



Identifying Reactive Intermediates Formed during Catalytic Upgrading of Bio-Crude

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Submitted by:

Abigail Goyette, Chemical Engineering

Samuel Presutti, Chemical Engineering

Bruno Schardong, Chemical Engineering

Advised By:

Associate Professor Michael T. Timko, Chemical Engineering

Abstract

Over the last couple of years there has been a growing interest in transitioning from traditional fuels to more renewable sources such as biofuels. However, biocrude straight from the reactor is not usable as a fuel source and needs to be upgraded through exposure to a catalyst. The reactants and products are known for this process, but the intermediates are not. Lowering the severity of conditions specifically temperature can allow for these intermediates to be identified through the use of GC-MS and other analytical techniques. 2 grams of biocrude made from hospital food waste was treated with 1 gram of a commercial catalyst (CoMo/Al₂O₃) for an hour at varying temperatures (350°C, 325°C, 300°C) to observe the intermediates produced when lowering the severity of operating temperatures. At lower operating temperatures, a greater presence of acids, alcohols, and esters was observed.

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1.0 Introduction

Over the past couple of years there has been a growing need for a replacement to traditional fuel sources. A potential replacement could come from biofuels made from renewable sources such as food waste and other biomasses. However, biofuel is not a good fuel source as there are many issues with the fuel regarding its properties. Biofuels taken straight from the refineries have low energy density, shelf life, and a high moisture content. To overcome these issues, the biocrude can be upgraded to reduce the moisture content and remove the impurities found in the fuels. There are three types of upgrading techniques that can be used on biocrude which include the following, thermochemical, biochemical, and physiochemical.

Thermochemical techniques tend to be the most effective and they involve the use of supplementary hydrogen and catalysts to treat biocrude¹. A common thermochemical technique that uses catalysts in the process is hydrodeoxygenation where oxygen is removed without any supplementary hydrogen. One catalyst that is used for this process is CoMo/Al₂O₃ and this catalyst is one of the most common ones that are used in industry³. The reactants and products are known for this reaction but there has been little research into the intermediates of the reaction. A study was developed to see if using milder reaction conditions will allow for the intermediates to be identified.

The reaction condition that was chosen to be changed was the reactor temperature and this was lowered for the different trials. The reactor temperatures that were used in the experiments were 350, 325, and 300 degrees Celsius. The other experimental conditions were kept the same for each trial including the reactor pressure, and the reactants. The biocrude used in the trials came from hospital food waste and the catalyst was a commercial CoMo/Al₂O₃ called Alfa Aesar. All the samples were analyzed, and GC-MS was used to identify the different components of the biocrude. The results from this analysis were looked at to see if any trends developed across the three temperatures. These trends and compounds were identified to see if the intermediates of the reaction were able to be found.

2.0 Background

General Information about Bio Crude

There has been a growing interest in the last decade to use less fossil fuel-based energy sources and move industry towards more renewable sources. Scientists and engineers have turned to different biomass feed sources to create substitute fuels such as biodiesel and bio-oil. These fuels are seen as an environmental solution to the problems surrounding traditional fuel sources. Some of the most common biomass feeds include wood, aquatic crops, and municipal and animal waste. The biomass would then be converted to bio-oil through either a thermochemical or biochemical process. The most common conversion process is to make ethanol and biodiesel from sugar, starches, and vegetable oil. Over the last couple of years there have been advancements in HTL technology and upgrading techniques for biocrude. Even with these advancements in technology, there are still issues with untreated biocrude¹.

Biocrude has the potential to be a replacement fuel source for traditional petroleum in response to the growing interest in using fewer fossil fuels. However, biocrude taken straight out of the reactor is unable to be used as a fuel source due to the properties of the crude. Typically, untreated biocrude has low energy density, high moisture content, and is not free flowing as a liquid. Also, there are issues with the viscosity of the crude at colder temperatures, the corrosiveness of the oil, and samples will begin to degrade if they are in storage over an extended period. To overcome these issues, different upgrading techniques can be used to alter the chemistry or physical properties of the bio crude samples ¹.

The most common upgrading techniques will upgrade the biocrude without the presence of oxygen and in conditions with high heat and pressure. Thermochemical processes usually use much higher temperatures and pressures than biochemical or physiochemical processes. The process will produce liquid products when the right catalyst is chosen to be used in the reaction. Upgrading biocrude will ensure that the crude will be able to be used as fuel source with less of the negative properties. To utilize this technology, the biocrude should be upgraded in good conditions using the right process ¹.

Upgrading Techniques: Utilizing Biocrude

Biocrude needs to be upgraded for it to be used as a type of transportation fuel. For upgrading biocrudes into usable fuels, there are three types of upgrading techniques, thermochemical, physiochemical, and biochemical. Out of three types, thermochemical processes tend to be the most effective, but they are the most expensive due to the process conditions. While physiochemical processes are less effective, they can be run using milder conditions and with another process. Biochemical processes can be an excellent choice for upgrading so long as it is the only upgrading option being used. Beyond the common three types, biocrude upgrading

techniques can be broken down further into three categories, dewatering, deoxygenation, and hydrogenation. Dewatering and deoxygenation refer to processes that reduce the water and oxygen content of the biocrude. Hydrogenation refers to processes that increase the hydrogen content of biocrude². Thermochemical processes include the following upgrading techniques, hydrocracking, catalytic cracking, and hydrodeoxygenation. All these techniques require the same basic conditions to run which include the use of high temperatures and pressures in the presence of hydrogen and catalysts. These specific conditions will help to change the characteristics of the biocrude during the upgrade process². Biochemical processes can alter the immediate properties of the end products using solvents and other biological treatments without adding any heat to the system. Physiochemical processes use electricity to improve the quality of the biocrude using either physical or chemical processes².

Thermochemical Processes: Catalytic Cracking, Hydrocracking, and Hydrodeoxygenation

As mentioned above some common thermochemical upgrading techniques include hydrocracking, catalytic cracking, and hydrodeoxygenation. Catalytic cracking upgrades the biocrude through the breaking down the untreated biocrude into low carbon aromatics and olefins. This technique has produced oil that has shown some promise of being a replacement for traditional fuel sources. Hydrocracking is a variation of the catalytic cracking technique with additional hydrogen, high temperatures, and catalysts being added to the biocrude to break down the larger carbon chains².

Hydrotreatments include the following upgrading processes, hydro-deoxygenation, hydrogenation, and hydrodesulfurization. Hydrogenation and hydrodesulfurization use similar techniques as the traditional refineries at temperatures that can range from 310-375 degrees Celsius. These processes use supplementary hydrogen gas and catalysts to remove oxygen and

sulfur as water and hydrogen sulfide. Hydrodeoxygenation removes oxygen from any oxygen containing species within the biocrude without using any supplementary hydrogen. Some metal catalysts can be used to improve the process, however, there are still many limiting factors that can affect the upgraded biocrude. These factors include low fuel costs, reusability, coking resistance, and effectiveness. There is one benefit of using hydrotreatments to upgrade the biocrude as the upgraded oil will have a low sulfur content after treatment ².

Physiochemical Processes: Electrochemical, Plasma, Ultrasonic cavitation, and Mechanical

Blending

Physiochemical upgrading techniques do not use any applied heat, catalysts, or chemicals to upgrade the biocrude. There are multiple benefits to using physical upgrading processes that include lower production hazards, fewer consumable inputs, and enhanced stability. This type of technology was just starting to emerge in the last three years, so it has not been proven to be more effective than thermochemical or biochemical processes. Some common physiochemical upgrading techniques include electrochemical, plasma, ultrasonic cavitation, and mechanical blending ².

The electrochemical process upgrades the biocrude without any additional hydrogen and can be run at a wide variety of temperatures and pressures. Hydrogen is one of the byproducts of this technique and it can be used for other upgrading techniques further along in the process. Electrochemical upgrading utilizes electricity to produce hydrogen protons on the anode side of an electrochemical cell. A cation exchange membrane allows for the protons to transfer to the cation side of the cell and hydrogenation takes place on this side of the cell. The only two requirements for the effectiveness of the process are the exact composition of the biocrude and the surrounding chemical environment ².

A common plasma upgrading technique is non-thermal plasma synergetic catalysis (NPSC) which uses an applied electrical field in the biocrude to ionize electrons and radicals. This type of process has lower energy requirements and environmental emissions than other upgrading techniques. However, the upgraded biocrude is still hydrogen deficient and there is a risk of any catalysts deactivating due to extensive coking ².

Ultrasonic cavitation uses an ultrasonic generator to convert 60Hz into 20Hz of high mechanical energy and the generator will run at average temperatures and pressures. The higher frequency energy will cause cavitations within the biocrude, specifically the air cavities of the oil. This technique can reduce the corrosiveness, viscosity, and instability of the untreated biocrude. The high oxygen and moisture content of the biocrude can be reduced with this technique through breaking the carbon-oxygen bonds and promoting carbon-hydrogen bonds with the use of catalysts and hydrogen donors ².

Mechanical blending is the process of blending together the untreated biocrude and either alcohols or hydrocarbons in small batches. There are some issues with this process that include the acidity and corrosiveness of the upgraded biofuel and a loss in performance of the biofuel in fuel separation and oxidation ².

Biochemical Processes: Esterification, Transesterification, and Catalytic Transfer Hydrogenation

In comparison to thermochemical processes, biochemical upgrading techniques operate at lower temperatures and pressures. Also, there is the benefit of having lower capital costs, small-scale suitability, and lower production hazards. One of the more common biochemical processes is esterification which involves the use of alcohol-based solvents to turn any carboxylic acids into esters. Introducing a catalyst into this process would reduce the acidity, water content, and viscosity of the biocrude at a much higher rate. Transesterification uses alcohols to replace long

chained carbons with short chained carbons within the ester groups. This process will also separate the excess water from the biocrude, reduce the viscosity, and increase the pH of the sample. However, there is a risk of the water being contaminated due to the high solvent concentration and lower biocrude concentrations. Another common biochemical upgrading technique is catalytic transfer hydrogenation where hydrogen rich compounds and catalysts are added to the untreated biocrude. This upgraded technique can be run at lower temperatures and pressures which avoids the common risks associated with using pure hydrogen².

Catalytic Upgrading of Biocrude: Hydrodeoxygenation

There are multiple forms of catalytic upgrading that can be used to treat biocrude which include cracking and hydrodeoxygenation. As mentioned above hydrodeoxygenation (HDO) is a process that removes oxygen from the biocrude as water without the use of supplementary hydrogen. Metal catalysts can be added to improve this type of process and the two common catalysts used are NiMo/Al₂O₃ and CoMo/Al₂O₃. The normal operating temperatures for this process range from 250 to 450 C and the right operating temperature should be chosen based on the kinetic requirements of the reaction. An important aspect of HDO processes is the consumption of hydrogen with different oxygen containing functional groups requiring different amounts of hydrogen. Some studies are looking into the effect of hydrogen consumption on deoxygenation of different functional groups and have found that functional groups such as ketones require less hydrogen while groups like furans require a much higher amount of hydrogen. This trend was shown in each study regardless of the catalyst chosen to be used in the HDO process. Each of the different catalysts used in HDO can be split into two distinct groups, sulfides/oxides, or transition metal catalysts³.

For sulfide/oxide catalysts, the two most researched catalysts are Co-MoS₂ and Ni-Mo S₂. The nickel and cobalt act as promoters by donating electrons to the molybdenum atoms which weakens the bond between molybdenum and sulfur. This creates a vacancy site on the metal and the oxygen from the biocrude can bond to this site. The important aspect is that the oxygen bonded to the metal catalyst must be removed from the biocrude as water for the reaction mechanism to work. There is evidence that has shown longer operating times can result in the activity of the catalyst being reduced as it transforms into an oxide form³.

Transitional metal catalysts used in HDO should be able to bifunctional where the metal would be able to activate the oxygen containing species and donate hydrogen to the oxygen species. Some common metal catalysts include Ru/C, Pd/C, and Pt/C. While these catalysts work well for HDO systems, they are expensive to use in industry and this makes them an unattractive choice. There are some alternatives that can be used in place of these more expensive catalysts such as nickel-based ones. These substitute catalysts are not as effective as the metal ones, but they are more stable than the cobalt catalysts and the cost of the nickel catalysts are much lower³. There have been different experiments looking into HDO and the effect that the catalysts can have on the process.

In 2015, there were experiments done looking into the performance of upgraded biocrude made from microalgae. The catalyst used in the upgrading process was Pt/Al₂O₃, and the experiments were run across a wide range of temperatures starting at 125 C and going up to 530 C. The results from these experiments showed that running the reactor at 400 C was the best temperature for the reaction as at this temperature there was the highest rate of reduction in the nitrogen content and O/C ratio and increased the C/H ratio. Also, the results showed that running the reactor at high temperatures should be avoided as there were concerns about recondensation

reactions taking place which could increase the amount of coke formed⁵. An increase in the amount of coke found could lead to a reduction in the upgraded bio-oil yields.

In 2019, researchers at the Pacific Northwest National Laboratory investigated the effect that different feed sources and catalysts had on the upgraded biocrude. The feed sources came from wet waste and the catalyst used was either CoMo/Al₂O₃ or NiMo/Al₂O₃ in either the guard bed or the main bed. The results from the experiments show that using CoMo/Al₂O₃ in both the guard and main bed with the WW06 sludge produced upgraded bio-oil with the most carbon and hydrotreated bio-oil. The worst combination was WW10 sludge with CoMo/Al₂O₃ in the guard bed and NiMo/Al₂O₃ in the main bed as this combo produced the least amount of hydrotreated bio-oil and the lowest amount of carbon in the samples. The results from these experiments show that using the same catalyst within both the guard and main bed worked better for upgrading the biocrude⁶.

3.0 Methodology

Experimental Parameters

The goal of the study was to determine the reactionary intermediates for the catalytic upgrading of hospital food waste biocrude. To determine these intermediates, the severity of the reaction conditions was lowered to allow for the biocrude to be upgraded under milder conditions. The temperature of the reactor was chosen to be the manipulated variable and all other conditions were kept the same. By running the reactor at lower temperatures, the biocrude may not have been upgraded completely, and other functional groups may be present in the oil sample. The initial temperature for the reactor was set to 350 degrees Celsius and the temperature was lowered by 25 degrees for each of the two subsequent trials. The catalyst used in each trial was a commercial version of a CoMo/Al₂O₃ catalyst called Alfa Aesar. The ratio of catalyst to biocrude was always 1 gram of catalyst for 2 grams of biocrude. For every trial, the reactor was pressurized with about 1000 psi of pure hydrogen gas. The biocrude was upgraded in the reactor

for 1 hour once the reactor reached its respective temperature for each trial: 350, 325, and 300 degrees Celsius. After one hour, the reactor was cooled to 40 degrees Celsius, and the oil and coke were removed from the reactor.

Using Dichloromethane (DCM), the upgraded biocrude and coke were flushed from the reactor. Gravitational filtration was used to separate the coke from the biocrude, and the DCM/biocrude mixture was transferred to a round bottom flask. To separate the DCM and upgraded biocrude, rotovaping was used as the main method for all the trials. Further analysis of the biocrude was performed once the sample was separated from the solvent.

Analytical Techniques

The analytic techniques that were chosen for the duration of the trials include Karl Fischer titrations, GC-MS, and elemental analysis. Karl-Fischer titrations investigated the moisture content of the biocrude samples with the samples being diluted in methanol and injected into the equipment. These titrations determined the amount of water found in the samples, and the results were used to determine whether the sample needs to be dried before undergoing elemental analysis. The elemental analysis was performed by an outside lab, and all samples were shipped to the lab once it was confirmed that they had the proper moisture content. All the biocrude samples were analyzed to determine the amount of carbon, hydrogen, oxygen, nitrogen, and sulfur in the biocrude. The results from this analysis were used to determine trends among the samples from each of the three temperatures.

The key analytical technique that was used in our study was the GC-MS analysis of each sample taken at three different temperatures. Each sample was diluted to be around 1-2 wt% biocrude in DCM and then injected into the machine to be analyzed. A chromatogram was

produced showing the intensity of the peaks versus the retention time. This plot was integrated for the first hundred peaks to be able to identify the compounds that the peaks represented. This process was crucial to understanding the compounds found in the biocrude and to begin to identify the intermediates of the reaction. Further analysis was done on the integrated peaks to determine both the type and amount of different functional groups found in the biocrude. Once the peaks and groups were identified, the trends between the three different temperatures were determined and the most common compounds were listed out.

Experimental Procedures:

First, the top and bottom halves of the empty reactor are each weighed out on a scale. Next, 2 grams of the bio-crude are weighed out and added to the reactor, followed by a gram of the fresh CoMo/Al₂O₃ catalyst. The full reactor is then weighed once again before adding clamps to ensure that the chamber is tightly sealed. After being weighed and sealed, the reactor chamber is hooked up to a hydrogen tank so that the air inside can be flushed out and replaced with hydrogen gas. The process of filling and flushing the gas inside the reactor should be done three times. After flushing the chamber three times, the reactor should be filled once again with hydrogen and pressurized to roughly 1000 PSI.

Once the reactor has been pressurized to 1000 PSI, the mixer, thermocouples, and cooling water tubes should be hooked up to the reactor and turned on. Begin heating the reactor to the desired temperature. Once the reactor has reached the desired temperature, record its initial temperature and pressure, and let the reactor run for one hour. After the one hour is up, the final temperature and pressure should be recorded, heating element should be turned off, and the reactor should be cooled in an ice bath until the internal temperature reaches 40 degrees Celsius or below. After cooling, the clamps should be removed and the weight of the full reactor must be

recorded. After the weight of the full reactor has been taken again, it is time to separate the newly refined oil from the coke and catalyst.

Using DCM, rinse out the reactor into a filter, separating the solid coke and catalyst from the liquid bio-oil and DCM. Weigh out a crucible as well as a round bottomed flask. The catalyst and coke can be transferred over to the crucible while the bio-oil and DCM will be poured into the round bottomed flask. Measure and record the weight of the coke and catalyst in the crucible before baking it in an oven overnight to remove the coke from the catalyst. In the morning, take the dry weight of the catalyst, which can be used to determine the weight of the coke for future results. Transfer the round bottomed flask over to a roto-evaporator, and set the water temperature to 50 degrees Celsius. Leave the mixture to run in the rotovap until it looks as though most of the DCM has evaporated. The final product should be much darker and more viscous; however, when in doubt, the team has found that the process takes about 15-20 minutes. A simplified diagram of the refinement process can be seen in Figure 1 below.

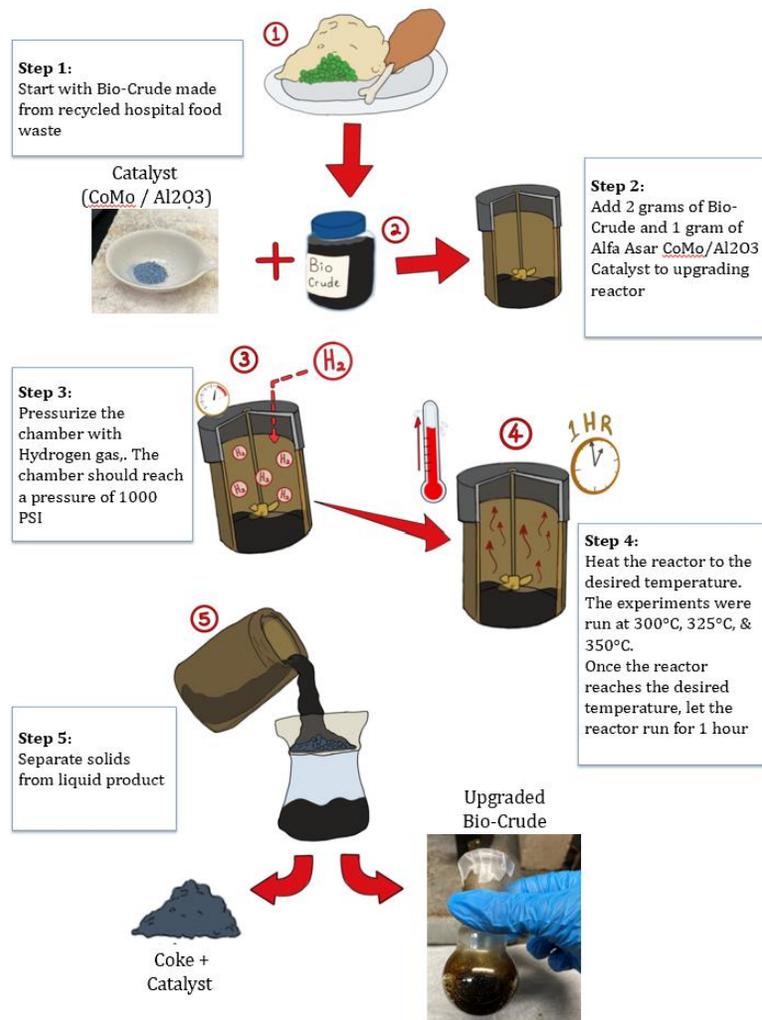


Figure 1: Simplified Diagram for the Major Steps Involved in Bio-Crude Upgrading

4.0 Results and Discussion

After the trials were run, the GC-MS data was graphed and analyzed for the three temperature ranges as seen in the figure below (Figure 2). All three temperature ranges showed peak values for both hexadecane (C₁₆H₃₄) and octadecane (C₁₈H₃₈). These results are somewhat consistent with the trends other researchers have observed while upgrading biocrude with CoMo/Al₂O₃ at temperatures of 350°C or above^{7,8}. The peaks for the 350 and 325 graphs are relatively similar; however, it can be noticed that between 325 C and 300 C not only does the concentration of both

octadecane and hexadecane decrease, but other peaks also become more prominent. The data recorded from the 325 trials were exposed to an argon leak when the samples were being recorded. The team did however manage to filter out the argon readings which ultimately did not affect the peak compositions of the graph, but do account for the irregular curve at the beginning of the graph. A noticeable increase of carboxylic acids and esters was observed during the 300-degree trials – specifically octadecenoic acid, ethyl ester ($C_{20}H_{38}O_2$) and hexadecenoic acid, ethyl ester ($C_{18}H_{36}O_2$), the other two peaks shown in the 300 degree data set of Figure 2. These results are somewhat consistent with the trends and graph shapes other researchers have observed, upgrading biocrude with $CoMo/Al_2O_3$ at 350 C or above^{7,8}.

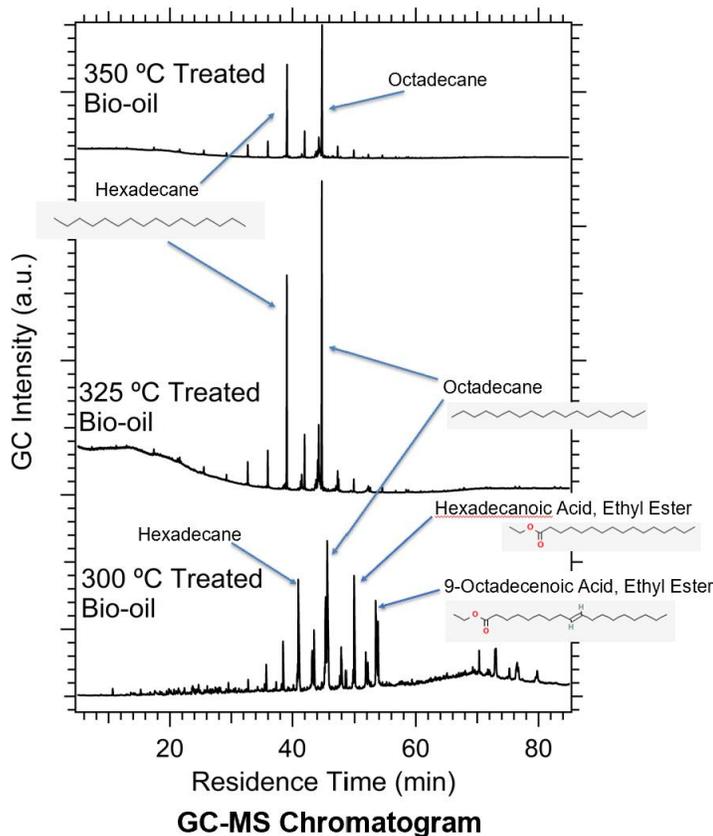


Figure 2: GC-MS Stacked Chromatogram for 350°C, 325°C, and 300°C with Peak Compounds Labeled.

	300°C	325°C	350°C
Hexadecane	13.75%	22.85%	20.13%

Octadecane	18.63%	35.19%	32.01%
Hexadecanoic Acid, Ethyl Ester	10.17%	0%	0%
9-Octadecenoic Acid, Ethyl Ester	12.08%	0%	0%
Hexadecane + Hexadecanoic Acid	23.75%	22.85%	20.13%
Octadecane + Octadecenoic Acid	30.71%	35.19%	23.01%

Table 1: Percent Concentration Comparisons of Hexadecane and Octadecane between all three Temperatures Tested

Based on the trends of the graphs, it is inferred that the difference in temperature between the 325 and 300 trials provides energy necessary to break down more of the ethyl esters into hexadecane and octadecane by cleaving off the oxygens. In the table above, Table 1, the concentrations of hexadecane, octadecane, hexadecenoic acid, ethyl ester, and 9-octadecenoic acid, ethyl ester are shown for all three temperatures. The concentrations of hexadecane and octadecane do drop by roughly 2% between the 325 and 350 trials, but that is not unusual. The temperature range for most biocrude upgrading is around 350 – 400°C in order to avoid burning bio-crude and producing coke^{1,6,7,8}. It is not without reason to suggest that some of the hexadecane and octadecane may have broken down or combusted during the refinement process. Additionally, it should be noted that if one were to add up the concentrations of hexadecane and hexadecenoic acid, ethyl ester from the 300 C trial, it adds up to be roughly the same as the concentration of hexadecane found in the 325°C trial. A similar correlation is observed when comparing the concentrations of 9-octadecenoic acid, ethyl ester and octadecane found in the 300-degree trial to the octadecane concentration of the 325 C trial. Furthermore, these two ethyl esters alone make up roughly 20% of the composition of the 300 C trial. If these two compounds did in fact undergo some sort of cleaving, forming hexadecane and octadecane respectively, they would make up a large portion of the loss of oxygen containing compounds in the transition between 300 and 325 degrees Celsius as seen in Figure 3 below. Note that in the diagram below, oxy refers to oxygen containing functional groups as a whole, including alcohols, esters, and carboxylic acids.

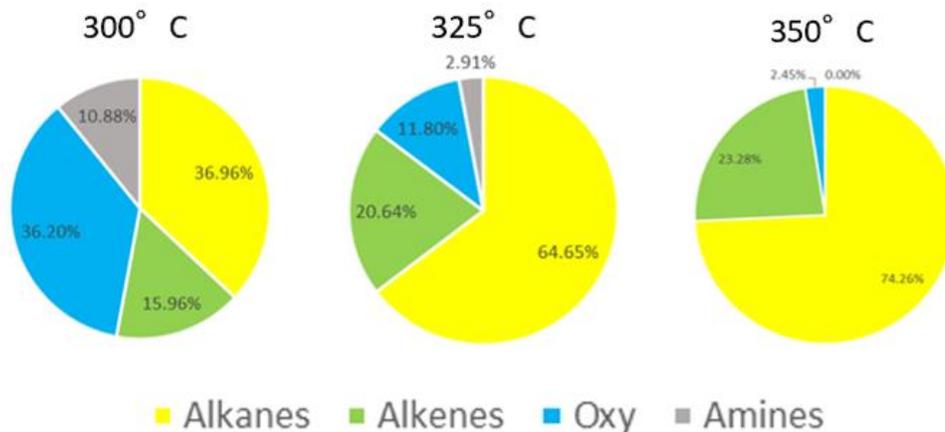


Figure 3: Pie charts showing the percentage of key functional groups identified for each temperature

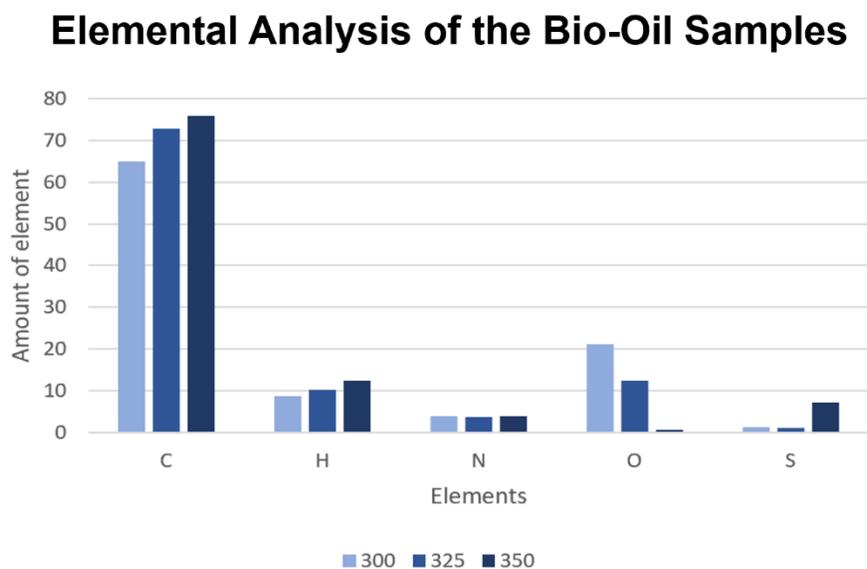


Figure 4: Elemental Analysis of Bio-Oil Samples for each Temperature

Based on the data shown in Figure 4, it is clear to see that as the upgrading temperature of the reactor increased, so did the concentrations of both carbon and hydrogen in the upgraded bio-oil. Alternatively, the increase in reactor temperature drove down the overall concentrations of oxygen present in the upgraded bio-oil, which was both beneficial and expected. The sudden spike in sulfur

found in the 350 degree data is believed to be a misnomer, and what most likely occurred was that the values of oxygen were mistaken for sulfur by the machine. Oxygen and Sulfur are rather similar and difficult to separate or distinguish from one another and at times react almost identically in the world of organic chemistry. None the less, the results from the elemental analysis paired with the functional group data in Figure 3 from GC-MS confirm that as the reactor temperature is increased, there is a decrease in oxygenated functional groups as well as oxygen as a whole within the upgraded bio-oil. In the 300-degree trials, there is almost an even split between the total concentration of alcohols, acids and esters and the number of alkanes present. The presence of oxygen containing groups is more than halved just by increasing the temperature of the reactor by 25 degrees. One thing that the team noticed was that the lower temperatures, beads of water could be seen resting on the surface of the oil. This could be the result of oxygen leaving the biocrude and reacting with the hydrogen gas; however, it was only observed to happen at the temperatures below 350°C. This unusual phenomenon was not mentioned in any of the papers that the team had read, but it could be a biproduct of operating the reactor at lower temperatures. It is possible that at temperatures below 350°C, there is enough energy present to remove the oxygen atoms and form water vapor, but not quite enough energy to prevent it from condensing atop the oil as the reactor cools.



Figure 5: Water Bubble formed on top of bio-oil from the 325 C trial

5.0 Conclusions and Recommendations

As mentioned above the overall trend of the results shows that as the reactor temperature increases the amount of carbon and hydrogen increases as well. The amount of oxygen decreases as the temperature goes up and the amount of nitrogen remains the same. This trend in the elemental analysis follows the results from the GC-MS analysis where the samples at the lowest temperature had the highest amount of oxygen containing species. The two most common compounds found in the samples were hexadecane and octadecane which proves that the upgraded biocrude would primarily produce long chained carbon species. The highest temperature samples have the highest percentage of alkanes for each of the three temperatures. The results from the 300 C and 325 C trials show how a higher temperature would be able to convert the oxygen containing species into alkenes and alkanes. The chained carbon species are desired for biofuels and the results of this study show that even at lower temperatures the biocrude may be upgraded to contain more of the carbon species.

If further research were to be conducted, it would be recommended to conduct tests throughout the temperature range of 300 to 325 degrees Celsius. This could help further the understanding of what

might be going on mechanistically, and could potentially show whether or not these results are a part of some greater trend. Additionally, running some samples at temperatures slightly below 300 degrees Celsius could also be beneficial in possibly discovering even more prerequisite mechanisms going on within the refinement process.

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7.0 Appendix

Experimental Procedures

FOR REACTION:

1. Grab reactor apparatus and remove from fume hood. Make sure it is empty, clean, and all remaining remnants of the last gasket are removed.
2. Weigh empty reactor w/ new gasket already inserted.
 - a. Be careful when placing in the new gasket.
3. Measure out catalyst and insert into reactor.
4. Put bio-crude into reactor while on scale.

5. Weight apparatus with biocrude and catalyst inside.
6. Lock up reactor with wrench.
7. Place reactor into slot and hook up the spinner and thermocouple.
8. Attach water pipes and turn on pump.
9. Flush with hydrogen.
 - a. Attach pipe to apparatus. Turn bearing with wrench until you feel resistance, then give another half turn.
 - b. Set the pressure coming out of the tank.
 - c. Open all valves allowing hydrogen into the reactor. Allow it to reach around 1100 PSI and flush. Repeat two-three more times.
 - d. TURN OFF HYDROGEN!
 - e. Close all valves and proceed to unscrew the pipe from the reactor.
10. Adjust heater so it is surrounding the crucible.
11. Turn on the stirrer.
12. Set heater temperature.
 - a. Once heater gets to around 100 degrees below the desired temp, turn down the heater by 50 degrees to prevent it from overshooting.
 - b. Once the overshooting occurs, raise the temperature back to the desired temp.
13. Wait.
14. Wait more.
15. Once process finishes, remove oven with glove and place to side.
16. Grab a bucket of ice with a little bit of water and place on reactor. Allow to cool to 40 degrees. Repeat if necessary.
17. release the gas into the GC column.
 - a. Leaving the valve near the GC column (computer) open, flush the reactor into the column in the fume hood until the column in the fume hood reaches 30 psi. Release that. Repeat two more times.
 - b. Fill column in fume hood to 60 psi and leave it.
 - c. Once the column in the fume hood cools, allow it to flow into the GC column for 10 psi.
18. Turn off water, detach pipes, and detach stirrer.
19. DEPRESSURIZE THE REACTOR
 - a. Open the back valve to bleed out the hydrogen head space
20. Remove reactor from slot carefully.
21. CAREFULLY remove brackets. They will be hot.
22. Take reactor and weigh whole apparatus to find mass loss.
23. Fill small container with DCM. Prepare pipette.
24. Flush the crucible with DCM to remove the bio-oil and transfer to ceramic filter.
 - a. Weigh the ceramic filter beforehand and add a paper liner.
 - b. Flush reactor crucible with DCM into secondary container.
 - c. Prepare vacuum apparatus and get a flask that is able to be used with the vacuum to catch the runoff.
 - d. Weigh the empty round bottom flask.
 - e. Attach the apparatus to the vacuum pump and turn on.
 - f. Wait for all Bio-oil solution to be vacuumed out and turn off pump.

g. Weigh both the filled crucible and filled round bottom flask to determine the mass.

25. Place catalyst and bio-oil into separate, pre-weighed containers and label.

ROTAVAPPING:

1. Crush dry ice and fill condenser.
2. Set temperature of water bath?
3. Make sure there is a large round bottom flask to catch the condensed DCM.
4. Find a small, clean round bottom flask for the diluted oil.
 - a. Weigh the empty round bottom flask. **MAKE SURE THE LIP IS ON THE SCALE!!!**
 - b. Try not to spill it. It's difficult.
5. Find the weird glass piece that makes sure it doesn't boil over.
6. Attach both pieces to the rotavapor via the vacuum pump.
 - a. Hold the small round bottom flask in place while turning on the pump.
7. Change the settings on the rotavapor to the correct solvent (DCM).
8. Lower the apparatus into the water bath.
9. Turn on spinner and slowly crank it to about 2/3 – 3/4 of the way.
10. Wait for all DCM to be evaporated.
11. Remove and weigh the round bottom flask.
12. Try to scrape out as much of the oil as possible into a separate container.

Excel Spreadsheets

Mass Balance:

Raw Data	11/9/2021	11/17/2021	11/30/2021	12/7/2021	2/6/2022	2/10/2022	2/17/2022	3/23/2022
Temperature (C)	350	350	325	325	325	300	300	300
Feed Type	HPW Bio crude	HPW Bio crude	HPW Bio crude	HPW Bio crude	HPW Bio crude	HPW Bio crude	HPW Bio crude	HPW Bio crude
Catalyst Type	Phillips 66 Activ	Alfa Aesar						
Catalyst (g)	1	1	1	1.1	1	1	1	1
Feed (g)	2	2	2	2	2	2	2	2.2
Empty Reactor Bottom	1918	1917.5	1917.5	1917.5	1917.5	1917.5	1917.5	1917.5
Empty Reactor Top	4928.5	4928	4929	4929	4928.5	4928.5	4928.5	4928.5
Full Reactor (Before Run)	6450	6449.5	6449	6449	6449.5	6449	6449	6449
Reactor Pressure - psi (Before Run)	1000	1000	1000	1000	1000	1000	1000	1000
Reactor Temperature - C (Before Run)	24.1	21.4	21.3	22.1	19.7	20.3	22.1	21.4
Empty Reactor Bottom (After Run/Weighted)	1918	1917.5	1917.5	1917.5	1917.5	1917.5	1917.5	1917.5
Empty Reactor Top (After Run)	4928.5	4928	4929	4929	4928	4928.5	4928	4928.5
Full Reactor (After Run)	6450.5	6449.5	6449	6449.5	6449	6449	6449	6449
Reactor Pressure - psi (After Run)	1000	1000	979	1000	1000	1000	980	1000
Reactor Temperature - C (After Run)	40	40	40	40	29	40	40	40
Funnel, FP & adapter (empty)	99.861	99.88	99.88	103.908	108.846	108.846	102.0791	103.9086
Funnel, FP & adapter (full, DCM washed, dried)	101.028	101.104	100.82	105.1113	110.086	97.8894	103.143	105.1152
DCM/Oil Flask (empty)	53.933	53.933	53.93	53.9847	51.508	51.513	51.5233	51.5125
DCM/Oil Flask (full)	104.72	88.86		105.48	88.24	111.7	78.3598	105.4135
Round bottom flask (empty)	69.73	69.708	69.72	69.7104	69.708	69.716	69.9236	69.7957
Round bottom flask (full)	71.37	71.33	71.29	72.144	71.5897	71.9933	71.573	71.8693
Product Distribution (g)								
Oil (wet) (g)	1.84	1.622	1.53	2.404	1.8757	2.2773	1.4484	2.0734
Mixture in Oil samples (%)	33.00%	4%	7%	4%	7%	4%	10%	28%
Coke removed from catalyst (%)	20.00%	33%	29%	23%				
Dry Oil basis (g)	1.83	1.55712	1.4229	2.30784	1.744401	2.186208	1.48356	1.92848
Coke (g)	0.2	0.19912	0.19112	0.276759	0.2976	0	0	0
Catalyst (g)	0.93	1.06488	1.1088	0.910541	0.7624	-0.9766	1.0999	1.2066
Water (g)	0.3	0.06488	0.1071	0.09616	0.131299	0.092082	0.16484	0.580552
Gas (gravimetrically determined)	0.0	0	0	0	0.5	0	0	0
Reactor Loss (g)	0.0	0	0	0	1	0	-0.3	0
All Losses (g)	0.53	0.22	0.14	-0.68	-0.17	-0.28	0.35	-0.07
Mass Yields (%)								
Oil (%)	60%	78%	71%	115%	87%	109%	74%	75%
Solid (%)	12%	8%	17%	14%	15%	0%	0%	0%
Water (%)	10%	1%	3%	2%	7%	5%	0%	2%
Gas (%)	0%	0%	0%	0%	0%	0%	0%	0%
Loss (%)	6%	11%	7%	-34%	-9%	-14%	18%	-4%
350C Run (11/9)								
Oil (%)	0.6442	0.7788	0.7145	1.1392	0.872205	1.091104	0.74178	0.746424
Solid (%)	0.1167	0.07956	0.1456	0.1383795	0.1488	0	0	0
Water (%)	0.1598	0.03244	0.05935	0.04808	0.0656495	0.045546	0.08242	0.290276
Gas (%)	0	0	0	0	0	0	0	0
Loss (%)	0.0683	0.10944	0.0894	-0.3403795	-0.08865	-0.13865	0.1758	-0.0387
	1	1	1	1	1	1	1	1

GC-MS Data:

**350C
Trial 1**

[MC Peak Table]												
# of Peaks	75											
Mass	TIC											
Peak#	RetTime	Proc.From	Proc.To	Mass	Area	Height	A/H	Conc.	Mark	Name	Ret. Index	
1	3.045	3.01	3.055	TIC	3123362	1168553	2.67	1.66		Argon		
2	3.065	3.055	3.07	TIC	981826	1100247	0.89	0.52	V	cis-Aconitic anhydride		
3-Jan	3.101	3.07	3.115	TIC	2631513	956846	2.75	1.39	V	1,3,5-Triazine, 2,4,6-tris(oxanomethyl)-		
4	3.13	3.115	3.21	TIC	4037371	861978	4.8	2.14	V	1-Benzyl-4-nitroimidazole		
5	3.245	3.21	3.205	TIC	1419416	411379	3.43	0.75	V	Argon		
6	3.28	3.265	3.285	TIC	345416	279940	1.23	0.18	V	1,2-Propadiene-1,3-dione		
7	3.3	3.285	3.305	TIC	261006	204057	1.28	0.14	V	1,3,5-Triazine, 2,4,6-tris(oxanomethyl)-		
8	3.335	3.305	3.355	TIC	281286	82948	3.39	0.15	V	Argon		
9	6.005	5.845	6.07	TIC	124747	18834	6.63	0.07	V	Propryne		
10	7.3	7.25	7.34	TIC	191060	67250	2.84	0.1		Toluene		
11	7.635	7.63	7.785	TIC	110934	24224	4.58	0.06		Argon		
12	8.53	8.495	8.585	TIC	187071	63665	2.94	0.1		Octane		
13	11.259	11.215	11.32	TIC	352632	97679	3.61	0.19		Ethylbenzene		
14	12.953	12.91	13.015	TIC	408425	115593	3.53	0.22	V	Undecane		
15	17.32	17.265	17.355	TIC	252522	63477	3.98	0.13		Phenol		
16	17.4	17.355	17.465	TIC	813421	240082	3.39	0.43	V	Undecane		
17	18.457	18.4	18.515	TIC	222197	49765	4.46	0.12		Bicyclo[2.2.2]oct-2-ene, 1-methylamino-		
18	19.886	19.845	19.96	TIC	134893	32257	4.18	0.07		Benzene, butyl-		
19	21.26	21.185	21.3	TIC	142149	39520	3.6	0.08		Phenol, 3-methyl-		
20	21.598	21.53	21.67	TIC	921810	257576	3.58	0.49		Undecane		
21	25.536	25.465	25.62	TIC	1236397	367725	3.36	0.66		Dodecane		
22	29.23	29.155	29.3	TIC	931080	265929	3.5	0.49		Tridecane		
23	33.705	33.61	33.795	TIC	3847357	1044933	3.68	2.04		Tetradecane		
24	33.87	33.795	33.955	TIC	325540	74133	4.39	0.17	V	Indole, 3-(piperidinomethyl)-		
25	34.41	34.375	34.465	TIC	120792	38049	3.17	0.06		Octane, 2-cyclohexyl-		
26	35.975	35.875	36.06	TIC	5255171	1407984	3.73	2.79		Pentadecane		
27	38.449	38.405	38.505	TIC	122596	45092	2.72	0.06		7-Heptadecene, 1-chloro-		
28	38.602	38.505	38.695	TIC	944775	133972	7.11	0.5		Octononanoic acid, 4-headacetyl ester		
29	38.839	38.695	38.89	TIC	1297923	170453	7.61	0.69	V	1-Hexadecanol		
30	38.91	38.89	38.97	TIC	398027	132149	3.01	0.21	V	Cetane		
31	39.108	38.97	39.175	TIC	3590615	813718	4.38	18.87	V	Hexadecane		
32	39.225	39.175	39.33	TIC	861091	233887	3.7	0.46	V	7-Hexadecene, (Z)-		
33	39.562	39.5	39.645	TIC	406921	111268	3.66	0.22		9-Nonadecene		
34	40.895	40.76	40.945	TIC	531971	79270	6.71	0.28		2-methyltetraacosane		
35	41.005	40.945	41.06	TIC	246581	54098	4.56	0.13	V	Cyclopentane, 1-butyl-2-pentyl-		
36	41.138	41.075	41.2	TIC	246989	65216	3.69	0.13		2-methyltetraacosane		
37	41.359	41.29	41.42	TIC	303669	73906	4.11	0.16		9-Octadecene, (E)-		
38	41.508	41.42	41.63	TIC	1531073	273789	5.59	0.81		8-Heptadecene		
39	41.827	41.785	41.88	TIC	145353	46864	3.1	0.08		8-Heptadecene		
40	41.982	41.885	42.065	TIC	9162104	2303584	3.98	4.86		Heptadecane		
41	42.12	42.065	42.2	TIC	330192	74342	4.44	0.18	V	Cyclotetradecane		
42	43.169	43.115	43.235	TIC	210792	55536	3.8	0.11		Heptadecane		
43	43.605	43.54	43.64	TIC	421896	105393	4	0.22		1,7-Dimethyl-4-(1-methylethyl)cyclodecane		
44	43.694	43.64	43.76	TIC	1313939	289961	4.71	0.71	V	Oleyl alcohol, triisopropylacetate		
45	43.847	43.76	43.93	TIC	2883861	584559	4.93	1.53	V	n-Pentadecanol		
46	43.995	43.93	44.04	TIC	983366	225617	4.36	0.52	V	3,3'-Bi-p-menthane		
47	44.126	44.04	44.215	TIC	4344591	639783	6.8	2.3	V	9-Tricosene, (Z)-		
48	44.293	44.215	44.365	TIC	10335218	1765815	5.85	5.48	V	9-Eicosene, (E)-		
49	44.375	44.365	44.425	TIC	292752	969621	3.01	1.55	V	n-Pentadecanol		
50	44.453	44.425	44.5	TIC	2701478	702349	3.85	1.43	V	7-Heptadecene, 1-chloro-		
51	44.531	44.5	44.585	TIC	2666672	591230	4.5	1.41	V	n-Heptadecanol-1		
52	44.61	44.585	44.665	TIC	1727341	479049	3.61	0.92	V	3-Octadecene, (E)-		
53	44.819	44.665	44.88	TIC	59174265	11623687	5.09	31.37	V	Octadecane		
54	44.901	44.88	45.04	TIC	1729652	516958	3.35	0.92	V	Cyclotetradecane		
55	45.12	45.04	45.18	TIC	548969	125132	4.39	0.29		Benzene, [1-methylundecyl]-		
56	45.246	45.18	45.34	TIC	883779	187662	4.71	0.47	V	9-Eicosene, (E)-		
57	45.449	45.365	45.605	TIC	812832	108748	7.47	0.43		Oxalic acid, cyclohexylmethyl, tridecyl ester		
58	45.828	45.73	46	TIC	843588	137386	6.14	0.45		Nonadecane, 9-methyl-		
59	46.387	46.35	46.44	TIC	103350	37480	2.76	0.05		2-methylheptacosane		
60	46.502	46.44	46.56	TIC	542568	142496	3.81	0.29		1-Cyclopentylcicosane		
61	46.625	46.56	46.695	TIC	566867	142796	3.97	0.3	V	Dodecylcyclohexane		
62	47.365	47.285	47.46	TIC	3825472	972277	3.91	2.03		Nonadecane		
63	47.843	47.725	47.95	TIC	893766	136527	7.06	0.47		Cyclononasiloxane, octadecamethyl-		
64	48.152	48.09	48.21	TIC	174245	48634	3.58	0.09		Tetradecanone		
65	48.871	48.77	48.95	TIC	2668492	669077	3.99	1.42		Heptacosane		
66	51.329	51.26	51.445	TIC	404702	93550	4.33	0.21		Cyclotetrasiloxane, hexadecamethyl-		
67	52.254	52.165	52.35	TIC	1178635	303743	3.88	0.62		Heptacosane		
68	54.422	54.36	54.47	TIC	274350	75587	3.63	0.15		Cyclononasiloxane, octadecamethyl-		
69	54.53	54.47	54.635	TIC	984770	248261	3.97	0.52	V	Heptacosane		
70	56.713	56.63	56.785	TIC	455144	117046	3.89	0.24		Heptacosane		
71	57.26	57.205	57.32	TIC	179150	51425	3.3	0.08		Cyclononasiloxane, octadecamethyl-		
72	58.806	58.725	58.885	TIC	418908	100729	4.16	0.22		Heptacosane		
73	59.933	59.88	60.01	TIC	132939	40945	3.25	0.07		Cyclononasiloxane, octadecamethyl-		
74	60.801	60.72	60.88	TIC	266678	57597	4.63	0.14		2-methylheptacosane		
75	67.844	67.765	67.94	TIC	278635	53732	5.19	0.15		Cholestane		

Trial 2

Peak#	Ret.Time	Proc.From	Proc.To	Mass	Area	Height	A/H	Conc.	Mark	Name	Ret. Index
1	3.049	3.01	3.055	TC	2848121	1020610	2.79	1.45		Argon	
2	3.085	3.055	3.09	TC	1805208	787911	2.29	0.92	V	Argon	
3	3.114	3.09	3.15	TC	2004314	606273	3.31	1.02	V	Argon	
4	3.2	3.15	3.205	TC	611331	45674	13.38	0.31	0.32% V	1,2-Propadiene-1,3-dione	
5	4.84	4.835	4.875	TC	144318	15799	9.13	0.07		Argon	
6	7.055	7.05	7.195	TC	101285	11571	8.75	0.05	V	Argon	
7	7.256	7.22	7.305	TC	299497	89069	3.36	0.15	0.16% V	Toluene	
8	7.414	7.305	7.42	TC	100330	30165	3.33	0.05	V	Argon	
9	8.489	8.435	8.54	TC	206737	74055	2.79	0.11	0.11% V	Hexane, 2,4-dimethyl-	
10	8.37	8.295	8.41	TC	116323	21639	5.38	0.06	V	Argon	
11	10.508	10.47	10.57	TC	139037	31921	4.36	0.07		Argon	
12	11.228	11.17	11.275	TC	268899	94915	2.83	0.14	0.14% V	Ethylbenzene	
13	12.918	12.875	13	TC	573530	176481	3.25	0.29	0.30% V	Undecane	
14	15.423	15.39	15.475	TC	170443	57970	2.64	0.09	0.09% V	Benzene, propyl-	
15	17.383	17.305	17.485	TC	1383755	385410	3.59	0.71	0.73% V	Undecane	
16	17.051	17.035	17.205	TC	121541	51689	2.35	0.06	0.06% V	1,3,5-Triazine, 2,4,6-tris(cyanomethoxy)-	
17	21.28	21.195	21.39	TC	606797	104705	5.8	0.31	0.32% V	2,2-dimethyl-3-vinylbicyclo[2.2.1]heptane	
18	21.46	21.43	21.53	TC	89222	32907	2.98	0.05	0.05% V	1,3,5-Triazine, 2,4,6-tris(cyanomethoxy)	
19	21.59	21.53	21.68	TC	1509122	449395	3.4	0.77	0.80% V	Undecane	
20	21.819	21.76	21.885	TC	276388	82058	3.37	0.14	0.15% V	2-Undecene, (E)-	
21	25.537	25.46	25.625	TC	883468	528029	3.47	0.94	0.97% V	Dodecane	
22	25.745	25.7	25.815	TC	147985	51031	2.9	0.08	0.08% V	2-Dodecene, (E)-	
23	29.234	29.15	29.305	TC	1636692	466324	3.51	0.84	0.87% V	Tetradecane	
24	32.707	32.615	32.79	TC	4827933	1316782	3.67	2.46	2.56% V	Tetradecane	
25	32.88	32.79	32.93	TC	284852	72488	3.93	0.15	0.15% V	4-Cyanoacetic acid, 6-ethyl-3-octyl ester	
26	34.413	34.355	34.495	TC	238389	67442	3.53	0.12	0.13% V	Cyclopentane, decyl-	
27	35.98	35.88	36.07	TC	8239175	2154126	3.82	4.2	4.37% V	Pentadecane	
28	36.134	36.075	36.175	TC	174290	51751	3.37	0.09	0.09% V	5-Octadecene, (E)-	
29	37.725	37.67	37.79	TC	204657	50438	4.05	0.1	0.11% V	n-Nonylcyclohexane	
30	38.444	38.39	38.51	TC	247059	78238	3.16	0.13	0.13% V	7-Heptadecene, 1-chloro-	
31	38.598	38.51	38.7	TC	1053446	168050	6.27	0.54	0.56% V	Cyclodecane	
32	38.74	38.7	38.79	TC	178963	54478	3.29	0.09	0.09% V	7-Heptadecene, 17-chloro-	
33	38.835	38.76	38.895	TC	627460	11462	5.63	0.31	0.33% V	n-Heptadecane-1	
34	38.915	38.895	38.965	TC	168042	68308	2.46	0.09	0.09% V	3-Dodecene, (E)-	
35	39.111	38.965	39.18	TC	37938469	8239038	4.6	19.36	20.13% V	Hexadecane	
36	39.224	39.18	39.335	TC	678387	184535	3.68	0.35	0.36% V	7-Hexadecene, (Z)-	
37	39.56	39.495	39.635	TC	367026	93238	3.94	0.19	0.19% V	7-Hexadecene, (Z)-	
38	40.874	40.745	40.945	TC	851672	108791	7.83	0.43	0.45% V	Dodecane, 2-cyclohexyl-	
39	40.988	40.945	41.065	TC	415819	101888	4.08	0.21	0.22% V	Cyclopentane, 1-pentyl-2-propyl-	
40	41.14	41.07	41.2	TC	332380	88383	3.76	0.17	0.18% V	1-Decanol, 2-octyl-	
41	41.365	41.2	41.43	TC	1158829	218143	5.3	0.59	0.61% V	9-Octadecene, (E)-	
42	41.506	41.43	41.635	TC	3438296	640122	5.37	1.75	1.82% V	8-Heptadecene	
43	41.84	41.785	41.89	TC	152809	51816	2.95	0.08	0.08% V	Cycloptadecane	
44	41.994	41.89	42.085	TC	1424641	3504080	4.06	7.27	7.50% V	Heptadecane	
45	42.12	42.085	42.185	TC	380171	105076	3.59	0.19	0.20% V	Cyclodecane	
46	42.316	42.255	42.385	TC	236678	65431	3.62	0.12	0.13% V	Benzene, 1,4-didecyl-	
47	43.163	43.09	43.235	TC	397794	90117	4.41	0.2	0.21% V	Heptadecane	
48	43.605	43.545	43.635	TC	363124	106277	3.42	0.19	0.19% V	1-Nonadecene	
49	43.701	43.635	43.76	TC	1423821	291187	4.89	0.73	0.76% V	Diethyl stochad, trifluoroacetate	
50	43.854	43.76	43.93	TC	2706519	571032	4.74	1.38	1.44% V	Cyclodecane, octyl-	
51	43.994	43.93	44.045	TC	688098	159049	4.33	0.35	0.37% V	3,3-Bi-p-menthane	
52	44.115	44.045	44.215	TC	365318	580169	6.3	1.86	1.94% V	9-Eicosene, (E)-	
53	44.292	44.215	44.495	TC	1251610	1617419	7.74	6.39	6.64% V	9-Eicosene, (E)-	
54	44.551	44.495	44.66	TC	2492208	384972	6.47	1.27	1.32% V	Cyclopentane, 1-butyl-2-pentyl-	
55	44.817	44.66	45.03	TC	60331750	11668848	5.17	30.78	32.01% V	Octadecane	
56	45.124	45.03	45.17	TC	629900	143899	4.38	0.32	0.33% V	Benzene, [1-methylundecyl]-	
57	45.248	45.17	45.33	TC	680927	128927	5.28	0.35	0.36% V	1-Decanol, 2-hexyl-	
58	45.45	45.33	45.615	TC	859911	121620	7.07	0.44	0.46% V	Oxalic acid, cyclohexylmethyl tetradecyl ester	
59	45.828	45.745	46.015	TC	1038855	170390	6.1	0.53	0.55% V	Henicosane	
60	46.294	46.225	46.34	TC	188265	51182	3.87	0.1	0.11% V	Benzene, [1,1,4,6,6-pentamethylheptyl]-	
61	46.394	46.34	46.45	TC	214668	67368	3.19	0.11	0.11% V	2-methyltricosane	
62	46.502	46.45	46.57	TC	459813	114660	4.01	0.23	0.24% V	Cyclopentane, decyl-	
63	46.623	46.57	46.69	TC	442468	117710	3.76	0.23	0.23% V	Dodecylcyclohexane	
64	46.91	46.85	47.01	TC	319128	75225	4.24	0.16	0.17% V	9-Tricosene, (Z)-	
65	47.236	47.185	47.28	TC	136962	41622	3.29	0.07	0.07% V	Hexane, 2-phenyl-3-propyl-	
66	47.371	47.28	47.455	TC	5043388	1285277	3.92	2.57	2.68% V	Henicosane	
67	47.798	47.72	47.865	TC	325554	79264	4.11	0.17	0.17% V	Henicosane	
68	49.155	49.08	49.22	TC	220664	61194	3.61	0.11	0.12% V	Tritetracontane	
69	49.871	49.775	49.965	TC	3110984	798783	3.9	1.59	1.65% V	Henicosane	
70	52.254	52.165	52.34	TC	1394083	343544	4.06	0.71	0.74% V	Henicosane	
71	54.535	54.44	54.63	TC	1106745	286094	3.87	0.56	0.59% V	Henicosane	
72	56.711	56.63	56.79	TC	573206	147409	3.92	0.3	0.31% V	Henicosane	
73	58.804	58.72	58.895	TC	548167	127885	4.29	0.28	0.29% V	Henicosane	
74	60.8	60.735	60.895	TC	337529	81777	4.13	0.17	0.18% V	Henicosane	
75	62.738	62.66	62.825	TC	305190	69562	4.39	0.16	0.16% V	Tetratetracontane	

325 C
Trial 1

Peak #	Ret. Time	Proc. From	Proc. To	Mass	Area	Height	A/N	Conc.	Mark	Name	Ret.	Index
1	3.041	3.01	3.05	TIC	2745721	1202324	2.28	2.48	Argon			
2	3.106	3.05	3.075	TIC	1748019	1170068	1.49	1.58	V	3-Butyn-1-ol		
3	3.105	3.075	3.115	TIC	2673624	1114119	2.4	2.41	V	Allene		
4	3.112	3.115	3.135	TIC	1276566	1087751	1.18	1.15	V	Argon		
5	3.159	3.135	3.17	TIC	2121381	1010088	2.1	1.93	V	Argon		
6	3.176	3.17	3.195	TIC	1444755	980583	1.47	1.3	V	Argon		
7	3.205	3.195	3.24	TIC	2436915	930053	2.62	2.2	V	Argon		
8	3.26	3.24	3.265	TIC	1273875	841475	1.51	1.15	V	3-Butyn-1-ol		
9	3.27	3.265	3.275	TIC	493448	829654	0.59	0.45	V	1,2-Propadiene-1,3-dione		
10	3.28	3.275	3.305	TIC	1418039	810325	1.75	1.28	V	1,3,5-Triaz 2,4,6-tris(cyanomethoxy)-		
11	3.32	3.305	3.345	TIC	1745915	747927	2.33	1.58	V	Borane carbonyl		
12	3.355	3.345	3.37	TIC	1003342	67247	1.48	0.91	V	Propyne		
13	3.415	3.37	3.43	TIC	2178986	590445	3.69	1.97	V	Argon		
14	3.435	3.43	3.44	TIC	329209	550491	0.6	0.3	V	Argon		
15	3.445	3.44	3.45	TIC	317058	537152	0.59	0.29	V	Argon		
16	3.465	3.45	3.46	TIC	310015	523800	0.59	0.28	V	Argon		
17	3.465	3.46	3.48	TIC	594200	510357	1.16	0.54	V	Propyne		
18	3.51	3.48	3.525	TIC	1180039	430990	2.74	1.07	V	2,5-Furandi hydro-3-methylene-		
19	3.541	3.525	3.56	TIC	793109	383593	2.07	0.72	V	1,2-Propadiene-1,3-dione		
20	3.57	3.56	3.585	TIC	499693	242647	1.46	0.45	V	3-Butyn-1-ol		
21	3.59	3.585	3.595	TIC	181248	304439	0.6	0.16	V	2-Propanol 1-methoxy		
22	3.6	3.595	3.645	TIC	783384	295615	2.65	0.71	V	1-(2-Chlorophenyl)-1,2,3,4-tetrahydro-3-methoxycarbonyl-9H-indolo[2,3-c]pyridine		
23	3.65	3.645	3.67	TIC	313197	222940	1.4	0.28	V	Argon		
24	3.705	3.68	3.72	TIC	325499	143695	2.27	0.29	V	Allene		
25	3.775	3.72	3.78	TIC	228288	39020	5.85	0.21	V	Allene		
26	6.855	6.72	6.875	TIC	155565	28390	5.48	0.14	V	Argon		
27	7.247	7.215	7.31	TIC	715993	54331	3.98	0.19	V	Toluene		
28	8.485	8.41	8.51	TIC	165682	46388	4.1	0.15	V	1,2,5-Oxadiazole		
29	9.841	9.76	9.895	TIC	124011	27741	4.47	0.11	V	Argon		
30	10.155	10.15	10.29	TIC	186203	25634	7.26	0.17	V	Argon		
31	12.915	12.885	12.98	TIC	194161	57244	3.39	0.18	V	Nonane		
32	17.371	17.28	17.45	TIC	693309	142993	4.86	0.63	V	Undecane		
33	17.66	17.595	17.69	TIC	134025	34238	3.91	0.12	V	3-Butyn-1-ol		
34	21.26	21.245	21.28	TIC	125138	74489	1.68	0.11	V	3-Butyn-1-ol		
35	21.325	21.28	21.355	TIC	168811	46073	4.13	0.15	V	Argon		
36	21.581	21.51	21.685	TIC	460644	117200	3.93	0.42	S	Undecane		
37	25.524	25.445	25.615	TIC	577540	156507	3.69	0.52	V	Dodecane		
38	29.22	29.15	29.285	TIC	438423	129753	3.38	0.4	V	Tridecane		
39	32.692	32.6	32.78	TIC	1811998	506882	3.57	1.64	V	Tetradecane		
40	35.858	35.875	36.045	TIC	2863045	785247	3.65	2.68	V	Heptadecane		
41	38.427	38.385	38.5	TIC	128717	36970	3.48	0.12	V	7-Heptade 1-chloro-		
42	38.587	38.505	38.685	TIC	338650	66100	5.12	0.31	V	9-Octadec (E)-		
43	38.83	38.765	38.92	TIC	420680	100597	4.18	0.38	V	9-Octadec (E)-		
44	39.069	38.955	39.155	TIC	17562084	4328256	4.06	15.85	V	Hexadecane		
45	39.55	39.43	39.62	TIC	133610	33196	4.02	0.12	V	5-Octadec (E)-		
46	41.121	41.07	41.185	TIC	134600	39259	3.43	0.12	V	1-Decanol 2-octyl-		
47	41.333	41.255	41.415	TIC	626210	147025	4.26	0.57	V	8-Heptadecane		
48	41.49	41.415	41.61	TIC	1382873	269584	5.13	1.25	V	8-Heptadecane		
49	41.962	41.87	42.05	TIC	4794352	1212912	3.95	4.33	V	Heptadecane		
50	42.1	42.05	42.17	TIC	189877	44699	4.25	0.17	V	Cyclopentadecane		
51	43.596	43.535	43.63	TIC	135279	43308	3.47	0.14	V	1,7-Dimethyl-4-(1-methylethyl)cyclododecane		
52	43.684	43.63	43.75	TIC	538657	112111	4.8	0.49	V	Oleyl alcohol, trifluoroacetate		
53	43.836	43.75	43.905	TIC	1052530	219755	4.79	0.95	V	Cyclopent 1-butyl-2-pentyl-		
54	43.976	43.905	44.02	TIC	417396	90602	4.61	0.38	V	3,3'-Bi-p-menthane		
55	44.099	44.02	44.185	TIC	2863330	507933	5.62	1.58	V	9-Tricosen (E)-		
56	44.268	44.185	44.485	TIC	8028098	1206783	6.65	7.25	V	9-Eicosen (E)-		
57	44.542	44.485	44.64	TIC	1232655	218509	5.64	1.11	V	n-Heptadecanol-1		
58	44.769	44.64	44.84	TIC	27132417	6287863	4.32	24.49	V	Octadecane		
59	44.865	44.84	44.955	TIC	619817	174614	3.55	0.56	V	Octadecane		
60	45.096	45.03	45.155	TIC	277167	70338	3.94	0.25	V	Benzene, (1-methylundecyl)-		
61	45.233	45.155	45.295	TIC	248258	52343	4.75	0.22	V	9-Eicosen (E)-		
62	45.439	45.37	45.57	TIC	735588	34265	6.88	0.21	V	Malonic acid, di(10-chloro ester)		
63	46.055	46.53	46.665	TIC	110654	41397	3.88	0.14	V	Dodecylcyclohexane		
64	46.888	46.79	46.98	TIC	213586	48629	4.39	0.19	V	2,5-Nonadecene		
65	47.08	47.06	47.195	TIC	122760	15639	7.85	0.11	V	9-Octadec (E)-		
66	47.354	47.27	47.43	TIC	1774862	468317	3.79	1.6	V	Hexacosane		
67	47.508	47.435	47.61	TIC	433278	94958	4.57	0.39	V	Pentadecanitrile		
68	49.852	49.77	49.945	TIC	1172943	295842	3.96	1.06	V	Hexacosane		
69	52.232	52.16	52.32	TIC	449086	114066	3.94	0.41	V	Hexacosane		
70	54.518	54.445	54.6	TIC	402374	102672	3.92	0.36	V	Hexacosane		
71	56.7	56.64	56.775	TIC	174413	45689	3.82	0.16	V	Hexacosane		
72	58.791	58.725	58.86	TIC	187716	50899	3.69	0.17	V	Hexacosane		
73	76.18	76.1	76.255	TIC	170379	32220	5.29	0.15	V	Tetracontane		
74	76.87	76.81	76.975	TIC	161304	29180	5.53	0.15	V	Dotriacontane		
75	83.54	83.49	83.665	TIC	139683	20352	6.86	0.13	V	Tetraiacontane		

Trial 2

[MC Peak Table]												
# of Peaks												
Mass	RetTime	Proc.From	Proc.To	Mass	Area	Height	A/H	Conc.	Mark	Name	Ret. Index	
1	3.056	3.01	3.055 TIC		188845	241911	7.8	2.44		Argon		
2	4.14	4.13	4.175 TIC		46674	26466	1.76	0.06		Argon		
3	4.189	4.175	4.31 TIC		100252	27196	3.69	0.13	V	Argon		
4	4.485	4.47	4.625 TIC		98135	17916	5.48	0.13		Argon		
5	4.658	4.625	4.665 TIC		24095	21262	1.13	0.03		Argon		
6	4.792	4.78	4.82 TIC		38278	29120	1.31	0.05		Argon		
7	5.105	5.08	5.125 TIC		32520	20858	1.56	0.04		Propyne		
8	5.57	5.565	5.605 TIC		24605	10431	2.36	0.03		Argon		
9	5.62	5.605	5.655 TIC		33348	24142	1.38	0.04	V	3-Butyn-1-ol		
10	7.14	7.125	7.145 TIC		6236	15774	0.4	0.01		1,2-Propadiene-1,3-dione		
11	7.21	7.145	7.25 TIC		73803	10219	7.22	0.1	V	Propyne		
12	7.273	7.25	7.29 TIC		101367	58655	1.73	0.13	V	Argon		
13	7.355	7.28	7.36 TIC		80213	17016	5.01	0.11	V	3-Butyn-1-ol		
14	7.395	7.36	7.405 TIC		40632	27332	1.49	0.05	V	Argon		
15	7.425	7.405	7.43 TIC		25138	23559	1.07	0.03	V	Propyne		
16	7.526	7.43	7.585 TIC		160947	29806	5.4	0.21	V	Argon		
17	7.725	7.72	7.845 TIC		84458	18525	4.56	0.11	V	Argon		
18	7.911	7.845	7.93 TIC		28916	17419	1.66	0.04	V	Allene		
19	8.064	8.045	8.07 TIC		21372	26355	0.81	0.03		Argon		
20	8.085	8.07	8.115 TIC		37952	13938	2.72	0.05	V	Argon		
21	8.125	8.115	8.14 TIC		17328	19904	0.87	0.02		Argon		
22	8.15	8.14	8.26 TIC		140300	28403	4.94	0.18		Argon		
23	8.265	8.26	8.28 TIC		20755	15044	1.38	0.03	V	Argon		
24	8.296	8.28	8.335 TIC		48341	26627	1.82	0.06	V	Argon		
25	8.405	8.345	8.41 TIC		57085	14567	3.92	0.07		3-Butyn-1-ol		
26	8.505	8.41	8.525 TIC		24612	16413	1.5	0.03	V	a5-Triazine-3,5[2H,4H]-dione, 6-(dimethylamino)-		
27	8.851	8.72	8.88 TIC		142241	27516	5.17	0.18		Argon		
28	9.181	9.165	9.195 TIC		18799	22875	0.82	0.02		Argon		
29	9.22	9.205	9.25 TIC		38439	16865	2.34	0.05		Argon		
30	9.266	9.25	9.305 TIC		37606	22964	1.64	0.05	V	Argon		
31	9.96	9.935	9.99 TIC		12265	10120	1.21	0.02		Argon		
32	10.385	10.37	10.39 TIC		11836	19838	0.6	0.02		Argon		
33	10.494	10.39	10.56 TIC		63378	18296	3.46	0.08	V	Argon		
34	10.83	10.82	10.845 TIC		110212	18889	5.83	0.14		Argon		
35	10.95	10.945	11.015 TIC		60969	16417	3.71	0.08	V	Argon		
36	11.02	11.015	11.145 TIC		125651	18026	6.97	0.16	V	Argon		
37	11.105	11.145	11.205 TIC		53944	23634	2.98	0.07	V	Argon		
38	11.236	11.205	11.3 TIC		211832	61566	3.44	0.27	V	Ethylbenzene		
39	11.33	11.3	11.35 TIC		49015	23061	2.13	0.06	V	Argon		
40	12.615	12.555	12.62 TIC		37157	16279	2.28	0.05		Argon		
41	12.935	12.895	12.965 TIC		92250	35484	2.6	0.12		Undecane		
42	15.965	15.96	15.99 TIC		18151	24208	0.75	0.02		Argon		
43	17.325	17.275	17.34 TIC		116547	46478	2.51	0.15		4-Spiroheptanone, 5,5-dichloro-		
44	17.384	17.34	17.45 TIC		401928	80568	3.81	0.52	V	Decane		
45	18.003	17.985	18.02 TIC		25145	21335	1.18	0.03		Argon		
46	19.215	19.205	19.365 TIC		109864	18345	5.99	0.14		Argon		
47	20.155	20.15	20.23 TIC		49981	17420	2.87	0.06		Argon		
48	21.276	21.185	21.32 TIC		316560	60882	5.2	0.41		Phenol, 3-methyl-		
49	21.375	21.32	21.395 TIC		87349	21198	4.12	0.11	V	Allene		
50	21.589	21.54	21.64 TIC		235537	86112	2.74	0.31		Heptadecane, 2,6-dimethyl-		
51	25.534	25.475	25.59 TIC		415265	129709	3.2	0.54		Dodecane		
52	29.225	29.17	29.285 TIC		354541	109935	3.23	0.46		Tridecane		
53	32.697	32.62	32.785 TIC		1650564	451277	3.66	2.14		Tetradecane		
54	35.966	35.885	36.045 TIC		2766424	725029	3.82	3.58		Pentadecane		
55	38.841	38.78	38.91 TIC		381453	103670	3.68	0.49		3-Eicosene, (E)-		
56	38.077	38.96	39.16 TIC		16762116	4381809	4.01	21.7		Hexadecane		
57	41.343	41.265	41.42 TIC		651223	150995	4.31	0.84		8-Heptadecene		
58	41.497	41.42	41.63 TIC		1383244	278745	4.96	1.79	V	8-Heptadecene		
59	41.974	41.88	42.06 TIC		4208841	1077925	3.92	5.47		Nonadecane		
60	42.125	42.06	42.175 TIC		179754	36336	4.95	0.23	V	5-Octadecene, (E)-		
61	43.691	43.635	43.75 TIC		258487	75336	3.43	0.33		Oleyl alcohol, trifluoroacetate		
62	43.846	43.75	43.915 TIC		667305	168303	3.96	0.86		Cyclopentane, 1-butyl-2-pentyl-		
63	44.105	44.025	44.19 TIC		2684078	541818	4.95	3.48		9-Eicosene, (E)-		
64	44.276	44.19	44.42 TIC		7348000	1235895	5.94	9.52	V	9-Eicosene, (E)-		
65	44.445	44.42	44.49 TIC		540422	163183	3.31	0.7	V	1-Tetradecanol, 14-chloro-		
66	44.554	44.49	44.65 TIC		1096408	209013	5.25	1.42	V	1-Nonadecene		
67	44.775	44.65	44.855 TIC		2534747	6032257	4.2	32.81		Nonadecane		
68	44.875	44.855	44.965 TIC		473232	156437	3.02	0.61	V	Cyclotetradecane		
69	45.106	45.05	45.17 TIC		196139	52823	3.71	0.25		Benzene, (1-methylundecyl)-		
70	47.361	47.285	47.44 TIC		1409666	370015	3.81	1.83		Heptacosane		
71	47.516	47.44	47.62 TIC		984556	236383	4.35	1.28		Hexadecanenitrile		
72	48.866	48.785	48.95 TIC		962843	243109	3.96	1.25		Heptacosane		
73	52.249	52.205	52.315 TIC		206291	66580	3.1	0.27		Heptacosane		
74	52.553	52.485	52.625 TIC		300668	75656	3.97	0.39		Heptadecanenitrile		
75	54.528	54.47	54.6 TIC		289151	82096	3.52	0.37		Heptacosane		

**300 C
Trial 1**

retention time	average	start time	end time	Area	Compound name
10.614	10.555	10.765	10.8712		Toluene
15.205	15.151	15.311	15.6704		Diethylbenzene
18.345	18.291	18.425	18.6512		Nonane
21.335	21.195	21.305	21.6512		1,2-Diethyl-3-methylbenzene
21.355	21.305	21.455	21.6012		1,3-Diethyl-2-methylbenzene
22.1	22.105	22.305	22.6012		1,2-Diethyl-4-methylbenzene
23.241	23.205	23.41	23.6012		Decane
23.581	23.505	23.63	23.6468		1,2-Dimethylbenzene
23.688	23.61	23.135	23.7708		1,2-Diethyl-3-methylbenzene
24.65	24.61	24.68	24.7272		1,2-Diethyl-4-methylbenzene
24.648	24.58	24.785	24.82017		1,2-Diethyl-3-methylbenzene
25.574	25.505	25.675	25.9168		1,2-Diethyl-4-methylbenzene
26.059	26.005	26.125	26.18809		Undecane
26.3	26.28	26.36	26.4272		1,2-Diethyl-3,6-dimethylbenzene
27.395	27.365	27.465	27.6162		1,2-Dimethylbenzene
27.945	27.88	28.05	28.18888		1,2-Diethyl-4-methylbenzene
28.185	28.105	28.21	28.68131		1,2-Diethyl-3,6-dimethylbenzene
28.517	28.465	28.595	28.8851		1,2-Dimethylbenzene
29.045	28.995	29.085	29.1018		1,2-Diethyl-3,6-dimethylbenzene
30.365	30.265	30.465	31.1784		1,2-Diethyl-4-methylbenzene
30.67	30.61	30.745	30.8915		1,2-Diethyl-3-propylbenzene
32.738	32.68	32.81	33.1112		1,2-Diethylbenzene
34.294	34.25	34.365	34.6116		1,2-Diethyl-4-methylbenzene
35.665	35.615	35.835	36.1809		1,2-Diethylbenzene
37.245	37.195	37.275	37.7089		0,0-Diacetyl-3-(1H-indol-3-yl)-N-(4-methylphenyl)-2-one
37.333	37.275	37.41	37.9782		0,0-Diacetyl-2,3-dimethylbenzene
38.205	38.155	38.21	38.6560		1,2-Diethylbenzene
38.3	38.25	38.35	38.6116		0,0-Diacetyl-1,2-dimethylbenzene
38.615	38.565	38.615	38.6809		1,2-Diethylbenzene
40.127	40.07	40.205	40.6116		0,0-Diacetyl-1,2-dimethylbenzene
40.46	40.41	40.745	40.8915		0,0-Diacetyl-1,2-dimethylbenzene
40.774	40.735	40.805	41.1816		0,0-Diacetyl-1,2-dimethylbenzene
40.836	40.805	40.88	41.1816		0,0-Diacetyl-1,2-dimethylbenzene
40.895	40.88	41.31	41.8117		0,0-Diacetyl-1,2-dimethylbenzene
41.574	41.52	41.61	41.6509		0,0-Diacetyl-1,2-dimethylbenzene
42.89	42.845	42.93	43.0609		0,0-Diacetyl-1,2-dimethylbenzene
43.03	42.97	43.065	43.7884		0,0-Diacetyl-1,2-dimethylbenzene
43.1	43.045	43.115	43.5402		0,0-Diacetyl-1,2-dimethylbenzene
43.164	43.115	43.11	43.1921		0,0-Diacetyl-1,2-dimethylbenzene
43.369	43.31	43.41	43.5208		0,0-Diacetyl-1,2-dimethylbenzene
43.456	43.41	43.605	43.6770		0,0-Diacetyl-1,2-dimethylbenzene
44.17	44.148	44.81	44.8114		0,0-Diacetyl-1,2-dimethylbenzene
45.038	44.92	45.085	45.1796		0,0-Diacetyl-1,2-dimethylbenzene
45.14	45.085	45.11	45.1796		0,0-Diacetyl-1,2-dimethylbenzene
45.295	45.17	45.41	45.4109		0,0-Diacetyl-1,2-dimethylbenzene
45.505	45.46	45.515	45.7028		0,0-Diacetyl-1,2-dimethylbenzene
45.54	45.515	45.61	45.6116		0,0-Diacetyl-1,2-dimethylbenzene
46.325	46.27	46.39	46.382		0,0-Diacetyl-1,2-dimethylbenzene
47.21	47.205	47.345	47.0411		0,0-Diacetyl-1,2-dimethylbenzene
47.381	47.345	47.465	47.6116		0,0-Diacetyl-1,2-dimethylbenzene
47.485	47.445	47.58	47.6207		0,0-Diacetyl-1,2-dimethylbenzene
47.678	47.648	47.785	47.8608		0,0-Diacetyl-1,2-dimethylbenzene
47.894	47.785	47.955	48.1789		0,0-Diacetyl-1,2-dimethylbenzene
47.984	47.955	48.225	48.7043		0,0-Diacetyl-1,2-dimethylbenzene
48.025	48.4	48.71	48.7116		0,0-Diacetyl-1,2-dimethylbenzene
48.645	48.595	48.705	48.626		0,0-Diacetyl-1,2-dimethylbenzene
50.071	49.965	50.195	49.9109		0,0-Diacetyl-1,2-dimethylbenzene
51.792	51.685	51.84	51.6549		0,0-Diacetyl-1,2-dimethylbenzene
51.981	51.94	52.07	51.9102		0,0-Diacetyl-1,2-dimethylbenzene
52.14	52.07	52.275	49.1460		0,0-Diacetyl-1,2-dimethylbenzene
53.614	53.52	53.685	53.6772		0,0-Diacetyl-1,2-dimethylbenzene
53.878	53.815	53.935	53.8161		0,0-Diacetyl-1,2-dimethylbenzene
54.054	54	54.115	42.0774		0,0-Diacetyl-1,2-dimethylbenzene
57.288	57.235	57.345	42.0207		0,0-Diacetyl-1,2-dimethylbenzene
57.614	57.67	57.67	46.5543		0,0-Diacetyl-1,2-dimethylbenzene
57.775	57.67	57.835	38.7266		0,0-Diacetyl-1,2-dimethylbenzene
58.345	58.295	58.465	39.0508		0,0-Diacetyl-1,2-dimethylbenzene
60.164	60.115	60.255	58.0334		0,0-Diacetyl-1,2-dimethylbenzene
60.544	60.475	60.595	40.7034		0,0-Diacetyl-1,2-dimethylbenzene
60.885	60.835	61.06	41.8950		0,0-Diacetyl-1,2-dimethylbenzene
62.514	62.39	62.59	74.004		0,0-Diacetyl-1,2-dimethylbenzene
63.108	63.13	63.265	59.7766		0,0-Diacetyl-1,2-dimethylbenzene
63.331	63.28	63.4	37.8989		0,0-Diacetyl-1,2-dimethylbenzene
64.496	64.425	64.61	11.0529		0,0-Diacetyl-1,2-dimethylbenzene
65.075	65.02	65.145	61.6438		0,0-Diacetyl-1,2-dimethylbenzene
65.588	65.54	65.56	49.7128		0,0-Diacetyl-1,2-dimethylbenzene
67.333	67.285	67.395	42.9549		0,0-Diacetyl-1,2-dimethylbenzene
67.771	67.705	67.875	42.1066		0,0-Diacetyl-1,2-dimethylbenzene
68.013	67.96	68.005	46.1861		0,0-Diacetyl-1,2-dimethylbenzene
68.129	68.005	68.205	57.1501		0,0-Diacetyl-1,2-dimethylbenzene
68.211	68.18	68.26	140.771		0,0-Diacetyl-1,2-dimethylbenzene
68.58	68.53	68.615	42.1066		0,0-Diacetyl-1,2-dimethylbenzene
70.086	70.015	70.215	140.743		0,0-Diacetyl-1,2-dimethylbenzene
70.296	70.215	70.38	40.9102		0,0-Diacetyl-1,2-dimethylbenzene
70.424	70.39	70.475	18.8867		0,0-Diacetyl-1,2-dimethylbenzene
71.084	71.025	71.175	14.7880		0,0-Diacetyl-1,2-dimethylbenzene
71.975	71.93	72.04	41.6271		0,0-Diacetyl-1,2-dimethylbenzene
72.087	72.04	72.18	74.385		0,0-Diacetyl-1,2-dimethylbenzene
72.729	72.665	72.78	12.5019		0,0-Diacetyl-1,2-dimethylbenzene
72.879	72.78	72.86	54.9290		0,0-Diacetyl-1,2-dimethylbenzene
73.04	72.98	73.11	60.1062		0,0-Diacetyl-1,2-dimethylbenzene
73.205	73.17	73.27	45.005		0,0-Diacetyl-1,2-dimethylbenzene
75.206	75.11	75.34	32.5170		0,0-Diacetyl-1,2-dimethylbenzene
76.21	76.13	76.385	20.1319		0,0-Diacetyl-1,2-dimethylbenzene
76.41	76.385	76.43	97.1338		0,0-Diacetyl-1,2-dimethylbenzene
76.688	76.43	76.525	22.8323		0,0-Diacetyl-1,2-dimethylbenzene

Trial 2

mol	Area	Height							
10.81	TC	1057519	0.32	35552	0.42	4.88			0.32% Toluene
15.345	TC	763224	0.23	172149	0.33	4.43			0.23% Ethylbenzene
18.432	TC	290463	0.09	88061	0.17	3.27			0.09% Naphthalene
19.535	TC	511880	0.15	109107	0.21	4.69			0.15% 6-Methyl-1-(phenylmethyl)-2,2,6-tetrahydropyridin-3-ol
20.75	TC	549251	0.18	128574	0.25	4.61			0.18% 2-Cyclopentyl-1-one, 4,4-dimethyl-
21.345	TC	321379	0.11	74243	0.14	4.33			0.11% Pyrene, 2-methyl-5-methyl-
21.465	TC	595453	0.18	140564	0.27	4.24	V		0.18% 2,3,4-Trimethylpyridine
22.33	TC	403736	0.12	71464	0.14	5.65			0.12% 2-Cyclopentyl-1-one, 2,3-dimethyl-
22.46	TC	634249	0.19	166568	0.32	3.82	V		0.19% Decane
23.64	TC	861654	0.27	200836	0.38	4.39			0.27% Benzene, butyl-
24.74	TC	1311743	0.39	261100	0.51	5.65	V		0.39% Phenol, 2-methyl-
24.915	TC	1553137	0.47	187271	0.38	7.87	V		0.47% 1H-Pyridine, 1-phenyl-
24.955	TC	1079028	0.32	163927	0.31	6.63	V		0.32% 1H-Pyridine, 2-carbamethoxy-, 1-ethyl-
24.935	TC	316588	0.11	52852	0.11	5.99			0.10% Trimethylamine (N-6) bis(trifluoromethyl)ethylborane trimethylamine
24.425	TC	673255	0.21	142204	0.27	4.75	V		0.20% Spiro[2.3]heptan-5-one, 4,4-dimethyl-
24.595	TC	820863	0.26	168843	0.22	7.88	V		0.26% Pyrene, 1-(4-oxocyclohex-1-yl)-
24.805	TC	1634113	0.48	263433	0.51	6.2	V		0.48% 1H-Pyridine, 3-ethyl-2,4-dimethyl-
26.155	TC	581446	0.18	186446	0.36	3.12			0.18% Undecane
26.095	TC	778288	0.23	107445	0.21	7.24			0.23% Phenol, 2,5-dimethyl-
26.975	TC	607987	0.18	121748	0.24	4.83			0.18% Pyridine, 1-methyl-3-(1,1-dimethylethyl)-
27.11	TC	432243	0.13	96964	0.18	4.51	V		0.13% Naphthalene-6,8a-dimethoxy-oxanthrone
27.51	TC	445958	0.13	110861	0.21	4.62			0.13% Benzene, pentyl-
28.025	TC	593783	0.18	151265	0.29	3.93			0.18% Phenol, 4-ethylmethoxy-
28.285	TC	555887	0.17	118419	0.23	4.69			0.17% Pyridine, 1-methyl-3-(1,1-dimethylethyl)-
29.62	TC	1291302	0.39	316502	0.41	4.69			0.39% Toluene
30.795	TC	711886	0.22	112788	0.27	6.46			0.22% Naphthalene, 2-acetyl-8-dimethyl-
32.85	TC	1404911	0.42	367973	0.71	3.82			0.42% Hexadecane
34.37	TC	340833	0.11	205612	0.19	3.39			0.10% 1H-Indole, 3-methyl-
35.49	TC	843463	0.25	218433	0.42	3.86	V		0.25% Decanoic acid, ethyl ester
35.58	TC	371895	0.11	116196	0.22	3.22	V		0.11% 1-Tetradecene
35.845	TC	4611267	1.21	824815	1.58	4.86			1.21% Hexadecane
37.445	TC	1265981	0.31	237004	0.45	5.35			0.31% 1H-Indole, 2,3-dimethyl-
38.285	TC	1607023	0.31	184615	0.46	5.66			0.31% 1-Tetradecene (E)
38.39	TC	619382	0.19	180723	0.35	3.39	V		0.19% 1-Tetradecene
38.035	TC	958409	0.28	1541981	2.96	6.22			2.89% Pentadecane
40.22	TC	610263	0.19	147856	0.28	4.13			0.19% 1,1,1,5-Tetraethyl-2-hexadecene-1-ol
40.675	TC	381036	0.11	18274	0.07	9.96			0.11% Hexan-3-one, 1-(4-(6-fluorophenyl)pyrimidin-5-yl)-
40.81	TC	278804	0.09	10946	1.03	5.17	V		0.09% 8-Hydroxodecane
40.895	TC	2941942	0.89	851184	1.63	3.46	V		0.89% Ceteane
41.34	TC	3608164	0.89	3536224	6.78	10.5V			0.89% Hexadecane
43.175	TC	2188209	0.72	882707	1.31	2.67			0.72% Heptadecane
43.34	TC	6156911	1.85	1071375	2.65	5.74	V		1.85% Heptadecane
43.635	TC	779378	0.21	103718	0.38	3.84	V		0.21% 1-Tetradecene
43.695	TC	10799228	3.25	1792512	3.46	6.16			3.25% Heptadecane
44.225	TC	323742	0.11	93323	0.18	3.42	V		0.10% Undecanoic acid, 10-methyl-, methyl ester
44.86	TC	778463	0.21	179314	0.31	4.84			0.21% 1,1,1,5-Tetraethyl-2-hexadecene-1-ol
45.155	TC	881658	0.27	196728	0.38	4.48	V		0.27% 9-Eicosene (E)
45.205	TC	2718226	0.82	657327	1.26	4.25	V		0.82% 11-Hydroxyoctadecanoic acid, n-undecyl ester
45.355	TC	7225001	2.18	2531324	4.85	2.85	V		2.18% 8-Octadecene (E)
45.56	TC	2262024	0.81	2888726	5.53	7.86	V		0.81% 8-Hydroxodecane
45.67	TC	5103788	15.39	4612226	8.99	10.845V			15.39% Octadecane
47.345	TC	307009	0.09	76961	0.15	3.89			0.09% Cyclopentane, umbellifer-
47.815	TC	2062097	0.62	260598	0.89	5.76			0.62% Nonadecane
47.995	TC	6642844	2	1270473	2.44	5.23	V		2.00% Tetradecanitrile
48.24	TC	4649366	1.4	888971	1.7	5.23	V		1.40% Heptadecane
48.745	TC	2329297	0.7	517621	1.09	4.69			0.70% Hexadecanoic acid, methyl ester
49.675	TC	558878	0.17	154837	0.3	3.61			0.17% Octadecanone
49.83	TC	2891564	0.82	577360	1.07	5.18	V		0.82% Ethyl 9-hexadecanoate
50.165	TC	3033010	0.13	3536897	6.78	8.58	V		0.13% Hexadecanoic acid, ethyl ester
51.96	TC	7202336	2.17	1073931	2.06	6.71	V		2.17% Octanitrile
52.08	TC	1431997	0.42	245474	0.68	4.63	V		0.42% 1-Octenyl-2,3-dimethyl-
52.27	TC	3165090	0.95	679046	1.3	4.63			0.95% Octadecanitrile
52.735	TC	466669	0.14	241486	0.27	3.32			0.14% Methyl stearate
53.48	TC	1124468	0.38	2657775	5.09	2.3			0.38% (E)-9-Octadecenoic acid ethyl ester
53.77	TC	1838893	0.54	2188575	4.21	8.36	V		0.54% (E)-9-Octadecenoic acid ethyl ester
53.98	TC	10503200	3.16	1954739	3.83	5.26	V		3.16% Octadecanoic acid, ethyl ester
54.11	TC	450246	0.14	97043	0.19	4.64	V		0.14% Tetradecanamide
54.18	TC	421099	0.13	99189	0.19	4.31			0.13% N-Methylpiperidocarbamide
55.305	TC	298895	0.09	87676	0.17	3.42			0.09% N-Cyclohexylpiperidocarbamide
55.71	TC	287395	0.09	87588	0.17	3.28			0.09% Tricosane
57.98	TC	286739	0.12	83716	0.16	4.24			0.12% Octadecanamide (Z)-
57.975	TC	338495	0.11	88973	0.19	3.43	V		0.10% Phenyl 3-deoxy-beta-D-ribo-hekso-pyranoside
58.42	TC	512724	0.14	143081	0.27	3.72			0.14% N-Octylmorpholine
60.27	TC	756607	0.21	117705	0.23	6.43			0.21% Hexanoic acid, methyl ester
63.975	TC	361618	0.11	100025	0.19	3.62	V		0.11% 1-Hexanone, 6-(1,5-dimethylpyrrol-2-yl)-6-methyl-
64.625	TC	496487	0.15	86132	0.17	5.74			0.15% Octadecane
65.03	TC	482096	0.14	88205	0.13	7.61	V		0.14% Cholest-4-ene
65.18	TC	781361	0.24	161106	0.31	4.79	V		0.24% N-Hydroxyheptadecanamide, (E)-alpha-
65.675	TC	262529	0.09	79990	0.16	3.83			0.09% 1-Tryptophan, N-(3-ethyl-L-alpha-glutamyl)-, dibutyl ester
68.1	TC	422845	0.14	118605	0.23	3.82	V		0.14% Tetradecanoic acid, hexadecyl ester
69.305	TC	820035	0.21	183346	0.35	4.67	V		0.21% Hexadecane
69.655	TC	379518	0.11	114284	0.22	3.26			0.11% 2-methyltetradecane
70.215	TC	380729	0.11	14627	0.27	5.88	V		0.11% Benzeneamine, 4-(4-oxo-6-phenylmethyl)phenyl-
70.265	TC	375275	0.11	135846	0.24	2.98	V		0.11% Lanoster-3-one, 5,11,18-epoxy-
70.41	TC	3513476	1.06	741646	1.42	4.74	V		1.06% Hexadecanoic acid, hexadecyl ester
70.5	TC	134027	0.11	78689	0.15	4.18	V		0.10% Eicosane
71.795	TC	504481	0.15	153142	0.29	3.29			0.15% Tetradecanone
72.02	TC	576239	0.17	137382	0.26	4.18	V		0.17% 10-Hydroxocostane
72.205	TC	411820	0.12	90265	0.18	4.23	V		0.12% Eicosane
72.8	TC	289795	0.09	81733	0.16	3.55	V		0.09% Methoxyacetamide, N-propyl-N-ethyl-
73.96	TC	6200765	1.87	847084	1.62	7.32	V		1.87% Oleyl stearate
74.275	TC	6407182	1.93	877481	1.68	7.3	V		1.93% Hexadecanoic acid, octadecyl ester
74.38	TC	2160239	0.69	302459	0.58	7.12	V		0.69% Octadecanamide, N-decyl-
74.965	TC	1580721	0.48	200811	0.58	5.25			0.48% 2-Methyl-5-hexadecene-4-ol fumarate
76.41	TC	946254	0.28	367298	0.7	2.58	V		0.28% (L)-1-Bocehydroxy-L-carboxylic acid, 4'-butyl-, 4-pentylcholesterol ester
76.485	TC	1991839	0.4	657161	0.88	4.36	V		0.40% Oleyl stearate
76.61	TC	3197707	0.96	511582	0.98	6.25	V		0.96% Oleic acid, ethoxy ester
76.645	TC	517204	0.14	268846	0.51	1.98	V		0.14% 10-Indene, 2-Butyl-5-hexylcyclohexyl-