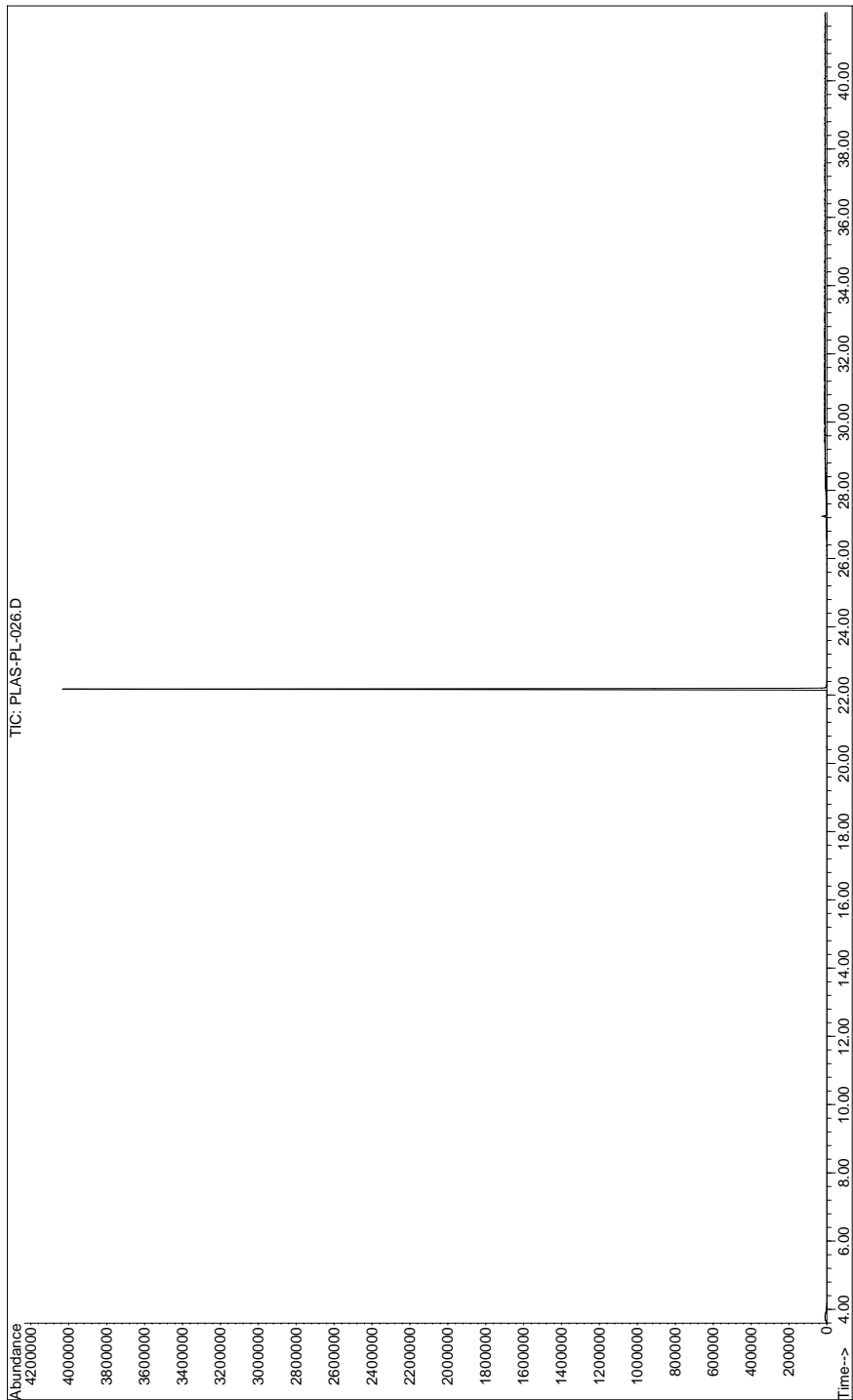
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Santicizer*[®] 141 - PLAS-PL-026

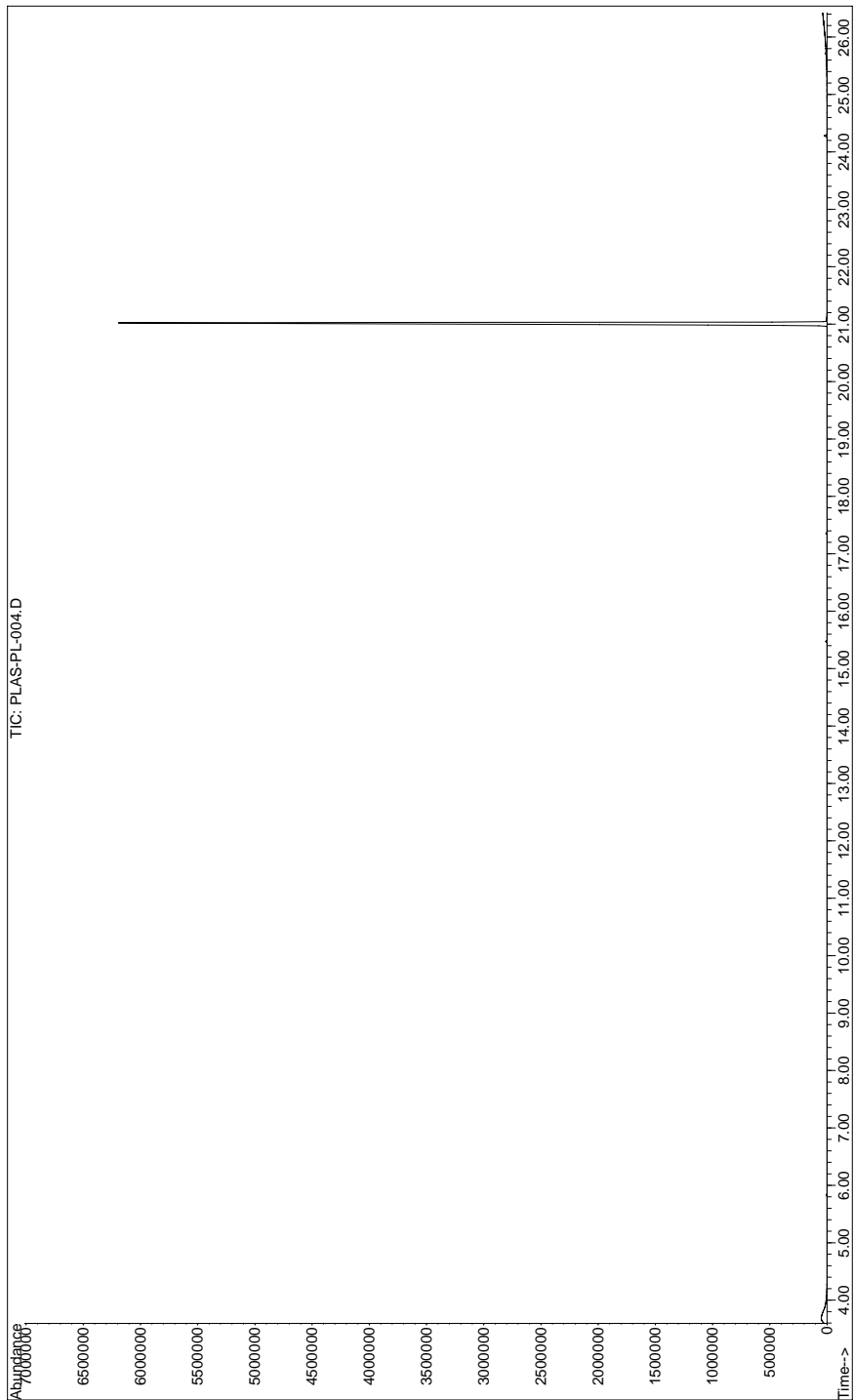
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Santicizer® 160 - PLAS-PL-004*

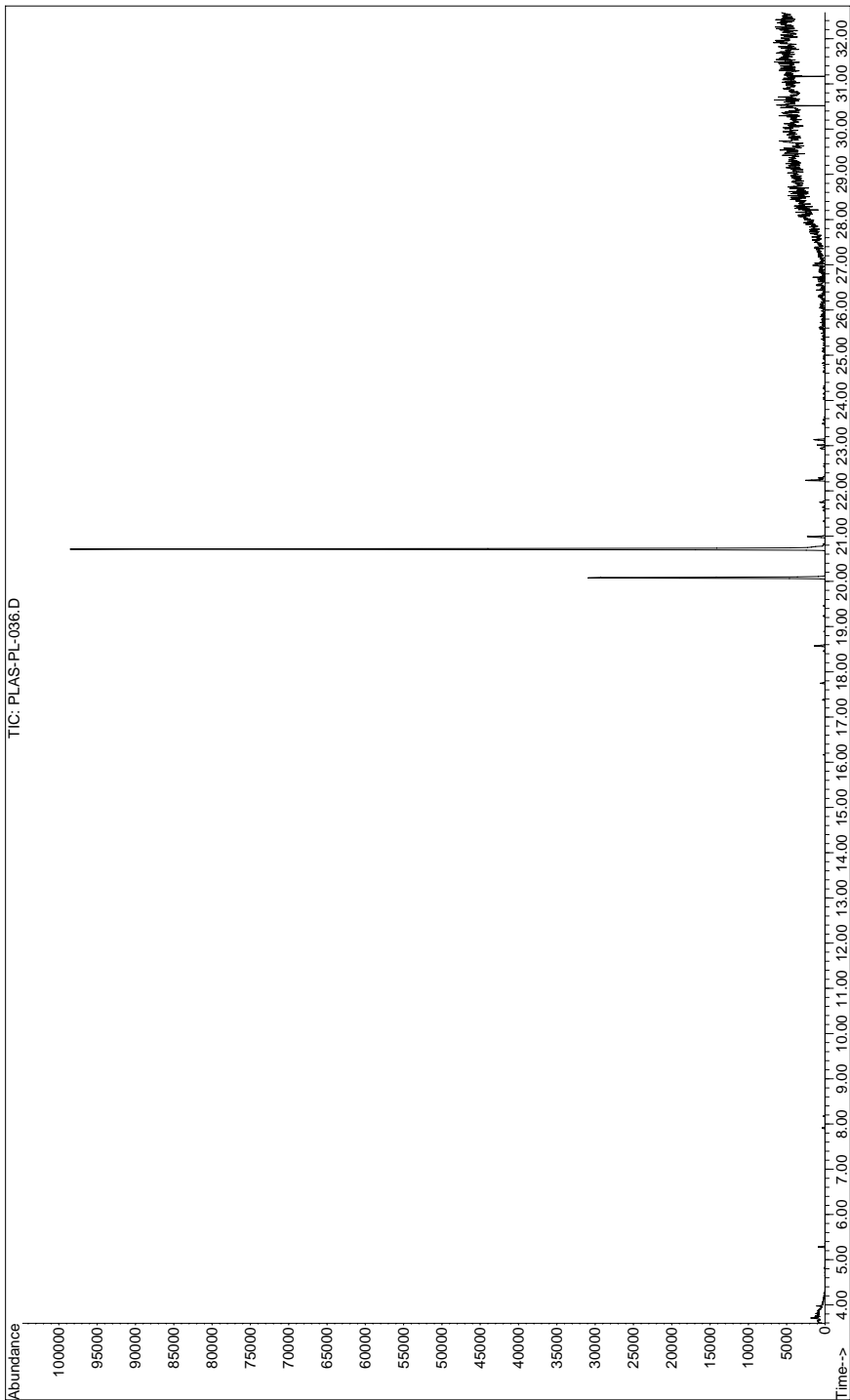
Analytical Conditions Summary 60 °C (0 min) to 330 °C (20 min) @ 10 °C/min Inj Temp=230 °C, Det=MSD



Analytical Information

Chromatogram for *Vinsol[®] resin - PLAS-PL-036*

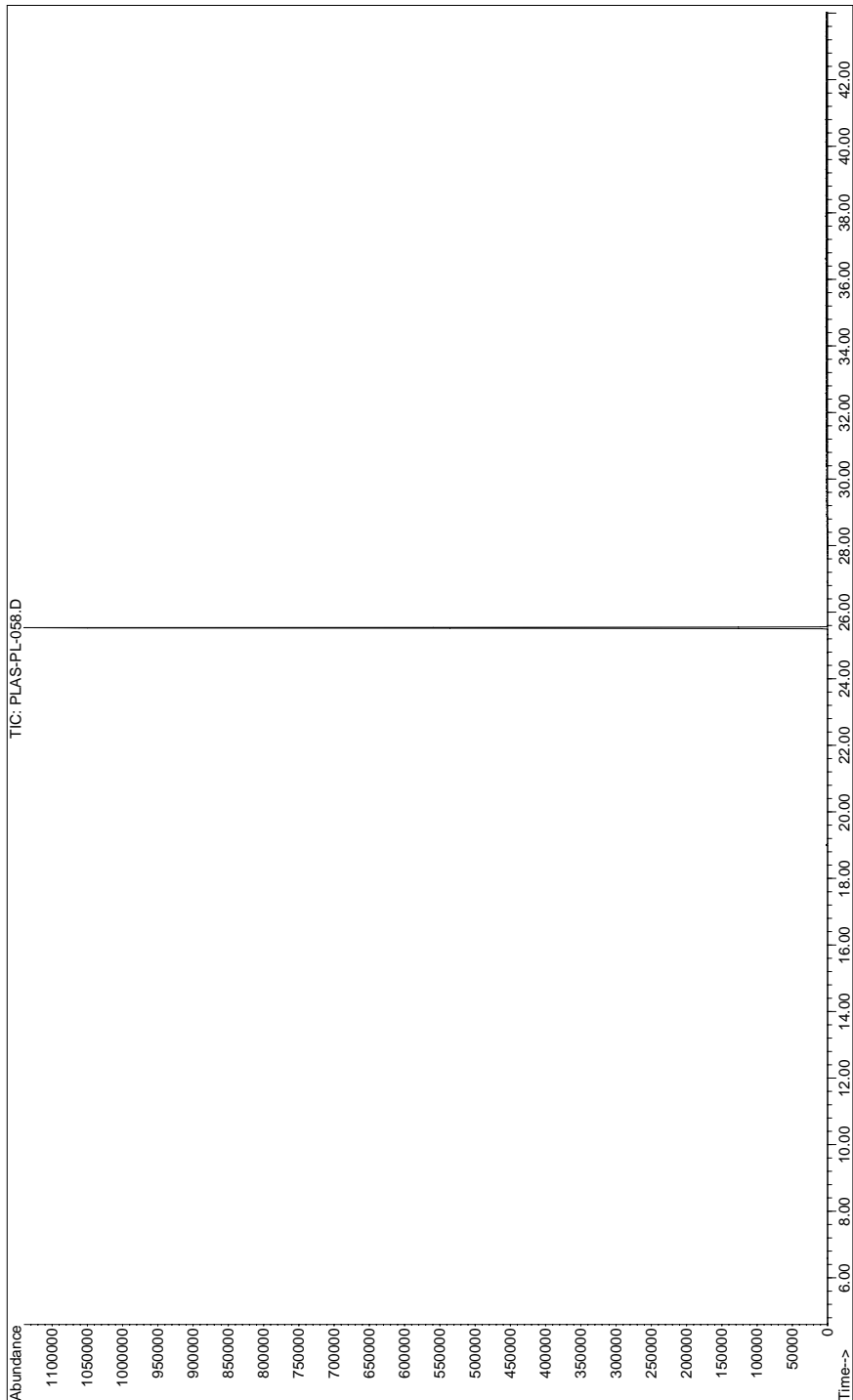
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 15 °C/min



Analytical Information

Chromatogram for *Witamol 500* - *PLAS-PL-058*

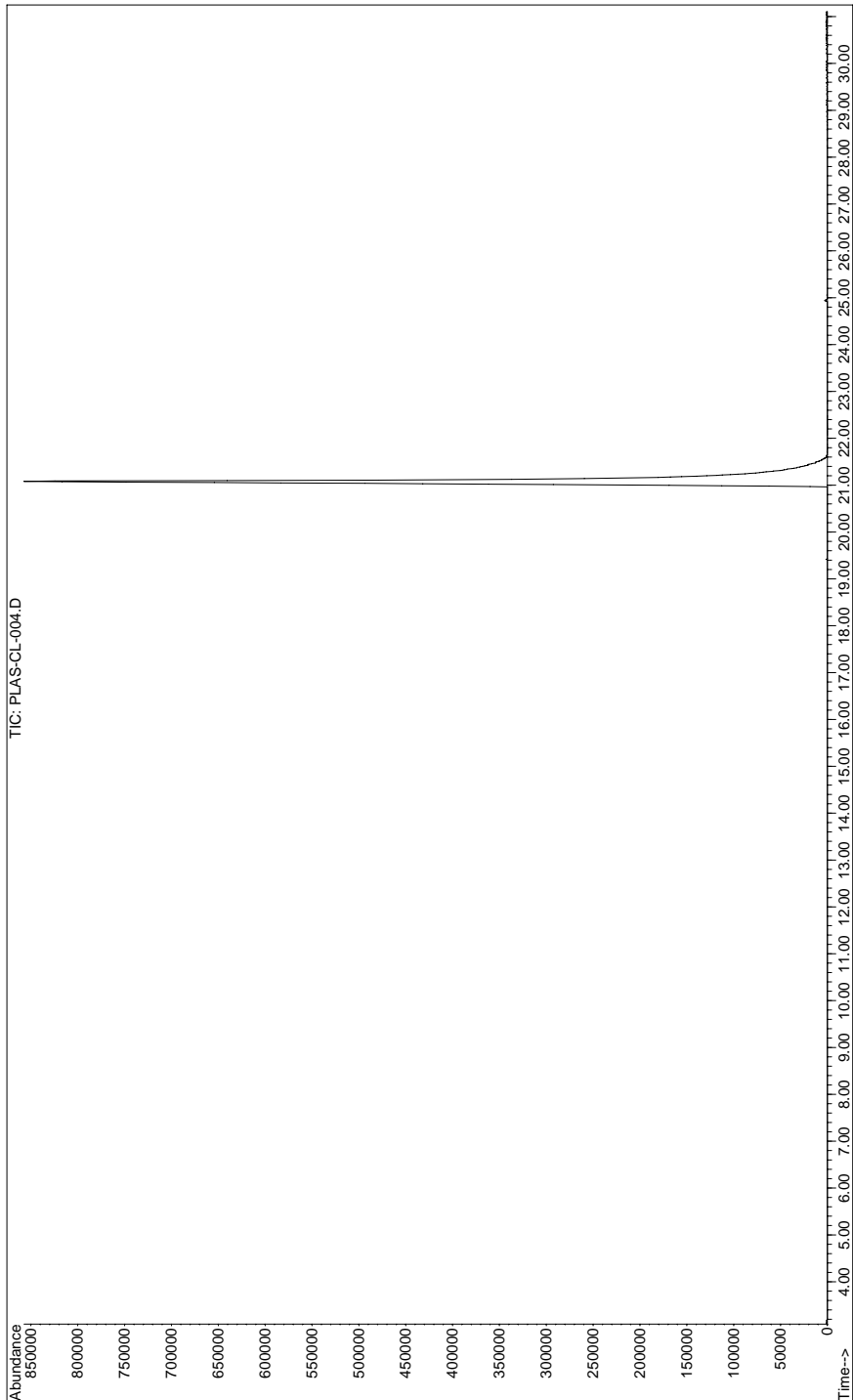
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Perkacit*[®] DPG - PLAS-CL-004

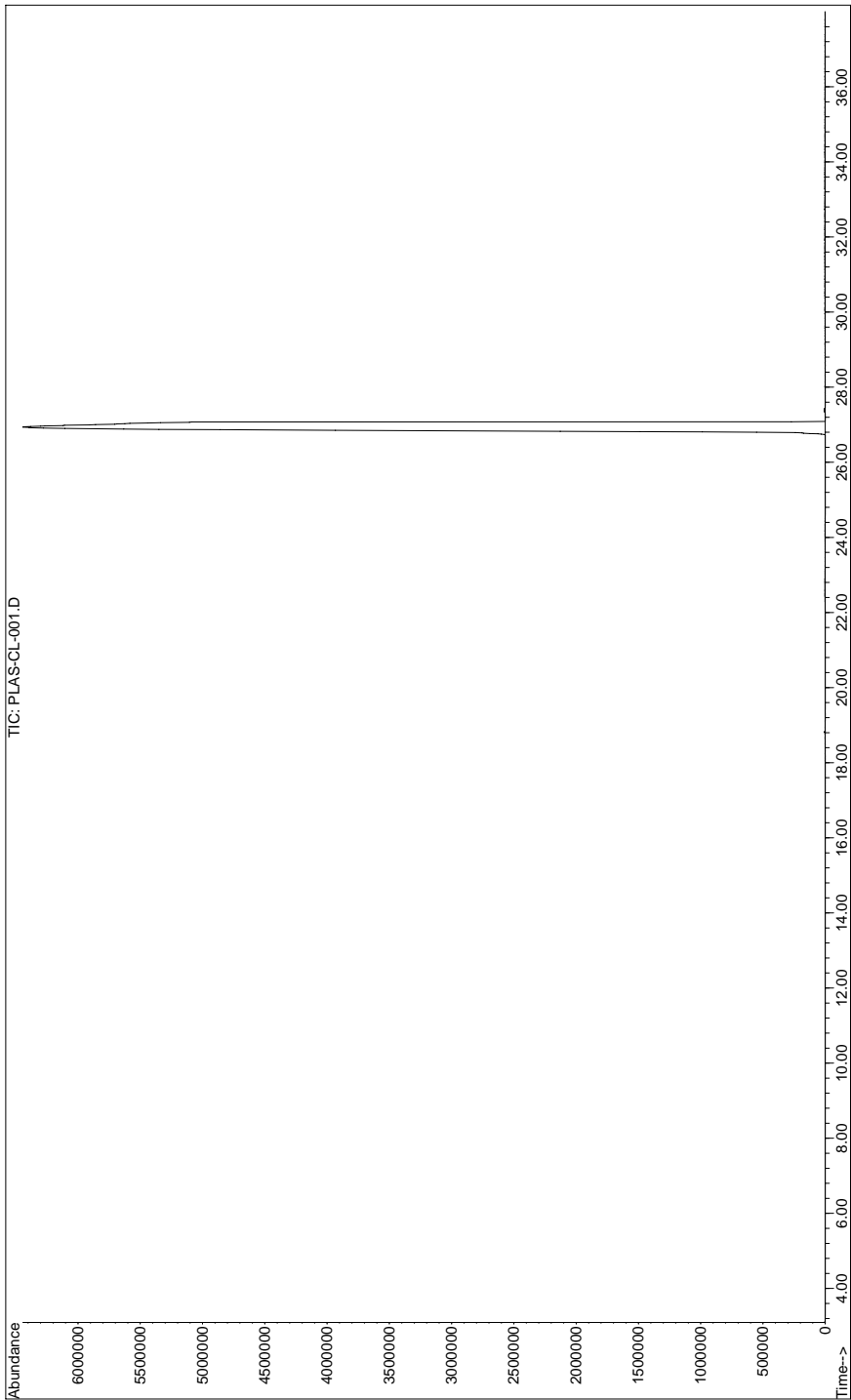
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Perkacit*[®] MBTS - PLAS-CL-001

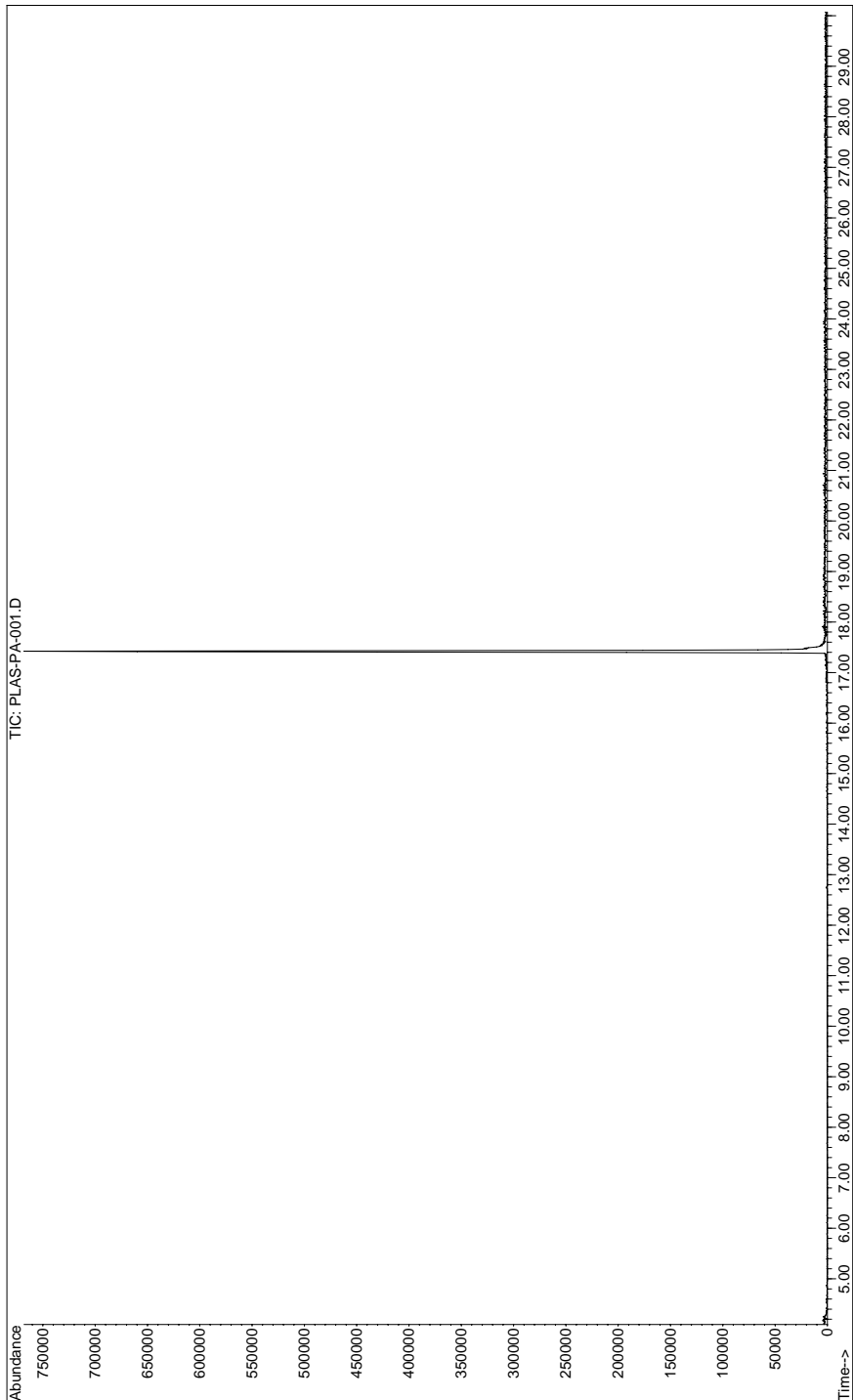
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for Kemamide® E ultra - PLAS-PA-001

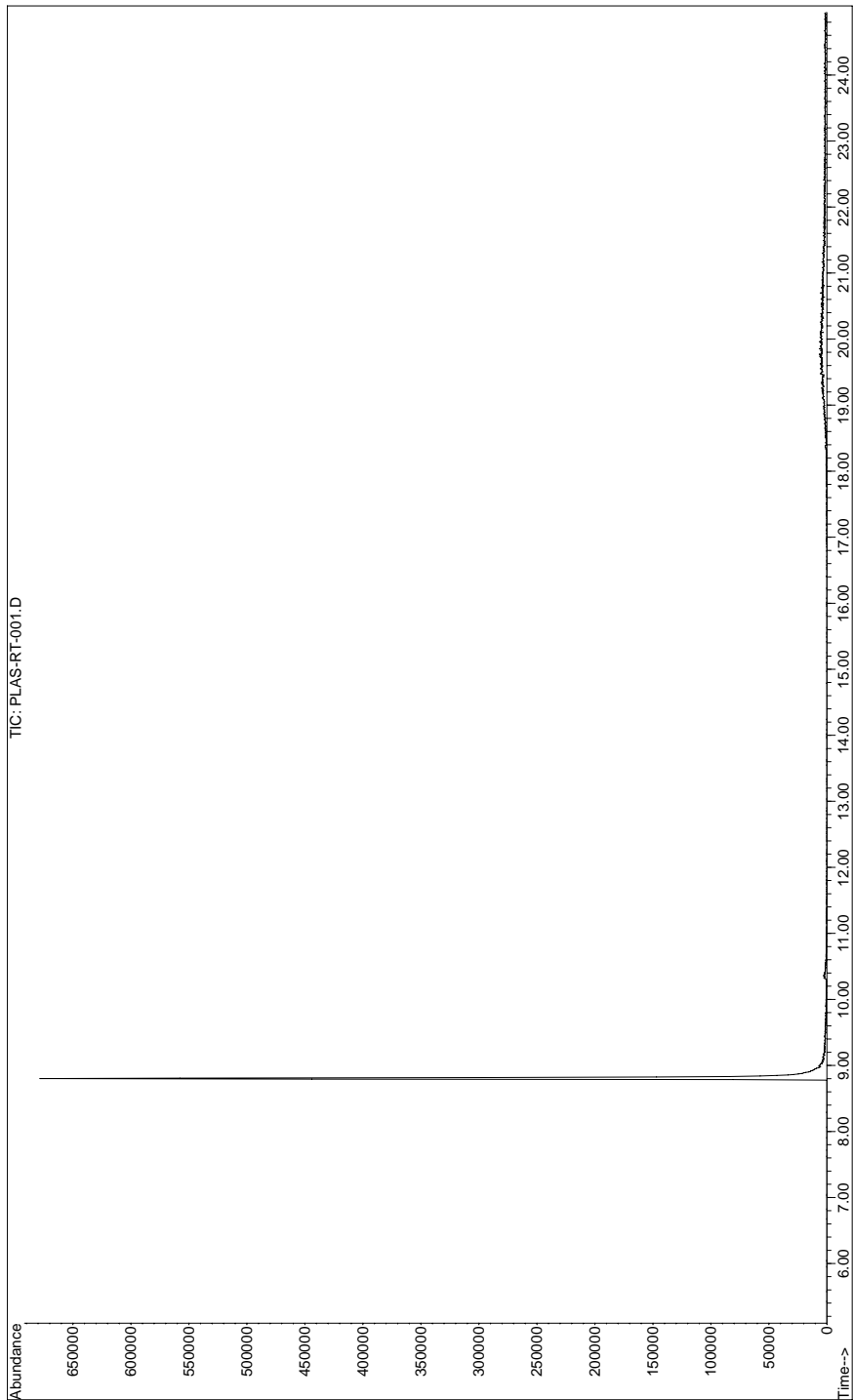
Analytical Conditions Summary 50 °C (0 min) to 350 °C (40 min) @ 15 °C/min Det=MSD



Analytical Information

Chromatogram for Retarder AK - PLAS-RT-001

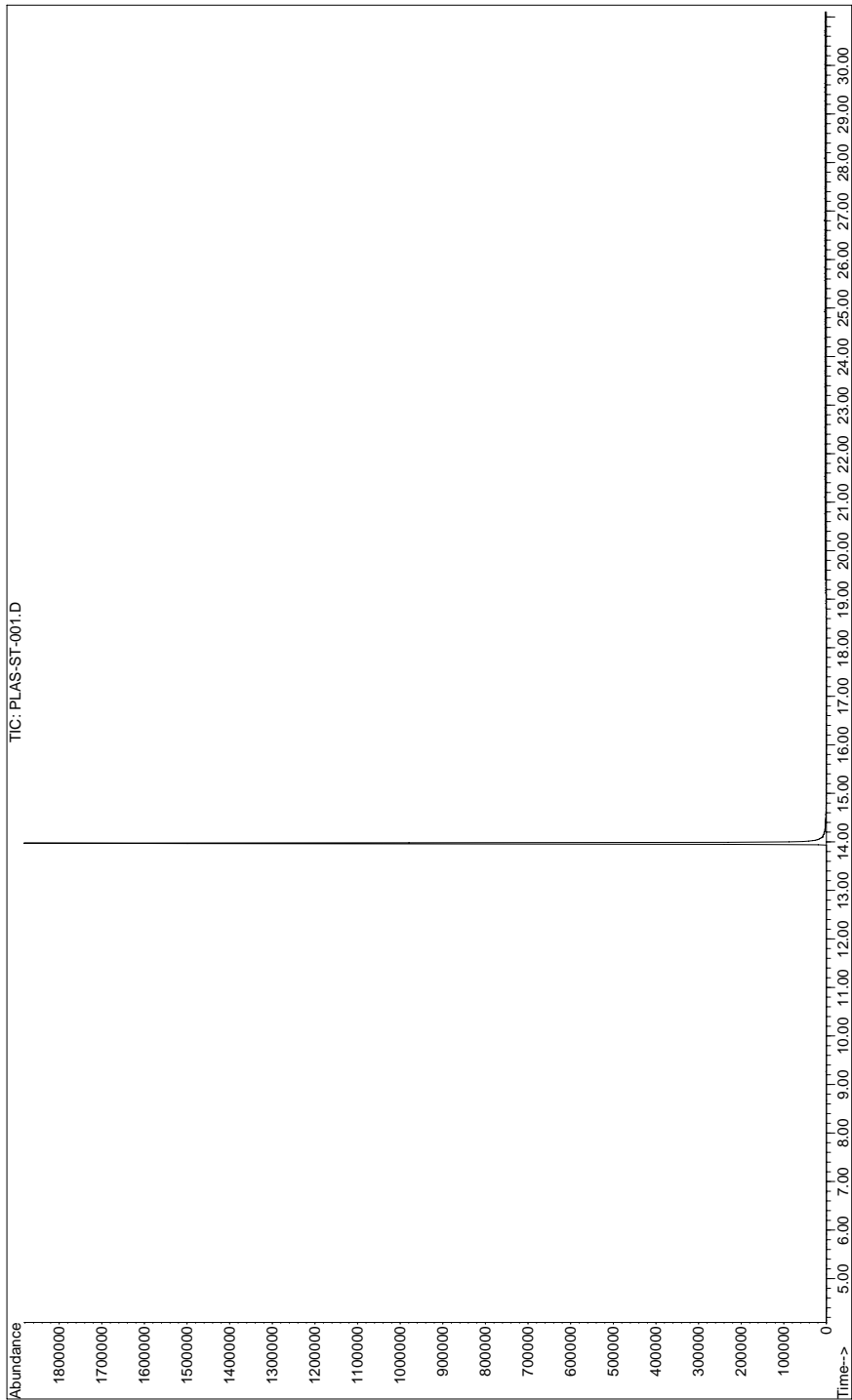
Analytical Conditions Summary 50 °C (0 min) to 330 °C (20 min) @ 10 °C/min
Inj Temp=250 °C, Det=MSD



Analytical Information

Chromatogram for *Stearic Acid RG (rubber grade)* - PLAS-ST-001

Analytical Conditions Summary 50 °C (0 min) to 340 °C (40 min) @ 15 °C/min Det=MSD



Definitions and Abbreviations

ABS	Acrylonitrile butadiene styrene
ACGIH	American Conference of Governmental Industrial Hygienists
ADI	Allowable daily intake
BCF	Bioconcentration Factor. The concentration of a chemical in a tissue per concentration of the chemical in water (reported as L/kg). BCF>1000 is considered a high potential for bioconcentration, between 1000 and 250 is considered moderate and <250 is considered low. <i>See also</i> Pow
	BCF is related to Pow by the following equation:
	$\log(BCF) = 0.79\log(Pow) - 0.4$
BR	Polybutadiene rubber
BW	Body weight
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CFR	Code of Federal Regulations
CM	Chlorinated polyethylene
CR	Neoprene
DMP	Dimethyl phthalate
CSM	Chlorosulfonated polyethylene
CWA	Clean Water Act
DMP	Dimethyl phthalate
DOT	Department of Transportation
E	Emulsifiable (as used in the solubility section)
ENR	Epoxidized natural rubber
EPM	Ethylene propylene rubber <i>see also</i> EPDM
EPDM	Ethylene propylene rubber <i>see also</i> EPM
EVA	Ethylene vinyl acetate
FDA	Food and Drug Administration (US). < www.fda.gov >
GRAS	Generally regarded as safe
HDPE	High density polyethylene
HRGC	High resolution gas chromatography
HRMS	High resolution mass spectrometry
IARC	International Agency for Research on Cancer
LC50	Lethal Concentration, 50% (median lethal concentration)
LD50	Lethal Dose, 50% (median lethal dose)
LDPE	Low density polyethylene

NBR	Nitrile-butadiene rubber
NIOSH	National Institute for Occupational Safety and Health
NOAEL	No observed adverse effect level
NOEL	No observed effect level
NTP	National Toxicology Program
NR	Natural rubber
OECD	Organization for Economic Co-operation and Development. < www.oecd.org >
OSHA	Occupational Safety and Health Administration
PBDE	Polybrominated diphenyl ether
PCP	Polychloroprene
PE	Polyethylene
PET	Polyethylene terephthalate
PETG	Polyethylene terephthalate glycol
PMMA	Poly(methyl methacrylate)
Polyols	A collective term for polyester, polyether, and aliphatic-multifunctional alcohols. All Polyols have more than one multifunctional alcohol group.
POM	Polyoxymethylene
POP	Persistent organic pollutant
Pow/Kow	log Pow or Kow are the partition coefficients of n-octanol/water. Substances with log Pow >3 are typically judged to have the potential to bioaccumulate. <i>See also</i> BCF
PP	Polypropylene
PS	Polystyrene
PVC	Polyvinyl chloride
RTECS	Registry of Toxic Effects of Chemical Substance
SBR	Styrene-butadiene rubber
SIS	Styrene-isoprene-styrene
TDLo	Lowest Published Toxic Dose
TPV	Thermoplastic vulcanizate
TSCA	Toxic Substances Control Act
U	Unknown (as used in the solubility section)
UR	Butyl rubber
UV	Ultraviolet

SUBJECT INDEX

A

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149	193	66	70		420.14	100	62	12	10		Hercoflex [®] 900, 236
149	263	77	133	57	336.38	100	37	16	14	12	Morflex [®] 190, 269
149	279	104	261	390	390.56	100	12	4	2	1	Polycizer [®] 162, 283
149	321	150	57	474	474.72	100	11	11	8	1	Jayflex [®] L11P-E Plasticizer, 257
151	257	274	124	108	274.29	100	30	29	15	12	Uvinul [®] 3049, 57
157	115	203	111	277	276.32	100	35	17	9	1	Citroflex [®] 2, 201
157	203	115	213	273	318.32	100	42	21	12		Citroflex [®] A-2, 205
158	159	115	157	173	173.25	100	12	8	7	5	Naugard [®] Q Extra, 145
161	203	129	218	175	784.08	100	77	52	51	44	Irganox [®] 3114 FF, 103
163	77	50	92	194	194.19	100	19	11	11	6	Hi-Point [®] PD-1, 239
163	77	164	76	194	210.22	100	18	10	9	7	2-Butanone peroxide (in DMP), 187
163	119	153	197	79	538.94	100	53	48	42	38	Silquest [®] A-1289, 163
163	134	175	119	221	221.37	100	66	46	44	1	Silquest [®] A-1100, 161
163	135	178	91	77	699.92	100	47	35	16	13	Cyanox [®] 1790, 71
163	199	79	63	276	276.55	100	23	23	9	7	Silquest [®] A-137, 165
164	163	106	77	51	164.23	100	65	32	12	10	Antioxidant 60, 69
167	69	108	63	123	167.25	100	23	15	15	11	Accelerator MBT, MBT/MG, 29

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171	55	255	152	83	356.54	100	86	78	41	31	Plastolein 9050, 281
171	71	55	112	283	412.65	100	40	33	28	6	Plasthall® DOZ, 279
175	190	58	235	176	699.92	100	77	63	20	15	Cyanox® 1790, 72
177	161	149	57	340	340.55	100	75	51	44	39	Cyanox® 2246, 75
177	220	135	67	149	775.32	100	52	42	41	36	Ethanox® 330, 85
182	223	57	238	149	238.38	100	53	52	39	35	Accelerator BBTS, 33
185	57	70	112	297	426.67	100	74	47	29	4	Witamol 500, 301
185	129	55	111	258	258.35	100	95	84	71	1	Polycizer® W 260, 293
185	129	57	259	351	276.32	100	73	27	25	1	Citroflex® 4, 203
185	129	259	57	403	402.54	100	56	52	26	1	Citroflex® A-4, 207
191	57	192	206	91	604	100	21	15	15	7	Alkanox® P27, 63
191	175	163	57	368	368.55	100	68	56	46	39	Cyanox® 425, 77
191	206	57	91	419	604.69	100	16	11	5	1	Ultranox® 626, 157
193	149	104	50	475	~800	100	39	35	8	1	Paraplex® G-30, 277
193	208	91	77	73	699.92	100	36	19	16	13	Cyanox® 1790, 73
194	193	195	192	209	N/A	100	21	21	11	11	Naugard® A, 121
205	220	57	206	145	600-700	100	24	16	16	12	Lowinox® CPL, 48
205	220	57	145	177	220.35	100	42	20	18	14	Naugard® BHT, 125
211	268	183	167	253	362.50	100	49	19	14	11	Jayflex® 77, 245
211	268	183	105	253	268.40	100	46	16	15	10	Santoflex® 6PPD, 43
213	137	214	77	51	214.22	100	80	67	46	30	Uvinul® 3000, 51
213	228	119	91	65	228.29	100	22	16	10	7	Bisphenol A, 193
213	326	43	137	105	326.43	100	37	36	33	32	Uvinul® 3008, 53
219	57	232	203	552	552.79	100	88	63	47	46	Irganox® MD 1024, 107
219	57	304	203	638	638.92	100	51	42	40	38	Irganox® 259, 101
219	191	234	57	220	775.32	100	27	26	18	16	Ethanox® 330, 86
219	218	217	108	115	219.28	100	64	51	23	16	Naugard® PANA, 133
219	263	58	163	203	263.42	100	26	19	12	12	Ethanox® 703, 93
221	250	222	192	71	250.38	100	19	16	10	8	Lowinox® AH25, 115

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226	225	165	227	152	N/A	100	45	28	16	10	Vinsol [®] resin, 299
227	151	228	77	51	228.26	100	81	66	38	21	Uvinul [®] 3040, 55
232	301	141	797	959	959.22	100	61	60	22	9	Decabromodiphenyl ether, 178
233	247	234	262	57	N/A	100	28	18	17	15	Naugard [®] PS-35, 143
233	247	262	57	217	262.43	100	29	17	10	6	Isonox [®] 132, 109
233	248	234	205		775.32	100	24	17	16		Ethanox [®] 330, 87
233	304	234	43	107	304.58	100	39	17	16	15	Santoflex [®] 77PD, 45
240	239	165	241	152	N/A	100	45	26	18	13	Vinsol [®] resin, 299
247	57	261	248	332	332.57	100	32	25	19	4	Isonox [®] 232, 112
247	261	57	55	332	332.57	100	64	63	23	5	Isonox [®] 232, 113
251	250	94	249	252	362.40	100	24	18	16	13	Santicizer [®] 141, 294, 295
260	261	183	167	77	260.36	100	21	17	16	15	Naugard [®] J, 129
266	98	194	123	85	~255	100	31	28	24	19	Halowax 1001, 183
266	267	337	250	322	N/A	100	23	15	10	7	Naugard [®] PS-30, 140
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266	281	267	97	125	N/A	100	32	21	15	7	Naugard [®] PS-30, 139
277	57	292	147	219	1177.65	100	41	37	28	23	Naugard [®] B-25, 123
277	193	278	379	462	462.62	100	22	17	8	1	Morflex [®] 560, 273
277	292	147	219	57	642.93	100	39	24	22	21	Irganox [®] 1035, 97
277	292	147	57	219	1177.65	100	38	32	26	22	Ethanox [®] 310, 83
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292	289	293	220	222	N/A	100	84	49	49	26	Aroclor 1242, 179
300	242	108	122	166	332.48	100	56	37	16	12	Perkacit [®] MBTS, 307
322	323	250	393	57	N/A	100	27	17	14	6	Naugard [®] PS-30, 141
326	325	169	215	94	368.37	100	88	25	23	20	Imol S-140, 241
331	332	158	346	315	173.25	100	27	18	6	6	Naugard [®] Q Extra, 146
354	165	104	181	368	368.37	100	32	16	13	1	Imol S-140, 242
358	164	149	136	302	358.54	100	98	84	26	7	Irganox [®] 1081, 99
358	343	359	136	164	358.54	100	41	25	21	13	Lowinox [®] TBM-6, 117

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371	372	355	170	178	173.25	100	29	22	20	15	Naugard® Q Extra, 147
382	91	165	103	179	368.37	100	31	30	29	24	Imol S-140, 243
390	405	391	406	187	405.57	100	54	31	18	15	Naugard® 445, 119
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406	404	465	563	297	564.72	100	99	90	89	20	2,2',4,4',5-Pentabromodiphenyl ether, 173
409	424	367	57	219	424.66	100	80	28	25	14	Ethanox® 702, 91
430	165	205	57	121	430.71	100	71	8	6	4	Irganox® E 201, 105
430	428	432	358	288	N/A	100	94	65	63	30	Aroclor 1260, 181
441	57	442	147	646	646.92	100	82	31	23	12	Naugard® B-25, 123
460	57	177	215	445	600-700	100	78	38	38	32	Lowinox® CPL, 49
466	57	468	116	467	467.45	100	60	57	29	26	Naugard® NBC, 131
466	57	468	467	116	467.45	100	64	53	28	24	Naugard® NBC, 131
484	74	486	482	62	643.62	100	87	72	62	49	2,2',4,4',5,5'-Hexabromodiphenyl ether, 175
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