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Qualitative Chemical Analysis of Elf Bar E-Liquids and their Effect on Phenotypic Characteristics of Arabidopsis Thaliana

Genevieve Neuwirth
University of Lynchburg

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Senior Honors Project

Submitted in partial fulfillment of the graduation requirements of the Westover Honors College

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Abstract

After their initial market introduction in 2003, the popularity and use of e-cigarettes have exponentially increased. There are three main components that have contributed to this: marketing, ease of access, and emerging flavors. The marketing industry uses claims that e-cigarettes are a 'safer' and 'healthier' alternative to cigarettes as a way to entice previous smokers into using this product. With the increase in popularity, there is also an increase in demand, which has led to the creation of stores designed to target customers and sell e-cigarettes and similar products at convenient locations. Finally, the emerging flavors have enticed many nonsmokers to start with e-cigarettes, as they are fun to try and taste good, without the aftertaste of traditional cigarettes. However, e-liquids contain flavor compounds that pose health risks to humans. These compounds, especially when smoked, produce toxic aldehydes and volatile organic compounds that impact the respiratory system as well as other systems within the body.

As the use of e-cigarettes has increased, so has the waste produced. As of 2018, approximately 58,000,000 e-cigarettes and vapes were sold within the United States; 19.7 million of which were single-use. These are often thrown away or littered, posing a threat to the environment with various plastics, circuiting, and residues of the various e-liquids within these devices. Some of the e-liquid waste and pollution, especially from unused e-cigarettes, is toxic enough to be considered hazardous waste. The aim of this study is to observe the effects of e-liquid interaction with the model plant species and weed *Arabidopsis thaliana* and observe the phenotypic stress response that is produced. Eight of the most popular Elf Bar e-cigarettes were chosen, as they are the most popular flavored e-cigarette currently on the market. Qualitative analysis of samples was performed using FTIR, H^1 NMR, and GC/MS in order to obtain the general chemical composition of the different e-liquids. Once complete, dilutions and neat e-liquids were introduced to *A. thaliana* plants grown in soil as well as on plant agar. It was found that the dilutions used (0.5%, 0.75%, and 1.0%) were too low to induce any type of stress response when systematically introduced to the mature plants in soil and the seedling in plant agar. The only phenotypic change observed with the dilutions occurred with a single-leaf treatment of a 1% dilution, where the leaf became bleached and withered while the rest of the plant flourished. With neat e-liquid introduction to seedlings in plant agar, bleaching, and death occurred within 24 hours of the treatment, indicating that e-liquids are toxic to plants and have the potential to negatively impact the environment with continued littering and improper waste disposal.

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Introduction

Background

The electronic cigarette, more commonly known as an e-cigarette, is well known throughout today's society. They were first patented in 1965, many years before they became a public phenomenon. That year, Herbert A. Gilbert first came up with, and invented a "smokeless non-tobacco cigarette."[1] His ultimate goal was to "replace burning tobacco with heated, moist, flavored air."[1] At this time, new evidence was emerging within the scientific community showing the negative health effects that by-products of the burned tobacco (such as tar) were having on human health.[1] It wasn't until about 2003 that e-cigarettes were officially introduced into mainstream markets, and while they did not gain traction for the first few years, their popularity soon skyrocketed.[2]

This major increase in popularity was due to three main components: marketing, access, and emerging flavors.[3] Multimedia marketing of these e-cigarettes was beginning to emerge and there was always one consistent image being portrayed -- that these e-cigarettes were a "safer" alternative to traditional cigarettes and that they promote smoking cessation.[1-4,6-8,10-12] This marketing ploy was based around the fact that these newer devices did not contain tobacco or, in turn, produce any tobacco byproducts. Since the health effects of e-cigarettes on humans were (and still are) unknown, it encouraged those trying to live healthy lifestyles or quit smoking to purchase them.[3] While this was the main reason for its rise in popularity, the ease of access and emerging flavors also played a large role. Over time, in order to keep up with the consumer demand, individual stores dedicated to selling products such as e-cigarettes emerged. This, along with a surplus of products within gas stations and grocery stores, gave many people easy access to purchase these items.[3] The final component to the rise in popularity of e-cigarettes is the

emergence of new and interesting flavors. There was a major shift from traditional cigarette flavors such as tobacco to newer flavors such as chocolate pudding or cherry limeade. These flavors made smoking e-cigarettes incredibly enjoyable and tended to entice a younger crowd to begin smoking. These factors caused a drastic increase in popularity for the e-cigarettes, to the point where in 2011 to 2013 the amount of first-time smokers tripled in number and in 2014 the number of e-cigarette users far surpassed the number of traditional cigarette smokers.[2,3] Due to this, there was almost a 300% increase of e-cigarette sales between November 2016 to August of 2020.[4] This, as well as the increase in sales of flavored e-cigarettes, can be seen in Figure 1.[4] However, the popularity increase (while great for marketing and manufacturing) left regulations far behind.

In 2016, the Food and Drug Administration (FDA) classified all e-cigarettes and e-liquids as tobacco products and began to require Premarket Tobacco Product Applications (PMTA).[5] Although these products do not contain tobacco, they were categorized in this way due to their similarity in usage and regulations to traditional cigarettes. These applications were required for each e-liquid and e-cigarette component by 2020.[5] These applications must show that the product aids in the protection of public health and offers a greater benefit to smokers than the risk posed to the youth, among other criteria.[5] While the FDA is currently still receiving applications, at this time they have denied over 1 million products, including popular brands such as flavored JUUL pods, due to their application failure.[5] Many of the products that have been banned as the marketing and flavoring of products entices younger people into trying this product, resulting in over 3.6 billion youth and young adults being or becoming smokers in 2018.[6] This is dangerous to public health, as nicotine is addictive and the long-term health effects of smoking e-cigarettes are unknown at this time, as this is the first generation to be continuously using these products.

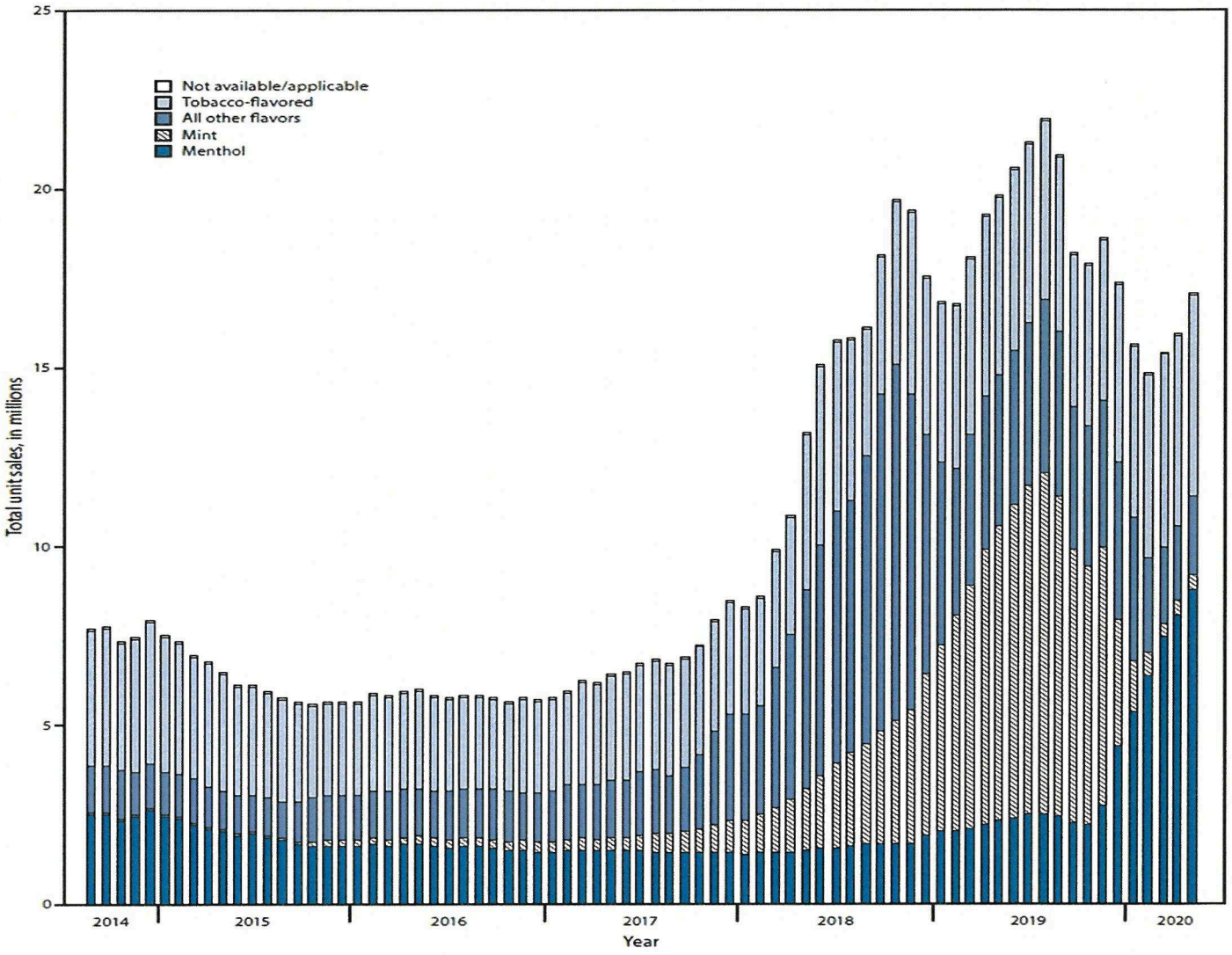


Figure 1: Retail sales data provided by CDC and obtained through Information Resources, Inc. for convenience stores, gas stations, grocery stores, drugstores/pharmacies, mass merchandiser outlets, club stores, dollar stores, and military sales; data from the Internet and vape shops were not collected. Each bar in the figure represents a 4-week aggregate interval. The "All other flavors" category includes fruit, clove/spice, chocolate, alcoholic drink (such as wine, cognac, or other cocktails), candy/desserts/other sweets, or some other flavor. Unknown flavors were excluded from this figure (<0.1%).[4]

Components

All e-cigarettes have the same basic components: a tank or pod for e-liquid storage, a power source, a heating element, and a means of aerosol production.[5] In most cases the power source consists of a lithium battery, and the heating element tends to be some sort of coil. The e-cigarette is activated either by a button or airflow sensor that activates the battery.[7,9] This causes the coil to heat up and draws the e-liquid over it, creating an aerosol. Even with these basic components and inner workings, e-cigarettes have drastically evolved since their beginning.[7,9] As of today there are four generations of e-cigarettes and, in the future, there is a potential for further evolution. The first generation was dubbed the 'cigalike' as it was an exact replica of the traditional cigarette, from its shape and size to its color. However, it had little capacity for e-liquid and was therefore disposable, with very inefficient nicotine delivery.[5] The second generation looked different from a traditional cigarette in order to accommodate various changes. These were both disposable and rechargeable, and unlike the first generation, had a larger capacity to hold e-liquids as well as the ability to refill or replace cartridges.[5] Due to the increase of e-liquids, they had a much more effective and efficient nicotine delivery.[5] The third generation gave the user more control with the power (wattage) of the battery as well as the temperature of the coil, both of which influenced how much aerosol was produced and, in conjunction, allowed the consumer to regulate their nicotine intake.[5] The final and most recent fourth generation has a variety of both refillable and disposable types. Many disposable ones have pre-filled cartridges or pods that are limited to a certain amount of 'puffs,' but are reusable and rechargeable until they run out.[5] In addition, some of the newer e-liquids contain nicotine salts which, along with allowing for efficient and effective nicotine delivery, makes the smoke less irritating to the lungs for a smoother inhale.[5]

In the same way that all e-cigarettes have basic components, so do e-liquids. The general vehicle consists of a propylene glycol (PG) and vegetable glycerin (VG) mixture.[1,8] These give the e-liquid its viscous nature, carries the flavor and nicotine, and allows for the production of aerosol. The ratio of PG and VG is dependent upon what the company is trying to achieve. A higher amount of PG will contribute to more flavor intensity with less aerosol production. On the other hand, a higher amount of VG will promote the production of more aerosol with less flavor intensity.[1,8] Nicotine is another basic component, with its potency measured in mg per mL of e-liquid.[5] The final component is the flavoring compounds. There are many different varieties and mixtures of these compounds, which are based upon the flavor that a company is trying to achieve with chemicals alone.[5]

Thermal Decomposition and E-liquid Toxicity

As the e-liquids are heated over the coil and vaporized, thermal decomposition of the various chemical compounds begins to occur. The heat of the coil breaks the bonds of compounds at certain temperatures, which creates byproducts that have a vastly different effect than the original chemical.[1] In the vehicle alone, thermal decomposition is the cause of four different byproducts that are considered dangerous. PG is typically used in a large variety of foods and cosmetics and is labelled as 'safe' by the FDA.[10] However, it is known that when PG is heated the bonds break and it changes from an aliphatic alcohol into both acetone and acetalaldehyde.[11] Similarly, VG also ends up breaking into acrolein and formaldehyde.[11] Three of these byproducts (formaldehyde, acrolein, and acetaldehyde) are toxic aldehydes and have been labelled as a harmful constituents by the FDA, as they can cause a myriad of health issues.[12] However, the vehicle is not the only part of e-liquids that produce harmful byproducts;

nicotine and all the other flavoring compounds do as well. It was found that in the aerosol of an e-cigarette, not only are there toxic aldehydes present but also various volatile organic compounds, nitrosamines, metal nanoparticle, phenols, free radicals, and a host of other potentially harmful compounds.[1,6,11,12] These compounds are incredibly harmful and can produce both acute and chronic health issues, including but not limited to cardiac and respiratory inflammation, impairment of DNA repair, cytotoxicity, respiratory and cardiovascular disease, tumors, and a delayed immune response.[2,6,8,11-13] Throughout a multitude of studies, it was found that there are always some type of thermal decomposition product within the aerosol of an e-cigarette. When examined with a consistent coil temperature, power (wattage), PG:VG ratio and nicotine strength, flavored e-liquids produced many more byproducts than e-liquids with little to no flavoring compounds added.[2,12] It was also found that there was a significant difference in the amounts of byproducts with a higher power, temperature, puff duration, and nicotine strength from the same e-liquid, as all of these factors contribute to the breaking of bonds within the compounds of the e-liquid.[2,5-9,11-13]

Although e-cigarette aerosols produce a multitude of toxic byproducts, in a 2018 study it was found that both the aerosols and neat e-liquids have statistically similar levels of toxicity to three types of human cells.[9] These cell types included human kidney, smooth epithelial respiratory, and alveolar basal cells. After treating cells and observing viability using fluorescent imaging, it was found that e-liquids with the same PG:VG ratio and nicotine strength have different toxicity levels, which is ultimately dependent upon the chemical compounds added.[9] Of the 148 e-liquids tested in this study, many had at least one unknown and unidentifiable constituent while some had up to ten. Along with this, there were chemical compounds found within the various samples that are known to cause negative health effects when aerosolized,

such as vanillin, cinnamate, and diacetyl.[9,13] While it is unclear exactly why the e-liquids and aerosols have the same cytotoxicity, though it may be due to the chemical compounds added into the e-liquids. While most, if not all compounds, are labelled as safe for product use by the FDA, some are found at concentrations over 100 times what the FDA has tested.[5,9] It was also found that the nicotine content of e-liquids could be up to 30% greater than the label claim, contributing to the toxic effect of the e-liquids.[5,7,9] Even without knowing the exact reasoning, the simple conclusion is that both e-liquids and the aerosols they produce are harmful to human health.

Environmental Impact

With the increase in popularity of e-cigarettes, there has been a noticeable increase in the amount that is littered. However, the environmental impact of such an industry tends to be overlooked by manufacturers and marketing companies, as considering this aspect may cause them to lose money.[14,15] Aside from e-cigarettes, about 2/3 of the 6.25 trillion cigarettes that are sold annually are littered.[14] This waste of traditional cigarettes has contributed to major issues such as clogged sewer drains impacting parks and outdoor recreation areas which has a negative affect on both human and animal life.[14,15] While this is a cause for concern, the current and potential impact of e-cigarette littering is a lot worse. As of 2018, over 58 million e-cigarettes and refills are being sold annually, with around 19.2 million of them being designated as single use, meaning that a large amount of e-cigarettes are either being littered or not disposed of properly.[14,15]

E-cigarettes contain pollutants such as endocrine disrupting plastics, residues of concentrated nicotine extracts, and electronic circuitry that pose biohazard risks. Not only does

the electronic waste have the potential to cause fires if sparks are produced from circuitry and wires, but the batteries can leach heavy metals and acid onto the ground and the small components may pose a choking hazard to children and animals.[14] The e-liquid itself is also dangerous as, according to federal regulations, if nicotine is meant to be the main active ingredient and over 50% of a substance is littered, it is considered hazardous material.[15] All of these issues can occur if e-cigarettes are littered or even disposed of improperly. The proper disposal method is to take the e-cigarette apart, separate the components, and then follow regulations for the electronic waste , batteries, and hazardous materials.[15] This is difficult for the average person to achieve and, while some companies offer disposal services, they are not easily accessible to the public or they have arbitrary requirements that make it difficult to take advantage of the services.[14] This indicates that littering and incorrect disposal techniques will continue, contributing negatively to the environment. As e-cigarettes continue to grow in popularity and regulations fail to be implemented, it will lead to an environmental impact whose full extent is unknown at this time. In conjunction, it is important to fully understand how e-liquids may contribute to this impact and what negative effects they might have on ecosystems if they are indeed littered.

Arabidopsis thaliana

Arabidopsis thaliana is a member of the Brassicaceae family, more commonly known as the 'mustard' family.[16] Crops such as cabbage, broccoli, and horseradish are also a part of the same family, although *A. thaliana* is, in all technical terms, a weed. This plant is a model plant, which makes it an excellent choice to use in experiments. It is able to survive in a multitude of climates and countries, including, but not limited to, high elevations, the tropics, a cold tundra,

and all of the continents, excluding Antarctica.[16] Along with its durability, *A. thaliana* is suitable for growing in laboratory settings. It is small in size and is quick to germinate and mature, completing the process in around 4 weeks, allowing for more testing and analysis to take place rather than a longer waiting period. There are also a multitude of genetic benefits that accompany this plant. It has a small, diploid genome which has allowed it to be fully sequenced and partially annotated and allows for greater genetic diversity amongst the population.[16] Each plant produces thousands of seeds, promoting self-fertilization and allowing for genetic manipulation experiments, such as mutagenesis of the seeds and various others.[16]

Arabidopsis thaliana has proven to be ideal for experimentation for its growth patterns and survival capabilities as well as the ease of evaluating phenotypic changes and stress responses.[16,17] There are four visible stress responses that *A. thaliana* might exhibit: bleaching or a loss of color in the leaves, loss or slowing of germination, diminished root length, or diminished plant growth.[17] The change in growth patterns and discoloration of leaves are easily visible, as a mature plant will produce multiple rosettes of small leaves. As it grows, the youngest leaves will develop at the top of the plant with the older ones beneath them.[16] Seed germination rates and roots are more difficult to ascertain, especially when the plants are grown within soil. All of these indicators, though not always visible, allow for a better understanding and visualization of how *A. thaliana* responds to stress.

Experimental Rationale

To evaluate the detrimental impact e-cigarettes may have on the environment when littered, neat e-liquids were extracted from Elf Bars, the most popular flavored e-cigarettes currently on the market. The top eight flavors (Sweet Menthol, Blue Razz Ice, Grape energy,

Lemon Mint, Watermelon Ice, Tropical Rainbow Blast, Kiwi Passionfruit Guava, and Sour Candy) were chosen for the experiment. The neat e-liquids were qualitatively analyzed using FTIR, H^1 NMR, and GC/MS. This allows for a better understanding of the exact chemical composition of the e-liquids, as outside of the vehicle composition, Elf Bar does not publish their ingredients list for consumers to view.

Once the chemical composition analysis was performed, three dilutions (0.5%, 0.75%, and 1.0%) of Elf Bar e-liquids were created in deionized water (water purified through ion exchange) and used to treat *Arabidopsis thaliana* plants in both soil and plant agar. *A. thaliana* was chosen due to it being a model plant with a fast growth rate, as well as it being a roadside weed. When e-cigarettes are littered it is typically done on the sides of roads or sidewalks where weeds are the most prevalent and most affected by the waste. Phenotypic stress responses, primarily bleaching and a reduced growth rate, will be observed in the plants and compared based upon the flavoring of the e-liquid. The reactions of the plants to various flavors will be monitored to see whether particular flavoring compounds or the e-liquid vehicle have an adverse effect,. Currently, there are no studies addressing the effects that e-liquids might have on the environment, though it is a pressing matter with the popularity and waste increase of e-cigarettes.

Methods

Flavored E-cigarettes and E-liquid Extraction

Flavored e-cigarettes were purchased online through Element Vape. All e-cigarettes were rechargeable, disposable pods, all being the same size (79mm x 41 mm x 19mm) and having a 5000-puff capacity with 13 mL e-liquid capacities. The battery capacity was 650 mAh with a type-c charging port. All e-liquids had a nicotine strength of 50 mg/mL. E-liquids were extracted by opening the Elf-bar with pliers, extracting the sponge, and squeezing the contents into small vials which were labeled and sealed.

FTIR Analysis of E-liquid

Qualitative e-liquid analysis was completed using a Thermo Nicolet model iS10. The instrument used a KBr beam splitter with a range of 4000-650 wavenumbers (cm^{-}) and an optimal velocity of 0.3165. Each e-liquid was scanned 16 times at a resolution of 8 using ATR corrections. Samples consisted of neat e-liquids and were directly placed upon the crystal for analysis by a DTGS KBr detector.

H^1 NMR Analysis of E-liquid

Analysis of e-liquid samples was performed using a Magritek Spinsolve 60 Carbon H^1 NMR. When running the samples, the receiver gain was set to 25.0 with 4 scans per sample. The instrument had a relaxation delay of 36.3698 and a pulse width of 13.4000. The samples were prepared by adding 650 µL of 99.8% chloroform and 10 µL of the neat e-liquids into NMR tubes. The signals were detected using a spectrometer frequency of 62.07 with a spectral width of 5000.0.

GC/MS Analysis of E-liquid

Qualitative e-liquid analysis was performed using a Shimadzu GCMS-QP2010 gas chromatograph/mass spectrometer, using a Shimadzu SH-Rxi-5Sil MS capillary column (30m, 0.25 ID, 0.25 DF) and helium carrier gas. Using a Shimadzu AOC-20i Auto-Injector, the instrument operated in constant flow mode at 1 mL/min He with the oven heating from 50 to 275 C at 20 C/min and then holding for 5 minutes. Samples were prepared at a 1.0% dilution by adding 1 mL of neat e-liquid to a 100 mL volumetric flask and bringing it to volume with 99.8% chloroform-D and inverting it 10 times to ensure proper mixture. Full scan mass spectra were acquired from Shimadzu GC/MS solution software. Compound identification and data analysis were completed by Agilent Chemstation. Information was collected for all eight e-liquid flavors and analyzed.

Arabidopsis thaliana in Soil

An equal ratio of Miracle-Gro potting soil and perlite were mixed together within a container and moistened with tap water. Small 2" square pots were filled with this mixture and placed within a large, clean plant tray for watering. *Arabidopsis thaliana* seeds were transferred using slightly damp tweezers to pick them up and place them into each pot. The plants were placed in a 4° C fridge, where they were stratified for at least 48 hours before being transferred into a growth chamber set to 22° C, running on a short-day light cycle with lights illuminated from 8 AM to 7 PM. The plants were watered from the bottom as needed. Approximately 2-3 weeks into the growth process, the pots were thinned of plants until only one *A. thaliana* plant was left.

At approximately 4 weeks of growth the plants were treated with varying dilutions of the e-liquids in water at 0.5%, 0.75% and 1.0% dilutions. These solutions were created by adding 500 µL, 750 µL, and 1 mL of individual e-liquids into 100 mL volumetric flasks with DI water and inverting to mix the solution. Plants were treated with 10 mL of each dilution as well as one drop of the 1.0% dilution upon a marked leaf of the control plant that was not being treated. Observations occurred over a 1–2-week period following treatment to observe any phenotypic changes.

***Arabidopsis thaliana* in Agar**

To sterilize the seeds, they were placed within plastic microcentrifuge tubes and covered with 1 mL of 70% ethanol for 2 minutes. Using a pipette, the ethanol was carefully removed until there was only a thin layer left and done so that no seeds were lost in the process. A 10% bleach and 0.1% triton-X 100 solution was made by mixing 1.5 mL of bleach and 15 mL of DI water in a plastic conical tube. 16.5 µL of Triton X-100 was added, and the tube was then slowly inverted in order to ensure proper mixture. 1 mL of the solution was used to cover the seeds and left for 20 minutes with periodic mixing. The bleach solution was carefully removed in a sterile laminar flow hood. The seeds were then rinsed with sterile DI water by adding 1 mL, inverting it, and discarding the water. This was done a total of 4 times, with the sterile DI water from the fourth being left in with the seeds.

Plant growth media was prepared containing ½ Murashige and Skoog (MS) plant growth media and 1.0% sucrose. The solution was adjusted to a pH of 5.7 with KOH. 4 g/L Gelzan was added as a solidifying agent. The mixture was autoclaved for 20 minutes and was then allowed to

cool to 60°C in a hot water bath. The molten media was poured in a thick layer in 10 cm square Petri plates and allowed to solidify and dry in a sterile hood.

A 200 µL pipette was used to draw up the sterilized seeds suspended in sterile water, and once there were some in the tip, it was taken off the pipette and held horizontally so as not to spill the seeds. Holding the tip at about a 45° angle, it was carefully dabbed onto the agar plate in order to deposit one seed at a time. Once all seeds were placed, the agar plate was sealed with 3M Micropore tape (to allow airflow) and placed in a 4° C fridge to be cold treated for 48 hours, after which they were transferred into the growth chamber with the same growing conditions as previously stated.

The first set of seedlings grown on agar were treated after 7 days of growth within the chamber, all of them being treated with 10 µL of 0.5%, 0.75%, and 1.0% dilutions of both Sweet Menthol and Blue Razz Ice. The second batch of seedlings were treated at 6 days after growth with either neat e-liquid or 20 µL of a 1.0% dilution of the following flavors: Sweet Menthol, Blue Razz Ice, Lemon Mint, Tropical Rainbow Blast, or Sour Candy. Observations occurred over a one week period to observe any phenotypic changes.

Results

Composition Analysis with FTIR

All eight of the neat e-liquid samples were tested to create an interferogram, which shows how the absorbance changes at various wavenumbers. This instrument creates a light beam at different wavenumbers to vibrationally excite the molecules. A detector analyzes how much light was absorbed at each wavenumber, giving peaks for various vibrational excitation of bonds. The data shown in Figure 2 shows that all eight of the samples have a similar chemical composition and very little, if any, differences between the samples. The peak between 3000 and 3500 cm^{-} depicts a single bond stretch either between O-H or N-H, and the peak right before 3000 cm^{-} also shows that there is a single bond stretch, only between C-H. A very small peak directly after 1500 cm^{-} may indicate the presence of a double bond that could be between two carbons, a carbon and oxygen, or carbon and nitrogen though it is difficult to determine due to the size of said peak. However, there is clear evidence of both bending and rocking within the skeletal fingerprint region (500 – 1500 cm^{-}), which could be found in the following bonds: C-Cl, C-O, C-C, and C-N.

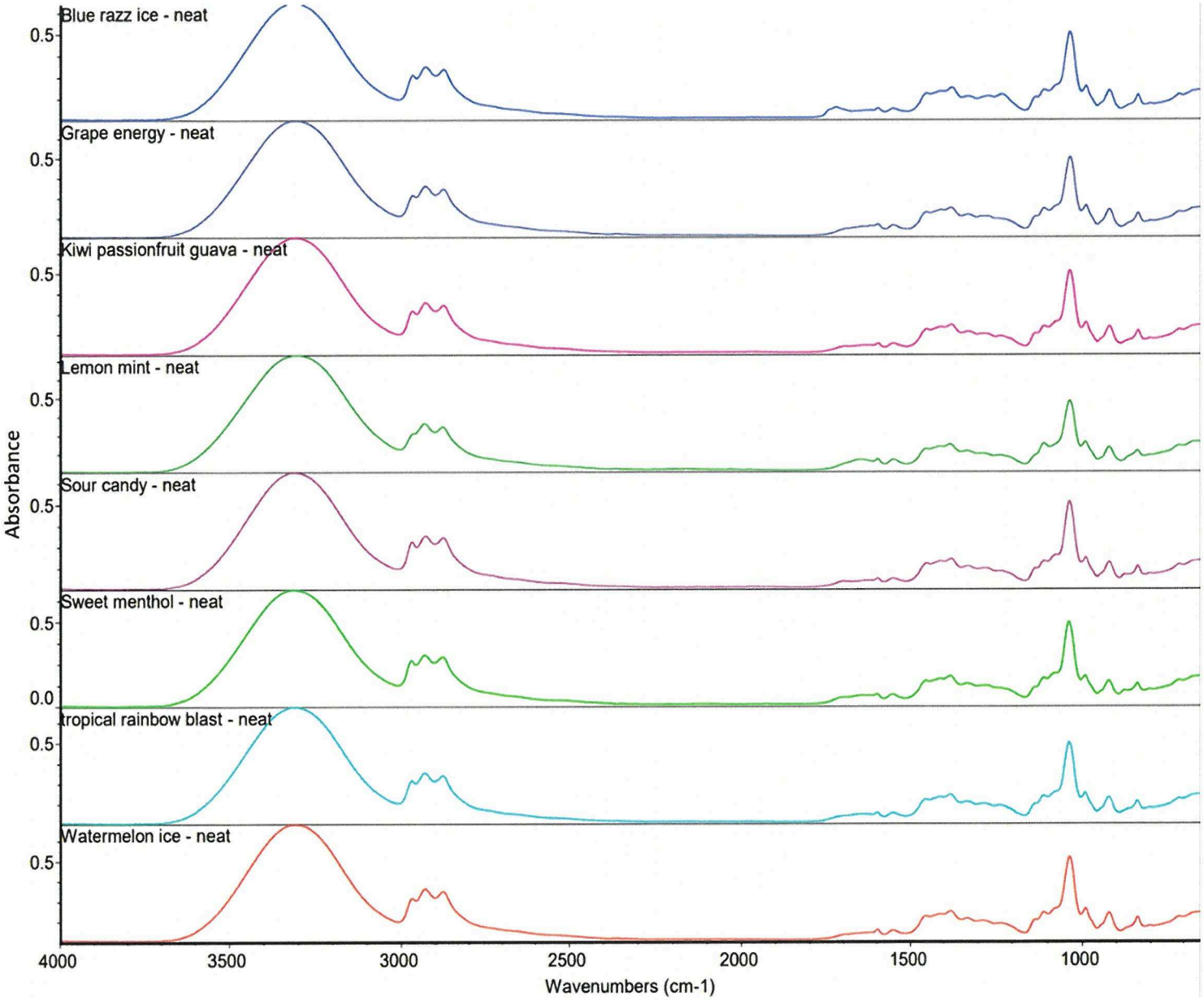


Figure 2: Fourier Transform Infrared (FTIR) interferogram of all eight e-liquids, showing the absorbances at specific wavenumbers (cm^{-})

Composition Analysis with H^1 NMR

All e-liquid samples created within the NMR tubes were run to create the spectra in Figure 3, which indicates the chemical shift of each compound vs the intensity of said compound. This instrument uses electromagnetic radiation to excite the nucleus (assuming it has a magnetic moment) of a compound and measures the resonance of that excited nucleus relaxing back to the ground state. The peaks at various frequencies, or the chemical shift, give an indication of what functional groups may be present within the sample. The initial peak at around 7.25 ppm is indicative of chloroform, which was the solvent used in all of our compounds. However, this peak is the only one whose identity is truly known. The peaks between 5.0-5.5 ppm for watermelon ice, lemon mint, grape energy, and sweet menthol are indicative of vinylic or phenolic hydrogen atoms. Of all the peaks, these are the only ones that differ from the rest of the samples, as the other peaks are present throughout all 8-e-liquids. This shows that the four flavors listed above have a specific compound that the others do not have. The next peaks from about 3.0-4.0 ppm show that all samples have compounds containing either an alcohol, an alcohol hydroxyl, an alkyl halide, or an ether. The peaks between 2.0-3.0 ppm show that there could be alcohol hydroxyl, a ketone, benzylic hydrogens, or acetylenic hydrogens present within the samples. Finally, the peaks between 1.0-1.5 ppm indicate the presence of an alcohol hydroxide or a 1° or 2° alkyl.

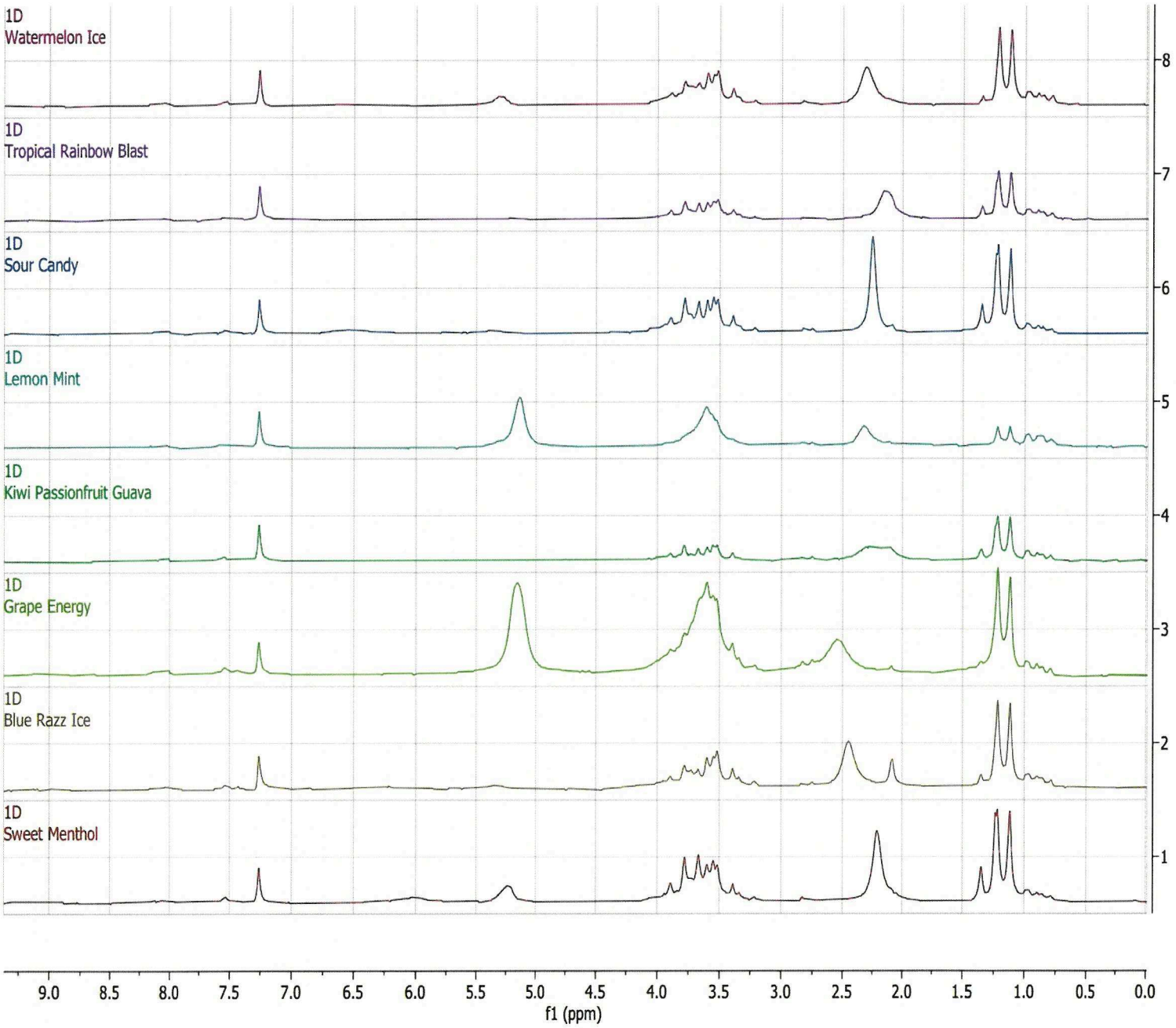


Figure 3: Proton Nuclear Magnetic Resonance (H^1 NMR) spectra showing the intensity of nuclear resonance at varying chemical shifts (ppm)

Composition Analysis with GC/MS

E-liquid samples at a 1.0% dilution with 99.8% chloroform-D were run through GC/MS to create the chromatogram in Figure 4 as well as all chromatograms in Appendix A. This instrument vaporizes the sample, and an inert gas (helium) pushes it through a column where it interacts with the stationary phase. As compounds elute from the column, the MS records the time of elution (retention time) as well as the abundance of the compound. The data is then analyzed with a program which provides the identity of each compound when possible. Table 1 gives the identities of each compound at their respective retention time. Other tables corresponding to each e-liquid can be found below their respective chromatograms in Appendix A.

Safety Data Sheets (SDS) were found for all compounds throughout the e-liquid samples. Using these, the chemical compounds were separated into three categories: not hazardous, hazardous and flammable, and hazardous and toxic, the first two categories can be found in Tables 2 and 3. The hazardous and toxic compounds are listed in Table 4 based upon the LD50 for oral toxicity in rats from most toxic to least toxic.

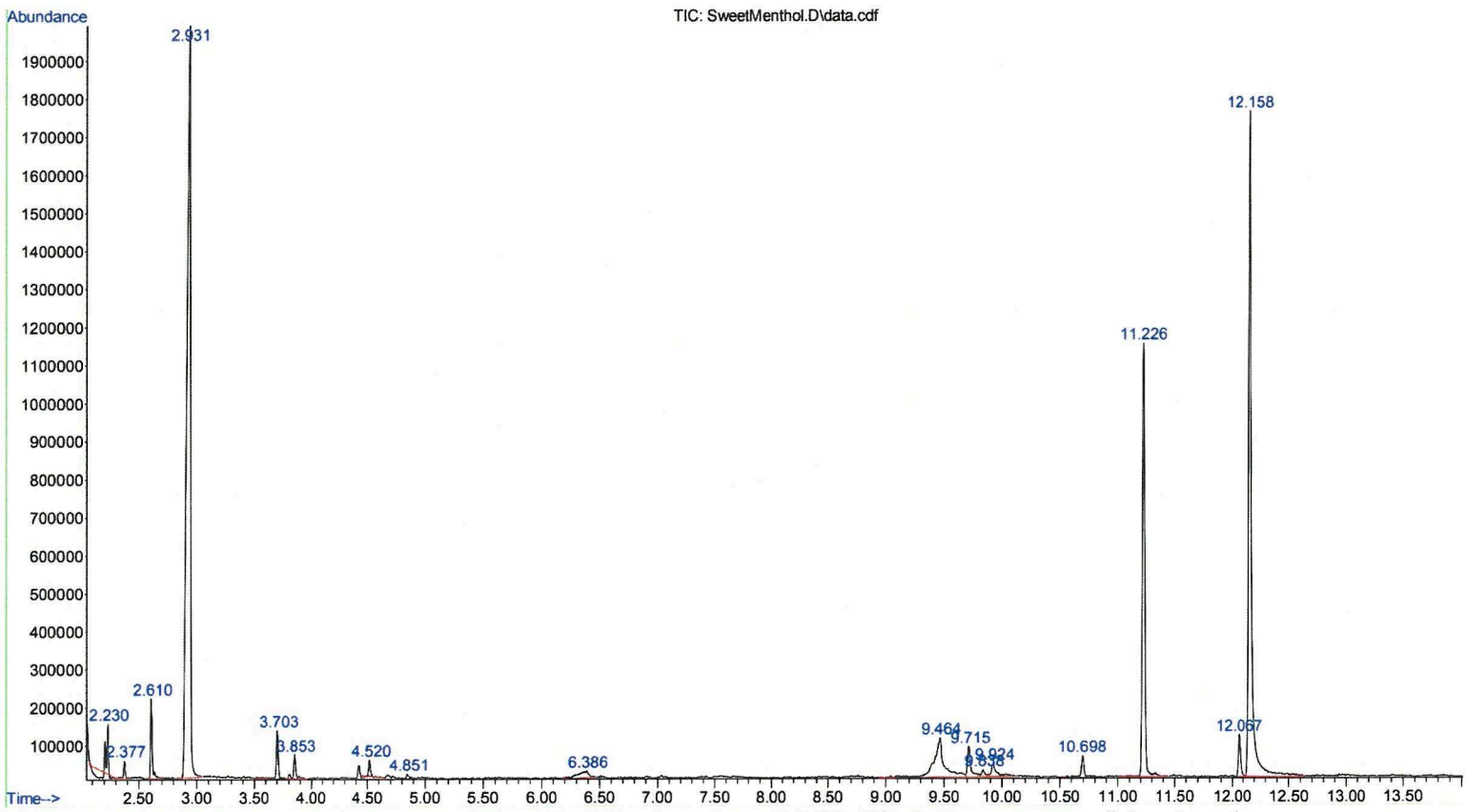


Figure 4: Gas-Chromatography Mass Spectroscopy (GC/MS) chromatogram of the abundance of various compounds as well as their retention times (min). All eight e-liquid chromatograms are scaled to the lowest peak with PG, VG, and nicotine all being the most abundant and having peaks off of chromatogram. These can be found in Appendix A

Table 1: The various compounds found within the Sweet Menthol e-liquid and their retention times. All eight chromatograms were simplified in this way and can be found in Appendix A. The library searches found in Appendix B aided in the creation of all eight tables.

Sweet Menthol	
Retention Time	**Identity**
2.230	2-chloro-2-methyl butane
2.377	3-penten-2-ol
2.611	ethyl propionate
2.931	propylene glycol
3.705	ethyl butyrate
3.852	2-hexanol
4.521	cis-3-hexanol
4.852	isoamyl acetate
6.385	glycerin
9.465	benzoic acid
9.714	menthol
9.839	ethylene glycol
9.924	ethyl maltol
10.697	carvone
11.224	quinoline
12.066	methyl anthranilate
12.159	nicotine

Table 2: Eight compounds from all e-liquid samples that were found to be non-hazardous according to the Occupational Safety and Health Administration (OSHA) in 2012 and their SDS's

Not Hazardous
propylene glycol
glycerin
ethyl propionate
triacetin
isoamyl acetate
diacetin
ethyl caproate
methyl cinnamate

Table 3: 12 compounds from all e-liquid samples that were found to be hazardous according to OSHA 2012. These were found to be flammable and are not toxic to humans or animals according to their SDS's

Hazardous, Flammable
2-chloro-2-methylbutane
tyramine
3-penten-2-ol
glycine
2-methyl butyl acetate
ethyl valerate
ethyl cinnamate
hexyl acetate
methyl(propyl) acetylene
ethyl 2-methylbutyrate
diethyl malonate
methyl beta-phenyl acetate

Table 4: Compounds from all e-liquid samples that were classified as hazardous by OSHA in 2012 and were found to have a negative effect on human health. These are ordered from most to

least toxic according to the LD50 (mg/Kg) for oral toxicity in rats, taken from their SDS's. Those that have dashes were classified as hazardous but did not have a recorded LD50 value.

Hazardous, Toxic	LD50 (mg/Kg)
nicotine	50.0
o-cresol	121.0
allyl hexanoate	218.0
quinoline	262.0
ethylene glycol	500.1
allyl cyclohexyl propionate	600.0
1-hexanol	720.0
benzene ethanol	810.0
ethyl maltol	1150.0
4-(4-hydroxyphenyl)-2-butanone	1320.0
maltol	1410.0
ethyl vanillin	1590.0
butanoic acid	1632.0
benzoic acid	2250.0
carbon tetrachloride	2350.0
2-heptanol	2580.0
ethyl succinate	2710.0
2-ethoxyethanol	2800.0
methyl anthranilate	2910.0
menthol	3300.0
carvone	3710.0
vanillin	3978.0
menthomenthene	4300.0
carvomenthol	4300.0
cis-3-hexanol	4700.0
limonene	5200.0
strawberry aldehyde	5470.0
toluene	5580.0
ethyl butyrate	13000.0
penta chloro aminobenzene	> 2000.0
geranyl propionate	> 5000.0
gamma decalactone	> 5000.0
eicosane	> 5000.0
citronellyl butyrate	> 5000.0
butyl cinnamate	> 5000.0
2, 3-butanediol	> 5000.0
3-methoxy-1-butanol	-
2-hexanol	-
2, 7-dimethyl-quinoline	-
1, 4-hexadiene	-

Treatment of Soil-liquid Dilutions

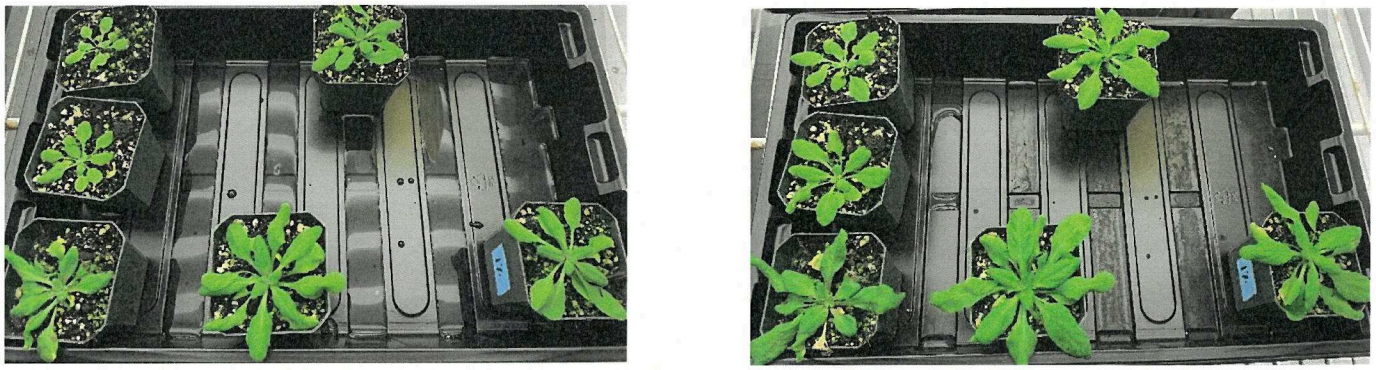
Arabidopsis **Grown Plants with E-**

thaliana plants grown in a Miracle-Gro and perlite mixture were allowed to

germinate and grow for a total of four weeks, being thinned out to 1 plants per pot between two and three weeks of growth. At four weeks, twelve plants were separated into two separate trays. This was to ensure that if there was water runoff from the e-liquid, it would not contaminate other plants. Each tray was dedicated to one e-liquid, one for Sweet Menthol and one for Blue Razz Ice. These flavors were chosen at the time due to obtaining GC/MS chromatograms before all other samples. Three of the plants were systematically treated with 10 mL of varying dilutions of the same e-liquid (i.e., one plant was treated with a 0.5% dilution, another with 0.75% and so on). These volumes of dilution were added to the soil evenly across the surface. The final three plants were all subject to a single-leaf application of the diluted e-liquid, where a healthy leaf was marked with sharpie and between three and five drops were placed on the leaf to dry. The plants were watered as needed over a two-week period as observations were made.

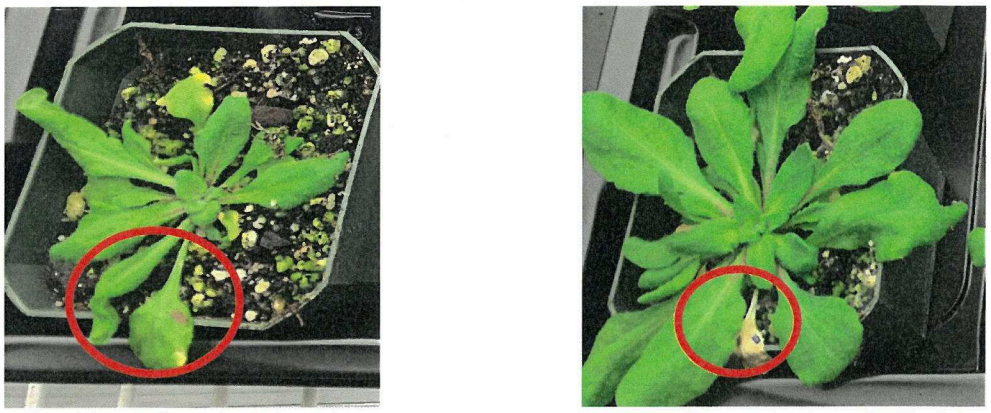
After two weeks, it was assumed that the plants would not show any other potential signs of phenotypic changes outside of what previously occurred and that the diluted e-liquid had run its course. Figure 5 shows the plants after being treated with 10 mL of Sweet Menthol e-liquid dilutions as well as completing the single-leaf treatment. It was observed that, with the systematic application of both Sweet Menthol and Blue Razz Ice there were no outward phenotypic changes due to a stress response throughout the two weeks. However, there was an indication of a stress response with the single-leaf application, as seen in Figure 6. A healthy leaf of one *A. thaliana* plant that was treated with a 1.0% Sweet Menthol dilution withered completely while the rest of the plant remained healthy. Other photos of before and after can be

found in Appendix C1 with comparable results of no phenotypic changes or visible stress responses.



A B

Figure 5: The *A. thaliana* plants after being systematically and single-leaf treated with Sweet Menthol e-liquid dilutions before (A) and after (B) a ten day period. The line of three plants on the left side of both images are those that obtained the single-leaf treatment (front to back: 1.0%, 0.75%, 0.5%). The other plants were those systematically treated with 10 mL of dilutions (left to right: 0.5%, 0.75%, 1.0%)



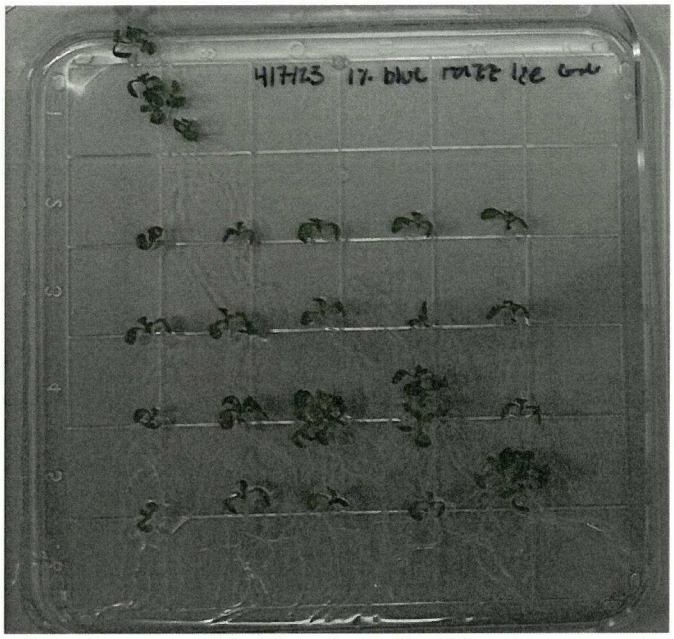
A B

Figure 6: An *A. thaliana* plant subjected to a single-leaf treatment of a 1.0% Sweet Menthol dilution, on the circled leaf with the black mark. After 10 days, the singular leaf completely withered while the rest of the plant continued to flourish under normal conditions

Treatment of Agar-Grown Seedlings with E-liquid Dilutions

Arabidopsis thaliana plants grown within plant agar were allowed to germinate for seven days before being treated with 10 μL of the varying dilutions (0.5%, 0.75%, and 1.0%) of Sweet Menthol and 0.75% and 1.0% dilutions of Blue Razz Ice. Each individual seedling was directly treated with the 10 μL dosage and was allowed to absorb it all before being placed back within the growth chamber. Observations took place over the following week. During this first trial, no phenotypic changes or negative stress responses were observed as seen in Figure 7 and Appendix C2. The only change that was seen was mold within the 0.5% Sweet Menthol plate over time (Figure 8), which elicited a negative stress response, excluding the data from the first trial.

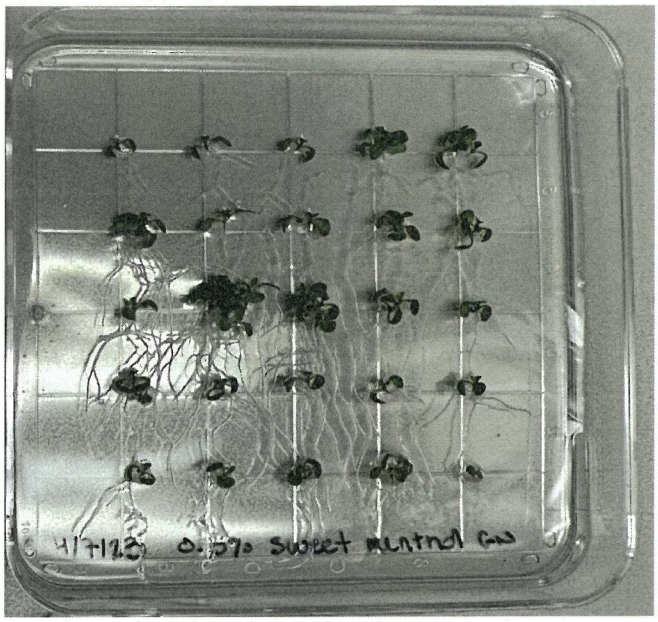
The next trial subjected seedlings to 20 μL of the 1.0% dilution and the neat e-liquid for the following flavors: Sweet Menthol, Blue Razz Ice, Lemon Mint, Sour Candy, and Tropical Rainbow Blast. Once treated, the seedlings were placed back into the growth chamber and were observed for a week. Those treated with the 1.0% dilution had no apparent stress response as seen in Figure 9 and Appendix C3. However, the plants treated with the neat e-liquid died within a 24-hour period after treatment, as seen in both Figure 10 and Appendix C4.



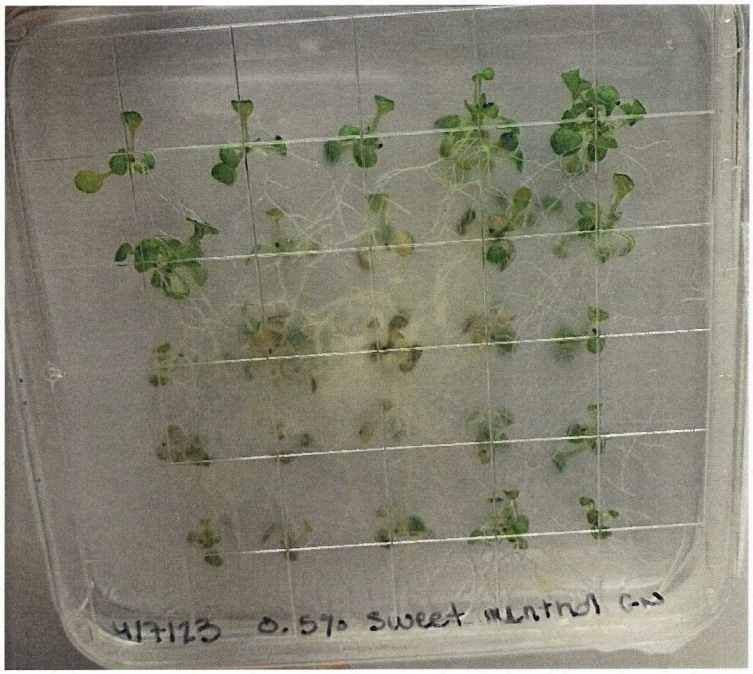
A

B

Figure 7: Before (A) and after (B) adding 10 µL of Blue Razz Ice e-liquid at a 1.0% dilution and allowing one week for germination. No negative phenotypic changes or stress responses were observed

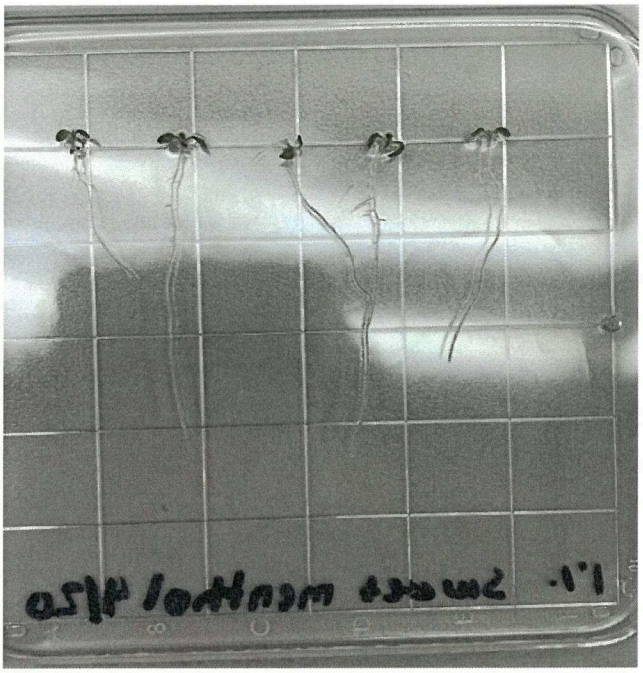


A

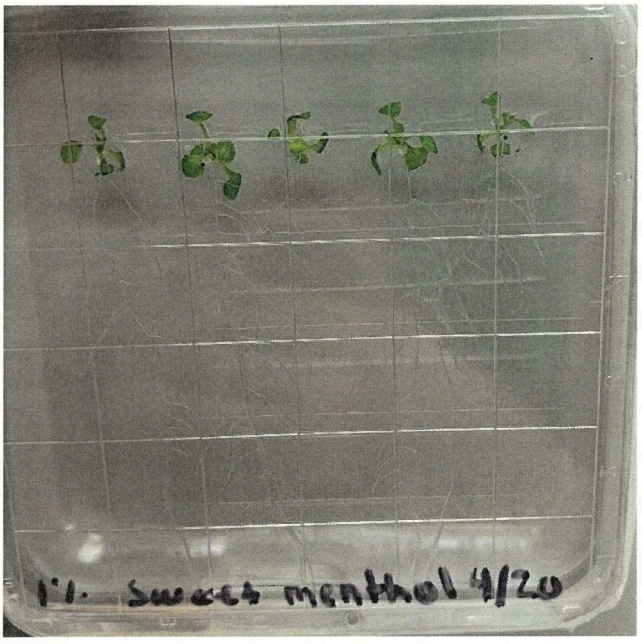


B

Figure 8: Before (A) and after (B) images of *A. thaliana* exposed to 10 µL of 0.5% Sweet Menthol dilution and allowing one week for germination. A negative stress response was seen in the plants, but is due to mold that formed, excluding the results



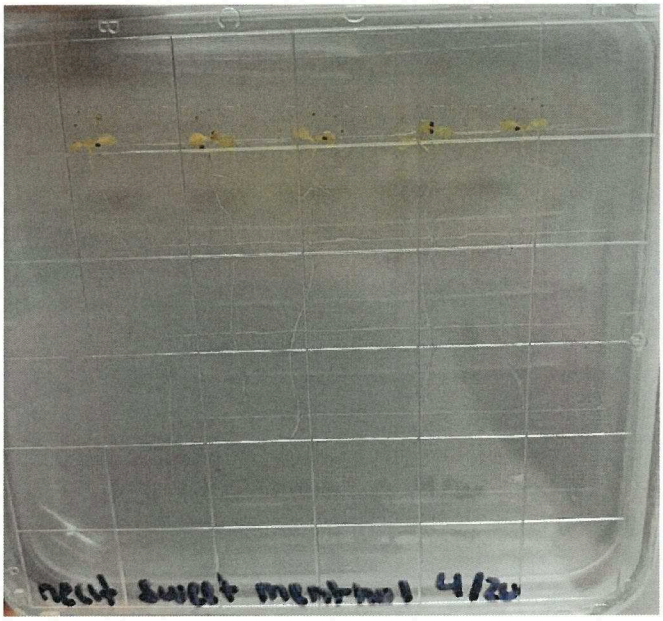
A



B

Figure 9: Before (A) and after (B) adding 20 µL of Sweet Menthol e-liquid at a 1.0% dilution and allowing one week for germination. No negative phenotypic changes or stress responses were observed

A



B

Figure 10: Before (A) and after (B) adding 20 µL of neat Sweet Menthol. Plant death occurred within a 24-hour period, as shown by bleaching and growth stopping

Discussion

Analysis of Chemical Compounds in E-liquid Samples

A qualitative chemical analysis was completed for eight different Elf Bar e-liquids: Sweet Menthol, Blue Razz Ice, Lemon Mint, Grape Energy, Sour Candy, Tropical Rainbow Blast, and Kiwi Passionfruit Guava. In the process to gain a full understanding of chemical compounds within each e-liquid, the use of FTIR, H^1 NMR, and GC/MS instrumentation were utilized in order to gain a full understanding of the chemical compounds within each e-liquid. However, as seen in Figures 2 and 3, FTIR and H^1 NMR spectra showed extraordinarily little, if any, differences between the eight e-liquid samples. FTIR interferogram in Figure 2 shows almost no differentiation between any of the peaks. In the H^1 NMR spectra in Figure 3, besides the extra peaks in Watermelon Ice, Lemon Mint, Grape Energy, and Sweet Menthol between 5.0 and 5.5 ppm, the only differentiation appears to be in the intensity of the signals recorded. These intensities, while they could be indicative of varying amounts of certain functional groups within the sample, could also be a result of the changing environment around the instrument as it is sensitive to things such as vibrations. The subtle variation in results for both instrumentation could also have been due to their detection limits and the concentrations of compounds within the samples; they just may not have been able to properly detect them due to a higher limit of detection (LOD). Overall, the FTIR and H^1 NMR data were unable to be used properly in the identification of the chemical compounds within the samples, leading to the use of GC/MS.

In comparison, the GC/MS chromatograms for all eight e-liquid samples were extraordinarily accurate and able to pick up a multitude of chemical compounds within each sample, as seen in Figure 4 and Appendix A. Between all of the samples there were 11 consistent chemical compounds which can be assumed to be the base vehicle of the e-liquid. These

compounds were 2-chloro-methyl butane, 3-penten-2-ol, propylene glycol, ethyl butyrate, 2-hexanol, cis-3-hexanol, glycerin, benzoic acid, ethyl maltol, quinoline, and nicotine. Along with these constants, each e-liquid sample also had their own unique peaks, ranging from about six to 13 of these, as well as a total of nine unknown compounds between all eight samples. As the various chromatograms and corresponding library searches (Appendix B) as well as Table 1 and Appendix A can be difficult to decipher, Tables 2-4 were created to garner a better understanding of the data collected.

Tables 2-4 give a representation of all known compounds from across the eight separate e-liquid samples, and their potential effects on organisms around them (as found within their SDS's). Table 2 shows that, of the 60 total known compounds within the samples, only eight pose no hazards, as classified by OSHA in 2012. Table 3 shows the 12 compounds that, while labelled as hazardous by OSHA 2012, are only flammable and have no known side effects on humans or animals. Finally, Table 4 contains the most interesting and dangerous of the compounds. 40 out of the 60 compounds (67%) were classified as hazardous by OSHA 2012 and also have negative, and in many cases severe, toxicological side effects of humans and animals. These potential hazards include respiratory and cardiovascular irritation if inhaled, severe skin and eye damage, reproductive system damage, and specific targeted organ toxicity (both acute and chronic) just to name a few. The LD50 for the oral toxicity of rats were found for all of these compounds and were listed from the most toxic to the least toxic in Table 4, placing compounds with unknown LD50 values at the bottom of the table.

When looking at the LD50 for oral toxicity in rats, a surprising number (top 9) indicate that, to kill 50% of the subjects, they would need to ingest less than 1 gram of the compound. These values are much different than an LD50 for humans, however. In the case of humans,

compounds like nicotine and menthol, the first of which is within this top nine most hazardous, have an LD50 of 0.5-1.0 mg/Kg and 50-500 mg/Kg, respectively. This means that, for an average human weighing around 60 Kg, between 30-60 mg of nicotine would be toxic and around 0.83-8.33 mg of menthol would cause toxicity in humans. These compounds, while tested for oral toxicity in rats and in some cases known to have negative effects on humans, have yet to be tested on plants either in a broad sense (such as e-liquid introduction) or specifically (individual chemical compound introduction). However it can be assumed that those compounds that have an especially high LD50 in Table 4 would also have some detrimental effect on other organisms within the environment.

Arabidopsis thaliana **and Response to E-liquids**

When e-cigarettes are littered, there is a potential that e-liquid is able to seep out of the shell and interact with the environment around them. This could be an interaction between organisms and neat e-liquid, or a dilution of the e-liquid due to rain and various water runoff. Currently, there are no studies looking into these interactions and the effect that the e-liquid may have on the surrounding environment. However, there is one study that completed high performance assays on human cells using e-liquid.[9] It was found that low dilutions of e-liquids (1.0% and below) had a cytotoxic effect on these human cells within a 24 hour period, resulting in major cell death with various e-liquid flavors.[9] While this was done on human cells, it can be assumed that e-liquids would also have a negative impact on the environment. The research that has been outlined and performed in this paper was aimed to not only analyze the chemical compounds of various e-liquids, but to also observe how different flavors might cause phenotypic stress in plants from both diluted and neat e-liquid introduction.

Throughout experimentation, *A. thaliana* was grown in both soil and plant agar and treated with either dilutions or neat e-liquids. The plants in soil were treated with 10 mL of e-liquid dilutions (0.5%, 0.75%, and 1.0%), specifically the Sweet Menthol and Blue Razz Ice e-liquids. In plant agar, the first trial of plants were treated with 10 μL of e-liquid dilutions, 0.5-1.0% of Sweet Menthol and 0.75-1.0% of Blue Razz Ice, where it was allowed to absorb into the agar and left to grow. In the second trial, agar seedling were treated with 20 μL of both 1.0% and neat e-liquids of Sweet Menthol, Blue Razz Ice, Lemon Mint, Sour Candy, and Tropical Rainbow Blast.

In both the soil and plant agar experiments, when systematic treatment with any amount of any e-liquid dilutions was performed, there were no phenotypic stress responses exhibited by the *A. thalaiana* over the course of one to two weeks. The single-leaf treatments of the plants also exhibited little to no stress response save for one leaf as seen in Figure 6. In this case the leaf treated with 1.0% Sweet Menthol dilution completely withered and showed bleaching (loss of leaf color) while the rest of the plant flourished. The systematic treatment of dilutions on the seedlings grown in agar also exhibited no stress response to the treatment. However, when treated with a small amount of the neat e-liquid (20 μL) the seedlings exhibited extreme stress responses within a 24 hour period that included bleaching and complete death. Though the previous studies with human cells showed cell death at these dilutions (0.5%, 0.75%, and 1.0%), they did not cause phenotypic stress responses in with mature or seedling *A. thaliana* plants, while neat e-liquids did. Due to these results it cannot be determined whether different e-liquid flavoring compounds have differing toxic effect, but only that neat e-liquids will have a generalized toxic effect on seedlings.

Future Aims

The study performed was a very broad and introductory assessment of how e-liquids might be chemically analyzed and how these e-liquids may affect both mature and germinating *A. thalaiana* plants. In order to truly understand the negative environmental effects that may occur, specific concentration thresholds for the survival versus death of seedlings for the e-liquids must be determined. Once this is determined, different e-liquid samples should be diluted to slightly above and below this threshold in order to identify potential differential effects of flavoring compounds on plant growth. This would also allow for observation of how they impact seed germination, using a control plate with water rather than an e-liquid dilution.

From there, individual chemical compounds can be isolated from all e-liquid samples and quantified using instrumentation such as GC/MS to understand how much of each component is present within e-liquids. These could then be individually tested on seedlings grown in plant agar to observe the stress response to individual compounds. Plant agar would be used for clear observation of root response to induced stress, as well as growth, germination, and leaf color responses. This will aid in the determination of what compounds are toxic to plants and whether it is mainly the vehicle or the unique chemical compounds found throughout the e-liquid samples. These results may eventually be used to alter the chemical composition of e-liquids to make them safer for both human health and the environment.

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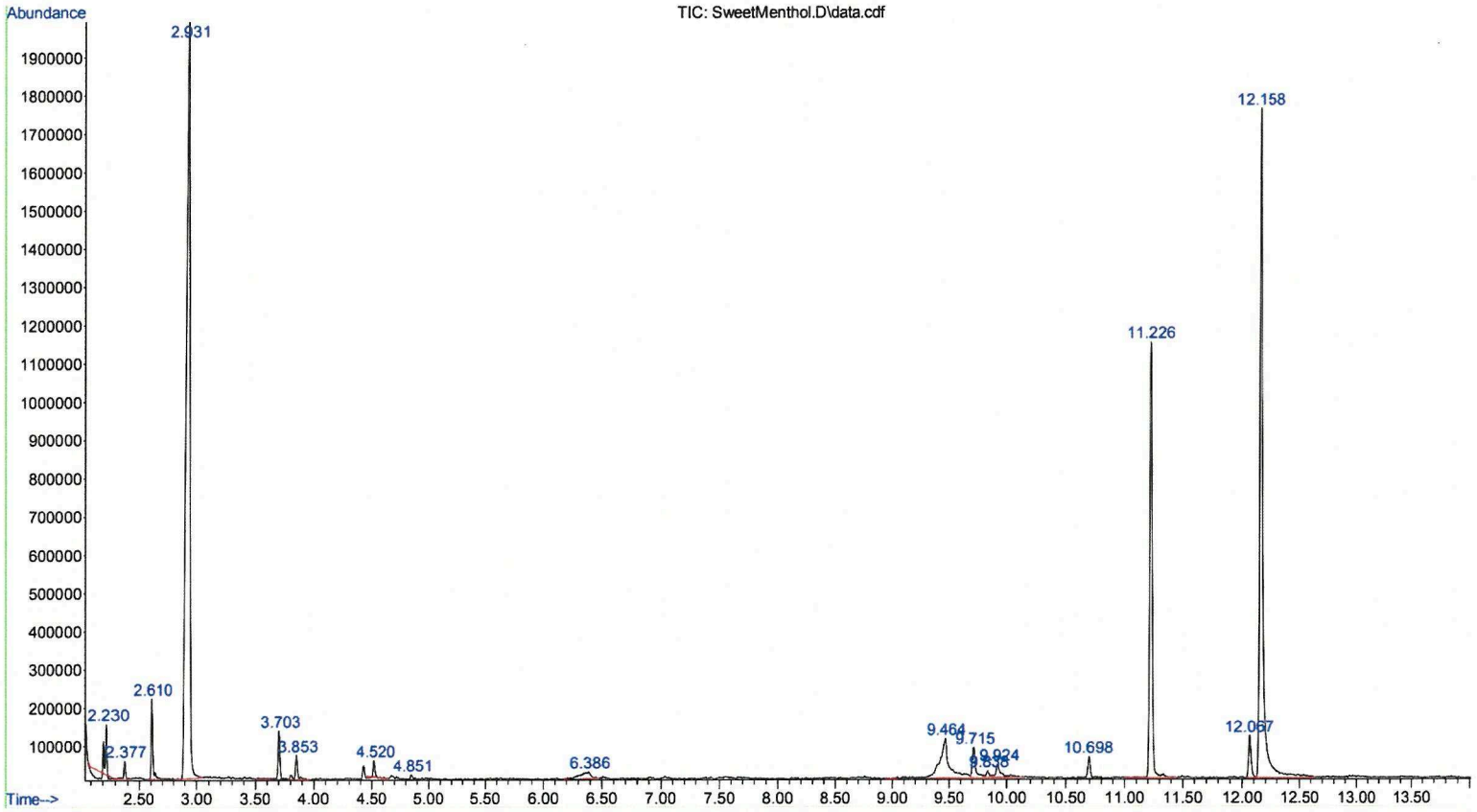
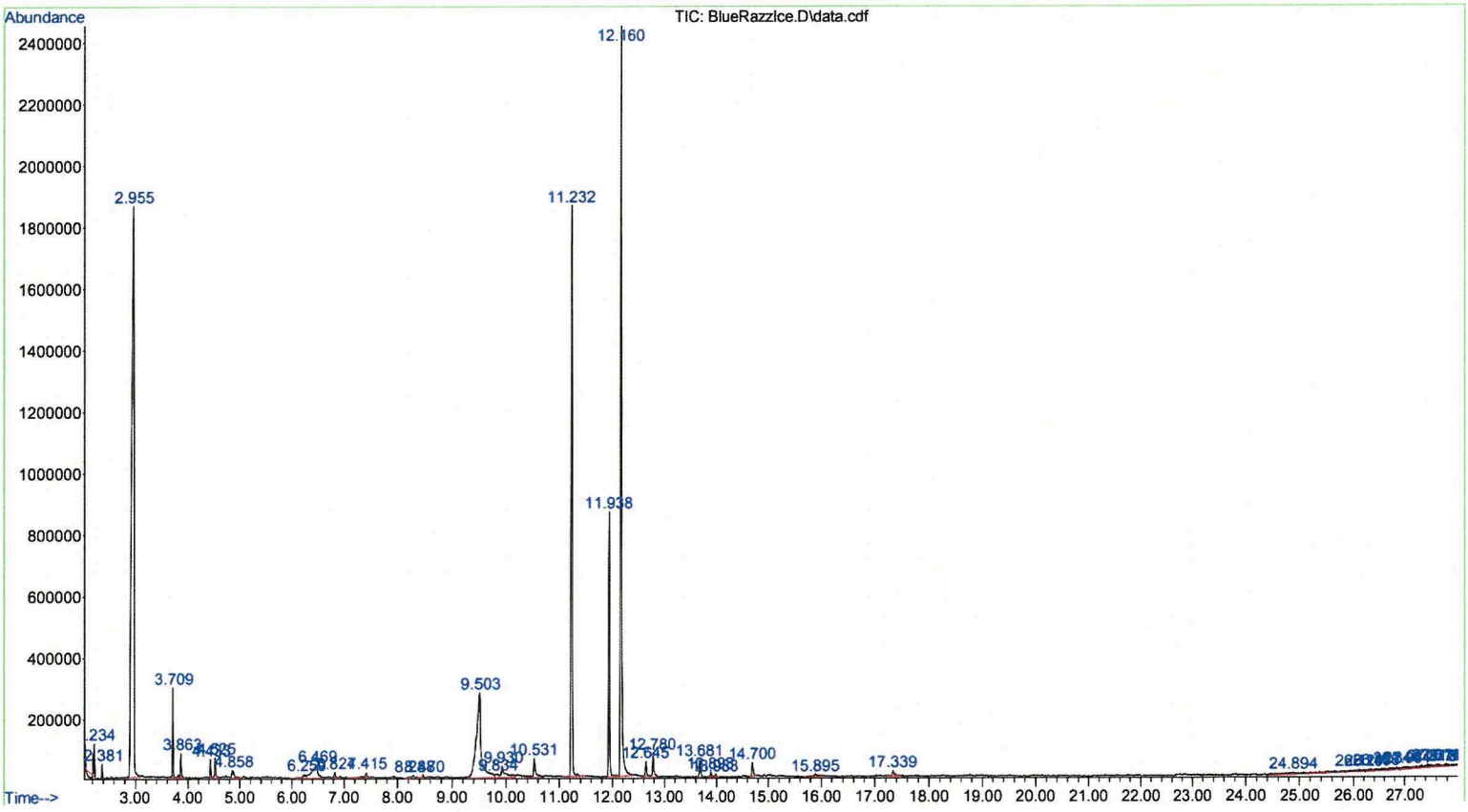
Appendix A: GC/MS Chromatograms Scaled to Smallest Peak and Chemical Compounds

A1: Sweet Menthol chromatogram and corresponding table of chemical compounds



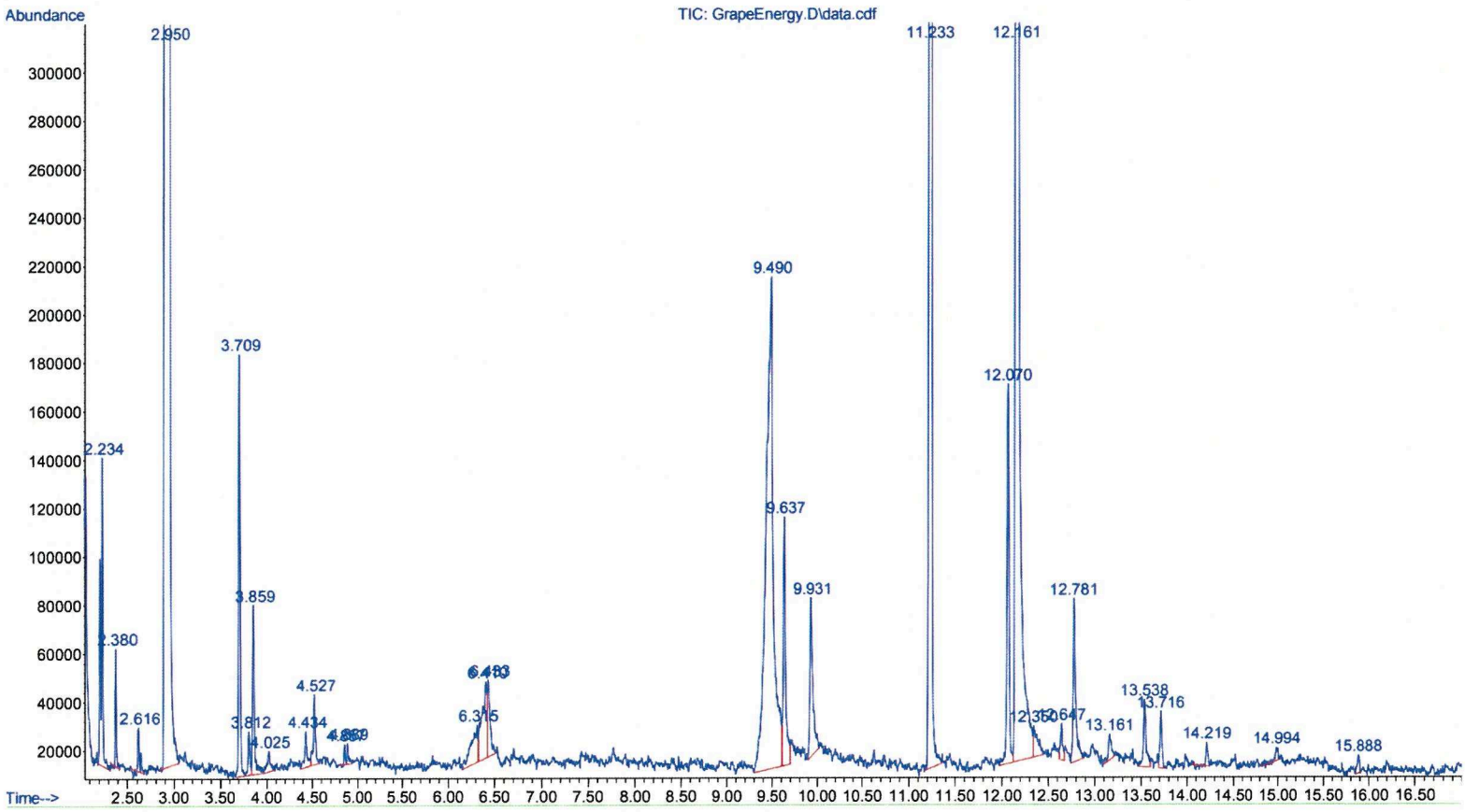
Sweet Menthol	
Retention Time	**Identity**
2.230	2-chloro-2-methyl butane
2.377	3-penten-2-ol
2.611	ethyl propionate
2.931	propylene glycol
3.705	ethyl butyrate
3.852	2-hexanol
4.521	cis-3-hexanol
4.852	isoamyl acetate
6.385	glycerin
9.465	benzoic acid
9.714	menthol
9.839	ethylene glycol
9.924	ethyl maltol
10.697	carvone
11.224	quinoline
12.066	methyl anthranilate
12.159	nicotine

A2: Blue Razz Ice chromatogram and corresponding table of chemical compounds



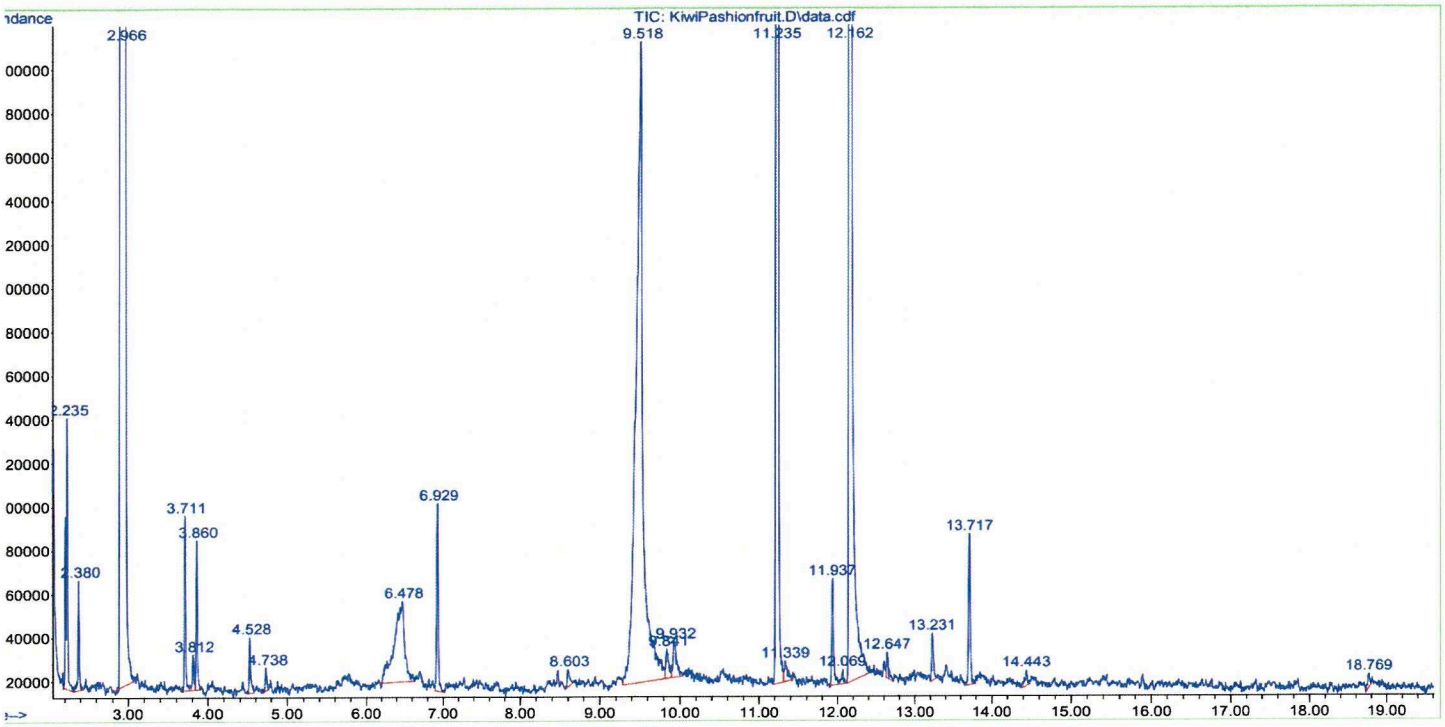
Blue Razz Ice	
Retention Time	**Identity**
2.234	2-chloro-2-methyl butane
2.382	3-penten-2-ol
2.954	propylene glycol
3.708	ethyl butyrate
3.863	2-hexanol
4.526	cis-3-hexanol
4.858	isoamyl acetate
6.470	glycerin
6.824	ethyl caproate
7.414	o-cresol
9.502	benzoic acid
9.833	ethylene glycol
9.929	ethyl maltol
10.530	diacetin
11.233	quinoline
11.938	triacetin
12.159	nicotine
12.647	methyl cinnamate
12.780	vanillin
13.681	gamma decalactone
13.893	unknown 1
14.701	4-(4-hydroxyphenyl)-2-butanone
15.897	unknown 2
17.339	unknown 3

A3: Grape Energy chromatogram and corresponding table of chemical compounds



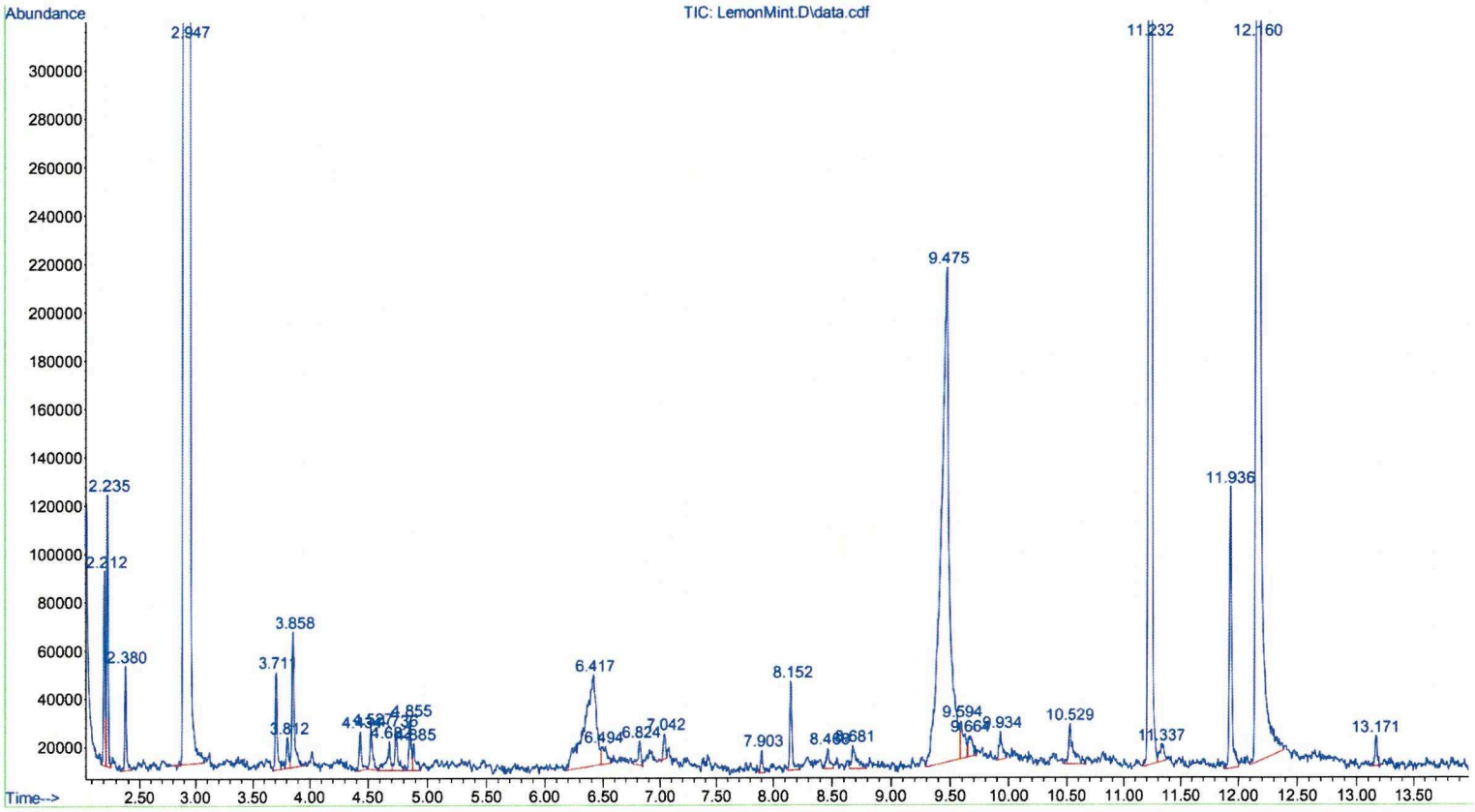
Grape Energy	
Retention Time	**Identity**
2.234	2-chloro-2-methyl butane
2.379	3-penten-2-ol
2.617	ethyl propionate
2.948	propylene glycol
3.710	ethyl butyrate
3.812	3-methoxy-1-butanol
3.858	2-hexanol
4.025	eicosane
4.436	tyramine
4.526	cis-3-hexanol
4.858	isoamyl acetate
4.889	2-methyl butyl acetate
6.433	glycerin
9.490	benzoic acid
9.638	ethyl succinate
9.932	ethyl maltol
11.233	quinoline
12.069	methyl anthranilate
12.162	nicotine
12.647	methyl cinnamate
12.783	vanillan
13.160	methyl beta-phenyl acetate
13.539	ethyl vanillan
13.718	ethyl cinnamate
14.219	butyl cinnamate
14.993	unknown 8
15.888	2, 7-dimethyl-quinoline

A4: Kiwi Passionfruit Guava chromatogram and corresponding table of chemical compounds



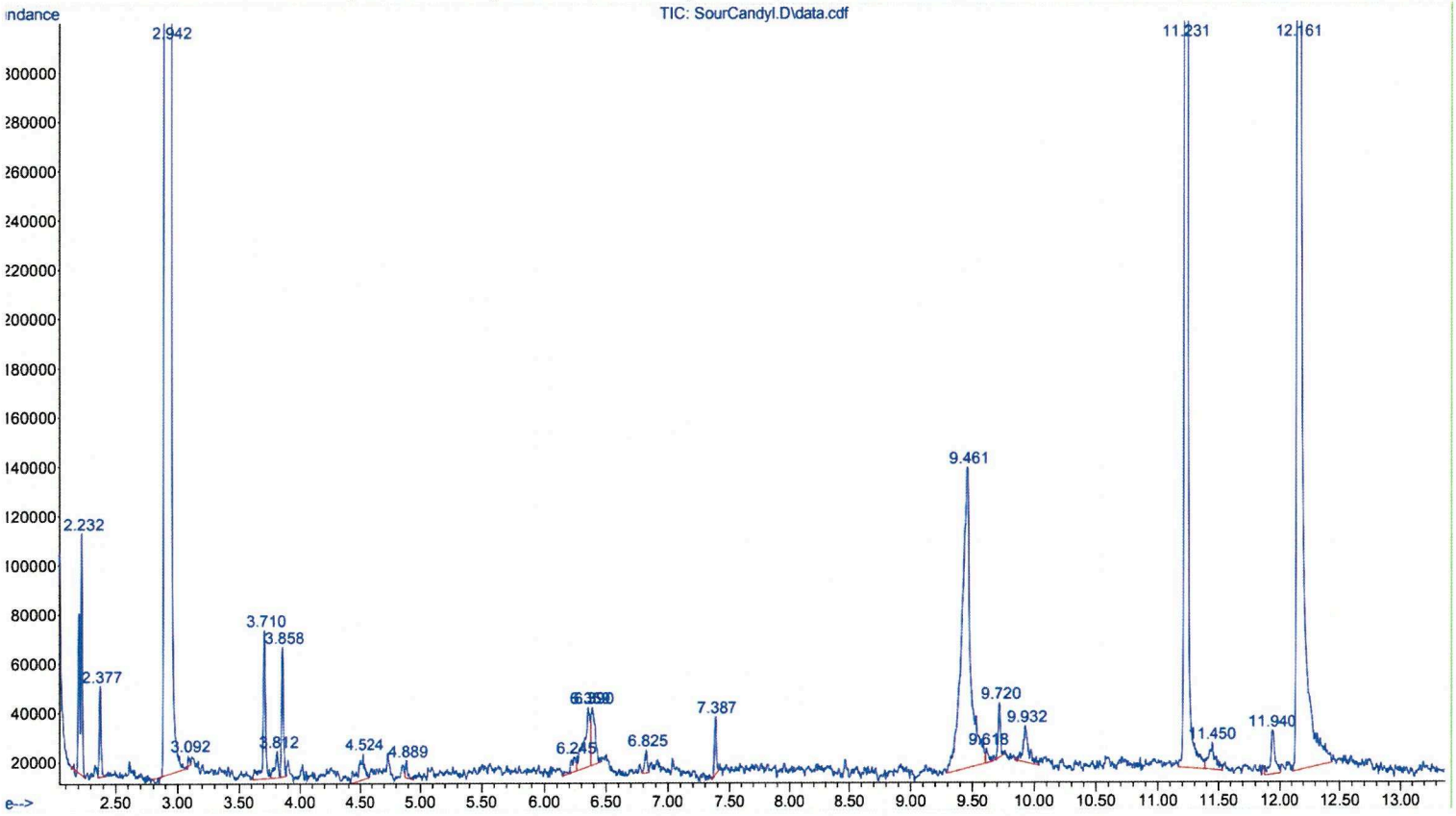
Kiwi Passionfruit Guava	
Retention Time	**Identity**
2.234	2-chloro-2-methyl butane
2.379	3-penten-2-ol
2.965	propylene glycol
3.710	ethyl butyrate
3.812	3-methoxy-1-butanol
3.861	2-hexanol
4.529	cis-3-hexanol
4.739	1-hexanol
6.478	glycerin
6.929	1, 4-hexadiene
8.604	maltol
9.519	benzoic acid
9.932	ethyl maltol
11.236	quinoline
11.340	carvomenthol
11.938	triacetin
12.069	methyl anthranilate
12.162	nicotine
12.647	methyl cinnamate
13.230	strawberry aldehyde
13.718	ethyl cinnamate
14.443	penta chloro aminobenzene

A5: Lemon Mint chromatogram and corresponding table of chemical compounds



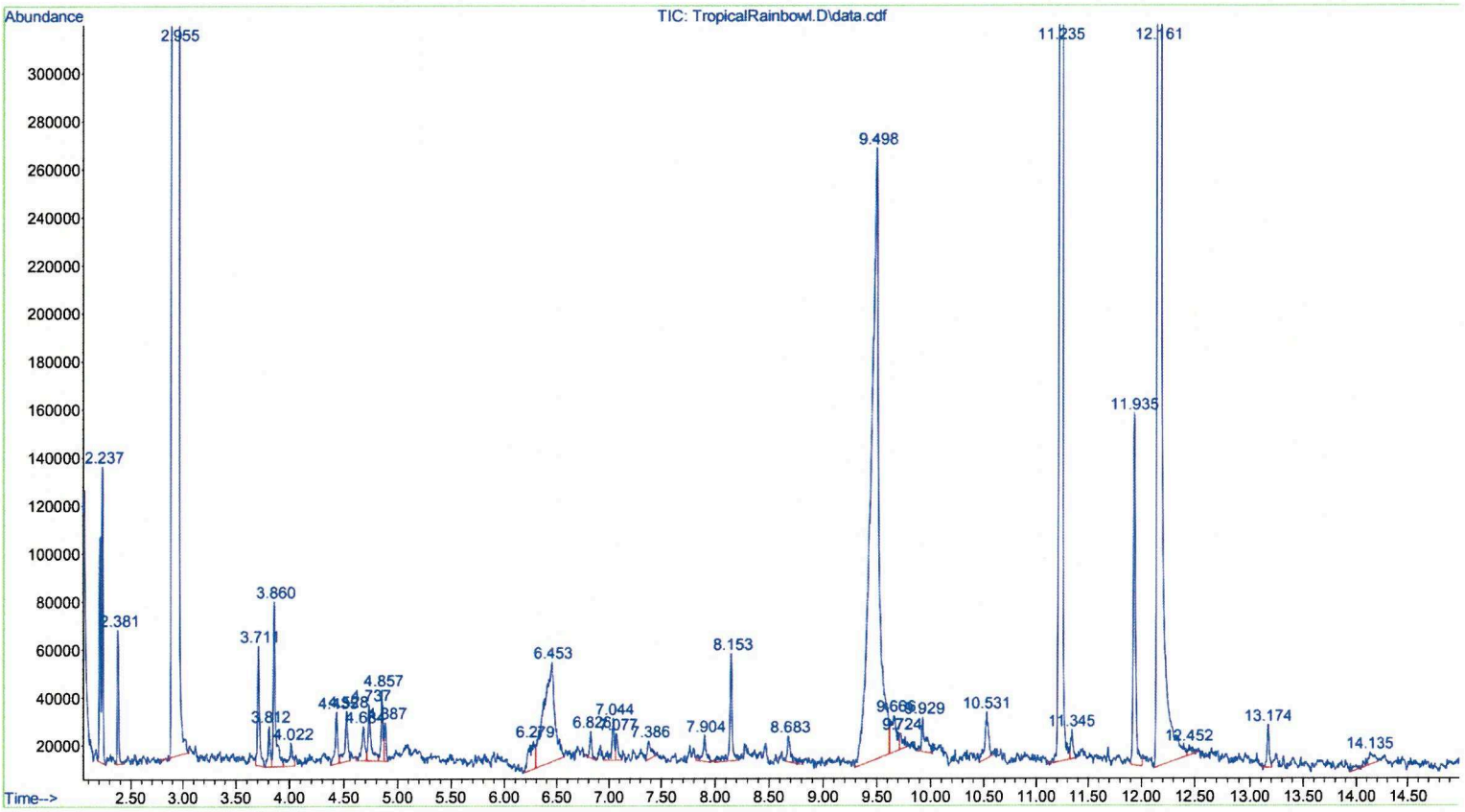
Lemon Mint	
Retention Time	**Identity**
2.212	carbon tetrachloride
2.234	2-chloro-2-methyl butane
2.382	3-penten-2-ol
2.948	propylene glycol
3.710	ethyl butyrate
3.812	3-methoxy-1-butanol
3.858	2-hexanol
4.433	ethyl 2-methyl-butyrate
4.526	cis-3-hexanol
4.682	unknown 5
4.736	1-hexanol
4.855	isoamyl acetate
4.866	2-heptanol
6.416	glycerin
6.824	ethyl valerate
7.042	hexyl acetate
7.904	diethyl malonate
8.153	allyl hexanoate
8.467	unknown 9
8.680	toluene
9.476	benzoic acid
9.935	ethyl maltol
10.530	glycine
11.233	quinoline
11.338	carvomenthol
11.935	triacetin
12.159	nicotine
13.171	allyl cyclohexyl propionate

A6: Sour Candy chromatogram and corresponding table of chemical compounds



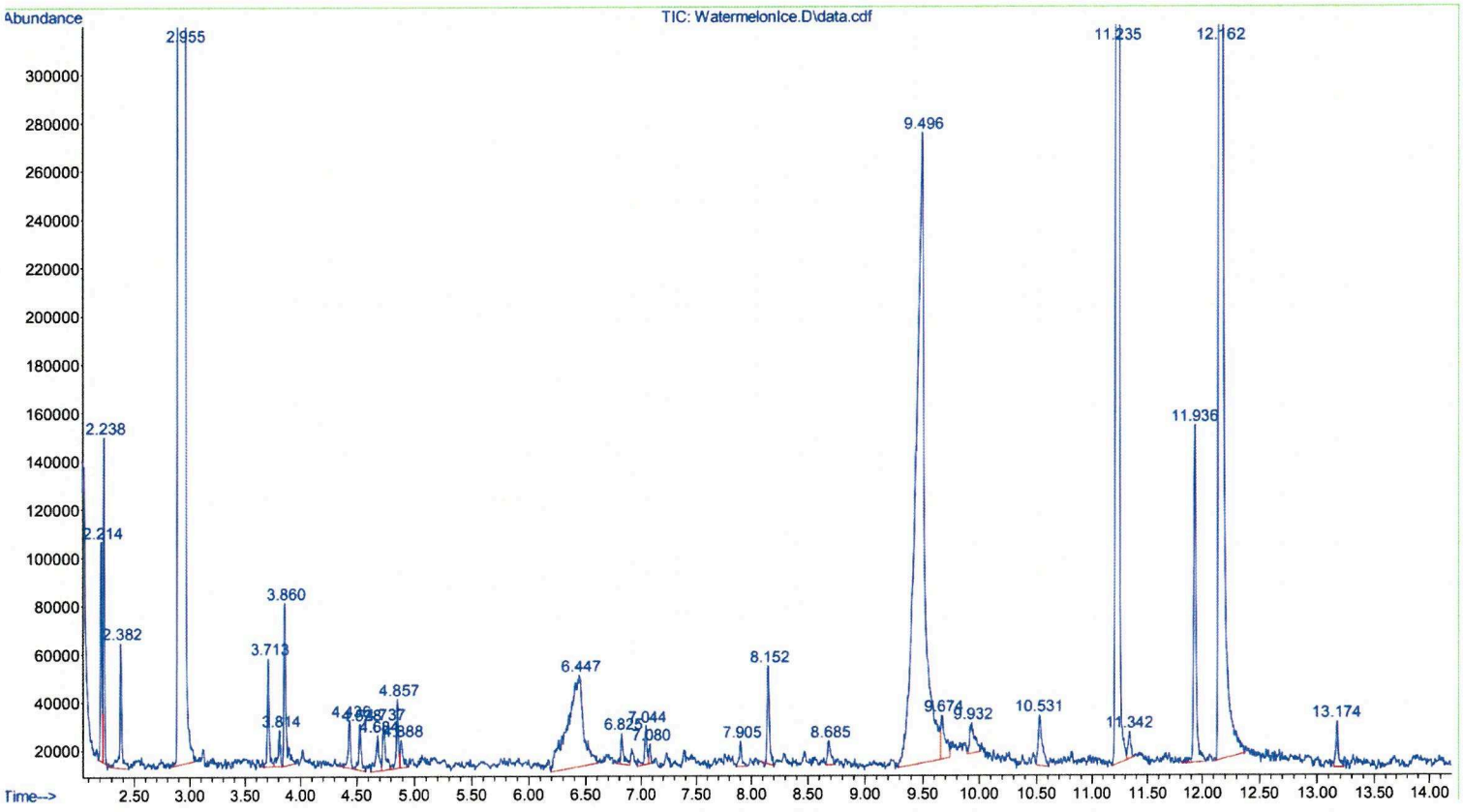
Sour Candy	
Retention Time	**Identity**
2.231	2-chloro-2-methyl butane
2.379	3-penten-2-ol
2.943	propylene glycol
3.093	2, 3-butanediol
3.710	ethyl butyrate
3.812	3-methoxy-1-butanol
3.858	2-hexanol
4.524	cis-3-hexanol
4.889	2-ethoxyethanol
6.391	glycerin
6.824	ethyl caproate
7.388	limonene
9.462	benzoic acid
9.720	menthol
9.932	ethyl maltol
11.230	quinoline
11.451	unknown 4
11.941	triacetin
12.162	nicotine

A7: Tropical Rainbow Blast chromatogram and corresponding table of chemical compounds



Tropical Rainbow Blast	
Retention Time	**Identity**
2.237	2-chloro-2-methyl butane
2.382	3-penten-2-ol
2.952	propylene glycol
3.710	ethyl butyrate
3.812	3-methoxy-1-butanol
3.861	2-hexanol
4.022	eicosane
4.360	tyramine
4.529	cis-3-hexanol
4.685	unknown 5
4.736	1-hexanol
4.858	isoamyl acetate
4.886	2-methyl butyl acetate
6.453	glycerin
6.824	ethyl valerate
7.045	hexyl acetate
7.076	methyl(propyl) acetylene
7.385	geranyl propionate
8.153	allyl hexanoate
8.683	benzene ethanol
9.499	benzoic acid
9.929	ethyl maltol
10.530	uknown 6
11.236	quinoline
11.346	menthomenthene
11.935	triacetin
12.162	nicotine
12.451	unknown 7
13.174	allyl cyclohexyl propionate
14.134	butanoic acid

A8: Watermelon Ice chromatogram and corresponding table of chemical compounds



Watermelon Ice	
Retention Time	**Identity**
2.214	carbon tetrachloride
2.237	2-chloro-2-methyl butane
2.382	3-penten-2-ol
2.957	propylene glycol
3.713	ethyl butyrate
3.815	3-methoxy-1-butanol
3.861	2-hexanol
4.436	ethyl 2-methyl-butyrate
4.529	cis-3-hexanol
4.685	unknown 5
4.736	1-hexanol
4.858	isoamyl acetate
4.889	2-methyl butyl acetate
6.447	glycerin
6.824	ethyl valerate
7.079	hexyl acetate
7.904	diethyl malonate
8.153	allyl hexanoate
8.686	toluene
9.496	benzoic acid
9.932	ethyl maltol
10.530	glycine
11.236	quinoline
11.340	citronellyl butyrate
11.935	triacetin
12.162	nicotine
13.174	allyl cyclohexyl propionate

Appendix B: GC/MS Library Search Raw Data

B1: Sweet Menthol Library Search

Data Path : D:\CDF file conversions\
Data File : SweetMenthol.D Acq On :
20230331154620+0000
Operator : Admin
Sample : 1% in CHCl3
Misc : 1% in CHCl3
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1
Search Libraries: C:\Database\Flavor2.L Minimum Quality: 55
C:\Database\WILEY275.L Minimum Quality: 55
C:\Database\demo.l
Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.231	0.53	C:\Database\demo.l	No matches found		
2	2.376	0.42	C:\Database\WILEY275.L			
			3-Penten-2-ol (CAS) $$ 2-PENTEN-4-	3386	001569-50-2	72
			OL $$ Methyl propenyl carbinol $$			
			.alpha.,.gamma.-Dimethylallyl alco		hol $$ PENT-3-EN-	
			2-OL $$ 3-Penten	2-ol,cis+trans		
			3-Penten-2-ol (CAS) $$ 2-PENTEN-4-	3385	001569-50-2	72
			OL $$ Methyl propenyl carbinol $$			
			.alpha.,.gamma.-Dimethylallyl alco		hol $$ PENT-3-EN-	
			2-OL $$ 3-Penten	2-ol,cis+trans		
			3-Penten-2-ol (CAS) $$ 2-PENTEN-4-	3381	001569-50-2	72
			OL $$ Methyl propenyl carbinol $$			
			.alpha.,.gamma.-Dimethylallyl alco		hol $$ PENT-3-EN-	
			2-OL $$ 3-Penten	2-ol,cis+trans		
3	2.611	1.92	C:\Database\Flavor2.L			
			Ethyl propionate	287	000105-37-3	56
			isobutyl alcohol			
62	000078-83-1	3	Isobutylpropionate	130	000540-42-1	2
4	2.931	35.64	C:\Database\WILEY275.L			
			1,2-Propanediol (CAS) $$ Propylene	2014	000057-55-6	78
			glycol $$			
PG 12 $$ 1,2-PROPANDIOL			$$ Sirlene $$ 2,3-Propanediol $$			2-
Hydroxypropanol $$ Methylethyl g			lycol $$ Methyl glycol $$ Monoprop			
ylene glycol $$ 1,2-Propylene glyc			ol $$ 1,2-Dihydroxypropane $$ Meth			
			ylethylene glycol			
			PROPYLENE GLYCOL $$ 1,2-PROPANEDIO	2035	000057-55-6	78
			L $$ 1,2-DIHYDROXYPROPANE			

2-Propanol (CAS) $$ Isopropyl alco 741 000067-63-0 9 hol $$ PRO
$$ propan-2-ol $$ Isoho l $$ Propol $$ Lutosol $$ Alcojel $$ Avantin
$$ Imsol A $$ Petrohol $$ Hartosol $$ Avantine $$ Takineo col $$ i-
Propanol $$ Isopropanol $ $ Alcosolve 2 $$ Isopropenol $$ Co mbi-
Schutz $$ Iso

5 3.705 1.33 C:\Database\WILEY275.L
ETHYL BUTANOATE $$ ETHYL BUTYRATE 13265 000105-54-4 94
ETHYLBUTANOATE 13286 000000-00-0 91
Butanoic acid, ethyl ester (CAS) $ 13025 000105-54-4 91
$ Ethyl butyrate $$ Butyric acid e thyl ester
$$ Butyric ether $$ Eth yl butanoate $$ Ethyl n-
butyrate $ $ Butyric acid, ethyl ester $$ Eth
yl ester of butanoic acid $$ Ethyl n-butanoate $$ n-
Butyric acid eth yl ester $$ Butyr

6 3.852 0.83 C:\Database\WILEY275.L
2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7750 000626-93-7 64
$$ n-Butylmethylcarbinol $$ Hexan ol-(2) $$ sec-
Hexyl alcohol
Ethene, 1,1'-[oxybis(2,1-ethanediy 43676 000764-99-8 56 loxy)]bis-
(CAS) $$ BIS(2-VINYLOXY ETHYL) ETHER $$ Divinylcarbitol $$
Bis[2-(vinyloxy)ethyl] ether $$ E ther, bis[2-(vinyloxy)ethyl] $$ 3,
6,9-Trioxaundeca-1,10-diene $$ Die thylene glycol divinyl ether $$ Di
vinyl ether dieth
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7804 000108-11-2 50
ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta nol $$
Isobutylmethylmethanol $$ I sobutylmethylcarbinol $$
Methyliso butyl carbinol $$ 4-Methyl-2-penty
l alcohol $$ 1,3-Dimethyl-1-butano l $$ 4-methyl 2-p

7 4.521 0.32 C:\Database\WILEY275.L
1,3-Pentadiene, 2-methyl- (CAS) $$ 2430 001118-58-7 72
2-Methyl-1,3-pentadiene $$ 1,3-Di methyl-1,3-
butadiene $$ 2,4-Dimeth yl-1,3-butadiene $$
CH2=C(CH3)CH=C HCH3 $$ 2-Methyl-1,3-
pentadiene,c&
C2H5CH=CHCH=CH2 $$ 1,3-Hexadiene,c 2495 000592-48-3 72
&t $$ 1,3-Hexadiene $$ 1,3-Hexadie ne cis +
trans $$ 1,3-Hexadiene(c,
t)
Cyclohexene (CAS) $$ Cyclohex-1-en 2479 000110-83-8 72 e $$
Cyclohexene ring $$ Tetrahydr obenzene $$ Benzene, tetrahydro- $ $
Benzene tetrahydride $$ 1,2,3,4-
Tetrahydrobenzene $$ Cykloheksen $

$ Hexanaphthylene $$ UN 2256
8 4.852 0.18 C:\Database\WILEY275.L
1-Butanol, 3-methyl-, acetate (CAS 20841 000123-92-2 64
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$
Isopentyl acet ate $$ 3-Methylbutyl acetate $$ 3
Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20838 000123-92-2 64
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$
Isopentyl acet ate $$ 3-Methylbutyl acetate $$ 3
Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20842 000123-92-2 64
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$
Isopentyl acet ate $$ 3-Methylbutyl acetate $$ 3
Methyl-1-butyl ac

9 6.385 0.96 C:\Database\WILEY275.L
Ethanol, 2-amino- (CAS) $$ Ethanol 789 000141-43-5 64 amine $$
MEA $$ ETHANOL-2-AMINE $$ Olamine $$ Colamine $$ Glycinol $
$ Aminoethanol $$ Ethylolamine $$
Thiofaco M-50 $$ 2-Aminoethanol $$
Monoethanolamine $$ 2-Amino-l-eth anol $$ 2-
Aminoethan-1-ol $$ 2-Hyd roxyethylamine $$
2(1H)-PYRIDINONE, 3,5,6-TRICHLORO- 141286 000000-00-0 25
N(METHYLTHIOMETHYL)-
DICHLOROFUROXAN 39108 000000-00-0 9

10 9.465 5.27 C:\Database\Flavor2.L
Benzoic acid 361 000065-85-0 59 2,3,5-Trimethylpyrazine
172 014667-55-1 5 p-Methylanisole 231 000104-93-8 1

11 9.714 1.30 C:\Database\Flavor2.L
L-Menthol 38 002616-51-5 91
Citronellyl butyrate 332 000141-16-2 50 Menthyl acetate;
d,L-methyl-2-(met 377 000089-48-5 43 hylethyl)cyclohexyl acetate

12 9.839 0.29 C:\Database\WILEY275.L
1,2-Ethanediol, 1-(2,3,4,4a,4b,5,6 194469 005940-00-1 56

,7,8,8a,9,10-dodecahydro-7-hydroxy -2,4b,8,8-
tetramethyl-2-phenanthre nyl)-, [2S-[2.alpha.(S*),4a.beta.,
4b.alpha.,7.alpha.,8a.beta.]]- (CA
S) $$ 1,2-Ethanediol, 1-(2,3,4,4a,
4b,5,6,7,8,8a,9,10-dodecahydro-7-h ydroxy-2,4b,8,8-t
Benzenemethanol, .alpha.-methyl-, 48753 000093-92-5 52 acetate
(CAS) $$ 1-Phenylethyl ace tate $$ Styralyl acetate $$ Garden ol $$
Gardeniol II $$ sec-Phenylet hyl acetate $$ .alpha.-Phenylethyl
acetate $$ .alpha.-Methylbenzyl a cetate $$ Methylphenylcarbinol ace
tate $$ Methyl ph
Benzenepropanoic acid, methyl este 48719 000103-25-3 46 r (CAS)
$$ Methyl hydrocinnamate $ $ .beta.-Phenylpropionic acid meth yl
ester $$ Methyl 3-phenylpropion ate $$ Methyl 3-phenylpropanoate $
$ Methyl .beta.-phenylpropionate $
$ Hydrocinnamic acid, methyl ester
$$ Methyl benzen

13 9.924 0.92 C:\Database\WILEY275.L
ETHYL MALTOL 27547 004940-11-8 87
4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27523 004940-11-8 81
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$ 3-Hydroxy-2-ethyl-4-
pyrone $$ 3-Hy droxy-2-ethyl-1,4-pyrone $$ 3-Hydr oxy-2-
ethyl-.gamma.-pyrone $$ 2-Et hyl-3-hydroxy-4H-pyran-4-one $$ 3
Hydroxy-2-ethyl-4
ETHYL MALTOL 27559 000000-00-0 81

14 10.697 0.97 C:\Database\Flavor2.L
Carvone 204 000099-49-0 89 p-Methylphenyl acetate
242 000140-39-6 25 Anisole 367 000100-66-3 10

15 11.224 13.96 C:\Database\demo.l No matches found

16 12.066 1.37 C:\Database\Flavor2.L
Methyl anthranilate 265 000134-20-3 94
4'-Methylacetophenone 252 000122-00-9 2
Phenethylamine 115 000064-04-0 1

17 12.159 25.51 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47262 000054-11-5 94 yl)-, (S)-
(CAS) $$ Nicotine $$ 1 METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
$ Flux Maag $$ L-Nicotine $$ (-)-N icotine $$ XL All Insecticide $$ 3
-(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3 -(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47257 000054-11-5 91 yl)-, (S)-
(CAS) $$ Nicotine $$ 1 METHYL-2-(3-PYRIDYL)-PYRROLIDINE $

$ Flux Maag $$ L-Nicotine $$ (-)-N icotine $$ XL All Insecticide $$ 3
-(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3 -(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47269 000054-11-5 91 yl)-, (S)-
(CAS) $$ Nicotine $$ 1 METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
$ Flux Maag $$ L-Nicotine $$ (-)-N icotine $$ XL All Insecticide $$ 3
-(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
18 23.938 0.56 C:\Database\demo.l
No matches found
19 24.255 0.64 C:\Database\demo.l
No matches found

20 24.745 0.33 C:\Database\demo.l
No matches found
21 24.938 0.51 C:\Database\demo.l
No matches found

22 25.428 1.04 C:\Database\demo.l
No matches found

23 25.969 0.87 C:\Database\demo.l
No matches found

24 26.411 0.91 C:\Database\demo.l
No matches found

25 27.612 3.42 C:\Database\demo.l
No matches found
DEFAULT.M Mon Apr 03 20:30:17 2023

B2: Blue Razz Ice Library Search

Data Path : D:\CDF file conversions\
Data File : BlueRazzIce.D

Acq On : 20230331180411+0000
Operator : Admin
Sample : 1% in CHCl3
Misc : 1% in CHCl3
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1
Search Libraries: C:\Database\Flavor2.L Minimum Quality: 55
C:\Database\WILEY275.L Minimum Quality: 55
C:\Database\demo.l

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.234	0.35	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $ 8548 000594-36-5 56 $ tert-Amyl chloride $$ 2-Chloro-2 -methylbutane $$ tert-Pentyl chlor ide $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1- Dimethylpropyl chloride $$ 2-Methy l-2-chlorobutane $$ 2-Chloro-2-met hyl-butane Butane, 2-chloro-2-methyl- (CAS) $ 8551 000594-36-5 53 $ tert-Amyl chloride $$ 2-Chloro-2 -methylbutane $$ tert-Pentyl chlor ide $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1- Dimethylpropyl chloride $$ 2-Methy l-2-chlorobutane $$ 2-Chloro-2-met hyl-butane Butane, 2-chloro-2-methyl-			

(CAS) $ 8552 000594-36-5 50
$ tert-Amyl chloride $$
2-Chloro-2
-methylbutane $$ tert-Pentyl chlor
ide $$ Tertiary pentyl chloride $$
2-Methyl-2-chlorobutane r $$
1,1-
Dimethylpropyl chloride $$
2-Methy
l-2-chlorobutane $$
2-Chloro-2-met
hyl-butane

2 2.382 0.26 C:\Database\WILEY275.L
4-Penten-2-ol (CAS) $$
PENT-4-EN-2 3393 000625-31-0 64
-OL $$ 1-Penten-4-ol $$
4-Hydroxyp
ent-1-ene $$ CH2=CHCH2CH(OH)CH3
2-METHYLBUT-3-EN-2-OL
3496 000000-00-0 59

(24R)-6.beta.-methoxy-3.alpha.,5-c 244576
088802-40-8 53
yclo-5.alpha.-ergostan-23-one

3 2.954 31.24 C:\Database\WILEY275.L
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 78
glycol $$ PG 12 $$
1,2-PROPANDIOL
$$ Sirlene $$
2,3-Propanediol $$
2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop
ylene glycol $$ 1,2-Propylene glyc
ol $$ 1,2-Dihydroxypropane $$ Meth ylethylene glycol
PROPYLENE GLYCOL $$
1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE 1,2-Propanediol (CAS) $$ Propylene
2015 000057-55-6 9 glycol $$ PG 12 $$
1,2-PROPANDIOL
$$ Sirlene $$
2,3-Propanediol $$
2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop

ylene glycol $$ 1,2-Propylene glyc
ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol

4 3.708 1.76 C:\Database\Flavor2.L
Ethyl butyrate 81 000105-54-4 59
Ethyl isobutyrate 188 000097-62-1 42
Butyl butyrate
270 000109-21-7 33

5 3.863 0.71 C:\Database\demo.l
No matches found 6 4.433 0.43
C:\Database\Flavor2.L
Ethyl-2methylbutyrate 82 007452-79-1 58
Ethyl propionate
287 000105-37-3 1

7 4.526 0.59 C:\Database\Flavor2.L cis-3-Hexenol
197 000928-96-1 74
cis-3-Hexenyl acetate
161 003681-71-8 9
cis-3-Hexenylpropionate
135 003647-74-2 4

8 4.858 0.42 C:\Database\Flavor2.L
Isoamyl acetate 366 000123-92-2 56
2-Methylbutylacetate 121 000624-41-9 4
Hexyl acetate
299 000142-92-7 4

9 6.260 0.26 C:\Database\demo.l
No matches found

10 6.470 1.79 C:\Database\demo.l
No matches found

11 6.824 0.19 C:\Database\WILEY275.L
Hexanoic acid, ethyl ester
(CAS) $ 31003 000123-66-0 59
$ ETHYL N-CAPROATE $$ Ethyl caproa
te $$ Ethyl hexanoate $$ Hexanoic
acid, ethyl ester, mixt. with soyb
ean oil epoxide $$ Ethyl ester of

hexanoic acid $$ Caproic acid ethy
l ester $$ n-Caproic acid ethyl es
ter $$ Acetic aci
Hexanoic acid, ethyl ester
(CAS) $ 31002 000123-66-0 47
$ ETHYL N-CAPROATE $$ Ethyl caproa
te $$ Ethyl hexanoate $$ Hexanoic
acid, ethyl ester, mixt. with soyb
ean oil epoxide $$ Ethyl ester of
hexanoic acid $$ Caproic acid ethy
l ester $$ n-Caproic acid ethyl es
ter $$ Acetic aci
Hexanoic acid, ethyl ester
(CAS) $ 31004 000123-66-0 43
$ ETHYL N-CAPROATE $$ Ethyl caproa
te $$ Ethyl hexanoate $$ Hexanoic
acid, ethyl ester, mixt. with soyb
ean oil epoxide $$ Ethyl ester of
hexanoic acid $$ Caproic acid ethy
l ester $$ n-Caproic acid ethyl es
ter $$ Acetic aci

12 7.414 0.29 C:\Database\WILEY275.L Phenol, 2-methyl- (CAS) $$ o-Creso
9117 000095-48-7 64
l $$ o-Toluol $$ 2-Cresol $$ o-Oxy
toluene $$ o-Methylphenol $$ 2-Met
hylphenol $$ o-Hydroxytoluene
$$ o
-Methylphenylol $$
2-Hydroxytoluen e $$ 1-Hydroxy-2-methylbenzene $$
o-Cresylic acid $$
1-HYDROXY-2-MET
HYLBENZENE(2-METH
Xanthine,
1,3-dipropyl-8-[4-[.beta 269838 000000-00-0 59

.-[(benzyloxycarbonylamino)acetyla mino]

(4S,5R)-4.beta.-allyl-2,4.alpha.-d 89047
126784-63-2 49
imethyl-5-propen-2-ylcyclohexen-3 one $$ (5S,6R)-6-allyl-6-
methyl ca
rvone $$ 2-Cyclohexen-1-one,
2,6-d

imethyl-5-(1-methylethenyl)-6-(2-p ropenyl)-, (5S-cis) 13 8.289 0.38
C:\Database\WILEY275.L Hexanoic acid, 3-hydroxy-, methyl 32352 021188-
58-9 64
ester (CAS) $$ Methyl
3-hydroxyhex
anoate $$ METHYL
.BETA.-HYDROXY HE
XANOATE $$ METHYL ESTER OF 3-HYDRO
XY-HEXANOIC ACID $$ Methyl
3-hydro
xycaproate Disulfide, propyl 1-(propylthio)et 95035
069078-86-0 37 hyl (CAS) $$ 5-Methyl-4,6,7-trithi
adecane
Disulfide, propyl 1-(propylthio)et 95034 069078-86-0 37
hyl (CAS) $$ 5-Methyl-4,6,7-trithi adecane

14 8.470 0.10 C:\Database\WILEY275.L
CIS-SABINENEHYDRATE
40576 015826-82-1 58
CIS-SABINENEHYDRATE 40577 015826-82-1 52
CIS-OCIMENE
25362 027400-71-1 50

15 9.502 9.02 C:\Database\WILEY275.L
Benzoic acid (CAS) $$
Retardex $$ 15531 000065-85-0 90
HA 1 $$ Tenn-Plas $$ Retarder
BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid
$$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV
$$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar Benzoic acid (CAS) $$
Retardex $$ 15527 000065-85-0 90
HA 1 $$ Tenn-Plas $$ Retarder
BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid
$$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV
$$ P

henylformic acid $$ Benzeneformic
acid $$ Phenylcar Benzoic acid (CAS) $$
Retardex $$ 15539 000065-85-0 86
HA 1 $$ Tenn-Plas $$ Retarder
BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid
$$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV
$$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

16 9.833 0.24 C:\Database\Flavor2.L
Benzoic acid 361 000065-85-0 72
2,3,5-Trimethylpyrazine
172 014667-55-1 43
p-Methylanisole
231 000104-93-8 2

17 9.929 1.11 C:\Database\WILEY275.L
3-Ethyl-2-formylthiophene
27471 000000-00-0 59
4H-Pyran-4-one, 3-hydroxy-2,6-dime 27528 002298-99-9 53 thyl-
(CAS) $$ METHYL MALTOL
$$ ME
THYL ALLOMALTOL
2-methylmercaptophenol
27478 000000-00-0 43

18 10.530 1.01 C:\Database\WILEY275.L
1,2,3-Propanetriol, diacetate (CAS 60170 025395-31-7 78
) $$ Diacetin $$ Acetin, di-
$$ Di
acetylglycerol $$ Glycerin diaceta
te $$ Glyceryl diacetate $$ Glycer
ol diacetate $$ Glycerine diacetat
e $$ Glycerol 1,3-diacetate DIACETIN
60187 000000-00-0 78
Ketone, methyl
2-methyl-1,3-oxothi 32114 033266-06-7 9 olan-2-yl (CAS) $$
2-(ETHYLENE-1'-
OXY-2'-THIO)-BUTAN-3-ONE $$
2-(Eth

ylene-1'-oxy-2'thio)-butan-3-one $
$
2-(1-oxoethyl)-2-methyl-1,3-oxat hiolane $$ Ethanone,
1-(2-methyl-1
,3-oxathiolan-2-yl)- $$ Ketone, me
thyl 2-methyl-1,3

19 11.233 14.68 C:\Database\demo.l
No matches found

20 11.938 6.41 C:\Database\Flavor2.L
Triacetin
33 000102-76-1 83

21 12.159 21.44 C:\Database\WILEY275.L
Nicotine $$ Black leaf $$ Black le 47308 016760-37-5 94 af 40 $$
Destruxol orchid spray $$
Emo-nik $$ ENT 3,424 $$ Flux maag
$$ Fumetobac $$ Mach-nic $$
1-Met
hyl-2-(3-pyridyl)pyrrolidine $$ 3-
(N-Methylpyrrolidino)pyridine
$$ L

-3-(1-Methyl-2-pyrrolidyl)pyridine
$$ (-)-3-(1-Meth
Pyridine,
3-(1-methyl-2-pyrrolidin 47262 000054-11-5 94 yl)-, (S)- (CAS) $$ Nicotine
$$ 1-

METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
$ Flux Maag $$ L-Nicotine $$
(-)-N
icotine $$ XL All Insecticide
$$ 3

-(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$
(-)-3
-(N-Methylpyrroli
Pyridine,
3-(1-methyl-2-pyrrolidin 47269 000054-11-5 94 yl)-, (S)- (CAS) $$ Nicotine
$$ 1-

METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
$ Flux Maag $$ L-Nicotine $$
(-)-N
icotine $$ XL All Insecticide
$$ 3

-(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$
(-)-3
-(N-Methylpyrroli

22 12.647 0.49 C:\Database\Flavor2.L
Methyl cinnamate
48 000103-26-4 64

23 12.780 0.83 C:\Database\Flavor2.L
Vanillin
24 000121-33-5 86

24 13.681 0.56 C:\Database\Flavor2.L gamma-Decalactone
196 000706-14-9 80
gamma-Undecalactone
352 000104-67-6 72
gamma-Octalactone
216 000104-50-7 53

25 13.893 0.18 C:\Database\Flavor2.L beta-Ionone
267 014901-07-6 76
beta-Damascone
41 023726-91-2 9

26 13.984 0.10 C:\Database\WILEY275.L
6,6-dimethyl-1-vinylfulven $$
1,3- 22288 102835-72-3 80
Cyclopentadiene,
1-ethenyl-5-(1-me
thylethylidene)-
(E)-4-(1'-PROPENYL)TOLUENE $$
Benz 22193 002077-30-7 80 ene, 1-methyl-4-(1-propenyl)-,
(E) - (CAS) $$ Toluene, p-propenyl-, (
E)- $$ trans-1-p-Tolylpropene
$$ 4

-Methyl-trans-.beta.-methylstyrene
(Z)-4-(1'-PROPENYL)TOLUENE $$
Benz 22191 002077-29-4 80 ene, 1-methyl-4-(1-propenyl)-,
(Z) - (CAS) $$ Toluene, p-propenyl-, (
Z)- $$ cis-1-p-Tolylpropene
$$ cis

-p-Methyl-.beta.-methylstyrene

27 14.701 0.41 C:\Database\WILEY275.L

4-(4-HYDROXYPHENYL)-2-BUTANONE 49039
000000-00-0 80
2-Butanone,
4-(4-hydroxyphenyl)- (48774 005471-51-2 80
CAS) $$ 4-(p-Hydroxyphenyl)-2-buta
none $$ METHYL
P-HYDROXY-.BETA.-PH
ENETHYL KETONE $$ Rheosmin $$ Rasp
berry ketone $$
(p-Hydroxybenzyl)a cetone $$ 4-(4-
Hydroxyphenyl)-2-bu tanone $$ 1-(p-
Hydroxyphenyl)-3-bu
tanone $$ 2-Butan
Phenol,
4-(1,1-dimethylpropyl)- (C 49248 000080-46-6
80
AS) $$ p-(1,1-Dimethylpropyl)pheno l $$
Amilfenol $$
4-t-Amylphenol $
$ tert-Amylphenol $$ p-tert-Amylph
enol $$ 4-tert-Amylphenol $$ p-ter
t-Pentylphenol $$
4-tert-Pentylphe
nol $$ Phenol, p-tert-pentyl-
$$ 4
-(1,1-Dimethylpro

28 15.897 0.28 C:\Database\demo.l
Barbital
5 000057-44-3 9
Pentobarbital
8 000076-74-4 7

29 17.339 0.32 C:\Database\demo.l

No matches found

30 24.892 0.62 C:\Database\demo.l
No matches found

31 26.113 1.19 C:\Database\demo.l
No matches found

32 26.298 0.13 C:\Database\demo.l
No matches found

33 26.456 0.20 C:\Database\demo.l
No matches found

34 26.845 0.50 C:\Database\demo.l
No matches found

35 27.060 0.39 C:\Database\demo.l
No matches found

36 27.513 0.72 C:\Database\demo.l
No matches found 37 27.615 0.17 C:\Database\demo.l
No matches found

38 27.788 0.16 C:\Database\WILEY275.L

2-Oxo-4-nitrosomethyl-6-trifluoro- 92085
000000-00-0 90
methyl-1,2-dihydropyrimidine

2,3-dimethyl-4-azaphenanthrene 92617
000000-00-0 37
Cyclotrisiloxane, hexamethyl-
(CAS 106849 000541-05-9 37
) $$
1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$
HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr
imer

39 27.887 0.04 C:\Database\demo.l

No matches found DEFAULT.M Mon Apr 03 20:39:17 2023

B3: Grape Energy Library Search

C:\Database\WILEY275.L Minimum Quality: 40 C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.234	1.19	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8548	000594-36-5	56
			Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8551	000594-36-5	53
			Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8549	000594-36-5	50
2	2.379	0.25	C:\Database\WILEY275.L 3-Penten-2-ol (CAS) $$ 2-PENTEN-4-OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-Dimethylallyl alcohol $$ PENT-3-EN-2-OL $$ 3-Penten-2-ol,cis+trans	3386	001569-50-2	80
			3-Penten-2-ol (CAS) $$ 2-PENTEN-4-OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-Dimethylallyl alco	3385	001569-50-2	80

hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-
ol,cis+trans
4-Penten-2-ol (CAS) $$ PENT-4-EN-2 3393 000625-31-0 78
-OL $$ 1-Penten-4-ol $$ 4-Hydroxyp
ent-1-ene $$ CH2=CHCH2CH(OH)CH3

3 2.617 0.12 C:\Database\WILEY275.L
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Propanoic acid, ethyl ester (CAS) 7466 000105-37-3 49
$$ Ethyl propanoate $$ Ethyl propi
onate $$ Propionic ether $$ Propio nic
ester $$ Propionic acid ethyl ester $$
Propionic acid, ethyl est er $$ Ethyl ester
of propanoic aci d $$ Ethyl-propionat $$
C2H5COOC2H
5 $$ Propionate d
ETHYL PROPIONATE 7596 000105-37-3 49
Propanoic acid, ethyl ester (CAS) 7473 000105-37-3 47
$$ Ethyl propanoate $$ Ethyl propi
onate $$ Propionic ether $$ Propio nic
ester $$ Propionic acid ethyl ester $$
Propionic acid, ethyl est er $$ Ethyl ester
of propanoic aci d $$ Ethyl-propionat $$
C2H5COOC2H
5 $$ Propionate d

4 2.948 37.92 C:\Database\WILEY275.L
PROPYLENE GLYCOL $$ 1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 78
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
1,2-Propanediol (CAS) $$ Propylene 2007 000057-55-6 64
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g

lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol

5 3.710 1.23 C:\Database\WILEY275.L
ETHYL BUTANOATE $$ ETHYL BUTYRATE 13265 000105-54-4 93
Butanoic acid, ethyl ester (CAS) $ 13021 000105-54-4 91
$ Ethyl butyrate $$ Butyric acid e
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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thyl ester $$ Butyric ether $$ Eth yl butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13024 000105-54-4 64
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr

6 3.812 0.15 C:\Database\Flavor2.L
isobutyl alcohol 62 000078-83-1 1

7 3.858 0.60 C:\Database\WILEY275.L
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7804 000108-11-2 59
ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty l
alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p
2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7753 000626-93-7 45
$$ n-Butylmethylcarbinol $$ Hexan
ol-(2) $$ sec-Hexyl alcohol
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7805 000108-11-2 45
ethyl-2-pentanol $$ MIC $$ MAOH $$ MIBC $$ 3-MIC $$

2-Methyl-4-penta nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso butyl carbinol $$ 4-
Methyl-2-penty l alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p

8 4.025 0.14 C:\Database\WILEY275.L
Octane, 4-methyl- (CAS) $$ 4-Methy 19810 002216-34-4 80
loctane $$ Isononane
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

{3,4,6,7-.eta.(4)-(1-ethoxytricycl 218718 137125-05-4 62
o[3.3.1.0(2,8)]nona-3,6-diene)}rho dium
N-EICOSANE 163902 000112-95-8 38

9 4.436 0.18 C:\Database\WILEY275.L
Ethyl 3-methyloxiranecarboxylate 20545 000000-00-0 64
Ethyl 3-methyloxiranecarboxylate i 20546 000000-00-0 59
somer
Thiophene, tetrahydro-3-methyl- (C 7666 004740-00-5 59
AS) $$ 3-Methylthiacyclopentane $$
3-Methylthiolane $$ 3-Methyltetra
hydrothiophene $$ Tetrahydro-3-met
hylthiophene $$ 3-METHYL-TETRAHYDR
OTHIOPHEN $$ 3-methyl-1-thia-cyclo pentane
$$ 3-Methylthiophane

10 4.526 0.29 C:\Database\WILEY275.L
1,3-Pentadiene, 2-methyl- (CAS) $$ 2430 001118-58-7 80
2-Methyl-1,3-pentadiene $$ 1,3-Di methyl-
1,3-butadiene $$ 2,4-Dimeth yl-1,3-butadiene $$
CH2=C(CH3)CH=C
HCH3 $$ 2-Methyl-1,3-pentadiene,c&
1,4-Hexadiene (CAS) $$ 1,4-Hexadie 2413 000592-45-0 80
ne,c&t $$ 1,4-Hexadiene cis-trans
Cyclopentane, methylene- (CAS) $$ 2470 001528-30-9 72
Methylenecyclopentane $$ METHYLENE
-CYCLOPENTANE $$ METHYLENE CYCLOPE
NTANE

11 4.858 0.04 C:\Database\WILEY275.L

1-Butanol, 3-methyl-, acetate (CAS 20837 000123-92-2 72
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20842 000123-92-2 72
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20841 000123-92-2 59
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac

12 4.889 0.07 C:\Database\WILEY275.L
Tetradecanoic acid, methyl ester (127995 000124-10-7 42
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 $$
MYRISTIC A
1-Butanol, 2-methyl-, acetate (CAS 20830 000624-41-9 35
) $$ 2-Methylbutyl acetate $$ 2-ME
THYL-1-ACETOXYBUTANE $$ 2-Methyl-1
-butyl acetate $$ 2-METHYL BUTYL A
CETATE $$ Acetic acid 2-methylbuty l
ester
1-Butanol, 2-methyl-, acetate (CAS 20828 000624-41-9 35

) $$ 2-Methylbutyl acetate $$ 2-ME
THYL-1-ACETOXYBUTANE $$ 2-Methyl-1
-butyl acetate $$ 2-METHYL BUTYL A
CETATE $$ Acetic acid 2-methylbuty 1
ester

13 6.314 0.47 C:\Database\Flavor2.L
n-Propyl acetate 227 000109-60-4 1
Ethyl acetate 92 000141-78-6 1
Hexyl acetate 299 000142-92-7 1

14 6.410 0.73 C:\Database\WILEY275.L
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Ethanol, 2-amino- (CAS) $$ Ethanol 789 000141-43-5 50
amine $$ MEA $$ ETHANOL-2-AMINE $$
Olamine $$ Colamine $$ Glycinol $
$ Aminoethanol $$ Ethylolamine $$
Thiofaco M-50 $$ 2-Aminoethanol $$
Monoethanolamine $$ 2-Amino-l-eth anol
$$ 2-Aminoethan-1-ol $$ 2-Hyd
roxyethylamine $$
NITROMETHANE 776 000000-00-0 50
1,2,3-Propanetriol (CAS) $$ Glycer 4510 000056-81-5 39
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy
nthetic glycerin

15 6.433 0.42 C:\Database\Flavor2.L
Isopropyl acetate 268 000108-21-4 1
Ethyl acetate 92 000141-78-6 1
Hexyl acetate 299 000142-92-7 1

16 9.490 7.20 C:\Database\WILEY275.L
Benzoic acid, anhydride (CAS) $$ B 112391 000093-97-0 83
enzoic anhydride $$ Benzoyl anhydr
ide $$ Benzoic acid anhydride
Benzoic acid (CAS) $$ Retardex $$ 15536 000065-85-0 80

HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15530 000065-85-0 78
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic Search Libraries:
C:\Database\WILEY275.L Minimum Quality:
40 C:\Database\Flavor2.L
Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

acid $$ Phenylcar

17 9.638 1.19 C:\Database\WILEY275.L
Butanedioic acid, diethyl ester (C 58585 000123-25-1 86
AS) $$ Clorius $$ Diethyl succinat e $$ Ethyl succinate $$
Succinic a cid, diethyl ester $$ Diethyl este r of
butanedioic acid $$ Diethyl b utanedioate $$ Diethylester
kyseli
ny jantarove
Butanedioic acid, diethyl ester (C 58587 000123-25-1 80
AS) $$ Clorius $$ Diethyl succinat e $$ Ethyl succinate $$
Succinic a cid, diethyl ester $$ Diethyl este r of
butanedioic acid $$ Diethyl b utanedioate $$ Diethylester
kyseli
ny jantarove
Butanedioic acid, diethyl ester (C 58588 000123-25-1 78
AS) $$ Clorius $$ Diethyl succinat e $$ Ethyl succinate $$
Succinic a cid, diethyl ester $$ Diethyl este r of
butanedioic acid $$ Diethyl b utanedioate $$ Diethylester
kyseli
ny jantarove

18 9.932 0.94 C:\Database\WILEY275.L

4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27523 004940-11-8 58
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$ 3-
Hydroxy-2-ethyl-4-pyrone $$ 3-Hy droxy-2-ethyl-1,4-
pyrone $$ 3-Hydr oxy-2-ethyl-.gamma.-pyrone $$ 2-Et
hyl-3-hydroxy-4H-pyran-4-one $$ 3 Hydroxy-2-ethyl-4
ETHYL MALTOL 27559 000000-00-0 58
4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27525 004940-11-8 53
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$ 3-Hydroxy-2-
ethyl-4-pyrone $$ 3-Hy droxy-2-ethyl-1,4-pyrone $$ 3-Hydr
oxy-2-ethyl-.gamma.-pyrone $$ 2-Et hyl-3-hydroxy-4H-
pyran-4-one $$ 3 Search Libraries: C:\Database\WILEY275.L
Minimum Quality: 40 C:\Database\Flavor2.L
Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Hydroxy-2-ethyl-4

19 11.233 16.53 C:\Database\Flavor2.L
Quinoline 174 000091-22-5 4
3-Hexenoic acid 36 004219-24-3 2

20 12.069 1.56 C:\Database\WILEY275.L
Benzoic acid, 2-amino-, methyl est 36529 000134-20-3 87
er (CAS) $$ Methyl anthranilate $$
Methyl o-aminobenzoate $$ o-Carbo
methoxyaniline $$ Methyl 2-aminobe
nzoate $$ 2-(Methoxycarbonyl)anili ne
$$ Anthranilic acid methyl este r $$
Anthranilic acid, methyl este
r $$ 2-Aminobenzo
Benzoic acid, 2-amino-, methyl est 36527 000134-20-3 86
er (CAS) $$ Methyl anthranilate $$
Methyl o-aminobenzoate $$ o-Carbo
methoxyaniline $$ Methyl 2-aminobe
nzoate $$ 2-(Methoxycarbonyl)anili ne
$$ Anthranilic acid methyl este r $$
Anthranilic acid, methyl este
r $$ 2-Aminobenzo
Benzoic acid, 2-amino-, methyl est 36530 000134-20-3 86

er (CAS) $$ Methyl anthranilate $$
Methyl o-aminobenzoate $$ o-Carbo
methoxyaniline $$ Methyl 2-aminobe
nzoate $$ 2-(Methoxycarbonyl)anili ne
$$ Anthranilic acid methyl este r $$
Anthranilic acid, methyl este r $$ 2-
Aminobenzo

21 12.162 23.95 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47262 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Nicotine $$ Black leaf $$ Black le 47308 016760-37-5 91
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

af 40 $$ Destruxol orchid spray $$ Emo-nik $$ ENT 3,424 $$ Flux maag
$$ Fumetobac $$ Mach-nic $$ 1-Met hyl-2-(3-pyridyl)pyrrolidine $$ 3 (N-
Methylpyrrolidino)pyridine $$ L
-3-(1-Methyl-2-pyrrolidyl)pyridine
$$ (-)-3-(1-Meth
Pyridine, 3-(1-methyl-2-pyrrolidin 47257 000054-11-5 91
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli

22 12.349 0.26 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47256 000054-11-5 64
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N

icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
NICOTINE-1-N-OXIDE 62215 000000-00-0 43
Pyridine, 3-(1-methyl-2-pyrrolidin 77937 002055-29-0 38
yl)-, N,1-dioxide, (S)- (CAS) $$ D
ioxynicotine $$ Nicotine dioxide $ $
Nicotine, 1,1'-dioxide $$ S-(-)
Nicotine-1,1'-dioxide $$ Pyridine,
3-(1-methyl-2-pyrrolidinyl)-, N,1
-dioxide $$ Pyridine, 3-(1-methyl 2-
pyrrolidinyl)-,

23 12.647 0.16 C:\Database\WILEY275.L
2-Propenoic acid, 3-phenyl-, methy 47040 000103-26-4 56
l ester (CAS) $$ Cinnamic acid met hyl ester $$ Methyl
cinnamate $$ M ethyl cinnamylate $$ Methyl 3-phen
ylpropenoate $$ Cinnamic acid, met hyl ester $$ Methyl 3-
phenyl-2-pro
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

---

penoate $$ Methyl 3-phenylacrylate
$$ Methyl ester
2-Propenoic acid, 3-phenyl-, methy 47031 000103-26-4 53
l ester (CAS) $$ Cinnamic acid met hyl ester $$ Methyl
cinnamate $$ M ethyl cinnamylate $$ Methyl 3-phen
ylpropenoate $$ Cinnamic acid, met hyl ester $$ Methyl 3-
phenyl-2-pro penoate $$ Methyl 3-phenylacrylate
$$ Methyl ester
METHYL CINNAMATE 47206 000000-00-0 50

24 12.783 0.83 C:\Database\WILEY275.L
Benzaldehyde, 4-hydroxy-3-methoxy- 37171 000121-33-5 91
(CAS) $$ Vanillin $$ VANILLINE $$
Lioxin $$ Vanilin $$ Vanillaldehy de $$
Vanillic aldehyde $$ 2-Metho xy-4-
formylphenol $$ 4-Formyl-2-me
thoxyphenol $$ p-Hydroxy-m-methoxy
benzaldehyde $$ 3-Methoxy-4-hydrox

ybenzaldehyde $$
Benzaldehyde, 4-hydroxy-3-methoxy- 37172 000121-33-5 91
(CAS) $$ Vanillin $$ VANILLINE $$
Lioxin $$ Vanilin $$ Vanillaldehy de $$
Vanillic aldehyde $$ 2-Metho xy-4-
formylphenol $$ 4-Formyl-2-me
thoxyphenol $$ p-Hydroxy-m-methoxy
benzaldehyde $$ 3-Methoxy-4-hydrox
ybenzaldehyde $$
Benzaldehyde, 4-hydroxy-3-methoxy- 37176 000121-33-5 91
(CAS) $$ Vanillin $$ VANILLINE $$
Lioxin $$ Vanilin $$ Vanillaldehy de $$
Vanillic aldehyde $$ 2-Metho xy-4-
formylphenol $$ 4-Formyl-2-me
thoxyphenol $$ p-Hydroxy-m-methoxy
benzaldehyde $$ 3-Methoxy-4-hydrox
ybenzaldehyde $$

25 13.160 0.15 C:\Database\WILEY275.L
Methyl 2,3-Dihydro-2-methylbenzofu 75901 079950-40-6 43
ran-4-carboxylate $$ 4-Benzofuranc
arboxylic acid, 2,3-dihydro-2-meth Search Libraries:
C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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yl-, methyl ester (CAS)
Benzenamine, 3,5-dimethyl- $$ 3,5- 15309 000108-69-0 30
Xylidine $$ 3,5-Dimethylaniline $$
m-Xylidine $$ 3,5-Dimethylbenzene
amine $$ 3,5-Xylidene $$ 3,5-Xylyl amine
$$ 5-Amino-1,3-dimethylbenze ne $$ 5-
Amino-1,3-xylene $$ 3,5-Di
methylphenylamine $$ 3,5-Dimethylb
enzenamine $$ 1-A
Benzenepropanoic acid, .alpha.-hyd 64289 013674-16-3 30
roxy-, methyl ester (CAS) $$ METHY
L .BETA.-PHENYLLACTATE $$ Methyl
2 -hydroxy-3-phenylpropionate $$ Lac
tic acid, 3-phenyl-, methyl ester $$ .beta.-
Phenyllactic acid methyl ester $$ L-Methyl
3-phenyllactate

$$ Methyl phenyl

26 13.539 0.36 C:\Database\WILEY275.L
ETHYL VANILLIN 50871 000000-00-0 80
Benzaldehyde, 3-ethoxy-4-hydroxy- 50767 000121-32-4 80
(CAS) $$ 3-Ethoxy-4-hydroxybenzald
ehyde $$ Ethovan $$ Vanirom $$ Eth
avan $$ Vanilal $$ Vanillal $$ Bou
rbonal $$ Ethylprotal $$ Quantrova nil
$$ Ethylvanillin $$ Ethyl vani llin $$ 4-
Hydroxy-3-ethoxybenzalde
hyde $$ Protocate
[1.alpha.(S*),5.beta.]-1-(Phenylsu 145991 067009-05-6 70
lfinyl)bicyclo[3.3.1]nonan-3-one

27 13.718 0.23 C:\Database\WILEY275.L
ETHYL CINNAMATE 60672 000103-36-6 86
2-Propenoic acid, 3-phenyl-, ethyl 60566 000103-36-6 81
ester (CAS) $$ Ethyl cinnamate $$ Cinnamic acid ethyl
ester $$ Cinn amic acid, ethyl ester $$ Ethyl 3
phenylpropenoate $$ Ethyl 3-phenyl acrylate $$ Ethyl 3-
phenyl-2-prope noate $$ Ethyl trans-cinnamate $$
Ethyl .beta.-phen
2-Propenoic acid, 3-phenyl-, ethyl 60564 000103-36-6 64
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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ester (CAS) $$ Ethyl cinnamate $$ Cinnamic acid ethyl ester $$ Cinn amic
acid, ethyl ester $$ Ethyl 3 phenylpropenoate $$ Ethyl 3-phenyl acrylate $$
Ethyl 3-phenyl-2-prope noate $$ Ethyl trans-cinnamate $$
Ethyl .beta.-phen

28 14.219 0.05 C:\Database\WILEY275.L
1-methylethyl E-3-phenyl-2-propeno 74409 000000-00-0 72
ate
BUTYL CINNAMATE 88875 000000-00-0 47
2-Propenoic acid, 3-phenyl- (CAS) 33772 000621-82-9 47
$$ Cinnamic acid $$ Phenylacrylic
acid $$ 3-Phenylacrylic acid $$ 3
Phenyl-2-propenoic acid $$ tert-.b eta.-

Phenylacrylic acid $$ Zimtsae ure $$ 3-
Phenylpropenoic acid $$ K
yselina skoricove

29 14.993 0.08 C:\Database\WILEY275.L
2,7-dimethyl-2,6-octadien-4-ol 40525 000000-00-0 53 1,2-
Cyclopentanediol, 1-(1-methyle 31126 056335-92-3 53
thyl)-, trans- (CAS) $$ trans-1-Is opropyl-1,2-
cyclopentanediol
2(3H)-Furanone, dihydro-5-pentyl- 42147 000104-61-0 53
(CAS) $$ 4-Hydroxynonanoic acid la
ctone $$ Prunolide $$ Nonlacton $$
Nonlakton $$ 4-Nonanolide $$ Nona n-
1,4-olide $$ .gamma.-Nonanolide $$ 4-
Pentyl-butanolide $$ .gamma.
Nonalactone $$ .gamma.-Nonanolacto ne
$$ .gamma.-Amy

30 15.888 0.09 C:\Database\WILEY275.L
Quinoline, 2,7-dimethyl- (CAS) $$ 43273 000093-37-8 64
m-Toluquinaldine $$ 2,7-Dimethylqu inoline
2.alpha.-ethyl-3.alpha.-trimethyls 249336 121709-28-2 64
ilyloxy-10.beta.-hydroxy-20-norgib
berell-16-ene-7,19-dioic acid 7-m ethyl
ester 19,10-lactone $$ Gibba Search Libraries:
C:\Database\WILEY275.L Minimum
Quality: 40 C:\Database\Flavor2.L
Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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ne-1,10-dicarboxylic acid, 3-ethyl
-4a-hydroxy-1-methyl-8-methylene-2
-[(trimethylsilyl)oxy]-, 1,4a-lact one,
10-methyl es
2,4,5-Trifluorobenzonitrile 43013 098349-22-5 59

31 25.938 0.08 C:\Database\Flavor2.L
No matches found

32 26.340 0.17 C:\Database\Flavor2.L
No matches found

33 26.403 0.12 C:\Database\Flavor2.L
No matches found

34 26.456 0.05 C:\Database\Flavor2.L
No matches found

35 26.547 0.11 C:\Database\Flavor2.L
No matches found

36 26.629 0.23 C:\Database\Flavor2.L
No matches found

37 26.692 0.04 C:\Database\WILEY275.L
Tetrasiloxane, decamethyl- (CAS) $ 185153 000141-62-8 43
$ Decamethyltetrasiloxane $$ [(CH3
)3SiOSi(CH3)2]2O $$ KF 96L1.5
Cyclotrisiloxane, hexamethyl- (CAS 106849 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
1,1,1,3,5,5,5-Heptamethyltrisiloxa 106884 001873-88-7 37
ne $$ Bis(trimethylsiloxy)methylsi
lane $$ Hydromethylsiloxane $$ Tri
siloxane, 1,1,1,3,5,5,5-heptamethy
l
38 26.952 0.10 C:\Database\WILEY275.L
3,3-Diethoxy-1,1,1,5,5,5-hexamethy 174413 000000-00-0 42
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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ltrisiloxane
3-CHLORO-5-PHENYL-1,2,4-TRIAZINE 2 92138 061178-01-6 38
-OXIDE $$ 1,2,4-Triazine, 3-chloro
-5-phenyl-, 2-oxide (CAS)
[4-(dimethoxyboryl)phenyl]trimethy 107233 107134-80-5 37
lsilane

39 27.063 0.16 C:\Database\WILEY275.L
2-Oxo-4-nitrosomethyl-6-trifluoro- 92085 000000-00-0 43 methyl-1,2-
dihydropyrimidine

3,3-Diethoxy-1,1,1,5,5,5-hexamethy 174413 000000-00-0 38
ltrisiloxane
2,3-dimethyl-4-azaphenanthrene 92617 000000-00-0 38

40 27.176 0.27 C:\Database\WILEY275.L
3,4-di(4-trimethylsiloxyphenyl)hex 239950 000000-00-0 50
ane
1H-Indole, 1-methyl-2-phenyl- (CAS 92600 003558-24-5 47
) $$ 1-Methyl-2-phenylindole $$ 2
Phenyl-N-methylindole $$ Indole, 1 -
methyl-2-phenyl- $$ N-Methyl-2-ph
enylindole
N-ethyl-1,3-dithioisoindoline $$ 1 92199 035373-06-9 47
H-Isoindole-1,3(2H)-dithione, 2-et
hyl
41 27.224 0.21 C:\Database\Flavor2.L
No matches found

42 27.363 0.42 C:\Database\Flavor2.L
No matches found

43 27.516 0.10 C:\Database\WILEY275.L
(-)-18-noramborx 108517 105561-28-2 43
Cyclotrisiloxane, hexamethyl- (CAS 106849 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
3,3-Diisopropoxy-1,1,1,5,5,5-hexam 195153 018082-56-9 37
ethyltrisiloxane
Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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44 27.635 0.29 C:\Database\Flavor2.L
No matches found

45 27.796 0.14 C:\Database\WILEY275.L
2-Oxo-4-nitrosomethyl-6-trifluoro- 92085 000000-00-0 42 methyl-1,2-
dihydropyrimidine
Dibenzoxazabicycloundecane $$ 1H-2 206379 087166-99-2 32

,6,10-(Epoxymethyno)-3-benzazacycl
ododecine, 2,3,4,5-tetrahydro-9,12
,13-trimethoxy-3-methyl-, (+)- (CA
S)
Cyclotrisiloxane, hexamethyl- (CAS 106848 000541-05-9 30
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer

46 27.842 0.11 C:\Database\WILEY275.L
Benz[e]azulene-3,8-dione, 5-[(acet 210271 025536-74-7 42
yloxy)methyl]-3a,4,6a,7,9,10,10a,1 0b-octahydro-3a,10a-
dihydroxy-2,10
-dimethyl-, (3a.alpha.,6a.alpha.,1
0.beta.,10a.beta.,10b.beta.)-(+)-
Cyclotrisiloxane, hexamethyl- (CAS 106845 000541-05-9 27
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
Tetrasiloxane, decamethyl- (CAS) $ 185153 000141-62-8 27
$ Decamethyltetrasiloxane $$ [(CH3
)3SiOSi(CH3)2]2O $$ KF 96L1.5

B4: Kiwi Passionfruit Guava Library Search

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.234	1.03	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8548	000594-36-5	56
			Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8551	000594-36-5	42
			Pentane, 3-chloro- (CAS) $$ 3-Chloropentane $$ 1-Ethylpropyl chlorid	8537	000616-20-6	38
2	2.379	0.32	C:\Database\WILEY275.L Methyl 2(Z)-Pentenyl Ether	7008	000000-00-0	72
			3-Buten-2-ol, 2-methyl- (CAS) $$ 2-methyl-3-buten-2-ol $$ Dimethylvinylcarbinol $$ Vinyldimethylcarbinol $$ Dimethylvinylmethanol $$ 1,1-Dimethyl-2-propenol $$ 1,1-Dimethylallyl alchol $$ 1,1-Dimethylallyl	3413	000115-18-4	72

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint2.e

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

---

l alcohol $$ .alpha.,.alpha.-Dimet
hylallyl alcohol
2-METHYLBUT-3-EN-2-OL 3496 000000-00-0 64

3 2.965 37.57 C:\Database\WILEY275.L
PROPYLENE GLYCOL $$ 1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 56
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
1-Propanol, 2-ethoxy- (CAS) $$ 2-E 8231 019089-47-5 43
thoxy-1-propanol $$ Propylene glyc ol monoethyl ether, .alpha.

4 3.710 0.54 C:\Database\WILEY275.L
Butanoic acid, ethyl ester (CAS) $ 13032 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth yl
ester $$ Butyr
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Butanoic acid, ethyl ester (CAS) $ 13033 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth

yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13022 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr

5 3.812 0.15 C:\Database\WILEY275.L
Propanoic acid, 2-hydroxy-2-methyl 13959 002110-78-3 47
-, methyl ester (CAS) $$ 2-HYDROXY
ISOBUTYRIC ACID-METHYL ESTER $$ Me
thyl 2-methyllactate $$ Methyl 2-h
ydroxyisobutyrate $$ Methyl .alpha .-
hydroxyisobutyrate $$ Methyl 2-h ydroxy-2-
methylpropionate $$ Lacti
c acid, 2-methyl-
TRANS- 3,5-DIDEUTERO HYDROXY CYCLO 6561 040524-90-1 47
PENTENE $$ 4-Cyclopentene-1,3-diol
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

-d2, trans- (CAS)
2-Pentanol, 2-methyl- (CAS) $$ 2-M 7795 000590-36-3 47
ethyl-2-pentanol $$ 2-Hydroxy-2-me thylpentane $$ 1,1-
Dimethylbutanol $$ 2-Methyl-2-hydroxypentane $$ 2
-Methylpentan-2-ol $$ UN 2560

6 3.861 0.50 C:\Database\Flavor2.L
2-Heptanol 180 000543-49-7 1
Isopropyl alcohol 35 000067-63-0 1
2-Pentanol 178 006032-29-7 1

7 4.529 0.22 C:\Database\WILEY275.L
4-Hexen-1-ol, (E)- (CAS) $$ TRANS- 6802 000928-92-7 72
HEX-4-EN-1-OL $$ trans-4-Hexen-1-o
l $$ trans-4-Hexenol $$ (E)-4-Hexe

n-1-ol $$ E-4-hexenol $$ 4-Hexen-1
-ol
4-Hexen-1-ol, (Z)- (CAS) $$ CIS-HE 6795 000928-91-6 72
X-4-EN-1-OL $$ Z-4-hexenol $$ cis 4-
Hexen-1-Ol
4-Hexen-1-ol, (Z)- (CAS) $$ CIS-HE 6796 000928-91-6 72
X-4-EN-1-OL $$ Z-4-hexenol $$ cis 4-
Hexen-1-Ol

8 4.739 0.08 C:\Database\WILEY275.L
5,6,7,8-TETRACHLORO-1,4-DIHYDRO-1, 193466 060857-28-5 59
4,9-TRIMETHYLNAPTHOLEN-1,4-IMINE $
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$ Naphthalen-1,4-imine, 5,6,7,8-te trachloro-1,4-dihydro-
1,4,9-trimet
hyl- (CAS)
4-METHYL-1-PENTANOL 7894 000000-00-0 45
1-HEXANOL 7890 000000-00-0 45

9 6.478 1.99 C:\Database\WILEY275.L
NITROMETHANE 776 000000-00-0 50
1,2,3-Propanetriol (CAS) $$ Glycer 4510 000056-81-5 39
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy
nthetic glycerin
1,2,3-Propanetriol (CAS) $$ Glycer 4511 000056-81-5 9
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy
nthetic glycerin

10 6.929 0.69 C:\Database\WILEY275.L
2,4-Hexadiene (CAS) $$ Bipropenyl 2426 000592-46-1 56
$$ Dipropenyl $$ 1,4-Dimethylbutad

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

---

iene $$ CH3CH=CHCH=CHCH3
1,4-Hexadiene (CAS) $$ 1,4-Hexadie 2413 000592-45-0 56
ne,c&t $$ 1,4-Hexadiene cis-trans
1,3-Pentadiene, 3-methyl-, (Z)- (C 2431 002787-45-3 56
AS) $$ (Z)-3-Methyl-1,3-pentadiene
$$ cis-3-Methyl-1,3-pentadiene $$
3-Methyl-1,3-pentadiene $$ (E)-CH
2=CHC(CH3)=CHCH3

11 8.604 0.09 C:\Database\WILEY275.L
1,2-Diethyl-5-undecylpyrrolidine 162764 000000-00-0 52
4H-Pyran-4-one, 3-hydroxy-2-methyl 17506 000118-71-8 52
- (CAS) $$ Maltol $$ VELTOL $$ 2-M
ethyl-3-hydroxypyrone $$ Palatone $$
Larixic acid $$ Larixinic acid $$ 3-
Hydroxy-2-methylpyrone $$ 3-H
ydroxy-2-methyl-4-pyrone $$ 3-Hydr
oxy-2-methyl-4-pyranone $$ 3-Hydro
xy-2-methyl-1,4-p
Phloroglucinol $$ 1,3,5-Benzenetri 17523 000108-73-6 52
ol (CAS) $$ BENZENE, 1,3,5-TRIHYDR OXY $$
Benzene-s-triol $$ Phlorogl ucin $$ sym-Trihydroxybenzene
$$ 1 ,3,5-Trihydroxybenzene $$ Phlorogl ucine
$$ s-Trihydroxybenzene $$ Be nzene, trihydroxy $$
Benzene, 1,3,
5-trihydroxy- $$

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

12 9.519 10.28 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15530 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15536 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15527 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

13 9.842 0.19 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15536 000065-85-0 58
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

Benzoic acid (CAS) $$ Retardex $$ 15533 000065-85-0 58
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15530 000065-85-0 52
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

14 9.932 0.30 C:\Database\WILEY275.L
4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27524 004940-11-8 47
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

3-Hydroxy-2-ethyl-4-pyrone $$ 3-Hy droxy-
2-ethyl-1,4-pyrone $$ 3-Hydr oxy-2-ethyl-.gamma.-
pyrone $$ 2-Et hyl-3-hydroxy-4H-pyran-4-one $$ 3
Hydroxy-2-ethyl-4
ETHYL MALTOL 27547 004940-11-8 35
2,4(1H,3H)-Pyrimidinedione, 1,3-di 27363 000874-14-6 30
methyl- (CAS) $$ 1,3-Dimethyluraci 1 $$ N,N'-
Dimethyluracil $$ N1,N3 Dimethyluracil $$ Uracil, 1,3-dime
thyl- $$ 1,3-DIMETHYL-2,4-(1H,3H)P YRIMIDINDIONE
$$ 2,4-Dihydroxy-1,3
-dimethylpyrimidine

15 11.236 17.61 C:\Database\Flavor2.L
Quinoline 174 000091-22-5 4
3-Hexenoic acid 36 004219-24-3 2

16 11.340 0.17 C:\Database\WILEY275.L
Carvomenthol $$ Cyclohexanol, 2-me 42616 000499-69-4 46
thyl-5-(1-methylethyl)-, (1.alpha. ,2.beta.,5.alpha.)- (CAS) $$
CIS-5
-ISOPROPYL-TRANS-2-METHYL-1-CYCLOH
EXANOL
Neoisocarvomenthol $$ Cyclohexanol 42620 042846-32-2 38
, 2-methyl-5-(1-methylethyl)-, (1. alpha.,2.alpha.,5.alpha.)- (CAS)
$
$ CIS-5-ISOPROPYL-CIS-2-METHYL-1-C
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

YCLOHEXANOL
Spirosolan-3-ol, (3.beta.,5.alpha. 240452 000077-59-8 38
,22.beta.,25S)- (CAS) $$ Tomatidin
e $$ (22S,25S)-5.ALPHA.-SPIROSTAN
3.BETA.-OL $$ Tomatidin $$ 5.alpha
.-Tomatidan-3.beta.-ol $$ TOMATIDI
NE ((22S,25S)-5ALPHA-SPIROSTAN-3BE
TA-OL)

17 11.938 0.46 C:\Database\Flavor2.L
Triacetin 33 000102-76-1 78

18 12.069 0.07 C:\Database\WILEY275.L
methyl anthranilate 36589 000134-20-3 74
Benzoic acid, 2-amino-, methyl est 36530 000134-20-3 72
er (CAS) $$ Methyl anthranilate $$
Methyl o-aminobenzoate $$ o-Carbo
methoxyaniline $$ Methyl 2-aminobe
nzoate $$ 2-(Methoxycarbonyl)anili ne
$$ Anthranilic acid methyl este r $$
Anthranilic acid, methyl este r $$ 2-
Aminobenzo
Benzene, (1,1-dimethyldecyl)- (CAS 131652 027854-40-6 47
) $$ Undecane, 2-methyl-2-phenyl-

19 12.162 25.63 C:\Database\WILEY275.L
Nicotine $$ Black leaf $$ Black le 47308 016760-37-5 94
af 40 $$ Destruxol orchid spray $$
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Emo-nik $$ ENT 3,424 $$ Flux maag
$$ Fumetobac $$ Mach-nic $$ 1-Met hyl-
2-(3-pyridyl)pyrrolidine $$ 3 (N-
Methylpyrrolidino)pyridine $$ L
-3-(1-Methyl-2-pyrrolidyl)pyridine
$$ (-)-3-(1-Meth
Pyridine, 3-(1-methyl-2-pyrrolidin 47262 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47269 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli

20 12.647 0.13 C:\Database\WILEY275.L
METHYL CINNAMATE 47173 000103-26-4 76
2-Propenoic acid, 3-phenyl-, methy 47033 000103-26-4 74 1
ester (CAS) $$ Cinnamic acid met hyl ester $$ Methyl
cinnamate $$ M
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
ethyl cinnamylate $$ Methyl 3-phen ylpropenoate $$ Cinnamic acid, met hyl ester $$ Methyl 3-phenyl-2-pro penoate $$ Methyl 3-phenylacrylate $$ Methyl ester						
			2-Propenoic acid, 3-phenyl-, methy	47035	000103-26-4	72
l ester (CAS) $$ Cinnamic acid met hyl ester $$ Methyl cinnamate $$ M ethyl cinnamylate $$ Methyl 3-phen ylpropenoate $$ Cinnamic acid, met hyl ester $$ Methyl 3-phenyl-2-pro penoate $$ Methyl 3-phenylacrylate $$ Methyl ester						
21	13.230	0.19	C:\Database\WILEY275.L			
			Oxiranecarboxylic acid, 3-methyl-3	91053	000077-83-8	49
-phenyl-, ethyl ester (CAS) $$ ETH YL METHYL PHENYL GLYCIDATE $$ Frae seol $$ Aldehyde C16 $$ Strawberry aldehyde $$ Ethyl methylphenylgly cidate $$ 3-Methyl-3-phenylglycidi c acid ethyl ester $$ Ethyl .alpha ,.beta.-epoxy-.b						
			Benzaldehyde, ethenyl- (CAS) $$ Vi	22101	043145-54-6	47
nylbenzaldehyde						
			E-2-phenyl-2-methyl-3-ethoxycarbon	91113	000000-00-0	43
yl-1-oxa-cyclopropane						

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
22	13.718	0.61	C:\Database\WILEY275.L			
			ETHYL CINNAMATE	60670	000103-36-6	94
			ETHYL CINNAMATE	60672	000103-36-6	94
2-Propenoic acid, 3-phenyl-, ethyl				60565	000103-36-6	91
ester (CAS) $$ Ethyl cinnamate $$ Cinnamic acid ethyl ester $$ Cinn amic acid, ethyl ester $$ Ethyl 3						

phenylpropenoate $$ Ethyl 3-phenyl
acrylate $$ Ethyl 3-phenyl-2-prope noate
$$ Ethyl trans-cinnamate $$
Ethyl .beta.-phen

23 14.443 0.09 C:\Database\WILEY275.L
Carbamic acid, (1-phenylethyl)-, 2 180737 054934-73-5 93
-methyl-5-(1-methylethyl)cyclohexy
l ester (CAS) $$ MENTHYL N-(1-PHEN
YLETHYL)-CARBAMATE $$ MENTHYL-N-(1
-PHENYLETHYL)-CARBAMATE
Carbamic acid, (.alpha.-methylbenz 180739 033027-13-3 56
yl)-, p-menth-3-yl ester (CAS)
Benzenamine, 2,3,4,5,6-pentachloro 146701 000527-20-8 53
- (CAS) $$ PCA $$ Pentachloroanili
ne $$ Pentachloroaminobenzene $$ 2
,3,4,5,6-Pentachloroaniline $$ Ani line,
2,3,4,5,6-pentachloro- $$ 2, 3,4,5,6-
Pentachlorobenzenamine

24 18.770 0.07 C:\Database\Flavor2.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

No matches found

25 26.111 0.02 C:\Database\Flavor2.L
No matches found

26 26.516 0.12 C:\Database\Flavor2.L
No matches found

27 26.881 0.08 C:\Database\Flavor2.L
No matches found

28 27.151 0.10 C:\Database\WILEY275.L
Dibenzoxazabicycloundecane $$ 1H-2 206379 087166-99-2 40
,6,10-(Epoxymethyno)-3-benzazacycl
ododecine, 2,3,4,5-tetrahydro-9,12

,13-trimethoxy-3-methyl-, (+)- (CA
S)
N-(4,4-DIDEUTERIO-4-PHENYL-BUTYL)P 161032 053429-01-9 35
HTHALIMIDE
Cyclotetrasiloxane, octamethyl- (C 174361 000556-67-2 25
AS) $$ 1,1,3,3,5,5,7,7-OCTAMETHYL-
CYCLOOCTASILOXANE $$ OCTAMETHYL-(C
YCLIC TETRAMER) CYCLOTETRASILOXANE
$$ Octamethylcyclotetrasiloxane $
$ NUC Silicone VS 7207 $$ Octameth
yl-cyclotetrasiloxane $$ Oktamethy
lcyklotetrasiloxa

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

29 27.233 0.08 C:\Database\Flavor2.L
No matches found

30 27.442 0.26 C:\Database\Flavor2.L
No matches found

31 27.471 0.11 C:\Database\WILEY275.L
Hexahydropyridine, 1-methyl-4-[4,5 92495 000000-00-0 86
-dihydroxyphenyl]-
[3-(dimethoxyboryl)phenyl]trimethy 107232 107134-79-2 35
lsilane
Cyclotrisiloxane, hexamethyl- (CAS 106849 000541-05-9 32
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer

32 27.558 0.08 C:\Database\Flavor2.L
No matches found

33 27.695 0.14 C:\Database\WILEY275.L
2-(4'-NITRO-2'-THIENYL)PYRIMIDINE 92109 057059-15-1
43 $$ Pyrimidine, 2-(4-nitro-2-thieny l)- (CAS)

Benz[e]azulene-3,8-dione, 5-[(acet 210271 025536-74-7 42
yloxy)methyl]-3a,4,6a,7,9,10,10a,1 0b-octahydro-3a,10a-
dihydroxy-2,10 ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			-dimethyl-, (3a.alpha.,6a.alpha.,1			
			0.beta.,10a.beta.,10b.beta.)-(+)-			
			N-ethyl-1,3-dithioisoindoline $$ 1	92199	035373-06-9	38
			H-Isoindole-1,3(2H)-dithione, 2-et			
			hyl			
34	27.717	0.04	C:\Database\Flavor2.L			
			No matches found			

B5: Lemon Mint Library Search

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.212	0.58	C:\Database\WILEY275.L TRICHLOROACETYL CHLORIDE	63666	000000-00-0	78
Methane, tetrachloro- (CAS) $$ Car				36815	000056-23-5	74
bon tetrachloride $$ R 10 $$ Unive rm $$ Carbona $$ Tetrasol $$ Fluko ids $$ Freon 10 $$ Fasciolin $$ Te trafinol $$ Necatorina $$ Benzinof orm $$ Tetraform $$ Perchlorometha ne $$ Tetrachlorocarbon $$ Tetrach loromethane $$ Ca						
Methane, tetrachloro- (CAS) $$ Car				36817	000056-23-5	74
bon tetrachloride $$ R 10 $$ Unive rm $$ Carbona $$ Tetrasol $$ Fluko ids $$ Freon 10 $$ Fasciolin $$ Te trafinol $$ Necatorina $$ Benzinof orm $$ Tetraform $$ Perchlorometha ne $$ Tetrachlorocarbon $$ Tetrach loromethane $$ Ca						
2	2.234	0.79	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $	8548	000594-36-5	56
$ tert-Amyl chloride $$ 2-Chloro-2 -methylbutane $$ tert-Pentyl chlor ide $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1- Dimethylpropyl chloride $$ 2-Methy l-2-chlorobutane $$ 2-Chloro-2-met hyl-butane						

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40

C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Butane, 2-chloro-2-methyl- (CAS) $ 8549 000594-36-5 53
$ tert-Amyl chloride $$ 2-Chloro-2
-methylbutane $$ tert-Pentyl chlor ide
$$ Tertiary pentyl chloride $$ 2-
Methyl-2-chlorobutane r $$ 1,1
Dimethylpropyl chloride $$ 2-Methy l-
2-chlorobutane $$ 2-Chloro-2-met
hyl-butane
Butane, 2-chloro-2-methyl- (CAS) $ 8551 000594-36-5 50
$ tert-Amyl chloride $$ 2-Chloro-2
-methylbutane $$ tert-Pentyl chlor
ide $$ Tertiary pentyl chloride $$
2-Methyl-2-chlorobutane r $$ 1,1
Dimethylpropyl chloride $$ 2-Methy l-
2-chlorobutane $$ 2-Chloro-2-met
hyl-butane

3 2.382 0.37 C:\Database\WILEY275.L
3-Penten-2-ol (CAS) $$ 2-PENTEN-4- 3385 001569-50-2 72
OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-
Dimethylallyl alco
hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-
ol,cis+trans
3-Buten-2-ol, 2-methyl- (CAS) $$ 2 3415 000115-18-4 72
-methyl-3-buten-2-ol $$ Dimethylvi
nylcarbinol $$ Vinyldimethylcarbin ol
$$ Dimethylvinylmethanol $$ 1,1 -
Dimethyl-2-propenol $$ 1,1-Dimeth ALS Vial :
0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

---

ylallyl alchol $$ 1,1-Dimethylally l alcohol $$ .alpha.,.alpha.-Dimet

hylallyl alcohol
2-METHYLBUT-3-EN-2-OL 3496 000000-00-0 72

4 2.948 34.91 C:\Database\WILEY275.L
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 78
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
2-Propanol (CAS) $$ Isopropyl alco 740 000067-63-0 9
hol $$ PRO $$ propan-2-ol $$ Isoho l $$ Propol $$ Lutosol
$$ Alcojel $$ Avantin $$ Imsol A $$ Petrohol $$
Hartosol $$ Avantine $$ Takineo col $$ i-Propanol $$
Isopropanol $ $ Alcosolve 2 $$ Isopropenol $$ Co
mbi-Schutz $$ Iso
2-Propanol (CAS) $$ Isopropyl alco 741 000067-63-0 9
hol $$ PRO $$ propan-2-ol $$ Isoho l $$ Propol $$ Lutosol
$$ Alcojel $$ Avantin $$ Imsol A $$ Petrohol $$
Hartosol $$ Avantine $$ Takineo col $$ i-Propanol $$
Isopropanol $
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$ Alcosolve 2 $$ Isopropenol $$ Co
mbi-Schutz $$ Iso

5 3.710 0.45 C:\Database\WILEY275.L
Butanoic acid, ethyl ester (CAS) $ 13032 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13033 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl

butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13022 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth yl
ester $$ Butyr
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

6 3.812 0.14 C:\Database\Flavor2.L
isobutyl alcohol 62 000078-83-1 1

7 3.858 0.66 C:\Database\WILEY275.L
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7806 000108-11-2 59
ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty 1
alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7805 000108-11-2 45
ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty 1
alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7807 000108-11-2 45

ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty l
alcohol $$ 1,3-Dimethyl-1-butano ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

l $$ 4-methyl 2-p

8 4.433 0.19 C:\Database\WILEY275.L
ETHYL 2-METHYLBUTYRATE 20970 000000-00-0
64 Butanoic acid, 2-methyl-, ethyl es 20735 007452-79-1 64
ter (CAS) $$ Ethyl 2-methylbutyrat e $$ Ethyl 2-
methylbutanoate $$ Et hyl .alpha.-methylbutyrate $$ Buty
ric acid, 2-methyl-, ethyl ester $
$ 2-Methylbutanoic acid ethyl este
Ethanamine, N-ethyl-N-nitroso- (CA 7394 000055-18-5 47
S) $$ Diethylnitrosamine $$ DENA $
$ N-Nitrosodiethylamine $$ Diethyl
nitrosamide $$ Nitrosodiethylamine $$
N,N-Diethylnitrosoamine $$ Die
thylamine, N-nitroso- $$ N-Nitroso -
N,N-diethylamine $$ N-Ethyl-N-nit
roso-ethylamine $

9 4.526 0.23 C:\Database\WILEY275.L
CIS 3 HEXENYL CIS 3 HEXENOATE $$ 3 80892 061444-38-0 64
-Hexenoic acid, 3-hexenyl ester, (
Z,Z)- $$ cis-3-Hexenyl cis-3-hexen oate
Cyclopentene, 4-methyl- (CAS) $$ 4 2469 001759-81-5 64
-Methylcyclopentene $$ 1-Methyl-3
cyclopentene
3-Hexen-1-ol, formate, (Z)- (CAS) 19161 033467-73-1 64
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$$ cis-3-Hexenyl formate $$ cis-.b
eta.-Hexenyl formate $$ cis-3-Hexe n-1-ol
formate $$ .beta.,.gamma.-H exenyl
methanoate

10 4.682 0.22 C:\Database\Flavor2.L
No matches found

11 4.736 0.27 C:\Database\WILEY275.L
Formic acid, hexyl ester (CAS) $$ 20854 000629-33-4 64
n-Hexyl formate $$ Hexyl formate $
$ n-Hexyl methanoate
1-HEXANOL 7890 000000-00-0 64
Cyclopentane, methyl- (CAS) $$ Met 2975 000096-37-7 64
hylcyclopentane $$ UN 2298

12 4.855 0.22 C:\Database\WILEY275.L
1-Butanol, 3-methyl-, acetate (CAS 20836 000123-92-2 72
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac
5H-Dibenzo[a,d]cycloheptene-5-prop 147195 000438-60-8 40
anamine, N-methyl- (CAS) $$ PROTRI PTYLINE
(ANTIDEPRESSANT) $$ MK 240
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$$ Triptil $$ Amimetilina $$ Prot
riptyline $$ Protryptyline $$ 5-(3 -

Methylaminopropyl)-5H-dibenzo[a,d
]cycloheptene $$ 5H-Dibenzo[a,d]cy
cloheptene-5-prop
1-Butanol, 3-methyl-, acetate (CAS 20833 000123-92-2 32
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac

13 4.886 0.16 C:\Database\Flavor2.L
2-Heptanol 180 000543-49-7 9
2-Methylbutylacetate 121 000624-41-9 9
Pyruvic acid; 2-oxopropanoic acid 393 000127-17-3 5

14 6.416 2.30 C:\Database\Flavor2.L
Lauryl acetate 7 000112-66-3 10
Ethyl acetate 92 000141-78-6 1
Hexyl acetate 299 000142-92-7 1

15 6.493 0.20 C:\Database\WILEY275.L
1,2-Ethanediol, 1-(2-phenyl-1,3,2- 92999 074807-80-0 50
dioxaborolan-4-yl)-, [S-(R*,R*)]-
(CAS) $$ L-THREIT, 1,2-O-(PHENYLBO
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

RANDIYL)- $$ 1,2-Ethanediol, 1-(2
phenyl-1,3,2-dioxaborolan-4-yl)-, [s-
(R@,R@)]- $$ 1,3,2-Dioxaborolan e, 1,2-
ethanediol deriv.
Propylamine, N,N,2,2-tetramethyl-, 21449 013993-87-8 47
N-oxide (CAS) $$ DIMETHYL-NEOPENT
YLAMINE OXIDE
Propanoic acid, 2-mercapto-, ethyl 22676 019788-49-9 45
ester (CAS) $$ Ethyl 2-mercaptopr opionate $$ ETHYL
MERCAPTOPROPIONA

TE $$ 2-THIOPROPANOIC ACID, ETHANO
L ESTER $$ Propionic acid, 2-merca pto-,
ethyl ester $$ ethyl 2-merca ptopropanoate $$
Ethyl 2-thiolprop anoate $$ Ethyl .

16 6.824 0.14 C:\Database\WILEY275.L
Undecanoic acid, ethyl ester (CAS) 99805 000627-90-7 64
$$ Ethyl undecylate $$ Ethyl unde
canoate $$ n-Undecanoic acid ethyl
ester
ETHYL CAPROATE $$ ETHYL N-HEXANOAT 31178 000123-66-0 53
3-methylbutyl 3-acetylpropanoate 70785 000000-00-0 38

17 7.042 0.11 C:\Database\WILEY275.L
HEXYL ACETATE 31189 000142-92-7 78
Acetic acid, hexyl ester (CAS) $$ 31085 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$$ Hexyl acetate $$ Hexyl ethanoa
te $$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate
$$ Acetic acid n-hexyl ester $$ n-
Hexyl ethanoate $$ Hexy
l alcohol, acetat
N-HEXYL ACETATE 31177 000142-92-7 59

18 7.904 0.09 C:\Database\WILEY275.L
Propanedioic acid, diethyl ester (45055 000105-53-3 80
CAS) $$ Diethyl malonate $$ Maloni
c ester $$ Dicarbethoxymethane $$
Ethyl malonate $$ Diethyl propaned
ioate $$ Carbethoxyacetic ester $$
Malonic acid diethyl ester $$ Mal onic
acid, diethyl ester $$ Methan
edicarboxylic aci
Propanedioic acid, diethyl ester (45053 000105-53-3 72

CAS) $$ Diethyl malonate $$ Maloni
c ester $$ Dicarbethoxymethane $$
Ethyl malonate $$ Diethyl propaned
ioate $$ Carbethoxyacetic ester $$
Malonic acid diethyl ester $$ Mal onic
acid, diethyl ester $$ Methan
edicarboxylic aci
Propanedioic acid, ethyl-, bis(1-m 129352 057983-52-5 42
ethylpropyl) ester (CAS)

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
19	8.153	0.42	C:\Database\WILEY275.L ALLYL CAPROATE $$ ALLYL HEXANOATE	42257	000123-68-2	78
			Hexanoic acid, 2-propenyl ester (C	42081	000123-68-2	72
			AS) $$ Allyl caproate $$ PROP-2-EN YL HEXANOATE $$ Allyl hexanoate $$ Hexanoic acid, allyl ester $$ 2-P ropenyl hexanoate $$ 2-Propenyl n hexanoate $$ Allylester kyseliny k apronove			
			Hexanoic acid, 2-propenyl ester (C	42080	000123-68-2	64
			AS) $$ Allyl caproate $$ PROP-2-EN YL HEXANOATE $$ Allyl hexanoate $$ Hexanoic acid, allyl ester $$ 2-P ropenyl hexanoate $$ 2-Propenyl n hexanoate $$ Allylester kyseliny k apronove			
20	8.467	0.14	C:\Database\Flavor2.L No matches found			
21	8.680	0.25	C:\Database\Flavor2.L No matches found			
22	9.476	8.50	C:\Database\WILEY275.L Benzoic acid (CAS) $$ Retardex $$	15536	000065-85-0	90
			HA 1 $$ Tenn-Plas $$ Retarder BA $			

$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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arboxybenzene $$ Benzoate $$ Benzo esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15527 000065-85-0 90
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15529 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

23 9.592 0.34 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15528 000065-85-0 80
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

henylformic acid $$ Benzeneformic
acid $$ Phenylcar
2-CHLOROETHYL BENZOATE 68348 000000-00-0 72
Benzoic acid (CAS) $$ Retardex $$ 15531 000065-85-0 64
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

24 9.663 0.21 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15526 000065-85-0 50
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15528 000065-85-0 49
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15538 000065-85-0 47
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C

arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

25 9.935 0.18 C:\Database\WILEY275.L
2 METHYL THIO 5 METHYL PYRAZINE 27394 000000-00-0 52
Pyrazine, 2-methyl-6-(methylthio)- 27391 002884-13-1 52
(CAS) $$ 2-Methylthio-6-methylpyr
azine
2-Hydroxy-5-nitropyridine (CAS) $$ 27300 005418-51-9 43
5-Nitro-2-hydroxypyridine $$ 5-Ni
tro-2-pyridinol $$ 5-Nitro-2-pyrid
inone $$ 5-Nitro-2(1H)-pyridinone $$
5-Nitro-2-pyridone $$ 5-Nitro-2 (1H)-
pyridone $$ 2-Pyridinol, 5-ni tro- $$ 5-
Nitro-2-pyridol $$ 2(1H)
-Pyridinone, 5-ni

26 10.530 0.40 C:\Database\WILEY275.L
Glycine, ethyl ester hydrochloride 7971 000000-00-0 53
Silane, ethoxytrimethyl- (CAS) $$ 14027 001825-62-3 40
ETHANOL TMS ETHER $$ TRIMETHYL-ETH
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

OXYSILANE $$ ETHANOL TRIMETHYLSILY
L ETHER $$ Trimethylethoxysilane $
$ Ethoxytrimethylsilane $$ Ethyl t
rimethylsilyl ether $$ Silane, tri
methylethoxy- $$ Trimethylsilyl et
hyl ether $$ Trim
Silane, ethoxytrimethyl- (CAS) $$ 14024 001825-62-3 40
ETHANOL TMS ETHER $$ TRIMETHYL-ETH
OXYSILANE $$ ETHANOL TRIMETHYLSILY
L ETHER $$ Trimethylethoxysilane $
$ Ethoxytrimethylsilane $$ Ethyl t
rimethylsilyl ether $$ Silane, tri
methylethoxy- $$ Trimethylsilyl et

hyl ether $$ Trim

27 11.233 19.40 C:\Database\Flavor2.L
Quinoline 174 000091-22-5 4
3-Hexenoic acid 36 004219-24-3 2

28 11.338 0.16 C:\Database\WILEY275.L
Cyclohexene, 3-methyl-6-(1-methyle 26757 001124-26-1 50
thyl)-, trans- (CAS) $$ trans-p-Me
nth-2-ene $$ p-Menth-2-ene, trans $$ (+)-
TRANS-P-MENTH-2-ENE $$ tra ns-3-
Isopropyl-6-methylcyclohexene
Camphane $$ Bicyclo[2.2.1]heptane, 26814 000464-15-3 49
1,7,7-trimethyl- (CAS) $$ Bornane
$$ Bornylane $$ 1,7,7-Trimethylbi
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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cyclo[2.2.1]heptane
.+/-.-4-Acetyl-1-methylcyclohexene 26627 070286-20-3 49
$$ Ethanone, 1-(4-methyl-3-cycloh
exen-1-yl)-, (.+-.)
29 11.935 1.38 C:\Database\WILEY275.L
1,2,3-Propanetriol, triacetate (CA 102718 000102-76-1 53
S) $$ Triacetin $$ Glycerol triace
tate $$ Vanay $$ Glyped $$ Enzacti n
$$ Triacetine $$ Fungacetin $$ A cetin,
tri- $$ Kesscoflex TRA $$ G lycerin
triacetate $$ Glyceryl tri acetate $$
1,2,3-Propanetriol tria cetate $$
Glycero
1,2,3-Propanetriol, triacetate (CA 102717 000102-76-1 43
S) $$ Triacetin $$ Glycerol triace
tate $$ Vanay $$ Glyped $$ Enzacti n
$$ Triacetine $$ Fungacetin $$ A cetin,
tri- $$ Kesscoflex TRA $$ G lycerin
triacetate $$ Glyceryl tri acetate $$
1,2,3-Propanetriol tria cetate $$
Glycero

TRIACETIN 102723 000102-76-1 43

30 12.159 24.27 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47269 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47262 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Nicotine $$ Black leaf $$ Black le 47308 016760-37-5 94
af 40 $$ Destruxol orchid spray $$
Emo-nik $$ ENT 3,424 $$ Flux maag $$
Fumetobac $$ Mach-nic $$ 1-Met hyl-2-
(3-pyridyl)pyrrolidine $$ 3 (N-
Methylpyrrolidino)pyridine $$ L
-3-(1-Methyl-2-pyrrolidyl)pyridine
$$ (-)-3-(1-Meth

31 13.171 0.14 C:\Database\Flavor2.L
Allyl cyclohexyl propionate 372 002705-87-5 45
Isoborneol (Isomer 2) 85 000124-76-5 9
Allyl heptanoate 370 000142-19-8 8

32 26.689 0.24 C:\Database\Flavor2.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

No matches found

33 26.779 0.19 C:\Database\Flavor2.L
No matches found

34 26.864 0.15 C:\Database\Flavor2.L
No matches found

35 26.893 0.10 C:\Database\Flavor2.L
No matches found

36 27.066 0.31 C:\Database\WILEY275.L
N-ethyl-1,3-dithioisoindoline $$ 1 92199 035373-06-9 43
H-Isoindole-1,3(2H)-dithione, 2-et
hyl-
Spiro[cyclopenta[c]pyran-7(1H),2'- 149325 103384-82-3 43
[1,3]dioxane]-7a(4aH)-carboxylic a
cid, 1-oxo-, methyl ester, cis-
1H-Indole, 1-methyl-2-phenyl- (CAS 92599 003558-24-5 43
) $$ 1-Methyl-2-phenylindole $$ 2
Phenyl-N-methylindole $$ Indole, 1 -
methyl-2-phenyl- $$ N-Methyl-2-ph
enylindole

37 27.116 0.29 C:\Database\Flavor2.L
No matches found

38 27.323 0.19 C:\Database\Flavor2.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

No matches found

39 27.408 0.10 C:\Database\WILEY275.L
Methanol, [4-(1,1-dimethylethyl)ph 107650 054889-98-4 43
enoxy]-, acetate (CAS) $$ P-TERT-B
UTYLPHENOXYMETHYL ACETATE $$ METHY
L P-TERT-BUTYLPHENOXYACETATE
Cyclotrisiloxane, hexamethyl- (CAS 106844 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
1,3-dimethyl-4-azaphenanthrene 92616 000000-00-0 43

40 27.491 0.22 C:\Database\WILEY275.L
Hexahydropyridine, 1-methyl-4-[4,5 92495 000000-00-0 42
-dihydroxyphenyl]-
N-METHYLDEACETYLCOLCHICINE $$ Benz 222417 000477-30-5
32 o[a]heptalen-9(5H)-one, 6,7-dihydr o-1,2,3,10-
tetramethoxy-7-(methyla mino)-, (S)- (CAS) $$ NSC-3096 $$
NSC 3096 $$ Omain $$ Omaine $$ Kol kamin $$ Colcemid $$
Colchamin $$ Kolchamin $$ Colchamine $$ Demecol
cine $$ Ciba 1266
Cyclotrisiloxane, hexamethyl- (CAS 106848 000541-05-9 30
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer

41 27.539 0.12 C:\Database\Flavor2.L
No matches found

42 27.646 0.13 C:\Database\Flavor2.L
No matches found

43 27.941 0.11 C:\Database\WILEY275.L

Dibenzoxazabicycloundecane $$ 1H-2 206379 087166-99-2 43
,6,10-(Epoxymethyno)-3-benzazacycl
ododecine, 2,3,4,5-tetrahydro-9,12
,13-trimethoxy-3-methyl-, (+)- (CA
S)
Cyclotrisiloxane, hexamethyl- (CAS 106844 000541-05-9 35
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
1,3-dimethyl-4-azaphenanthrene 92616 000000-00-0 30

B6: Sour Candy Library Search

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.231	1.16	C:\Database\WILEY275.L Pentane, 3-chloro- (CAS) $$ 3-Chlo ropentane $$ 1-Ethylpropyl chlorid Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2 -methylbutane $$ tert-Pentyl chlor $$ Tertiary pentyl chloride $$ Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methy 2-chlorobutane $$ 2-Chloro-2-met hyl-butane Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2 -methylbutane $$ tert-Pentyl chlor $$ Tertiary pentyl chloride $$ Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methy 2-chlorobutane $$ 2-Chloro-2-met hyl-butane	8537 8548 8552	000616-20-6 000594-36-5 000594-36-5	64 64 50
2	2.379	0.30	C:\Database\WILEY275.L 3-Penten-2-ol (CAS) $$ 2-PENTEN-4- OL $$ Methyl propenyl carbinol $$ Dimethylallyl alco hol $$ PENT-3-EN-2-OL $$ 3-Penten ol,cis+trans 4-Penten-2-ol (CAS) $$ PENT-4-EN-2 -OL $$ 1-Penten-4-ol $$ 4-Hydroxyp	3379 3393	001569-50-2 000625-31-0	78 72

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint2.e

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

ent-1-ene $$ CH2=CHCH2CH(OH)CH3
3-Buten-2-ol, 2-methyl- (CAS) $$ 2 3412 000115-18-4 72
-methyl-3-buten-2-ol $$ Dimethylvi
nylcarbinol $$ Vinyldimethylcarbin ol
$$ Dimethylvinylmethanol $$ 1,1 -
Dimethyl-2-propenol $$ 1,1-Dimeth
ylallyl alchol $$ 1,1-Dimethylally l
alcohol $$ .alpha.,.alpha.-Dimet
hylallyl alcohol

3 2.943 43.24 C:\Database\WILEY275.L
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 78
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
PROPYLENE GLYCOL $$ 1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE
1,2-Propanediol (CAS) $$ Propylene 2016 000057-55-6 64
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ylethylene glycol

4 3.093 0.03 C:\Database\WILEY275.L
DIOXYLUCIFERIN $$ 4(5H)-Thiazolone 149073 037657-63-9 95
, 5-hydroxy-2-(6-hydroxy-2-benzoth
iazolyl)- (CAS)
2,3-Butanediol (CAS) $$ Butane-2,3 4367 000513-85-9 64

-diol $$ 2,3-BUTANDIOL $$ 2,3-Buty
lene glycol $$ 2,3-Dihydroxybutane $$
Dimethylethylene glycol $$ D-2 ,3-
Butane diol $$ Dimethylene glyc ol
URACIL, N,N'-BIS(METHOXYMETHYL)- 84362 000000-00-0 64

5 3.710 0.73 C:\Database\WILEY275.L
Butanoic acid, ethyl ester (CAS) $ 13024 000105-54-4 83
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13026 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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yl ester of butanoic acid $$ Ethyl n-butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13033 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr

6 3.812 0.17 C:\Database\WILEY275.L
2-Hydroxy-2,4-dimethyl-3-pentanone 20912 003212-67-7 52
(CAS) $$ 3-Pentanone, 2-hydroxy-2
,4-dimethyl-

1-Butanol, 3-methoxy- (CAS) $$ 3-M 8218 002517-43-3 50
ethoxy-1-butanol $$ 3-Methoxybutan
ol $$ Methoxybutanol
2-Propanol, 1-methoxy-2-methyl- (C 8230 003587-64-2 50
AS) $$ 1-METHOXY-2-METHYL-2-PROPAN
OL $$ 1,1-Dimethyl-2-methoxyethano

7 3.858 0.49 C:\Database\WILEY275.L
2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7752 000626-93-7 59
$$ n-Butylmethylcarbinol $$ Hexan
ol-(2) $$ sec-Hexyl alcohol
Butane, 1,2,4-trimethoxy- (CAS) $$ 33685 020637-48-3 42
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

BUTANE-1,2,4-TRIOL-TRIMETHYL ETHE
R $$ DL-1,2,4-TRIMETHOXYBUTANE $$
1,2,4-TRIMETHOXY-BUTANE
2-Heptadecanol (CAS) $$ HEPTADECAN 141161 016813-18-6 39
OL-2

8 4.524 0.33 C:\Database\WILEY275.L
1,1'-AZOXY-BIS-(2.ALPHA.-CHLORO-TR 247218 072193-56-7 62
ANS,TRANS-5,9-CYCLODODECADIENE) $$
Diazene, bis(12-chloro-4,8-cyclod
odecadien-1-yl)-, 1-oxide, [1R*(1R
,4E,8E,12R),4E,8E,12R*]- (CAS) $
$ Cyclododecane, diazene deriv. (C
AS)
Cyclopentene, 3-methyl- (CAS) $$ 3 2465 001120-62-3 58
-Methylcyclopentene
Bicyclo[3.1.0]hexane (CAS) $$ Nort 2483 000285-58-5 53
hujane $$ Norsabinane

9 4.889 0.08 C:\Database\WILEY275.L
3-Ethyl-2-heptanol 31510 019780-39-3 47
Ethane, 1,2-diethoxy- (CAS) $$ 1,2 14171 000629-14-1 47
-Diethoxyethane $$ Glyme-1 $$ Diet
hyl cellosolve $$ 2-Ethoxyethyl et hyl

ether $$ Ethylene glycol dieth yl ether
$$ diethoxyethane $$ Diet hylether
ethylenglykolu $$ Ethyl g lyme $$ UN
1153
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			2,3-O-Cyclohexylidene-4-C-(2-metho	202096	085254-54-2	47
			xymethoxyphenyl)-D-ribo-tetronolac			
			tones $$ Spiro[cyclohexane-1,2'-fu			
			ro[3,4-d][1,3]dioxol]-4'(3'aH)-one ,			
			dihydro-6'-[2-(methoxymethoxy)ph			
			enyl]-, [3'aR-(3'a.alpha.,6'.alpha			
			.,6'a.alpha.)]- (CAS)			
10	6.246	0.14	C:\Database\WILEY275.L			
			1-Propanone, 3-[[(methylthio)methy	142040	055030-38-1	42
			l]sulfonyl]-1-phenyl- (CAS) $$ 3-(			
			METHYLTHIOMETHYLSULPHONYL)PROPIOPH			
			ENONE			
			2,6-Dihydroxy-7-methylpurine $$ 7-	50367	000552-62-5	36
			Methylxanthine $$ 1H-Purine-2,6-di			
			one, 3,7-dihydro-7-methyl- $$ Hete			
			roxanthin $$ Heteroxanthine $$ Xan thine,			
			7-methyl- $$ 7-Methylxanthi			
			Ethanol, 2,2'-thiobis- (CAS) $$ DI	15424	000111-48-8	36
			ETHYL 2,2-DIHYDROXY SULFIDE $$			
			2,2 '-Thiodiethanol $$ Tedegyl $$ Thio			
			diglycol $$ Thiodiethanol $$ Kromf ax			
			Solvent $$ 2,2'-Thiodiglycol $$ 2,2'-			
			Thiobisethanol $$ .beta.-Thi odiglycol $$			
			Thiodiethylene glycol			
			$$ Ethanol, 2,2'			
11	6.359	0.69	C:\Database\Flavor2.L			

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Isopropyl acetate	268	000108-21-4	1
Ethyl acetate				92	000141-78-6	1
n-Propyl acetate				227	000109-60-4	1
12	6.391	0.49	C:\Database\WILEY275.L			
			1,2,3-Propanetriol (CAS) $$ Glycer	4509	000056-81-5	50
ol $$ Glyrol $$ Glycerin $$ Osmogl				yn $$ Glysanin $$		
Glycerine $$ Gly			ceritol $$ Glycyl alcohol $$ Trihy			
droxypropane $$ Propanetriol $$ Gl				ycerin suppositories $$		
1,2,3-Trih			ydroxypropane $$ Propantriol $$ Sy			
			nthetic glycerin			
			1,2,3-Propanetriol (CAS) $$ Glycer	4512	000056-81-5	39
ol $$ Glyrol $$ Glycerin $$ Osmogl				yn $$ Glysanin $$		
Glycerine $$ Gly			ceritol $$ Glycyl alcohol $$ Trihy			
droxypropane $$ Propanetriol $$ Gl				ycerin suppositories $$		
1,2,3-Trih			ydroxypropane $$ Propantriol $$ Sy			
			nthetic glycerin			
			Propane, 2-fluoro-2-methyl- (CAS)	2067	000353-61-7	39
			$$ 2-Fluoro-2-methylpropane $$ ter			
			t-Butyl fluoride			
13	6.824	0.11	C:\Database\WILEY275.L			
			ETHYL CAPROATE $$ ETHYL N-HEXANOAT	31178	000123-66-0	53
			Undecanoic acid, ethyl ester (CAS)	99805	000627-90-7	43

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			$$ Ethyl undecylate $$ Ethyl unde			
			canoate $$ n-Undecanoic acid ethyl			
			ester			
			Phenol-d5	4841	000000-00-0	38
14	7.388	0.24	C:\Database\WILEY275.L			

dl-Limonene $$ Cyclohexene, 1-meth 25064 000138-86-3 95
yl-4-(1-methylethenyl)- (CAS) $$ 1
-P-MENTHA-1,8-DIENE $$ Limonene $C
inen $$ Nesol $$ Cinene $$ Limonen $$
Eulimen $$ Dipenten $$ Cajeput en $$
Kautschin $$ Cajeputene $$. alpha.-
Limonene $$ p-Mentha-1,8-di
ene $$ 4-Isoprope dl-Limonene $$ Cyclohexene, 1-
meth 25059 000138-86-3 95
yl-4-(1-methylethenyl)- (CAS) $$ 1
-P-MENTHA-1,8-DIENE $$ Limonene $C
inen $$ Nesol $$ Cinene $$ Limonen $$
Eulimen $$ Dipenten $$ Cajeput en $$
Kautschin $$ Cajeputene $$. alpha.-
Limonene $$ p-Mentha-1,8-di
ene $$ 4-Isoprope dl-Limonene $$ Cyclohexene, 1-
meth 25055 000138-86-3 95
yl-4-(1-methylethenyl)- (CAS) $$ 1
-P-MENTHA-1,8-DIENE $$ Limonene $C
inen $$ Nesol $$ Cinene $$ Limonen $$
Eulimen $$ Dipenten $$ Cajeput en $$
Kautschin $$ Cajeputene $$.
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

alpha.-Limonene $$ p-Mentha-1,8-di
ene $$ 4-Isoprope

15 9.462 5.25 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15531 000065-85-0 91
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15527 000065-85-0 83
HA 1 $$ Tenn-Plas $$ Retarder BA $

$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15538 000065-85-0 81
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic acid
$$ Phenylcar
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

16 9.618 0.08 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15526 000065-85-0 46
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid, ammonium salt (CAS) 15545 001863-63-4 46
$$ Ammonium benzoate
1,2,4-Trioxolane, 3-phenyl- (CAS) 37194 023253-30-7 45
$$ STYRENE OZONIDE $$ 3-Phenyl-1,2
,4-trioxolane $$ Benzene, ethenyl
, ozonide

17 9.720 0.26 C:\Database\WILEY275.L
L-(-)-Menthol $$ Cyclohexanol, 5-m 42602 002216-51-5 64
ethyl-2-(1-methylethyl)-, [1R-(1.a
lpha.,2.beta.,5.alpha.)]- (CAS) $$ (-
)-Menthol $$ l-Menthol $$ (R)-(

-)-Menthol $$ Menthol, (1R,3R,4S)-
(-)- $$ (-)-Menthyl alcohol $$ U.s
.p. menthol $$ 1-Menthol $$ (1R,3R
,4S)-(-)-MENTHOL
1-Methyl-bicyclo[4.1.1]octan-7-one 26562 005212-78-2 49
$$ Bicyclo[4.1.1]octan-7-one, 1-m
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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ethyl-
Cyclohexane, 1-methyl-4-(1-methyle 26782 001124-25-0 46
thenyl)-, trans- (CAS) $$ TRANS-8
MENTHENE $$ trans-p-Menth-8-ene $$ p-
Menth-8-ene, trans- $$ trans-1 Isopropenyl-
4-methylcyclohexane

18 9.932 0.40 C:\Database\WILEY275.L
4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27524 004940-11-8 50
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$ 3-
Hydroxy-2-ethyl-4-pyrone $$ 3-Hy droxy-2-ethyl-1,4-
pyrone $$ 3-Hydr oxy-2-ethyl-.gamma.-pyrone $$ 2-Et
hyl-3-hydroxy-4H-pyran-4-one $$ 3 Hydroxy-2-ethyl-4
ETHYL MALTOL 27547 004940-11-8 50
2 METHYL THIO 5 METHYL PYRAZINE 27394 000000-00-0 46

19 11.230 17.11 C:\Database\Flavor2.L
Quinoline 174 000091-22-5 7
3-Hexenoic acid 36 004219-24-3 2

20 11.451 0.35 C:\Database\Flavor2.L
No matches found

21 11.941 0.40 C:\Database\WILEY275.L
1,2,3-Propanetriol, triacetate (CA 102717 000102-76-1 86
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			S) $$ Triacetin $$ Glycerol triace			
tate $$ Vanay $$ Glyped $$ Enzacti				n		
$$ Triacetine $$ Fungacetin $$ A				cetin,		
tri- $$ Kesscoflex TRA $$ G				lycerin		
triacetate $$ Glyceryl tri				acetate $$		
1,2,3-Propanetriol tria						
			cetate $$ Glycero			
			TRIACETIN	102723	000102-76-1	64
			1,2,3-Propanetriol, triacetate (CA	102716	000102-76-1	56
			S) $$ Triacetin $$ Glycerol triace			
tate $$ Vanay $$ Glyped $$ Enzacti				n		
$$ Triacetine $$ Fungacetin $$ A				cetin,		
tri- $$ Kesscoflex TRA $$ G				lycerin		
triacetate $$ Glyceryl tri				acetate $$		
1,2,3-Propanetriol tria				cetate $$		
Glycero						
22	12.162	23.14	C:\Database\WILEY275.L			
			Pyridine, 3-(1-methyl-2-pyrrolidin	47262	000054-11-5	94
			yl)-, (S)- (CAS) $$ Nicotine $$ 1-			
			METHYL-2-(3-PYRIDYL)-PYRROLIDINE			
$			$ Flux Maag $$ L-Nicotine $$ (-)-N			
icotine $$ XL All Insecticide $$ 3				-(N-		
Methylpyrollidino)pyridine $$						
			Nicotin $$ S-(-)-Nicotine $$ (-)-3			
			-(N-Methylpyrroli			
			Pyridine, 3-(1-methyl-2-pyrrolidin	47256	000054-11-5	93
yl)-, (S)- (CAS) $$ Nicotine $$ 1-						

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			METHYL-2-(3-PYRIDYL)-PYRROLIDINE			
$			$ Flux Maag $$ L-Nicotine $$ (-)-N			

icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47264 000054-11-5 91
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli

23 24.595 0.19 C:\Database\WILEY275.L
1-[(2-trimethylsiloxy)vinyl]-4-tri 161524 126210-57-9
43 methylsiloxy-2,6-dideuteriobenzene $$
Silane, trimethyl[4-[1-[(trime
thylsilyl)oxy]ethenyl]phenoxy-2,6
d2]-
1,1,1,3,5,5,5-Heptamethyltrisiloxa 106885 001873-88-7 38
ne $$ Bis(trimethylsiloxy)methylsi
lane $$ Hydromethylsiloxane $$ Tri
siloxane, 1,1,1,3,5,5,5-heptamethy
l-
4' METHYL-2 PHENYLINDOLE 92601 000000-00-0 27

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

24 24.974 0.14 C:\Database\Flavor2.L
No matches found

25 25.963 0.07 C:\Database\Flavor2.L
No matches found

26 26.139 0.20 C:\Database\Flavor2.L
No matches found

27 26.334 0.18 C:\Database\WILEY275.L

Hexahydropyridine, 1-methyl-4-[4,5 92495 000000-00-0 46
-dihydroxyphenyl]-
Cyclotrisiloxane, hexamethyl- (CAS 106844 000541-05-9 38
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
3,4-di(4-trimethylsiloxyphenyl)hex 239950 000000-00-0 35
ane

28 26.465 0.08 C:\Database\Flavor2.L
No matches found

29 26.496 0.15 C:\Database\Flavor2.L
No matches found

30 26.640 0.41 C:\Database\Flavor2.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

No matches found

31 26.796 0.22 C:\Database\Flavor2.L
No matches found

32 26.915 0.24 C:\Database\Flavor2.L
No matches found

33 27.040 0.21 C:\Database\Flavor2.L
No matches found

34 27.108 0.12 C:\Database\Flavor2.L
No matches found

35 27.153 0.27 C:\Database\WILEY275.L
Dibenzoxazabicycloundecane $$ 1H-2 206379 087166-99-2 43
,6,10-(Epoxymethyno)-3-benzazacycl
ododecine, 2,3,4,5-tetrahydro-9,12
,13-trimethoxy-3-methyl-, (+)- (CA

S)
Arsenous acid, tris(trimethylsilyl 206537 055429-29-3 38
) ester (CAS) $$ TRIMETHYLSILYL AR
SINATE
BENZENE, 1,4-BIS(TRIMETHYLSILYL)- 107558 000000-00-0 32

36 27.253 0.34 C:\Database\Flavor2.L
No matches found

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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37 27.391 0.17 C:\Database\Flavor2.L
No matches found

38 27.448 0.22 C:\Database\Flavor2.L
No matches found

39 27.558 0.37 C:\Database\Flavor2.L
No matches found

40 27.627 0.10 C:\Database\WILEY275.L
Cyclotrisiloxane, hexamethyl- (CAS 106844 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
Cyclotrisiloxane, hexamethyl- (CAS 106848 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
Cyclotrisiloxane, hexamethyl- (CAS 106849 000541-05-9 38
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
41	27.675	0.53	C:\Database\Flavor2.L No matches found			
42	27.805	0.14	C:\Database\Flavor2.L No matches found			
43	27.836	0.07	C:\Database\Flavor2.L No matches found			
44	27.890	0.36	C:\Database\Flavor2.L No matches found			

B7: Tropical Rainbow Blast Library Search

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.237	1.26	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8553	000594-36-5	64
			Butane, 2-chloro-2-methyl- (CAS) $ $ tert-Amyl chloride $$ 2-Chloro-2-methylbutane $$ tert-Pentyl chloride $$ Tertiary pentyl chloride $$ 2-Methyl-2-chlorobutane r $$ 1,1 Dimethylpropyl chloride $$ 2-Methyl-2-chlorobutane $$ 2-Chloro-2-methyl-butane	8548	000594-36-5	64
			4,4-Dimethyl-1-hexene $$ 1-Hexene, 4,4-dimethyl	11209	001647-08-1	43
2	2.382	0.33	C:\Database\WILEY275.L 3-Penten-2-ol (CAS) $$ 2-PENTEN-4-OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-Dimethylallyl alcohol $$ PENT-3-EN-2-OL $$ 3-Penten-2-ol,cis+trans	3386	001569-50-2	78
			3-Penten-2-ol (CAS) $$ 2-PENTEN-4-OL $$ Methyl propenyl carbinol $$	3385	001569-50-2	78

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

.alpha.,.gamma.-Dimethylallyl alco
hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-
ol,cis+trans
4-Penten-2-ol (CAS) $$ PENT-4-EN-2 3393 000625-31-0 78
-OL $$ 1-Penten-4-ol $$ 4-Hydroxyp
ent-1-ene $$ CH2=CHCH2CH(OH)CH3

3 2.954 33.20 C:\Database\WILEY275.L
PROPYLENE GLYCOL $$ 1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 56
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
2-Propanol (CAS) $$ Isopropyl alco 740 000067-63-0 9
hol $$ PRO $$ propan-2-ol $$ Isoho 1 $$ Propol $$ Lutosol
$$ Alcojel $$ Avantin $$ Imsol A $$ Petrohol $$
Hartosol $$ Avantine $$ Takineo col $$ i-Propanol $$
Isopropanol $ $ Alcosolve 2 $$ Isopropenol $$ Co
mbi-Schutz $$ Iso

4 3.710 0.44 C:\Database\WILEY275.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ETHYLBUTANOATE 13286 000000-00-0 72
Butanoic acid, ethyl ester (CAS) $ 13025 000105-54-4 72
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr

ETHYL BUTANOATE $$ ETHYL BUTYRATE 13265 000105-54-4 70

5 3.812 0.15 C:\Database\WILEY275.L
Butanoic acid, 2-hydroxy-, ethyl e 21827 052089-54-0 40
ster (CAS) $$ ETHYL 2-HYDROXY
BUTY RATE $$ Ethyl .alpha.-hydroxybutyr
ate $$ ETHYL 2 HYDROXY BUTYRATE
2-Pentanol, 2-methyl- (CAS) $$ 2-M 7795 000590-36-3 40
ethyl-2-pentanol $$ 2-Hydroxy-2-me thylpentane $$ 1,1-
Dimethylbutanol $$ 2-Methyl-2-hydroxypentane $$ 2
-Methylpentan-2-ol $$ UN 2560
3-Ethyl-2-methyl-2-heptanol 44310 000000-00-0 40

6 3.861 0.70 C:\Database\WILEY275.L
2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7743 000626-93-7 59
$$ n-Butylmethylcarbinol $$ Hexan
ol-(2) $$ sec-Hexyl alcohol
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7806 000108-11-2 59
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ethyl-2-pentanol $$ MIC $$ MAOH $$ MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty l alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p
2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7752 000626-93-7 45
$$ n-Butylmethylcarbinol $$ Hexan
ol-(2) $$ sec-Hexyl alcohol

7 4.022 0.16 C:\Database\WILEY275.L
Eicosane (CAS) $$ n-Eicosane 163880 000112-95-8 43
Docosane (CAS) $$ n-Docosane $$ C2 186059 000629-97-0 43
2H46 STANDARD $$ Normal-docosane
2-Docosanone, 4,21,21-trimethyl-, 220142 018607-44-8 38
L-(-)- (CAS) $$ (-)-2-OXO-4L,21,21
-TRIMETHYLDOCOSANE

8 4.436 0.22 C:\Database\WILEY275.L
Silanamine, 1,1,1-trimethyl-N-[2-[162466 054965-31-0 50

4-[(trimethylsilyl)oxy]phenyl]ethy
l]- (CAS) $$ TYRAMINE-DITMS $$ 4-T
RIMETHYLSILYLOXYPHENETHYL-N-TRIMET
HYLSILYLAMINE $$ Phenylethanolamin
e, di(trimethylsilyl)-
BETA AMINO ISOBUTYRIC DI-TMS 131805 000000-00-0 40
Ethylene Thiourea 7325 000096-45-7 40
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

9 4.529 0.26 C:\Database\WILEY275.L
Cyclopentene, 1-methyl- (CAS) $$ 1 2461 000693-89-0 72
-Methylcyclopentene $$ 1-Methyl-1
cyclopentene $$ methylcyclopentene
$$ 1-Methyl-1-cyclopentane
Cyclopropane, 1,2-dimethyl-3-methy 2455 062338-02-7 72
lene- (CAS)
Cyclopentene, 1-methyl- (CAS) $$ 1 2460 000693-89-0 64
-Methylcyclopentene $$ 1-Methyl-1
cyclopentene $$ methylcyclopentene
$$ 1-Methyl-1-cyclopentane

10 4.685 0.20 C:\Database\Flavor2.L
No matches found

11 4.736 0.32 C:\Database\WILEY275.L
1-HEXANOL 7890 000000-00-0 59
1-Hexanol (CAS) $$ n-Hexanol $$ Am 7734 000111-27-3 59
ylcarbinol $$ n-Hexan-1-ol $$ Hexy
l alcohol $$ Hexanol $$ Pentylcarb inol $$
Caproyl alcohol $$ n-Hexyl alcohol $$ 1-
Hexyl alcohol $$ 1-H ydroxyhexane $$ n-
C6H13OH $$ Hexan
-1-ol $$ Hexanol-(1) $$ Epal 6 $$
UN 2282
1-Hexanol (CAS) $$ n-Hexanol $$ Am 7731 000111-27-3 59
ylcarbinol $$ n-Hexan-1-ol $$ Hexy
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

l alcohol $$ Hexanol $$ Pentylcarb inol $$ Caproyl alcohol $$ n-Hexyl alcohol $$ 1-Hexyl alcohol $$ 1-H ydroxyhexane $$ n-C6H13OH $$ Hexan -1-ol $$ Hexanol-(1) $$ Epal 6 $$ UN 2282

12 4.858 0.25 C:\Database\WILEY275.L
1-Butanol, 3-methyl-, acetate (CAS 20836 000123-92-2 72) $$ Isoamyl acetate $$ 3-METHYL B UTYL ACETATE $$ ETHANOIC ACID, 3-M ETHYL BUTANOL ESTER $$ Pear oil $$ Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$ Isopentyl acet ate $$ 3- Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20841 000123-92-2 72) $$ Isoamyl acetate $$ 3-METHYL B UTYL ACETATE $$ ETHANOIC ACID, 3-M ETHYL BUTANOL ESTER $$ Pear oil $$ Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$ Isopentyl acet ate $$ 3- Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20837 000123-92-2 56) $$ Isoamyl acetate $$ 3-METHYL B UTYL ACETATE $$ ETHANOIC ACID, 3-M ETHYL BUTANOL ESTER $$ Pear oil $$
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Banana oil $$ i-Amyl acetate $$ I soamyl ethanoate $$ Isopentyl acet ate $$

3-Methylbutyl acetate $$ 3 Methyl-1-
butyl ac

13 4.886 0.14 C:\Database\WILEY275.L
N,N-Dimethylformamide diisopropyl 59651 018503-89-4 43
acetal $$ N,N-Dimethylformamide di -i-propylacetal $$
Methanamine, N, N-dimethyl-1,1-bis(1-methylethoxy)
2-METHYL-BUTYL ACETATE 20932 000624-41-9 25
Isopentyl acetate $$ ISO AMYL ACET 20924 000123-92-2 25
ATE $$ PEAR ETHER

14 6.280 0.30 C:\Database\WILEY275.L
1,2,3-Propanetriol (CAS) $$ Glycer 4512 000056-81-5 45
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy
nthetic glycerin
Ethanol, 2-amino- (CAS) $$ Ethanol 789 000141-43-5 45
amine $$ MEA $$ ETHANOL-2-AMINE $$
Olamine $$ Colamine $$ Glycinol $
$ Aminoethanol $$ Ethylolamine $$
Thiofaco M-50 $$ 2-Aminoethanol $$
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Monoethanolamine $$ 2-Amino-l-eth
anol $$ 2-Aminoethan-1-ol $$ 2-Hyd
roxyethylamine $$
Ethanol, 2-[2-(2-mercaptoethoxy)et 50418 056282-36-1 45
hoxy]- (CAS) $$ MONOTHIOL TRIETHYL
ENE GLYCOL

15 6.453 2.10 C:\Database\WILEY275.L
1,2,3-Propanetriol (CAS) $$ Glycer 4509 000056-81-5 56
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy

nthetic glycerin
Tungsten, [1,2-bis(methylthio)etha 241194 038536-75-3 9
ne-S,S']tetracarbonyl-, (OC-6-22)-
(CAS) $$ .PI.-2,5-DITHIAHEXANE-TE
TRACARBONYL TUNGSTEN
NITROMETHANE 776 000000-00-0 9

16 6.824 0.10 C:\Database\Flavor2.L
delta-Octalactone 175 000698-76-0 32
Isoamyl hexanoate 371 002198-61-0 16
Ethyl valerate 141 000539-82-2 14

17 7.045 0.21 C:\Database\WILEY275.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

HEXYL ACETATE 31232 000000-00-0 78
Acetic acid, hexyl ester (CAS) $$ 31088 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
$$ Hexyl acetate $$ Hexyl ethanoa te
$$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate
$$ Acetic acid n-hexyl ester $$ n-
Hexyl ethanoate $$ Hexy
l alcohol, acetat
Acetic acid, hexyl ester (CAS) $$ 31085 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
$$ Hexyl acetate $$ Hexyl ethanoa te
$$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate
$$ Acetic acid n-hexyl ester $$ n-
Hexyl ethanoate $$ Hexy
l alcohol, acetat

18 7.076 0.11 C:\Database\WILEY275.L
1,1'-AZOXY-BIS-(2.ALPHA.-CHLORO-TR 247218 072193-56-7 87
ANS,TRANS-5,9-CYCLODODECADIENE) $$

Diazene, bis(12-chloro-4,8-cyclod
odecadien-1-yl)-, 1-oxide, [1R*(1R
,4E,8E,12R),4E,8E,12R*]- (CAS) $
$ Cyclododecane, diazene deriv. (C
AS)
2-Ethyl-1,3-butadiene 2440 000000-00-0 42
2-Hexyne (CAS) $$ Methyl(propyl)ac 2397 000764-35-2 38
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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etylene $$ 1-Methyl-2-propylacetyl
ene $$ Hex-2-yne $$ C3H7C.$.CCH3

19 7.385 0.12 C:\Database\WILEY275.L
Geranyl propionate $$ 2,6-Octadien 95768 000105-90-8 83
-1-ol, 3,7-dimethyl-, propanoate,(
E)- (CAS) $$ trans-3,7-Dimethyl-2,
6-octadienyl propionate $$ 2,6-Oct
adien-1-ol, 3,7-dimethyl-, propion ate,
(E)- $$ 2,6-Octadien-1-ol, 3, 7-
dimethyl-, propanoate, (E)- $$ g eranyl
propanoate
.DELTA.3-Carene $$ Bicyclo[4.1.0]h 25254 013466-78-9 64
ept-3-ene, 3,7,7-trimethyl- (CAS)
$$ (+)-3-CARENE $$ .delta.-3-caren e
$$ 3-Carene $$ .DELTA.(sup3)-Car ene
$$ CAR-3-ENE $$ D-3-carene $$ 3,7,7-
Trimethylbicyclo[4.1.0]hept 3-ene $$
.delta. 3-carene $$ 3,7,7
-Trimethylbicyclo
.GAMMA.-TERPINENE 25353 000099-85-4 45

20 7.904 0.17 C:\Database\WILEY275.L
2-PENTADECYL-4,6-DIMETHYL-1,3-DIOX 197138 056599-77-0 50
ANE (POLAR ISOMER)
DIETHYL MALONATE 45089 000105-53-3 38
Methyl 3-((methylsulphonyl)acetyl) 92723 076078-75-6 38
propanoate
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
21	8.153	0.50	C:\Database\WILEY275.L Hexanoic acid, 2-propenyl ester (C AS) $$ Allyl caproate $$ PROP-2-EN YL HEXANOATE $$ Allyl hexanoate $$ Hexanoic acid, allyl ester $$ 2-P ropenyl hexanoate $$ 2-Propenyl n hexanoate $$ Allylester kyseliny k apronove	42082	000123-68-2	86
			Hexanoic acid, 2-propenyl ester (C AS) $$ Allyl caproate $$ PROP-2-EN YL HEXANOATE $$ Allyl hexanoate $$ Hexanoic acid, allyl ester $$ 2-P ropenyl hexanoate $$ 2-Propenyl n hexanoate $$ Allylester kyseliny k apronove	42081	000123-68-2	78
			2-propenyl hexanoate	42234	000000-00-0	78
22	8.683	0.18	C:\Database\WILEY275.L Benzeneethanol (CAS) $$ Phenethyl alcohol $$ PEA $$ PHENETHYL ALCOLH OL $$ Phenethanol $$ .beta.-PEA $$ Benzyl carbinol $$ 2-Phenylethano l $$ Ethanol, 2-phenyl- $$ 2-Phene thyl alcohol $$ .beta.-Phenylethan ol $$ .beta.-Phenethyl alcohol $$ .beta.-Hydroxyeth	15786	000060-12-8	53
			Benzeneethanol (CAS) $$ Phenethyl	15785	000060-12-8	53

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

alcohol $$ PEA $$ PHENETHYL ALCOLH
OL $$ Phenethanol $$ .beta.-PEA $$
Benzyl carbinol $$ 2-Phenylethano 1 $$
Ethanol, 2-phenyl- $$ 2-Phene thyl alcohol
$$ .beta.-Phenylethan ol $$ .beta.-
Phenethyl alcohol $$
.beta.-Hydroxyeth
Benzeneethanol (CAS) $$ Phenethyl 15787 000060-12-8 52
alcohol $$ PEA $$ PHENETHYL ALCOLH
OL $$ Phenethanol $$ .beta.-PEA $$
Benzyl carbinol $$ 2-Phenylethano 1 $$
Ethanol, 2-phenyl- $$ 2-Phene thyl alcohol
$$ .beta.-Phenylethan ol $$ .beta.-
Phenethyl alcohol $$
.beta.-Hydroxyeth

23 9.499 9.09 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15531 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15538 000065-85-0 80
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo esaeure
GK $$ Benzoesaeure GV $$ P henylformic acid
$$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15537 000065-85-0 72
HA 1 $$ Tenn-Plas $$ Retarder BA $

$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

24 9.666 0.40 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15536 000065-85-0 58
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15525 000065-85-0 52
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

esaeure GK $$ Benzoesaeure GV $$ P henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15542 000065-85-0 52
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

25 9.726 0.10 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15538 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $

$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15537 000065-85-0 83
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

---

acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15531 000065-85-0 83
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

26 9.929 0.24 C:\Database\WILEY275.L
Benzaldehyde, 3-fluoro-4-hydroxy- 27440 000000-00-0 50
ETHYL MALTOL 27559 000000-00-0 45
4H-Pyran-4-one, 2-ethyl-3-hydroxy- 27523 004940-11-8 45
(CAS) $$ Ethyl maltol $$ VELTOL P
LUS $$ 2-Ethylpyromeconic acid $$ 3-
Hydroxy-2-ethyl-4-pyrone $$ 3-Hy droxy-2-ethyl-1,4-
pyrone $$ 3-Hydr oxy-2-ethyl-.gamma.-pyrone $$ 2-Et
hyl-3-hydroxy-4H-pyran-4-one $$ 3 Hydroxy-2-ethyl-4

27 10.530 0.32 C:\Database\Flavor2.L
No matches found

28 11.236 19.85 C:\Database\Flavor2.L
Quinoline 174 000091-22-5 7
3-Hexenoic acid 36 004219-24-3 2
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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29 11.346 0.12 C:\Database\WILEY275.L
(2,4,4,4,16,16-D6)-3.ALPHA.,17.BET 172140 000000-00-0 89
A.-DIHYDROXY-5.BETA.-ANDROSTANE
Cyclohexene, 4-methyl-1-(1-methyle 26769 000500-00-5 46
thyl)- (CAS) $$ 1-METHYL-4-ISOPROP
YL-3-CYCLOHEXENE $$ (-)-P-MENTH-3
ENE $$ 3-p-Menthene $$ p-Menth-3-e ne $$
Menthomenthene $$ .DELTA.3-p -Menthene
$$ 1-Isopropyl-4-methylc yclohexene $$ 4-
Methyl-1-(1-methyl
ethyl)cyclohexene
4,4-Dimethyl-5-ethylcyclopent-2-en 26394 081825-20-9 45
-1-one $$ 2-Cyclopenten-1-one, 5-e
thyl-4,4-dimethyl- (CAS)

30 11.935 1.45 C:\Database\WILEY275.L
1,2,3-Propanetriol, triacetate (CA 102718 000102-76-1 90
S) $$ Triacetin $$ Glycerol triace
tate $$ Vanay $$ Glyped $$ Enzacti n
$$ Triacetine $$ Fungacetin $$ A cetin,
tri- $$ Kesscoflex TRA $$ G lycerin
triacetate $$ Glyceryl tri acetate $$
1,2,3-Propanetriol tria cetate $$
Glycero
TRIACETIN 102723 000102-76-1 78
1,2,3-Propanetriol, triacetate (CA 102716 000102-76-1 56
S) $$ Triacetin $$ Glycerol triace
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

tate $$ Vanay $$ Glyped $$ Enzacti n $$ Triacetine $$ Fungacetin $$ A
cetin, tri- $$ Kesscoflex TRA $$ G lycerin triacetate $$ Glyceryl tri acetate
$$ 1,2,3-Propanetriol tria cetate $$ Glycero

31 12.162 25.10 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47256 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47269 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47259 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE $
$ Flux Maag $$ L-Nicotine $$ (-)-N
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

icotine $$ XL All Insecticide $$ 3 -(N-Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli

32 12.451 0.06 C:\Database\Flavor2.L
No matches found

33 13.174 0.17 C:\Database\WILEY275.L
ALLYL CYCLOHEXYL PROPIONATE 80891 002705-87-5 72
Pyrrolidine, 1-(1-oxopentadecyl)- 174271 056630-55-8 44
(CAS) $$ PENTADECANOYLPYRROLIDINE
Pyrrolidine, 1-(13-methyl-1-oxotet 174273 056630-52-5 25
radecyl)- (CAS) $$ 13-METHYLTETRAD
ECANOYLPYRROLIDINE $$ N-13-METHYL-
TETRADECANOYL PYRROLIDINE

34 14.134 0.19 C:\Database\WILEY275.L
Methyl .alpha.-(diphenylphosphinoy 237491 127208-07-5 53
l)-N-phenylsuccinamate $$ Methyl . beta.-
(diphenylphosphinoyl)-N-phen ylsuccinamate $$ Butanoic
acid, 2 (diphenylphosphinyl)-4-oxo-4-(phen
ylamino)-, methyl ester
1-Phthalazinecarbonitrile, 2-benzo 145186 013925-27-4 49 yl-
1,2-dihydro- (CAS) $$ 2-BENZOYL
-1,2-DIHYDROPHALAZINE-1-CARBONITRI
LE $$ 2-BENZOYL-1,2-DIHYDRO-1-PHTH
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ALAZINECARBONITRILE $$ 2-BENZOYL-1
,2-DIHYDROPHTHALAZINE-CARBONITRILE
Methyl .alpha.-(diphenylphosphinoy 237492 127208-07-5 49
l)-N-phenylsuccinamate $$ Methyl . beta.-
(diphenylphosphinoyl)-N-phen ylsuccinamate $$ Butanoic
acid, 2 (diphenylphosphinyl)-4-oxo-4-(phen
ylamino)-, methyl ester

35 18.781 0.24 C:\Database\WILEY275.L
Thiopropazate $$ 1-Piperazineethan 249086 000084-06-0 59
ol, 4-[3-(2-chloro-10H-phenothiazi
n-10-yl)propyl]-, acetate (ester) (CAS)
$$ Dartal $$ Dartalan $$ Thi opropazat
$$ Perphenazine acetate $$ 1-
Piperazineethanol, 4-[3-(2-ch
lorophenothiazin-10-yl)propyl]-, a

cetate (ester) $$
9,10-Anthracenedione, 1,8-dihydrox 199128 000081-55-0 15
y-4,5-dinitro- $$ Anthraquinone, 1 ,8-dihydroxy-
4,5-dinitro- $$ 1,8-D ihydroxy-4,5-dinitroanthraquinone
$$ 1,8-Dinitro-4,5-dihydroxyanthra quinone $$ 4,5-
Dinitrochrysazin $$ 4,5-Dihydroxy-1,8-dinitroanthraqu
inone $$ NCI-C607 steroisomer 1,10,11,13,14-pentaflu
183927 128822-13-9 11 oro-tetracyclo[8.4.0.0(2,9).0(11,1
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

4)]tetradec-12-ene

36 24.717 0.09 C:\Database\Flavor2.L
No matches found

37 26.680 0.06 C:\Database\Flavor2.L
No matches found

38 27.204 0.52 C:\Database\WILEY275.L
1-Amino-1-ortho-chlorophenyl-2-(2- 162556 069737-10-6 43
quinoxalinyl)ethene $$ Benzenemeth anamine, 2-chloro-
.alpha.-(2-quino xalinylmethylene)- (CAS)
Arsenous acid, tris(trimethylsilyl 206537 055429-29-3 35
) ester (CAS) $$ TRIMETHYLSILYL AR
SINATE
N-METHYL-2-IODO-PYRROLE 92072 000000-00-0 27

39 27.253 0.17 C:\Database\WILEY275.L
Hexahydropyridine, 1-methyl-4-[4,5 92495 000000-00-0 42
-dihydroxyphenyl]-
Dibenzoxazabicycloundecane $$ 1H-2 206379 087166-99-2 35
,6,10-(Epoxymethyno)-3-benzazacycl
ododecine, 2,3,4,5-tetrahydro-9,12
,13-trimethoxy-3-methyl-, (+)- (CA
S)
2,4,6(1H,3H,5H)-Pyrimidinetrione, 121357 000052-31-3 30
5-(1-cyclohexen-1-yl)-5-ethyl- (CA
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			S) $$ Cyclobarbital $$ Adorm $$ Ir			
			ifan $$ Palinum $$ Amnosed $$ Cavo		nyl	
			$$ Hexemal $$ Namuron $$ Pralu		min $$	
			Sonaform $$ Fanodorm $$ Hyp		noval $$	
			Praelumin $$ Fanodormo $$			
			Pro-Sonil $$ Cyc			
40	27.340	0.20	C:\Database\WILEY275.L			
			Hexahydropyridine, 1-methyl-4-[4,5	92495	000000-00-0	42
			-dihydroxyphenyl]-			
			2-(5'-NITRO-3'-THIENYL)PYRIMIDINE	92107	057059-17-3	
30			$$ Pyrimidine, 2-(5-nitro-3-thieny		l)- (CAS)	
			5-NITROBENZOFURAN-2-CARBOXYLIC ACI	92132	000000-00-0	27
41	27.471	0.04	C:\Database\WILEY275.L			
			Hexahydropyridine, 1-methyl-4-[4,5	92495	000000-00-0	46
			-dihydroxyphenyl]-			
			Arsenous acid, tris(trimethylsilyl	206537	055429-29-3	38
			) ester (CAS) $$ TRIMETHYLSILYL AR			
			SINATE			
			Spiro[cyclopenta[c]pyran-7(1H),2'-	149325	103384-82-3	38
			[1,3]dioxane]-7a(4aH)-carboxylic a			
			cid, 1-oxo-, methyl ester, cis-			
42	27.527	0.15	C:\Database\Flavor2.L			
			No matches found			

B8: Watermelon Ice Library Search

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	2.214	0.52	C:\Database\WILEY275.L Methane, tetrachloro- (CAS) $$ Carbon tetrachloride $$ R 10 $$ Universal $$ Carbona $$ Tetrasol $$ Fluko $$ Freon 10 $$ Fasciolin $$ Tetrafol $$ Necatorina $$ Benzinoform $$ Tetraform $$ Perchloromethane $$ Tetrachlorocarbon $$ Tetrachloromethane $$ Ca	36815	000056-23-5	83
			Methane, tetrachloro- (CAS) $$ Carbon tetrachloride $$ R 10 $$ Universal $$ Carbona $$ Tetrasol $$ Fluko $$ Freon 10 $$ Fasciolin $$ Tetrafol $$ Necatorina $$ Benzinoform $$ Tetraform $$ Perchloromethane $$ Tetrachlorocarbon $$ Tetrachloromethane $$ Ca	36816	000056-23-5	78
			Methane, tetrachloro- (CAS) $$ Carbon tetrachloride $$ R 10 $$ Universal $$ Carbona $$ Tetrasol $$ Fluko $$ Freon 10 $$ Fasciolin $$ Tetrafol $$ Necatorina $$ Benzinoform $$ Tetraform $$ Perchloromethane $$ Tetrachlorocarbon $$ Tetrachloromethane $$ Ca	36814	000056-23-5	74
2	2.237	0.77	C:\Database\WILEY275.L Butane, 2-chloro-2-methyl- (CAS) $	8549	000594-36-5	50

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$ tert-Amyl chloride $$ 2-Chloro-2
-methylbutane $$ tert-Pentyl chlor ide
$$ Tertiary pentyl chloride $$ 2-
Methyl-2-chlorobutane r $$ 1,1
Dimethylpropyl chloride $$ 2-Methy l-
2-chlorobutane $$ 2-Chloro-2-met
hyl-butane
Butane, 2-chloro-2-methyl- (CAS) $ 8550 000594-36-5 47
$ tert-Amyl chloride $$ 2-Chloro-2
-methylbutane $$ tert-Pentyl chlor ide
$$ Tertiary pentyl chloride $$ 2-
Methyl-2-chlorobutane r $$ 1,1
Dimethylpropyl chloride $$ 2-Methy l-
2-chlorobutane $$ 2-Chloro-2-met
hyl-butane
Butane, 2-chloro-2-methyl- (CAS) $ 8553 000594-36-5 47
$ tert-Amyl chloride $$ 2-Chloro-2
-methylbutane $$ tert-Pentyl chlor
ide $$ Tertiary pentyl chloride $$ 2-
Methyl-2-chlorobutane r $$ 1,1
Dimethylpropyl chloride $$ 2-Methy l-
2-chlorobutane $$ 2-Chloro-2-met
hyl-butane

3 2.382 0.45 C:\Database\WILEY275.L
3-Penten-2-ol (CAS) $$ 2-PENTEN-4- 3386 001569-50-2 80
OL $$ Methyl propenyl carbinol $$
.alpha.,.gamma.-Dimethylallyl alco
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-ol,cis+trans
3-Penten-2-ol (CAS) $$ 2-PENTEN-4- 3385 001569-50-2 80
OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-
Dimethylallyl alco
hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-
ol,cis+trans
3-Penten-2-ol (CAS) $$ 2-PENTEN-4- 3379 001569-50-2 72

OL $$ Methyl propenyl carbinol $$ .alpha.,.gamma.-
Dimethylallyl alco
hol $$ PENT-3-EN-2-OL $$ 3-Penten 2-
ol,cis+trans

4 2.957 34.10 C:\Database\WILEY275.L
1,2-Propanediol (CAS) $$ Propylene 2014 000057-55-6 78
glycol $$ PG 12 $$ 1,2-PROPANDIOL $$ Sirlene $$ 2,3-
Propanediol $$ 2-Hydroxypropanol $$ Methylethyl g
lycol $$ Methyl glycol $$ Monoprop ylene glycol $$ 1,2-
Propylene glyc ol $$ 1,2-Dihydroxypropane $$ Meth
ylethylene glycol
PROPYLENE GLYCOL $$ 1,2-PROPANEDIO 2035 000057-55-6 78
L $$ 1,2-DIHYDROXYPROPANE
2-Propanol (CAS) $$ Isopropyl alco 741 000067-63-0 9
hol $$ PRO $$ propan-2-ol $$ Isoho l $$ Propol $$ Lutosol
$$ Alcojel $$ Avantin $$ Imsol A $$ Petrohol
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

$$ Hartosol $$ Avantine $$ Takineo
col $$ i-Propanol $$ Isopropanol $ $
Alcosolve 2 $$ Isopropenol $$ Co
mbi-Schutz $$ Iso

5 3.713 0.39 C:\Database\WILEY275.L
Butanoic acid, ethyl ester (CAS) $ 13033 000105-54-4 64
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl
ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
Butanoic acid, ethyl ester (CAS) $ 13032 000105-54-4 64
$ Ethyl butyrate $$ Butyric acid e
thyl ester $$ Butyric ether $$ Eth yl
butanoate $$ Ethyl n-butyrate $ $
Butyric acid, ethyl ester $$ Eth yl

ester of butanoic acid $$ Ethyl n-
butanoate $$ n-Butyric acid eth
yl ester $$ Butyr
PROPYL BUTYRATE 20930 000105-66-8 59

6 3.815 0.16 C:\Database\Flavor2.L
No matches found

7 3.861 0.65 C:\Database\WILEY275.L
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

2-Hexanol (CAS) $$ n-C4H9CH(OH)CH3 7754 000626-93-7 45
$$ n-Butylmethylcarbinol $$ Hexan
ol-(2) $$ sec-Hexyl alcohol
2,4-Pentanediol (CAS) $$ 2,4-Amyle 8207 000625-69-4 39
ne glycol $$ Pentane-2,4-diol $$ 2 ,4-
Pentanediol (dl+meso) $$ dl-2,4
-Pentanediol $$ Isoamylene alcohol
$$ Pentanediol-2,4
2-Pentanol, 4-methyl- (CAS) $$ 4-M 7804 000108-11-2 38
ethyl-2-pentanol $$ MIC $$ MAOH $$
MIBC $$ 3-MIC $$ 2-Methyl-4-penta
nol $$ Isobutylmethylmethanol $$ I
sobutylmethylcarbinol $$ Methyliso
butyl carbinol $$ 4-Methyl-2-penty l
alcohol $$ 1,3-Dimethyl-1-butano
l $$ 4-methyl 2-p

8 4.436 0.21 C:\Database\WILEY275.L
Butanoic acid, 2-methyl-, ethyl es 20740 007452-79-1 53
ter (CAS) $$ Ethyl 2-methylbutyrat e $$ Ethyl 2-
methylbutanoate $$ Et hyl .alpha.-methylbutyrate $$ Buty
ric acid, 2-methyl-, ethyl ester $
$ 2-Methylbutanoic acid ethyl este
OCTANOIC ACID, 2-METHYL-, ETHYLEST 70996 000000-00-0 52
ER
OCTANOIC ACID, 2-METHYL-, ETHYLEST 70997 000000-00-0 50
ER

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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9 4.529 0.22 C:\Database\WILEY275.L
CIS-3-HEXENOL 6975 000928-96-1 64
3-Hexen-1-ol, (Z)- (CAS) $$ cis-3- 6778 000928-96-1 64
Hexene-1-ol $$ Z-3-Hexenol $$ Leaf
alcohol $$ 3-(Z)-Hexenol $$ cis-3 -Hexenol
$$ Blatteralkohol $$ cis 3-Hexen-1-ol $$ (Z)-
Hex-3-en-1-ol
$$ Blatteralkohol (German) $$ .bet
a.,.gamma.-Hexenol $$ HEXEN-30L-1
$$ 3-Hexen-1-ol $
CIS-3-HEXENYL FORMATE 19279 033467-73-1 59

10 4.685 0.22 C:\Database\Flavor2.L
No matches found

11 4.736 0.25 C:\Database\WILEY275.L
Cyclopropane, propyl- (CAS) $$ Pro 2962 002415-72-7 59
pylcyclopropane $$ Propane, 1-cycl opropyl-
Cyclopropane, propyl- (CAS) $$ Pro 2963 002415-72-7 59
pylcyclopropane $$ Propane, 1-cycl opropyl-
1-Hexanol (CAS) $$ n-Hexanol $$ Am 7737 000111-27-3 50
ylcarbinol $$ n-Hexan-1-ol $$ Hexy
l alcohol $$ Hexanol $$ Pentylcarb
inol $$ Caproyl alcohol $$ n-Hexyl
alcohol $$ 1-Hexyl alcohol $$ 1-H ALS Vial :
0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ydroxyhexane $$ n-C6H13OH $$ Hexan
-1-ol $$ Hexanol-(1) $$ Epal 6 $$
UN 2282

12 4.858 0.25 C:\Database\WILEY275.L
1-Butanol, 3-methyl-, acetate (CAS 20841 000123-92-2 72
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20838 000123-92-2 56
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3 Methyl-1-butyl ac
1-Butanol, 3-methyl-, acetate (CAS 20836 000123-92-2 56
) $$ Isoamyl acetate $$ 3-METHYL B
UTYL ACETATE $$ ETHANOIC ACID, 3-M
ETHYL BUTANOL ESTER $$ Pear oil $$
Banana oil $$ i-Amyl acetate $$ I soamyl
ethanoate $$ Isopentyl acet ate $$ 3-
Methylbutyl acetate $$ 3-
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Methyl-1-butyl ac

13 4.889 0.14 C:\Database\Flavor2.L
2-Methylbutylacetate 121 000624-41-9 12
Propionic acid 54 000079-09-4 9
Heptanal 239 000111-71-7 9

14 6.447 2.56 C:\Database\WILEY275.L
Propane, 2-fluoro-2-methyl- (CAS) 2068 000353-61-7 40

$$ 2-Fluoro-2-methylpropane $$ ter
t-Butyl fluoride
1,2,3-Propanetriol (CAS) $$ Glycer 4509 000056-81-5 9
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$ Glysanin $$
Glycerine $$ Gly ceritol $$ Glycyl alcohol $$ Trihy
droxypropane $$ Propanetriol $$ Gl ycerin suppositories $$
1,2,3-Trih ydroxypropane $$ Propantriol $$ Sy
nthetic glycerin
1,2,3-Propanetriol (CAS) $$ Glycer 4512 000056-81-5 9
ol $$ Glyrol $$ Glycerin $$ Osmogl yn $$
Glysanin $$ Glycerine $$ Gly ceritol $$ Glycyl alcohol $$
Trihy droxypropane $$ Propanetriol $$ Gl ycerin
suppositories $$ 1,2,3-Trih ydroxypropane $$ Propantriol
$$ Sy
nthetic glycerin

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

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15 6.824 0.16 C:\Database\Flavor2.L
Ethyl heptanoate 309 000106-30-9 16
2-Isobutylthiazole 209 018640-74-9 10 delta-
Octalactone 175 000698-76-0 10

16 7.045 0.17 C:\Database\WILEY275.L
Acetic acid, hexyl ester (CAS) $$ 31081 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
$$ Hexyl acetate $$ Hexyl ethanoa te
$$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate
$$ Acetic acid n-hexyl ester $$ n-
Hexyl ethanoate $$ Hexy
l alcohol, acetat
Acetic acid, hexyl ester (CAS) $$ 31087 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
$$ Hexyl acetate $$ Hexyl ethanoa te
$$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate

$$ Acetic acid n-hexyl ester $$ n-
Hexyl ethanoate $$ Hexy
l alcohol, acetat
Acetic acid, hexyl ester (CAS) $$ 31083 000142-92-7 78
1-Hexyl acetate $$ n-Hexyl acetate
$$ Hexyl acetate $$ Hexyl ethanoa te
$$ Acetic acid hexyl ester $$ H exyl
ester of acetic acid $$ Capro yl acetate
$$ Acetic acid n-hexyl ALS Vial : 0 Sample
Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

ester $$ n-Hexyl ethanoate $$ Hexy
l alcohol, acetat

17 7.079 0.06 C:\Database\WILEY275.L
2-HEXENYL ACETATE $$ TRANS-2-HEXEN 29576 002497-18-9 86
YL ACETATE
TRANS-2-HEXENYL ACETATE 29579 002497-18-9 72
2-Hexen-1-ol, acetate, (E)- (CAS) 29420 002497-18-9 64
$$ trans-2-Hexenyl acetate $$ E-2
hexenyl acetate $$ 2-Hexen-1-ol ac etate
$$ Hex-2-enyl acetate $$ 2-H exenyl
acetate $$ 2-Hexen-1-yl-ace tate $$ (E)-2-
Hexenyl acetate $$ (
E)-2-Hexen-1-yl acetate

18 7.904 0.12 C:\Database\WILEY275.L
DIETHYL MALONATE 45090 000105-53-3 72
Propanedioic acid, diethyl ester (45051 000105-53-3 72
CAS) $$ Diethyl malonate $$ Maloni
c ester $$ Dicarbethoxymethane $$
Ethyl malonate $$ Diethyl propaned
ioate $$ Carbethoxyacetic ester $$
Malonic acid diethyl ester $$ Mal onic
acid, diethyl ester $$ Methan
edicarboxylic aci
Propanedioic acid, diethyl ester (45054 000105-53-3 72

CAS) $$ Diethyl malonate $$ Maloni
c ester $$ Dicarbethoxymethane $$ ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Ethyl malonate $$ Diethyl propaned ioate $$ Carbethoxyacetic ester $$ Malonic acid diethyl ester $$ Mal onic acid, diethyl ester $$ Methan edicarboxylic aci			
19	8.153	0.39	C:\Database\WILEY275.L 4-METHYLTHIAZOLE	6160	000000-00-0	53
			ALLYL CAPROATE $$ ALLYL HEXANOATE	42257	000123-68-2	45
			Hexanoic acid, thio-, S-butyl este r (CAS) $$ NOR-BUTYL THIOL NOR-HEX ANOATE $$ Hexanethioic acid, S-but yl ester	72465	002432-79-3	42
20	8.686	0.13	C:\Database\WILEY275.L Benzene, methyl- (CAS) $$ Toluene $$ CP 25 $$ Methylbenzene $$ Toluo l $$ Methacide $$ Antisal 1a $$ Me thylbenzol $$ Phenylmethane $$ MET HYLBENZENE(TOLUENE) $$ Benzene, me thyl $$ Methane, phenyl- $$ NCI-C0 Tolueen $$ Toluen $$ Toluo lo $$ Rcra waste	4566 7272	000108-88-3	46
			Benzeneethanol (CAS) $$ Phenethyl alcohol $$ PEA $$ PHENETHYL ALCOLH OL $$ Phenethanol $$ .beta.-PEA $$ Benzyl carbinol $$ 2-Phenylethano l $$ Ethanol, 2-phenyl- $$ 2-Phene ALS Vial : 0	15787	000060-12-8	43

Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex

Integration Events: ChemStation Integrator - autoint2.e

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

thyl alcohol $$ .beta.-Phenylethan ol $$ .beta.-Phenethyl alcohol $$
.beta.-Hydroxyeth
Benzeneethanol (CAS) $$ Phenethyl 15783 000060-12-8 43
alcohol $$ PEA $$ PHENETHYL ALCOLH
OL $$ Phenethanol $$ .beta.-PEA $$
Benzyl carbinol $$ 2-Phenylethano 1 $$
Ethanol, 2-phenyl- $$ 2-Phene thyl alcohol
$$ .beta.-Phenylethan ol $$ .beta.-
Phenethyl alcohol $$
.beta.-Hydroxyeth

21 9.496 9.81 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15536 000065-85-0 90
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15527 000065-85-0 90
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic ALS Vial : 0
Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15528 000065-85-0 87
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C

arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

22 9.675 0.35 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15529 000065-85-0 58
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15538 000065-85-0 58
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid 2-bromoethyl ester $$ 113656 000939-54-8 52
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

2-Bromoethyl benzoate

23 9.932 0.28 C:\Database\WILEY275.L
Benzoic acid (CAS) $$ Retardex $$ 15533 000065-85-0 45
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15525 000065-85-0 43
HA 1 $$ Tenn-Plas $$ Retarder BA $

$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar
Benzoic acid (CAS) $$ Retardex $$ 15539 000065-85-0 38
HA 1 $$ Tenn-Plas $$ Retarder BA $
$ Benzoic aicd $$ Solvo powder $$
Salvo liquid $$ Dracylic acid $$ C
arboxybenzene $$ Benzoate $$ Benzo
esaeure GK $$ Benzoesaeure GV $$ P
henylformic acid $$ Benzeneformic
acid $$ Phenylcar

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
24	10.530	0.36	C:\Database\WILEY275.L			
			2-methyl-2-(ethoxycarbonyl)-1,3-ox	60149	000000-00-0	56
athiolane						
			2-methyl-2-benzyl-1,3-oxathiolane	78043	017642-77-2	40
			$$ 1,3-Oxathiolane, 2-methyl-2-(ph			
enylmethyl)- $$ 1,3-Oxathiolane, 2						
			-benzyl-2-methyl-			
			ethoxytrimethylsilane $$ Silane, e	14033	034746-77-5	38
			thoxytri(methyl-d3)- $$ Ethoxytri(			
methyl-d3)silane						
25	11.236	19.85	C:\Database\Flavor2.L			
			Quinoline	174	000091-22-5	4
			3-Hexenoic acid	36	004219-24-3	2
26	11.340	0.13	C:\Database\Flavor2.L			
			Citronellyl butyrate	332	000141-16-2	12
			Citronellyl propionate	186	000141-14-0	10
			L-Menthol	38	002616-51-5	9
27	11.935	1.44	C:\Database\WILEY275.L			

1,2,3-Propanetriol, triacetate (CA 102718 000102-76-1 90
S) $$ Triacetin $$ Glycerol triace
tate $$ Vanay $$ Glyped $$ Enzacti n
$$ Triacetine $$ Fungacetin $$ A cetin,
tri- $$ Kesscoflex TRA $$ G lycerin
triacetate $$ Glyceryl tri acetate $$
1,2,3-Propanetriol tria ALS Vial : 0 Sample
Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

cetate $$ Glycero
TRIACETIN 102723 000102-76-1 83
1,2,3-Propanetriol, triacetate (CA 102716 000102-76-1 50
S) $$ Triacetin $$ Glycerol triace
tate $$ Vanay $$ Glyped $$ Enzacti n
$$ Triacetine $$ Fungacetin $$ A cetin,
tri- $$ Kesscoflex TRA $$ G lycerin
triacetate $$ Glyceryl tri acetate $$
1,2,3-Propanetriol tria cetate $$
Glycero

28 12.162 24.56 C:\Database\WILEY275.L
Pyridine, 3-(1-methyl-2-pyrrolidin 47265 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
Pyridine, 3-(1-methyl-2-pyrrolidin 47269 000054-11-5 94
yl)-, (S)- (CAS) $$ Nicotine $$ 1-
METHYL-2-(3-PYRIDYL)-PYRROLIDINE
$ $ Flux Maag $$ L-Nicotine $$ (-)-N
icotine $$ XL All Insecticide $$ 3 -(N-
Methylpyrollidino)pyridine $$
Nicotin $$ S-(-)-Nicotine $$ (-)-3
-(N-Methylpyrroli
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
			Nicotine $$ Black leaf $$ Black le af 40 $$ Destruxol orchid spray $$ Emo-nik $$ ENT 3,424 $$ Flux maag $$ Fumetobac $$ Mach-nic $$ 1-Met hyl-2-(3-pyridyl)pyrrolidine $$ 3 (N-Methylpyrrolidino)pyridine $$ L -3-(1-Methyl-2-pyrrolidyl)pyridine $$ (-)-3-(1-Meth	47308	016760-37-5	94
29	13.174	0.19	C:\Database\WILEY275.L Cyclohexanepropanoic acid, 2-prope nyl ester (CAS) $$ ALLYL 3-CYCLOHE XYLPROPIONATE $$ Allyl cyclohexylp ropionate $$ Allyl cyclohexaneprop ionate $$ Cyclohexanepropionic aci d, allyl ester $$ Ananolide $$ ALL YL(3-CYCLOHEXYL)PROPIONATE $$ 3-Al lylcyclohexyl pro	80765	002705-87-5	49
			.beta.-Necrodol $$ (1S,4R)-1-(Hydr oxymethyl)-3-methylene-4,5,5-trime thylcyclopentane $$ epi-.beta.-Nec rodol $$ Cyclopentanemethanol, 2,2 ,3-trimethyl-4-methylene-, (1R-tra ns)- $$ (-)-.beta.-Necrodol	40701	104086-70-6	49
			(-)-.beta.necrodol	40702	000000-00-0	49
30	26.439	0.20	C:\Database\WILEY275.L 3,4-di(4-trimethylsiloxyphenyl)hex	239950	000000-00-0	43

ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
ane						
			2,4,6(1H,3H,5H)-Pyrimidinetrione,	121357	000052-31-3	35

5-(1-cyclohexen-1-yl)-5-ethyl- (CA
S) $$ Cyclobarbital $$ Adorm $$ Ir ifan
$$ Palinum $$ Amnosed $$ Cavo nyl $$
Hexemal $$ Namuron $$ Pralu min $$
Sonaform $$ Fanodorm $$ Hyp noval $$
Praelumin $$ Fanodormo $$
Pro-Sonil $$ Cyc
1,3-dimethyl-4-azaphenanthrene 92616 000000-00-0 35

31 26.720 0.16 C:\Database\WILEY275.L
11H-Dibenzo[b,e][1,4]diazepin-11-o 162634 013450-70-9 53
ne, 5,10-dihydro-5-[3-(methylamino
)propyl]- (CAS) $$ 5-(3-METHYLAMIN
OPROPYL)-5,10-DIHYDRO-11H-DIBENZO
[B,E][1,4]DIAZEPIN-11-ONE
Benz[e]azulene-3,8-dione, 5-[(acet 210271 025536-74-7 42
yloxy)methyl]-3a,4,6a,7,9,10,10a,1 0b-octahydro-3a,10a-
dihydroxy-2,10
-dimethyl-, (3a.alpha.,6a.alpha.,1
0.beta.,10a.beta.,10b.beta.)-(+)-
Hexahydropyridine, 1-methyl-4-[4,5 92495 000000-00-0 42
-dihydroxyphenyl]-

32 27.253 0.18 C:\Database\WILEY275.L
3,3-Diethoxy-1,1,1,5,5,5-hexamethy 174413 000000-00-0 40
ltrisiloxane
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

Cyclotrisiloxane, hexamethyl- (CAS 106844 000541-05-9 27
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
THYMOL-TMS 107840 000000-00-0 27

33 27.380 0.13 C:\Database\WILEY275.L
Cyclotrisiloxane, hexamethyl- (CAS 106846 000541-05-9 43

) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
Imidazole, 5-bromo-4-nitro-2-methy 89856 000000-00-0 43
l-
2,4,6(1H,3H,5H)-Pyrimidinetrione, 121357 000052-31-3 37
5-(1-cyclohexen-1-yl)-5-ethyl- (CA
S) $$ Cyclobarbital $$ Adorm $$ Ir ifan
$$ Palinum $$ Amnosed $$ Cavo nyl $$
Hexemal $$ Namuron $$ Pralu min $$
Sonaform $$ Fanodorm $$ Hyp noval $$
Praelumin $$ Fanodormo $$
Pro-Sonil $$ Cyc

34 27.465 0.17 C:\Database\Flavor2.L
No matches found
ALS Vial : 0 Sample Multiplier: 1 Samp. Amt.: 1

Search Libraries: C:\Database\WILEY275.L Minimum Quality: 40
C:\Database\Flavor2.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: ChemStation Integrator - autoint2.e

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

---

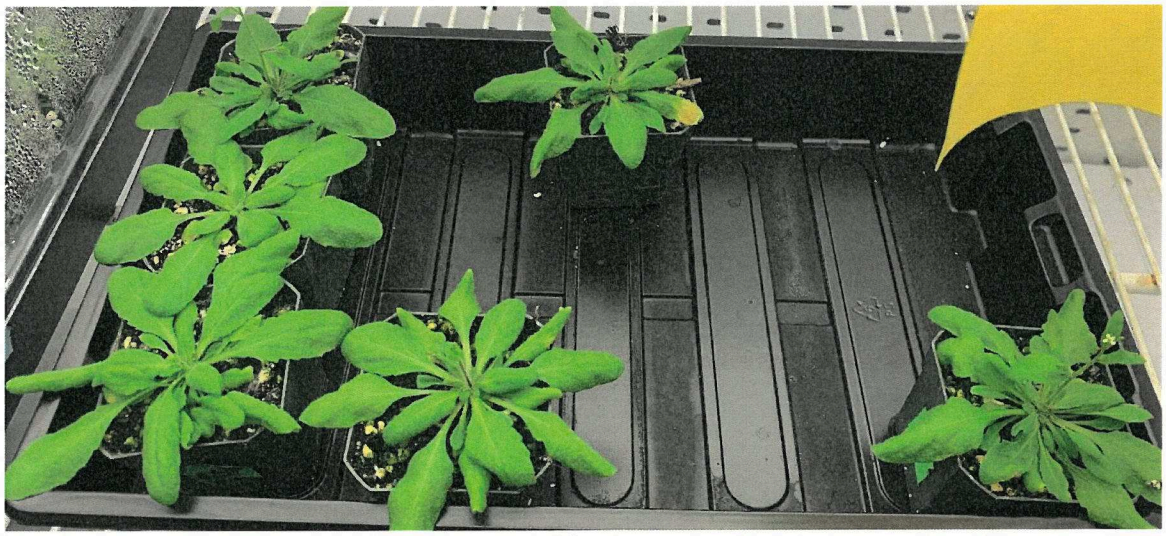
35 27.590 0.13 C:\Database\Flavor2.L
No matches found

36 27.822 0.11 C:\Database\WILEY275.L
Cyclotrisiloxane, hexamethyl- (CAS 106845 000541-05-9 43
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris
iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer
Benz[e]azulene-3,8-dione, 5-[(acet 210271 025536-74-7 42
yloxy)methyl]-3a,4,6a,7,9,10,10a,1 0b-octahydro-3a,10a-
dihydroxy-2,10
-dimethyl-, (3a.alpha.,6a.alpha.,1
0.beta.,10a.beta.,10b.beta.)-(+)-
Cyclotrisiloxane, hexamethyl- (CAS 106848 000541-05-9 38
) $$ 1,1,3,3,5,5-HEXAMETHYL-CYCLOH
EXASILOXANE $$ Hexamethylcyclotris

iloxane $$ HEXAMETHYL-CYCLOTRISILO
XANE $$ Dimethylsiloxane cyclic tr imer

Appendix C: Before and After Images of *Arabidopsis thaliana* in Soil and Agar

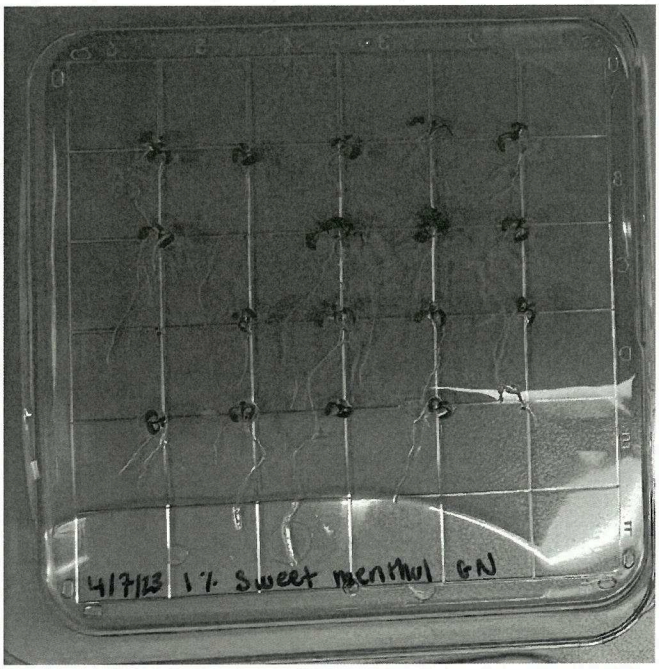
C1: Before and after images of *A. thaliana* in soil two weeks after being treated with Blue Razz Ice dilutions. The line of three plants on the left side of both images are those that obtained the single-leaf treatment (front to back: 0.5%, 0.75%, 1.0%). The other plants were those systematically treated with 10 mL of dilutions (left to right: 0.5%, 0.75%, 1%)



Before

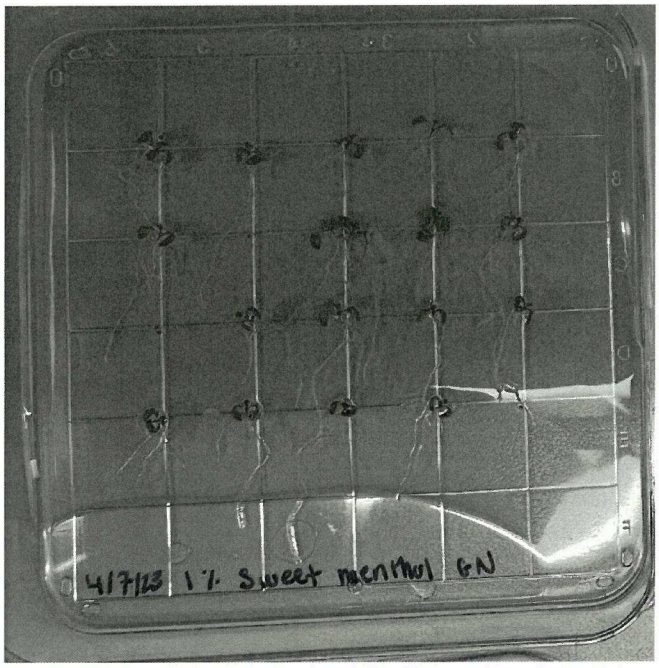
After

C2: Before and after images of the first trial of dilution introduction with plant agar. 10 µL of 0.75% Sweet Menthol, 1.0% Sweet Menthol, and 0.75% Blue Razz Ice were added to individual seedlings and observed for one week.



Before (0.75% Sweet Menthol)

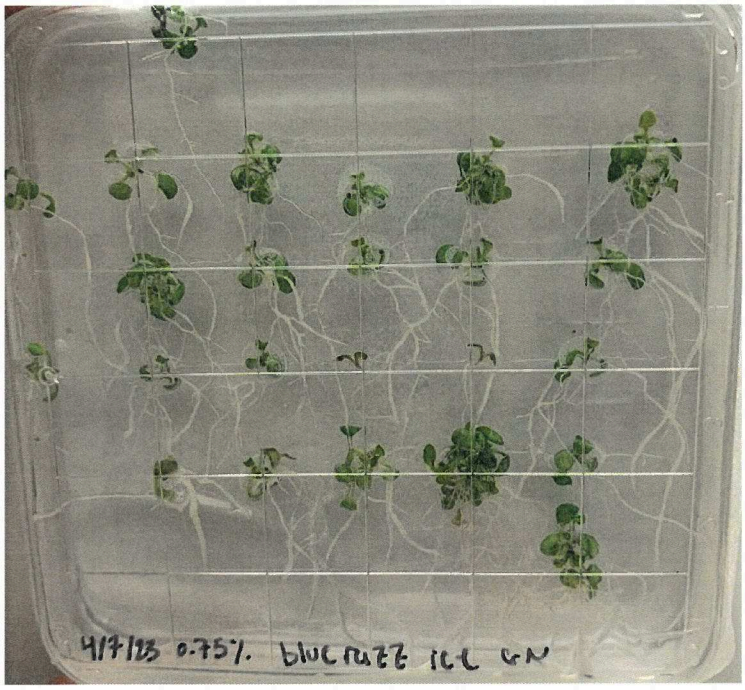
After (0.75% Sweet Menthol)



Before (1.0% Sweet Menthol)

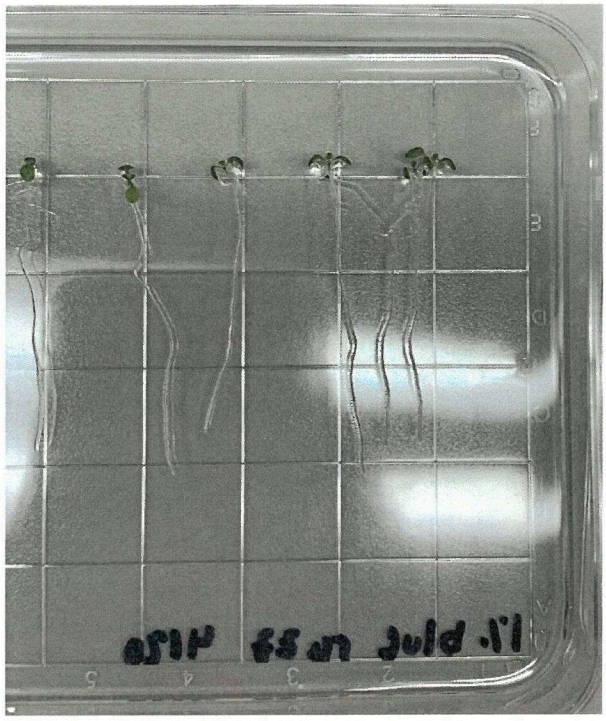
After (1.0% Sweet Menthol)

Before (0.75% Blue Razz Ice)

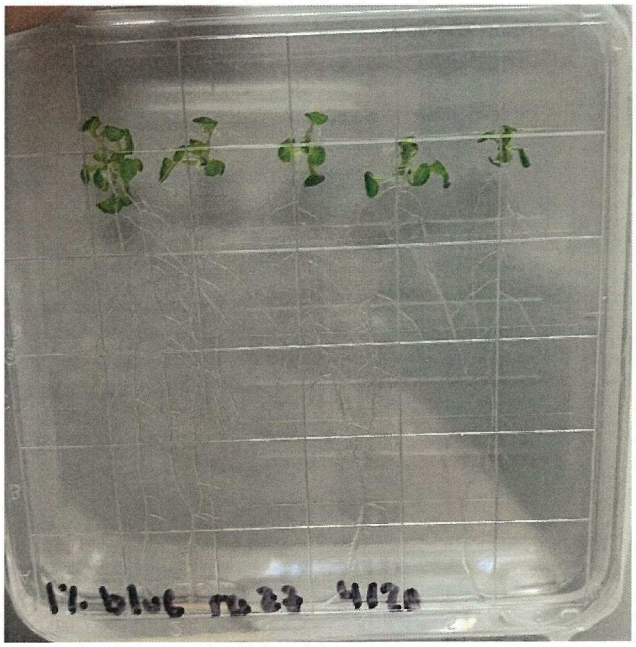


After (0.75% Blue Razz Ice)

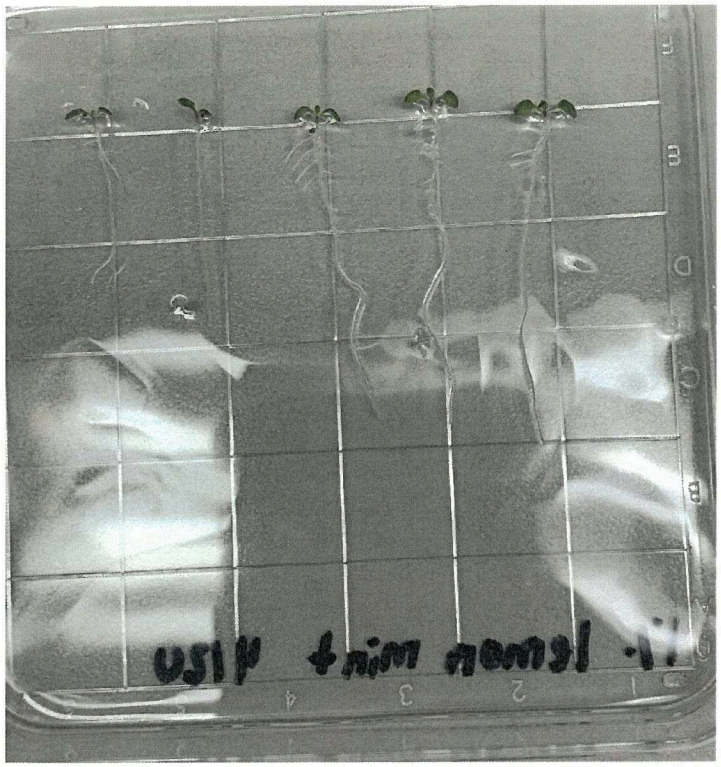
C3: Before and after images of the second trial of dilution introduction with plant agar. 20 μL of Blue Razz Ice, Lemon Mint, Sour Candy, and Tropical Rainbow Blast, all 1.0% dilutions, were used to treat individual seedlings and observed for one week



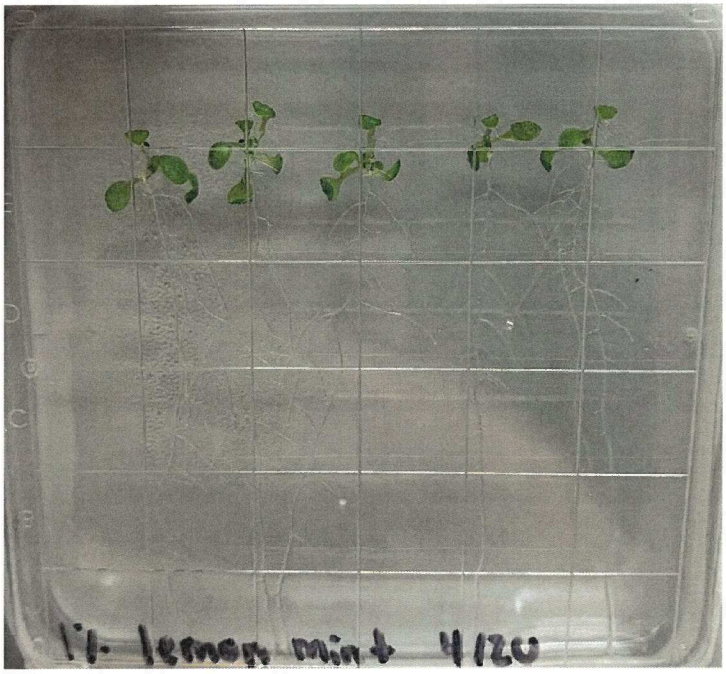
Before (1.0% Blue Razz Ice)



After (1.0% Blue Razz Ice)

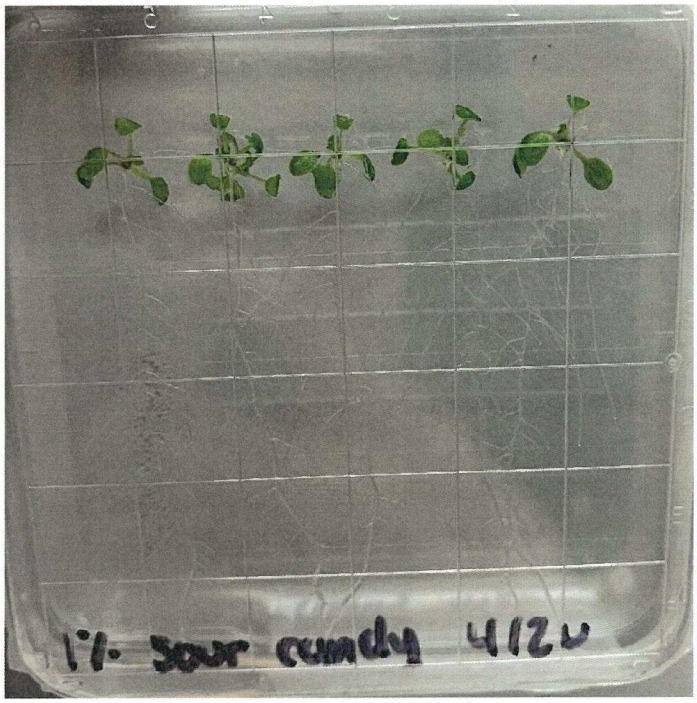


Before (1.0% Lemon Mint)

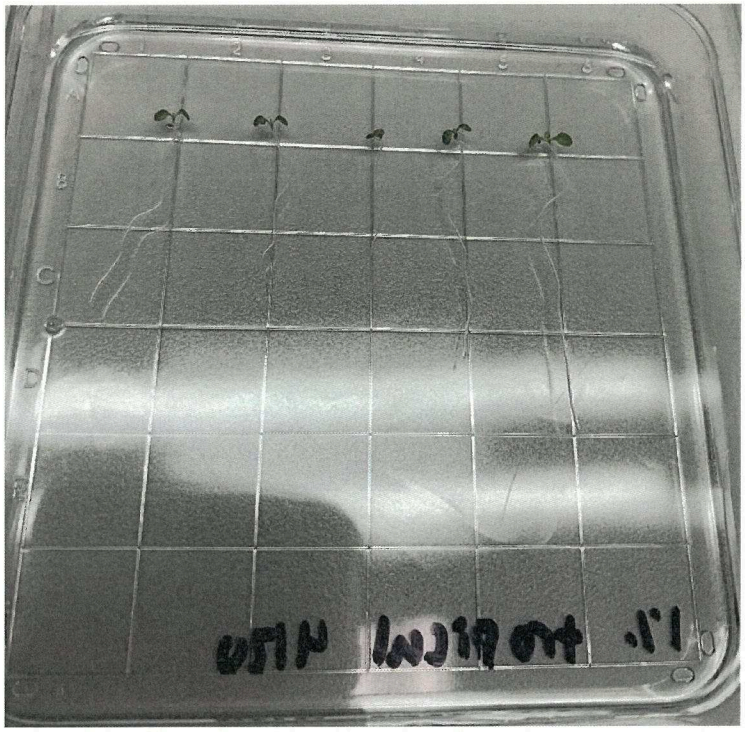


After (1.0% Lemon Mint)

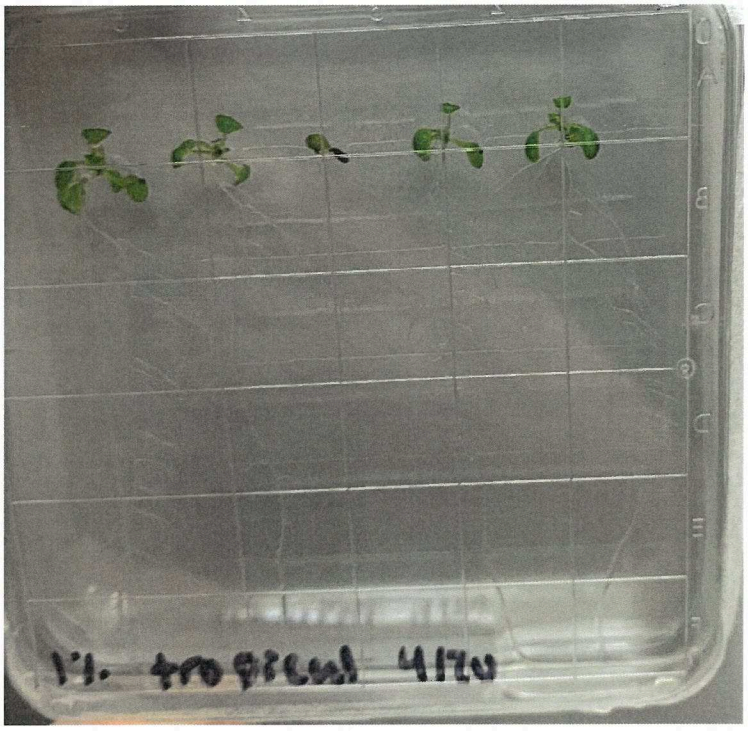
Before (1.0% Sour Candy)



After (1.0% Sour Candy)



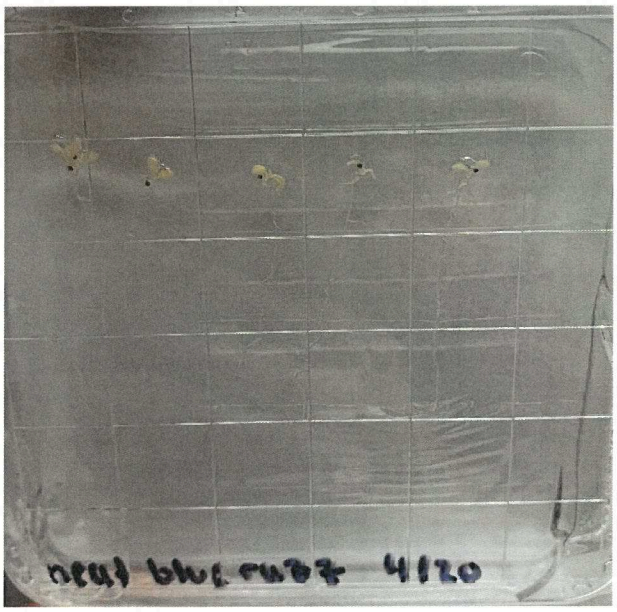
Before (1.0% Tropical Rainbow Blast)



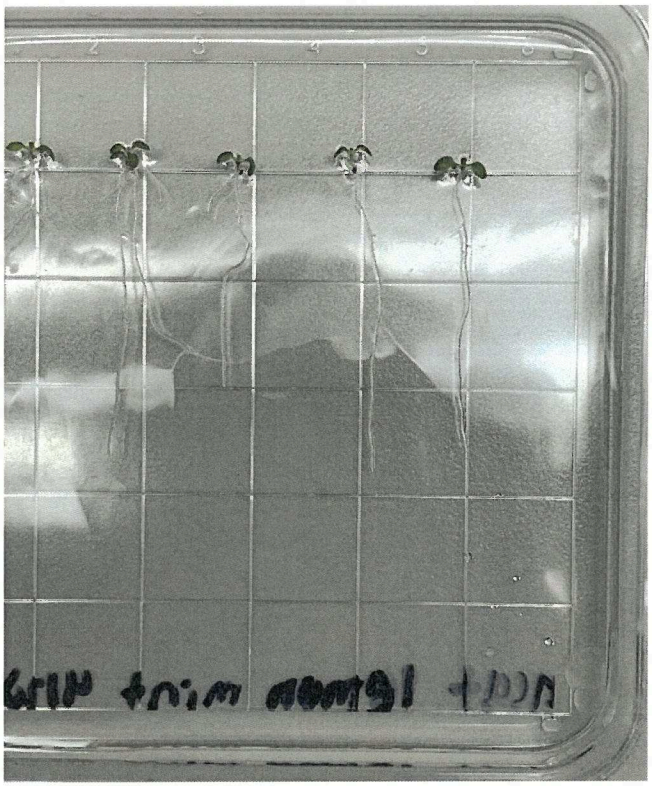
After (1.0% Tropical Rainbow Blast

C4: Before and after images of the second trial of dilution introduction with plant agar. 20 µL of Blue Razz Ice, Lemon Mint, Sour Candy, and Tropical Rainbow Blast neat e-liquids were used to treat individual seedlings and observed for one week. Bleaching and plant death occurred within a 24-hour period

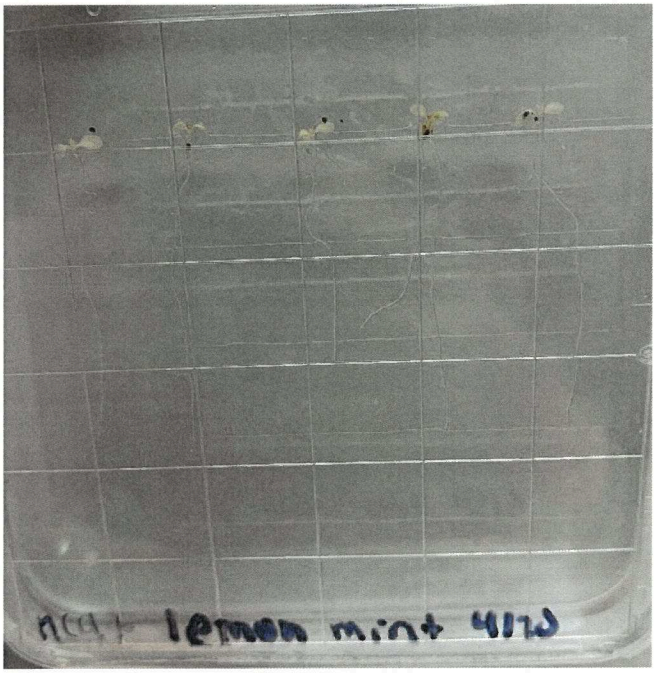
Before (Neat Blue Razz Ice)



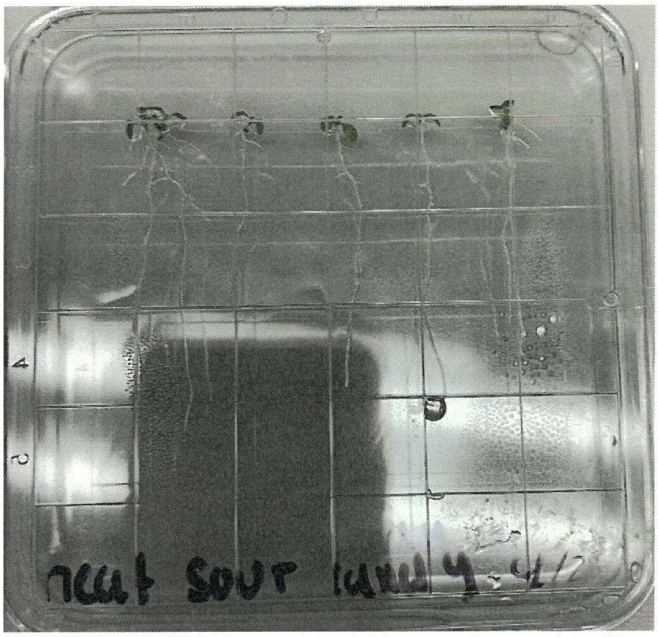
After (Neat Blue Razz Ice)



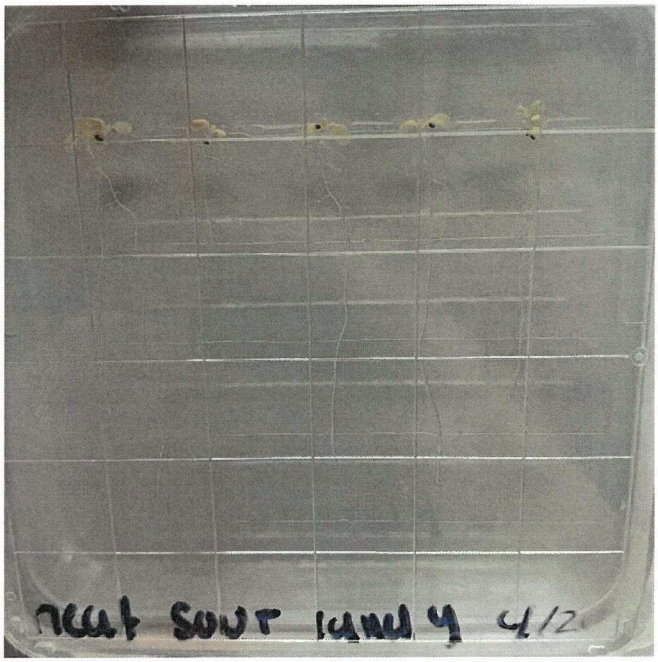
Before (Neat Lemon Mint)



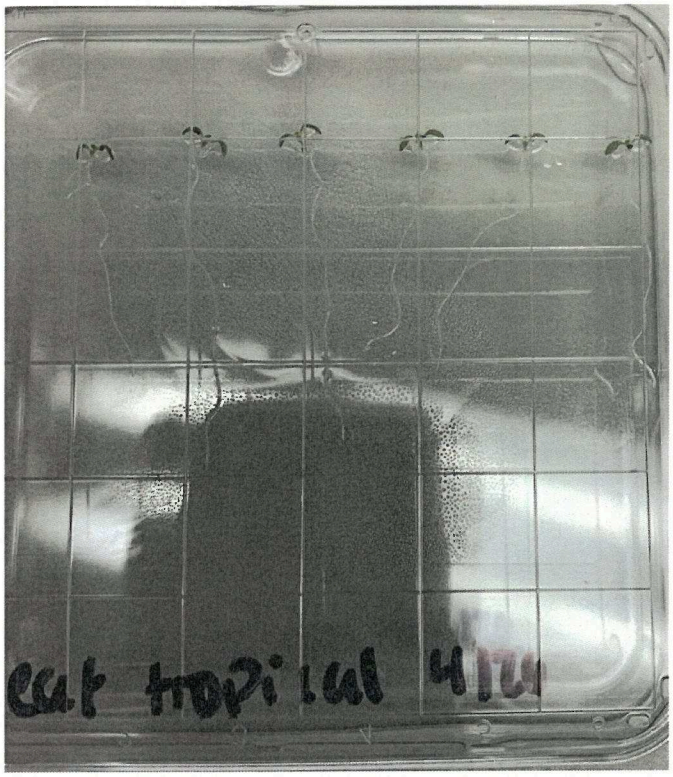
After (Neat Lemon Mint)



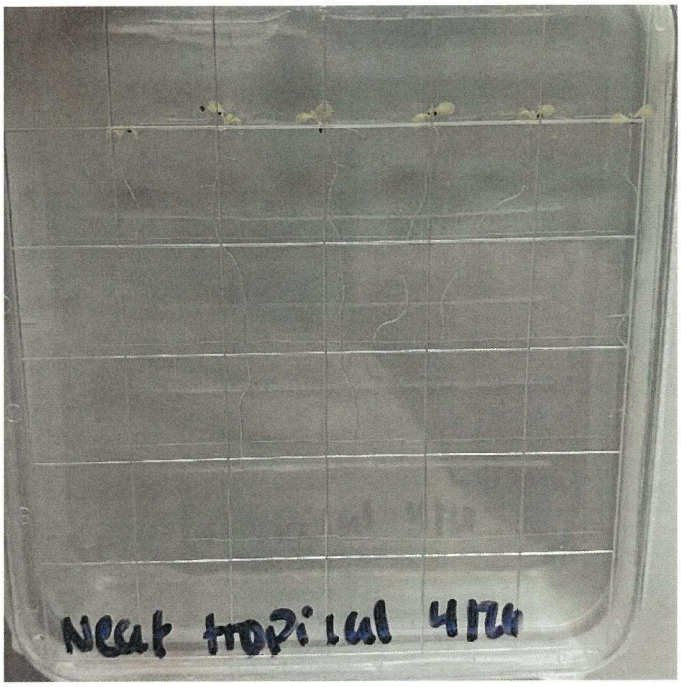
Before (Neat Sour Candy)



After (Neat Sour Candy)



Before (Neat Tropical Rainbow Blast)



After (Neat Tropical Rainbow Blast)