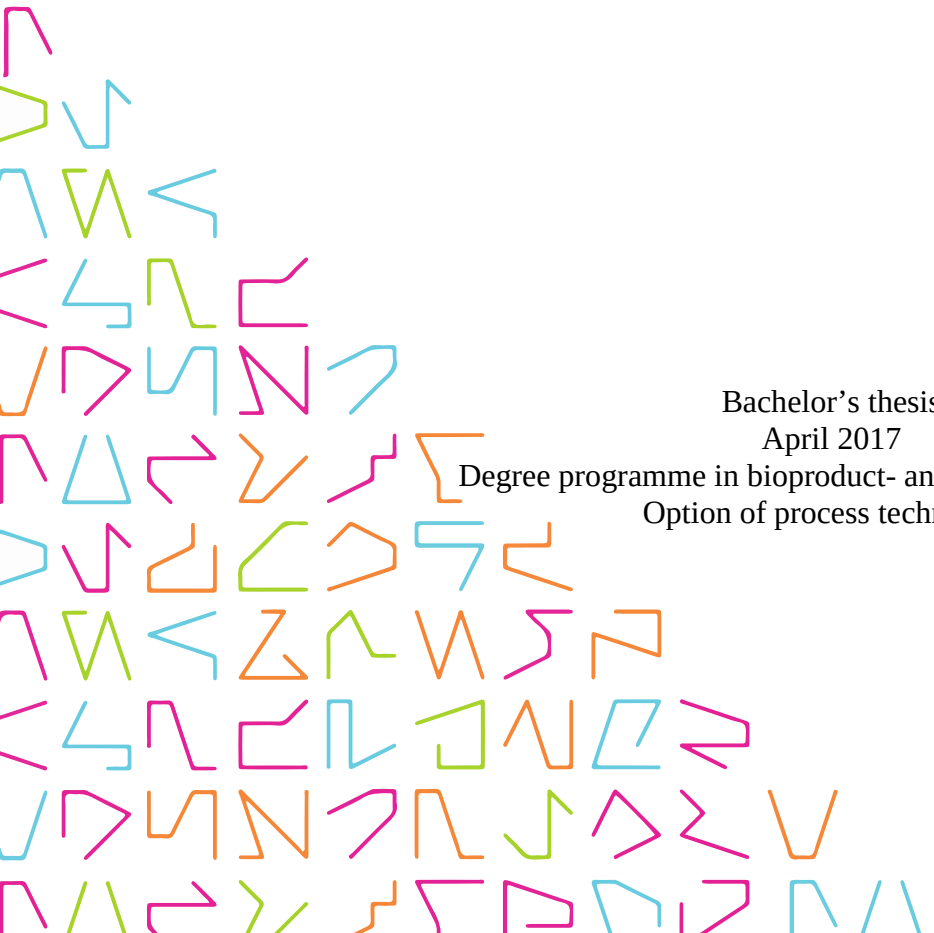
TAMPEREEN
AMMATTIKORKEAKOULU

FATTY ACID COMPOSITION AND SHELF LIFE OF CRICKET FLOUR

Ville Kontio



Bachelor's thesis
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ABSTRACT

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Fatty Acid Composition and Shelf Life of Cricket Flour

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This thesis was made for Finsect Oy to determine the fatty acid composition of their cricket flour product. In addition common packaging methods, use of food additives, and fat extraction were researched to find a prominent way of extending the current shelf life.

In theoretical part of this thesis the nutritional content of crickets and the main causes of spoilage were researched to choose the correct procedures for determination of fatty acid composition. The shelf life prolongation methods were researched by investigating the packaging methods, commonly used preservatives and antioxidants in foods, and industrial fat extraction procedures that are used by food stuff industry currently.

In the practical part the fat extracted from cricket flour was tested using a gas chromatograph. From the results of the analysis could be acquired the fatty acid composition of cricket fat, early changes in fatty acid composition, and an approximate of fatty acid decrease rate. Although, the shelf life could not be determined in this work some useful information for future tests was uncovered.

Key words: shelf life, spoilage, preservation

CONTENTS

ABBREVIATIONS AND TERMS

Adepocytes	Animal fat cells
Organoleptic	Sensing through odor, flavor, sight, and touch
GC	Gas Chromatograph
MS	Mass Spectrometer

1 INTRODUCTION

It is estimated that by the year 2050 the earth's population will rise up to over 9 billion which also means that the need of food will rise also. At the moment 40 % of earth's land area is used for food production, therefore, new and more efficient methods of food production are needed. Especially in production of protein based foods. (Huldén, 2015, 7)

One auspicious way to fulfill the growing need for protein is insects. Insects are in every way more efficient source of food than their vertebrated counterparts. This efficiency consists of 2 things: upholding body heat and the utilizable portion of the body. Insects do not use energy to uphold their body heat since they are cold-blooded. Also 80 % of e.g. a house crickets' (Acheta domesticus) body can be used for food when the number for cattle is 40 % and for chicken and pork 55 %. (Huldén, 2015, 167-170)

The use of insects in food industry is not yet allowed in the EU-area but it seems that laws concerning the use of insects for nutritional purposes will be alleviated. The use of insects in foods will fall under EUs regulation (EC) No 258/97 on novel foods and it will be applicable for use from 1.1.2018. (European Parliament, 2016, 1)

Finsect Oy is one of the pioneering companies that has brought the cricket production to Finland and the purpose of this thesis is to determine cricket flour's current shelf life and research some promising methods to prolong the shelf life. The greatest problem for shelf life of ground crickets is fat spoilage, in other words rancidification.

In theoretical part of this thesis different kinds of shelf life prolongation methods are examined by comparing the use of food additives and possible packaging methods. The possibility of removing easily spoiling fat is also investigated. Practical part of thesis consists of testing the current shelf life and determining the fatty acid composition of house cricket flour.

2 CONTENTS OF GROUND CRICKETS

The nutritional content of house crickets varies depending on the source but generally it is a food with high amounts of protein along with healthy fatty acids, carbohydrates and essential minerals. A major factor determining the nutritional content is the given feed. On average 100 g of house cricket flour contains 67.8 g of protein, 5.5 g of carbohydrates and 5.6 g of fat which adds up to 350 kilocalories in energy. (European Journal of Clinical Nutrition, 2016, 289; Finsect Oy, 2017)

2.1 Proteins and amino acids

Proteins are a cornerstone of nutrition. They are organic compounds that are comprised of amino acids and their quality depends on the types of amino acids they consist of. Table 1 presents the 13 amino acids contained in house crickets of which seven are essential for human metabolism. The essential amino acids for human metabolism are histidine, isoleucine, leucine, lysine, methionine, phenylalanine, threonine, tryptophan and valine. In addition house crickets also contain arginine, cysteine and glutamine which are specified as a conditionally essential amino acids which are needed during illness or stress. (The Food and Agricultural Organization of the United Nations, 2013, 68; Nature Education, 2010; MedPlus, 2015)

TABLE 1. Amino acid composition of house crickets (Finke 2002)

Amino acids	g/16 g nitrogen
Alanine	8.8 (8.8, 8.9)
Arginine	6.1 (6.1, 6.1)
Aspartic acid	7.7 (7.1, 8.4)
Cystine	0.8 (0.8, 0.8)
Methionine	1.4 (1.3, 1.5)
Lysine	5.4 (5.4, 5.4)
Isoleucine	4.4 (4.3, 4.6)
Leucine	9.8 (9.5, 10.0)
Phenylalanine	3.0 (2.8, 3.2)
Threonine	3.6 (3.6, 3.6)
Tryptophan	0.6 (0.5, 0.6)
Glutamic acid	10.4 (10.4, 10.5)
Histidine	2.3 (2.2, 2.3)

Proteins are formed from amino acids by peptide bonds. Proteins have multiple purposes in the cell which is determined by the sequence of different amino acids they comprise of. In figure 1 is shown the synthesis of proteins from amino acids. (Solunetti, 2006, Proteiinit)

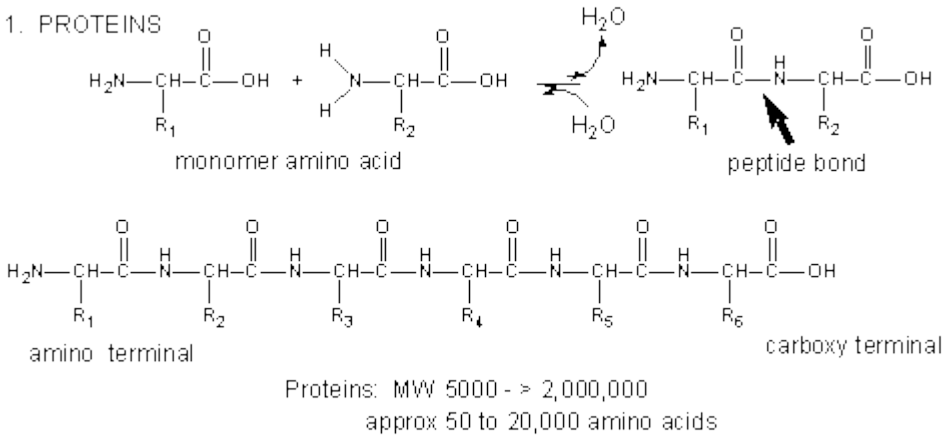


FIGURE 1. Protein formation from amino acids (Jakubowski 2016)

From nutritional point of view proteins are necessary for growth, repair and maintenance of body. It is estimated that a full grown adult's need for protein in a day is 0.6- 0.75 g per kilogram of bodyweight. The body can utilize excess protein intake as energy where 1 g of protein equals to 4 kcal of energy. (British Nutrition Foundation, 2016, Protein)

2.2 Carbohydrates

Carbohydrates in house crickets consist of glucose, in the form of glycogen which is a multi-branched polysaccharide and it is stored in the adepocytes of house cricket and it can easily be degraded to glycolytic fuel when needed. The 2 dimensional structure of glycogen can be seen from figure 2. (Solunetti, 2006, Glykogeeni)

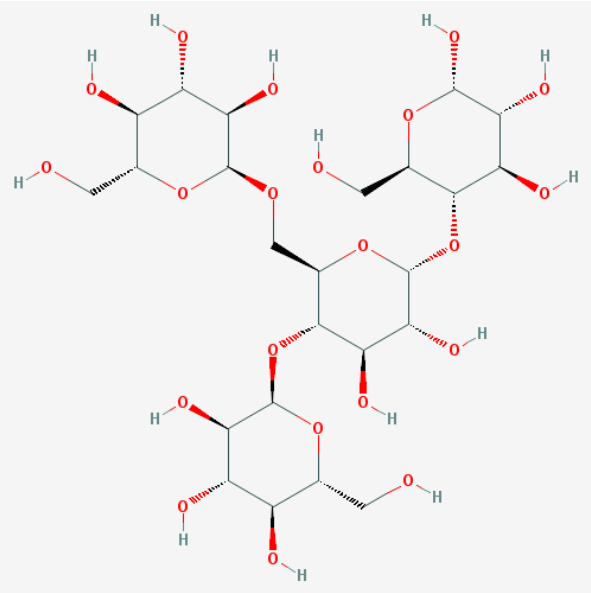


FIGURE 2. Structure of glycogen (PubChem 2009)

In animals carbohydrates are formed from sugars and starch to glycogen. It is a vital source of energy for body's tissues containing around 3.75 kcal of energy per 1 g. The daily need of carbohydrates for an average adult is 252g for men and 198 for women. This covers 47.5 % and 48.3 % of the required daily energy consumption. (British Nutrition Foundation, 2016, Carbohydrates)

2.3 Fats

Fats in house crickets are found in the form of triglycerides (triacylglycerol). Triglycerides are also stored in the adepocytes along with glycogen. They are the most common form of lipids and act as the energy reserve of animals. (Solunetti, 2006, Asyyliglyserolit)

Triglycerides consist of a glycerol molecule that has esterified with three fatty acid molecules. The formation and structure of triglycerides is shown in figure 3. The fatty acids found in house crickets are linoleic-, oleic-, palmitic-, stearic-, palmitoleic-, myristic- and linolenic acids. Linoleic, oleic palmitic and stearic acids compose the majority of fatty acids found in house crickets along with smaller amounts of palmitoleic, myristic and linolenic acids. (Hutchins & Martin, 1968)

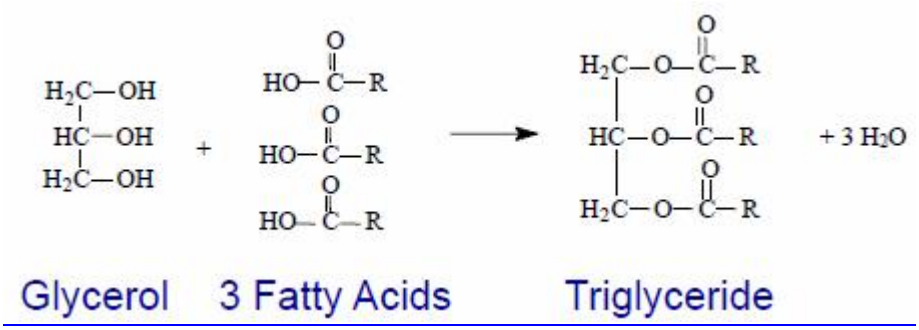


FIGURE 3. Formation and structure of triglycerides

In addition of being an energy reserve in the body, fats help in the absorption of certain vitamins and minerals as well as playing a key part in a variety of different bodily functions. Fats can be classified as monounsaturated-, polyunsaturated-, saturated- and trans fats. Mono- and polyunsaturated fats are considered to be good fats while trans fats are the most unhealthy option and saturated fats fall somewhere in-between. (Harvard Medical School, 2015)

2.3.1 Unsaturated fats

Unsaturated fats consist of monounsaturated and polyunsaturated fats. They have the least amount of hydrogen atoms bonded to carbon chains. Unsaturation refers to double bonds between carbon atom, therefore, it is not saturated with hydrogen atoms. Unsaturated fats are usually in liquid form at room temperature. Unsaturated fatty acids found in house crickets are linoleic-, linolenic-, oleic- and palmitoleic acids. (Harvard Medical School, 2015; Chemra, 2016)

2.3.2 Saturated fats

Saturated fats are solid at room temperature. In saturated fats carbon atoms have bonded to as many hydrogen atoms as possible which means that there are no double bonds between carbon atoms. Saturated fatty acids found in house crickets are palmitic-, stearic- and myristic acids. (Harvard Medical School, 2015; Chemra, 2016)

2.3.3 Trans fats

Trans fats are an industrially manufactured type of fat through hydrogenation. Hydrogenation process saturates the healthy unsaturated fats and oils with hydrogen atoms. This process is used to prevent rancidity. Trans fats are linked to several life threatening conditions such as heart disease and diabetes. Even 2 % daily calorie intake from trans fats can raise the risk of heart disease by 23 %. (Harvard Medical School, 2015)

2.4 Minerals

Along with proteins, carbohydrates and fats house crickets also contain a variety of essential minerals and fiber. Of house crickets' body mass 7 % is comprised of crude fiber and roughly 3 % consists of minerals such as phosphorus, potassium, calcium, magnesium and sulfur. Also in addition to these minerals, smaller amounts of zinc, manganese, iron, copper, aluminum and sodium can be found. (Defoliart, Nagakagi & Sunde, 1986, 1368)

3 SPOILING OF CRICKET FLOUR

Cricket flour can spoil in various ways which are hydrolytic, oxidative, microbial and enzymatic spoilage. The general spoiling of fats causing unwanted color, flavors and odors, is commonly referred to as rancidity.

3.1 Hydrolytic spoilage

In hydrolytic spoiling the triglycerides go through hydrolyzation process where the triglyceride molecule breaks, freeing the fatty acids from their ester bonds with the glycerol molecule. This hydrolytic spoilage of triglycerides is represented in figure 4.

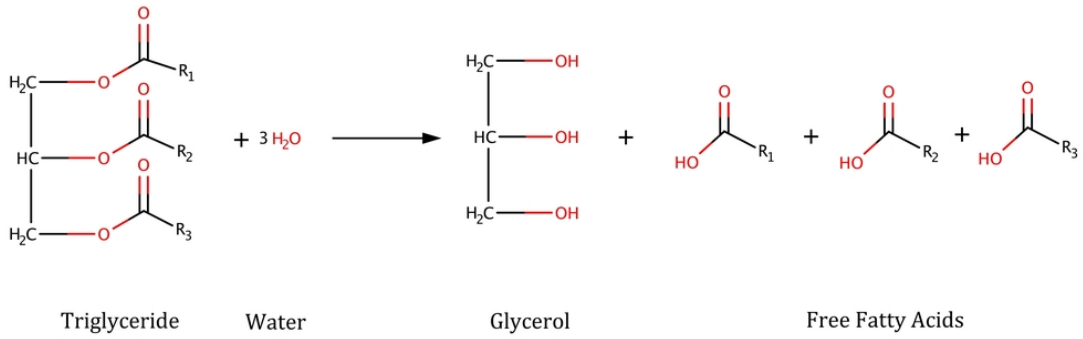


FIGURE 4. Hydrolysis of triglycerides (Nordic Food Lab 2016)

Especially short chained fatty acids can be easily detected in small quantities through foul smell or taste. The presence of water acts as a catalyst to hydrolytic spoilage. (Mattila, Piironen & Ollilainen, 2001, 115)

3.2 Oxidative spoilage

Oxidative spoilage results from exposure to oxygen in air. This is the most common type of spoiling and it consists of three phases which are presented in figure 5. In the initiation phase lipid free radicals are formed. These free radicals then react with the oxygen in air forming peroxyl radicals. The peroxyl radicals react with surrounding lipid molecules to

form hydroperoxides in propagation phase. In termination phase the free radicals react with each other to form a wide range of different non-radical compounds such as aldehydes and ketones that can be easily detected organoleptically. (World Food Logistics Organization, 2008, 1-3; Dave & Ghaly, 2011, 490-491)

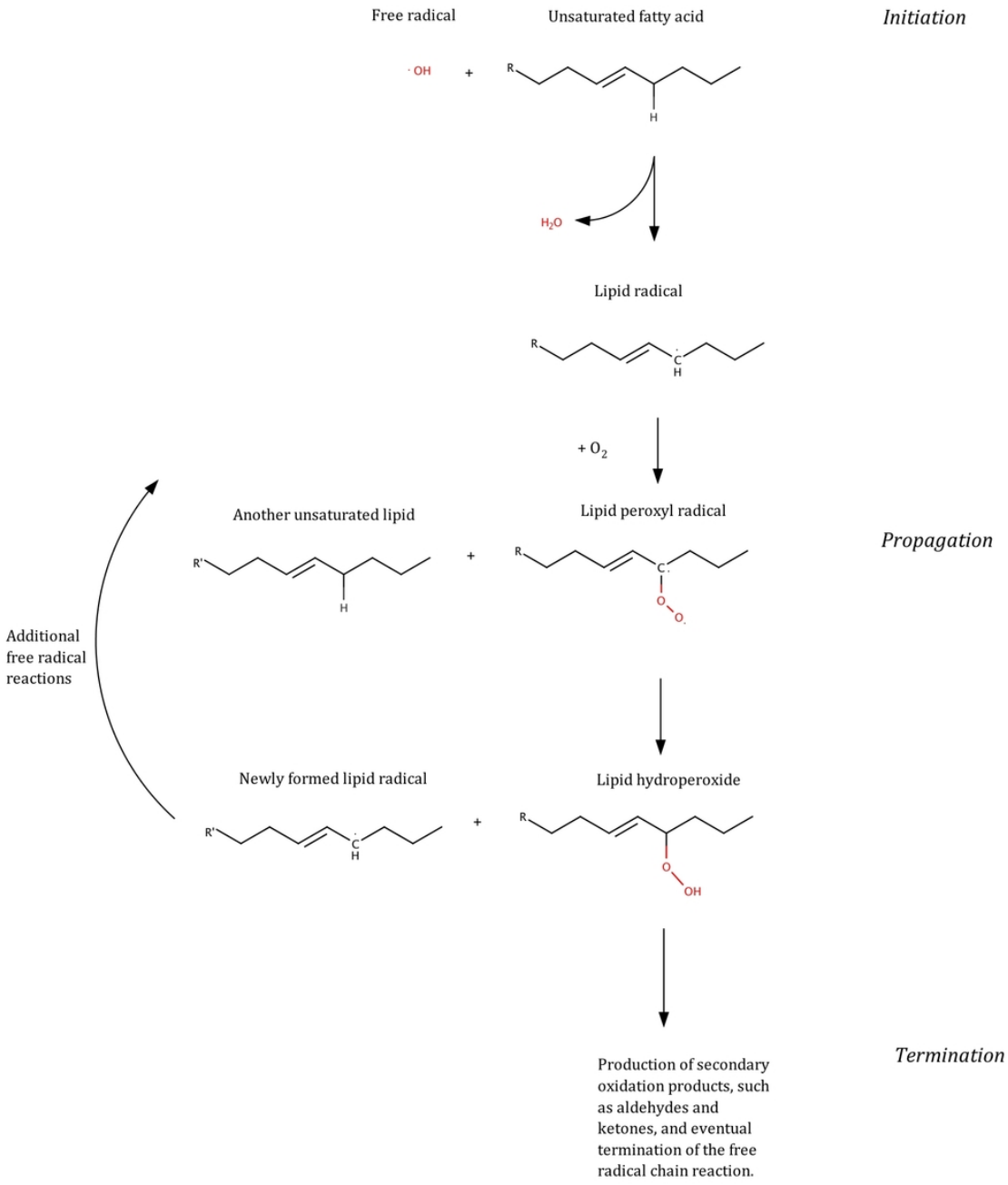


FIGURE 5. Process of oxidative spoilage (Nordic Food Lab 2016)

The oxidation process is affected by many factors. In the initiation phase light, heat, metal ions or enzymes can work as a catalyst in the process. Also the fatty acid composition and

presence of antioxidants as well as prooxidants in the product have an effect on the oxidation process. Oxidative spoilage affects the product's flavor, odor, color, composition and nutritional value and can even produce toxic compounds. . (World Food Logistics Organization, 2008, 1-3; Dave & Ghaly, 2011, 490-491)

3.3 Microbial and enzymatic spoilage

Microbial spoilage is caused by microorganisms like bacteria, mold and yeasts and the rapidity of spoilage depends greatly on initial shelf life, handling hygiene, storage temperature, and initial amount of microorganisms found in the product. In addition to foul odor and flavor caused by hydrolytic- and oxidative the bacteria, molds, and yeasts may cause sliminess, discoloration, souring, and gases. (Garg, Lohani & Umesh, 2009)

Enzymatic spoilage is caused by enzymes that are produced by all living things. Enzymes can work as a catalyst in spoiling process by speeding up the chemical reactions causing rancidity. Enzymes can already be found in the product but bacterial growth can produce enzymes as well. (Garg, Lohani & Umesh, 2009)

Microbial and enzymatic spoilage can be controlled through proper storaging and handling. Low temperatures, lack of air, and hygienic handling of product may extend the shelf life of product considerably. (Garg, Lohani & Umesh, 2009)

4 POSSIBLE METHODS OF PRESERVATION

Prolongation of shelf life of the product can be approached from three different angles which are: removal of the spoiling ingredient, addition of preserving agent and removal of external factors.

4.1 Solvent extraction

Different separation methods are widely used in food industry. The general aims of separation are to better the color or flavor, separate essential ingredients, prolong shelf life, extract or separate aroma- and coloring agents, salvage byproducts for utilization or wastewater cleansing. In the process an organic solvent is in liquid form or near its boiling point so that it percolates through the solid phase dissolving desired compounds. The solvent is then removed from the product through distillation or vacuum vaporization. (Hyvönen… 2010, 317)

4.1.1 Extractor types

Extractors are usually categorized on the basis of the depth of the material bed. In figure 6 are presented the three most common types of extractors which are vertical loop extractor, straight line extractors and round extractors. (Anderson, 2011)

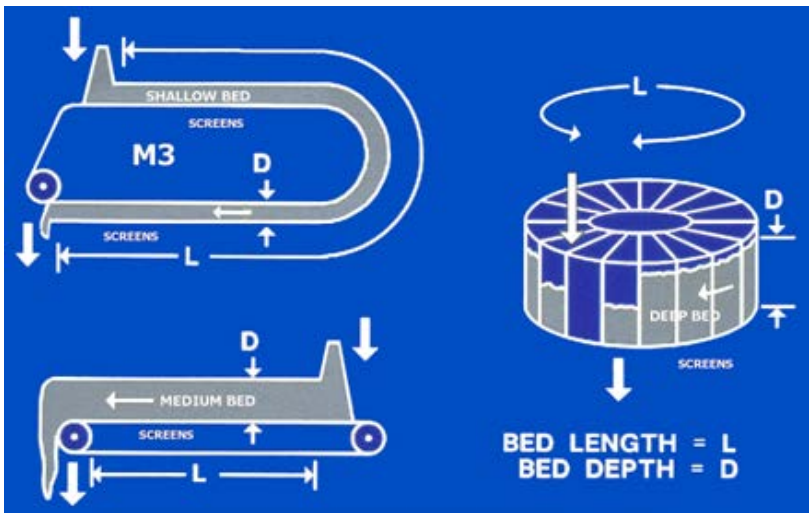


FIGURE 6. Three most common types of solvent extractors (Anderson 2011)

Vertical loop extractors have the shallowest bed (0.3-1 m). The shallowness of the bed is compensated in length which is approximately 50 times as long as it is deep. Due to the great length of vertical loop extractors they are curved into a loop to save space. In straight-line extractors the depth of bed is 0.9-1.8m and the length of bed is usually about 15 times the depth of the bed. Round extractors have the deepest beds (1.6-2.9 m). The round extractor is divided to cells where the material is placed for extraction. (Anderson, 2011)

The solvent extractors are expensive and large industrial machines that also require high amounts of material and solvent for the process. Some extractors may have a daily extraction capacity for 9000 tons of material which makes it beneficial only when the production capacity reaches a certain point. (Anderson, 2011)

4.1.2 Extraction solvents

Extraction solvents used in processing of foodstuffs and food ingredients are highly regulated. The EU has allowed the use of various different chemicals in solvent extraction some of which are allowed for all uses in compliance with good manufacturing practices but the rest have specific conditions of use and maximum residue limits that can be found in the extracted foodstuffs or food ingredients. Propane, butane, ethyl acetate, ethanol, carbon dioxide, acetone and nitrous oxides are extraction solvents allowed for all uses. Dimethyl ether's condition of use is specified for preparation of defatted animal protein products and it has a maximum residue limit of 0.009 mg/kg in the final product. (EUR-Lex, 2009)

4.2 Use of food additives

In Europe food additives are known as E numbers. They have multiple purposes such as adding or restoring color and prolonging the shelf life of products. The Scientific Committee on Food (SCF) and the European Food Safety Authority (EFSA) authorize all food additives that are considered safe for consumption. (Evira, 2016; European Commission, 2017)

SCF determines an ADI-value (Acceptable Daily Intake) for all food additives in the EU area. ADI-value expresses the acceptable amount of specific food additive that is safe to consume daily through one's whole life. ADI values are presented as milligrams of additive per kilogram of bodyweight daily (mg/kg/d). (Mattila, Piironen & Ollilainen, 2001, 184)

4.2.1 Preservatives

Preservatives are chemical agents added to foods that improve their shelf life by preventing the development and growth of microorganisms, like bacteria, molds and yeasts. Preservatives also help to preserve the flavor and nutritional value of product. (Evira, 2009, 25)

Some common preservatives used in foods are sorbic acid, benzoic acid, propionic acid, lactic acid, sodium nitrite and sulphurous acid and its salts. Most of the preservatives used in foods are naturally occurring but they may be chemically produced. In table 2 are listed all the currently EU allowed preservatives and their E numbers. For shelf life prolongation of meat products sodium nitrate (E 251) and potassium nitrate (E 252) are commonly used preservatives. (Louekari, Salminen & Von Wright, 1994, 61-63; Evira, 2009, 26-29)

TABLE 2. Currently EU approved preservatives and their E numbers (Food Standards Agency 2016, edited)

Preservatives			
E200	Sorbic acid	E228	Potassium hydrogen sulphite
E202	Potassium sorbate	E234	Nisin
E203	Calcium sorbate	E235	Natamycin
E210	Benzoic acid	E239	Hexamethylene tetramine
E211	Sodium benzoate	E242	Dimethyl dicarbonate
E212	Potassium benzoate	E243	Ethyl lauroyl arginate
E213	Calcium benzoate	E249	Potassium nitrite
E214	Ethyl p-hydroxybenzoate	E250	Sodium nitrite
E215	Sodium ethyl p-hydroxybenzoate	E251	Sodium nitrate
E218	Methyl p-hydroxybenzoate	E252	Potassium nitrate
E219	Sodium methyl p-hydroxybenzoate	E280	Propionic acid
E220	Sulphur dioxide	E281	Sodium propionate
E221	Sodium sulphite	E282	Calcium propionate
E222	Sodium hydrogen sulphite	E283	Potassium propionate
E223	Sodium metabisulphite	E284	Boric acid
E224	Potassium metabisulphite	E285	Sodium tetraborate; borax
E226	Calcium sulphite	E1105	Lysozyme
E227	Calcium hydrogen sulphite		

4.2.2 Antioxidants

The food additives preventing the oxidation of fats are called antioxidants which disrupt the oxidation process by working as an electron or a proton donor to free radicals. Free radicals are bound to antioxidant creating an intermediate product which leads to stabile compounds. The working principle of antioxidants is presented in figure 7. In addition to fat preservation antioxidants also assist the preservation of A-, D-, E- and B2-vitamins. (Louekari, Salminen & Von Wright, 1994, 66-67; Evira, 2009, 25, 30)

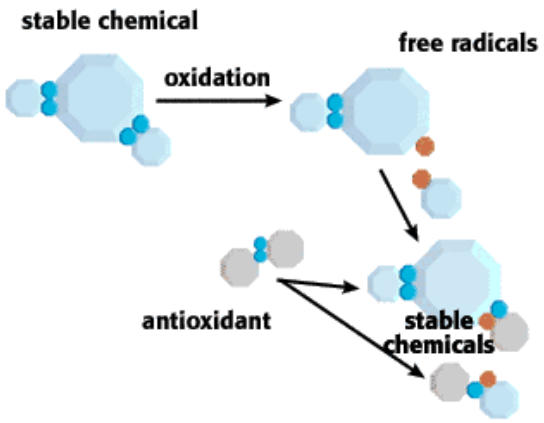


FIGURE 7. Working principle of antioxidants (Chemistry58, 2017)

There are 18 antioxidants that are currently EU approved for use in foods which are presented in table 3. Generally these antioxidants are naturally occurring in various fruits and vegetables with some exceptions and they can generally be added to all foods where use of food additives is allowed. Even though antioxidants are naturally occurring they are usually chemically produced. Probably the most known and used antioxidants are ascorbic acid and tocopherols, commonly known as C- and E-vitamins. (Evira, 2009, 30-35; Food Standards Agency 2016)

TABLE 3. Currently EU approved antioxidants (Food Standards Agency 2016)

Antioxidants	
E300	Ascorbic acid
E301	Sodium ascorbate
E302	Calcium ascorbate
E304	Fatty acid esters of ascorbic acid
E306	Tocopherols
E307	Alpha-tocopherol
E308	Gamma-tocopherol
E309	Delta-tocopherol
E310	Propyl gallate
E311	Octyl gallate
E312	Dodecyl gallate
E315	Erythorbic acid
E316	Sodium erythorbate
E319	Tertiary-butyl hydroquinone (TBHQ)
E320	Butylated hydroxyanisole (BHA)
E321	Butylated hydroxytoluene (BHT)
E392	Extracts of rosemary
E586	4-Hexylresorcinol

4.3 Packaging

Packaging prolongs the shelf life of products by removing the effect of external factors such as oxygen, heat and light which can catalyze the spoiling process of fats. Oxygen can be removed from the package or it can be replaced with an inert gas that diminishes

the oxidation process and growth of aerobic organisms. Effect of heat and light can be minimized by use packaging materials that have light reflecting or insulating properties.

4.3.1 Vacuum packaging

The vacuum packaging procedure is fairly simple. The product is placed in the package and then air is removed from the package via suction. Lack of air in the package minimizes oxidative and microbial spoilage. All air cannot be removed from the package in vacuum packaging which means that small amounts of oxygen is left in it that allows minor spoilage of the product. (Modified Atmosphere Packaging, 2012)

The preservation effect of vacuum packaging depends highly on the products nutritional content and storing temperature. For example vacuum packaging may extend the shelf-life of beef stored in fridge from 2-3 days to 30-40 days. When stored in a freezer at a temperature of -18 °C the shelf life of meat may be prolonged from 6 months to 24-36 months. (Vakuumikauppa, 2017)

There is a large variety of different vacuum packaging machines ranging from small scale machines for personal use to large machines for industrial food packaging purposes. The vacuum packaging machines for personal use are fairly cheap ranging from 50 € to 2000 €. The prices of industrial vacuum packaging machines, shown in picture 1, are upwards from 500 €.

PICTURE 1. Double chamber vacuum packaging machine (Henkovac 2014)

4.3.2 Modified atmosphere packaging (MAP)

Modified atmosphere packaging bases on replacing air to an inert gas in the package. It is also known as gas flushing, protective atmosphere packaging and reduced oxygen packaging. (Bergslien…, 2002, 62)

Oxygen, nitrogen and carbon dioxide are the most commonly used gases in modified atmosphere packaging. The optimal mixture is comprised of these gases for a specific product to enhance its shelf life. For oxygen sensitive foods a mixture of carbon dioxide and nitrogen is common for their ability to inhibit growth of microorganisms. Oxygen is added to gas mixture for preserving the red color for meats. (Bergslien…, 2002, 63)

MAP technology is already widely used in the food industry. Usually all meat products and convenience foods are packed using MAP. In picture 2 is shown a common package of minced meat packed using MAP technology.

PICTURE 2. Minced meat packed using MAP technology (Atria 2017)

Although MAP has many good qualities it does create some disadvantages such as added expenses through needed equipment, training, product safety establishment and even transport costs due to increased pack volume. However, when compared to vacuum packaging MAP does give some liberty when choosing the packaging material and the shape of the package. (Bergslien…, 2002, 63)

5 PROCEDURES TO DETERMINE SHELF LIFE

To determine the shelf life of cricket flour the fat had to be extracted from the product using soxhlet method. Four different tests for determining oxidative and hydrolytic fat spoilage were chosen and the decay rate of fatty acids was observed using gas chromatography-mass spectrometry.

5.1 Soxhlet extraction

Soxhlet extraction is a method of solid-liquid extraction where solute is separated from solid sample with the aid of solvent. In figure 8 is shown that soxhlet extraction apparatus comprises of 4 main parts: round bottomed boiling flask, extraction chamber, reflux condenser and heating mantle. In addition rubber tubing for the reflux condenser and an extraction thimble for the sample are needed. (SFS-EN 1528-2:1996; Royal Society of Chemistry, 2017)

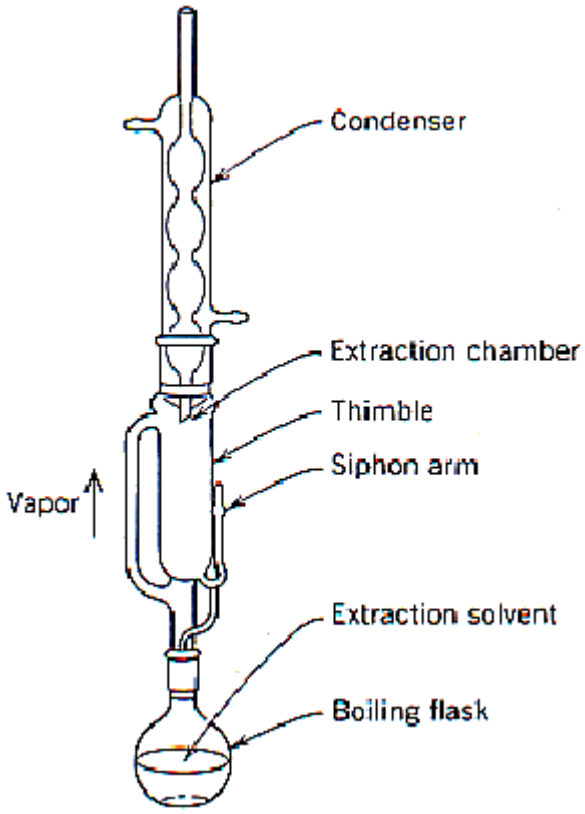


FIGURE 8. Soxhlet extraction apparatus (Oleoresins 2016)

The operational principle of soxhlet extraction is fairly simple. Solvent placed in the boiling flask is heated with heating mantle to its boiling point. Solvent vapor travels to the extraction chamber where it is condensed and accumulates slowly filling up the chamber. Solvent dissolves part of the desired compound in the sample. When solvent level in the extraction chamber reaches a critical point siphon arm empties it back to the boiling flask and the process starts all over. (García-Ayuso & Luque de Castro, 1998; Royal Society of Chemistry, 2017)

5.2 Acid value

Determination of acid value is a titrimetric method that allows the monitoring of hydrolytic spoilage in fats. Acid value determines the amount of free fatty acids present in the sample. It is a neutralization titration where acid value implies the amount of potassium hydroxide in milligrams required to neutralize the free fatty acids. The acid value for still usable animal fats can be 2.5 at most. (SFS-EN 14104:2003; Nielsen, 2003, 235)

5.3 Peroxide value

Peroxide value defines the ongoing oxidative spoilage. Determination of peroxide value is an iodometric titration that defines the milliequivalents of peroxide contained in a kilogram of sample. Peroxides created by the oxidative spoiling process are a transient product that will continue to react and create stable products. Due to this ephemerality a low peroxide value may indicate the beginning of oxidation process or advanced oxidation so it is recommended that peroxide value is determined over a specific time. A product that hasn’t started to oxidize should have peroxide value of 0 and a peroxide value of over 20 correlates poor quality. (SFS-EN ISO 3960:2017; Mattila, Piironen & Ollilainen, 2001, 116-117; Nielsen, 2003, 237-238)

5.4 Anisidine and Totox value

Anisidine value measures the oxidative spoilage of sample. The method determines the α- and β-unsaturated aldehydes, especially 2-alkenals and 2,4-dienals in the sample. Aldehydes react with anisidine producing a chromogen which is then measured with a spectrophotometer. The aldehydes measured by this method are the secondary oxidation products of hydroperoxides. For this reason anisidine value determination is a suitable determination that supplements the determination of peroxide value. (SFS-EN ISO 6885:2016; Mattila, Piironen & Ollilainen, 2001, 118; Nielsen, 2003, 238)

Totox value predicates the combined amount of hydroperoxides and α- and β-unsaturated aldehydes present in the sample. Totox value is calculated from the results of anisidine- and peroxide values. The connection between anisidine-, peroxide-, and totox values is presented in figure 9. (Nielsen, 2003, 238)

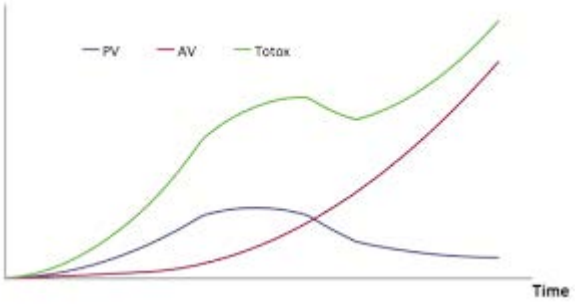


FIGURE 9. Visual presentation of connection between peroxide-, anisidine- and totox values (Chris Masterjohn 2015)

5.5 Iodine value

Iodine value determines the unsaturation in the sample by measuring the ratio between the amount of carbon-carbon double bonds and fat. It is defined by the amount of iodine in grams absorbed by 100 grams of the sample. Iodine absorption increases simultaneously with the degree of unsaturation. (SFS-EN ISO 3961:2013; Mattila, Piironen & Ollilainen, 2001, 114; Nielsen, 2003, 233-234)

5.6 Gas chromatography mass spectrometry

Gas chromatography mass spectrometry (GC/MS) is a combination of two techniques which allows the separation, identification and quantification of complex of chemicals. It is an optimal method for investigating the presence of organic compounds with a relatively low molecular weight. (Bull, 2008; EAG Laboratories, 2017)

5.6.1 Gas chromatography

Figure 10 shows that gas chromatography consists of three parts: injector, column and detector. Injector injects the sample solution into the inlet of gas chromatography where it is vaporized. Inert carrier gas then sweeps the vaporized sample into the column which is located in an oven that keeps it at a constant temperature. Different compounds are identified according to their retention time which means the time it takes specific compounds to make their way through the column to the detector. Identification occurs by comparing the retention times of compounds in the sample to the existing database. (EAG Laboratories, 2017; Opetushallitus, kaasukromatografia)

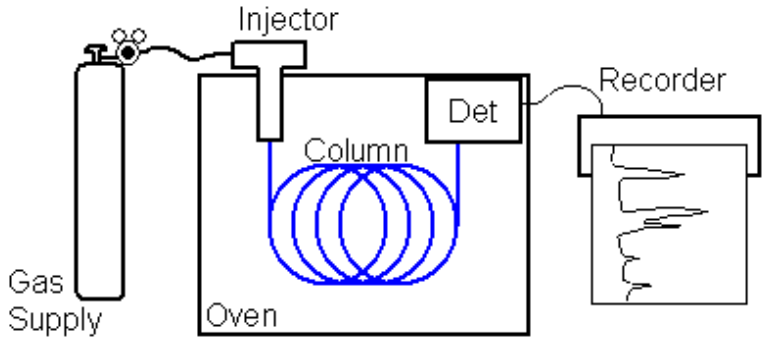


FIGURE 10. Schematics of a gas chromatograph (Kutztown University 2017)

5.6.2 Mass spectrometry

Mass spectrometry is an efficient method to identify and measure the concentration of organic compounds. The working principle of MS is shown in figure 11 where the compounds in the vaporized sample are fragmented or ionized with the help of an electron beam. These ions are then accelerated, sorted according to their masses and directed through a powerful magnetic field to a detector. The amount of effect the magnetic field

has on the ionized molecules course of direction depends on the molecules weight. The detector can therefore determine the mass and quantity of these ions. (EAG Laboratories, 2017; Opetushallitus, 2017)

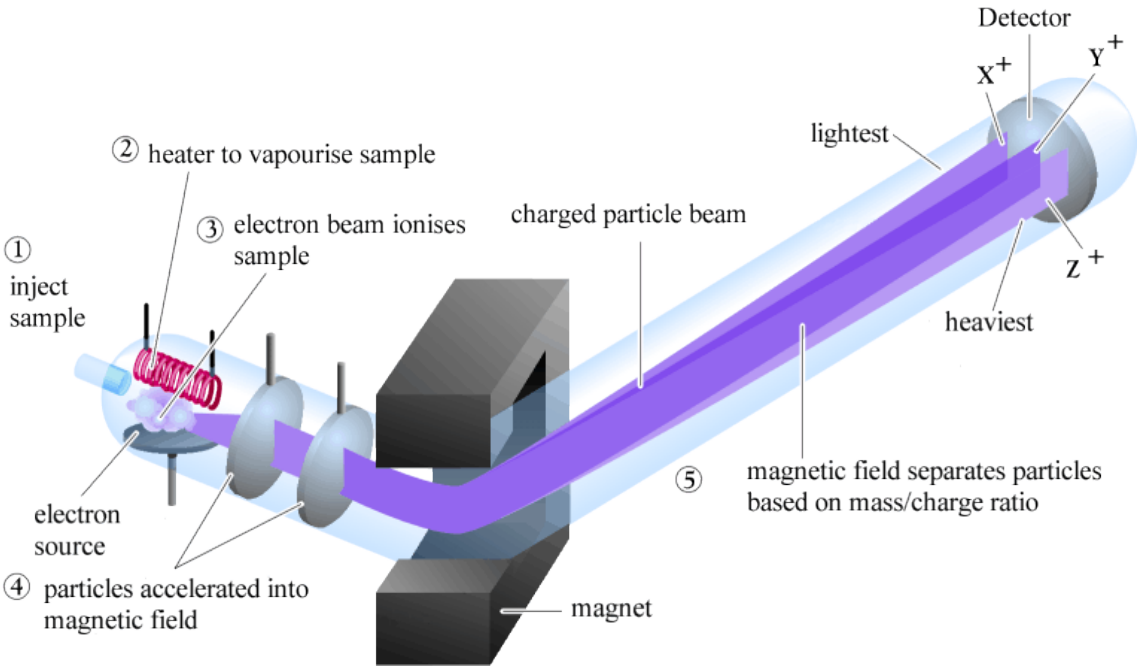


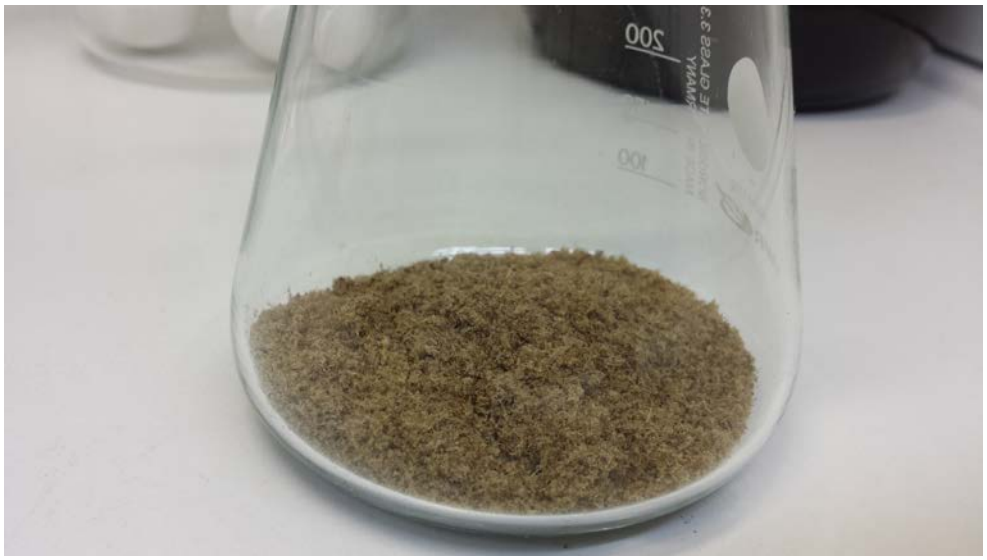
FIGURE 11. Working principle of mass spectrometry (Ian Hunt 2017)

6 SHELF LIFE DETERMINATION

The house crickets were boiled and dried between 15.3.2017-17.3.2017 and ground to flour 22.3.2017. After sample preparation the cricket flour was left to be for two weeks after which the fat was extracted on three different occasions with one week in-between and the quality was tested.

6.1 Sample preparation

Approximately 200 g of house crickets were acquired for the testing of preservation. The crickets were prepared by boiling, drying and vacuum packaging until they were ground in to a fine flour with Kenwood Blend-X Pro blender. Cricket flour was then transferred into an air-tight glass bottle and it was stored at room temperature in the dark. Glass bottle was opened only to acquire samples for testing to minimize the cricket flours exposure to oxygen.



PICTURE 3. Cricket flour prepared for fat extraction (Ville Kontio 2017)

6.2 Soxhlet extraction

Fat was extracted from ground house crickets by soxhlet extraction and the extraction apparatus was constructed according to SFS-Standard. At first three concurrent extractions were performed to ensure the functionality of soxhlet extraction for this specific process. When functionality was verified the amount of concurrent extractions could be decreased. On second time two concurrent extractions were performed and on the third time only one.

PICTURE 4. Soxhlet extraction apparatus (Ville Kontio 2017)

The apparatus was comprised of a heating mantle, 500 ml round-bottomed boiling flask, 200 ml extraction chamber and a reflux condenser with rubber tubing. 250 ml of diethyl ether was used as a solvent per extraction. Diethyl ether is an efficient organic solvent and its low boiling point minimized the negative effects of temperature on the sample.

In every extraction between 20 to 25 grams of sample was placed in the extraction thimble. After the first three concurrent soxhlet extractions it was discovered that circa 60 grams of cricket flour sample yielded approximately 9 grams of fat for testing.

6.3 Acid, anisidine, iodine and peroxide values

Acid-, anisidine-, iodine-, and peroxide values were to be tested from the fat extracted from cricket flour sample. Potassium hydroxide solution (0,1 M) for the acid value determination and potassium iodate solution needed in peroxide value determination were prepared in advance to hasten the procedures.

However these tests could not be done due to the surprisingly low fat yield of 9 g from the cricket flour fat extraction. The tests required altogether 45 g of fat sample in order to be tested (acid value: 20 g, peroxide value: 5 g, anisidine value: 10 g, iodine value: 10 g). Because of the low fat yield these tests were discarded.

6.4 Gas chromatography-mass spectrometry

To compensate for the discard of acid-, peroxide-, anisidine-, and iodine values GC/MS (gas chromatography-mass spectrometry) was chosen for the testing of fat spoilage. GC/MS was chosen for its low requirement of fat sample and accurate measurements to determine different molecules and their quantity

The GC/MS used in this work was a 6890N Network GC System coupled with 5973Network Mass Selective Detector from Agilent Technologies. GC/MS system was equipped with an automatic injector.

PICTURE 5. Agilent Technologies GC/MS system (Ville Kontio 2017)

6.4.1 Sample and standard preparation

In order to analyze the fat sample acquired from ground house crickets the free fatty acids were to be freed from triglycerides through hydrolyzation. The free fatty acids were then esterified to improve the gas chromatographic properties. Standard curve was made by creating methyl ester compounds from myristic-, palmitic-, stearic- and oleic acids.

On the first tests two different test series were produced to find the optimal way to prepare the sample for GC/MS analyzation. The first test series was prepared by dissolving 0.1 g of the sample and standard acids to 2 ml of heptane after which they were tansesterified with 2 M methanolic solution of potassium hydroxide. The other test series was prepared by dissolving the sample and standard acids to 2 ml of diethyl ether and esterifying them with the same 2 M methanolic potassium hydroxide solution. After methylation the solutions were centrifuged at 3000 rpm for 10 minutes to separate methyl esters from rest of the sample matrix.

After the first GC/MS run it was discovered that in the series of heptane solutions the standard acids had not been transesterified. In the series of diethyl ether solutions the fat samples had not been transesterified. For the different solvents used in the test series' the results were not comparable.

The incomparability of these series' meant that a standard curve could not be obtained for the mass spectrometry to determine the quantity of different compounds found in the sample. This meant that the decay of fats had to be calculated from the decline of relative intensity of fatty acid methyl esters contained in the fat sample.

6.4.2 Gas chromatograph settings

The setpoint of oven of gas chromatograph was 40 °C where it was held for 2 minutes and it was set to heat up 10 °C per minute until it reached the temperature of 260 °C. The temperature of 260 °C was held for 2 minutes after which the heating rate grew to 50 °C per minute until it reached the temperature of 300 °C where it was held for 1 minute. The equilibration time was set at 0.50 min and maximum temperature at 325 °C.

The column used was DB-5ms and it was set to be at constant flow of helium. The volume of helium flow was 1.0 ml per minute where its average flow velocity was 40 cm per second.

The injector used was Agilent technologies 7683 Series Injector with the syringe size of 10 µl and injection volume was set at 1 µl. Pre injection process consisted of 3 sample washes, 3 solvent washes with both A and B solvents and 6 sample pumps. After injection the syringe was washed 3 times in both A and B solvents.

At the inlet of GC the temperature was set to 250 °C at a pressure of 16.4 psi and the total flow of helium was at 53.7 ml per minute.

7 RESULTS

Acid-, peroxide-, anisidine,- and iodine values could not be determined due to low yield of fat but two different results were acquired from the gas chromatographic-mass spectrometric analysis. The decrease rate of fatty acids and the fatty acid composition in cricket flour. GC/MS analysis provided an explicit determination of fatty acid composition and the concentration of contents.

7.1 Fatty acid composition

Overall there were no major changes in the fatty acid composition but between 29.3.2017 and 5.4.2017 the amount of oleic acid started to decrease rapidly. Correspondingly elaidic acid which is a trans isomer of oleic acid had started to occur in the analyses during this time. Therefore, it could be concluded that oleic acid had started to isomerate into elaidic acid. The transformation rate of oleic acid to elaidic acid is shown in figure 12.

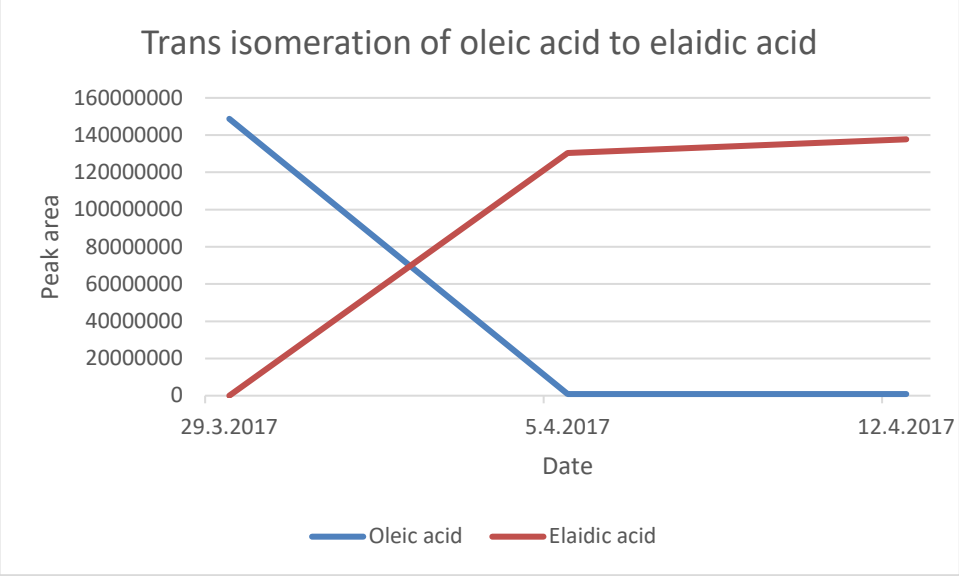


FIGURE 12. Trans isomeration of oleic acid to elaidic acid

Fatty acid composition was calculated by comparing the average peak area of methylated products of fatty acids in all GC/MS analyses to the total peak area. In table 4 the average peak area for each fatty acid methyl ester was calculated from all GC/MS analyses. The fatty acid composition can be x directly from the fatty acid methyl ester composition since

they are direct products of fatty acids in cricket fat. The combined values of elaidic and oleic acid were used to calculate the amount of oleic acid.

TABLE 4. Estimated fatty acid distribution in house cricket fat

Fatty acid methyl esters	**Average peak area**	**Fatty acid**	**%**
Methyl laurate	319070,8	Lauric acid	0,1
Methyl myristate	3820256,4	Myristic acid	0,9
Methyl palmitate	112862075,4	Palmitic acid	25,5
Methyl palmitoleate	7549766,8	Palmitoleic acid	1,7
Methyl linoleate	120526784,2	Linoleic acid	27,2
Methyl oleate	137723053,2	Oleic acid	31,1
Methyl stearate	58102507,8	Stearic acid	13,1
Methyl arachate	2023121,4	Arachic acid	0,5
Total	**442926636**		100,0

The calculations show that palmitic-, linoleic-, oleic- and stearic acids are the major fatty acids of house cricket fat with smaller amounts of lauric-, myristic-, palmitoleic-, and arachic acids. In addition traces of various fatty acids such as ricinoleic-, pentadecanoic-7,10-hexadecadienoic-, and isoheptanedacoic acids could be found.

7.2 Decrease rate of fatty acids

Decrease of fatty acids presented in figure 12 was acquired from the results of GC/MS analysis (appendices 1-15). In determining the decrease rate of fatty acids, four major fatty acid methyl esters were investigated. Table 5 was composed from library report and integrated peak area values of the four major fatty acids in the sample at three different dates. The percentual decrease rate of fatty acids was calculated with the average peak values between tests. Peak area means the concentration of certain compounds found in the sample. The retention times of compounds remained consistent throughout all GC/MS analyses.

TABLE 5. Peak values of fatty acids and calculated percentual decrease rate

	Average integrated area			Average 1	Average 2	Decrease rate
Compound	29.3.2017	5.4.2017	12.4.2017	(29.3-5.4)	(5.4-12.4)	(%/week)
Palmitic acid	157147737	136673890	145418070	146910814	141045980	4,0
Linoleic acid	167560150	145851886	154933969	156706018	150392927	4,0
Stearic acid	63119237	54829126	58867525	58974182	56848325,5	3,6
Oleic/elaidic acid	148750700	131314088,5	138618195	140032394	134966142	3,6

Figure 12 is a visual presentation showing the decrease of fatty acids in the fat sample from the information in table 5.

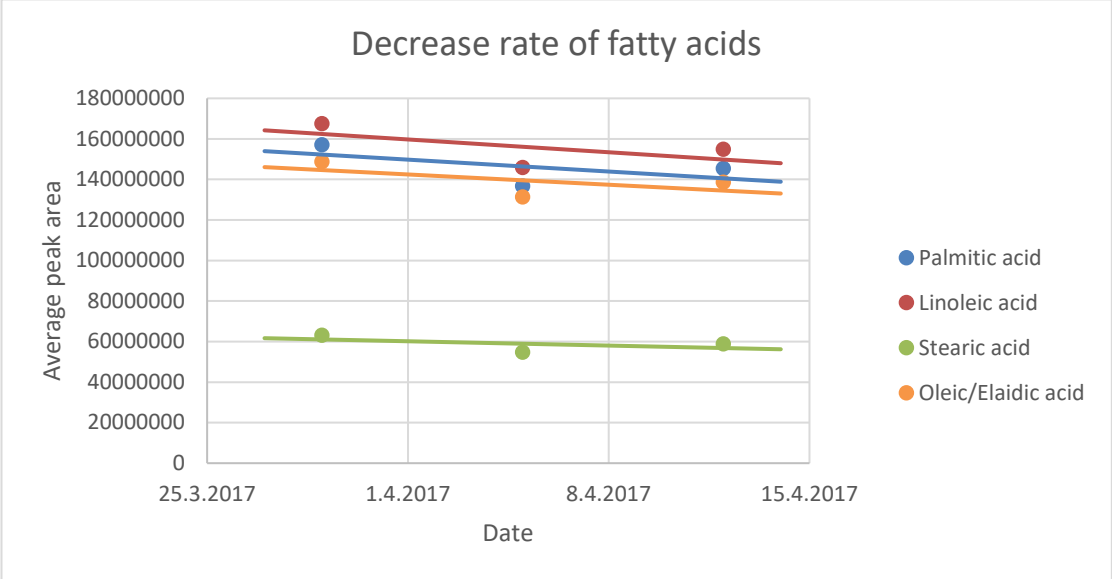


FIGURE 12. Decrease of fatty acid content over three weeks

8 CONCLUSIONS

Although the shelf life of cricket flour could not be determined the work did reveal some useful information on the rate of spoilage, fatty acid composition and quality of fats. The timespan of 4 weeks was too short for shelf life determination. In the future if acid-, peroxide-, anisidine-, and iodine are to be tested at least 300 g of cricket product should be reserved for a series of tests. Also the timespan for the tests should be extended to 6-12 months for proper results as fat spoilage is shown to be a fairly slow process.

The fat quality of crickets was found to be relatively healthy containing a large portion of unsaturated linoleic- and oleic acids along with saturated palmitic- and stearic acids. It can be seen that oleic acid starts to spoil first and quite fast, transforming to elaidic acid which is a trans fat that causes negative effect on the product's nutritional value. The calculated decrease rates of major fatty acids present a momentary rate between second and fourth week of shelf life.

Aldehyde and ketone compounds produced by oxidative spoilage could be detected ever since the first test where olealdehyde and few different ketones were found. In later GC-MS analyses a large variety of different aldehyde- and ketone compounds could be found in small amounts. However, the reliability of identifying aldehyde- and ketone compounds was too low to enable precise determination of compounds and their quantity.

For the prolongation of shelf life the most prominent methods are use of additives and MAP (Modified Atmosphere Packaging). Vacuum packaging poses a problem when the product is in flour form as it could be sucked into the equipment causing failure.

Food additives such as antioxidants could be used to decrease fat spoilage through oxidation and if problems occur from microbial spoilage preservatives could be added. Food additives are an inexpensive and easy method to extend shelf life. However, the right food additives should be considered since food additives are usually seen having a negative connotation. Some possible antioxidants used for preservation could be ascorbic acid and tocopherols which are commonly known as C- and E-vitamin.

MAP is a prominent way to extend shelf life of the product by reducing oxidation and microbial growth in the product and it does not have an effect on the products nutritional value. MAP's advantage over vacuum packaging is also the freedom in choosing the shape and materials of the package. Nevertheless, MAP machines are industrial machines which causes the initial costs of packaging to be high.

Fat extraction becomes an applicable method for shelf life prolongation only in great production capacities. The cost of industrial extractors are high and they require large volumes of organic solvents. Also the waste management and energy consumption add to a considerable rises in costs.

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APPENDICES

Appendix 1. Sample 1, 29.3.2017, GC Analysis

```
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Sample Name: Hnayte
Misc Info  :
Vial Number: 6
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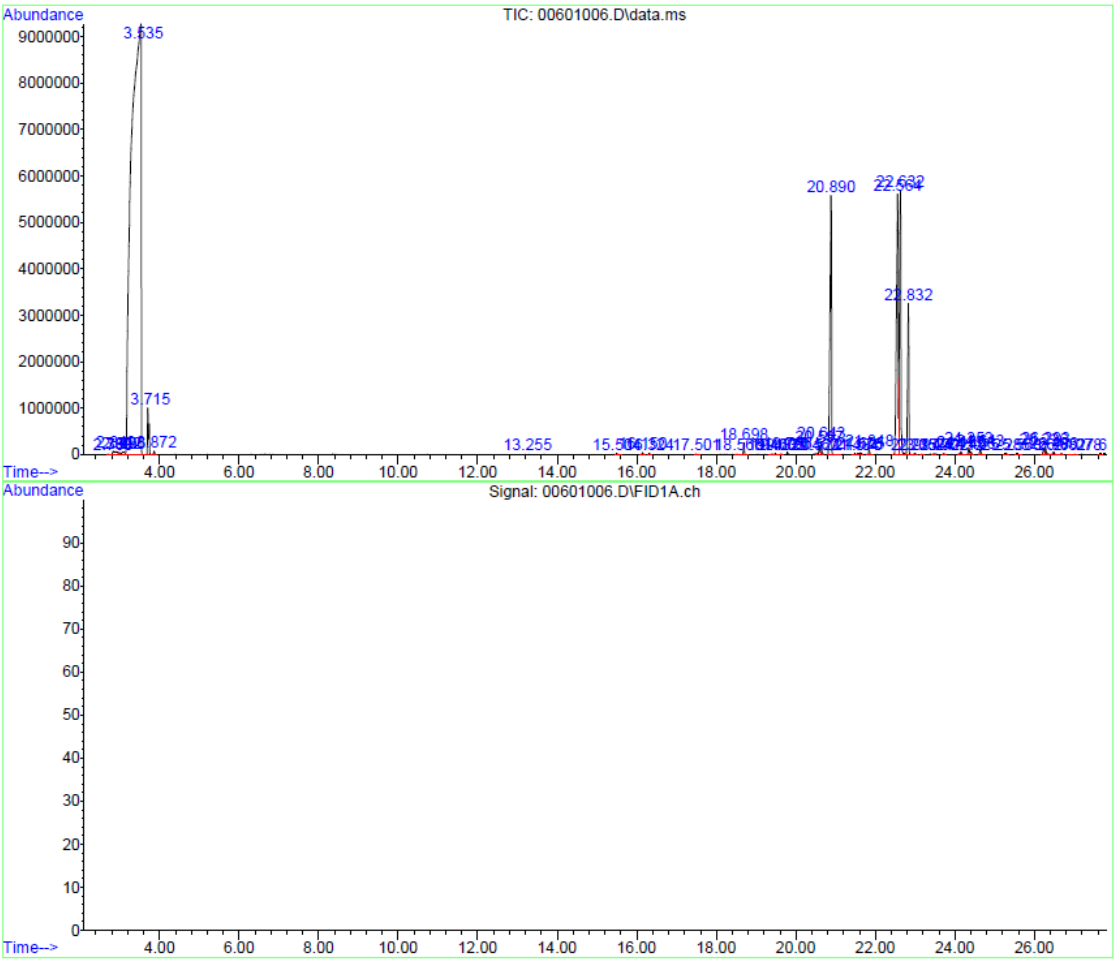

Appendix 2. Sample 1, 29.3.2017, Integrated peak areas

TIC: 00601006.D\data.ms
Hnayte

Peak #	Ret Time	Type	Width	Area	Start Time	End Time
1	2.768	BV	0.082	378151	2.670	2.799
2	2.849	VV	0.097	5088105	2.799	2.973
3	2.992	VV	0.039	859029	2.973	3.016
4	3.096	VV	0.098	2687565	3.016	3.142
5	3.535	VV	0.198	1574179115	3.142	3.669
6	3.715	VV	0.036	18942513	3.669	3.836
7	3.872	VV	0.025	966624	3.836	3.924
8	13.255	BB	0.046	128248	13.178	13.328
9	15.504	VB	0.035	289485	15.460	15.629
10	16.150	BB	0.027	524678	16.092	16.203
11	16.324	BB	0.027	329939	16.286	16.379
12	17.501	BB	0.032	143526	17.452	17.572
13	18.566	BV	0.026	82407	18.478	18.601
14	18.698	PB	0.027	4037805	18.648	18.793
15	19.400	BV	0.033	92500	19.339	19.450
16	19.487	PB	0.028	243731	19.450	19.542
17	19.633	BB	0.034	143588	19.561	19.699
18	19.796	BV	0.037	713958	19.718	19.856
19	20.467	BV	0.024	126457	20.430	20.492
20	20.521	VV	0.025	292988	20.492	20.552
21	20.597	VV	0.028	3346891	20.552	20.619
22	20.643	VV	0.030	4691282	20.619	20.715
23	20.890	PV	0.047	157147737	20.796	21.114
24	21.484	VV	0.030	269515	21.429	21.520
25	21.570	VV	0.034	428428	21.520	21.589
26	21.625	VV	0.042	946817	21.589	21.682
27	21.848	VV	0.045	1834927	21.772	21.936
28	22.564	VV	0.050	167560150	22.435	22.590
29	22.632	VV	0.044	148750700	22.590	22.763
30	22.832	VV	0.033	63119237	22.763	22.951
31	22.997	VV	0.045	511413	22.951	23.048
32	23.157	VV	0.054	279148	23.116	23.212
33	23.490	VV	0.056	338649	23.422	23.521
34	23.722	VV	0.031	312706	23.684	23.777
35	24.112	VV	0.035	232304	24.057	24.126
36	24.155	VV	0.034	1166045	24.126	24.259
37	24.353	VV	0.032	2835226	24.303	24.387
38	24.406	VV	0.036	1062212	24.387	24.474
39	24.643	VV	0.035	2166559	24.581	24.762
40	25.285	VV	0.043	506190	25.229	25.360
41	25.568	VV	0.056	437298	25.507	25.683
42	26.236	PV	0.031	2116931	26.163	26.257
43	26.283	VV	0.035	3383375	26.257	26.398
44	26.486	VV	0.032	1044553	26.447	26.597
45	26.682	VV	0.029	242400	26.641	26.720
46	27.078	PV	0.093	184734	26.819	27.097
47	27.660	VV	0.036	73674	27.626	27.692

Appendix 3. Sample 1, 29.3.2017, Library search report

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
Operator : AKK
Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.768	0.02	C:\Database\wiley7n.l			
			2-METHYLPIPERAZINE	144769	000000-00-0	78
			Furan, tetrahydro-2,5-dimethyl-	8562	001003-38-9	64
			Piperazine, 2-methyl-	8133	000109-07-9	64
2	2.849	0.23	C:\Database\wiley7n.l			
			Hexane, 3-methyl-	8699	000589-34-4	91
			Hexane, 3-methyl-	8697	000589-34-4	91
			Hexane, 3-methyl- (CAS) $$ 3-Methylhexane $$ 2-Ethylpentane	8701	000589-34-4	90
3	2.992	0.04	C:\Database\wiley7n.l			
			Pentane, 3-ethyl- $$ 3-Ethylpentan	8703	000617-78-7	78
			Pentane, 3-ethyl- (CAS) $$ 3-Ethylpentane	8705	000617-78-7	78
			Pentane, 3-ethyl- (CAS) $$ 3-Ethylpentane	8706	000617-78-7	56
4	3.096	0.12	C:\Database\wiley7n.l			
			1-Butanol, 2-ethyl- (CAS) $$ 2-Ethyl-1-butanol $$ 3-Methylolpentane $$ Pseudohexyl alcohol $$ 2-Ethylbutyl alcohol $$ 2-Ethylbutanol $$ 2-Ethylbutanol-1 $$ sec-Hexyl alcohol $$ sec-Pentyl carbinol $$ 3-Pentyl carbinol $$ 2-Ethylbutan-1-ol $$ Ethylbutanol	9669	000097-95-0	40
			Heptane, 3,4-dimethyl-	25198	000922-28-1	36
			Pentane, 3-ethyl- (CAS) $$ 3-Ethylpentane	8705	000617-78-7	25
5	3.535	72.37	C:\Database\wiley7n.l			
			Heptane (CAS) $$ n-Heptane $$ Skellysolve c $$ Heptyl hydride $$ Dipropylmethane $$ n-C7H16 $$ Eptani $$ Heptan $$ Heptanen $$ Gettysolve-C $$ UN 1206	8677	000142-82-5	90
			Heptane (CAS) $$ n-Heptane $$ Skellysolve c $$ Heptyl hydride $$ Dipropylmethane $$ n-C7H16 $$ Eptani $$ Heptan $$ Heptanen $$ Gettysolve-C $$ UN 1206	8675	000142-82-5	90
			Heptane	8673	000142-82-5	78
6	3.715	0.87	C:\Database\wiley7n.l			
			Cyclobutanone, 2,2-dimethyl- (CAS) $$ 2,2-Dimethylcyclobutanone	7062	001192-14-9	72
			Cyclopentane, 1,3-dimethyl-, cis-	7461	002532-58-3	59
			Cyclopentane, 1,2-dimethyl-, cis- (CAS) $$ 1,cis-2-Dimethylcyclopentane $$ cis-1,2-Dimethylcyclopentan	7454	001192-18-3	58
7	3.872	0.04	C:\Database\wiley7n.l			
			Cyclopentane, ethyl- $$ Ethylcyclopentane	7448	001640-89-7	91
			Cyclopentane, ethyl-	7451	001640-89-7	91
			Cyclopentane, ethyl-	7447	001640-89-7	91
8	13.255	0.01	C:\Database\wiley7n.l			
			Cyclohexasiloxane, dodecamethyl- $ $ Dodecamethylcyclohexasiloxane	352523	000540-97-6	64
			Cyclohexasiloxane, dodecamethyl-	352522	000540-97-6	64
			1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane	352530	038147-00-1	36

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
Operator : AKK
Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
9	15.504	0.01	C:\Database\wiley7n.l			
			1,1,1,3,5,7,9,9,9-Nonamethylpentasiloxane	291181	084409-41-6	38
			2,4-Diamino-N,N,5-trimethyl-6-quinolinesulfonamide	226507	000000-00-0	27
			2-Methyl-5-(4'-methylphenyl)sulfonyl-4-nitroimidazole $$ 1H-Imidazole, 2-methyl-4-[(4-methylphenyl)sulfonyl]-5-nitro- (CAS)	226497	113121-75-8	16
10	16.150	0.02	C:\Database\wiley7n.l			
			Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl- (CAS) $$ 4-Methyl-2,6-di-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT-4-METHYLPHENOL $$ Buks $$ Ional $$ Ionole $$ Deenax $$ Dalpac $$ Stavox $$ Vianol $$	144843	000128-37-0	96
			BUTYL HYDROXY TOLUENE	145122	000128-37-0	96
			Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl- (CAS) $$ 4-Methyl-2,6-di-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT-4-METHYLPHENOL $$ Buks $$ Ional $$ Ionole $$ Deenax $$ Dalpac $$ Stavox $$ Vianol $$	144838	000128-37-0	95
11	16.324	0.02	C:\Database\wiley7n.l			
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Methelene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136176	000111-82-0	97
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Methelene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136165	000111-82-0	97
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Methelene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136172	000111-82-0	96
12	17.501	0.01	C:\Database\wiley7n.l			
			Benzoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester $$ .beta.-Resorcylic acid (tms) $$ 2,4-Bis(trimethylsiloxy)trimethylsilybenzoate	313244	010586-16-0	50
			Dimethyl cis-6-(methylthio)-6,7,10,11,12,12a-hexahydro-9H-pyrido[1',	333468	000000-00-0	38

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
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ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2':1,2]pyrazino[4,3-a]indole-11-malonate			
			Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester $$ Gentisic acid (tms)	313248	003618-20-0	33
13	18.566	0.00	C:\Database\wiley7n.l			
			METHYL ESTER OF RICINOLEIC ACID $$ Methyl 12-hydroxy-9-octadecenoate $$ methyl ricinoleate $$ methyl 12-hydroxy-9-octadecenoate (Z) $$ Ricinoleic acid methyl ester $$ 9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]- $$ Flexricin P-1 $$ Methyl rici	263144	000141-24-2	59
			10-Undecenoyl chloride (CAS) $$ Undecylenoyl chloride $$ 10-Undecylenoyl chloride $$ .omega.-Undecylenic acid chloride	117665	038460-95-6	43
			Oxacyclotridecan-2-one	112765	000947-05-7	43
14	18.698	0.19	C:\Database\wiley7n.l			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176783	000124-10-7	97
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176765	000124-10-7	96
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176781	000124-10-7	96
15	19.400	0.00	C:\Database\wiley7n.l			
			Methyl 9-methyltetradecanoate	195519	000000-00-0	96
			methyl 13-methyltetradecanoate	195518	000000-00-0	94
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ PENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentadecanoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pendecanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	93
16	19.487	0.01	C:\Database\wiley7n.l			
			methyl 13-methyltetradecanoate	195518	000000-00-0	81
			Tridecanoic acid, 12-methyl-, methyl ester $$ Methyl isomyristate $$ Methyl 12-methyltridecanoate	176788	005129-58-8	72

Library Search Report

Data Path : C:\mødchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
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Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195467	005129-66-8	72
17	19.633	0.01	C:\Database\wiley7n.l			
			9-Dodecenoic acid, methyl ester, (E)-	133398	055030-26-7	50
			10-Undecenoic acid, methyl ester (CAS) $$ Methyl 10-undecenoate $$ M ETHYL UNDEC-10-ENOATE $$ Methyl un decenate $$ Methyl undecenoate $$ Methyl 10-undecenate $$ Undecenoic acid, methyl ester $$ Undecylenic acid, methyl ester $$ 10-Hendecen oic acid, methyl	112523	000111-81-9	43
			methyl Z-4-decenoate $$ methyl (Z) -4-decenoate	92711	000000-00-0	22
18	19.796	0.03	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	98
			Pentadecanoic acid, methyl ester	195449	007132-64-1	96
			Pentadecanoic acid, methyl ester	195454	007132-64-1	95
19	20.467	0.01	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213909	000112-39-0	97
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213891	000112-39-0	95
			Hexadecanoic acid, methyl ester	213889	000112-39-0	95
20	20.521	0.01	C:\Database\wiley7n.l			
			7,10-Hexadecadienoic acid, methyl ester	208525	016106-03-9	98
			Hexadecadienoic acid, methyl ester (CAS) $$ Methyl hexadecadienoate	208528	029961-54-4	70
			Ethyl linoleate $$ LINOLEIC ACID, ETHYL ESTER $$ ETHYL 9,12-OCTADECA DIENOATE $$ Linoleic acid ethyl es ter $$ 9,12-Octadecadienoic acid (Z,Z)-, ethyl ester $$ Ethyl cis,ci s-9,12-octadecadienoate $$ Ethyl l inolate $$ Mandenol $$ LINOLSAEURE , ETHYLESTER	258924	000544-35-4	64
21	20.597	0.15	C:\Database\wiley7n.l			

Library Search Report

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Data File : 00601006.D
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Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	99
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
22	20.643	0.22	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
23	20.890	7.22	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	99
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213888	000112-39-0	98
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213893	000112-39-0	97
24	21.484	0.01	C:\Database\wiley7n.l			
			Hexadecanoic acid, 15-methyl-, methyl ester $$ Methyl isoheptadecanoate $$ Methyl 15-methylhexadecanoate	231378	006929-04-0	94
			Heptadecanoic acid, methyl ester	231340	001731-92-6	94
			Heptadecanoic acid, methyl ester	231339	001731-92-6	93
25	21.570	0.02	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	94
			Hexadecanoic acid, 14-methyl-, methyl ester	231377	002490-49-5	94
			Tetradecanoic acid, 12-methyl-, methyl ester (CAS) $$ Methyl 12-methyltetradecanoate	195468	005129-66-8	92

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
Operator : AKK
Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
26	21.625	0.04	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228711	010152-61-1	91
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	83
			9-Octadecenoic acid (Z)-, methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ Methyl cis-9-octadecenoate $$ Methyl oleate $$ (Z)-9-Octadecenoic acid methyl ester $$ Methyl-o-octadecenoate $$ cis-9-Octyldecenoic acid, methyl ester $$	245468	000112-62-9	64
27	21.848	0.08	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	98
			Heptadecanoic acid, methyl ester	231336	001731-92-6	98
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ Methyl margarate $$ Margaric acid methyl ester $$ n-Heptadecanoic acid methyl ester $$ HEPTADECANCARBONSAEUREMETHYLESTER	231335	001731-92-6	96
28	22.564	7.70	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid, methyl ester	243170	002462-85-3	99
			10,13-Octadecadienoic acid, methyl ester	243108	056554-62-2	99
			9,12-Octadecadienoic acid, methyl ester, (E,E)-	243102	002566-97-4	99
29	22.632	6.84	C:\Database\wiley7n.l			
			13-Octadecenoic acid, methyl ester, (Z)-	245518	013058-55-4	99
			9-Octadecenoic acid (Z)-, methyl ester (CAS) $$ Methyl oleate $$ Methyl cis-9-octadecenoate $$ Oleic acid methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHYL ESTER $$ (Z)-9-	245466	000112-62-9	99
			9-Octadecenoic acid, methyl ester (CAS) $$ METHYL OCTADEC-9-ENOATE $$ Methyl 9-octadecenoate $$ METHYL OLEATE	245474	002462-84-2	99
30	22.832	2.90	C:\Database\wiley7n.l			
			Octadecanoic acid, methyl ester $$ Stearic acid, methyl ester $$ n-Octadecanoic acid, methyl ester $$ Kemester 9718 $$ Methyl n-octadecanoate $$ Methyl octadecanoate $$ Methyl stearate $$ Metholene 2218 $$ Emery 2218 $$ Kemester 9018 $$ Methyl ester of oc	247760	000112-61-8	98
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester	247763	000112-61-8	98

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
Operator : AKK
Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			$$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es			
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247769	000112-61-8	97
31	22.997	0.02	C:\Database\wiley7n.l			
			6,9-Octadecadienoic acid, methyl ester (CAS) $$ METHYL 6,9-OCTADECADIENOATE	243096	056599-55-4	93
			7,10-Octadecadienoic acid, methyl ester	243097	056554-24-6	93
			8,11-Octadecadienoic acid, methyl ester	243099	056599-58-7	93
32	23.157	0.01	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213899	000112-39-0	35
			Nonanoic acid, 9-oxo-, methyl este	95130	001931-63-1	35
			Methyl 9-methyltetradecanoate	195520	000000-00-0	32
33	23.490	0.02	C:\Database\wiley7n.l			
			Cyclododecanone, 2-methylene-	106914	003045-76-9	46
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211106	001120-25-8	46
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	38
34	23.722	0.01	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester $$ Methyl nonadecanoate $$ n-Nonadecanoic acid methyl ester	263309	001731-94-8	96
			Nonadecanoic acid, methyl ester	263311	001731-94-8	95
			Hexadecanoic acid, methyl ester	213889	000112-39-0	93
35	24.112	0.01	C:\Database\wiley7n.l			
			8,11,14-Eicosatrienoic acid, (Z,Z,Z)- $$ cis-8,11,14-Eicosatrienoic Acid $$ Dihomo-.gamma.-linolenic acid	256725	001783-84-2	64
			7,10,13-Eicosatrienoic acid, methyl ester $$ Methyl eicosa-7,10,13-trienoate	271819	030223-51-9	64
			9-Chloro-9-methylbicyclo[6.1.0]non-4-ene	73385	142926-32-7	64
36	24.155	0.05	C:\Database\wiley7n.l			

Library Search Report

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Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

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Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Bicyclo[10.1.0]tridec-1-ene	84411	054766-91-5	64
			1,5-Cyclodecadiene, (E,Z)- $$ cis, trans-1,5-Cyclodecadiene $$ trans, cis-1,5-Cyclodecadiene $$ 1,5-Cyclodecadiene, (Z,E)- $$ (E,Z)-1,5-Cyclodecadiene	32091	001124-78-3	55
			5-Undecyne	50449	002294-72-6	55
37	24.353	0.13	C:\Database\wiley7n.l			
			Hexadecanoic acid (CAS) $$ Palmitic acid $$ Palmitinic acid $$ n-Hexadecoic acid $$ n-Hexadecanoic acid $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic acid $$ Prifrac 2960 $$ Coconut oil fatty acids $$ Cetylic acid $$ Emersol 140 $$ Emersol 143	195437	000057-10-3	46
			2-(METHYL-D3)-CYCLONONANONE $$ Cyclononanone, 2-methyl-d3- (CAS)	53597	032454-54-9	41
			Myristoyl chloride $$ Tetradecanoyl chloride	181495	000112-64-1	38
38	24.406	0.05	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linoleate $$ METHYL CIS-9,CIS-12-OCTADECADIENOATE $$ Methyl octadecadienoate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoate $$ Methyl 9-ci	243135	000112-63-0	91
			11-Eicosenoic acid, methyl ester	275547	003946-08-5	89
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	68
39	24.643	0.10	C:\Database\wiley7n.l			
			Eicosanoic acid, methyl ester $$ Methyl arachate $$ Methyl eicosanoate $$ Arachidic acid methyl ester	277451	001120-28-1	98
			Eicosanoic acid, methyl ester	277450	001120-28-1	97
			Eicosanoic acid, methyl ester	277452	001120-28-1	97
40	25.285	0.02	C:\Database\wiley7n.l			
			Z-14-Octadecen-1-ol acetate	261160	000000-00-0	64
			(s)(+)-Z-13-Methyl-11-pentadecen-1-ol acetate	228745	000000-00-0	58
			E-6-Octadecen-1-ol acetate	261154	000000-00-0	53
41	25.568	0.02	C:\Database\wiley7n.l			
			17-Pentatriacontene	366689	006971-40-0	58
			17-Pentatriacontene (CAS)	366690	006971-40-0	58
			Cyclopentane, 1,1'-[3-(2-cyclopentylethyl)-1,5-pentanediyl]bis- $$ 1,5-Dicyclopentyl-3-(2-cyclopentylethyl)pentane	254898	055255-85-1	38
42	26.236	0.10	C:\Database\wiley7n.l			
			Cyclododecyne	65443	001129-90-4	93
			Bicyclo[10.1.0]tridec-1-ene	84411	054766-91-5	93
			Isopropyl linoleate $$ 9,12-Octadecadienoic acid (Z,Z)-, 1-methylethyl ester	273683	022882-95-7	70

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Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
43	26.283	0.16	C:\Database\wiley7n.l			
			9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal	208774	002423-10-1	93
			7,11-Hexadecadienal	168609	000000-00-0	47
			9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester $$ Olein, 2-mono- $$ .beta.-Monoolein $$ Glycerol 2-monooleate $$ 2-Monoolein $$ 2-Monooleoylglycerol $$ 2-Oleoyl glycerol ether $$ 2-Oleoylglycerol	303308	003443-84-3	38
44	26.486	0.05	C:\Database\wiley7n.l			
			Octadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester $$ Stearin, 2-mono- $$ .beta.-Glyceryl monostearate $$ .beta.-Monostearin $$ Glycerol-.beta.-monostearate $$ Stearic acid .beta.-monoglyceride $$ 2-Monostearin $$ 2-Monostearoylglycerol $$ 1,2,3-Pr	304826	000621-61-4	35
			2-XYLENE-D10 $$ 1,2-XYLENE-D10	10737	000000-00-0	27
			Hexadecanedioic acid $$ n-Tetradecane-.omega.,.omega.'-dicarboxylic acid $$ Hexadecane-1,16-dioic acid $$ Thapsic acid $$ 1,14-Tetradecanedicarboxylic acid $$ 1,16-Hexadecanedioic acid	233336	000505-54-4	14
45	26.682	0.01	C:\Database\wiley7n.l			
			Docosanoic acid, methyl ester	302040	000929-77-1	98
			Docosanoic acid, methyl ester	302034	000929-77-1	98
			Docosanoic acid, methyl ester	302033	000929-77-1	98
46	27.078	0.01	C:\Database\wiley7n.l			
			1,1,1,3,5,5,5-Heptamethyltrisiloxane $$ Bis(trimethylsiloxy)methylsilane $$ Hydromethylsiloxane $$ Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-	146455	001873-88-7	43
			1,1,1,3,5,5,5-Heptamethyltrisiloxane $$ Bis(trimethylsiloxy)methylsilane $$ Hydromethylsiloxane $$ Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-	146454	001873-88-7	43
			Cyclotrisiloxane, hexamethyl- (CAS) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOHEXASILOXANE $$ Hexamethylcyclotrisiloxane $$ HEXAMETHYL-CYCLOTRISILOXANE $$ Dimethylsiloxane cyclic trimer	146393	000541-05-9	38
47	27.660	0.00	C:\Database\wiley7n.l			
			Cyclotrisiloxane, hexamethyl- (CAS) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOHEXASILOXANE $$ Hexamethylcyclotrisiloxane $$ HEXAMETHYL-CYCLOTRISILOXANE $$ Dimethylsiloxane cyclic trimer	146393	000541-05-9	43
			Cyclotrisiloxane, hexamethyl-	146396	000541-05-9	43
			Cyclotrisiloxane, hexamethyl- $$ Dimethylsiloxane cyclic trimer $$ H	146392	000541-05-9	43

Library Search Report

Data Path : C:\msdchem\1\data\170404VK\
Data File : 00601006.D
Acq On : 4 Apr 2017 19:17
Operator : AKK
Sample : Hnayte
Misc :
ALS Vial : 6 Sample Multiplier: 1

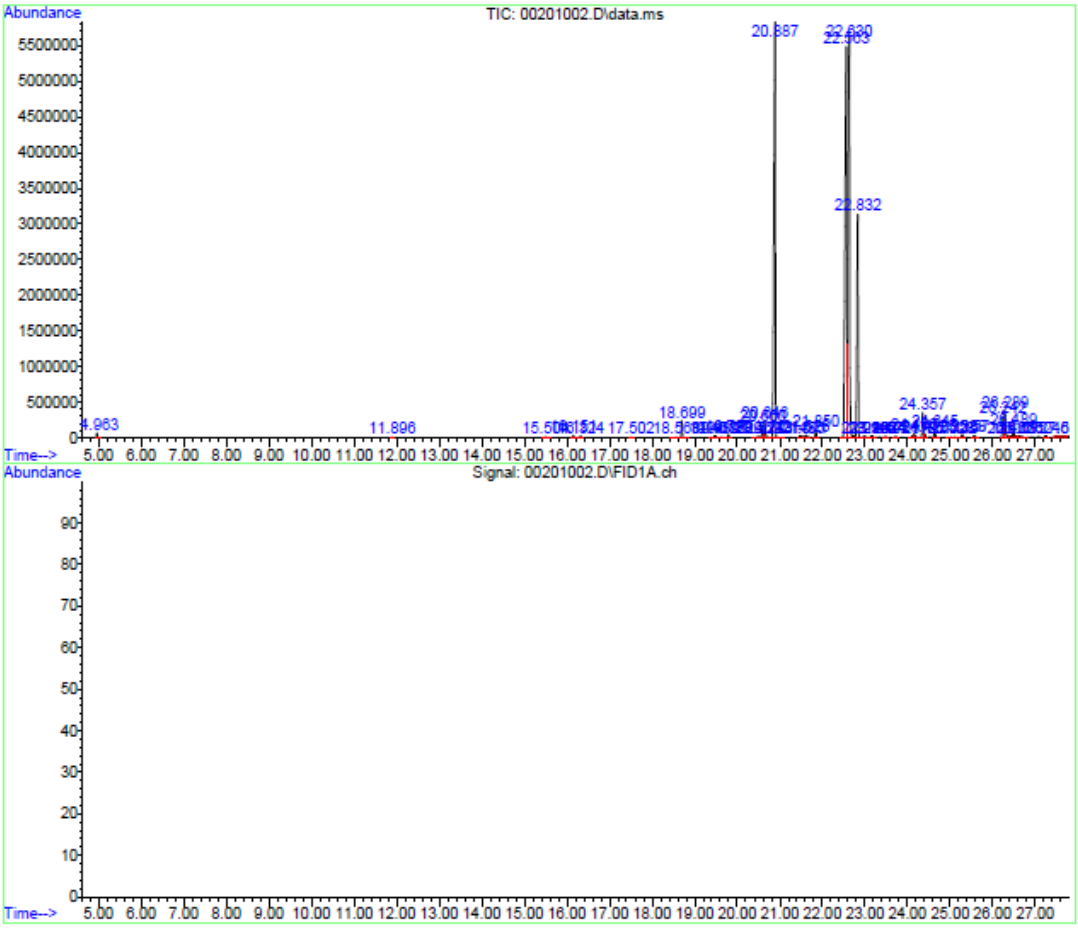
Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			examethylcyclotrisiloxane			

Appendix 4. Sample 1, 5.4.2017, GC Analysis

```
File       :C:\msdchem\1\data\170406VK\00201002.D
Operator   : AKK
Acquired   :  5 Apr 2017  16:32     using AcqMethod 170404VK.M
Instrument :    Inst 2
Sample Name: Hnaytel
Misc Info  :
Vial Number: 2
```



Appendix 5. Sample 1, 5.4.2017, Integrated peak areas

TIC: 00201002.D\data.ms
Hnayte1

Peak #	Ret Time	Type	Width	Area	Start Time	End Time
1	4.963	BB	0.041	882988	4.921	5.059
2	11.896	BB	0.023	80472	11.849	11.932
3	15.504	BV	0.033	175652	15.410	15.609
4	16.151	BV	0.026	431044	16.094	16.201
5	16.324	PB	0.027	310792	16.201	16.372
6	17.502	BB	0.033	92460	17.445	17.579
7	18.568	VV	0.045	91677	18.440	18.601
8	18.699	PB	0.028	3667013	18.652	18.851
9	19.401	BV	0.035	92002	19.341	19.434
10	19.489	PV	0.027	216622	19.434	19.555
11	19.635	VB	0.039	134166	19.555	19.684
12	19.799	BB	0.028	663930	19.720	19.850
13	20.469	BV	0.024	121363	20.359	20.493
14	20.523	VV	0.027	275094	20.493	20.555
15	20.600	VV	0.029	3024038	20.555	20.622
16	20.646	VV	0.031	4310671	20.622	20.714
17	20.743	VV	0.033	86722	20.714	20.797
18	20.887	VV	0.042	138176729	20.797	21.107
19	21.486	PV	0.030	221300	21.435	21.512
20	21.571	VV	0.043	459756	21.512	21.592
21	21.626	VV	0.042	852484	21.592	21.684
22	21.850	VV	0.028	1609653	21.799	21.896
23	22.563	VV	0.046	148421317	22.432	22.589
24	22.630	VV	0.064	132006625	22.589	22.764
25	22.832	VV	0.031	55604757	22.764	22.914
26	22.996	VV	0.039	492321	22.946	23.049
27	23.145	VV	0.039	264147	23.109	23.172
28	23.193	VV	0.049	290649	23.172	23.273
29	23.492	VV	0.051	298447	23.434	23.539
30	23.726	PB	0.030	221847	23.677	23.785
31	24.118	BV	0.025	177632	24.013	24.129
32	24.160	VV	0.037	1027855	24.129	24.289
33	24.357	VV	0.030	6245100	24.289	24.396
34	24.410	VV	0.032	796501	24.396	24.460
35	24.645	VV	0.036	1952456	24.580	24.764
36	25.028	VV	0.054	213922	24.916	25.063
37	25.119	VV	0.079	298862	25.063	25.220
38	25.288	VV	0.044	966090	25.220	25.355
39	25.571	VV	0.040	625955	25.506	25.644
40	26.242	PV	0.031	5448148	26.185	26.264
41	26.289	VV	0.033	8116570	26.264	26.402
42	26.425	VV	0.034	272062	26.402	26.450
43	26.489	VV	0.030	2292446	26.450	26.539
44	26.626	VV	0.057	331103	26.585	26.655
45	26.685	VV	0.037	373485	26.655	26.814
46	27.245	VV	0.033	82448	27.204	27.290
47	27.639	PV	0.126	999207	27.413	27.732

Appendix 6. Sample 1, 5.4.2017, Library search report

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	4.963	0.17	C:\Database\wiley7n.l Octane $$ n-Octane $$ n-C8H18 $$ O ktan $$ Oktanen $$ Ottani $$ UN 12 62 $$ Isooctane	15631	000111-65-9	90
			Octane (CAS) $$ n-Octane $$ Octane (DOT) $$ Isooctane $$ n-C8H18 $$ Oktan $$ Oktanen $$ Ottani $$ UN 1 262	15629	000111-65-9	72
			Octane (CAS) $$ n-Octane $$ Octane (DOT) $$ Isooctane $$ n-C8H18 $$ Oktan $$ Oktanen $$ Ottani $$ UN 1 262	15635	000111-65-9	72
2	11.896	0.02	C:\Database\wiley7n.l Octane	15632	000111-65-9	43
			Hexane, 2,3,4-trimethyl-	25228	000921-47-1	39
			Ether, heptyl hexyl	115828	007289-40-9	33
3	15.504	0.03	C:\Database\wiley7n.l 1,1,1,3,5,7,9,9,9-Nonamethylpentas iloxane	291181	084409-41-6	43
			3.ALPHA.,19-DIACETOXYDPONGIA-13(16),14-DIEN-2-ONE $$ 18-Nor-16-oxaan drosta-13(17),14-dien-2-one, 3-(ac etyloxy)-4-[(acetyloxy)methyl]-4,8 -dimethyl-, (3.alpha.,4.beta.,5.al pha.)- (CAS) $$ Phenanthro[1,2-c]f uran, 18-nor-16-oxaandrosta-13(17) ,14-dien-2-one de	340967	071302-24-4	12
			1h-Pyrrole-3,4-diacetic acid, 2-ac etoxymethyl-5-methoxycarbonyl-, di methyl ester	290681	000000-00-0	12
4	16.151	0.08	C:\Database\wiley7n.l Phenol, 2,6-bis(1,1-dimethylethyl) -4-methyl- (CAS) $$ 4-Methyl-2,6-d i-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4 K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT -4-METHYLPHENOL $$ Buks $$ Ional $ $ Ionole $$ Deenax $$ Dalpac $$ St avox $$ Vianol $$	144841	000128-37-0	97
			Phenol, 2,6-bis(1,1-dimethylethyl) -4-methyl- (CAS) $$ 4-Methyl-2,6-d i-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4 K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT -4-METHYLPHENOL $$ Buks $$ Ional $ $ Ionole $$ Deenax $$ Dalpac $$ St avox $$ Vianol $$	144850	000128-37-0	97
			BUTYL HYDROXY TOLUENE	145122	000128-37-0	95
5	16.324	0.06	C:\Database\wiley7n.l Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136176	000111-82-0	91
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$	136169	000111-82-0	83

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnayte1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci			
			Dodecanoic acid, methyl ester	136163	000111-82-0	81
6	17.502	0.02	C:\Database\wiley7n.l			
			1,3,5,7,9-Pentaethyl-1,9-dibutoxyp entasiloxane	368434	073420-35-6	38
			Benzoic acid, 2,4-bis[(trimethylsi lyl)oxy]-, trimethylsilyl ester (C AS) $$ TRISTRIMETHYLSILYL 2,4-DIHY DROXYBENZOIC ACID $$ 2,4-DIHYDROXY BENZOIC ACID 3TMS $$ trimethylsily l [(2,4-di(trimethylsiloxy)phenyl] -methanoate $$ .beta.-Resorcylic a cid (tms) $$ 2,4-	313242	010586-16-0	36
			Propanoic acid, 3-[bis[(trimethyls ilyl)oxy]phosphinyl]-, trimethylsi lyl ester (CAS) $$ PHOSPHONOPROPIO NIC ACID-TRITMS ESTER $$ TRISTRIME THYLSILYL PHOSPHONOPROPIONATE	313098	053044-28-3	36
7	18.568	0.02	C:\Database\wiley7n.l			
			Methyl ricinoleate $$ Ricinoleic a cid methyl ester $$ 9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]- $$ Flexricin P-1 $$ Methy l ricinolate	263143	000141-24-2	38
			10-Undecenoic acid, methyl ester (CAS) $$ Methyl 10-undecenoate $$ M ETHYL UNDEC-10-ENOATE $$ Methyl un decenate $$ Methyl undecenoate $$ Methyl 10-undecenate $$ Undecenoic acid, methyl ester $$ Undecylenic acid, methyl ester $$ 10-Hendecen oic acid, methyl	112523	000111-81-9	27
			10-Undecenoic acid, methyl ester (CAS) $$ Methyl 10-undecenoate $$ M ETHYL UNDEC-10-ENOATE $$ Methyl un decenate $$ Methyl undecenoate $$ Methyl 10-undecenate $$ Undecenoic acid, methyl ester $$ Undecylenic acid, methyl ester $$ 10-Hendecen oic acid, methyl	112521	000111-81-9	27
8	18.699	0.70	C:\Database\wiley7n.l			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176765	000124-10-7	95
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176781	000124-10-7	95

3(10)

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester	176766	000124-10-7	95
9	19.401	0.02	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ PENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentadecanoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pendecanoate $$ n-Pentadecanoic acid methyl ester	195451	007132-64-1	94
			Methyl 9-methyltetradecanoate	195519	000000-00-0	93
			methyl 13-methyltetradecanoate	195518	000000-00-0	91
10	19.489	0.04	C:\Database\wiley7n.l			
			Tetradecanoic acid, 12-methyl-, methyl ester (CAS) $$ Methyl 12-methyltetradecanoate	195468	005129-66-8	94
			Tetradecanoic acid, 12-methyl-, methyl ester $$ Methyl 12-methyltetradecanoate	195466	005129-66-8	86
			Tridecanoic acid, 12-methyl-, methyl ester $$ Methyl isomyristate $$ Methyl 12-methyltridecanoate	176788	005129-58-8	72
11	19.635	0.03	C:\Database\wiley7n.l			
			Eicosenoic acid, methyl ester	275549	027070-40-2	68
			Eicosenoic acid, methyl ester (CAS) $$ METHYL EICOSENOATE	275550	027070-40-2	47
			Chloromethyl 5-chlorodedecanoate	227713	000000-00-0	35
12	19.799	0.13	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ PENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentadecanoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pendecanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	97
			Pentadecanoic acid, methyl ester	195449	007132-64-1	96
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ PENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentadecanoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pendecanoate $$ n-Pentadecanoic acid methyl ester	195457	007132-64-1	96
13	20.469	0.02	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 2216 $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Methyl palmitate $$ Uniphat A60	213890	000112-39-0	94

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Hexadecanoic acid, methyl ester	213900	000112-39-0	94
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213909	000112-39-0	94
14	20.523	0.05	C:\Database\wiley7n.l			
			7,10-Hexadecadienoic acid, methyl ester	208525	016106-03-9	98
			9,12-Octadecadien-1-ol (CAS) $$ OCTADECA-9,12-DIEN-1-OL	208785	001577-52-2	95
			Hexadecadienoic acid, methyl ester (CAS) $$ Methyl hexadecadienoate	208528	029961-54-4	91
15	20.600	0.58	C:\Database\wiley7n.l			
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
16	20.646	0.82	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	99
17	20.743	0.02	C:\Database\wiley7n.l			
			Oxacyclohexadecan-2-one	174119	000106-02-5	50
			Hexadecenoic acid, Z-11-	192904	002416-20-8	50
			Cyclopentadecanone, 2-hydroxy-	174133	004727-18-8	50
18	20.887	26.38	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	99
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213888	000112-39-0	97

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnayte1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213893	000112-39-0	97
19	21.486	0.04	C:\Database\wiley7n.l			
			Hexadecanoic acid, 15-methyl-, met hyl ester $$ Methyl isoheptadecano ate $$ Methyl 15-methylhexadecanoa te	231378	006929-04-0	94
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	93
			Heptadecanoic acid, methyl ester	231340	001731-92-6	93
20	21.571	0.09	C:\Database\wiley7n.l			
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	95
			Hexadecanoic acid, 14-methyl-, met hyl ester $$ Methyl 14-methylhexad ecanoate	231376	002490-49-5	95
			Heptadecanoic acid, methyl ester	231340	001731-92-6	94
21	21.626	0.16	C:\Database\wiley7n.l			
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245467	000112-62-9	93
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211101	001120-25-8	87
			1-Oxaspiro[2.2]pentane, 5-isopropy lidene-2,2,4,4-tetramethyl-	68056	015448-69-8	83
22	21.850	0.31	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	97
			Heptadecanoic acid, methyl ester	231336	001731-92-6	96
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ M ethyl margarate $$ Margaric acid m ethyl ester $$ n-Heptadecanoic aci d methyl ester $$ HEPTADECANCARBON SAEUREMETHYLESTER	231335	001731-92-6	95
23	22.563	28.34	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linol eate $$ METHYL CIS-9,CIS-12-OCTADE CADIENOATE $$ Methyl octadecadieno ate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoa te $$ Methyl 9-ci	243127	000112-63-0	99
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243128	000112-63-0	99
			9,12-Octadecadienoic acid, methyl	243170	002462-85-3	99

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ester			
24	22.630	25.20	C:\Database\wiley7n.l			
			8-Octadecenoic acid, methyl ester, (E)- (CAS) $$ TRANS-8-OCTADECENOIC METHYL ESTER $$ Methyl trans-8-octadecenoate	245465	026528-50-7	99
			9-Octadecenoic acid, methyl ester, (E)- $$ Elaidic acid, methyl ester $$ Methyl elaidate $$ Methyl trans-9-octadecenoate $$ (E)-9-Octadecenoic acid methyl ester	245486	001937-62-8	99
			9-Octadecenoic acid (Z)-, methyl ester	245471	000112-62-9	99
25	22.832	10.62	C:\Database\wiley7n.l			
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247763	000112-61-8	98
			Octadecanoic acid, methyl ester $$ Stearic acid, methyl ester $$ n-Octadecanoic acid, methyl ester $$ Kemester 9718 $$ Methyl n-octadecanoate $$ Methyl octadecanoate $$ Methyl stearate $$ Metholene 2218 $$ Emery 2218 $$ Kemester 9018 $$ Methyl ester of oc	247760	000112-61-8	98
			Octadecanoic acid, methyl ester	247756	000112-61-8	97
26	22.996	0.09	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243132	000112-63-0	98
			10,13-Octadecadienoic acid, methyl ester	243108	056554-62-2	95
			11,14-Octadecadienoic acid, methyl ester	243110	056554-61-1	93
27	23.145	0.05	C:\Database\wiley7n.l			
			Ethyl linoleate $$ LINOLEIC ACID, ETHYL ESTER $$ ETHYL 9,12-OCTADECADIENOATE $$ Linoleic acid ethyl ester $$ 9,12-Octadecadienoic acid (Z,Z)-, ethyl ester $$ Ethyl cis,cis-9,12-octadecadienoate $$ Ethyl linolate $$ Mandenol $$ LINOLSAEURE, ETHYLESTER	258924	000544-35-4	60
			3-Phenyl-1,4(E)-dodecadiene	168721	000000-00-0	52
			Cyclohexene, 4-(4-ethylcyclohexyl)-1-pentyl-	203503	000000-00-0	49
28	23.193	0.06	C:\Database\wiley7n.l			
			Ethyl Oleate	261113	000111-62-6	91
			Ethyl Oleate $$ 9-Octadecenoic acid (Z)-, ethyl ester $$ Oleic acid, ethyl ester $$ (Z)-9-Octadecenoic acid ethyl ester $$ Ethyl cis-9-octadecenoate	261107	000111-62-6	72
			Ethyl Oleate	261112	000111-62-6	70

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
29	23.492	0.06	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-octyl -, methyl ester	261100	010152-62-2	52
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	52
			9-Octadecenoic acid (Z)-, methyl ester (CAS) $$ Methyl oleate $$ Methyl cis-9-octadecenoate $$ Oleic acid methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHYL ESTER $$ (Z)-9-	245467	000112-62-9	49
30	23.726	0.04	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester (CAS) $$ Methyl nonadecanoate $$ Nonadecanoic acid methyl ester $$ METHYL N-NONADECANOATE $$ n-Nonadecanoic acid methyl ester	263308	001731-94-8	97
			Nonadecanoic acid, methyl ester $$ Methyl nonadecanoate $$ n-Nonadecanoic acid methyl ester	263309	001731-94-8	96
			Nonadecanoic acid, methyl ester	263311	001731-94-8	95
31	24.118	0.03	C:\Database\wiley7n.l			
			2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)-	127817	054594-42-2	60
			5-Decen-1-ol, (E)- (CAS) $$ (E)-dec-5-en-1-ol $$ (E)-5-Decen-1-ol $$ trans-5-Decen-1-ol	55897	056578-18-8	43
			5-Decen-1-ol, (E)- $$ (E)-5-Decen-1-ol	55896	056578-18-8	43
32	24.160	0.20	C:\Database\wiley7n.l			
			METHYL TETRADECADIENOATE	171135	000000-00-0	64
			1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.beta.,4a.beta.,7.beta.,7a.beta.,7b.alpha.)]- $$ Ledane	124906	028580-43-0	49
			anti(10,11)-Tricyclo[4.3.1.1(2,5)]-undecan-10-one $$ Tricyclo[4.3.1.1(2,5)]undecan-10-one, (1.alpha.,2.beta.,5.beta.,6.alpha.)- (CAS) $$ Tricyclo[4.3.1.12,5]undecan-10-one, (1.alpha.,2.beta.,5.beta.,6.alpha.)- (CAS)	65149	085219-11-0	49
33	24.357	1.19	C:\Database\wiley7n.l			
			o-Xylene-d10	10736	000000-00-0	30
			Dodecanoic acid (CAS) $$ Lauric acid $$ Abl $$ Neo-fat 12 $$ Vulvic acid $$ Univol u-314 $$ Aliphat no. 4 $$ Neo-fat 12-43 $$ Dodecylic acid $$ Ninol aa62 extra $$ Lauros tearic acid $$ n-Dodecanoic acid $$ 1-Undecanecarboxylic acid $$ Univol U 314 $$ Luna	115386	000143-07-7	25
			1-Propanone, 1-phenyl-3-(1-piperidyl)-	140058	000000-00-0	14

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnaytel
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
29	23.492	0.06	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-octyl -, methyl ester	261100	010152-62-2	52
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	52
			9-Octadecenoic acid (Z)-, methyl ester (CAS) $$ Methyl oleate $$ Methyl cis-9-octadecenoate $$ Oleic acid methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHYL ESTER $$ (Z)-9-	245467	000112-62-9	49
30	23.726	0.04	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester (CAS) $$ Methyl nonadecanoate $$ Nonadecanoic acid methyl ester $$ METHYL N-NONADECANOATE $$ n-Nonadecanoic acid methyl ester	263308	001731-94-8	97
			Nonadecanoic acid, methyl ester $$ Methyl nonadecanoate $$ n-Nonadecanoic acid methyl ester	263309	001731-94-8	96
			Nonadecanoic acid, methyl ester	263311	001731-94-8	95
31	24.118	0.03	C:\Database\wiley7n.l			
			2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)-	127817	054594-42-2	60
			5-Decen-1-ol, (E)- (CAS) $$ (E)-dec-5-en-1-ol $$ (E)-5-Decen-1-ol $$ trans-5-Decen-1-ol	55897	056578-18-8	43
			5-Decen-1-ol, (E)- $$ (E)-5-Decen-1-ol	55896	056578-18-8	43
32	24.160	0.20	C:\Database\wiley7n.l			
			METHYL TETRADECADIENOATE	171135	000000-00-0	64
			1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1a.alpha.,4.beta.,4a.beta.,7.beta.,7a.beta.,7b.alpha.)]- $$ Ledane	124906	028580-43-0	49
			anti(10,11)-Tricyclo[4.3.1.1(2,5)]-undecan-10-one $$ Tricyclo[4.3.1.1(2,5)]undecan-10-one, (1.alpha.,2.beta.,5.beta.,6.alpha.)- (CAS) $$ Tricyclo[4.3.1.12,5]undecan-10-one, (1.alpha.,2.beta.,5.beta.,6.alpha.)- (CAS)	65149	085219-11-0	49
33	24.357	1.19	C:\Database\wiley7n.l			
			o-Xylene-d10	10736	000000-00-0	30
			Dodecanoic acid (CAS) $$ Lauric acid $$ Abl $$ Neo-fat 12 $$ Vulvic acid $$ Univol u-314 $$ Aliphat no. 4 $$ Neo-fat 12-43 $$ Dodecylic acid $$ Ninol aa62 extra $$ Lauros tearic acid $$ n-Dodecanoic acid $$ 1-Undecanecarboxylic acid $$ Univol U 314 $$ Luna	115386	000143-07-7	25
			1-Propanone, 1-phenyl-3-(1-piperidyl)-	140058	000000-00-0	14

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnayte1
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Thiophene, 2-nitro- $$ 2-Nitrothio phene	25311	000609-40-5	14
43	26.489	0.44	C:\Database\wiley7n.l			
			o-Xylene-d10	10736	000000-00-0	38
			d-Gulopyranoside, 2,3:4,6-di-O-(et hylboranediyl)-1-O-methyl-	212670	000000-00-0	35
			Dodecanoic acid (CAS) $$ Lauric ac id $$ Abl $$ Neo-fat 12 $$ Vulvic acid $$ Univol u-314 $$ Aliphat no . 4 $$ Neo-fat 12-43 $$ Dodecylic acid $$ Ninol aa62 extra $$ Lauros tearic acid $$ n-Dodecanoic acid $ $ 1-Undecanecarboxylic acid $$ Uni vol U 314 $$ Luna	115386	000143-07-7	20
44	26.626	0.06	C:\Database\wiley7n.l			
			Phenol, 2,2'-[(1-methyl-1,2-ethane diyl)bis(nitrilomethylidyne)]bis- $$ o-Cresol, .alpha.,.alpha.'-(pro pylenedinitrilo)di- $$ Cuvan 80 $$ DMD $$ Keromet MD $$ N,N'-Bis(sal icylidene)-1,2-diaminopropane $$ N ,N'-Disalicylidene-1,2-diaminoprop ane $$ N,N'-Disal	228407	000094-91-7	22
			6-bromo-3-(2'-hydroxyethyl)quinoli n-2(1H)-one	209039	000000-00-0	22
			(S)-(E)-(-)-4-Acetoxy-1-phenyl-2-d odecen-1-one	267542	000000-00-0	12
45	26.685	0.07	C:\Database\wiley7n.l			
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl doc osanoate $$ Behenic acid methyl es ter $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302031	000929-77-1	97
			Docosanoic acid, methyl ester	302034	000929-77-1	97
			Docosanoic acid, methyl ester	302035	000929-77-1	96
46	27.245	0.02	C:\Database\wiley7n.l			
			Phenol, 2,2'-[(1-methyl-1,2-ethane diyl)bis(nitrilomethylidyne)]bis- $$ o-Cresol, .alpha.,.alpha.'-(pro pylenedinitrilo)di- $$ Cuvan 80 $$ DMD $$ Keromet MD $$ N,N'-Bis(sal icylidene)-1,2-diaminopropane $$ N ,N'-Disalicylidene-1,2-diaminoprop ane $$ N,N'-Disal	228407	000094-91-7	50
			Gibberellin A3 $$ Gibb-3-ene-1,10- dicarboxylic acid, 2,4a,7-trihydro xy-1-methyl-8-methylene-, 1,4a-lac tone, (1.alpha.,2.beta.,4a.alpha., 4b.beta.,10.beta.)- (CAS) $$ GA3 $ $ GA $$ Gibberellin X $$ Gibberell ic acid $$ 4a,1-(Epoxymethano)-7,9 a-methanobenz[a]a	294997	000077-06-5	47
			Galactitol, hexaacetate, D- (CAS) $$ GALACTITOL-1,2,3,4,5,6-HEXAACET ATE	348804	014330-96-2	37
47	27.639	0.19	C:\Database\wiley7n.l			
			Silicic acid, diethyl bis(trimethy lsilyl) ester	244286	003555-45-1	38
			2-Ethylacridine	125906	000000-00-0	30

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00201002.D
Acq On : 5 Apr 2017 16:32
Operator : AKK
Sample : Hnayte1
Misc :
ALS Vial : 2 Sample Multiplier: 1

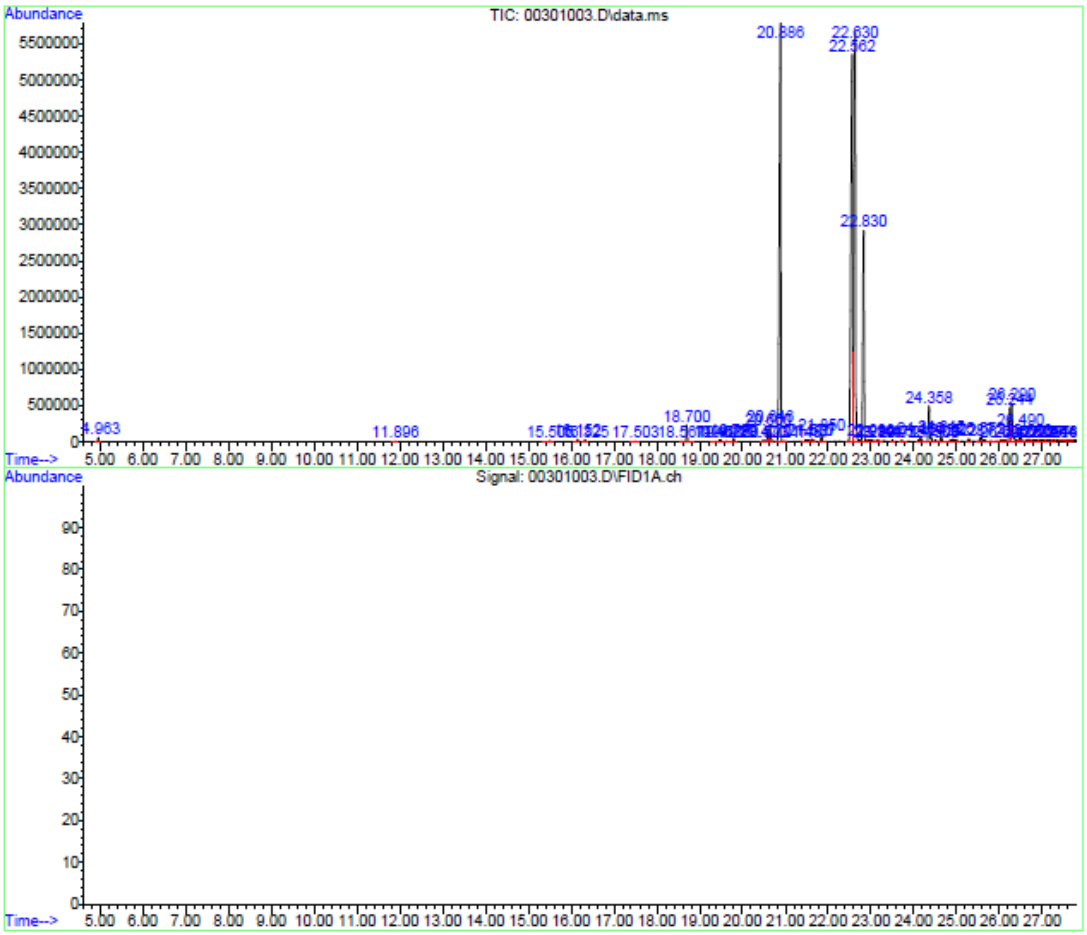
Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Cyclotrisiloxane, hexamethyl- (CAS) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOHEXASILOXANE $$ Hexamethylcyclotrisiloxane $$ HEXAMETHYL-CYCLOTRISILOXANE $$ Dimethylsiloxane cyclic trimer	146397	000541-05-9	27

Appendix 7. Sample 2, 5.4.2017, GC Analysis

```
File       :C:\msdchem\1\data\170406VK\00301003.D
Operator   : AKK
Acquired   :  5 Apr 2017  17:13     using AcqMethod 170404VK.M
Instrument :    Inst 2
Sample Name: Hnayte2
Misc Info  :
Vial Number: 3
```



Appendix 8. Sample 2, 5.4.2017, Integrated peak areas

TIC: 00301003.D\data.ms
Hnayte2

Peak #	Ret Time	Type	Width	Area	Start Time	End Time
1	4.963	PV	0.039	887028	4.894	5.015
2	11.896	BB	0.024	89091	11.830	11.932
3	15.505	BB	0.034	197717	15.336	15.572
4	16.152	BB	0.027	443736	16.057	16.196
5	16.325	BB	0.026	316564	16.261	16.363
6	17.503	BB	0.034	101674	17.399	17.574
7	18.567	VV	0.025	87148	18.529	18.603
8	18.700	PB	0.027	3642789	18.652	18.842
9	19.402	PV	0.029	108329	19.267	19.448
10	19.490	PB	0.028	242249	19.448	19.567
11	19.635	BV	0.034	140184	19.572	19.710
12	19.799	PV	0.029	667655	19.710	19.844
13	20.470	BV	0.025	140657	20.405	20.495
14	20.523	VV	0.026	289513	20.495	20.554
15	20.600	PV	0.029	3011998	20.554	20.622
16	20.646	VV	0.030	4155611	20.622	20.718
17	20.886	PV	0.042	135171051	20.798	21.030
18	21.487	VV	0.038	361163	21.375	21.510
19	21.570	VV	0.041	628884	21.510	21.592
20	21.627	VV	0.046	978640	21.592	21.688
21	21.850	VV	0.030	1702109	21.789	21.927
22	22.562	VV	0.046	143282455	22.427	22.588
23	22.630	VV	0.042	128790428	22.588	22.764
24	22.830	VV	0.032	54053495	22.764	22.912
25	22.996	VV	0.060	1116870	22.912	23.057
26	23.144	VV	0.035	359068	23.113	23.168
27	23.191	VV	0.063	537885	23.168	23.277
28	23.493	VV	0.042	295411	23.468	23.536
29	23.725	VV	0.041	390036	23.673	23.823
30	24.160	VV	0.053	1717102	24.051	24.292
31	24.358	VV	0.037	10591498	24.292	24.475
32	24.500	VV	0.033	206613	24.475	24.525
33	24.645	VV	0.036	1802766	24.582	24.698
34	24.922	VV	0.111	2161672	24.751	25.066
35	25.287	VV	0.044	896488	25.229	25.361
36	25.572	VV	0.084	2413305	25.470	25.812
37	26.095	PV	0.103	1125872	25.812	26.190
38	26.244	VV	0.033	8652373	26.190	26.266
39	26.290	VV	0.039	12331627	26.266	26.407
40	26.425	VV	0.035	307822	26.407	26.450
41	26.490	VV	0.031	3427833	26.450	26.588
42	26.683	VV	0.051	902713	26.588	26.740
43	26.815	VV	0.075	819522	26.740	26.897
44	27.046	VV	0.063	215570	26.954	27.061
45	27.087	VV	0.084	521550	27.061	27.208
46	27.244	VV	0.042	140537	27.208	27.295
47	27.462	PV	0.043	144617	27.405	27.501
48	27.665	VV	0.051	163773	27.547	27.705

Appendix 9. Sample 2, 5.4.2017, Library search report

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	4.963	0.17	C:\Database\wiley7n.l			
			Octane $$ n-Octane $$ n-C8H18 $$ O ktan $$ Oktanen $$ Ottani $$ UN 12 62 $$ Isooctane	15631	000111-65-9	90
			Octane (CAS) $$ n-Octane $$ Octane (DOT) $$ Isooctane $$ n-C8H18 $$ Oktan $$ Oktanen $$ Ottani $$ UN 1 262	15635	000111-65-9	90
			Heptane, 2,4-dimethyl- $$ 2,4-Dime thylheptane	25184	002213-23-2	78
2	11.896	0.02	C:\Database\wiley7n.l			
			Dodecane	74391	000112-40-3	91
			Dodecane (CAS) $$ n-Dodecane $$ Ba 51-090453 $$ Adakane 12 $$ Isodod ecane $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ n-Dodecane min $$ N-Dodecan $$ Duodecane $$ ACETIC ACI D 3-HYDROXY-7-ISOPROPENYL-1,4A-DIM ETHYL-2,3,4,4A,5,6,7,8-OCTAHYDRO-N AP	74407	000112-40-3	91
			Dodecane	74390	000112-40-3	90
3	15.505	0.04	C:\Database\wiley7n.l			
			2,4-Diamino-N,N,5-trimethyl-6-quin olinesulfonamide	226507	000000-00-0	22
			TRIMETHYLSILYL ESTER OF 4-METHYL-2 -TRIMETHYLSILYLOXY-BENZOIC ACID	244578	000000-00-0	12
			TRIMETHYLSILYL ESTER OF 5-METHYL-2 -TRIMETHYLSILYLOXY-BENZOIC ACID	244579	000000-00-0	12
4	16.152	0.08	C:\Database\wiley7n.l			
			Phenol, 2,6-bis(1,1-dimethylethyl) -4-methyl- (CAS) $$ 4-Methyl-2,6-d i-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4 K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT -4-METHYLPHENOL $$ Buks $$ Ional $ $ Ionole $$ Deenax $$ Dalpac $$ St avox $$ Vianol $$	144850	000128-37-0	97
			Phenol, 2,6-bis(1,1-dimethylethyl) -4-methyl- (CAS) $$ 4-Methyl-2,6-d i-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4 K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT -4-METHYLPHENOL $$ Buks $$ Ional $ $ Ionole $$ Deenax $$ Dalpac $$ St avox $$ Vianol $$	144843	000128-37-0	95
			Phenol, 2,6-bis(1,1-dimethylethyl) -4-methyl- (CAS) $$ 4-Methyl-2,6-d i-tert-butylphenol $$ BHT $$ P 21 $$ CAO 3 $$ AO 29 $$ CAO 1 $$ AO 4 K $$ DBPC $$ P 21 $ $$ 2,6-DI-TERT -4-METHYLPHENOL $$ Buks $$ Ional $ $ Ionole $$ Deenax $$ Dalpac $$ St avox $$ Vianol $$	144845	000128-37-0	95
5	16.325	0.06	C:\Database\wiley7n.l			
			Undecanoic acid, 10-methyl-, methy l ester	136187	005129-56-6	86
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho	136177	000111-82-0	86

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci			
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136175	000111-82-0	86
6	17.503	0.02	C:\Database\wiley7n.l			
			6-Aza-5,7,12,14-tetrathiapentacene	302266	000000-00-0	40
			1,3,5,7,9-Pentaethylbicyclo[5.3.1] pentasiloxane	322197	073420-26-5	33
			1,3,5,7-Tetraethyl-1-ethylbutoxysi loxycyclotetrasiloxane	351705	073420-30-1	28
7	18.567	0.02	C:\Database\wiley7n.l			
			METHYL ESTER OF RICINOLEIC ACID $$ Methyl 12-hydroxy-9-octadecenoate $$ methyl ricinoleate $$ methyl 1 2-hydroxy-9-octadecenoate (Z) $$ R icinoleic acid methyl ester $$ 9-O ctadecenoic acid, 12-hydroxy-, met hyl ester, [R-(Z)]- $$ Flexricin P -1 $$ Methyl rici	263144	000141-24-2	53
			10-Undecenoyl chloride (CAS) $$ Un decylenoyl chloride $$ 10-Undecyle noyl chloride $$ .omega.-Undecylen ic acid chloride	117665	038460-95-6	32
			4H-Cyclopentacycloocten-4-one, dec ahydro-	68109	055723-95-0	25
8	18.700	0.69	C:\Database\wiley7n.l			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176778	000124-10-7	98
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176765	000124-10-7	96
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176783	000124-10-7	96
9	19.402	0.02	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester (	195451	007132-64-1	97

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester			
			Methyl 9-methyltetradecanoate	195519	000000-00-0	90
			Pentadecanoic acid, methyl ester	195454	007132-64-1	74
10	19.490	0.05	C:\Database\wiley7n.l			
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195467	005129-66-8	70
			Tetradecanoic acid, 12-methyl-, me thyl ester $$ Methyl 12-methyltetr adecanoate	195466	005129-66-8	58
			Methyl 9-methyltetradecanoate	195519	000000-00-0	58
11	19.635	0.03	C:\Database\wiley7n.l			
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	46
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211101	001120-25-8	43
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211106	001120-25-8	35
12	19.799	0.13	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester	195454	007132-64-1	97
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	96
			Pentadecanoic acid, methyl ester	195449	007132-64-1	96
13	20.470	0.03	C:\Database\wiley7n.l			
			Tridecanoic acid, methyl ester (CA S) $$ Methyl tridecanoate $$ METHY L N-TRIDECANOATE $$ Tridecanoic ac id methyl ester $$ Methyl ester of tridecanoic acid $$ n-Tridecanoic acid methyl ester	157240	001731-88-0	96
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	96
			Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ Metholene 2216 $$ Methyl hexadecan oate $$ Methyl n-hexadecanoate $$ Methyl palmitate $$ Uniphat A60	213890	000112-39-0	95

4(10)

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
14	20.523	0.05	C:\Database\wiley7n.l Hexadecadienoic acid, methyl ester (CAS) $$ Methyl hexadecadienoate	208528	029961-54-4	95
			Hexadecadienoic acid, methyl ester $$ Methyl hexadecadienoate	208527	029961-54-4	95
			7,10-Hexadecadienoic acid, methyl ester	208525	016106-03-9	94
15	20.600	0.57	C:\Database\wiley7n.l 7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211106	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	98
16	20.646	0.78	C:\Database\wiley7n.l 9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211101	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmitoleic acid, methyl ester	211106	001120-25-8	99
17	20.886	25.47	C:\Database\wiley7n.l Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	99
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213888	000112-39-0	97
			Hexadecanoic acid, methyl ester (CAS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadecanoate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213893	000112-39-0	97
18	21.487	0.07	C:\Database\wiley7n.l Hexadecanoic acid, 14-methyl-, methyl ester $$ Methyl 14-methylhexad	231376	002490-49-5	97

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ecanoate			
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195468	005129-66-8	95
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195467	005129-66-8	93
19	21.570	0.12	C:\Database\wiley7n.l			
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	95
			Methyl 10-Methylhexadecanoate	231361	000000-00-0	89
			Tetradecanoic acid, 12-methyl-, me thyl ester $$ Methyl 12-methyltetr adecanoate	195466	005129-66-8	89
20	21.627	0.18	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228711	010152-61-1	93
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228710	010152-61-1	87
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245467	000112-62-9	64
21	21.850	0.32	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	98
			Heptadecanoic acid, methyl ester	231336	001731-92-6	98
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ M ethyl margarate $$ Margaric acid m ethyl ester $$ n-Heptadecanoic aci d methyl ester $$ HEPTADECANCARBON SAEUREMETHYLESTER	231335	001731-92-6	97
22	22.562	27.00	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linol eate $$ METHYL CIS-9,CIS-12-OCTADE CADIENOATE $$ Methyl octadecadieno ate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoa te $$ Methyl 9-ci	243127	000112-63-0	99
			9,12-Octadecadienoic acid, methyl ester	243170	002462-85-3	99
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243128	000112-63-0	99
23	22.630	24.27	C:\Database\wiley7n.l			
			9-Octadecenoic acid, methyl ester, (E)- $$ Elaidic acid, methyl este r $$ Methyl elaidate $$ Methyl tra ns-9-octadecenoate $$ (E)-9-Octade cenoic acid methyl ester	245486	001937-62-8	99
			METHYLELAIDATE $$ ELAIDINSAEUREMET HYLESTER	245483	000112-62-9	99
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met	245469	000112-62-9	99

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			hyl cis-9-octadecenoate $$ Oleic acid methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHYL ESTER $$ (Z)-9-			
24	22.830	10.18	C:\Database\wiley7n.l			
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247763	000112-61-8	98
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247777	000112-61-8	98
			Octadecanoic acid, methyl ester $$ Stearic acid, methyl ester $$ n-Octadecanoic acid, methyl ester $$ Kemester 9718 $$ Methyl n-octadecanoate $$ Methyl octadecanoate $$ Methyl stearate $$ Metholene 2218 $$ Emery 2218 $$ Kemester 9018 $$ Methyl ester of oc	247760	000112-61-8	98
25	22.996	0.21	C:\Database\wiley7n.l			
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linoleate $$ METHYL CIS-9,CIS-12-OCTADECADIENOATE $$ Methyl octadecadienoate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoate $$ Methyl 9-ci	243127	000112-63-0	95
			8,11-Octadecadienoic acid, methyl ester	243098	056599-58-7	90
			8,11-Octadecadienoic acid, methyl ester	243099	056599-58-7	90
26	23.144	0.07	C:\Database\wiley7n.l			
			Linoleic acid ethyl ester	258929	000544-35-4	86
			Ethyl linoleate $$ LINOLEIC ACID, ETHYL ESTER $$ ETHYL 9,12-OCTADECADIENOATE $$ Linoleic acid ethyl ester $$ 9,12-Octadecadienoic acid (Z,Z)-, ethyl ester $$ Ethyl cis,cis-9,12-octadecadienoate $$ Ethyl linolate $$ Mandenol $$ LINOLSAEURE, ETHYLESTER	258925	000544-35-4	78
			9,12-Octadecadienoic acid, ethyl ester	258969	007619-08-1	78
27	23.191	0.10	C:\Database\wiley7n.l			
			Cyclohexaneethanol, .beta.,4-dimethyl-, cis- $$ p-Menthan-9-ol, cis-	56048	005113-95-1	43
			7-Tetradecanol	136582	003981-79-1	27

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Cyclohexanol, 5-methyl-2-(1-methyl ethenyl)-, [1R-(1.alpha.,2.beta.,5 .alpha.)]- $$ p-Menth-8-en-3-ol, (1R,3R,4S)-(-)- $$ (-)-Isopulegol $ $ L-isopulegol $$ Isopulegol	52950	000089-79-2	27
28	23.493	0.06	C:\Database\wiley7n.l			
			6(Z),9(E)-Heptadecadiene $$ (6Z,9E)-Heptadeca-6,9-diene	168722	000000-00-0	60
			9-Octadecenoic acid (Z)-, 2,3-dihy droxypropyl ester $$ Olein, 1-mono - $$ .alpha.-Monoolein $$ Aldo HMO $$ Aldo MO $$ Glycerin 1-monoolea te $$ Glycerol .alpha.-cis-9-octad ecenate $$ Glycerol .alpha.-monool eate $$ Glycerol 1-monooleate $$ G lyceryl Monooleat	303305	000111-03-5	52
			9-Octadecenoic acid (Z)-, 2-hydrox y-1-(hydroxymethyl)ethyl ester $$ Olein, 2-mono- $$ .beta.-Monoolein $$ Glycerol 2-monooleate $$ 2-Mon oolein $$ 2-Monooleoylglycerol $$ 2-Oleoyl glycerol ether $$ 2-Oleoy lglycerol	303308	003443-84-3	52
29	23.725	0.07	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester (C AS) $$ Methyl nonadecanoate $$ Non adecanoic acid methyl ester $$ MET HYL N-NONADECANOATE $$ n-Nonadecan oic acid methyl ester	263308	001731-94-8	93
			Nonadecanoic acid, methyl ester $$ Methyl nonadecanoate $$ n-Nonadec anoic acid methyl ester	263309	001731-94-8	93
			Nonadecanoic acid, methyl ester	263311	001731-94-8	90
30	24.160	0.32	C:\Database\wiley7n.l			
			Bicyclo[10.1.0]tridec-1-ene	84412	054766-91-5	70
			Bicyclo[10.1.0]tridec-1-ene	84411	054766-91-5	70
			METHYL TETRADECADIENOATE	171135	000000-00-0	64
31	24.358	2.00	C:\Database\wiley7n.l			
			Dodecanoic acid (CAS) $$ Lauric ac id $$ Abl $$ Neo-fat 12 $$ Vulvic acid $$ Univol u-314 $$ Aliphat no . 4 $$ Neo-fat 12-43 $$ Dodecylic acid $$ Ninol aa62 extra $$ Lauros tearic acid $$ n-Dodecanoic acid $ $ 1-Undecanecarboxylic acid $$ Uni vol U 314 $$ Luna	115386	000143-07-7	38
			Tridecanedioic acid, dimethyl este r (CAS) $$ METHYL TRIDECANE-1,13-D IOATE $$ 1,11-UNDECANE DICARBOXYLI C ACID DIMETHYL ESTER $$ Methyl br assylate $$ Dimethyl brassylate $$ Dimethyl tridecanedioate $$ Dimet hyl tridecane-1,13-dioate $$ Tride canedioic acid di	215841	001472-87-3	27
			4-Cyclopropylmethylbenzonitrile	56962	000000-00-0	27
32	24.500	0.04	C:\Database\wiley7n.l			
			5-(3-METHYL-BUTYL)-3-MERCAPTO-4-ME THYL-1,2,4-TRIAZOLE $$ 3H-1,2,4-Tr iazole-3-thione, 2,4-dihydro-4-met	93791	066921-10-6	27

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			hyl-5-(3-methylbutyl)- (CAS)			
			Butanedioic acid, 2,3-dimethyl-, d ibutyl ester	197443	056051-57-1	27
			Benzonitrile, 4-(4-butylcyclohexyl)-, trans-	175429	061204-00-0	22
33	24.645	0.34	C:\Database\wiley7n.l			
			Eicosanoic acid, methyl ester $$ M ethyl arachate $$ Methyl eicosanoa te $$ Arachidic acid methyl ester	277451	001120-28-1	98
			Eicosanoic acid, methyl ester	277449	001120-28-1	96
			Hexadecanoic acid, 15-methyl-, met hyl ester $$ Methyl isoheptadecano ate $$ Methyl 15-methylhexadecanoa te	231378	006929-04-0	96
34	24.922	0.41	C:\Database\wiley7n.l			
			Hexacosane	311168	000630-01-3	96
			Tetratriacontane $$ n-Tetratriacon tane	363627	014167-59-0	70
			Eicosane (CAS) $$ n-Eicosane	228991	000112-95-8	64
35	25.287	0.17	C:\Database\wiley7n.l			
			E-6-Octadecen-1-ol acetate	261154	000000-00-0	64
			Z-14-Octadecen-1-ol acetate	261160	000000-00-0	62
			E-5-Octadecen-1-ol acetate	261153	000000-00-0	53
36	25.572	0.45	C:\Database\wiley7n.l			
			17-Pentatriacontene	366689	006971-40-0	87
			17-Pentatriacontene (CAS)	366690	006971-40-0	87
			1-Nonadecene	208864	018435-45-5	86
37	26.095	0.21	C:\Database\wiley7n.l			
			Tetratetracontane $$ n-Tetratetrac ontane	383557	007098-22-8	80
			Heptacosane, 1-chloro-	340109	062016-79-9	80
			Nonadecane (CAS) $$ n-Nonadecane	211484	000629-92-5	80
38	26.244	1.63	C:\Database\wiley7n.l			
			Isopropyl linoleate $$ 9,12-Octade cadienoic acid (Z,Z)-, 1-methyleth yl ester	273683	022882-95-7	70
			9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl e ster $$ Linolein, 2-mono- $$ .beta .-Monolinolein	301826	003443-82-1	68
			4-Tetradecyne	107092	060212-33-1	64
39	26.290	2.32	C:\Database\wiley7n.l			
			9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylalde hyde $$ Z-9-Octadecenal	208774	002423-10-1	96
			2-Methyl-Z,Z-3,13-octadecadienol	226325	000000-00-0	92
			9-Oxabicyclo[6.1.0]nonane $$ Cyclo octane, 1,2-epoxy- $$ Cyclooctene, oxide $$ 1,2-Epoxycyclooctane $$ Epoxycyclooctane	22927	000286-62-4	62
40	26.425	0.06	C:\Database\wiley7n.l			
			Pentanoic acid, 4-methyl-5-[(2,3,4 ,6-tetra-O-acetyl-D-glucopyranosyl)oxy]-, methyl ester	362798	056246-40-3	35
			Hexanedioic acid, bis(2-methylprop yl) ester	197427	000141-04-8	25

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2,2-Dimethyl-1-oxa-2-silacyclotrid ecanone-13	176267	020470-88-6	25
41	26.490	0.65	C:\Database\wiley7n.l			
			Dodecanoic acid (CAS) $$ Lauric ac id $$ Abl $$ Neo-fat 12 $$ Vulvic acid $$ Univol u-314 $$ Aliphat no . 4 $$ Neo-fat 12-43 $$ Dodecylic acid $$ Ninol aa62 extra $$ Lauros tearic acid $$ n-Dodecanoic acid $ $ 1-Undecanecarboxylic acid $$ Uni vol U 314 $$ Luna	115386	000143-07-7	35
			2-(METHYL-D3)-CYCLONONANONE $$ Cyc lononanone, 2-methyl-d3- (CAS)	53597	032454-54-9	30
			Cyclononanone	36152	003350-30-9	25
42	26.683	0.17	C:\Database\wiley7n.l			
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl doc osanoate $$ Behenic acid methyl es ter $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302041	000929-77-1	95
			Docosanoic acid, methyl ester	302040	000929-77-1	93
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl doc osanoate $$ Behenic acid methyl es ter $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302031	000929-77-1	83
43	26.815	0.15	C:\Database\wiley7n.l			
			2,4-Dimethyl-6-(2-furyl)pyridine	77574	078563-67-4	18
			Metanilic acid	77201	000121-47-1	18
			Metanilic acid	77199	000121-47-1	18
44	27.046	0.04	C:\Database\wiley7n.l			
			Cyclotrisiloxane, hexamethyl-	146391	000541-05-9	38
			1,3-Bis(trimethylsilyl)benzene	147371	002060-89-1	38
			Indole-2-one, 2,3-dihydro-N-hydrox y-4-methoxy-3,3-dimethyl-	125469	000000-00-0	38
45	27.087	0.10	C:\Database\wiley7n.l			
			Ethyl 2-(2-chloroacetamido)-3,3,3- trifluoro-2-(4-fluoroanilino)propi onate	302693	000000-00-0	22
			2',4'-DIMETHYLOXANILIC ACID N'-VER ATRYLIDENEHYDRAZIDE	302366	000000-00-0	22
			8-Methylisothiazolo[4,5-c]-2,1,3-b enzothiadiazole $$ Isothiazolo[3,4 -e]-2,1,3-benzothiadiazole, 4-meth yl- (CAS)	125155	074801-78-8	18
46	27.244	0.03	C:\Database\wiley7n.l			
			Phenol, 2,2'-[(1-methyl-1,2-ethane diyl)bis(nitrilomethylidyne)]bis- $$ o-Cresol, .alpha.,.alpha.'-(pro pylenedinitrilo)di- $$ Cuvan 80 $$ DMD $$ Keromet MD $$ N,N'-Bis(sal icylidene)-1,2-diaminopropane $$ N ,N'-Disalicylidene-1,2-diaminoprop ane $$ N,N'-Disal	228407	000094-91-7	47
			Silicic acid, diethyl bis(trimethy lsilyl) ester	244286	003555-45-1	42
			Galactitol, hexaacetate, D- (CAS) $$ GALACTITOL-1,2,3,4,5,6-HEXAACET	348804	014330-96-2	37

Library Search Report

Data Path : C:\msdchem\1\data\170406VK\
Data File : 00301003.D
Acq On : 5 Apr 2017 17:13
Operator : AKK
Sample : Hnayte2
Misc :
ALS Vial : 3 Sample Multiplier: 1

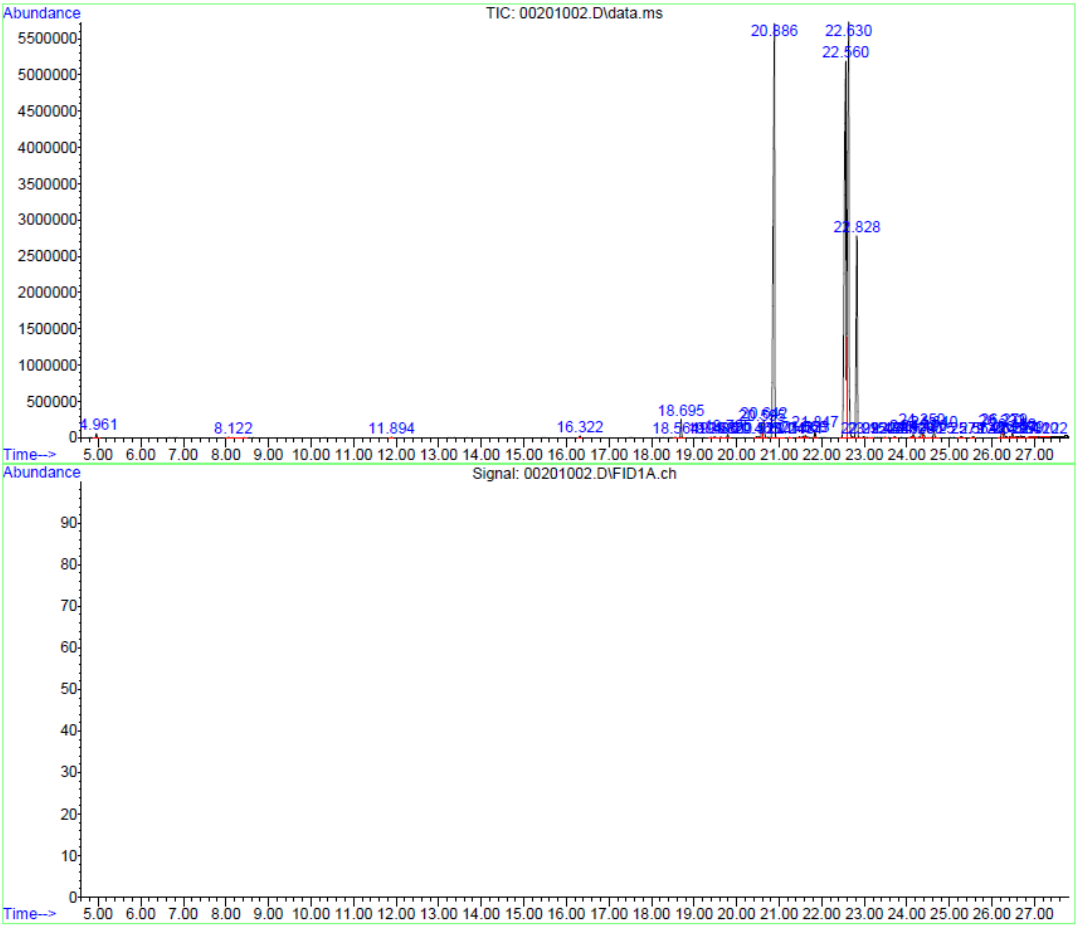
Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ATE			
47	27.462	0.03	C:\Database\wiley7n.l			
			Silane, 1,4-phenylenebis[trimethyl - $$ Silane, p-phenylenebis[trimethyl- $$ p-Bis(trimethylsilyl)benzene $$ Benzene, p-bis(trimethylsilyl)- $$ Silane, p-biphenylylenebis[trimethyl- $$ 1,4-Bis(trimethylsilyl)benzene $$ p-Phenylenebis(trimethylsilane) $$ Si	147366	013183-70-5	43
			Silicic acid, diethyl bis(trimethylsilyl) ester	244286	003555-45-1	40
			Gibberellin A3 $$ Gibb-3-ene-1,10-dicarboxylic acid, 2,4a,7-trihydroxy-1-methyl-8-methylene-, 1,4a-lactone, (1.alpha.,2.beta.,4a.alpha.,4b.beta.,10.beta.)- (CAS) $$ GA3 $$ GA $$ Gibberellin X $$ Gibberellic acid $$ 4a,1-(Epoxymethano)-7,9a-methanobenz[a]a	294997	000077-06-5	40
48	27.665	0.03	C:\Database\wiley7n.l			
			2,3,4-Trimethoxyphenylacetonitrile	125480	068913-85-9	35
			2-Ethylacridine	125906	000000-00-0	35
			3,3,4-TRIMETHYL-2,2-DIPHENOXYTHIETANE $$ Thietane, 3,3,4-trimethyl-2,2-diphenoxy- (CAS)	249842	050468-87-6	32

Appendix 10. Sample 1, 12.4.2017, GC Analysis

```
File       :C:\msdchem\1\data\170418VK\00201002.D
Operator   : AKK
Acquired   : 18 Apr 2017  14:22     using AcqMethod 170404VK.M
Instrument :     Inst 2
Sample Name: N1heptaani
Misc Info  :
Vial Number: 2
```



Appendix 11. Sample 1, 12.4.2017, Integrated peak areas

TIC: 00201002.D\data.ms
N1heptaani

Peak #	Ret Time	Type	Width	Area	Start Time	End Time
1	4.961	BB	0.025	788866	4.902	5.022
2	8.122	BB	0.112	437545	7.992	8.482
3	11.894	BB	0.035	78222	11.849	11.932
4	16.322	BB	0.037	305267	16.280	16.363
5	18.564	PV	0.022	79615	18.531	18.597
6	18.695	PB	0.026	3753748	18.597	18.768
7	19.398	BV	0.026	95441	19.351	19.438
8	19.486	PV	0.027	222258	19.438	19.544
9	19.630	VB	0.026	124143	19.591	19.674
10	19.795	BB	0.026	679256	19.711	19.841
11	20.465	BV	0.026	113169	20.414	20.489
12	20.518	VV	0.026	269911	20.489	20.550
13	20.595	PV	0.030	3059385	20.550	20.618
14	20.642	VV	0.033	4264261	20.618	20.711
15	20.886	VV	0.045	140798245	20.790	21.108
16	21.247	VV	0.036	109695	21.193	21.299
17	21.481	VV	0.037	232728	21.420	21.517
18	21.568	VV	0.034	389036	21.517	21.588
19	21.623	VV	0.058	840768	21.588	21.682
20	21.847	PV	0.040	1594653	21.791	21.896
21	22.560	VV	0.049	150979677	22.426	22.585
22	22.630	VV	0.063	134550550	22.585	22.760
23	22.828	VV	0.033	56727179	22.760	22.940
24	22.992	VV	0.036	367435	22.940	23.047
25	23.154	VV	0.047	169520	23.112	23.208
26	23.488	VV	0.045	202230	23.463	23.532
27	23.719	VV	0.033	252447	23.661	23.766
28	24.109	VV	0.031	192738	24.044	24.121
29	24.152	VV	0.034	929475	24.121	24.251
30	24.290	VV	0.032	135994	24.251	24.305
31	24.350	VV	0.035	2758404	24.305	24.383
32	24.400	VV	0.040	977763	24.383	24.518
33	24.640	VV	0.035	2103903	24.518	24.754
34	25.279	VV	0.044	476116	25.205	25.346
35	25.564	PV	0.037	387374	25.503	25.623
36	26.233	PV	0.030	2230452	26.144	26.255
37	26.279	VV	0.035	2933171	26.255	26.388
38	26.425	VV	0.035	194449	26.388	26.446
39	26.482	VV	0.030	1136156	26.446	26.540
40	26.574	VV	0.046	240697	26.540	26.639
41	26.679	VV	0.056	674341	26.639	26.843
42	27.010	VV	0.078	155016	26.843	27.054
43	27.222	VV	0.081	425345	27.133	27.364

Appendix 12. Sample 1, 12.4.2017, Library search report

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	4.961	0.15	C:\Database\wiley7n.l			
			Octane $$ n-Octane $$ n-C8H18 $$ O ktan $$ Oktanen $$ Ottani $$ UN 12 62 $$ Isooctane	15631	000111-65-9	90
			Heptane, 2,4-dimethyl-	25185	002213-23-2	78
			Heptane, 2,4-dimethyl- $$ 2,4-Dime thylheptane	25184	002213-23-2	78
2	8.122	0.08	C:\Database\wiley7n.l			
			Methane, nitro- (CAS) $$ Nitrometh ane $$ Nitrocarbol $$ CH3NO2 $$ Ni trometan $$ UN 1261	834	000075-52-5	4
			Methanamine, N-methoxy- (CAS) $$ O ,N-Dimethylhydroxylamine $$ Methox ymethylamine $$ N-Methoxymethylami ne $$ N-methoxy-N-methylamine $$ M ethylamine, N-methoxy- $$ Methoxya mine, N-methyl- $$ N,O-Dimethylhyd roxylamine $$ Hydroxylamine, N,O-d imethyl- $$ N-Met	855	001117-97-1	4
			Methane, nitro- (CAS) $$ Nitrometh ane $$ Nitrocarbol $$ CH3NO2 $$ Ni trometan $$ UN 1261	833	000075-52-5	4
3	11.894	0.02	C:\Database\wiley7n.l			
			Dodecane	74391	000112-40-3	83
			Dodecane $$ n-Dodecane $$ Adakane 12 $$ Ba 51-090453 $$ CH3(CH2)10CH 3 $$ Bihexyl $$ Dihexyl $$ n-Dodec ane min $$ Duodecane $$ Isododecan	74403	000112-40-3	83
			Dodecane (CAS) $$ n-Dodecane $$ Ba 51-090453 $$ Adakane 12 $$ Isodod ecane $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ n-Dodecane min $$ N- Dodecan $$ Duodecane $$ ACETIC ACI D 3-HYDROXY-7-ISOPROPENYL-1,4A-DIM ETHYL-2,3,4,4A,5,6,7,8-OCTAHYDRO-N AP	74407	000112-40-3	80
4	16.322	0.06	C:\Database\wiley7n.l			
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136169	000111-82-0	96
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136165	000111-82-0	96
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dode canoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metho lene 2296 $$ Methyl laurinate $$ M ethyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136172	000111-82-0	96

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
5	18.564	0.02	C:\Database\wiley7n.l			
			Z-8-Pentadecen-1-ol acetate	211151	000000-00-0	35
			Muskolactone $$ Oxacyclohexadecan-2-one (CAS) $$ .OMEGA.-PENTADECANOLIDE $$ Cyclopentadecanolide $$ Exaltolide $$ Thibetolide $$ Muskalactone $$ Pentadecanolide $$ 2-Pentadecalone $$ Pentadecalactone $$ 1,15-Pentadecanolide $$ 15-Hydroxypentadecanoic acid	174118	000106-02-5	27
			1-Cyclohexylnonene	128096	114614-84-5	22
6	18.695	0.73	C:\Database\wiley7n.l			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176778	000124-10-7	98
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176768	000124-10-7	98
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetradecanoate $$ Myristic acid methyl ester $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl ester $$ Tetradecanoic acid methyl ester $$ MYRISTIC A	176765	000124-10-7	97
7	19.398	0.02	C:\Database\wiley7n.l			
			Methyl 9-methyltetradecanoate	195519	000000-00-0	94
			methyl 13-methyltetradecanoate	195518	000000-00-0	78
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metholene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136172	000111-82-0	64
8	19.486	0.04	C:\Database\wiley7n.l			
			Tetradecanoic acid, 12-methyl-, methyl ester (CAS) $$ Methyl 12-methyltetradecanoate	195467	005129-66-8	95
			Tetradecanoic acid, 12-methyl-, methyl ester (CAS) $$ Methyl 12-methyltetradecanoate	195468	005129-66-8	94
			methyl 13-methyltetradecanoate	195518	000000-00-0	87
9	19.630	0.02	C:\Database\wiley7n.l			
			9-Dodecenoic acid, methyl ester, (E)-	133398	055030-26-7	46
			Eicosenoic acid, methyl ester (CAS	275550	027070-40-2	43

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			) $$ METHYL EICOSENOATE			
			1,5-Naphthalenedione, octahydro-4a -methyl-, trans-(.+-.)-	86837	002906-90-3	42
10	19.795	0.13	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	98
			Pentadecanoic acid, methyl ester	195449	007132-64-1	97
			Pentadecanoic acid, methyl ester	195454	007132-64-1	96
11	20.465	0.02	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	97
			Hexadecanoic acid, methyl ester $$ Palmitic acid, methyl ester $$ n- Hexadecanoic acid methyl ester $$ Metholene 2216 $$ Methyl hexadecan oate $$ Methyl n-hexadecanoate $$ Methyl palmitate $$ Uniphat A60	213890	000112-39-0	94
			Hexadecanoic acid, methyl ester	213902	000112-39-0	94
12	20.518	0.05	C:\Database\wiley7n.l			
			7,10-Hexadecadienoic acid, methyl ester	208525	016106-03-9	99
			Z-11(12-Cyclopropyl)dodecen-1-ol a cetate	208567	000000-00-0	94
			Hexadecadienoic acid, methyl ester $$ Methyl hexadecadienoate	208527	029961-54-4	94
13	20.595	0.59	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211106	001120-25-8	99
14	20.642	0.82	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Me thyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
15	20.886	27.21	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl	213911	000112-39-0	99

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213893	000112-39-0	97
			Hexadecanoic acid, methyl ester	213889	000112-39-0	97
16	21.247	0.02	C:\Database\wiley7n.l			
			METHYL 11-(2,3-DIDEUTEROCYCLOPENTA N-1-YL)UNDECANOATE	211175	033422-41-2	43
			Cyclopentaneundecanoic acid, methy l ester $$ Methyl dihydrohydnocarp ate	211110	025779-85-5	37
			Decanoic acid, methyl ester (CAS) $$ Methyl caprate $$ Methyl decano ate $$ Capric acid methyl ester $$ Uniphat A30 $$ Metholene 2095 $$ Methyl caprinate $$ Methyl-n-capra te $$ Decanoic acid methyl ester $ $ Methyl n-caprate $$ Methyl n-dec anoate $$ n-Capri	95548	000110-42-9	28
17	21.481	0.04	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	98
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	98
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ M ethyl margarate $$ Margaric acid m ethyl ester $$ n-Heptadecanoic aci d methyl ester $$ HEPTADECANCARBON SAEUREMETHYLESTER	231341	001731-92-6	97
18	21.568	0.08	C:\Database\wiley7n.l			
			Hexadecanoic acid, 14-methyl-, met hyl ester $$ Methyl 14-methylhexad ecanoate	231376	002490-49-5	95
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	94
			Hexadecanoic acid, 15-methyl-, met hyl ester $$ Methyl isoheptadecano ate $$ Methyl 15-methylhexadecanoa te	231378	006929-04-0	93
19	21.623	0.16	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228711	010152-61-1	93
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245467	000112-62-9	93

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228710	010152-61-1	87
20	21.847	0.31	C:\Database\wiley7n.l Heptadecanoic acid, methyl ester	231340	001731-92-6	98
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ M ethyl margarate $$ Margaric acid m ethyl ester $$ n-Heptadecanoic aci d methyl ester $$ HEPTADECANCARBON SAEUREMETHYLESTER	231335	001731-92-6	98
			Heptadecanoic acid, methyl ester	231336	001731-92-6	98
21	22.560	29.18	C:\Database\wiley7n.l 9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243128	000112-63-0	99
			10,13-Octadecadienoic acid, methyl ester	243108	056554-62-2	99
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linol eate $$ METHYL CIS-9,CIS-12-OCTADE CADIENOATE $$ Methyl octadecadieno ate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoa te $$ Methyl 9-ci	243127	000112-63-0	99
22	22.630	26.00	C:\Database\wiley7n.l 13-Octadecenoic acid, methyl ester , (Z)-	245518	013058-55-4	99
			8-Octadecenoic acid, methyl ester, (E)- (CAS) $$ TRANS-8-OCTADECENOI C METHYL ESTER $$ Methyl trans-8-o ctadecenoate	245465	026528-50-7	99
			METHYLELAIDATE $$ ELAIDINSAEUREMET HYLESTER	245483	000112-62-9	99
23	22.828	10.96	C:\Database\wiley7n.l Octadecanoic acid, methyl ester (C AS) $$ Methyl stearate $$ Methyl o ctadecanoate $$ Methyl n-octadecan oate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic aci d methyl ester $$ Methyl-octadecan oate $$ Methyl es	247763	000112-61-8	98
			Octadecanoic acid, methyl ester (C AS) $$ Methyl stearate $$ Methyl o ctadecanoate $$ Methyl n-octadecan oate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic aci d methyl ester $$ Methyl-octadecan oate $$ Methyl es	247777	000112-61-8	98
			Octadecanoic acid, methyl ester (C AS) $$ Methyl stearate $$ Methyl o ctadecanoate $$ Methyl n-octadecan oate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic aci d methyl ester $$ Methyl-octadecan oate $$ Methyl es	247752	000112-61-8	97
24	22.992	0.07	C:\Database\wiley7n.l			

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243134	000112-63-0	95
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243132	000112-63-0	93
			6,9-Octadecadienoic acid, methyl ester (CAS) $$ METHYL 6,9-OCTADECADIENOATE	243096	056599-55-4	93
25	23.154	0.03	C:\Database\wiley7n.l			
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247751	000112-61-8	43
			Nonanoic acid, 9-oxo-, methyl ester $$ Azelaaldehydic acid, methyl ester $$ Methyl azelaaldehydate $$ Methyl azelaaldehydrate $$ Methyl 8-formyloctanoate $$ Methyl 9-oxononanoate $$ 9-Oxononanoic acid methyl ester	95128	001931-63-1	38
			11-Dodecenoic acid, 10-hydroxy-, methyl ester	156931	106753-87-1	35
26	23.488	0.04	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-octyl-, methyl ester	261100	010152-62-2	81
			Z-7-Tetradecenoic acid	154487	000000-00-0	47
			9-Octadecenoic acid (Z)-, methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ Methyl cis-9-octadecenoate $$ Methyl oleate $$ (Z)-9-Octadecenoic acid methyl ester $$ Methyl-o-octadecenoate $$ cis-9-Octyldecenoic acid, methyl ester $$	245468	000112-62-9	38
27	23.719	0.05	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester (CAS) $$ Methyl nonadecanoate $$ Nonadecanoic acid methyl ester $$ METHYL N-NONADECANOATE $$ n-Nonadecanoic acid methyl ester	263312	001731-94-8	95
			Nonadecanoic acid, methyl ester	263307	001731-94-8	94
			Nonadecanoic acid, methyl ester	263310	001731-94-8	93
28	24.109	0.04	C:\Database\wiley7n.l			
			2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)-	127817	054594-42-2	49
			Santolina triene	32329	002153-66-4	38
			1-ethenyl-1-isopropenylcyclohexane	47424	116927-19-6	38
29	24.152	0.18	C:\Database\wiley7n.l			
			(7R,8S)-cis-anti-cis-7,8-Epoxytricyclo[7.3.0.0(2,6)]dodecane	84103	073285-35-5	86
			METHYL TETRADECADIENOATE	171135	000000-00-0	83
			Bicyclo[10.1.0]tridec-1-ene	84411	054766-91-5	64
30	24.290	0.03	C:\Database\wiley7n.l			
			1-Hentetracontanol	381314	040710-42-7	43

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2-Azabicyclo[2.2.2]octan-3-one	21826	003306-69-2	43
			1,1-dichloro-2-dodecanol $$ 2-Dode canol, 1,1-dichloro- (CAS)	191924	096502-91-9	43
31	24.350	0.53	C:\Database\wiley7n.l			
			Hexadecanoic acid (CAS) $$ Palmiti c acid $$ Palmitinic acid $$ n-Hex adecoic acid $$ n-Hexadecanoic aci d $$ Pentadecanecarboxylic acid $$ 1-Pentadecanecarboxylic acid $$ P rifrac 2960 $$ Coconut oil fatty a cids $$ Cetylic acid $$ Emersol 14 0 $$ Emersol 143	195437	000057-10-3	38
			2-(METHYL-D3)-CYCLONONANONE $$ Cyc lononanone, 2-methyl-d3- (CAS)	53597	032454-54-9	30
			Myristoyl chloride $$ Tetradecanoy l chloride	181495	000112-64-1	25
32	24.400	0.19	C:\Database\wiley7n.l			
			11-Eicosenoic acid, methyl ester	275547	003946-08-5	81
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245476	000112-62-9	53
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245467	000112-62-9	49
33	24.640	0.41	C:\Database\wiley7n.l			
			Eicosanoic acid, methyl ester $$ M ethyl arachate $$ Methyl eicosanoa te $$ Arachidic acid methyl ester	277451	001120-28-1	99
			Eicosanoic acid, methyl ester (CAS) $$ Arachidic acid methyl ester $ $ Methyl arachate $$ Methyl eicosa noate $$ METHYL N-EICOSANOATE $$ E ICOSANOIC ACID METHYL ESTER	277460	001120-28-1	98
			Eicosanoic acid, methyl ester	277458	001120-28-1	98
34	25.279	0.09	C:\Database\wiley7n.l			
			2(1H)-Naphthalenone, octahydro-4a- methyl-7-(1-methylethyl)-, (4a.alp ha.,7.beta.,8a.beta.)-	127817	054594-42-2	80
			Z-14-Octadecen-1-ol acetate	261160	000000-00-0	58
			Z-7-Octadecen-1-ol acetate	261166	000000-00-0	49
35	25.564	0.07	C:\Database\wiley7n.l			
			17-Pentatriacontene (CAS)	366690	006971-40-0	60
			1-Dotriacontanol $$ n-Dotriacontan ol $$ Dotriacontanol	360217	006624-79-9	60
			17-Pentatriacontene	366689	006971-40-0	60
36	26.233	0.43	C:\Database\wiley7n.l			
			Isopropyl linoleate $$ 9,12-Octade cadienoic acid (Z,Z)-, 1-methyleth	273683	022882-95-7	70

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			yl ester			
			LINOLEIC ACID, BUTYL ESTER	286980	000000-00-0	62
			3,4-Octadiene, 7-methyl-	21461	037050-05-8	58
37	26.279	0.57	C:\Database\wiley7n.l			
			2-Methyl-Z,Z-3,13-octadecadienol	226325	000000-00-0	59
			9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal	208774	002423-10-1	53
			10-Octadecenoic acid, methyl ester	245511	013481-95-3	44
38	26.425	0.04	C:\Database\wiley7n.l			
			3-Trifluoroacetoxytetradecane	260468	000000-00-0	47
			HEXADECYL ESTER OF GALLIC ACID	329042	000000-00-0	47
			1-Eicosanol	248010	000629-96-9	42
39	26.482	0.22	C:\Database\wiley7n.l			
			o-Xylene-d10	10736	000000-00-0	38
			Tridecanedioic acid, dimethyl ester (CAS) $$ METHYL TRIDECANE-1,13-DIOATE $$ 1,11-UNDECANE DICARBOXYLIC ACID DIMETHYL ESTER $$ Methyl brassylate $$ Dimethyl brassylate $$ Dimethyl tridecanedioate $$ Dimethyl tridecane-1,13-dioate $$ Tridecanedioic acid di	215841	001472-87-3	22
			ethyl N-piperidine acetate $$ 1-Piperidineacetic acid, ethyl ester (CAS) $$ Ethyl 1-piperidineacetate $$ Ethyl N-piperidinylacetate $$ Ethyl piperidinoacetate	74930	023853-10-3	18
40	26.574	0.05	C:\Database\wiley7n.l			
			Hexadecanoic acid, 2,3-dihydroxypropyl ester $$ Palmitin, 1-mono- $$ .alpha.-Monopalmitin $$ Glycerol 1-monopalmitate $$ Glycerol 1-palmitate $$ Glyceryl palmitate $$ Palmitic acid .alpha.-monoglyceride $$ 1-Monopalmitin $$ 1,2,3-P	281035	000542-44-9	64
			Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester	378933	000761-35-3	52
			Hexadecanoic acid, 1-(hydroxymethyl)-1,2-ethanediyl ester $$ Palmitin, 1,2-di- $$ Dipalmitin $$ Glycerol 1,2-dipalmitate $$ 1,2-Dipalmitin $$ 1,2-Dipalmitoylglycerol	378934	000761-35-3	35
41	26.679	0.13	C:\Database\wiley7n.l			
			Docosanoic acid, methyl ester	302035	000929-77-1	89
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl docosanoate $$ Behenic acid methyl ester $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302041	000929-77-1	64
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl docosanoate $$ Behenic acid methyl ester $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302036	000929-77-1	53
42	27.010	0.03	C:\Database\wiley7n.l			
			Cyclotrisiloxane, hexamethyl-	146391	000541-05-9	38

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00201002.D
Acq On : 18 Apr 2017 14:22
Operator : AKK
Sample : N1heptaani
Misc :
ALS Vial : 2 Sample Multiplier: 1

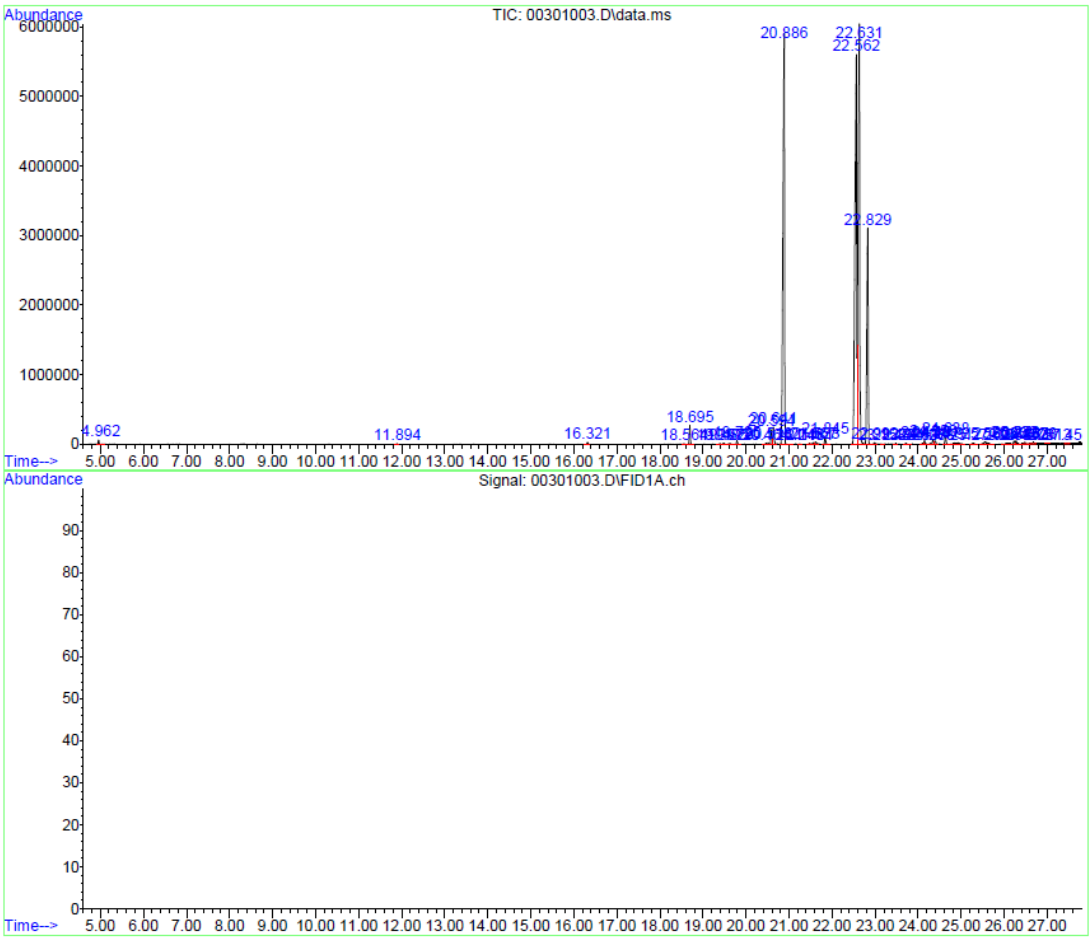
Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			N-(2-Acetylcyclopentylidene)cycloh exylamine	125785	000000-00-0	38
			Indole-2-one, 2,3-dihydro-N-hydrox y-4-methoxy-3,3-dimethyl-	125469	000000-00-0	35
43	27.222	0.08	C:\Database\wiley7n.l			
			Silicone grease, Siliconfett	392047	000000-00-0	74
			5,6,8,9-TETRAMETHOXY-2-METHYLPEPER O(3,4,5-JK)-9,10-DIHYDROPHENANTHRA CENE $$ 4H-Dibenz[de,g]isoquinolin e, 5,6,6a,7-tetrahydro-1,2,9,10-te tramethoxy-5-methyl- (CAS)	302480	074199-94-3	43
			N-Cyano-N',N',N'',N''-tetramethyl- 1,3,5-triazinetriamine	125166	074150-88-2	27

Appendix 13. Sample 2, 12.4.2017, GC Analysis

```
File       :C:\msdchem\1\data\170418VK\00301003.D
Operator   : AKK
Acquired   : 18 Apr 2017  15:03     using AcqMethod 170404VK.M
Instrument :    Inst 2
Sample Name: N2heptaani
Misc Info  :
Vial Number: 3
```



Appendix 14. Sample 2, 12.4.2017, Integrated peak areas

TIC: 00301003.D\data.ms
N2heptaani

Peak #	Ret Time	Type	Width	Area	Start Time	End Time
1	4.962	BB	0.025	820426	4.911	5.106
2	11.894	BB	0.034	76193	11.849	11.932
3	16.321	BB	0.027	332792	16.252	16.363
4	18.564	PB	0.034	83698	18.527	18.601
5	18.695	BB	0.026	3999927	18.638	18.796
6	19.397	BV	0.024	108627	19.323	19.438
7	19.485	PV	0.046	260420	19.438	19.551
8	19.629	VV	0.040	156754	19.551	19.709
9	19.795	VB	0.026	745362	19.709	19.887
10	20.464	BV	0.026	131153	20.368	20.489
11	20.518	VV	0.026	304429	20.489	20.549
12	20.594	VV	0.030	3322586	20.549	20.617
13	20.641	VV	0.033	4562111	20.617	20.710
14	20.886	VV	0.043	150037895	20.789	21.078
15	21.246	VV	0.042	120092	21.198	21.296
16	21.481	VV	0.037	248264	21.416	21.513
17	21.567	VV	0.036	440653	21.513	21.588
18	21.623	VV	0.043	910066	21.588	21.682
19	21.845	VV	0.044	1804912	21.775	21.957
20	22.562	VV	0.052	158888260	22.437	22.587
21	22.631	VV	0.063	140935005	22.587	22.760
22	22.829	VV	0.033	61007871	22.760	22.940
23	22.992	VV	0.041	583817	22.940	23.052
24	23.153	VV	0.052	170516	23.120	23.204
25	23.488	VV	0.048	262347	23.420	23.520
26	23.720	VV	0.031	276497	23.667	23.826
27	24.107	VV	0.031	183740	24.050	24.120
28	24.151	VV	0.031	954791	24.120	24.214
29	24.288	VV	0.043	270238	24.214	24.309
30	24.350	VV	0.039	1393405	24.309	24.377
31	24.401	VV	0.035	1044251	24.377	24.451
32	24.638	VV	0.033	2089923	24.577	24.734
33	24.912	VV	0.134	1906476	24.734	25.072
34	25.279	VV	0.052	462954	25.202	25.374
35	25.560	VV	0.081	1920340	25.438	25.762
36	26.073	VV	0.091	954040	25.949	26.184
37	26.232	VV	0.030	779728	26.184	26.253
38	26.278	VV	0.034	986039	26.253	26.367
39	26.422	PV	0.031	183142	26.367	26.450
40	26.482	VV	0.031	456706	26.450	26.542
41	26.575	PV	0.025	71276	26.542	26.594
42	26.678	VV	0.050	646944	26.594	26.738
43	27.013	BV	0.049	196968	26.954	27.070
44	27.454	PV	0.043	125014	27.405	27.519

Appendix 15. Sample 2, 12.4.2017, Library search report

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	4.962	0.15	C:\Database\wiley7n.l			
			Octane (CAS) $$ n-Octane $$ Octane (DOT) $$ Isooctane $$ n-C8H18 $$ Oktan $$ Oktanen $$ Ottani $$ UN 1262	15635	000111-65-9	90
			Octane	15633	000111-65-9	83
			Heptane, 2,4-dimethyl-	25186	002213-23-2	83
2	11.894	0.01	C:\Database\wiley7n.l			
			Dodecane	74390	000112-40-3	91
			Dodecane	74391	000112-40-3	91
			Dodecane (CAS) $$ n-Dodecane $$ Ba 51-090453 $$ Adakane 12 $$ Isododecane $$ CH3(CH2)10CH3 $$ Bihexyl $$ Dihexyl $$ n-Dodecane min $$ N-Dodecan $$ Duodecane $$ ACETIC ACID 3-HYDROXY-7-ISOPROPENYL-1,4A-DIMETHYL-2,3,4,4A,5,6,7,8-OCTAHYDRO-NAP	74407	000112-40-3	91
3	16.321	0.06	C:\Database\wiley7n.l			
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metholene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136172	000111-82-0	96
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metholene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136169	000111-82-0	95
			Dodecanoic acid, methyl ester (CAS) $$ Methyl laurate $$ Methyl dodecanoate $$ Methyl n-dodecanoate $$ Lauric acid methyl ester $$ Metholene 2296 $$ Methyl laurinate $$ Methyl dodecylate $$ Uniphat A40 IN 511 $$ Lauric acid, methyl ester $$ Dodecanoic aci	136162	000111-82-0	94
4	18.564	0.02	C:\Database\wiley7n.l			
			Methyl ricinoleate $$ Ricinoleic acid methyl ester $$ 9-Octadecenoic acid, 12-hydroxy-, methyl ester, [R-(Z)]- $$ Flexricin P-1 $$ Methyl ricinolate	263143	000141-24-2	50
			10-Undecenoyl chloride (CAS) $$ Undecylenoyl chloride $$ 10-Undecylenoyl chloride $$ .omega.-Undecylenic acid chloride	117665	038460-95-6	35
			chloromethyl 4-chloroundecanoate $$ Undecanoic acid, 4-chloro-, chloromethyl ester (CAS) $$ 4-Chloroundecanoic acid chloromethyl ester	210102	080418-90-2	22
5	18.695	0.73	C:\Database\wiley7n.l			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl	176778	000124-10-7	98

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A			
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176783	000124-10-7	97
			Tetradecanoic acid, methyl ester (CAS) $$ Methyl myristate $$ Methyl tetradecanoate $$ Methyl n-tetrad ecanoate $$ Myristic acid methyl e ster $$ Uniphat A50 $$ Metholeneat 2495 $$ Myristic acid, methyl est er $$ Tetradecanoic acid methyl es ter $$ MYRISTIC A	176780	000124-10-7	97
6	19.397	0.02	C:\Database\wiley7n.l			
			Methyl 9-methyltetradecanoate	195519	000000-00-0	56
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester	195448	007132-64-1	50
			Heptadecanoic acid, 16-methyl-, me thyl ester (CAS) $$ Methyl isostea rate $$ Methyl 16-methylheptadecan oate	247859	005129-61-3	45
7	19.485	0.05	C:\Database\wiley7n.l			
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195467	005129-66-8	95
			Tetradecanoic acid, 12-methyl-, me thyl ester (CAS) $$ Methyl 12-meth yltetradecanoate	195468	005129-66-8	90
			methyl 13-methyltetradecanoate	195518	000000-00-0	76
8	19.629	0.03	C:\Database\wiley7n.l			
			Spiro[4.5]decane	34355	000176-63-6	44
			9-Dodecenoic acid, methyl ester, (E)-	133398	055030-26-7	38
			6-Nonenoic acid, methyl ester	73417	020731-21-9	35
9	19.795	0.14	C:\Database\wiley7n.l			
			Pentadecanoic acid, methyl ester	195449	007132-64-1	96
			Pentadecanoic acid, methyl ester	195454	007132-64-1	95
			Pentadecanoic acid, methyl ester (CAS) $$ Methyl pentadecanoate $$ P ENTADECANOIC ACID-METHYL ESTER $$ Methyl n-pentadecanoate $$ Pentade canoic acid methyl ester $$ Methyl 2-ethyltridecanoate $$ methyl pen decanoate $$ n-Pentadecanoic acid methyl ester	195447	007132-64-1	93

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
10	20.464	0.02	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213905	000112-39-0	95
			Pentadecanoic acid, 14-methyl-, me thyl ester	213933	005129-60-2	94
			Pentadecanoic acid, 14-methyl-, me thyl ester	213934	005129-60-2	94
11	20.518	0.06	C:\Database\wiley7n.l			
			Hexadecadienoic acid, methyl ester $$ Methyl hexadecadienoate	208527	029961-54-4	93
			7,10-Hexadecadienoic acid, methyl ester	208525	016106-03-9	91
			Hexadecadienoic acid, methyl ester (CAS) $$ Methyl hexadecadienoate	208528	029961-54-4	86
12	20.594	0.61	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211101	001120-25-8	99
			7-Hexadecenoic acid, methyl ester, (Z)-	211115	056875-67-3	99
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
13	20.641	0.84	C:\Database\wiley7n.l			
			9-Hexadecenoic acid, methyl ester, (Z)-	211103	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211101	001120-25-8	99
			9-Hexadecenoic acid, methyl ester, (Z)- $$ Methyl palmitoleate $$ Me thyl palmitoleinate $$ Palmitoleic acid, methyl ester	211104	001120-25-8	99
14	20.886	27.52	C:\Database\wiley7n.l			
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213911	000112-39-0	99
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-	213893	000112-39-0	97
			Hexadecanoic acid, methyl ester (C AS) $$ Methyl palmitate $$ Methyl	213891	000112-39-0	97

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			hexadecanoate $$ Methyl n-hexadeca noate $$ Uniphat A60 $$ Metholene 2216 $$ Palmitic acid methyl ester $$ Palmitic acid, methyl ester $$ n-Hexadecanoic acid methyl ester $$ PALMITIC ACID-			
15	21.246	0.02	C:\Database\wiley7n.l			
			Methyl 9-oxo-8,8-dideuterionon oate	95373	000000-00-0	47
			Decanoic acid, 8-methyl-, methyl e ster $$ Methyl ester of 8-methylde canoic acid	115395	005129-64-6	37
			10-Undecenoic acid, methyl ester (CAS) $$ Methyl 10-undecenoate $$ M ETHYL UNDEC-10-ENOATE $$ Methyl un decenate $$ Methyl undecenoate $$ Methyl 10-undecenate $$ Undecenoic acid, methyl ester $$ Undecylenic acid, methyl ester $$ 10-Hendecen oic acid, methyl	112522	000111-81-9	37
16	21.481	0.05	C:\Database\wiley7n.l			
			Hexadecanoic acid, 14-methyl-, met hyl ester $$ Methyl 14-methylhexad ecanoate	231376	002490-49-5	96
			Heptadecanoic acid, methyl ester	231336	001731-92-6	94
			Hexadecanoic acid, 15-methyl-, met hyl ester $$ Methyl isoheptadecano ate $$ Methyl 15-methylhexadecanoa te	231378	006929-04-0	93
17	21.567	0.08	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231340	001731-92-6	94
			Hexadecanoic acid, 14-methyl-, met hyl ester	231377	002490-49-5	93
			Heptadecanoic acid, methyl ester $ $ Margaric acid methyl ester $$ Me thyl heptadecanoate $$ Methyl marg arate $$ n-Heptadecanoic acid meth yl ester	231337	001731-92-6	91
18	21.623	0.17	C:\Database\wiley7n.l			
			Cyclopropaneoctanoic acid, 2-hexyl -, methyl ester	228711	010152-61-1	93
			9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245467	000112-62-9	58
			9-Hexadecenoic acid, methyl ester, (Z)- (CAS) $$ Methyl palmitoleate $$ Methyl palmitoleinate $$ Palmi toleic acid, methyl ester	211101	001120-25-8	58
19	21.845	0.33	C:\Database\wiley7n.l			
			Heptadecanoic acid, methyl ester	231336	001731-92-6	95
			Heptadecanoic acid, methyl ester	231339	001731-92-6	95
			Heptadecanoic acid, methyl ester (CAS) $$ Methyl heptadecanoate $$ M ethyl margarate $$ Margaric acid m	231335	001731-92-6	94

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			ethyl ester $$ n-Heptadecanoic aci d methyl ester $$ HEPTADECANCARBON SAEUREMETHYLESTER			
20	22.562	29.14	C:\Database\wiley7n.l 9,12-Octadecadienoic acid (Z,Z)-, methyl ester (CAS) $$ Methyl linol eate $$ METHYL CIS-9,CIS-12-OCTADE CADIENOATE $$ Methyl octadecadieno ate $$ Linoleic acid methyl ester $$ Linoleic acid, methyl ester $$ Methyl cis,cis-9,12-octadecadienoa te $$ Methyl 9-ci	243127	000112-63-0	99
			9,12-Octadecadienoic acid (Z,Z)-, methyl ester	243128	000112-63-0	99
			9,12-Octadecadienoic acid, methyl ester	243170	002462-85-3	99
21	22.631	25.85	C:\Database\wiley7n.l 9-Octadecenoic acid (Z)-, methyl e ster (CAS) $$ Methyl oleate $$ Met hyl cis-9-octadecenoate $$ Oleic a cid methyl ester $$ Oleic acid, me thyl ester $$ Emery oleic acid est er 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHY L ESTER $$ (Z)-9-	245469	000112-62-9	99
			9-Octadecenoic acid, methyl ester, (E)- $$ Elaidic acid, methyl este r $$ Methyl elaidate $$ Methyl tra ns-9-octadecenoate $$ (E)-9-Octade cenoic acid methyl ester	245486	001937-62-8	99
			METHYLELAIDATE $$ ELAIDINSAEUREMET HYLESTER	245483	000112-62-9	99
22	22.829	11.19	C:\Database\wiley7n.l Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl o ctadecanoate $$ Methyl n-octadecan oate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic aci d methyl ester $$ Methyl-octadecan oate $$ Methyl es	247777	000112-61-8	99
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl o ctadecanoate $$ Methyl n-octadecan oate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic aci d methyl ester $$ Methyl-octadecan oate $$ Methyl es	247763	000112-61-8	98
			Octadecanoic acid, methyl ester $$ Stearic acid, methyl ester $$ n-O ctadecanoic acid, methyl ester $$ Kemester 9718 $$ Methyl n-octadeca noate $$ Methyl octadecanoate $$ M ethyl stearate $$ Metholene 2218 $ $ Emery 2218 $$ Kemester 9018 $$ M ethyl ester of oc	247760	000112-61-8	98
23	22.992	0.11	C:\Database\wiley7n.l Ethyl linoleate $$ LINOLEIC ACID, ETHYL ESTER $$ ETHYL 9,12-OCTADECA	258924	000544-35-4	93

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			DIENOATE $$ Linoleic acid ethyl ester $$ 9,12-Octadecadienoic acid (Z,Z)-, ethyl ester $$ Ethyl cis,cis-9,12-octadecadienoate $$ Ethyl linolate $$ Mandenol $$ LINOLSAEURE, ETHYLESTER			
			6,9-Octadecadienoic acid, methyl ester (CAS) $$ METHYL 6,9-OCTADECADIENOATE	243096	056599-55-4	91
			Cyclopentanol, 1-(1-methylene-2-propenyl)-	33800	078158-11-9	89
24	23.153	0.03	C:\Database\wiley7n.l			
			Octadecanoic acid, 11-methyl-, methyl ester	263398	074484-77-8	58
			Octadecanoic acid, methyl ester (CAS) $$ Methyl stearate $$ Methyl octadecanoate $$ Methyl n-octadecanoate $$ Stearic acid methyl ester $$ Kemester 9718 $$ Stearic acid, methyl ester $$ n-Octadecanoic acid methyl ester $$ Methyl-octadecanoate $$ Methyl es	247751	000112-61-8	50
			Nonadecanoic acid, methyl ester (CAS) $$ Methyl nonadecanoate $$ Nonadecanoic acid methyl ester $$ METHYL N-NONADECANOATE $$ n-Nonadecanoic acid methyl ester	263312	001731-94-8	43
25	23.488	0.05	C:\Database\wiley7n.l			
			9-Octadecenoic acid (Z)-, methyl ester (CAS) $$ Methyl oleate $$ Methyl cis-9-octadecenoate $$ Oleic acid methyl ester $$ Oleic acid, methyl ester $$ Emery oleic acid ester 2301 $$ OLEIC ACID-METHYL ESTER $$ (Z)-9-OCTADECENOIC ACID, METHYL ESTER $$ (Z)-9-	245467	000112-62-9	49
			11-Hexadecenoic acid, methyl ester	211109	055000-42-5	49
			methyl dihydromalvalate	245489	000000-00-0	49
26	23.720	0.05	C:\Database\wiley7n.l			
			Nonadecanoic acid, methyl ester $$ Methyl nonadecanoate $$ n-Nonadecanoic acid methyl ester	263309	001731-94-8	99
			Nonadecanoic acid, methyl ester	263307	001731-94-8	98
			Nonadecanoic acid, methyl ester (CAS) $$ Methyl nonadecanoate $$ Nonadecanoic acid methyl ester $$ METHYL N-NONADECANOATE $$ n-Nonadecanoic acid methyl ester	263308	001731-94-8	98
27	24.107	0.03	C:\Database\wiley7n.l			
			Spiro[2.4]heptane, 1,5-dimethyl-6-methylene-	32097	062238-24-8	74
			(Z)-4-Vinylcyclooctene $$ Cyclooctene, 4-ethenyl-, (Z)- (CAS) $$ cis-4-Vinylcyclooctene	32358	043044-21-9	70
			1,5-Cyclodecadiene, (E,Z)- $$ cis, trans-1,5-Cyclodecadiene $$ trans, cis-1,5-Cyclodecadiene $$ 1,5-Cyclodecadiene, (Z,E)- $$ (E,Z)-1,5-Cyclodecadiene	32091	001124-78-3	60

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
28	24.151	0.18	C:\Database\wiley7n.l			
			Bicyclo[10.1.0]tridec-1-ene	84411	054766-91-5	64
			Tricyclo[5.2.1.0(2,6)]decane, 4-methyl-	47445	000000-00-0	62
			TRICYCLO[5.2.1.0(2,6)]DECANE, 4-METHYL-	47375	000000-00-0	62
29	24.288	0.05	C:\Database\wiley7n.l			
			Bacteriochlorophyll-c-stearyl	390640	000000-00-0	87
			2-Pentadecanol $$ sec-Pentadecyl alcohol	157551	001653-34-5	87
			1-Octadecanol $$ n-Octadecanol $$ n-Octadecyl alcohol $$ n-1-Octadecanol $$ Aldol 62 $$ Alfol 18 $$ Atalco S $$ Cachalot S-43 $$ Crodacol-S $$ Lanol S $$ Lorol 28 $$ Octadecan-1-ol $$ Octadecyl alcohol $$ Sipol S $$ Siponol S $$ Siponol SC $$ Stearol $$ S	214154	000112-92-5	83
30	24.350	0.26	C:\Database\wiley7n.l			
			2-(METHYL-D3)-CYCLONONANONE $$ Cyclononanone, 2-methyl-d3- (CAS)	53597	032454-54-9	20
			Cyclohexanone, 2-butyl-	53375	001126-18-7	15
			Cyclononanone	36150	003350-30-9	15
31	24.401	0.19	C:\Database\wiley7n.l			
			11-Eicosenoic acid, methyl ester	275547	003946-08-5	99
			methyl dihydromalvalate	245489	000000-00-0	62
			Cyclopropaneoctanoic acid, 2-hexyl-, methyl ester	228710	010152-61-1	60
32	24.638	0.38	C:\Database\wiley7n.l			
			Eicosanoic acid, methyl ester	277452	001120-28-1	99
			Eicosanoic acid, methyl ester	277458	001120-28-1	98
			Eicosanoic acid, methyl ester	277450	001120-28-1	98
33	24.912	0.35	C:\Database\wiley7n.l			
			Hexacosane, 9-octyl- $$ 9-n-Octylhexacosane	363626	055429-83-9	83
			Hexatriacontane	369896	000630-06-8	81
			Hexacosane, 13-dodecyl- $$ 13-n-Dodecylhexacosane	374601	055517-73-2	80
34	25.279	0.08	C:\Database\wiley7n.l			
			2(1H)-Naphthalenone, octahydro-4a-methyl-7-(1-methylethyl)-, (4a.alpha.,7.beta.,8a.beta.)-	127817	054594-42-2	66
			(+-)-Tridec-2-en-12-ol $$ 12-Tridecen-2-ol, (.+-.)- (CAS)	113120	131871-11-9	62
			Octadec-9Z-enol	211407	000000-00-0	46
35	25.560	0.35	C:\Database\wiley7n.l			
			1-Docosene	259091	001599-67-3	91
			17-Pentatriacontene	366689	006971-40-0	83
			17-Pentatriacontene (CAS)	366690	006971-40-0	83
36	26.073	0.17	C:\Database\wiley7n.l			
			Octacosane $$ n-Octacosane	329266	000630-02-4	86
			Hexacosane $$ n-Hexacosane	311169	000630-01-3	86
			Docosane $$ n-Docosane $$ Normal-docosane	261311	000629-97-0	83
37	26.232	0.14	C:\Database\wiley7n.l			

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			(Z,Z)-heptadeca-8,11-dien-1-yl iodide	307520	000000-00-0	58
			5-Dodecyne $$ 5-C12H22	68426	019780-12-2	52
			9,12-Octadecadienoic acid (Z,Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester $$ Linolein, 2-mono- $$ .beta.-Monolinolein	301826	003443-82-1	52
38	26.278	0.18	C:\Database\wiley7n.l			
			9-Octadecenal, (Z)- $$ Olealdehyde $$ cis-9-Octadecenal $$ Oleylaldehyde $$ Z-9-Octadecenal	208774	002423-10-1	90
			9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester $$ Olein, 2-mono- $$ .beta.-Monoolein $$ Glycerol 2-monooleate $$ 2-Monoolein $$ 2-Monooleoylglycerol $$ 2-Oleoyl glycerol ether $$ 2-Oleoylglycerol	303308	003443-84-3	35
			DI-(9-OCTADECENOYL)-GLYCEROL $$ 9-Octadecenoic acid (Z)-, 2-hydroxy-1,3-propanediyl ester	383671	002465-32-9	25
39	26.422	0.03	C:\Database\wiley7n.l			
			1-Docosanol	277578	000661-19-8	58
			17-Pentatriacontene (CAS)	366690	006971-40-0	58
			4-Trifluoroacetoxytetradecane	260469	000000-00-0	58
40	26.482	0.08	C:\Database\wiley7n.l			
			Decanoic acid, 4-oxo-	95299	000000-00-0	27
			o-Xylene-d10	10736	000000-00-0	27
			Ethene, chlorotrifluoro-	16062	000079-38-9	11
41	26.575	0.01	C:\Database\wiley7n.l			
			Hexadecanoic acid, 2-hydroxy-1-(hydroxymethyl)ethyl ester $$ Palmitin, 2-mono- $$ Palmitic acid .beta.-monoglyceride $$ 2-Hexadecanoyl glycerol $$ 2-Monopalmitin $$ 2-Monopalmitoyl-sn-glycerol $$ 1,2,3-Propanetriol 2-hexandecanoyl ester $$ Glycerol .beta.	281038	023470-00-0	38
			1-Methyl-3-methylene-1-silacyclobutane $$ Silacyclobutane, 1-methyl-3-methylene- (CAS)	6918	084602-64-2	18
			2H-Pyran, 3,4-dihydro-6-methyl- (CAS) $$ 2-Methyl-.delta.2-dihydropyran $$ 6-Methyl-3,4-dihydro-2H-pyran	7209	016015-11-5	18
42	26.678	0.12	C:\Database\wiley7n.l			
			Docosanoic acid, methyl ester	302040	000929-77-1	90
			Docosanoic acid, methyl ester (CAS) $$ Methyl behenate $$ Methyl docosanoate $$ Behenic acid methyl ester $$ Behenic acid, methyl ester $$ n-Docosanoic acid methyl ester	302031	000929-77-1	89
			Docosanoic acid, methyl ester	302034	000929-77-1	86
43	27.013	0.04	C:\Database\wiley7n.l			
			2-Ethylacridine	125906	000000-00-0	27
			Thiocarbamic acid, N,N-dimethyl, S-1,3-diphenyl-2-butenyl ester	261852	000000-00-0	27
			1,3-Bis(trimethylsilyl)benzene	147371	002060-89-1	27

Library Search Report

Data Path : C:\msdchem\1\data\170418VK\
Data File : 00301003.D
Acq On : 18 Apr 2017 15:03
Operator : AKK
Sample : N2heptaani
Misc :
ALS Vial : 3 Sample Multiplier: 1

Search Libraries: C:\Database\wiley7n.l Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint1.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
44	27.454	0.02	C:\Database\wiley7n.l			
			Silicic acid, diethyl bis(trimethy lsilyl) ester	244286	003555-45-1	53
			Gibberellin A3 $$ Gibb-3-ene-1,10- dicarboxylic acid, 2,4a,7-trihydro xy-1-methyl-8-methylene-, 1,4a-lac tone, (1.alpha.,2.beta.,4a.alpha., 4b.beta.,10.beta.)- (CAS) $$ GA3 $ $ GA $$ Gibberellin X $$ Gibberell ic acid $$ 4a,1-(Epoxymethano)-7,9 a-methanobenz[a]a	294997	000077-06-5	43
			Galactitol, hexaacetate, D- (CAS) $$ GALACTITOL-1,2,3,4,5,6-HEXAACET ATE	348804	014330-96-2	35