Effective laundering conditions for ignitable liquid
decontamination of fire scene clothing used by the Bureau of
Alcohol, Tobacco, Firearms, and Explosives

Rebecca K. Whitney

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Effective laundering conditions for ignitable liquid decontamination of fire scene clothing used by the Bureau of Alcohol, Tobacco, Firearms, and Explosives

A thesis submitted in partial fulfillment of the requirements for the degree of Master of Science in Forensic Science at Virginia Commonwealth University.

by

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<td>ASTM</td>
<td>American Society for Testing and Materials</td>
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<td>ATF</td>
<td>Alcohol, Tobacco, Firearms, and Explosives, Bureau of</td>
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<td>C-strip</td>
<td>activated carbon strip</td>
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<td>CS₂</td>
<td>carbon disulfide</td>
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<td>CFI</td>
<td>certified fire investigator</td>
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<td>EIP</td>
<td>extracted ion profile</td>
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<td>GC</td>
<td>gas chromatograph</td>
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<td>GC-MS</td>
<td>gas chromatograph mass spectrometer</td>
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<td>m/z</td>
<td>mass to charge ratio</td>
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<td>mL</td>
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<td>Persil ProClean Stain Fighter Power Caps detergent</td>
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<td>PNA</td>
<td>polynuclear aromatics</td>
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<td>SAM</td>
<td>standard accelerant mixture</td>
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<td>TIC</td>
<td>total ion chromatogram</td>
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<td>µL</td>
<td>microliter</td>
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Abstract

Ignitable liquids such as gasoline and diesel fuel are common accelerants encountered by Certified Fire Investigators (CFIs). These ignitable liquids can be identified by gas chromatography-mass spectroscopy; the presence of particular peaks in appropriate abundances and patterns indicates the presence of compounds found in ignitable liquids. The Bureau of Alcohol, Tobacco, Firearms, and Explosives (ATF) issues clothing to its CFIs for wear during fire scene investigation. Previous research has identified a method to decontaminate the tools used by CFIs, but no explicit protocol to decontaminate scene clothing has been determined. This study investigated the use of Tide Ultra Stain Release, Persil ProClean Stain Fighter and Persil ProClean Stain Fighter Power Caps along with rigorous washing machine and dryer conditions to decontaminate 100% cotton fabrics (t-shirt material and ATF-issued pants) and 90:10 cotton:polyester ATF-issued shirts spiked with a Standard Accelerant Mixture (SAM, 1:1 gasoline:diesel fuel). Samples were collected in epoxy-lined metal paint-type cans and extracted using activated charcoal strips overnight at 60 °Celsius. The volatile compounds were then eluted from the charcoal strips using a small amount of carbon disulfide. The resulting liquid was then run on a gas chromatograph-mass spectrometer using a method consistent with the ATF fire debris method. The first phase of this study aimed to establish a method to prevent cross-contamination between wash and dry cycles for all three detergents using 100% cotton broadcloth. It was determined that two wash cycles with Tide Ultra Stain Release and two dry cycles were sufficient. The second phase aimed to determine a procedure to sufficiently remove ignitable liquids in trace and gross amounts beyond the point of identification using all three detergents and 100% cotton t-shirt material. One and two dry cycles were also investigated. It was determined that trace amounts could be sufficiently removed with a single dry cycle using Tide Ultra Stain Release and Persil ProClean Stain Fighter. In the third phase, the effectiveness of the previously established procedures were tested on ATF-issued 100% cotton fire scene clothing and 90:10 cotton:polyester shirts, in small and moderate load sizes, with trace amounts of SAM. This study found that under rigorous washing and drying conditions trace amounts of SAM could be sufficiently removed from ATF-issued clothing of both fabric types using Tide Ultra Stain Release and Persil ProClean Stain Fighter.
Introduction

Ignitable liquids are “any liquids or the liquid phases of any materials that are capable of fueling a fire, including a flammable liquid, combustible liquid, or any other material that can be liquefied and burned” [1]. It is important for an understanding of fire to note that solids and liquids themselves do not undergo combustion, but it is their vapors that can ignite [1]. Ignitable liquids are often used as accelerants, which by definition, are any materials used to start or speed up the spread of a fire [1]. Ignitable liquids, such as gasoline and diesel fuel, are often used as accelerants because they are inexpensive, easy to obtain, and provide means to both easily ignite and hasten the development of a fire [2].

Automotive gasoline and diesel fuel are two of the most common ignitable liquids to be used as accelerants, because they are both readily available to consumers. Gasoline is the most common due to it being relatively inexpensive and efficient as an accelerant [2]. Gasoline is an ignitable liquid produced from light fractions of crude oil and contains a variety of hydrocarbon classes from C$_4$ to C$_{12}$ range, largely aromatics with boiling points between 32°C and 205°C [1,2]. These aromatic compounds include alkylbenzenes, naphthalenes, and indanes [2]. Automotive gasoline, in particular, is a blend of the resulting petroleum products from several different oil refinement processes [2]. Diesel fuel is an ignitable liquid produced from heavier fractions of crude oil than gasoline and classified as a heavy petroleum distillate (HPD) [1]. HPDs contain a Gaussian distribution of alkanes and naphthalene-based aromatic compounds in the carbon number range C$_{10}$ to C$_{23}$, covering the boiling point range from 190°C to 340°C [1,3]. While diesel fuel is also readily available at public gas stations, it is not as efficient as gasoline as an accelerant because it does not ignite as easily [1].
Following the suppression and overhaul of a fire, fire investigators may take control of the scene with the intent of determining the origin and cause of the fire [4]. Contamination of fire debris evidence can occur at several points during the investigative process. This can greatly affect the weight of the evidence in court and can occur if the evidence is improperly collected, stored, or shipped [5]. Evidence being collected for fire debris analysis should be collected using clean gloves, tools and evidence packaging containers. Only containers that safely preserve evidence for transport, protect against the loss of ignitable liquid residues, and prevent contamination should be used [2]. Common containers for fire debris are metal paint cans, as they are inexpensive and well-structured to protect debris and any volatiles [2]. Contamination concerns prior to use may be alleviated by storing the empty metal cans with the lids on [2]. An empty paint can may be submitted as a blank to verify a lack of contamination of that lot at the manufacturing level [2].

Another concern is that contamination may occur during scene processing and evidence collection if an accelerant is absorbed by the scene clothing, gear, or tools worn or used by a Certified Fire Investigator (CFI) at one scene and transferred onto evidence at a separate scene [5]. The prevention of such contamination is so crucial that it is included as a standard for professional qualification of a fire investigator in NFPA 1033: “ensuring cross-contamination and investigator-inflicted damage to evidentiary items is avoided and the chain of custody is established” [6]. Bureau of Alcohol, Tobacco, Firearms, and Explosives (ATF) CFIs and National Response Team members may launder the designated gear they are required to wear to fire scenes, consisting of 100% cotton pants, a 100% cotton jacket, and a 100% cotton or 90% cotton-10% polyester long sleeve shirt, for decontamination purposes although there is no standard protocol [7]. Previous work with decontamination of ignitable liquids has included
revisiting ATF’s procedure for decontaminating tools used during fire debris collection [8] The
previous decontamination procedure for ATF involved scrubbing each tool with Dawn dish
detergent, followed by rinsing with a strong stream of water [8]. This study found that Dawn dish
detergent alone was not effective at removing ignitable liquids from tools, but evaporation of the
ignitable liquid from the tools did occur if they were allowed to sit overnight [8]. This study
recommended a heavy-duty cleaning product, Simple Green Pro HD, be used to clean tools [8].
However, Simple Green Pro HD cannot be used on fire scene apparel due to its ability to
deteriorate fabric [8].

Laundry detergents are used to remove trace materials from fabric more efficiently than
water alone. Laundry detergents contain builders to soften water, surfactants to remove oils, and
sometimes bleach to remove plant material [9]. Surfactants work to improve the wetting ability
of the water by decreasing the surface tension and increasing the spreading and penetrating
properties, loosening and removing debris, and solubilizing the debris in the liquid [10,11].
Builders soften water, increase efficiency of surfactants, manage pH, and suspend debris in the

Fabric composition is also a factor that can affect the performance of laundry detergents.
Cotton is a natural fiber that is highly hydrophilic [9]. A previous study examined the persistence
of a standard accelerator mixture (SAM; 1:1 gasoline:diesel fuel) on several fiber types using
Tide Original detergent. SAM is often used in ignitable liquid research because it covers a wide
range of volatile compounds, heavy and light, commonly seen in fire debris. On cotton washed
with Tide Original, the aliphatic content of the SAM mixture persisted more than the aromatic
content of the ignitable liquids, and heavier compounds were retained more than lighter
compounds [9]. Polyester is a synthetic fiber that is not very hydrophilic [9]. Research on the
persistence of SAM on polyester when laundered with Tide Original showed that the aromatic content persisted more than the aliphatic content of the ignitable liquids [9]. For all fabric types and laundering conditions, the addition of a drying step decreased the presence of ignitable liquid compounds proportionally, but ultimately it was concluded that a single wash cycle with Tide Original was not effective at ignitable liquid decontamination of cotton and polyester fabrics, even with this addition of one drying cycle [9]. This previous study highlights the need for a sufficient decontamination protocol for ATF fire scene clothing.

In this experiment, effectiveness of three detergents was tested on 100% white cotton t-shirt material and the ATF-issued 100% cotton pants and 90% cotton-10% polyester long sleeve shirts. It utilized the two highest rated and only recommended liquid detergents by Consumer Reports, in addition to the highest rated pod detergent: Tide Ultra Stain Release, Persil ProClean Stain Fighter and Persil ProClean Stain Fighter Power Caps [12]. Effectiveness of the removal of SAM spiked on clothing was evaluated through standard fire debris extraction and analysis protocol of the clothing material following laundering procedures. Fire debris analysis is an important aspect of fire investigation, as it is the scientific examination of the evidence collected at the scene in order to identify any ignitable liquids that may be present [2]. A gas chromatograph-mass spectrometer (GC-MS) is used for fire debris analysis based on the instrument’s ability to separate and then identify components in ignitable liquids [2]. In order to analyze a sample using a GC-MS, the compounds must be extracted from the substrate. Activated charcoal strips are commonly used in adsorption-elution extractions, as they are an efficient adsorbent for volatilized compounds due to the large number of adsorption sites available [2]. Activated charcoal strips can be suspended from the lid of a metal can and when the can is heated, ignitable liquid residues will volatilize and adsorb onto the charcoal strip [2].
The charcoal strips are then rinsed with an appropriate solvent, such as carbon disulfide (CS$_2$), to elute the ignitable compounds from the strip [2]. This particular extraction method is named passive headspace concentration in American Society for Testing and Materials (ASTM) procedure E1412 but is known as passive adsorption-elution within the forensic science community [13]. This method is the most common and widely accepted method among fire debris chemists due to the sensitivity and efficiency of the activated charcoal strips [14]. After this process, the volatilized compounds are removed from the charcoal strip with a solvent for analysis on the GC-MS.

GC-MS is only used for qualitative purposes, to determine the presence or absence of ignitable liquids, when analyzing ignitable liquids recovered from fire debris [14]. Ignitable liquids are difficult to quantify because their components evaporate or are consumed during the fire, therefore the original amount of ignitable liquid present cannot be determined [14,15]. Even quantification of the ignitable liquids that may be present in a sample container cannot be achieved as the activated charcoal strips commonly used for fire debris analysis do not possess unlimited adsorption sites, and when ignitable liquids are present in high concentrations, displacement of lighter compounds on the charcoal strip by heavier compounds has been noted to occur [16]. To qualitatively identify ignitable liquids, diagnostic patterns must be recognized in the total ion chromatogram (TIC). Alkane, aromatic, polynuclear aromatic, and indanes are some of the classes of compounds that may be examined as extracted ion profiles (EIPs) to indicate the presence and type of an ignitable liquid when seen in particular patterns [2].

In this experiment, Tide Ultra Stain Release, Persil ProClean Stain Fighter and Persil ProClean Stain Fighter Power Caps will be tested on various 100% cotton fabrics spiked with trace and gross amounts of SAM under vigorous washing and drying conditions. The aim of this
experiment is to develop a procedure for ATF CFIs to use to successfully launder their fire scene clothing between wear at each fire scene to remove any potential ignitable liquid contamination.
Research Materials & Methods

Sample Preparation

The conditions for the washer and dryer were the most vigorous available on each appliance. The front load, high efficiency consumer grade washer, a Frigidaire Affinity (model FAFW3801LW3, serial number 4C22806256, Charlotte, NC), was set to a normal cycle, with hot temperature, at the max spin speed, and with a heavy soil level. With these settings applied, one wash cycle was 58 minutes. An exact temperature of the hot water cycle cannot be determined as the water temperature is affected by water heater settings and other water usage during the wash cycle [17]. As this experiment was performed in an apartment complex where water usage is not metered and billed to residents, this information is unknown. The dryer, also a Frigidaire Affinity (model FAQE7001, serial number 4D22002948, Charlotte, NC), was set to a 90-minute dry time with maximum heat. The exact temperature of this setting was not specified by the manufacturer [18]. For the liquid detergents, the volume used was to the top fill line inscribed on each detergent’s cap, and two power-caps (pods) were used for the detergent packs. These were the maximum detergent amounts directed to be used per the manufacturer’s instructions. The pods were placed in the washing machine after the addition of the fabric and the liquid detergent was dispensed using the dispenser drawer on the machine. The detergents tested were Tide Ultra Stain Release liquid detergent (Tide Ultra), Persil ProClean Stain Fighter liquid detergent (Persil Liquid), and Persil ProClean Stain Fighter Power Caps detergent (Persil Pods). Spike volumes of SAM (1:1 gasoline:diesel, Exxon, Columbia, MD) were 10mL for the gross amount and 100 µL for the trace amount. The amount of fabric in each load varied based on the phase in the experiment and is described below. Spiked cloth or clothing samples were
prepared and sealed for analysis in clean, epoxy-lined, metal paint-type cans. In addition, comparison samples of each fabric, clothing and detergent type were prepared, packaged, and extracted following the same procedures as described in this section to establish the sample background/matrix contributions from each for data analysis purposes.

*Phase One – Cross-Contamination Prevention Between Wash/Dry Cycles*

Bulk 100% cotton broadcloth (JoAnn Fabrics), a cost-effective cotton material, was cut to 33 x 38 cm pieces, which was a similar size as the pre-cut t-shirt rags to be used in a later phase. The significance of the size of the pieces of broadcloth was only to provide consistency in the amount of fabric in each load across the first two phases. SAM was introduced to the washer and dryer by spiking a piece of cloth with the gross volume of liquid, which was 10 mL, and washing and drying it with 14 additional pieces of un-spiked cloth. Each spiked cloth was previously marked by cutting out a notch from one of the sides of the rectangular piece. Subsequent unspiked “blank” loads of 15 pieces of cloth were cycled through the washer or dryer, and one cloth from each load was collected at random for extraction and analysis. This was repeated for each type of detergent and was used to evaluate cross-contamination, where no carryover would occur between spiked loads in the following phases.

After analysis of these samples (detailed in the Data Analysis section) it was determined that the next subsequent load cycled through the dryer for each detergent was free of ignitable liquid components, but this was not the case for the washer. Two loads of broadcloth using Tide Ultra was sufficient to establish the clean slate with no ignitable liquid components present between spiked samples. Subsequent loads were found to be ineffective at preventing ignitable liquid carry over for Persil Liquid and Persil Pods, so a “wipe-down” procedure was tested
utilizing 409 All Purpose Cleaner and Dawn Ultra dish detergent following the spiked load. The inside of the washing machine was sprayed liberally with 409 All Purpose Cleaner and then wiped down with a clean, dry paper towel. This included the drum, gaskets, and door. The washing machine was then wiped down with a paper towel with Dawn Ultra dish detergent and warm water on it. Finally, the washing machine was wiped down with a clean, wet paper towel to remove any residual dish detergent. Even with the addition of this “wipe-down” step, Persil Liquid and Persil Pods could not be used to establish a clean slate between spiked samples in a reasonable amount of wash cycles. Therefore, for the remainder of the project, two wash cycles using the maximum amount of Tide Ultra and un-spiked cotton broadcloth, followed by two dry cycles, were performed between all spiked samples. This procedure was followed to prevent cross-contamination regardless of which detergent was being used for the test samples themselves.

Phase Two – Persistence of SAM on 100% Cotton T-Shirt Material

One ULINE 100% cotton premium white t-shirt rag, approximately 33 x 38 cm, was marked with a notch and spiked with 100 µL SAM. The spiked rag was added to the washer with 14 additional rags and was washed with Tide Ultra and then dried with one drying cycle. The spiked rag was collected and packaged for analysis after drying. This procedure was repeated in triplicate for each detergent, utilizing two drying cycles for each. The procedure was then repeated with a spike volume of 10 mL SAM, in triplicate with one drying cycle, followed by in triplicate with two drying cycles.
Phase Three – Persistence of SAM on Fire Scene Clothing

Small Load Size – One pair of ATF-issued 100% cotton navy scene pants was cut in half in order to fit in the metal cans used for collection. The pants were cut vertically through the center of the pair to separate the left and right legs. One half was spiked with 100 µL SAM and was added to the washer with an un-spiked, ATF-issued 100% cotton navy t-shirt. This small load of laundry was washed with Tide Ultra and dried. The half pair of pants was collected for analysis after drying. This procedure was repeated in triplicate for each detergent, and then again with an ATF-issued 90:10 cotton:polyester blend gray scene shirt spiked with the SAM mixture. Only the trace volume of 100 µL SAM and one drying cycle were used for this phase based on results of Phase Two testing.

Moderate Load Size – The same type of scene pants and shirts tested above were evaluated in a larger size load of laundry. The pants were again cut in half and spiked with 100 µL SAM. The spiked clothing was added to the washer with other ATF-issued apparel of consisting of two 100% cotton navy t-shirts, one navy tactical-type jacket and two additional pairs of scene pants. This larger load of laundry was washed with Tide Ultra and dried, and the half pair of pants was collected for analysis. This procedure was repeated in triplicate for each detergent, and again with a spiked 90:10 cotton:polyester blend gray scene shirt. Only the trace volume of SAM and one drying cycle were used.

Passive Headspace Concentration

The metal cans were opened to insert half an activated charcoal strip (C-strip) for extraction. The C-strip (Albrayco Technologies, Inc., Cromwell, CT) was suspended in the
headspace of each can using a paperclip and magnet. The lids of the metal cans were then resealed. The cans were placed into a Yamoto Constant Temperature Oven (model DKN602C, serial number J1312239, Santa Clara, CA) at 60° Celsius overnight, approximately ten hours. The can was removed and allowed to cool before the C-strip was transferred to a GC vial (Agilent Technologies, lot number 18211373, Santa Clara, CA). Next, 400 μL of CS₂ (Fisher Chemical, C573-500, lot number 186320, Waltham, MA) was added to the GC vial using a Pipetman P200 pipet (VCU Department of Forensic Science pipet number DH54647), and the vial was capped and shaken manually and gently for approximately 30 seconds to elute the adsorbed volatiles from the surface of the C-strip. The solution was transferred using a disposable glass pipette (Corning, lot number 12318525, Corning, NY) and pipette bulb to a new GC vial with an autosampler vial insert for instrumental analysis. The insert reduced the capacity of the GC vial in order to maximize sample removal by the autosampler needle.

**Gas Chromatography-Mass Spectrometry**

Samples were analyzed on an Agilent 6890N Gas Chromatograph (serial number CN10313022, Santa Clara, CA) with an Agilent 5973 Network Mass Selective Detector Mass Spectrometer (serial number US30955326, Santa Clara, CA) and an Agilent 7683 Series Injector (Santa Clara, CA) with a J&W DB-1MS capillary column (Agilent, Santa Clara, CA). The method used for this analysis was RWHITNEY_ATF which was designed based on the ATF’s fire debris method. The method RWHITNEY_ATF can be found in Appendix 1 and includes method control parameters, instrument control parameters, and data analysis parameters.

A quality control standard, E-1618 test mix (Restek, Bellefonte, PA) in CS₂ was run at the beginning of each analysis. This standard was consistent with the recommendations of
ASTM to ensure the instrument was functioning properly for fire debris analysis [19]. This standard contains the following compounds: $n$-Hexane, $n$-Octane, $n$-Decane, $n$-Dodecane, $n$-Tetradecane, $n$-Hexadecane, $n$-Octadecane, $n$-Eicosane, 2-Ethyltoluene, 3-Ethyltoluene, Toluene, 1,2,4-Trimethylbenzene, and $p$-Xylene [20]. The total ion chromatogram for E-1618 test mix can be seen in Figure 1.

A negative control, pentane (Alfa Aeser, lot number R09C704, Haverhill, MA), was run in between samples to ensure that no carryover of ignitable liquid components occurred on the column during the analysis.
Data Analysis

The total ion chromatograms (TIC) for each sample were viewed using the Agilent GC-MS ChemStation software (version number G1701EA E.02.021431, Santa Clara, CA). Each TIC was then separated into the following EIPs: alkanes, olefins/cycloparaffins, aromatics, indanes, and polynuclear aromatics (PNAs), which are the classes of compounds examined to identify ignitable liquids [21]. The ions selected for the alkane class were 57, 71, 85, and 99 m/z. The ions selected for the olefin/cycloparaffin class were 55, 69, and 83 m/z. The ions selected for the aromatic class were 91, 105, 119, and 133 m/z. The ions selected for the indane class were 117, 131, and 145 m/z. The ions selected for the PNA class were 128, 142, and 156 m/z.

Phase One – Cross-Contamination Prevention

This first phase of the experiment aimed to prevent carryover, therefore the TICs associated with these samples were screened for any peaks consistent with the peaks seen in the SAM TIC (Figure 2), which fall into the above-mentioned categories of compounds. Laundry conditions for the subsequent phases were adjusted based on the results.

Phase Two – Persistence of SAM on 100% Cotton T-Shirt Material

This second phase of the experiment aimed to remove enough SAM from the cotton material such that no ignitable liquids could be identified. The TICs associated with these samples were screened for series of peaks that could be identified as an ignitable liquid such as gasoline or an HPD. Separating the TICs into the above-mentioned extracted ion profiles allowed
for each group to be filtered and examined separately, although it is the totality of the data in the TIC and EIPs that were used to draw a conclusion. In order for gasoline to be identifiable, the data was examined for the presence of the following diagnostic patterns: broad range of aromatic compounds (e.g. C_{1-}, C_{2-}, C_{3-}, and C_{4-}alkylbenzenes) in the TIC (Figure 3) and as the most abundant EIP, PNAs and indanes which were better visualized in the EIPs, and the presence of aliphatic compounds [2]. The ratios of these compounds may change over the amount of time gasoline is exposed to the air, shifting to a higher abundance of the heavier compounds, with a lower abundance of the lighter compounds as evaporation occurs [2]. If aliphatics were absent and the aromatics were present in a narrower range, an aromatic product was considered. In order for an HPD to be identifiable, the following characteristic patterns had to be present: clear, Gaussian distribution of spiking n-alkanes, less abundant branched and cyclic alkanes, as well as aromatic compounds (Figure 4) [2]. The pairs of C_{17} and C_{18} with pristane and phytane should also be present in “appropriate ratios” (Figure 4) [2]. Comparisons to reference ignitable liquids were performed as deemed necessary.

*Phase Three – Persistence of SAM on Fire Scene Clothing*

The third phase of the experiment aimed to remove enough SAM from the 100% cotton fire scene pants and the 90:10 cotton:polyester shirt, such that no ignitable liquids could be identified. The data analysis was performed in the same manner as Phase Two data analysis described above for both the small and moderate load sizes.
Results

All comparison samples of each fabric, clothing, and detergent type were prepared, packaged, and extracted following the same procedures as the spiked samples to establish the sample background/matrix contributions showed no peaks of interest. The fabric and clothing substrate samples were broadcloth from the first order (Figure 5), broadcloth from the second order (Figure 6), 100% cotton t-shirt material (Figure 7), 100% cotton ATF fire scene pants (Figure 8), and the 90:10 cotton:polyester ATF shirt (Figure 9). These fabrics were not laundered. The detergent samples were collected by washing clean cotton broadcloth from the first order with each detergent type. These substrate samples were also subjected to a drying cycle to replicate the conditions the detergent compounds would be subjected to. These detergent substrate samples were Tide Ultra (Figure 10), Persil Liquid (Figure 11), and Persil Pods (Figure 12).

Phase One – Cross-Contamination Prevention

Tide Ultra – Two loads of clean broadcloth using Tide Ultra was efficient to establish a clean slate in the washing machine with no ignitable liquid components present between spiked samples (Figure 13). Only one load of clean broadcloth was needed to establish a clean slate in the dryer with no ignitable liquid components present between spiked samples, however two cycles were performed as a precaution.

Persil Liquid – Persil Liquid could not be used to establish a clean slate between spiked samples in no more than two wash cycles. Alkanes and aromatics, components of both gasoline
and HPDs, were present in the TIC and EIPs (Figure 14). Even with two wash cycles and the use of Dawn Ultra dish detergent and 409 All Purpose Cleaner to wipe down the interior of the washing machine between spiked loads, the alkane and aromatic peaks persisted and had the potential to accumulate over time; therefore Tide Ultra was used in between spiked samples washed with Persil Liquid to prevent cross-contamination.

Persil Pods – Similar data was obtained for Persil Pods as with Persil Liquid. Due to the persistence of alkanes and aromatics, even with the additional use of Dawn Ultra dish detergent and 409 All Purpose Cleaner to clean the washer, Persil Pods could not be used to establish a clean slate between spiked samples in a reasonable amount of wash cycles (Figure 15). As such, Tide Ultra was used in between spiked samples washed with Persil Pods to prevent cross-contamination.

Phase Two – Testing with 100% Cotton T-Shirt Material
Testing was performed in triplicate. The results are shown in Table 1 and the trends observed in each sample group will be discussed.

Trace Amount of SAM: 100 µL

Tide Ultra – The cotton t-shirt material, spiked with 100 µL SAM and washed with the maximum amount of Tide Ultra, resulted in no identifiable ignitable liquid patterns. Aromatic peaks, specifically C₁, C₂, and C₃-alkylbenzenes, were visible in the TIC for samples processed with one drying cycle but were ultimately too weak to lead to a positive conclusion in two of the three replicates (Figure 16). No aromatic or alkane peaks were present in the third sample as seen
in Figure 17. With the incorporation of a second drying cycle, the abundance of aromatics in the TIC was reduced even further in two of the three replicates, and again, no aromatic or alkane peaks were present in the third sample. Tide Ultra sufficiently removed the SAM to a point beyond identification of an ignitable liquid; therefore, Tide Ultra was used in the next phase of the experiment.

*Persil Liquid* – The cotton t-shirt material, spiked with 100 µL SAM and washed with the maximum amount of Persil Liquid, showed aromatic and alkane peaks consistent with ignitable liquids. Aromatic peaks including C_2 and C_3-alkylbenzenes were present in two out of three replicates when a single drying cycle was performed (Figure 18). When two drying cycles were performed, one replicate showed C_2-alkylbenzenes only and two showed C_2 and C_3-alkylbenzenes. For all cases, the presence of these aromatic peaks was too weak to support an identification. Alkanes peaks were present in the TIC but were not in a pattern consistent with an ignitable liquid. The abundance of these alkanes was greatly reduced by the addition of a second drying cycle. Persil Liquid was sufficient to remove the SAM to a point beyond identification of an ignitable liquid; therefore, Persil Liquid was used in the next phase of the experiment.

*Persil Pods* – The cotton t-shirt material spiked with 100 µL SAM and washed with the maximum amount of Persil Pods followed by one drying cycle, resulted in peaks in an abundance and pattern consistent with an ignitable liquid in two of the three replicates. A light to medium aromatic product was identified because aromatic peaks, specifically C_1-, C_2- and C_3-alkylbenzenes, were present in high abundance, but in a narrower boiling point range than seen in gasoline (Figure 19). Additionally, the other gasoline components such as alkanes, PNAs and
indanes were absent in these samples, resulting in the aromatic product classification. With the addition of a second drying cycle, the abundance of the aromatic peaks in the TIC was generally reduced, but an aromatic product was still identifiable in two of the three replicates. Even though the third sample had no identifiable ignitable liquid patterns, Persil Pods were deemed to be ineffective at thoroughly and consistently removing SAM to a point beyond identification of an ignitable liquid; therefore, Persil Pods were not used in Phase Three of the experiment.

**Gross Amount of SAM: 10 mL**

*Tide Ultra* – The cotton t-shirt material, spiked with 10 mL SAM and washed with the maximum amount of Tide Ultra, resulted in peaks in an abundance and pattern consistent with ignitable liquids. For the samples processed with one drying cycle, alkanes were present in a Gaussian distribution consistent with an HPD in two of the three replicates (Figure 20). The HPD identification was further supported by the presence and appropriate abundance of pristane, phytane, and lower branched alkanes present in the characteristic patterns. In the third sample, the n-alkanes in the TIC were not sufficiently abundant or in a clear Gaussian distribution (Figure 21). Performance was not improved by the addition of a second drying cycle where all replicates resulted in positive HPD identifications. Tide Ultra was not sufficient to remove a gross volume of SAM to a point beyond identification of an ignitable liquid; therefore, no further testing of Tide Ultra was conducted with gross volumes of SAM.

*Persil Liquid* – Ignitable liquids were identified in all samples at this spike volume, regardless of the number of drying cycles. For each set of triplicate samples, gasoline and an HPD were identified in two of the three samples. Clear patterns of broad aromatics present in the
characteristic patterns and separate heavy range n-alkanes in a Gaussian distribution were visible in the TIC (Figure 22). The gasoline and HPD classifications were further supported by the presence of additional components in the EIPs as detailed in previous sections. An HPD was identified in the third replicate prepared with one drying cycle, and no aromatics were present in the TIC (Figure 23). This was not the case for the third replicate prepared with two drying cycles. An abundant broad aromatic pattern was clear in the TIC and had additional support for a gasoline identification in the EIPs, but not enough support was present for a separate HPD identification (Figure 24). Heavy alkanes were present in the TIC, but not in a clear Gaussian distribution and the spectra were not sufficient to confirm the presence of pristane or phytane. Persil Liquid was not effective at removing gross volumes of SAM to a point beyond identification of an ignitable liquid; therefore, no further testing of Persil Liquid with gross spike volumes was conducted.

**Persil Pods** – All samples were prepared at the same time and were extracted and analyzed at a later date. Although Persil Pods were not effective at removing the trace SAM volume, samples were still generated with the gross volume. The cotton t-shirt material, spiked with 10 mL SAM and washed with the maximum amount of Persil Pods, resulted in peaks in an abundance and pattern consistent with ignitable liquids with the incorporation of a single drying cycle. Aromatics, specifically C\textsubscript{1}-, C\textsubscript{2}-, and C\textsubscript{3}-alkylbenzenes, were present in high abundance in two out of three of these replicates, with additional support for gasoline in these same replicates visible in the appropriate EIPs. One of these also had a separate Gaussian distribution of n-alkanes with enough support to identify a separate HPD pattern (Figure 25). The replicate that only contained indicators of gasoline can be seen in Figure 26. The remaining replicate had no
indicators of gasoline, but a Gaussian distribution of n-alkanes consistent with an HPD (Figure 27). With the addition of a second drying cycle, a Gaussian distribution of n-alkanes was visible in two out of three replicates with a severely reduced abundance compared to the results of the single drying cycle. One had sufficient support for an HPD identification, but in the other one of these replicates the Gaussian distribution was too weak to be distinguished from the baseline, and no further support for an ignitable liquid was present (Figure 28). In the third replicate, no support for an HPD was present, but C₁-, C₂-, and C₃-alkylbenzenes were present in high abundance, with additional support in the EIPs to substantiate a gasoline identification. Persil Pods were not sufficient to remove the SAM to a point beyond identification of an ignitable liquid; therefore, Persil Pods were not used in the next phase of the experiment.

Phase Three – Persistence of SAM on Fire Scene Clothing

The results are shown in Tables 2 and 3, and the detailed results of each sample group are discussed below. Only 100 µL SAM was used in this phase and only one dry cycle was performed.

Small Load Size

Tide Ultra – The 100% cotton fire scene pants washed with the maximum amount of Tide Ultra resulted in no peaks in an abundance or pattern consistent with ignitable liquids. No gasoline, HPD, or aromatic product could be identified. (Figure 29).

The 90:10 cotton:polyester ATF-issued shirt washed with the maximum amount of Tide Ultra resulted in few peaks in a pattern consistent with ignitable liquids. C₁, C₂, and C₃-
alkylbenzenes were present in their characteristic ignitable liquid patterns in all three replicates; however, these peaks were ultimately too weak to substantiate an ignitable liquid identification (Figure 30). Also present in these samples were some weak spiking n-alkanes, which were only visible in the EIP, not the TIC. No identifications of ignitable liquids could be made.

**Persil Liquid** – The 100% cotton fire scene pants washed with the maximum amount of Persil Liquid resulted in no visible ignitable liquid patterns in the TICs. In two of the three replicates, C_1_, C_2_, and C_3_-alkylbenzenes were present in very low abundance but were only seen the in EIP. In all three replicates some n-alkanes were present, but not in significant abundance or a characteristic pattern. (Figure 31).

The 90:10 cotton:polyester ATF-issued shirt washed with the maximum amount of Persil Liquid resulted in no peaks consistent with ignitable liquids. There were no diagnostic patterns of aromatics or alkanes in any of the three replicates (Figure 32).

**Moderate Load Size**

**Tide Ultra** – The 100% cotton fire scene pants, spiked with 100 µL SAM and washed with the maximum amount of Tide Ultra, resulted in no peaks in an abundance or pattern consistent with ignitable liquids. No gasoline, HPD, or aromatic product could be identified. Tide Ultra was sufficient to remove the SAM to a point beyond identification of an ignitable liquid. (Figure 33).

The 90:10 cotton:polyester ATF-issued shirt, spiked with 100 µL SAM and washed with the maximum amount of Tide Ultra, resulted in no peaks in the TIC in an abundance or pattern consistent with ignitable liquids. Only very weak C_1_, C_2_ and C_3_-alkylbenzenes were visible in the
EIP of each replicate. No gasoline, HPD, or aromatic product could be identified. Tide Ultra was sufficient to remove the SAM to a point beyond identification of an ignitable liquid. (Figure 34).

*Persil Liquid* – The 100% cotton fire scene pants spiked with 100 µL SAM and washed with the maximum amount of Persil Liquid, resulted in no ignitable liquid being identified. No peaks in a pattern or abundance consistent with gasoline, HPD, or an aromatic product were present. Persil Liquid was sufficient to remove the SAM to a point beyond the identification of an ignitable liquid. (Figure 35).

The 90:10 cotton:polyester ATF-issued gray shirt, spiked with 100 µL SAM and washed with the maximum amount of Persil Liquid, resulted in no peaks in an abundance or pattern consistent with ignitable liquids in the TICs. No gasoline, heavy petroleum distillate, or aromatic product could be identified; however very weak C₁, C₂, and C₃-alkylbenzenes were present in the EIP only in two of the replicates (Figure 36). Persil Liquid was sufficient to remove the SAM to a point beyond identification of an ignitable liquid.
Conclusion

As demonstrated in this study, the manufacturer-recommended maximum amount, as designated on the provided measuring cup/container lid, of Tide Ultra and Persil Liquid were each effective at removing trace levels of SAM such that no ignitable liquids could be identified on ATF-issued fire scene clothing when laundered under rigorous washing and drying conditions. This research allows the Bureau of Alcohol, Tobacco, Firearms, and Explosives to establish a protocol for its CFIs on how to decontaminate their scene clothing from trace amounts of ignitable liquids if they choose to launder their scene clothing themselves. It must be noted that these liquid detergents did not perform satisfactorily on 100% cotton white t-shirt material at gross spike volumes, where gasoline and/or HPDs were identifiable after laundering.

All three detergents showed some evidence of performance variability, with results inconsistent across the three replicates. This was especially evident in the results of testing with Persil Pods. This pod detergent was not effective at the removal of ignitable liquids at trace or gross spike volumes, resulting in positive identifications of light to medium aromatic products, gasoline and/or HPDs. The variability seen in the results of the pod detergent may be attributed to the pod’s position in the washing machine. If the pod became trapped in the center of the load of laundry it may not have been fully exposed to the water necessary to break the pod down and release the detergent for an efficient wash. Laundry positioning of the spiked fabric may also have affected the trends seen in the replicates. If the spiked fabric remained outside the load of fabrics during the rotation of the washer and/or dryer it would be more exposed to the water and detergent, possibly resulting in the removal of more SAM or certain components of SAM. If the spiked fabric migrated into the center of the load of fabrics during the rotation of the washer
and/or dryer it could have been more protected from the water and detergent. The addition of a second drying cycle generally resulted in decreased abundances of compounds that supported an identification when only one drying cycle was performed. However, variation within these replicates may be due to laundry positioning of the spiked fabric, pod detergent, or both.

There are many avenues of further research that could be conducted to expand on any of the main aspects of this experiment. The effectiveness of less rigorous laundering conditions could be explored, as well as testing on different fiber types and blends that could be used in scene clothing by other fire investigators. Only one model of Frigidaire brand appliances was used in this experiment. The effectiveness of different models of washers and dryers in addition to the performance variation between brands could be tested. Additionally, there are numerous other detergents available to consumers, and more extensive research could be conducted looking at a larger selection of detergents. The ATF will be conducting research on the efficiency of multiple wash cycles using Tide Original liquid detergent as well as the efficiency of dry cleaning for the decontamination of fire scene clothing worn by ATF CFIs.
References

8. Evans M, Trimmer SE. An examination of decontamination procedures utilized by the Bureau of Alcohol, Tobacco, Firearms and Explosives. Fire&Arson Investigator 2017;10-15
# Tables & Figures

Table 1. Results for Phase Two.

<table>
<thead>
<tr>
<th>Detergent</th>
<th>100 µL</th>
<th>10 mL</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1 Dry</td>
<td>2 Dry</td>
</tr>
<tr>
<td>Tide Ultra</td>
<td>3- NEGATIVE</td>
<td>3- NEGATIVE</td>
</tr>
<tr>
<td>Persil Liquid</td>
<td>3- NEGATIVE</td>
<td>3- NEGATIVE</td>
</tr>
<tr>
<td>Persil Pods</td>
<td>2- AROMATIC 1- NEGATIVE</td>
<td>2- AROMATIC 1- NEGATIVE</td>
</tr>
</tbody>
</table>

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Table 2. Results for Phase Three, small load size.

<table>
<thead>
<tr>
<th>Detergent</th>
<th>Small Load Size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100% Cotton</td>
</tr>
<tr>
<td>Tide Ultra</td>
<td>3- NEGATIVE</td>
</tr>
<tr>
<td>Persil Liquid</td>
<td>3- NEGATIVE</td>
</tr>
</tbody>
</table>
Table 3. Results for Phase Three, moderate load size.

<table>
<thead>
<tr>
<th>Detergent</th>
<th>Moderate Load Size</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>100% Cotton</td>
</tr>
<tr>
<td>Tide Ultra</td>
<td>3- NEGATIVE</td>
</tr>
<tr>
<td>Persil Liquid</td>
<td>3- NEGATIVE</td>
</tr>
</tbody>
</table>
Figure 1. The total ion chromatogram of the E-1618 test mix in carbon disulfide used as a quality control standard.
Figure 2. The total ion chromatograph of standard accelerant mixture diluted in carbon disulfide. Standard accelerant mixture is equal parts automotive gasoline and diesel fuel.
Figure 3. The total ion chromatograph of automotive gasoline diluted in carbon disulfide.
Figure 4. The total ion chromatograph of diesel fuel diluted in carbon disulfide.
Figure 5. The total ion chromatogram of the first order of broadcloth substrate, unlaunched.
Figure 6. The total ion chromatogram of the second order of broadcloth substrate, unlaundred.
Figure 7. The total ion chromatogram of the 100% cotton t-shirt material substrate, unlaunched.
Figure 8. The total ion chromatogram of the 100% cotton ATF fire scene pants substrate, unlaunched.
Figure 9. The total ion chromatogram of the 90:10 cotton:polyester ATF shirt substrate, unlaundered.
Figure 10. The total ion chromatogram of Tide Ultra detergent on first order broadcloth, washed and dried.
Figure 11. The total ion chromatogram of Persil Liquid detergent on first order broadcloth, washed and dried.
Figure 12. The total ion chromatogram of Persil Pods detergent on first order broadcloth, washed and dried.
Figure 13. The total ion chromatograph showing the results of the second wash cycle of unspiked broadcloth with Tide Ultra following a load spiked with 10 mL SAM and washed with Tide Ultra.
Figure 14. The total ion chromatograph showing the results of the second wash cycle of unspiked broadcloth with Persil Liquid following a load spiked with 10 mL SAM and washed with Persil Liquid, as well as a wipe down of the washer.
Figure 15. The total ion chromatograph showing the results of the second wash cycle of unspiked broadcloth with Persil Pods following a load spiked with 10 mL SAM and washed with Persil Pods, as well as a wipe down of the washer.
Figure 16. A total ion chromatograph showing results consistent with two of three replicates for Phase Two, trace amount of SAM, washed with Tide Ultra. These samples were negative for ignitable liquids.
Figure 17. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, trace amount of SAM, washed with Tide Ultra. This sample was negative for ignitable liquids.
Figure 18. A total ion chromatograph showing results consistent with two of three replicates for Phase Two, trace amount of SAM, washed with Persil Liquid. These samples were negative for ignitable liquids.
Figure 19. A total ion chromatograph showing results consistent with two of three replicates for Phase Two, trace amount of SAM, washed with Persil Pods. These samples were positive for ignitable liquids.
Figure 20. A total ion chromatograph showing results consistent with two of three replicates for Phase Two, gross amount of SAM, washed with Tide Ultra. These samples were positive for HPD.
Figure 21. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Tide Ultra. This sample was negative for ignitable liquids.
Figure 22. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Liquid. This sample was positive for gasoline and HPD.
Figure 23. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Liquid. This sample was positive for gasoline and HPD.
Figure 24. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Liquid. This sample was positive for gasoline.
Figure 25. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Pods. This sample was positive for gasoline and HPD.
Figure 26. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Pods. This sample was positive for gasoline.
Figure 27. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Pods. This sample was positive for HPD.
Figure 28. A total ion chromatograph showing results consistent with one of three replicates for Phase Two, gross amount of SAM, washed with Persil Pods. This sample went through two drying cycles and is negative for ignitable liquids.
Figure 29. A total ion chromatograph showing results consistent with all replicates for the 100% cotton fire scene pants, Phase Three, small load, washed with Tide Ultra. These samples were negative for ignitable liquids.
Figure 30. A total ion chromatograph showing results consistent with all replicates for the cotton:polyester shirt, Phase Three, small load, washed with Tide Ultra. These samples were negative for ignitable liquids.
Figure 31. A total ion chromatograph showing results consistent with all replicates for the 100% cotton fire scene pants, Phase Three, small load, washed with Persil Liquid. These samples were negative for ignitable liquids.
Figure 32. A total ion chromatograph showing results consistent with all replicates for the cotton:polyester shirt, Phase Three, small load, washed with Persil Liquid. These samples were negative for ignitable liquids.
Figure 33. A total ion chromatograph showing results consistent with all replicates for the 100% cotton fire scene pants, Phase Three, moderate load, washed with Tide Ultra. These samples were negative for ignitable liquids.
Figure 34. A total ion chromatograph showing results consistent with all replicates for the cotton:polyester shirt, Phase Three, moderate load, washed with Tide Ultra. These samples were negative for ignitable liquids.
Figure 35. A total ion chromatograph showing results consistent with all replicates for the 100% cotton fire scene pants, Phase Three, moderate load, washed with Persil Liquid. These samples were negative for ignitable liquids.
Figure 36. A total ion chromatograph showing results consistent with all replicates for the cotton:polyester shirt, Phase Three, moderate load, washed with Persil Liquid. These samples were negative for ignitable liquids.
Vita

Rebecca Kaye Whitney was born on September 2, 1995 in Ellsworth, Maine. Ms. Whitney is a second year Master of Science Student in the FEPAC accredited Forensic Science program at Virginia Commonwealth University in Richmond, Virginia. Ms. Whitney furthered her education by participating in classes offered by the University of Maine at Machias in Machias, Maine, Husson University in Bangor, Maine, and the University of Maine flagship campus in Orono, Maine. Ms. Whitney earned her Bachelor of Science Degree in Chemistry from Elmira College in Elmira, New York, graduating Summa Cum Laude in June 2018. Ms. Whitney earned a place on the Dean’s List seven out of eight semesters during her time at Elmira College. Ms. Whitney was also inducted into the Elmira College chapters of the following honor societies: Phi Eta Sigma, Gamma Sigma Epsilon, and Omicron Delta Kappa.
Appendix 1

GC-MS Method for RWHITNEY_ATF.
Method Information for: C:\MSDCHEM\1\METHODS\RWHITNEY_ATF.M

Method Sections To Run:

( ) Save Copy of Method With Data
( ) Instrument Control Pre-Run Cmd/Macro =
( ) Data Analysis Pre-Run Cmd/Macro =
(X) Data Acquisition
( ) Data Analysis
( ) Instrument Control Post-Run Cmd/Macro =
( ) Data Analysis Post-Run Cmd/Macro =

Method Comments:
This is the default method

END OF METHOD CONTROL PARAMETERS

------------------------
INSTRUMENT CONTROL PARAMETERS: GC#3

C:\MSDCHEM1\METHODS\WHITNEY_ATF.M
Tue Jul 23 16:21:10 2019

Control Information
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Sample Inlet : GC
Injection Source : GC ALS
Mass Spectrometer : Enabled

No Sample Prep method has been assigned to this method.

6890 GC METHOD

OREN
Initial temp: 40 C (On)
Initial time: 2.00 min
Ramps:
  # Rate Final temp Final time
 1  5.00  120  0.00
 2 12.00  300  5.00
 3  0 (Off)
Post temp: 50 C
Post time: 0.00 min
Run time: 38.00 min

FRONT INLET (SPLIT/SPLITLESS)
Mode: Split
Initial temp: 250 C (On)
Pressure: 9.1 psi (On)
Split ratio: 20:1
Split flow: 23.9 mL/min
Total flow: 27.8 mL/min
Gas saver: On
Saver flow: 20.0 mL/min
Saver time: 2.00 min
Gas Type: Helium

COLUMNS

COLUMN 1
Capillary Column
Model Number: 122-0132
Description: DB-1ms
Max temperature: 325 C
Nominal length: 30.0 m
Nominal diameter: 250.00 um
Nominal film thickness: 0.25 um
Mode: constant flow
Initial flow: 1.2 mL/min
Nominal init pressure: 9.1 psi
Average velocity: 40 cm/sec
Inlet: Front Inlet
Outlet: MSD
Outlet pressure: vacuum

FRONT DETECTOR (FID)
Temperature: 250 C (Off)
Hydrogen flow: 40.0 mL/min (Off)
Air flow: 450.0 mL/min (Off)
Mode: Constant makeup flow
Makeup flow: 45.0 mL/min (Off)
Makeup Gas Type: Nitrogen
Flame: Off
Electrometer: Off
Lit offset: 2.0

SIGNAL 1
Save Data: Off

SIGNAL 2
Save Data: Off

BACK DETECTOR (NO DET)

COLUMNS

COLUMN 2
(not installed)

BACK INLET (SPLIT/SPLITLESS)
Mode: Split
Initial temp: 0 C (Off)
Pressure: 0.0 psi (Off)
Total flow: 45.0 mL/min
Gas saver: Off
Gas type: Helium
THERMAL AUX 2
  Use: MSD Transfer Line Heater
  Initial temp: 300 C (On)

AUX PRESSURE 3
  Gas Type: Helium
  Initial pressure: 0.0 psi (Off)

AUX PRESSURE 4
  Gas Type: Helium
  Initial pressure: 70.2 psi (Off)

AUX PRESSURE 5
  Gas Type: Helium
  Initial pressure: 0.0 psi (Off)

VALVES
  Valve 1 Switching Off

POST RUN
  Post Time: 0.00 min

INJECTOR 1
  Solvent Wash Mode: A, B-B2
  Waste Bottle Use: A Only
  Sample Volume (uL): 1.000
  Syringe Size (uL): 10.0
  Pre washes from bottle A: 0
  Pre washes from bottle B: 0
  Post washes from bottle A: 10
  Post washes from bottle B: 10
  Viscosity delay (seconds): 0
  Pre injection dwell (min): 0.00
  Post injection dwell (min): 0.00
  Sample skim depth (mm): 0.0 (Off)
  Plunger Speed: Variable
  Draw Speed (uL/min): 300
  Dispense Speed (uL/min): 3000
  Inject Speed (uL/min): 3000
  Solvent save: Off

TIME TABLE
  Time(min) Parameter & Setpoint

Column 1 Inventory Number:
Column 2 Inventory Number:

MS ACQUISITION PARAMETERS

General Information
-----------------
Tune File: atune.u
Acquisition Mode: Scan

MS Information
---------------
Solvent Delay: 2.00 min

EMV Mode: Gain Factor
Gain Factor: 1.00
Resulting EM Voltage: 1624

[Scan Parameters]

Low Mass: 33.0
High Mass: 300.0
Threshold: 50
Sample #: 3
A/D Samples: 8
Plot 2 low mass: 50.0
Plot 2 high mass: 550.0

[MS Zones]

MS Source: 230 C maximum 250 C
MS Quad: 150 C maximum 200 C

Timed Events
-----------

RWHITNEY_ATF.M Tue Jul 23 16:21:09 2019 Instrumentation Facility
### MS Acquisition Parameters

<table>
<thead>
<tr>
<th>Time (min)</th>
<th>State (MS On/Off)</th>
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</thead>
<tbody>
<tr>
<td>2.00</td>
<td>On</td>
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</table>

END OF MS ACQUISITION PARAMETERS

---

**TUNE PARAMETERS for SN: US30955326**

Trace Ion Detection is OFF.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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<tbody>
<tr>
<td>EMISSION</td>
<td>34.610</td>
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<tr>
<td>ENERGY</td>
<td>69.922</td>
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<td>REPELLEL</td>
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<td>IONFOCUS</td>
<td>83.514</td>
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<td>ENTRANCE_LE</td>
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<td>EMVOLTS</td>
<td>1670.588</td>
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<td>Actual EMV</td>
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<tr>
<td>GAIN FACTOR</td>
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<td>AMUGAIN</td>
<td>2176.000</td>
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<tr>
<td>AMOFFSET</td>
<td>133.000</td>
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<tr>
<td>FILAMENT</td>
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<td>DCPOLARITY</td>
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<td>ENTLSENSOFFS</td>
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<tr>
<td>MASSGAIN</td>
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<tr>
<td>MASSOFFSET</td>
<td>-8.000</td>
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</table>

END OF TUNE PARAMETERS

---

END OF INSTRUMENT CONTROL PARAMETERS
DATA ANALYSIS PARAMETERS

Method Name: C:\MSDCHEM\l\METHODS\RWHITNEY_ATF.M

Percent Report Settings
-----------------------
Sort By: Signal
Output Destination
    Screen: Yes
    Printer: No
    File: No
Integration Events: AutoIntegrate
Generate Report During Run Method: Yes
Signal Correlation Window: 0.020

Qualitative Report Settings
---------------------------
Peak Location of Unknown: Apex
Library to Search Minimum Quality
C:\Database\NIST14.L 0
Integration Events: AutoIntegrate
Report Type: Summary
Output Destination
    Screen: Yes
    Printer: No
    File: No
Generate Report During Run Method: Yes

Quantitative Report Settings
-----------------------------
Report Type: Summary
Output Destination
    Screen: Yes
    Printer: No
    File: No
Generate Report During Run Method: Yes

Calibration Last Updated:
Reference Window: 10.00 Percent
Non-Reference Window: 5.00 Percent
Correlation Window: 0.02 minutes
Default Multiplier: 1.00
Default Sample Concentration: 0.00

Compound Information

*** Empty Quantitation Database ***

END OF DATA ANALYSIS PARAMETERS

Tue Jul 23 16:21:11 2019