A Chemical Analysis of Flavor Differences in Chocolate Coconut Rum Porter

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Abstract

The origin of the batch-to-batch inconsistency in flavor of Purgatory Beer Company's Fiero Coconut Rum porter was investigated by extracting organic compounds from desirable and undesirable batches of porter and quantifying them using GC-MS. The concentration and occurrence of key flavor compounds were compared between the samples and showed that the undesirable batch contained more unpleasant organoleptic compounds and was more acidic. Based on the marked inconsistency in chemical profile between batches, the team recommended quality control be improved through more accurate monitoring and consistent control of the fermentation temperature, oxygenation of wort and beer, order of ingredient addition to the fermentation broth, reuse of yeast, and filtration of water.

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1. Introduction

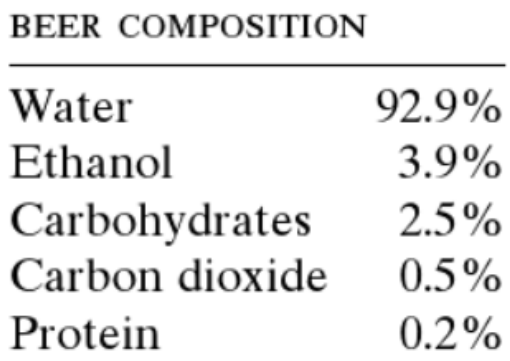
A porter is a full-bodied, malty beer characterized by a rich, dark color and distinctive flavors such as coffee, nuts, cocoa, and caramel. Purgatory Beer Company created its own version of a porter, known as the Fiero Coconut Rum Porter. Its flavors include the coffee, nut, and caramel flavors of a standard porter, combined with coconut, rum, and chocolate.

Purgatory Beer Company serves its Fiero Coconut Rum Porter with generally positive reviews. However, customers started to notice taste consistency problems between batches. Using GC-MS, the differences in chemical profile between batches qualitatively deemed by Purgatory Beer Company as a desired and undesired were characterized. The desired flavor of the “good batch” of porter was characterized by a rich, slightly bitter dark cocoa flavor, with coconut and rum undertones, while the undesired flavor of the “bad batch” was likened to Coca-Cola due to an uncharacteristically sweet, slightly spicy taste.

2. Background

2.1 Brewing Process

Beer is a beverage made from fermenting starches without concentrating the alcohol content. Although numerous minor components contribute to the flavor of beers, in general, American beers are composed of approximately 92.9% water, 3.9% ethanol, and smaller concentrations of carbohydrates, proteins, and carbon dioxide (Figure 1).[1]



BEER COMPOSITION	
Water	92.9%
Ethanol	3.9%
Carbohydrates	2.5%
Carbon dioxide	0.5%
Protein	0.2%

Figure 1. Beer Composition[1]

In general, beer is brewed in five distinct steps: malting, mashing, boiling, fermenting, and maturation. During the malting step, barley is steeped by immersion in aerated water. By the end of steeping, a root emerges from the barley called a chit. Next, germination occurs, which converts proteins and glucans into amino acids and glucose. The barley is then dried and aged to produce malted barley. Malted barley contains all the sugars necessary for fermentation.[2]

The malted grain is milled for improved sugar extraction and mixed with hot water to form the mash in a vessel called a mash tun. The mash is mixed and kept at a steady temperature around 149°F for optimal extraction of sugars.[2]

The leftover malted barley is separated from the mash to produce wort, which is usually achieved by draining the mash tun through a filter on the base of the vessel. The wort contains all the necessary sugars and amino acids that are needed for fermentation.[2]

The wort is transferred to a kettle to boil, which stops enzymatic activity and leaves behind insoluble proteins. Boiling also helps to sterilize the batch of beer. Hops are added during this

stage, which contribute greatly to the bitterness and aroma of beer. The wort is then cooled using a heat exchanger and oxygenated by agitation or by pumping O_2 directly into the wort.[2]

The next step in the process is fermentation, where sugars are converted to alcohol by yeast. Other compounds known as flavor compounds are also produced during fermentation, which can significantly alter the taste of the beer. During fermentation, the temperature is regulated as the yeast converts sugars and other compounds. Fermentation varies depending on the type of alcoholic beverage being created. In general, it usually takes a few days to a week for ales to ferment, while drinks like lagers may require multiple weeks to complete fermentation.[2]

After fermentation is complete, a secondary fermentation is often used to add carbon dioxide to the beer by introducing simple sugars into the liquid. When these simple sugars are broken down by the yeast, carbon dioxide is released into the beer. In commercial breweries, the beer is then filtered using diatomaceous earth or cellulose to remove the yeast (microbreweries usually skip this step) and is finally ready for packaging and consumption.[2]

The typical ingredients for making beer are water, malt, hops, yeast and adjuncts. “Adjuncts” refer to any material that provides starch or sugar to supplement the amount provided by the malt.[2]

2.1.1 Malt

Malt is a key ingredient used in the production of beer. It provides complex carbohydrates and sugars needed for the fermentation to occur while simultaneously providing flavor components and impacting the color of the final product.[3] Malt is comprised of the seeds of grains that are allowed to sprout and then killed using heat to prevent the germination process from proceeding too far. Typically, most malt used for beer comes from barley seeds, although oats, rye, millet and other grain types are sometimes used, depending on which type of beer one is creating[1]. The malting process consists of three steps: steeping, germination, and drying.

The first step, steeping, occurs by alternating the seeds between being submerged and drained to increase the internal moisture content from around 12% to about 44%[2]. Steeping typically takes between 40 and 48 hours.[2] Once the water content has reached the appropriate levels, the germination process begins.

Germination occurs when the water activates the pre-existing enzymes in the seeds and stimulates the embryo in the seed to release hormones, which in turn tell the cells inside the seed to produce more enzymes.[2] These enzymes then break down the seed's protein and carbohydrate matrix which releases the seed's internal starch reserves. Germination usually occurs in a temperature-controlled vessel containing humid air where the seeds are continuously stirred. The germinating seeds are typically kept in the germination vessel for 4 to 5 days before they are ready for the drying process.

The drying process occurs when the seeds are removed from the germination vessel and moved into a kiln where they remain in 180-190°F air for 2-4 hours[2]. The temperatures supplied by the kiln end the germination process before the seeds consume too much of the starch for their own growth. Brewers can control the extent of germination which in turn controls the flavor and color characteristics of their malts by varying the moisture content, time, and temperature of each individual stage of the malting process.[2]

2.1.2 Hops

The flowers of the hop plant, *Humulus lupulus*, are used to flavor beer. The hop flowers significantly impact the flavor of beer and provide beer with its characteristic bitter taste. Hops flavor is highly subjective to growing temperature, soil, moisture, and a variety of other climate issues. Some brewers use a mixture of different hop varieties so that the proportions can be modified to counter local and seasonal variations. Some small craft brewers are unable to keep wide varieties of hops on hand, so the tastes of their beer are inconsistent compared to larger scale breweries[1]. Often, the synergistic interaction of the many low-concentration flavor compounds derived from hops is the most influential factor on the difference in taste and smell between beer varieties.[3]

2.1.3 Yeast

Yeast is a single-cell fungus that is used to convert starches released by the malt into alcohol in a process known as fermentation. During fermentation, the yeast breaks down starches contained in the malt to create energy for its own biological processes. This process releases ethanol and carbon dioxide as byproducts that are not useful to the yeast, but are vital ingredients in brewing.[1] The most common yeast used in beer production is *saccharomyces cerevisiae*, although hundreds of

other species have been identified. Yeast strains are classified into two categories, top-fermenting yeast and bottom-fermenting yeast.

Top-fermenting yeasts are typically used to make ales and porters and receive their nickname from the fact that as they ferment, they float to the surface of the fermentation vessel. These strains should be used between a temperature range of 10°C and 25°C and yield a final product that is high in the concentration of esters.[4]

Bottom-fermenting yeasts are typically used to produce lager beers, and their name is derived from that fact that during the fermentation process, they settle down to the bottom of the fermentation vessel. These strains should be used between a temperature range of 7°C and 15°C to maximize their effect on the production alcohols.[4]

2.1.4 Specifics of Brewing Porters

Porters are complex beers chiefly characterized by a strong, dark malt flavor. The recipe for a typical chocolate porter like the Fiero Coconut Rum Porter calls for around 85% percent of the solid ingredients to be malt. Malts such as amber malt, brown malt, chocolate malt, black malt, and pale malt are all combined in porters, which are commonly composed of 60% of pale malt and smaller percentages of other malts (Figure 2). Addition of cacao rather than using excess chocolate malt often provides a richer, more chocolate-like flavor profile.[6] The remaining solid ingredients are brown sugar (10%) and flaked oats (5%). Additional ingredients, around 0.2-0.4 oz/gal of porter, are added after the primary fermentation is complete to distinguish a porter.

60%	pale malt
12%	CaraMunich/CaraVienne
6%	melanoidin malt
3%	wheat malt
6%	flaked oats
9%	brown sugar
3%	chocolate malt (Carafa)
1%	black patent malt
1 oz. low cohumulone, high alpha acid hop (first wort or 45 min boil)	
1 oz. low alpha hop (20 min boil)	
Ferment in low- to mid- 60s.	
Add cacao nibs and vanilla beans to secondary, age 1-2 weeks depending on desired level of flavor and aroma extraction.	
Bottle condition for best results.	

Figure 2. Example of Typical Commercial Porter Recipe[5]

Cacao is preferred over baker's or milk chocolate because it lacks the high lipid content present in other forms of chocolate. This high lipid content is deleterious to the formation of the porter's head and seriously harms the beer's shelf life because lipids such as cocoa butter will go rancid as the beer ages and is exposed to oxygen.

The boiling stage is often split into two steps — the first being a 45-60 minute boil with high alpha acid, low cohumulone hops to acquire the bitter taste of alpha acids without the harsh bitterness of cohumulone, and the second being a shorter, 15-30 minute boil with low alpha acid hops to add a slightly spicy dimension without excess bitterness (see 1.3).[5]

Two-stage fermentation is often used with porters due to their complex flavor profiles and the need for careful regulation of the brewing process. Two-stage fermentation allows for the removal of any sediment and precipitate that may form in the primary fermentation, including spent yeast, off-flavors, and particles that may harm the coloration or opacity of the beer.[5] Furthermore, the beer can age in the secondary fermentation vessels for up to two weeks and be mixed with custom flavors, such as cacao, vanilla, or coconut rum, which will not harm the yeast or compete with other sugar sources to be the primary sources of fermentation. Fermentation temperatures are typically maintained around 60°F, which is too low for the extraction of undesired lipids from fatty secondary flavor compounds like cacao or vanilla beans.[5] The higher alcohol content of the secondary fermentation broth also aids in the extraction of flavor compounds from their source ingredients.

2.2 Flavor Compounds

The taste of alcoholic beverages is largely controlled by various chemicals known as flavor compounds. Many of these flavor compounds are formed during fermentation, but some exist in the ingredients before fermentation, while others are formed during aging and other processing steps.[8]

Every flavor compound that is present in beer has an associated flavor threshold, which is the concentration at which human taste receptors can detect its presence. To study the impacts of various flavor compounds on the taste of beer, a parameter known as a flavor unit was defined. Flavor units are the ratio of the concentration of a particular flavor compound in a sample to the

flavor threshold concentration. Flavor units allow for comparison of tastes associated with unique compounds.[8]

Flavor compounds are generally divided into three levels that describe their concentration in beer according to flavor units: primary, secondary, and tertiary. Primary flavor compounds are found in concentrations of more than 2 flavor units, secondary flavor compounds range from 0.5-2.0 flavor units, and tertiary compounds are present in doses less than 0.5 flavor units.[8] Flavor compounds of less than 1 flavor unit produce flavors when combined with other tertiary compounds, which act together to provide a unique flavor element.

2.2.1 Primary flavor compounds

Primary flavor compounds found in most beers include ethanol, carbon dioxide, and bittering compounds from hops (hop acids). These compounds are found in varying amounts in different styles of beer, but the base flavors of most beers are due to primary flavor compounds (Table 1).

Ethanol, the primary alcohol in beer, generally comprises approximately 4-6% of a beer's volume, although stouts and porters typically contain more ethanol (8-14% by volume). As its concentration increases, the burning taste and fragrant, somewhat strong odor of an alcoholic beverage increases. High fermentation temperatures, large sources of sugar for fermentation, and high yeast attenuation — or a high percentage of sugar consumption by the yeast — will drive fermentation and produce more ethanol. Ethanol concentrations that are inappropriate for certain styles of beer will harm the beer's taste and can be avoided by ensuring the consistency of these fermentation variables.[8]

Carbon dioxide, which is produced by yeast during fermentation and sometimes artificially added to beers, provides the "bite" of a beer: a tart, dry, slightly sour taste that induces a pleasurable sensation on the tongue.[9] The amount of CO_2 dissolved in a beer can be controlled by how much CO_2 is allowed to escape into the atmosphere during and immediately after fermentation and by regulation of the beer's temperature and container pressure. If more CO_2 is desired, sugar can be added to the beer before bottling to induce further fermentation by the yeast, and the beer can be kept cold and pressurized to improve CO_2 solubility in it. Higher CO_2 concentrations usually improve the taste of a beer by making its flavors more palatable, and are relatively similar among

beer types.[9] The exception are porters and stouts, which should have slightly less (1.5-2.2 volumes) dissolved CO_2 than most other beers, including lagers and ales (2.2-2.6 volumes).

Hop acids are subdivided into humulones (alpha-acids) and lupulones (beta-acids). Hop acids are barely soluble in water and have a very slight bitter taste but constitute up to 25% of the dry weight of hops. The amount and variety of hop acids in any given batch of hops also depends entirely on the type of hops used and the way that they are was grown.[10]

Beta-acids[10] are the more undesirable of the two types, as they are easily decomposed by oxidation, creating products that "possess unpleasant organoleptic characteristics." However, the effect of **alpha-acids** on flavor is more complex. The thermal isomerization of alpha acids into iso-alpha-acids (isohumulones) produces both *cis* and *trans* epimers, with the *cis* epimers being at least five-times more stable in terms of half-life than the *trans* epimers (Figure 3).

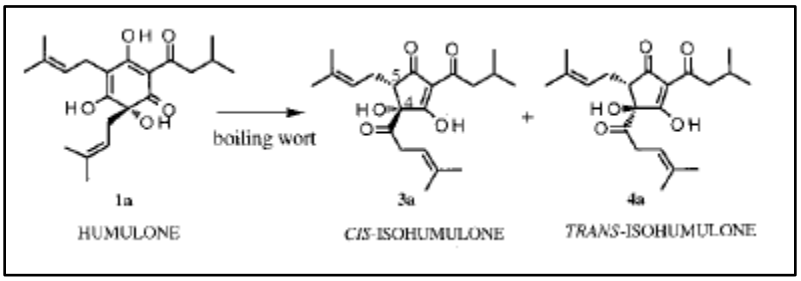


Figure 3. Isohumulone production during wort boiling[11]

A higher concentration of *cis*-isohumulones is desirable due to the much greater chemical (and thus flavor) stability of the beer, although the bitter taste of all isohumulones means that a very high concentration of them will harm beer flavor. Changing the isohumulone content of a beer can be used to make a beer more or less bitter and is most closely correlated with hop variety and amount. The bitterness can also be masked somewhat with sweetness provided by sugars.[7] Bittering elements such as beta acids are highest in bitter beers like IPAs and lowest in stouts and lagers.[11]

Isovaleric acid concentration in beer increases with the age of the hops used. Some varieties of fresh hops have a relatively small concentration of isovaleric acid (under 0.1 mg/L) that provides a slightly spicy odor to beer, which is desirable in IPAs and other bitter beers, but not in most porters. However, at concentrations above 1.5 mg/L, isovaleric acid will give beer a stale, cheesy odor.[11] Certain strains of yeast, such as *Brettanomyces*, also tend to produce excess isovaleric acid,

as does exposing the hops to too much air (O_2 catalyzes isovaleric acid production). Ensuring pure strains of yeast are used when brewing, using fresh hops, and minimizing exposure to oxygen are necessary to prevent buildup of isovaleric acid in beers.

Acetic acid, the main flavor compound in vinegar, is also naturally found in beers as a byproduct of fermentation. It provides beer with a sour flavor in low concentrations, but as its concentration increases, the vinegar-like flavor and odor become overpowering and can ruin the beer.[12] Excess acetic acid is usually a result of using wild-type yeasts (which naturally produce more acetic acid than normal brewer's yeasts) or bacterial contamination. Acetic acid-producing bacteria such as *Actinobacteria* are often found in batches that have been excessively oxygenated. Ensuring pure batches of yeast and closely following sanitation protocol is essential for avoiding excess amounts of acetic acid from forming during fermentation.

Acetaldehyde is involved in fermentation reactions and provides a tart, apple or pumpkin-like flavor and odor to beer. However, it can result in a noticeably unpleasant, rotten apple-like taste if the flavor threshold is greatly exceeded. There are multiples factors that can cause excess acetaldehyde to linger after the fermentation process, including low quality or insufficient yeast, high temperatures during fermentation, adding the yeast too quickly, or high oxygen levels in the wort.[7] A low acetaldehyde concentration is essential for a traditional porter flavor profile.

Table 1. Primary flavor compounds in beer

Flavor Compound	Class	Flavor/Odor	Desirability	Source(s) of Excess
Ethanol	Alcohol	Burning taste; fragrant, strong odor	4-6% in lagers and ales; 8-14% in stouts and porters	**High** fermentation temps **Excess** sugar sources **High** yeast attenuation
Carbon dioxide	Acid	Tart, dry, sour taste	1.5-2.2 volumes in stouts and porters; 2.2-2.6 volumes in all others	**Excess** sugar sources **Low** temp, high pressure storage **Limited** exposure of beer to atmosphere
Alpha acids (humulones)	Acid	Bitter, herbal, or hoppy flavor and odor	Desirable in IPAs and bitter beers; less desirable in stouts and porters	**Dependent** on hop variety and amount
Beta acids (lupulones)	Acid	Bitter, herbal, or hoppy flavor and odor	Desirable at ½ concentration of alpha acids; least desirable in stouts	**Dependent** on hop variety and amount
Valeric acid	Fatty acid	Spicy odor at low concentration; Stale, cheese-like odor at high concentration	Desirable in IPAs & other bitter beers at low concentration	**Use** of old hops **Wild** yeast contamination **Excessive** oxygenation
Acetic acid	Acid	Vinegar-like odor and taste	Undesirable at high concentration	**Bacterial** contamination **Wild** yeast contamination **Excessive** oxygenation
Acetaldehyde	Aldehyde	Green apple or pumpkin taste and smell; rotten apple at high concentration	Undesirable at high concentration	**Insufficient** yeast **Poor** quality yeast **Insufficient** fermentation time

2.2.2 Secondary flavor compounds

Secondary flavor compounds are generally the factor that distinguishes one style of beer from another. Fusel alcohols, esters (fruit flavors), phenols, and peptides are common secondary flavors compounds (Table 2).

Fusel alcohols are aliphatic and aromatic alcohols that constitute a large proportion of beer flavor compounds and include 1-propanol, 2-methyl-1-propanol, 2-methyl-1-butanol, 3-methyl-1-butanol, and phenylethyl alcohol. They are a natural byproduct of fermentation, in which the yeast's breakdown of amino acids and sugars occasionally yields keto acids that subsequently are decarboxylated and reduced to fusel alcohols.[7] Their "hot, spicy, solvent-like flavor and alcohol burn" would be inappropriate for milder beers like lagers, but are appropriate for strong ales and porters, though an excess of fusel alcohols would detract from any beer type due to an overly alcoholic taste.[13] Excess fusel alcohols tend to form from high temperatures and excess aeration of yeast during fermentation, especially with limited yeast nutrients. These conditions promote rapid yeast growth with limited nutrients to support this growth, which "stresses" yeast and promotes their biosynthetic pathways that produce fusel alcohols.[10] To limit fusel alcohol concentration, the fermentation temperature and exposure of the fermentation vessels to air should both be closely regulated.

Isoamyl acetate (banana oil) is a common ester flavor compound present in all beers. A byproduct of fermentation, its effect on flavor varies by concentration, and its desirability by beer type. It is important in many lagers, ales, and wheat beers, though is not typical to porters as it provides the fruity flavor and smell of a banana or pear.[14] High temperatures and low oxygen levels during fermentation tend to drive the production of esters like isoamyl acetate.

4-vinyl guaiacol (4VG) and most other phenols have a strong influence on beer flavor, providing a spicy and clove-like taste and smell at low concentrations that becomes off-putting and medicinal at high concentrations.[15] It is a distinctive flavor in wheat and smoked beers, as well as many stouts. Its production is heavily controlled by yeast strain and by mashing conditions (which control the release of its precursor molecule, ferulic acid). If it appears in a beer brewed from a yeast strain that is not known for producing 4VG, then its presence is likely from bacterial contamination or an inconsistent batch of yeast that contains other strains.

Polyphenols in a beer are mainly linked to the variety and quality of hops used. Polyphenols oxidize and polymerize easily, further changing a beer's taste, smell, and appearance as it ages. Large polyphenol chains, for instance, make a beer hazy due to their insolubility at room temperature and result in colloidal instability.[11] High amounts of polyphenols, especially catechins, have also been linked to an increased astringent response and an increased bitter and "metallic" taste, though other studies have shown little to no negative impact on flavor.[11] Conversely, the anti-oxidative properties of polyphenols impart upon beers a chemical stability that can extend their shelf life, preventing other flavor compounds from being oxidized and harming the beer's flavor as it ages. The overall polyphenol concentration may not necessarily harm a beer's taste, though high amounts of certain polyphenols, such as catechins, may do so. If a beer's taste is suspected to be harmed by a high polyphenol content, tests can be performed comparing the original beer and beer treated with polyvinylpyrrolidone (PVPP), which forms hydrogen bonds with polyphenols and removes them.[11]

Table 2. Secondary flavor compounds in beer

Flavor Compound	Class	Flavor/Odor	Desirability	Source(s) of Excess
Fusel alcohols	Alcohol	Hot, spicy flavor; alcohol "burn"	Desirable in porters and ales; undesirable in lagers and in excess	**High** fermentation temps **Excess** aeration of yeast **Inadequate** yeast nutrients
Isoamyl acetate	Ester	Banana- or pear-like flavor and odor (fruity)	Desirable in many lagers and ales	**High** fermentation temps **Low** yeast oxygenation
4-vinyl guaiacol (4VG)	Phenol	Spicy, clove-like odor and flavor; medicinal taste at high concentrations	Desirable at low concentrations in wheat beers, ales, and stouts	**Use** of wild or specialty yeasts **Bacterial** contamination of raw materials **Poor** sanitation
Polyphenols	Phenol	Astringent, tart, metallic taste; hazy appearance	Undesirable above low concentrations	**Overhopping** **Excessive** steeping of grain **Excessive** crushing or milling of grains

2.2.3 Tertiary flavor compounds

Tertiary flavor compounds may introduce a new flavor to a beer despite being below the flavor threshold, due to the additive properties of combining various tertiary flavor compounds, or synergism.[1] Alone, they do not impart a noticeable difference in flavor. Due to their complex interactions with other flavor compounds and largely unnoticeable flavor effects, this project focused primarily on identifying differences in primary and secondary flavor compounds between the good and bad porter, as they have definitive and individual effects on beer flavor.

2.2.4 Off-flavors

There are certain compounds that will always negatively impact the flavor of a beer. Known as "off-flavors," their presence can generally be attributed to a lack of consistent quality control at any stage of brewing. Many off-flavors have a low flavor threshold and are thus easily detected.

TCA (2,4,6-trichloroanisole), or "cork taint," is one easily detectable off-flavor. This cyclic ether is naturally produced by fungi and bacteria, so its presence in beer usually suggests mold contamination.[17] Storage of raw materials (especially grain) in damp areas, or poor humidity control during fermentation, can lead to contamination of the beer with TCA. Its extremely low flavor threshold means its moldy odor can be detected very easily by humans, even if present in low concentrations.[17]

Butanoic (butyric) acid is an off-flavor which has a putrid, rancid odor somewhat similar to vomit when present above its flavor threshold. It is normally found in beer at low concentrations as a byproduct of fermentation, but at concentrations above 2 mg/L, its smell becomes severely off-putting. Usually, excessive butanoic acid arises from bacterial contamination, especially at the wort production stage, or from raw materials — some studies suggest that improper quality control in the manufacture of cane sugar syrup leads to abnormal amounts of butanoic acid in the ingredient.[18]

Chlorophenols (often 2,6-dichlorophenol) are an especially pungent off-flavor that arises from exposure of equipment or ingredients to chlorinated water. It produces the smell and taste of mouthwash or disinfectant and can be detected at concentrations as low as 0.0002 mg/L.[19] To avoid contamination of beer with chlorophenols, any cleaning solutions or water used in between brews should be thoroughly rinsed from all equipment and vessels. To avoid chlorophenols in raw materials, only high-quality ingredients from clean facilities should be used.[19]

Sulfur-containing compounds are common in beer ingredients like hops and can react upon aging to form unwanted flavor compounds like dimethyl sulfide. Sulfur possesses a very low flavor threshold, allowing even the trace amounts commonly found in aging beer to cause an unpleasant taste or odor.[1]

Trans-2-nonenal is one such organosulfur compound, caused by the oxidation and aging of beer. It gives beer an unpleasantly musty odor, often described as "stale or old wet cardboard."[17] It is difficult to prevent its overall production in a beer, other than by minimizing headspace in bottles. However, early production of trans-2-nonenal can be combatted by minimizing excessive aeration of wort and fermented beer during transfer from vessel to vessel.

Other common sulfur-containing compounds include **mercaptan**, a skunky-smelling thiol that is caused by exposing beer to excess sunlight; **dimethyl sulfide (DMS)**, which is caused by bacterial contamination of raw ingredients or high temperatures of wort and beer during fermentation; and **hydrogen sulfide**, a poisonous gas generated by certain yeast strains in minute but flavor-harming amounts.[21]

Another pair of significant off-flavors are **ferrous sulfate**, which is a salt that gives beer a metallic flavor and odor due to contamination of the beer or its raw materials by rust and **2,3-butanedione**, which is a diacetyl that gives beers a buttery and slick taste due to poor quality yeast and insufficient and incomplete fermentation. Like most off-flavors, they can be avoided by ensuring routine cleanliness of equipment, usage of high-quality and new raw materials, and careful quality control of the fermentation stage variables (including time, temperature, air supply, and quality and age of yeast).[1]

Table 3. Potential off-flavors in beer

Flavor Compound	**Class**	**Flavor/Odor**	**Desirability**	**Source(s) of Excess**
2,4,6-trichloroanisole (TCA)	Ether	Moldy cellar odor	Undesirable	**Fermentation** and/or storage of grain in damp areas
Butanoic acid	Fatty acid	Putrid, rancid odor	Undesirable above 2 mg/L[18]	**Bacterial** contamination during wort production **Beer** spoiling
2,6-dichlorophenol	Phenol	Strong mouthwash odor and flavor	Undesirable	**Exposure** of equipment or ingredients to chlorinated water
Ferrous sulfate	Inorganic salt	Metallic or penny-like flavor and odor	Undesirable	**Dirty** and/or poor quality piping and vessels **Improperly** stored grains **Metal** packaging of ingredients
Trans-2-nonenal	Fatty aldehyde	Old cardboard or paper flavor and odor	Undesirable	**Excessive** oxygenation of wort or beer after fermentation **Excessive** aeration **Aging** of beer
Mercaptan	Organosulfur compound	Skunky odor Coffee odor	Undesirable	**Exposure** of beer to light after bottling

Flavor Compound	Class	Flavor/Odor	Desirability	Source(s) of Excess
Dimethyl sulfide (DMS)	Organosulfur compound	Cabbage, corn, tomato, and/or shellfish odors	Small amounts in pale lagers and ales	**High** wort and fermentation temperatures **Sulfur-containing** ingredients (i.e. coconut) **Bacterial** contamination
Hydrogen sulfide	Gas	Rotten egg, burning match	Less than 0.005 mg/L in pale lagers and ales	**Using** lager yeast strains **Inadequate** air supply to yeast[21]
2,3-butanedione	Diacetyl	Buttery taste, slick feeling on tongue	Small amounts in stouts and ales Undesirable in lagers	**Short** boiling time **High** yeast flocculation **Low** fermentation temps **Low** yeast oxygenation **Poor** quality yeast

2.3 Reactions in Beer

Once bottled, beer is not a static mixture. Beers still contain some yeast and may continue to ferment, and the exposure of beer to air or light can induce chemical reactions that change the appearance and flavor profile of a beer over time. All beer ages, but the process is accelerated if the beer contains excess oxygen or lipids, which promote runaway oxidation reactions in the beer that make it less bitter and sweeter. Frequently, the beer can begin tasting metallic, burnt, overly bitter, stale (like cardboard), or "catty" (a flavor known as *ribes*), collectively termed staling.[1]

The presence of excess oxygen in beer can be attributed to any stage of its production. Even early stages like milling and mashing can force excess oxygen into grain if the process is too vigorous, but the biggest areas of concern are movement and storage of wort and beer during wort boiling and fermentation. High flow rates, inadequately covered vessels, and high pressure and

temperature systems can force extra oxygen into wort or beer. At the bottling stage, leaving too much head space also adds to the risk of oxidation.

Large amounts of lipids in beer, which can arise from failure to remove spent grain and trub (fatty debris in wort) and from using fatty ingredients like cacao or coconut, can both turn rancid and be oxidized by O_2. For example, linoleic acid, a lipid prevalent in barley, is readily oxidized by reactive oxygen species and forms the fatty aldehyde trans-2-nonenal, which gives beer a stale, cardboard-like flavor and odor (see 1.3.4).[1] The presence of metallic ions in the beer can also accelerate free radical formation if they form enzyme complexes (such as superoxide dismutase). Metallic ions like iron can easily contaminate beer from poor quality or dirty piping, equipment, and raw materials, and can harm beer flavor outright, in addition to aiding in oxidation reactions.

To ensure maximum beer stability, oxygen, lipid, and metallic ion content in beer should be minimized. Careful control over temperature and pressure involving wort and fermentation broth are required to ensure temperatures and pressures do not become high enough to force O_2 to dissolve in the beer. Gentle mixing, low flow rates, and infrequent and gentle wort or broth transfers are necessary to minimize aeration. Additionally, fermentation vessels should be carefully sealed, with only a small orifice for gas exchange open to the environment, to keep O_2 no higher than the required amount. Packaging and bottling of beer should be done gently and with minimal splashing to avoid aeration of the beer. Pumping CO_2 into containers before adding beer can also drive out O_2. Flavorless compounds known as free radical traps can also be added to beers to react with oxygen radicals and effectively prevent oxidation reactions. This is a common practice with winemakers, who frequently add bisulfite ions to their products to prevent oxidation.[1]

To limit lipid content in beers, fatty ingredients should be substituted with less fatty ones (such as using cocoa powder instead of chocolate) and fermentation performed at lower temperatures to minimize lipid extraction from the ingredients. Effective lautering (separation of wort from grains) and separation of trub from unfermented wort are also essential to keep these heavy fats out of beer.[21] Boiling wort for at least 10-30 minutes before hopping improves separation of trub from wort by giving time for coagulated proteins and lipids to precipitate out of solution.[21] It can also be more easily removed by adding coagulants such as Irish moss or carrageenan to the wort during boiling. Lastly, using clean equipment and piping and pure water sources eliminates any metallic ions that may also accelerate oxidation.

One other major class of reactions that occur in beer are Maillard (browning) reactions, which are undesirable in excess in most beers except for porters and stouts due to the nutty- and malty-flavored melanoidins that they produce.[21] Melanoidins are large, dark colored molecules that are produced by the reaction of sugars with amino acids into Schiff bases, which further react to form highly flavored molecules like furaneol and maltol.[1] Melanoidin production is favored by high temperature and dry conditions, so they are mainly produced during high temperature grain roasting. Melanoidins can be largely retained during wort boiling if the boil is incomplete or the wort is kept at a high gravity. Excess melanoidin concentration can give beer an undesirable "extract tang" that is worsened by oxidation, so boiling time and wort gravity should be closely monitored and regulated to ensure that their concentration is not too high, even for porters.

3. Methodology

3.1 Extraction

To determine the presence and concentrations of organic compounds in the beer, multiple organic extractions were performed on both beer samples using two solvents; dichloromethane (DCM) and tetrahydrofuran (THF). For each extraction, 5 mL samples of the porter, 5 mL of water, and 5 mL of solvent were added to polypropylene centrifuge tubes. Salt (2.25 g for extractions using DCM and 3.55 g for extractions using THF) was also added to drive the desired organic compounds out of the porter/water layer and into the organic solvent layer. The two different solvents were used to supplement the data of one another and to maximize the number of organic compounds extracted from the porter because some organics have a higher affinity to one solvent than to the other. Without using multiple solvents, some organic compounds would avoid detection. For example, higher molecular weight compounds (especially those derived from hops) may be more easily extracted by THF than by DCM.[23]

The centrifuge tubes were shaken for 10 minutes using a wrist action shaker machine and then centrifuged at 3750 RPM for 15 minutes. In the experiments using the solvent dichloromethane, a clear organic layer formed in the bottom of each centrifuge tube. This clear layer contained the dichloromethane and the organic compounds that were extracted from the porter. Conversely, when performing extraction using the solvent tetrahydrofuran, a slightly murky layer containing the THF and the organic compounds extracted from the porter formed at the top of the centrifuge tube.

The organic layers (bottom for DCM, top for THF) were then carefully withdrawn from the centrifuge tubes using a pipette and filtered through 0.45 µm hydrophobic PTFE filters. The subsequent filtered products were placed in GC-MS vials for testing. The GC-MS method is detailed in Appendix A and ineffective extraction methods explained in Appendix B.

3.2 Observations During Extraction

During the dichloromethane extractions, there were clear visible differences in the physical characteristics of the porter layers between the desirable and undesirable porter batches. The

desirable batch displayed three distinct layers: a clear, transparent organic layer formed at the bottom; a murky layer containing some bubbles formed in the middle; and an opaque, dark water/porter layer formed at the top (Figure 4). The undesirable batch, however, did not distinctly display these three layers. Instead, the layers blend together, forming an opaque, dark water/porter layer on the top, and a slightly lighter, but still rather dark and murky layer that traveled to the bottom of the tube (Figure 4). The undesirable batch, when subjected to the same extraction treatment as the desirable batch (including same intensity and duration of mixing and shaking), appeared to form a much larger and more viscous emulsion that spread indiscriminately between the water layer and solvent layer.

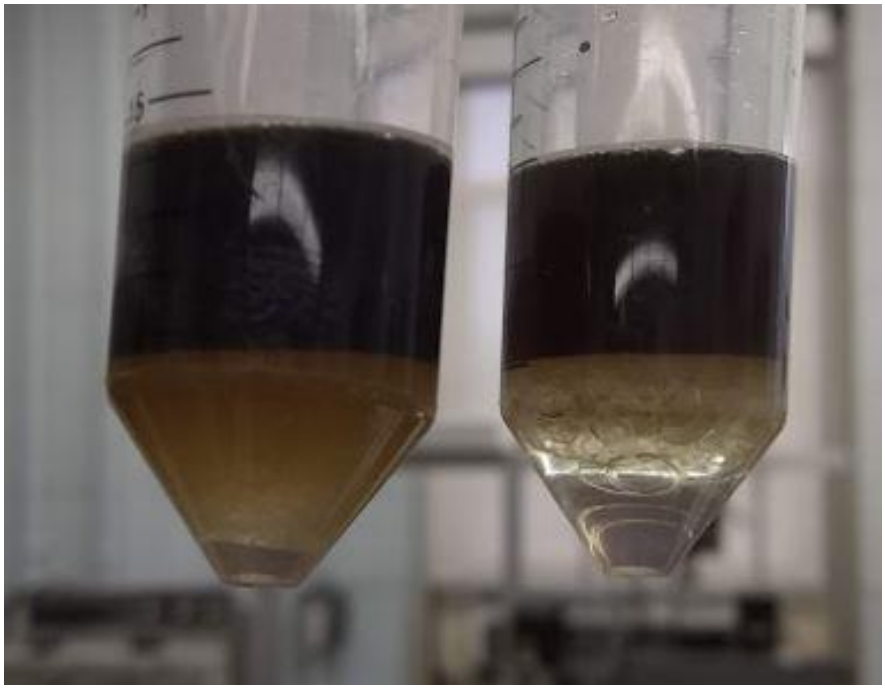


Figure 4. Visible Difference Between Undesirable (left) and Desirable (right) Batches in DCM

When the dichloromethane extractions were performing after letting the beer age in a refrigerator for two months, the visible difference between the desirable and undesirable porters became less distinct. Both the desirable and undesirable porters only exhibited two distinct layers, an opaque, dark water/porter layer on the top, and a slightly lighter, but still rather dark brown layer that traveled to the bottom of the tubes (Figure 5). This appeared to be similar to the original test extraction results for the undesirable porter and suggested that over time, the chemical composition

of the desirable porter batch changed and caused its physical properties to become more like the those of the undesirable porter.

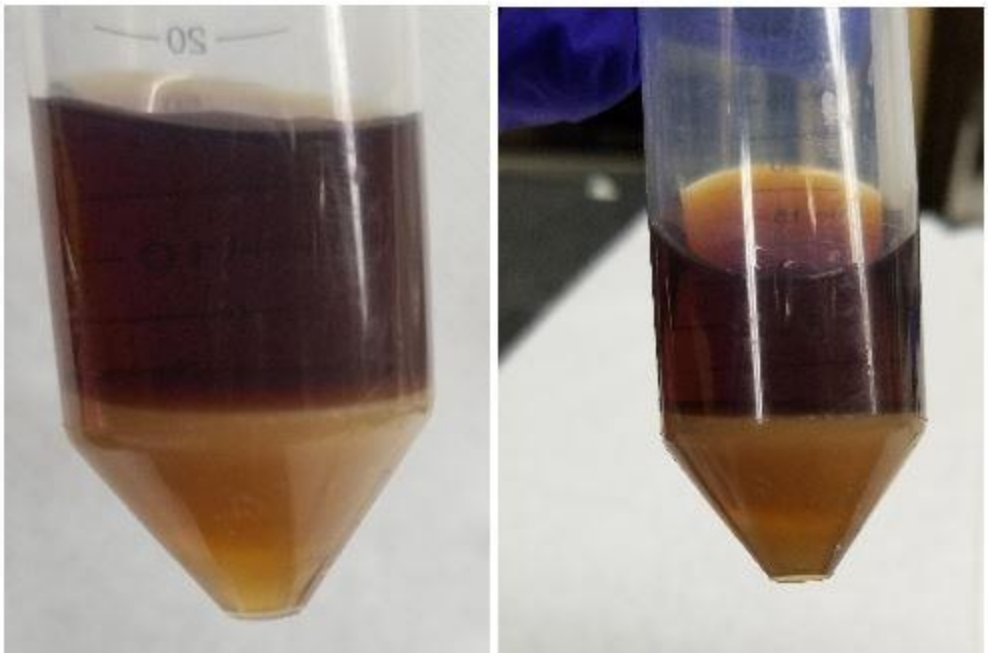


Figure 5. Visible Difference Between Undesirable (left) and Desirable (right) Batches in DCM after Two Months of Aging

4. Results and Analysis

4.1 Overall Chemical Composition Comparison from DCM Extraction

Chemicals identified in the beer samples were categorized by functional group, including acids, alcohols, esters, and amines. Because all the runs used the same GC-MS method, the areas obtained using GC analysis were representative of the relative concentration of a compound and could be compared between runs. Full GC-MS results can be found in Appendix C.

Table 4. Overall Chemical Composition, DCM Extraction 2/17/19

Compound Class	Desirable Batch (Area)	Undesirable Batch (Area)	Difference
Acid	28.20	34.64	+22.8%
Alcohol	34.53	49.69	+43.9%
Amine	7.96	3.04	-61.8%
Ester	12.98	20.90	+61.0%

The DCM extraction on 2/17/18 showed that the undesirable batch of porter had a significantly higher proportion of acids, alcohols, and esters (22.8%, 43.9%, and 61.0% more, respectively). It showed a decrease in the amount of amines present in the undesirable batch, but due to the identification of only a very small number of amines by the mass spectrometer, this result is statistically insignificant (Table 4).

Table 5. Overall Chemical Composition, DCM Extraction 3/19/19

Compound Class	Desirable Batch (Area)	Undesirable Batch (Area)	Difference
Acid	8.59	15.58	+81.33%
Alcohol	24.55	24.68	+0.50%
Amine	4.92	6.40	+30.24%
Ester	6.73	5.27	-21.68%

The DCM extraction that was executed on 3/19/19 yielded similar results to the trial from a month earlier. The undesirable batch once again contained more acids, alcohols, and amines (81.3%, 0.5%, and 30.2% more, respectively), but a lower amount of esters (Table 5).

4.2 Overall Chemical Composition Comparison from THF Extraction

Our first THF extraction yielded results that differed from the DCM extraction, which is likely because a slightly different profile of compounds was extracted (see 2.1). The undesirable batch of porter contained a lower concentration of acids, alcohols, esters, and amines than the desirable batch (30.9%, 5.7%, 12.3%, and 15.1% less, respectively). The absence of these major classes of flavor compounds in the undesirable batch suggests that compounds in other classes such as alkanes, alkenes, and amides were at higher concentrations in the undesirable batch (Table 6).

Table 6. Overall Chemical Composition, THF Extraction 2/26/19

Compound Class	Desirable Batch (Area)	Undesirable Batch (Area)	Difference
Acid	42.53	29.41	-30.9%
Alcohol	47.88	45.17	-5.7%
Amine	9.92	8.43	-15.1%
Ester	8.39	7.36	-12.3%

Table 7. Overall Chemical Composition, THF Extraction 3/19/19

Compound Class	Desirable Batch (Area)	Undesirable Batch (Area)	Difference
Acid	19.86	20.97	+5.57%
Alcohol	37.11	31.01	-16.43%
Amine	6.31	10.82	+71.44%
Ester	7.06	3.24	-54.15%

Our second extraction using THF showed slightly more acidic compounds in the undesirable porter, which is inconsistent with results from the earlier THF trial (Table 7). However, the alcohol concentration comparison was similar to the previous trial (16.4% less alcohol in the undesirable batch). Amine concentration was 71.4% higher in the undesirable batch in this extraction, unlike

the previous extraction (15.1% less in undesirable batch). Ester concentration was considerably lower in the undesirable batch in the second extraction (54% less esters in undesirable batch).

Again, the overall low overall areas of both amines and esters in both THF extractions means there is a high margin of error, as very small variations in areas can skew the percent difference considerably. These variations can arise from inclusion of false positive compounds or incorrectly identified compounds from the mass spectrometer to human error in properly identifying the most appropriate class for various complex compounds.

Overall GC-MS data suggests that the desirable batch contains less acidic compounds than the undesirable batch (Table 8). All extractions yielded results consistent with this claim except for the first THF extraction. Overall beer acidity can change the taste, with highly acidic beers tasting sour. A description of the taste of the undesirable porter designated the flavor as resembling Coca-Cola, so it is unlikely that the increased acidity is the sole reason for the taste difference. However, acidity differences may contribute to the overall flavor profile change of the porter.

Table 8. Acidic Compound Comparison

Run	Desirable Batch Acid (Area)	Undesirable Batch Acid (Area)
DCM 1	28.2	34.64
DCM 2	8.59	15.58
THF 1	42.53	29.41
THF 2	19.86	20.97

The relative amounts of alcohol in desirable and undesirable samples varied between DCM and THF extraction methods, which suggests that the desirable and undesirable batches may contain different types of alcohols. The concentrations of various alcohols are compared below in Section 4.3.

Esters exhibit inconsistent results between trials of the same extraction method, which may be attributed to aging. Many esters are formed due to exposure to oxygen, which oxidizes compounds in the beer, forming carboxylic acids and, ultimately, esters. Due to the differing chemical profile

between the desirable and undesirable batches as well as varying exposure to oxygen, esters may have formed or reacted at different rates in both batches. However, GC-MS analysis did not provide sufficient data to prove this definitively occurred in the beer.

Extraction methods aimed to provide a consistent profile of flavor compounds from the desirable and undesirable samples. Therefore, the relative amounts of extracted compounds were not representative of the ratios present in the beer but did allow for comparison between samples. Trials using different extraction methods were not compared because compounds were not extracted equally due to the different groups of compounds that are attracted to each solvent. Conversely, DCM and THF were both used for extraction in an attempt extract different profiles of compounds, as DCM and THF interact with various compounds differently.

Misidentification of compounds by the GC-MS is possible because many compounds exhibit similar mass to charge ratios, which may have led to errors in total area due to incorrect classification. Multiple trials were evaluated and averaged to account for area variance. Only trials that used the exact same extraction and GC-MS methods were compared.

4.3 Individual Flavor Compound Area Comparison

Fusel alcohols 2-methyl-1-propanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and phenylethyl alcohol are fermentation byproducts that produce a hot, spicy, or unpleasant alcoholic taste when present in excess. No significant differences were observed between the relative concentrations of most of these species using the DCM and THF extraction methods (Tables 9 & 10). However, the undesirable batch did have over twice as much 2-methyl-2-butanol (amylene hydrate) as the desirable batch, although future extractions showed none of it in either batch. The overall consistency in concentration between the desirable and undesirable batches suggests that fusel alcohols are unlikely to be the main culprit in flavor differences, although 2-methyl-2-butanol may play a small role.

It is possible that the undesirable batch originally contained more fusel alcohols than the desirable batch and some of the fusel alcohols reacted with carboxylic acids present in the beer to form esters.[1] For example, 3-methyl-1-butanol readily condenses with carboxylic acids to form 3-methyl-1-butanol acetate, or isoamyl acetate, which was identified in only undesirable porter batch

samples (see 4.4). Unfortunately, the team was not able to run GC-MS analyses on the porter immediately after it was brewed in order to prove this hypothesis. The fusel alcohol concentrations shown below are from several months after brewing and may not necessarily be indicative of initial fusel alcohol concentrations in the porter. Future studies should test multiple samples of brews immediately to avoid this uncertainty.

Table 9. Overall Chemical Composition, THF Extraction 3/19/19

Compound	Desirable Batch (Area)	Undesirable Batch (Area)
2-methyl-1-propanol	2.40	2.39
2-methyl-1-butanol	3.54	3.54
2-methyl-2-butanol	1.64	3.72
3-methyl-1-butanol	3.33	3.32
Phenylethyl Alcohol	6.74	6.71

Table 10. Fusel Alcohol Area Comparison, THF Extractions

Compound	Desirable Batch (Area)	Undesirable Batch (Area)
2-methyl-1-propanol	2.17	2.06
2-methyl-1-butanol	3.63	3.63
3-methyl-1-butanol	3.38	3.39
Phenylethyl Alcohol	6.48	6.53

Acetic Acid was present at a 26% higher concentration in the undesirable batch than the desirable batch according to the 2/17/19 DCM extraction (Table 11). Acetic acid, also known as vinegar, can create a foul taste at high concentrations. Acetic acid can be inadvertently formed in large amounts during the brewing process due to bacterial contamination, wild yeast contamination, or excessive oxygenation.

Table 11. Acetic Acid Area Comparison, DCM Extraction 2/17/19

Compound	Desirable Batch (Area)	Undesirable Batch (Area)
Acetic Acid	6.76	8.53

However, future extractions failed to show any acetic acid in either batch of beer, so the sample size for this trend is small (values are averages of four undesirable samples and three desirable samples). Acetic acid is present in all beers, so it is likely that the mass spectrometer failed to properly identify the compound in later extractions.

Ethyl acetate was found in consistent amounts between DCM runs with a variance of 5%. In large amounts, ethyl acetate can be considered an off-flavor, especially in a porter. Like many esters, ethyl acetate generally contributes a fruit-like flavor. However, due to the consistency between desirable and undesirable porter samples, it is unlikely that ethyl acetate formation is contributing to the inconsistency in taste (Table 12).

Table 12. Ethyl Acetate Area Comparison

Compound	Desirable Batch (Area)	Undesirable Batch (Area)
Ethyl Acetate	2.55	2.33

Organosulfur compounds were found to be present in both the desirable and undesirable porters. The team observed that two different types of coconut flavoring were used in the process, one of which was sulfured. GC-MS results did not show significant quantities of organosulfur compounds, so it is unlikely that organosulfur compounds drastically affect flavor.

Organochlorides had a 19.5% higher concentration in the desirable batch of porter (Table 13). Exposure of equipment to chlorinated water can lead to the formation of many types of organochlorine compounds, including **chlorophenols**, which cause the beer to have the smell and taste of mouthwash or disinfectant in concentrations as low as 0.0002 mg/L.[19] Although chlorine concentration was higher in the desirable batch of porter, compounds containing chlorine are often associated with off flavors and overall concentration should be kept consistently to a minimum. Equipment should be sanitized using cleaning solutions and thoroughly rinsed with water between

batches to avoid any build-up of chlorine-containing compounds in the system and water supplies into breweries should be filtered to reduce their chlorine concentration.

Table 13. Organochloride Area Comparison

Compound	Desirable Batch (Area)	Undesirable Batch (Area)	Difference
Organochlorides	74.5	60	-19.5%

4.4 Comparison of Presence or Absence of Individual Flavor Compounds

GC-MS results were screened for specific off-flavors that almost always harm the flavor of a beer, as well as flavors that only appear in one batch or the other. If a specific organoleptic compound was found mainly or only in one batch, it likely contributed to the porter's flavor consistencies and could help uncover root causes of the reoccurrence of undesirable batches.

Isoamyl acetate and **maltol**, two standard beer flavor compounds, were found mainly in the undesirable batch from the first DCM extraction. **Isoamyl acetate** (3-methyl-1-butanol acetate), found in 100% of the undesirable batch samples but only 33% of the desirable batch samples, provides a fruity, banana-like flavor to beers but can be off-putting in excess. **Maltol**, found in 75% of the undesirable batch samples but only 33% of the desirable batch samples, is a naturally-occurring flavor compound from roasted malts. Its sweet flavor can impart a cotton candy or caramel-like aroma to a beer, and can be detrimental in excess.[24] Even though the average peak areas for these compounds were relatively similar between batches, both of them mainly appeared in undesirable batch samples, which suggested they were more routinely prevalent in the undesirable batch (Appendices C & D). The presence of more flavor compounds in the undesirable batches can have a compounding, synergistic effect, as their interactions can create entirely new and undesirable flavor profiles.

Ammonium chloride, **N-aminopyrrolidine**, and **2-methylpyrazine** were three flavor compounds identified only in undesirable batch samples. **Ammonium chloride** is a salty food additive found in nutritive media for yeast that can confer a salty, spicy, somewhat medicinal

taste. Found in 75% of the undesirable batch samples but none of the desirable batch samples, ammonium chloride could add to the cola-like flavor of the undesirable batch due to the spicy flavor it provides. It usually is found in candies and dried foods, so it is very possible to be present in some amount in any of the grains (especially chocolate or caramel malts) or marshmallows. If slightly different sets of ingredients were used for each batch, then it is possible a single ingredient contained ammonium chloride and was responsible for its presence in the undesirable batch.

N-aminopyrrolidine belongs to a class of compounds known as pyrrolidines, which possess unpleasant fishy odors. Meanwhile, **2-methylpyrazine** provides a nutty, roasted cocoa flavor and smell, but in higher amounts can smell and taste musty or old. While these flavors were inconsistent with the cola-like taste of the undesirable batch, they certainly could have played a role in making the batch taste slightly unpleasant. Both were present in 50% of the undesirable batch samples but none of the desirable batch samples.

Other organoleptic compounds present in around 30% of the undesirable batch samples but in none of the desirable batch samples included **butanoic acid**, **piperidine carboxamide**, and **dioxopropanoic (pyruvic) acid**. **Butanoic acid** is usually indicative of bacterial contamination of some stage of brewing or of the beer aging. Since the organic extractions were all performed two to five months after brewing, the butanoic acid presence was most likely a result of aging. Meanwhile, the presence of piperidines and pyruvic acid in only the undesirable batch could have been due to an incomplete fermentation. **Piperidines** are biogenic amines with a pepper-like flavor and odor that result from the decarboxylation of amino acids during protein metabolism by yeast, while **pyruvic acid** is an intermediate in the breakdown of carbohydrates, lipids, and proteins.

The low rate of occurrence of these compounds mean that they may have been false positives. However, they appeared in undesirable batch samples from different extraction dates and using different solvents, so there was some measure of reproducibility in finding these compounds.

The inability to show the same organoleptic compounds in every organic extraction of the undesirable batch made it difficult to connect the undesirable flavor to specific compounds. Nevertheless, the undesirable batch samples overall had far more organoleptic compounds

present than the desirable batch samples, which suggested that the problem was more complex than a single troublesome flavor compound and was likely due to the synergistic interaction of the aforementioned flavor compounds in the undesirable batch (Appendices C & D).

5. Conclusions

Purgatory Beer Company's Coconut Rum Porter was tested for differences in flavor compounds between a desirable and undesirable batch using GC-MS. The results of GC-MS testing showed inconsistency between desirable and undesirable porters. The inconsistency between the two samples in GC-MS results suggests that one or more phases of the brewing process require increased control and standardization. Results showed that raw ingredients, fermentation temperature, water quality, and oxidation may have contributed to the introduction of undesired flavor compounds. Qualitative observation as well as GC-MS results suggested that the porter is highly susceptible to the effects of oxidation and aging.

The use of two different solvents for extraction of organic compounds (DCM and THF) resulted in a wider range of flavor compounds detected using GC-MS. Inconsistencies in trends between these two methods were observed, which suggests that the two solvents extracted certain compounds in varying amounts. Overall, GC-MS results provided guidance to further examine portions of the porter's brewing process to achieve a consistent, desirable product. Based on these conclusions, the team developed a set of recommendations that can be found in Section 6.

6. Recommendations

6.1 Control of Fermentation Variables

The difference in chemical profile between the desirable and undesirable batches is most likely linked to inconsistent control of certain process variables during fermentation. As organisms with a very specific range of optimal conditions, yeast can change how they metabolize carbohydrates, lipids, and proteins depending on the conditions to which they are subjected. While GC-MS analysis did not show specific chemical compounds as being solely responsible for the flavor differences between the two batches, the undesirable batch contained more overall acids and more flavor-influencing compounds. As such, the team recommends that Purgatory Beer Company ensure careful, consistent control over several key fermentation variables: temperature, order of ingredient addition, aeration or oxygenation during and between fermentations, and storage of yeast when not fermenting.

6.1.1 Temperature Control

Beer fermentation temperature has a significant impact on the flavor profile of a beer. Many primary flavor components such as ethanol, carbon dioxide, acetaldehyde, and fusel alcohol concentrations are significantly influenced by the beer's fermentation temperature. According to the distributor of the type of yeast used in the Fiero Coconut Rum Porter, the ideal fermentation temperature range is 65-68°F. The standard fermentation temperature that Purgatory Beer Company uses for this porter is 69°F, which is slightly above the ideal temperature range provided by the distributor. By operating the fermentation outside of the suggested temperature for the yeast, a certain degree of inconsistency is added into the brewing process.

There was a clear trend of increased acidity and increased flavor compounds (many with negative organoleptic effects) in the undesirable batch, and the overall chemical profile was considerably different between batches. The fact that so many more organoleptic compounds appeared in the undesirable batch suggests that at least one fermentation variable was not consistently controlled between porter batches. Inconsistent temperature, especially when outside of the of the optimal range, can drive the yeast to use alternate metabolic pathways and produce compounds that they would not normally produce, and potentially kill them.

Additionally, although the difference between the actual and suggested fermentation temperature is only a few degrees Fahrenheit, the increased fermentation temperature promotes the production of ethanol, acetaldehyde, and fusel alcohols. These compounds have significant impacts on the flavor of the beer, so if more of them are produced, the actual flavor can vary significantly from what was expected. The team recommends that the temperature used for fermentation is lowered to 66°F and is carefully regulated every time the Fiero Coconut Rum Porter is brewed.

Purgatory Beer Company previously expressed concern about the accuracy of fermenter thermometers. Given the importance of controlling temperature, the team recommends ensuring that all thermometers used be accurate and frequently checked for proper functioning to allow for careful monitoring of the fermentation process. Multiple thermometers located at various stages and multiple levels in the fermenters ensure that even if mixtures are not well-mixed, a more accurate temperature reading for an entire vessel can be acquired. Yeast also acts like an insulator, so yeast cakes can often be 10 to 15°F above the temperature of the beer that they are fermenting.[26] Electronic or remote-reading thermometers are preferable, as they provide much more accurate readings than dial or liquid-in-glass thermometers.[1] Additionally, opening and closing of the doors at Purgatory during brewing can also cause temperature fluctuations in the fermenters, especially if they are not well-insulated.

GC-MS analysis showed isoamyl acetate (banana oil), a result of running fermentation at an elevated temperature, primarily in the undesirable batch samples (Appendix D). Additionally, multiple intermediates of metabolic processes, including pyruvic acid, pyrrolidines, and piperidines, appeared mostly in the undesirable batch, which suggests that not all of the yeast were able to fully carry out fermentation, or that their metabolic pathways were altered in some way due to being at an increased temperature.

Lowering and carefully maintaining the fermentation temperature to 66°F would not only allow the yeast to operate in their ideal temperature range, but it would also lower the risk of producing higher concentrations of undesirable primary flavor components. If the temperature is maintained at exactly 66°F from batch to batch, it reduces the likelihood of inconsistencies occurring during fermentation, thereby reducing the likelihood of inconsistencies in flavor from occurring from one batch to another.

6.1.2 Addition of Flavor Compounds During Secondary Fermentation

Depending on the type of beer being created, some brewers will break the fermentation process into two subsequent stages that allow for the unique customization of a beer's flavor. The team recommends whenever brewing a porter, Purgatory Beer Company should use two-stage fermentation and the flavoring should be added during the second stage. The first stage, known as primary fermentation, is where most of the starch is converted to alcohol by yeast. During primary fermentation, custom flavoring ingredients should be left out of the vessel because these flavorings will introduce new types of sugar into the brewing liquid that will compete with the starches of the malt and oats to be the primary energy sources for the yeast. If the yeast begins to convert the new and artificial sugars instead of the starch from the malt, the chemicals, alcohol content, and taste produced by the yeast may vary significantly from one batch to the next.

After the yeast has converted most of the starches into alcohol, the liquid is moved to a new vessel where secondary fermentation begins. During secondary fermentation, the custom flavors, such as cacao, vanilla, or coconut rum should be added into the fermentation vessel. By waiting to add the flavoring ingredients until after the majority of fermentation has taken place, they will not harm the yeast or compete with other sugar sources to be the primary sources of fermentation. Additionally, the higher alcohol content of the secondary fermentation broth also aids in the extraction of flavor compounds from their source ingredients, yielding more flavorful alcohol than if the flavors were added during primary fermentation. Based on these benefits, the team strongly urges the use of two-stage fermentation whenever crafting a porter and recommends waiting until stage two to add in the flavoring ingredients.

6.1.3 Control of Oxygenation and Aeration

Another key variable during fermentation is the amount of O_2 that is provided to the yeast during fermentation. Too little oxygenation of the yeast will severely limit yeast growth and cell membrane formation, poor yeast attenuation, and inconsistent or incomplete fermentations. It also skews metabolic pathways to form more potentially undesirable esters like isoamyl acetate or highly undesirable diacetyls like 2,3-butanedione (Tables 2 and 4). Conversely, too much oxygenation of the yeast can also change the metabolic pathways of the yeast, and often causes the production of many acids, such as valeric acid and acetic acid. It also promotes a variety of

oxidation reactions to occur as the beer ages in storage or bottles, most of which alter and potentially harm a beer's flavor profile.

The team recommends that Purgatory Beer Company maintain the dissolved oxygen content of fermentation broths around 10 ppm.[27] Oxygen levels of wort and beer before, during, and after fermentation should be monitored using dissolved O_2 meters.

Additionally, to minimize aeration of the wort and beer when transferring them between vessels, vigorous mixing and splashing should be kept to a minimum. One specific area of concern for aeration is when transferring beer from the primary fermenter to the secondary fermenter, where there is a high potential for introduction of excess oxygen before fermentation is complete if the beer is transferred with a high flow rate. The turbid fluid flow of higher rates allows O_2 to more easily dissolve in the beer. Establishing a dedicated line between one fermenter to another through which the beer may be routed in a controlled manner would help minimize aeration.

6.1.4 Controlled Yeast Reuse

Reuse of yeast is a common way for breweries to reduce costs and reduce the time required to activate the yeast for each successive brew. However, there are several important steps that must be taken to ensure that the yeast is able to survive for several brews and that they are separated from potentially flavor-harming contaminants. Due to significant inconsistency between the chemical profiles of the desirable and undesirable batches of porter, the team suggests that the reuse of yeast either be terminated or more tightly controlled.

The myriad array of organoleptic compounds detected by GC analysis in the undesirable batch are emblematic of contamination of the beer by other flavors or compounds that should not be in a finished porter, often caused by an incomplete separation of the yeast from the trub and old beer before reuse. The trub contains many biochemical compounds that harm the flavor and stability of a beer and can be carried over into a new beer if they are not fully removed from the yeast. Purgatory's porter has marshmallows, cocoa, and coconut, which contain heavy lipids that can go rancid or oxidize quickly and that will be found in the trub. Yeast should also not be reused for different beer types, as flavor compounds from one type of beer will remain in the yeast when it is used for an entirely different type of beer and harm its flavor.[26]

The yeast should be removed shortly after fermentation has completed and the beer has chilled in order to keep its temperature low and stable, as high temperatures during storage seriously hamper the yeast's lifespan. After cleaning and separation from the trub, the yeast should be stored in smooth-walled containers to avoid bacterial buildup in the grooves of other types of containers. The container should be sealed from the environment to prevent excess oxygenation of the yeast and the entry of bacteria, all of which can harm further brews. Lastly, the container should be daily opened briefly to allow for any built-up CO_2 to be released — both the high pressure of too much stored CO_2, and the chemical interactions of CO_2 with yeast cell walls can kill yeast and ultimately harm future brews.[26]

The yeast should be stored for no more than two weeks before being reused, as many of them begin to die past that duration, which harms the efficiency and taste of future brews. If the yeast is kept for too long before reuse, fermentation will be significantly less efficient and may not be fully completed in new brews. This can leave unfermented sugars in the beer which give it an uncharacteristic, soda-like flavor, consistent with the observations by Purgatory. Unfortunately, the presence and concentration of such sugars could not be detected via the team's limited analytical methods, although the pyruvic acid and piperidines detected by GC-MS are typical products of incomplete fermentation.

6.1.5 Improved Fermentation Monitoring Tools

New technologies developed specifically for use by micro- or nanobreweries like Purgatory can improve the monitoring of various process variables and thus quality control. The team recommends that Purgatory investigate the use of improved fermentation monitoring tools in order to improve the consistency between beer batches and to more easily see the effects of changing certain variables, like fermentation temperature, in small increments.

One such technology is a remote fermentation monitoring sensor developed by BoxcarCentral, which detects the formation of CO_2 bubbles in tanks and uses it to determine the current fermentation rate.[28] It also provides more accurate and precise temperature readings than standard thermometers.

Another novel sensor technology is an acoustic-based sensor developed by TZero Labs, which measures changes in the density of the fermentation broth by monitoring the changes in the speed of sound waves traveling through the liquid.[28] As fermentation progresses, the density of the broth decreases as starches are converted to alcohols, so density is directly related to the progress of fermentation. This allows brewers to monitor beer density in real-time and to determine how far along a fermentation is, without taking any manual measurements.

In addition to improving consistency, these sensors can be used to monitor the effects of changing certain ingredients, process variables, or orders of process steps on fermentation, even in small increments. It adds a level of control to the experimentation that is uncommon in brewing.

6.2 Use of Unsulfured Coconut

The Fiero Coconut Rum Porter requires coconut to be added to the beer during fermentation (usually during the secondary fermentation if two stages are used), which will provide the beer with its characteristic coconut flavor. Based on available sources of coconut online, brewers can either purchase sulfured or unsulfured coconut to add to their beer. It can contribute to the production of undesirable sulfur-containing compounds such as dimethyl sulfide that detract from the taste of the beer. If a brewer switches back and forth between using sulfured and unsulfured coconut from one batch to another, the taste of the beer may be significantly impacted by the varying sulfur content.

While GC-MS analysis of both batches did not show an appreciable increase in organosulfur compounds in the undesirable batch, the team nevertheless suggests that Purgatory Beer Company buys unsulfured coconut to use in their porters to reduce the overall concentration of sulfur-containing compounds in their beer. By using unsulfured coconut, the taste of the Fiero Coconut Rum Porter may both improve beer taste and become more consistent from batch to batch.

6.3 Filtration of Water

Purgatory Beer Company uses municipal water provided by the Whitinsville Water Company. Town water must adhere to strict state and federally regulated guidelines to ensure the safety of anyone drinking the water; however, these usually only provide a maximum allowable

concentration for specific chemicals and not exact amounts that must be present in the water. This "allowable range" for the concentration of certain chemicals and toxins in the water means that the chemical composition of city water is constantly fluctuating. Although Whitinsville town water falls into the safe-to-consume range, based on their water quality testing results from 2018, significant fluctuations can be detected within certain chemicals in the water (see Appendix E).

One of the more significant fluctuations in the Whitinsville water supply is the concentration of chlorine. The maximum concentration of chlorine allowed in the water supply is 4 parts per million before it becomes dangerous for consumption, while the detected range varied from 0.03-1.51 parts per million during monthly test samples taken by the water company.[25] While a difference of 1.5 parts per million of chlorine may seem insignificant on the surface, this is nearly half of the allowable concentration before chlorine may cause adverse health effects upon consumption. Additionally, the data representing this range of concentrations was collected monthly, which shows that the concentration of chlorine in the water supply to Purgatory Beer Company fluctuates regularly.

Based on the GC-MS data collected, the amount of organochlorines in the desirable and undesirable porter batches differ from one another by 19.5%. This varied chlorine concentration could be caused by the lack of a filter on the water supply being used at Purgatory Beer Company. The team recommends that the brewery filters the water using an activated carbon filter to regulate chemical composition and decrease inconsistency between batches while brewing.

6.4 Minimize Effects of Aging

How a beer ages and its storage conditions have a significant impact on the shelf-life and quality of a beer's taste over time. When the DCM extraction was performed on fresh, new samples of the desirable and undesirable porters, distinct differences were observed between the samples. Initially, the desirable sample of porter displayed three separate layers: a clear, transparent organic layer formed at the bottom; a murky layer containing some bubbles formed in the middle; and an opaque, dark water/porter layer formed at the top (Figure 4). The layers of the undesirable batch blended together, forming an opaque, dark water/porter layer on the top, and a slightly lighter, but still rather dark and murky layer that traveled to the bottom of the tube (Figure 4). After being in a sealed growler in a fridge for several months, the DCM extraction was run again and both the desirable and undesirable porters displayed similar observable physical characteristics to the original extraction results for the undesirable porter (Figure 5).

This shows that over the course of a few months of being in a sealed container, in a cold storage area, the chemical composition of the porter changed in some way to make it behave physically similar to the undesirable porter. Although the team was unable to determine a definitive cause for this change since the viscous semisolid beer layer could not be analyzed by GC-MS, something inside the porter is changing over time and causing it to become more like the undesirable porter. The team recommends that the Fiero Coconut Rum Porter be sold relatively quickly after being brewed rather than being kept for sale at a later date. By preventing the porter from aging, the porter will likely exhibit less of the undesirable characteristics and flavors.

6.5 Improvements for Future Studies

One of the scientific limitations of this experiment was the team's limited access to advanced analytical chemistry equipment. Gas chromatography cannot separate all types of compounds and is often limited to more polar fermentation products and volatile compounds. Since it separates compounds by vaporization, non-volatile or heavy compounds will not be detected, or may not even be allowed to enter the GC depending on their viscosity. There is also the chance that compounds of similar chemical properties co-elute, which causes misidentification or no identification of certain compounds.

During the team's extraction, much of the extraction samples were discarded and heavily filtered to avoid harming the GC's delicate instrumentation with dark, viscous, sludge-like compounds extracted from the beer. Any compounds contained in the discarded layer were not tested by the GC, so their effect on flavor profile or stability remained unknown.

Future teams studying the flavor profiles of a beer may wish to a variety of equipment to test the beer. Two dimensional GC, or GC*GC, may be used to prevent co-elution of compounds and acquire a better picture of a sample's chemical profile. High performance liquid chromatography (HPLC) is also a viable way to separate and identify heavier and nonvolatile compounds in the extraction samples, since it does not rely on vaporization to separate compounds.[28]

Another limitation of the study was the use of extraction method. The liquid-liquid extraction used by the team is unable to extract many of the relatively large hop acids from the beer. The team used two solvents (THF and DCM) to extract a larger class of compounds, but the method is inherently limited in the types of flavor compounds it extracts, which are mainly alcohols and lower molecular weight acids. Headspace solid phase microextraction (HS-SPME) is considered the most effective method for extracting both the standard flavor constituents of a beer and its many hop compounds and is easily interfaced with a GC for analysis.[29]

Lastly, extractions should be performed immediately upon acquisition of beer samples to prevent the effects of aging from distorting the chemical profile of a beer. The same growlers of porter were used for several months of testing by the team, and this likely contributed to inconsistency in the results and made it more difficult to develop a chemical profile of the beer that is closer to its profile upon serving.

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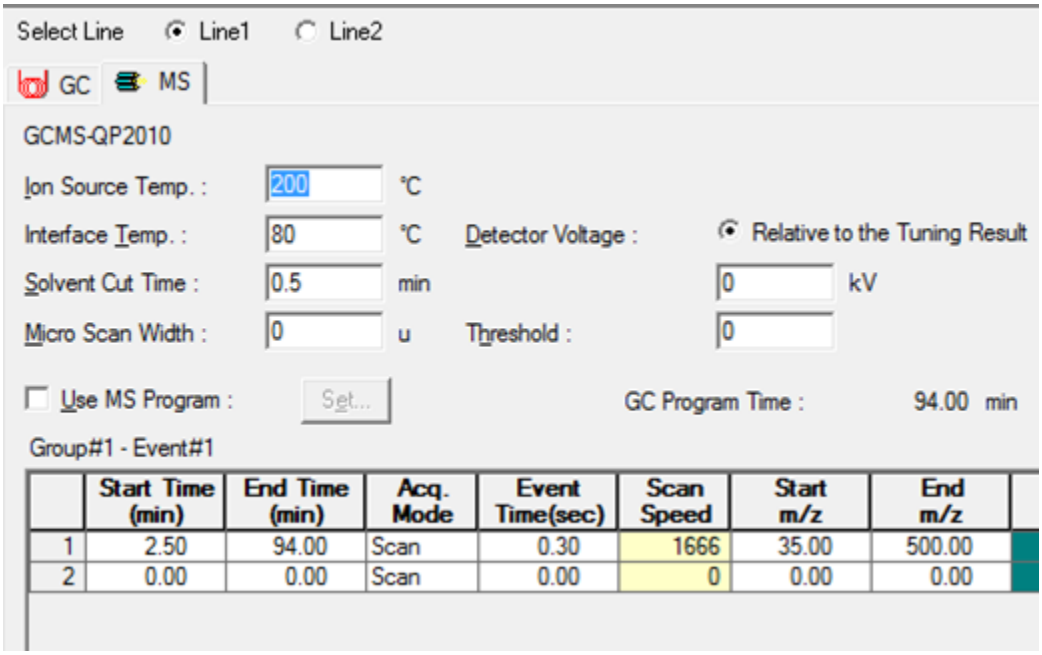
Appendices

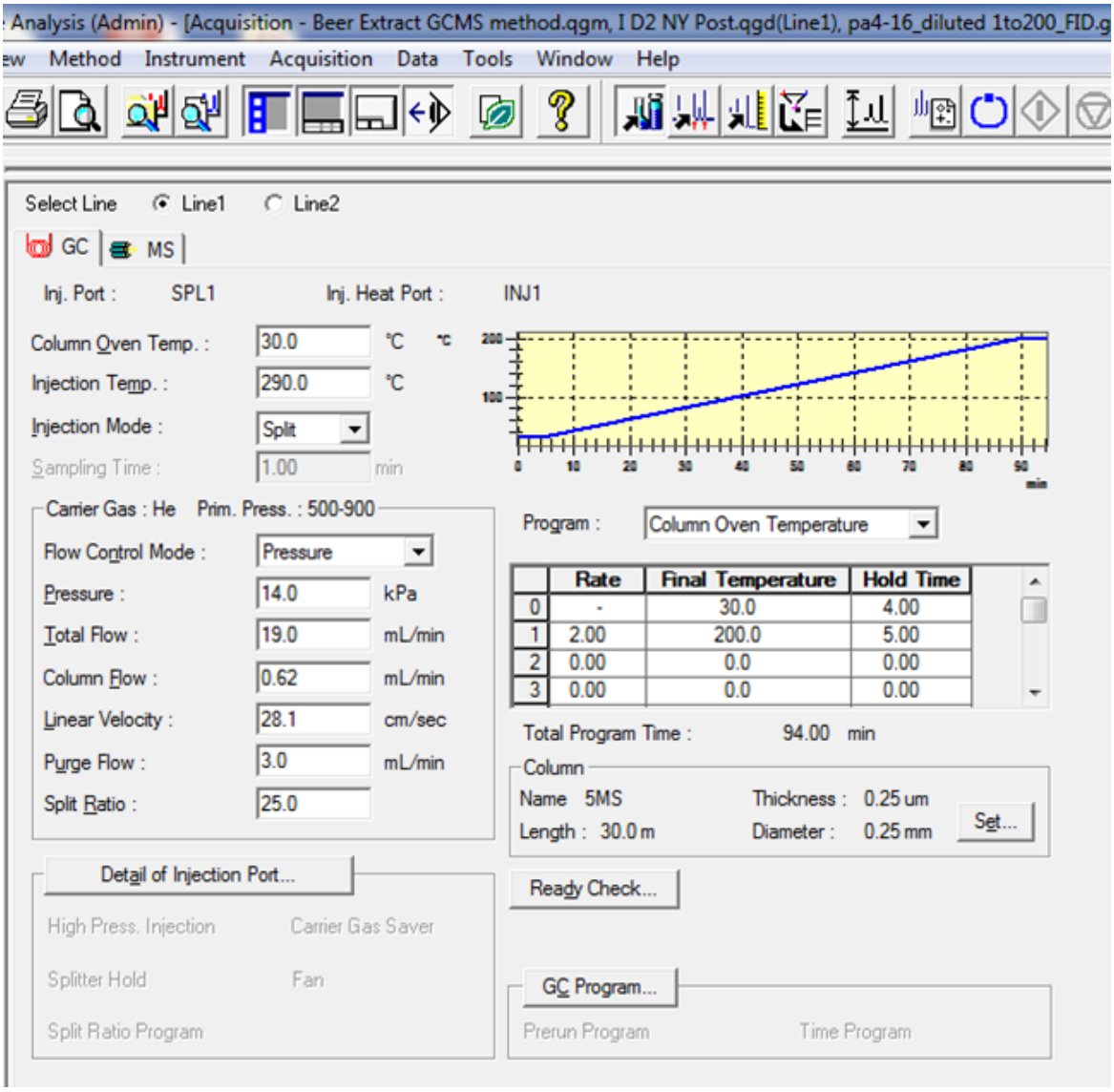
Appendix A: GC-MS Method

The samples of extracted organic compounds were analyzed using GC-MS. A specific method for analyzing the samples was developed by graduate student Alex Maag in the Timko Lab and injected 3 microliter samples of every sample into the GC. The carrier gas, helium, had a flow rate of 19.0 mL/min in split injection mode. The samples were automatically injected at 290℃. The oven temperature was maintained at 30℃ for four minutes, then ramped up to 200℃ for five minutes.

Subsequent analysis of mass spectra used a peak integration slope parameter of 350 for the first two DCM and THF runs, and 400 for the last two DCM and THF runs in order to cut down on the amount of low-concentration, potentially inaccurate compounds in the results. Figures 6 shows the exact method used.



	Start Time (min)	End Time (min)	Acq. Mode	Event Time(sec)	Scan Speed	Start m/z	End m/z
1	2.50	94.00	Scan	0.30	1666	35.00	500.00
2	0.00	0.00	Scan	0.00	0	0.00	0.00


Analysis (Admin) - [Acquisition - Beer Extract GCMS method.qgm, I D2 NY Post.qgd(Line1), pa4-16_diluted 1to200_FID.g
Method Instrument Acquisition Data Tools Window Help
Select Line Line1 Line2
GC MS
Inj. Port : SPL1
Inj. Heat Port : INJ1
Column Oven Temp. : 30.0 °C
Injection Temp. : 290.0 °C
Injection Mode : Split
Sampling Time : 1.00 min
Carrier Gas : He Prim. Press. : 500-900
Flow Control Mode : Pressure
Pressure : 14.0 kPa
Total Flow : 19.0 mL/min
Column Flow : 0.62 mL/min
Linear Velocity : 28.1 cm/sec
Purge Flow : 3.0 mL/min
Split Ratio : 25.0
Detail of Injection Port...
High Press. Injection
Carrier Gas Saver
Splitter Hold
Fan
Split Ratio Program
Program : Column Oven Temperature
Rate Final Temperature Hold Time
0 - 30.0 4.00
1 2.00 200.0 5.00
2 0.00 0.0 0.00
3 0.00 0.0 0.00
Total Program Time : 94.00 min
Column
Name 5MS
Thickness : 0.25 um
Length : 30.0 m
Diameter : 0.25 mm
Set...
Ready Check...
GC Program...
Prerun Program
Time Program

Appendix B: Initial Ineffective Extraction Method

In order to determine the prevalence of organic compounds using gas chromatography in combination with mass spectrometry an extraction using dichloromethane was performed. 5 mL samples of the porter were added to a centrifuge tube along with 5 mL of water and 1 mL (instead of the 5 mL used for final experimentation) of dichloromethane. Additionally, 2.25 grams of salt was also added to drive the desired organic compounds out of the porter and into the organic dichloromethane layer.

The centrifuge tube was shaken for 10 minutes using a wrist action shaker machine and then centrifuged at 3000 RPMs for 10 minutes. A clear organic layer formed in the bottom of centrifuge tube, which contained the dichloromethane and the organic compounds that were extracted from the porter.

The problem with this methodology was that the volume of the clear organic layer was too small to properly filter. When the layer was extracted and pushed through a filter, the filter absorbed much of the liquid and did not leave enough of the sample to run GC-MS testing on. In order to correct this problem, higher volumes of dichloromethane (5 mL) were added during the initial extraction instead of using the initially planned 1 mL of dichloromethane.

Appendix C: GC-MS Results

GC-MS Results Comparison, DCM Extraction 2/17/19

O1, O2, O3 = undesirable batch samples; N2, N3, N4 = desirable batch samples

Chemical	O1	O2	O3	O4	N2	N3	N4
.alpha.-Aminoisobutyronitrile	X	X	1.78	X	X	X	X
.alpha.-D-Glucopyranoside, methyl 2-(acetylamino)-2-deoxy-3-O-(trimethylsilyl)-, cyclic butylboronate	2.05	X	X	X	X	X	X
.beta.-Chloroethylurea	X	X	X	X	X	X	0.67
(2-Acetyl-1-naphthyloxy)difluoroborane	X	X	X	X	X	1.12	X
(2,2-Dichlorocyclopropyl)methanol	X	1.87	X	X	X	X	X
(3,5-Dimethyl-piperidin-1-yl)-(2-iodo-phenyl)-methanone	8.31	X	X	X	X	X	X
(R)-(+)-2,2,2-Trifluoro-N-(3-pyrrolidinyl)acetamide	2.09	X	X	X	X	X	X
(S)-5-Hydroxymethyl-2[5H]-furanone	X	X	X	X	X	1.77	X
[4,4']Bipiperidinyl	X	X	X	1.61	X	X	X
1-(4-Chlorophenyl)-2-[2-(2,2,2-trifluoro-1-hydroxy-1-trifluoromethylethyl)-1-naphthyl]urea	9.85	X	X	X	X	X	X
1-Butanamine, N-butyl-N-nitroso-	X	X	X	X	X	X	2.49
1-Butaneboronic acid	X	X	X	X	0.64	X	X
1-Butanethiol	X	0.51	X	X	X	X	X
1-Butanol, 2-methyl-	3.61	3.56	3.48	3.56	3.66	3.51	3.51
1-Butanol, 3-methyl-	3.29	3.37	3.34	3.36	3.38	3.38	3.36
1-Butanol, 3-methyl-, acetate	3.83	4.18	3.12	3.72	3.89	X	X
1-Buten-3-yne, 1-chloro-, (Z)-	X	X	X	X	X	X	6.55
1-Butene, 2,3-dimethyl-	X	X	X	X	X	X	3.93
1-Heptanol, 2,4-diethyl-	X	3.63	X	X	X	X	X
1-Nonanol, 4,8-dimethyl-	X	X	X	X	X	X	3.67
1-Octadecene	X	X	3.15	X	X	X	X
1-Octanol, 2,7-dimethyl-	X	4.11	X	X	X	X	X
1-Pentanol, 2,4-dimethyl-, (.+/-.)-	X	X	X	X	1.76	X	X
1-Propanol, 2-methyl-	2.57	2.27	2.7	2.56	2.43	2.85	2.75
1-Propanol, 3-(methylthio)-	X	X	X	2.16	X	X	X
1,1-Dichloro-2-methyl-3-(4,4-diformyl-1,3-butadien-1-yl)cyclopropane	X	3.22	X	X	X	X	X
1,10-Diaminodecane	0.39	X	X	6	X	1.26	5.19

1,2-Cyclopropanedicarboxylic acid, cis-	X	X	X	5.9	X	X	X
1,2-Disilacyclopentane, 1,1,2,2-tetramethyl-	X	1.34	X	X	X	X	X
1,2,4-Cyclopentanetriol	X	0.79	X	X	X	X	X
1,2,4-Triazole, 4-(4-dimethylamino-3-nitrobenzylidenamino)-	X	1.64	X	X	X	X	X
1,3-Butanediol, (R)-	0.94	X	X	X	X	X	X
1,3-Dioxolane, 2-heptyl-4-phenyl-	X	X	X	X	X	2.33	X
1,3,2-Oxaazaborinane, 3-cyclohexyl-2-isopropyl-	X	X	X	X	X	2.01	X
1,3:2,4:5,7-Trimethylene-.beta.-sedoheptitol	0.87	X	X	X	X	X	X
1,4-Eicosanediol	X	X	X	1.47	X	X	X
1,6-Dimethyl-7-oxo-1,2,3,7-tetrahydroimidazo[1,2-a]pyrimidine	X	4.76	X	X	X	X	X
1H-1,2,3-Triazole-1,5-diamine, 3-nitro-	X	X	X	1.83	X	X	X
1H-Imidazole-1-ethanol, .alpha.-methyl-	X	X	X	X	0.31	X	4.5
1H-Pyrazole-4-carboxylic acid, 1-(2-chloroethyl)-5-methyl-	X	X	X	X	2.36	X	X
1R-Ethoxy-3-cis-methoxy-2-cis-methylcyclohexane	X	X	0.56	X	X	X	X
2-(2,4-Dichlorophenoxy)-N-(4-nitro-1,8-naphthalimido)acetamide	X	X	X	X	X	0.39	X
2-(3-Methylphenoxy)octahydro-1H-1,3,2-benzodiazaphosphole 2-oxide	X	X	X	X	X	1.64	X
2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazolyl)-5-nitrobenzoic acid	X	X	X	0.32	X	X	X
2-(Chloromethyl)-5-oxo-1,2-oxaphospholane 2-oxide	X	X	X	X	X	X	1.95
2-Butenediamide, (E)-	X	X	X	X	1.05	X	X
2-Butyne-1,4-diol, diformate	1.86	X	X	X	X	X	X
2-Dimethyl(trimethylsilyl)silyloxytetradecane	X	X	X	X	X	0.3	X
2-Furanmethanol	4.4	4.93	4.56	4.08	4.22	4.74	3.41
2-Hexenedioic acid, 2,4-dichloro-5-oxo-	4.11	5.25	9.58	X	X	3.11	X
2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, (E)-	X	0.89	X	X	X	X	X
2-Methyl-2-pentyl methylphosphonofluoridate	X	X	X	X	X	2.61	X
2-Nonenoic acid	X	X	0.71	X	X	X	X
2-Oxa-8-azaspiro[5.5]undecane-1,3,7-trione	X	X	X	X	X	0.88	X
2-Pentanone, 4-hydroxy-	X	3.45	X	X	X	X	X
2-Pentenal, (E)-	4.83	X	X	X	X	X	X
2-Piperidinone, 1-methyl-	2.13	X	X	X	X	X	X
2-Propanol, 1-(4-methylphenyl)-3-ureido-	4.79	X	X	X	X	X	X
2-Propen-1-one, 1,3-diphenyl-, (E)-	X	X	X	X	X	0.73	X

2-Pyridineethanol, .alpha.-methyl-	X	X	X	X	X	X	3.58
2-Pyrrolidinone, 3-(1-hydroxyethyl)-	X	X	X	X	X	2.73	X
2-Quinuclidinecarboxylic acid, 3-oxo-, ethyl ester	X	1.93	0.86	X	X	X	X
2-Thiopheneacetic acid, 2,2-dimethylpropyl ester	1.96	X	X	X	X	X	X
2,2-Dimethyl-1-propyl methylphosphonofluoridate	X	X	1.16	X	X	X	X
2,3-Butanediol	X	X	2.58	X	X	X	X
2,3-Dichloropropionitrile	2.76	X	X	X	X	X	X
2,3-Dioxopropanoic acid, 3-(2,5-dichlorothien-3-yl)-, 2-(4-methoxyphenyl)hydrazone	X	X	X	1.48	X	X	X
2,4-Dimethyl-1-heptene	4.41	3.98	3.42	4.13	3.58	4.14	4.02
2,5-Piperazinedione, 3-benzyl-6-isopropyl-	X	X	1.18	X	X	X	X
2.3-dimethyl-1-pyrroline 1-oxide	0.59	X	X	X	X	X	X
2H-1,4-Benzodiazepin-2-one, 7-chloro-1,3-dihydro-5-phenyl-1-(trimethylsilyl)-	X	X	X	X	X	2.89	X
2H-Thiazolo[2,3-c][1,2,4]triazol-3-one, 6-methyl-5,6-dihydro-	X	X	X	X	X	1.17	X
3-(Ethyl-hydrazono)-butan-2-one	X	X	X	X	X	0.72	X
3-(Methylthio)propyl acetate	X	X	X	0.94	X	X	X
3-Amino-1,2,4-triazole-5-carboxylic acid	X	X	X	X	X	X	3.78
3-Cyclopentylpropionic acid, nonyl ester	X	4.61	X	X	X	X	X
3-Furanmethanol	X	X	X	X	X	1.76	X
3-Heptanol	X	X	X	X	X	3.7	X
3-Pentanol, 2,2-dimethyl-	X	X	X	3.87	X	X	X
3,3-Dichloropropyne	X	X	X	X	X	2.68	X
3,3,5-Trimethylcyclohexyl acrylate	X	X	X	1.78	X	X	X
3,3',4,4'-Tetranitrodiphenylsulfoxide	X	X	X	2.28	X	X	X
3,5-Hexadien-2-ol, 2-methyl-	1.03	X	X	X	X	X	X
3',4'-Dichloro-3-(propionylhydrazono)butyranilide	X	X	X	X	1.22	X	X
4-(3-Chloro-phenyl)-9-methyl-2-trifluoromethyl-2H-pyrido[1,2-a][1,3,5]triazine-2-carboxylic acid methyl ester	0.6	X	X	X	X	X	X
4-(Dimethylhydrazono)-3,5,5-trimethylhexan-2-ol	X	X	X	X	X	0.97	X
4-[(2-Hydroxy-5-nitrobenzyl)amino]isoxazolidin-3-one	X	1.07	X	X	X	X	X
4-Amino-1-propylpiperidine	X	X	X	X	3.67	X	X
4-Bromo-N-(piperidinomethyl)phthalimide	X	X	X	X	X	X	0.85
4-Chloropyridine	1.01	X	X	X	X	X	X
4-Ethyl-5-methylthiazole	X	X	2.11	X	X	X	X

4-Hexadecanol	X	X	X	X	X	X	1.83
4-Isopropyl-1,3-cyclohexanedione	X	X	X	X	X	X	3.74
4-Nitropyridazine 1-oxide	X	X	X	5.36	X	X	X
4-Piperidinecarboxamide	9.85	X	X	X	X	X	X
4-Pyridinemethanol, hexahydro-.alpha.,.alpha.-dimethyl-	0.71	X	X	X	X	X	X
4-Pyrimidinamine, 2-(methylthio)-	X	X	0.97	X	X	X	X
4,5-Dichloro-1,3-dioxolan-2-one	X	X	X	2.99	X	X	X
4H-Naphtho[1,2-b]pyran-4-one, 5-methoxy-2-methyl-	X	X	X	X	8.07	X	X
5-Bromo-6-carboxy-2,4-dihydroxypyrimidine	X	X	0.98	X	X	X	X
5-Chloromethyl-[1,2,3]oxadiazole	X	X	X	2.02	X	X	X
5-Chloromethyl-2-oxazolidinone	X	2.26	X	X	X	X	X
5-Methyl-1,3-diazaadamantan-6-spiro-5'-imidazolidin-2',4'-dione	X	X	X	0.82	X	X	X
5-Morpholin-4-yl-2-(4-nitrophenyl)-3H-imidazol-4-carboxylic acid, methyl ester	X	8.22	X	X	X	X	X
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[(aminophenylacetyl)amino]-3-chloro-8-oxo-, [6R-[6.alpha.,7.beta.(R*)]	X	X	X	X	0.33	X	X
5,6-Dihydro-4-methoxy-2H-pyran	3.83	X	X	X	X	X	X
6-Bromohexanoic acid, decyl ester	X	X	X	X	0.67	X	X
6-Methylnicotinamide	X	X	X	4.67	X	X	X
7-Hexyltridecan-1-ol	X	2.09	X	X	X	X	X
8-[N-Aziridylethylamino]-2,6-dimethyloctene-2	X	X	X	X	5.57	X	X
8,9,9,10,10,11-Hexafluoro-4,4-dimethyl-3,5-dioxatetracyclo[5.4.1.0(2,6).0(8,11)]dodecane	X	X	X	X	X	X	0.69
9-Dodecyn-1-ol, dimethyl(dimethyl(dimethyl(pyrid-3-ylmethoxy)silyloxy)silyloxy)silyl ether	X	X	2.64	X	X	X	X
Acetamide, 2-(1-pyrrolidinyl)-N-(2-methyl-4-quinolinyl)-	X	X	X	6.05	X	X	X
Acetamide, 2-chloro-N-(2-cyano-3-thienyl)-	4.6	X	X	X	X	X	X
Acetamide, 2,2-dichloro-	X	X	X	2.7	X	X	X
Acetic acid	10.79	9.82	8.63	4.87	5.68	7.37	7.24
Acetic acid, 10-oxotricyclo[4.2.1.1(2,5)]deca-3,7-dien-9-yl ester	X	X	X	X	3.93	X	X
Acetic acid, chloro-, 1-methylbutyl ester	X	X	X	X	X	0.85	X
Acetic acid, dichloro-	0.75	X	X	X	X	1.77	X
Acetic acid, hydrazino-, ethyl ester	X	X	X	X	X	1.07	X
Ammonium Chloride	X	2.06	2.74	7.91	X	X	X
Amylene hydrate	5.42	1.7	2.7	5.07	1.81	4.73	X

Aniline, 2-(3-methoxy-1-propynyl)-	**2.49**	**X**	**X**	**X**	**X**	**X**	**X**
Benzene, 1-ethoxy-4-methyl-	**X**	**X**	**X**	**1.52**	**X**	**X**	**X**
Benzene, 1,3-bis(1,1-dimethylethyl)-	**X**	**5.35**	**4.25**	**4.94**	**X**	**X**	**5.22**
Benzeneethanol, 4-hydroxy-	**6.39**	**X**	**X**	**X**	**X**	**X**	**X**
Benzenesulfonic acid	**X**	**X**	**X**	**X**	**4.24**	**X**	**X**
Benzoic acid, 2,3,6-trichloro-	**X**	**X**	**X**	**X**	**1.9**	**X**	**X**
Bis(tributyltin)	**X**	**X**	**8.2**	**X**	**X**	**X**	**X**
Borane, methyldipropyl-	**1.54**	**X**	**X**	**X**	**X**	**X**	**X**
Bromoacetic acid, hexyl ester	**X**	**X**	**X**	**X**	**X**	**0.97**	**X**
Butanediamide, 2-methylene-	**0.48**	**X**	**X**	**X**	**X**	**X**	**X**
Butanoic acid, 2-methyl-, octyl ester	**X**	**X**	**X**	**1.88**	**X**	**X**	**X**
Butanoic acid, 4-hydroxy-	**X**	**4.04**	**X**	**X**	**X**	**X**	**X**
Butyrolactone	**5.8**	**X**	**X**	**X**	**X**	**X**	**X**
Caprolactam	**X**	**9.47**	**X**	**X**	**X**	**X**	**X**
Carbaminic acid, N-(3-chlorophenyl)-, oxyranylmethyl ester	**X**	**X**	**X**	**5.65**	**X**	**X**	**X**
Carbonyl-.pi.-cyclopentadienyl-trichlorgermyl-bis-trimethylphosphan-tungsten	**X**	**X**	**X**	**X**	**9.26**	**X**	**X**
Chloromethanesulfonyl chloride	**X**	**1.26**	**3.79**	**X**	**X**	**X**	**X**
Chloromethyl thiocyanate	**X**	**X**	**2.24**	**X**	**X**	**X**	**X**
Cholesta-9(11),20(22)-diene-3,23-dione, 6-hydroxy-, (5.alpha.,6.alpha.)-	**X**	**X**	**X**	**X**	**0.64**	**X**	**X**
Cycloheptasiloxane, tetradecamethyl-	**X**	**X**	**X**	**X**	**X**	**X**	**1.56**
Cyclohexasiloxane, dodecamethyl-	**X**	**X**	**X**	**X**	**X**	**1.71**	**X**
Cyclononasiloxane, octadecamethyl-	**X**	**X**	**X**	**X**	**0.81**	**X**	**X**
Cyclopropanecarboxylic acid,pentyl ester	**X**	**X**	**X**	**X**	**X**	**5.44**	**X**
d-Arabinosamine, N-(3-carboxyphenyl)-	**X**	**X**	**0.62**	**X**	**X**	**X**	**X**
D-Aspartic acid	**X**	**X**	**X**	**X**	**1.13**	**X**	**X**
D-erythro-Pentose, 2-deoxy-	**X**	**X**	**X**	**4.82**	**X**	**X**	**X**
D-Glucitol, 4-O-methyl-, pentaacetate	**X**	**X**	**7.54**	**X**	**X**	**X**	**X**
Decaborane, ethyl-	**1.96**	**X**	**X**	**X**	**X**	**X**	**X**
Decaborane(14)	**X**	**X**	**X**	**X**	**X**	**X**	**1.67**
Dichloroacetic acid, 2-octyl ester	**0.69**	**X**	**X**	**X**	**X**	**X**	**X**
Dichloroacetic acid, cyclopentyl ester	**X**	**X**	**X**	**1.73**	**X**	**X**	**X**
Dichloroacetic acid, tridecyl ester	**X**	**X**	**X**	**X**	**3.85**	**X**	**X**

Diethylamine, 2,2'-dichloro-	X	X	X	X	X	X	1.46
Dimethylmalonic acid, hexadecyl 2-isopropoxyphenyl ester	X	X	X	X	X	X	1.22
Docosanoic acid, docosyl ester	X	5.3	5.33	4.76	X	X	X
Eicosanoic acid, phenylmethyl ester	X	0.55	X	X	X	X	X
Ethanone, 1-[4-(4,6-dimethyl-2-pyrimidylamino)-1,2,3-triazol-5-yl]-	X	1.2	X	X	X	X	X
Ether, chloromethyl dichloromethyl	X	X	0.69	X	X	X	X
Ethosuximide	2.61	X	X	X	X	X	X
Ethyl .alpha.-hydroxymyristate	X	X	X	X	X	X	0.6
Ethyl 2-(2-chloroacetamido)-3,3,3-trifluorolactate	X	X	X	2.14	X	X	X
Ethyl Acetate	2.85	2.38	2.82	2.73	3.1	3.28	3.42
Ethylene, 1,2-dichloro-, (E)-	7.15	6.98	7.47	6.96	7.04	7.11	7.22
Fumaramic acid	X	X	X	X	X	X	1.29
Fumaric acid, isobutyl 2-propylphenyl ester	0.38	X	X	X	X	X	X
Heptane, 1-(methylthio)-	X	X	X	1.67	X	X	X
Heptane, 2,5,5-trimethyl-	5.11	4.87	X	X	X	X	X
Heptane, 4-methyl-	3.65	X	2.68	3.05	3.18	X	3.11
Hexahydropyrimidine-2,4,6-trione, 5-(2-thiazolylhydrazono)-	3.81	X	X	X	X	X	X
Hexanedioyl dichloride	X	3.56	4.83	X	2	1.36	X
Hexanoic acid, 2,2-dimethylpropyl ester	X	X	X	X	X	X	2.88
Hydrogen chloride	3.85	X	X	X	X	X	X
Hydroxyproline	X	X	X	X	X	8.24	X
Imidazolidin-4-one, 1-(4-morpholinocarbonyl)-	X	X	X	2	X	X	X
Isopropyl myristate	9.08	8.97	X	X	X	X	X
Isopropyl palmitate	0.29	X	X	X	X	X	X
Isoxazole, 5-amino-3-butyl-4-propyl-	7.12	X	X	X	X	X	X
L-Alanine, N-[N-[N-(trifluoroacetyl)-L-valyl]glycyl]-, methyl ester	X	X	X	X	1.04	X	X
l-Norvalyl-l-norvaline, n-propargyloxycarbonyl-, heptyl ester	X	X	X	0.74	X	X	X
Lactic acid	3.57	X	X	X	X	X	X
Maltol	X	1.02	4.59	3.9	4.44	X	X
Methane-d, trichloro-	2.92	1.53	X	1.47	4.77	1.16	X
Methane-D2-, dichloro-	X	2.07	X	X	X	X	X
Methane, bromochloro-	2.02	X	X	X	X	X	X

Methanimidamide, N'-(2-cyanophenyl)-N,N-dimethyl-	X	X	X	1.58	X	X	X
Methanol-D4	X	X	X	X	X	3.02	X
Methylene chloride	X	4.05	14	2.14	5.29	4.97	6.27
Methylphosphonyl dichloride	X	X	X	X	X	X	0.51
N-[2,2,2-Trifluoro-1-(isopropylamino)-1-(trifluoromethyl)ethyl]butyramide	X	X	X	2.19	X	X	X
N-Aminopyrrolidine	X	4.57	X	0.51	X	X	X
N,N'-(Hexamethylenebis(oxy-p-phenylenetrimethylene))diacetamide	X	X	X	6.03	X	X	X
N,N'-(Oxydi-4,1-phenylene)bis(2,2,2-trichloroacetamide)	X	X	X	X	X	3.83	X
Nonane, 4,5-dimethyl-	X	X	3.11	X	X	X	X
Octane, 3,3-dimethyl-	X	X	X	X	X	X	3.98
p-Menth-8(10)-ene-2,9-diol	3.4	X	X	X	X	X	X
Paromomycin	X	X	X	X	1.68	X	X
Pentane, 2,3,4-trimethyl-	X	3.57	X	X	X	X	X
Pentanoic acid, 1,1-dimethylpropyl ester	9.5	X	X	X	X	X	X
Pentanoic acid, 3-methyl-	X	X	X	X	X	X	1.18
Pentanoic acid, 3-oxo-4-phenylseleno-, methyl ester	X	X	X	X	X	8.29	X
Phenylethyl Alcohol	6.84	6.89	6.86	6.73	6.84	6.64	6.94
Phosphinic acid, [(methyl)(formyl)amino]methyl(2-phenylethyl)-	X	2.71	X	X	X	X	X
Propane, 2-ethoxy-2-methyl-	2.05	X	X	X	3.53	X	3.14
Propanenitrile, 2,2,3-trichloro-	X	X	X	X	X	X	0.57
Propanenitrile, 3-chloro-2,3-dihydroximino-	X	X	0.59	X	X	X	X
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	4.29	4.23	4.33	4.32	4.56	4.58	4.42
Pyrazine-2-carboxamide, N-cyclooctyl-	X	X	X	X	X	1.43	X
Pyrazine, methyl-	X	2.47	2.08	X	X	X	X
Pyrazole-1-carboxamide, 4-bromo-N-chloroacetyl-	X	X	X	3.06	X	X	X
Pyridinium, 1-(2-hydrazino-2-oxoethyl)-, chloride	X	X	X	1.21	X	X	X
Silane, [(cholestan-3-yl)oxy]trimethyl-	X	X	3.29	X	X	X	X
Silane, dimethyldi-2-propenyl-	X	X	X	X	X	0.35	X
Spiro-[6,6-dichlorobicyclo[3.1.0]hexane-2,2'-[1,3]dioxolane]	X	X	X	X	0.32	X	X
Spiropentane	X	X	1.12	X	X	X	X
t-Butyl 1-piperaziencarboxylate	X	X	X	7.68	X	X	X
Tetrahydro-3,4,5-trimethoxy-6-methoxymethyl-2H-pyran-2-one	X	X	X	X	X	X	8.3

Thiocyanic acid, methyl ester	**X**	**X**	**X**	**X**	**X**	**1.48**	**X**
Trichloroacetic Acid	**X**	**1.61**	**X**	**X**	**1.34**	**X**	**X**
Trichloroacetic acid, tridecyl ester	**X**	**3.11**	**X**	**X**	**X**	**X**	**X**
Trichloroethylene	**X**	**2.35**	**2.01**	**2.03**	**2.56**	**2.6**	**X**
Trichloromethane	**3.97**	**6.82**	**7.73**	**3.58**	**3.79**	**3.4**	**3.44**
Tryptophol	**5.82**	**7.45**	**X**	**6.8**	**X**	**5.98**	**X**

GC-MS Results Comparison, DCM Extraction 3/19/19

O1, O2, O3 = undesirable batch samples; N1, N2, N3 = desirable batch samples

Chemical	**O1**	**O2**	**O3**	**N1**	**N2**	**N3**
(3-Chloro-propyl)-urea			3.59			
1-(4-Acetamidoanilino)-3,7-dimethylbenzo[4,5]imidazo[1,2-a]pyridine-4-carbonitrile	3.46		1.61			0.36
1-Butanol, 2-methyl-	3.57	3.44	3.55	3.54	3.44	3.59
1-Butanol, 3-methyl-	3.24	3.29	3.33	3.32	3.28	3.28
1-Butanol, 3-methyl-					3.28	
1-Butanol, 3-methyl-, acetate			4.55		3.57	
1-Cyanomethyl-1H-indole-2-carboxylic acid	2.68					
1-Propanol, 2-methyl-	2.12	2.14	2.4	2.13	2.08	2.13
1,10-Diaminodecane						0.59
1,2-Propadiene-1,3-dione				1.07	0.61	1.23
1,2,5-Oxadiazole	2.68					1.3
1,3-Dioxolane, 2-heptyl-4-phenyl-			0.27	3.97	3.87	
1,3-Methylene-d-arabitol			0.64			
1,3,5-Triazine, 2,4,6-tris(cyanomethoxy)-		1.91	4.6	1.08		
1,3(4H)-Benzothiazin-4-one, 2,3-dihydro-3-methyl-2-benzoylmethylene-						0.46
1,5-Diacetyl-3,7-bis(3-chloropropionyl)-octahydro-1,3,5,7-tetraazocine				2.31		
1H-1,2,4-Triazole-3-carboxamide, N-(4H-1,2,4-triazol-4-yl-)-	0.94	1.32				
1H-Pyrrole-3-propanoic acid, 5-(ethoxycarbonyl)-2,4-dimethyl-, methyl ester						0.9
2-(1H-Benzo[g]indol-3-yl)-1-methylethylamine		1.8				
2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazolyl)-5-nitrobenzoic acid	0.32		4.42			

2-(Chloromethyl)oxazolo[4,5-c]quinolin-4(5H)-one		1.74				
2-(E)-Heptenoic acid, (4S)-4-[((S)-alanyl)amino]-6-methyl-	4.59					
2-Butyne-1,4-diol						0.3
2-Butyne-1,4-diol, diformate				2.13		
2-Cyanosuccinonitrile						6.06
2-Furanmethanol		3.77				
2-Hexenedioic acid, 2,4-dichloro-5-oxo-				4.07	3.75	
2-Isopropoxyethylamine					3.66	
2-Pyrrolidinone, 1-methyl-						2.72
2,3-Dioxopropanoic acid, 3-(2,5-dichlorothien-3-yl)-, 2-(4-methoxyphenyl)hydrazone		1.85				
2,4-Dimethyl-1-heptene		3.2	2.43	4.04	3.39	3.65
2,6-Pyridinediamine, 3-(phenylazo)-		6.53				
3-(.beta.-Chlorophenethylsulfonyl)-N-(p-tolyl)benzamide					5.37	
3-(1,2-Dibromoethyl)-1,1,2,2-tetrafluorocyclobutane					2.12	
3-(2,4-Dichlorophenyl)-2-(4-nitrostyryl)-4(3H)-quinazolinone				0.51		
3-Butyn-1-ol	7.14	2.11	5.5	2.28	12.93	2.38
3-Butynoic acid	0.96			1.5	0.35	1
3,3-Dimethyl-1-(toluene-4-sulfinyl)butan-2-one			5.83			
3,6-Dioxo-octahydro-1,2,7,8-tetrathia-9-azaanthracene-10-carboxylic acid, methyl ester		0.72				
3H-Isobenzofuran-1-one, 3-[4-(tetrahydrofuran-2-carbonyl)piperazin-1-yl]-	3.55					
4-Bromo-N-(piperidinomethyl)phthalimide	3.64					
4-Nitropyridazine 1-oxide	3.36			3.18	4.55	
4-Penten-1-ol			4.25			
4-Spirohexanone, 5,5-dichloro-	5.97	0.79		4.51	1.94	
4H-1,2,4-Triazol-4-amine, N-(4-chlorophenyl)methylene-				0.6		
5-Aminoisoxazole				4.49		
5-Fluoroorotic acid			6.32			
5-Thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid, 7-[(aminophenylacetyl)amino]-3-chloro-8-oxo-, [6R-[6.alpha.,7.beta.(R*)]		3.72				
7-Chloro-3-[4-cylcohexylphenyl]-3,4-dihydro-10-hydroxy-1,9(2H,10H)-acridinedione						5.84
7-Chloro-4-p-chlorobenzenesulfonylquinoline				2.58		

7,7-Dibromobicyclo[2.2.1]heptane-1-carboxylic acid, methyl ester				0.76		
Acetamide, N-(.alpha.-methylphenethyl)-	1.58					
Acetamide, N-[4-(chlorodifluoromethoxy)phenyl]-2-pyrrolidin-1-yl-					3.06	
Acetic acid, cyano-		0.81				
Allene					0.26	1.89
Argon	12.23	0.29	0.98		8.15	1.41
Benzaldehyde, 3,5-dichloro-2-hydroxy-, 2,2-dimethylhydrazone				6		
Benzene, 1-ethenyl-3-nitro-	1.03					
Benzeneacetamide						4.02
Borane carbonyl						1.05
Bromchlorenone					1.11	
Butanoic acid, 3-benzyloxy-3-(1,1,-dimethylethoxycarbonyl)-1-methylpropyl ester			0.71			
Butanoyl chloride, 3-methyl-				7.63	0.34	
Chlorodibromoacetaldehyde				0.75		
Chloromethyl 6-chloroundecanoate			0.63			
Chloromethyl(propyl)dichlorosilane	1.39					1.95
Chloromethylmethyl sulfide	0.54		0.4	2.68	0.31	3.38
cis-Aconitic anhydride				2.68		
Cyclotetrasiloxane, (iodomethyl)heptamethyl-	6.84					
dl-2-Formamido-2-methylbutyric acid			1.05			
Ethanedial, 2-[(2-trifluoromethyl-4-methoxyphenyl)amino]-,1-oxime				0.94		
Ethene, 1,1-dichloro-						1.41
Ether, 2-chloro-1-methylethyl isopropyl				3.76		
Ethyl 2-(2-chloroacetamido)-3,3,3-trifluorolactate				0.91		
Ethyl 2-chloro-3,3,3-trifluoro-2-isovaleramidopropionate			3.1			
Ethyl Acetate	1.83	1.83	1.87	1.88	1.85	1.78
Ethylene, 1,2-dichloro-, (E)-	1.38	1.41	1.32	1.28	1.38	
Fumaric acid, cyclohexylmethyl isohexyl ester		1.79				
Glycylglycine ethyl ester					5.07	
Heptane, 4-methyl-				3.06	3.27	2.81
Hydrogen chloride					0.9	
Iodoacetonitrile						2.76

Methane, oxybis[dichloro-				1.59		1.84
Methoxyacetic acid, hexyl ester			1.37			
Methylene chloride		1.12				1.89
Morpholine, 4-[[(dimethylamino)thioxomethyl]thio]-						0.59
N-(5-Bromo-2-pyridyl)-2,4-dichloro-N-[1-(1H-1,2,4-triazol-1-yl)ethyl]benzamide	0.42			5.43		
N-Aminopyrrolidine					1.49	
N-Trifluoroacetylimidazole						2.35
O-Benzyl-N-carbobenzyloxy-aspartic acid		1.07				
Octane, 3,3-dimethyl-						3.99
Pentane, 1-chloro-				1.28		
Perhydro-htx-2-one, 2-depentyl-, acetate ester				0.68		
Phenylethyl Alcohol	6.44	6.58	6.61	6.36	6.8	6.84
Phosphoramidous dichloride, dimethyl-		1.38				
Piperazine, 1-(2,5-dichlorophenyl)-4-(4-fluorobenzenesulfonyl)-					0.92	
Piperazine, 2,6-dimethyl-				1.6	4.21	
Piperidine-1-thiocarboxamide, N-(3-hydroxyphenyl)-		3.93				
Pregnane-3,8,12,14,17,20-hexol, (3.beta.,5.alpha.,12.beta.,14.beta.,17.alpha.,20S)-		0.66				
Propanal, 2,2-dimethyl-, oxime		1.86			2.87	
Propane					0.92	
Propane, 2-ethoxy-2-methyl-				1.13		
Propanenitrile, 3-(5-diethylamino-1-methyl-3-pentynyloxy)-		2.57				
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	4.3	4.33	3.97	4.35	4.23	4.21
Propyne		5.26		7.77		
Pyrazine, methoxy-, 1-oxide		0.88				
Quinoline, 6-bromo-			2.92			
Silane, [(cholestan-3-yl)oxy]trimethyl-		2.52				
Silane, dimethyl(3-phenylprop-2-enyloxy)hexyloxy-				5.66		
Spiro[4.5]decane-7,9-dione, 8-(4-bromobenzylidene)-6,10-dioxa-					0.5	
Sulphonyl diacetonitrile					1.2	
Tetraborane(10)			5.15			
Thebenine			0.91			
Thiophene, 3-(methylthio)-				4.76		

Toluene, 5-nitro-2-(4-nitrobenzylidenamino)-				2.39		
trans-.beta.-Chloroacrylic acid				0.65		
Trichloroethylene						1.69
Trichloromethane	1.63	1.61			2.04	
Trifluoromethanesulfonyl imidazole	3.62					1.85
Trifluoromethanesulfonyl imidazole					1.96	
Urea, N-nitroso-N-propyl-						

GC-MS Results Comparison, THF Extraction 2/24/19

O1, O2 = undesirable batch samples; N1, N2, N3 = desirable batch samples

Chemical	O1	O2	N1	N2	N3
.alpha.-[3'-(Phenyl)isoxazolyl]-.alpha.-(Z)-sulfinyl-N-(4-methylphenylsulfonyl)morpholinoacetamidin					2.48
.alpha.-Aminoisobutyronitrile			0.9		1.02
.beta.-D-Fructopyranose, pentaacetate				6.08	
(-)-(5)-Bromouridine		2.19			
(2R,4R)-(-)-Pentanediol		6.32			
(3-Chloro-propyl)-urea	0.98				
(3-Trifluoromethylphenyl)carbamic acid, 4-methylsulfanylphenyl ester	1.57				
(S)-Isopropyl lactate			5.9		
[1,2,4]Triazolo[4,3-b][1,2,4]triazin-7-ol, 3-tert-butyl-3,6-dimethyl-2,3-dihydro-					4.76
1-(2-Aminoethylamino)-2-propanol		0.8			
1-[N-Aziridyl]propane-2-thiol				9.63	
1-Amino-7-guanidino-hept-3-yne	3.89				
1-Butanamine, N-ethyl-N-methyl-	1.36				
1-Butanol, 2-methyl-	3.46	3.75	3.61	4	3.67
1-Butanol, 3-methyl-	3.46	3.41	3.31	3.48	3.43
1-Butanol, 3-methyl-, acetate		4.24			
1-Butanol, 4-ethoxy-				2.6	
1-Butyl-1-methoxy-3-dimethylaminocyclohexane (cis)				4.68	
1-Dimethylcarbamidoyl-2-benzoyl-3,3-dimethyldiaziridine					1.18
1-Methoxymethylthiopropane					4.12

1-Pentanol, 2-[(tert.butoxycarbonyl)amino)-	1.29				
1-Pentanol, 5-cyclopropylidene-		6.72			
1-Pentene, 5-chloro-			0.39		
1-Propene, 2-methoxy-	9.47			2.64	
1-Propene, 3-methoxy-					0.78
1-Propyne, 3-[(1-methylethyl)thio]-				5.19	
1-Pyrrol1-[1-(2-methoxyethyl)-1H-tetrazol-5-yl]-butylmorpho-4-pyridin-4-ylmethylpiperazine				3.23	
1,1-Dibutoxy-isobutane	2.31				
1,1-Dichloro-2-methyl-3-(4,4-diformyl-1,3-butadien-1-yl)cyclopropane		2.58			
1,2,4-Cyclohexanetriol, (1.alpha.,2.alpha.,4.beta.)-			6.32		
1,2,4-Triazine-3,5(2H,4H)-dione, 6-(2-oxopropylthio)-			2.07		
1,2,4,5-Tetrazine, hexahydro-1,2,4,5-tetramethyl-		0.79			0.72
1,3-Butanediol, (R)-				1	
1,3-Cyclopentadiene-1,3-dicarboxylic acid, 5-(1-hydroxyethylidene)-2-methyl-, dimethyl ester					0.57
1,3-Dimethyldiaziridine					0.7
1,3-Dioxolan-4-one, 2-t-butyl-5-methyl-5-(4,4-dimethoxypentyl)-					0.76
1,3-Dioxolane, 4-ethyl-		1.2	1.79		
1,3,4-Thiadiazolidine-3,4-dicarboxylic acid, 2-spiro-2'-adamantyl-, dimethyl ester				1.45	
1,3,5-Triethyl-1-(ethylbutoxysiloxy)cyclotrisiloxane		1.44			
1,4-Butanediol				1.72	
1,4-Dioxan-2-ol				5.37	
1,4-Pentanediol	6.34				
1,5-Heptadiene-3,4-diol, 2-methyl-		1.06			
1,5-Hexanediol	0.57				
1,5,6,7-Tetramethylbicyclo[3.2.0]hept-6-en-3-ylideneemicarbazide				3.85	
1(2H)-Naphthalenone, 8a-chlorooctahydro-		0.58			
10-Hydroxy-5,7-dimethoxy-2,3-dimethyl-1,4-anthracenedione			4.75		
10-Oxa-3-azatricyclo[5.2.1.0(1.5)]dec-8-ene-6-carboxylic acid, 2-allyl-3-benzyl-4-oxo-,	1.89				
1H-Imidazole-1-ethanol, .alpha.-methyl-	0.31				2.04
1H-Indole-3-ethanamine, N-methyl-			1.02		
1H-Indole-5-sulfonamide, 1-acetyl-N,N-diethyl-2,3-dihydro-	0.36				

1H-Pyrazole-3-carboxylic acid, 4-bromo-1-methyl-					2.44
1H-Pyrazole, 4-amino-1-(4-bromobenzyl)-3,5-dimethyl-		0.44			
1H-Pyrrole, 2,5-dihydro-1-nitroso-			0.88		
1H-Tetrazole			0.59		
2-(2-Hydroxy-2-methyl-4-phenyl-but-3-ynylamino)hexanoic acid				11.39	
2-(3-Methylphenoxy)octahydro-1H-1,3,2-benzodiazaphosphole 2-oxide	6.7				
2-[2-Aminothiazol-4-yl]-2-hydroxyiminoacetic acid		1.62			
2-[4-(2-Chloro-5-nitrobenzamido)phenyl]-6-methylbenzothiazole		2.51			
2-Azido-4-iodo-butanoic acid, methyl ester		0.99			
2-Bromovaleric acid					1.45
2-Buten-1-ol, 3-methyl-	0.53				
2-Butenal				3.86	
2-Butene-1,4-diol, (Z)-			7.93		
2-Butene, 1,4-dibromo-			3.04		
2-Butenediamide, (Z)-			0.96		
2-Chloroethyl isopropyl sulfide	2.77				
2-Cyclohexylamino-3-nitropyridine		2.73			
2-Dimethyl(chloromethyl)silyloxypentadecane			2.86		
2-Fluoropropene		2.81	3.95	2.49	4.81
2-Furancarboxylic acid, pentadecyl ester		2.27			
2-Furanmethanol		4.01	1.09		
2-Hexenedioic acid, 2,4-dichloro-5-oxo-	1.5				
2-Methyl-3-dimethylamino-2-isopropylthio(2H)azirine	1.11				
2-Methyl-pentanoic acid [4-(2-methyl-pentanoylsulfamoyl)-phenyl]-amide			2.39		
2-Oxabicyclo[2.2.0]hex-5-en-3-one		0.84			
2-Oxetanone, 4-methyl-		1.2			
2-Oxoacetic acid, ethyl ester, oxime			2.8		
2-Pentanol, 3-chloro-4-methyl-, (R*,S*)-(.+/-.)-					4.45
2-Propanamine, N-ethyl-				3.1	
2-Propanol, 1-hydrazino-					1.48
2-Propanol, 1-methoxy-					3.2
2-Propanol, 2-methyl-	2.08	1.97	2.06	2.16	2.61

2-Propanone, 1-hydroxy-, oxime			**0.32**		
2-Propenamide, N-[4-(acetylamino)butyl]-3-[3,4-bis(acetyloxy)phenyl]-					**0.63**
2-Pyrrolidinone, 1-methyl-					**3.96**
2-Trifluoroacetoxydodecane			**0.94**	**0.89**	
2-Trifluoroacetoxypentadecane				**5.18**	
2,1,3-Benzoxazole, 4,6-dichloro-7-nitro-				**1.07**	
2,2-Diethylacetamide				**1.01**	
2,2,2-Trichloro-1-(2-nitrophenylthioamino)ethanol			**2.61**		
2,2'-Urea-N,N'-bis(ethyl 3,3,3-trifluorolactate)					**1.13**
2,3-Butanediol			**4.51**		**5.13**
2,3-Butanediol, [R-(R*,R*)]-		**4.02**	**2.49**	**7.61**	
2,3-Dioxopropanoic acid, 3-(2,5-dichlorothien-3-yl)-, 2-(4-methoxyphenyl)hydrazone				**2.15**	
2,3,6-Trichlorobenzoyl chloride					**2.12**
2,3,6,6-Tetramethyl-2,3,4,5,5a,6,7,8-octahydro-1H-benzo[c]azepine					**2.01**
2,4-Bis(hydroxylamino)-6-methylpyrimidine				**1.02**	
2,4-Dimethyl-1-heptene	**2.9**	**4.51**	**3.94**	**2.71**	**3.6**
2'-Acetonaphthone, 1',2'.alpha.,3',4',4'a,5',6',7',8',8'a.alpha.-decahydro-5'.beta.-hydroxy-4'a.beta.,8'.beta.-dimethyl-, (.+-.				**2.9**	
2H-1,2,4-Benzothiadiazine-7-sulfonamide, 6-chloro-3,4-dihydro-N,N,2,4-tetramethyl-, 1,1-dioxide			**1.97**		
3-(2,4-Dichlorophenyl)-2-(4-nitrostyryl)-4(3H)-quinazolinone				**1.04**	
3-[2-Iodoethyl]-2-oxazolidinone				**3.13**	
3-Azabutyl-1-ol, 4-cyclopropyl-3,3-dimethyl-, bromide	**1.86**				
3-Butenamide			**0.62**		
3-Ethylamino-5-hexene-2-ol			**2.93**		
3-Hexanol, 2-methyl-5-nitro-, (R*,R*)-			**5.27**		
3-Isopropylsulfanyl-1-(4-nitro-phenyl)-pyrrolidine-2,5-dione		**5.69**			
3-Isoxazolecarboxamide, 4,5-dihydro-5-methyl-5-(4-methyl-5-oxo-3-cyclohexenyl)-		**3.03**			
3,3,5-Tributoxy-1,1,1,7,7,7-hexamethyl-5-(trimethylsiloxy)tetrasiloxane	**2.78**				**4.1**
3,3'-Nitro-4,4'-aminodiphenylsulfoxide	**8.8**				
3,4-Dihydroxybenzyl alcohol,tris(trimethylsilyl)-	**9.05**				
4-(1-Methoxyiminoethyl)-2,2,5,5-tetramethyl-3-imidazoline-3-oxide-1-oxyl					**1.07**

4-[5-(Diethylaminosulfonyl)-2-(2-furyl)-1-benzimidazolyl]butyric acid			**2.07**		
4-Amino-6-morpholino-5-nitropyrimidine		**1.78**			
4-Chloro-1-butanol				**3.39**	
4-Heptanone, 3-methyl-		**3.99**			
4-Hydroxy-2,2,7,7-tetramethyl-octahydro-2H-dibenzofuran-1,8-dione				**0.36**	
4-Penten-2-ol		**2.29**			
4-Pentenamide, N,N-diethyl-4-methyl-2-methylene-					**2.16**
4-Pentyn-2-ol			**6.37**		
4-Pyrimidinol, 2-acetonylthio-					**5.32**
4-Thiazolemethanol, 2-(4-chlorophenyl)-			**4.82**		
4(3H)-Pteridinone, 3-methoxy-2-methyl-			**2.86**		
4(3H)-Quinazolinone, 2-phthalimidoylmethyl-3-(1,5-dimethyl-2-phenyl-pyrazol-3-one-4-yl)-				**8.6**	
4H-Pyrano[2,3-d]pyrimidine-6-carbonitrile, 7-amino-1,5-dihydro-2-methyl-4-oxo-5-(3-pyridinyl)-			**2.59**		
5-(3-Thienyl)-2H-1,2,3,4-tetrazole		**0.4**			
5-[4-(Dimethylamino)cinnamoyl]acenaphthene		**3.78**			
5-Amino-2-methyl-2H-tetrazole		**0.64**			
5-Cyclopropylcarbonyloxypentadecane				**0.76**	
5-Dimethyl(chloromethyl)silyloxytridecane					**1.64**
5-Dimethylaminomethyleneamino-4-methyl-2,1,3-benzothiadiazole				**6.49**	
5-Methylhexahydro-1,3,5-triazine-2-thione					**0.37**
5,6-Dicarbadecaborane(12), 5,6-dimethyl-				**6.72**	
5,6-Dihydro-6-methyluracil					**1.95**
5H-[1,3,4]Thiadiazolo[3,2-a]pyrimidin-5-one, 6-amino-2-ethyl-7-methyl-					**0.69**
5H-2,3,4a,6,7a-Pentaazacyclopenta[cd]indene-1,4(2H,3H)-dione, 2-(1,1-dimethylethyl)tetrahydro-6-(2-hydroxyethyl)-				**1.11**	
7-Chloro-3-[2,4-dichlorophenyl]-3,4-dihydro-1H-thioxanthene-1,9(2H)-dioone					**0.59**
9-(2-(2-Methyl-5-pyridyl)ethyl)-6-bromo-3-methyl-1,2,3,4-tetrahydro-.gamma.-carboline	**0.26**				
9-Dimethylamino-10-ethoxycarbonyl-9-aza[3.3.2]propellane	**2.05**				
Acetamide, N-(aminoiminomethyl)-			**0.97**		
Acethydrazide, 2-tert-butylamino-N2-(3-hydroxy-1-methyl-2-butenylideno)-		**1.41**			

Acetic acid, (2-propenylthio)-		**6.7**			
Acetonitrile, 2-[(1-ethyl-1H-1,2,3,4-tetrazol-5-yl)thio]-			**2.46**		**3.46**
Allyl chloroformate			**4.92**		
Allyl fluoride	**4.24**				
Aluminum, tripropyl-			**2.49**		
Anthracene, 9,10-dinitro-	**7.47**				
Anthranilic acid, N-dimethylaminomethylene-, methyl ester			**1.93**		
Benzene, 1,3-bis(1,1-dimethylethyl)-			**2.84**		
Benzeneethanamine, .alpha.-methyl-N-(1-methylethyl)-			**2.2**		
Benzeneethanamine, 3,4-dibenzyloxy-2-fluoro-.beta.-hydroxy-N-methyl-				**1.6**	
Benzeneethanol, 4-hydroxy-		**5.6**		**1.77**	**6.89**
Benzoic acid, 2,4,5-trichloro-			**0.93**		
Benzoic acid, 4-methyl-, tert-butyldimethylsilyl ester					**0.77**
Boronic acid, ethyl-	**10.15**	**2.75**			
Butan-1-one, 1-(4-benzyl-1-piperidyl)-2-ethyl-					**5.81**
Butanal			**0.85**		**0.62**
Butanamide, N-(aminocarbonyl)-2-ethyl-				**0.74**	
Butane, 1-chloro-4-methoxy-					**2.93**
Butane, 2,3-dimethyl-					**1.48**
Butanedioic acid, chloro-, bis(1-methylpropyl) ester					**4.41**
Butanedioic acid, methylene-		**5.39**			
Butanoic acid, 2-butoxy-1-methyl-2-oxoethyl ester				**1.11**	
Butanoic acid, 2,3-dichloro-	**6.33**				
Butanol, 3-[(tert.butyloxycarbonyl)amino]-			**2.09**		
Butanoyl chloride	**3.35**				
Butylated Hydroxytoluene	**6.68**	**6.72**	**6.75**	**6.84**	**6.79**
Carbamic acid, (.alpha.-methylbenzyl)-, 1-ethyl-1-methylpentyl ester	**1.76**				
Carbamic acid, N-aminocarbonylmethyl-, isobutyl(ester)		**1**			
Carbonic acid, hexadecyl methyl ester					**2.47**
Carbonic acid, propargyl 2,2,2-trichloroethyl ester					**3.07**
Chloromethyl 4-chlorodecanoate				**5.23**	
Chol-7-ene, (5.beta.)-					**0.54**

Cholesta-5,7,9(11)-trien-3-ol, (3.beta.)-			**8.15**		
Cholestan-7-ol, 8,14-epoxy-3-(phenylmethoxy)-, (3.beta.,5.alpha.,7.alpha.,8.alpha.)-	**4.87**				
cis-Aconitic anhydride				**3.86**	
Cyclic-isopropylidene cyclopropane-1,1-dicarboxylate		**1.71**			
Cyclodecasiloxane, eicosamethyl-	**3.89**				
Cycloheptasiloxane, tetradecamethyl-	**1.6**				
Cyclohexanecarboxamide, N,N-dimethyl-2-oxo-	**0.92**				
Cyclohexanone, 2,3-dimethyl-2-(3-oxobutyl)-		**1.68**			
Cyclohexasiloxane, dodecamethyl-	**0.76**			**4.92**	
Cyclononasiloxane, octadecamethyl-	**16.27**				
Cyclopentane, 1,3-dimethyl-, cis-	**1.26**				
D-Galactonic acid, .gamma.-lactone				**5.11**	
Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl propyl ester				**8.24**	
Diisopropanolnitrosamine		**0.45**			
Diprop-2-ynyl phthalate	**1.3**				
dl-Serine, N-acetyl-, methyl ester, acetate (ester)					**5.75**
Dutadrupine				**0.91**	
Ethanamine, N-ethyl-N-methyl-					**1.31**
Ethanamine, N-ethyl-N-nitroso-				**7.27**	
Ethanol, 2-(2-ethoxyethoxy)-, acetate			**1.58**		
Ethanol, 2-(4-methylthiazol-2-yl)thio-	**3.88**				
Ethanol, 2,2'-(nitrosoimino)bis-					**5.94**
Ethanone, 2-(5-methoxy-1-methyl-2-benzimidazolyl)thio-1-phenyl-	**7.42**				
Ether, 1-butylvinyl methyl				**3.89**	
Ethyl 2-(2-chloroacetamido)-3,3,3-trifluorolactate	**3.37**				
Ethyl 3-methyl-8-[p-sulfamylbenzylamino]pyrido[2,3-b]pyrazin-6-carbamate			**2.08**		
Ethyl isopropyl dimethylphosphoramidate	**3.92**				
Formaldehyde, dimethylhydrazone				**4.52**	
Formic acid, 1-methylethyl ester					**2.81**
Fumaric acid, 2-methoxyethyl octadecyl ester				**4.33**	
Fumaric acid, hexyl 5-methoxy-3-methylpentyl ester					**2.04**
Furan, tetrahydro-2-methyl-	**2.36**	**2.21**	**6.45**	**6.39**	**2.49**

Furan, tetrahydro-3-methyl-	**2.56**	**2.86**	**2.79**	**2.86**	**2.82**
Furazan-3-carbohydrazide, 4-amino-N2-(4-fluorobenzylideno)-		**6.73**			
Furazan-3-carboxamide, oxime, 4-amino-N,N-dimethyl-				**5.2**	
Glutaraldehyde			**7.11**		
Glycine, N-(dithiocarboxy)-N-methyl-			**2.59**		
Glycylglycine ethyl ester		**2.97**			
Heptane, 2,5,5-trimethyl-				**3.19**	
Heptane, 4-methyl-	**3.03**	**2.84**	**3.19**	**2.67**	**2.82**
Hexahydro-1,3,5-trinitroso-1,3,5-triazine				**1.13**	
Hexane, 1-(1-ethoxyethoxy)-	**3.84**				
Hexane, 2-chloro-					**1.44**
Hexanoic acid, ethyl ester			**0.37**		
Histidine, 1,N-dimethyl-4-nitro-			**0.92**		
Hydrazine, 2-propenyl-			**5.01**		
Hydrazinecarboxamide, 2-(2-thienylmethylene)-				**1**	
Hydrazinecarboximidamide, 2-isopropylideno-N-nitro-				**2.54**	
Hydroperoxide, hexyl			**3.97**		
Imidazole-4-carboxylic acid, 1-methyl-		**2.23**			
Imidazole-4,5-dicarboxamide				**5.43**	
Isobutylene epoxide	**3.09**	**6.23**	**2.77**	**2.97**	**2.87**
l-Alanyl-l-valine, N-ethoxycarbonyl-, ethyl ester					**0.66**
L-Lactic acid		**2.72**	**2.06**	**6.07**	**9.12**
Lilac aldehyde A			**5.38**		
Methoxyacetic acid, 2-butyl ester			**0.45**		
Methoxyacetic acid, 2-octyl ester	**2.26**				
Methoxyacetyl chloride			**5.11**		**4.46**
Methyltartronic acid					**3.56**
Methylzinc propoxide	**1.92**				
Molybdenum tetracarbonyl-[N-butylL-N,N-bis(2-phosphinoethyl)amino]-					**7.62**
N-(2-Fluoro-phenyl)-3-(pentanoyl-hydrazono)-butyramide		**1.05**			
N-Aminopyrrolidine		**2.03**			
N-Formyl-3,4-methylenedioxyamphetamine	**0.68**				

N-Isopropyl-1-phenyl-5-chloropentylamine			**1.58**		
N-Nitroso-2-ethyl-1,3-tetrahydrooxazine	**0.4**				
n-Octadecanoic acid, pentamethyldisilyl ester	**1.17**				
N-Sec-butyl-3-[(4-fluoro-benzoyl)-hydrazono]-butyramide					**1.75**
N,N-Dimethylformamide dipropyl acetal	**1.28**				
N,N-Dimethylformamide ethylene acetal			**3.4**		
N,N'-Diethyloxamide			**3.72**		
N,N'-Dodecamethylenebis(p-toluenesulfonamide)					**4.63**
N'-(4-Cyano-5H-pyrido[4,3-b]indol-3-yl)-N,N-dimethyl-formamidine					**5.08**
N1-Cyclohexylpiperidine-1-carbothioamide				**2.79**	
Neopentyl-.beta.-phenylpropionate				**0.54**	
Nicotinonitrile, 2-chloro-4-(methoxymethyl)-6-methyl-5-nitro-				**7**	
Nonane, 2,6-dimethyl-		**3.99**			
Octadecyl 3-(4'-hydroxyphenyl)propanoate			**0.36**		
Oxalic acid, 6-ethyloct-3-yl hexyl ester					**7.14**
Oxirane, butyl-					**7.57**
Oxirane, trimethyl-		**12.05**			
Paraldehyde					**1.1**
Paromomycin		**2.12**			
Pentaborane(9), bromo-					**0.78**
Pentane, 3-chloro-				**3.47**	
Pentanoic acid, 5-methoxy-, phenyl ester		**1.38**			
Phenoltetrabromophthalein			**8.99**		
Phenylethyl Alcohol	**6.53**	**6.78**	**6.51**	**6.56**	**6.88**
Phosphonic acid, (1-chloro-1-phenylethyl)-		**0.4**			
Phosphoramidous dichloride, dimethyl-				**0.82**	
Piperazine, 1-ethyl-4-(4-piperidyl)-		**2.48**			
Piperazine, 2,6-dimethyl-	**0.75**			**3.8**	
Piperidine, 3-(bromomethyl)-				**4**	
Pregnane-3,20-dione dioxime			**1.27**		
Pregnane-3,20-dione, 17-[(trimethylsilyl)oxy]-, bis(O-methyloxime), (5.alpha.)-					**0.69**
Propan-2-ol, 1-methoxy-3-(2-methyl-4-nitro-5-imidazolylthio)-					**5.28**

Propanamide, 2-methyl-				**2.05**	
Propanamide, 3-bromo-			**2.55**		
Propanamide, N,N-dimethyl-				**0.92**	
Propane, 1-chloro-3-methoxy-	**7.14**				
Propane, 1-isothiocyanato-	**2.83**				
Propanoic acid, 2-hydroxy-, ethyl ester					**4.45**
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	**6.62**	**4.66**	**4.41**	**4.58**	
Propanoic acid, 2,3-dibromo-					**4.78**
Propanoic acid, 3-hydroxy-				**0.69**	
Propennitrile, 2-(benzoxazol-2-yl)-3-hydroxy-					**8.78**
Purine, 6-carboxamido-9-.beta.-d-ribofuranosyl-					**5.3**
Pyrazolo[3,4-b]pyridin-3(2H)-one, 4-trifluoromethyl-2,6-diphenyl-					**0.91**
Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 1-ethyl-5-(2-furanyl)-	**0.49**				
Pyrimidine, 2-(2,4-difluorophenoxy)-	**0.96**				
Pyrrol3-[4-(3-tert-butoxycarbonylamino-3-phenyl-propionyl)-piperazin-1-yl]-3-oxo-1-phenyl- propylmorpho-carbamic acid tert-buty			**2.64**		
Silane, [(cholestan-3-yl)oxy]trimethyl-				**0.81**	
Silane, dimethyl-2-propenyl[(6a,7,8,10a-tetrahydro-6,6,9-trimethyl-3-propyl-6H-dibenzo[b,d]pyran-1-yl)oxy]-, (6aR-trans)-	**3.76**				
Spiro(adamantane)-2,2'-(1,3-dithiolane), 4-methanesulfonate			**2.66**		
Succinic acid, butyl cyclohex-2-enylmethyl ester	**1.77**				
Tetradecane, 1-chloro-				**15.03**	
Tetraethyl 4,4'-(1,3-phenylene)bis(1,4-dihydro-2,6-dimethyl-3,5-pyridinedicarboxylate)	**0.67**				
Tetrahydrofuran	**6.02**	**0.95**		**10.33**	
Tetrahydrofuran-2-carboxylic acid, (4-pyridin-4-ylmethylphenyl)amide		**0.37**			
Thiazole, 2-bromo-4-methyl-				**1.16**	
Thiazolidin-4-one, 2-(4-tert-butyl-cyclohexylidenhydrazono)-5-methyl-			**1.17**		
Thieno[2,3-b]pyridine-2-carboxamide, 3-amino-6-methyl-		**0.92**			
Thiodiacetonitrile			**2.46**		
Thiophene-2-carbonitrile, 3-methyl-4-(3-dimethylamino-1-oxo-2-propenyl)-5-methylthio-		**0.32**			
trans-2,3-Epoxyoctane					**2.99**
trans-Cyclohexane-1,3-dicarboxamide			**7.02**		

Triacontane, 1-bromo-		**2.2**			
Tricyclo[7.2.0.0(2,6)]undecan-5-ol, 2,6,10,10-tetramethyl-		**9.14**			
Trimethylene glycol monomethyl ether	**1.81**				
Tungsten, pentacarbonyl-(2,3-.eta.-2-norbornene)		**7.6**			
Urea, 1-methylcyclopropyl-	**0.27**	**3.23**	**14.99**		
Urea, N-tert-butyl-N',N'-dimethyl-		**1.6**			
Z,Z,Z-1,4,6,9-Nonadecatetraene				**1.25**	

GC-MS Results Comparison, THF Extraction 3/19/19

O1, O2 = undesirable batch samples; N1, N2, N3 = desirable batch samples

Chemical	O1	O2	O3	N1	N2	N3
[1,3,4]Thiadiazole, 2-amino-5-(pyridin-3-ylmethylsulfanyl)-		0.38				
1-Butanol, 2-methyl-	3.63	3.63	3.68	3.36	3.55	3.59
1-Butanol, 3-methyl-	3.37	3.36	3.34	3.35	3.37	3.33
1-Penten-3-ol, 2-methyl-						2.46
1-Pentene, 5-chloro-				2.34		
1-Propene, 2-methoxy-	2.32					
1,2,4,5-Tetrazine-3,6-diamine			12.4			
1,3-Dioxolane, 4-ethyl-					2.23	
1,3-Dioxolane, 4-methyl-			3.59			
1,3,5-Triazine, 2,4,6-tris(cyanomethoxy)-						1.57
1,4-Pentanediol			7.78			
1H-Benzimidazole, 2-(difluoromethyl)-		23.64				
2-(1-Chloro-2,3,3-trifluoro-cyclobutyl)-cyclopropanecarboxylic acid methyl ester				1.12		
2-(4,5-Dihydro-3-methyl-5-oxo-1-phenyl-4-pyrazolyl)-5-nitrobenzoic acid				0.59		
2-Fluoropropene	3.91	4.1	3.71	3.84		
2-Furanmethanol					4.01	4.49
2-Heptyn-1-ol			4.05			
2-Hexanol, 3-methyl-						13.65
2-Oxetanone, 4-methyl-		2.27				
2-Oxetanone, 4-methylene-			4.13			
2-Pentanol, 3-chloro-2-methyl-				2.16		

2-Pentanol, 3-chloro-4-methyl-, (R*,S*)-(.+/-.)-					10.59	
2-Propanol, 1-(1-methylethoxy)-				1.88		
2-Propanol, 1-[(1-methyl-2-propynyl)oxy]-	2.9					
2-Propanol, 2-methyl-			2.13		2.02	1.99
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate					5.01	
2,2'-Ethylenediphenol						4.98
2,3-Butanediol		4.76				
2,3-Butanediol, [R-(R*,R*)]-	2.61		3.34	4.22	3.27	3.35
2,3-Epoxybutane			2.94			
2,4-Bis(hydroxylamino)-6-methylpyrimidine	0.46					
2,4-Dimethyl-1-heptene	4.16	3.52	3.46	3.66	4.09	3.23
2,4-Pentanediamine, 2-methyl-		5.04				
2,4-Pentanediol			2.75			
2,4,6,8-Tetraazabicyclo[3.3.0]octan-3-one, 7-nitroimino-			5.69			
2,5-Furandione, dihydro-3-methyl-	2.8					
2,5-Furandione, dihydro-3-methylene-				5.49		
2,5-Hexanediol	1.48					
2,6-Pyridinedicarboxylic acid, butyl 2-methylhex-3-yl ester				0.6		
2H-Pyran-2,6(3H)-dione, dihydro-	3.57					
2H-Thiopyran-3(6H)-one			0.43			
3-Amino-1-azabicyclo[2.2.2]octane				0.83		
3-Buten-1-ol				3.26		
3-Butyn-1-ol		1.51				1.82
3-Methyl-2-trichloromethyl-oxazolidin-5-one						7.6
4-(5-Bromosalicylideneamino)-N-(2-thiazolyl)benzenesulfonamide					7.91	
4-Chloro-1-butanol			8.49			
4-Methyl-1,3,2-dioxathiane 2-oxide			4.95			
4-Pentyn-2-ol			2.05			2.68
5-Amino-2-methyl-2H-tetrazole		3.57				
5,7-Dioxa-1-octene, 1-chloro-4-isopropyl-3-methyl-	1.63					
6-Aminocaproic acid, N-isobutoxycarbonyl-, butyl ester						5.01
7-Benzhydrylidene-5-methylenebicyclo[2.2.1]hept-2-ene				7.42		
Acetamide, N-ethyl-						4.4

Acetic acid, cyano-	2.26					
Acetic acid, hydrazino-, ethyl ester			2.35			
Acetoacetic acid, 1,3-dithio-, S-isopropyl ester			1.26			
Allyl fluoride					3.66	4.23
Argon			8			
Benzaldehyde, (1,4-dihydro-6-methyl-4-oxo-2-pyrimidinyl)hydrozone		8.99				
Benzene-1,3-diamine, 5-[3,4,4,4-tetrafluoro-1,3-di(trifluoromethyl)-2-heptafluoroisopropyl-1-butenyloxy-						3.36
Benzene, 1,3-bis(1,1-dimethylethyl)-					4.28	
Benzeneethanol, 4-hydroxy-			3.63			
Benzyl mandelate			2.23			
Borane carbonyl		1.02				
Boronic acid, ethyl-			6.12			
Butanal		3.08				
Butanal, 3-methyl-				1.96		
Butanedioic acid, methyl-					0.38	
Butanoic acid, 2-propenyl ester						1.44
Butyl glyoxylate				2.14		
Butylated Hydroxytoluene	6.71	6.66	6.75	6.71	6.87	6.67
Carbamic acid, nitrosopropyl-, ethyl ester					2.09	
Chloroacetyl-L-leucine	8.26					
Chloroacetylamine, N-[2-n-octyl]-						1.83
Chloroxuron				3.67		
Cinchoninanilide, 1,2-dihydro-6,7-dimethoxy-2-oxo-			7.87			
cis-Aconitic anhydride				1.85		
Cyclononasiloxane, octadecamethyl-			3.25			
Cyclopentane, 1,3-dimethoxy-, cis-					6.82	
Decaborane(14)	6.81			6.83		
Dichlofenthion			8.15			
Dichloroacetamide, N-heptyl-N-octyl-						2.34
Didemnin B				4.97		
DL-Asparagine	3.57					
Docosanoic acid, docosyl ester					5.73	

Ethanedial, dioxime	2.57					
Ethanol, 2-(vinyloxy)-			1.74			
Formaldehyde, dimethylhydrazone			1.69		1.71	
Formic acid, 1-methylethyl ester	3.24					
Furan, tetrahydro-2-methyl-	5.1	6.08	2.97	4.58	3.66	3.99
Furan, tetrahydro-3-methyl-	2.76	2.74	2.68	2.6	2.65	2.59
Furazan-3,4-diol			7.99			
Heptane, 4-methyl-	2.58		4.78	2.69	3.15	2
Hexanoic acid, 2-methylphenyl ester	2.86					
Iron, dicarbonyl(.eta.5-2,4-cyclopentadien-1-yl)[2,3,5,6-tetrafluoro-4-(trifluoromethyl)phenyl]-						9.07
Isobutylene epoxide	2.6	4.66		2.84	2.71	2.76
Isonipecotic acid, N-pentafluorobenzoyl-, decyl ester				8.92		
L-Lactic acid	8.37	6.58	5.11	4.2	5.92	6.14
Loperamide						1.57
Methanol, (4-amino-1,2,5-oxadiazol-3-yl)(imino)-	3.46					
Methyl propyl ether						1.95
Methyldiallylamine		5.39				
Methylmalonic acid	2.26					
Molybdenum, [(4a,4b,8a,9,9a-.eta.)-9H-fluoren-9-yl]tris(.eta.3-2-propenyl)					9.07	
Molybdenum, tetracarbonyl[N,N'-1,2-ethanediylidenebis[2-propanamine]-N,N']-, (oc-6-22)-		8.05				
Molybdenum, tetrakis(.eta.3-2-propenyl)-		6.62				
Morpholine, 2,6-dimethyl-		2.5				
N-Chloro-2-carbomethoxyaziridine					1.65	
N-Methoxymethyl-N-methylacetamide	5.8					
Nonane, 2,6-dimethyl-						4.84
Oxazolidine				6.63		
Oxirane, ethyl-	2.78					
p-Dioxane, methylene-						1.97
Paromomycin					3.16	
Pentane, 1-chloro-						2.52
Pentane, 2,2'-oxybis-			3.61			
Pentane, 3-chloro-	5.45					

Pentanoic acid, 5-(acetylamino)-4-oxo-, methyl ester				2.35		
Phenylethyl Alcohol	6.47	6.34	6.54	6.11	6.39	6.44
Phosphinothionic acid, bis(1-methylethyl)-		0.84				
Propanal, 2-methyl-						4.34
Propanal, 2,2-dimethyl-, oxime	6.4					
Propane, 1-chloro-3-methoxy-						4.22
Propane, 1-ethoxy-2-methyl-	2.61					
Propanoic acid, 2-hydroxy-, ethyl ester			4.59	4.24		4.55
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	4.3	4.5			4.17	
Propanoic acid, 2-methyl-					2.13	
Pyrido[2,3-d]thiazolo[3,2-b]pyridazin-4-ium, 3-methyl-, perchlorate						2.74
S-1-Propenylmethanethiosulfonate						1.33
Salicylaldehyde, thiocarbazone	8.86					
Spirost-8-en-11-one, 3-hydroxy-, (3.beta.,5.alpha.,14.beta.,20.beta.,22.beta.,25R)-		0.68				
Stannane, ethyltrimethyl-						6.82
Tetrahydrofuran	7.14	6.91	2.23	12.32	0.87	9.45
Tetrahydrofurfuryl chloride	2.87					
Thiazolidin-4-one, 5-ethyl-2-imino-						0.7
Thiodiacetonitrile					1.53	

Appendix D: Example Organoleptic Compound Comparison

O1, O2, O3, O4 = undesirable batch samples; N2, N3, N4 = desirable batch samples

Chemical	O1	O2	O3	O4	N2	N3	N4
1-Butanol, 2-methyl-	✓	✓	✓	✓	✓	✓	✓
1-Butanol, 3-methyl-	✓	✓	✓	✓	✓	✓	✓
2-Furanmethanol	✓	✓	✓	✓	✓	✓	✓
Acetic acid	✓	✓	✓	✓	✓	✓	✓
Ethyl Acetate	✓	✓	✓	✓	✓	✓	✓
Phenylethyl Alcohol	✓	✓	✓	✓	✓	✓	✓
Propanoic acid, 2-hydroxy-, ethyl ester, (S)-	✓	✓	✓	✓	✓	✓	✓
2H-Thiazolo[2,3-c][1,2,4]triazol-3-one, 6-methyl-5,6-dihydro-						✓	
3-Furanmethanol						✓	
8-[N-Aziridylethylamino]-2,6-dimethyloctene-2					✓		
Benzenesulfonic acid					✓		
Pentanoic acid, 3-methyl-							✓
Pentanoic acid, 3-oxo-4-phenylseleno-, methyl ester						✓	
Pyrazine-2-carboxamide, N-cyclooctyl-						✓	
Thiocyanic acid, methyl ester						✓	
2H-Thiazolo[2,3-c][1,2,4]triazol-3-one, 6-methyl-5,6-dihydro-						✓	
(3,5-Dimethyl-piperidin-1-yl)-(2-iodo-phenyl)-methanone	✓						
[4,4']Bipiperidinyl				✓			
1-Butanethiol		✓					
1-Heptanol, 2,4-diethyl-		✓					
1-Octanol, 2,7-dimethyl-		✓					
1-Propanol, 3-(methylthio)-				✓			
1,3:2,4:5,7-Trimethylene-.beta.-sedoheptitol	✓						
1,4-Eicosanediol				✓			
2-Pentanone, 4-hydroxy-		✓					
2-Piperidinone, 1-methyl-	✓						
2,3-Dioxopropanoic acid, 3-(2,5-dichlorothien-3-yl)-, 2-(4-methoxyphenyl)hydrazone				✓			
3-(Methylthio)propyl acetate				✓			
3,3',4,4'-Tetranitrodiphenylsulfoxide				✓			
4-Piperidinecarboxamide	✓						
Aniline, 2-(3-methoxy-1-propynyl)-	✓						
Benzeneethanol, 4-hydroxy-	✓						
Bis(tributyltin)			✓				
Butanoic acid, 2-methyl-, octyl ester				✓			
Butanoic acid, 4-hydroxy-		✓					
Butyrolactone	✓						
Chloromethanesulfonyl chloride		✓	✓				
D-Glucitol, 4-O-methyl-, pentaacetate			✓				
Eicosanoic acid, phenylmethyl ester		✓					
Fumaric acid, isobutyl 2-propylphenyl ester	✓						
Heptane, 1-(methylthio)-				✓			
Lactic acid	✓						
p-Menth-8(10)-ene-2,9-diol	✓						
Pentanoic acid, 1,1-dimethylpropyl ester	✓						
1-Butanol, 3-methyl-, acetate	✓	✓	✓	✓	✓		
Maltol		✓	✓	✓	✓		
Ammonium Chloride		✓	✓	✓			
N-Aminopyrrolidine		✓		✓			
Pyrazine, methyl-		✓	✓				

KEY	
	New and old
	Only new (1 instance)
	Only old (1 instance)
	Mostly old (3+ old to 1 new)
	Only old (2+ instances)

Appendix E: Whitinsville Water Quality Testing Results[25]

4. IMPORTANT DEFINITIONS

Maximum Contaminant Level (MCL) – The highest level of a contaminant that is allowed in drinking water. MCLs are set as close to the MCLGs as feasible using the best available treatment technology.

Maximum Contaminant Level Goal (MCLG) –The level of a contaminant in drinking water below which there is no known or expected risk to health. MCLGs allow for a margin of safety.

Maximum Residual Disinfectant Level (MRDL) -- The highest level of a disinfectant (chlorine, chloramines, chlorine dioxide) allowed in drinking water. There is convincing evidence that addition of a disinfectant is necessary for control of microbial contaminants.

Maximum Residual Disinfectant Level Goal (MRDLG) -- The level of a drinking water disinfectant (chlorine, chloramines, chlorine dioxide) below which there is no known of expected risk to health.
MRDLG's do not reflect the benefits of the use of disinfectants to control microbial contaminants.

Action Level (AL) – The concentration of a contaminant which, if exceeded, triggers treatment or other requirements that a water system must follow.

90^{th} Percentile – Out of every 10 homes sampled, 9 were at or below this level.

ppm = parts per million, or milligrams per liter (mg/l)
ppb = parts per billion, or micrograms per liter (ug/l)
ppt = parts per trillion, or nanograms per liter
pCi/l = picocuries per liter (a measure of radioactivity)
NTU = Nephelometric Turbidity Units
ND = Not Detected
N/A = Not Applicable
mrem/year = millimrems per year (a measure of radiation absorbed by the body)

Secondary Maximum Contaminant Level (SMCL) – These standards are developed to protect the aesthetic qualities of drinking water and are not health based.

Massachusetts Office of Research and Standards Guideline (ORSG) – This is the concentration of a chemical in drinking water, at or below which, adverse health effects are unlikely to occur after chronic (lifetime) exposure. If exceeded, it serves as an indicator of the potential need for further action.

5. WATER QUALITY TESTING RESULTS

What Does This Data Represent?
The water quality information presented in the table(s) is from the most recent round of testing done in accordance with the regulations. All data shown was collected during the last calendar year unless otherwise noted in the table(s).

	Date(s) Collected	90^{TH} percentile	Action Level	MCLG	# of sites sampled	# of sites above Action Level	Possible Source of Contamination
Lead (ppb)	2015	1.9	15	0	60	0	Corrosion of household plumbing systems; Erosion of natural deposits
Copper (ppm)	2015	0.36	1.3	1.3	60	0	Corrosion of household plumbing systems; Erosion of natural deposits; Leaching from wood preservatives

Regulated Contaminant	Date(s) Collected	Highest Result or Highest Running Average Detected	Range Detected	MCL or MRDL	MCLG or MRDLG	Violation (Y/N)	Possible Source(s) of Contamination
Inorganic Contaminants							
Barium (ppm)	May 2014	0.02	0-0.02	2	2	N	Discharge of drilling wastes; discharge from metal refineries; erosion of natural deposits
Nitrate (ppm)	May 2017	0.47	0.1-0.47	10	10	N	Runoff from fertilizer use; leaching from septic tanks; sewage; erosion of natural deposits
Disinfectants and Disinfection By-Products							
Total Trihalomethanes (TTHMs) (ppb)	*Quarterly*	14.9	5.46-14.9	80	-----	N	Byproduct of drinking water chlorination
Haloacetic Acids (HAA5) (ppb)	*Quarterly*	10	3.17-10	60	-----	N	Byproduct of drinking water disinfection
Chlorine (ppm) (free)	*Monthly*	0.764 (ave)	0.03-1.51	4	4	N	Water additive used to control microbes
Radioactive Contaminants							
Radium 226 & 228 (pCi/L) (combined values)	April 2016	0.5	0.5	5	0	N	Erosion of natural deposits
Gross Alpha (pCi/L)	April 2016	1.6	0.04-1.6	15	0	N	Erosion of natural deposits

Unregulated contaminants are those for which there are no established drinking water standards. Secondary Contaminants are non-health based standards.

Unregulated and Secondary Contaminants	Date(s) Collected	Result or Range Detected	Average Detected	SMCL	ORSG	Possible Source
Inorganic Contaminants						
Sodium (ppm)	May 2017	6.8	6.8	-----	20	Natural sources; runoff from use as salt on roadways; by-product of treatment process
Secondary Contaminants						
Iron (ppm)	*2017*	0 - 0.065	0.0065	0.3	---	Naturally occurring, corrosion of cast iron pipes
Manganese (ppm)	*2017*	0 - 0.009	0.008	0.05	---	Erosion of natural deposits
Total Hardness (ppm)	*April 2015*	8.1 - 40	24.05	-----	---	Erosion of natural deposits
Potassium (ppm)	*April 2015*	7.7 - 21	14.35	-----	---	Naturally present in the environment

* The EPA has established a lifetime health advisory (HA) value of 0.3 mg/L for manganese to protect against concerns of potential neurological effects, and a one-day and 10-day HA of 1 mg/L for acute exposure.