Determination of the Influence of Polyurethane Lining on Potable Water Quality

by

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ABSTRACT

The corrosion of the drinking water distribution system is a serious problem in the United States. The annual cost to repair damages related to corrosion for public utilities in the United States are estimated at $22 billion. Polyurethane can be used as an in situ pipe liner which reduces the overall cost to rehabilitate water mains. Polyurethane is gaining popularity as a drinking water pipe liner. Not much is known about the effects of polyurethane to reline potable pipes. Polyurethane has only recently begun to be approved by the U.S. Environmental Protection Agency for use in drinking water piping, although it has been used in the United Kingdom since 1999.

The American National Standards Institute/National Sanitation Foundation 61 Drinking Water System Components – Health Effects (ANSI/NSF 61) for pipe and pipe liners was used to investigate changes in water quality in contact with polyurethane lining material. In addition, the exposure time was extended to 30 days and odor analysis was performed. Polyurethane coupons were placed in headspace free borosilicate glass vessels with a surface area to volume ratio of 0.39. The water was pH 8 and comprised of salts: $MgSO_4$, $NaHCO_3$, $CaSO_4$, $CaC1_2$, Na_2SiO_3 and KNO_3 in a ratio typical of standard drinking water. Three types of disinfectant were used: no disinfectant, chlorine and monochloramine. The water was removed, sampled and replaced on days 1, 2, 4, 9, 11, 14, 15, 19, 21 and 30. The sample water was tested for pH, temperature, total organic carbon concentration (TOC), disinfectant residual, ammonia concentration as $N\text{-}NH_3$, hardness as combined Ca and Mg concentrations, alkalinity and temperature on days when the sample water was

changed. Total solids (TS), odor, trihalomethanes (THMs), haloacetic acids (HAAs), and semivolatile organic carbons (SVOCs) were tested on days 1, 4, 9, and 14.

The polyurethane lining had major impacts on pH, odor and haloacetic acids throughout the 30 day experiment. A 2-3 pH unit decrease to pH 6 was constant for all conditions tested. Odor panelists described the odor for both chlorinated and monochloraminated waters as "chlorinous" and either pleasant as "sweet chemical" or putrid as "locker room". Haloacetic acids were formed and increased in concentration (by approximately 30 μg/L, which is half the US EPA regulated value of 60 μg/L). Trihalomethane formation was not seen. Total organic carbon leached from the polyurethane liners reached 0.65 mg/L above background on day 1 but by day 15 was only >0.1 mg/L above background. Chlorine and monochloramine were consumed by the polyurethane and increased exposure time leads to decreased disinfectant residual.

It is important for water utilities to know how a lining material will affect the water quality. It has been shown that other polymeric lining materials have impacted the disinfection by-products as well as producing odor. Water treatment facilities are responsible for the water quality throughout the infrastructure and with Environmental Protection Agency regulations becoming stricter they cannot afford to not know the impact of polymeric lining materials in their system.

ACKNOWLEDGEMENTS

I would like to begin my acknowledgements by thanking the Civil and Environmental Department at Virginia Tech for welcoming me making it my home for the past three years. I will miss you all. I would also like to thank my advisor Andrea M. Dietrich for giving me an opportunity to work on such an expansive project. I would also like to thank my committee members; Dr. John C. Little (for a bit!), Dr. Marc Edwards and Dr. Lindsey Marr for their insightful guidance and flexibility. I couldn't have completed this work without the help of Jody Smiley and Julie Petruska for their patience and advice. Tom Wertalik for his helpful advice on the apparatuses and thrifty suggestions. Betty Wingate and Beth Lucas for their friendly smiles and solutions to any administrative problems.

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My family for always supporting me through these past years. Your love and advice allowed me to accomplish my goals and pushed me to go even further. Brian Huddle for your wonderful presence in my life and all that you do for me.

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This thesis is presented in the Virginia Tech manuscript format. The first chapter is a review of the literature related to the chemistry of polyurethane and related polymers. The second chapter is a report formatted for the American Water Works Association Research Foundation (AwwaRF) which explains the experimental findings for the effects of polyurethane coatings on the water chemistry of potable water. The disinfectant (no disinfectant, chlorine and monochloramine) used was varied while measuring pH, temperature, alkalinity, disinfectant residual, ammonia, elemental analysis, total solids, total organic carbon, trihalomethanes, odor analysis, haloacetic acids and semi volatile organic compounds were measured over the course of 30 days. An additional project was performed where the data and the calculations are presented in Appendix A. Henry's constant was measured for geosmin varying time, fulvic acid and temperature.

1. CHAPTER I

1.1 LITERATURE REVIEW

1.1.1 IN SITU LINING OF DRINKING WATER PIPE

The corrosion of the drinking water distribution system is a serious problem worldwide. The annual cost to repair damages related to corrosion for public utilities in the United States are estimated at $22 billion (Brongers, 2002). One solution would be to reline leaking pipes through *in situ* relining. For polyurethane this involves surface preparation through abrasive blast cleaning then applying the polyurethane coating to coat and seal the interior of the pipe (USA Corp of Engineers, 2001). Epoxy lining is the most common polymer lining material used to coat *in situ* piping especially the relining of copper piping (Heim, 2007). Epoxy was first used as a coating for pipes 40 years ago to prevent corrosion in Japanese industrial factories. Epoxy lining is used in a variety of applications such as shipboard pipe remediation by the navy (USA Corp of Engineers, 2001).

Polyurethane (100% solids) is gaining popularity as a potable water pipe lining material due to its low application costs (faster application and lower labor costs) and lack of solvents (Guan, 2001). Solvent based epoxies were a common lining material; however, due to VOC pollution as a result of the solvents used epoxy was no longer a solution (Guan, 2001). The leaching of the endocrine disruptor, bisphenol A, from epoxy lining materials to water is an example of the health effects of this material (Yeo and Kang, 2006). By using solventless materials or 100% solid polyurethanes these health effects can be reduced (Guan, 2001). For the last 17 years polyurethane (100% solids) has been developed for optimum properties when in contact with drinking water (Guan, 2001). Polyurethane (100% solids) is smoother and more abrasive resistant than cement mortar. Therefore, the pipe will have increased efficiency and lower operational costs associated with the pipe (Guan, 2001). Polyurethane has also been shown to keep metal piping from further corrosion while maintaining resistance to chemicals, degradation, and impact (Guan, 2001).

Lining materials for potable water must be certified under protocol American National Standards Institute/National Sanitation Foundation 61 Drinking Water System Components – Health Effects (ANSI/NSF 61) for use as a lining material and United States Food and Drug Administration (USFDA) 21 177.1680 for contact with consumable goods. Polyurethane is used in Australia, Great Britain and Canada; however, it has not made a significant transition to the United States. Not much is known about the use of polyurethane in the application of relining potable pipes.

1.1.2 FORMATION CHEMISTRY FOR POLYURETHANES AND RELATED POLYMERS

1.1.2.1 History of Polyurethane

Polyurethane was first developed at the beginning of World War II but not used in commercial applications until the early 1950s. One of the first urethane polymers was developed by Otto Bayer (Figure 1-1) (Frisch and Reegen, 1973). The reaction involves 1-5 naphthalene diisocyanate and poly(ethylene adipate) with 1,4 butane diol acting as a chain extender, to produce the polyurethane. The extender allows a chain to form beyond the copolymer product shown in the reaction below (Figure 1-1). The polyurethane segment shown was not used commercially and thus does not have a specified use (Figure 1-1). Bayer and his team noticed the particular nature of polyurethane and its lightweight fibrous nature. The group found that with subtle alterations polyurethanes could be used in airplane and nautical construction, thermal insulation, toys, artificial limbs and shoe soles. Polyurethane has been used in foams (polyurethane foam) as an insulator and can be recycled to be used as carpet underlay (Frisch and Reegen, 1978). Polyurethane has also been used as fabric (Suen *et al.*, 2008), adhesives (Dilik *et al.*, 2007), chairs, "synthetic wood," and as a replacement for aluminum castings (Frisch and Reegen, 1973).

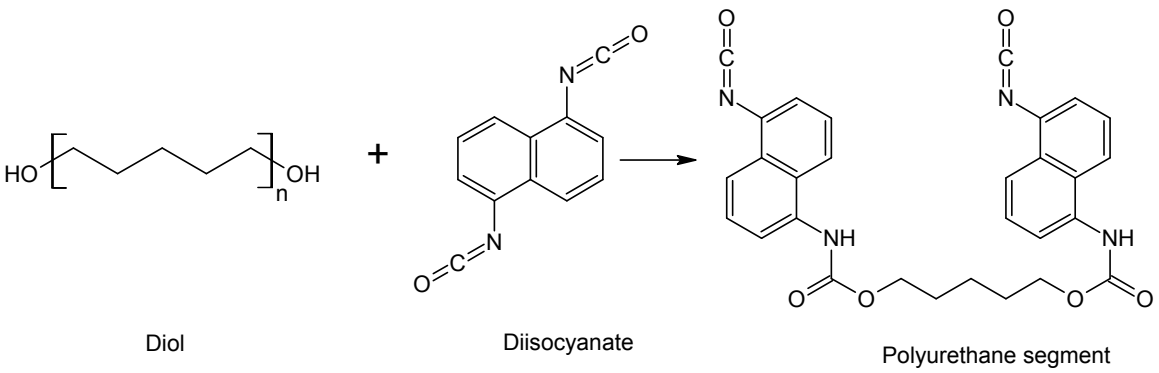

Figure 1-1. First recorded reaction for polyurethane (Frisch and Reegen, 1973).

1.1.2.2 Basic Chemistry of Polyurethane

Polyurethanes, like most polymers, are used in conjunction with anti-plasticizers (which harden the polymer) and plasticizers (which make the polymer more moldable). These compounds can heavily influence the characteristics of the polymer. However, they will not be discussed greatly within this literature review due to their abundance and numerous characteristics. In the water industry, the addition of antioxidants to a polymer to resist oxidation from disinfectants is commonly used (Frisch and Reegen, 1973). The chemical resistance or the leaching of these compounds could be detected when analyzing the polymer's interaction with an aqueous solution.

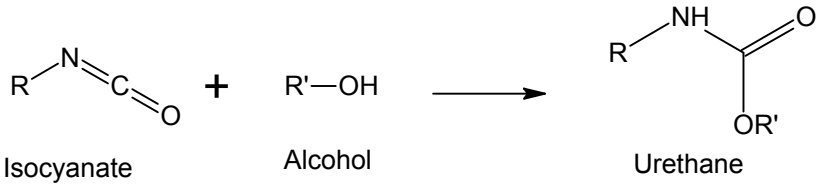

Figure 1-2. General reaction for a urethane linkage (Oertel and Abele, 1985).

Polyurethanes are typically formed using an isocyanate (-N=C=O) and any compound with an acidic hydrogen (Figure 1-2). The term urethane was originally given to the compound ethyl carbamate but then was extended to the whole class of compounds (Oertel and Abele, 1985). Polyurethanes can be formed without the use of isocyanates; however, isocyanates are the most common reagent due to the simplicity of the reaction. The reaction shown is a primary isocyanate and a primary alcohol forming a urethane linkage rather than a true *poly*urethane (Figure 1-2). In order to form chains or chain

branching two or more functional groups for both alcohol and isocyanate ligands would be needed.

Polyurethanes can have several properties due to the variety of the reactants that can be used to form them. Polyurethanes can both be flexible (e.g. polyurethane foam) as well as rigid (used in structural materials as previously described). The polymeric characteristics can also be altered using different R group combinations (refer to Figure 1-2). If either of the R groups are a long carbon-hydrogen chain then the polymer will have van der Waals forces interacting between the chains and therefore be more amorphous. Amorphous regions or "soft segments" are not rigid and have chain movement at lower temperatures. The temperature at which the polymer begins to "flow" is referred to as the glass transition temperature, T_g (Oertel and Abele, 1985).

"Hard segments" can be incorporated into the polymer by choosing R groups that have stronger interactions between the chains. This can be accomplished with several techniques. Chains that have charges associated with atoms in the chain can form polyelectrolytes and ionomers. Polyelectrolytes contain several ionic centered atoms that are evenly distributed throughout the chain. Ionomers contain ionic centers as well but are characterized by long nonpolar regions separating them (Kebir *et al.*, 2007). Both of these polymers have ionic interactions between the chains and have coulumbic forces associated with them. Coulumbic forces are much stronger than van der Waals forces forming stronger interactions and "hard" segments. The ionic centers and long C-H chains form both "hard" and "soft" regions, respectively, within the polymer. Their structure can be thought of as a rigid structure surrounded by mobile flowing chains, similar to a skeleton surrounded by soft tissue. The morphology just described can be varied based on the ratios and amounts of "hard" and "soft" segments (Oertel and Abele, 1985).

Hydrogen bonding can also be used to strengthen the interactions between the chains of the polyurethane (Ding *et al.*, 2008). This is normally accomplished using several functional groups or short side chains. Any electron rich oxygen, nitrogen and less

commonly fluorine can be on the chain and interact with hydrogens to strengthen the "bond" between the chains (Oertel and Abele, 1985).

All of the above interactions consist of linear chains with no cross-linking. The general reaction given for urethane illustrated a monoisocyanate and monoalcohol (Figure 1-2). If a compound has at least 3 reactive functional groups (tri-) and is paired with a compound with at least 2 functional groups (di-) then cross-linking will occur. Cross-linking is an important aspect of polymers because it can often be, but not always, linked to the rigidity of the polymer. The cross-linking often restricts the movement of the polymer increasing the T_g and decreasing its amorphous characteristics. The length of the chains and hence the amount of amorphous characteristics of the polymer can alter the rigidity of the structure which makes a cross-linked polymer more amorphous. Therefore, cross-linking does not always lead to increased rigidity (Dolmaire *et al.*, 2006). It is also important to note that if there are other acidic hydrogens on the polymer, not just an alcohol group, the polymer can further react to form a more extensive lattice structure. The reactivity decreases as the cross-linking increases due to the steric hindrance as the chain branching forms. The steric hindrance restricts chain movement and lowers the probability that the remaining functional groups will interact with each other (Shafee and Naguib, 2003).

1.1.2.3 Differences in Chemistry of Polyurea and Polyurethane Foam

Polyurethane is a general term that is often given to polyurethane, polyureas (Figure 1-3) or a combination of the two polymers with "sections" or domains containing either (Figure 1-4) (Oertel and Abele, 1985). The reactions to form polyurethane and polyureas are very similar; polyureas form through a reaction with an amine rather than an alcohol. Thus the chemistry of the two polymers can be vastly different as a result. Unlike the polyurethanes, polyureas have an additional acidic hydrogen from the amine group and can react further with an isocyanate. The reaction below is a single urea segment were the R groups can contain additional segments forming a polyurea (Oertel and Abele, 1985).

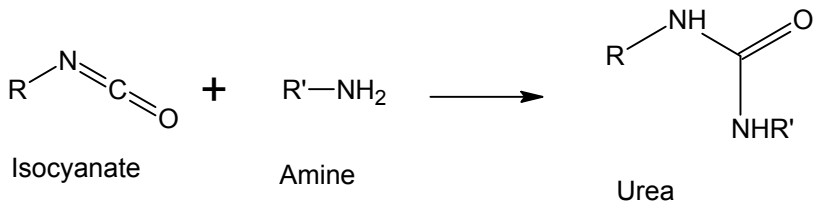

Figure 1-3. Basic polyurea reaction (Oertel and Abele, 1985).

Polyurethane foam is formed similarly to polyurethane but with the addition of water and typically carbamic acid is used to react with an isocyanate (Figure 1-5) (Oertel and Abele, 1985). All of the previously discussed chemistry can be applied to polyurethane foam as well. However, there is an important product formed in this reaction. Carbon dioxide, which is formed during the reaction, conglomerates to form "pockets" of empty space in polyurethane to give a very large surface area to volume ratio. This increase in surface area to volume ratio enables a greater chemical interaction between polyurethane and whatever comes into contact with it. The increase in interaction exaggerates the absorptive properties of polyurethane. This is studied heavily as a means of removing contaminants from food (Lemos *et al.*, 2007b, Meligi, 2008, Zoran *et al.*, 2007), water (Farag *et al.*, 2007, Kuz'mina *et al.*, 2008, Kocincova *et al.*, 2007, T. V. Nguyen, 2006) and air (Lemos *et al.*, 2007b, Oertel and Abele, 1985). Polyurethane foam can have moldable and flexible characteristics as well as a rigid structure (Dolmaire *et al.*, 2006) giving a wide range of uses and forms.

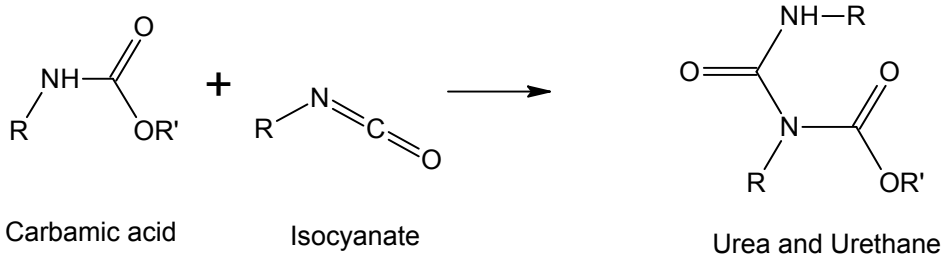

Figure 1-4. A polymer with polyurethane and polyurea domains (Oertel and Abele, 1985).

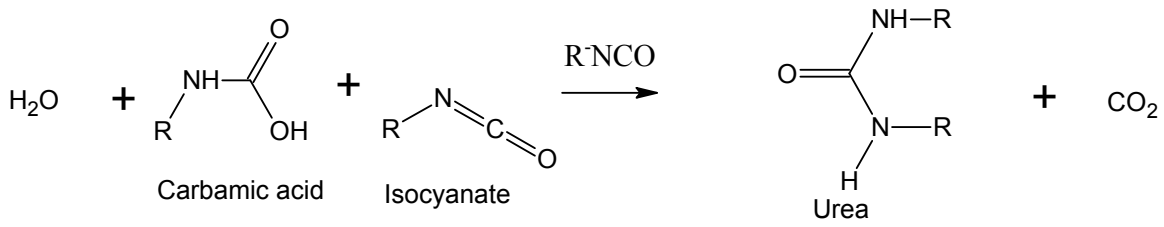

Figure 1-5. Basic Polyurethane foam reaction (Oertel and Abele, 1985).

1.1.2.4 Health Concerns of Isocyanate

Isocyanates are very toxic and can lead to respiratory illnesses and skin irritation which has led the Environmental Protection Agency (EPA) to fund several initiatives to better understand health concerns as well as methods of prevention (EPA, 1997). Polyurethane is extremely common in several mass produced goods and is also heavily regulated by the U.S. Department of Labor under Occupational Safety & Health Administration (OSHA) (OSHA, 2006). Elastic, paint, foam-blowing, foam mattresses and under-carpet padding are just a few examples of materials with varying forms of polyurethane. All require isocyanates in their production therefore it is very common for isocyanates to be present in these factories. Isocyanates have been shown to be carcinogenic in animals and a possible human carcinogen, as well as a skin, throat, eye and lung irritant. OSHA Section 5(a)(1) regards isocyanates as a hazard and requires employers to provide "a place of employment which are free from recognized hazards that are likely…to cause death or serious physical harm to his employees".

Concerns of unreacted isocyanates leaching from polyurethane as it degrades can be avoided by forcing the polyurethane reaction to go to completion. Therefore there are no unreacted isocyanates present to leach out of the polyurethane. It is also possible to use another reactant, other than an isocyanate, with fewer health concerns. These techniques are most popular in the biomedical field where polyurethane is being investigated as a material in organ and joint replacement. The biomedical studies are concerned primarily with blood clots forming around the implant. The degradation of polyurethane can potentially form amides that are very toxic (Spaans *et al.*, 1998).

Though isocyanates are dangerous to work with and should be handled with extreme caution, they are more hazardous in the air or in small particulates than through ingestion. OSHA only discusses the inhalation hazards of isocyanates and not through ingestion. Once isocyanates react to form polyurethane, a large network of the polymer is formed and is therefore not as hazardous. If there was some isocyanate within the polymer that then migrated to an aqueous solution there are no health warnings to suggest that it would have the same health effects given by OSHA. In fact polyurethane has even been used in car air filters with no reported health effects (Oertel and Abele, 1985).

1.1.2.5 Biomedical Applications of Polyurethane

Polyurethane has been found to be an excellent material to use for joint replacement as well as regeneration of biomaterials in the human body (Spaans *et al.*, 1998). When the polyurethane is carefully synthesized and fully reacted it can be used in the body without harmful reactants, such as isocyanates leaching from the polyurethane. The diversity of chemistry allows polyurethane to be used in applications ranging from an artificial knee cap to a biomaterial for tissue scaffolding.

Spaans et al. discovered a new approach to synthesize polyurethane through a reaction of ε-caprolactone and 1,4-butanediisocyanate with hard segments, giving it enough mechanical strength to serve as joint replacement (Spaans *et al.*, 1998). The polyurethane is also produced as a foam to act as a scaffolding for biological material to grow. Degradation of the polyurethane was analyzed to determine the products formed as well as its interactions in an aqueous solution. Ester linkages in the polyurethane are generally thought to be more susceptible to hydrolytic scission than urethane linkages (Spaans *et al.*, 1998). Spaans et al. found carboxylic end groups were also shown to hydrolyze the ester linkages. However, by the calculation of reaction mechanism rates, the urethane linkages react through hydrolysis as well and therefore degrade more quickly than previously reported. Soft segments were confirmed to be the main source of degradation as is typically predicted in polymer chemistry. The degradation of polyurethane could be analyzed to determine its degradation in an aqueous solution using the same techniques.

Mooney, D. J. et al. synthesized a polyurethane porous sponge using poly(lactic-co-glycolic acid) without using organic solvents (Mooney *et al.*, 1996). The synthesis of polyurethane is readily performed in an organic solvent. Organic solvents are toxic to cells and decrease factors needed to grow tissue. Thus it is vital to form a porous polyurethane to be used as a biomaterial scaffolding without the use of organic solvents. The porous structure was synthesized using a gaseous technique with a pore diameter of up to 100 μm (Mooney *et al.*, 1996). It was hypothesized that by increasing the crystalline material used to form the polyurethane a larger structure could be produced. The new chemistry involved in the synthesis would increase the possibilities in the chemistry of polyurethanes.

Kébir, N. et al. developed antibacterial ionic polyurethanes from the reaction of cis-1,4-polyisoprene cationomers with ammonium groups and isophorone diisocyanate (Kebir *et al.*, 2007). In joint replacement resulting infections are resistant to antibiotics and can lead to the removal of the implant. Many techniques can be used to reduce the likelihood of bacteria spreading on the implant such as decreasing surface friction to reduce bacteria adhesion and decrease the affinity of bacteria to the polyurethane to decrease sorption of bacteria into the polymer. *Pseudomonas aeruginosa* in an aqueous solution was used to determine the disinfectant capabilities of the polyurethane (Kebir *et al.*, 2007). It was theorized that the weak cross-linking density released bactericidal moieties formed from ammonium, hydroxide and carboxylic acids functionalities. The stability of the polyurethane in water was determined by the amount of water sorbed after a 2 week immersion. The surface chemistry was varied using different telechelic oligomer reagents and characterized by surface polarity, surface charges, density and hard and soft segments. Scanning electronic microscopy (SEM), atomic force microscopy (AFM), Fourier transform infrared spectroscopy (FTIR) and dynamic mechanical thermal analysis (DMA) were performed to determine these characteristics. Kébir et al. (2007) illustrated the flexibility in the surface chemistry by small alterations in the reactants used. The surface could be made hydrophilic or hydrophobic as well as alter the thermal properties of the polyurethane.

1.1.2.6 Food Industry and Air Quality Applications of Polyurethane

Polyurethane foam has a large surface area to volume ratio which is associated with increased ability to sorb compounds into the polymer. By varying the surface chemistry the foam can target specific compounds with a high affinity to sorb into the polyurethane foam. The large sorption potential of metals into polyurethane foam has led to the sorption of metals and then removal to determine the concentration of metals in liquid and solid foods as well as air quality (Lee and Lee, 2008, Lemos *et al.*, 2007b, Lemos *et al.*, 2007a, Farag *et al.*, 2007).

Lemos et al. summarized the use of polyurethane foam as a means to extract compounds from solution for analysis of the concentration in liquids and gases (Lemos *et al.*, 2007b).

1.1.2.7 Drinking Water Industry and Possible Impacts from Polyurethane

Epoxy lining material was the first polymer lining material to be used commonly (Warren, 2000). However, the discovery of bisphenol A and TOC leaching from the epoxy into the drinking water forced utilities to look for an alternative (Warren, 2000). In 1999, polyurethane was used for its fast cure time and thus the reduction of non-operational time (Warren, 2000). Polyurethane is just recently having the research performed in other fields applied to problems associated with drinking water (Farag *et al.*, 2007, T. V. Nguyen, 2006).

Nguyen, T.V. et al. analyzed techniques to remove arsenic from drinking water. An iron coated polyurethane foam was used to successfully extract arsenic from drinking water (T. V. Nguyen, 2006).

Farag et al. (2007) used polyurethane foams to separate gold (I and III) from silver and other base metals by investigating the sorption properties of such metals to the polyurethane foam. Ion exchange polyurethane foams (IEPUFs), commercial unloaded polyurethane foams (PUFs) and first order reaction rates were used to characterize the

sorption rate of the gold ions. Gold ions were removed from polyurethane columns using 1.0 M perchloric acid. The IEPUFs were more effective at sorbing the gold ions from the ionized water. 95% separation of gold from other base metals (Ag, Fe, Ni, Cu and Zn) from wastewater was achieved. Farag et al. illustrate the extent to which polyurethane surface chemistry can be altered to remove specific metals in aqueous solutions.

2. CHAPTER II

2.1 POLYURETHANE LINING AND ITS INFLUENCE ON WATER QUALITY

2.1.1 ABSTRACT

Polyurethane is gaining popularity over epoxy as a drinking water pipe liner in lieu of costly repairs to old or damaged pipe. Due to the leaching of the endocrine disruptor, bisphenol A, from epoxy lining materials and high application costs, polyurethane has become the practical solution. Polyurethane has been used in other countries (such as Canada) and has recently been approved by the US EPA for use in drinking water piping. The methodology in this study was expanded and based on "American National Standards Institute/National Sanitation Foundation 61 Drinking Water System Components – Health Effects" (ANSI/NSF 61) for pipe and pipe liners were used. The exposure time was extended from 19 to 30 days and odor analysis was performed. The short term impacts of polyurethane lining on drinking water quality and aesthetics were measured by assessing changes in pH, nitrogen-ammonia, alkalinity, total organic carbon (TOC), disinfectant residual (chlorine and monochloramine), hardness (as calcium and magnesium), total solids, odor, trihalomethanes (THMs), haloacetic acids (HAAs), semi-volatile organic compounds (SVOCs) and elemental analysis were measured. Polyurethane coupons were placed in contact with a standard water in a head-space free glass apparatus. Water was extracted and water quality parameters measured on testing days; the water was replaced with fresh water on testing days. The polyurethane lining had a significant impact on pH, odor and haloacetic acids throughout the 30 day experiment. A 2-3 pH unit decrease to pH 6 was constant for all conditions tested. Odor panelists described the odor for both chlorinated and monochloraminated waters as "chlorinous" and either pleasant as "sweet chemical" or putrid as "locker room". Haloacetic acids were formed and increased in concentration (by approximately 30 μg/L, EPA regulated at 60 μg/L). THM formation was not seen. Total organic carbon leached from the polyurethane liners and reached 0.65 mg/L above background on day 1 but by day 15 was only >0.1 mg/L above background. Chlorine and monochloramine were consumed by the polyurethane where increased exposure time leads to decreased

disinfectant residual. Polyurethane impacted water quality; however, all parameters measured (except those mentioned above) had a minimum impact and returned to background levels within the 30 day time period.

2.1.2 Introduction

The corrosion of the drinking water distribution system is a serious problem worldwide. The annual cost to repair damages related to corrosion for public utilities in the United States are estimated at $22 billion (Brongers, 2002). A solution would be to reline leaking pipes through *in situ* relining. In situ relining involves surface preparation through abrasive blast cleaning and then applying lining material to coat and seal the interior of the pipe (USA Corp of Engineers, 2001). Epoxy lining is the most common polymer lining material used to coat *in situ* piping especially in copper piping (Heim, 2007). Epoxy was first used as a coating for pipes 40 years ago to prevent corrosion in Japanese industrial factories. Epoxy lining is used in a variety of applications including shipboard pipe remediation by the navy (USA Corp of Engineers, 2001).

Polyurethane (100% solids) is gaining popularity as a potable water pipe lining material due to its low application costs (faster application and lower labor costs) and lack of solvents (Guan, 2001). Solvent based epoxies were a common lining material for steel pipe; however, due to VOC pollution as a result of the solvents used epoxy was no longer a solution (Guan, 2001). The leaching of the endocrine disruptor, bisphenol A, from epoxy lining materials to water is an example of the health effects of this material (Yeo and Kang, 2006). By using solventless materials or 100% solid polyurethanes can reduce these health effects (Guan, 2001). For the last 17 years polyurethane (100% solids) has been developed for optimum properties when in contact with drinking water (Guan, 2001). 100% solids polyurethane is smoother and better abrasive resistance than cement mortar therefore, the pipe will have increased efficiency and lower operational costs (Guan, 2001). Polyurethane has also been shown to keep metal piping from further corrosion while maintaining resistance to chemicals, degradation, and impact (Guan, 2001).

Lining materials for potable water must be certified under protocol American National Standards Institute/National Sanitation Foundation 61 Drinking Water System Components – Health Effects (ANSI/NSF 61) for use as a lining material and United

States Food and Drug Administration (USFDA) 21 177.1680 for contact with consumable goods. Polyurethane is used in Australia, Great Britain and Canada; however, it has not made a significant transition to the United States. Polyurethane is similar to epoxy in that two compounds are mixed to form a strong, durable, cross-linked polymer (Dekker, 1988, Frisch and Reegen, 1973). Cement can also be used as a potable pipe lining material. It is not a polymer and therefore has very different characteristics from polyurethane and epoxy. Limited data are available for use of polyurethane to reline potable pipes, although it has been used for consumer products for decades (Frisch and Reegen, 1973).

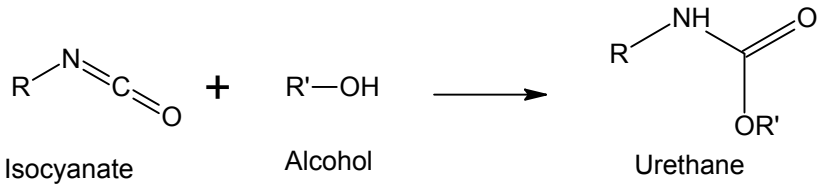

Figure 2-1. General reaction for a urethane linkage (Oertel and Abele, 1985).

Polyurethanes are typically formed using an isocyanate (-N=C=O) and any compound with an acidic hydrogen (Figure 2-1). The term urethane was originally given to the compound ethyl carbamate but then was extended to the whole class of compounds (Oertel and Abele, 1985). Polyurethanes can be formed without the use of isocyanates, however; isocyanates are the most common reagent due to the simplicity of the reaction. The reaction is shown as a single urethane linkage forming from a primary isocyanate and a primary alcohol and thus is not a true polyurethane (Figure 1-2). In order to form chains or chain branching a tertiary reagent reacting with a secondary reagent would be needed to form a lattice structure. This can be accomplished through the alterations of R groups (refer to Figure 2-1).

Polyurethanes, like most polymers, are used in conjunction with anti-plasticizers (which harden the polymer) and plasticizers (which make the polymer more moldable). These compounds can heavily influence the characteristics of the polymer. There are an abundance of plasticizers and anti-plasticizers used to form polyurethanes. They are often proprietary, and thus their specific identities are unavailable. In the water industry

it is most likely that antioxidants would be added to the polymer to resist oxidation from disinfectants and are commonly used in other polymeric piping materials (Frisch and Reegen, 1973). Therefore the chemical resistance or the leaching of these compounds could be detected in analyzing the polymer's interaction with an aqueous solution.

Polyurethanes can have a variety of properties due to the variety of the chemistry that can be used to form them. Polyurethanes can be very hard and used in the structural materials previously described, as well as soft materials as in polyurethane foam. The polymeric characteristics can also be altered using different R group combinations. If either of the R groups is a long carbon-hydrogen chain then the polymer will have van der Waals forces interacting between the chains and therefore be more amorphous. Amorphous regions, or "soft segments", are not rigid and have chain movement at lower temperatures. The temperature at which the polymer begins to flow is referred to as the glass transition temperature, T_g (Oertel and Abele, 1985).

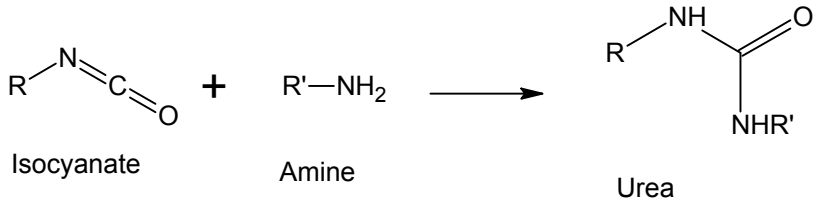

Figure 2-2. Basic urea reaction (Oertel and Abele, 1985).

Polyurethane is a general term that is often given to polyurethane, polyureas (Figure 2-2) or a combination of the two polymers with "sections" or domains containing either (Figure 2-3) (Oertel and Abele, 1985). The reactions are very similar and can have similar reactants; however, polyureas contain amine groups and can have vastly different chemistry as a result. Unlike the polyurethanes, polyureas have an acidic hydrogen on the additional secondary amine group and therefore are able to react further, similarly to the reaction seen with the polyurethane and polyurea copolymer. The reaction below is again a single urea segment, and combining these segments into chains and branching units will form polyureas (Oertel and Abele, 1985).

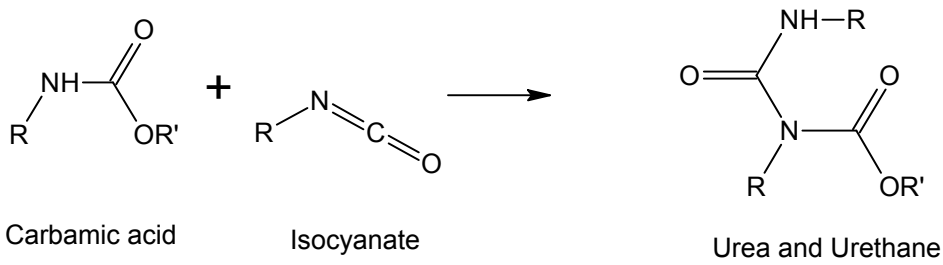

Figure 2-3. A polymer with polyurethane and polyurea domains (Oertel and Abele, 1985).

Isocyanates are used in the production of polyurethane. They are very toxic and can lead to respiratory illnesses and skin irritation which has led the Environmental Protection Agency (EPA) to fund several initiatives to better understand health concerns as well as methods of prevention (EPA, 1997). Polyurethane is extremely common in several mass produced goods and is also heavily regulated by the U.S. Department of Labor under the Occupational Safety & Health Administration (OSHA) (OSHA, 2006). Elastic, paint, foam-blowing, foam mattresses and under-carpet padding are just of the few examples of materials, varying forms of polyurethane, that require isocyanates in their production; therefore it is very common for isocyanates to be present in these factories. Isocyanates have been shown to be carcinogenic in animals and a possible human carcinogen, as well as a skin, throat, eye and lung irritant. OSHA Section 5(a)(1) regards isocyanates as a hazard and requires employers to provide "a place of employment which [is] free from recognized hazards that are likely…to cause death or serious physical harm to his employees".

Concerns about unreacted isocyanates leaching from polyurethane as it degrades can be avoided by forcing the polyurethane reaction to go to completion. Therefore there are no unreacted isocyanates left to leach out of the polyurethane. It is also possible to use another reactant with fewer health concerns. These techniques are most popular in the biomedical field where polyurethane is being investigated as a material in organ and joint replacement. The biomedical studies are concerned primarily with blood clots forming around the implant. The degradation of polyurethane can potentially form amides that are very toxic (Spaans *et al.*, 1998).

Though isocyanates are dangerous to work with and should be handled with extreme precaution they are more hazardous in the air or in small particulates. All of the hazards and warnings were for their inhalation and not in the ingestion as would occur in a drinking water system. If there was some isocyanate within the polymer that then migrated to an aqueous solution there are no health warnings to suggest that it would have the same health effects given by OSHA. In fact polyurethane has even been used in car air filters with no reported health effects (Oertel and Abele, 1985).

Polyurethane has been found to be an excellent material to use for joint replacement as well as regeneration of biomaterials in the human body when using the appropriate reactants and methods (Spaans *et al.*, 1998). When the polyurethane is carefully synthesized and fully reacted it can be used in the body without harmful reactants, such as isocyanates, leaching from the polyurethane. The diversity of characteristics allows polyurethane to be synthesized to have the appropriate characteristics for each use.

Polyurethane is just recently having the research performed in other fields applied to problems associated with drinking water (Farag *et al.*, 2007, T. V. Nguyen, 2006). Nguyen, T.V. et al. analyzed techniques to remove arsenic from drinking water (T. V. Nguyen, 2006). Iron coated polyurethane foam was used to successfully extract arsenic from drinking water.

It is important for water utilities to know how a lining material will affect the water quality of their influent before it is used. It has been shown that other polymeric lining materials have impacted the disinfection by-products as well as odor (Heim, 2007). Water treatment facilities are responsible for the water quality throughout the infrastructure, and with EPA regulations becoming stricter they cannot afford to not know the impact of polymeric lining materials in their system.

2.1.3 Objectives

The objective of this research was to measure the short term impact of polyurethane lining on drinking water quality and aesthetics by assessing changes in pH, nitrogen-

ammonia, alkalinity, total organic carbon (TOC), disinfectant residual, hardness (as calcium and magnesium), total solids, odor, trihalomethanes (THMs), haloacetic acids (HAAs), semi-volatile organic compounds (SVOCs) and elemental analysis.

2.1.4 Materials and Methods

2.1.4.1 Polyurethane Preparation

A single polyurethane was tested. Coating of the glass coupons with polyurethane was achieved and performed through the cooperation and coordination of Madison Chemical (Madison Chemical Industries Inc., 490 McGeachie Drive, Milton, Ontario L9T 3Y5). Clean sand-blasted 8cm x 8cm glass coupons were coated on all sides with polyurethane in accordance with procedures recommended by the manufacturer. This polyurethane consists of two components in a 1:1 mixture that was applied using heated airless plural spray equipment. After the recommended 48 hour curing time, the polyurethane-coated coupons were washed and prepared as specified in NSF 61. The coupons were exposed to a 200 mg/L Cl_2 dose of chlorine for 30 minutes and rinsed, then the leaching tests for the polyurethane-coated coupons began.

Figure 2-4. Immersion test apparatus with coupons. (Photo by Heather Johnson)

2.1.4.2 Test Waters for Leaching of Lining Materials

Three water types were tested so as to investigate the different disinfectants that are typical of USA drinking waters. The composition of the pH 8, low alkalinity/low hardness reference water was prepared by adding salts to Nanopure® reagent water (Table 2-1).

Eleven liters of each water type were prepared for each water change/sampling date. Chlorinated test water was prepared by adding NaOCl. Chloraminated test water was prepared by first adding NH_4OH while being continuously stirred. After 5 minutes of mixing, NaOCl was quickly added and the water was shaken vigorously for 30 seconds. pH was adjusted as necessary by adding hydrochloric acid. The chloraminated water pH fluctuated between 8 and 9 depending on the amount of pH adjustment after addition of ammonium hydroxide.

The three water types were:

- pH = 8.0, low alkalinity/hardness, no disinfectant.
- pH = 8.0, low alkalinity/hardness, 2.0 mg/L chlorine.
- pH = 8.0, low alkalinity/hardness, 4.0-6.0 mg/L monochloramine.

Table 1. Reference Water Composition.

Chemical	Molarity	Concentration (mg/L)
$MgSO_4$*	0.0003292	39.64
$NaHCO_3$	0.000677	56.89
$CaSO_4$*	0.0001452	19.78
$CaC1_2$*	0.0001415	15.70
Na_2SiO_3*	$9.1485*10^{-5}$	11.16
KNO_3	$9.8902*10^{-5}$	10.00
HCl	0.0002	7.29
Alkalinity	-	35
Hardness	-	61.67

*added as hydrates

2.1.4.3 Test Vessels for Leaching of Lining Materials

The prepared polyurethane coupons were placed in a fully enclosed container to simulate contact with water in an enclosed pipe (Figure 2-4). Triplicate all glass immersion test vessels of approximately 3 L volume containing coupons were prepared for each water type. The ratio of lining material surface area to potable water mimicked a 4 inch diameter pipe (0.40 cm^2/mL). Coupons were held upright by perfluoroethylene support racks. A control for each water type, that contained no coupons, was also prepared. All vessels were maintained headspace free through the experiment. Temperature was between 21-23 ˚C. During the leaching procedure, all test vessels were stored in the dark.

2.1.4.4 Protocol for Water Changes and Analyses

Table 2. Typical Frequency and Quality Control for Chemical Water Quality Parameters for Bench Scale Testing of Lining Materials.

Parameter	Measurement Frequency (Day)
TOC	1, 2, 4, 9, 11, 14, 15
Disinfectant Residual	1, 2, 4, 9, 11, 14, 15, 19, 21, 30
Ammonia	1, 2, 4, 9, 11, 14, 15
Hardness	1, 2, 4, 9, 11, 14, 15, 19, 21, 30
Alkalinity	1, 2, 4, 9, 11, 14, 15, 19, 21, 30
pH	1, 2, 4, 9, 11, 14, 15, 19, 21, 30
Temperature	1, 2, 4, 9, 11, 14, 15, 19, 21, 30
Total Solids	1, 4, 9, 14
Odor	1, 4, 9, 14
THMs	1, 4, 9, 14
HAA5[1]	1, 4, 9, 14
SVOCs[1]	1, 4, 9, 14
Elements	1, 2, 4, 9, 14, 15

[1] A single sample was analyzed that was a composite from the triplicate sample for each water combination.

The leaching protocol was adapted from ANSI/NSF 61 which evaluates the leaching of organic and inorganic components from materials in contact with drinking water. The leaching test was performed for 30 days and the frequency for measuring different water quality parameters are presented (Table 2-2). Water was changed on the days indicated and sub-samples of the water were obtained to measure selected analytes as indicated (Table 2-2).

The sample water was tested for pH, total organic carbon concentration (TOC), disinfectant residual, ammonia concentration as $N\text{-}NH_3$, hardness as combined Ca and Mg concentrations, alkalinity (as $CaCO_3$), temperature and pH on days when the sample

water is changed. Total solids (TS), odor, trihalomethanes (THMs), haloacetic acids (HAA5) and semi-volatile organic compounds (SVOCs) were determined on days 1, 4, 9, and 14.

The specific sampling protocols and measurement methods used to determine the water quality parameters are presented (Table 2-3).

Table 3. Measurement Method and Sampling Procedures.

Parameter	Standard Method[1]	Instrumentation	Sample Container/ Replicates[2]	Preservation /Storage	Maximum Holding Time
TOC	SM 5310c	TOC analyzer	glass/3	In dark, 4°C ± 2°C	28 days
Disinfectant Residual	SM 2350	HACH colorimeter	glass/3	4°C ± 2°C	< 24 hours
Ammonia	SM 4500	HACH colorimeter	glass/3	H_2SO_4 to pH<2, 4°C ± 2°C	7 days
Hardness	SM 2340b	ICP-MS[3]	glass/3	HCl or H_2SO_4 to pH<2, 4°C ± 2°C	6 months
Alkalinity	SM 2320	HACH colorimeter	glass/3	4°C ± 2°C	14 days
pH	SM 2310	pH meter	glass/3	N/A	immediately
Temperature	SM 2550	Thermometer	glass/3	N/A	immediately
Total Solids	SM 2540	Evaporation	glass/3	4°C ± 2°C	7 days
Odor	SM 2170	FPA	odor free glass/1	4°C ± 2°C	<2 days
THMs	SM 6232D	Purge & Trap	glass/3	Ascorbic Acid (20mg/ 40 mL), 4°C ± 2°C	7 days
HAA_5	SM 6251	Extraction	glass/1	Dechlorinate, 4°C ± 2°C	9 days
SVOCs	SM 6410	GC/MS	glass/1	Dechlorinate, 4°C ± 2°C	7 days until extraction
Metals/Elements	SM 3125	ICP-MS	glass/3	HNO_3 to pH<2, 4°C ± 2°C	6 months

[1.] SM = Standard Methods for the Examination of Water and Wastewater

[2] Quantity of Samples is number of samples per triplicate lining material and water types; 3 = each replicate will be measured; 1 = composite of triplicates

[3] Hardness = sum of calcium and magnesium concentrations

2.1.4.5 Methods

2.1.4.5.1 pH and Temperature

Temperature and pH were measured using Standard Method 4500-H^+ using a Corning 315 pH/ion probe that was calibrated using standard pH solutions 4, 7 and 11 (BioWorld).

2.1.4.5.2 Total Alkalinity

Alkalinity was measured using Standard Method 2320. H_2SO_4 (CAS# 7664-93-9) at 0.0190 N concentration was titrated into 100 mL sample to pH 4.5.

2.1.4.5.3 Disinfectant Residual

Disinfectant Residual was measured using Standard Method 2350 with a HACH® kit (HACH, free chlorine CAT# 21055-69, total chlorine CAT#21056-69) measuring free and total chlorine. Free chlorine was used to measure the chlorinated sample water. Monochloramine was calculated using free and total chlorine (Total – Free = Monochloramine).

2.1.4.5.4 Nitrogen-Ammonia (N-NH_3)

Nitrogen-Ammonia (N-NH_3) was measured using Standard Method 4500 with a HACH® kit using salicylate (HACH, CAT# 26522-99) and cyanurate reagents (HACH, CAT# 26531-99).

2.1.4.5.5 Solids

Total Solids (TS) were measured using Standard Method 2540B and a 0.5 μm filter was used to separate a water sample into dissolved solids and suspended solids.

2.1.4.5.6 Elemental Analysis and Hardness

Selected trace metals (Sodium (Na), Magnesium (Mg), Aluminum (Al), Potassium (K), Vanadium (V), Chromium (Cr), Iron (Fe), Manganese (Mn), Cobalt (Co), Nickel (Ni), Copper (Cu), Zinc (Zn), Arsenic (As), Molybdenum (Mo), Cadmium (Cd), Tin (Sn), Barium (Ba), and Lead (Pb)) , non-metals (Sulfur (S), Phosphorous (P), Chlorine (Cl), and Silicon (Si, a semi-metal) were measured. Standard Method 3125 was used and the

samples were analyzed on ThermoElectron Corporation inductively coupled plasma mass spectrometer (ICP-MS) X-Series. Hardness, as the sum of calcium and magnesium concentrations, was measured by using the elemental analysis results.

2.1.4.5.7 Total Organic Carbon (TOC)

Total organic carbon (TOC) was measured using Standard Method 5310C using a Shimadzu TOC-V Total Organic Carbon Analyzer. The samples were acidified to < pH 2 using Nitric acid (CAS# 7697-37-2). Two measurements were taken from each replicate, if the samples were not within 20% a third sample was taken and an average was calculated to give the TOC concentration for that sample.

2.1.4.5.8 Trihalomethanes (THMs)

Trihalomethanes (THMs) were analyzed using Standard Method 6232D using Tre Metrics 9001 gas chromatograph, Tracor 1000 Hall® Detector, Purge & Trap Autosampler Tekmar 2016 and Purge & Trap Concetrator Tekmar 3000. The column used was a DB-624 with helium as the carrier gas with the initial oven temperature at 45 ºC and held for 3 minutes, increasing at 11 ºC/min with a maximum oven temperature of 200 ºC. Standard curve was performed for each run unless run sequentially (THM-521-1 Ultra 5000 µg/mL standard).

2.1.4.5.9 Haloacetic acids (HAA5)

The HAA5 extractions were performed following EPA Method 552.3 using liquid-liquid extraction, derivitization, and gas chromatography with electron capture detection. The standard (Methylated Haloacetic Acid Standard, Chem Service, West Chester, PA) contained concentrations of HAA5 ranging from 20 µg/L-60 µg/L. The GC column used was a DB-1701 (30 m length, 0.25 diam., 0.25 µm film) with helium as the carrier gas and nitrogen as the makeup gas. Initial oven temperature was 35 ˚C, which was held for 10 min and increased at 5.7 ˚C/min to 75 ˚C and held for 5 min. Temperature was again increased at 5 ˚C/min to 100 ˚C and held for 5 min, then increased at 20 ˚C/min to 140 ˚C and held for 5 min. After being removed and equilibrating to room temperature, the samples were identified and quantified using procedural standard calibration.

2.1.4.5.10 Semi-volatile organic compounds (SVOCs)

Semi-volatile organic compounds (SVOCs) were measured using Standard Method 6410B which is a liquid-liquid extraction using methylene chloride followed by concentration using a Kaderna-Danish apparatus at 75 ˚C water bath. The samples were analyzed using a gas chromatograph-mass spectrometer (GC-MS) using a DB-5 column (30.0 m x 250 µm x 0.30 µm). The initial oven temperature was 40 ºC and was held for 3 minutes then increased by 8 ºC/min to 200 ºC and held for one minute. The column was then heated by 10 ºC/min to 300 ºC and held for 11 minutes. The targeted compounds were then identified using standard NIST mass spectra. Non-targeted compounds were tentatively identified based on library matching of mass spectra. For selected compounds, chemical standards were purchased and retention times and mass spectra were compared to confirm their qualitative identity and measure quantitative amounts.

2.1.4.5.11 Odor Analysis

Odor analysis was performed using the Flavor Profile Analysis (FPA) using Standard Method 2170 where participants underwent a one day training session to learn the Flavor Profile Analysis method. The study protocol was approved by the Institutional Review Board for Research Involving Human Subjects at Virginia Tech (Appendix B). The FPA intensity scale is 0: odor free (OF), 1:threshold, 2:very weak, 4:weak, 8:moderate, 10:strong, 12: very strong. The weak intensity corresponds to the sweetness of canned fruit (for comparison, FPA taste intensity of 8 is moderate and corresponds to canned soda while an FPA intensity of 12 is strong and corresponds to syrup or jelly).

2.1.4.5.12 Trihalomethane Sorption/Formation Experiment

An issue for leaching tests, including those described in NSF-61, is that DBPs can form in the water during leaching and then be re-sorbed into the lining material and consequently not measured. This phenomenon was investigated for selected trihalomethanes. The formation of trihalomethanes from the reaction of TOC leached from the lining material and added chlorine used for disinfection was investigated by placing coated coupons in reference water with no disinfectant and allowing TOC leaching to occur over a 72 hour period under headspace free conditions at room temperature. The TOC was then measured from aliquots of the leached water that were

placed in headspace free VOA vials with the addition of free chlorine. The surface area to volume ratio of the polyurethane coupons to test water was 408.8 cm^2/L. At 0, 24, and 72 hour time intervals, 0.0250 N sodium thiosulfate solution (VWR, CAS #7737-18-5) solution was added to quench the THM formation reaction. The samples were then analyzed for TOC, disinfectant residual and THMs.

To investigate if THMs could sorb into the lining material, coated coupons were immersed headspace free for up to 72 hours in reference water containing 100 µg/L standard THM solution (THM-521-1 Ultra 5000 µg/mL standard) with no free chlorine. Lining material coupons were placed in the test apparatus with the standard water without disinfectant for 96 hours under headspace free conditions. The sorption of trihalomethanes into the lining material was tested by determining the concentration of THMs in the water over time.

2.1.4.5.13 Statistical Analysis

Statistical analysis was performed using both a linear and logarithmic regression analysis and 2-way ANOVA using the using the statistical program R version 2.6.2, where an $\alpha = 0.05$. A p value was generated where if $p > 0.05$ the data are statistically significant and $p < 0.05$ the data are not statistically significant. Logarithmic analysis could not always be used due to the negative values which cannot be analyzed logarithmically and therefore decreased the data points available.

2.1.5 QA/QC Procedures

Quality control (QC) samples were collected/analyzed. Method Blanks (MB), Check Sample (CS), Matrix Spike (MS) and Surrogate Standards (SS) were performed for each batch of samples for every 20 (or less) samples received.

2.1.6 Results

2.1.6.1 Introduction

pH, total alkalinity, hardness (as calcium and magnesium), elemental analysis, total solids, disinfectant residual, ammonia, total organic carbon (TOC), trihalomethanes (THMs), haloacetic acids (HAAs), semi-volatile organic compounds (SVOCs), odor and leaching tests were perform to analyze the impact of polyurethane in-situ lining on the drinking water quality. These tests were conducted over the course of 30 days and analyzed according the NSF 61 standards.

2.1.6.2 Part 1: Inorganic Water Quality Parameters

2.1.6.2.1 pH

Regardless of the disinfectant type, the presence of polyurethane caused the leachate pH to decrease 2-3 pH units to approximately pH 6. Because pH is a log scale, a 2-3 unit change in pH corresponds to a 100-1000 fold change in $[H^+]$. Values near pH 6 persisted throughout the 30 day exposure period to polyurethane with very small standard deviations in pH measurement (Figure 2-5). To provide evidence of sample variation, the data (Figure 2-5) contain error bars but are covered by the data point symbols. All of the initial water conditions began with a pH of 8 for no disinfectant and chlorine or pH 9 for monochloramine. The controls with no polyurethane were able to maintain their target pH values throughout the 30 day test period (Figure 2-5).

The waters were changed and pH measured on days: 1, 2, 4, 9, 11, 14, 15, 19, 21, and 30. The initial pH for monochloramine-containing water was 9, which dropped to about pH 6 in the presence of polyurethane making the polyurethane-induced change in pH more dramatic for monochloramine than for chlorine or no disinfectant.

Statistical analysis was performed using linear regression where only exposure time statistically impacted the change in pH ($p = 0.013$). The type of disinfectant used, chlorine or monochloramine, had no impact on the change of pH ($p = 0.879$ and 0.083, respectively).

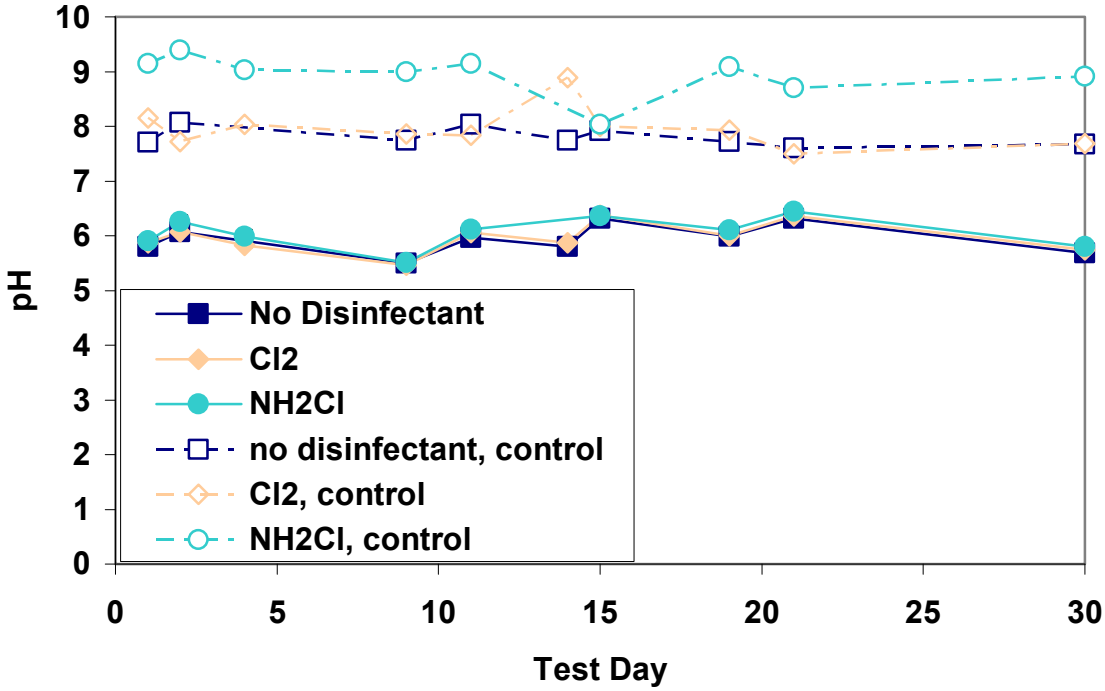

Figure 2-5. pH as a function of time as measured by test day and water change. Control waters did not contain polyurethane coupons.

2.1.6.2.2 Total Alkalinity

The total alkalinity was not significantly different in the presence of polyurethane compared to the corresponding control water with no polyurethane (Figure 2-6). Statistical analysis was performed using linear regression where the presence of monochloramine held no statistical impact ($p = 0.121$). The presence of chlorine ($p = 0.014$) and exposure time ($p = 0.004$) had a decreasing slope over time when corrected for the controls. However, the change in alkalinity was ~3 mg $CaCO_3$/L and therefore a minor impact to the water quality.

The measured alkalinity was slightly higher for the monochloraminated test water and pH control due to addition of ammonium hydroxide. No major impact to alkalinity in the presence of polyurethanes for the no disinfectant, chlorine or monochloramine containing waters was seen. On day 30 the control for the chloraminated water is noticeably lower

than in previous days. There was no measured change in the dissolved salts in the test water. The decrease is most likely due to random error.

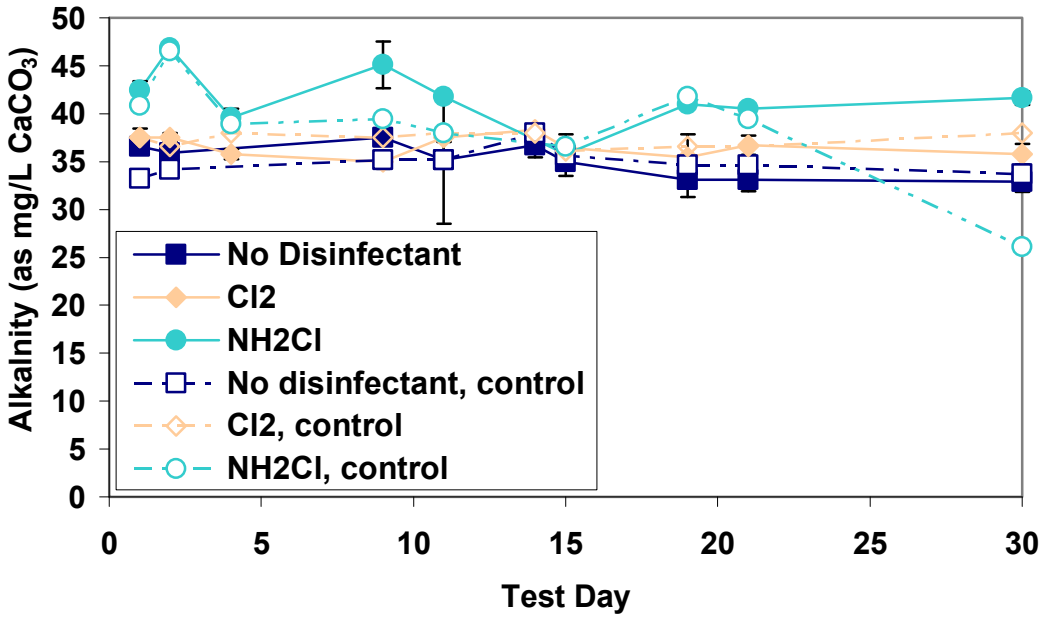

Figure 2-6. Alkalinity as a function of time for the three sample waters and their controls.

2.1.6.2.3 Hardness

Similar to alkalinity, the presence of polyurethane did not affect water hardness (Figure 2-7). The concentrations of calcium and magnesium, which constitute hardness, in leachate water were not statistically different from their corresponding control waters without polyurethane for no disinfectant, chlorinated or monochloraminated water types ($p = 0.264$, 0.721 and 0.329, respectively). The hardness did not change over the 30 day exposure time ($p = 0.127$).

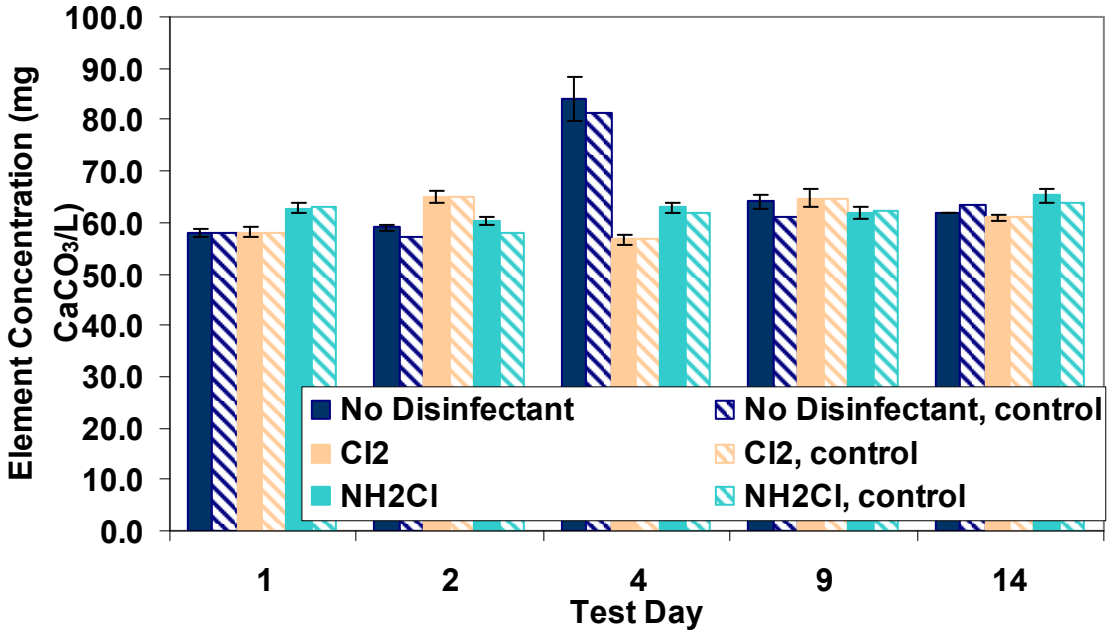

Figure 2-7. Calcium and Magnesium concentrations for test waters in contact with polyurethane and their controls as a function of time (Test Day). Error bars represent standard deviations.

2.1.6.2.4 Elemental Analyses

Metals and non-metals were measured by ICP-MS. There was no substantial change (change < 10% wt/wt) in the concentration of Ba, Sn, Na, Si, K, Cd, V, Co, As and Mo in any test water containing polyurethane coupons compared to its corresponding control water without polyurethane.

Selected trace metals and non-metals, in the µg/L range, are shown to depict the data collected for the elemental analysis in the samples compared to those of the respective control. An element was considered to leach from the polymer if its concentration was higher than the control and adsorbed into the polymer if the concentration was lower than the control. Five elements, two non-metals (sulfur and phosphorous) and three metals (aluminum, iron, and zinc) were the most vaired in all three disinfectant treatments of the polyurethane and were used for comparison (Figures 2-8, 2-9 and 2-10). Standard deviation bars were placed on the graphs to give an indication of how meaningful the differences between the control and the sample water. Most of the changes seen in the data at within the standard deviation; therefore, this data falls within measuring error and

therefore are not significant changes. The sorption or leaching of zinc does seem to be significant from the control water.

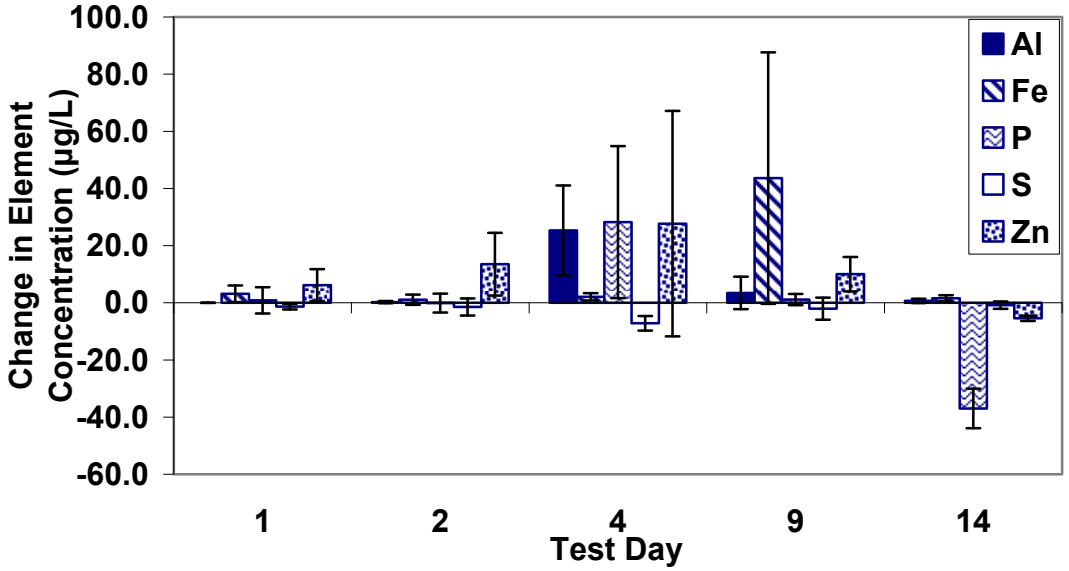

Figure 2-8. Concentrations of selected elements in no disinfectant water in contact with polyurethane coupons. The element concentrations in the control water (without polyurethane coupons) were subtracted from the test data.

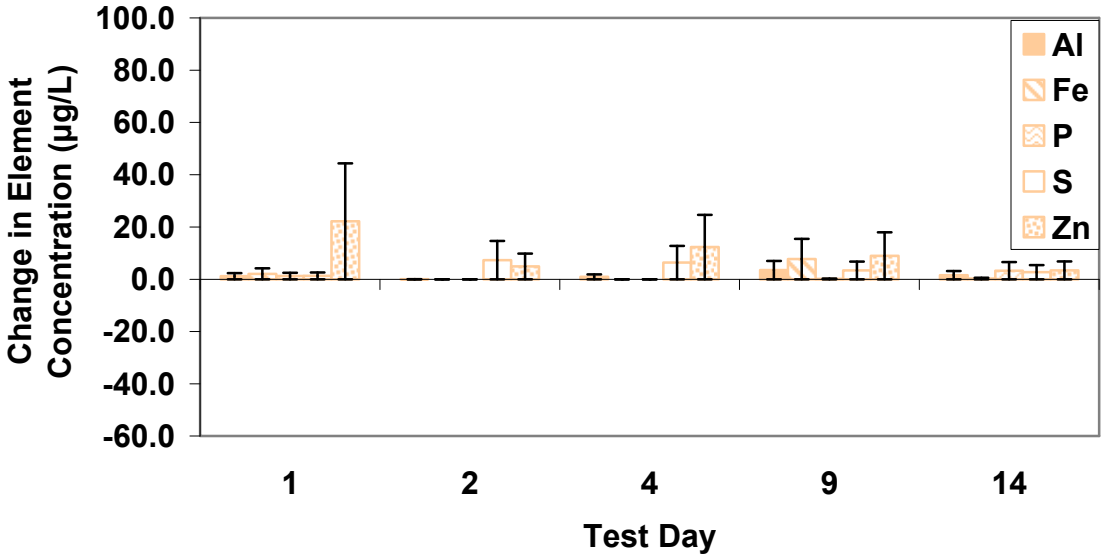

Figure 2-9. Concentrations of selected elements in 2 mg/L Cl_2 water in contact with polyurethane coupons. The element concentrations in the control water (without polyurethane coupons) were subtracted from the test data.

The data indicate that the three water types had different trends in the decrease or increase of selected elements. Overall there was no consistent change within the metals

and the differences are within statistical error and therefore are not significant. Other elements that were leached from the polymer (> 10% wt/wt change), in this water were Pb and Cu with Cl, Cr, Mn and Ni and showed no significant change in concentration (data not shown).

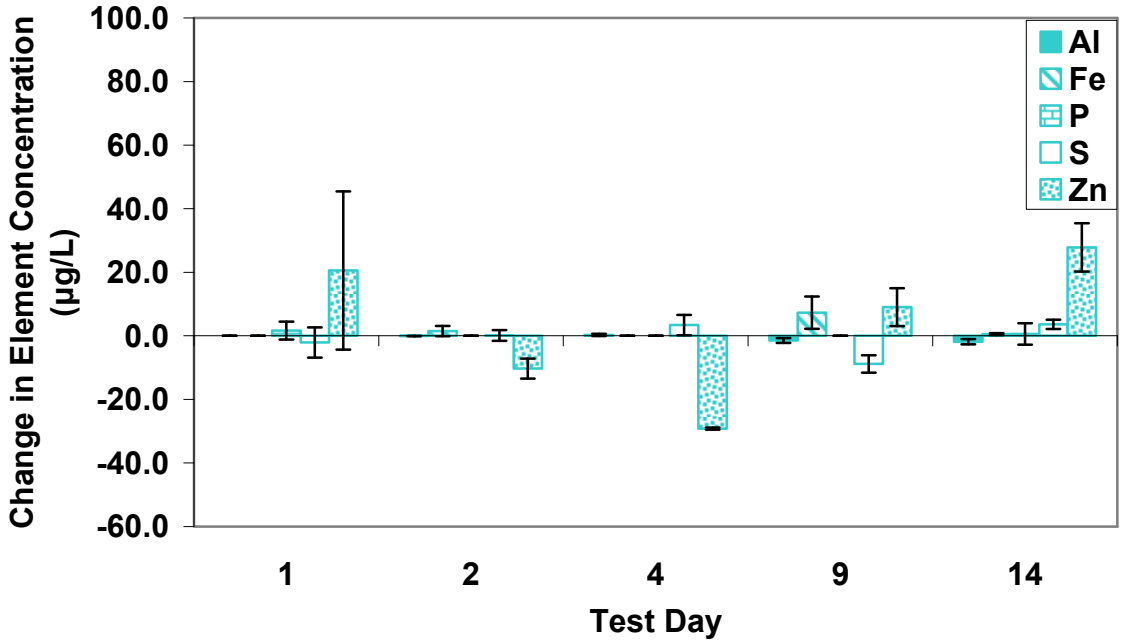

Figure 2-10. Concentrations of selected elements in 5-6 mg/L NH_2Cl water in contact with polyurethane coupons. The element concentrations in the control water (without polyurethane coupons) were subtracted from the test data.

The chlorinated water both increased and decreased element concentrations with respect to the controls throughout the testing period (Figure 2-9). The elements did not have general trends but the elements that were both "leached" and "sorbed" from the polymer (> 10% wt/wt change) were Al, Cr, Fe, Ni, P, S, Cu and Zn. The water with monochloramine both increased and decreased elemental concentrations but to a lesser extent than the chlorinated water (Figure 2-10). Again there was not a trend in all of the elements thus both "sorbed" and "leached" (> 10% wt/wt change), and include: P, Cr, Fe, Ni, S, Al and Zn.

Of the metals measured, several had USEPA regulatory limits, as MCLs or Action Levels, or guidelines through secondary maximum contaminant levels (Table 2-4). No measured

values for any metal in any test water with polyurethane exceeded USEPA regulated or guideline limits.

Table 4. Elements with Maximum Contaminant Level (MCL), Secondary Maximum Contaminant Level (SMCL) and Action Level (AL) Regulated by the EPA (EPA, 2003).

Element	Symbol	AL (mg/L)	SMCL (mg/L)	MCL (mg/L)
Aluminum	Al		0.05-0.2	0.2
Chromium	Cr			0.1
Iron	Fe		0.3	
Manganese	Mn		0.05	
Copper	Cu	1.3	1.0	
Zinc	Zn		5	
Arsenic	As			0.05
Cadmium	Cd			0.005
Nickel (EPA, 1995)	Ni		0.1	
Lead	Pb	0.015		

2.1.6.2.5 Total and Dissolved Solids

The presence of polyurethane did not add or remove measurable amounts of solids (data not shown). The values for total solids and dissolved solids were similar indicating that only dissolved solids were present in the control waters or waters containing polyurethane coupons. Linear regression analysis was performed and water with no disinfectant, chlorine and chloramine ($p = 0.059$, 0.632 and 0.655, respectively) as well as exposure time ($p = 0.350$) had no significant impact on the total solids.

2.1.6.2.6 Disinfectant Residual

Data for chlorine and monochloramine disinfectant loss in mg/L as Cl_2 are shown (Figures 2-11 and 2-12). The water with no disinfectant is not shown as there was no change in the disinfectant concentration. The data are shown as disinfectant residual in mg/L Cl_2 for both chlorine and monochloramine disinfectant as well as the control concentrations. The residuals in the controls were higher than the test water residuals, indicating that the polyurethane is causing the disinfectant to degrade more quickly than it would otherwise. As expected, free chlorine decayed to a greater extent than monochloramine. Statistical analysis was performed where monochloramine and chlorine were statistically different with respect to the controls over time ($p < 0.001$ for both).

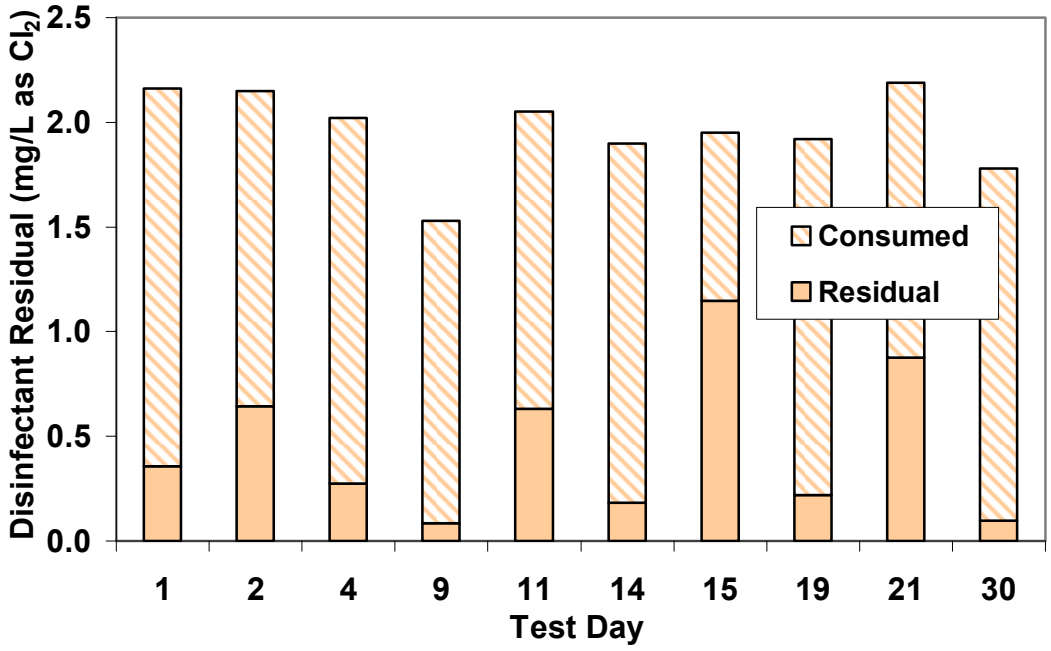

Figure 2-11. Chlorine decay, showing residual disinfectant, and consumed disinfectant, as a function of time without the correction for the controls.

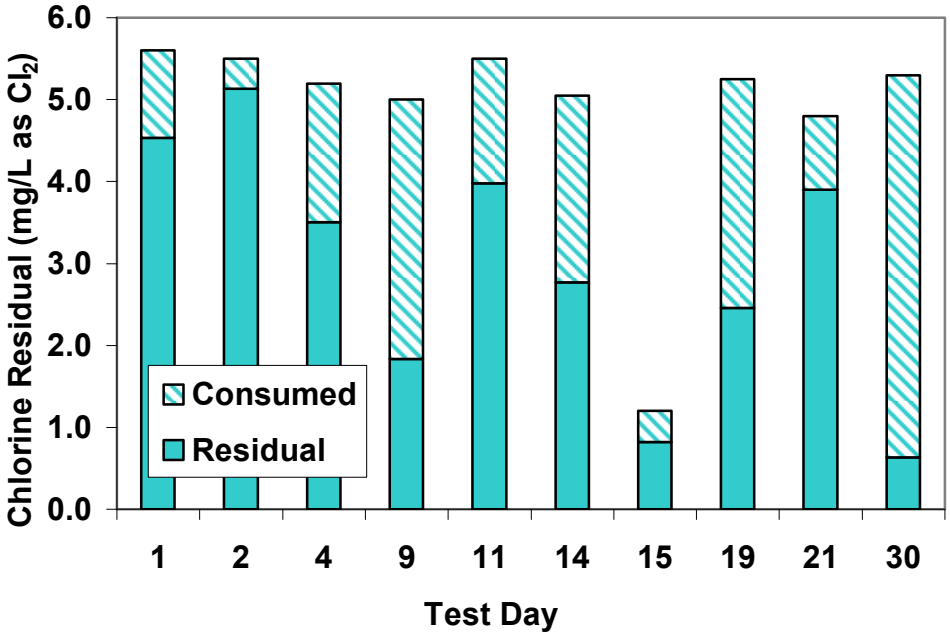

Figure 2-12. Monochloramine decay, showing residual disinfectant, and consumed disinfectant, as a function of time, without the correction for controls.

When the disinfectant consumed per day exposed (mg as Cl_2/L/exposure time) is graphed, the reaction rate of the chlorine with polyurethane decreases with time (Figure 2-13). For chlorine, the rate of decay is variable but overall shows a significant decreasing trend over time ($p < 0.001$). The decay rate was the highest in the first few days, then leveled off by day 9 (Figure 2-13). Therefore, within a few weeks after lining, the chlorine consumption by the polyurethane will lessen. With monochloramine there was more variation but with an overall downward trend with respect to time ($p < 0.001$). There was a high residual on day 2 where the control decreased dramatically after one day. The decrease in the sample chloramine decay was slightly lower than what was seen on day 1. Once this outlier point is taken into account, a trend can be seen, where there is a slight decrease over time. It is also important to note that the chlorinated water had the greatest percent decay when compared to the monochloraminated water. This statement will be discussed further in the discussion section.

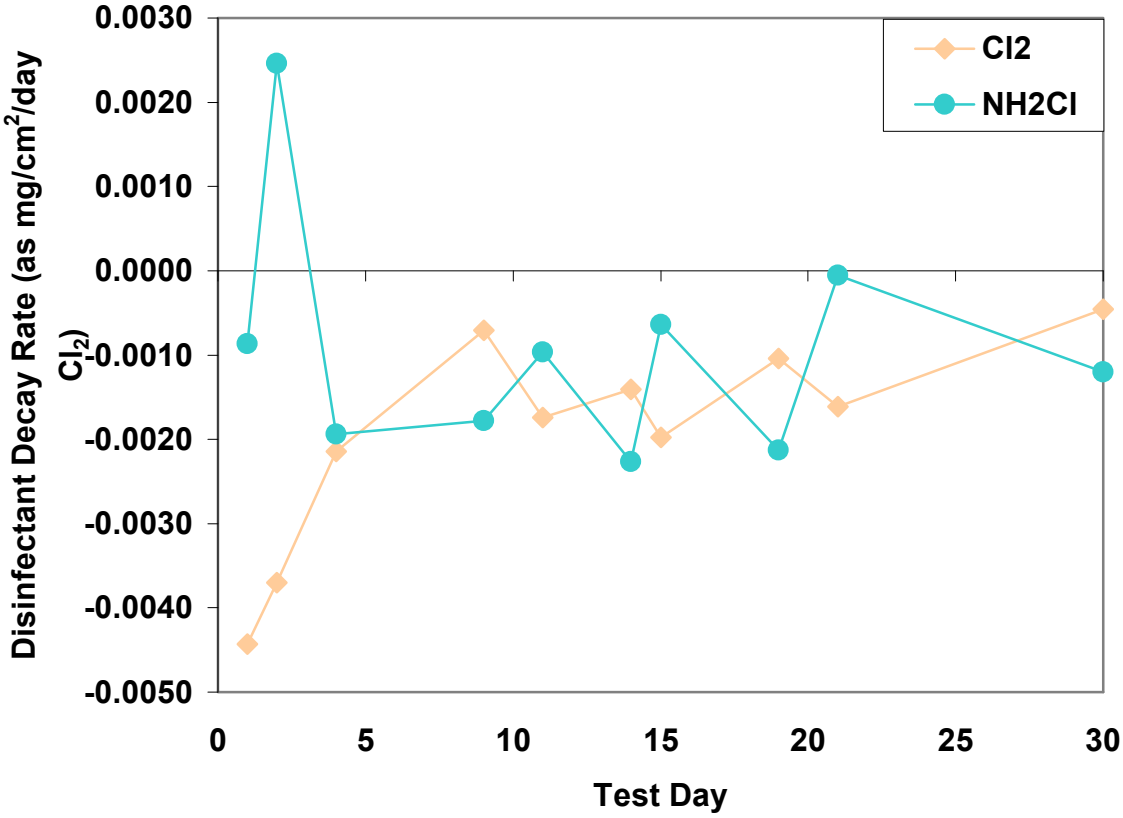

Figure 2-13. Chlorine and Monochloramine decay corrected for the controls (mg/cm^2/time of exposure) function of time.

2.1.6.2.7 Ammonia

Only the chloraminated water and its control contained measurable ammonia, which was formed by the decay of monochloramine (Figure 2-14). The test and control waters had similar concentrations of ammonia. From statistical analysis it is shown that the presence of polyurethane and the length of time the water was exposed to the coupons had no effect on ammonia production ($p = 0.945$ and 0.903). These data are consistent with chloramine residual which indicate that the rate of monochloramine decay was fairly stable (Figure 2-13).

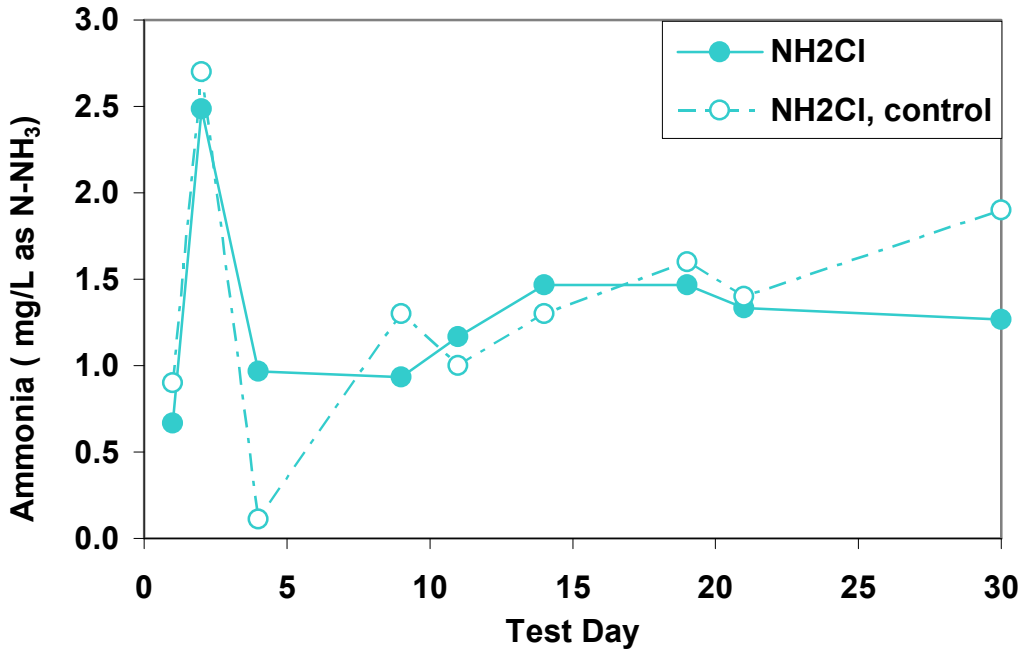

Figure 2-14. Ammonia (mg/L as N), with water: pH 8, 5-6 mg/L NH_2Cl, as a function of time (Test Day).

2.1.6.3 Part 2: Organic Water Quality Parameters

2.1.6.3.1 Total Organic Carbon

Data for TOC are shown below (Figure 2-15). The TOC in test waters are all higher than their controls especially after polyurethane exposure times exceeding 1 day. It is important to note that the TOC in the controls decrease from ~0.5 mg/L to ~0.2 mg/L over 15 days, likely due to changes in TOC in Nanopure® water used to prepare the reference water. Comparison to the controls seems to illustrate that the test water TOC notably increases when exposed to the polyurethane coupons for longer time periods. Yet, when statistical analysis was performed it was found that the increase was not statistically significant ($p = 0.130$). The large variation in the data most likely led to the lack of statistical confirmation. Over 15 days and six water changes the TOC levels in waters with polyurethane coupons decreased but were still above the controls for no disinfectant, chlorinated and chloraminated (concentration above control = 0.0381, 0.0872 and 0.0854 mg/L TOC, respectively) (Figure 2-15). The convergence of TOC leaching over 15 days is significant using regression on a linear scale ($p = 0.028$). Disinfectant (chlorine and

monochloramine) did not have a significant impact on TOC leached ($p = 0.189$ and 0.997).

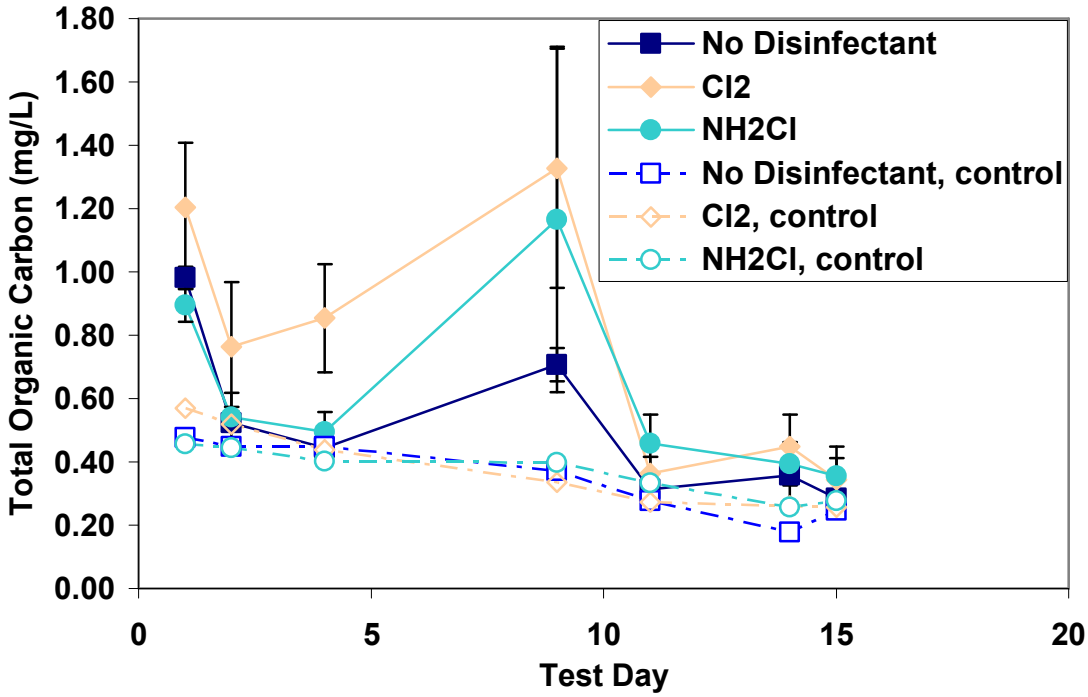

Figure 2-15. Total Organic Carbon (TOC, mg/L) as a function of time for all three water types with controls. Error bars represent standard deviation.

A trend in the leaching of TOC with disinfectant type was noted with the most TOC leached in the presence of chlorine, then in the presence of monochloramine, and the least TOC leached in the presence of no disinfectant. Although this relative amount of TOC leaching is apparent it is not statistically significant due to the moderate variability between replicates (Figure 2-15). The convergence of the TOC leached to the concentration found in the controls shows that the decrease in leached TOC was not likely due to the decay of the polymer from disinfectant but to leachable TOC in the polymer.

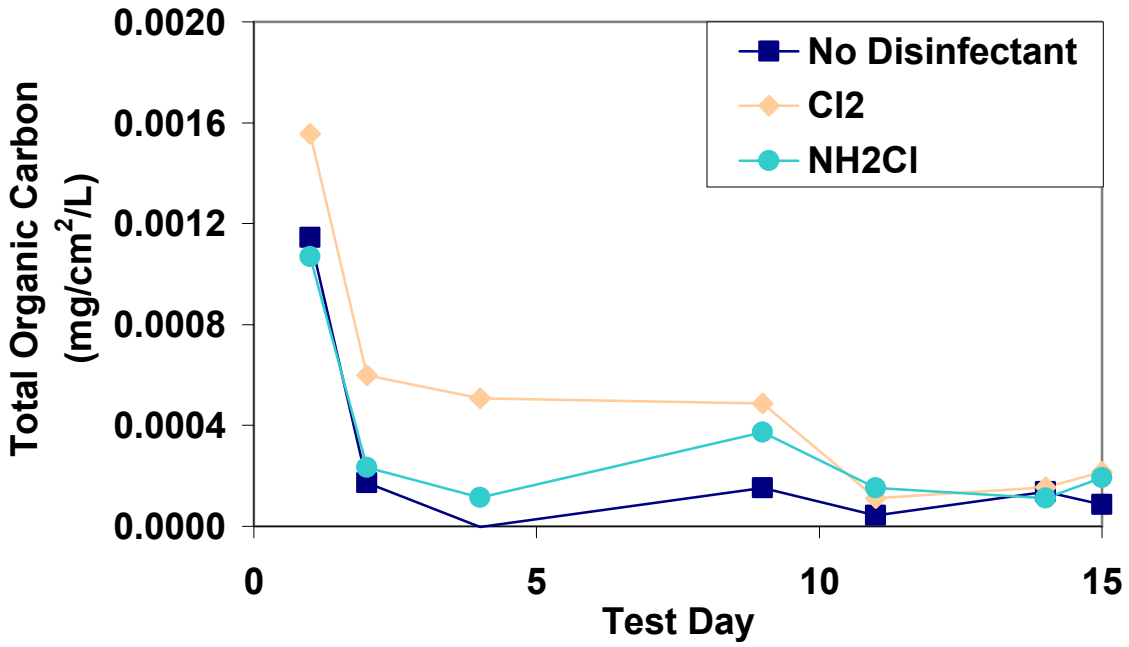

Figure 2-16. The rate of Total Organic Carbon leachate (TOC, mg/cm^2/day) as a function of time for all three waters and corrected for TOC measured in controls.

When plotted as a rate of TOC leaching, the data indicate that the rate of TOC leaching during the initial four days of contact with water is higher than the rate after four days (Figure 2-16).

2.1.6.3.2 Trihalomethanes

THM formation did not occur within the first 14 days of the polyurethane leaching test for any of the test water conditions. As expected, THMs were not detected in the water which had no disinfectant or the water which contained monochloramine. The chlorinated waters contained only < 2 µg/L chloroform in both the chlorine test water and its control. As was stated previously, about 0.2 mg/L TOC was in the reference water and therefore, some formation of THMs could occur in the control.

Additional experiments were performed to determine if THMs could be formed from the leached TOC and possibly sorb into the polyurethane. TOC was extracted from the polyurethane coupons with disinfectant-free water, then chlorine was added to this water in glass VOA vials and the THM formation was monitored. Although the TOC was

about 1 mg/L and the free chlorine was not detectable after 24 hours, no THMs were detected. Thus, THM formation does not occur for TOC leached from this polyurethane lining.

Table 5. Sorption of THMs from aqueous solution and into polyurethane after a 72 hour contact time; initial THM concentration was 100 µg/L (0.245 µg/cm^2).

Replicate	Aqueous Concentration, µg/cm^2				
	$CHCl_3$	**$CHCl_2Br$**	**$CHClBr_2$**	**$CHBr_3$**	**TOC**
1	0.16	0.13	0.12	0.12	14.0
2	0.21	0.18	0.17	0.15	16.6
3	0.20	0.17	0.16	0.18	16.6
MEAN ± SD	0.19 ± 0.028	0.16 ± 0.028	0.15 ± 0.027	0.15 ± 0.029	15.8 ± 1.50

The absorption of THMs into polyurethane was also investigated. Reference water without disinfectant and containing 100 µg/L THMs was exposed to the polyurethane coupons for 3 days, after which THMs were measured in triplicate samples. The THMs decreased by 21.3, 34.8, 38.6 and 40.2% for $CHCl_3$, $CHCl_2Br$, $CHClBr_2$ and $CHBr_3$, respectively (Table 2-5). Interestingly, as the number of bromines in the THM molecule increased, so did the amount of absorption of that THM into the polyurethane. The structure of the polyurethane is unknown and therefore it is difficult to speculate why the presence of bromine increases sorption into the polyurethane. Bromine has a larger electron field and would interact with a large electron field on the surface of the polyurethane. This is one possible explanation. A One-way ANOVA test was performed ($\alpha = 0.05$) on the data where the analytes measured were statistically different from one another ($p < 0.001$).

During the leaching study approximately 15.8 µg/cm^2 or 6.44 mg/L TOC was leached from the coupons. This was a much larger concentration than was seen during the study (1.75 mg/L maximum). During the 30 testing period, water changes were performed frequently in the first few days. The frequent water changes would minimize changes seen in the maximum amount of TOC leached from the polyurethane. Therefore, the

increase in TOC seen during the leaching test is indicative of the TOC levels if the coupons were in contact with the potable water for three days.

2.1.6.3.3 Haloacetic Acids (HAA5)

The HAA5 are comprised of monochloroacetic acid (MCAA), dichloroacetic acid (DCAA), trichloroacetic acid (TCAA), monobromoacetic acid (MBAA) and dibromoacetic acid (DBAA). The EPA regulates total HAA5 species concentration to 60 μg/L (EPA, 2003). The major HAA species that formed was MCAA, with lesser amounts of DCAA and TCAA. There was no bromide added to the water therefore it is logical that none of the species containing bromine were detected. The amount of HAA5 was minimal and the same for both the no disinfectant test water with polyurethane coupons and its control; thus, polyurethane does not leach HAA5. The monochloraminated test water formed approximately 5 μg/L more HAA5 than its corresponding control; this would be due to the presence of free chlorine in equilibrium with the ammonia and monochloramine. Limited HAA5 formed in the disinfected control waters due to the background level of TOC in the reference water.

Substantial amounts of HAA5 formed (approximately 30 μg/L) in the chlorinated water in the presence of the polyurethane coupons when compared to the controls (Figure 2-17). When the data were plotted as a rate of HAA5 formation in terms of $\mu g/cm^3$/day HAA5 (Figure 2-18), the chlorinated water had the highest rate between days 1 and 4 and then decreased. This is consistent with the TOC data that indicated that the rate of TOC leaching was the greatest in the initial contact of polyurethane with test water. It is also consistent with the higher rate of chlorine decay in the first days of the test. MCAA comprised most of the HAA5 (85%) that were present which is to be expected in chlorinated waters if haloacetic acids are formed (Bayless, 2008). Day 9 also formed large amounts of HAA5 compounds (approximately 30 μg/L) which is most likely due to the high TOC leached on this day as well as the long contact time (5 days).

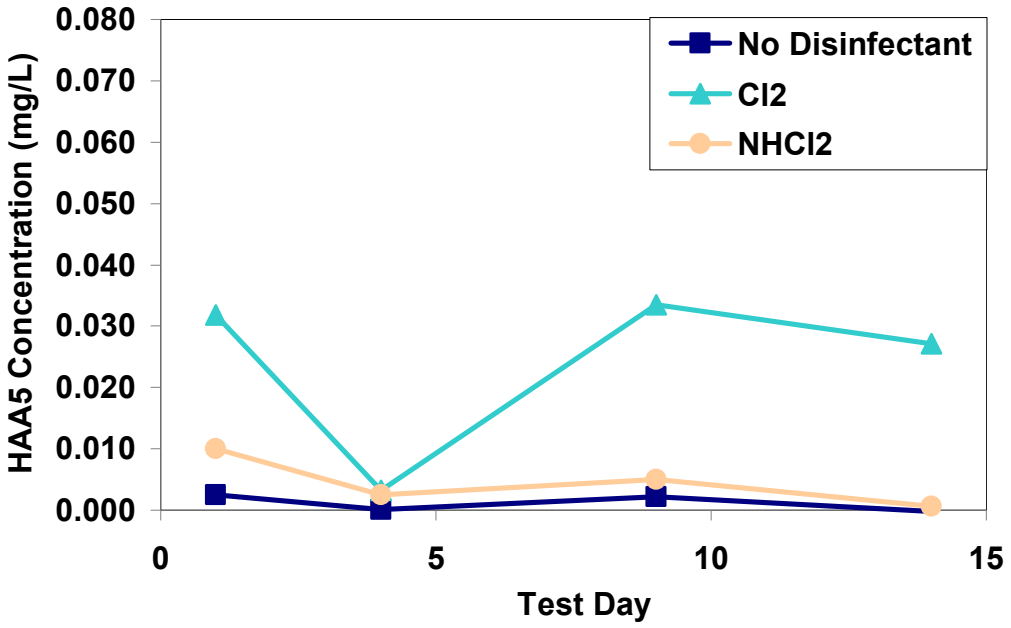

Figure 2-17. HAA_5 concentrations as a function of exposure time for all three water types and corrected for controls.

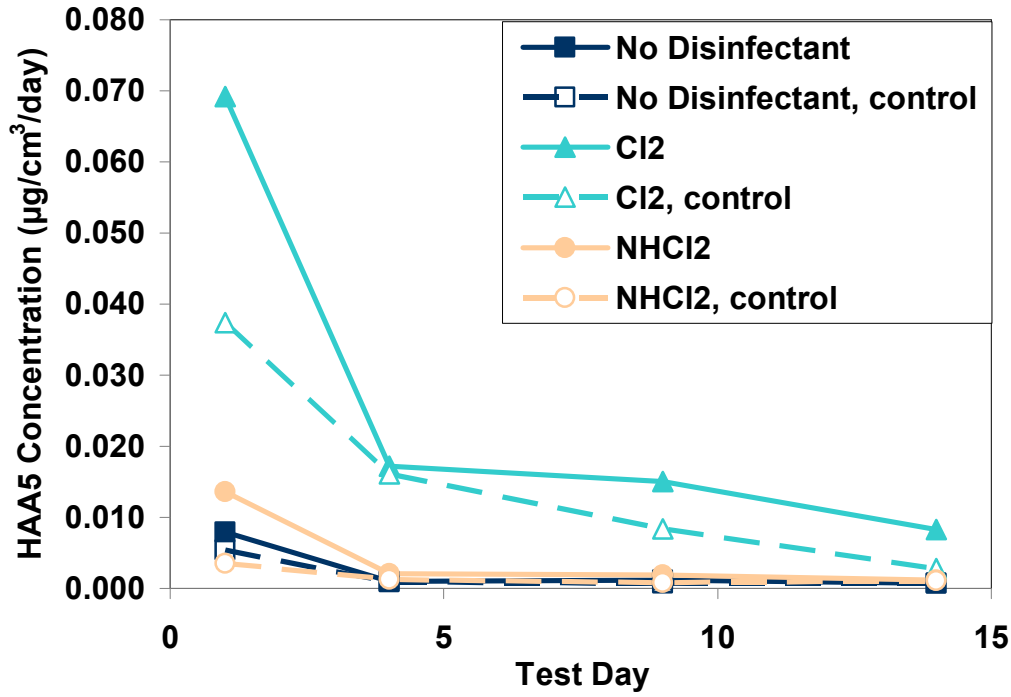

Figure 2-18. HAA_5 rate of leaching over time, as $\mu g/cm^3$/exposure time for all three water types.

2.1.6.3.4 Semi-Volatile Organic Chemicals (SVOCs)

SVOCs are a specific group of organic compounds that are extractable using methylene chloride liquid-liquid extraction and detectable by gas chromatograph-mass spectrometry (GC-MS). An organic compound found in the test waters in contact with polyurethane coupons and not found in the corresponding control is chlorophenylisoscyanate (Table 2-6). This compound was detected in all the chlorinated samples and the day 1 chloraminated sample; it was not detected in the no disinfecatant water. The compound 2,4,-di-t-butyphenol was also detected and confirmed with a standard. This compound was present in both samples and controls and therefore not related to th the presence of polyurethane. Properties of these compounds are presented in Table 2-7. The compounds were not found in all of the waters or found in both the samples and controls and therefore it cannot be conclusively stated that these compounds are leached from the polyurethane.

Table 6. Summary of organic chemicals found in the GC-MS Chromatograms of the leachate water with polyurethane coupons and corresponding controls. A numerical value indicates a measured concentration and confirmation of identification with a chemical standard. A check mark indicates that the compound was detected and tentatively identified based on ≥ 90% library matching with NIST mass spectra.

Sample ID (CAS #)		**No Disinfectant (µg/L)**					**Cl_2 (µg/L)**					**NH_2Cl (µg/L)**			
Sampling Day		1 d[1]	4 d	9 d	14 d		1 d	4 d	9 d	14 d		1 d	4 d	9 d	14 d
Chlorophenyl isocyanate (3320-83-0)	Sample						✓	✓	✓	✓		✓			
	Control														
2,4-Di-,tert-butylphenol[2] (96-76-4)	Sample	3.27	5.70				0.79			3.85		1.79		1.85	2.80
	Control	0.63		0.76				3.80				2.08			

[1] Sampling Day

[2]Identification confirmed by GC/MS retention time and mass spectrum match that of a purchased standard.

Table 7. Properties of organic compounds detected by GC-MS.

Compound Name (CAS #)	Odor Descriptor	Color	Acute Oral LD_{50}	Acute Dermal LD_{50}	Irritant?
Chlorophenyl isocyanate (2004) (3320-83-0)[1]	slight corn oil	pale yellow	4977 mg/kg[2]	>2000 mg/kg[3]	no[3]
2,4-Di-,tert-butylphenol (2005) (96-76-4)	N/A[5]	pale yellow	700 mg/kg[4]	2200 mg/kg[3]	possible

[1]Identification tentative based on match of mass spectrum of sample and NIST library.

Toxicology test animal: [2]rat; [3]rabbit; [4]mouse

[5] N/A = Not Available

2.1.6.3.5 Odor

Water samples from all treatments were evaluated for odor by 3-6 members of a human panel trained in Flavor Profile Analysis (Standard Method 2170). The FPA intensity scale is: 0 is odor free (OF), 4 is weak and 8 is moderate. Many drinking water customers begin to complain when a non-chlorinous odor intensity reaches 2 or above (Burlingame and Mackey, 2007).

There were distinct odors associated with the polyurethane coupons. To some of the panelists there was a "putrid" smell which was also described as a "smelly locker room", "wet socks" and "organic". Another set of panelists described the odor as "pleasant" or "sweet chemical" and "vegetative". These descriptors were found in all of the samples; yet, the prominence of the odors varied in each water type. The chlorine smell was also seen in both the water with chlorine and chloramines. In fact several of the samples (most notably day 1, 9 and 30) had concentrations of chlorine < 0.10 mg/L Cl_2 and therefore were not likely to be the source of such a strong odor. The controls samples were only described as "chlorinous". Therefore, the increase in odor intensity comes

from the interaction of the test water and the polyurethane. The odors did not exceed an odor intensity of 8 in the odor panel or a "moderate" intensity.

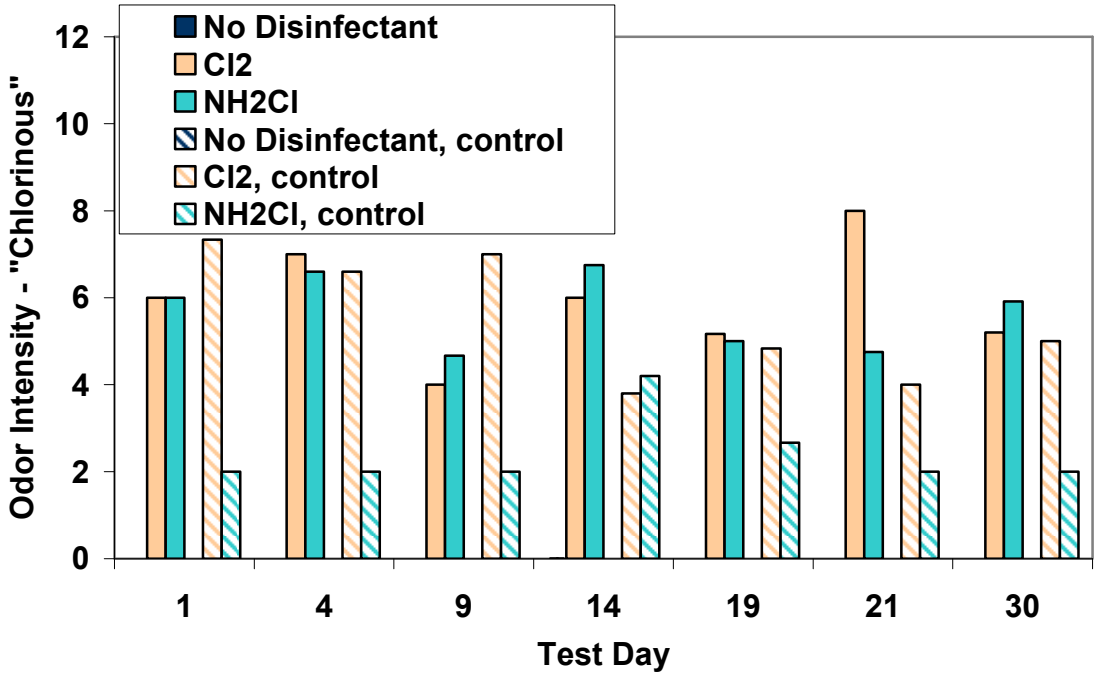

Figure 2-19. Odor intensity with controls, for "chlorinous" odor, as a function of time.

The presence of the pleasant smell was what separated the water odors most appreciably (Figures 2-20). With no disinfectant present the "pleasant odor" was detected on the first day. The chlorinated test water did not detect the "pleasant" odor until day 4, and not until day 9 in the presence of monochloramine (Figure 2-20). The pleasant odor was also the most difficult to characterize and to detect and was described as: organic, vegetative, pleasant, sweet, sweet chemical, beets and burning meat (still described as a pleasant odor). The panelists often took several "sniffs" to be able to describe the odor accurately. Over the course of the tests there was not a decrease in the average intensity of the waters; therefore it is not possible to determine how long these odors will be present in the water.

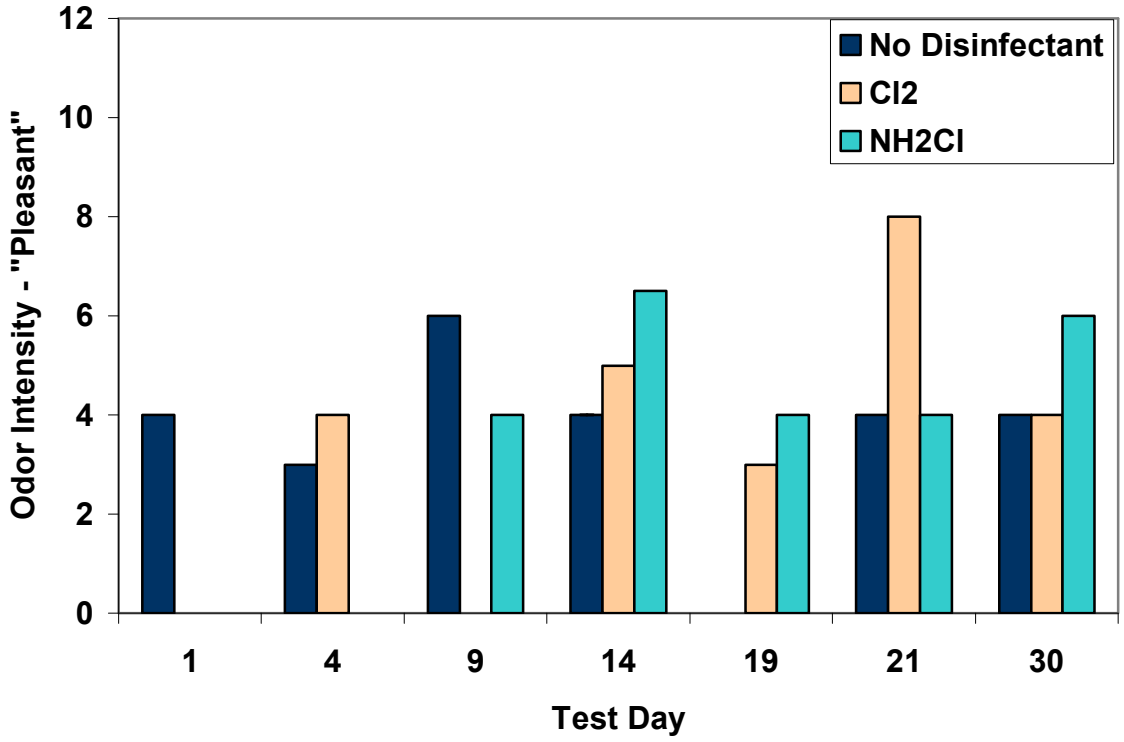

Figure 2-20. Odor intensity, for “pleasant” odor, as a function of time.

The odors detected in the FPA test cannot be directly related to the SVOC identified. Additionally, perception of odor is related to the composite of all compounds present, and many odorants are detectable by the human nose at ng/L concentrations (Burlingame and Mackey, 2007), which is lower than the detection limit of the SVOC method used. The extraction process used to measure SVOCs would not have extracted smaller chained molecules (volatile organic compounds) that could be responsible for these odors; more tests should be performed to confirm this.

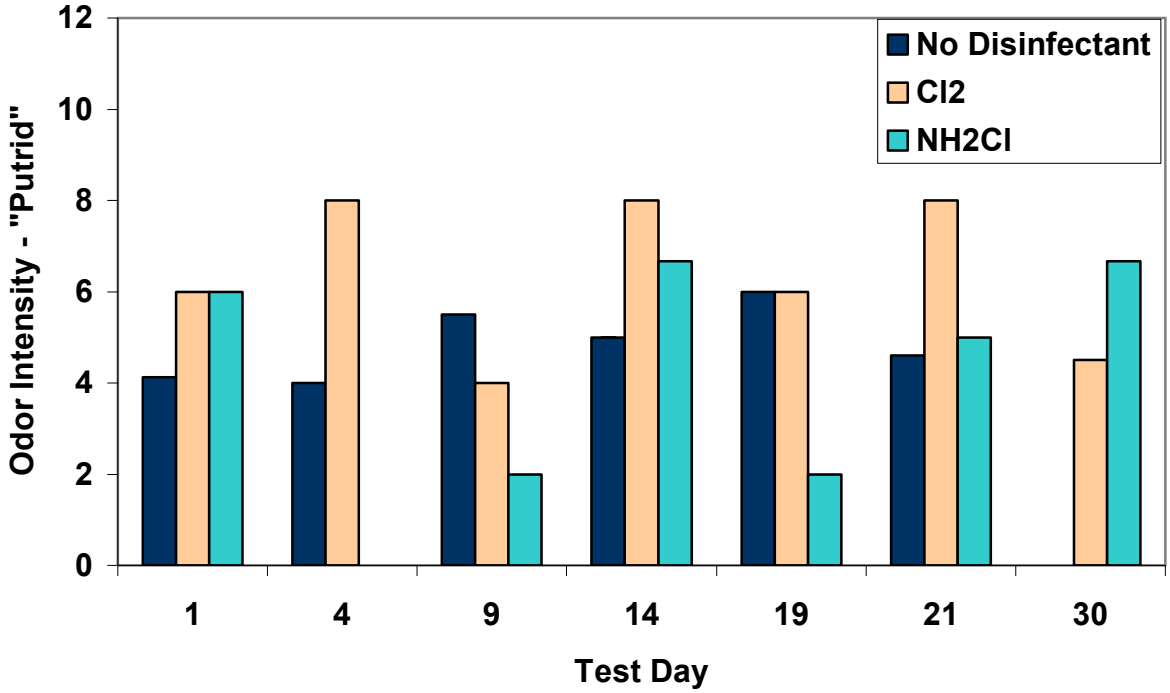

Figure 2-21. Odor intensity, for "putrid" odor, as a function of time.

2.1.6.3.6 Physical Changes to Polyurethane Coupons

A color change was noted after the polyurethane was exposed to the test waters (Figure 2-22). The chlorine-exposed polyurethane coupons had the most noticeable change followed by those exposed to monochloramine (which is always in equilibrium with free chlorine). The change was a "graying" and darkening of the purplish color of the unexposed polyurethane. Though no physical or chemical analyses were preformed on the polyurethane material, the color change strongly supports the idea that chlorine reacted with the polyurethane. This could be the source of an increased leaching of TOC and odors.

Figure 2-22. Polyurethane coupons after exposed to no disinfectant (1), monochloramine (2) and chlorine (3). (Photo by Heather Johnson)

2.1.6.4 Discussion

In the presence of polyurethane lining, the aqueous pH decreased to 6 regardless of disinfectant used. It is possible that short chained carboxylic acids are leached from the polymer. Larger chained carboxylic acids were found to leach from other polyurethanes (Kebir *et al.*, 2007). While larger chained carboxylic acids were not found, the liquid-liquid extraction method used does not extract smaller more volatile compounds and therefore would not be detected. Parallel studies were conducted using the same test waters with epoxy and cement lining materials. Epoxy coupons did not impact pH, while cement (due to the leaching of calcium carbonate) increased the pH to 11 until day 9.

TOC was leached from polyurethane; however by day 15, the TOC leached decreased to background levels. On day 14 the leachate was exposed to the coupons for 3 days and there was an increase in TOC leached. It is possible that polyurethane could still leach TOC with extended exposure times. Alkalinity was not altered and if the TOC leached contained acidic compounds there should be a respective decrease in alkalinity, which was not seen. Therefore, when the TOC leachate is fully characterized a better assessment could be made. Similarly to polyurethane, epoxy leached TOC, and reached background level at 14 exposure days as well. Most of the TOC was leached from the epoxy by the second exposure day unlike polyurethane that had the most TOC leached on the ninth exposure day. The epoxy has more soft segments (shown by its "spongy" texture) than polyurethane. Therefore the most logical result is that the epoxy would leach more TOC over a longer period of time. However, the data illustrate the contrary.

This is an excellent example of how polymer chemistry does not always follow what one would "expect". Cement had increased TOC that did not go to background until day 9. Cement used to line potable water piping still contains organic material and therefore when in contact with water the organic material is leached into the water.

Chlorine residual was decreased to <0.10 mg/L Cl_2 for the first 9 days as well as extended exposure times (> 2 days). Monochloramine residual was also decreased on extended exposure times as seen on days 4, 9, 14, 19 and 30. Chloramines (product) are formed from the reaction of chlorine and ammonium (reactants) to form an equilibrium. Typically, free chlorine composes 10% of disinfectant residual for monochloramine. It is possible that chloramine degrades through the degradation of chlorine. The degradation of chlorine would shift the equilibrium and reduce chloramine and form more chlorine. Epoxy, again, reacted similarly to polyurethane by decreasing the amount of chlorine residual which, with both polymers, is decreased by reaction, in part, to form disinfection by-products (DBPs). Cement also had decreased levels of chlorine; but, its cause is most likely due to the large amount of inorganic particulate matter in the water.

Nitrogen-ammonia was only found in chloraminated water. For monochloramine, there was no trend in the disinfectant degradation and ammonia measured. Humar et al. studied the impact of water quality on the extraction of metals from wood treated with chromated copper borate (Humar *et al.*, 2004). An increase in ammonia concentration increased the amount of copper and chromate in the leachate. In this experiment, copper and chromate were found within 0.1% of the EPA limit. However, for the future research of polyurethane in the presence of chloramine, it is an important note. A decrease in chloramine residual implies an increase in ammonia concentration. Although, it is not a strong correlation, polyurethane has many different types of surface chemistry, it could impact the future polyurethane research. Epoxy and cement-mortar, along with polyurethane, showed little impact on ammonia concentrations.

Alkalinity had little variation; this variation was not dependant on pH, disinfectant used or exposure time. Polyurethane had no impact on water quality when alkalinity is

considered. The large impact to pH and the lack of impact on alkalinity is conflicting. Yet, it has been reported in previous polymer lining studies where pH changed and alkalinity did not (Whelton and Dietrich, 2008). Epoxy did not impact the alkalinity. Cement mortar, which had a large amount of lime leached from the coupons to exceed 500 mg/L as $CaCO_3$, but by the fifteenth exposure day the alkalinity was to background level.

Polyurethane was shown to not impact hardness or any other elements or metals that would impact health. No trends within the elements leached or sorbed into the polyurethane were found. Polyurethane foam has been used to sorb toxins, especially elements, from liquid food products to determine their concentration (Haugen *et al.*, 2004, Klein, 1985, T. V. Nguyen, 2006). Desorption of elements from the polyurethane foam is difficult and has been studied extensively to optimize desorption and typically uses organic solvents and extreme conditions, such as $pH < 2$. Desorbed compounds and elements would need to be analyzed for each polyurethane but will most likely require specific solvents and extreme conditions as well. Epoxy also held no trends in the elemental analysis. Cement increased the hardness due to the $CaCO_3$ dissolving into the water, as mentioned previously.

Total solids were comprised of dissolved solids, and did not have a statistically significant change due to the polyurethane coupons in the water. Hardness, as calcium and magnesium, was also not shown to significantly change in the presence of the polyurethane coupons. Elemental analysis had some variation but no metal or element exceeded EPA regulated levels. Epoxy did not show any impacts to total solids. Cement mortar would increase the pH and therefore decrease the solubility of the calcium carbonate leached from the coupons. The leachate was supersaturated which resulted in a hazy translucent appearance. On the thirtieth exposure day the hardness was still above background level; however, the hazy appearance of the water was no longer noticeable. Epoxy did not have a significant impact on total solids. It is important to note that polyurethane and epoxy both did not impact elemental analysis as well as total solids.

Cement mortar coupons leached a large amount of metals which resulted in a large increase in elemental analysis, specifically calcium and magnesium.

Trihalomethanes were not detected in chlorinated water in the presence of polyurethane coupons. Formation of THMs from TOC extracted from the polyurethane was also shown not to form any THMs. This supports the lack of THMs in the presence of polyurethane and chlorine. It is also hard to say they leach out; however, in the short term polyurethane could potentially decrease the THMs to improve water quality. Trihalomethanes were formed in the presence of cement mortar coupons as well as epoxy coupons, where both coupons increased TOC. Both of these formations occurred at pH > 8, which are more favorable conditions for THM formation, and not what is seen in the polyurethane coupons. The analysis has not be finalized and therefore cannot be discussed quantitatively.

Haloacetic acids were formed, mainly as monochloroacetic acid (MCAA), to the concentration of 30 μg/L in chlorinated water, where HAA_5 are regulated to 60 μg/L (EPA, 2003). The test waters with chloramine and no disinfectant formed HAAs at or below the 10 μg/L level. Therefore, the HAAs formed under these conditions represent 50% of the total HAA5 allotment for the water treatment facilities and could cause a water treatment plant to exceed the EPA regulated levels. HAA_5 concentration did not decrease within 15 days, therefore, it cannot be stated from this research when and how much the HAA formation concentration would decrease. Previous research determined TOC to leach from phenolic based polyurethanes for 46 days (Yokoyama *et al.*, 2007). The presence of TOC leaching from the polyurethane leaves the ability of chlorine in the water to react to form HAAs. HAAs were present in epoxy coupons as well but less than in polyurethane coupons, which due to the pH conditions most likely. Polyurethane coupons only formed HAAs where epoxy coupons formed both THMs and HAAs. The combination of pH and the composition of TOC in the leachate will impact the quantity and quality of the formation of DBPs.

The odor from the polyurethane coupons with both chlorinated and monochloraminated waters had an odor descriptor of "chlorinous" and either pleasant as "sweet chemical" or putrid as "locker room". If the panelist detected the chorine odor then the other odors were masked. The controls samples were only described as "chlorinous". Therefore, the increase in odor intensity comes from the interaction of the test water and the polyurethane. The panelists are most likely detecting different odorous compounds. There was no correlation between the organic found in the leachate and the odors described by the panelists. Strong odors were also associated with epoxy and cement mortar, "burning plastic" and "wet cement" respectively. By the fourteenth exposure day these odors were minimal.

2.1.6.5 Conclusions

- In the presence of polyurethane, the test water pH was reduced from pH 8 to approximately pH 6. The pH drop was observed within 24 hours and persisted for 30 days. The source of the pH drop is not known. Changes in concentrations of metals and non metals, or SVOCs measured cannot account for the 2-3 pH unit decrease. Analytes that were not measured in this study, such as strong acid anions, carbon dioxide, or volatile organic acids, should be investigated. If metal piping is not coated further in the piping infrastructure, the pH of 6 would increase the rate of corrosion of that pipe (Edwards and Dudi, 2004). The US EPA suggests that the pH to be within 6.5-8.5 where the polyurethane reduces the pH to below the required limit (EPA, 2003).
- Free chlorine was consumed in the presence of polyurethane and its consumption was greater than that for monochloramine. The rate of chlorine decay was greater during days 1-4 than in later exposure times.
- Organic carbon was leached from polyurethane, with a greater amount leached in the presence of chlorine than for no disinfectant or monochloramine. However, due to the large standard deviation this increase was not statistically different and more replicates should be performed to confirm or reject this. TOC leached to approximately 1 mg/L in the first 24 hour contact period; afterwards, the rate of

TOC leaching declined over time for all disinfectant treatment types. The TOC leached has the potential to promote biofilm growth. After 15 days of exposure TOC leached to approximately 0.1 mg/L above background indicating that the TOC leached will lessen after 2 weeks of use. Leached TOC reacted with free chlorine to form up to 30 ug/L HAAs but no THMs were detected. The low pH of 6 would favor HAA formation over THM formation.

- Weak to moderate odor intensities were released from the polyurethane and persisted for the 30 days of this study. These odor intensities would be objectionable to consumers. The odor was described as "pleasant" or "putrid" by different people on the odor panel. While the presence of a disinfectant caused a "chlorinous" odor, the disinfectant did not substantially alter the intensity or descriptors of the polyurethane odors. The identity of the odorants was not determined.

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4. APPENDIX A – DATA FOR HENRY'S LAW CONSTANTS

Percent decrease of Henry's law constant with TOC (n=3)

Compounds, Temp., and conc. / TOC (mg/L)	Geosmin				Trichloromethane
	25 ºC		40 ºC		40 ºC
	100ng/L *	122µg/L	100ng/L	122µg/L	80µg/L
0	0	0	0	0	0
1	22.2	13.2	17.5	19.7	-2.0
2	29.6	16.9	31.4	21.8	9.0
5	29.6	21.6	26.5	11.8	10.3

* Result from previous study by Pinar Omür-Ozbek and Dietrich 2005

Summary of Conditions for Henry's Law Constant of Geosmin versus TOC Trial 1

Vol of Vial	0.575	L
Vol of Headspace	0.375	L
Vol of Liquid	0.2	L
Vol of Std Added	2.00E-05	L
[Std added]	1.00E+06	ng/L
Mass in flask	2.00E+01	ng/L
Temp	40	°C
Conc	100	ng/L

Chart Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 1

[TOC]	**m**	**Std Dev**
mg/L		
0	0.00705	0.00056
1	0.00572	0.00118
2	0.00484	0.00175
5	0.00518	0.00045

Graph Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 1

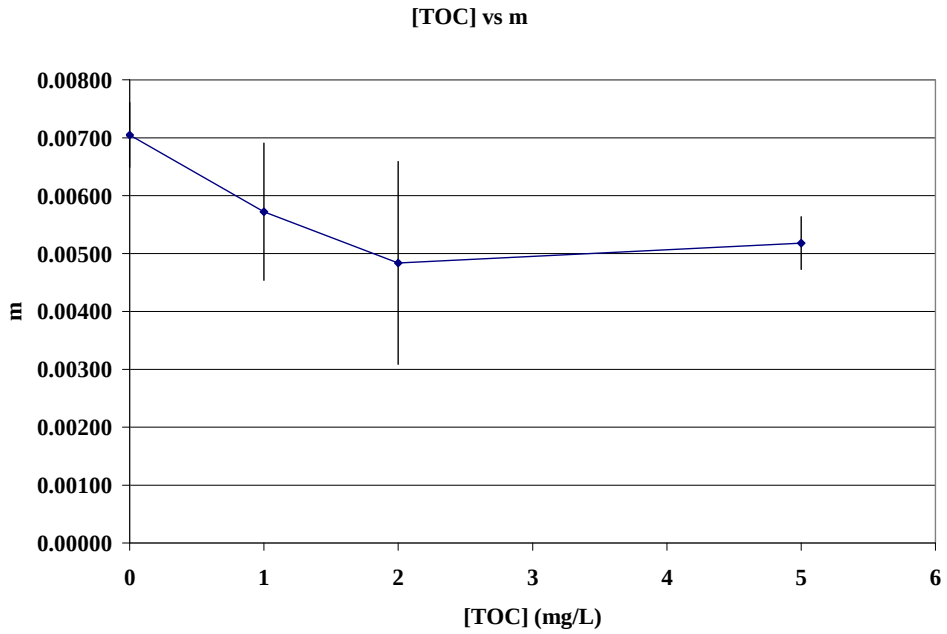


Chart Summarizing Anova statistical test on Results for Henry's Law Constant Trial 1

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Column 1	3	0.021	0.00705	3.1223E-07
Column 2	3	0.017	0.00581	1.40374E-06
Column 3	3	0.015	0.00484	3.06207E-06
Column 4	2	0.01	0.00518	2.06625E-07

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	8.2E-06	3	2.7E-06	1.960134185	0.2086	4.3468
Within Groups	9.76E-06	7	1.4E-06			
Total	1.8E-05	10				

Summary of Conditions for Henry's Law Constant of Geosmin versus TOC Trial 2

Vol of Vial	0.043	L
Vol of Headspace	0.033	L
Vol of Liquid	0.01	L
Vol of Std Added	2.45E-05	L
[Std added]	5.00E+04	µg/L

Mass in flask	1.23E+00	µg/L
Temp	40	°C
Conc	122	µg/L

Chart Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 2

[TOC]	**m**	**Std Dev**
mg/L		
0	0.02507	0.00167
1	0.02013	0.00160
2	0.01960	0.00161
5	0.02370	0.00157

Graph Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 2

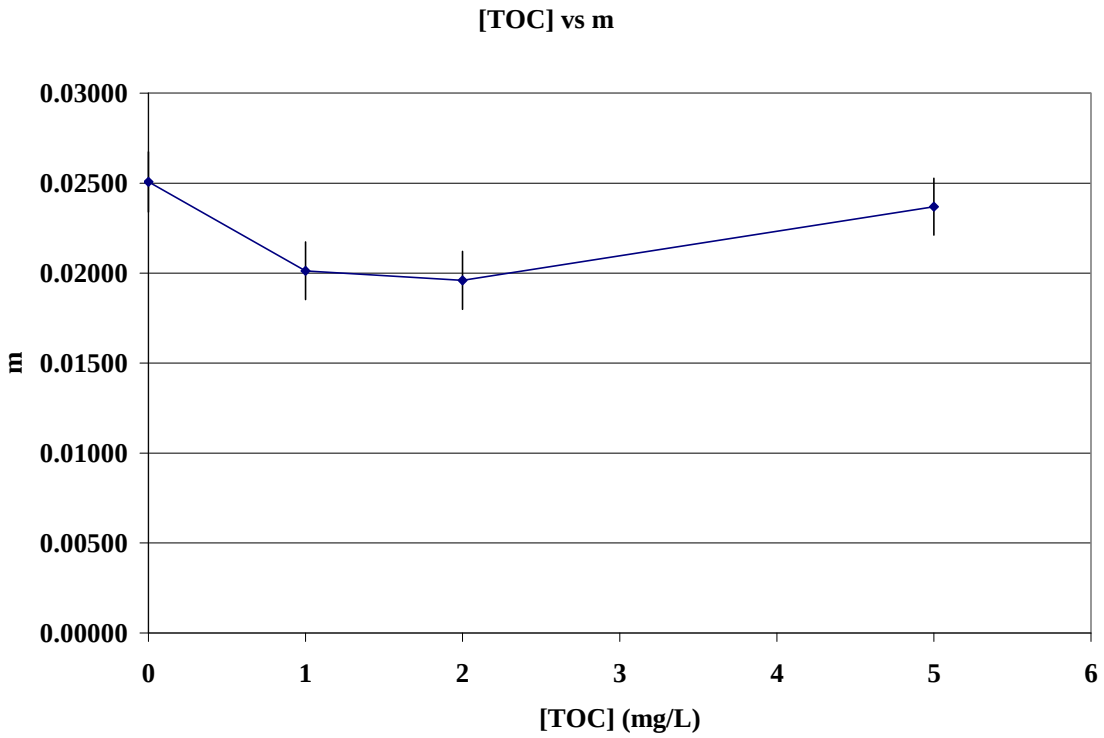


Chart Summarizing Anova statistical test on Results for Henry's Law Constant Trial 2

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Column 1	3	0.0752	0.0251	2.79E-6
Column 2	3	0.0604	0.0201	2.57E-6
Column 3	3	0.0888	0.0296	0.0003022
Column 4	3	0.0663	0.0221	8.80E-6

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	0.000153	3	5.10E-5	0.645	0.608	4.07
Within Groups	0.000633	8	7.91E-5			
Total	0.000786	11				

Summary of Conditions for Henry's Law Constant of Geosmin versus TOC Trial 3

Vol of Vial	0.043	L
Vol of Headspace	0.033	L
Vol of Liquid	0.01	L
Vol of Std Added	2.45E-05	L
[Std added]	5.00E+04	µg/L
Mass in flask	1.23E+00	µg/L
Temp	25	°C
Conc	122	µg/L

Chart Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 3

[TOC]	**m**	**Std Dev**
mg/L		
0	0.00529	0.00048
1	0.00459	0.00031
2	0.00440	0.00011
5	0.00415	0.00026

Graph Summarizing Results y of Data and Conditions for Henry's Law Constant Trial 3

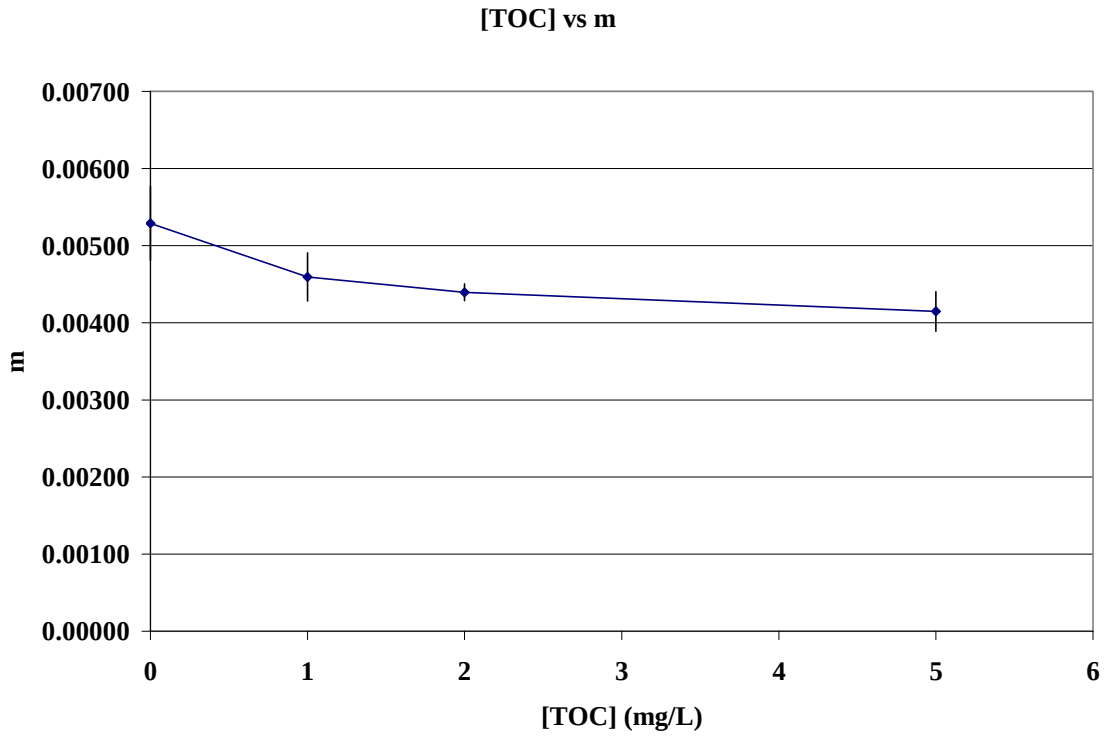


Chart Summarizing Anova statistical test on Results for Henry's Law Constant Trial 3

SUMMARY

Groups	*Count*	*Sum*	*Average*	*Variance*
Column 1	3	0.01587	0.005291	2.33E-7
Column 2	3	0.01378	0.004594	9.73E-8
Column 3	3	0.01319	0.004396	1.168E-8
Column 4	3	0.01244	0.004147	6.54E-8

ANOVA

Source of Variation	*SS*	*df*	*MS*	*F*	*P-value*	*F crit*
Between Groups	2.17E-6	3	7.23E-7	7.111	0.01204	4.066
Within Groups	8.14E-7	8	1.017E-7			
Total	2.98E-6	11				
Total	2.98E-6					

5. IRB APPROVAL FOR HUMAN SUBJECTS

VirginiaTech

Office of Research Compliance
Institutional Review Board
1880 Pratt Drive (0497)
Blacksburg, Virginia 24061
540/231-4991 Fax: 540/231-0959
E-mail: moored@vt.edu
www.irb.vt.edu
FWA00000572(expires 7/20/07)
IRB # is IRB00000667.

DATE: January 23, 2007

MEMORANDUM

TO: Andrea M. Dietrich
Pinar Omur
Heather Johnson

FROM: David M. Moore

Approval date: 2/2/2006
Continuing Review Due Date:1/18/2007
Expiration Date: 2/1/2007

SUBJECT: **IRB Amendment Approval:** "Taste and Odor Testing of Plumbing Materials" , IRB # 06-042

This memo is regarding the above referenced protocol which was previously granted approval by the IRB on February 2, 2006. You subsequently requested permission to amend your IRB application. Since the requested amendment is nonsubstantive in nature, I, as Chair of the Virginia Tech Institutional Review Board, have granted approval for requested protocol amendment, effective as of January 22, 2007. The anniversary date will remain the same as the original approval date.

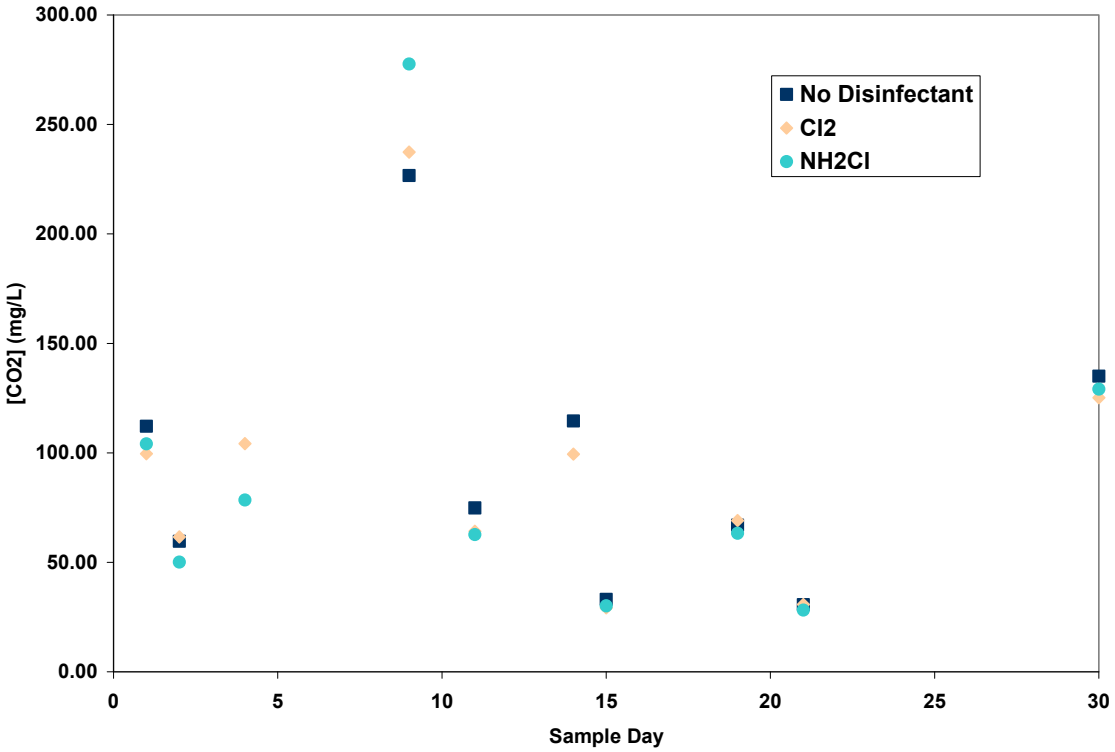
As an investigator of human subjects, your responsibilities include the following:

1. Report promptly proposed changes in previously approved human subject research activities to the IRB, including changes to your study forms, procedures and investigators, regardless of how minor. The proposed changes must not be initiated without IRB review and approval, except where necessary to eliminate apparent immediate hazards to the subjects.
2. Report promptly to the IRB any injuries or other unanticipated or adverse events involving risks or harms to human research subjects or others.
3. Report promptly to the IRB of the study's closing (i.e., data collecting and data analysis complete at Virginia Tech). If the study is to continue past the expiration date (listed above), investigators must submit a request for continuing review prior to the continuing review due date (listed above). It is the researcher's responsibility to obtained re-approval from the IRB before the study's expiration date.
4. If re-approval is not obtained (unless the study has been reported to the IRB as closed) prior to the expiration date, all activities involving human subjects and data analysis must cease immediately, except where necessary to eliminate apparent immediate hazards to the subjects.

cc: File
Department Reviewer: William R. Knocke

6. CARBON DIOXIDE AND PH DISCUSSION

CO_2 concentration (mg/L) required to cause the decrease seen in pH in water in contact with polyurethane coupons



The pH dropping while the alkalinity remained constant can only be explained by the addition of CO_2 to the system. If you recall a form of polyurethane is polyurethane foam where the addition of water to the system yields CO_2 to give a foam consistency. The reaction is a 100% solids two component reaction therefore not a polyurethane foam. The CO_2 would form in a 1:1 molar ratio with the number of polyurethane linkages formed. The polyurethane analyzed was polyurethane and not polyurethane foam and therefore hydrolysis would not be the mechanism to produce CO_2. Therefore, the source of the carbon dioxide cannot be known without further analysis of the structure of the polyurethane. Carbon dioxide was not analyzed for by ANSI/NSF 61. However, the concentration of CO_2 that would have given such pH decreases were calculated (Figure above). At most 300 mg/L CO_2 would be needed; CO_2 is soluble to the 2000 mg/L

(Oldenburg and Lewicki, 2005). Therefore, CO_2 is soluble to this level but where did the CO_2 come from. However, there were no visual changes to the surface of the polyurethane (not including discoloration). Surface analysis would need to be performed to confirm or reject this hypothesis.

Calculations:

CALCULATIONS:

$$[CO_2] = \left|10^{-pH_{INI}} - 10^{-pH_{FIN}}\right| \bullet Alkalinity\left(as\frac{mgCaCO_3}{L}\right) \bullet \frac{1g}{1000mg} \bullet \frac{1molCO_2}{100gCaCO_3} \bullet \frac{2molH^+}{1molCaCO_3} \bullet 10^{-pKa_{CO_2}}$$

where $pKa_{CO2} = 6.35$

Calculations for CO_2 produced in water with no disinfectant

	No Disinfectant				
	pH			Alkalinity	$[CO_2]$
Test Day	Average	Control	Initial	Average	mg/L
1	5.80	7.71	7.85	36.58	112.21
2	6.07	8.07	8.03	35.94	59.56
4	4.55	5.52	7.99		
9	5.50	7.74	6.94	37.53	226.61
11	5.96	8.04	8.03	35.15	74.82
14	5.80	7.75	8.02	36.73	114.53
15	6.31	7.91	8.01	34.99	33.06
19	5.98	7.72	8.02	33.09	67.02
21	6.32	7.61	8.03	33.09	30.64
30	5.68	7.67	8.04	32.93	134.96

Calculations for CO_2 produced in chlorinated water

	Chlorine				
	pH			Alkalinity	$[CO_2]$
Test Day	Average	Control	Initial	Average	mg/L
1	5.87	8.16	8.04	37.53	99.58
2	6.07	7.72	8.01	37.53	61.62
4	5.83	8.03	8.01	35.78	104.22
9	5.46	7.86	7.98	34.99	237.39
11	6.06	7.84	8.02	37.53	64.18
14	5.88	8.89	7.93	38.32	99.38
15	6.38	8.00	8.00	36.42	29.19
19	6.00	7.93	8.00	35.47	69.11
21	6.36	7.50	8.00	36.73	30.81
30	5.75	7.68	8.02	35.78	125.16

Calculations for CO_2 produced in monochloraminated water

	Monochloramine				
	pH			Alkalinity	$[CO_2]$
Test Day	Average	Control	Initial	Average	mg/L
1	5.901	9.142	8.04	42.43	104.16
2	6.258	9.394	8.03	46.87	50.07
4	5.993	9.032	8.03	39.58	78.46
9	5.505	8.991	8.743	45.13	277.53
11	6.113	9.152	8	41.80	62.66
14	5.228	9.699	8.031		
15	6.360	8.036	7.999	35.78	30.09
19	6.100	9.085	7.97	41.01	63.26
21	6.439	8.705	7.963	40.53	28.17
30	5.800	8.907	7.988	41.64	129.08

7. SVOC GC-MS SPECTRA SUMMARIES

No Disinfectant
Day 1
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\007.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 9:03 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 9

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	15.67	0.72	C:\Database\NIST98.L			
			Nonanoic acid	113427	000112-05-0	96
			Nonanoic acid	113428	000112-05-0	95
			Nonanoic acid	20156	000112-05-0	93
2	19.54	0.47	C:\Database\NIST98.L			
			1-Undecanol	13829	000112-42-5	91
			1-Tridecanol	13019	000112-70-9	87
			Cyclodecane	13064	000293-96-9	86
3	20.08	0.44	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	125776	000096-76-4	94
			Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4	93
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	93
4	20.87	0.50	C:\Database\NIST98.L			
			.alpha.-D-Glucose	25791	000492-62-6	38
			Nonanoic acid	20156	000112-05-0	38
			D-Glucose, 6-O-.alpha.-D-galact...	25771	000585-99-9	37
5	21.47	1.25	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	80
			Di-n-butyl Phthalate	28	000084-74-2	9
6	22.50	3.91	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	96
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	12
			Diacenaphtho[1,2-b:1',2'-d]thio...	128736	000203-42-9	9
7	23.37	0.43	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	96
			Heptadecane	112321	000629-78-7	90
			Hexadecane	112409	000544-76-3	87
8	24.90	0.82	C:\Database\NIST98.L			
			Octadecane	112350	000593-45-3	98
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	97
9	25.01	0.79	C:\Database\NIST98.L			
			Hexadecane, 2,6,10,14-tetramethyl-	17086	000638-36-8	49
			Tritetracontane	17076	007098-21-7	49
			Dodecane, 2,6,10-trimethyl-	112559	003891-98-3	49
10	25.21	0.61	C:\Database\NIST98.L			

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			Isopropyl Myristate	110206	000110-27-0	83
			Isopropyl Myristate	4614	000110-27-0	49
			Tetradecanoic acid	114898	000544-63-8	30
11	25.75	3.51	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	9
			Benzyl butyl Phthalate	36	000085-68-7	2
12	26.01	0.69	C:\Database\NIST98.L			
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	95
			Cyclotetradecane	111326	000295-17-0	95
			1-Heptadecanol	13564	001454-85-9	91
13	26.26	1.02	C:\Database\NIST98.L			
			Nonadecane	16515	000629-92-5	98
			Nonadecane	112380	000629-92-5	92
			Nonadecane	112381	000629-92-5	92
14	26.38	0.94	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	42
			Benzyl butyl Phthalate	36	000085-68-7	16
			Di-n-butyl Phthalate	28	000084-74-2	12
15	26.77	0.49	C:\Database\NIST98.L			
			Oxirane, tetradecyl-	108844	007320-37-8	41
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	38
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	38
16	26.99	15.31	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	94
			Diethyl Phthalate	14	000084-66-2	7
17	27.51	1.16	C:\Database\NIST98.L			
			Eicosane	112345	000112-95-8	95
			Heptadecane	16420	000629-78-7	91
			Dotriacontane	112351	000544-85-4	91
18	27.76	0.63	C:\Database\NIST98.L			
			1-Hentetracontanol	16591	040710-42-7	18
			Cyclohexanol, 1R-4-acetamido-2,...	5394	1000153-72-8	14
			D-Glucopyranoside, 4-O-decyl-	6569	1000158-00-4	14
19	28.49	0.76	C:\Database\NIST98.L			
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	90
			1-Eicosanol	112640	000629-96-9	90
			1-Octadecanol	5273	000112-92-5	87
20	29.06	0.58	C:\Database\NIST98.L			
			Heptafluorobutyric acid, n-octa...	5522	1000216-79-5	70
			1-Hentetracontanol	16591	040710-42-7	58
			17-Pentatriacontene	5525	006971-40-0	58
21	29.19	0.48	C:\Database\NIST98.L			
			Piperidine, 1-phenpropioloyl-	58581	1000128-53-6	35
			2H-Azepine-2-thione, hexahydro-	121794	007203-96-5	30
			2H-Azepine-2-thione, hexahydro-	58333	007203-96-5	30
22	29.29	4.59	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	96
			n-Hexadecanoic acid	114901	000057-10-3	86
			Octadecanoic acid	6590	000057-11-4	83

23	29.50	0.67	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	81
			Hexadecanamide	113298	000629-54-9	81
			Dodecanamide	19649	001120-16-7	68
24	29.56	1.04	C:\Database\NIST98.L			
			Hexadecanoic acid, 1,1-dimethyl...	15255	031158-91-5	91
			Eicosanoic acid	5652	000506-30-9	50
			2H-Pyran-2-one, tetrahydro-3,6-...	3446	003720-22-7	30
25	29.71	0.61	C:\Database\NIST98.L			
			Docosane	16531	000629-97-0	92
			Dotriacontane	112351	000544-85-4	87
			Tetratetracontane	16486	007098-22-8	87
26	29.78	5.42	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
27	31.22	2.73	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	98
			Diethyl Phthalate	14	000084-66-2	40
			Di-n-butyl Phthalate	28	000084-74-2	38
28	31.30	4.84	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	98
			9-Octadecenamide, (Z)-	113301	000301-02-0	93
			9-Octadecenamide, (Z)-	19657	000301-02-0	90
29	31.52	3.71	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	95
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	91
			Diisooctyl adipate	58242	001330-86-5	91
30	31.61	3.86	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	91
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	58
			2-Propanone, ethylhydrazone	15402	007422-99-3	25
31	32.25	0.45	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	71908	034006-76-3	38
			Butane, 1-isothiocyanato-	108447	000592-82-5	15
			Dimethyl phthalate	124365	000131-11-3	14
32	32.48	2.10	C:\Database\NIST98.L			
			1-Heneicosyl formate	16592	077899-03-7	94
			Cyclohexadecane	14275	000295-65-8	93
			1-Eicosanol	112640	000629-96-9	91
33	32.82	4.78	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	50
			Di-n-butyl Phthalate	28	000084-74-2	43
34	33.11	0.74	C:\Database\NIST98.L			
			Naphthalene-2,6-dicarboxylic ac...	99513	1000192-39-7	38
			4-[p-Chlorophenoxy]-6-methoxy-8...	99543	1000214-52-6	38
			Benzaldehyde, 3-methyl-, (2,4-d...	99495	002880-05-9	38
35	33.36	0.50	C:\Database\NIST98.L			
			Eicosane	112565	000112-95-8	46
			Tetracosane, 1-bromo-	16525	006946-24-3	43
			Nonahexacontanoic acid	17028	040710-32-5	43

36	34.08	0.51	C:\Database\NIST98.L				
			[8,8'-Biisoquinoline]-7,7'-diol...	105272	025383-49-7	18
			Methyl 3-(1-pyrrolo)thiophene-2...	84784	074772-16-0	15
			Methadone N-oxide	84766	1000120-80-7	14
37	35.04	21.49	C:\Database\NIST98.L				
			Erucylamide	19656	000112-84-5	90
			Erucylamide	113300	000112-84-5	81
			9-Octadecenamide, (Z)-	19657	000301-02-0	72
38	35.37	1.19	C:\Database\NIST98.L				
			Squalene	114263	007683-64-9	46
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	46
			1,5,9-Decatriene, 2,3,5,8-tetra...	22365	1000149-59-0	46
39	36.16	0.95	C:\Database\NIST98.L				
			Propanamide, N-(3-methoxyphenyl...	17665	056619-93-3	11
			Propionamide, 2,2-dimethyl-N-(5...	18128	086436-38-6	7
			Imidazole, 4-bromo-1-methyl-5-n...	3825	1000126-15-1	7
40	36.25	0.48	C:\Database\NIST98.L				
			Tricosane	16532	000638-67-5	46
			Eicosane	112345	000112-95-8	42
			Pentatriacontane	112346	000630-07-9	42
41	36.37	3.28	C:\Database\NIST98.L				
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	49
			Acetic acid, (dodecahydro-7-hyd...	100955	000468-74-6	28
			4-(1,1'-Biphenyl-2-yl)-7-chloro...	100860	1000112-24-1	9
42	39.62	0.54	C:\Database\NIST98.L				
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	43
			Cyclotrisiloxane, hexamethyl-	84874	000541-05-9	43
			Silicic acid, diethyl bis(trime...	84851	003555-45-1	37

Tue Jan 15 16:54:08 2008

No Disinfectant
Day 1
Sample

Information from Data File:
File: D:\DATA\HEATHER\010708\011.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 12:51 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 13

Search Libraries: C:\Database\NIST98.L Minimum Quality: 35

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	7.30	0.16	C:\Database\NIST98.L			
			Phenol, 2-fluoro-	50680	000367-12-4	90
			Phenol, 4-fluoro-	120185	000371-41-5	22
			Phenol, 3-fluoro-	120187	000372-20-3	12
2	9.67	0.39	C:\Database\NIST98.L			
			Glycocyanidine	43063	000503-86-6	72
			Hexanoic acid, anhydride	118572	002051-49-2	59
			2-Pyrrolidinone, 4-methyl-	914	1000197-00-3	45
3	14.21	0.20	C:\Database\NIST98.L			
			Ethanol, 2-(2-butoxyethoxy)-	112444	000112-34-5	86
			Ethanol, 2-[2-(2-butoxyethoxy)e...	110872	000143-22-6	50
			2-(2-Hexyloxyethoxy)ethanol	4911	000112-59-4	42
4	14.90	0.19	C:\Database\NIST98.L			
			Ethanol, 2-phenoxy-	40669	000122-99-6	94
			Carbonic acid, neopentyl phenyl...	40591	013183-19-2	59
			Urocanic acid	40719	000104-98-3	59
5	15.26	0.30	C:\Database\NIST98.L			
			Hexanedioic acid, dimethyl ester	113348	000627-93-0	91
			3-Pentenoic acid, methyl ester	13752	000818-58-6	35
			Butanedioic acid, 2,3-dimethyl-...	113327	028306-68-5	22
6	15.69	0.25	C:\Database\NIST98.L			
			Nonanoic acid	20156	000112-05-0	64
			Heptanoic acid	113406	000111-14-8	43
			Ethanone, 1-(4,5-dihydro-2-thia...	5931	1000248-99-5	38
7	17.42	0.90	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	64
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	45
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	38
8	17.83	1.80	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	83
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	78
			Butanoic acid, butyl ester	114541	000109-21-7	72

9	18.50	0.35	C:\Database\NIST98.L			
			Benzenamine, 2,4,6-trichloro-	81952	000634-93-5	98
			Benzenamine, 2,3,4-trichloro-	82457	000634-67-3	93
			Benzenamine, 3,4,5-trichloro-	81968	000634-91-3	83
10	18.87	1.68	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	59
			2-Propanol, 1-[2-(2-methoxy-1-m...	19665	020324-33-8	59
			2-Propanol, 1,1'-[(1-methyl-1,2...	19307	001638-16-0	53
11	19.32	0.26	C:\Database\NIST98.L			
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	46
			Hexasiloxane, 1,1,3,3,5,5,7,7,9...	27715	000995-82-4	38
			Pentasiloxane, dodecamethyl-	97318	000141-63-9	37
12	19.55	0.22	C:\Database\NIST98.L			
			1-Dodecanol	13544	000112-53-8	91
			Cycloundecane, 1,1,2-trimethyl-	15270	062376-15-2	86
			5-Tetradecene, (E)-	111257	041446-66-6	80
13	20.09	1.43	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	97
			Pentanoic acid, 5-hydroxy-, 2,4...	80726	1000164-49-3	78
			Pentanedioic acid, (2,4-di-t-bu...	80725	1000164-44-5	78
14	20.89	0.22	C:\Database\NIST98.L			
			Talopyranoside, methyl 4-acetam...	5856	015856-46-9	38
			Mannopyranoside, methyl 4-aceta...	5855	015856-45-8	35
			2-Acetyl-2-thiazoline	5930	1000121-56-5	18
15	21.47	1.08	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	38
			Phenmetrazine	114096	000134-49-6	37
			Butyric acid, 1-propylpentyl ester	24329	020286-46-8	23
16	21.65	0.26	C:\Database\NIST98.L			
			Hexadecane	112409	000544-76-3	95
			Hexatriacontane	112335	000630-06-8	60
			Tricosane	109661	000638-67-5	53
17	22.06	0.19	C:\Database\NIST98.L			
			Silane, [[4-(1,2-bis[(trimethyl...	103450	056114-62-6	43
			Benzoic acid, 2,5-bis(trimethyl...	128840	003618-20-0	35
			N-(Trifluoroacetyl)-N,O,O',O''-...	27961	1000072-26-7	35
18	22.51	1.60	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	94
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	10
19	22.80	1.78	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	96
			1,4-Naphthoquinone, 6-acetyl-2,...	127595	013379-24-3	56
			Pyrazine, 2,5-bis(1,1-dimethyle...	76399	018709-51-8	30
20	23.01	0.28	C:\Database\NIST98.L			
			Cyclododecane	111537	000294-62-2	94
			Hexadecanol	5280	029354-98-1	91
			1-Hexadecanol	109484	036653-82-4	91

21	23.57	2.32	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	47
			2-Pentanol, 3-ethyl-2-methyl-	19421	019780-63-3	43
			Nonanamide	19654	001120-07-6	37
22	24.35	0.47	C:\Database\NIST98.L			
			2,3,5,6-Detetrahydrocyclohexano...	87517	1000130-27-1	96
			Phenol, 2,6-bis(1,1-dimethyleth...	126888	004130-42-1	96
			3,5-di-tert-Butyl-4-hydroxybenz...	126889	001620-98-0	94
23	24.51	0.79	C:\Database\NIST98.L			
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	56
			2-Azido-17-(1,5-dimethylhexyl)-...	5160	1000210-24-9	22
			Heptasiloxane, 1,1,3,3,5,5,7,7,...	27374	019095-23-9	22
24	24.90	0.75	C:\Database\NIST98.L			
			Octadecane	112333	000593-45-3	98
			Heneicosane	17094	000629-94-7	90
			Docosane	16531	000629-97-0	90
25	24.99	0.42	C:\Database\NIST98.L			
			Tetratriacontane	16431	014167-59-0	83
			Heptacosane	16471	000593-49-7	83
			Hexatriacontane	112334	000630-06-8	83
26	25.17	1.06	C:\Database\NIST98.L			
			Formic acid, 2,4,6-tri-t-butyl-...	92594	1000194-52-1	56
			11H-Indeno[1,2-b]quinoline, 2-m...	92644	1000214-21-7	50
			4-O-Nitrophenylhydrazono-3-meth...	92623	1000148-19-3	50
27	25.48	0.61	C:\Database\NIST98.L			
			Cyclopentadecane	13210	000295-48-7	60
			2-Pentadecanone, 6,10,14-trimet...	109744	000502-69-2	49
			Nonahexacontanoic acid	17028	040710-32-5	49
28	25.76	1.53	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	67019	017851-53-5	86
			1,2-Benzenedicarboxylic acid, b...	123451	000084-69-5	86
			Dibutyl phthalate	123427	000084-74-2	78
29	25.92	0.55	C:\Database\NIST98.L			
			Ethanol, 2-(octadecyloxy)-	16507	002136-72-3	38
			Nonahexacontanoic acid	17028	040710-32-5	30
			7-Nonenamide	19655	090949-53-4	20
30	26.06	0.51	C:\Database\NIST98.L			
			3-Tetradecanol	19356	001653-32-3	38
			3-Hexadecanol	113255	000593-03-3	35
			Benzenethiol, 4-(1,1-dimethylet...	67961	002396-68-1	35
31	26.26	0.62	C:\Database\NIST98.L			
			Nonadecane	112380	000629-92-5	97
			Dotriacontane	112351	000544-85-4	90
			Tetratetracontane	16486	007098-22-8	90
32	26.38	0.50	C:\Database\NIST98.L			
			1-(4-Butoxy-2,6-dimethylphenyl)...	67120	1000190-22-9	50
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	46
			2-Methyl-6-tert-octylphenol	67087	019546-31-7	38

33	26.51	0.69	C:\Database\NIST98.L				
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	37	
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	25	
			Pentasiloxane, dodecamethyl-	115143	000141-63-9	12	
34	26.76	0.58	C:\Database\NIST98.L				
			Benzoic acid, 2-benzoyl-, methy...	71765	000606-28-0	53	
			3-Methyl-2-(2-oxopropyl)furan	16777	087773-62-4	51	
			Oxirane, tetradecyl-	108844	007320-37-8	38	
35	27.00	4.54	C:\Database\NIST98.L				
			Dibutyl phthalate	123426	000084-74-2	96	
			1,2-Benzenedicarboxylic acid, b...	67019	017851-53-5	92	
			1,2-Benzenedicarboxylic acid, b...	66775	000084-69-5	83	
36	27.17	1.71	C:\Database\NIST98.L				
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	58	
			2-Methyl-tridecane-2,12-diol	19413	1000187-03-5	38	
			2,4,6,8,9,10-Hexathiatricyclo[3...	19863	057274-38-1	38	
37	27.51	1.48	C:\Database\NIST98.L				
			Eicosane	112345	000112-95-8	92	
			Tetradecane, 2,6,10-trimethyl-	16537	014905-56-7	83	
			Heptacosane	16471	000593-49-7	70	
38	27.73	0.66	C:\Database\NIST98.L				
			1,3-Pentadiene, 1,1-diphenyl-, ...	126412	015295-31-5	38	
			Ethanone, 1-(9-anthracenyl)-	126411	000784-04-3	38	
			Butylated Hydroxytoluene	84224	000128-37-0	35	
39	27.95	0.41	C:\Database\NIST98.L				
			.beta.-D-Mannofuranoside, 3,6,9...	19843	1000155-77-2	47	
			Methane, diethoxy-	108344	000462-95-3	43	
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	43	
40	28.29	3.60	C:\Database\NIST98.L				
			Azadibenzopyrene	99857	104219-69-4	9	
			5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4	9	
			Hydromorphinol	99808	002183-56-4	9	
41	28.50	0.53	C:\Database\NIST98.L				
			Cyclohexadecane	14275	000295-65-8	96	
			1-Octadecanol	5273	000112-92-5	94	
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	94	
42	28.65	0.24	C:\Database\NIST98.L				
			Heneicosane	112581	000629-94-7	50	
			Hexatriacontane	112334	000630-06-8	49	
			Pentatriacontane	112346	000630-07-9	49	
43	28.78	0.30	C:\Database\NIST98.L				
			Triallylmethylsilane	42227	001112-91-0	50	
			Heneicosane, 11-cyclopentyl-	112276	006703-81-7	45	
			1-Hentetracontanol	16591	040710-42-7	38	
44	29.06	0.88	C:\Database\NIST98.L				
			3-Tridecanol	19339	010289-68-6	38	
			Silane, ethyldimethyl-	19594	000758-21-4	35	
			2-Octanol, 2-methyl-6-methylene-	19419	1000132-19-1	32	

45	29.30	2.92	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	87
			Octadecanoic acid, 2-(2-hydroxy...	4373	000106-11-6	72
			Heptadecanoic acid	114893	000506-12-7	68
46	29.50	0.84	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	94
			Dodecanamide	19649	001120-16-7	78
			Nonanamide	19654	001120-07-6	72
47	29.78	2.96	C:\Database\NIST98.L			
			p-Terphenyl-d14	92199	001718-51-0	99
			2H-Pyran-2-one, 6-[2-E-(2-hydro...	92165	132405-77-7	59
			cis-5-Methyl-6-phenyl-5,6-dihyd...	92129	1000212-27-8	47
48	30.15	1.30	C:\Database\NIST98.L			
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	53
			2,4,6,8,9,10-Hexathiatricyclo[3...	19863	057274-38-1	43
			Silane, (chloromethyl)dimethyl-	19630	003144-74-9	38
49	30.70	0.27	C:\Database\NIST98.L			
			Tetracosane, 1-bromo-	16525	006946-24-3	46
			Octadecane, 1-chloro-	16321	003386-33-2	46
			Octadecane	16439	000593-45-3	43
50	30.96	1.57	C:\Database\NIST98.L			
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	38
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	25
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	22
51	31.31	3.93	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			Tetradecanamide	19652	000638-58-4	72
			Hexadecanamide	113298	000629-54-9	56
52	31.61	2.11	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	74
			2,5-Hexanediol	110870	002935-44-6	25
			2-Propanone, ethylhydrazone	15402	007422-99-3	25
53	32.16	2.16	C:\Database\NIST98.L			
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	27
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	25
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	25
54	32.48	1.45	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	96
			1-Docosene	111438	001599-67-3	94
			1-Octadecene	112298	000112-88-9	93
55	32.82	1.79	C:\Database\NIST98.L			
			Bis(2-ethylhexyl) phthalate	66784	000117-81-7	91
			1,2-Benzenedicarboxylic acid, d...	123512	027554-26-3	91
			Phthalic acid, diisooctyl ester	66787	001330-91-2	86
56	33.28	3.46	C:\Database\NIST98.L			
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	47
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	45
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	27

57	34.01	0.84	C:\Database\NIST98.L				
			3-Pentanol, 2-methyl-	113304	000565-67-3	38	
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	32	
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	32	
58	34.39	3.47	C:\Database\NIST98.L				
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	59	
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	42	
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	25	
59	35.05	15.06	C:\Database\NIST98.L				
			Erucylamide	19656	000112-84-5	90	
			9-Octadecenamide, (Z)-	19657	000301-02-0	56	
			7-Nonenamide	19655	090949-53-4	47	
60	35.37	0.79	C:\Database\NIST98.L				
			Squalene	114263	007683-64-9	97	
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	74	
			4,9,13,17-Tetramethyl-4,8,12,16...	23043	056882-09-8	64	
61	35.63	3.35	C:\Database\NIST98.L				
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	45	
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	30	
			Mercaptoacetic acid, bis(trimet...	26922	006398-62-5	16	
62	36.37	0.79	C:\Database\NIST98.L				
			13H-Benz[6,7]indolo[3,2-c]quino...	101046	004240-59-9	35	
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	22	
			Methane, tert-butoxyisopropoxy-	16926	004346-01-4	22	
63	36.63	0.77	C:\Database\NIST98.L				
			2-Heptanol, 2-methyl-	113196	000625-25-2	35	
			2-Dodecanol, 2-methyl-	19343	001653-37-8	35	
			Oxirane, 3-ethyl-2,2-dimethyl-	19363	001192-22-9	35	
64	37.06	2.62	C:\Database\NIST98.L				
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	38	
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	35	
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	35	
65	37.39	0.44	C:\Database\NIST98.L				
			9-Octadecenamide, (Z)-	19657	000301-02-0	46	
			Octadecanamide	19648	000124-26-5	38	
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	35	
66	38.80	2.79	C:\Database\NIST98.L				
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	38	
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	32	
			Pentasiloxane, dodecamethyl-	115143	000141-63-9	25	
67	39.63	0.23	C:\Database\NIST98.L				
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	47	
			Tetrasiloxane, decamethyl-	126458	000141-62-8	22	
			1,1,1,3,5,5,5-Heptamethyltrisil...	84726	001873-88-7	22	
68	40.39	2.06	C:\Database\NIST98.L				
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	43	
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	42	
			2-Propanol, 1-(1-methyl-2-(2-pr...	19368	055956-25-7	38	

69	40.95	1.91	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	53
			1,2-Benzenedicarboxylic acid, b...	65838	002078-22-0	22
			Hexasiloxane, 1,1,3,3,5,5,7,7,9...	27715	000995-82-4	18
70	43.69	0.89	C:\Database\NIST98.L			
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	38
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	35
			Pentasiloxane, dodecamethyl-	97318	000141-63-9	30

Fri Oct 24 11:45:47 2008

No Disinfectant
Day 4
Control

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\006.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 8:06 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 8

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	9.65	0.95	C:\Database\NIST98.L			
			Glycocyanidine	43063	000503-86-6	72
			Hexanoic acid, anhydride	118546	002051-49-2	45
			Hexanoic acid, 1,2,3-propanetri...	43039	000621-70-5	39
2	10.20	0.71	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	59
3	13.61	0.57	C:\Database\NIST98.L			
			Benzoic Acid	119309	000065-85-0	95
			Benzoic Acid	119310	000065-85-0	90
			Benzoic Acid	119125	000065-85-0	90
4	15.68	0.72	C:\Database\NIST98.L			
			Nonanoic acid	20156	000112-05-0	95
			Nonanoic acid	113428	000112-05-0	93
			Nonanoic acid	113398	000112-05-0	87
5	17.41	1.23	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	56
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	45
			Propanoic acid, 2-methyl-, 2-me...	114586	000097-85-8	33
6	17.76	4.02	C:\Database\NIST98.L			
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	96
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	94
7	17.82	1.32	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	78
			Butanoic acid, butyl ester	109895	000109-21-7	72
			Butanoic acid, butyl ester	114541	000109-21-7	72
8	19.54	0.41	C:\Database\NIST98.L			
			1-Dodecanol	111442	000112-53-8	91
			1-Tridecanol	13019	000112-70-9	91
			1-Undecanol	13829	000112-42-5	91
9	21.47	1.43	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			Butyric acid, thio-, S-decyl ester	24338	002432-55-5	38
			Butane, 1-bromo-2-methyl-	114514	010422-35-2	33

Page 1

10	22.37	0.36	C:\Database\NIST98.L			
			Benzophenone	46089	000119-61-9	81
			Benzophenone	119052	000119-61-9	81
			Benzophenone	119171	000119-61-9	81
11	22.50	4.39	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	60
			2-Bromo-4-chloro-5,8-dimethoxy-...	102208	104506-11-8	9
			Estra-1,3,5(10)-triene-2,17-dio...	102217	065969-01-9	9
12	22.80	2.92	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	86
			1,2-Benzenedicarboxylic acid, 4...	76484	069094-40-2	44
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	38
13	23.07	1.16	C:\Database\NIST98.L			
			Phenol, 2,4-di-t-butyl-6-nitro-	90753	1000128-93-2	97
			1,3,2-Oxazaborolidine, 3,4-dime...	90718	026574-29-8	72
			7,7-Dimethyl-1,4-dioxo-2,3,4,5,...	90678	051799-98-5	59
14	23.37	0.84	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	98
			Heptadecane	112320	000629-78-7	96
			Heptadecane	112322	000629-78-7	93
15	24.90	0.70	C:\Database\NIST98.L			
			Octadecane	112330	000593-45-3	98
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	93
16	24.99	0.62	C:\Database\NIST98.L			
			Heptacosane	16471	000593-49-7	90
			Hexadecane, 2,6,10,14-tetramethyl-	112575	000638-36-8	87
			Tetratetracontane	16486	007098-22-8	87
17	25.48	0.40	C:\Database\NIST98.L			
			Oxirane, [(dodecyloxy)methyl]-	16338	002461-18-9	49
			Cyclododecanol, 1-ethenyl-	13267	006244-49-1	43
			1-Decanol, 2-hexyl-	112269	002425-77-6	38
18	25.76	1.33	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	64
			Benzyl butyl Phthalate	36	000085-68-7	9
			Diethyl Phthalate	14	000084-66-2	9
19	26.26	0.72	C:\Database\NIST98.L			
			Nonadecane	112382	000629-92-5	96
			Nonadecane	112381	000629-92-5	95
			Nonadecane	112380	000629-92-5	93
20	26.38	0.80	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	81
			3H-Cyclopenta[1,3]cyclopropa[1,...	84281	066708-18-7	43
			Ethanone, 1-(5,6,7,8-tetrahydro...	84211	071596-88-8	41
21	27.00	7.81	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	80
			Diethyl Phthalate	14	000084-66-2	7
22	27.51	0.68	C:\Database\NIST98.L			
			Eicosane	112345	000112-95-8	96
			Heptacosane	16471	000593-49-7	91
			Tritetracontane	17076	007098-21-7	91

23	27.94	0.43	C:\Database\NIST98.L			
			1,3-Diphenyl-2-azafluorene	101235	1000216-51-5	58
			Iron, (.eta.-4-naphthalene)(.et...	101232	1000161-39-4	47
			Buphanitine	101227	004673-18-1	40
24	28.49	0.50	C:\Database\NIST98.L			
			Cyclotetradecane	13185	000295-17-0	98
			1-Octadecene	112298	000112-88-9	96
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	94
25	29.06	0.70	C:\Database\NIST98.L			
			2,7-Methanonaphthalen-3-amine, ...	17907	1000186-49-9	10
			1-Propanesulfonic acid, methyl ...	4067	002697-50-9	10
			Cyclohexanamine, N,N'-1,2-ethan...	14145	003673-06-1	10
26	29.30	4.85	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	93
			Octadecanoic acid	109378	000057-11-4	81
			Octadecanoic acid	6590	000057-11-4	78
27	29.50	0.78	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	76
			Hexadecanamide	19647	000629-54-9	70
			Tetradecanamide	19652	000638-58-4	62
28	29.78	6.88	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
29	31.22	0.85	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	98
			Diethyl Phthalate	14	000084-66-2	42
			Di-n-butyl Phthalate	28	000084-74-2	9
30	31.31	3.75	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			9-Octadecenamide, (Z)-	113301	000301-02-0	91
			9-Octadecenamide, (Z)-	19657	000301-02-0	86
31	31.53	0.93	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	87
			Diisooctyl adipate	58242	001330-86-5	60
32	31.61	0.84	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	90
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	80
			2H-Pyran, tetrahydro-2-[(2-nitr...	34285	096039-96-2	35
33	32.48	1.72	C:\Database\NIST98.L			
			1-Eicosanol	112640	000629-96-9	95
			1-Docosene	111438	001599-67-3	94
			1-Octadecanol	111484	000112-92-5	94
34	32.82	2.06	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	40
35	33.37	1.35	C:\Database\NIST98.L			
			Eicosane	16454	000112-95-8	60
			Heneicosane	112581	000629-94-7	35
			Pentatriacontane	112346	000630-07-9	35

36	35.05	18.24	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	93
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
			Hexadecanamide	113298	000629-54-9	64
37	35.37	0.82	C:\Database\NIST98.L			
			Docosa-2,6,10,14,18-pentaen-22-...	23027	1000163-04-7	49
			Squalene	114263	007683-64-9	47
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	46
38	35.48	0.52	C:\Database\NIST98.L			
			1H-Indole, 2-methyl-3-phenyl-	126477	004757-69-1	38
			1-(t-Butyldimethylsilyl)-3,7-di...	25757	1000192-68-9	35
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	35
39	36.09	0.90	C:\Database\NIST98.L			
			Propanamide, N-(3-methoxyphenyl...	17665	056619-93-3	18
			2,4-Di-tert-butyl-6-(tert-butyl...	2241	1000224-34-5	12
			1-(2-Hydroxyphenyl)-4-(2,6-xyly...	1330	1000224-28-5	10
40	36.15	0.70	C:\Database\NIST98.L			
			Spiro[bicyclo[3.3.0]oct-6-ene-3...	557	1000156-60-3	11
			4,6-Bis(t-butyl)-2-(dimethylben...	16197	144688-99-3	10
			2-(2,2-Dimethyl-propionyl)-6,7-...	15743	1000193-35-7	10
41	36.25	0.60	C:\Database\NIST98.L			
			Eicosane	16454	000112-95-8	86
			Pentadecane	16493	000629-62-9	50
			Hexatriacontane	112334	000630-06-8	50
42	36.38	3.30	C:\Database\NIST98.L			
			2,2-Dimethyl-propionic acid, 10...	17942	1000189-34-4	12
			Propanamide, 2,2-dimethyl-N-(4-...	17554	021354-40-5	12
			Propanamide, 2,2-dimethyl-N-(3-...	17553	032597-29-8	12
43	37.48	0.38	C:\Database\NIST98.L			
			Eicosane	16454	000112-95-8	86
			Eicosane	112565	000112-95-8	46
			Eicosane, 9-octyl-	5630	013475-77-9	46
44	37.64	2.89	C:\Database\NIST98.L			
			Benzene, 1,4-bis(3-phenylindol-...	106699	1000164-74-0	27
			1H-Isoindole-1,3(2H)-dione, 5,5...	106698	033734-37-1	27
			1,3,5-Triazine-2,4,6-triamine, ...	106696	033933-66-3	27
45	39.02	0.38	C:\Database\NIST98.L			
			1-Octadecanol	5273	000112-92-5	42
			1-Octadecanol	111484	000112-92-5	42
			1-Eicosanol	112640	000629-96-9	42
46	41.60	10.59	C:\Database\NIST98.L			
			Benzene, 1,4-bis(3-phenylindol-...	106699	1000164-74-0	35
			1,3,5-Triazine-2,4,6-triamine, ...	106696	033933-66-3	25
			5-Hydroxy-N-(4-diethylaminophen...	106694	1000110-48-8	9
47	43.14	0.93	C:\Database\NIST98.L			
			Silicic acid, diethyl bis(trime...	84851	003555-45-1	25
			Benzene, 1,4-bis(3-phenylindol-...	106699	1000164-74-0	14
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	14

No Disinfectant
Day 4
Sample

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\01070 8\003.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 5:14 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 5

Search Libraries: C:\Database\NIST98.L Minim um Quality: 35
C:\Database\NIST98.L Minim um Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Q	ual
1	17.41	0.62	C:\Database\NIST98.L				
"Propanoic acid, 2-methyl-, 2,2-..."				24402	074367-33-2		64
"2,2,4-Trimethyl-1,3-pentanediol..."				24399	006846-50-0		59
"Propanoic acid, 2-methyl-, 3-hy..."				24534	074367-34-3		38
2	17.75	0.64	C:\Database\NIST98.L				
"1,1'-Biphenyl, 2-fluoro-"			124940	000321-60-8		96	
"1,1'-Biphenyl, 2-fluoro-"			74959	000321-60-8		96	
"1,1'-Biphenyl, 4-fluoro-"			74960	000324-74-3		96	
3	17.82	0.85	C:\Database\NIST98.L				
"Butanoic acid, butyl ester"			114541	000109-21-7		72	
"Propanoic acid, 2-methyl-, 3-hy..."				24534	074367-34-3		72
"Propanoic acid, 2-methyl-, hexy..."				109360	002349-07-7		47
4	20.08	1.70	C:\Database\NIST98.L				
"Phenol, 2,4-bis(1,1-dimethyleth..."				125781	000096-76-4		95
"Phenol, 2,4-bis(1,1-dimethyleth..."				125782	000096-76-4		95
"Phenol, 2,4-bis(1,1-dimethyleth..."				125783	000096-76-4		93
5	21.47	1.08	C:\Database\NIST98.L				
"2-Hexen-4-ol, 5-methyl-"			24320	1000163-45-		9 38	
Phenmetrazine	114496	000134-49-6		37			
"2,2,4-Trimethyl-1,3-pentanediol..."				24399	006846-50-0		37
6	22.50	1.49	C:\Database\NIST98.L				
"Phenol, 2,4,6-tribromo-"			102083	000118-79-6		91	
"Iron, (.eta.5-2,4-cyclopentadie..."				102184	012149-23-4		10
"Estra-1,3,5(10)-triene-2,17-dio..."				102217	065969-01-9		9
7	22.81	4.64	C:\Database\NIST98.L				
"2,5-Cyclohexadiene-1,4-dione, 2..."				1509	004584-63-8		98
"Pyrazine, 2,5-bis(1,1-dimethyle..."				76399	018709-51-8		20
"Octamethyl-1,3-cyclohexadiene"			76425	1000110-41-		8 20	
8	24.52	0.58	C:\Database\NIST98.L				
"Cyclononasiloxane, octadecamethyl-"				115158	000556-71-8		72
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."				26950	038147-00-1		25
"Heptasiloxane, 1,1,3,3,5,5,7,7,..."				27374	019095-23-9		14
9	24.60	0.79	C:\Database\NIST98.L				
"Phenol, 2-(1,1-dimethylethyl)-4..."				80516	005806-73-5		87
"Phenol, 2,4-bis(1,1-dimethyleth..."				125781	000096-76-4		72
"Phenol, 2,4-bis(1,1-dimethyleth..."				125783	000096-76-4		64

Page 1

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10  25.17  2.58 C:\Database\NIST98.L
4-O-Nitrophenylhydrazono-3-meth...      92623   1000148-19-     3 42
8-Methoxy-11H-benzo[a]carbazole 92655   1000212-76-     8 38
"Phenol, 2,4,6-tris(1,1-dimethyl..."    92595   000732-26-3     38

11  25.76  1.36 C:\Database\NIST98.L
"1,2-Benzenedicarboxylic acid, b..."    123451  000084-69-5     86
"1,2-Benzenedicarboxylic acid, b..."    123453  000084-69-5     83
"1,2-Benzenedicarboxylic acid, b..."    66775   000084-69-5     83

12  26.51  0.54 C:\Database\NIST98.L
"Eseroline, 7-bromo-, methylcarb..."    3850    114546-23-5     90
"Cyclodecasiloxane, eicosamethyl-"      27712   018772-36-6     60
"Octasiloxane, 1,1,3,3,5,5,7,7,9..."    27373   019095-24-0     43

13  27.00  5.10 C:\Database\NIST98.L
n-Hexadecanoic acid     109985  000057-10-3     95
"1,2-Benzenedicarboxylic acid, b..."    67019   017851-53-5     86
Dibutyl phthalate       123493  000084-74-2     86

14  28.15  1.28 C:\Database\NIST98.L
2-Nitrofluoranthene     92640   013177-29-2     56
4-O-Nitrophenylhydrazono-3-meth...      92623   1000148-19-     3 50
"Phenol, 2,4,6-tris(1,1-dimethyl..."    127581  000732-26-3     50

15  28.21  0.80 C:\Database\NIST98.L
"Heptasiloxane, hexadecamethyl-"        27486   000541-01-5     28
"Pentasiloxane, dodecamethyl-"  115143  000141-63-9     27
"Benzoic acid, 2,5-bis(trimethyl..."    115317  003618-20-0     25

16  28.30  7.63 C:\Database\NIST98.L
Azadibenzopyrene        99857   104219-69-4     9
"5-[[[3,4,5-Trimethoxyphenyl]imi..."    99851   1000212-37-     4  9
Hydromorphinol  99808   002183-56-4     9

17  29.30  2.13 C:\Database\NIST98.L
Octadecanoic acid       114902  000057-11-4     97
Octadecanoic acid       6590    000057-11-4     94
Octadecanoic acid       109378  000057-11-4     83

18  29.50  0.68 C:\Database\NIST98.L
Hexadecanamide  19647   000629-54-9     95
Hexadecanamide  113298  000629-54-9     94
Dodecanamide    19649   001120-16-7     86

19  29.66  1.21 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     62
"9,12,15-Octadecatrienoic acid, ..."    25608   055521-22-7     41
"Cyclodecasiloxane, eicosamethyl-"      27712   018772-36-6     36

20  29.78  1.92 C:\Database\NIST98.L
p-Terphenyl-d14 92199   001718-51-0     94
"2H-Pyran-2-one, 6-[2-E-(2-hydro..."    92165   132405-77-7     59
"Cyclopentene, 3-methylene-2-phe..."    92106   1000157-28-     3 58

21  30.96  1.79 C:\Database\NIST98.L
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."    26950   038147-00-1     39
"9,12,15-Octadecatrienoic acid, ..."    25608   055521-22-7     25
"Trisiloxane, 1,1,1,5,5,5-hexame..."    26961   003555-47-3     25

22  31.03  0.62 C:\Database\NIST98.L
"Isopropyl-[2-(4-methoxy-2,6-dim..."    103705  1000189-65-     2 80
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"1-Anthracenamine, N-methyl-9,10..." 103706 055334-26-4 9
"Cobalt, .eta.-5-fluorenyl-penta..." 103692 1000153-46- 4 7

23 31.32 6.63 C:\Database\NIST98.L
"9-Octadecenamide, (Z)-" 113302 000301-02-0 96
"9-Octadecenamide, (Z)-" 113301 000301-02-0 86
Tetradecanamide 113299 000638-58-4 64

24 31.53 0.92 C:\Database\NIST98.L
"Hexanedioic acid, bis(2-ethylhe..." 121807 000103-23-1 92
"Hexanedioic acid, bis(2-ethylhe..." 58246 000103-23-1 62
Diisooctyl adipate 58242 001330-86-5 62

25 31.62 0.71 C:\Database\NIST98.L
"Ethanol, 2-butoxy-, phosphate (..." 112451 000078-51-3 90
"Ethanol, 2-butoxy-, phosphate (..." 16713 000078-51-3 46
"2-Propanone, ethylhydrazone" 15402 007422-99-3 27

26 32.16 2.60 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-" 115158 000556-71-8 64
"Heptasiloxane, hexadecamethyl-" 27486 000541-01-5 25
"3-Isopropoxy-1,1,1,7,7,7-hexame..." 26784 071579-69-6 25

27 32.48 1.69 C:\Database\NIST98.L
1-Heneicosyl formate 16592 077899-03-7 93
1-Eicosanol 112640 000629-96-9 93
1-Octadecanol 111484 000112-92-5 90

28 32.82 1.84 C:\Database\NIST98.L
Bis(2-ethylhexyl) phthalate 66784 000117-81-7 91
Bis(2-ethylhexyl) phthalate 123452 000117-81-7 91
Bis(2-ethylhexyl) phthalate 123509 000117-81-7 90

29 33.00 1.30 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-" 115158 000556-71-8 58
"3,6-Dioxa-2,4,5,7-tetrasilaocta..." 87890 004342-25-0 43
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..." 26950 038147-00-1 38

30 33.28 3.06 C:\Database\NIST98.L
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..." 26950 038147-00-1 47
"Cyclononasiloxane, octadecamethyl-" 115158 000556-71-8 42
"Heptasiloxane, hexadecamethyl-" 27486 000541-01-5 22

31 34.40 3.40 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-" 115158 000556-71-8 64
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..." 26950 038147-00-1 42
"3-Isopropoxy-1,1,1,7,7,7-hexame..." 26784 071579-69-6 32

32 35.07 25.63 C:\Database\NIST98.L
Erucylamide 19656 000112-84-5 93
"9-Octadecenamide, (Z)-" 19657 000301-02-0 64
Hexadecanamide 19647 000629-54-9 50

33 35.37 0.65 C:\Database\NIST98.L
Squalene 114263 007683-64-9 97
"1,5,9-Undecatriene, 2,6,10-trim..." 22381 062951-96-6 58
"2,6,10,14,18,22-Tetracosahexaen..." 114266 000111-02-4 58

34 35.63 3.18 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-" 115158 000556-71-8 72
"Cyclodecasiloxane, eicosamethyl-" 27712 018772-36-6 43
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..." 26950 038147-00-1 40

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35  37.06  2.32 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"     115158  000556-71-8     72
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."     26950   038147-00-1     42
"3-Isopropoxy-1,1,1,7,7,7-hexame..."     26784   071579-69-6     37

36  37.73  1.19 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"     115158  000556-71-8     64
"Mercaptoacetic acid, bis(trimet..."     26922   006398-62-5     32
"Pentasiloxane, dodecamethyl-"  97318    000141-63-9     30

37  38.80  1.54 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"     115158  000556-71-8     83
"Eseroline, 7-bromo-, methylcarb..."     3850    114546-23-5     59
"Pentasiloxane, dodecamethyl-"  115143   000141-63-9     35

38  39.01  0.83 C:\Database\NIST98.L
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."     26950   038147-00-1     42
"Cyclononasiloxane, octadecamethyl-"     115158  000556-71-8     38
"Pentasiloxane, dodecamethyl-"  115143   000141-63-9     22

39  40.96  0.81 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"     115158  000556-71-8     72
"Pentasiloxane, dodecamethyl-"  97318    000141-63-9     27
"Pentasiloxane, dodecamethyl-"  115143   000141-63-9     27

40  43.73  1.69 C:\Database\NIST98.L
"Trisiloxane, 1,1,1,5,5,5-hexame..."     26961   003555-47-3     25
"Pentasiloxane, dodecamethyl-"  115143   000141-63-9     22
"3-Isopropoxy-1,1,1,7,7,7-hexame..."     26784   071579-69-6     16

Tue Jan 15 16:01:07 2008
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No Disinfectant
Day 9
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\017.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 6:34 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 19

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

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			Diethylacetamide	25025	1000127-23-4	42
			Butanamide, N-ethyl-	35346	013091-16-2	37
			1-Propene, 3-methoxy-	108850	000627-40-7	27
2	5.41	0.68	C:\Database\NIST98.L			
			Cyclohexane, 1,4-dimethoxy-2-me...	35350	029887-66-9	38
			N,N-Dimethylvaleramide	116938	006225-06-5	27
			2-Butanone, oxime	109078	000096-29-7	27
3	5.95	2.30	C:\Database\NIST98.L			
			2-Hexanol, 3-methyl-	11546	002313-65-7	39
			Dimethyl-cyano-phosphine	11633	031641-57-3	10
			Oxirane, trimethyl-	109726	005076-19-7	9
4	6.26	0.66	C:\Database\NIST98.L			
			Butane, 2,3-dichloro-2-methyl-	29395	000507-45-9	86
			Propane, 1,1-dichloro-	29392	000078-99-9	50
			Propane, 2-bromo-1-chloro-	115667	003017-95-6	38
5	8.33	0.90	C:\Database\NIST98.L			
			2-Butenal, 3-methyl-	116598	000107-86-8	58
			2-Butenal, 3-methyl-	33657	000107-86-8	53
			1-Methoxy-6,6-dimethyl-cyclohex...	33750	1000144-64-5	52
6	9.03	0.97	C:\Database\NIST98.L			
			Cyclohexane, 1-methyl-2-propyl-	14506	004291-79-6	72
			Pyridine, 2-fluoro-	118348	000372-48-5	64
			Cyclohexane, 1-methyl-4-(1-meth...	111721	001678-82-6	64
7	20.10	1.00	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	125782	000096-76-4	97
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	96
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	96
8	22.52	3.44	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	94
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
			Pregn-4-ene-3,20-dione, 15-hydr...	102024	000600-73-7	9
9	24.90	0.91	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	98
			Pentacosane	109667	000629-99-2	90

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10	24.99	0.78	C:\Database\NIST98.L			
			Dotriacontane	112351	000544-85-4	87
			Tetratriacontane	16431	014167-59-0	87
			Octacosane	16409	000630-02-4	86
11	25.21	0.79	C:\Database\NIST98.L			
			Isopropyl Myristate	110206	000110-27-0	58
			Nonanoic acid, 1-methylethyl ester	7782	1000132-17-3	27
			Methanimine, 1-(1,4,4-trimethyl...	44401	042448-53-3	14
12	25.75	1.82	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	4
			Benzyl butyl Phthalate	36	000085-68-7	1
13	26.06	0.64	C:\Database\NIST98.L			
			Heptafluorobutyric acid, n-pent...	5520	1000216-79-3	53
			17-Pentatriacontene	5525	006971-40-0	49
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	46
14	26.27	0.86	C:\Database\NIST98.L			
			Nonadecane	112381	000629-92-5	97
			Nonadecane	16515	000629-92-5	95
			Nonadecane	112382	000629-92-5	93
15	26.38	0.85	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	64
			3H-Cyclopenta[1,3]cyclopropa[1,...	84281	066708-18-7	38
			Butylated Hydroxytoluene	126413	000128-37-0	35
16	27.00	7.53	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	90
			Diethyl Phthalate	14	000084-66-2	9
17	27.16	0.85	C:\Database\NIST98.L			
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	49
			1-Decanol, 2-hexyl-	112269	002425-77-6	45
			17-Pentatriacontene	5525	006971-40-0	41
18	27.51	1.15	C:\Database\NIST98.L			
			Eicosane	112345	000112-95-8	96
			Hexatriacontane	112335	000630-06-8	91
			Pentacosane	109667	000629-99-2	90
19	28.29	0.83	C:\Database\NIST98.L			
			Verapamil	128484	000052-53-9	64
			Verapamil	99859	000052-53-9	50
			2-Deoxyribofuranose, 1(O)-(t-bu...	99860	1000193-96-2	40
20	29.30	4.54	C:\Database\NIST98.L			
			Octadecanoic acid	109378	000057-11-4	83
			Octadecanoic acid	109986	000057-11-4	64
			Octadecanoic acid	114902	000057-11-4	64
21	29.50	1.14	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	68
			Tetradecanamide	19652	000638-58-4	58
			Octadecanamide	19648	000124-26-5	53
22	29.78	6.56	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
23	31.23	1.11	C:\Database\OWML.L			

			Benzyl butyl Phthalate	36	000085-68-7	90
			Diethyl Phthalate	14	000084-66-2	12
			Di-n-butyl Phthalate	28	000084-74-2	2
24	31.31	6.28	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			9-Octadecenamide, (Z)-	113301	000301-02-0	93
			Tetradecanamide	113299	000638-58-4	64
25	31.52	1.81	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	87
			Diisooctyl adipate	58242	001330-86-5	87
26	31.61	1.14	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	90
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	52
			Dodecane, 3-methyl-	112340	017312-57-1	22
27	32.51	2.37	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	98
			1-Eicosanol	112640	000629-96-9	94
			1-Heneicosyl formate	16592	077899-03-7	94
28	32.82	4.61	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	38
29	33.12	0.64	C:\Database\NIST98.L			
			9(10H)-Acridinone, 1-hydroxy-2,...	99584	007008-68-6	35
			9-Acridanone, 4-hydroxy-1,2,3-t...	99541	017014-63-0	30
			7-(4-Chlorophenyl)-1,2,3,4-tetr...	100906	1000105-69-8	25
30	33.76	0.66	C:\Database\NIST98.L			
			Heptasiloxane, 1,1,3,3,5,5,7,7,...	27374	019095-23-9	37
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	22
			1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1	11
31	33.92	1.27	C:\Database\NIST98.L			
			2-Ethylacridine	84846	1000147-64-9	11
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	11
			1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1	11
32	33.99	1.25	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	43
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	37
			Silane, [[4-[1,2-bis[(trimethyl...	128841	056114-62-6	12
33	34.08	0.81	C:\Database\NIST98.L			
			1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1	25
			N-Cyano-N',N',N'',N''-tetrameth...	84777	074150-88-2	25
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	22
34	35.04	30.64	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	91
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
			7-Nonenamide	19655	090949-53-4	59
35	35.36	1.12	C:\Database\NIST98.L			
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	25
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	22
			3-Hydroxy-.beta.-damascone	23371	102488-09-5	12

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36  36.14  1.41 C:\Database\NIST98.L
              Propanamide, N-(3-methoxyphenyl...  17665 056619-93-3 14
              Propanamide, N-(4-methoxyphenyl...  17557 056619-94-4 14
              14-Oxabicyclo[10.3.0]pentadecan...   2747 1000163-86-0 10

37  36.35  3.77 C:\Database\NIST98.L
              Phenanthro[3,2-b]furan-4-carbox... 100976 019941-61-8 16
              Androst-4-en-3-one, 17-acetoxy-... 100966 1000189-52-8 10
              4H-1-Benzopyran-4-one, 3,5,7-tr... 101040 000480-19-3  9

38  39.11  0.69 C:\Database\NIST98.L
              Silane, 1,4-phenylenebis[trimet...  84731 013183-70-5 35
              1,3-Bis(trimethylsilyl)benzene      84730 002060-89-1 35
              Cyclotrisiloxane, hexamethyl-       84874 000541-05-9 27

                    Tue Jan 15 17:58:02 2008
```

No Disinfectant
Day 9
Sample

tmpfrbrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\016.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 5:37 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 18

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	6.18	4.81	C:\Database\NIST98.L			
			N-Hydroxymethylacetamide	4703	000625-51-4	7
			Formamide, N-methyl-	113277	000123-39-7	5
			Ethanol, O-acetimidoyl-	5839	1000130-65-6	5
2	7.32	0.55	C:\Database\NIST98.L			
			Phenol, 2-fluoro-	50680	000367-12-4	91
			Phenol, 3-fluoro-	120187	000372-20-3	27
			1,4-Cyclohexanedione	50578	000637-88-7	14
3	8.68	1.60	C:\Database\NIST98.L			
			3-Hexanol, 4-methyl-	113235	000615-29-2	59
			3-Hexanol, 4-methyl-	19352	000615-29-2	59
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	42
4	9.69	0.86	C:\Database\NIST98.L			
			Cyclopropane, isothiocyanato-	118526	056601-42-4	64
			2-Pyrrolidinone, 4-methyl-	914	1000197-00-3	59
			Hexanoic acid, anhydride	118546	002051-49-2	50
5	10.21	0.78	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	86
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	86
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	58
6	13.49	0.55	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	90
			1-Propanol, 2-(2-hydroxypropoxy)-	19322	000106-62-7	72
			Methane, diethoxy-	108343	000462-95-3	72
7	13.57	0.52	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	90
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	78
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	78
8	15.71	0.55	C:\Database\NIST98.L			
			Nonanoic acid	20156	000112-05-0	64
			Nonanoic acid	113428	000112-05-0	53
			Butanoic acid, 3-methyl-, 1-met...	110081	032665-23-9	37
9	17.42	1.25	C:\Database\NIST98.L			
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	59
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	50
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	38

Page 1

10	17.76	2.03	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	96
11	17.83	1.60	C:\Database\NIST98.L			
			Butanoic acid, butyl ester	109895	000109-21-7	78
			Butanoic acid, butyl ester	114541	000109-21-7	78
			Propanoic acid, 2-methyl-, 2-et...	36107	074367-31-0	59
12	18.79	0.80	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	59
			2-Propanol, 1-methoxy-2-methyl-	19309	003587-64-2	50
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	42
13	18.88	1.57	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	59
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	56
			2-Propanol, 1,1'-[(1-methyl-1,2...	19307	001638-16-0	53
14	18.96	0.89	C:\Database\NIST98.L			
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	59
			2-Butanol, 3-methoxy-	113137	053778-72-6	52
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	50
15	19.55	0.60	C:\Database\NIST98.L			
			Cyclodecane	13064	000293-96-9	95
			Cyclodecane	111288	000293-96-9	95
			1-Dodecanol	111442	000112-53-8	95
16	21.47	1.55	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			Methylamine, N-(1-methylhexylid...	24533	022058-71-5	47
			Butyric acid, thio-, S-decyl ester	24338	002432-55-5	47
17	22.51	2.14	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	97
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	12
			Benzene, 1,1',1'',1'''-(1,2-eth...	128732	000632-51-9	9
18	23.08	1.01	C:\Database\NIST98.L			
			Phenol, 2,4-di-t-butyl-6-nitro-	90753	1000128-93-2	97
			Benzodifuroxanofurazan	90607	1000110-71-3	59
			7,7-Dimethyl-1,4-dioxo-2,3,4,5,...	90678	051799-98-5	59
19	23.37	0.86	C:\Database\NIST98.L			
			Heptadecane	112320	000629-78-7	86
			Heptadecane	16420	000629-78-7	83
			Heptadecane	112322	000629-78-7	46
20	23.49	1.17	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	50
			4-Hydroxy-3-hexanone	113140	004984-85-4	50
			3,5-Dioxahexaldoxin-2,6-dione-,...	5834	081539-54-0	43
21	23.57	1.19	C:\Database\NIST98.L			
			2-Butanol, 3-methoxy-	19505	053778-72-6	46
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	43
			2-Butanol, 3-methoxy-	113137	053778-72-6	43
22	24.90	0.72	C:\Database\NIST98.L			
			Octadecane	112333	000593-45-3	96
			Octadecane	16439	000593-45-3	96

				Octadecane	112330	000593-45-3 96
23	24.99	0.63	C:\Database\NIST98.L			
				Hexatriacontane	112335	000630-06-8 86
				Tetratetracontane	112365	007098-22-8 80
				Heptacosane, 1-chloro-	16427	062016-79-9 80
24	25.75	1.71	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 64
				Diethyl Phthalate	14	000084-66-2 9
				Benzyl butyl Phthalate	36	000085-68-7 1
25	26.07	0.67	C:\Database\NIST98.L			
				Ethanone, 2,2-dimethoxy-1,2-dip...	67798	024650-42-8 43
				Benzylamine, .alpha.-methyl-m-n...	67797	1000187-78-7 38
				6H-Purin-6-one, 2-amino-1,7-dih...	123597	000073-40-5 35
26	26.26	0.76	C:\Database\NIST98.L			
				Nonadecane	112381	000629-92-5 98
				Nonadecane	112380	000629-92-5 96
				Nonadecane	16515	000629-92-5 96
27	26.38	1.18	C:\Database\NIST98.L			
				7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4 93
				Ethene,-1-(4-diethylaminophenyl...	84389	1000221-95-1 38
				3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9 38
28	27.01	7.62	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 60
				Diethyl Phthalate	14	000084-66-2 1
29	27.51	0.97	C:\Database\NIST98.L			
				Eicosane	112345	000112-95-8 95
				Eicosane	112565	000112-95-8 95
				Heptacosane	16471	000593-49-7 91
30	29.08	0.58	C:\Database\NIST98.L			
				Methyl 15-oxohexadecanoate	5774	099706-71-5 38
				2-Naphthalenemethanol, decahydr...	19927	051317-08-9 25
				3-Acetoxypentadecane	4233	1000245-62-1 22
31	29.31	5.76	C:\Database\NIST98.L			
				Octadecanoic acid	114902	000057-11-4 96
				Octadecanoic acid	109378	000057-11-4 87
				Pentadecanoic acid	114896	001002-84-2 86
32	29.51	1.11	C:\Database\NIST98.L			
				Hexadecanamide	113298	000629-54-9 76
				Hexadecanamide	19647	000629-54-9 76
				Tetradecanamide	19652	000638-58-4 62
33	29.78	4.09	C:\Database\OWML.L			
				Terphenyl-d14	34	001718-51-0 99
34	31.23	1.01	C:\Database\OWML.L			
				Benzyl butyl Phthalate	36	000085-68-7 99
				Diethyl Phthalate	14	000084-66-2 38
				Di-n-butyl Phthalate	28	000084-74-2 25
35	31.31	5.39	C:\Database\NIST98.L			
				9-Octadecenamide, (Z)-	113302	000301-02-0 97
				9-Octadecenamide, (Z)-	113301	000301-02-0 91
				7-Nonenamide	19655	090949-53-4 64

36	31.53	1.11	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Diisooctyl adipate	58242	001330-86-5	81
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	70
37	31.61	1.67	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	81
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	49
			2-Propanone, ethylhydrazone	15402	007422-99-3	30
38	32.50	2.62	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	98
			Cyclohexadecane	14275	000295-65-8	95
			1-Heneicosyl formate	16592	077899-03-7	95
39	32.82	2.50	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	90
			Di-n-octyl phthalate	40	000117-81-0	40
			Di-n-butyl Phthalate	28	000084-74-2	37
40	33.16	0.53	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	109752	000301-02-0	47
			9-Octadecenamide, (Z)-	19657	000301-02-0	46
			Dodecanamide	19649	001120-16-7	38
41	35.05	25.12	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	90
			Erucylamide	113300	000112-84-5	89
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
42	35.37	0.71	C:\Database\NIST98.L			
			Docosa-2,6,10,14,18-pentaen-22-...	23027	1000163-04-7	46
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	43
			2,6,10-Dodecatrien-1-ol, 3,7,11...	23046	004602-84-0	43
43	36.10	0.67	C:\Database\NIST98.L			
			Propanamide, N-(4-methoxyphenyl...	17557	056619-94-4	18
			2-t-Butyl-5-chloromethyl-3-meth...	17941	1000192-88-5	9
			Butanedioic acid, chloro-, bis(...	17739	057983-51-4	8
44	36.36	3.09	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	10
			4H-1-Benzopyran-4-one, 3,5,7-tr...	101040	000480-19-3	9
			2-Propyn-1-one, 1-(2-thienyl)-,...	100982	056588-20-6	9
45	37.63	2.38	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	40
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	25
			Pentasiloxane, dodecamethyl-	115143	000141-63-9	22
46	39.05	0.53	C:\Database\NIST98.L			
			Hexahydropyridine, 1-methyl-4 [...	84723	094427-47-1	49
			1-Dotriacontanol	16786	006624-79-9	25
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	15

Tue Jan 15 17:53:37 2008

No Disinfectant
Day 14
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\018.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 7:32 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 20

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	5.94	0.96	C:\Database\NIST98.L			
			1-Methoxy-5-heptafluorobutyrylo...	11866	1000216-63-3	40
			Butane, 1-bromo-4-methoxy-	110863	004457-67-4	39
			2-Pentanol, 4-methyl-	110825	000108-11-2	9
2	6.26	1.66	C:\Database\NIST98.L			
			Butane, 2,3-dichloro-2-methyl-	29395	000507-45-9	90
			4-Ethynyl-4-vinyl-1,6-heptadiene	29556	1000118-58-4	9
			Propane, 1,1-dichloro-	29392	000078-99-9	9
3	6.53	0.80	C:\Database\NIST98.L			
			Silane, tetramethyl-	114850	000075-76-3	12
			Silane, tetramethyl-	114826	000075-76-3	9
			Isopropyl 5,11-dihydroxy-3,7,11...	25305	1000223-34-1	9
4	7.32	1.72	C:\Database\NIST98.L			
			Phenol, 2-fluoro-	50680	000367-12-4	91
			Phenol, 4-fluoro-	50723	000371-41-5	22
			Phenol, 4-fluoro-	120186	000371-41-5	12
5	8.36	0.51	C:\Database\NIST98.L			
			Cyclopentene, 1,2,3,3,4-pentame...	55761	1000152-27-1	90
			Cyclopentene, 1,2,3,4,5-pentame...	55801	1000154-28-6	90
			5-t-Butyl-4-methylimidazole	56050	1000129-14-1	80
6	8.68	0.50	C:\Database\NIST98.L			
			.beta.-Methoxyethoxymethyl chlo...	11722	003970-21-6	72
			Silane, ethyldimethyl-	19594	000758-21-4	56
			Ethanol, 2-(2-methoxyethoxy)-	110890	000111-77-3	53
7	9.69	1.72	C:\Database\NIST98.L			
			Glycocyanidine	43063	000503-86-6	64
			2(3H)-Furanone, 5-hexyldihydro-...	43041	125133-98-4	56
			trans-4-Hydroxy-3-methyldecanoi...	43036	147254-33-9	56
8	10.20	1.70	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	64
9	10.88	0.55	C:\Database\NIST98.L			
			1-Butanol, 3-methyl-, nitrate	2253	000543-87-3	28
			1-Hexanol, 2-ethyl-	112637	000104-76-7	27
			1-Hexanol, 2-ethyl-	112165	000104-76-7	27

Page 1

10	12.13	1.28	C:\Database\NIST98.L			
			Benzene-d5-, nitro-	32381	004165-60-0	72
			1,2-Benzenedicarbonitrile	121767	000091-15-6	9
			6-Amino-1,3,5-triazine-2,4(1H,3...	57996	000645-93-2	9
11	16.72	0.76	C:\Database\NIST98.L			
			Phthalic anhydride	44822	000085-44-9	95
			Phthalic anhydride	118873	000085-44-9	91
			Phthalic anhydride	115649	000085-44-9	91
12	17.42	1.60	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	59
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	45
			Propanoic acid, 2-methyl-, 2-me...	114586	000097-85-8	33
13	17.76	2.90	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	96
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	94
14	17.83	1.92	C:\Database\NIST98.L			
			Butanoic acid, butyl ester	109895	000109-21-7	78
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	74
			Butanoic acid, hexyl ester	109931	002639-63-6	74
15	18.25	2.58	C:\Database\NIST98.L			
			Vanillin	123636	000121-33-5	95
			Benzaldehyde, 3-hydroxy-4-methoxy-	67910	000621-59-0	95
			Vanillin	123724	000121-33-5	95
16	19.75	0.60	C:\Database\NIST98.L			
			Ethanone, 1-(4-hydroxy-3-methox...	67962	000498-02-2	91
			Ethanone, 1-(4-hydroxy-3-methox...	123645	000498-02-2	90
			Ethanone, 1-[4-(methylthio)phen...	67954	001778-09-2	72
17	20.91	0.70	C:\Database\NIST98.L			
			Dodecanoic acid	114899	000143-07-7	70
			Dodecanoic acid	114903	000143-07-7	55
			Dodecanoic acid	25776	000143-07-7	55
18	21.47	2.72	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	34
			Butane, 1-bromo-2-methyl-	114514	010422-35-2	33
19	22.51	2.58	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	94
			Estra-1,3,5(10)-triene-4,17-dio...	102213	065968-98-1	10
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
20	22.80	0.55	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	64
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	55
			1,4-Benzenediol, 2,5-bis(1,1-di...	126923	000079-74-3	47
21	23.07	0.82	C:\Database\NIST98.L			
			Phenol, 2,4-di-t-butyl-6-nitro-	90753	1000128-93-2	76
			1,3,2-Oxazaborolidine, 3,4-dime...	90718	026574-29-8	50
			1,2,3,4-Tetrahydroisoquinoline,...	90738	1000128-00-6	47
22	23.37	1.25	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	97
			Heptadecane	112320	000629-78-7	97

				Hexatriacontane	112335	000630-06-8 70
23	24.90	0.75	C:\Database\NIST98.L			
				Octadecane	16439	000593-45-3 98
				Octadecane	112333	000593-45-3 93
				Octacosane	112312	000630-02-4 91
24	24.98	0.52	C:\Database\NIST98.L			
				Hexatriacontane	112334	000630-06-8 83
				Tetratetracontane	16486	007098-22-8 81
				Hexadecane, 2,6,10,14-tetramethyl-	112575	000638-36-8 74
25	25.16	1.93	C:\Database\NIST98.L			
				4H-1,3,2-Dioxaborin, 6-ethenyl-...	67890	074630-05-0 60
				2H-Pyran-2-carboxylic acid, 5-e...	67701	019776-81-9 58
				4-(Methylthio)thiobenzoic acid,...	67709	1000192-53-9 50
26	25.75	1.37	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 78
				Diethyl Phthalate	14	000084-66-2 9
27	26.26	0.65	C:\Database\NIST98.L			
				Nonadecane	112382	000629-92-5 96
				Nonadecane	112380	000629-92-5 95
				Nonadecane	112576	000629-92-5 94
28	26.38	1.32	C:\Database\NIST98.L			
				7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4 93
				1,3-Pentadiene, 1,1-diphenyl-, ...	126412	015295-31-5 55
				1,3-Pentadiene, 1,1-diphenyl-, ...	84396	015295-31-5 51
29	27.00	22.55	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 95
				Di-n-octyl phthalate	40	000117-81-0 38
				Diethyl Phthalate	14	000084-66-2 9
30	27.16	0.74	C:\Database\NIST98.L			
				Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4 55
				Oxirane, hexadecyl-	109681	007390-81-0 52
				Ethanol, 2-(hexadecyloxy)-	112374	002136-71-2 46
31	27.51	0.89	C:\Database\NIST98.L			
				Eicosane	112565	000112-95-8 96
				Eicosane	112345	000112-95-8 95
				Eicosane	109630	000112-95-8 93
32	29.07	0.54	C:\Database\NIST98.L			
				Trifluoroacetic acid, n-tetrade...	4218	1000216-79-0 46
				14-Pentadecenoic acid	13939	017351-34-7 46
				2-Pentenoic acid, 4-methyl-, me...	108835	050652-78-3 43
33	29.30	4.42	C:\Database\NIST98.L			
				Octadecanoic acid	114902	000057-11-4 99
				Octadecanoic acid	109378	000057-11-4 80
				Pentadecanoic acid	114896	001002-84-2 70
34	29.50	0.70	C:\Database\NIST98.L			
				Hexadecanamide	19647	000629-54-9 70
				Tetradecanamide	19652	000638-58-4 64
				Hexadecanamide	113298	000629-54-9 52
35	29.56	0.59	C:\Database\NIST98.L			
				Hexadecanoic acid, butyl ester	15257	000111-06-8 52

			Octadecanoic acid	109986	000057-11-4	41
			Hexadecanoic acid, 1,1-dimethyl...	15255	031158-91-5	38
36	29.78	3.77	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
37	31.22	1.55	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	99
			Diethyl Phthalate	14	000084-66-2	33
			Di-n-butyl Phthalate	28	000084-74-2	9
38	31.31	4.73	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			9-Octadecenamide, (Z)-	113301	000301-02-0	83
			Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	64
39	31.53	1.04	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	87
			Diisooctyl adipate	58242	001330-86-5	87
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	87
40	31.61	0.73	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	74
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	58
			Heptadecane, 3-methyl-	17051	006418-44-6	22
41	32.51	1.56	C:\Database\NIST98.L			
			Cyclohexadecane	14275	000295-65-8	98
			1-Heneicosyl formate	16592	077899-03-7	94
			1-Eicosanol	112640	000629-96-9	94
42	32.82	5.78	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	37
43	33.11	0.48	C:\Database\NIST98.L			
			9-Acridanone, 4-hydroxy-1,2,3-t...	99541	017014-63-0	58
			9(10H)-Acridinone, 1-hydroxy-2,...	99584	007008-68-6	49
			Sulazepam	99575	002898-13-7	43
44	33.38	0.73	C:\Database\NIST98.L			
			2,4-Di-tert-butylthiophenol	84717	019728-43-9	25
			Pentasiloxane, dodecamethyl-	97318	000141-63-9	22
			Tetrasiloxane, decamethyl-	27371	000141-62-8	14
45	35.04	7.60	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	93
			Erucylamide	113300	000112-84-5	87
			9-Octadecenamide, (Z)-	109752	000301-02-0	76
46	35.36	0.88	C:\Database\NIST98.L			
			2,6,10,14,18-Pentamethyl-2,6,10...	23038	075581-03-2	83
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	52
			Docosa-2,6,10,14,18-pentaen-22-...	23027	1000163-04-7	52
47	36.11	0.48	C:\Database\NIST98.L			
			1,1,1,3,5,5,5-Heptamethyltrisil...	84726	001873-88-7	38
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	27
			Silane, trimethyl[5-methyl-2-(1...	84732	055012-80-1	27
48	36.35	2.26	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	22

			2-Propyn-1-one, 1-(2-thienyl)-,...	100982	056588-20-6	22
			10,11-(3'-6'-Dihydrobenzo)[3.2]...	100973	1000202-32-4	9
49	39.10	0.51	C:\Database\NIST98.L			
			1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1	50
			Silane, 1,4-phenylenebis[trimet...	84731	013183-70-5	47
			1,1,1,3,5,5,5-Heptamethyltrisil...	84726	001873-88-7	43
50	39.69	0.56	C:\Database\NIST98.L			
			Silane, 1,4-phenylenebis[trimet...	84731	013183-70-5	43
			Propiophenone, 2'-(trimethylsil...	84849	033342-87-9	43
			Cyclotrisiloxane, hexamethyl-	126480	000541-05-9	40

Tue Jan 15 18:02:57 2008

No Disinfectant
Day 14
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\023.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 12:17 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 25

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	27.00	3.10	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	94
			Diethyl Phthalate	14	000084-66-2	10
2	29.79	3.28	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
3	31.32	2.98	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	95
			9-Octadecenamide, (Z)-	113301	000301-02-0	91
			Tetradecanamide	113299	000638-58-4	64
4	32.52	1.83	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	97
			Cyclotetradecane	13185	000295-17-0	94
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	94
5	32.84	70.69	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	99
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	37
6	35.04	14.89	C:\Database\NIST98.L			
			Erucylamide	113300	000112-84-5	93
			Erucylamide	19656	000112-84-5	93
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
7	36.36	3.23	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	27
			Bicyclo[5.3.0]decan-2-one, 9-(d...	100989	1000151-00-6	12
			Butanoic acid, heptafluoro-, 4-...	100964	055521-08-9	10

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Chlorine
Day 1
Control

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\002.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 4:16 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 4

Search Libraries: C:\Database\NIST98.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	10.20	0.24	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	86
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	86
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	52
2	16.37	0.35	C:\Database\NIST98.L			
			Cyclohexasiloxane, dodecamethyl-	27931	000540-97-6	94
			Cyclohexasiloxane, dodecamethyl-	115309	000540-97-6	80
			Acetic acid, [bis[(trimethylsil...	102689	053044-27-2	38
3	17.41	0.39	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	59
			3-Hexenoic acid, 5-hydroxy-2-me...	6424	110678-36-9	33
			Oxirane, propyl-	108847	001003-14-1	32
4	17.76	0.65	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	93
5	17.82	0.46	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	80
			Butanoic acid, butyl ester	109895	000109-21-7	72
			Butanoic acid, butyl ester	114541	000109-21-7	72
6	19.32	0.94	C:\Database\NIST98.L			
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	60
			3-Isopropoxy-1,1,1,7,7,7-hexame...	26784	071579-69-6	27
			Tetrasiloxane, 3,5-diethoxy-1,1...	27899	072439-78-2	22
7	21.47	0.37	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 1-(1...	24401	074381-40-1	50
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	36
			Butane, 1-bromo-2-methyl-	114514	010422-35-2	33
8	22.06	1.07	C:\Database\NIST98.L			
			Silane, [[4-[1,2-bis[(trimethyl...	103450	056114-62-6	40
			Silane, [[4-[1,2-bis[(trimethyl...	128841	056114-62-6	40
			1,3,5,7-Tetraethyl-1-ethylbutox...	103472	073420-30-1	38
9	24.52	1.45	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	72
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	36
			Cyclohexasiloxane, dodecamethyl-	27931	000540-97-6	27

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10	25.76	0.29	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	67019	017851-53-5	90
			1,2-Benzenedicarboxylic acid, b...	123428	000084-78-6	90
			1,2-Benzenedicarboxylic acid, b...	66726	000084-78-6	86
11	26.38	0.24	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	95
			1,3-Pentadiene, 1,1-diphenyl-, ...	126412	015295-31-5	47
			Ethanone, 1-(5,6,7,8-tetrahydro...	84211	071596-88-8	46
12	26.52	1.88	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	38
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	37
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	35
13	27.01	2.92	C:\Database\NIST98.L			
			n-Hexadecanoic acid	114901	000057-10-3	97
			n-Hexadecanoic acid	109985	000057-10-3	91
			Tetradecanoic acid	114897	000544-63-8	90
14	28.21	2.71	C:\Database\NIST98.L			
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	68
			Chromium, tricarbonyl-.eta.-6-(...	103435	1000162-19-6	64
			Cycloheptasiloxane, tetradecame...	27714	000107-50-6	49
15	29.30	1.91	C:\Database\NIST98.L			
			Octadecanoic acid	6590	000057-11-4	93
			Octadecanoic acid	109378	000057-11-4	83
			Pentadecanoic acid	114896	001002-84-2	70
16	29.67	4.17	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	72
			9,12,15-Octadecatrienoic acid, ...	25608	055521-22-7	35
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	28
17	29.78	0.82	C:\Database\NIST98.L			
			p-Terphenyl-d14	92199	001718-51-0	99
			2-Benzylbiphenyl	92149	1000118-48-9	59
			Cyclopropane, 2-methylene-1-phe...	92107	1000157-34-1	59
18	30.97	6.19	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	53
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	50
			3-Isopropoxy-1,1,1,7,7,7-hexame...	26784	071579-69-6	25
19	31.31	0.57	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	93
			9-Octadecenamide, (Z)-	113301	000301-02-0	91
			Tetradecanamide	19652	000638-58-4	72
20	31.53	0.34	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	94
			Diisooctyl adipate	58242	001330-86-5	91
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	83
21	32.17	8.69	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	27
			Benzoic acid, 2,5-bis(trimethyl...	103449	003618-20-0	25
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	22
22	32.48	0.32	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	99
			Cyclohexadecane	14275	000295-65-8	98

			1-Heneicosyl formate	16592	077899-03-7	95
23	32.83	1.85	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, d...	123512	027554-26-3	91
			Bis(2-ethylhexyl) phthalate	66784	000117-81-7	91
			Bis(2-ethylhexyl) phthalate	123509	000117-81-7	91
24	33.28	10.96	C:\Database\NIST98.L			
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	30
			Dibutanoylmorphine	103463	066641-03-0	25
			2,4,6(1H,3H,5H)-Pyrimidinetrion...	103442	052937-67-4	15
25	34.40	11.77	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	64
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	38
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	18
26	35.04	2.33	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	91
			Erucylamide	113300	000112-84-5	76
			7-Nonenamide	19655	090949-53-4	59
27	35.64	11.24	C:\Database\NIST98.L			
			Eseroline, 7-bromo-, methylcarb...	3850	114546-23-5	91
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	64
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	32
28	36.37	0.30	C:\Database\NIST98.L			
			13H-Benz[6,7]indolo[3,2-c]quino...	101046	004240-59-9	16
			Benzoic acid, 3,5-dicyclohexyl-...	100954	055125-23-0	12
			Tris(3-fluorophenyl)phosphine	100984	023039-94-3	9
29	37.08	10.10	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	74
			Eseroline, 7-bromo-, methylcarb...	3850	114546-23-5	59
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	43
30	38.82	7.28	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	64
			Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	41
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	38
31	40.98	5.08	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	74
			Mercaptoacetic acid, bis(trimet...	26922	006398-62-5	38
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	37
32	43.73	2.12	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	80
			Heptasiloxane, hexadecamethyl-	27486	000541-01-5	30
			Dibutanoylmorphine	103463	066641-03-0	25

Tue Jan 15 15:50:14 2008

Chlorine
Day 1
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\008.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 10:00 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 10

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	6.15	0.40	C:\Database\NIST98.L			
			2-Butanol, 2,3-dimethyl-	113317	000594-60-5	9
			Ethanol, O-acetimidoyl-	5839	1000130-65-6	5
			1,2-Butanediol	113157	000584-03-2	5
2	7.30	0.85	C:\Database\NIST98.L			
			Phenol, 2-fluoro-	50680	000367-12-4	91
			Phenol, 4-fluoro-	120185	000371-41-5	22
			Phenol, 4-fluoro-	120186	000371-41-5	12
3	8.67	0.38	C:\Database\NIST98.L			
			Ethanol, 2-(2-methoxyethoxy)-	110890	000111-77-3	83
			Ethanol, 2-(2-methoxyethoxy)-	11464	000111-77-3	83
			Ethanol, 2-[2-(2-methoxyethoxy)...	11712	000112-35-6	64
4	9.67	0.71	C:\Database\NIST98.L			
			Hexanoic acid, anhydride	43066	002051-49-2	64
			Hexanoic acid, anhydride	118546	002051-49-2	64
			Glycocyanidine	43063	000503-86-6	64
5	10.20	1.12	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	64
6	10.85	0.75	C:\Database\NIST98.L			
			1-Hexanol, 2-ethyl-	15889	000104-76-7	90
			1-Hexanol, 2-ethyl-	112146	000104-76-7	83
			1-Hexanol, 2-ethyl-	112147	000104-76-7	74
7	10.89	0.35	C:\Database\NIST98.L			
			Butanedioic acid, dimethyl ester	51620	000106-65-0	78
			Butanedioic acid, dimethyl ester	111493	000106-65-0	78
			Butanedioic acid, dimethyl ester	120347	000106-65-0	64
8	11.00	1.32	C:\Database\NIST98.L			
			Benzyl Alcohol	115958	000100-51-6	96
			Benzyl Alcohol	30979	000100-51-6	96
			Benzyl Alcohol	115957	000100-51-6	94
9	12.13	0.63	C:\Database\NIST98.L			
			Benzene-d5-, nitro-	32381	004165-60-0	43
			1H-Imidazole, 2-methyl-	116286	000693-98-1	38
			Piperidine, 4-methyl-1-nitroso-	3307	015104-03-7	9

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10	13.13	2.07	C:\Database\NIST98.L			
			Pentanedioic acid, dimethyl ester	113343	001119-40-0	90
			Pentanedioic acid, dimethyl ester	113131	001119-40-0	83
			Pentanedioic acid, dimethyl ester	19807	001119-40-0	83
11	13.27	0.56	C:\Database\NIST98.L			
			Benzene, 1-chloro-2-isocyanato-	68548	003320-83-0	97
			Benzene, chloroisocyanato-	68619	051134-03-3	87
			Benzene, 1-chloro-3-isocyanato-	68620	002909-38-8	87
12	13.57	0.42	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	86
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	78
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	78
13	15.26	1.22	C:\Database\NIST98.L			
			Hexanedioic acid, dimethyl ester	113348	000627-93-0	91
			Hexanedioic acid, dimethyl ester	19850	000627-93-0	91
			Hexanedioic acid, dimethyl ester	113264	000627-93-0	91
14	15.71	0.98	C:\Database\NIST98.L			
			Nonanoic acid	113428	000112-05-0	95
			Nonanoic acid	20156	000112-05-0	94
			Nonanoic acid	113427	000112-05-0	90
15	17.41	1.61	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	59
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	59
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	38
16	17.76	1.91	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	96
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
17	17.83	1.86	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	74
			Butanoic acid, butyl ester	114541	000109-21-7	72
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	72
18	18.78	0.39	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	64
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	64
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	59
19	18.87	0.70	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	64
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	64
			2-Butanol, 3-methoxy-	19505	053778-72-6	52
20	18.96	0.39	C:\Database\NIST98.L			
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	64
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	59
			2-Propanol, 1-[2-(2-methoxy-1-m...	19665	020324-33-8	50
21	19.30	0.38	C:\Database\NIST98.L			
			Butylated Hydroxyanisole	124493	025013-16-5	70
			Phenol, 3-(1,1-dimethylethyl)-4...	124524	000088-32-4	64
			Butylated Hydroxyanisole	72597	025013-16-5	64
22	19.54	0.41	C:\Database\NIST98.L			
			Cyclododecane	111542	000294-62-2	97
			1-Dodecanol	111442	000112-53-8	94

			Cyclodecane	111288	000293-96-9	93
23	20.89	0.51	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	93
			n-Decanoic acid	113414	000334-48-5	62
			n-Decanoic acid	113415	000334-48-5	62
24	21.47	1.96	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	74
			Di-n-butyl Phthalate	28	000084-74-2	10
25	21.62	0.96	C:\Database\NIST98.L			
			2-Pentanol, 2,3-dimethyl-	19399	004911-70-0	50
			2-Propanol, 1-[2-(2-methoxy-1-m...	19665	020324-33-8	50
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	50
26	22.37	0.40	C:\Database\NIST98.L			
			Benzophenone	46089	000119-61-9	93
			Benzophenone	119383	000119-61-9	93
			Benzophenone	119171	000119-61-9	76
27	22.51	1.79	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	94
			2-Bromo-4-chloro-5,8-dimethoxy-...	102208	104506-11-8	12
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	10
28	22.80	0.81	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	46
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	42
			Octamethyl-1,3-cyclohexadiene	76425	1000110-41-8	35
29	23.37	0.46	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	97
			Heptadecane	112320	000629-78-7	96
			Heptadecane	112322	000629-78-7	91
30	23.56	0.46	C:\Database\NIST98.L			
			d-Ribo-tetrofuranose, 4-c-cyclo...	19644	030571-50-7	38
			Ethane, 1,2-diethoxy-	19316	000629-14-1	38
			Butane, 2-methoxy-	19272	006795-87-5	38
31	24.23	0.62	C:\Database\NIST98.L			
			Tetradecanoic acid	114898	000544-63-8	98
			Tetradecanoic acid	114897	000544-63-8	98
			Tetradecanoic acid	113420	000544-63-8	93
32	24.90	0.49	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octadecane	112330	000593-45-3	98
			Octadecane	112333	000593-45-3	91
33	24.99	0.49	C:\Database\NIST98.L			
			Tritetracontane	17076	007098-21-7	72
			Dotriacontane	112351	000544-85-4	68
			Hexadecane	112409	000544-76-3	64
34	25.20	0.45	C:\Database\NIST98.L			
			Isopropyl Myristate	110206	000110-27-0	38
			2-Imidazolidinethione, 1-acetyl...	44413	067845-09-4	35
			Isopropyl Myristate	4614	000110-27-0	30
35	25.76	3.19	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78

				Diethyl Phthalate	14	000084-66-2 39
				Benzyl butyl Phthalate	36	000085-68-7 4
36	26.01	0.64	C:\Database\NIST98.L			
				Ethyl pentadecyl ether	19394	1000130-85-3 68
				1,2-Octadecanediol	16347	020294-76-2 38
				E-15-Heptadecenal	4195	1000130-97-9 38
37	26.38	0.43	C:\Database\OWML.L			
				Diethyl Phthalate	14	000084-66-2 50
				Di-n-butyl Phthalate	28	000084-74-2 38
				Benzyl butyl Phthalate	36	000085-68-7 9
38	27.00	7.45	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 94
				Diethyl Phthalate	14	000084-66-2 10
39	27.50	1.67	C:\Database\NIST98.L			
				Thiazole, 5-ethyl-2-methyl-	57685	019961-52-5 43
				3-Octen-2-ol, 2-methyl-, (Z)-	24462	018521-07-8 41
				Thiazole, 2,4,5-trimethyl-	121695	013623-11-5 38
40	27.81	0.40	C:\Database\NIST98.L			
				4-Isopropyl-5-methylhexa-2,4-di...	2959	1000191-04-3 35
				6-Methylcyclohexathiazole	50511	096963-10-9 25
				Benzoic acid, 2-amino-5-chloro-	68722	000635-21-2 18
41	28.15	0.50	C:\Database\NIST98.L			
				4-Hydroxy-2-hydroxyaminopyrimidine	57681	1000111-25-4 30
				Pyridine, 2-chloro-4-methyl-	57621	003678-62-4 25
				p-Chloroaniline	121728	000106-47-8 25
42	28.29	0.44	C:\Database\NIST98.L			
				2-Deoxyribofuranose, 1(O)-(t-bu...	99860	1000193-96-2 59
				1H-Indole-2,3-dione, 1-(tert-bu...	99838	1000143-18-8 39
				Silylamine, 1,1,1-trimethyl-N-[...	99852	033285-85-7 38
43	28.48	0.33	C:\Database\NIST98.L			
				Cyclohexadecane	14275	000295-65-8 96
				1-Octadecene	111277	000112-88-9 93
				1-Heneicosyl formate	16592	077899-03-7 91
44	29.05	0.39	C:\Database\NIST98.L			
				Methyl 15-methoxyhexadecanoate	19540	1000110-17-9 47
				2-Dodecanol, 2-methyl-	19343	001653-37-8 47
				Methyl trifluoroacetate	113295	000431-47-0 47
45	29.30	2.86	C:\Database\NIST98.L			
				Octadecanoic acid	114902	000057-11-4 97
				Octadecanoic acid	6590	000057-11-4 83
				Pentadecanoic acid	114896	001002-84-2 64
46	29.50	0.56	C:\Database\NIST98.L			
				Hexadecanamide	19647	000629-54-9 90
				Hexadecanamide	113298	000629-54-9 87
				9-Octadecenamide, (Z)-	19657	000301-02-0 86
47	29.78	2.22	C:\Database\OWML.L			
				Terphenyl-d14	34	001718-51-0 99
48	31.22	1.38	C:\Database\OWML.L			
				Benzyl butyl Phthalate	36	000085-68-7 99
				Di-n-octyl phthalate	40	000117-81-0 38

			Di-n-butyl Phthalate	28	000084-74-2	38
49	31.31	3.81	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113301	000301-02-0	93
			9-Octadecenamide, (Z)-	113302	000301-02-0	91
			9-Octadecenamide, (Z)-	19657	000301-02-0	87
50	31.53	1.11	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	78
			Hexanedioic acid, dioctyl ester	58241	000123-79-5	55
			Diisooctyl adipate	58242	001330-86-5	53
51	31.61	2.39	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	81
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	43
			2-Propanone, ethylhydrazone	15402	007422-99-3	14
52	31.74	2.91	C:\Database\NIST98.L			
			1-Propanol, 2-(2-hydroxypropoxy)-	19322	000106-62-7	50
			2-Pentanol, 2,3-dimethyl-	19399	004911-70-0	50
			Butanoic acid, 2-hydroxy-, ethy...	19292	052089-54-0	50
53	32.47	1.82	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	99
			1-Docosene	111438	001599-67-3	94
			1-Eicosanol	112640	000629-96-9	94
54	32.82	1.97	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	38
55	33.16	0.41	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	19657	000301-02-0	70
			9-Octadecenamide, (Z)-	109752	000301-02-0	53
			7-Nonenamide	19655	090949-53-4	52
56	34.02	2.66	C:\Database\NIST98.L			
			2-Heptanol, 2-methyl-	113196	000625-25-2	43
			2-Heptanol, 2-methyl-	113195	000625-25-2	43
			2-Hexanol, 2-methyl-	113176	000625-23-0	38
57	34.10	1.15	C:\Database\NIST98.L			
			4-O-Acetyl-2,5-di-O-methyl-3,6-...	19455	1000101-80-3	38
			2-[5-(1-Hydroxy-1-methylethyl)-...	19466	1000190-33-6	38
			4-Hydroxy-3-hexanone	19313	004984-85-4	38
58	34.23	0.59	C:\Database\NIST98.L			
			1,4-Di-O-acetyl-2,5-di-O-methyl...	19333	1000101-82-1	38
			3-Tetradecanol	113172	001653-32-3	37
			2-Pentanone, 5-methoxy-	5841	017429-04-8	35
59	35.05	16.42	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	90
			Hexadecanamide	19647	000629-54-9	59
			9-Octadecenamide, (Z)-	19657	000301-02-0	56
60	35.37	0.40	C:\Database\NIST98.L			
			2,6,10-Dodecatrien-1-ol, 3,7,11...	23046	004602-84-0	55
			9-Octadecenamide, (Z)-	19657	000301-02-0	38
			Erucylamide	19656	000112-84-5	35
61	36.38	1.22	C:\Database\NIST98.L			

			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	35
			Methyl 15-methoxyhexadecanoate	19540	1000110-17-9	27
			2-Hexanol, 2,3-dimethyl-	19357	019550-03-9	27
62	36.59	4.62	C:\Database\NIST98.L			
			Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3	43
			Ethane, 1,2-diethoxy-	19316	000629-14-1	43
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	43
63	39.02	0.39	C:\Database\NIST98.L			
			1-Dotriacontanol	16786	006624-79-9	60
			17-Pentatriacontene	5525	006971-40-0	60
			1-Docosanol	109619	000661-19-8	55
64	40.45	6.85	C:\Database\NIST98.L			
			.alpha.-D-Xylo-Hex-5-enofuranos...	19430	007284-07-3	38
			4-Hydroxy-3-hexanone	19313	004984-85-4	38
			2-Propanol, 1-methoxy-2-methyl-	19309	003587-64-2	38

Tue Jan 15 16:59:35 2008

Chlorine
Day 4
Control

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\005.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 7:09 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 7

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	17.41	0.49	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	35
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	33
			trans-2,3-Epoxydecane	5384	054125-39-2	27
2	17.76	0.90	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	96
3	17.82	0.44	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	80
			Butanoic acid, butyl ester	114541	000109-21-7	72
			Butanoic acid, butyl ester	109895	000109-21-7	72
4	20.08	0.69	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	94
			Phenol, 2,4-bis(1,1-dimethyleth...	125776	000096-76-4	93
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	93
5	21.20	0.55	C:\Database\NIST98.L			
			Benzene, 1,4-dichloro-2-ethenyl-	74996	001123-84-8	27
			2-Chlorobenzo[b]thiophene-3-ace...	75027	1000136-82-7	25
			Phenol, 4-bromo-	74993	000106-41-2	25
6	21.47	0.55	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	36
			3-Methyl-hepta-1,6-dien-3-ol	24386	1000192-46-9	33
7	22.83	17.17	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	93
			Octamethyl-1,3-cyclohexadiene	76425	1000110-41-8	38
			1,4-Naphthoquinone, 6-acetyl-2,...	127595	013379-24-3	35
8	24.60	1.82	C:\Database\NIST98.L			
			Phenol, 2-(1,1-dimethylethyl)-4...	80516	005806-73-5	91
			Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4	78
			3,4-Dimethyl-2-(3-methyl-butyry...	80691	071940-29-9	64
9	24.95	0.47	C:\Database\NIST98.L			
			Thiophene, 2-(butylthio)-	52184	003988-71-4	53
			4-Imidazolidinone, 5-(1-methylp...	52186	056830-83-2	45
			4-Imidazolidinone, 5-(2-methylp...	52185	056805-19-7	32

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10	25.17	6.66	C:\Database\NIST98.L			
			1,3,5,2-Oxaazoniaazaboratin, 2,...	92662	1000160-64-7	59
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	56
			Phenol, 2,4,6-tris(1,1-dimethyl...	92595	000732-26-3	38
11	25.76	0.49	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	40
			Benzyl butyl Phthalate	36	000085-68-7	1
12	27.01	3.64	C:\Database\NIST98.L			
			n-Hexadecanoic acid	114901	000057-10-3	98
			n-Hexadecanoic acid	109985	000057-10-3	96
			Tetradecanoic acid	113420	000544-63-8	89
13	28.15	2.96	C:\Database\NIST98.L			
			2-Nitrofluoranthene	92640	013177-29-2	45
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	39
			Phenol, 2,4,6-tris(1,1-dimethyl...	127577	000732-26-3	36
14	28.31	20.10	C:\Database\NIST98.L			
			Azadibenzopyrene	99857	104219-69-4	9
			5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4	9
			Hydromorphinol	99808	002183-56-4	9
15	29.31	2.66	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	95
			Octadecanoic acid	109378	000057-11-4	87
			Octadecanoic acid	6590	000057-11-4	83
16	29.78	1.27	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	98
17	31.03	1.38	C:\Database\NIST98.L			
			Morphine, 7-hydroxy-6,6-dimetho...	103696	1000124-39-9	45
			Isopropyl-[2-(4-methoxy-2,6-dim...	103705	1000189-65-2	40
			Kobalt, bis[3-(dimethylamino)pr...	103681	1000158-82-2	39
18	31.31	2.39	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	98
			9-Octadecenamide, (Z)-	19657	000301-02-0	90
			9-Octadecenamide, (Z)-	113301	000301-02-0	87
19	31.52	0.53	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	68
			Hexanedioic acid, dioctyl ester	58241	000123-79-5	64
20	31.85	0.51	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1-phenylethyl)-	98181	002769-94-0	70
			4-Androsten-6.beta.-ol-3,17-dione	99759	1000126-77-1	50
			Methanone, [1,4-dimethyl-7-(1-m...	99692	039665-56-0	43
21	31.99	0.51	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1-phenylethyl)-	98181	002769-94-0	76
			1-Hydroxy-3,7,8-trimethoxyxanth...	98185	1000140-88-5	47
			1-Hydroxy-3,7,8-trimethoxyxanth...	98184	1000110-64-5	47
22	32.48	1.42	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1-phenylethyl)-	98181	002769-94-0	91
			Cycloeicosane	13708	000296-56-0	78
			Cyclohexadecane	14275	000295-65-8	62

23	32.84	19.28	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	99
			Di-n-octyl phthalate	40	000117-81-0	53
			Di-n-butyl Phthalate	28	000084-74-2	37
24	35.05	9.56	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	93
			Erucylamide	113300	000112-84-5	81
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
25	35.37	1.88	C:\Database\NIST98.L			
			Squalene	114263	007683-64-9	99
			Squalene	114269	007683-64-9	93
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	91
26	37.92	0.72	C:\Database\NIST98.L			
			1-Azaspiro[4.5]dec-3-ene, 2-(di...	105071	100942-44-7	38
			(2-Methoxy-1,3,2-thiozin)[5,10,...	105075	1000128-12-1	32
			4,5-2H-Oxazole-5-one, 4-[3,5-di...	47557	1000130-25-1	32
27	38.15	0.96	C:\Database\NIST98.L			
			Z-14-Nonacosane	7508	1000131-18-9	35
			7-Chloro-3-[2,4-dichlorophenyl]...	105083	1000213-14-3	32
			1-Azaspiro[4.5]dec-3-ene, 2-(di...	105071	100942-44-7	32

Tue Jan 15 16:15:10 2008

Chlorine
Day 4
Sample

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Information from Data File:
     File:          D:\DATA\HEATHER\010708\013.D
     Operator:      Heather Johnson
     Date Acquired:  8 Jan 2008   2:45 am
     Method File:   OMML
     Sample Name:
     Misc Info:
     Vial Number:   15

Search Libraries:   C:\Database\NIST98.L              Minimum Quality:  35

Unknown Spectrum:   Apex
Integration Events: RTE Integrator - RTEINT.P
```

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	5.94	0.12	C:\Database\NIST98.L			
			2-Pentanol, 4-methyl-	110801	000108-11-2	39
			2,3-Butanediol, 1,4-dimethoxy-	11837	119613-19-3	38
			2-Hexanol, 5-methyl-	110852	000627-59-8	38
2	9.68	0.12	C:\Database\NIST98.L			
			Glycocyanidine	43063	000503-86-6	64
			Hexanoic acid, 1,2,3-propanetri...	43039	000621-70-5	39
			Phenol-d6-	43198	013127-88-3	38
3	13.28	0.45	C:\Database\NIST98.L			
			Benzene, 1-chloro-2-isocyanato-	68548	003320-83-0	95
			Benzene, chloroisocyanato-	68619	051134-03-3	93
			Benzene, 1-chloro-4-isocyanato-	68625	000104-12-1	91
4	13.77	0.11	C:\Database\NIST98.L			
			Octanoic Acid	113422	000124-07-2	38
			Butanoic acid, 3-methyl-, 1-met...	110081	032665-23-9	25
			Heptanoic acid	113419	000111-14-8	17
5	15.69	0.33	C:\Database\NIST98.L			
			2,3-Dimethyl-pyrrolo(2,3-b)pyra...	65651	1000146-46-8	38
			1H-Indol-4-ol, 3-methyl-	65646	001125-31-1	38
			1,3-Oxathiane, 2,4,6-trimethyl-...	20238	022425-90-7	35
6	16.86	0.22	C:\Database\NIST98.L			
			2-Propanol, 1,1'-[(1-methyl-1,2...	19307	001638-16-0	72
			Dipropylene glycol	113236	025265-71-8	64
			2-Butanol, 3-methoxy-	113137	053778-72-6	59
7	17.42	0.23	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	53
			Butanoic acid, 1-methyloctyl ester	24366	069727-42-0	38
			Ether, hexyl pentyl	6425	032357-83-8	38
8	17.83	0.38	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	90
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	64
			Butanoic acid, hexyl ester	109931	002639-63-6	56

9	18.87	0.73	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	64
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	59
			2-Propanol, 1,1'-[(1-methyl-1,2...	19307	001638-16-0	53
10	19.30	0.13	C:\Database\NIST98.L			
			Benzenethiol, 4-(1,1-dimethylet...	72721	015570-10-2	62
			9H-Fluorene, 2-methyl-	72713	001430-97-3	58
			3-tert-Butyl-4-hydroxyanisole	124527	000121-00-6	53
11	19.55	0.18	C:\Database\NIST98.L			
			1-Tridecanol	13019	000112-70-9	91
			Cyclododecane	111351	000294-62-2	91
			1-Undecanol	13829	000112-42-5	91
12	20.55	0.13	C:\Database\NIST98.L			
			Benzaldehyde, 2-chloro-4-hydroxy-	123882	056962-11-9	50
			Benzaldehyde, 2-chloro-3-hydroxy-	69298	056962-10-8	46
			Benzenamine, 4-chloro-N,N-dimet...	68965	000698-69-1	43
13	20.90	0.13	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	72
			Lauric anhydride	114892	000645-66-9	53
			n-Decanoic acid	113414	000334-48-5	43
14	21.47	0.67	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 1-(1...	24401	074381-40-1	43
			Phenmetrazine	114496	000134-49-6	38
			3-Methyl-hepta-1,6-dien-3-ol	24386	1000192-46-9	38
15	21.64	1.47	C:\Database\NIST98.L			
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	50
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	50
			Hexanamide	113230	000628-02-4	47
16	22.07	0.17	C:\Database\NIST98.L			
			Diazene, [1-(2,2-dimethylhydraz...	19854	061940-94-1	53
			Silane, octyl-	19805	000871-92-1	38
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	32
17	22.51	1.51	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	91
			2-Bromo-4-chloro-5,8-dimethoxy-...	102208	104506-11-8	12
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
18	22.81	0.19	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	80
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	55
			Boron, diethyl(5-ethyl-4,6-nona...	87941	136705-03-8	52
19	23.08	0.29	C:\Database\NIST98.L			
			Phenol, 2,4-di-t-butyl-6-nitro-	90753	1000128-93-2	96
			1,3,2-Oxazaborolidine, 3,4-dime...	90718	026574-29-8	72
			9,10-Anthracenedione, 1-ethyl-	127306	024624-29-1	53
20	23.37	0.27	C:\Database\NIST98.L			
			Heptadecane	112322	000629-78-7	42
			Hexatriacontane	112335	000630-06-8	38
			Eicosane	112344	000112-95-8	30

21	23.56	0.75	C:\Database\NIST98.L			
			Ethane, 1,2-diethoxy-	108349	000629-14-1	47
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	38
			Butanamide, 3-methyl-	113229	000541-46-8	37
22	24.36	0.18	C:\Database\NIST98.L			
			Quinoline, 6-methyl-2-phenyl-	87477	027356-46-3	38
			Phenethenyl hydrocyanic ether, ...	126877	112369-98-9	35
			Carbamodithioic acid, dibutyl-,...	16284	038351-44-9	27
23	24.44	0.19	C:\Database\NIST98.L			
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	52
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	50
			2,5,8,11,14-Pentaoxapentadecane	113269	000143-24-8	50
24	24.90	0.37	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octacosane	112312	000630-02-4	90
			Docosane	16531	000629-97-0	90
25	25.02	0.39	C:\Database\NIST98.L			
			1-Butanol, 3-methoxy-, acetate	5857	004435-53-4	50
			2-Propanol, 1-(isooctyloxy)-2-m...	19578	056282-27-0	38
			3-Tetradecanol	113170	001653-32-3	35
26	25.21	0.60	C:\Database\NIST98.L			
			2-Propanol, 1-[2-(2-methoxy-1-m...	19665	020324-33-8	43
			Hydrazine, 1,1-dimethyl-2-propyl-	19823	052728-54-8	43
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	35
27	25.48	0.27	C:\Database\NIST98.L			
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	35
			3-Hexadecanol	113255	000593-03-3	35
			3-Tetradecanol	19356	001653-32-3	27
28	25.75	1.45	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	67019	017851-53-5	52
			1,2-Benzenedicarboxylic acid, b...	123453	000084-69-5	50
			Dibutyl phthalate	123485	000084-74-2	47
29	25.93	3.38	C:\Database\NIST98.L			
			3-Hexanol	113251	000623-37-0	53
			Butanamide, 3-methyl-	113229	000541-46-8	53
			2-Heptanol, 2-methyl-	113195	000625-25-2	53
30	26.38	1.24	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	93
			1,3-Pentadiene, 1,1-diphenyl-, ...	126412	015295-31-5	44
			3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9	30
31	26.77	0.30	C:\Database\NIST98.L			
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	30
			Silane, trimethyl(6-methyl-5-he...	22989	061685-11-8	27
			Cyclohexanol, dodecyl-	17142	055000-30-1	25
32	27.00	2.29	C:\Database\NIST98.L			
			n-Hexadecanoic acid	114901	000057-10-3	95
			Dibutyl phthalate	123493	000084-74-2	74
			Tridecanoic acid	114895	000638-53-9	64

33	27.23	1.00	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	47
			Cyclohexane, (ethoxymethoxy)-	19366	054699-29-5	46
			2-(3,4-Dibromo-4-methylcyclohex...	19797	110202-13-6	27
34	27.50	1.70	C:\Database\NIST98.L			
			Thiazole, 4-ethyl-2-methyl-	121703	032272-48-3	30
			Nonadecane, 9-methyl-	16462	013287-24-6	25
			5-Iodo-nonane	4431	1000143-48-8	22
35	27.83	0.83	C:\Database\NIST98.L			
			2-Chloro-4-hydroxybenzonitrile	68684	003336-16-1	42
			1H-Benzotriazole, 5-chloro-	68515	000094-97-3	38
			Benzene, chloroisocyanato-	68619	051134-03-3	38
36	28.15	0.63	C:\Database\NIST98.L			
			3-Pentenoic acid, 2,2-diethyl-	57558	038477-07-5	38
			4-Hydroxy-2-hydroxyaminopyrimidine	57681	1000111-25-4	30
			Thiazole, 4-ethyl-2-propyl-	57743	041981-68-4	30
37	28.30	0.47	C:\Database\NIST98.L			
			Verapamil	128484	000052-53-9	25
			l-Arabinose, 2,3:4,5-di-O-ethyl...	99819	1000154-65-6	25
			3-Heptadecanol	19340	084534-30-5	10
38	28.50	0.57	C:\Database\NIST98.L			
			Cyclohexadecane	14275	000295-65-8	95
			1-Eicosanol	112640	000629-96-9	78
			1-Octadecanol	5273	000112-92-5	55
39	28.66	0.98	C:\Database\NIST98.L			
			Octanal, 7-hydroxy-3,7-dimethyl-	113222	000107-75-5	43
			Ethane, 1,2-diethoxy-	19316	000629-14-1	38
			Propanamide, N-(1-cyclohexyleth...	10877	1000142-14-4	35
40	29.11	3.50	C:\Database\NIST98.L			
			Butane, 2-methoxy-3-methyl-	19275	062016-49-3	47
			Butanoic acid, 2-hydroxy-, ethy...	19292	052089-54-0	47
			2-Hydroxy-2,4-dimethyl-3-pentanone	19402	003212-67-7	47
41	29.30	3.90	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	95
			Tetradecanoic acid	114897	000544-63-8	83
			1-Trimethylsily-2-(dimethyl-n-p...	19894	1000214-91-7	43
42	29.52	0.83	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	64
			Tetradecanamide	113299	000638-58-4	64
			Nonanamide	19654	001120-07-6	59
43	29.78	2.48	C:\Database\NIST98.L			
			p-Terphenyl-d14	92199	001718-51-0	99
			Cyclopentene, 3-methylene-2-phe...	92106	1000157-28-3	64
			Cyclopropane, 2-methylene-1-phe...	92107	1000157-34-1	59
44	30.15	1.32	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	53
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	45
			2-Hexanol, 2-methyl-	113192	000625-23-0	43

45	30.70	0.65	C:\Database\NIST98.L			
			Silane, 1-butenyltrimethyl-	19848	018291-95-7	46
			Dotriacontane	112352	000544-85-4	38
			Octadecane, 1-chloro-	112584	003386-33-2	30
46	31.00	0.49	C:\Database\NIST98.L			
			Benzocyclobutene, 1-triisopropy...	19987	1000161-78-6	38
			Cyclooctanemethanol, .alpha.,.a...	19347	016624-06-9	35
			1-Propene, 3-[2-(2-methoxyethox...	19353	013752-97-1	35
47	31.31	2.89	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	95
			Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	72
			Hexadecanamide	113298	000629-54-9	56
48	31.79	9.62	C:\Database\NIST98.L			
			3-Pentanol, 2-methyl-	113303	000565-67-3	43
			Oxirane, tetramethyl-	113273	005076-20-0	43
			Diazene, [1-(2,2-dimethylhydraz...	19854	061940-94-1	40
49	32.48	1.75	C:\Database\NIST98.L			
			1-Octadecene	112297	000112-88-9	95
			1-Heneicosyl formate	16592	077899-03-7	93
			Cyclohexadecane	14275	000295-65-8	93
50	32.82	1.14	C:\Database\NIST98.L			
			Bis(2-ethylhexyl) phthalate	66784	000117-81-7	91
			1,2-Benzenedicarboxylic acid, d...	123512	027554-26-3	91
			Di-n-octyl phthalate	123444	000117-84-0	70
51	33.16	0.68	C:\Database\NIST98.L			
			1-Butanol, 3-methoxy-, acetate	5857	004435-53-4	53
			Hexadecanamide	113298	000629-54-9	50
			Tetradecanamide	19652	000638-58-4	50
52	33.37	0.64	C:\Database\NIST98.L			
			1-Ethoxypentan-3-ol	19516	100910-92-7	35
			Silane, octyl-	19805	000871-92-1	35
			9-Octadecenamide, (Z)-	19657	000301-02-0	35
53	34.01	9.95	C:\Database\NIST98.L			
			2-Heptanol, 2-methyl-	113195	000625-25-2	37
			2-Hexanol, 2,5-dimethyl-, (S)-	113201	003730-60-7	37
			3-Hydroxy-3-methyl-2-butanone	113156	000115-22-0	32
54	34.73	0.51	C:\Database\NIST98.L			
			Silane, diethyldimethyl-	19725	000756-81-0	27
			Silane, octyl-	19805	000871-92-1	27
			1,4-Di-O-acetyl-2,5-di-O-methyl...	19333	1000101-82-1	27
55	35.05	9.25	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	90
			9-Octadecenamide, (Z)-	19657	000301-02-0	72
			2-Octanol, 2-methyl-6-methylene-	19419	1000132-19-1	46
56	36.62	10.79	C:\Database\NIST98.L			
			3-Pentanol, 2-methyl-	113303	000565-67-3	38
			2,3-Butanediol, 2,3-dimethyl-	113190	000076-09-5	38
			Oxirane, tetramethyl-	113273	005076-20-0	38

57	37.47	1.38	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	109752	000301-02-0	42
			1,3-Dioxolane, 2,2-dimethyl-4,5...	19922	051064-64-3	37
			D-Ribofuranose, 2,3-O-(1-methyl...	19485	004099-88-1	37
58	39.03	0.53	C:\Database\NIST98.L			
			1-Dotriacontanol	16786	006624-79-9	46
			1-Hentetracontanol	16591	040710-42-7	41
			Acetic acid, octadecyl ester	109492	000822-23-1	41
59	39.63	0.25	C:\Database\NIST98.L			
			1,2-Benzisothiazole-3-acetic ac...	84760	029876-70-8	37
			Acetic acid, [4-(1,1-dimethylet...	84742	088530-52-3	35
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	27
60	40.51	8.76	C:\Database\NIST98.L			
			Butane, 2-methoxy-3-methyl-	19275	062016-49-3	38
			Butanoic acid, 2-hydroxy-, ethy...	19292	052089-54-0	38
			Oxirane, tetramethyl-	113273	005076-20-0	38
61	41.56	0.83	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	35
			1,1,2-Trimethyldisilane	19435	1000216-84-5	25
			3-Hexanol, 1,5-dimethoxy-2,4-di...	19515	013897-22-8	25
62	42.09	0.85	C:\Database\NIST98.L			
			Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3	35
			1,8-Nonanediol, 8-methyl-	19401	054725-73-4	22
			7-Octen-2-ol, 2,6-dimethyl-	19349	018479-58-8	22
63	42.70	0.47	C:\Database\NIST98.L			
			1,3-Bis(dimethyl-n-pentylsilyl)...	19895	1000214-94-5	35
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	27
			Ethane, 1,2-diethoxy-	19316	000629-14-1	27
64	42.98	0.52	C:\Database\NIST98.L			
			Silane, ethyldimethyl-	19594	000758-21-4	32
			Silane, trimethyl-	113305	000993-07-7	27
			1-Trimethylsily-2-(dimethyl-n-p...	19894	1000214-91-7	25
65	43.37	0.36	C:\Database\NIST98.L			
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	27
			Silane, [2-(2-methoxyethoxy)eth...	19671	062199-57-9	25
			1,3-Bis(dimethyl-n-pentylsilyl)...	19895	1000214-94-5	25
66	43.78	0.27	C:\Database\NIST98.L			
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	35
			Silane, trimethyl-	19663	000993-07-7	30
			1,3-Bis(dimethyl-n-pentylsilyl)...	19895	1000214-94-5	27

Fri Oct 24 11:51:34 2008

Chlorine
Day 9
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\01070 8\014.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 3:43 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 16

Search Libraries: C:\Database\OWML.L Minim um Quality: 35
C:\Database\NIST98.L Minim um Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Q	ual
1	19.32	0.44	C:\Database\NIST98.L				
"Cycloheptasiloxane, tetradecame..."				27714	000107-50-6		93
"Pentasiloxane, dodecamethyl-"			115143	000141-63-9		37	
"Hexasiloxane, 1,1,3,3,5,5,7,7,9..."				27715	000995-82-4		35
2	21.47	0.37	C:\Database\NIST98.L				
"2-Hexen-4-ol, 5-methyl-"			24320	1000163-45-		9 47	
"Propanoic acid, 2-methyl-, 1-(1..."				24401	074381-40-1		42
"Butyric acid, thio-, S-decyl ester"				24338	002432-55-5		38
3	22.06	0.86	C:\Database\NIST98.L				
"n-Nonadecanoic acid, pentamethy..."				10264	1000217-02-		3 38
"Benzeneacetic acid, .alpha.,3,4..."				128844	037148-65-5		38
"Phenethylamine, N-methyl-.beta...."				115313	010538-85-9		35
4	22.51	0.41	C:\Database\NIST98.L				
"Phenol, 2,4,6-tribromo-"			102083	000118-79-6		53	
"Iron, (.eta.5-2,4-cyclopentadie..."				102184	012149-23-4		10
"Estra-1,3,5(10)-triene-4,17-dio..."				102213	065968-98-1		9
5	24.52	1.27	C:\Database\NIST98.L				
"Cyclononasiloxane, octadecamethyl-"				115158	000556-71-8		53
"Cyclohexasiloxane, dodecamethyl-"				27931	000540-97-6		43
"2-Azido-17-(1,5-dimethylhexyl)-..."				5160	1000210-24-		9 35
6	25.76	0.46	C:\Database\OWML.L				
Di-n-butyl Phthalate			28	000084-74-2		56	
Diethyl Phthalate			14	000084-66-2		39	
7	26.51	1.48	C:\Database\NIST98.L				
"Cyclodecasiloxane, eicosamethyl-"				27712	018772-36-6		60
3-Trimethylsilyloxystearic acid...				26930	1000079-42-		6 23
"9,12,15-Octadecatrienoic acid, ..."				25608	055521-22-7		22
8	27.00	1.66	C:\Database\OWML.L				
Di-n-butyl Phthalate			28	000084-74-2		92	
Diethyl Phthalate			14	000084-66-2		7	
9	28.21	2.05	C:\Database\NIST98.L				
"Benzoic acid, 2,4-bis[(trimethy..."				103446	010586-16-0		46
"Benzeneacetic acid, .alpha.,3,4..."				128844	037148-65-5		43
Dibutanoylmorphine			103463	066641-03-0		42	
10	29.30	0.59	C:\Database\NIST98.L				

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Tetradecanoic acid      114897  000544-63-8     93
Octadecanoic acid       6590    000057-11-4     93
Tetradecanoic acid      114898  000544-63-8     89

11  29.67  3.17 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     72
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."    26950   038147-00-1     38
"Cyclohexasiloxane, dodecamethyl-"      27931   000540-97-6     14

12  29.78  0.74 C:\Database\OWML.L
Terphenyl-d14   34      001718-51-0     99

13  30.61  0.26 C:\Database\NIST98.L
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."    26950   038147-00-1     12
"Octasiloxane, 1,1,3,3,5,5,7,7,9..."    27373   019095-24-0     10
"Hexasiloxane, 1,1,3,3,5,5,7,7,9..."    27715   000995-82-4     10

14  30.96  5.05 C:\Database\NIST98.L
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."    26950   038147-00-1     47
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     38
"Heptasiloxane, hexadecamethyl-"        27486   000541-01-5     27

15  31.23  0.26 C:\Database\OWML.L
Benzyl butyl Phthalate  36      000085-68-7     99
Diethyl Phthalate       14      000084-66-2     37
Di-n-butyl Phthalate    28      000084-74-2     25

16  31.31  0.81 C:\Database\NIST98.L
"9-Octadecenamide, (Z)-"        113302  000301-02-0     96
"9-Octadecenamide, (Z)-"        113301  000301-02-0     93
"9-Octadecenamide, (Z)-"        19657   000301-02-0     90

17  31.61  0.55 C:\Database\NIST98.L
"Ethanol, 2-butoxy-, phosphate (..."    112451  000078-51-3     90
"Ethanol, 2-butoxy-, phosphate (..."    16713   000078-51-3     46
"2-Propanone, ethylhydrazone"   15402   007422-99-3     30

18  31.90  0.27 C:\Database\NIST98.L
"1,8-Nonanediol, 8-methyl-"     19401   054725-73-4     30
2-Pentacosanone 19602   075207-54-4     27
"Silane, trimethylpropyl-"      25713   003510-70-1     27

19  32.16  7.57 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     53
"1,1,1,5,7,7,7-Heptamethyl-3,3-b..."    26950   038147-00-1     43
Dibutanoylmorphine      103463  066641-03-0     25

20  32.48  0.37 C:\Database\NIST98.L
"5-Eicosene, (E)-"      13710   074685-30-6     98
1-Heptadecene   13024   006765-39-5     96
1-Heptadecene   118308  006765-39-5     94

21  32.82  1.02 C:\Database\OWML.L
Bis(2-ethylhexyl) phthalate     39      000117-81-7     91
Di-n-octyl phthalate    40      000117-81-0     50
Di-n-butyl Phthalate    28      000084-74-2     43

22  33.11  0.32 C:\Database\NIST98.L
"9-Acridanone, 4-hydroxy-1,2,3-t..."    99541   017014-63-0     49
"9(10H)-Acridinone, 1-hydroxy-2,..."    99584   007008-68-6     38
.alpha.-Hydroxystearic acid     110445  001330-70-7     35

23  33.28 10.21 C:\Database\NIST98.L
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"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     50
"Heptasiloxane, hexadecamethyl-"        27486   000541-01-5     25
"2,4,6(1H,3H,5H)-Pyrimidinetrion..."    103442  052937-67-4     15

24  34.40 11.55 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     58
"Trisiloxane, 1,1,1,5,5,5-hexame..."    26961   003555-47-3     38
"Pentasiloxane, dodecamethyl-"  115143  000141-63-9     35

25  35.05  3.86 C:\Database\NIST98.L
Erucylamide     19656   000112-84-5     91
"9-Octadecenamide, (Z)-"        19657   000301-02-0     64
7-Nonenamide    19655   090949-53-4     50

26  35.63 11.80 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     59
"Trisiloxane, 1,1,1,5,5,5-hexame..."    26961   003555-47-3     43
"Cyclodecasiloxane, eicosamethyl-"      27712   018772-36-6     38

27  37.07 11.33 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     64
"Eseroline, 7-bromo-, methylcarb..."    3850    114546-23-5     53
"3,6-Dioxa-2,4,5,7-tetrasilaocta..."    87890   004342-25-0     37

28  38.82  9.55 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     74
"Mercaptoacetic acid, bis(trimet..."    26922   006398-62-5     32
"Trisiloxane, 1,1,1,5,5,5-hexame..."    26961   003555-47-3     30

29  40.99  7.40 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     74
"Mercaptoacetic acid, bis(trimet..."    26922   006398-62-5     38
"Cyclodecasiloxane, eicosamethyl-"      27712   018772-36-6     30

30  43.73  4.31 C:\Database\NIST98.L
"Cyclononasiloxane, octadecamethyl-"    115158  000556-71-8     72
"3,6-Dioxa-2,4,5,7-tetrasilaocta..."    87890   004342-25-0     43
"Cyclodecasiloxane, eicosamethyl-"      27712   018772-36-6     43

Tue Jan 15 17:43:21 2008
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Chlorine
Day 9
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\012.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 1:48 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 14

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	9.68	0.34	C:\Database\NIST98.L			
			Hexanoic acid, anhydride	118546	002051-49-2	59
			Glycocyanidine	43063	000503-86-6	59
			2-Pyrrolidinone, 1-methyl-	43090	000872-50-4	59
2	13.27	0.56	C:\Database\NIST98.L			
			Benzene, 1-chloro-2-isocyanato-	68548	003320-83-0	97
			Benzene, chloroisocyanato-	68619	051134-03-3	94
			Benzene, 1-chloro-4-isocyanato-	68625	000104-12-1	91
3	15.69	0.61	C:\Database\NIST98.L			
			Nonanoic acid	20156	000112-05-0	95
			Nonanoic acid	113428	000112-05-0	95
			Nonanoic acid	113427	000112-05-0	74
4	17.42	0.51	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	72
			1-Methylcycloheptanol	24425	003761-94-2	38
			3-Hexenoic acid, 5-hydroxy-2-me...	6424	110678-36-9	33
5	17.75	0.84	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	95
6	17.83	0.63	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	80
			Butanoic acid, butyl ester	114541	000109-21-7	72
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	53
7	18.87	0.33	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	64
			2-Propanol, 1-[2-(2-methoxy-1-m...	19665	020324-33-8	59
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	50
8	19.55	0.32	C:\Database\NIST98.L			
			1-Decene	111296	000872-05-9	95
			Cyclodecane	111288	000293-96-9	93
			Cyclodecane	13064	000293-96-9	93
9	20.89	0.34	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	94
			Lauric anhydride	114892	000645-66-9	74
			Undecanoic acid	20158	000112-37-8	50

Page 1

10	21.47	0.97	C:\Database\NIST98.L			
			Phenmetrazine	114496	000134-49-6	43
			Propanoic acid, 2-methyl-, 1-(1...	24401	074381-40-1	43
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	37
11	21.65	0.60	C:\Database\NIST98.L			
			4-Hydroxy-3-hexanone	19313	004984-85-4	50
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	50
			Ethane, 1,2-diethoxy-	108349	000629-14-1	50
12	22.37	0.36	C:\Database\NIST98.L			
			Benzophenone	119383	000119-61-9	60
			Benzophenone	46089	000119-61-9	60
			Benzophenone	119052	000119-61-9	60
13	22.51	1.87	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	53
			Estra-1,3,5(10)-triene-4,17-dio...	102213	065968-98-1	9
			Anthracene, 9,10-diphenyl-	102075	001499-10-1	9
14	22.81	2.64	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	95
			1,4-Naphthoquinone, 6-acetyl-2,...	127595	013379-24-3	59
			1,2-Benzenedicarboxylic acid, 4...	76484	069094-40-2	47
15	23.08	0.88	C:\Database\NIST98.L			
			Phenol, 2,4-di-t-butyl-6-nitro-	90753	1000128-93-2	97
			7,7-Dimethyl-1,4-dioxo-2,3,4,5,...	90678	051799-98-5	59
			dl-5-Benzyloxytryptophan	90613	1000129-42-0	53
16	23.37	0.41	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	96
			Heptadecane	112320	000629-78-7	95
			Heptadecane	109557	000629-78-7	91
17	24.23	0.40	C:\Database\NIST98.L			
			Tetradecanoic acid	114897	000544-63-8	96
			Tetradecanoic acid	114898	000544-63-8	95
			Tetradecanoic acid	113420	000544-63-8	91
18	24.44	0.33	C:\Database\NIST98.L			
			6-Methyl-5-[1-piperidinyl]-2,4-...	84786	1000212-53-0	38
			2-Ethylacridine	84846	1000147-64-9	38
			1,4-Benzenediol, 2,5-bis(1,1-di...	84896	000088-58-4	32
19	24.90	0.53	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octadecane	112330	000593-45-3	98
			Octadecane	112333	000593-45-3	93
20	24.99	0.37	C:\Database\NIST98.L			
			Hexadecane, 2,6,10,14-tetramethyl-	112575	000638-36-8	70
			Tetratetracontane	112365	007098-22-8	64
			Tetratriacontane	16431	014167-59-0	62
21	25.17	0.35	C:\Database\NIST98.L			
			4-Amino-2,6-diphenylpyrimidine	92663	041270-99-9	59
			4-Iodo-2,6-dimethyl-phenylamine	127578	004102-53-8	58
			1,3,5,2-Oxaazoniaazaboratin, 2,...	92662	1000160-64-7	53
22	25.76	1.68	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	36
			Di-n-butyl Phthalate	28	000084-74-2	9

			Benzyl butyl Phthalate	36	000085-68-7	1
23	25.92	1.25	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	50
			Cyclooctanemethanol, .alpha.,.a...	19347	016624-06-9	50
			Methyl 17-methoxy-10-methoxycar...	19542	1000110-20-7	50
24	26.03	0.79	C:\Database\NIST98.L			
			2-Hexanol, 2,3-dimethyl-	19357	019550-03-9	50
			Butanamide, 3,3-dimethyl-	113267	000926-04-5	47
			1,8-Nonanediol, 8-methyl-	19401	054725-73-4	46
25	26.12	0.38	C:\Database\NIST98.L			
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	50
			2-Pentanone, 5-methoxy-	5841	017429-04-8	49
			2-Hexanol, 2,5-dimethyl-, (S)-	19345	003730-60-7	47
26	26.26	0.49	C:\Database\NIST98.L			
			Nonadecane	112382	000629-92-5	91
			Nonadecane	112381	000629-92-5	83
			Pentatriacontane	112346	000630-07-9	76
27	26.38	1.09	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	76
			1,3-Pentadiene, 1,1-diphenyl-, ...	126412	015295-31-5	48
			3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9	38
28	27.01	7.70	C:\Database\NIST98.L			
			n-Hexadecanoic acid	114901	000057-10-3	98
			Tetradecanoic acid	114897	000544-63-8	95
			n-Hexadecanoic acid	109985	000057-10-3	95
29	27.50	1.69	C:\Database\NIST98.L			
			Eicosane	109630	000112-95-8	70
			Thiazole, 5-ethyl-2-methyl-	57685	019961-52-5	50
			Octacosane	112312	000630-02-4	38
30	27.92	0.34	C:\Database\NIST98.L			
			1,3-Diphenyl-2-azafluorene	101235	1000216-51-5	45
			Iron, (.eta.-4-naphthalene)(.et...	101232	1000161-39-4	45
			1,3-Diphenyl-4-azafluorene	101229	1000216-52-1	45
31	28.16	0.53	C:\Database\NIST98.L			
			Carbamic acid, (4-chlorophenyl)...	8555	002239-92-1	38
			o-Chloroaniline	57726	000095-51-2	25
			3-Pentenoic acid, 2,2-diethyl-	57558	038477-07-5	25
32	28.29	0.48	C:\Database\NIST98.L			
			Verapamil	128483	000052-53-9	50
			Verapamil	128484	000052-53-9	50
			Verapamil	99859	000052-53-9	39
33	28.50	0.36	C:\Database\NIST98.L			
			1-Octadecene	112298	000112-88-9	96
			Cyclohexadecane	14275	000295-65-8	91
			1-Octadecanol	5273	000112-92-5	90
34	29.11	2.00	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	50
			Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	49
			Hexanamide, 4-ethyl-5,5-dimethyl-	19851	054789-39-8	47
35	29.31	6.51	C:\Database\NIST98.L			

				Octadecanoic acid	114902	000057-11-4 98
				Octadecanoic acid	109378	000057-11-4 87
				Octadecanoic acid	6590	000057-11-4 83
36	29.51	0.59	C:\Database\NIST98.L			
				Hexadecanamide	113298	000629-54-9 58
				Pentadecanamide, 15-bromo-	19651	1000163-86-1 53
				Tetradecanamide	113299	000638-58-4 53
37	29.78	3.46	C:\Database\OWML.L			
				Terphenyl-d14	34	001718-51-0 99
38	30.70	0.37	C:\Database\NIST98.L			
				Octadecane, 1-chloro-	112584	003386-33-2 38
				Tridecanol, 2-ethyl-2-methyl-	17034	1000115-66-1 38
				Tetracontane	17096	004181-95-7 35
39	31.22	0.80	C:\Database\OWML.L			
				Benzyl butyl Phthalate	36	000085-68-7 96
				Diethyl Phthalate	14	000084-66-2 10
				Di-n-butyl Phthalate	28	000084-74-2 4
40	31.31	3.71	C:\Database\NIST98.L			
				9-Octadecenamide, (Z)-	113302	000301-02-0 96
				9-Octadecenamide, (Z)-	113301	000301-02-0 93
				Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1 64
41	31.53	1.21	C:\Database\NIST98.L			
				Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1 50
				Diisooctyl adipate	58242	001330-86-5 49
				Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1 43
42	31.62	1.67	C:\Database\NIST98.L			
				Oxepane, 2,2,4-trimethyl-	113210	023120-44-7 47
				3-[2-Ethoxycarbonyl-2-methyl)pr...	19971	021153-32-2 46
				Butane, 1-ethoxy-	113144	000628-81-9 43
43	31.79	4.57	C:\Database\NIST98.L			
				Diazene, [1-(2,2-dimethylhydraz...	19854	061940-94-1 53
				Pentane, 2-methoxy-	19506	006795-88-6 47
				2-Hydroxy-2,4-dimethyl-3-pentanone	19402	003212-67-7 47
44	32.48	1.54	C:\Database\NIST98.L			
				1-Heneicosyl formate	16592	077899-03-7 93
				1-Eicosanol	112640	000629-96-9 93
				1-Docosanol	109619	000661-19-8 91
45	32.82	1.33	C:\Database\OWML.L			
				Bis(2-ethylhexyl) phthalate	39	000117-81-7 91
				Di-n-octyl phthalate	40	000117-81-0 50
				Di-n-butyl Phthalate	28	000084-74-2 37
46	32.97	0.38	C:\Database\NIST98.L			
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8 27
				Hydrazinecarboxylic acid, 1,1-d...	15839	000870-46-2 10
				4H-Pyrido[1,2-a]pyrimidine-3-ca...	87940	064399-29-7 10
47	34.09	5.66	C:\Database\NIST98.L			
				Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3 43
				2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7 43
				Butane, 2-methoxy-	19272	006795-87-5 43
48	34.22	1.18	C:\Database\NIST98.L			

				2-Hexanol, 2,3-dimethyl-	19357	019550-03-9 43
				2-Pentanone, 5-methoxy-	5841	017429-04-8 35
				2-Propanol, 1-(isooctyloxy)-2-m...	19578	056282-27-0 35
49	35.05	15.28	C:\Database\NIST98.L			
				Erucylamide	19656	000112-84-5 91
				9-Octadecenamide, (Z)-	19657	000301-02-0 64
				Hexadecanamide	113298	000629-54-9 56
50	35.37	0.53	C:\Database\NIST98.L			
				Docosa-2,6,10,14,18-pentaen-22-...	23027	1000163-04-7 46
				2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4 46
				2,6,10,14,18-Pentamethyl-2,6,10...	23038	075581-03-2 46
51	36.12	0.76	C:\Database\NIST98.L			
				Hydrazinecarboxylic acid, 1,1-d...	15839	000870-46-2 30
				4-Keto-3,3-dimethylhexanoic aci...	16935	1000129-20-1 27
				2-Pentanone, 5-methoxy-	5841	017429-04-8 27
52	36.37	3.70	C:\Database\NIST98.L			
				Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8 10
				2-Hydroxy-2,4-dimethyl-hept-6-e...	19337	1000192-56-0 10
				2-Heptanol, 2-methyl-	19423	000625-25-2 10
53	36.63	5.42	C:\Database\NIST98.L			
				Cyclohexanemethanol, .alpha.,.a...	113275	000498-81-7 38
				Oxirane, 3-ethyl-2,2-dimethyl-	113167	001192-22-9 38
				Butanoic acid, 2-hydroxy-, ethy...	19292	052089-54-0 38
54	37.67	0.44	C:\Database\NIST98.L			
				Silane, trimethyl[5-methyl-2-(1...	84732	055012-80-1 35
				1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9 27
				Acetic acid, [4-(1,1-dimethylet...	84742	088530-52-3 25
55	39.02	0.40	C:\Database\NIST98.L			
				1-Dotriacontanol	16786	006624-79-9 35
				17-Pentatriacontene	5525	006971-40-0 20
				1-Tricosene	16349	018835-32-0 20
56	39.65	0.33	C:\Database\NIST98.L			
				1,1,1,3,5,5,5-Heptamethyltrisil...	84726	001873-88-7 38
				1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9 35
				Cyclotrisiloxane, hexamethyl-	126481	000541-05-9 35
57	40.38	2.47	C:\Database\NIST98.L			
				2-Propanol, 1-methoxy-2-methyl-	19309	003587-64-2 38
				Butane, 2-methoxy-	19272	006795-87-5 38
				Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3 38
58	40.48	3.97	C:\Database\NIST98.L			
				4-O-Acetyl-2,5-di-O-methyl-3,6-...	19455	1000101-80-3 35
				2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7 35
				Oxirane, tetramethyl-	19436	005076-20-0 35
59	41.54	0.34	C:\Database\NIST98.L			
				3-Pentanol, 2-methyl-	113304	000565-67-3 35
				1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9 27
				2-Ethylacridine	84846	1000147-64-9 25
60	43.71	0.43	C:\Database\NIST98.L			
				Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0 38
				1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1 14
				2-Methyl-6-(5-methyl-2-thiazoli...	84743	1000225-39-3 11

Chlorine
Day 14
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\022.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 11:20 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 24

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	22.52	2.65	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	60
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	10
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
2	24.90	1.00	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	93
			Octadecane	112330	000593-45-3	93
3	24.99	0.83	C:\Database\NIST98.L			
			Hexadecane, 2,6,10,14-tetramethyl-	112575	000638-36-8	87
			Hexadecane, 2,6,10,14-tetramethyl-	17086	000638-36-8	86
			Tetratetracontane	112365	007098-22-8	86
4	25.76	2.03	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	64
			Diethyl Phthalate	14	000084-66-2	40
			Benzyl butyl Phthalate	36	000085-68-7	9
5	26.27	0.89	C:\Database\NIST98.L			
			Nonadecane	112382	000629-92-5	96
			Nonadecane	112576	000629-92-5	93
			Nonadecane	112381	000629-92-5	93
6	26.39	0.79	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	38
			3,5-Cyclohexadiene-1,2-dione, 3...	112724	003383-21-9	18
			4a,7-Methano-4aH-naphth[1,8a-b]...	108926	067999-56-8	14
7	27.01	8.47	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	70
8	27.51	1.42	C:\Database\NIST98.L			
			Eicosane	16454	000112-95-8	95
			Hexadecane	112410	000544 76 3	95
			Eicosane	112345	000112-95-8	93
9	29.30	4.55	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	96
			Octadecanoic acid	109378	000057-11-4	87
			Octadecanoic acid	6590	000057-11-4	83
10	29.50	1.30	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	95

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				Dodecanamide	19649	001120-16-7 87
				Hexadecanamide	113298	000629-54-9 72
11	29.79	11.03	C:\Database\OWML.L			
				Terphenyl-d14	34	001718-51-0 99
12	31.24	1.01	C:\Database\OWML.L			
				Benzyl butyl Phthalate	36	000085-68-7 74
				Diethyl Phthalate	14	000084-66-2 14
				Di-n-butyl Phthalate	28	000084-74-2 2
13	31.32	7.54	C:\Database\NIST98.L			
				9-Octadecenamide, (Z)-	113302	000301-02-0 96
				9-Octadecenamide, (Z)-	113301	000301-02-0 91
				Pentadecanamide, 15-bromo-	19651	1000163-86-1 56
14	31.53	1.32	C:\Database\NIST98.L			
				Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1 64
				Diisooctyl adipate	58242	001330-86-5 60
				Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1 58
15	31.62	1.79	C:\Database\NIST98.L			
				Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3 72
				Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3 58
				2-Propanone, ethylhydrazone	15402	007422-99-3 27
16	32.50	3.61	C:\Database\NIST98.L			
				5-Eicosene, (E)-	13710	074685-30-6 99
				1-Heptadecene	13024	006765-39-5 96
				1-Docosene	111438	001599-67-3 95
17	32.82	4.06	C:\Database\OWML.L			
				Bis(2-ethylhexyl) phthalate	39	000117-81-7 90
				Di-n-octyl phthalate	40	000117-81-0 50
				Di-n-butyl Phthalate	28	000084-74-2 37
18	33.12	1.00	C:\Database\NIST98.L			
				9-Acridanone, 2-hydroxy-1,3,4-t...	99586	017014-62-9 50
				Sulazepam	99575	002898-13-7 45
				9-Acridanone, 4-hydroxy-1,2,3-t...	99541	017014-63-0 32
19	33.39	0.73	C:\Database\NIST98.L			
				3-Tetradecanol	19356	001653-32-3 38
				3-Hexadecanol	113255	000593-03-3 35
				9-Octadecenamide, (Z)-	109752	000301-02-0 30
20	35.05	35.66	C:\Database\NIST98.L			
				Erucylamide	19656	000112-84-5 93
				9-Octadecenamide, (Z)-	19657	000301-02-0 64
				Hexadecanamide	19647	000629-54-9 64
21	35.25	1.16	C:\Database\NIST98.L			
				9-Octadecenamide, (Z)-	19657	000301-02-0 64
				Erucylamide	19656	000112-84-5 55
				7-Nonenamide	19655	090949-53-4 52
22	35.36	0.90	C:\Database\NIST98.L			
				2-Methyl-5,5-diphenyl-4-(methyl...	84809	024133-96-8 38
				1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9 38
				2-Ethylacridine	84846	1000147-64-9 25
23	36.14	1.16	C:\Database\NIST98.L			
				Propanamide, N-(4-methoxyphenyl...	17557	056619-94-4 10

				Ethyl 2-butyramido-3,3,3-triflu...	9559	1000224-16-2	10
				1-(4-Acetamidoanilino)-3,7-dime...	4048	1000226-07-9	9
24	36.36	4.01	C:\Database\NIST98.L				
				Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	30
				13H-Benz[6,7]indolo[3,2-c]quino...	101046	004240-59-9	10
				Propanamide, N-(3-methoxyphenyl...	17665	056619-93-3	10
25	39.09	1.11	C:\Database\NIST98.L				
				1-Dotriacontanol	16786	006624-79-9	60
				1-Eicosanol	112640	000629-96-9	55
				1-Docosanol	109619	000661-19-8	55

Tue Jan 15 18:31:55 2008

Chlorine
Day 14
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\019.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 8:29 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 21

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	14.40	0.74	C:\Database\NIST98.L			
			1-Methylpyrrolo[1,2-a]pyrazine	59716	064608-59-9	53
			2H-Cyclopenta[d]pyridazine, 2-m...	59625	022291-85-6	50
			5-Aminoindole	59718	005192-03-0	40
2	17.44	0.62	C:\Database\NIST98.L			
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	59
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	50
			Oxirane, propyl-	108847	001003-14-1	32
3	17.84	0.88	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	90
			Butanoic acid, butyl ester	114541	000109-21-7	72
			Butanoic acid, butyl ester	109895	000109-21-7	72
4	20.10	1.47	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	95
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	95
			Phenol, 2,4-bis(1,1-dimethyleth...	125776	000096-76-4	93
5	21.47	1.34	C:\Database\NIST98.L			
			Butyric acid, thio-, S-decyl ester	24338	002432-55-5	38
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	38
			Phenmetrazine	114496	000134-49-6	37
6	21.66	1.15	C:\Database\NIST98.L			
			Oxirane, 3-ethyl-2,2-dimethyl-	113175	001192-22-9	47
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	43
			Pentane, 1-ethoxy-	19288	017952-11-3	43
7	22.51	1.02	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	55
			Phosphine, acetyldimethyl-	7821	018983-86-3	16
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	12
8	22.81	2.11	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	96
			Boron, diethyl(5-ethyl-4,6-nona...	87941	136705-03-8	46
			Naphtho[1,2-b]furan-2,8(3H,4H)-...	92791	018409-93-3	35
9	23.37	1.04	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	97
			Heptadecane	112320	000629-78-7	96
			Heptadecane	109557	000629-78-7	95

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10	24.89	0.81	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	99
			Octadecane	112330	000593-45-3	98
			Octadecane	112333	000593-45-3	98
11	24.99	0.80	C:\Database\NIST98.L			
			Tetratriacontane	16431	014167-59-0	90
			Heptadecane, 2,3-dimethyl-	5578	061868-03-9	87
			Heptacosane	16471	000593-49-7	87
12	25.17	0.75	C:\Database\NIST98.L			
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	64
			Phenol, 2,4,6-tris(1,1-dimethyl...	127577	000732-26-3	50
			Phenol, 2,4,6-tris(1,1-dimethyl...	127575	000732-26-3	50
13	25.76	1.66	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	39
			Benzyl butyl Phthalate	36	000085-68-7	9
14	25.92	1.31	C:\Database\NIST98.L			
			2-Methyl-tridecane-2,12-diol	19413	1000187-03-5	47
			3-Tetradecanol	113172	001653-32-3	47
			7-Nonenamide	19655	090949-53-4	38
15	26.04	1.55	C:\Database\NIST98.L			
			Cyclohexane, (ethoxymethoxy)-	19366	054699-29-5	43
			2-Methyl-2-decanol	19566	003396-02-9	43
			2-Pentanone, 5-methoxy-	5841	017429-04-8	43
16	26.26	0.92	C:\Database\NIST98.L			
			Nonadecane	112381	000629-92-5	96
			Nonadecane	16515	000629-92-5	96
			Nonadecane	112382	000629-92-5	95
17	26.38	0.68	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	87
			2-Pentene, 2-cyano-3-(diethylbo...	66870	1000160-60-3	25
			Diethyl Phthalate	123514	000084-66-2	25
18	27.02	6.49	C:\Database\NIST98.L			
			n-Hexadecanoic acid	114901	000057-10-3	97
			Heptadecanoic acid	114893	000506-12-7	76
			n-Decanoic acid	113415	000334-48-5	64
19	27.51	1.59	C:\Database\NIST98.L			
			Eicosane	112565	000112-95-8	96
			Eicosane	112345	000112-95-8	83
			Eicosane	109630	000112-95-8	78
20	28.16	0.72	C:\Database\NIST98.L			
			4-Iodo-2,6-dimethyl-phenylamine	92614	004102-53-8	47
			4-Amino-2,6-diphenylpyrimidine	92663	041270-99-9	42
			1,3,5,2-Oxaazoniaazaboratin, 2,...	92662	1000160-64-7	42
21	28.29	1.37	C:\Database\NIST98.L			
			2-Deoxyribofuranose, 1(O)-(t-bu...	99860	1000193-96-2	39
			Azadibenzopyrene	99857	104219-69-4	9
			5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4	9
22	28.51	0.71	C:\Database\NIST98.L			
			1-Heptadecene	13024	006765-39-5	98
			1-Octadecene	112297	000112-88-9	96

			Z-8-Hexadecene	1696	1000130-87-5	95
23	29.11	0.85	C:\Database\NIST98.L			
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	50
			2-Octanol, 2-methyl-6-methylene-	19419	1000132-19-1	50
			Methyl trifluoroacetate	113295	000431-47-0	50
24	29.31	4.34	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	98
			Octadecanoic acid	6590	000057-11-4	70
			Pentadecanoic acid	114896	001002-84-2	70
25	29.51	0.93	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	95
			Dodecanamide	19649	001120-16-7	90
			Hexadecanamide	113298	000629-54-9	87
26	29.78	3.28	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
27	31.32	7.29	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			9-Octadecenamide, (Z)-	113301	000301-02-0	91
			9-Octadecenamide, (Z)-	19657	000301-02-0	78
28	31.53	0.91	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	89
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	49
			Diisooctyl adipate	58242	001330-86-5	49
29	31.62	1.37	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	41
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	35
			Mannosamine hydrochloride	19653	1000127-68-8	35
30	31.85	2.96	C:\Database\NIST98.L			
			Diazene, [1-(2,2-dimethylhydraz...	19854	061940-94-1	50
			4-Hydroxy-3-hexanone	19313	004984-85-4	47
			Dodecanamide	19649	001120-16-7	43
31	32.50	2.96	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	99
			1-Octadecene	112297	000112-88-9	98
			1-Octadecene	112298	000112-88-9	97
32	32.82	2.17	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	40
			Di-n-butyl Phthalate	28	000084-74-2	37
33	33.91	0.71	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	43
			Pentane, 2-methoxy-	19506	006795-88-6	38
			4-Hydroxy-3-hexanone	19313	004984-85-4	38
34	34.02	0.71	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	43
			Diazene, [1-(2,2-dimethylhydraz...	19854	061940-94-1	43
			2-Hexanol, 2-methyl-	113176	000625-23-0	38
35	34.09	1.85	C:\Database\NIST98.L			
			Ethane, 1,2-diethoxy-	19316	000629-14-1	43
			2-Pentanol, 2,3-dimethyl-	19399	004911-70-0	38

				Oxirane, tetramethyl-	19436	005076-20-0 38
36	34.25	1.08	C:\Database\NIST98.L			
				1-Decanol, 5,9-dimethyl-	1776	091482-38-1 43
				.alpha.-D-Xylo-Hex-5-enofuranos...	19430	007284-07-3 38
				2-Hexanol, 2,5-dimethyl-, (S)-	19345	003730-60-7 38
37	35.07	30.46	C:\Database\NIST98.L			
				Erucylamide	19656	000112-84-5 90
				Erucylamide	113300	000112-84-5 89
				9-Octadecenamide, (Z)-	19657	000301-02-0 72
38	36.34	0.92	C:\Database\NIST98.L			
				1-Butanol, 3-methoxy-, acetate	5857	004435-53-4 38
				3-Tridecanol	19339	010289-68-6 35
				3-Heptadecanol	19340	084534-30-5 27
39	36.58	1.13	C:\Database\NIST98.L			
				Pentane, 2-methoxy-	19506	006795-88-6 38
				Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3 35
				2-Pentanol, 2,3-dimethyl-	19399	004911-70-0 35
40	36.68	3.37	C:\Database\NIST98.L			
				Ethane, 1,2-diethoxy-	19316	000629-14-1 38
				Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3 38
				O-Menthan-8-ol	19544	1000160-38-8 35
41	39.05	0.99	C:\Database\NIST98.L			
				Cyclooctacosane	16340	000297-24-5 96
				1-Hexacosanol	16618	000506-52-5 90
				13-Tertadecen-1-ol acetate	6938	1000130-79-8 86
42	40.61	1.99	C:\Database\NIST98.L			
				Dimethylallyl(n-octyl)silane	19967	081272-81-3 38
				3,5-Dioxahexaldoxin-2,6-dione-,...	5834	081539-54-0 38
				1,4-Di-O-acetyl-2,5-di-O-methyl...	19333	1000101-82-1 27

Tue Jan 15 18:09:58 2008

Chloramine
Day 1
Control

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\001.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 3:17 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 3

Search Libraries: C:\Database\NIST98.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	17.41	0.67	C:\Database\NIST98.L			
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	59
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	35
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	32
2	17.82	1.25	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	80
			Butanoic acid, butyl ester	114541	000109-21-7	56
			Butanoic acid, hexyl ester	109931	002639-63-6	50
3	19.54	0.90	C:\Database\NIST98.L			
			Cyclodecane	111288	000293-96-9	95
			Cyclooctane, 1,2-dimethyl-	13072	013151-94-5	93
			Cyclodecane	13064	000293-96-9	93
4	20.08	2.29	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	96
			Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4	96
			Phenol, 2,4-bis(1,1-dimethyleth...	125782	000096-76-4	90
5	21.47	2.64	C:\Database\NIST98.L			
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			Pentanoic acid, 2,2,4-trimethyl...	24310	1000140-77-5	42
			Phenmetrazine	114496	000134-49-6	40
6	22.37	0.57	C:\Database\NIST98.L			
			Benzophenone	46089	000119-61-9	60
			Benzophenone	119383	000119-61-9	49
			Benzophenone	119052	000119-61-9	47
7	22.80	2.08	C:\Database\NIST98.L			
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	46
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	42
			Chromone, 6-hydroxy-2-methyl-5-...	87870	030095-72-8	38
8	23.00	0.83	C:\Database\NIST98.L			
			Cyclododecane	111788	000294-62-2	93
			1-Heptadecanol	13564	001454-85-9	91
			1-Pentadecanol	13330	000629-76-5	91
9	23.37	0.89	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	97
			Heptadecane	112320	000629-78-7	96
			Heptadecane	112322	000629-78-7	93

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10	24.90	1.43	C:\Database\NIST98.L			
			Octadecane	112330	000593-45-3	98
			Octadecane	112333	000593-45-3	98
			Octadecane	16439	000593-45-3	98
11	24.99	1.30	C:\Database\NIST98.L			
			Tetratriacontane	16431	014167-59-0	91
			Tetratetracontane	112365	007098-22-8	86
			Heptacosane	16471	000593-49-7	86
12	25.17	1.45	C:\Database\NIST98.L			
			8-Methoxy-11H-benzo[a]carbazole	92655	1000212-76-8	72
			Phenol, 2,4,6-tris(1,1-dimethyl...	127575	000732-26-3	64
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	64
13	25.48	0.76	C:\Database\NIST98.L			
			1-Decanol, 2-hexyl-	112269	002425-77-6	52
			Octadecane, 1-bromo-	17754	000112-89-0	43
			Pentatriacontane	112346	000630-07-9	38
14	25.76	3.24	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	123451	000084-69-5	86
			1,2-Benzenedicarboxylic acid, b...	66726	000084-78-6	78
			1,2-Benzenedicarboxylic acid, b...	66775	000084-69-5	78
15	25.91	0.60	C:\Database\NIST98.L			
			Tridecane, 7-cyclohexyl-	16791	013151-92-3	53
			Tridecane, 6-cyclohexyl-	17259	013151-91-2	53
			Dodecane, 5-cyclohexyl-	16789	013151-85-4	46
16	26.01	1.01	C:\Database\NIST98.L			
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	87
			2-Tetradecanol	11548	004706-81-4	86
			1-Nonadecene	42210	018435-45-5	83
17	26.27	1.41	C:\Database\NIST98.L			
			Nonadecane	112380	000629-92-5	95
			Nonadecane	112382	000629-92-5	94
			Nonadecane	16515	000629-92-5	93
18	26.38	0.62	C:\Database\NIST98.L			
			1-Methyl-1-hydroxymethyladamantane	66863	001200-78-8	38
			Dodecane, 1,2-dibromo-	1718	055334-42-4	38
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	38
19	26.76	0.78	C:\Database\NIST98.L			
			Cyclopentadecane	13210	000295-48-7	86
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	64
			1-Hentetracontanol	16591	040710-42-7	58
20	26.99	8.93	C:\Database\NIST98.L			
			Dibutyl phthalate	123426	000084-74-2	96
			Dibutyl phthalate	123493	000084-74-2	95
			1,2-Benzenedicarboxylic acid, b...	67019	017851-53-5	94
21	27.17	1.18	C:\Database\NIST98.L			
			1-Octadecene	4293	000112-88-9	83
			E-15-Heptadecenal	4195	1000130-97-9	83
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	72
22	27.51	1.43	C:\Database\NIST98.L			
			Eicosane	112345	000112-95-8	97
			Pentatriacontane	112346	000630-07-9	95

				Eicosane	112565	000112-95-8 94
23	28.15	0.52	C:\Database\NIST98.L			
				4-Amino-2,6-diphenylpyrimidine	92663	041270-99-9 53
				Cyclohexanone, 4-methyl-, (4-ni...	92602	025117-42-4 53
				Phenol, 2,4,6-tris(1,1-dimethyl...	127577	000732-26-3 53
24	28.29	2.82	C:\Database\NIST98.L			
				Azadibenzopyrene	99857	104219-69-4 39
				5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4 9
				2-Deoxyribofuranose, 1(O)-(t-bu...	99860	1000193-96-2 9
25	28.49	0.74	C:\Database\NIST98.L			
				Phosphonic acid, dioctadecyl ester	13890	019047-85-9 91
				Isoheptadecanol	33115	057289-07-3 90
				Octadecanol	33113	026762-44-7 90
26	29.28	1.26	C:\Database\NIST98.L			
				Octadecanoic acid	114902	000057-11-4 70
				Octadecanoic acid	109378	000057-11-4 52
				Octadecanoic acid	6590	000057-11-4 52
27	29.50	0.71	C:\Database\NIST98.L			
				Hexadecanamide	113298	000629-54-9 87
				Hexadecanamide	19647	000629-54-9 87
				Tetradecanamide	113299	000638-58-4 72
28	29.78	6.95	C:\Database\NIST98.L			
				p-Terphenyl-d14	92199	001718-51-0 99
				2-Benzylbiphenyl	92149	1000118-48-9 64
				Cyclopentene, 3-methylene-2-phe...	92106	1000157-28-3 58
29	31.23	1.37	C:\Database\NIST98.L			
				Benzyl butyl phthalate	123466	000085-68-7 91
				Benzyl butyl phthalate	123465	000085-68-7 90
				Benzyl butyl phthalate	66846	000085-68-7 52
30	31.31	31.31	C:\Database\NIST98.L			
				9-Octadecenamide, (Z)-	113302	000301-02-0 96
				9-Octadecenamide, (Z)-	113301	000301-02-0 91
				9-Octadecenamide, (Z)-	19657	000301-02-0 90
31	31.53	3.86	C:\Database\NIST98.L			
				Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1 95
				Diisooctyl adipate	58242	001330-86-5 91
				Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1 90
32	31.61	2.48	C:\Database\NIST98.L			
				Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3 91
				Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3 52
				Butane, 1-(ethenyloxy)-	108661	000111-34-2 38
33	32.48	2.30	C:\Database\NIST98.L			
				5-Eicosene, (E)-	13710	074685-30-6 97
				1-Eicosanol	112640	000629-96-9 95
				1-Docosene	111438	001599-67-3 94
34	32.82	5.09	C:\Database\NIST98.L			
				1,2-Benzenedicarboxylic acid, d...	123512	027554-26-3 91
				Bis(2-ethylhexyl) phthalate	66784	000117-81-7 91
				Bis(2-ethylhexyl) phthalate	123509	000117-81-7 91
35	35.04	26.11	C:\Database\NIST98.L			

			Erucylamide	19656	000112-84-5	87
			Erucylamide	113300	000112-84-5	81
			9-Octadecenamide, (Z)-	19657	000301-02-0	59
36	35.37	2.32	C:\Database\NIST98.L			
			2,6,10,14,18,22-Tetracosahexaen...	114266	000111-02-4	74
			Squalene	114263	007683-64-9	72
			2,6,10-Dodecatrien-1-ol, 3,7,11...	114131	000106-28-5	59

Tue Jan 15 15:51:43 2008

Chloramine
Day 1
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\009.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 10:57 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 11

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	8.67	0.32	C:\Database\NIST98.L			
			Ethanol, 2-(2-methoxyethoxy)-	110890	000111-77-3	83
			Ethanol, 2-(2-methoxyethoxy)-	11464	000111-77-3	78
			.beta.-Methoxyethoxymethyl chlo...	11722	003970-21-6	45
2	9.65	0.28	C:\Database\NIST98.L			
			Hexanoic acid	113410	000142-62-1	78
			Propanedioic acid, propyl-	20103	000616-62-6	72
			Heptanoic acid	113411	000111-14-8	64
3	10.20	1.29	C:\Database\NIST98.L			
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0	90
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0	64
4	10.89	0.49	C:\Database\NIST98.L			
			Butanedioic acid, dimethyl ester	111493	000106-65-0	78
			Butanedioic acid, dimethyl ester	51620	000106-65-0	78
			Butanedioic acid, dimethyl ester	120347	000106-65-0	64
5	11.00	0.96	C:\Database\NIST98.L			
			Benzyl Alcohol	30979	000100-51-6	94
			Benzyl Alcohol	115958	000100-51-6	94
			Benzyl Alcohol	115957	000100-51-6	91
6	13.12	1.42	C:\Database\NIST98.L			
			Pentanedioic acid, dimethyl ester	113343	001119-40-0	90
			Pentanedioic acid, dimethyl ester	113342	001119-40-0	78
			Pentanedioic acid, dimethyl ester	118675	001119-40-0	72
7	13.64	0.38	C:\Database\NIST98.L			
			Benzoic Acid	119309	000065-85-0	94
			Benzoic Acid	119125	000065-85-0	94
			Benzoic Acid	119310	000065-85-0	90
8	13.79	0.43	C:\Database\NIST98.L			
			Octanoic Acid	113422	000124-07-2	72
			Octanoic Acid	113421	000124-07-2	64
			Octanoic Acid	20165	000124-07-2	64
9	14.90	0.28	C:\Database\NIST98.L			
			Ethanol, 2-phenoxy-	118054	000122-99-6	95
			Ethanol, 2-phenoxy-	40669	000122-99-6	94
			Ethanol, 2-phenoxy-	118055	000122-99-6	91

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10	15.26	0.97	C:\Database\NIST98.L			
			Hexanedioic acid, dimethyl ester	113264	000627-93-0	91
			Hexanedioic acid, dimethyl ester	19850	000627-93-0	91
			Hexanedioic acid, dimethyl ester	113348	000627-93-0	90
11	15.73	1.38	C:\Database\NIST98.L			
			Nonanoic acid	20156	000112-05-0	94
			Nonanoic acid	113428	000112-05-0	93
			Nonanoic acid	113427	000112-05-0	91
12	17.41	1.14	C:\Database\NIST98.L			
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	59
			Propanoic acid, 2-methyl-, 2-me...	114586	000097-85-8	50
			Propanoic acid, 2-methyl-, 2,2-...	24402	074367-33-2	45
13	17.52	0.61	C:\Database\NIST98.L			
			n-Decanoic acid	113415	000334-48-5	72
			n-Decanoic acid	20154	000334-48-5	72
			n-Decanoic acid	113413	000334-48-5	70
14	17.76	0.75	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	96
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	93
15	17.83	1.36	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	80
			Butanoic acid, butyl ester	109895	000109-21-7	72
			Butanoic acid, butyl ester	114541	000109-21-7	72
16	19.30	0.37	C:\Database\NIST98.L			
			Phenol, 3-(1,1-dimethylethyl)-4...	124524	000088-32-4	60
			Butylated Hydroxyanisole	72597	025013-16-5	59
			3-tert-Butyl-4-hydroxyanisole	72598	000121-00-6	55
17	19.54	0.58	C:\Database\NIST98.L			
			Cyclopropane, nonyl-	13662	074663-85-7	95
			1-Decene	111296	000872-05-9	91
			1-Dodecanol	111442	000112-53-8	91
18	20.09	0.78	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	95
			Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4	93
			Phenol, 2,4-bis(1,1-dimethyleth...	125783	000096-76-4	93
19	20.89	0.56	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	97
			Lauric anhydride	114892	000645-66-9	80
			Heptanoic acid	113419	000111-14-8	43
20	21.47	1.70	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	74
			Di-n-butyl Phthalate	28	000084-74-2	9
21	21.64	0.43	C:\Database\NIST98.L			
			2-Pentanone, 5-methoxy-	5841	017429-04-8	43
			Oxirane, 3-ethyl-2,2-dimethyl-	113175	001192-22-9	43
			Methyl 16-methoxyheptadecanoate	19541	1000110-18-2	38
22	22.37	0.37	C:\Database\NIST98.L			
			Benzophenone	119383	000119-61-9	76
			Benzophenone	46089	000119-61-9	76
			Benzophenone	119052	000119-61-9	68

23	22.80	1.91	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	70
			1,4-Naphthoquinone, 6-acetyl-2,...	127595	013379-24-3	56
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	38
24	23.37	0.39	C:\Database\NIST98.L			
			Heptadecane	112320	000629-78-7	98
			Heptadecane	16420	000629-78-7	98
			Heptadecane	112322	000629-78-7	93
25	23.57	0.27	C:\Database\NIST98.L			
			2-Hydroxy-2-methylundec-5-en-3-one	19355	1000191-46-2	38
			5-Ethyl-3-nonanol	16991	019780-71-3	37
			1-Butanol, 3-methoxy-, acetate	5857	004435-53-4	27
26	24.23	0.93	C:\Database\NIST98.L			
			Tetradecanoic acid	114897	000544-63-8	98
			Tetradecanoic acid	114898	000544-63-8	96
			Tetradecanoic acid	113420	000544-63-8	95
27	24.35	0.29	C:\Database\NIST98.L			
			Phenol, 2,6-bis(1,1-dimethyleth...	126888	004130-42-1	86
			3,5-di-tert-Butyl-4-hydroxybenz...	87462	001620-98-0	84
			3,5-di-tert-Butyl-4-hydroxybenz...	126889	001620-98-0	83
28	24.60	0.31	C:\Database\NIST98.L			
			Phenol, 2-(1,1-dimethylethyl)-4...	80516	005806-73-5	62
			Phenol, 2,5-bis(1,1-dimethyleth...	125777	005875-45-6	50
			Phenol, 2,4-bis(1,1-dimethyleth...	125782	000096-76-4	50
29	24.90	0.78	C:\Database\NIST98.L			
			Octadecane	112330	000593-45-3	98
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	98
30	24.99	0.80	C:\Database\NIST98.L			
			Pentatriacontane	112346	000630-07-9	76
			Hexadecane, 2,6,10,14-tetramethyl-	17086	000638-36-8	68
			Hexadecane, 2,6,10,14-tetramethyl-	112575	000638-36-8	68
31	25.17	1.11	C:\Database\NIST98.L			
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	64
			8-Methoxy-11H-benzo[a]carbazole	92655	1000212-76-8	59
			Phenol, 2,4,6-tris(1,1-dimethyl...	92595	000732-26-3	50
32	25.28	0.38	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	53
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	47
			2-Propanol, 1,1'-[(1-methyl-1,2...	19307	001638-16-0	47
33	25.48	0.31	C:\Database\NIST98.L			
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	42
			Dodecane, 1,1'-oxybis-	16642	004542-57-8	41
			1-Decanol, 2-hexyl-	112269	002425-77-6	38
34	25.76	2.82	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	50
			Benzyl butyl Phthalate	36	000085-68-7	9
35	25.92	0.62	C:\Database\NIST98.L			
			2-Methyl-tridecane-2,12-diol	19413	1000187-03-5	50

				3-Tridecanol	19339	010289-68-6 47
				3-Pentadecanol	19358	053346-71-7 47
36	26.01	0.77	C:\Database\NIST98.L			
				1,2-Octadecanediol	16347	020294-76-2 60
				Octadecanol	33113	026762-44-7 55
				1-Nonadecene	108523	018435-45-5 55
37	26.27	0.72	C:\Database\NIST98.L			
				Nonadecane	112382	000629-92-5 97
				Nonadecane	16515	000629-92-5 96
				Nonadecane	112381	000629-92-5 93
38	26.38	0.89	C:\Database\NIST98.L			
				7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4 55
				Diethyl Phthalate	67077	000084-66-2 38
				Phenanthrene, tetradecahydro-4,...	66871	056292-68-3 38
39	27.01	11.50	C:\Database\NIST98.L			
				n-Hexadecanoic acid	114901	000057-10-3 97
				n-Hexadecanoic acid	109985	000057-10-3 92
				Heptadecanoic acid	114893	000506-12-7 89
40	27.15	0.61	C:\Database\NIST98.L			
				1-Nonadecene	108523	018435-45-5 74
				Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4 50
				Cyclopentane, (4-octyldodecyl)-	109588	005638-09-5 49
41	27.30	0.36	C:\Database\NIST98.L			
				18,19-Secoyohimban-19-oic acid,...	16341	005523-49-9 43
				2-Butanone, 4-(2,6,6-trimethyl-...	4528	039721-65-8 25
				Isojasmone	42256	011050-62-7 25
42	27.51	1.25	C:\Database\NIST98.L			
				Eicosane	112565	000112-95-8 95
				Eicosane	109630	000112-95-8 94
				Eicosane	112345	000112-95-8 94
43	27.76	0.33	C:\Database\NIST98.L			
				1-Hentetracontanol	16591	040710-42-7 38
				3-Octadecene, (E)-	22895	007206-19-1 35
				9-Octadecene, (E)-	13709	007206-25-9 25
44	28.16	0.46	C:\Database\NIST98.L			
				4-Iodo-2,6-dimethyl-phenylamine	92614	004102-53-8 43
				2-Amino-4,6-diphenylpyrimidine	92665	040230-24-8 38
				5,8-Dimethoxy-6-methyl-2-nitros...	92652	099316-37-7 37
45	28.29	2.11	C:\Database\NIST98.L			
				Azadibenzopyrene	99857	104219-69-4 9
				5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4 9
				Hydromorphinol	99808	002183-56-4 9
46	28.49	0.60	C:\Database\NIST98.L			
				1-Octadecene	112297	000112-88-9 98
				1-Octadecene	112298	000112-88-9 96
				1-Octadecene	111277	000112-88-9 93
47	28.66	0.31	C:\Database\NIST98.L			
				Nonahexacontanoic acid	17028	040710-32-5 42
				Octadecane, 1-chloro-	112584	003386-33-2 30
				Hexatriacontane	112334	000630-06-8 30

48	29.06	1.60	C:\Database\NIST98.L			
			Octan-2-one, 3,6-dimethyl-	5044	1000132-45-2	42
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	27
			Heptafluorobutyric acid, n-pent...	5520	1000216-79-3	15
49	29.31	9.34	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	97
			Octadecanoic acid	109378	000057-11-4	72
			Pentadecanoic acid	114896	001002-84-2	70
50	29.52	1.03	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	58
			Tetradecanamide	19652	000638-58-4	58
			Nonanamide	19654	001120-07-6	52
51	29.71	0.30	C:\Database\NIST98.L			
			Docosane	109660	000629-97-0	89
			Docosane	16531	000629-97-0	87
			Docosane	112393	000629-97-0	64
52	29.78	2.87	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
53	31.03	0.29	C:\Database\NIST98.L			
			Isopropyl-[2-(4-methoxy-2,6-dim...	103705	1000189-65-2	38
			3-Methoxy-3,6.alpha.-dipentyl-5...	103711	059251-88-6	25
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	14
54	31.22	0.90	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	99
			Diethyl Phthalate	14	000084-66-2	25
			Di-n-butyl Phthalate	28	000084-74-2	17
55	31.31	2.90	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113301	000301-02-0	93
			9-Octadecenamide, (Z)-	113302	000301-02-0	86
			9-Octadecenamide, (Z)-	19657	000301-02-0	83
56	31.53	1.21	C:\Database\NIST98.L			
			Diisooctyl adipate	58242	001330-86-5	60
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	60
			1,3-Disilacyclobutane, 1,1,3,3-...	121822	001627-98-1	47
57	31.61	1.28	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	43
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	30
			Oxirane, (ethoxymethyl)-	1096	004016-11-9	27
58	31.74	0.53	C:\Database\NIST98.L			
			Silane, triethyl-	19733	000617-86-7	43
			1,8-Nonanediol, 8-methyl-	19401	054725-73-4	43
			O-Menthan-8-ol	19544	1000160-38-8	43
59	31.78	0.96	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	47
			1,4-Di-O-acetyl-2,5-di-O-methyl...	19333	1000101-82-1	47
			Methyl 16-methoxyheptadecanoate	19541	1000110-18-2	47
60	32.47	2.05	C:\Database\NIST98.L			
			1-Docosene	111438	001599-67-3	95
			1-Octadecanol	111484	000112-92-5	94
			1-Heptadecene	13024	006765-39-5	92

61	32.82	1.97	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	90
			Di-n-octyl phthalate	40	000117-81-0	50
			Di-n-butyl Phthalate	28	000084-74-2	43
62	33.16	0.33	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	109752	000301-02-0	49
			7-Nonenamide	19655	090949-53-4	46
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	43
63	33.91	0.27	C:\Database\NIST98.L			
			Oxirane, 3-ethyl-2,2-dimethyl-	19363	001192-22-9	38
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	37
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	37
64	34.09	0.28	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	37
			1,3-Bis(dimethyl-n-pentylsilyl)...	19895	1000214-94-5	37
			2,4,6,8,9,10-Hexathiatricyclo[3...	19863	057274-38-1	32
65	34.23	0.39	C:\Database\NIST98.L			
			3-Hexadecanol	113255	000593-03-3	38
			1,3-Dioxolane, 4-hexyl-2,2-dime...	20022	054934-58-6	35
			3-Heptadecanol	19340	084534-30-5	35
66	35.05	13.30	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	93
			9-Octadecenamide, (Z)-	19657	000301-02-0	86
			Hexadecanamide	113298	000629-54-9	64
67	35.47	0.27	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	19657	000301-02-0	35
			3-Tetradecanol	19356	001653-32-3	27
			1H-Indole, 2-methyl-3-phenyl-	126477	004757-69-1	22
68	36.15	0.66	C:\Database\NIST98.L			
			Propanamide, N-(3-methoxyphenyl...	17665	056619-93-3	15
			Thiocyanic acid, ethyl ester	108008	000542-90-5	10
			Hydrazinecarboxylic acid, 1,1-d...	15839	000870-46-2	10
69	36.36	2.46	C:\Database\NIST98.L			
			4H-1-Benzopyran-4-one, 3,5,7-tr...	101040	000480-19-3	12
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	11
			1-Butanol, 3-methoxy-, acetate	5857	004435-53-4	10
70	36.61	1.58	C:\Database\NIST98.L			
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	43
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	40
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	38
71	37.46	0.35	C:\Database\NIST98.L			
			Thiocyanic acid, ethyl ester	108008	000542-90-5	35
			Silane, octyl-	19805	000871-92-1	35
			2,5,8,11-Tetraoxatetradecan-13-...	19675	020324-34-9	27
72	39.03	0.74	C:\Database\NIST98.L			
			1-Dotriacontanol	16786	006624-79-9	50
			1-Eicosanol	112640	000629-96-9	50
			17-Pentatriacontene	5525	006971-40-0	45
73	39.64	0.36	C:\Database\NIST98.L			
			Dodecahydropyrido[1,2-b]isoquin...	84738	1000195-30-7	45
			Acetamide, N-[2-[2-[2-[(2-nitro...	84712	069395-33-1	27

			1,2-Benzisothiazole-3-acetic ac...	84760	029876-70-8 27
74	40.90	3.45	C:\Database\NIST98.L		
			Dodecanamide	19649	001120-16-7 80
			Nonanamide	19654	001120-07-6 72
			Tetradecanamide	19652	000638-58-4 64
75	42.94	0.32	C:\Database\NIST98.L		
			Silane, diethyldimethyl-	19725	000756-81-0 25
			Cyclohexane, (ethoxymethoxy)-	19366	054699-29-5 22
			3-Tridecanol	19339	010289-68-6 22
76	43.82	0.28	C:\Database\NIST98.L		
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0 35
			3-Hexanol, 1,5-dimethoxy-2,4-di...	19515	013897-22-8 32
			Dimethylallyl(n-octyl)silane	19967	081272-81-3 27

Tue Jan 15 17:05:31 2008

Chloramine
Day 4
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\010.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 11:54 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 12

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	5.71	0.28	C:\Database\NIST98.L			
			Acetic acid, chloro-, 2-butoxye...	15971	1000131-74-3	45
			1,8-Nonadien-3-ol	16734	1000111-56-0	45
			Acetic acid, chloro-, 1,1-dimet...	16914	000107-59-5	28
2	5.87	0.83	C:\Database\NIST98.L			
			Oxirane, 3-ethyl-2,2-dimethyl-	113175	001192-22-9	39
			2-Octanol, 2-methyl-	19442	000628-44-4	9
			Butanamide	113228	000541-35-5	9
3	5.94	0.35	C:\Database\NIST98.L			
			Butane, 1-methoxy-	11673	000628-28-4	53
			2-Hexanol, 3-methyl-	11546	002313-65-7	39
			Hexane, 1-methoxy-	110868	004747-07-3	39
4	6.25	7.73	C:\Database\NIST98.L			
			Butane, 2,3-dichloro-2-methyl-	29395	000507-45-9	90
			Propane, 1,1-dichloro-	29392	000078-99-9	9
			Propane, 2-bromo-1-chloro-	115667	003017-95-6	9
5	6.53	0.37	C:\Database\NIST98.L			
			Butane, 2-methoxy-2-methyl-	25351	000994-05-8	28
			3-Hexanol, 2,4-dimethyl-	25553	013432-25-2	25
			Epi-Inositol	25800	000488-58-4	12
6	6.64	0.41	C:\Database\NIST98.L			
			Acetamide, 2-chloro-	11080	000079-07-2	33
			.beta.-Myrcene	108895	000123-35-3	9
			Acetamide, 2-chloro-	110641	000079-07-2	7
7	6.81	0.29	C:\Database\NIST98.L			
			Butane, 1,2-dichloro-2-methyl-	36612	023010-04-0	64
			Decane, 1-chloro-	4520	001002-69-3	33
			Hexane, 1-chloro-	111394	000544-10-5	33
8	6.86	0.24	C:\Database\NIST98.L			
			Acetic acid, 3-methoxy-2-butyl ...	19385	1000151-29-7	38
			2-Butanol, 2,3-dimethyl-	113200	000594-60-5	9
			2-Butanol, 3-methoxy-	19505	053778-72-6	9
9	7.31	0.30	C:\Database\NIST98.L			
			Phenol, 2-fluoro-	50680	000367-12-4	86
			Ethyl Chloride	107943	000075-00-3	43
			Ethyl Chloride	113564	000075-00-3	32

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10	7.40	0.32	C:\Database\NIST98.L		
			2-Thiazolidinethione	120680	000096-53-7 35
			Hydrazinecarbothioamide, N-ethyl-	113439	013431-34-0 25
			Ethane, 1,2-dichloro-1,1-difluoro-	43095	001649-08-7 22
11	7.50	0.25	C:\Database\NIST98.L		
			Propane, 2,2-bis(ethylthio)-	44581	014252-45-0 27
			1-Ethoxy-3,3-diethyltriazene 2-...	44656	091725-44-9 17
			3-Pentyn-2-ol, 5-chloro-	4042	1000250-38-8 17
12	8.18	1.98	C:\Database\NIST98.L		
			Cyclopentane, 1,1-dichloro-	21604	031038-06-9 47
			Cyclopentane, 1,3-dichloro-, cis-	21600	026688-51-7 43
			1-Butyne, 3-chloro-3-methyl-	21047	001111-97-3 43
13	8.24	0.56	C:\Database\NIST98.L		
			s-Dichloroethyl ether	117836	000111-44-4 78
			s-Dichloroethyl ether	39932	000111-44-4 56
			Cyclopropane, 1-bromo-1-chloro-...	39986	024071-59-8 56
14	8.39	0.62	C:\Database\NIST98.L		
			2-(2-Bromoethyl)-3-methyl-oxirane	34127	1000193-47-0 38
			1-Pentanol, 5-[(tetrahydro-2H-p...	34370	076102-74-4 35
			Cyclohexanol, 1,3-dimethyl-, cis-	34193	015466-94-1 35
15	8.68	0.32	C:\Database\NIST98.L		
			Ethanol, 2-(2-methoxyethoxy)-	11464	000111-77-3 56
			Ethanol, 2-(2-methoxyethoxy)-	110890	000111-77-3 53
			Ethanol, 2-[2-(2-methoxyethoxy)...	11712	000112-35-6 50
16	9.62	0.38	C:\Database\NIST98.L		
			Hexanoic acid	113410	000142-62-1 64
			Hexanoic acid	113407	000142-62-1 53
			Hexanoic acid	113409	000142-62-1 50
17	9.94	0.24	C:\Database\NIST98.L		
			1,3-Cyclopentanedione, 2-chloro-	59720	014203-19-1 25
			Methylphosphonothioicchlorofluo...	59761	1000226-51-3 22
			3H-1,2-Dithiol-3-one, 4-methyl-	59616	003620-10-8 12
18	10.20	0.73	C:\Database\NIST98.L		
			Ethanol, 2-(2-ethoxyethoxy)-	110887	000111-90-0 86
			Ethanol, 2-(2-ethoxyethoxy)-	110886	000111-90-0 86
			Ethanol, 2-(2-ethoxyethoxy)-	11716	000111-90-0 58
19	10.67	0.28	C:\Database\NIST98.L		
			1-Propene, 1-chloro-	1587	000590-21-6 64
			1-Propene, 3-chloro-	1586	000107-05-1 59
			1-Propene, 2-chloro-	1590	000557-98-2 59
20	10.85	1.00	C:\Database\NIST98.L		
			1-Hexanol, 2-ethyl-	112637	000104-76-7 86
			1-Hexanol, 2-ethyl-	112146	000104-76-7 78
			1-Hexanol, 2-ethyl-	15889	000104-76-7 64
21	11.07	0.94	C:\Database\NIST98.L		
			Propanal, 2,3-dichloro-2-methyl-	29244	010141-22-7 59
			1-Propene, 1-chloro-	1587	000590-21-6 53
			Butanoic acid, 2,3-dichloro-, m...	29242	054460-97-8 45
22	11.23	1.17	C:\Database\NIST98.L		
			5-Chloro-beznofurazan oxide	29367	1000144-38-6 56
			Butanoic acid, 2,3-dichloro-, m...	29242	054460-97-8 45

			Propanal, 2,3-dichloro-2-methyl-	29244	010141-22-7	38
23	11.73	0.29	C:\Database\NIST98.L			
			D-Mannoheptulose	20082	003615-44-9	32
			(1R,3R,4R,5R)-(-)-Quinic acid	20081	000077-95-2	23
			1,4-Dithiane-2,5-dione, 3,6-dim...	20227	070400-95-2	22
24	12.13	1.10	C:\Database\NIST98.L			
			Benzene-d5-, nitro-	32381	004165-60-0	47
			Dehydromevalonic lactone	32276	002381-87-5	28
			Piperidine, 4-methyl-1-nitroso-	3307	015104-03-7	10
25	12.95	0.24	C:\Database\NIST98.L			
			N-Formylmorpholine	357	004394-85-8	50
			N-Methylpivalamide	16002	006830-83-7	33
			3H-1,2,4-Triazole-3-thione, 2,4...	120346	024854-43-1	32
26	13.08	0.52	C:\Database\NIST98.L			
			Cyclopentasiloxane, decamethyl-	115315	000541-02-6	83
			Cyclopentasiloxane, decamethyl-	103462	000541-02-6	72
			Cyclopentasiloxane, decamethyl-	128838	000541-02-6	72
27	13.59	0.29	C:\Database\NIST98.L			
			Benzoic Acid	119309	000065-85-0	90
			Benzoic Acid	119310	000065-85-0	87
			Benzoic Acid	46847	000065-85-0	86
28	13.76	0.27	C:\Database\NIST98.L			
			Octanoic Acid	113421	000124-07-2	59
			Octanoic Acid	20165	000124-07-2	53
			Octanoic Acid	113422	000124-07-2	53
29	14.40	0.28	C:\Database\NIST98.L			
			Xenon	59698	007440-63-3	38
			2(3H)-Thiophenone, dihydro-5-th...	59532	053951-47-6	38
			1H-Benzimidazole, 2-methyl-	122087	000615-15-6	38
30	15.69	0.68	C:\Database\NIST98.L			
			Nonanoic acid	113427	000112-05-0	86
			Nonanoic acid	20156	000112-05-0	64
			Nonanoic acid	113428	000112-05-0	59
31	17.42	1.01	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	38
			Heptanoic acid, 2-methyl-2-buty...	4432	1000160-11-4	37
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	35
32	17.76	2.53	C:\Database\NIST98.L			
			1,1'-Biphenyl, 2-fluoro-	74959	000321-60-8	96
			1,1'-Biphenyl, 2-fluoro-	124940	000321-60-8	95
			1,1'-Biphenyl, 4-fluoro-	74960	000324-74-3	93
33	17.83	1.11	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 2-et...	114627	074367-31-0	78
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	64
			Propanoic acid, 2-methyl-, buty...	109936	000097-87-0	50
34	19.42	0.25	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	76501	000719-22-2	96
			2,5-Cyclohexadiene-1,4-dione, 2...	125160	000719-22-2	95
			2,5-Cyclohexadiene-1,4-dione, 2...	125134	000719-22-2	87
35	19.56	0.39	C:\Database\NIST98.L			

			Cyclodecane	111288	000293-96-9	93
			Cyclodecane	13064	000293-96-9	93
			1-Dodecanol	111442	000112-53-8	91
36	20.89	0.50	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	76
			Dodecanoic acid	114899	000143-07-7	76
			Lauric anhydride	114892	000645-66-9	58
37	21.47	1.04	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 1-(1...	24401	074381-40-1	53
			2-Hexen-4-ol, 5-methyl-	24320	1000163-45-9	47
			2,2,4-Trimethyl-1,3-pentanediol...	24399	006846-50-0	36
38	21.65	0.26	C:\Database\NIST98.L			
			Heptadecane, 2,6,10,15-tetramet...	17067	054833-48-6	87
			Hexadecane	112410	000544-76-3	86
			Octadecane	112333	000593-45-3	86
39	22.37	0.34	C:\Database\NIST98.L			
			Benzophenone	119171	000119-61-9	81
			Benzophenone	46089	000119-61-9	81
			Benzophenone	119383	000119-61-9	81
40	22.51	1.78	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	94
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	12
			Androst-4-ene-3,17-dione-18-oic...	102056	1000195-76-9	9
41	22.81	1.96	C:\Database\NIST98.L			
			Boron, diethyl(5-ethyl-4,6-nona...	87941	136705-03-8	49
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	46
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	38
42	23.02	0.36	C:\Database\NIST98.L			
			Phosphonic acid, dioctadecyl ester	13890	019047-85-9	91
			5-Octadecene, (E)-	13707	007206-21-5	91
			1-Pentadecene	109475	013360-61-7	91
43	23.37	0.51	C:\Database\NIST98.L			
			Heptadecane	16420	000629-78-7	98
			Heptadecane	112320	000629-78-7	97
			Heptadecane	109557	000629-78-7	95
44	24.23	0.51	C:\Database\NIST98.L			
			Tetradecanoic acid	114897	000544-63-8	95
			Tetradecanoic acid	113420	000544-63-8	94
			Tetradecanoic acid	114898	000544-63-8	81
45	24.90	0.58	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	93
			Hexadecane	112409	000544-76-3	91
46	24.99	0.48	C:\Database\NIST98.L			
			Tetratetracontane	112365	007098-22-8	83
			Tritetracontane	17076	007098-21-7	80
			Pentatriacontane	112346	000630-07-9	72
47	25.21	0.28	C:\Database\NIST98.L			
			Isopropyl Myristate	110206	000110-27-0	49
			9,9-Dimethoxybicyclo[3.3.1]nona...	5530	117132-08-8	43
			Nonanoic acid, 1-methylethyl ester	7782	1000132-17-3	30

48	25.48	0.25	C:\Database\NIST98.L			
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	43
			1-Dotriacontanol	16786	006624-79-9	41
			Muscimol, [5-(Aminomethyl)isoxa...	690	1000201-01-8	38
49	25.76	1.38	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	64
			Diethyl Phthalate	14	000084-66-2	40
			Benzyl butyl Phthalate	36	000085-68-7	2
50	26.03	0.24	C:\Database\NIST98.L			
			1-Heptadecanol	13564	001454-85-9	74
			1-Eicosanol	112640	000629-96-9	74
			3-Eicosene, (E)-	16986	074685-33-9	68
51	26.26	0.44	C:\Database\NIST98.L			
			Nonadecane	112381	000629-92-5	96
			Nonadecane	112382	000629-92-5	95
			Nonadecane	16515	000629-92-5	94
52	26.38	1.07	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	93
			.alpha.-Cedrene oxide	84384	1000159-39-1	60
			3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9	60
53	27.00	9.73	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	53
			Diethyl Phthalate	14	000084-66-2	7
54	27.51	0.55	C:\Database\NIST98.L			
			Eicosane	112345	000112-95-8	94
			Eicosane	112565	000112-95-8	94
			Pentacosane	109667	000629-99-2	91
55	28.23	0.27	C:\Database\NIST98.L			
			2,15-Hexadecanedione	5791	018650-13-0	27
			Menthol, 1'-(butyn-3-one-1-yl)-...	4392	1000156-95-3	27
			3-Methyl-2-(2-oxopropyl)furan	16777	087773-62-4	15
56	28.29	0.25	C:\Database\NIST98.L			
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	25
			3-Methyl-2-(2-oxopropyl)furan	16777	087773-62-4	15
			Trifluoroacetic acid,n-tridecyl...	4217	1000216-78-8	14
57	28.51	0.76	C:\Database\NIST98.L			
			1-Octadecene	112298	000112-88-9	98
			1-Octadecene	112297	000112-88-9	98
			1-Octadecanol	5273	000112-92-5	95
58	28.78	0.28	C:\Database\NIST98.L			
			1-Hentetracontanol	16591	040710-42-7	49
			1-Dotriacontanol	16786	006624-79-9	46
			Cyclopentane, 1,1'-[3-(2-cyclop...	2576	055255-85-1	38
59	29.08	0.25	C:\Database\NIST98.L			
			Heptafluorobutyric acid, n-octa...	5522	1000216-79-5	49
			3-Heptafluorobutyroxypentadecane	1716	1000245-50-1	46
			Trifluoroacetic acid, n-octadec...	5521	1000216-79-4	46
60	29.30	6.70	C:\Database\NIST98.L			
			Octadecanoic acid	6590	000057-11-4	93
			Octadecanoic acid	114902	000057-11-4	92

			Pentadecanoic acid	114896	001002-84-2	86
61	29.50	1.13	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	70
			Hexadecanamide	113298	000629-54-9	64
			Dodecanamide	19649	001120-16-7	52
62	29.78	4.96	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
63	30.23	0.31	C:\Database\NIST98.L			
			Ethanol, 2-(tetradecyloxy)-	112367	002136-70-1	25
			Nonahexacontanoic acid	17028	040710-32-5	22
			11-Undecanolide	14557	1000132-46-4	18
64	31.22	0.42	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	72
			Diethyl Phthalate	14	000084-66-2	32
			Di-n-butyl Phthalate	28	000084-74-2	2
65	31.53	1.23	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Diisooctyl adipate	58242	001330-86-5	90
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	90
66	31.61	0.96	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	74
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	74
			Butane, 1,1'-[oxybis(2,1-ethane...	17205	000112-73-2	43
67	31.77	0.24	C:\Database\NIST98.L			
			.alpha.-L-Lyxo-Hexopyranoside, ...	19816	032385-07-2	32
			Hexane, 1-(ethoxymethoxy)-	19456	1000141-99-4	25
			3-Tridecanol	19339	010289-68-6	25
68	32.50	1.33	C:\Database\NIST98.L			
			3-Eicosene, (E)-	16986	074685-33-9	95
			1-Heneicosyl formate	16592	077899-03-7	87
			1-Eicosanol	112640	000629-96-9	87
69	32.82	11.59	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	98
			Di-n-octyl phthalate	40	000117-81-0	40
			Di-n-butyl Phthalate	28	000084-74-2	37
70	34.09	0.42	C:\Database\NIST98.L			
			Octaverine	105278	000549-68-8	35
			Methadone N-oxide	84766	1000120-80-7	14
			4-Pyrimidinecarboxylic acid, 1,...	105273	016135-24-3	12
71	35.14	3.29	C:\Database\NIST98.L			
			Pentanamide	113232	000626-97-1	64
			Undecanamide, 11-bromo-	19650	1000163-84-6	64
			Pentadecanamide, 15-bromo-	19651	1000163-86-1	64
72	35.49	0.37	C:\Database\NIST98.L			
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	43
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	27
			2-Ethylacridine	84846	1000147-64-9	27
73	35.99	0.34	C:\Database\NIST98.L			
			2,3,4-Trimethoxyphenylacetonitrile	84840	068913-85-9	43
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	38

			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	38
74	36.14	0.66	C:\Database\NIST98.L			
			2-t-Butyl-5-chloromethyl-3-meth...	17941	1000192-88-5	12
			t-Butyl-1-thio-.beta.-d-glucofu...	17745	1000127-29-5	9
			Acetic acid, 3,5-diacetoxy-2-br...	9447	1000194-80-2	7
75	36.36	2.26	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	38
			Acetic acid, 3,5-diacetoxy-2-br...	9447	1000194-80-2	10
			Propanamide, 2,2-dimethyl-N-(3-...	17553	032597-29-8	10
76	39.09	0.33	C:\Database\NIST98.L			
			Hexahydropyridine, 1-methyl-4-[...	84723	094427-47-1	52
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	43
			Cyclotrisiloxane, hexamethyl-	126480	000541-05-9	35
77	40.91	10.55	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	72
			Undecanamide, 11-bromo-	19650	1000163-84-6	72
			Pentadecanamide, 15-bromo-	19651	1000163-86-1	72
78	41.54	0.31	C:\Database\NIST98.L			
			3-Tridecanol	19339	010289-68-6	27
			1-Butanol, 3-methoxy-, acetate	5857	004435-53-4	27
			3-Hexanol, 1,5-dimethoxy-2,4-di...	19515	013897-22-8	25

Tue Jan 15 17:10:41 2008

Chloramine
Day 4
Sample

TMPLIBRP.TXT

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\004.D
Operator: Heather Johnson
Date Acquired: 7 Jan 2008 6:12 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 6

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	27.00	1.68	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	83
			Diethyl Phthalate	14	000084-66-2	9
2	28.50	0.67	C:\Database\NIST98.L			
			Cyclotetradecane	111326	000295-17-0	72
			2-Dodecanol	110819	010203-28-8	72
			1-Tridecene	111270	002437-56-1	72
3	29.08	0.96	C:\Database\NIST98.L			
			6-[[[3,4-Dichlorophenyl]methyla...	9339	1000227-15-8	9
			1,2-O-Isopropylidene-3-O-tosyl-...	5875	1000213-83-7	9
			Stannane, (1,1-dimethylethyl)tr...	17913	035569-21-2	7
4	29.18	0.49	C:\Database\NIST98.L			
			Propionic acid, 2-diethylborylo...	17707	1000149-82-1	22
			1-Chloro-2-methyl-2-phenyl-1-(2...	58576	1000222-74-1	10
			2,6-Piperazinedione, monooxime	58232	056700-84-6	10
5	29.78	1.34	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	96
6	31.22	1.92	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	90
			Diethyl Phthalate	14	000084-66-2	32
			Di-n-butyl Phthalate	28	000084-74-2	9
7	31.53	4.90	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	94
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	91
			Hexanedioic acid, mono(2-ethylh...	58234	004337-65-9	72
8	31.62	0.72	C:\Database\NIST98.L			
			Epoxy-linalooloxide	5864	1000007-96-5	38
			Butanoic acid, 4-ethoxy-, methy...	113309	029006-04-0	37
			1-Octadecanamine	108203	000124-30-1	23
9	32.82	3.72	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	87
			Di-n-butyl Phthalate	28	000084-74-2	47
			Di-n-octyl phthalate	40	000117-81-0	9
10	32.98	2.55	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	59
			1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	25

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				Pentasiloxane, dodecamethyl-	97318	000141-63-9	22
11	34.24	0.65	C:\Database\NIST98.L				
				Eicosane	16454	000112-95-8	50
				13-Methylhentriacontane	16385	1000131-19-4	47
				Octadecane, 3-ethyl-5-(2-ethylb...	109659	055282-12-7	47
12	34.60	0.59	C:\Database\NIST98.L				
				Silicic acid, diethyl bis(trime...	84851	003555-45-1	38
				Propiophenone, 2'-(trimethylsil...	84849	033342-87-9	38
				Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	38
13	35.18	0.79	C:\Database\NIST98.L				
				Eicosane	16454	000112-95-8	42
				Eicosane	112565	000112-95-8	42
				Octadecane, 1-chloro-	112584	003386-33-2	38
14	36.16	12.06	C:\Database\NIST98.L				
				Spiro[bicyclo[3.3.0]oct-6-ene-3...	557	1000156-60-3	11
				Ethyl 2-acetamido-3,3,3-trifluo...	9561	1000224-78-8	9
				Isolongifolan-8-ol	3146	001139-08-8	9
15	36.38	23.42	C:\Database\NIST98.L				
				2-Propyn-1-one, 1-(2-thienyl)-,...	100982	056588-20-6	9
				Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	9
				Bicyclo[5.3.0]decan-2-one, 9-(d...	100989	1000151-00-6	9
16	37.69	17.60	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	46
				trans-2,3-Methylenedioxy-b-meth...	84750	086029-47-2	25
				Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	22
17	38.93	0.71	C:\Database\NIST98.L				
				Cyclotrisiloxane, hexamethyl-	126480	000541-05-9	35
				Cyclotrisiloxane, hexamethyl-	126461	000541-05-9	27
				4-Phenyl-3,4-dihydroisoquinoline	84818	006187-58-2	27
18	41.58	23.03	C:\Database\NIST98.L				
				Benzene, 1,4-bis(3-phenylindol-...	106699	1000164-74-0	35
				1H-Isoindole-1,3(2H)-dione, 5,5...	106698	033734-37-1	25
				1,3,5-Triazine-2,4,6-triamine, ...	106696	033933-66-3	17
19	43.15	0.90	C:\Database\NIST98.L				
				Silicic acid, diethyl bis(trime...	84851	003555-45-1	32
				Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	25
				Cyclotrisiloxane, hexamethyl-	126480	000541-05-9	22
20	43.72	1.30	C:\Database\NIST98.L				
				Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	83
				Heptasiloxane, 1,1,3,3,5,5,7,7,...	27374	019095-23-9	42
				1-Monolinoleoylglycerol trimeth...	27370	054284-45-6	32

Tue Jan 15 16:08:00 2008

Chloramine
Day 9
Control

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\015.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 4:40 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 17

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - RTEINT.P

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	21.47	0.85	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	92
			Di-n-butyl Phthalate	28	000084-74-2	4
2	22.52	0.85	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	98
			7-Bromo-2,3-dihydro-5-phenyl-1H...	102209	034099-70-2	10
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	10
3	22.81	0.49	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	93
			Boron, diethyl(5-ethyl-4,6-nona...	87941	136705-03-8	58
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	50
4	24.89	0.71	C:\Database\NIST98.L			
			Octadecane	112330	000593-45-3	98
			Octadecane	16439	000593-45-3	98
			Octadecane	112333	000593-45-3	94
5	24.98	0.63	C:\Database\NIST98.L			
			Pentatriacontane	112346	000630-07-9	91
			Nonadecane, 2,3-dimethyl-	5612	075163-99-4	91
			Dotriacontane	112351	000544-85-4	90
6	25.21	0.43	C:\Database\NIST98.L			
			Isopropyl Myristate	110206	000110-27-0	64
			Isopropyl Myristate	4614	000110-27-0	46
			Tetradecanoic acid	114898	000544-63-8	22
7	25.47	0.42	C:\Database\NIST98.L			
			Oxirane, [(dodecyloxy)methyl]-	16338	002461-18-9	49
			Cyclohexanone, 4-(1,1-dimethylp...	24668	016587-71-6	38
			1-Decanol, 2-hexyl-	112269	002425-77-6	38
8	25.76	1.44	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Diethyl Phthalate	14	000084-66-2	40
			Benzyl butyl Phthalate	36	000085-68-7	2
9	26.27	0.75	C:\Database\NIST98.L			
			Nonadecane	112380	000629-92-5	95
			Nonadecane	112382	000629-92-5	95
			Nonadecane	16515	000629-92-5	90
10	26.38	0.61	C:\Database\NIST98.L			

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				7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	92
				Ethene,-1-(4-diethylaminophenyl...	84389	1000221-95-1	46
				3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9	38
11	27.01	8.22	C:\Database\OWML.L				
				Di-n-butyl Phthalate	28	000084-74-2	70
				Diethyl Phthalate	14	000084-66-2	1
12	27.51	0.87	C:\Database\NIST98.L				
				Eicosane	112345	000112-95-8	95
				Hexatriacontane	112335	000630-06-8	94
				Tetratetracontane	16486	007098-22-8	91
13	28.51	0.60	C:\Database\NIST98.L				
				1-Heptadecanol	13564	001454-85-9	94
				1-Nonadecene	42210	018435-45-5	94
				Cyclohexadecane	14275	000295-65-8	93
14	29.31	5.57	C:\Database\NIST98.L				
				Octadecanoic acid	114902	000057-11-4	87
				Pentadecanoic acid	114896	001002-84-2	83
				Octadecanoic acid	109378	000057-11-4	80
15	29.50	1.20	C:\Database\NIST98.L				
				Hexadecanamide	19647	000629-54-9	81
				Hexadecanamide	113298	000629-54-9	72
				Dodecanamide	19649	001120-16-7	72
16	29.66	0.41	C:\Database\NIST98.L				
				1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	32
				3-Isopropoxy-1,1,1,7,7,7-hexame...	26784	071579-69-6	17
				3-Trimethylsilyloxystearic acid...	26930	1000079-42-6	17
17	29.78	4.57	C:\Database\OWML.L				
				Terphenyl-d14	34	001718-51-0	99
18	30.96	0.40	C:\Database\NIST98.L				
				1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	64
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	40
				3-Trimethylsilyloxystearic acid...	26930	1000079-42-6	32
19	31.23	1.07	C:\Database\OWML.L				
				Benzyl butyl Phthalate	36	000085-68-7	99
				Diethyl Phthalate	14	000084-66-2	12
				Di-n-butyl Phthalate	28	000084-74-2	9
20	31.31	3.62	C:\Database\NIST98.L				
				9-Octadecenamide, (Z)-	113302	000301-02-0	95
				Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	64
				9-Octadecenamide, (Z)-	113301	000301-02-0	60
21	31.53	0.94	C:\Database\NIST98.L				
				Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
				Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	87
				Diisooctyl adipate	58242	001330-86-5	83
22	31.61	0.70	C:\Database\NIST98.L				
				Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	68
				Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	49
				Dodecane, 3-methyl-	16452	017312-57-1	27
23	32.16	0.55	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	42

				1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	25
				Heptasiloxane, hexadecamethyl-	27486	000541-01-5	22
24	32.49	1.91	C:\Database\NIST98.L				
				1-Heneicosyl formate	16592	077899-03-7	95
				1-Eicosanol	112640	000629-96-9	94
				Cycloeicosane	13708	000296-56-0	93
25	32.82	3.20	C:\Database\OWML.L				
				Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
				Di-n-octyl phthalate	40	000117-81-0	50
				Di-n-butyl Phthalate	28	000084-74-2	37
26	32.98	3.15	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	83
				Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	38
				1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	33
27	33.05	5.49	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	72
				3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	37
				Mercaptoacetic acid, bis(trimet...	26922	006398-62-5	32
28	33.27	1.43	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	58
				3-Isopropoxy-1,1,1,7,7,7-hexame...	26784	071579-69-6	25
				3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	16
29	33.36	1.17	C:\Database\NIST98.L				
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	53
				Pentasiloxane, dodecamethyl-	97318	000141-63-9	35
				Pentasiloxane, dodecamethyl-	115143	000141-63-9	35
30	34.09	0.61	C:\Database\NIST98.L				
				Octaverine	105278	000549-68-8	16
				1,2-Benzisothiazole-3-acetic ac...	84760	029876-70-8	14
				Lanost-8-ene	105263	006593-21-1	11
31	34.25	0.44	C:\Database\NIST98.L				
				Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	38
				1,2,4-Benzenetricarboxylic acid...	84894	043049-07-6	22
				1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	10
32	34.39	1.45	C:\Database\NIST98.L				
				Cyclodecasiloxane, eicosamethyl-	27712	018772-36-6	43
				Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	42
				1,1,1,5,7,7,7-Heptamethyl-3,3-b...	26950	038147-00-1	40
33	34.81	0.59	C:\Database\NIST98.L				
				1,2-Benzenedicarboxylic acid, d...	123527	000084-76-4	46
				1,2-Benzenedicarboxylic acid, b...	66802	020548-62-3	43
				1,2-Benzenedicarboxylic acid, d...	66803	028553-12-0	43
34	34.90	0.55	C:\Database\NIST98.L				
				1,2-Benzenedicarboxylic acid, b...	66802	020548-62-3	52
				1,2-Benzenedicarboxylic acid, d...	66803	028553-12-0	46
				1,2-Benzenedicarboxylic acid, d...	123527	000084-76-4	46
35	35.05	19.90	C:\Database\NIST98.L				
				Erucylamide	19656	000112-84-5	91
				Erucylamide	113300	000112-84-5	76
				9-Octadecenamide, (Z)-	19657	000301-02-0	59

36	35.37	1.07	C:\Database\NIST98.L			
			Didecyl phthalate	66744	000084-77-5	47
			1,2-Benzenedicarboxylic acid, d...	67001	025724-58-7	47
			1,2-Benzenedicarboxylic acid, b...	66750	000146-50-9	47
37	35.48	0.92	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, d...	66803	028553-12-0	64
			1,2-Benzenedicarboxylic acid, d...	66777	026761-40-0	52
			1,2-Benzenedicarboxylic acid, d...	123446	026761-40-0	50
38	35.63	1.75	C:\Database\NIST98.L			
			Stannane, tributylethyl-	126475	019411-60-0	46
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	38
			Pentasiloxane, dodecamethyl-	115143	000141-63-9	25
39	35.76	0.67	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	66750	000146-50-9	38
			1,2-Benzenedicarboxylic acid, d...	66803	028553-12-0	35
			1,2-Benzenedicarboxylic acid, b...	66780	000089-16-7	32
40	35.95	0.41	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	66750	000146-50-9	38
			1,2-Benzenedicarboxylic acid, d...	123446	026761-40-0	38
			Didecyl phthalate	66744	000084-77-5	38
41	36.09	1.22	C:\Database\NIST98.L			
			2-t-Butyl-6-[2-hydroxy-2-(2,4,6...	66734	1000192-88-0	14
			Benzothiazole, 2-methyl-	123474	000120-75-2	11
			Tricyclo[5.4.3.0(1,8)]tetradeca...	67121	1000197-61-7	10
42	36.36	2.54	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	30
			4H-1-Benzopyran-4-one, 3,5,7-tr...	101040	000480-19-3	12
			Propanamide, 2,2-dimethyl-N-(4-...	17554	021354-40-5	11
43	37.06	0.79	C:\Database\NIST98.L			
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	38
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	38
			Acetic acid, [4-(1,1-dimethylet...	84742	088530-52-3	18
44	37.73	6.55	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	56
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	46
			Mercaptoacetic acid, bis(trimet...	26922	006398-62-5	32
45	38.30	0.73	C:\Database\NIST98.L			
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	53
			2-Ethylacridine	84846	1000147-64-9	35
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	27
46	38.79	0.56	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	58
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	47
			Pentasiloxane, dodecamethyl-	97318	000141-63-9	27
47	38.92	0.42	C:\Database\NIST98.L			
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	64
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	27
			1,1,1,3,5,5,7,7,7-Nonamethyl-3-...	27713	038146-99-5	27
48	39.04	0.74	C:\Database\NIST98.L			
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	50
			Hexahydropyridine, 1-methyl-4-[...	84723	094427-47-1	41

			Heptasiloxane, 1,1,3,3,5,5,7,7,...	27374	019095-23-9	38
49	40.92	1.33	C:\Database\NIST98.L			
			3-Pentanol, 2-methyl-	113304	000565-67-3	35
			2-Pentanol, 3-chloro-2-methyl-	19396	074685-49-7	27
			1-Trimethylsily-2-(dimethyl-n-p...	19894	1000214-91-7	27
50	43.73	3.95	C:\Database\NIST98.L			
			Cyclononasiloxane, octadecamethyl-	115158	000556-71-8	50
			Trisiloxane, 1,1,1,5,5,5-hexame...	26961	003555-47-3	25
			3,6-Dioxa-2,4,5,7-tetrasilaocta...	87890	004342-25-0	22
51	44.04	0.57	C:\Database\NIST98.L			
			Octasiloxane, 1,1,3,3,5,5,7,7,9...	27373	019095-24-0	49
			Indole-2-one, 2,3-dihydro-N-hyd...	84802	1000129-52-1	22
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	22

Tue Jan 15 17:47:37 2008

Chloramine
Day 9
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\021.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 10:23 am
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 23

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	15.71	0.60	C:\Database\NIST98.L			
			Nonanoic acid	113428	000112-05-0	96
			Nonanoic acid	113427	000112-05-0	95
			Nonanoic acid	113398	000112-05-0	94
2	18.88	0.55	C:\Database\NIST98.L			
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	72
			2-Propanol, 1-[1-methyl-2-(2-pr...	19368	055956-25-7	59
			2-Propanol, 1-methoxy-2-methyl-	19309	003587-64-2	50
3	20.10	1.20	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	97
			Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4	96
			Phenol, 2,4-bis(1,1-dimethyleth...	125782	000096-76-4	96
4	21.47	0.58	C:\Database\OWML.L			
			Diethyl Phthalate	14	000084-66-2	95
			Di-n-butyl Phthalate	28	000084-74-2	9
5	22.51	2.18	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	96
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	10
			Ketone, 11-bromotricyclo[8.2.2....	102067	018931-44-7	10
6	22.81	1.98	C:\Database\NIST98.L			
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	95
			Boron, diethyl(5-ethyl-4,6-nona...	87941	136705-03-8	60
			1,4-Naphthoquinone, 6-acetyl-2,...	127595	013379-24-3	59
7	23.37	0.55	C:\Database\NIST98.L			
			Ethane, 1,2-diethoxy-	19316	000629-14-1	38
			3,5-Dioxahexaldoxin-2,6-dione-,...	5834	081539-54-0	38
			Ethane, 1,2-diethoxy-	108349	000629-14-1	38
8	23.49	1.14	C:\Database\NIST98.L			
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	53
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	42
			Hexaethylene glycol dimethyl ether	19827	001072-40-8	40
9	23.57	1.22	C:\Database\NIST98.L			
			Hexanamide	113230	000628-02-4	50
			2-Butanol, 3-methoxy-	19505	053778-72-6	49
			Ethane, 1,2-diethoxy-	19316	000629-14-1	40
10	24.45	0.61	C:\Database\NIST98.L			

				Indolizine, 2-(4-methylphenyl)-	84864	1000138-63-1 38
				1,4-Benzenediol, 2,5-bis(1,1-di...	84896	000088-58-4 38
				5-Methyl-2-phenylindolizine	84865	036944-99-7 35
11	24.61	0.52	C:\Database\NIST98.L			
				Phenol, 2-(1,1-dimethylethyl)-4...	80516	005806-73-5 87
				Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4 56
				Phenol, 2,4-bis(1,1-dimethyleth...	125781	000096-76-4 56
12	24.90	0.56	C:\Database\NIST98.L			
				Octadecane	112330	000593-45-3 98
				Octadecane	16439	000593-45-3 98
				Octadecane	112333	000593-45-3 94
13	24.99	0.56	C:\Database\NIST98.L			
				Hexatriacontane	16446	000630-06-8 72
				Tetratetracontane	16486	007098-22-8 68
				Hentriacontane	112561	000630-04-6 64
14	25.17	1.13	C:\Database\NIST98.L			
				Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3 72
				Phenol, 2,4,6-tris(1,1-dimethyl...	127577	000732-26-3 64
				1,3,5,2-Oxaazoniaazaboratin, 2,...	92662	1000160-64-7 50
15	25.76	1.73	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 64
				Diethyl Phthalate	14	000084-66-2 39
				Benzyl butyl Phthalate	36	000085-68-7 1
16	25.92	0.61	C:\Database\NIST98.L			
				Octanal, 7-hydroxy-3,7-dimethyl-	19446	000107-75-5 47
				3-Tetradecanol	113172	001653-32-3 38
				Octanal, 7-hydroxy-3,7-dimethyl-	113297	000107-75-5 35
17	26.05	1.33	C:\Database\NIST98.L			
				3-Heptadecanol	19340	084534-30-5 58
				3-Hexadecanol	113255	000593-03-3 38
				Trifluoroacetic acid, n-octadec...	5521	1000216-79-4 38
18	26.26	0.61	C:\Database\NIST98.L			
				Nonadecane	112382	000629-92-5 96
				Nonadecane	112380	000629-92-5 96
				Nonadecane	16515	000629-92-5 96
19	26.39	1.27	C:\Database\NIST98.L			
				7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4 93
				Ethanone, 1-(5,6,7,8-tetrahydro...	84211	071596-88-8 70
				1,3-Pentadiene, 1,1-diphenyl-, ...	84396	015295-31-5 60
20	27.01	7.53	C:\Database\OWML.L			
				Di-n-butyl Phthalate	28	000084-74-2 35
				Diethyl Phthalate	14	000084-66-2 9
21	27.30	0.55	C:\Database\NIST98.L			
				3-Hexanol, 1,5-dimethoxy-2,4-di...	19515	013897-22-8 59
				Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0 59
				Dimethylallyl(n-octyl)silane	19967	081272-81-3 59
22	27.51	0.82	C:\Database\NIST98.L			
				Eicosane	112565	000112-95-8 95
				Dotriacontane	112351	000544-85-4 90
				Heptadecane	16420	000629-78-7 87

23	27.94	0.51	C:\Database\NIST98.L			
			1,3-Diphenyl-2-azafluorene	101235	1000216-51-5	55
			1,3-Diphenyl-4-azafluorene	101229	1000216-52-1	37
			1H,6H-5,11b-Ethano[1,3]dioxolo[...	128634	003660-65-9	9
24	28.16	0.95	C:\Database\NIST98.L			
			4-Amino-2,6-diphenylpyrimidine	92663	041270-99-9	45
			Phenol, 2,4,6-tris(1,1-dimethyl...	127577	000732-26-3	45
			4-O-Nitrophenylhydrazono-3-meth...	92623	1000148-19-3	45
25	28.29	2.51	C:\Database\NIST98.L			
			Azadibenzopyrene	99857	104219-69-4	9
			5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4	9
			2-Deoxyribofuranose, 1(O)-(t-bu...	99860	1000193-96-2	9
26	28.52	0.65	C:\Database\NIST98.L			
			Cyclohexadecane	14275	000295-65-8	98
			1-Octadecene	112297	000112-88-9	96
			1-Octadecene	112298	000112-88-9	95
27	29.06	0.78	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	47
			Silacycloundec-6-yne, 1,1-dimet...	19470	017973-78-3	18
			1-Nonadecene	109267	018435-45-5	11
28	29.19	0.83	C:\Database\NIST98.L			
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	43
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	43
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	38
29	29.31	6.73	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	87
			Tetradecanoic acid	25385	000544-63-8	86
			Octadecanoic acid	6590	000057-11-4	83
30	29.51	1.31	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	72
			9-Octadecenamide, (Z)-	19657	000301-02-0	72
			Tetradecanamide	19652	000638-58-4	68
31	29.79	3.92	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
32	30.23	1.04	C:\Database\NIST98.L			
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	59
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	50
			1,3-Bis(dimethyl-n-pentylsilyl)...	19895	1000214-94-5	50
33	31.03	0.54	C:\Database\NIST98.L			
			Isopropyl-[2-(4-methoxy-2,6-dim...	103705	1000189-65-2	72
			Morphine, 7-hydroxy-6,6-dimetho...	103696	1000124-39-9	45
			Androst-4-ene-3,17-dione, 2-[(t...	103708	069688-13-7	39
34	31.23	0.73	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	99
			Diethyl Phthalate	14	000084-66-2	37
			Di-n-butyl Phthalate	28	000084-74-2	2
35	31.32	5.09	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	99
			9-Octadecenamide, (Z)-	113301	000301-02-0	91
			7-Nonenamide	19655	090949-53-4	64

36	31.53	0.83	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	70
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	70
			Hexanedioic acid, dioctyl ester	58241	000123-79-5	60
37	31.61	1.45	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	47
			2-Propanone, ethylhydrazone	15402	007422-99-3	22
			3-Pentanol, 3-ethyl-2-methyl-	110754	000597-05-7	22
38	31.80	0.80	C:\Database\NIST98.L			
			Pentane, 1-ethoxy-	19288	017952-11-3	53
			Octanal, 7-hydroxy-3,7-dimethyl-	113222	000107-75-5	50
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	47
39	31.85	0.93	C:\Database\NIST98.L			
			Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	47
			Butanamide, 3,3-dimethyl-	113267	000926-04-5	46
			2-Propanol, 1-[1-methyl-2-(2-pr...	113164	055956-25-7	43
40	32.50	3.30	C:\Database\NIST98.L			
			1-Heptadecene	118308	006765-39-5	99
			Cyclohexadecane	14275	000295-65-8	98
			5-Eicosene, (E)-	13710	074685-30-6	97
41	32.82	2.23	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	50
			Di-n-butyl Phthalate	28	000084-74-2	43
42	33.90	0.53	C:\Database\NIST98.L			
			2-Hexanol, 2,3-dimethyl-	19357	019550-03-9	35
			2-Pentanone, 5-methoxy-	5841	017429-04-8	30
			Cyclooctanemethanol, .alpha.,.a...	19347	016624-06-9	27
43	34.00	0.74	C:\Database\NIST98.L			
			2,5,8,11,14,17-Hexaoxaoctadecane	19609	001191-87-3	38
			1,4-Di-O-acetyl-2,5-di-O-methyl...	19333	1000101-82-1	38
			1,1,2-Trimethyldisilane	19435	1000216-84-5	38
44	34.09	1.01	C:\Database\NIST98.L			
			3-Pentanol, 2-methyl-	113304	000565-67-3	38
			Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3	38
			Dimethylallyl(n-octyl)silane	19967	081272-81-3	38
45	34.25	0.67	C:\Database\NIST98.L			
			1-Propanol, 2-(2-methoxypropoxy)-	19674	013588-28-8	38
			1,3-Dioxolane, 4-hexyl-2,2-dime...	20022	054934-58-6	35
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	35
46	35.05	23.46	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	90
			9-Octadecenamide, (Z)-	19657	000301-02-0	64
			Hexadecanamide	113298	000629-54-9	50
47	36.12	0.65	C:\Database\NIST98.L			
			Ethyl 2-acetamido-3,3,3-trifluo...	9561	1000224-78-8	9
			Ethyl 2-butyramido-3,3,3-triflu...	9558	1000224-16-1	9
			1-(4-Acetamidoanilino)-3,7-dime...	4048	1000226-07-9	8
48	36.35	2.30	C:\Database\NIST98.L			
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	14
			Imidazole, 2-bromo-4-methyl-5-n...	3826	105983-46-8	10

			3,6-Bis(2-methylphenyl)-2,5-dih...	101023	107680-83-1	9
49	36.65	3.68	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	38
			3-Pentanol, 2-methyl-	113304	000565-67-3	38
			2-Heptanol, 2-methyl-	113196	000625-25-2	35
50	38.15	0.49	C:\Database\NIST98.L			
			2-Ethylacridine	84846	1000147-64-9	35
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	18
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	14
51	39.06	0.79	C:\Database\NIST98.L			
			Cyclohexane, 1,1'-(2-methyl-1,3...	32855	002883-08-1	38
			2-Cyclohexen-1-ol, 1-methyl-	118347	023758-27-2	25
			1-Octadecanol	111484	000112-92-5	25
52	39.66	0.59	C:\Database\NIST98.L			
			Cholesterol	5250	000057-88-5	90
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	43
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	43
53	40.55	2.14	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	38
			Propanoic acid, 2-hydroxy-2-met...	19383	002110-78-3	38
			Oxirane, tetramethyl-	19436	005076-20-0	35

Tue Jan 15 18:25:16 2008

Chloramine
Day 14
Control

```
Information from Data File:
     File:          C:\MSDCHEM\1\DATA\020.D
     Operator:      Heather Johnson
     Date Acquired:  8 Jan 2008   9:26 am
     Method File:   OWML
     Sample Name:
     Misc Info:
     Vial Number:   22

Search Libraries:   C:\Database\NIST98.L              Minimum Quality:  35

Unknown Spectrum:   Apex
Integration Events: RTE Integrator - RTEINT.P
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Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	5.26	0.30	C:\Database\NIST98.L			
			Diethylacetamide	25025	1000127-23-4	38
			Methylene Chloride	12327	000075-09-2	27
			Ethanamine, N-ethyl-N-methyl-	24874	000616-39-7	25
2	5.93	0.34	C:\Database\NIST98.L			
			Butane, 1-methoxy-	11673	000628-28-4	50
			2,3-Butanediol, 1,4-dimethoxy-	11837	119613-19-3	45
			Lacthydrazide	11878	002651-42-5	40
3	6.55	0.13	C:\Database\NIST98.L			
			2-Propanol, 1,3-bis(dimethylami...	822	005966-51-8	9
			Permethylspermine	18762	057905-96-1	9
			N-(2-Cyanoethyl)-N-(3-dimethyla...	18767	1000223-07-4	9
4	8.33	0.13	C:\Database\NIST98.L			
			Furan, 2,3-dihydro-4-methyl-	33672	034314-83-5	32
			2-Butenal, 3-methyl-	116598	000107-86-8	32
			3,6,6-Trimethyl-cyclohex-2-enol	33801	1000193-83-0	30
5	9.03	0.14	C:\Database\NIST98.L			
			1-But-1-enylaziridine	2771	1000195-06-7	47
			2H-Pyrrol-2-one, 1,5-dihydro-1-...	3622	013950-21-5	40
			2,5-Dimethylpyrroline	42027	000822-64-0	38
6	13.84	0.17	C:\Database\NIST98.L			
			Butanoic acid, 3-oxo-, propyl e...	7127	001779-60-8	9
			Cyclobut-1-enylmethanol	14175	1000195-03-0	7
			.alpha.-D-Galactopyranoside, me...	17188	005540-31-8	7
7	15.71	0.37	C:\Database\NIST98.L			
			Nonanoic acid	113428	000112-05-0	72
			Octanoic Acid	113421	000124-07-2	42
			Hexanoic acid	113409	000142-62-1	38
8	17.52	0.28	C:\Database\NIST98.L			
			.alpha.-D-Glucose	25791	000492-62-6	12
			N-(3-Methylbutyl)acetamide	108191	013434-12-3	9
			Trisilane	20134	007783-26-8	9

9	17.85	0.14	C:\Database\NIST98.L			
			Propanoic acid, 2-methyl-, 3-hy...	24534	074367-34-3	40
			1,3-Pentanediol, 2,2,4-trimethyl-	111888	000144-19-4	32
			2,5-Dimethyl-5-hexen-3-ol	15181	067760-91-2	12
10	18.38	0.14	C:\Database\NIST98.L			
			Pyrrolidine, 1-(1,6-dioxooctade...	5465	056630-89-8	10
			3-Hydroxy-4-isopropyl-5,10-dime...	49133	093487-17-3	10
			Cyclohexanol, 3,3,5-trimethyl-	119891	000116-02-9	9
11	19.60	0.30	C:\Database\NIST98.L			
			1-Decene	111296	000872-05-9	95
			1-Dodecanol	111442	000112-53-8	91
			1-Undecanol	13829	000112-42-5	86
12	20.09	0.24	C:\Database\NIST98.L			
			2,4(3H,5H)-Furandione, 5-hexyl-...	5800	054852-79-8	23
			Benzeneacetic acid, 4-(1,1-dime...	80591	003549-23-3	22
			Phenol, 2,6-bis(1,1-dimethyleth...	125780	000128-39-2	22
13	20.89	0.26	C:\Database\NIST98.L			
			Dodecanoic acid	25776	000143-07-7	70
			Lauric anhydride	114892	000645-66-9	52
			n-Decanoic acid	113414	000334-48-5	35
14	21.33	0.20	C:\Database\NIST98.L			
			1,14-Tetradecanediol	14140	019812-64-7	25
			2-Propenoic acid, ethyl ester	111193	000140-88-5	25
			Cyclopropane, [(2-propenyloxy)m...	14659	018022-46-3	22
15	21.47	0.62	C:\Database\NIST98.L			
			Diethyl Phthalate	67077	000084-66-2	38
			Pentanoic acid, 2,2,4-trimethyl...	24310	1000140-77-5	37
			Methylamine, N-(1-methylhexylid...	24533	022058-71-5	35
16	22.52	1.67	C:\Database\NIST98.L			
			Phenol, 2,4,6-tribromo-	102083	000118-79-6	62
			4-[p-Chlorophenoxy]-6-methoxy-8...	102050	1000214-52-4	12
			Iron, (.eta.5-2,4-cyclopentadie...	102184	012149-23-4	12
17	22.81	0.31	C:\Database\NIST98.L			
			1,4-Benzenediol, 2,5-bis(1,1-di...	87823	000079-74-3	38
			Chromone, 6-hydroxy-2-methyl-5-...	87870	030095-72-8	38
			2,5-Cyclohexadiene-1,4-dione, 2...	1509	004584-63-8	25
18	23.06	0.29	C:\Database\NIST98.L			
			Trifluoroacetic acid, n-tetrade...	4218	1000216-79-0	68
			Hexadecanol	5280	029354-98-1	64
			Trifluoroacetic acid, n-heptade...	4324	1000216-79-2	62
19	23.37	0.90	C:\Database\NIST98.L			
			Heptadecane	112320	000629-78-7	90
			Hexatriacontane	112335	000630-06-8	53
			Tricosane	109661	000638-67-5	52
20	23.58	0.14	C:\Database\NIST98.L			
			3-Octene, (Z)-	108606	014850-22-7	38
			Benzene, 1-nitro-2-(octyloxy)-	109576	037682-29-4	32
			2-Undecenal	23718	002463-77-6	27

21	24.04	0.21	C:\Database\NIST98.L			
			Tetratetracontane	112573	007098-22-8	64
			Pentacosane	17109	000629-99-2	59
			Octacosane	16409	000630-02-4	59
22	24.24	0.33	C:\Database\NIST98.L			
			1-Octanol, 2-butyl-	112349	003913-02-8	46
			Nonahexacontanoic acid	17028	040710-32-5	46
			Octadecane, 1-bromo-	17754	000112-89-0	38
23	24.35	0.17	C:\Database\NIST98.L			
			Nonahexacontanoic acid	17028	040710-32-5	46
			1-Decanol, 2-hexyl-	16763	002425-77-6	38
			Octadecane, 1-chloro-	112584	003386-33-2	38
24	24.90	0.90	C:\Database\NIST98.L			
			Octadecane	16439	000593-45-3	98
			Heneicosane	17094	000629-94-7	91
			Pentacosane	109667	000629-99-2	91
25	25.21	0.36	C:\Database\NIST98.L			
			2,6-Bis[thiocarbamyl]-3-methylp...	20259	1000227-19-5	18
			1-Decanol, 2-hexyl-	112269	002425-77-6	15
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	15
26	25.48	0.56	C:\Database\NIST98.L			
			7-Oxabicyclo[4.1.0]heptane, 1,5...	6342	162239-52-3	46
			Tetradecane	112358	000629-59-4	38
			1-Bromodocosane	112328	006938-66-5	35
27	25.75	1.64	C:\Database\NIST98.L			
			1,2-Benzenedicarboxylic acid, b...	123451	000084-69-5	86
			1,2-Benzenedicarboxylic acid, b...	66726	000084-78-6	78
			Dibutyl phthalate	123493	000084-74-2	72
28	25.92	0.32	C:\Database\NIST98.L			
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	58
			1-Decanol, 2-hexyl-	112269	002425-77-6	43
			Ethanol, 2-(dodecyloxy)-	16546	004536-30-5	35
29	26.07	0.56	C:\Database\NIST98.L			
			Ethanone, 2,2-dimethoxy-1,2-dip...	123614	024650-42-8	47
			1-Octadecanol	5273	000112-92-5	20
			1-Nonadecene	108523	018435-45-5	20
30	26.38	1.84	C:\Database\NIST98.L			
			7,9-Di-tert-butyl-1-oxaspiro(4,...	17969	1000143-92-4	90
			3,5-Cyclohexadiene-1,2-dione, 3...	84221	003383-21-9	35
			Ethanone, 1-(5,6,7,8-tetrahydro...	84211	071596-88-8	30
31	26.59	0.20	C:\Database\NIST98.L			
			1-Heptadecene	118308	006765-39-5	41
			3-Methyl-2-(2-oxopropyl)furan	16777	087773-62-4	30
			Tetrapentacontane, 1,54-dibromo-	17122	1000156-09-4	30
32	26.77	0.18	C:\Database\NIST98.L			
			Heptadecane	112320	000629-78-7	59
			Nonahexacontanoic acid	17028	040710-32-5	38
			Benzoic acid, 2-benzoyl-, methy...	124371	000606-28-0	38

33	27.00	9.77	C:\Database\NIST98.L			
			n-Hexadecanoic acid	109985	000057-10-3	95
			Tetradecanoic acid	114897	000544-63-8	94
			Tridecanoic acid	114895	000638-53-9	89
34	27.51	1.38	C:\Database\NIST98.L			
			Eicosane	16454	000112-95-8	94
			Tricosane	109661	000638-67-5	91
			Pentacosane	109667	000629-99-2	91
35	28.22	0.43	C:\Database\NIST98.L			
			Methyl (1s*,2s*,5R*)-1,5-dimeth...	16983	1000143-89-6	46
			Bicyclo[3.1.1]heptan-2-one, 6,6...	32975	038651-65-9	25
			Cyclohexanone, 2,2-dimethyl-5-(...	2097	141033-65-0	18
36	28.54	0.95	C:\Database\NIST98.L			
			1-Heptadecene	118308	006765-39-5	99
			Cyclohexadecane	14275	000295-65-8	98
			1-Octadecene	112298	000112-88-9	98
37	29.07	0.32	C:\Database\NIST98.L			
			Cyclooctane, methyl-	111531	001502-38-1	46
			Heptafluorobutyric acid, n-octa...	5522	1000216-79-5	46
			5-Octadecene, (E)-	13707	007206-21-5	45
38	29.30	5.86	C:\Database\NIST98.L			
			Octadecanoic acid	114902	000057-11-4	91
			Pentadecanoic acid	114896	001002-84-2	76
			Tridecanoic acid	114895	000638-53-9	64
39	29.50	2.03	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	91
			Dodecanamide	19649	001120-16-7	72
			Tetradecanamide	113299	000638-58-4	64
40	29.78	9.15	C:\Database\NIST98.L			
			p-Terphenyl-d14	92199	001718-51-0	99
			1-(4-Hydroxyphenyl)-3,6-diazaho...	92099	1000216-01-8	72
			Triphenylmethane	127486	000519-73-3	64
41	30.26	0.53	C:\Database\NIST98.L			
			Cyclohexane, 1,4-dimethoxy-2-me...	35351	030363-88-3	45
			1-Propene, 3-[(4-nitrobutyl)thio]-	35582	1000115-55-4	43
			Thiocyanic acid, ethyl ester	35221	000542-90-5	43
42	30.70	0.39	C:\Database\NIST98.L			
			Ethanol, 2-(octadecyloxy)-	16507	002136-72-3	38
			Octadecane, 1-chloro-	112584	003386-33-2	38
			Tricosane	112394	000638-67-5	38
43	31.01	0.25	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	109752	000301-02-0	30
			3-Tetradecanol	19356	001653-32-3	25
			3-Hexadecanol	113255	000593-03-3	22
44	31.30	2.42	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	96
			Benzeneethanamine, 2-fluoro-.be...	19658	061338-98-5	59
			Dodecanamide	19649	001120-16-7	53

45	31.52	2.45	C:\Database\NIST98.L				
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93	
			Diisooctyl adipate	58242	001330-86-5	76	
			Hexanedioic acid, mono(2-ethylh...	58234	004337-65-9	68	
46	32.18	0.15	C:\Database\NIST98.L				
			2-Octen-1-ol, 7-ethoxy-3,7-dime...	35432	1000132-19-5	38	
			Ethane, isothiocyanato-	35424	000542-85-8	38	
			Butane, 2-ethoxy-2-methyl-	19732	000919-94-8	35	
47	32.51	2.60	C:\Database\NIST98.L				
			5-Eicosene, (E)-	13710	074685-30-6	99	
			1-Eicosanol	112640	000629-96-9	95	
			1-Heneicosyl formate	16592	077899-03-7	95	
48	32.82	9.97	C:\Database\NIST98.L				
			Bis(2-ethylhexyl) phthalate	66784	000117-81-7	91	
			1,2-Benzenedicarboxylic acid, d...	123512	027554-26-3	91	
			Phthalic acid, diisooctyl ester	66787	001330-91-2	78	
49	33.01	0.32	C:\Database\NIST98.L				
			Cyclopropanedecanoic acid, 2-oc...	13509	010152-64-4	47	
			Z-7-Hexadecen-1-ol acetate	6910	1000130-88-7	46	
			Cyclopropaneoctanoic acid, 2-he...	111346	010152-61-1	25	
50	33.38	0.51	C:\Database\NIST98.L				
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	25	
			1,3-Dioxolane, 4-hexyl-2,2-dime...	20022	054934-58-6	22	
			3-Tetradecanol	19356	001653-32-3	22	
51	33.64	0.13	C:\Database\NIST98.L				
			1H-Indole, 2-methyl-3-phenyl-	126477	004757-69-1	30	
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	27	
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	27	
52	34.09	0.46	C:\Database\NIST98.L				
			Octaverine	105278	000549-68-8	38	
			Iodoquinol	129014	000083-73-8	10	
			17.alpha.-Ethynyl-17.beta.-hydr...	105265	1000069-43-1	9	
53	34.27	0.39	C:\Database\NIST98.L				
			1,3-Dioxolane, 4-ethyl-5-octyl-...	23228	038274-73-6	30	
			Hexahydropyridine, 1-methyl-4-[...	84723	094427-47-1	30	
			1-Hentetracontanol	16591	040710-42-7	25	
54	34.58	0.24	C:\Database\NIST98.L				
			2,3,4-Trimethoxyphenylacetonitrile	84840	068913-85-9	38	
			1H-Indole, 2-methyl-3-phenyl-	126477	004757-69-1	35	
			Cyclotrisiloxane, hexamethyl-	126481	000541-05-9	35	
55	35.04	12.77	C:\Database\NIST98.L				
			Erucylamide	19656	000112-84-5	91	
			9-Octadecenamide, (Z)-	113301	000301-02-0	89	
			Heptanamide, 4-ethyl-5-methyl-	19661	054789-40-1	59	
56	36.13	3.43	C:\Database\NIST98.L				
			Propanamide, N-(3-methoxyphenyl...	17665	056619-93-3	10	
			Ethyl 2-acetamido-3,3,3-trifluo...	9561	1000224-78-8	9	
			Ethyl 2-acetamido-3,3,3-trifluo...	9560	1000224-78-7	9	

57	36.35	7.06	C:\Database\NIST98.L			
			Xanthine, 8-[2-cyclohexenyl]-1,...	101036	1000117-02-2	38
			Phenanthro[3,2-b]furan-4-carbox...	100976	019941-61-8	38
			Bicyclo[5.3.0]decan-2-one, 9-(d...	100989	1000151-00-6	9
58	39.09	0.95	C:\Database\NIST98.L			
			1-Dotriacontanol	16786	006624-79-9	35
			1-Hentetracontanol	16591	040710-42-7	30
			1-Octadecanol	5273	000112-92-5	25
59	39.68	0.31	C:\Database\NIST98.L			
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	47
			Cyclotrisiloxane, hexamethyl-	126480	000541-05-9	43
			2-Ethylacridine	84846	1000147-64-9	40
60	40.91	10.17	C:\Database\NIST98.L			
			Hexadecanamide	113298	000629-54-9	80
			Undecanamide, 11-bromo-	19650	1000163-84-6	64
			Pentadecanamide, 15-bromo-	19651	1000163-86-1	56
61	42.69	0.27	C:\Database\NIST98.L			
			1H-Indole, 5-methyl-2-phenyl-	84867	013228-36-9	38
			Ethane, 1-[4,4,4-trifluoro-1,3-...	84757	1000226-87-3	37
			1,3-Bis(trimethylsilyl)benzene	84730	002060-89-1	27

Mon Dec 08 11:00:14 2008

Chloramine
Day 14
Sample

tmplibrp.txt

Information from Data File:
File: C:\MSDCHEM\1\DATA\HEATHER\010708\024.D
Operator: Heather Johnson
Date Acquired: 8 Jan 2008 1:14 pm
Method File: OWML
Sample Name:
Misc Info:
Vial Number: 26

Search Libraries: C:\Database\OWML.L Minimum Quality: 35
C:\Database\NIST98.L Minimum Quality: 0

Unknown Spectrum: Apex
Integration Events: RTE Integrator - events.e

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	20.10	2.27	C:\Database\NIST98.L			
			Phenol, 2,4-bis(1,1-dimethyleth...	125782	000096-76-4	95
			Phenol, 2,4-bis(1,1-dimethyleth...	80518	000096-76-4	95
			Phenol, 2,4-bis(1,1-dimethyleth...	125776	000096-76-4	91
2	25.17	0.97	C:\Database\NIST98.L			
			8-Methoxy-11H-benzo[a]carbazole	92655	1000212-76-8	64
			Phenol, 2,4,6-tris(1,1-dimethyl...	127581	000732-26-3	56
			2-t-Butyl-3-methyl-4-oxo-5-phen...	92596	1000195-28-6	50
3	25.76	2.24	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	78
			Benzyl butyl Phthalate	36	000085-68-7	9
			Diethyl Phthalate	14	000084-66-2	9
4	26.07	1.62	C:\Database\NIST98.L			
			Ethanone, 2,2-dimethoxy-1,2-dip...	67798	024650-42-8	43
			Silane, trimethylphenoxy-	123651	001529-17-5	35
			3-Hexadecanol	113255	000593-03-3	30
5	26.27	1.22	C:\Database\NIST98.L			
			Nonadecane	112381	000629-92-5	98
			Nonadecane	112576	000629-92-5	97
			Nonadecane	112382	000629-92-5	96
6	27.00	2.60	C:\Database\OWML.L			
			Di-n-butyl Phthalate	28	000084-74-2	97
			Di-n-octyl phthalate	40	000117-81-0	38
			Diethyl Phthalate	14	000084-66-2	9
7	27.51	1.41	C:\Database\NIST98.L			
			Hexadecane	112410	000544-76-3	95
			Eicosane	112565	000112-95-8	93
			Eicosane	112345	000112-95-8	93
8	28.30	2.53	C:\Database\NIST98.L			
			Azadibenzopyrene	99857	104219-69-4	9
			5-[[[3,4,5-Trimethoxyphenyl]imi...	99851	1000212-37-4	9
			Hydromorphinol	99808	002183-56-4	9
9	29.19	0.91	C:\Database\NIST98.L			
			2-Methyl-tridecane-2,12-diol	19413	1000187-03-5	43
			3-Hexadecanol	19584	000593-03-3	38
			2,2-Dimethyl-hexahydro-benzo[1,...	19439	1000187-24-1	38

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10	29.50	1.20	C:\Database\NIST98.L			
			Hexadecanamide	19647	000629-54-9	95
			Hexadecanamide	113298	000629-54-9	90
			Tetradecanamide	113299	000638-58-4	72
11	29.79	8.16	C:\Database\OWML.L			
			Terphenyl-d14	34	001718-51-0	99
12	31.23	1.47	C:\Database\OWML.L			
			Benzyl butyl Phthalate	36	000085-68-7	91
			Diethyl Phthalate	14	000084-66-2	47
			Di-n-butyl Phthalate	28	000084-74-2	28
13	31.31	7.80	C:\Database\NIST98.L			
			9-Octadecenamide, (Z)-	113302	000301-02-0	98
			9-Octadecenamide, (Z)-	113301	000301-02-0	93
			Tetradecanamide	113299	000638-58-4	64
14	31.53	1.05	C:\Database\NIST98.L			
			Hexanedioic acid, bis(2-ethylhe...	121807	000103-23-1	93
			Diisooctyl adipate	58242	001330-86-5	62
			Hexanedioic acid, bis(2-ethylhe...	58246	000103-23-1	62
15	31.61	1.99	C:\Database\NIST98.L			
			Ethanol, 2-butoxy-, phosphate (...	112451	000078-51-3	90
			Ethanol, 2-butoxy-, phosphate (...	16713	000078-51-3	43
			1-Iodoundecane	16278	004282-44-4	25
16	31.85	0.96	C:\Database\NIST98.L			
			Butane, 2-methoxy-	19272	006795-87-5	46
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	43
			3-Tetradecanol	113172	001653-32-3	43
17	32.50	5.19	C:\Database\NIST98.L			
			5-Eicosene, (E)-	13710	074685-30-6	99
			1-Octadecene	112297	000112-88-9	98
			Cyclohexadecane	14275	000295-65-8	95
18	32.82	4.24	C:\Database\OWML.L			
			Bis(2-ethylhexyl) phthalate	39	000117-81-7	91
			Di-n-octyl phthalate	40	000117-81-0	50
			Di-n-butyl Phthalate	28	000084-74-2	43
19	34.11	1.03	C:\Database\NIST98.L			
			Methyl 17-methoxy-10-methoxycar...	19542	1000110-20-7	27
			2-Pentanone, 5-methoxy-	5841	017429-04-8	27
			.alpha.-D-Xylo-Hex-5-enofuranos...	19430	007284-07-3	27
20	34.24	1.06	C:\Database\NIST98.L			
			Heptacosane	109643	000593-49-7	66
			Heptacosane	16471	000593-49-7	64
			Tritetracontane	17076	007098-21-7	50
21	35.06	41.09	C:\Database\NIST98.L			
			Erucylamide	19656	000112-84-5	93
			Erucylamide	113300	000112-84-5	89
			9-Octadecenamide, (Z)-	19657	000301-02-0	72
22	35.37	2.85	C:\Database\NIST98.L			
			Geranyl vinyl ether	22320	1000132-11-4	43
			2,6,10,14-Hexadecatetraenoic ac...	23034	024035-35-6	38
			4,9,13,17-Tetramethyl-4,8,12,16...	23043	056882-09-8	38

23	36.37	1.35	C:\Database\NIST98.L			
			14-Oxabicyclo[10.3.0]pentadecan...	2747	1000163-86-0	15
			Hydrazinecarboxylic acid, 1,1-d...	15839	000870-46-2	9
			5.alpha.-androstan-3.Beta.,17.b...	10127	1000126-90-6	9
24	36.58	3.02	C:\Database\NIST98.L			
			Allyl(n-pentyl)dimethylsilane	19891	1000214-90-0	25
			1,1,2-Trimethyldisilane	19435	1000216-84-5	25
			2-Heptanol, 2-methyl-	19423	000625-25-2	22
25	39.06	1.80	C:\Database\NIST98.L			
			1-Eicosanol	112640	000629-96-9	91
			1-Dotriacontanol	16786	006624-79-9	70
			Cyclohexane, 1,1'-(2-methyl-1,3...	32855	002883-08-1	68

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