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Tank 241-BY-108 Vapor Sampling and Analysis Tank Characterization Report (WHC-SD-WM-ER-422)		ECN No. 623545

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7. Abstract Tank 241-BY-108 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in "Program Plan for the Resolution of Tank Vapor Issues" (Osborne and Huckaby 1994). Tank 241-BY-108 was vapor sampled in accordance with "Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution (Osborne et al., 1994).		

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## Tank 241-BY-108 Vapor Sampling and Analysis Tank Characterization Report

### X.0 INTRODUCTION

Tank BY-108 headspace gas and vapor samples were collected and analyzed to help determine the potential risks to tank farm workers due to fugitive emissions from the tank. The drivers and objectives of waste tank headspace sampling and analysis are discussed in *Program Plan for the Resolution of Tank Vapor Issues* (Osborne and Huckaby 1994). Tank BY-108 was vapor sampled in accordance with *Data Quality Objectives for Generic In-Tank Health and Safety Issue Resolution* (Osborne et al. 1994).

Tank BY-108 was vapor sampled in March 1994 using the *in situ* sampling (ISS) method, and again in October 1994 using the more robust vapor sampling system (VSS) method. There were problems with the March 1994 sampling event (i.e., some samples were radiolytically contaminated) and only the SUMMA™ canister samples were analyzed. Nearly all of results presented here are from the October 1994 sampling event.

### X.1 SAMPLING EVENT

Headspace gas and vapor samples were collected from tank BY-108 using the VSS on October 27, 1994 by WHC Sampling and Mobile Laboratories, (WHC 1995). Sample collection and analysis were performed as directed by *Tank 241-BY-108 Tank Characterization Plan* (Carpenter 1994). The tank headspace temperature was determined to be 25.7 °C. Air from the tank BY-108 headspace was withdrawn via a 7.9 m-long heated sampling probe mounted in riser 1, and transferred via heated tubing to the VSS sampling manifold. All heated zones of the VSS were maintained at approximately 50 °C.

Sampling media were prepared and analyzed by WHC, Oak Ridge National Laboratories (ORNL), and Pacific Northwest Laboratories (PNL). The 40 tank air samples and 2 ambient air control samples collected are listed in Table X-1 by analytical laboratory. Table X-1 also lists the 14 trip blanks and 2 field blanks that accompanied the samples.

A general description of vapor sampling and sample analysis methods is given by Huckaby (1995). The sampling equipment, sample collection sequence, sorbent trap sample air flow rates and flow times, chain of custody information, and a discussion of the sampling event itself are given in WHC 1995 and references therein.



## X.2 INORGANIC GASES AND VAPORS

Analytical results of sorbent trap and SUMMA<sup>TM,1</sup> canister tank air samples for selected inorganic gases and vapors are given in Table X-2 in parts per million by volume (ppmv). Inorganic analyte sorbent traps and SUMMA<sup>TM</sup> canisters were prepared and analyzed by PNL. Ligothke et al. (1995) describe sample preparation and analyses.

The relative standard deviations of the results, given in the last column in Table X-2, are typical for the analytical methods used. Relative standard deviations range from 8 % for ammonia, to 38 % for carbon dioxide results. The precision reported depends both on sampling parameters (e.g., sample flow rate and flow time for sorbent traps) and analytical parameters (e.g., sample preparation, dilutions, etc.), and the relative standard deviations suggest there were no significant problems in the field or in the laboratories.

### X.2.1 Ammonia, Hydrogen, and Nitrous Oxide

The reported ammonia concentration, 1040 ppmv, is the highest observed to date in the waste tanks, and is almost 42 times the National Institute of Occupational Safety and Health (NIOSH) 8-hr recommended exposure limit (REL) of 25 ppmv (NIOSH 1995).

Hydrogen and nitrous oxide are commonly detected gases in the waste tanks. Believed to be products of chemical reactions and radiolysis of the waste, they have been found above the 1 ppmv level in virtually all the tank headspaces sampled to date. In general, hydrogen is of concern as a fuel. The measured 399 ppmv of hydrogen in tank BY-108, however, represents only about 1 % of the lower flammability limit (LFL) for hydrogen in air, and is not a flammability concern at this level. The nitrous oxide concentration in tank BY-108, 641 ppmv, is about 25 times the NIOSH 8-hr REL of 25 ppmv (NIOSH 1995).

For comparison, the measured concentrations of ammonia, hydrogen, and nitrous oxide for tanks BY-104, BY-105, BY-106, BY-107, and BY-108 are given in Table X-3. There is a strong correlation between increased waste tank headspace organic vapor concentrations (the last column in Table X-3) and increased ammonia vapor concentrations, though this correlation is far from linear.

### X.2.2 Carbon Dioxide and Carbon Monoxide

The average measured headspace carbon dioxide concentration, 224 ppmv, is about one-half of the normal ambient air concentration of about 400 ppmv. Lower-than-ambient carbon dioxide concentrations are expected in the waste tank headspaces. Carbon dioxide introduced by air exchange with the atmosphere is readily absorbed by caustic supernatant and interstitial liquids of the waste tanks, and converted to carbonate in solution. It is reasonable

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<sup>1</sup> SUMMA is a trademark of Molectrics, Inc., Cleveland, Ohio.

to expect the level of carbon dioxide in a tank headspace will therefore depend on the tank's breathing rate, and the pH and surface area of aqueous waste (i.e., supernate, interstitial liquid, and condensate) in the tank. The 224 ppmv carbon dioxide concentration measured in tank BY-108 is typical of other tanks sampled to date.

Carbon monoxide in the tank BY-108 headspace, measured to be < 76 ppmv, is not well characterized. The method quantitation limit, 76 ppmv, is above the highest waste tank carbon monoxide concentration measured to date (26.7 ppmv in tank C-103, Huckaby and Story 1994). Elevated carbon monoxide concentrations are thought to be due to the decomposition of organic waste in the tanks.

### **X.2.3 Nitric Oxide, Nitrogen Dioxide, Water and Tritium**

Nitric oxide and nitrogen dioxide concentrations in the tank BY-108 headspace were determined to be  $\leq 0.03$  ppmv and  $\leq 0.02$  ppmv, respectively. These are both acid gases that would have very low equilibrium concentrations above the high pH waste in tank BY-108. Nitric oxide is commonly found at trace concentrations, presumably due to its formation from oxygen and nitrogen in the radiation field of the headspace. The NIOSH 8-hr REL is 25 ppmv for nitric oxide, and the 15-minute short term exposure limit (STEL) for nitrogen dioxide is 1 ppmv.

The water vapor concentration was measured by gravimetric analysis of 5 sorbent trap systems by PNL (McVeety et al. 1995). The water vapor concentration of tank BY-108 was determined to be about 13.4 mg/L, at the tank headspace temperature of 25.7 °C and pressure of 984 mbar (737.7 torr), (WHC 1995). This corresponds to a water vapor partial pressure of 18.5 mbar (13.9 torr), to a dew point of 16.3 °C, and to a relative humidity of 56 %. It was noted that less mass (water) had been trapped on each successive sample, yet no explanation has been offered for this observation. The relative standard deviation is also higher than typical for this measurement.

Tritium was tested for using silica gel sorbent traps. It is assumed that tritium ions produced by the waste combine with hydroxide ions to form tritium-substituted water. Evaporation of the tritium-substituted water would then result in airborne radioactive contamination. Silica gel sorbent traps adsorb virtually all (normal and tritium-substituted) water vapor from the sampled tank air, and are analyzed at the WHC 222-S laboratory. Analysis of the silica gel, which would have trapped approximately 15 mg of water vapor, indicated the total activity of the sample to be below the method detection limit of 50 pCi (WHC 1995).

### **X.3 ORGANIC VAPORS**

Organic vapors in the tank BY-108 headspace were sampled using SUMMA™ canisters, which were analyzed by PNL, and triple sorbent traps (TSTs), which were analyzed by ORNL. TST sample analyses indicated that benzene was above

accepted industrial hygiene limits for the workplace. Both laboratories used gas chromatography and mass spectrometry to separate, identify, and quantitate the analytes. Descriptions of sample device cleaning, sample preparations, and analyses are given by Jenkins et al. (1994) and McVeety et al. (1995). A quantitative measurement of the total organic vapor concentration by the U.S. Environmental Protection Agency (EPA) task order 12 (TO-12) method (EPA 1988) was also performed by Oregon Graduate Institute of Science and Technology (OGIST) on samples collected in March 1994 by the ISS method (Pingel 1994, Rasmussen 1994a). The total organic vapor concentration of the tank BY-108 headspace was determined to be very high, and may indicate the presence of an organic liquid phase in the tank.

SUMMA<sup>TM</sup> sample results should be considered to be the primary organic vapor data for tank BY-108. ORNL analyses of TST samples from this and other waste tanks generally agree with, support, and augment the SUMMA<sup>TM</sup> sample results. However, because certain WHC quality assurance requirements were not satisfied by ORNL, the quality assurance assessment of ORNL by Hendrickson (1995) should be reviewed before results unique to the TST samples are used for decision making.

### X.3.1 Positively Identified Organic Analytes

ORNL positively identified 23 of 27 target analytes selected by WHC. Four target analytes (vinylidene chloride, heptanenitrile, tributyl phosphate and dibutyl butylphosphonate) were below detection limits. The detected analytes, and their average concentrations from the analysis of 3 TSTs, are given in Table X-4. The 27 TST target analytes for tank BY-108 are an extended set of the tank C-103 target analytes, which were selected by a PNL panel of toxicology experts as being of potential toxicological concern (Mahlum et al. 1994). Three of the target analytes (acetone, dichloromethane and 1-butanol) were measured to be above the method's upper calibration limit. Also, 3 of the target analytes (propanenitrile, pentanenitrile and hexanenitrile) were positively identified by ORNL, but below the method quantitation limit.

Also given in Table X-4 are the organic compounds positively identified and quantitated in SUMMA<sup>TM</sup> canister samples by PNL. PNL performed analyses according to the EPA task order 14 (TO-14) methodology, but expanded the number of target analytes from 40 to 54 to include waste tank analytes of particular interest (EPA 1988, McVeety et al. 1995). Of the original 40 TO-14 analytes, 32 were determined to be below the 0.002 ppmv quantitation limit of the analyses (McVeety et al. 1995 provide the complete TO-14 analyte list), and 3 of the 15 additional target analytes (acetonitrile, propanenitrile and butanenitrile) were below the 0.005 ppmv method quantitation limit. Averages reported are from analyses of 3 SUMMA<sup>TM</sup> canister samples.

Eleven target analytes were common to both the ORNL and PNL analyses. Comparison of the results from the 2 laboratories indicates the following:

- 1) An acceptable agreement for acetone and certain nonpolar analytes (i.e., n-hexane, n-heptane, toluene, and n-decane);

- 2) TST analyses indicate dichloromethane to be present at an average concentration of 1.2 ppmv, while none was detected in SUMMA<sup>TM</sup> canister samples;
- 3) TST analyses indicate acetonitrile at 0.94 ppmv, and butanenitrile at 0.31 ppmv, while SUMMA<sup>TM</sup> analyses indicate each of these to be below their quantitation limit of 0.005 ppmv; and
- 4) the 2 methods disagree on the concentration of benzene by roughly a factor of 7.

The TST dichloromethane results are questionable. First, the individual TST sample results are relatively inconsistent; the individual results are 0.30, 2.3, and 1.0 ppmv, which average to 1.2 ppmv, have a standard deviation of 1.0 ppmv, and a relative standard deviation of 83 %. Second, if dichloromethane were present at the 1 ppmv level, it is very likely that SUMMA<sup>TM</sup> analyses would have detected it. Dichloromethane is an EPA T0-14 target analyte, and its recovery from SUMMA<sup>TM</sup> canisters has been well-studied (EPA 1988).

Though the discrepancy between the TST and SUMMA<sup>TM</sup> sample nitrile results is currently not understood, the reported concentrations are not above action limits. The 0.94 ppmv acetonitrile concentration measured in TST samples is well below its NIOSH 8-hr REL of 20 ppmv. Similarly, the 0.31 ppmv of butanenitrile measured in the TST samples is well below its NIOSH 8-hr REL of 8 ppmv (NIOSH 1995).

The benzene concentration in tank BY-108 was measured to be 0.18 ppmv in TST samples, and 0.025 ppmv in SUMMA<sup>TM</sup> canister samples. These conflicting values fall to either side of the NIOSH 8-hr REL for benzene of 0.1 ppmv (NIOSH 1995). Comparison of the pedigree of the TST and SUMMA<sup>TM</sup> methods would favor the SUMMA<sup>TM</sup> results; SUMMA<sup>TM</sup> canister sampling and analysis is performed according to the T0-14 method recommended by the EPA for benzene.

The most abundant analytes in Table X-4, neglecting the TST dichloromethane result, are 1-butanol, acetone, 1-propanol, n-hexane and tetrahydrofuran, each of which was measured to be above 1 ppmv. At the reported concentrations, the Table X-4 analytes do not individually or cumulatively represent a flammability hazard. None of the analytes in Table X-4, with the noted exception of benzene discussed above, is above NIOSH recommended workplace guidelines.

### **X.3.2 Tentatively Identified Organic Analytes**

In addition to targeted analytes, both ORNL and PNL analytical procedures allow the tentative identification of other organic vapors. By the nature of the samples and their analysis, virtually all 3 to 15 carbon organic compounds present in the tank headspace above analytical detection limits are observable. The PNL list of tentatively identified compounds, with estimated concentrations, is given in Table X-5, and the ORNL list of tentatively identified compounds, and their estimated concentrations, is given in Table X-

6. Estimated concentrations are in  $\text{mg}/\text{m}^3$ , based on dry air at 0 °C and 1.01 bar.

Both ORNL and PNL tentatively identify analytes by comparing the MS molecular fragmentation patterns with a library of known MS fragmentation patterns. This method allows an organic analyte to be identified (with reasonable certainty) as an alkane, a ketone, an aldehyde, etc., and also determines its molecular weight (which specifies the number of carbon atoms in the molecule). The method usually does not, however, allow the unambiguous identification of structural isomers, and this ambiguity increases with analyte molecular weight. Entries in Tables X-5 and X-6, particularly near the bottom of the tables where the analytes have higher molecular weights, illustrate this.

The ORNL and PNL methods used to tentatively identify and estimate concentrations are described by Jenkins et al. (1994) and McVeety et al. (1995), respectively, and should be reviewed before this data is used for decision making. Results in Tables X-5 and X-6 are presented in terms of observed peaks, and are not adjusted for the occurrence of split chromatographic peaks (e.g., Cmpd # 96 and 99 in Table X-6). In these instances, the estimated concentration of a compound appearing as a doublet or triplet is simply the sum of the individual peak estimates.

Concentrations given in Tables X-5 and X-6 should be considered rough estimates. The proper quantitation of all observed analytes is outside the scope and budget of these analyses, and the estimation of concentrations involves several important assumptions. The validity of each assumption depends on the analyte, and such factors as the specific configuration of the analytical instrumentation.

### X.3.3 Total Nonmethane Organic Compounds

OGIST measured the total nonmethane organic compound (TNMOC) concentration in 3 SUMMA™ canister samples collected on March 28, 1994 (Pingel 1994) using the EPA TO-12 method (Rasmussen 1994a). The sample mean was  $594 \text{ mg}/\text{m}^3$ , with a standard deviation of  $14 \text{ mg}/\text{m}^3$ . Though data on other tanks is very limited, this value is very high compared to other waste tanks sampled to date. Only tank C-103, estimated to have 3,000 to 5,000  $\text{mg}/\text{m}^3$  of TNMOC (Rasmussen and Einfeld 1994), is known to have a higher TNMOC concentration. For comparison, the TNMOC concentration in clean ambient air may range from 0.03 to 0.1  $\text{mg}/\text{m}^3$ , in polluted city air it may be 0.3 to 0.4  $\text{mg}/\text{m}^3$ . Table X-3 also gives the TNMOC concentrations of several other 241-BY farm tanks.

### X.3.4 Discussion of Organic Analytes

In general, the organic analytes observed in the waste tank headspaces are indicative of the types of volatile and semivolatile organic waste that reside in each tank. Examination of the data provides clues to both the current organic constituents and the chemical reactions that are taking place.

Some of the compounds listed in Tables X-4, X-5, and X-6 were introduced to the tank with process waste streams, and are detected in the headspace because the original inventory has not been completely evaporated or degraded. Examples of these are the semivolatile normal paraffinic hydrocarbons (NPHs), (i.e., n-dodecane, n-tridecane, n-tetradecane, n-pentadecane) and methyl-substituted decahydronaphthalenes that were used as diluents for tributyl phosphate.

Though there is no toxicological or flammability hazard associated with the 0.13 ppmv of trichlorofluoromethane measured in tank BY-108, its presence warrants an explanation. The origin of trichlorofluoromethane in the waste tanks has not been established, however, it has been used as a decontaminating (cleaning) solvent at the Hanford Site, and small amounts may have been placed in the waste tanks. Once there, its high density (1.47 g/mL) and low solubility in the aqueous liquid wastes would have caused it to pool at the bottom of the tank.

Most of the compounds in Tables X-4, X-5, and X-6 are believed to be chemical reaction and radiolytic reaction products of the semivolatile or nonvolatile organic waste stored in the tank. For example, 1-butanol is known to be formed by the hydrolysis of tributyl phosphate, and it has been suggested that the alcohols, aldehydes, ketones, nitriles, alkenes, and short chain alkanes are all degradation products of NPHs.

Neither TST nor SUMMA<sup>TM</sup> methods detected tributyl phosphate as a headspace constituent. The relatively high concentration of 1-butanol, however, is a strong indication that tributyl phosphate does exist in tank BY-108. That tributyl phosphate was not observed in the TST samples may be due to 1) the fact that tributyl phosphate has a very low vapor pressure, and 2) the tendency for tributyl phosphate to adsorb on the high efficiency particulate air (HEPA) filters used during sampling to protect the samples from radiological particulate contamination.

In the semivolatile region of Tables X-5 and X-6, there are many branched alkanes. The abundance of these, as well as the decahydronaphthalenes, was also noted in tank BY-107, to which tank BY-108 is attached.

It is interesting to note that while there are many ketones identified (particularly 2-alkanones, of which the homologous series from propanone to 2-nonanone, and several others exist), there are only 3 aldehydes identified. In other NPH-rich tanks (notably sludge tanks in 241-C farm, e.g., C-108, C-109, C-111 and C-112) the aldehydes and ketones are found in comparable numbers. This may be indicative of the oxidative properties of the waste, as the oxidation of an aldehyde to an acid is chemically easier than the oxidation of ketones.

Similarly, tank BY-108 has fewer nitriles than other NPH-rich tanks. Camaioni et al. (1994) point out that the hydrolysis of aldoximes produces aldehydes, while the dehydration of aldoximes produces nitriles. The observation that

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nitriles and aldehydes are found together in some tanks, and almost not at all in other NPH-rich tanks, appears to support the proposed aldoxime mechanism.

**Table X-1**  
**Tank BY-108 Gas and Vapor Sample Type and Number**

Laboratory	Sampling Device	Nominal Sample Volume (L)	Target Analytes	Number of Samples
Oak Ridge National Laboratories	Triple Sorbent Trap	0.05, 0.25 and 0.5	Organic vapors	12 tank air samples + 2 trip blanks + 2 field blanks
Pacific Northwest Laboratories	Acidified Carbon Sorbent Trap	3.0	Ammonia	6 tank air samples + 3 trip blanks
	Triethanolamine Sorbent Trap	3.0	Nitrogen Dioxide	6 tank air samples + 3 trip blanks
	Oxidation bed + Triethanolamine Sorbent Trap	3.0	Nitric Oxide	6 tank air samples + 3 trip blanks
	Silica Gel Sorbent Trap	3.0	Water vapor	6 tank air samples + 3 trip blanks
	SUMMA™ canister	6.0	Organic vapors	3 tank air samples + 2 ambient air samples
WHC 222-S Laboratory	Silica Gel Sorbent Trap	1.0	Tritium-Substituted Water Vapor	1 tank air sample



**Table X-2**  
**Tank BY-108 Inorganic Gas and Vapor Concentrations**

Compound	CAS <sup>1</sup> Number	Sample Type	Number of samples	Average (ppmv)	Standard Deviation (ppmv)	RSD <sup>2</sup> (%)
Ammonia, NH <sub>3</sub>	7664-41-7	Sorbent Trap	6	1040	80	8
Carbon Dioxide, CO <sub>2</sub>	124-38-9	SUMMA™	3	224	86	38
Carbon Monoxide, CO	630-08-0	SUMMA™	3	< 76	--	--
Hydrogen, H <sub>2</sub>	1333-74-0	SUMMA™	3	399	78	20
Nitric Oxide, NO	10102-43-9	Sorbent Trap	6	≤ 0.03	--	--
Nitrogen Dioxide, NO <sub>2</sub>	10102-44-0	Sorbent Trap	6	≤ 0.02	--	--
Nitrous Oxide, N <sub>2</sub> O	10024-97-2	SUMMA™	3	641	109	17
Water Vapor, H <sub>2</sub> O	7732-18-5	Sorbent Trap	6	18,800 (13.4 mg/L)	5,500 (3.9 mg/L)	29

1. CAS = Chemical Abstracts Service.

2. RSD = relative standard deviation.

**Table X-3**  
**Comparison of Selected Analytes**  
**in Tanks BY-104, BY-105, BY-106, BY-107 and BY-108**

Tank	Ammonia (ppmv)	Hydrogen (ppmv)	Nitrous Oxide (ppmv)	TNMOC <sup>1</sup> (mg/m <sup>3</sup> )
BY-104 <sup>2</sup>	248	295	201	60.8
BY-105 <sup>3</sup>	43	48	50	12.7
BY-106 <sup>4</sup>	74	46	71	9.9
BY-107 <sup>5</sup>	972	267	621	173
BY-108 <sup>6</sup>	1040	399	641	594

1. TNMOC = total nonmethane organic compounds.

2. Ammonia result is from Clauss et al. 1994; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994b.

3. Ammonia result is from Pool et al. 1995; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994c.

4. Ammonia result is from Lucke et al. 1995; hydrogen, nitrous oxide, and TNMOC results are from Rasmussen 1994d.

5. Ammonia, hydrogen, and nitrous oxide results are from Clauss et al. 1995; TNMOC result is from Rasmussen 1994a.

6. Ammonia, hydrogen, and nitrous oxide results are from McVeety et al. 1995; TNMOC result is from Rasmussen 1994a.

**Table X-4**  
**Tank BY-108 Organic Target Compound Average Concentrations**

Compound	CAS <sup>1</sup> Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD <sup>2</sup> (%)
Trichlorofluoromethane	75-69-4	SUMMA <sup>TM,3</sup>	0.128	0.064	5
Ethanenitrile (acetonitrile)	75-05-8	TST <sup>4</sup> SUMMA <sup>TM</sup>	0.94 < 0.005	0.18 --	19 --
Propanone (acetone) <sup>5</sup>	67-64-1	TST SUMMA <sup>TM</sup>	8.2 4.4	0.6 0.5	7 11
1-Propanol	71-23-8	SUMMA <sup>TM</sup>	6.8	0.1	2
Dichloromethane <sup>5</sup>	75-09-2	TST SUMMA <sup>TM</sup>	1.2 < 0.005	1.0 --	85 --
Propanenitrile <sup>5</sup>	107-12-0	TST SUMMA <sup>TM</sup>	< 0.059 < 0.005	-- --	-- --
Butanal	123-72-8	TST	0.87	0.66	75
2-Butanone	78-93-3	SUMMA <sup>TM</sup>	0.54	0.33	60
n-Hexane	110-54-3	TST SUMMA <sup>TM</sup>	2.3 1.5	0.1 0.04	3 2
Benzene	71-43-2	TST SUMMA <sup>TM</sup>	0.18 0.025	0.01 0.001	7 2
1-Butanol <sup>5</sup>	71-36-3	TST	58	5	8
Butanenitrile	109-74-0	TST SUMMA <sup>TM</sup>	0.31 < 0.005	0.04 --	12 --
2-Pentanone	107-87-9	TST	0.46	0.07	16
4-Methyl-2-pentanone	108-10-1	SUMMA <sup>TM</sup>	0.037	0.001	2
Cyclohexane	110-82-7	SUMMA <sup>TM</sup>	0.14	0.005	3
n-Heptane	142-82-5	TST SUMMA <sup>TM</sup>	0.89 0.52	0.03 0.01	3 2
Tetrahydrofuran	109-99-9	SUMMA <sup>TM</sup>	1.29	0.02	2
Toluene	108-88-3	TST SUMMA <sup>TM</sup>	0.10 0.045	0.02 0.002	17 3
Ethylbenzene	100-41-4	SUMMA <sup>TM</sup>	0.185	0.0005	0.3
m-Xylene + p-Xylene	108-38-3 106-42-3	SUMMA <sup>TM</sup>	0.077	0.003	4
o-Xylene	95-47-6	SUMMA <sup>TM</sup>	0.024	0.001	5

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Compound	CAS <sup>1</sup> Number	Sample Type	Average (ppmv)	Standard Deviation (ppmv)	RSD <sup>2</sup> (%)
Cyclohexanone	108-94-1	SUMMA <sup>TM</sup>	0.010	0.002	16
Pentanenitrile <sup>5</sup>	110-59-8	TST	< 0.054	--	--
		SUMMA <sup>TM</sup>	< 0.005	--	--
2-Hexanone	591-78-6	TST	0.16	0.02	15
n-Octane	111-65-9	TST	0.33	0.08	23
Hexanenitrile <sup>5</sup>	628-73-9	TST	< 0.034	--	--
2-Heptanone	110-43-0	TST	0.14	0.03	19
n-Nonane	111-84-2	TST	0.19	0.03	14
2-Octanone	111-13-7	TST	0.039	0.018	46
n-Decane	124-18-5	TST	0.21	0.10	46
		SUMMA <sup>TM</sup>	0.090	0.002	3
n-Undecane	1120-21-4	TST	0.48	0.09	19
n-Dodecane	112-40-3	TST	0.80	0.18	22
n-Tridecane	629-50-5	TST	0.73	0.22	30

1. CAS = Chemical Abstract Service.
2. RSD = relative standard deviation.
3. SUMMA<sup>TM</sup> canister results based on analyses of 3 samples.
4. TST results are based on analyses of 3 samples.
5. Two or more of the sample results fell outside the calibration range.

**Table X-5**  
**Tank BY-108 Tentatively Identified Organic Compounds in SUMMA™ Samples**

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
1	Propene	115-07-1	1.82	0.04
2	Propane	74-98-6	0.91	0.04
3	Cyclopropane	75-19-4	0.29	0.00
4	Isobutane	75-28-5	0.58	0.02
5	1-Butene	106-98-9	2.02	0.13
6	Butane	106-97-8	1.38	0.08
7	2-Methyl-1-Propene	115-11-7	0.22	0.00
8	Cyclobutane	287-23-0	0.40	0.01
9	Isopropyl Alcohol	67-63-0	0.22	0.01
10	1-Pentene	109-67-1	0.69	0.01
11	Pentane	109-66-0	1.37	0.09
12	4-Methyl-1-Pentene	691-37-2	0.53	0.04
13	2-Methylpentane	107-83-5	2.07	0.06
14	3-Methylpentane	96-14-0	0.40	0.01
15	1-Hexene	592-41-6	0.74	0.04
16	Methylcyclopentane	96-37-7	0.28	0.01
17	1-Butanol	71-36-3	12.60	0.75
18	2-Pentanone	107-87-9	1.66	0.07
19	3-Methylhexane	589-34-4	1.69	0.05
20	1-Heptene	592-76-7	1.14	0.11
21	Unknown C8 Alkene/Cycloalkane		0.34	0.03
22	Unknown C8 Alkane		1.26	0.03
23	2-Hexanone	591-78-6	0.66	0.04
24	Unknown C8 Alkene/Cycloalkane		0.21	0.01
25	1,2-Dimethylcyclohexane	583-57-3	0.25	0.01
26	1-Octene	111-66-0	0.31	0.01
27	Octane	111-65-9	1.36	0.05

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
28	2,6-dimethylheptane	1072-05-5	0.43	0.02
29	Unknown Alkene/Cycloalkane		0.41	0.02
30	2-Heptanone	110-43-0	0.32	0.02
31	Nonane	111-84-2	0.80	0.03
32	Unknown Ketone		0.75	0.04
33	Unknown C9 Alkene/Cycloalkane		0.27	0.02
34	Unknown C10 Alkane		0.25	0.01
35	2-Octanone	111-13-7	0.30	0.01
36	Unknown C10 Alkene/Cycloalkane		0.37	0.02
37	Unknown C10 Alkene/Cycloalkane		0.20	0.01
38	Unknown C10 Alkene/Cycloalkane		0.24	0.01
39	Unknown C11 Alkane		1.03	0.04
40	Unknown C11 Alkane		0.22	0.01
41	Unknown C10 Alkene/Cycloalkane		0.47	0.02
42	Unknown C11 Alkane		0.22	0.01
43	Unknown C11 Alkane		0.27	0.01
44	Unknown C11 Alkane		0.27	0.01
45	Decahydronaphthalene	91-17-8	0.32	0.01
46	1-Undecene	821-95-4	0.32	0.03
47	Undecane	1120-21-4	3.34	0.13
48	Unknown C11 Alkene/Cycloalkane		0.60	0.04
49	Unknown C12 Alkane		0.51	0.04
50	Unknown C12 Alkane		0.53	0.04
51	Naphthalene, decahydro-2-methyl-	2958-76-1	0.67	0.03

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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
52	Unknown C11 Alkene/Cycloalkane		0.80	0.05
53	Unknown C12 Alkane		0.52	0.02
54	Decahydro-2-Methylnaphthalene	2958-76-1	0.30	0.01
55	Unknown C12 Alkane		0.86	0.05
56	Unknown C12 Alkane		0.51	0.05
57	Unknown Alkyl Decahydronaphthalene		0.58	0.03
58	Dodecane	112-40-3	6.16	0.27
59	Unknown C12 Alkene/Cycloalkane		0.31	0.02
60	Decahydro-2,6-Dimethylnaphtal ene	1618-22-0	0.58	0.03
61	2,6-Dimethylundecane	17301-23-4	4.18	0.22
62	Unknown C13 Alkane		0.46	0.06
63	Unknown Alkyl Decahydronaphthalene		0.57	0.04
64	Unknown C13 Alkene/Cycloalkane		2.36	0.19
65	Unknown Alkyl Decahydronaphthalene		0.71	0.07
66	Unknown C12 Alkane		0.98	0.12
67	Unknown Alkane		0.70	0.09
68	Unknown C14 Alkane		4.92	0.34
69	Unknown C13 Alkene/Cycloalkane		0.38	0.03
70	Tridecane	629-50-5	5.30	0.36
71	Unknown C13 Alkene/Cycloalkane		0.33	0.03
72	Unknown C14 Alkene/Cycloalkane		0.91	0.06
73	Unknown Alkane		1.11	0.14
74	Unknown C14 Alkene/Cycloalkane		0.25	0.02

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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
75	Unknown C13 Alkene/Cycloalkane		0.99	0.10
76	2-Methyltridecane	1560-96-9	0.41	0.05
77	Unknown Alkane		0.23	0.03
78	2,6,10-Trimethyldodecane,	3891-98-3	2.43	0.24
79	Unknown C4 Alkyl Decahydronaphthalene		0.32	0.04
80	Tetradecane	629-59-4	1.95	0.25
81	Unknown C15 Alkene/Cycloalkane		0.41	0.14
Sum of tentatively identified compounds:			89.0	

1. CAS = Chemical Abstract Number.



**Table X-6**  
**Tank BY-108 Tentatively Identified Organic Compounds in TST Samples**

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
1	1-propene, 2-methyl	115-11-7	1.6	1.5
2	1-propene, 2-methyl	115-11-7	2.1	0.4
3	1-propene, 2-methyl	115-11-7	0.48	0.84
4	1-butene, 3-methyl	563-45-1	0.51	0.88
5	butane, 2-methyl	78-78-4	7.9	0.8
6	methane, trichlorofluro	75-69-4	11.9	13.0
7	cyclopropane, ethyl	1191-96-4	7.3	0.8
8	3-buten-1-ol	627-27-0	6.1	10.5
9	furan	110-00-9	0.55	0.96
10	oxirane, ethenyl	930-22-3	0.8	1.4
11	2-propanol	67-63-0	5.3	1.6
12	2-pentene, (Z)-	627-20-3	0.88	0.76
13	cyclobutane, methyl	598-61-8	0.92	0.80
14	1-pentene, 4-methyl	691-37-2	2.5	0.3
15	pentane, 2-methyl	107-83-5	15.1	0.9
16	1-propene, 2-fluoro	1184-60-7	0.47	0.82
17	pentane, 3-methyl	96-14-0	2.5	0.2
18	1-pentene, 2-methyl	763-29-1	2.6	1.6
19	1-hexene	592-41-6	3.0	2.6
20	2-butanone	78-93-3	0.66	1.14
21	cyclopentane, methyl	96-37-7	2.1	0.3
22	furan, tetrahydro	109-99-9	8.5	2.0
23	1,3-pentadiene, 2-methyl	1118-58-7	0.49	0.85
24	1-pentene, 3,4-dimethyl	7385-78-6	0.59	1.02
25	1-hexene, 5-methyl	3524-73-0	0.53	0.91
26	hexane, 2-methyl	591-76-4	1.34	0.05

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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
27	cyclopentane, 1,2-dimethyl-, trans-	822-50-4	0.324	0.305 2
28	cyclopropane, butyl	930-57-4	2.5	0.3
29	2-heptene	592-77-8	0.16	0.28
30	cyclohexane, methyl	108-87-2	1.13	0.06
31	mixture		0.14	0.24
32	propane, 2-nitro & others	79-46-9	0.14	0.23
33	1-heptene, 6-methyl	5026-76-6	0.25	0.43
34	1-heptene, 3-methyl	4810-09-7	0.52	0.46
35	heptane, 2,3,5-trimethyl	20278-85-7	0.65	1.12
36	heptane, 2,3,6-trimethyl-	4032-93-3	1.26	1.10
37	1-octene	111-66-0	0.74	0.65
38	heptane, 3-methyl	589-81-1	0.19	0.32
39	3-pentanol, 2-methyl and others	565-67-3	0.11	0.19
40	cyclohexane, 1,3-dimethyl-, cis-	638-04-0	0.11	0.20
41	cyclopentane, 1,1,3-trimethyl-	4516-69-2	0.24	0.21
42	hexanal, 3-methyl	19269-28-4	0.24	0.42
43	1-octene	111-66-0	0.18	0.31
44	2H-pyran-2-one, tetrahydro-5,6-dimethyl-	24405-16-1	0.81	0.72
45	1-octanol	111-87-5	0.12	0.20
46	hexamethylcyclotrisiloxane		0.13	0.22
47	heptane, 2,6-dimethyl	1072-05-5	0.56	0.07
48	cyclohexane, ethyl	1678-91-7	0.46	0.11
49	cyclohexane, 1,1,3-trimethyl	3073-66-3	0.82	0.19
50	1-nonene		0.31	0.27
51	heptane, 2,3-dimethyl	3074-71-3	0.09	0.16
52	benzene, ethyl and octane, 2-methyl		0.54	0.05
53	benzene, 1,2-dimethyl	95-47-6	0.40	0.69

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
54	benzene, 1,4-dimethyl	106-42-3	0.35	0.61
55	heptane, 3,5-dimethyl	926-82-9	0.073	0.126
56	octane, 3-methyl and c2-benzene		0.43	0.74
57	butane, 1,1'-oxybis	142-96-1	0.17	0.15
58	3-heptanone	106-35-4	0.68	0.10
59	benzene, 1,2-dimethyl	95-47-6	0.38	0.06
60	mixture		0.069	0.119
61	cyclohexane, 1-ethyl-4-methyl-, trans	6236-88-0	0.057	0.099
62	3,4-nonadiene	37050-03-6	0.48	0.14
63	heptane, 4-(1-methylethyl)-	52896-87-4	0.15	0.26
64	1-hexene, 4,5-dimethyl	16106-59-5	0.11	0.20
65	4-nonyne	20184-91-2	0.13	0.23
66	2-heptanone, 6-methyl	928-68-7	1.4	0.6
67	nonane, 4-methyl	17301-94-9	0.57	0.25
68	cyclohexane, 1,1,4,4-tetramethyl		0.41	0.12
69	2-octanol	123-96-6	0.40	0.20
70	3-buten-2-ol	598-32-3	4.8	3.9
71	2-heptyl furan		0.22	0.23
72	cyclohexane, 1-methyl-4-(1-methylethyl) & others		0.099	0.170
73	cyclopentanone, 2-methyl-4-(2-methylpropyl)	69770-96-3	0.16	0.27
74	cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	0.25	0.44
75	cyclohexane, 1-methyl-4-(1-methylethyl)cis	6069-98-3	0.23	0.22
76	cyclopentane, 1-methyl-3-(2-methylpropyl)	29053-04-1	0.57	0.16

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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
77	cyclotetrasiloxane, octamethyl	556-67-2	1.1	0.9
78	cyclohexane, 1,5-diethyl-2,3-dimethyl-	74663-66-4	0.52	0.25
79	nonane, 2,6-dimethyl	17302-28-2	2.2	1.1
80	octane, 6-ethyl-2-methyl	62016-19-7	0.19	0.20
81	1,4-pentadiene, 2,3,4-trimethyl & others		0.079	0.137
82	3-decyne	2384-85-2	0.51	0.17
83	cyclohexane, butyl	1678-93-9	1.46	0.39
84	cyclohexane, 1-ethyl-4-methyl, cis	4926-78-7	0.16	0.14
85	cyclohexane, cyclopropyl-	32669-86-6	0.19	0.17
86	1-ethyl-2,2,6-trimethylcyclohexane		0.55	0.14
87	decane, 5-methyl	13151-35-4	0.73	0.20
88	decane, 4-methyl	2847-72-5	0.78	0.21
89	decane, 2-methyl	6975-98-0	1.8	0.5
90	naphthalene, decahydro-, trans-	493-02-7	1.1	0.3
91	decane, 3-methyl	13151-34-3	1.1	0.2
92	cyclohexane, 1,2-diethyl-3-methyl		0.47	0.12
93	formic acid, 2,6-dimethyl-5-hepten-2-ol est		0.37	0.10
94	cyclohexane, 1-(cyclohexylmethyl)-4-methyl		0.80	0.19
95	c5-cyclohexane		0.69	0.14
96	5-undecene		1.0	0.3
97	2-nonanone and others	821-55-6	0.93	0.23
98	cyclohexane, 1-ethyl-2-propyl	62238-33-9	0.28	0.26
99	5-undecene		0.49	0.13
100	1-undecene, 4-methyl	74630-39-0	0.51	0.89
101	nonane, 3,7-dimethyl	17302-32-8	0.80	1.39
102	undecane, 5-methyl	1632-70-8	2.9	0.8

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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
103	bicyclo[4.1.0]heptane, 3-methyl-7-pentyl		0.41	0.09
104	undecane, 4-methyl	2980-69-0	0.36	0.09
105	naphthalene, decahydro-2-methyl	2958-76-1	2.2	0.6
106	undecane, 3,8-dimethyl	17301-30-3	1.0	0.9
107	undecane, 4,7-dimethyl	17301-32-5	0.77	1.34
108	dimethyl-decahydronaphthalene		0.25	0.24
109	2-undecene, 8-methyl	74630-44-7	0.38	0.12
110	1-dodecene	112-41-4	0.38	0.08
111	cyclopentane, (2-methylbutyl)-	53366-38-4	0.35	0.10
112	naphthalene, decahydro-2-methyl	2958-76-1	5.9	1.6
113	3-dodecene, (Z)-	7239-23-8	0.20	0.19
114	naphthalene, decahydro-2-methyl	2958-76-1	0.21	0.19
115	6-methylundecane	17302-33-9	3.4	0.9
116	undecane, 4-methyl	2980-69-0	1.9	0.5
117	undecane, 2-methyl	7045-71-8	3.8	1.0
118	undecane, 2,3-dimethyl	17312-77-5	0.97	0.28
119	undecane, 3-methyl	1002-43-3	2.1	0.6
120	4-undecene, 4-methyl	61142-40-3	0.86	0.18
121	decane, 2,3,6- trimethyl	62238-12-4	0.71	0.18
122	cyclododecane	294-62-2	1.4	0.3
123	naphthalene, decahydro-2,6-dimethyl-	1618-22-0	1.4	0.3
124	naphthalene, decahydro-2,3-dimethyl-	1008-80-6	0.11	0.11
125	cyclohexane, 1-methyl-2-pentyl	54411--01-7	0.53	0.11
126	5-heptenal, 2,6-dimethyl	106-72-9	0.42	0.11
127	undecane, 2,4-dimethyl	17312-80-0	0.16	0.15
128	undecane, 2,6-dimethyl	17301-23-4	7.5	1.7
129	undecane, 2,7-dimethyl	17301-24-5	0.40	0.37

## WHC-SD-WM-ER-422 REV. 1

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
130	undecane, 3,7-dimethyl	17301-29-0	0.24	0.42
131	dimethyl-decahydronaphthalene		1.0	0.2
132	cyclopentane, 1-pentyl-2-propyl	62199-51-3	0.26	0.05
133	cyclohexane, 2-butyl-1,1,3-trimethyl		3.0	0.6
134	1-octanol, 2-butyl	3913-02-8	0.35	0.08
135	naphthalene, decahydro-1,6-dimethyl	1750-51-2	0.36	0.08
136	(E,E)(3S,8S),3,8-dimethyldeca-4,6-diene		0.47	0.10
137	cyclohexane, (4-methylpentyl)-	61142-20-9	2.7	0.5
138	dodecane, 6-methyl	6044-71-9	0.80	0.15
139	dodecane, 5-methyl	17453-93-9	0.57	0.12
140	dodecane, 4-methyl	6117-97-1	1.8	0.4
141	undecane, 2,10-dimethyl	17301-27-8	3.3	0.7
142	mixture		0.45	0.10
143	dodecane, 4,6-dimethyl	61141-72-8	6.4	6.1
144	cyclohexane, 2,4-diethyl-1-methyl	61142-70-9	0.15	0.14
145	tridecane, 7-methyl	26730-14-3	3.9	6.8
146	2(3H)-benzofuranone,3a,4,5,6tetra hydro-3a,6,6-trimethyl	16778-26-0	0.73	0.20
147	cyclohexane, 1,2-diethyl-1-methyl	61141-79-5	0.24	0.25
148	6-tridecene, 7-methyl	24949-42-6	2.3	0.7
149	5-tetradecene, (E)-	41446-66-6	0.63	0.17
150	tridecane, 5-methyl	25117-31-1	0.32	0.31
151	undecane, 4,6-dimethyl	17312-82-2	0.47	0.44
152	tetradecane	629-59-4	0.22	0.38
153	undecane, 6,6-dimethyl	17312-76-4	0.30	0.51
154	dodecane, 2,5-dimethyl	56292-65-0	2.5	0.7
155	cyclopentane, 1-hexyl-3-methyl	61142-68-5	0.093	0.087

## WHC-SD-WM-ER-422 REV. 1

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
156	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl	54934-93-9	0.31	0.10
157	4-nonene, 2,3,3-trimethyl-, (E)-	63830-68-2	0.57	0.16
158	naphthalene, 2-butyldecahydro	6305-52-8	0.32	0.09
159	tetradecane	629-59-4	1.0	0.3
160	octane, 2-cyclohexyl	2883-05-8	2.6	0.8
161	tridecane, 4-methyl	26730-12-1	1.5	0.4
162	tridecane, 2-methyl	1560-96-9	2.0	0.6
163	undecane, 4,6-dimethyl	17312-82-2	0.037	0.064
164	decane, 2,3,5,8-tetramethyl		0.052	0.091
165	cyclohexane, 1-(cyclohexylmethyl)-2-ethyl		0.70	0.20
166	tridecane, 3-methyl	6418-41-3	0.25	0.44
167	dodecane, 3-methyl	17312-57-1	0.87	0.75
168	dodecane, 2,6,10-trimethyl	3891-98-3	7.3	2.1
169	cyclohexane, (2,2-dimethylcyclopentyl)-	61142-23-2	0.027	0.047
170	cyclohexane, 1-(cyclohexylmethyl)-2-methyl	54823-94-8	0.25	0.07
171	tetradecane	629-59-4	7.3	2.0
172	tridecane, 4,8-dimethyl	55030-62-1	1.5	1.4
173	tridecane, 3-ethyl	13286-73-2	0.089	0.154
174	pentadecane	629-62-9	1.2	1.7
175	pentadecane	629-62-9	0.32	0.55
176	alkyl-cyclohexane		0.45	0.15
177	heptadecane, 7-methyl	20959-33-5	0.17	0.29
178	c15-alkane		0.14	0.16
179	c15-alkane		0.16	0.15

Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
180	decane, 1,1'-oxybis	2456-28-2	0.65	0.63
181	1-octadecanol	112-92-5	0.45	0.78
182	dodecane, 2-methyl-8-propyl	55045-07-3	2.9	0.8
183	pentadecane, 2-methyl	1560-93-6	0.18	0.17
184	tetradecane, 3-methyl	18435-22-8	0.13	0.22
185	hexadecane, 2,6,10,14-tetramethyl	638-36-8	0.091	0.080
186	7-hexadecene, (Z)-	35507-09-6	0.22	0.06
187	2-pentanone, 4-cyclohexyliden-3,3-diethyl		0.11	0.10
188	pentadecane	629-62-9	1.6	0.5
189	dodecanoic acid	143-07-7	0.31	0.10
190	hexadecane	544-76-3	0.053	0.092
191	benzenamine, N-phenyl	122-39-4	0.23	0.06
192	tetradecanoic acid	544-63-8	2.1	1.7
193	hexacosane	630-01-3	0.099	0.172
194	benzenesulfonamide, N-butyl	3622-84-2	1.5	0.7
195	pentadecanoic acid	1002-84-2	0.36	0.14
196	1-hexadecanol	36653-82-4	0.097	0.174
197	1-hexadecene	629-73-2	0.049	0.085
198	alkane		0.53	0.92
199	alkane		2.2	3.6
200	9-hexadecenoic acid	2091-29-4	0.32	0.31
201	hexadecanoic acid	57-10-3	1.4	1.4
202	phthalate		0.081	0.140
203	hexadecanoic acid, 1-methylethyl ester	142-91-6	0.44	0.31



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Cmpd #	Compound	CAS <sup>1</sup> Number	Average (mg/m <sup>3</sup> )	Standard Deviation (mg/m <sup>3</sup> )
204	ethanol, 2-(tetradecyloxy)-	2136-70-1	0.70	1.22
205	alkane		0.09	0.15
206	5-eicosane, (E)	74685-30-6	0.23	0.39
207	1-hexadecene	629-73-2	0.25	0.43
208	octadecane	630-06-8	0.025	0.043
Sum of tentatively identified compounds:			251.9	

1. CAS = Chemical Abstract Service.

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