INSTALLATION RESTORATION PROGRAM

EVALUATION OF 2-BUTANONE IN GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE WESTHAMPTON BEACH, NEW YORK

Prepared for:

Air National Guard Readiness Center
Andrews Air Force Base, Maryland

and

Managed by:

Martin Marietta Energy Systems, Inc.
HAZWRAP Support Contractor Office
Oak Ridge, Tennessee

Prepared by:

ABB Environmental Services, Inc.
Portland, Maine
Project No. 6943-02

MARCH 1992

362308

EVALUATION OF 2-BUTANONE
IN GROUNDWATER SAMPLES

TABLE OF CONTENTS

Section	Title	Page No.
1.0	INTRODUCTION	1-1
2.0	BACKGROUND INFORMATION	2-1
2.1	GROUNDWATER SAMPLING AT THE FTA	2-1
2.2	THE USE OF 2-BUTANONE AT SCANGB	2-6
2.3	PREVIOUS STUDIES CONCERNING THE PRESENCE OF 2-BUTANONE	2-11
2.4	CHEMISTRY OF 2-BUTANONE	2-12
3.0	EVALUATION OF 2-BUTANONE IN METHYL HYDRATE DECONTAMINATION FLUID	3-1
3.1	SOLVENT PURITY BY DIRECT INJECTION	3-1
3.2	PURGE AND TRAP DATA	3-2
3.3	RESPONSE FACTOR FOR ETHANOL	3-2
4.0	EVALUATION OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN GROUNDWATER SAMPLES	4-1
4.1	ROUND 1	4-1
4.2	ROUND 2	4-1
4.3	ROUND 3	4-2
4.4	ROUND 4	4-2
4.5	ROUND 5	4-4
5.0	TEMPORAL COMPARISON OF 2-BUTANONE GROUNDWATER DATA	5-1
6.0	OCTOBER 1991 SAMPLING AND ANALYSIS OF MW-107B	6-1
7.0	STATISTICAL ANALYSIS OF 2-BUTANONE GROUNDWATER DATA	7-1
8.0	DISCUSSION	8-1

EVALUATION OF 2-BUTANONE
IN GROUNDWATER SAMPLES

TABLE OF CONTENTS
(continued)

Section	Title	Page No.
9.0	CONCLUSIONS AND RECOMMENDATIONS	9-1

GLOSSARY OF ACRONYMS AND ABBREVIATIONS

REFERENCES

APPENDICES

APPENDIX A - PHYSICOCHEMICAL CHARACTERISTICS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE

APPENDIX B - DIRECT INJECTION DATA FOR METHYL HYDRATE

APPENDIX C - PURGE AND TRAP ANALYSIS OF METHYL HYDRATE

APPENDIX D - ETHANOL STANDARDS

APPENDIX E - DATA VALIDATION GROUNDWATER SUMMARY TABLES FOR VOCS - SCANGB

EVALUATION OF 2-BUTANONE
IN GROUNDWATER SAMPLES

LIST OF FIGURES

Figure	Title	Page No.
2-1	Monitoring Well Location Map	2-10
4-1	Tentatively Identified Compounds Reported in MW-107B (Round 3)	4-3
4-2	Tentatively Identified Compounds Reported in MW-107B (Round 4)	4-5
7-1	Plot of 2-Butanone vs. Ethanol	7-2
7-2	Plot of 2-Butanone vs. Ethyl Acetate	7-3

EVALUATION OF 2-BUTANONE
IN GROUNDWATER SAMPLES

LIST OF TABLES

Table	Title	Page No.
2-1	Concentrations of 2-Butanone, Ethanol, and Ethyl Acetate in Round 1 Groundwater Samples	2-2
2-2	Concentrations of 2-Butanone, Ethanol, and Ethyl Acetate in Round 2 Groundwater Samples	2-3
2-3	Concentrations of 2-Butanone, Ethanol, and Ethyl Acetate in Round 3 Groundwater Samples	2-4
2-4	Concentrations of 2-Butanone, Ethanol, and Ethyl Acetate in Round 4 Groundwater Samples	2-5
2-5	Concentrations of 2-Butanone, Ethanol, and Ethyl Acetate in Round 5 Groundwater Samples	2-7
2-6	Monitoring Well Sample Designations	2-8
5-1	2-Butanone Concentrations in Monitoring Wells Sampled Multiple Times	5-2
6-1	Concentrations of 2-Butanone, Ethanol, Ethyl Acetate in MW-107B Samples Collected in October 1991	6-2
7-1	Kendall TAU Coefficients	7-5
7-2	Approximate Z-values	7-5
7-3	Approximate Probability Levels	7-5

1.0 INTRODUCTION

This report concerns the presence of 2-butanone, also known as methyl ethyl ketone, in groundwater samples collected at the Fire Training Area (FTA) at Suffolk County Airport during five phases of groundwater sampling between 1987 and 1991. The FTA, formerly operated by the Suffolk County Air National Guard Base (SCANGB), is the subject of investigations under the Air National Guard's Installation Restoration Program (IRP). These investigations are conducted by ABB Environmental Services (ABB-ES) for the Hazardous Waste Remedial Actions Program (HAZWRAP) Support Contractor Office.

This report links 2-butanone reported in groundwater samples with the use of methyl hydrate (Anachemia, Inc., Product No. AC-4099), a decontamination fluid used in IRP investigations at SCANGB before December 1989. Methyl hydrate is a commercial solvent mixture of ethanol and methanol. Through laboratory analyses, 2-butanone and ethyl acetate were identified as additional constituents of methyl hydrate, establishing a relationship between 2-butanone in groundwater samples and the presence of ethanol and ethyl acetate in those same samples. The relationship of 2-butanone, ethanol, and ethyl acetate was identified as a fingerprint of methyl hydrate. The fingerprint was observed in nearly all samples in which 2-butanone was reported, suggesting that the use of methyl hydrate during the decontamination of sampling equipment was responsible for the presence of 2-butanone, ethanol, and ethyl acetate in groundwater samples.

This study examines all groundwater samples collected in conjunction with IRP investigations at the FTA since April 1987. The data set includes samples collected with the use of methyl hydrate as a decontamination fluid (Rounds 1, 2, and 3), and samples collected without its use (Rounds 4 and 5). The conclusions of this report are based on the combined results of a four-part investigation, which included the following tasks:

- Several different lots of methyl hydrate were analyzed by direct injection gas chromatography/mass spectrometry (GC/MS) to characterize chemical composition. Samples of methyl hydrate in water were also analyzed by purge-and-trap GC/MS for comparison to groundwater sample data.

- Groundwater data from the FTA investigation were organized, reviewed, and summarized with reference to the presence of 2-butanone, ethanol, and ethyl acetate. When more than one sampling round was available from a particular monitoring well, data were examined for temporal trends.

- A statistical evaluation was performed on the data to test the relationship between 2-butanone, ethanol, and ethyl acetate reported in groundwater samples.

- Data collected during sampling Rounds 4 and 5, after methyl hydrate use was discontinued, were summarized and compared to analogous data from the previous three rounds.

- During Round 5, the monitoring well where 2-butanone was most persistent in earlier sampling rounds (MW-107B), was serially purged and sampled several times. Analyses showed that residual 2-butanone in the water column was removed by the purging procedures, and final samples collected at MW-107B did not contain 2-butanone.

As a result of this study, ABB-ES believes the 2-butanone reported in samples collected at the FTA is a sampling artifact resulting from the use of methyl hydrate as a decontamination fluid.

2.0 BACKGROUND INFORMATION

2.1 GROUNDWATER SAMPLING AT THE FTA

As part of IRP activities at SCANGB, two rounds of groundwater samples and a series of surface and subsurface soil samples were collected from the FTA in 1987. Three additional rounds of groundwater samples were collected in 1989 and 1991. The sampling events referred to in this report occurred as follows:

Round 1: The results of Round 1, conducted in April 1987, are presented in the Final Site Characterization Report (FSCR) for the FTA (U.S. Air Force Installation Restoration Program, 1989). Fourteen groundwater samples were collected from 10 monitoring wells and analyzed for Target Compound List (TCL) volatile organic compounds (VOCs) according to Contract Laboratory Program (CLP) protocols. Samples identified as containing 2-butanone are presented in Table 2-1. Complete analytical results are presented in Appendix E.

Round 2: Round 2 was conducted in July 1987, and like Round 1, was reported in the FSCR. Fifteen groundwater samples were collected from 11 monitoring wells and analyzed for TCL VOCs. Samples identified as containing 2-butanone are presented in Table 2-2. Complete analytical results are presented in Appendix E.

Round 3: Round 3 was conducted in August 1989 under an Additional Investigation Program authorized by HAZWRAP designed to specifically characterize 2-butanone at the FTA. The effort involved the collection of 24 groundwater samples from 22 monitoring wells and subsequent analysis for TCL VOCs. Samples identified as containing 2-butanone are presented in Table 2-3. Complete analytical results are presented in Appendix E.

Round 4: Round 4 was conducted in December 1989 in conjunction with the Additional Investigation Program and was the first field effort to substitute a solution of deionized (DI) water and Liquinox for methyl hydrate as a decontamination fluid. Twenty groundwater samples were collected from 18 monitoring wells and analyzed for TCL VOCs. Samples identified as containing 2-butanone are presented in Table 2-4. Complete analytical results are presented in Appendix E.

TABLE 2-1
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN ROUND 1 GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in μg/L)

WELL ID	SAMPLE DATE	2-BUTANONE	ETHANOL	ETHYL ACETATE
MW-101A	04/29/87	18	11 J	NI
MW-102	04/29/87	82	17 J	NI
MW-102 (Dup)	04/29/87	28	10 J	NI
MW-107A	04/30/87	65	32 J	NI
MW-107B	04/30/87	56,000	17,000 J	3,200 J

NOTES:

NI = Not Identified
μg/L = micrograms per liter
J = Estimated Data
Dup = Duplicate

TABLE 2-2
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN ROUND 2 GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in µg/L)

WELL ID	SAMPLE DATE	2-BUTANONE	ETHANOL	ETHYL ACETATE
MW-101A	07/09/87	312	140 J	12 J
MW-101B	07/09/87	1,400	230 J	96 J
MW-102	07/09/87	9 J	NI	NI
MW-103 (Dup)	07/08/87	10 U	16 J	NI
MW-104	07/09/87	18	12 J	NI
MW-104 (Dup)	07/08/87	19	NI	NI
MW-106	07/08/87	30	19 J	NI
MW-106 (Dup)	07/08/87	23	9 J	NI
MW-107A	07/08/87	24	18 J	NI
MW-107B	07/08/87	14,000	1,400 J	950 J
P-3	08/09/87	21	37 J	NI
SB-1	07/08/87	7.8 J	NI	NI

NOTES:

J = Estimated Data
NR = Not Identified
Dup = Duplicate
U = less than Quantitation Limit
µg/L = micrograms per liter
SB = Equipment Rinsate Blank
P = piezometer

TABLE 2-3
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN ROUND 3 GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in μg/L)

WELL ID	SAMPLE DATE	2-BUTANONE	ETHANOL	ETHYL ACETATE
MW-101A	02/07/89	320 J	1,100 J	10 J
MW-101A (Dup)	02/07/89	320 J	900 J	10 J
MW-101B	02/07/89	R	30 J	NI
MW-102	02/07/89	94 J	61 J	4 J
MW-103	02/07/89	24 J	21 J	NI
MW-103 (Dup)	02/07/89	38 J	26 J	NI
MW-104	02/07/89	150 J	220 J	NI
MW-105	02/07/89	460 J	75 J	NI
MW-106	02/07/89	40 J	37 J	NI
MW-107A	02/07/89	830 J	770 J	36 J
MW-107B	02/07/89	53,000 J	33,000 J	3,800 J
MW-107C	02/07/89	150 J	95 J	7 J
MW-9	02/08/89	14 J	19 J	NI
MW-10	02/08/89	5,700 J	1,900 J	350 J
MW-11	02/08/89	380 J	130 J	22 J
MW-14	02/08/89	2,600 J	880 J	160 J
MW-22	02/08/89	160	71 J	11 J
MW-24	02/08/89	10 J	10 J	NI
MW-OOX	02/08/89	140 J	62 J	5 J
P1	02/07/89	13,000 J	6,500 J	600 J
P2	02/07/89	26 J	35 J	NI
P3	02/07/89	170 J	140 J	7 J
P4	02/07/89	190 J	120 J	NI
MS-1	02/07/89	320 J	940 J	1,413 J
MSD-1	02/07/89	330 J	1,100 J	13 J

NOTES:

R = Rejected data.
J = Estimated Data
NI = Not Identified
Dup = Duplicate
MS = Matrix Spike Sample
MSD = Matrix Spike Duplicate Sample
μg/L = micrograms per liter
P = piezometer

TABLE 2-4
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN ROUND 4 GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in μg/L)

WELL ID	SAMPLE DATE	2-BUTANONE	ETHANOL	ETHYL ACETATE
MW-101A	12/12/89	10 U	15 J	NI
MW-107A	12/12/89	10	NI	NI
MW-107B	12/12/89	4,300 J	720 J	160 J
MW-202	12/12/89	10 U	52 J	NI

NOTES:

J = Estimated Data
NI = Not Identified
U = less than Quantitation Limit
μg/L = micrograms per liter

Round 5: Round 5, conducted in October 1991, was limited to the extensive purging and sampling of three monitoring wells (i.e., MW-107A, MW-107B, and MW-107C). An innovative purging and sampling technique was employed to verify that 2-butanone was not a genuine aquifer contaminant. The results of this study are summarized in Section 6.0. Samples identified as containing 2-butanone are presented in Table 2-5. Complete analytical results are presented in Appendix E.

Monitoring well designations to identify groundwater samples varied between sampling events. In this report, monitoring wells are designated with MW prefixes. Table 2-6 presents the designations used in the various sampling events, and their relationship to those used in this report. Monitoring well locations are illustrated in Figure 2-1.

ABB-ES personnel collected approximately 77 groundwater samples associated with the FTA throughout the five sampling rounds. These samples were analyzed for TCL VOCs according to CLP protocols. 2-Butanone was detected in approximately 50 percent of the samples, in concentrations ranging from 9 to 56,000 micrograms per liter (μg/L). Twenty-six of the samples were collected during Rounds 4 and 5 after the use of methyl hydrate as a decontamination fluid was discontinued. Results from these sampling events provided important data to evaluate the effects of methyl hydrate used in previous sampling programs.

2.2 THE USE OF 2-BUTANONE AT SCANGB

Although 2-butanone use has decreased in recent years, it is still commonly used at many military facilities. In addition to being a solvent for paint-stripping, 2-butanone is used in industry as a constituent of lacquers, thinners, and adhesives. 2-Butanone reportedly was burned with fuels at the FTA prior to 1971 (U.S. Air Force Installation Restoration Program, 1989). Although 2-butanone was reported in the groundwater samples, several observations were made that led to additional investigations. These observations, originally reported in the FSCR, were:

- 2-Butanone was reported in both upgradient and downgradient wells.
- Calculated groundwater velocity rates were estimated to be 300 feet per year. Consequently, any 2-butanone dissolved in groundwater in the vicinity of the FTA would travel beyond the farthest downgradient

TABLE 2-5
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN ROUND 5 GROUNDWATER SAMPLES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in μg/L)

Well ID	Sample Date	2-Butanone	Ethanol	Ethyl Acetate
MW-107B	10/03/91	1,600	4,400 J	900 J

NOTES:

J = Estimated Data

TABLE 2-6
MONITORING WELL SAMPLE DESIGNATIONS

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

WELL LOCATION	ROUND 1	ROUND 2	ROUND 3	ROUND 4	ROUND 5
MW-101A	JMW101AX01	JMW101AX02	SCGW101AXX03XX SCGW101AXX03DX	MW-101A	—
MW-101B	JMW101BX01	JMW101BX02	SCGW101BXX03XX	MW-101B	—
MW-102	JMW102XX01 JDUP1	JMW102XX02	SCGW102XXX03XX	MW-102	—
MW-103	JMW103XX01	JMW103XX02 JDUP1	SCGW103XXX03XX SCGW103XXX03DX	MW-103	—
MW-104	JMW104XX01	JMW104XX02 JDUP2	SCGW104XXX03XX	MW-104	—
MW-105	JMW105XX01 JREP2	JMW105XX02 JREP1	SCGW105XXX03XX	MW-105 MW-105D	—
MW-106	JMW106XX01 JDUP2	JMW106XX02 JREP2	SCGW106XXX03XX	MW-106	—
MW-107A	JMW107AX01	JMW107AX02	SCGW107AXX03XX	MW-107A	07MW017AXX 05XX
MW-107B	JMW107BX01	JMW107BX02	SCGW107BXX03XX	MW-107B	07MW107BX1 05XX 07MW107BX2 05XX 07MW107BX3 05XX
MW-107C	JMW107CX01	JMW107CX02	SCGW107CXX03XX	MW-107C	07MW107CXX 05XX
MW-201	—	—	—	MW-201	—
MW-202	—	—	—	MW-202 MW-202D	—
MW-203	—	—	—	MW-203	—
MW-204	—	—	—	MW-204	—
MW-OOX	—	—	SCGW00XXXX03XX	—	—
MW-9	—	—	SCGW9XXXXX03XX	—	—
MW-10	—	—	SCGW10XXXX03XX	—	—
MW-11	—	—	SCGW11XXXX03XX	—	—

TABLE 2-6
MONITORING WELL SAMPLE DESIGNATIONS

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

WELL LOCATION	ROUND 1	ROUND 2	ROUND 3	ROUND 4	ROUND 5
MW-14	—	—	SCGW14XXXX03XX	—	—
MW-22	—	—	SCGW22XXXX03XX	—	—
MW-23	—	—	SCGW23XXXX03XX	—	—
MW-24	—	—	SCGW24XXXX03XX	—	—
P1	—	—	SCGWP1XXXX03XX	—	—
P2	—	—	SCGWP2XXXX03XX	—	—
P3	—	JP3XXXXX02	—	—	—
P4	—	—	SCGWP4XXXX03XX	—	—
UST	—	JUCTANKX02	—	—	—

NOTES: UST = Underground Storage Tank

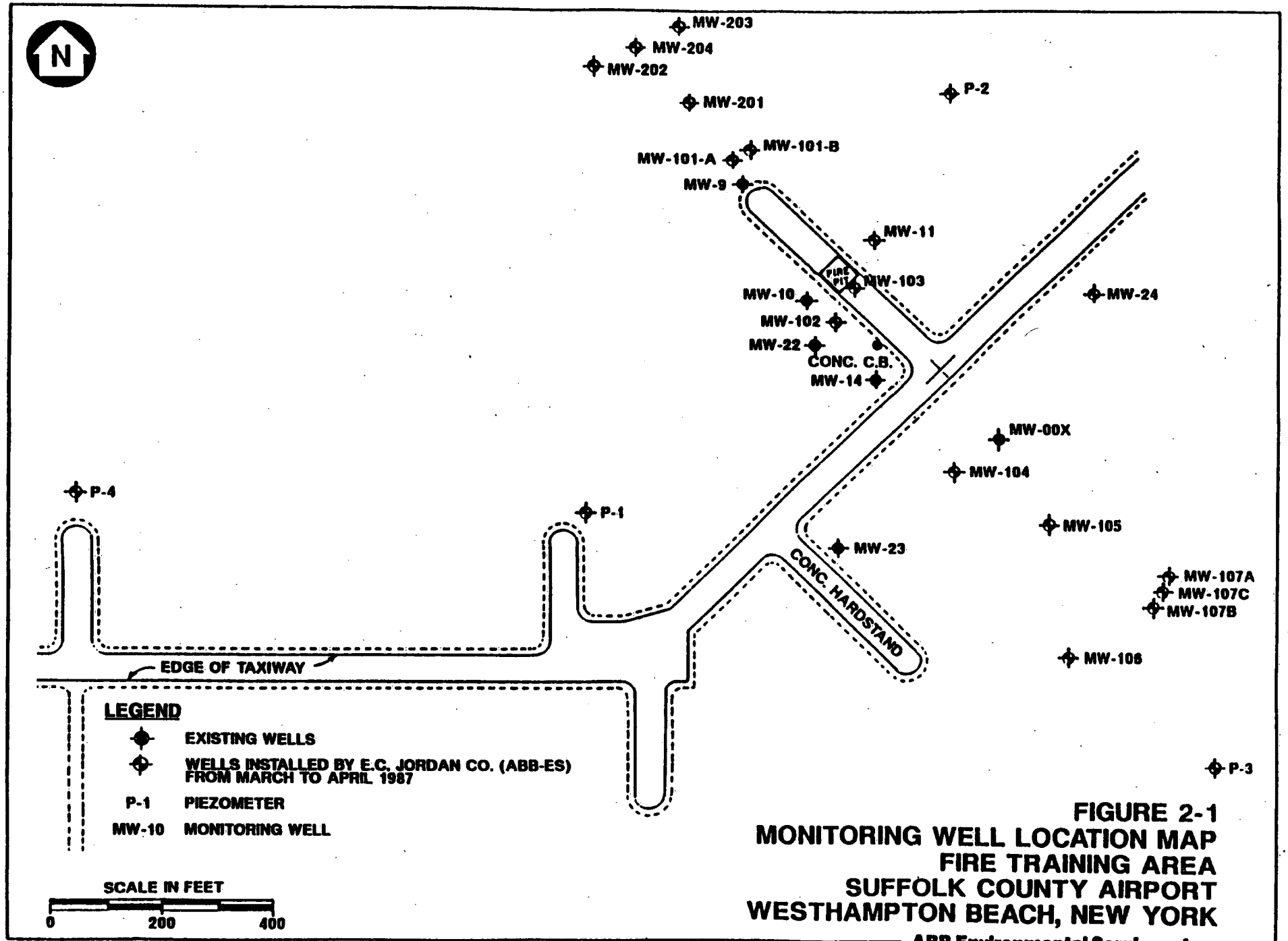


FIGURE 2-1
MONITORING WELL LOCATION MAP
FIRE TRAINING AREA
SUFFOLK COUNTY AIRPORT
WESTHAMPTON BEACH, NEW YORK

6943-02

ABB Environmental Services, Inc.

monitoring well within approximately six years. (Assuming that the SCANGB did not use 2-butanone at the FTA after 1971, it is unlikely that a source of 2-butanone could have persisted in groundwater, given estimated groundwater flow rates.)

- 2-Butanone concentrations and spatial patterns showed no definable distributions and no relation to site hydrology or any particular identifiable source.

- 2-Butanone was not reported above detection limits in any soil samples. At its higher groundwater concentrations, 2-butanone should have been detected in the associated soil column.

2.3 Previous Studies Concerning the Presence of 2-Butanone

Historically, the presence of 2-butanone in groundwater samples collected by ABB-ES during IRP investigations at military facilities presented problems because the compound did not conform to any spatial distribution patterns. This concern prompted two investigations to discuss the possibility that 2-butanone was not a site-related chemical parameter. These studies were conducted in 1988 by Andrew D. Sauter Consulting, ABB-ES (formerly E.C. Jordan Co.), and Martin Marietta Energy Systems, Inc. (Sauter and Downs, 1988; and Haase et al., 1988) in conjunction with IRP activities at the Massachusetts Military Reservation (MMR). Although no definitive explanations of the 2-butanone results were presented in the reports, both concluded that it was unlikely that 2-butanone was actually present in groundwater. The following possibilities were raised by the reports:

- 2-Butanone results could be either artificial or inaccurate due to limitations of the analytical methods.

- Contamination of the samples may have occurred during sample collection or at the laboratory.

- Variable 2-butanone concentrations observed in samples could be due to its degradation in the environment.

Although sampling procedures were considered a potential source of 2-butanone, both investigations lacked a comprehensive examination of the decontamination fluid.

2.4 CHEMISTRY OF 2-BUTANONE

With a vapor pressure of 90.6 millimeters (mm) Hg at 25°C and a boiling point of 79.6°C, 2-butanone will volatilize readily in the environment. If released into soils, 2-butanone could evaporate into the atmosphere and leach into groundwater. 2-Butanone is very soluble in water (2.68×10^5 milligrams per liter) and would be expected to migrate to and disperse within groundwater (see Appendix A). Once in the soil/groundwater system, 2-butanone will migrate with little retardation. Biodegradation does occur, and persistence in environments with microbial activity is not expected (Goyer, 1987).

Upon direct exposure to intense ultraviolet light, 2-butanone has been observed to photodegrade (Howard, 1990). However, under environmental conditions, photodegradation of 2-butanone in groundwater and during sample collection is not significant.

3.0 EVALUATION OF 2-BUTANONE IN METHYL HYDRATE DECONTAMINATION FLUID

To properly identify all the component compounds of methyl hydrate, samples from three lots were analyzed in the spring of 1990. Methyl hydrate lot numbers were not recorded during sampling events; therefore, ABB-ES was unable to correlate specific lot numbers with sampling events. The methyl hydrate analyses were performed by ABB-ES' Analytical Laboratory. Laboratory tests consisted of direct injection analysis of methyl hydrate by GC/MS and by purge-and-trap GC/MS analyses of methyl hydrate dilutions in water using U.S. Environmental Protection Agency (USEPA) methodologies. These analyses are discussed in the following subsections. Raw data from these analyses are presented in Appendices B through D.

3.1 SOLVENT PURITY BY DIRECT INJECTION

According to the product description provided by Anachemia, Inc., methyl hydrate is an industrial-grade mixture of 90 percent ethanol and 10 percent methanol. To further evaluate the chemical composition of methyl hydrate, aliquots from three lots were analyzed employing GC/MS. The aliquots were injected directly into the GC column, employing procedures commonly used in solvent purity testing. Different chemicals in the methyl hydrate were separated from one another in the GC column and appeared as separate peaks on the GC/MS chromatogram. Mass spectra and peak areas were then used to identify and quantitate the individual chemicals. Although methanol was reportedly in the methyl hydrate, methanol is not detectable by the GC/MS method; as a result, it was not evaluated. Copies of chromatograms, mass spectra, quantitation reports, spectral library comparisons, and examples of calculations are in Appendix B.

The direct injection GC/MS analysis of methyl hydrate indicated the presence of 2-butanone in all three lots tested. 2-Butanone was reported at 2.4 to 2.7 percent, relative to ethanol. Ethyl acetate was also detected in the three lots, ranging from 0.8 to 1 percent, as compared to ethanol. In addition to these compounds, several other compounds were identified at much lower concentrations in the methyl hydrate. Tentative identifications were attempted on eight additional peaks distinguishable on the chromatogram. The peaks were tentatively identified by computer matching as 2-methyl-2-propanol, acetic acid methyl ethyl ester, propanoic acid ethyl ester, and unknown methyl substituted ketones and alkanes.

3.2 PURGE AND TRAP DATA

Methyl hydrate was diluted with organic-free water to replicate groundwater sample analytical conditions and analyzed by purge-and-trap GC/MS. During the purge-and-trap GC/MS analyses, helium was passed through the sample and then through a polymer trap. VOCs carried by the helium stream were captured by the trap. The trap was then heated and the chemicals transferred to the GC column, where they were separated and evaluated (see Subsection 2.1). This method is described in the USEPA CLP Statement of Work (SOW) for organic analysis (USEPA, 1988a).

Three dilutions of methyl hydrate were analyzed with the concentration of 2-butanone at the mid-calibration range for the purge-and-trap GC/MS method (50 μg/L); two other analyses were performed with 2-butanone at higher concentrations. As a result of these analyses, a direct positive relationship between increasing concentrations of 2-butanone and increasing peak sizes of ethanol and ethyl acetate was apparent. Chromatograms, quantitation reports, and spectra are included in Appendix C. The relationship of 2-butanone, ethanol, and ethyl acetate was observed in the data from samples collected at SCANGB and is discussed in Section 4.0.

3.3 RESPONSE FACTOR FOR ETHANOL

To better interpret the concentration of ethanol reported in the samples, the approximate relative response factor (RRF) for the GC/MS analysis was calculated. The RRF is a comparison of the instrumental response of a compound (in this case, ethanol) to the response of a known concentration of an internal standard compound. In this case, the compound used for comparison was bromochloromethane, the first internal standard used in purge-and-trap GC/MS analyses as specified by the USEPA SOW. Response is measured by the areas of the chromatographic peak. An RRF of 1.0 indicates equal response of a target compound and an internal standard. Compounds that have RRFs higher than 1.0 respond well to the purge-and-trap GC/MS method and provide relatively large chromatographic peaks for a given concentration. Compounds that have RRFs lower than 1.0 yield smaller peaks for a given concentration. The difficulty of detecting compounds increases with decreasing RRFs. RRFs and internal standards are described in more detail in the USEPA SOW (USEPA, 1988a).

As calculated in Appendix D, the RRF of ethanol was quite low. An RRF of 0.00148 was calculated for ethanol using the average response of three ethanol standards at concentrations of 5,000, 10,000, and 20,000 μg/L. The RRFs calculated from the three ethanol standards are listed in the calibration summary in Appendix C. Raw data are included in Appendix D.

In CLP analyses, ethanol is not on the USEPA TCL. When present, ethanol would be reported as a tentatively identified compound (TIC) in sample data. The procedure used to calculate the concentration of TICs assumes that each TIC has an RRF of 1.0. Based on the low RRF values calculated for ethanol from the ABB-ES laboratory data, and the procedures routinely followed in CLP VOC data interpretation, concentrations of ethanol in sample data would be reported two to three orders of magnitude lower than the actual concentration. Ethyl acetate would also be evaluated as a TIC in samples analyzed by CLP methodologies. The RRF for ethyl acetate was not determined in this study.

In contrast to ethanol, 2-butanone is on the USEPA TCL, and reported 2-butanone concentrations are based on calibration standards defined in the USEPA SOW (USEPA, 1988a). Therefore, 2-butanone values reported in sample data should accurately represent the concentration in the sample.

4.0 EVALUATION OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE IN GROUNDWATER SAMPLES

The following subsections describe the presence of 2-butanone, ethanol, and ethyl acetate in five rounds of groundwater samples collected from the FTA. Full CLP deliverables were available from the five groundwater sampling events at SCANGB and were reviewed by ABB-ES personnel for the presence of ethanol and ethyl acetate in conjunction with 2-butanone. Non-target compound chromatographic peaks were compared to mass spectral libraries and reported as TICs. Ethanol and ethyl acetate were identified as TICs in many cases. Complementary data summary tables are presented in the following subsections for all samples containing one of these three compounds.

4.1 ROUND 1

2-Butanone, ethanol, and ethyl acetate results from Round 1 are listed in Table 2-1 for all samples containing one of the three compounds. 2-Butanone was reported in five of 14 (36 percent) samples collected during Round 1 at concentrations ranging from 18 to 56,000 μg/L. These values did not appear to follow any spatial distribution pattern. Four of these samples, MW-101A, MW-102, JDUP1 (designation for duplicate of MW-102), and MW-107A, possessed 2-butanone concentrations of less than 100 μg/L, while 2-butanone was reported at 56,000 μg/L in MW-107B. Ethanol, the primary fingerprint compound, was noted in all five (100 percent) samples containing 2-butanone. Ethyl acetate, the secondary fingerprint compound, was only noted in MW-107B, where 2-butanone was most concentrated. Neither of the fingerprint compounds were identified in samples where 2-butanone was not present.

4.2 ROUND 2

The samples collected in Round 2 showed a similar pattern of 2-butanone, ethanol, and ethyl acetate detection as observed in conjunction with the Round 1 data. 2-Butanone, ethanol, and ethyl acetate results for these samples are summarized in Table 2-2. Eleven out of 16 (69 percent) samples contained 2-butanone at concentrations ranging from 9J to 14,000 μg/L. These values did not appear to follow any spatial distribution pattern. Ethanol was reported in eight (73 percent)

of these 11 samples at concentrations ranging from 9 to 1,400 μg/L. Three (27 percent) of these samples contained ethyl acetate at concentrations ranging from 12 to 950 μg/L (i.e., MW-107B, MW-101B, and MW-101A). As expected, these three samples also had the highest reported concentrations of 2-butanone.

An equipment rinsate blank (designated as SB-1) contained 2-butanone at 7.8 μg/L. The presence of 2-butanone in this sample is important because it directly represents product introduced during decontamination procedures.

4.3 ROUND 3

Twenty-seven groundwater samples (1 MS/MSD) were collected during Round 3, and 24 contained 2-butanone. Of these, 22 (92 percent) exhibited the fingerprint compound ethanol, and 17 (71 percent) exhibited ethyl acetate. These values did not follow any spatial distribution pattern. A summary of the data for 2-butanone, as well as ethanol and ethyl acetate, is presented in Table 2-3. The same positive correlation between frequency of occurrence and relative concentrations of these three compounds that was apparent in the 1987 groundwater data was evident in the Round 3 data; that is, ethanol concentrations increased as 2-butanone concentrations increased, and ethyl acetate was detected in samples where 2-butanone and ethanol were reported at relatively high concentrations. A statistical analysis of these data is presented in Section 7.0.

In Round 3, several additional TIC compounds were reported in sample MW-107B, in which a particularly high concentration of 2-butanone (53,000 μg/L) was reported. The reported TICs in sample MW-107B are listed in Figure 4-1. The list of TICs includes acetic acid methylethyl ester and propanoic acid ethyl ester. These TICs were also detected during the direct injection analyses of methyl hydrate as discussed in Subsection 3.1 of this report, and detailed in Appendix B. The low concentrations of these TICs detected in this sample, relative to ethanol and 2-butanone, are similar to the relative concentrations reported in the laboratory analysis of methyl hydrate.

4.4 ROUND 4

During Round 4, 20 groundwater samples were collected without the use of methyl hydrate during decontamination procedures. Instead, DI water and Liquinox were used to decontaminate sampling equipment. Summary data from 20 samples are

FIGURE 4-1: TENTATIVELY IDENTIFIED COMPOUNDS REPORTED IN MW-107B (ROUND 3)

1E
VOLATILE ORGANICS ANALYSIS DATA SHEET
TENTATIVELY IDENTIFIED COMPOUNDS

EPA SAMPLE NO
SCGW107BX

Lab Name: COMPUCHEM LABS Contract: (10-86)-REV

Lab Code: COMPU Case No.: 16160 SAS No.: _____ SDG No.: 01

Matrix: (soil/water) WATER Lab Sample ID: 244461

Sample wt/vol: 0.50 (g/mL) ML Lab File ID: CN044461B09

Level: (low/med) LOW Date Received: 02/09/89

% Moisture: not dec. ____ Date Analyzed: 02/09/89

Column (pack/cap) PACK Dilution Factor: 1.0

Number TICs found: 8

CONCENTRATION UNITS:
(ug/L or ug/Kg) UG/L

CAS NUMBER	COMPOUND NAME	RT	EST. CONC.	Q
1.	INSTRUMENT ARTIFACT	2.03	160	J
2.	UNKNOWN	5.43	25000	J
3. 79-20-9	ACETICACID,METHYLESTER	9.15	100	J
4.	UNKNOWN BUTANOL	13.72	60	J
5. 141-78-6	ACETICACIDETHYLESTER	14.39	4400	J
6.	UNKNOWN	17.79	30	J
7.	UNKNOWN	18.60	70	J
8. 105-37-3	PROPANOICACID,ETHYLESTER	18.90	60	J

shown in Table 2-4. 2-Butanone was detected in only two samples (10 percent), in MW-107A at 10 μg/L and MW-107B at 4,300 μg/L. Ethanol and ethyl acetate were reported in MW-107B at 720 μg/L and 160 μg/L, respectively, but were absent from MW-107A. Methyl hydrate fingerprint compounds were most likely absent from MW-107B during Round 4 because methyl hydrate was not present at a concentration high enough that these compounds could be detected. Although ethanol was not reported by the laboratory as a TIC in MW-107A, the GC/MS data review identified a small peak at the expected retention time for ethanol. Because this peak represented less than 10 percent of the peak height of the nearest internal standard, it was not included as a TIC as described in CLP methodologies.

It should also be noted that ethanol was reported in samples from MW-101A and MW-202 at 15 μg/L and 52 μg/L, respectively, although no 2-butanone was present.

As with Round 3, the Round 4 sample from well MW-107B contained additional TICs identified during GC/MS analysis of methyl hydrate. A summary of these TICs is in Figure 4-2.

4.5 ROUND 5

Five groundwater samples were collected during the most recent round of sampling in October 1991; of these, three were from MW-107B. MW-107B was focused on during this last sampling event because it exhibited a relatively high concentration of 2-butanone throughout the previous four sampling rounds. During this final sampling round, special purging techniques were used to ascertain whether 2-butanone was a genuine aquifer contaminant. The sampling procedures and the results are described in detail in Section 6.0. Briefly, 2-butanone was only detected in one sample, the first collected, from MW-107B during Round 5. Ethanol and ethyl acetate were also identified in this sample at 4,400 and 900 μg/L, respectively. No compounds were detected in MW-107B after extensive purging of the well. Neither 2-butanone nor any of the fingerprint compounds were identified in the other wells sampled during Round 5. The significance of these findings is presented in Section 6.0.

FIGURE 4-2: TENTATIVELY IDENTIFIED COMPOUNDS REPORTED IN MW-107B (ROUND 4)

1E
VOLATILE ORGANICS ANALYSIS DATA SHEET
TENTATIVELY IDENTIFIED COMPOUNDS

EPA SAMPLE NO.
MW-107B

Lab Name: COMPUCHEM LABS Contract: (2-88)-REVS

Lab Code: COMPU Case No.: 18312 SAS No.: _____ SDG No.: 05

Matrix: (soil/water) WATER Lab Sample ID: 308916

Sample wt/vol: 5.0 (g/mL) ML Lab File ID: CN008916C11

Level: (low/med) LOW Date Received: 12/14/89

% Moisture: not dec. ____ Date Analyzed: 12/19/89

Column (pack/cap) CAP Dilution Factor: 1.0

Number TICs found: 8

CONCENTRATION UNITS:
(ug/L or ug/Kg) UG/L

CAS NUMBER	COMPOUND NAME	RT	EST. CONC.	Q
1. 64-17-5	ETHANOL	2.92	720	J
2. 141-78-6	ACETICACIDETHYLESTER	5.23	160	J
3. 554-12-1	PROPANOICACID,METHYLESTER	5.62	10	J
4. 14898-79-4	2-BUTANOL,(R)-	5.82	87	J
5. 71-36-3	1-BUTANOL	7.68	40	J
6. 105-37-3	PROPANOICACID,ETHYLESTER	7.92	10	J
7. 623-42-7	BUTANOICACID,METHYLESTER	8.20	7.0	J
8. 105-54-4	BUTANOICACID,ETHYLESTER	10.30	37	J

5.0 TEMPORAL COMPARISON OF 2-BUTANONE GROUNDWATER DATA

Fourteen monitoring wells from the FTA were sampled a minimum of two times from April 1987 to December 1989. In addition, these same 14 monitoring wells were sampled both with and without the use of methyl hydrate as a decontamination fluid. 2-Butanone data for these monitoring wells are summarized in Table 5-1. The most important transition is denoted in Table 5-1 with a bold vertical line indicating when the use of methyl hydrate was discontinued. In no instance did a concentration of 2-butanone increase from Round 3 to Round 4. In fact, the 2-butanone occurrence rate decreased from 93 percent (13/14) in Round 3 to 14 percent (2/14) in Round 4.

2-Butanone most likely was present in the form of residues in these monitoring well riser columns as a result of the heavy use of methyl hydrate during previous sampling rounds. Ethanol was identified in both MW-107A and MW-107B during Round 4, suggesting a residual concentration of methyl hydrate in Round 4 samples collected from these two wells.

TABLE 5-1
2-BUTANONE CONCENTRATIONS IN MONITORING WELLS SAMPLED MULTIPLE TIMES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in µg/L)

WELL LOCATION	ROUND 1	ROUND 2	ROUND 3	ROUND 4
P-1	--	--	13,000	10 U
P-2	--	--	26	10 U
P-3	--	31	170	10 U
P-4	--	--	190	10 U
MW-101A	18	312	320	10 U
MW-101B	10 U	1,400	R	10 U
MW-102	55	9	94	10 U
MW-103	10 U	10 U	31	10 U
MW-104	10 U	19	150	10 U
MW-105	10 U	8	460	10 U
MW-106	10 U	27	40	10 U
MW-107A	65	24	830	10
MW-107B	56,000	14,000	53,000	4,300
MW-107C	10 U	10 U	150	R

NOTES:

When duplicates were collected, an average of the two numbers was used.

"--" = indicates the well was not sampled during that round.
U = less than Quantitation Limit.
µg/L = micrograms per liter.
R = Rejected Data.

6.0 OCTOBER 1991 SAMPLING AND ANALYSIS OF MW-107B

To test the hypothesis that 2-butanone was introduced to monitoring wells as a component of methyl hydrate, a sampling experiment was developed and implemented at the FTA in October 1991 with an emphasis on MW-107B. MW-107B was chosen for this activity because it had particularly high concentrations of 2-butanone throughout all sampling events at SCANGB. It was hypothesized that if a well were to contain 2-butanone as a genuine contaminant (at least in part), MW-107B would be the most likely candidate. However, if 2-butanone was a residual contaminant, extensive purging of this well should remove residual 2-butanone.

The first stage of the test involved sampling the monitoring well using standard sampling procedures with Liquinox as a decontamination fluid. After purging three well volumes, standard protocol for well sampling, a sample was collected. This sample contained 2-butanone at 1,600 μg/L and the methyl hydrate fingerprint of both ethanol (4,400 μg/L) and ethyl acetate (900 μg/L). After collecting the first sample, the monitoring well was again purged for approximately 10 minutes. Discharged water was directed back down the well to thoroughly wash the inside walls. After 10 minutes of washing, seven additional well volumes were purged and the monitoring well was resampled. Neither 2-butanone, ethanol, nor ethyl acetate were identified in the second sample (see Table 6-1).

Because they did not have the benefit of CLP results on site, the field sampling crew repeated the procedure to ensure that 2-butanone had been decreased to the lowest possible concentration. Neither 2-butanone, ethanol, nor ethyl acetate were identified during the analysis of the final sample collected from MW-107B.

If 2-butanone had been a genuine aquifer contaminant, these field activities should have had little or no effect on 2-butanone concentrations. Instead, the washing eliminated detectable 2-butanone in MW-107B. Clearly, at least in MW-107B, 2-butanone is not an aquifer contaminant, but rather an artifact introduced during prior sampling rounds. TIC data from MW-107B indicated significant concentrations of both fingerprint compounds (i.e., ethanol and ethyl acetate) throughout Rounds 1 through 4. It can be concluded that methyl hydrate is accountable for all detectable 2-butanone in MW-107B.

TABLE 6-1
CONCENTRATIONS OF 2-BUTANONE, ETHANOL, ETHYL ACETATE IN MW-107B SAMPLES COLLECTED IN OCTOBER 1991

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

(all concentrations in µg/L)

	Round 1	Round 2	Round 3	Round 4	Round 5*	Round 5#A	Round 5#B
2-Butanone	56,000	14,000	53,000	4,300	1,600	10 U	10 U
Ethanol	17,000 J	1,400 J	33,000 J	720 J	4,400 J	10 U	10 U
Ethyl Acetate	3,200 J	950 J	3,800 J	160 J	900 J	10 U	10 U

NOTES:

Methyl hydrate was used for decontamination in conjunction with Rounds 1, 2, and 3. Liquinox and water were used in conjunction with Rounds 4 and 5.

*	=	standard three-well-volume purge
#A	=	three-well-volume purge/10-minute wash/seven-well-volume purge
#B	=	Same procedure as #A, repeated after #A
U	=	less than Quantitation Limit
µg/L	=	micrograms per liter
J	=	Estimated Data

It is inferred from this one experiment that monitoring wells sampled using methyl hydrate as a decontamination fluid could contain residual 2-butanone. Monitoring wells appear to be cleansed of residual 2-butanone by thorough purging and rinsing.

7.0 STATISTICAL ANALYSIS OF 2-BUTANONE GROUNDWATER DATA

To generate further evidence that methyl hydrate contamination is the cause of 2-butanone in groundwater samples at SCANGB, a statistical evaluation was performed on all groundwater data. These data included all 74 groundwater samples (three samples were excluded from statistical analysis as a result of validation flagging them as unusable [R] and associated 2-butanone, ethanol, and ethyl acetate results.

Because ethanol and ethyl acetate were reported as TICs, these concentrations were quantified based on a response factor of 1.0 (see Subsection 3.3). As a result, direct statistical comparison of concentration data is difficult. However, this inconsistency in quantitation does not preclude a correlation analysis of relative concentrations among 2-butanone, ethanol, and ethyl acetate. Plots of 2-butanone concentrations versus relative concentrations of ethanol and ethyl acetate are provided in Figures 7-1 and 7-2, respectively, illustrating that the concentrations of these constituents in groundwater appear to be positively correlated.

If methyl hydrate is the cause of 2-butanone contamination, then samples with high concentrations of 2-butanone would be expected to exhibit analogously high concentrations of ethanol and ethyl acetate as a result of these relative concentrations. Low 2-butanone concentrations would be associated with low ethanol and ethyl acetate concentrations. The Kendall Tau coefficient procedure, a nonparametric statistical procedure, was chosen to assess the relative correlation of the data. The Kendall Tau coefficient measures the degree of association between the relative magnitudes of two variables. In this case, the associations measured were those between 2-butanone and ethanol and 2-butanone and ethyl acetate. The procedure requires that the concentrations for each of the three compounds for each data point be ranked relative to all other respective concentrations. In order to calculate the Kendall Tau test statistic the relative concentration of each compound is ranked in ascending order. Let X_i denote the *ith* observation of the arbitrarily designated first compound and Y_i denote the *ith* observation of the second compound. When the X observations or ranks are written in natural order, the value of U may be found by simply counting the number of Y pairs that also appear in natural order. With the Y ranks listed in the order corresponding to the X observations that are in their natural order U is calculated by the sum of the Y ranks greater and to the right of each successive Y rank. The Kendall Tau test statistic is then calculated by the following equation:

FIGURE 7-1 PLOT OF 2-BUTANONE VS. ETHANOL

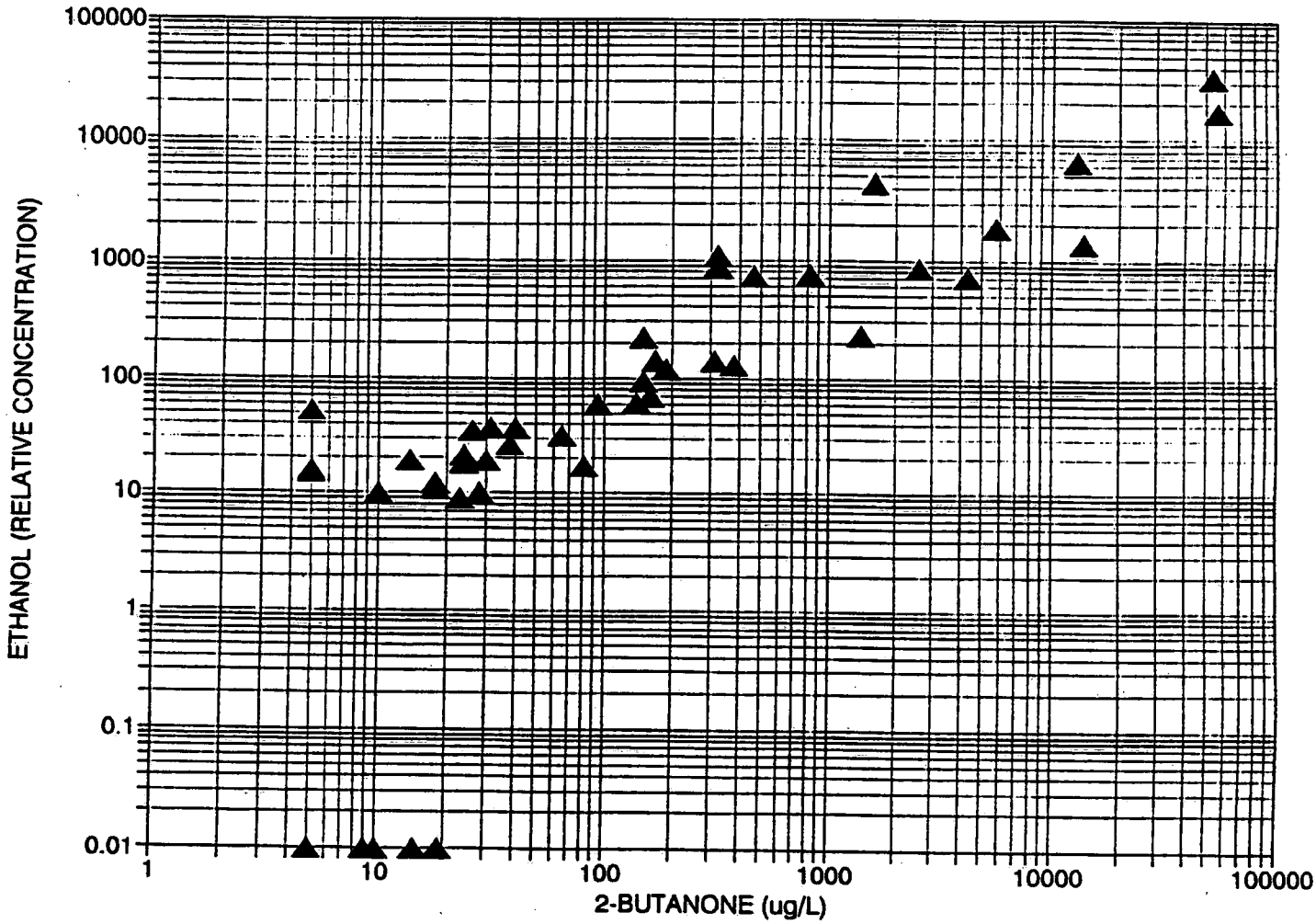
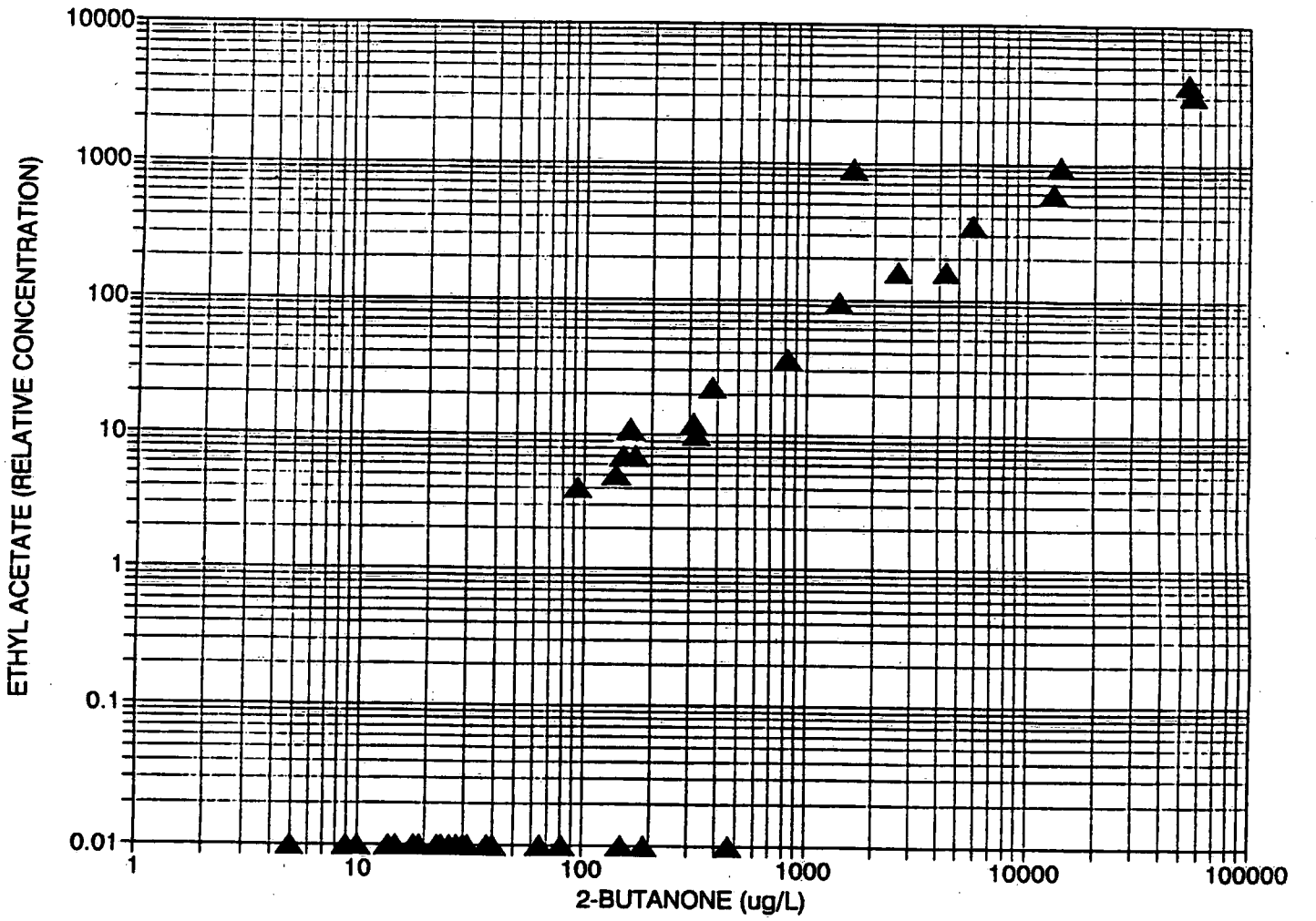


FIGURE 7-2 PLOT OF 2-BUTANONE VS. ETHYL ACETATE



$$T = \frac{4U}{n(n - 1)} - 1$$

A test statistic equal to zero indicates no correlation; equal to 1, a perfect positive correlation; and equal to -1, a perfect negative, or inverse, correlation.

For large sample sizes (i.e., greater than 60 data points), the probability level of the Kendall Tau test statistic (T) is approximated by the following equation:

$$Z = \frac{3T\sqrt{n(n - 1)}}{\sqrt{2 * (2n + 5)}}$$

T is the calculated Kendall Tau statistic, n is the sample size, and Z is the standard normal deviate. High probability percentages (close to 100 percent) indicate significant evidence that the data are correlated.

The Kendall Tau statistics for the comparisons of 2-butanone and ethanol and 2-butanone and ethyl acetate are in Table 7-1. The approximate standard normal values (Z-value) are in Table 7-2, and the approximate probability levels are in Table 7-3.

Test results indicate an extremely significant evidence of correlations between 2-butanone and ethanol and 2-butanone and ethyl acetate (i.e., all pairs of compounds). The probability that the ranks of the concentrations are due to random chance is essentially zero.

TABLE 7-1
KENDALL TAU COEFFICIENTS

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

COMPOUND	2-BUTANONE	ETHANOL	ETHYL ACETATE
2-Butanone	1.000	—	—
Ethanol	0.853	1.000	—
Ethyl Acetate	0.714	0.698	1.000

TABLE 7-2
APPROXIMATE Z-VALUES

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

COMPOUND	2-BUTANONE	ETHANOL	ETHYL ACETATE
2-Butanone	*	—	—
Ethanol	10.58	*	—
Ethyl Acetate	8.85	8.65	*

NOTE:

* There is always perfect correlation between a parameter and itself.

TABLE 7-3
APPROXIMATE PROBABILITY LEVELS

SUFFOLK COUNTY AIR NATIONAL GUARD BASE
WESTHAMPTON BEACH, NEW YORK

COMPOUND	2-BUTANONE	ETHANOL	ETHYL ACETATE
2-Butanone	100%	—	—
Ethanol	> 99.99%	100%	—
Ethyl Acetate	> 99.99%	> 99.99%	100%

8.0 DISCUSSION

Based on the laboratory analyses of methyl hydrate, a review of sample data collected at the SCANGB FTA between April 1987 and October 1991, and results of statistical analyses, a relationship between the chemical composition of methyl hydrate and compounds reported in the groundwater samples can be established. The data in this report demonstrate a clear link between the use of methyl hydrate during sampling equipment decontamination and the presence of 2-butanone in groundwater samples collected at the SCANGB FTA.

One possible method for the introduction of methyl hydrate into groundwater samples was through the use of submersible pumps for purging monitoring wells prior to sampling. Deep well submersible bladder pumps were used to purge the required well volumes of groundwater prior to bailing samples for analyses of VOCs. Between each sampling event, submersible pumps were decontaminated with a Liquinox/water solution, followed by a tap water rinse, a methyl hydrate rinse, and a thorough deionized water rinse. The methyl hydrate was placed in the receptacle used to carry the intake portion of the pump, and was then pumped through the pump and all associated tubing. The pump was left running until the methyl hydrate stopped discharging from the tubing; however, it is likely a small amount of methyl hydrate remained in the pump and tubing. A larger volume of deionized water was used as the final rinse, however adequate volumes of water to completely remove all the methyl hydrate may not have been used. Also, the internal components of the submersible pump are constructed in such a way that methyl hydrate residues probably were trapped in the system. The submersible pumps were lowered into the monitoring well until they reached the water table. During this time, the tubing was straightened and residual decontamination fluids were allowed to collect in the intake portion of the pump. The pumps were turned on after they were positioned in the water column and they were lowered through the water column to allow complete removal of groundwater in the water column. This procedure would allow methyl hydrate residues to enter the water column and therefore to have been collected during sampling.

Laboratory analyses of three lots of methyl hydrate identified its principal components as ethanol, 2-butanone, and ethyl acetate. Methanol, another major component of methyl hydrate, was not addressed during this investigation because it is not detected by the GC/MS method used for this investigation. These relative concentrations suggest that ethanol should appear in methyl-hydrate-contaminated

samples at the highest concentration of the three compounds. However, because of the low GC/MS response and the method of quantitation (see Subsection 3.3), ethanol is detected only in samples with significant (greater than 20 μg/L) concentrations of 2-butanone.

At the FTA, ethanol was present in 37 of 41 (90 percent) samples where 2-butanone was reported. The four samples that did not exhibit the methyl hydrate fingerprint had 2-butanone concentrations of 9, 10, 15, and 19 μg/L. Because of the low RRF of ethanol, the fingerprint would not be expected to be present when the concentration of 2-butanone is so low.

In addition, ethyl acetate was present in 22 of 44 (54 percent) samples when 2-butanone was detected. Ethyl acetate was reported in 100 percent of those samples that exhibited a 2-butanone concentration of more than 150 μg/L. Of the three compounds, ethyl acetate is present at the lowest concentrations in methyl hydrate (i.e., approximately 1 percent by volume). Lower concentrations of ethanol and 2-butanone reflect less sample contamination. Ethyl acetate may be below the instrument detection limit; if so, it would not be reported. Therefore, the lack of detectable concentrations of ethyl acetate does not invalidate the fingerprint.

A comparison was made between samples from SCANGB and the laboratory purge-and-trap analyses of methyl hydrate diluted in water. Appendix C contains the chromatograms of laboratory dilutions of methyl hydrate. The laboratory chromatograms are similar to chromatograms from field samples in which 2-butanone is present. The comparative concentrations vary between sampling periods and individual samples; however, the peaks for ethanol, 2-butanone, and ethyl acetate show a strong relationship to one another (see Section 7.0). This positive correlation is consistent with the theory that these three compounds originate from the same source; that is, methyl hydrate. The same pattern of relative concentration ratios was observed in groundwater data from investigations at other military installations where ABB-ES personnel used methyl hydrate as a decontamination fluid (e.g., MMR) (ABB-ES, 1991). It is unlikely that unrelated sites would have similar patterns of groundwater contamination. A feature common to all these sites is the decontamination fluid used during sample collection.

The relative concentrations of 2-butanone, ethanol, and ethyl acetate detected in FTA samples did show some variability, which could be due to several factors depending on the physicochemical properties of these compounds (see Appendix A). Because the volatilities and solubilities of these compounds differ, the concentrations

are affected by the ambient temperature, atmospheric conditions at the time of sampling, and the amount of water used to rinse sampling equipment. Because these factors do not remain constant throughout the year or even during an entire sampling event, some variability in the relative concentrations of these compounds is expected. In addition, ethanol, the primary fingerprint compound, is subject to hydrolysis (note: ethanol hydrolyses to ethyl acetate), which would affect the relative concentrations of the three compounds.

In addition to the statistical analysis and the fingerprint that links the use of methyl hydrate to 2-butanone in groundwater samples, other evidence described in this evaluation includes:

- the near elimination of detectable 2-butanone in monitoring wells between Rounds 3 and 4 (from 93 percent occurrence to 14 percent occurrence) after the use of methyl hydrate was discontinued (see Section 5.0);
- the elimination of 2-butanone in MW-107B after the sampling procedure was specially modified for testing purposes (see Section 6.0);
- the elimination of 2-butanone in all other wells between Rounds 4 and 5; and
- the presence of fingerprint compounds in only 3 of 39 (8 percent) samples when 2-butanone was not detected; therefore, this lack of false positives supports the integrity of the model.

9.0 CONCLUSIONS AND RECOMMENDATIONS

ABB-ES' evaluation of groundwater sample data collected at SCANGB FTA since April 1987 indicates that the presence of 2-butanone in groundwater samples is attributable to the use of commercial methyl hydrate as a decontamination fluid for sampling equipment. ABB-ES personnel used methyl hydrate for equipment decontamination while collecting of most of the affected samples (i.e., Rounds 1, 2, and 3). Analytical data from samples collected during this time indicate a high frequency of elevated concentrations of 2-butanone. The concentration and frequency of 2-butanone decreased during subsequent sampling rounds when methyl hydrate was not used as a decontamination fluid. 2-Butanone observed in samples collected during Rounds 4 and 5 apparently results from residual methyl hydrate introduced into the monitoring wells during previous sampling events. By Round 5, 2-butanone was eliminated from all wells except MW-107B. Extensive purging of the water column in the riser of MW-107B during Round 5 eliminated 2-butanone.

Evidence gathered by ABB-ES personnel supports the theory that the 2-butanone identified at SCANGB FTA was attributable to the use of methyl hydrate. The evidence includes laboratory analyses of undiluted and diluted methyl hydrate, which revealed that methyl hydrate consists primarily of approximately 90 percent ethanol, 2.5 percent 2-butanone, and 1 percent ethyl acetate. ABB-ES personnel reviewed CLP data packages for all sampling events at SCANGB FTA since April 1987, focusing on an evaluation of nontarget compounds reported as TICs.

In nearly all samples where 2-butanone was detected, ethanol was also detected. A strong positive correlation was observed among the concentrations of 2-butanone, ethanol, and ethyl acetate in all samples where they were detected. Furthermore, in samples with relatively high reported concentrations of 2-butanone, ethyl acetate was also observed. The chemical characterization of methyl hydrate and identification of ethanol and ethyl acetate in samples where 2-butanone was detected provided a fingerprint of methyl hydrate contamination. The much higher concentrations of 2-butanone observed in MW-107B, as compared to other monitoring wells, may be due to variations in the source and composition of the methyl hydrate, as well as sampling variabilities. Any doubt surrounding 2-butanone concentrations in this well were eliminated in October 1991 through the implementation of modified sampling techniques (see Section 6.0) that purged 2-butanone from the water column of MW-107B.

Finally, ABB-ES evaluated data from other sites where methyl hydrate was used as a decontamination fluid, and where water samples also contained 2-butanone. These evaluations revealed the same strong correlations among 2-butanone, ethanol, and ethyl acetate discussed herein (ABB-ES, 1991).

ABB-ES concludes that the 2-butanone reported in groundwater samples collected at SCANGB FTA is not site-related; rather, it is an artifact of sample collection. The 2-butanone data should not be used in any risk assessments conducted for the FTA.

ABB-ES recommends that methyl hydrate no longer be used for decontaminating sampling equipment. ABB-ES discontinued its use at SCANGB in 1989.

ABB-ES	ABB Environmental Services, Inc.
CLP	Contract Laboratory Program
DI	deionized water
FSCR	Final Site Characterization Report
FTA	Fire Training Area
GC	gas chromatography
HAZWRAP	Hazardous Waste Remedial Action Program
Hg	mercury
IRP	Installation Restoration Program
mm	millimeters
MMR	Massachusetts Military Reservation
MS	mass spectrometry
MW	monitoring well
NR	Not Reported
RRF	relative response factor
SCANGB	Suffolk County Air National Guard Base
SOW	Statement of Work
TCL	Target Compound List
TIC	tentatively identified compound
USEPA	U.S. Environmental Protection Agency
VOCs	volatile organics compounds
μg/L	micrograms per liter

ABB-Environmental Services, Inc. (ABB-ES) 1991. "Evaluation of 2-Butanone in Groundwater Samples: Task 2-4, Task 2-5, and Task 2-5B"; Installation Restoration Program; Massachusetts Military Reservation; prepared for HAZWRAP; Portland, Maine; March 1991.

Goyer, M.M., M.L. Bonfiglio, P.M. Capomaccio, D.L. Gerundolo, S.F. Goons, J.H. Hagopian, C.P. Loreti, W.J. Lyman, and J.H. Perwak, 1987. "The Installation Restoration Program Toxicology Guide"; Volume II; ADA191175; Harry G. Armstrong Aerospace Medical Research Laboratory; Wright-Patterson Air Force Base, Ohio.

Haase, S.C., B.C. Wallin, and M.S. Miller, 1988. "Evaluation of Methyl Ethyl Ketone (2-Butanone) Contamination at the Massachusetts Military Reservation"; E.C. Jordan Co., Oak Ridge, Tennessee and Portland, Maine; Martin Marietta Energy Systems, Inc., Oak Ridge, Tennessee.

Howard, P.H., 1990. Handbook of Environmental Fate and Exposure Data for Organic Chemicals; Vol. II, Solvents; Lewis Publishers; Chelsea, Michigan.

Lyman, W., W. Riehl, and D. Rosenblatt, 1982. Chemical Property Estimation Methods/Environmental Behavior of Organic Compounds; McGraw-Hill Book Company; New York, New York.

Sauter, A.D. and J.J. Downs, 1988. "On the Presence of 2-Butanone in MMR Groundwater: Observations, Conclusions and Recommendations"; HAZWRAP.

U.S. Air Force Installation Restoration Program, 1989. "Final Site Characterization Report - Suffolk County Airport Fire Training Area, Westhampton Beach, N.Y."; HAZWRAP; prepared by E.C. Jordan Co.; June 1989.

U.S. Environmental Protection Agency (USEPA), 1986. "Superfund Public Health Evaluation Manual"; Office of Emergency and Remedial Response; Washington, DC; USEPA/540/1-86/060; October 1986.

U.S. Environmental Protection Agency (USEPA), 1988a. "Contract Laboratory Program Statement of Work for Organic Analyses"; Analytical Operations Branch; Washington, DC; February 1988.

U.S. Environmental Protection Agency (USEPA), 1988b. "Region I Laboratory Data Validation: Functional Guidelines for Evaluating Organic Analyses"; prepared for the USEPA Hazardous Site Evaluation Division; Washington, DC; February 1, 1988 (modified November 1988).

U.S. Environmental Protection Agency (USEPA), 1989. "Risk Assessment Guidance for Superfund Volume 1"; Human Health Evaluation Manual (Part A); USEPA/540/1-89/002; December 1989.

APPENDIX A

PHYSICOCHEMICAL CHARACTERISTICS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE

APPENDIX A: PHYSICOCHEMICAL CHARACTERISTICS OF 2-BUTANONE, ETHANOL, AND ETHYL ACETATE

	MOLECULAR WEIGHT (g/mole)	WATER SOLUBILITY (mg/L)	VAPOR PRESSURE (mmHg)	HENRY'S LAW CONSTANT (atm-m^3/mole)	K_{oc} (mL/g)	BOILING POINT degrees Centigrade	BIODEGRADATION
Ethanol	46	1.00+06	59 at 25°C	4.48 E-05 (3)	2.2	78.5	moderately-relatively
2-Butanone	72	2.68+05	90.6 at 25°C	2.74 E-05 (1) 1.05E-05 (1)	4.5	79.6	relatively
Ethyl Acetate	88	6.40+04	69.0 at 19°C	1.2E-04 (1)	-	77	relatively

SOURCES: Howard, 1990; Lyman, et al., 1982; and USEPA, 1986.

APPENDIX B

DIRECT INJECTION DATA FOR METHYL HYDRATE

APPENDIX B

DIRECT INJECTION DATA FOR METHYL HYDRATE

Method Blank
Methyl Hydrate Lot C780708 - 2 ul Injection
Methyl Hydrate Lot C780811 - 2 ul Injection
Methyl Hydrate Lot C880524 - 2 ul Injection
Methyl Hydrate - 5 ul Injection Including Trace
Compound Spectra and Library Comparisons

Summary of Direct Injection Results for MEK and Ethyl Acetate in Methyl Hydrate

Lot No.	C-EE Sample Id	Percentage MEK	Percentage Ethyl Acetate
C780708	90018-017	2.4	0.8
C780811	90018-018	2.5	0.8
C880524	90018-019	2.7	1.0

An example calculation for Lot C780708 is presented below:

(Sample 90018-017)

$$\frac{\text{Area MEK}}{\text{Area of Ethanol}} * 100 = \text{Percent MEK}$$

$$\frac{141129}{5796672} * 100 = 2.43$$

$$\frac{\text{Area Ethyl Acetate}}{\text{Area of Ethanol}} * 100 = \text{Percent Ethyl Acetate}$$

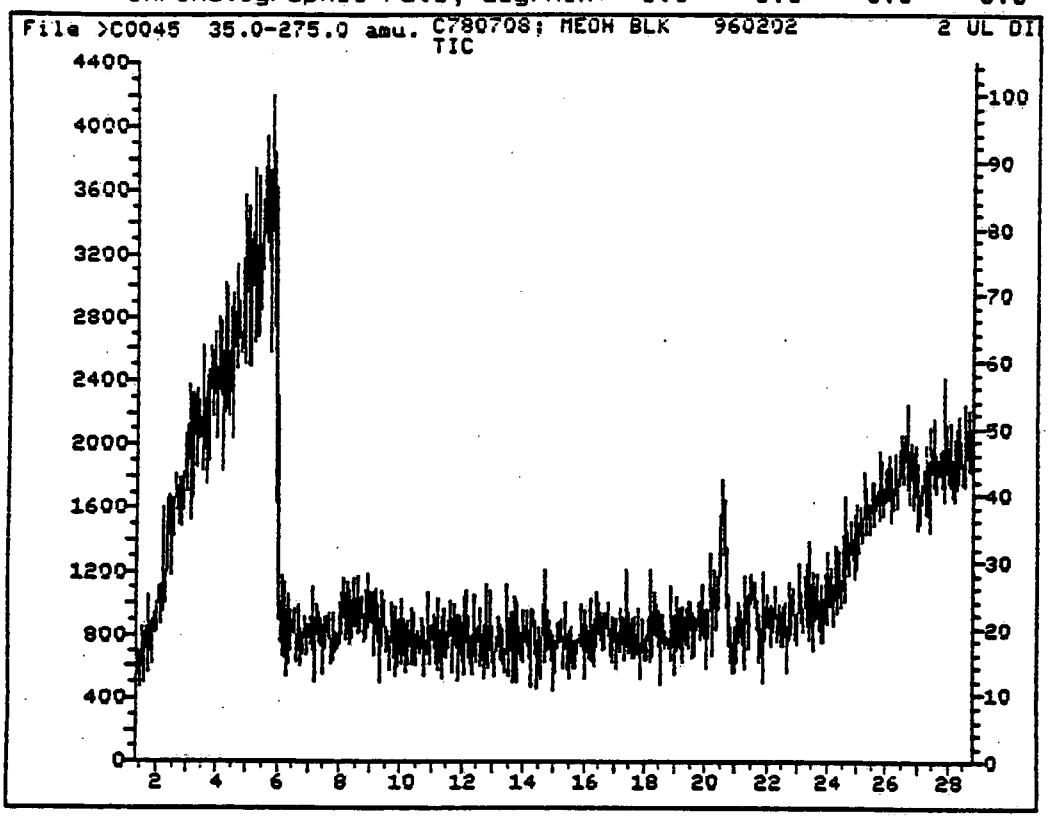
$$\frac{46272}{5796672} * 100 = 0.79$$

:MSH

MS data file header from : >C0045

Sample: C780708; MEOH BLK Operator: USER2 MS 1/23/90 13:13
Misc : 960202 2 UL DIRECT INJECTION
Sys. #: 2 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: M_CMH Tuning file: MT2000 No. of extra records: 2
Source temp.: 170 Analyzer temp.: 170 Transfer line temp. : 170

Chromatographic temperatures :	40.	230.	0.	0.	0.
Chromatographic times, min. :	4.0	1.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	8.0	0.0	0.0	0.0	0.0



Method Blank for Direct Injection

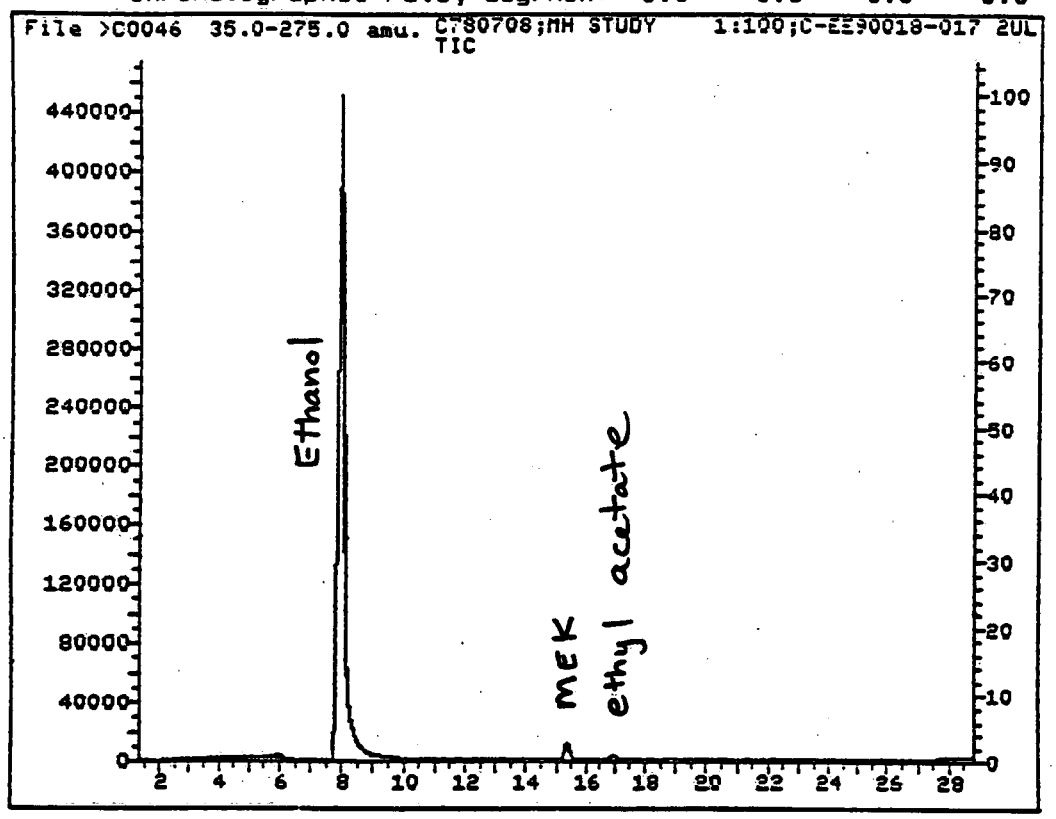
2 uL Methanol

:MSH

MS data file header from : >C0046

Sample: C780708;MH STUDY Operator: USER2 MS 1/23/90 13:50
Misc : 1:100;C-EE90018-017 2UL DIR INJECTION
Sys. #: 2 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: M_CMH Tuning file: MT2000 No. of extra records: 2
Source temp.: 170 Analyzer temp.: 170 Transfer line temp. : 170

Chromatographic temperatures :	40.	230.	0.	0.	0.
Chromatographic times, min. :	4.0	1.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	8.0	0.0	0.0	0.0	0.0



Lot C780708 Direct Injection
Data Package

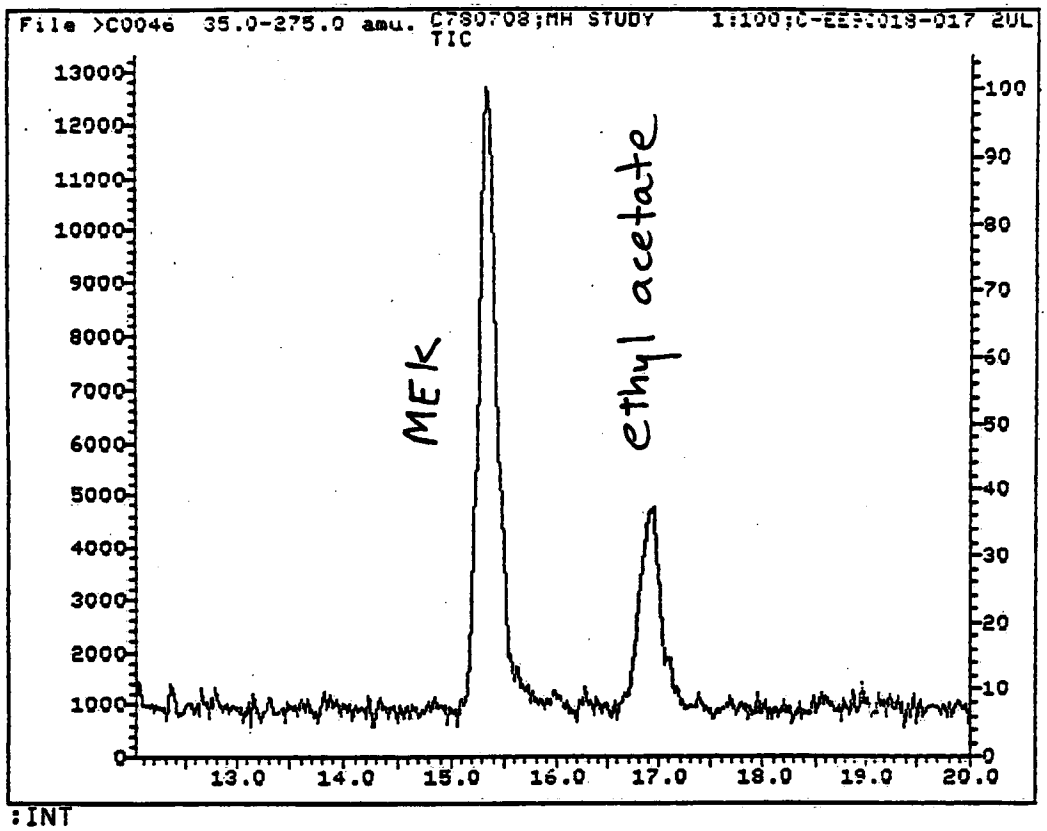
:INT

>C0046 C780708;MH STUDY 1:100;C-EE90018-017 2UL DIR INJECTION
35.0: 275.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 1 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
1	7.98	304	321	359	450710	5837517	5796672	100.00	100.000

ethanol

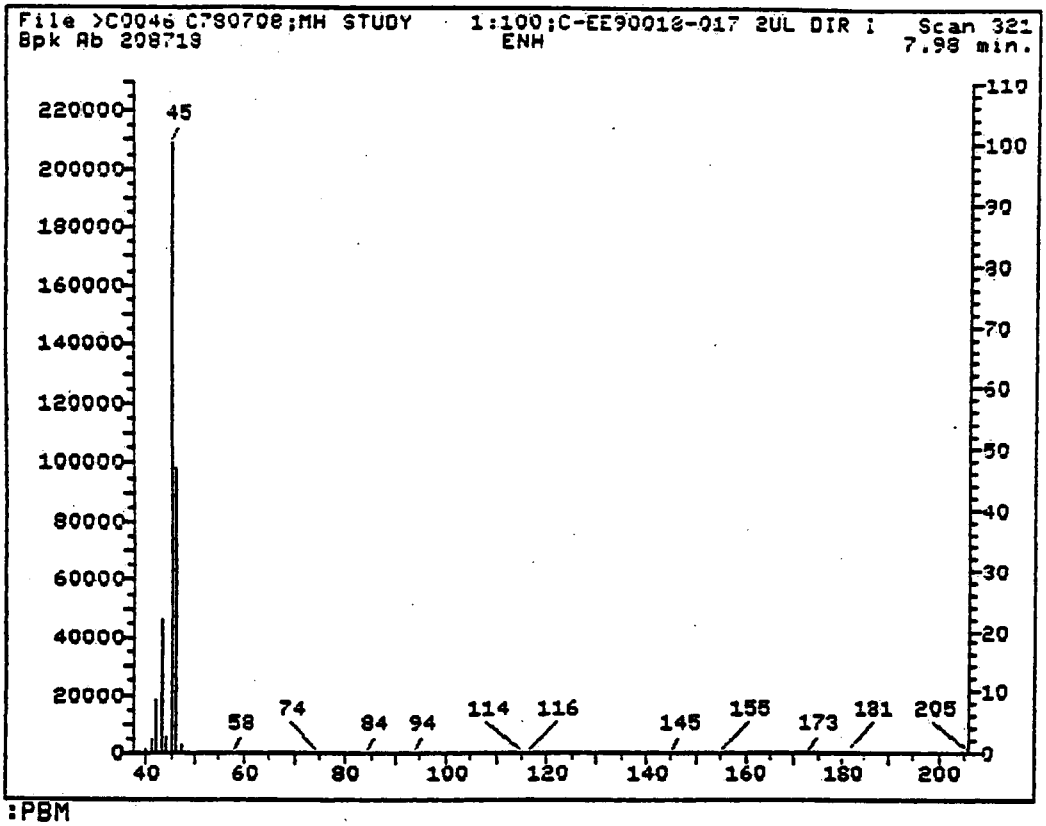
Sum of corrected areas: 5796672.



>C0046 C780708;MH STUDY 1:100;C-EE90018-017 2UL DIR INJECTION
35.0! 275.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 2 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

	Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
(MEK)	1	15.33	663	673	686	11703	169472	141129	100.00	75.309
ethyl acetate)	2	16.96	738	751	756	3797	69911	46272	32.79	24.691

Sum of corrected areas: 187401.

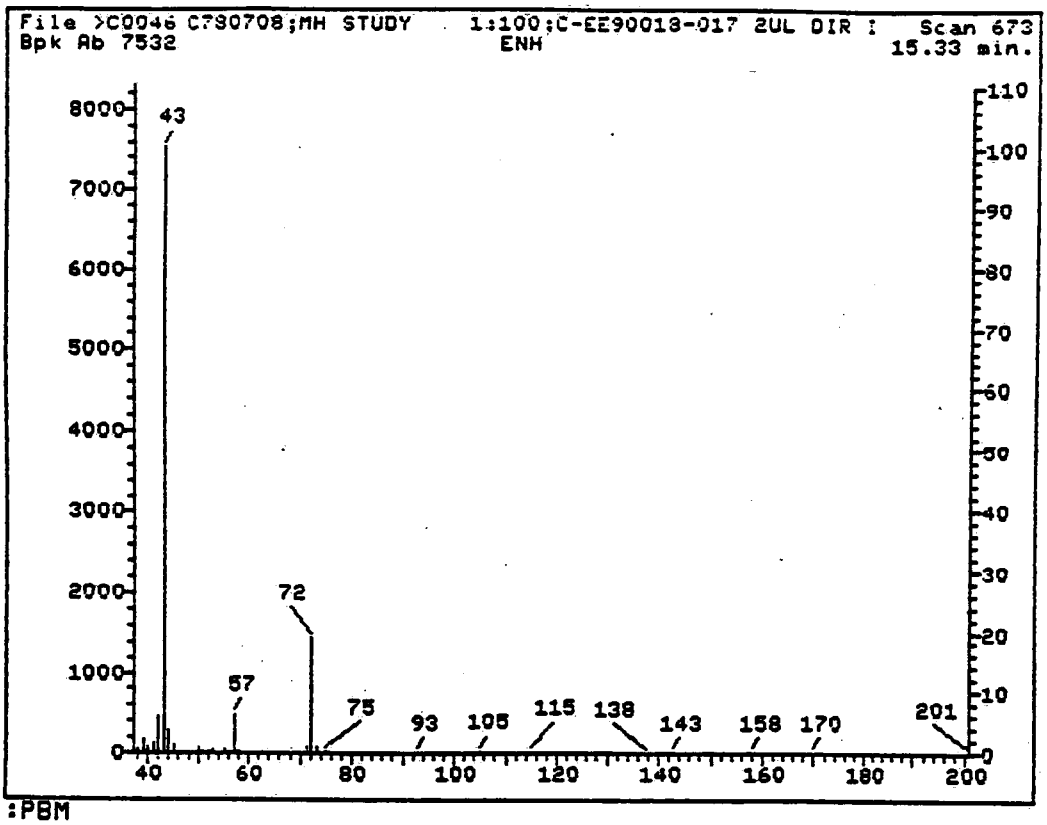


1. Ethanol (ACN)(SCI) 46 C2H6O
2. Methane, oxybis- (SCI) 46 C2H6O

Sample file: >C0046 Spectrum #: 321
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLS	TILT	%	CON	C_I	R_IV
1.	60*	64175	121	*BIGDB	24	43	1	0	204	14	30	14
2.	52*	115106	376	*BIGDB	24	62	0	0	100	18	20	17

Ethanol Spectra

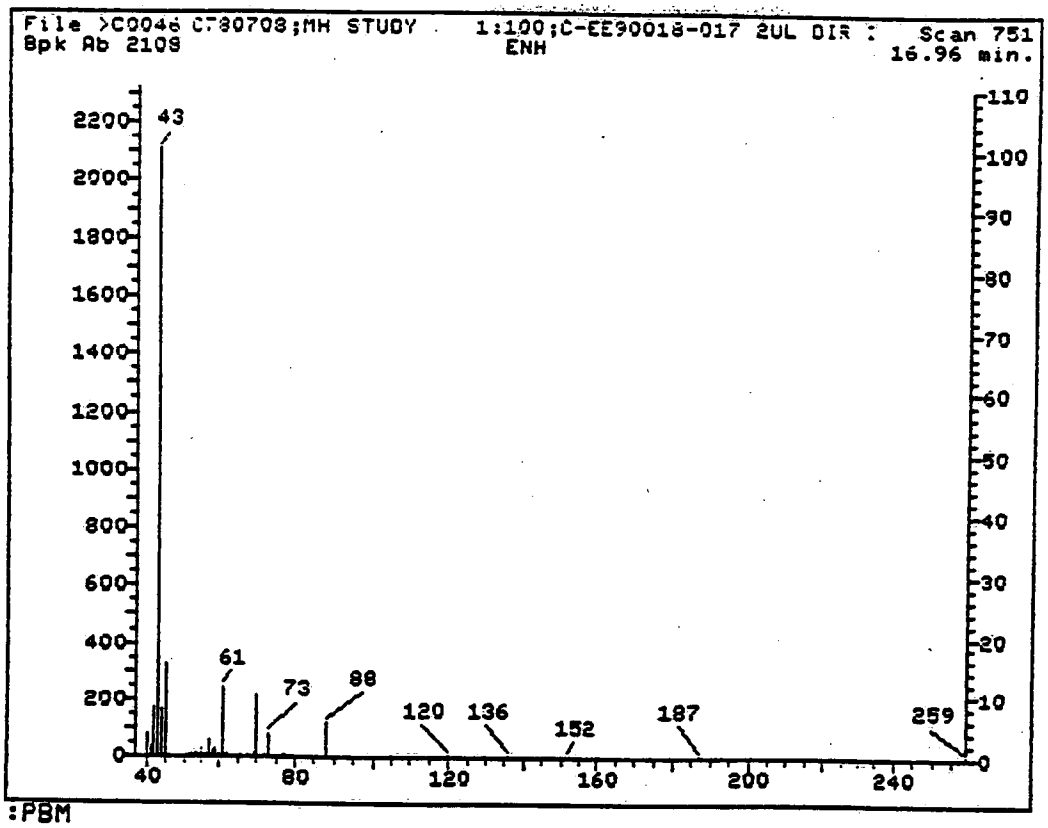


1. 2-Butanone (8CI9CI) 72 C4H8O

Sample file: >C0046 Spectrum #: 673
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	84*	78933	4050	"BI6DB	44	25	0	0	77	8	55	60

MEK Spectra



1. Propanoic acid, 2-oxo- (9CI) 88 C3H4O3
2. Acetic acid, ethyl ester 88 C4H8O2

Sample file: >C0046 Spectrum #: 751
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	37*	127173	11	*BIGDB	21	56	1	0	99	28	14	14
2.	11*	141786	6949	*BIGDB	29	48	1	0	36	61	2	16

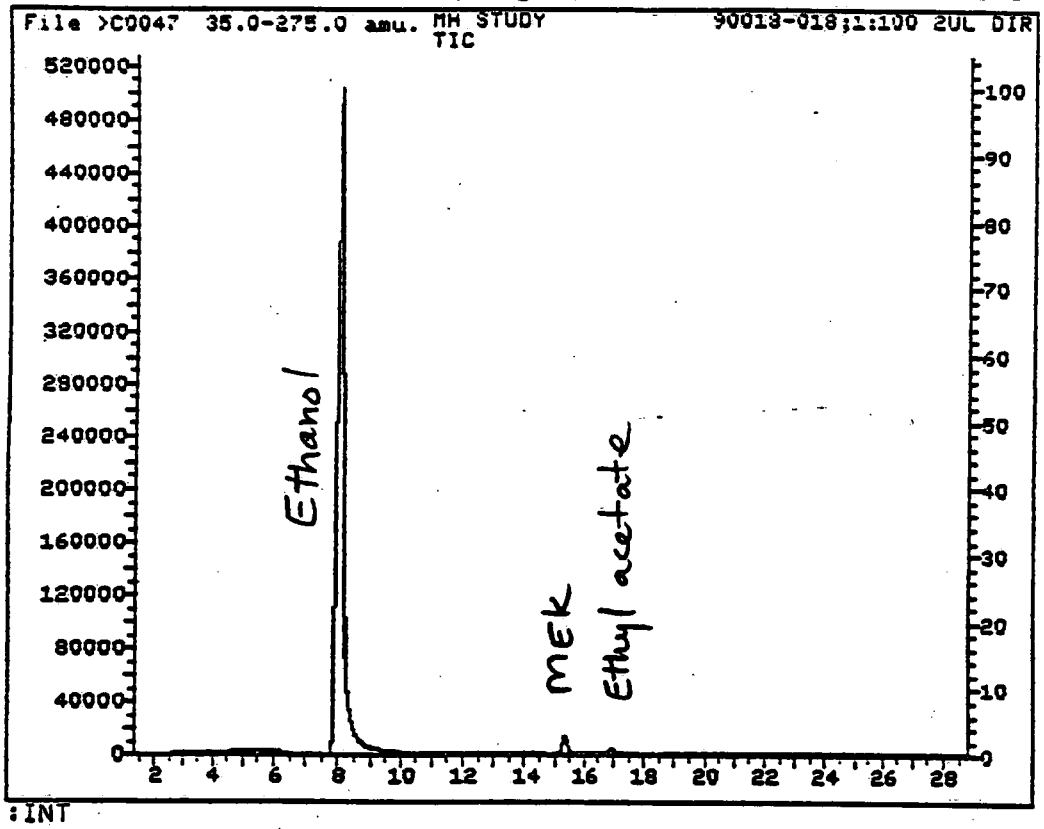
Ethyl acetate spectra

:MSH

MS data file header from : >C0047

Sample: MH STUDY Operator: USER6 MS 1/23/90 14:25
Misc : 90018-018;1:100 2UL DIR INJECTION
Sys. #: 2 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: M_CMH Tuning file: MT2000 No. of extra records: 2
Source temp.: 170 Analyzer temp.: 170 Transfer line temp. : 170

Chromatographic temperatures :	40.	230.	0.	0.	0.
Chromatographic times, min. :	4.0	1.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	8.0	0.0	0.0	0.0	0.0



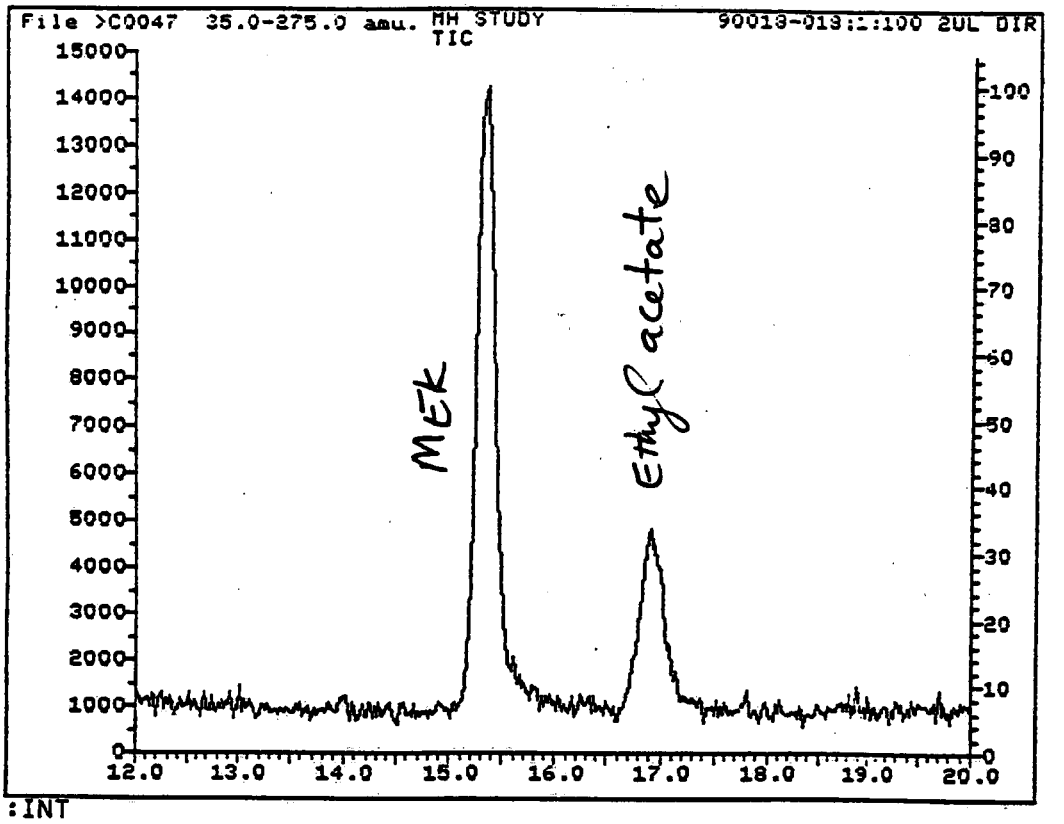
:INT

>C0047 MH STUDY 90018-018;1:100 2UL DIR INJECTION
35.0! 275.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 1 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

	Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
thanol)	1	8.07	307	325	366	502024	6610930	6578273	100.00	100.000

Sum of corrected areas: 6578273.

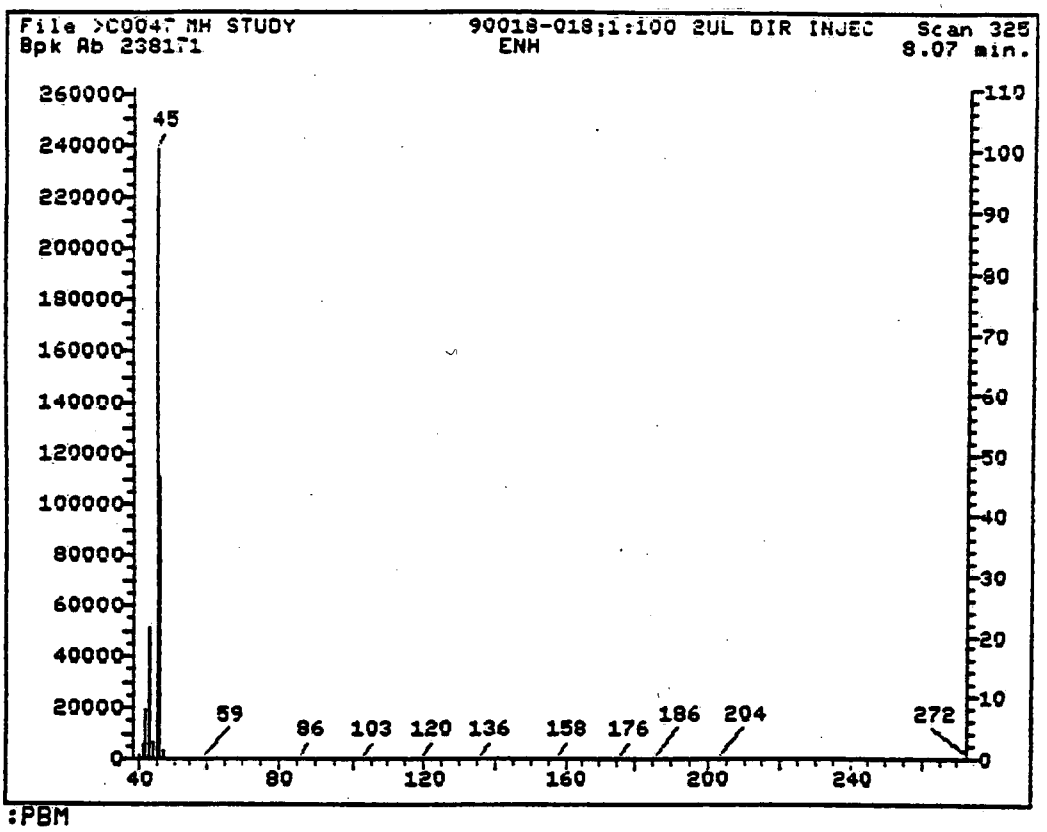
Lot C780811 Direct Injection
Data Package



>C0047 MH STUDY 90018-018;1:100 2UL DIR INJECTION
35.0: 275.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 2 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

	Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
(MEK)	1	15.35	661	674	685	13314	192055	164221	100.00	75.640
(yl acetate)	2	16.92	736	749	756	3902	76332	52887	32.20	24.360

Sum of corrected areas: 217108.

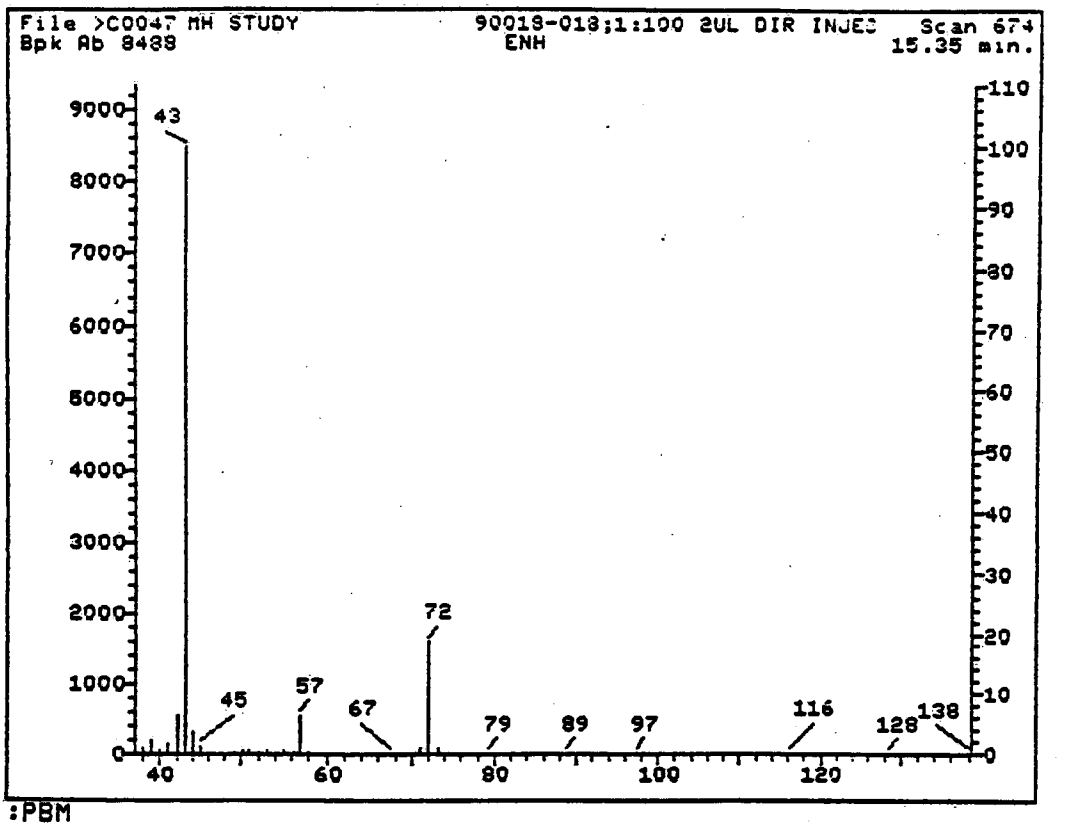


1. Ethanol (ACN)(SCI) 46 C2H6O
2. Methane, oxybis- (SCI) 46 C2H6O

Sample file: >C0047 Spectrum #: 325
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	70*	64175	121	*BIGDB	29	38	1	0	204	7	42	16
2.	52*	115106	376	*BIGDB	24	62	0	0	100	18	20	17

Ethanol Spectra

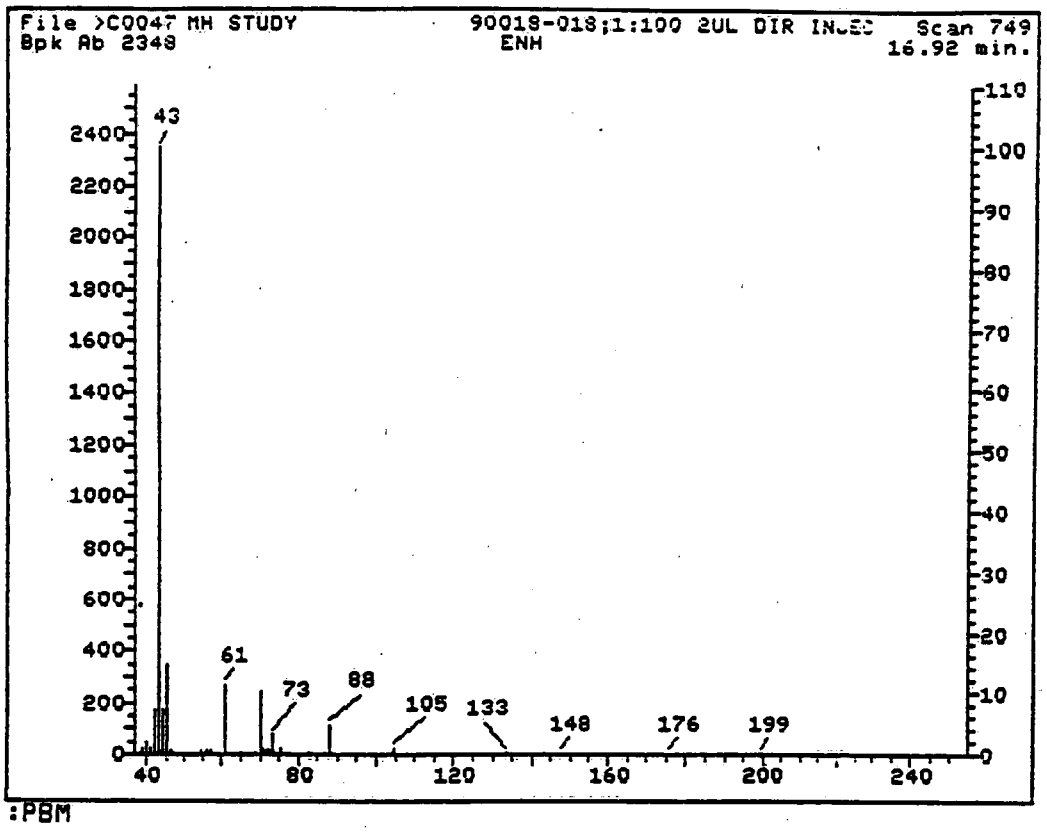


1. 2-Butanone (8CI9CI) 72 C4H8O

Sample file: >C0047 Spectrum #: 674
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	84*	78933	4050	*BIGDB	48	21	0	0	77	6	55	69

MEK Spectra



1. Propanoic acid, 2-oxo- (SCI) 88 C3H4O3
2. Acetic acid, ethyl ester 88 C4H8O2

Sample file: >C0047 Spectrum #: 749
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	43*	127173	11	*BIGDB	26	51	1	0	93	25	17	14
2.	11*	141786	6949	*BIGDB	30	47	1	0	31	62	2	16

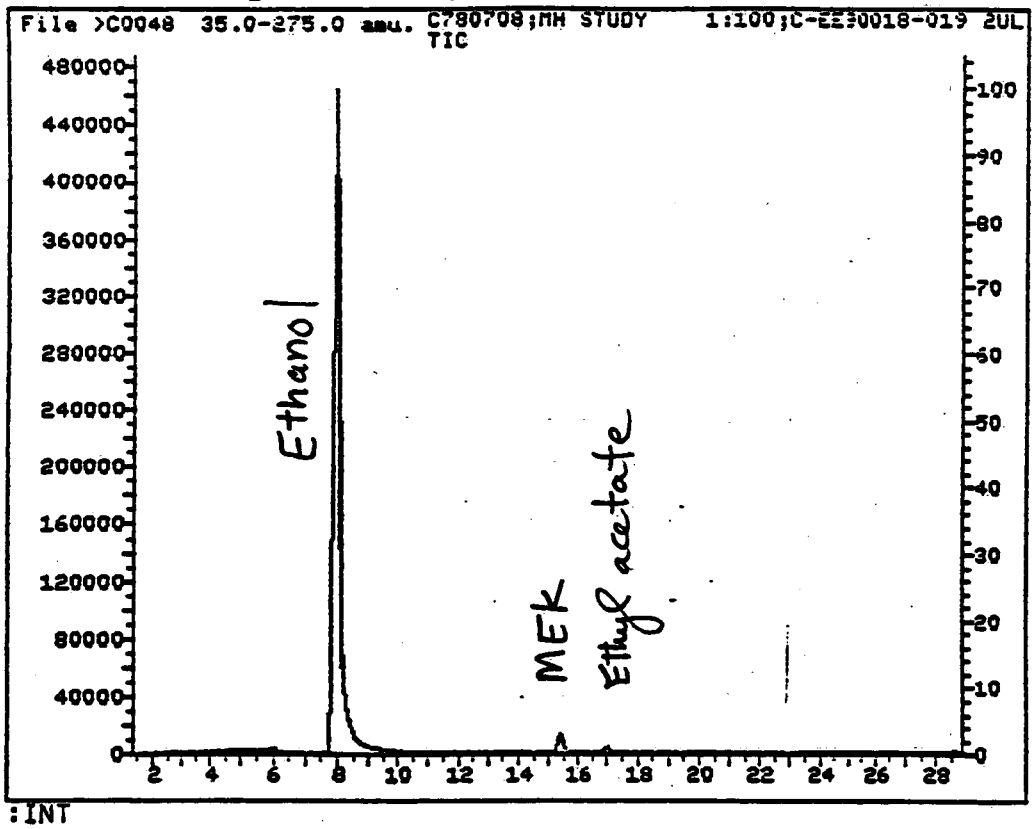
Ethyl acetate Spectra

:MSH

MS data file header from : >C0048

Sample: C780708;MH STUDY Operator: USER6 MS 1/23/90 15:01
Misc : 1:100;C-EE90018-019 2UL DIR INJECTION
Sys. #: 2 MS model: 96 SW/HW rev.: IA ALS # : 0
Method file: M_CMH Tuning file: MT2000 No. of extra records: 2
Source temp.: 170 Analyzer temp.: 170 Transfer line temp. : 170

Chromatographic temperatures :	40.	230.	0.	0.	0.
Chromatographic times, min. :	4.0	1.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	8.0	0.0	0.0	0.0	0.0



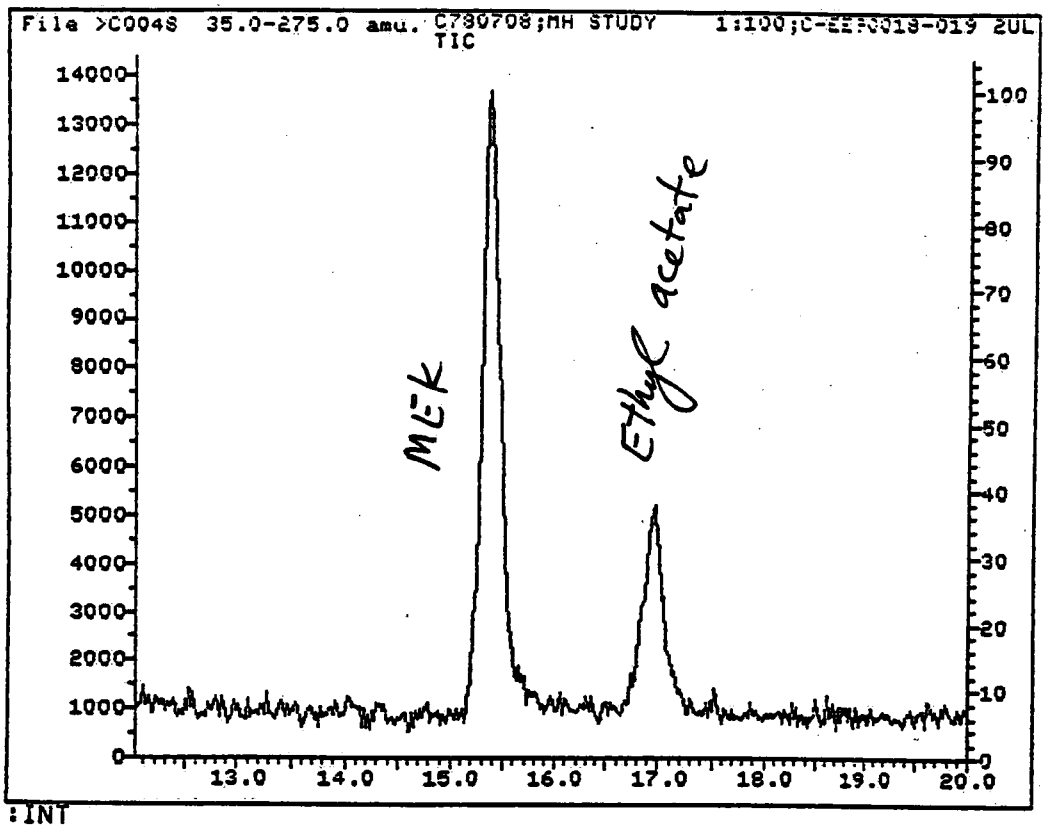
:INT

>C0048 C780708;MH STUDY 1:100;C-EE90018-019 2UL DIR INJECTION
35.0! 275.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 1 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
ethanol) 1	8.00	305	321	352	463788	6124025	6093239	100.00	100.000

Sum of corrected areas: 6093239.

Lot C880524 Direct Injection Data Package

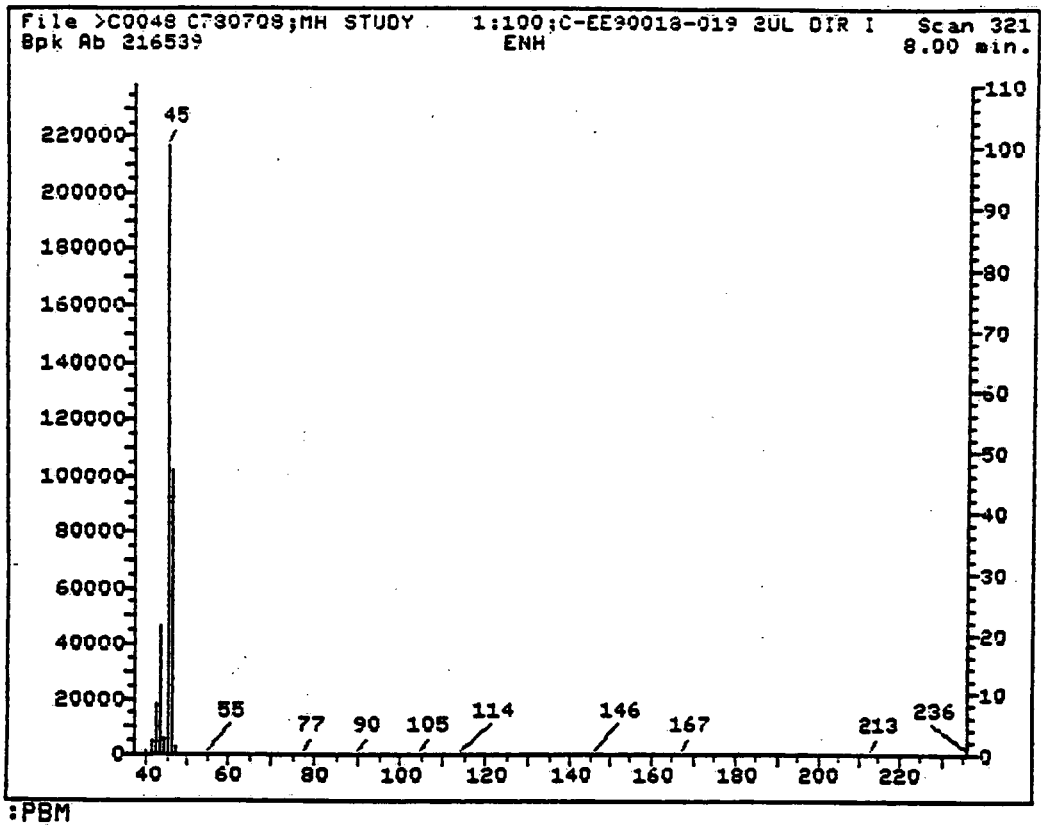


>C0048 C780708;MH STUDY 1:100;C-EE90018-019 2UL DIR INJECTION
35.0| 275.0 TIC

Upslope: .20 Area Reject: 5.00 % Max Peaks: 2 Bunching: 1
Dnslope: 0.00 Results File VDIR87 Sorted by Time/Area INT

	Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
(MEK)	1	15.37	663	674	687	12977	183544	161544	100.00	73.256
ethyl acetate)	2	16.97	741	751	765	4439	83725	58976	36.51	26.744

Sum of corrected areas: 220520.

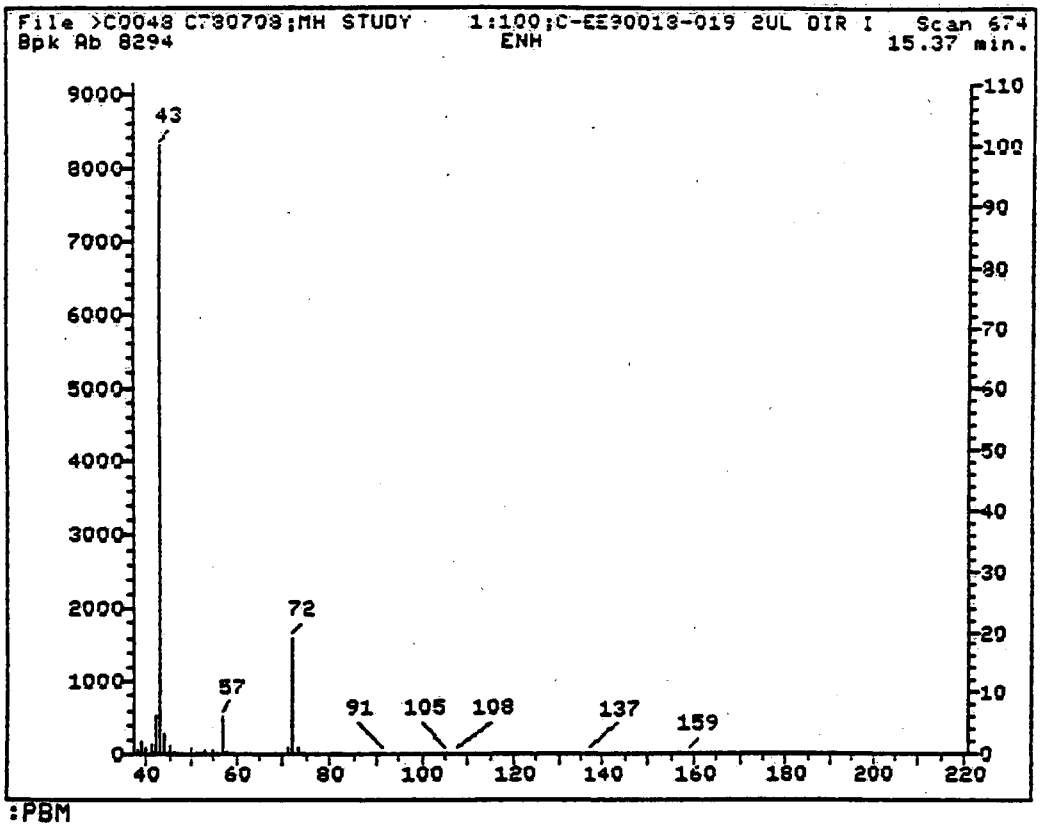


1. Ethanol (ACN)(SCI) 46 C2H6O
2. Methane, oxybis- (SCI) 46 C2H6O

Sample file: >C0048 Spectrum #: 321
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	70*	64175	121	*BIGDB	29	38	1	0	204	7	42	16
2.	52*	115106	376	*BIGDB	24	62	0	0	100	18	20	17

Ethanol Spectra



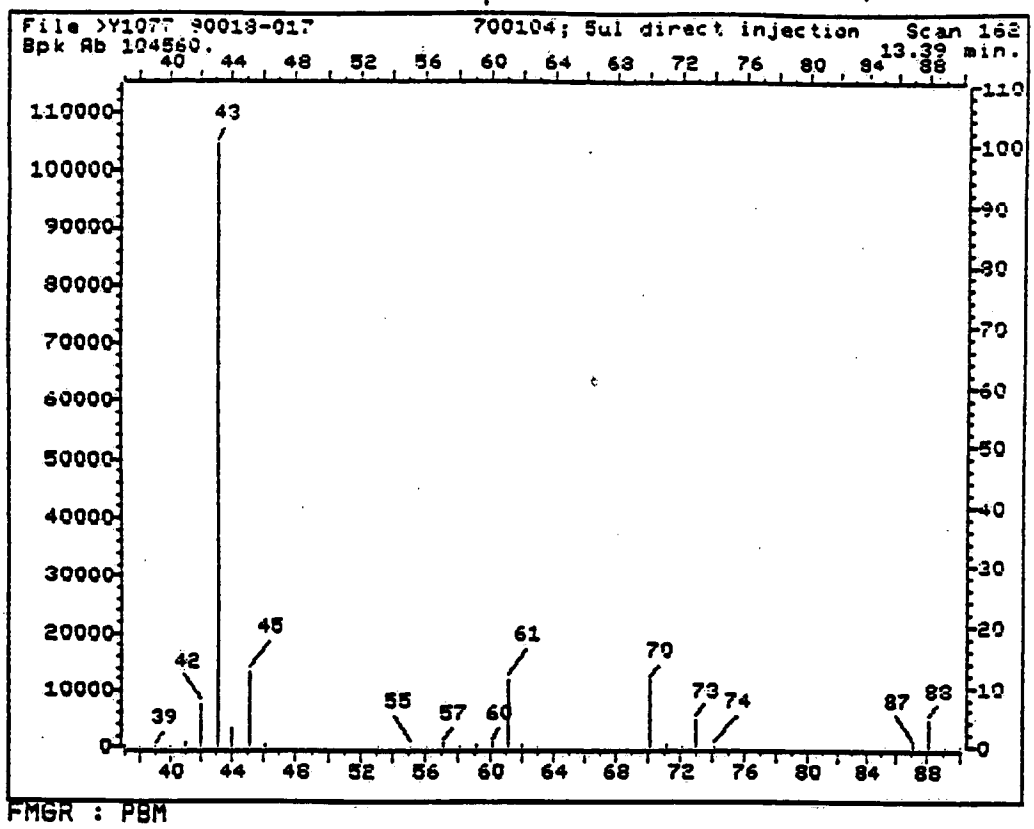
1. 2-Butanone (8CI9CI) 72 C4H8O

Sample file: >C0048 Spectrum #: 674
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	84*	78933	4050	*BIGDB	48	21	0	0	79	6	55	69

MEK Spectra

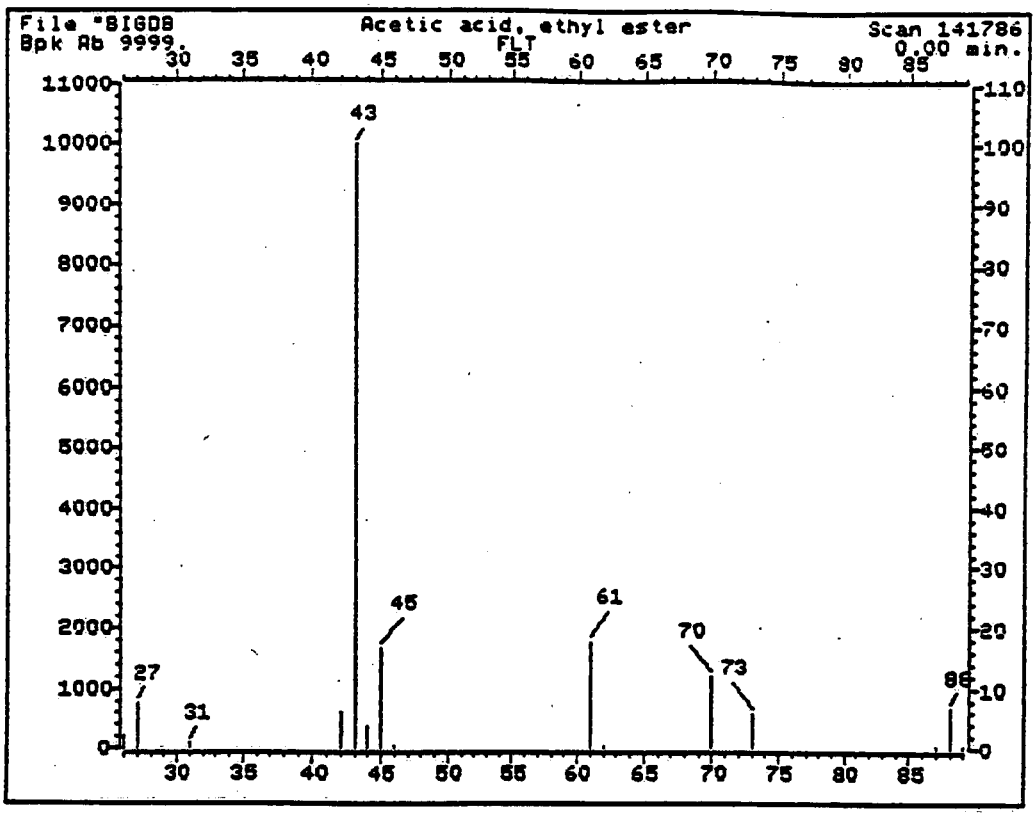
Ethyl acetate Spectra and Library Comparison



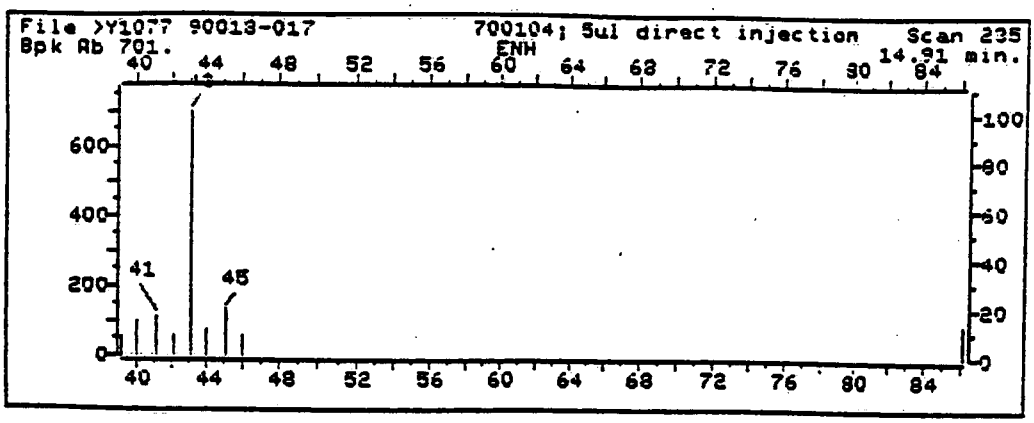
1.	Acetic acid, ethyl ester	88	C4H8O2
2.	Acetic acid, ethyl ester	88	C4H8O2
3.	Acetic acid, ethyl ester	88	C4H8O2
4.	Acetic acid, ethyl ester	88	C4H8O2
5.	Acetic acid, ethyl ester	88	C4H8O2
6.	Acetic acid, ethyl ester	88	C4H8O2
7.	Acetic acid, ethyl ester	88	C4H8O2
8.	3-(4,5-DICHLORO-2-CYANO-3,6-DIHYDROXY-1-PHENYL) INDO	318	C15H8Cl2N2O2
9.	Acetic acid, ethyl ester	88	C4H8O2
10.	Propanoic acid, 2-oxo-	88	C3H4O3
11.	Acetic acid, ethyl ester	88	C4H8O2
12.	Acetic acid, ethyl ester	88	C4H8O2

Sample file: >Y1077 Spectrum #: 162
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	.CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89*	141786	4341	*BIGDB	47	22	0	0	100	5	66	66
2.	86*	141786	4336	*BIGDB	51	26	0	0	88	9	59	73
3.	84*	141786	4337	*BIGDB	48	31	0	0	94	7	55	66
4.	84*	141786	4338	*BIGDB	44	36	0	0	88	7	55	60
5.	83*	141786	4344	*BIGDB	43	9	0	0	81	7	54	59
6.	76*	141786	4342	*BIGDB	44	39	2	0	86	7	45	23
7.	71*	141786	4192	*BIGDB	51	27	0	0	53	32	32	72
8.	70	0	4320	*BIGDB	47	28	2	0	70	7	42	16
9.	60*	141786	4343	*BIGDB	25	24	0	0	70	15	30	18
10.	52*	127173	660	*BIGDB	22	58	2	0	67	19	20	13
11.	42*	141786	4339	*BIGDB	43	35	1	0	65	34	16	25
12.	32*	141786	4340	*BIGDB	39	38	0	0	37	55	9	48


File *BIGDB
Bpk Ab 9999.
Acetic acid, ethyl ester
FLT
Scan 141786
0.00 min.
43
45
61
70
73
27
31
86

Methyl Substituted Ketone Spectra and Library Comparison. (Unknown Ketone)

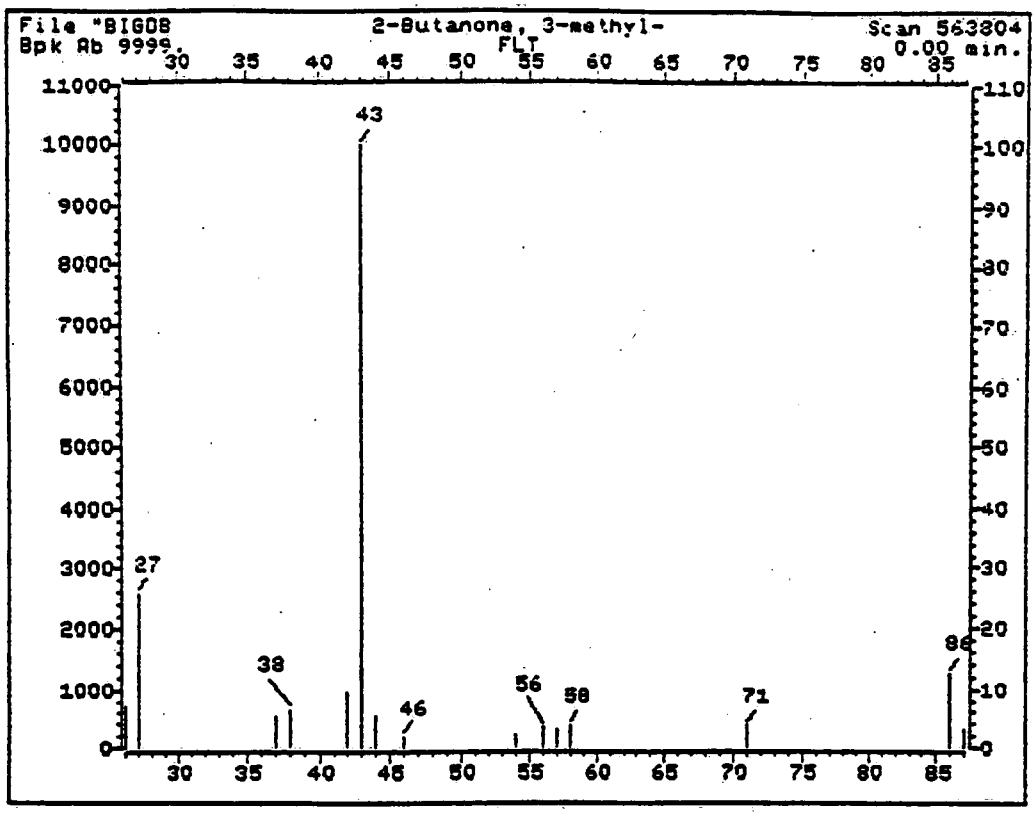


FMGR : PBM

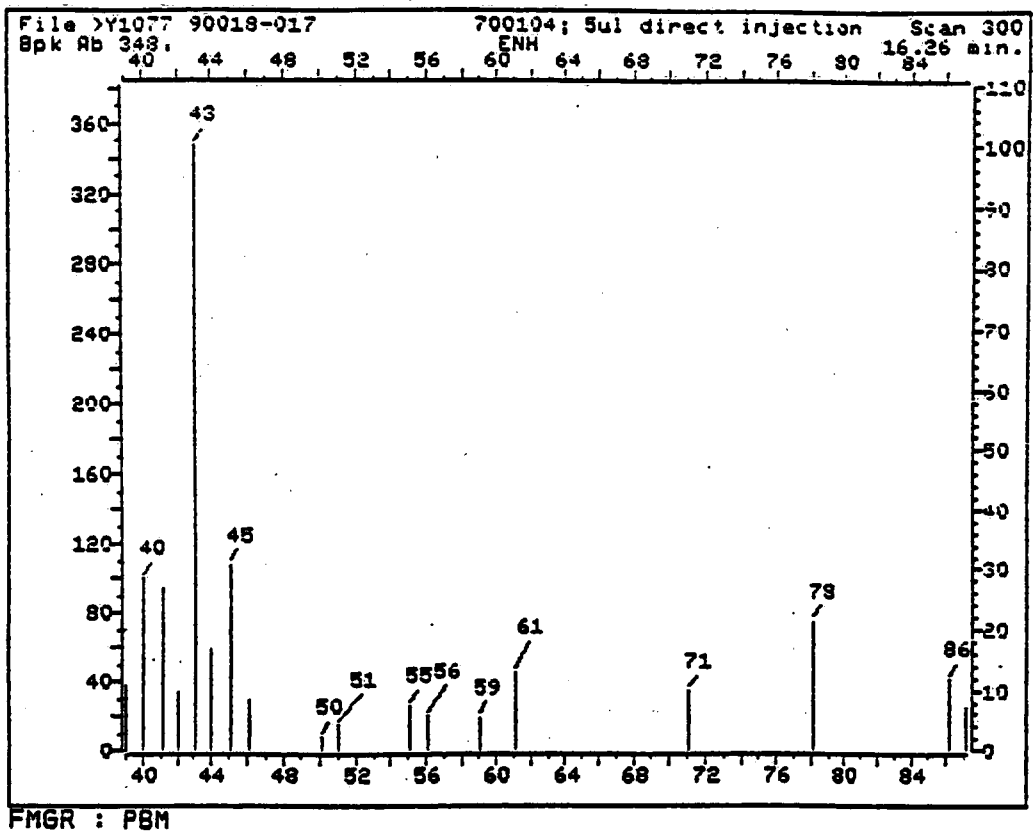
1.	2-Butanone, 3-methyl-	86 C5H10O
2.	2-Butanone, 3-methyl-	86 C5H10O
3.	2-Butanone, 3-methyl-	86 C5H10O
4.	2-Butanone, 3-methyl-	86 C5H10O
5.	2-Pentanone	86 C5H10O
6.	2-Butanone, 3-methyl-	86 C5H10O

Sample file: >Y1077 Spectrum #: 235
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	58*	563804	13209	*BIGDB	30	12	0	0	90	19	25	22
2.	43*	563804	13207	*BIGDB	25	42	2	0	100	25	17	14
3.	43*	563804	12890	*BIGDB	25	42	2	0	100	25	17	14
4.	42*	563804	13206	*BIGDB	21	39	2	0	100	25	17	13
5.	36*	107879	13219	*BIGDB	21	47	2	0	100	27	14	13
6.	36*	563804	13204	*BIGDB	21	52	2	0	84	29	14	13


File "BIGDB
Bpk Ab 9999.
2-Butanone, 3-methyl-
FLT
Scan 563804
0.00 min.
43
27
38
46
56
58
71
86

Acetic acid - methylethyl ester Spectra and Library Comparison



FMGR : PBM

1.	Acetic acid, 1-methylethyl ester	102 C5H10O2
2.	2-Pentanone	86 C5H10O
3.	2-Pentanone	86 C5H10O
4.	2-Butanone, 3-methyl-	86 C5H10O
5.	2-Pentanone	86 C5H10O
6.	2-Pentanone	86 C5H10O
7.	2-Butanone, 3-methyl-	86 C5H10O
8.	2-Butanone, 3-methyl-	86 C5H10O
9.	2-Pentanone	86 C5H10O
10.	2-Butanone, 3-methyl-	86 C5H10O
11.	Aziridine	43 C2H5N

Sample file: >Y1077 Spectrum #: 300
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

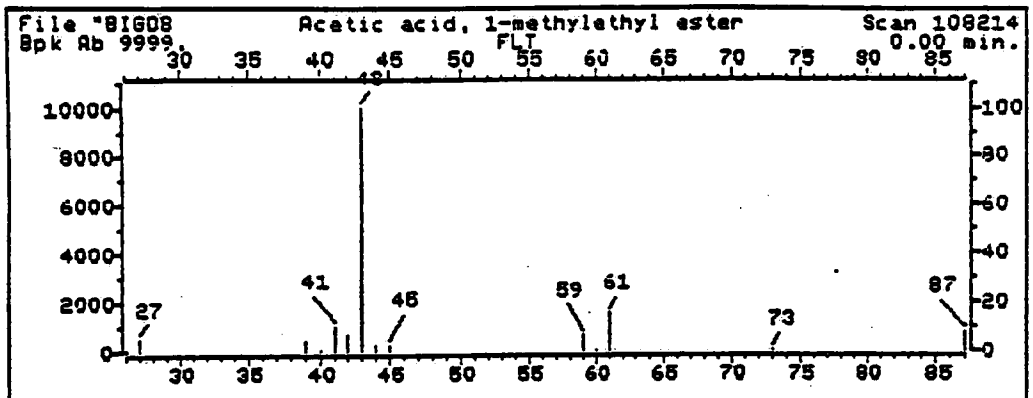
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	31	108214	4358	*BIGDB	41	38	1	0	80	33	12	14
2.	28*	107879	13222	*BIGDB	27	49	2	0	82	39	10	14
3.	28*	107879	13224	*BIGDB	24	52	2	0	100	40	10	14
4.	27*	563804	12890	*BIGDB	21	46	0	0	100	45	8	15
5.	26*	107879	13219	*BIGDB	26	42	2	0	100	44	8	14
6.	26*	107879	13218	*BIGDB	28	46	2	0	80	41	8	14
7.	26*	563804	13207	*BIGDB	21	46	1	0	100	44	8	14
8.	25*	563804	13206	*BIGDB	21	39	1	0	100	47	7	14
9.	25*	107879	12892	*BIGDB	21	54	2	0	78	43	8	13
10.	25*	563804	13208	*BIGDB	23	58	2	0	94	45	8	13
11.	20*	151564	13	*BIGDB	20	41	0	0	68	51	5	15

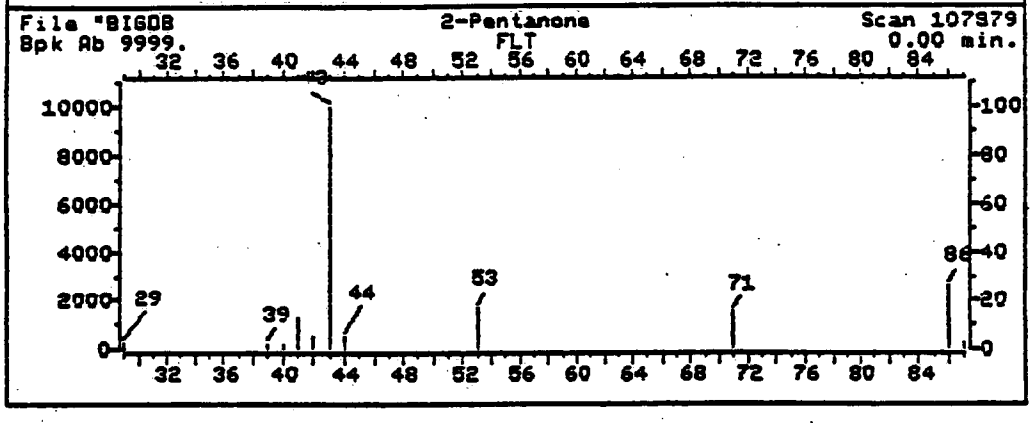
CAS #: 108214 found at record #: 4359

Rec.#: 108214 Reg.#: 108214 Xref.#: 0 Base : *BIGDB
Name: Acetic acid, 1-methylethyl ester
MW : 102.068 QI: 0 MF: C5H10O2

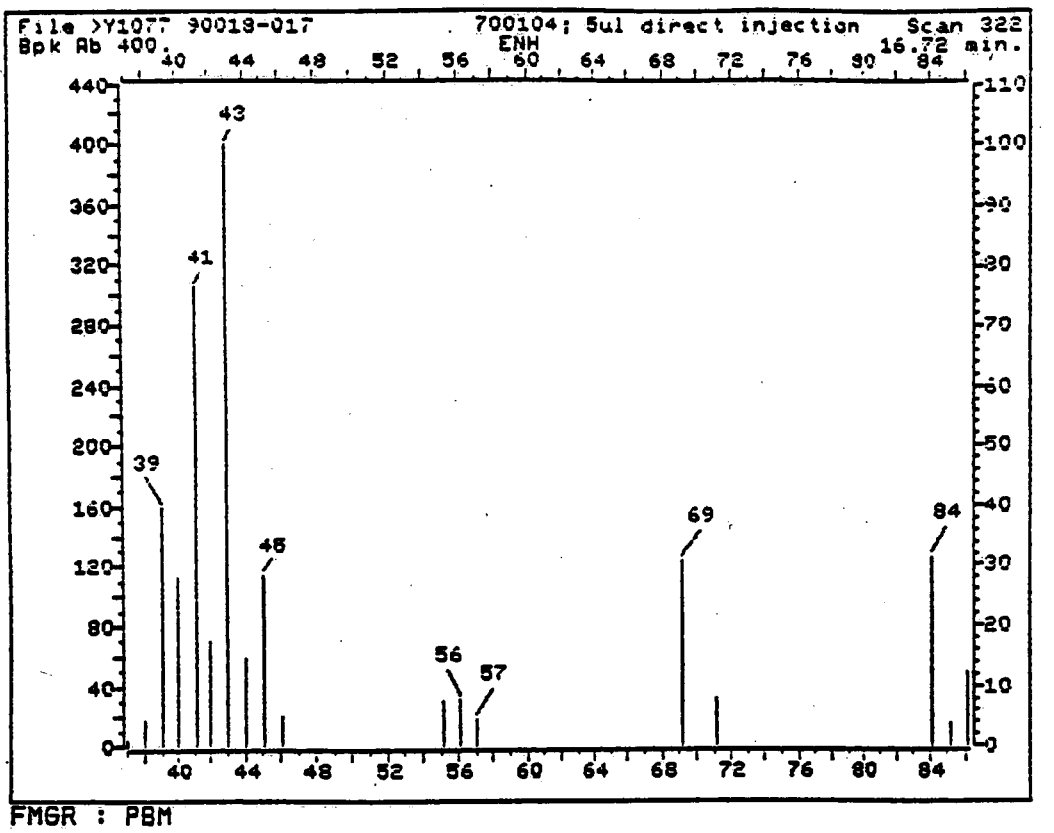
Rec.#: 108214 Lomass: 26 max K-value: 65 No. ions:14 IX: 0 0

m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.
26:	103	39:	430	41:	997	43:	9999	45:	241	60:	57	73:	55
27:	520	40:	50	42:	680	44:	260	59:	642	61:	1555	87:	746





Unknown Ketone Spectra and Library Comparison.



FMGR : PBM

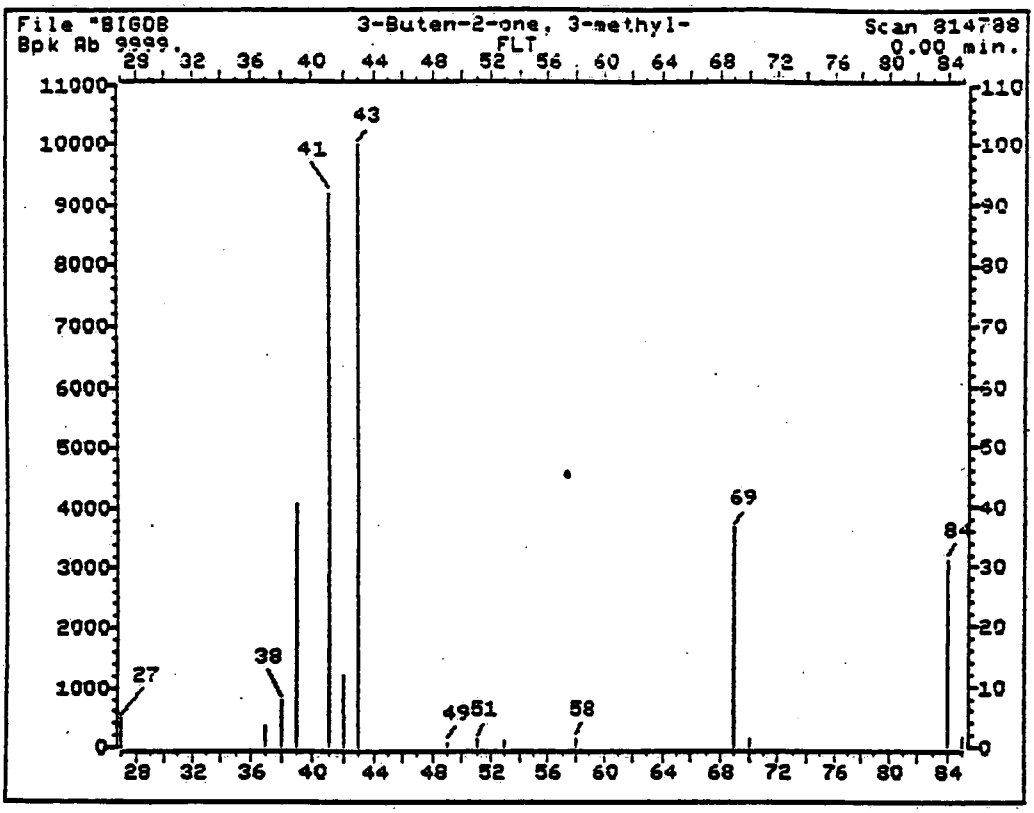
1.	3-Buten-2-one, 3-methyl-	84	C5H8O
2.	3-Buten-2-one, 3-methyl-	84	C5H8O
3.	3-Buten-2-one, 3-methyl-	84	C5H8O
4.	3-Buten-2-one, 3-methyl-	84	C5H8O
5.	3-Buten-2-one, 3-methyl-	84	C5H8O
6.	3-Buten-1-ol, 3-methyl-	86	C5H10O
7.	2-Butanone, 4-hydroxy-3-(hydroxymethyl)-3-methyl-	132	C6H12O3
8.	2-Pentanone	86	C5H10O
9.	2-Butanone, 3-methyl-	86	C5H10O
10.	2-Pentanone	86	C5H10O
11.	2-Butanone, 3-methyl-	86	C5H10O
12.	Butane, 2,3-dimethyl-	86	C6H14

Sample file: >Y1077 Spectrum #: 322

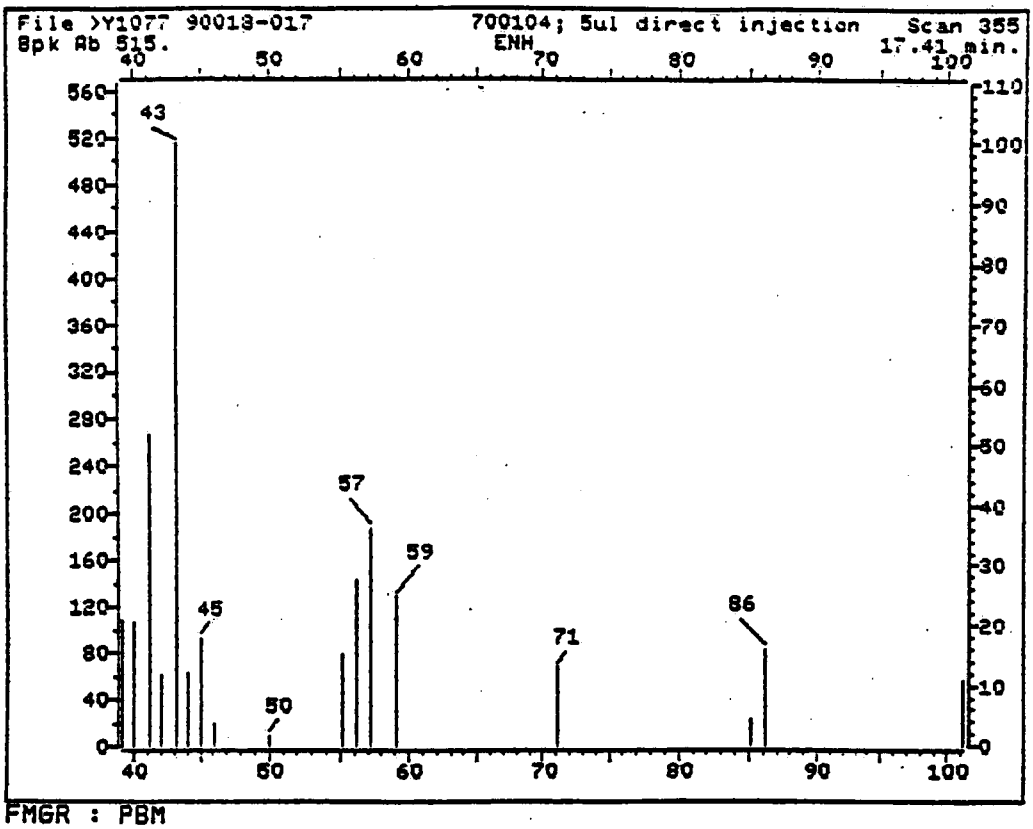
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	42*	814788	11682	*BIGDB	39	38	2	0	76	27	14	19
2.	41*	814788	11683	*BIGDB	36	32	2	0	76	29	14	18
3.	40*	814788	11679	*BIGDB	39	56	2	0	78	30	14	17
4.	35*	814788	11681	*BIGDB	44	38	1	0	67	42	12	26
5.	34*	814788	11144	*BIGDB	34	48	2	0	83	31	12	17
6.	25*	763326	358	*BIGDB	23	29	1	0	95	41	8	14
7.	25	6868979	11258	*BIGDB	43	46	2	0	70	48	7	13
8.	20*	107879	13218	*BIGDB	28	46	2	0	100	51	5	14
9.	20*	563804	12890	*BIGDB	21	46	1	0	100	51	5	14
10.	20*	107879	13219	*BIGDB	21	47	2	0	100	52	5	13

FMGR : CRT,FF


File "BIGOB
Bpk Ab 9999.
3-Buten-2-one, 3-methyl-
FLT
Scan 814788
0.00 min.
28 32 36 40 44 48 52 56 60 64 68 72 76 80 84
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
110
100
90
80
70
60
50
40
30
20
10
0
43
41
69
84
38
27
49
51
58

Unknown Ketone Spectra and Library Comparison.

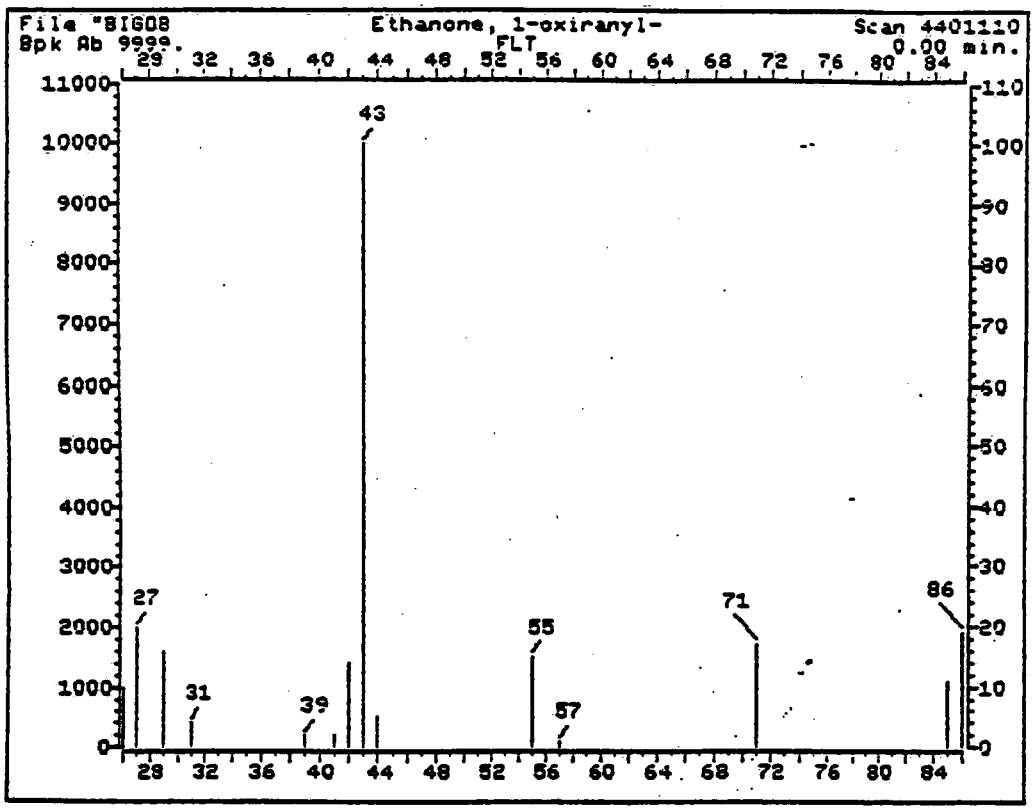


FMGR : PBM

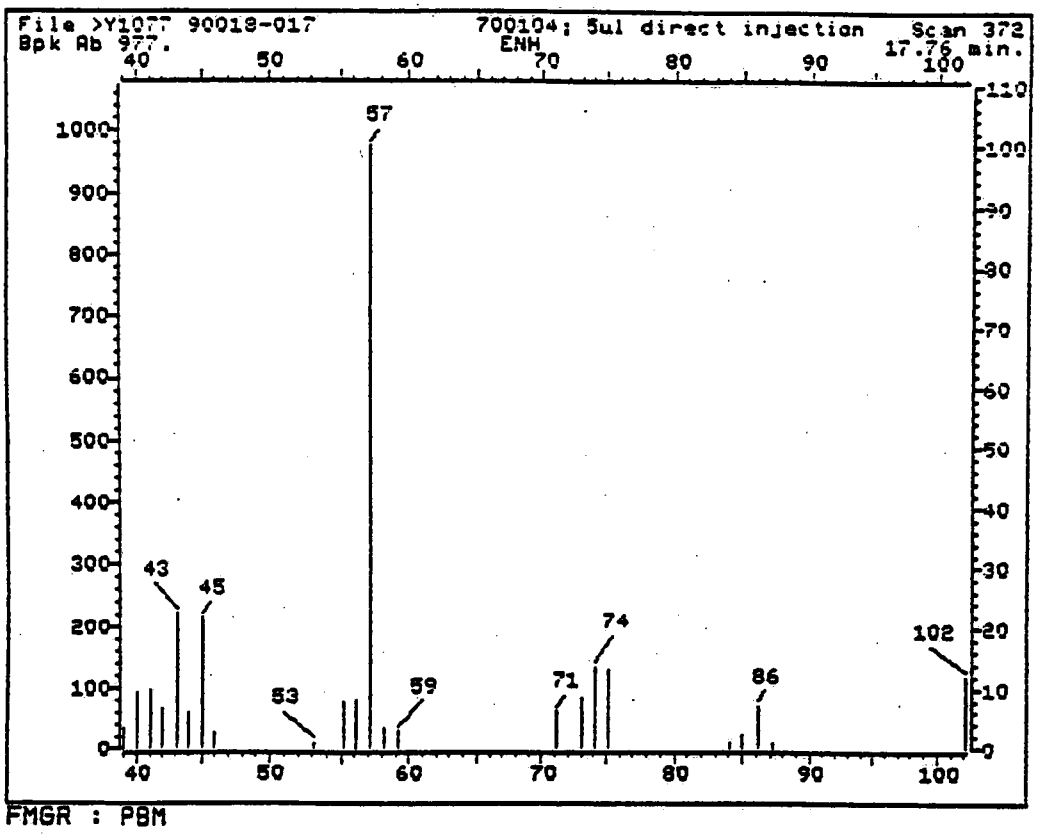
1. Ethanone, 1-oxiranyl-	86	C4H6O2
2. 2-Pentanone	86	C5H10O
3. 2-Butanone, 3-methyl-	86	C5H10O
4. 3-Buten-1-ol, 3-methyl-	86	C5H10O
5. 2-Pentanone	86	C5H10O
6. 2-Pentanone	86	C5H10O
7. 2-Pentanone	86	C5H10O
8. Propane, 2-nitro-	89	C3H7NO2

Sample file: >Y1077 Spectrum #: 355
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	29*	4401110	12878	*BIGDB	32	47	1	0	77	44	8	17
2.	26*	107879	12892	*BIGDB	22	53	1	0	100	44	8	14
3.	26*	563804	13208	*BIGDB	25	56	2	0	100	43	8	14
4.	25*	763326	358	*BIGDB	23	29	2	0	82	42	8	13
5.	25*	107879	13218	*BIGDB	24	50	2	0	95	46	7	14
6.	25*	107879	13222	*BIGDB	22	54	2	0	100	44	8	13
7.	25*	107879	13224	*BIGDB	20	56	2	0	100	43	8	13
8.	20	79469	42	*BIGDB	27	57	0	0	69	53	5	14


File "BIGDB
Bpk Ab 9999.
Ethanone, 1-oxiranyl-
FLT
Scan 4401110
0.00 min.
43
27
31
39
55
57
71
86

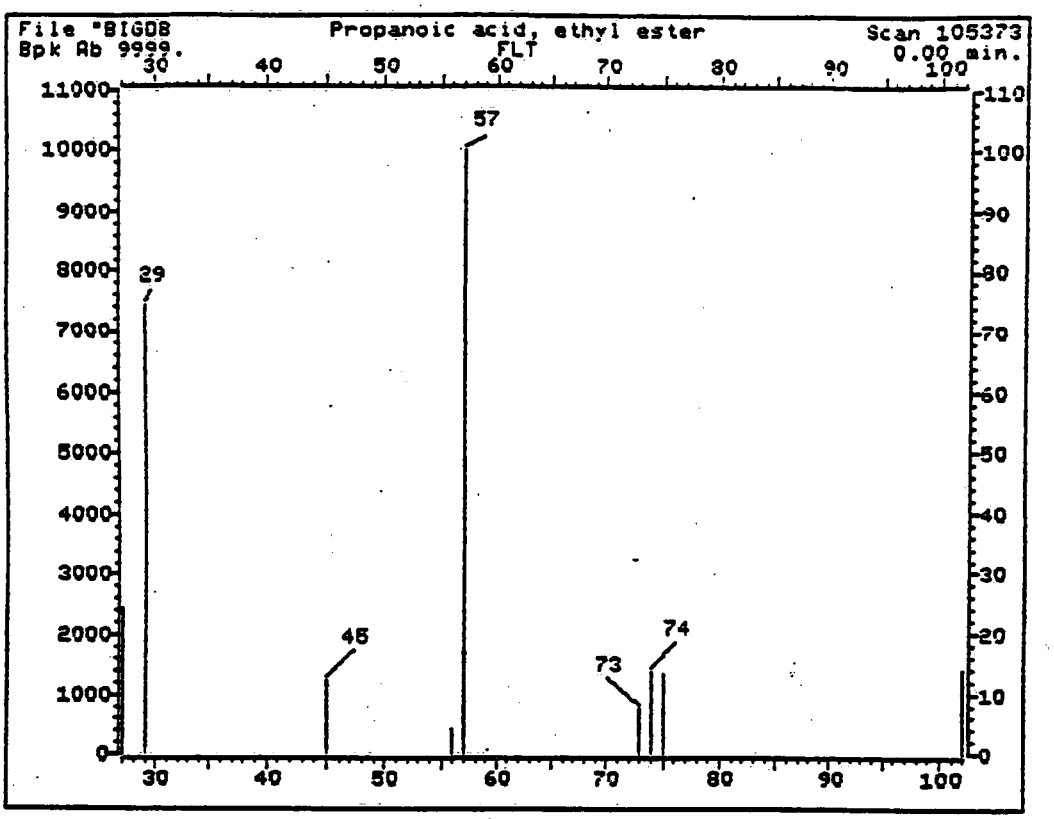
Propanoic acid ethyl ester Spectra and Library Comparison



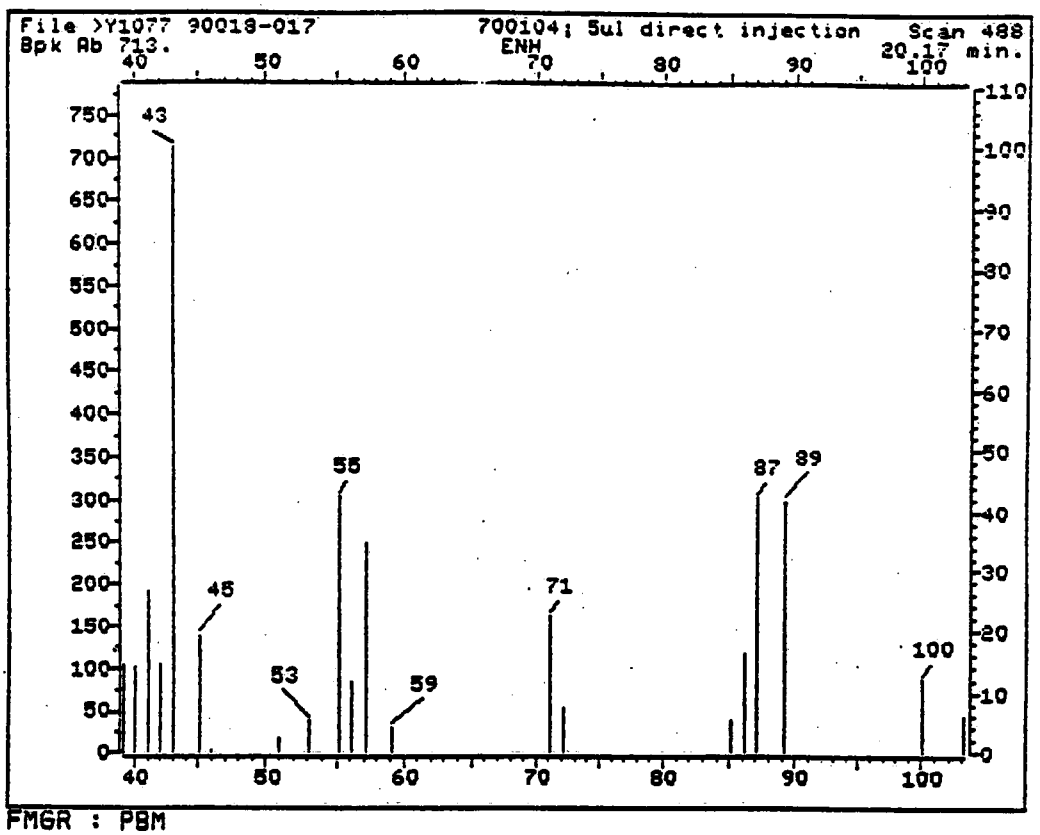
1.	Propanoic acid, ethyl ester	102 C5H10O2
2.	Propanoic acid, ethyl ester	102 C5H10O2
3.	Propanoic acid, ethyl ester	102 C5H10O2
4.	Propanoic acid, ethyl ester	102 C5H10O2
5.	Propanoic acid, ethyl ester	102 C5H10O2
6.	1-Penten-3-ol	86 C5H10O
7.	Borinic acid, diethyl-	86 C4H11BO
8.	1-Penten-3-ol	86 C5H10O
9.	Propanoic acid, ethyl ester	102 C5H10O2

Sample file: >Y1077 Spectrum #: 372
Search speed: 1 Tilting option: N No. of ion ranges searched: 46

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	67*	105373	2349	*BIGDB	43	40	1	0	154	12	34	25
2.	64*	105373	19926	*BIGDB	38	24	0	0	86	22	28	44
3.	58*	105373	2466	*BIGDB	40	45	1	0	117	19	25	23
4.	58*	105373	19924	*BIGDB	41	49	1	0	70	17	25	23
5.	58*	105373	2467	*BIGDB	29	44	0	0	146	19	25	21
6.	27*	616251	2452	*BIGDB	21	54	2	0	100	40	10	13
7.	25*	4426317	2343	*BIGDB	21	63	2	0	100	45	8	13
8.	25*	616251	61	*BIGDB	21	76	2	0	100	41	8	13
9.	20*	105373	19925	*BIGDB	24	37	0	0	52	51	5	17


File *BIGDB
Bpk Ab 9999.
Propanoic acid, ethyl ester
FLT
Scan 105373
0.00 min.
57
29
45
73
74

Unknown Spectra and Library Comparison.

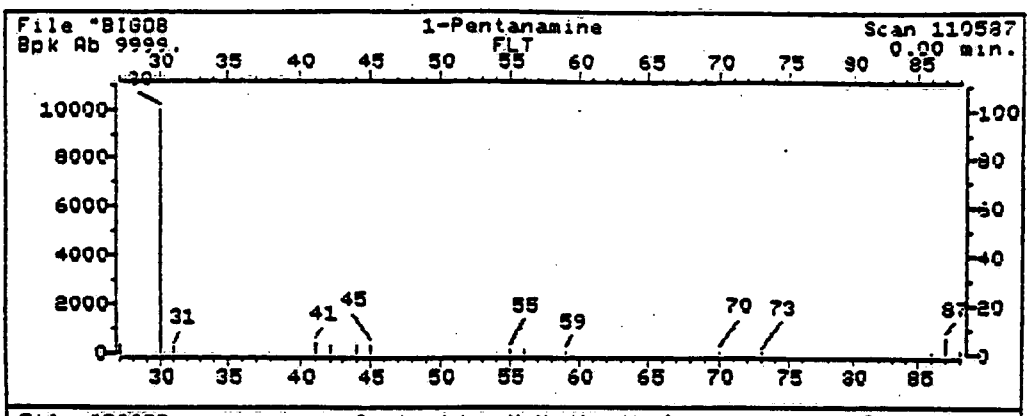


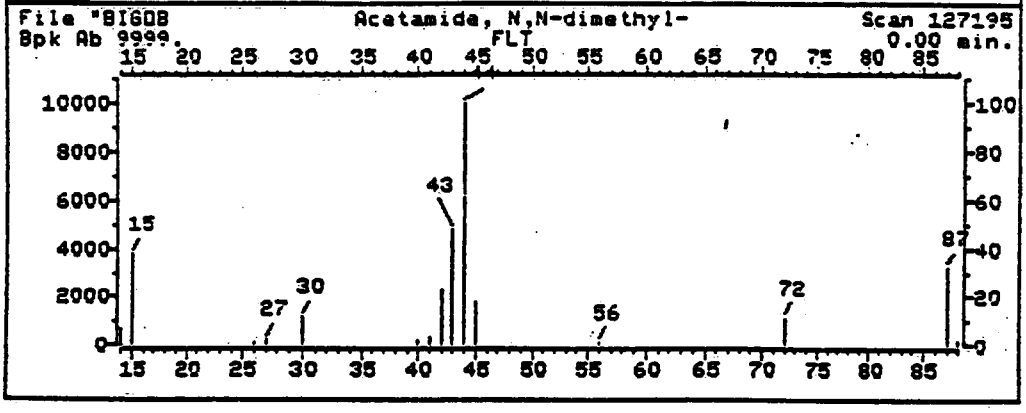
FMGR : PBM

1. 1-Pentanamine	87	C5H13N
2. 1-Pentanamine	87	C5H13N
3. Acetamide, N,N-dimethyl-	87	C4H9NO
4. Acetamide, N,N-dimethyl-	87	C4H9NO
5. 3-Penten-2-ol	86	C5H10O

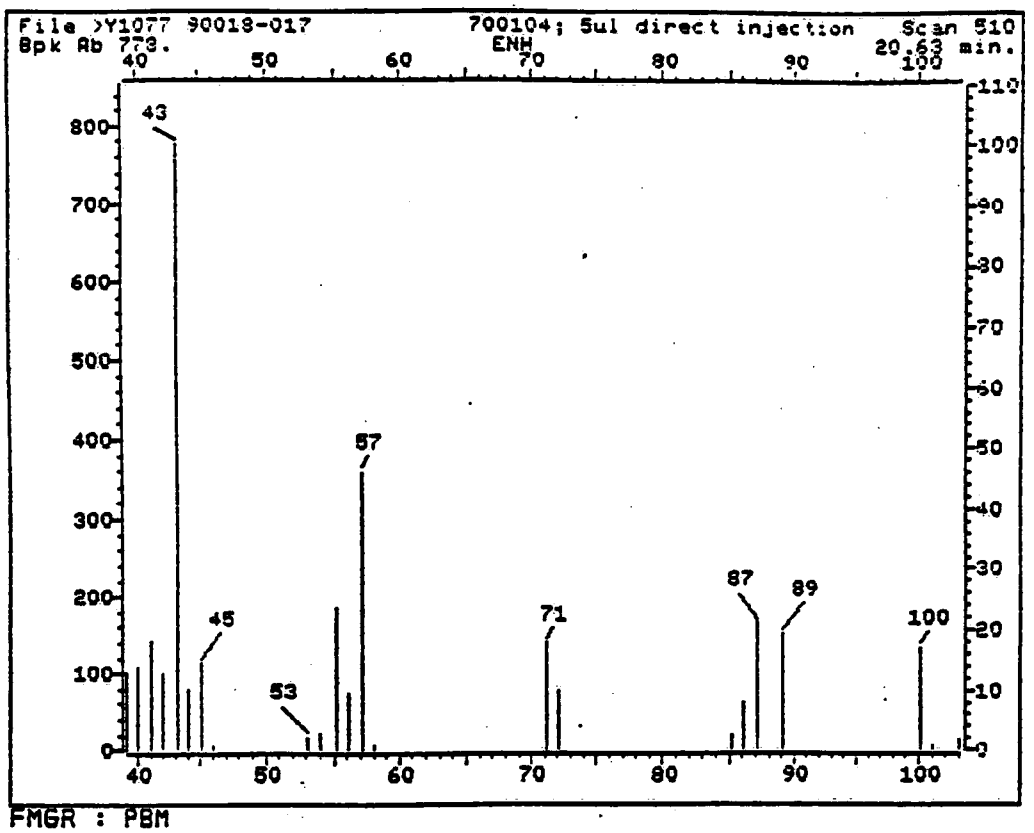
Sample file: >Y1077 Spectrum #: 488
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	15*	110587	101	*BIGDB	24	39	2	0	490	60	3	14
2.	15*	110587	156	*BIGDB	23	45	2	0	525	60	3	13
3.	15*	127195	13750	*BIGDB	23	68	3	0	61	60	3	12
4.	15*	127195	13752	*BIGDB	23	69	3	0	60	59	3	12
5.	11*	1569502	7613	*BIGDB	22	83	3	0	131	63	2	12


File *BIG08
Bpk Ab 9999.
1-Pentanamine
FLT
Scan 110587
0.00 min.
10000
8000
6000
4000
2000
0
100
80
60
40
20
0
30
31
41
45
55
59
70
73
87


File *BIG08
Bpk Ab 9999.
Acetamide, N,N-dimethyl-
FLT
Scan 127195
0.00 min.
10000
8000
6000
4000
2000
0
100
80
60
40
20
0
15
27
30
43
56
72
87

Unknown alkane Spectra and Library Comparison.



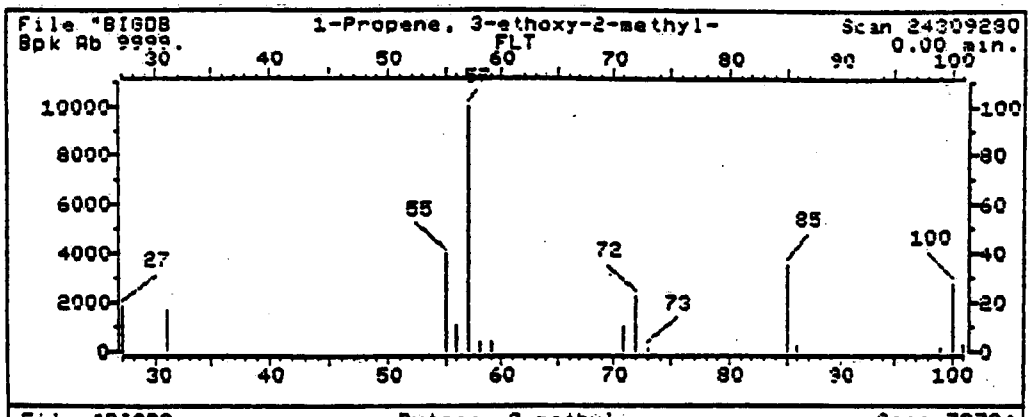
FMGR : PBM

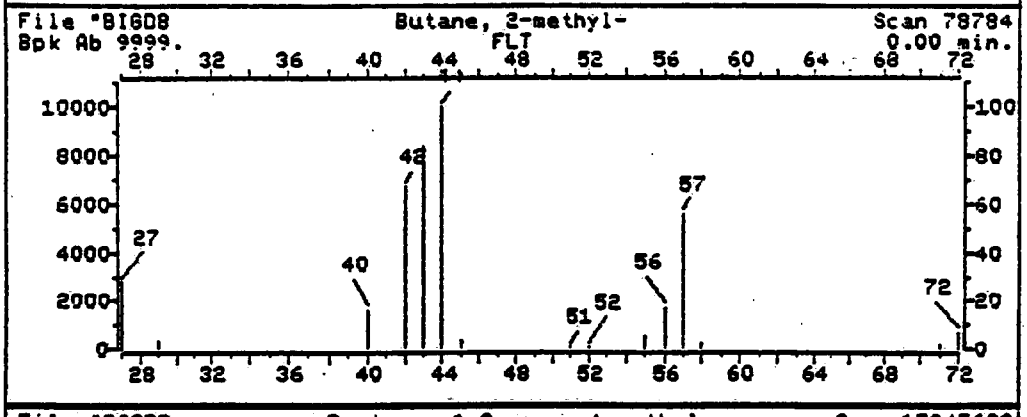
1. 1-Propene, 3-ethoxy-2-methyl-	100	C6H12O
2. Butane, 2-methyl-	72	C5H12
3. Pentane, 1,3-epoxy-4-methyl-	100	C6H12O
4. 3-Hexanone	100	C6H12O
5. 2,3-Pentanedione	100	C5H8O2
6. 2,3-Pentanedione	100	C5H8O2
7. 2,3-Pentanedione	100	C5H8O2

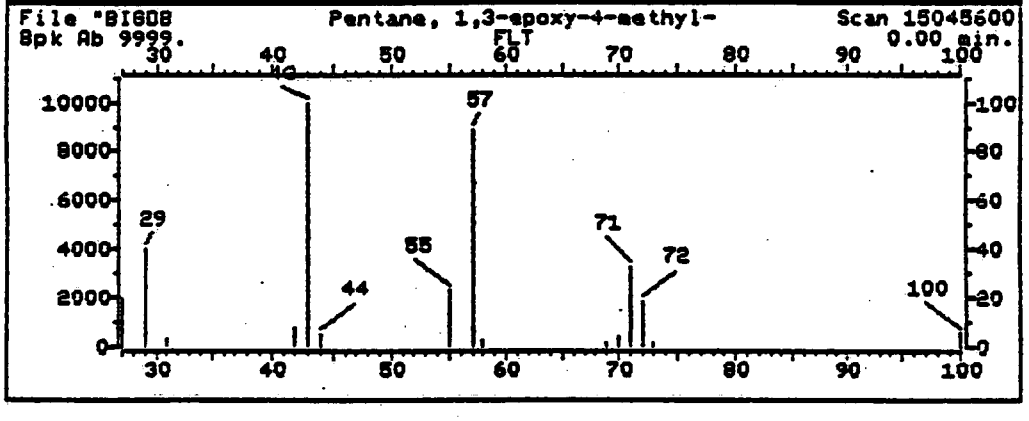
Sample file: >Y1077 Spectrum #: 510
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

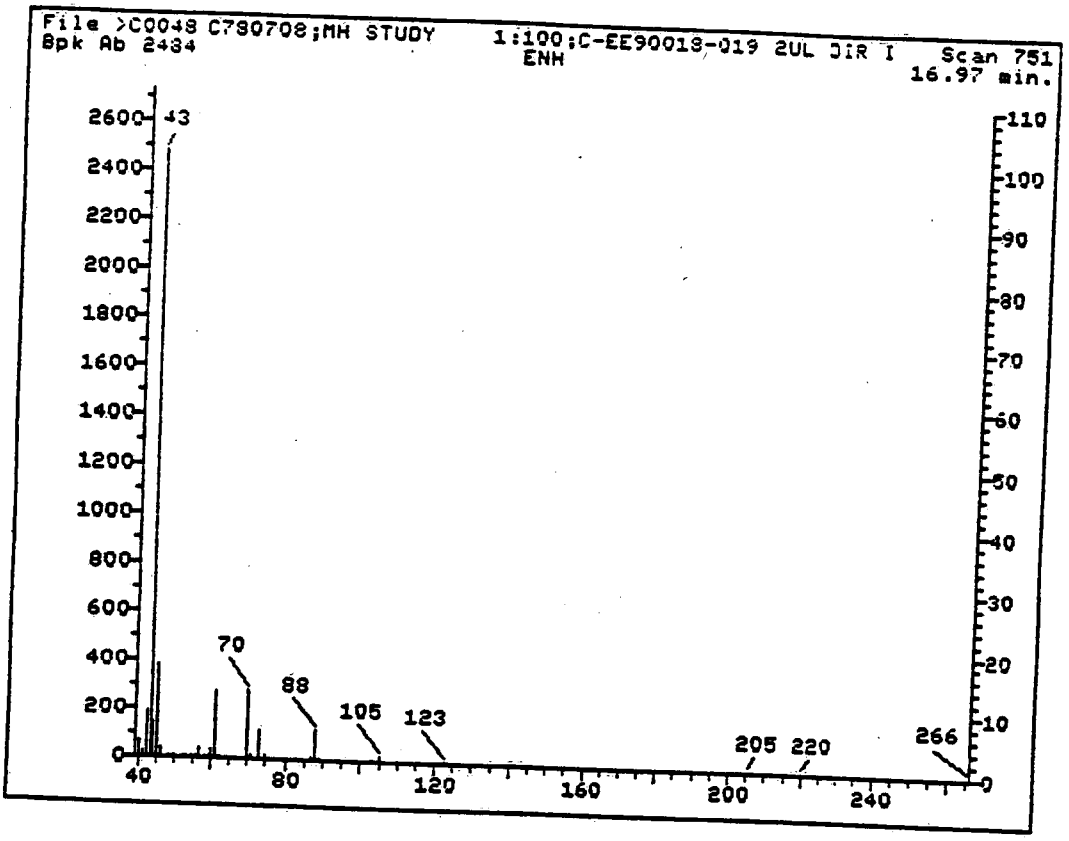
	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	24*	24309282	19029	*BIGDB	23	60	3	0	46	43	8	12
2.	20*	78784	8165	*BIGDB	22	62	3	0	74	54	5	12
3.	20*	15045600	7791	*BIGDB	21	66	2	0	51	54	5	13
4.	15*	589388	19289	*BIGDB	30	60	2	0	59	60	3	15
5.	11*	600146	19266	*BIGDB	27	52	1	0	100	61	2	15
6.	11*	600146	19009	*BIGDB	24	62	1	0	97	63	2	14
7.	11*	600146	19267	*BIGDB	22	64	2	0	130	61	2	13

FMGR :
FMGR :
FMGR :
FMGR :
FMGR :
FMGR :
FMGR :


File "BIGDB
Bpk Ab 9999.
1-Propene, 3-ethoxy-2-methyl-
FLT
Scan 24309230
0.00 min.
27
55
57
72
73
85
100


File "BIGDB
Bpk Ab 9999.
Butane, 2-methyl-
FLT
Scan 78784
0.00 min.
27
40
42
44
51
52
56
57
72


File "BIGDB
Bpk Ab 9999.
Pentane, 1,3-epoxy-4-methyl-
FLT
Scan 15045600
0.00 min.
29
44
55
57
71
72
100



Ethyl acetate Spectra

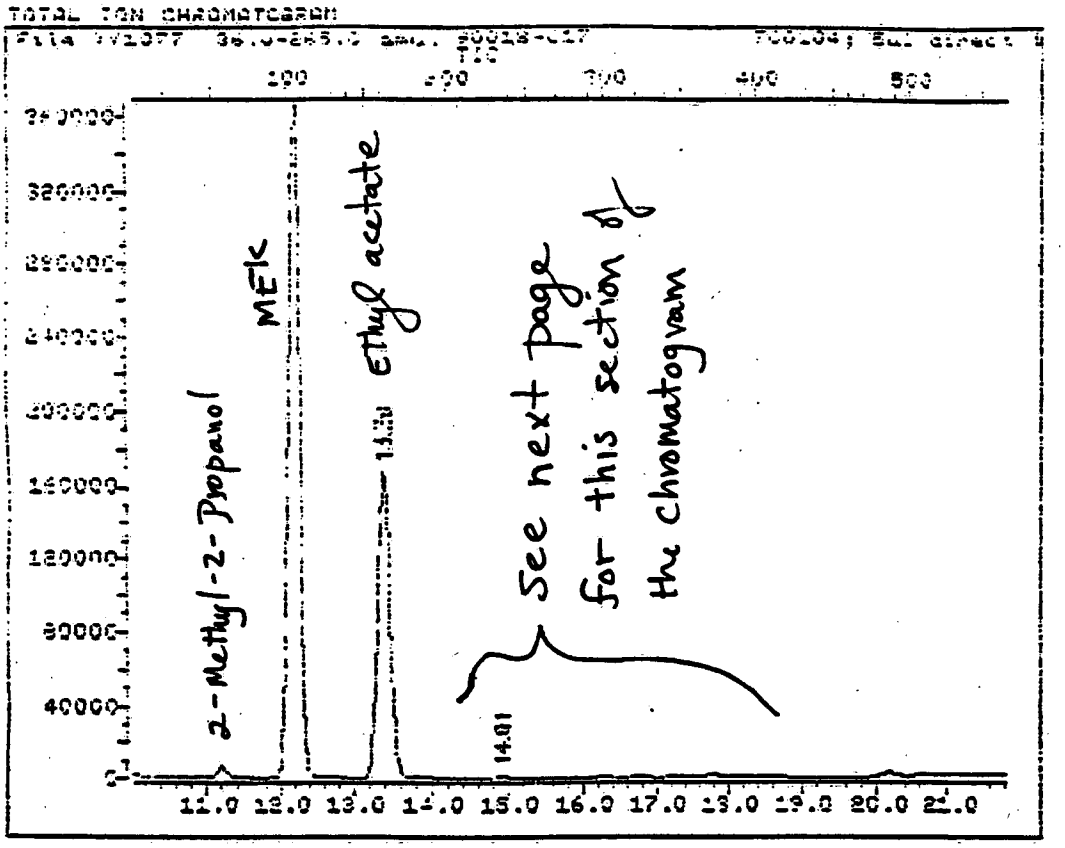
:PBM

1. Propanoic acid, 2-oxo- (SCI) 88 C3H4O3
2. Acetic acid, ethyl ester 88 C4H8O2

Sample file: >C0048 Spectrum #: 751
Search speed: 1 Tilting option: N No. of ion ranges searched: 42

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	43*	127173	11	*BIGDB	26	51	1	0	85	23	17	14
2.	41*	141786	6949	*BIGDB	35	42	0	0	39	43	14	36

5µl direct injection of methyl hydrate



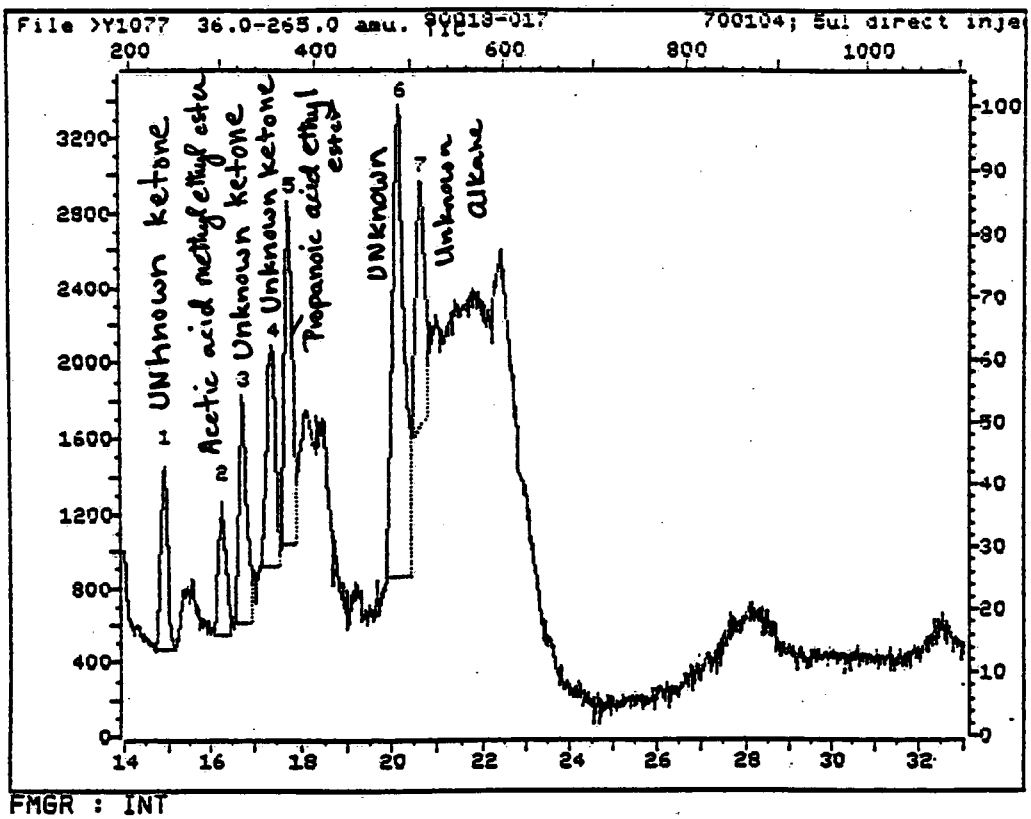
Data File: >Y1077::D2 Quant Output File: ^Y1077::D2
Name: 90018-017
Misc: 700104: 5ul direct injection

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: JFG
Quant Time: 900312 09:14
Injected at: 900312 07:15

TIC page 1 of 2

Methyl Hydrate - 5ul Injection Including Trace Compound Spectra and Library Comparisons.

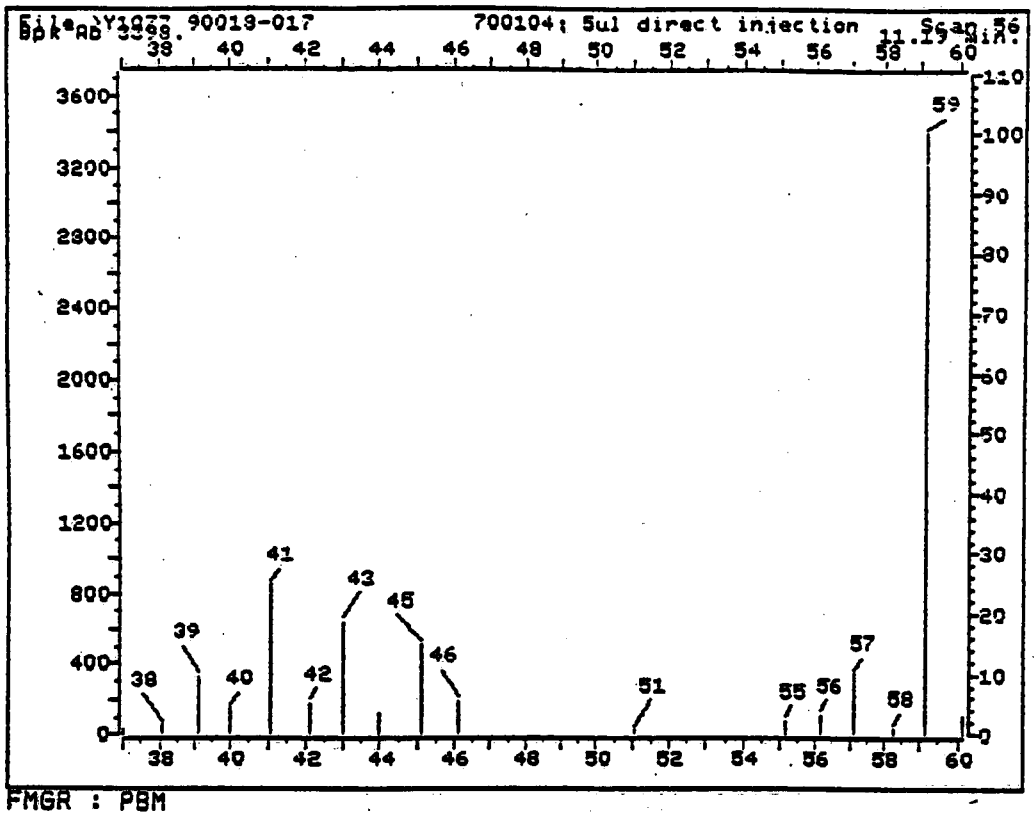


FMGR : INT

>Y1077 90018-017 700104; Sul direct injection
36.0; 265.0 TIC
Upslope: .20 Area Reject: 5.00 % Max Peaks: 7 Bunching: 1
Dnslope: 0.00 Results File VDIR71 Sorted by Time/Area INT

Peak #	R.T. min.	first scan	max scan	last scan	peak height	raw area	corr. area	corr. % max.	% of total
1	14.91	226	235	246	981	22273	10617	23.82	8.065
2	16.26	292	300	309	707	19856	8145	18.27	6.187
3	16.72	314	322	333	1218	29397	14909	33.45	11.326
4	17.41	343	355	363	1183	39109	16368	36.72	12.434
5	17.76	364	372	381	1832	42287	20405	45.78	15.501
6	20.17	474	488	500	2512	72485	44571	100.00	33.859
7	20.63	503	510	519	1371	49810	16623	37.30	12.628

Sum of corrected areas: 131638.

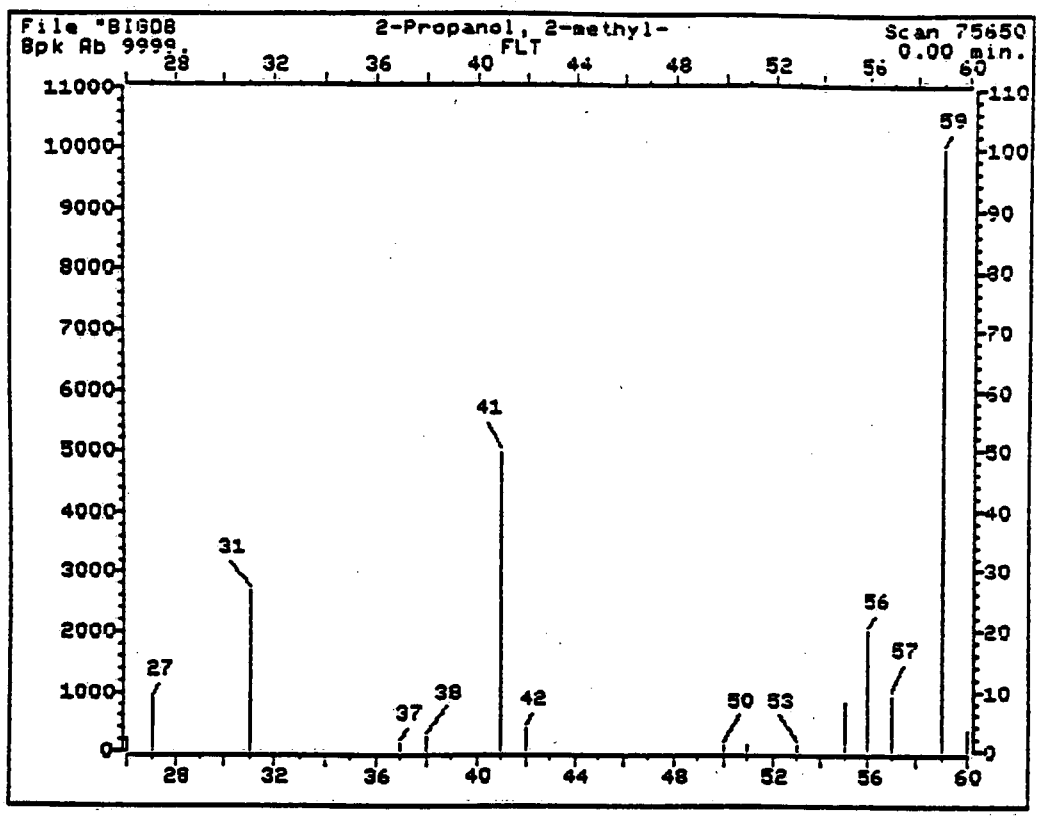


1. 2-Propanol, 2-methyl- 74 C4H10O
2. 2-Propanol, 2-methyl- 74 C4H10O
3. 2-Propanol, 2-methyl- 74 C4H10O
4. 2-Propanol, 2-methyl- 74 C4H10O
5. 2-Propanol, 2-methyl- 74 C4H10O

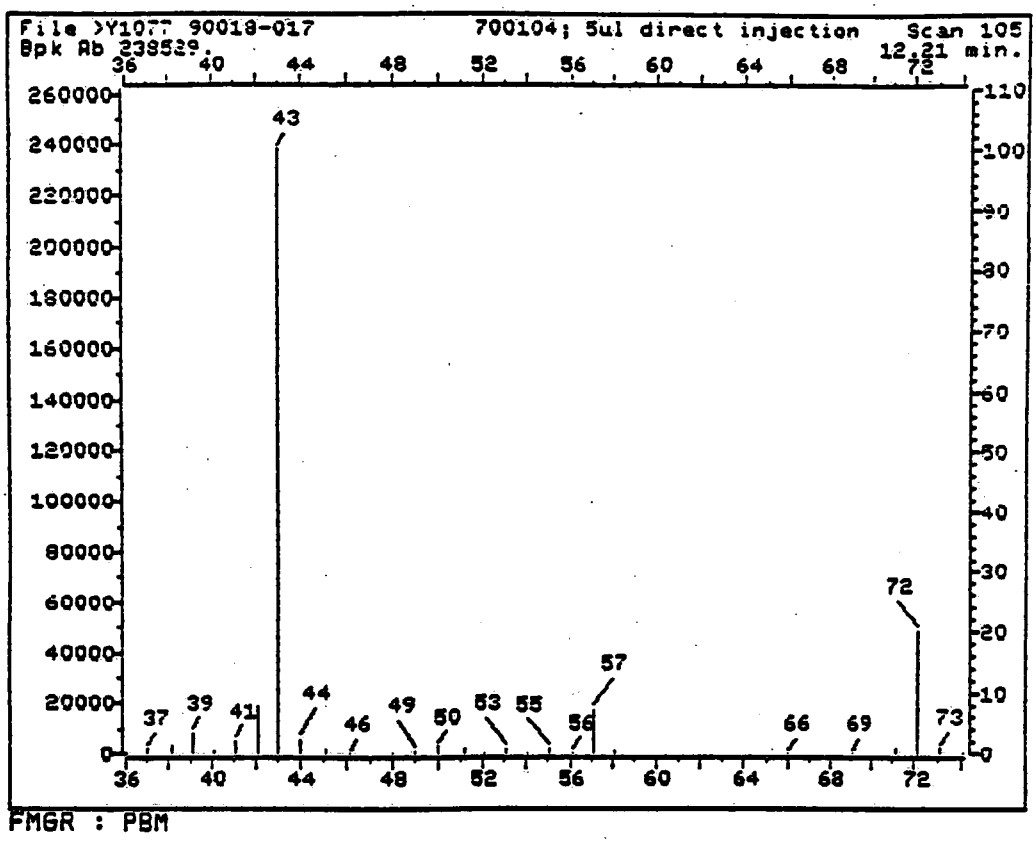
Sample file: >Y1077 Spectrum #: 56
Search speed: 1 Tilting option: N No. of ion ranges searched: 41

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	58	75650	3091	*BIGDB	45	31	0	0	97	20	25	26
2.	58	75650	3646	*BIGDB	42	29	0	0	95	20	25	23
3.	58	75650	3650	*BIGDB	40	37	0	0	77	18	25	22
4.	49	75650	3649	*BIGDB	39	35	0	0	94	22	22	21
5.	47	75650	3647	*BIGDB	35	38	0	0	91	22	17	18

2-Methyl-2-Propanol Spectra and Library Comparison


File *BIG08
Bpk Ab 9999.
2-Propanol, 2-methyl-
FLT
Scan 75650
0.00 min.
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
110
100
90
80
70
60
50
40
30
20
10
0
28
32
36
40
44
48
52
56
60
27
31
37
38
41
42
50
53
56
57
59

MEK Spectra



FMGR : PBM

1.	2-Butanone	72 C4H8O
2.	2-Butanone	72 C4H8O
3.	2-Butanone	72 C4H8O
4.	2-Butanone	72 C4H8O
5.	2-Butanone	72 C4H8O
6.	Propanal, 2-methyl-	72 C4H8O
7.	2-Butanone	72 C4H8O
8.	2-Butanone	72 C4H8O
9.	2-Butanone	72 C4H8O
10.	2-Butanone	72 C4H8O
11.	Propanal, 2-methyl-	72 C4H8O
12.	Butanal	72 C4H8O
13.	2-Butanone	72 C4H8O

Sample file: >Y1077 Spectrum #: 105
Search speed: 1 Tilting option: N No. of ion ranges searched: 40

	Prob.	CAS #	CON #	ROOT	.K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	89*	78933	8128	*BIGDB	47	26	0	0	85	4	66	66
2.	84*	78933	8122	*BIGDB	46	21	0	0	98	10	55	66
3.	76*	78933	8124	*BIGDB	31	37	0	0	73	10	45	24
4.	76*	78933	8121	*BIGDB	43	22	1	0	100	8	45	25
5.	76*	78933	7760	*BIGDB	43	25	1	0	98	10	45	25
6.	70*	78842	8109	*BIGDB	29	43	2	0	97	8	42	14
7.	70*	78933	8126	*BIGDB	37	33	1	0	98	10	42	19
8.	67*	78933	8123	*BIGDB	42	24	1	0	98	12	34	24
9.	60*	78933	8125	*BIGDB	36	31	1	0	88	12	30	19
10.	52*	78933	8127	*BIGDB	21	45	0	0	100	16	20	15

APPENDIX C

PURGE AND TRAP ANALYSIS OF METHYL HYDRATE

APPENDIX C

PURGE AND TRAP ANALYSIS OF METHYL HYDRATE

BFB Summary and Spectra
Initial Calibration Summary
50 ppb Calibration Standard

Method Blank
Methyl Hydrate Purge 1:100,000 Dilution
Methyl Hydrate Purge 1:50,000 Dilution
Methyl Hydrate Purge 1:10,000 Dilution
Methyl Hydrate Purge 1:5,000 Dilution

FMGR : TAB

>YB122 50 NG BFB 700104
487 SUB NRM ENH

File: >YB122 Scan #: 487 Retn. time: 10.10

m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.	m/z	Int.
40.05	-.063	51.00	6.504	74.10	14.947	94.10	10.944	175.05	6.004
43.95	2.877	61.00	3.002	75.10	50.594	95.10	100.000	176.05	76.360
45.05	2.251	68.10	10.944	80.90	1.001	96.10	7.255	177.05	4.190
49.00	2.939	69.00	9.443	88.00	4.565	174.05	76.298	207.15	1.313
50.10	20.513	73.10	4.503						

FMGR : TUNER,=BFB

GC/MS PERFORMANCE STANDARD

Bromofluorobenzene (BFB)

m/z	Ion Abundance Criteria	% Relative Abundance Base Peak	% Relative Abundance Appropriate Peak	Status
50	15-40% of mass 95	20.51	20.51	Ok
75	30-60% of mass 95	50.59	50.59	Ok
95	Base peak, 100% relative abundance	100.00	100.00	Ok
96	5-9% of mass 95	7.25	7.25	Ok
173	Less than 2% of mass 174	0.00	0.00	Ok
174	Greater than 50% of mass 95	76.30	76.30	Ok
175	5-9% of mass 174	6.00	7.87	Ok
176	95-101% of mass 174	76.36	100.08	Ok
177	5-9% of mass 176	4.19	5.49	Ok

Injection Date: 03/11/90
Injection Time: 08:10
Data File: >YB122
Scan: 487

ENH,-1:1
PS,100
SUB

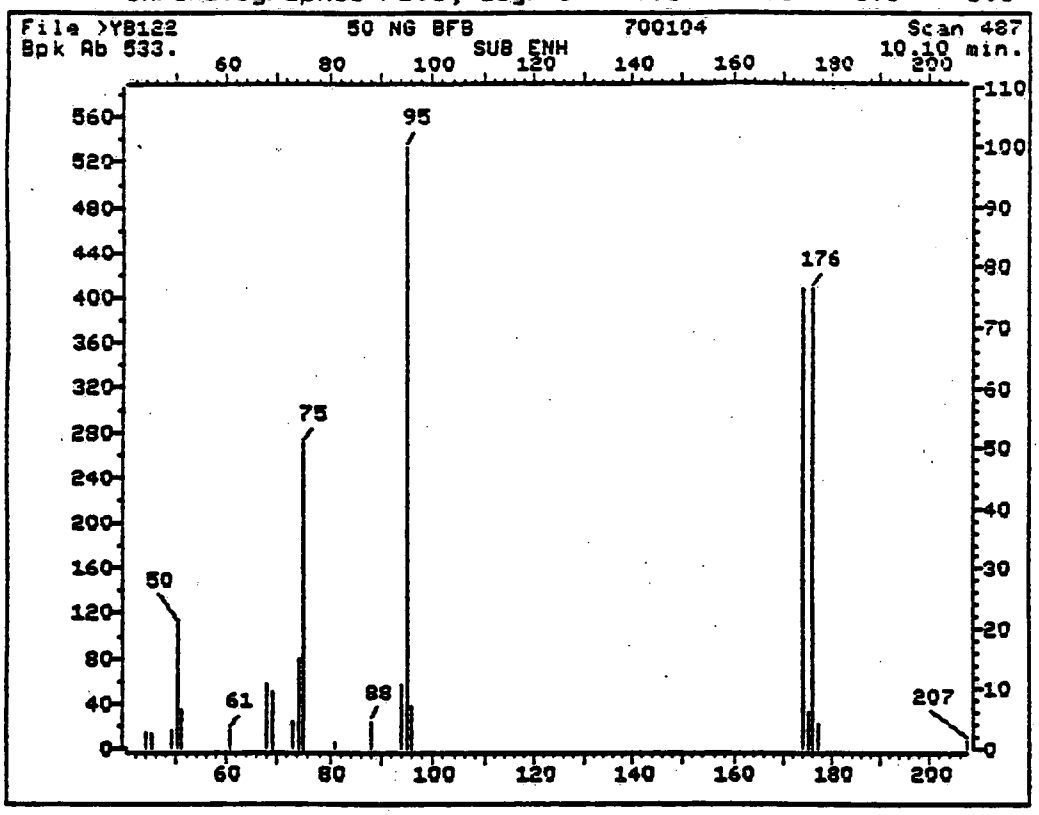
BFB Summary Page

FMGR : MSH

MS data file header from : >YB122

Sample: 50 NG BFB Operator: EJK SUPER GRP. 3/11/90 8:10
Misc : 700104
Sys. #: 1 MS model: 70 SW/HW rev.: IA ALS # : 0
Method file: M_YBFB Tuning file: MT4000 No. of extra records: 2
Source temp.: 0 Analyzer temp.: 170 Transfer line temp. : 0

Chromatographic temperatures :	200.	200.	0.	0.	0.
Chromatographic times, min. :	10.0	8.0	0.0	0.0	0.0
Chromatographic rate, deg/min:	1.0	0.0	0.0	0.0	0.0



BFB Spectra

Initial Calibration Summary and Ethanol Relative Response Factors.

Initial Calibration Data
HSL Compounds

Case No: _____ Instrument ID: 700104

Contractor: C-E ENVIRONMENTAL Calibration Date: 03/12/90

Contract No: _____

Minimum $\overline{RF}$ for SPCC is .300 Maximum % RSD for CCC is 30%

Laboratory ID:	YY1062	YY1063	YY1064	YY1065	YY1066					
Compound	RF 20.00	RF 50.00	RF 100.00	RF 150.00	RF 200.00	$\overline{RRT}$	$\overline{RF}$	%RSD	CCC	SPCC
Chloromethane	.94372	.80279	.86546	.77921	.73532	.157	.82530	9.837		**
Bromomethane	1.38060	1.21740	1.30021	.97772	.87161	.234	1.14951	18.933		
Vinyl Chloride	.94930	.88947	.91536	.89747	.72615	.294	.87555	9.894	*	
Chloroethane	.60410	.53428	.57645	.57469	.51896	.382	.56170	6.143		
thanol) – Ethanol	.00134	.00151	.00159	-	-	.504	.00148	8.626		(Conc=5000.0,10000.,20000
Methylene Chloride	.86626	.96119	1.02721	.99560	.89489	.620	.94903	7.110		
Acetone	.23545	.15582	.13233	.14877	.15666	.712	.16581	24.208		
Carbon Disulfide	1.94318	1.98205	2.14947	1.98680	2.76705	.791	2.16571	15.347		
1,1-Dichloroethene	.89356	.93260	1.01605	.96368	.86164	.945	.93351	6.447	*	
1,1-Dichloroethane	1.83901	2.13139	2.38193	2.00371	1.82926	1.088	2.03706	11.284		**
1,2-Dichloroethene (total)	1.06942	1.09715	1.15177	1.06421	1.00951	1.173	1.07841	4.818		
Chloroform	2.37103	2.67415	3.01031	2.65105	2.53463	1.240	2.64823	8.886	*	
1,2-Dichloroethane	1.57261	1.64124	1.65865	1.60850	1.63195	1.319	1.62259	2.851		
1,2-Dichloroethane-d4 (surr.)	1.51303	1.61805	1.60046	1.60631	1.54835	1.307	1.57724	2.937		
2-Butanone	.02998	.04795	.05211	.06257	.06857	1.322	.05224	28.509		
1,1,1-Trichloroethane	.70524	.64835	.72939	.62663	.68650	.683	.67922	6.144		
Carbon Tetrachloride	.59951	.65700	.78909	.65582	.65492	.701	.67127	18.466		
Vinyl Acetate	.54164	.54003	.62735	.57371	.35769	.720	.52808	19.248		
Bromodichloromethane	.77878	.75733	.86241	.74199	.80770	.733	.78964	6.025		
1,2-Dichloropropane	.33473	.35045	.41818	.34700	.34723	.800	.35952	9.274	*	
cis-1,3-Dichloropropene	.50305	.48941	.56505	.50242	.51966	.814	.51592	5.716		(Conc=25.6,64.0,128.0,192
Trichloroethene	.39433	.43003	.51274	.41584	.44447	.845	.43948	10.226		
Dibromochloromethane	.64344	.69455	.83295	.70602	.71562	.873	.71852	9.718		
1,1,2-Trichloroethane	.29969	.30740	.36940	.30496	.30497	.879	.31728	9.226		
Benzene	.78635	.74990	.80851	.68597	.71533	.868	.74921	6.688		
trans-1,3-Dichloropropene	.44226	.43862	.50154	.43211	.46732	.879	.45637	6.259		(Conc=14.4,36.0,72.0,108.
Bromoform	.50163	.49548	.54217	.49180	.55714	1.008	.51764	5.777		**
4-Methyl-2-Pentanone	.26235	.27752	.28624	.28606	.30510	.832	.28346	5.475		
2-Hexanone	.15933	.18122	.17532	.18450	.20215	.895	.18050	8.584		
Tetrachloroethene	.43581	.48918	.56155	.48294	.43641	.909	.48118	10.693		

RF - Response Factor (Subscript is amount in UG/L)

$\overline{RRT}$ - Average Relative Retention Time (RT Std/RT Istd)

$\overline{RF}$ - Average Response Factor

%RSD - Percent Relative Standard Deviation

CCC - Calibration Check Compounds (*) SPCC - System Performance Check Compounds (**)

Initial Calibration Data
HSL Compounds

Case No: _____ Instrument ID: 700104

Contractor: C-E ENVIRONMENTAL Calibration Date: 03/12/90

Contract No: _____

Minimum $\overline{RF}$ for SPCC is .300 Maximum % RSD for CCC is 30%

Laboratory ID:	XY1062	XY1063	XY1064	XY1065	XY1066					
Compound	RF 20.00	RF 50.00	RF 100.00	RF 150.00	RF 200.00	$\overline{RRT}$	$\overline{RF}$	% RSD	CCC	SPCC
1,1,2,2-Tetrachloroethane	.62035	.59247	.62950	.57999	.54584	.905	.59363	5.632		**
Toluene	.61985	.60467	.65390	.56308	.57595	.959	.60349	5.976	*	
Toluene-d8 (surr.)	1.10111	1.08367	1.15127	1.07497	.98967	.951	1.08014	5.423		
Chlorobenzene	.77790	.82626	.99681	.84687	.76380	1.005	.84233	11.019		**
Ethylbenzene	.39499	.37294	.40364	.36623	.37550	1.078	.38266	4.149	*	
Styrene	.83215	.81971	.89031	.79365	.80855	1.186	.82887	4.483		
Xylene (total)	.47742	.49059	.54939	.45732	.45649	1.192	.48624	7.835		
p-Bromofluorobenzene (surr.)	.78728	.75998	.83546	.76291	.70466	1.150	.77006	6.161		

RF - Response Factor (Subscript is amount in UG/L)

$\overline{RRT}$ - Average Relative Retention Time (RT Std/RT Istd)

$\overline{RF}$ - Average Response Factor

%RSD - Percent Relative Standard Deviation

CCC - Calibration Check Compounds (*) SPCC - System Performance Check Compounds (**)

50 ppb Calibration Standard Data Package

QUANT REPORT

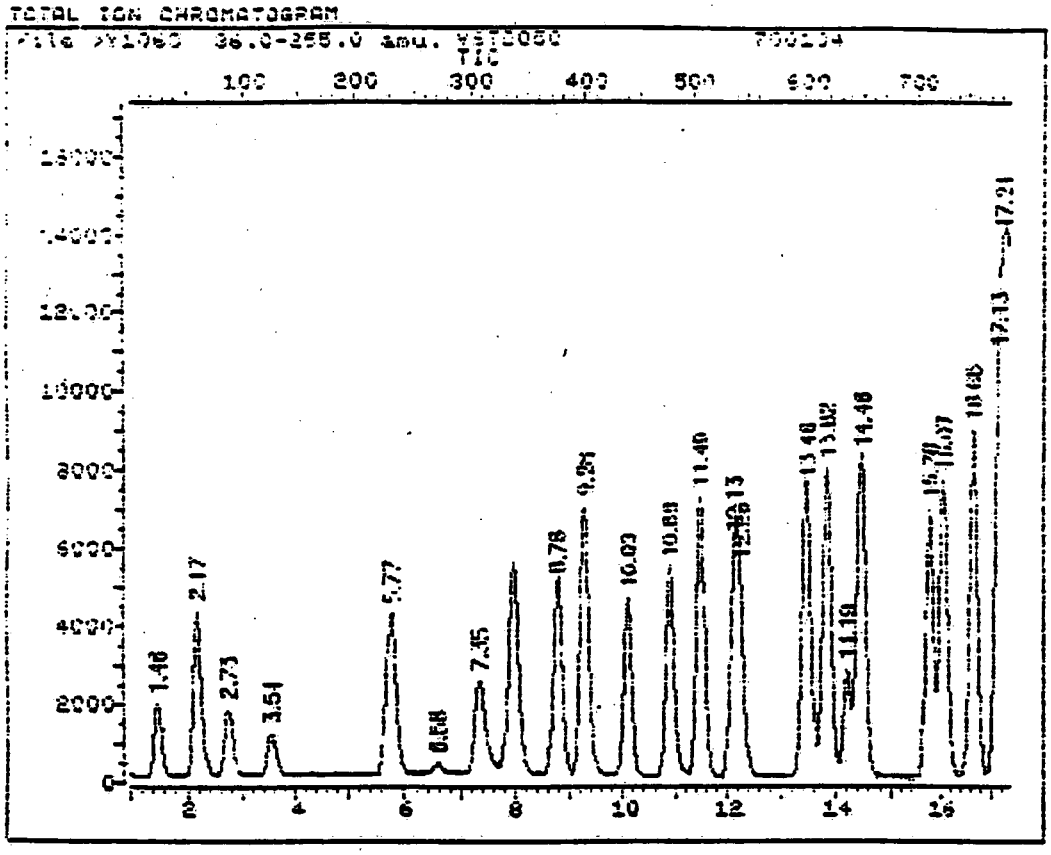
Operator ID: EJK Quant Rev: 6 Quant Time: 900512 09:36
Output File: [illegible] Injected at: 900311 12:35
Data File: [illegible] Dilution Factor: 1.00000
Name: 90T0030
Misc: 70P104

ID File: [illegible]
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900311 11:18

	Compound	R.T.	Q ion	Area	Conc	Units	Q
1)	*Bromochloromethane	9.25	128.0	12033	50.00	UG/L	94
2)	Chloromethane	1.46	50.0	9660	80.54	UG/L	76
3)	Bromomethane	2.17	94.0	14649	73.90	UG/L	81
4)	Vinyl Chloride	2.73	62.0	10703	76.04	UG/L	97
5)	Chloroethane	3.54	64.0	6429	66.46	UG/L	94
7)	Methylene Chloride	5.77	84.0	11566	44.50	UG/L	98
8)	Acetone	6.58	43.0	1875	16.20	UG/L	90
9)	Carbon Disulfide	7.35	76.0	23850	94.52	UG/L	97
10)	1,1-Dichloroethene	8.76	96.0	11222	42.99	UG/L	95
11)	1,1-Dichloroethane	10.09	63.0	25647	50.79	UG/L	96
12)	1,2-Dichloroethene (total)	10.88	96.0	13202	47.44	UG/L	84
13)	Chloroform	11.49	83.0	32178	50.02	UG/L	92
14)	1,2-Dichloroethane	12.26	62.0	19749	44.18	UG/L	89
15)	1,2-Dichloroethane-d4 (surr.)	12.13	65.0	19470	52.91	UG/L	92
16)	2-Butanone	12.26	72.0	577	42.98	UG/L	98
17)	*1,4-Difluorobenzene	19.75	114.0	42551	50.00	UG/L	91
18)	1,1,1-Trichloroethane	13.46	97.0	27588	42.31	UG/L	90
19)	Carbon Tetrachloride	13.82	117.0	27956	45.58	UG/L	96
20)	Vinyl Acetate	14.19	43.0	22979	49.15	UG/L	96
21)	Bromodichloromethane	14.46	83.0	32225	45.86	UG/L	90
22)	1,2-Dichloropropane	15.78	63.0	14912	49.08	UG/L	98
23)	cis-1,3-Dichloropropene	16.07	75.0	26656	52.47	UG/L	63
24)	Trichloroethene	16.65	130.0	18298	45.35	UG/L	92
25)	Dibromochloromethane	17.21	129.0	29554	46.87	UG/L	95
26)	1,1,2-Trichloroethane	17.34	97.0	13080	45.15	UG/L	81
27)	Benzene	17.13	78.0	31909	46.99	UG/L	67
28)	trans-1,3-Dichloropropene	17.36	75.0	13438	27.83	UG/L	64
29)	Bromoform	19.85	173.0	21083	40.02	UG/L	96
30)	*Chlorobenzene-d5	24.53	117.0	34660	50.00	UG/L	95
31)	4-Methyl-2-Pentanone	20.41	43.0	9619	368.35	UG/L	94
32)	2-Hexanone	21.95	43.0	6231	56.82	UG/L	83
33)	Tetrachloroethene	22.29	164.0	16955	45.82	UG/L	94
34)	1,1,2,2-Tetrachloroethane	22.18	83.0	20535	40.45	UG/L	90
35)	Toluene	23.53	92.0	20958	38.89	UG/L	93
36)	Toluene-d8 (surr.)	23.35	98.0	37560	48.23	UG/L	96
37)	Chlorobenzene	24.66	112.0	28638	45.41	UG/L	94
38)	Ethylbenzene	26.43	106.0	12926	41.18	UG/L	74
39)	Styrene	29.09	104.0	28411	43.82	UG/L	91
40)	Xylene (total)	29.24	106.0	17004	49.86	UG/L	72
40)	Xylene (total)	29.82	106.0	32869	96.38	UG/L	70
41)	p-Bromofluorobenzene (surr.)	23.21	95.0	26341	51.29	UG/L	86

* Compound is ISTD

TOTAL ION CHROMATOGRAM



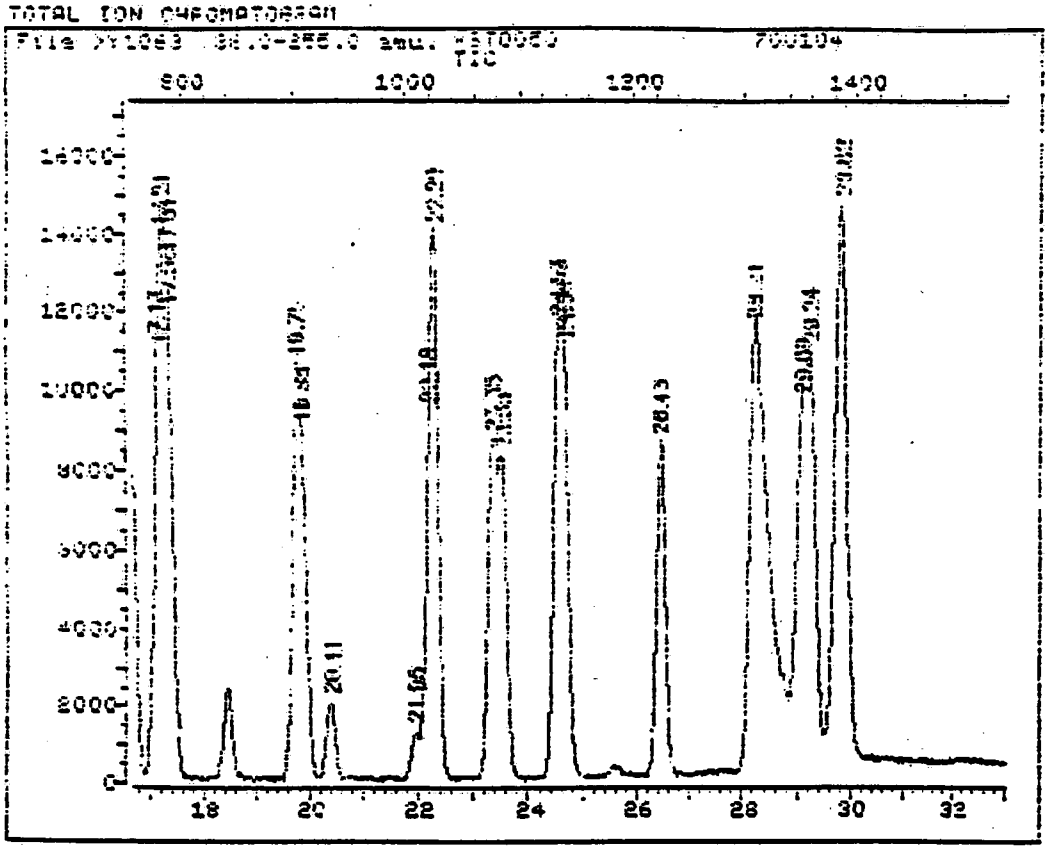
Data File: >Y1063::D2 Quant Output File: ^Y1063::D2
Name: VSTD050
Misc: 700104

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900311 11:18

Operator ID: EJK
Quant Time: 900312 05:26
Injected at: 900311 12:28

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



Data File: >Y1063::D2 Quant Output File: ^Y1063::D2
Name: VSTD050
Misc: 700104

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900311 11:18

Operator ID: EJK
Quant Time: 900312 05:26
Injected at: 900311 12:28

TIC page 2 of 2

QUANT REPORT

Operator ID: EJK
Output File: ^Y1068::D2
Data File: >Y1068::D2
Name: VBLK03
Misc: 700104

Quant Rev: 6
Quant Time: 900312 05:57
Injected at: 900311 15:47
Dilution Factor: 1.00000

ID File: I_YETC::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

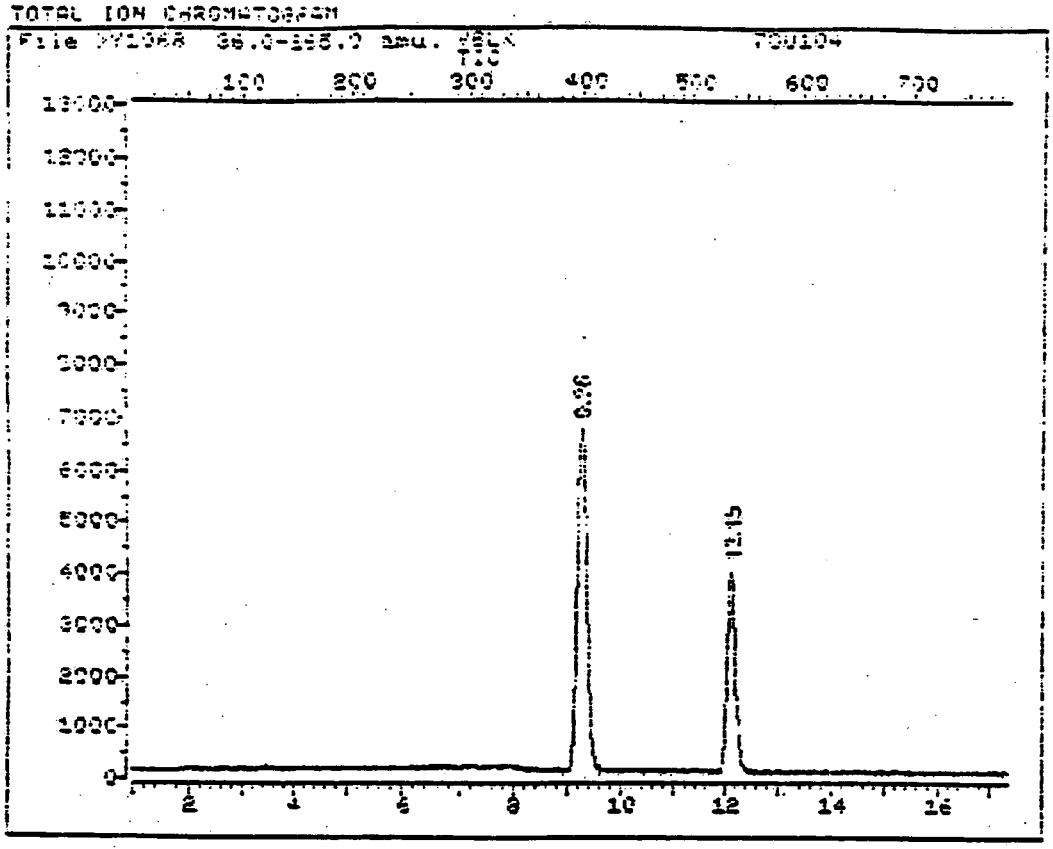
	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.26	128.0	11550	50.00	UG/L	97
15)	1,2-Dichloroethane-d4 (surr.)	12.15	65.0	16851	46.25	UG/L	80
17)	*1,4-Difluorobenzene	19.69	114.0	38486	50.00	UG/L	93
30)	*Chlorobenzene-d5	24.50	117.0	30928	50.00	UG/L	90
36)	Toluene-d8 (surr.)	23.31	98.0	33969	50.84	UG/L	94
41)	p-Bromofluorobenzene (surr.)	28.18	95.0	24313	51.04	UG/L	85

* Compound is ISTD

Method Blank Data Package

5 mL Purge and Trap

TOTAL ION CHROMATOGRAM



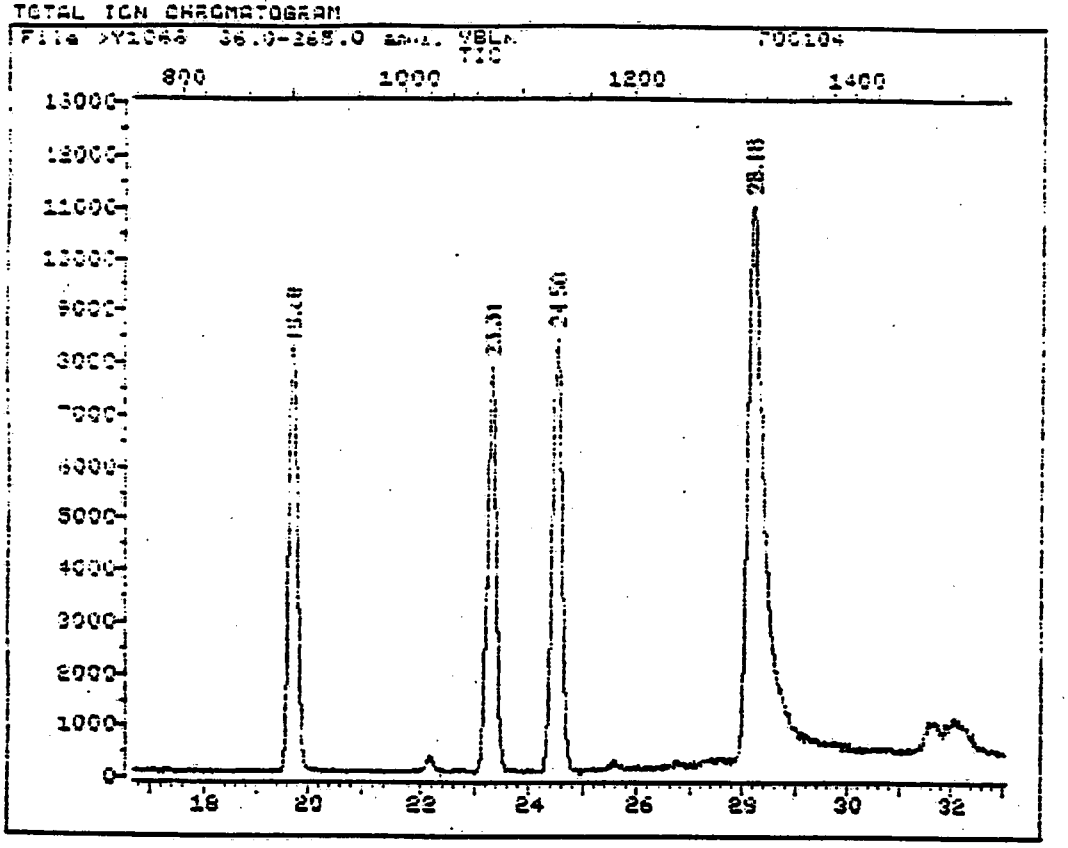
Data File: >Y1068::D2 Quant Output File: ^Y1068::D2
Name: VBLK
Misc: 700104

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900312 05:59
Injected at: 900311 15:47

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



Data File: >Y1068::D2 Quant Output File: ^Y1068::D2
Name: VBLK
Misc: 700104

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900312 05:59
Injected at: 900311 15:47

TIC page 2 of 2

QUANT REPORT

Operator ID: EJK
Output File: >Y10692::D1
Data File: >Y10692::D2
Name: 90018-017
Misc: 700104:1:100000 DL

Quant Rev: 6
Quant Time: 900314 15:00
Injected at: 900311 16:27
Dilution Factor: 1.00000

ID File: I_YET8::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

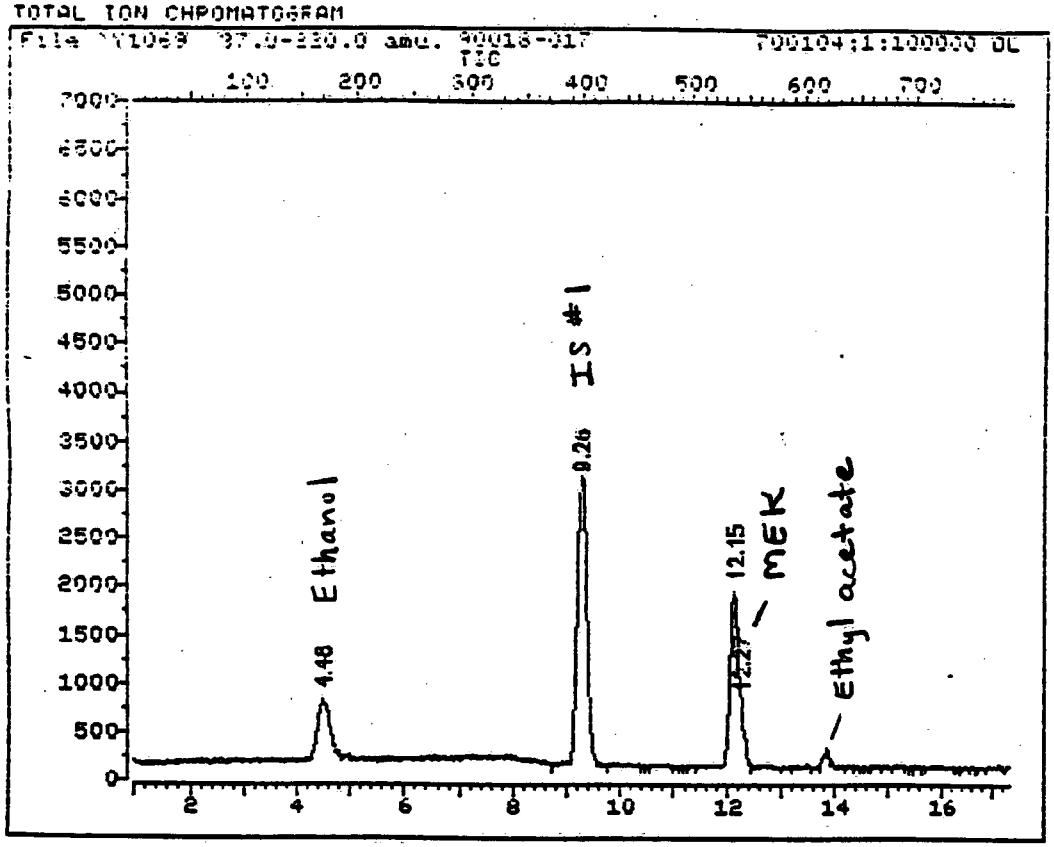
	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.26	128.0	5236	50.00	UG/L	97
6)	Ethanol	4.48	46.0	2082	13433.50	UG/L	73
15)	1,2-Dichloroethane-d4 (surr.)	12.15	65.0	7756	46.96	UG/L	84
16)	2-Butanone	12.27	72.0	364	66.54	UG/L	94
17)	*1,4-Difluorobenzene	19.69	114.0	17864	50.00	UG/L	91
30)	*Chlorobenzene-d5	24.49	117.0	14500	50.00	UG/L	97
36)	Toluene-d8 (surr.)	23.31	98.0	15770	50.34	UG/L	98
41)	p-Bromofluorobenzene (surr.)	28.18	95.0	11758	52.65	UG/L	95

* Compound is ISTD

Methyl Hydrate Purge and Trap Data Package

1:100,000 Dilution

TOTAL ION CHROMATOGRAM



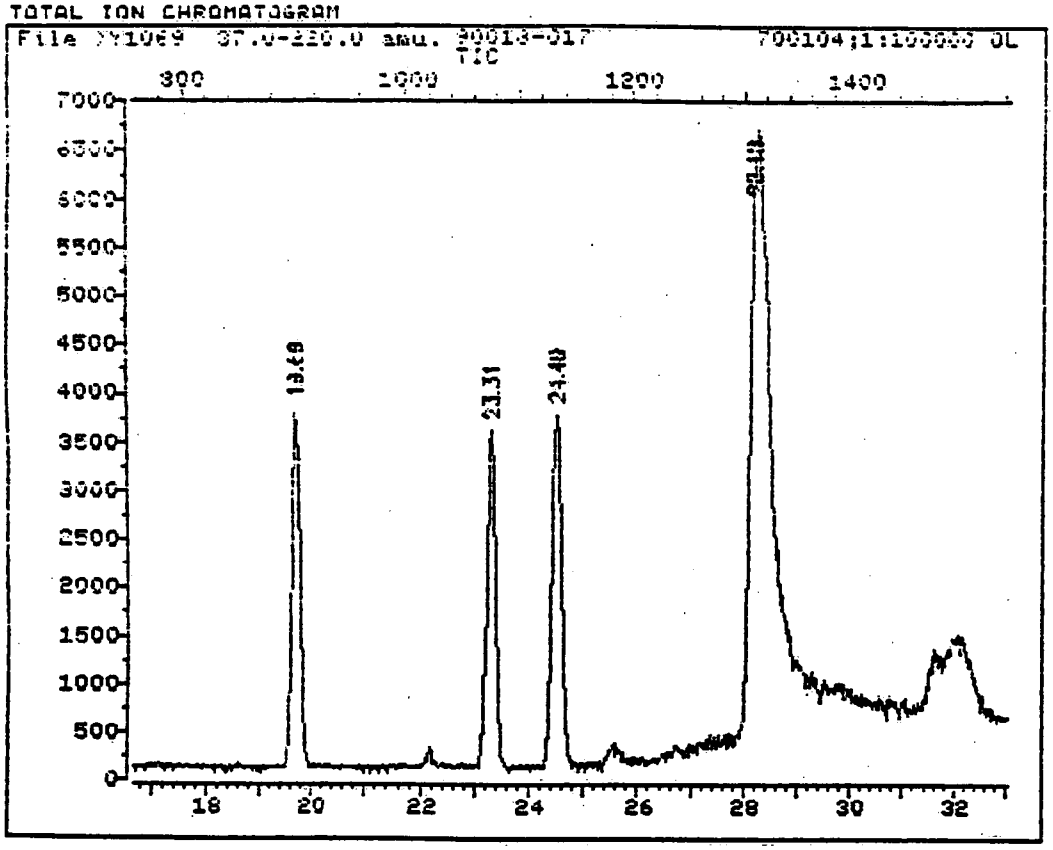
Data File: >Y1069::D2 Quant Output File: ^Y1069::D1
Name: 90018-017
Misc: 700104;1:100000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900314 15:00
Injected at: 900311 16:27

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



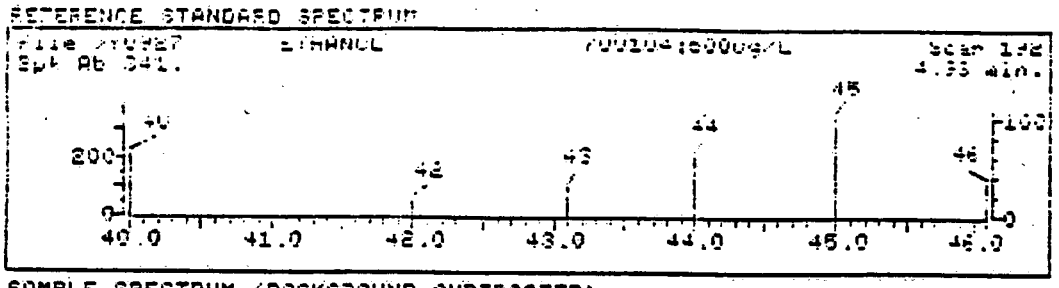
Data File: >Y1069::D2 Quant Output File: ^Y1069::D1
Name: 90018-017
Misc: 700104;1:100000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

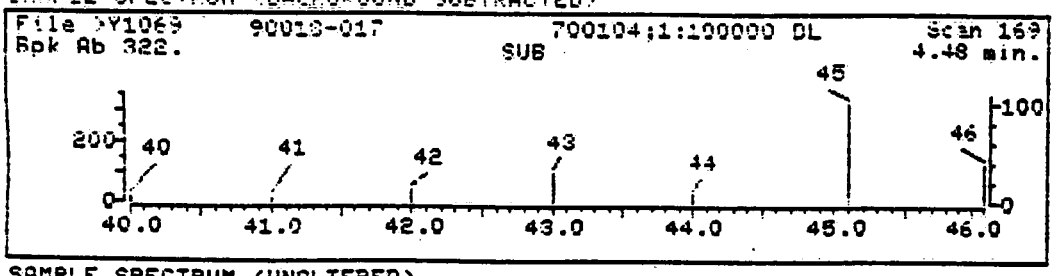
Operator ID: EJK
Quant Time: 900314 15:00
Injected at: 900311 16:27

TIC page 2 of 2

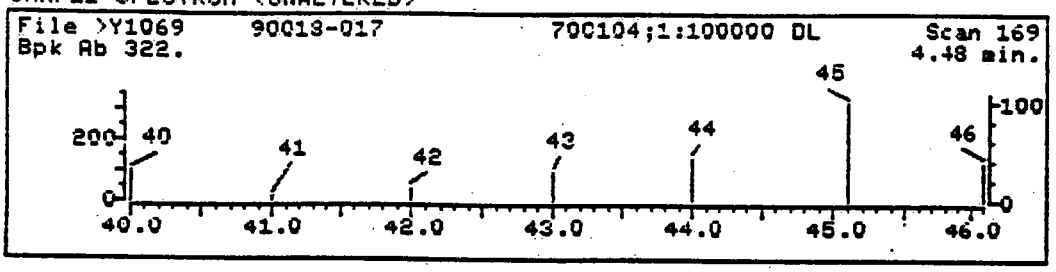
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



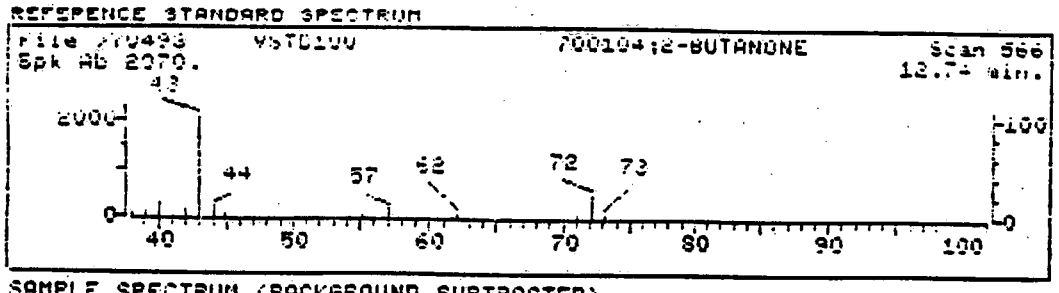
Data File: >Y1069::D2
Name: 90018-017
Misc: 700104:1:100000 DL
Quant Time: 900314 15:00
Injected at: 900311 16:27

Quant Output File: ^Y1069::D1

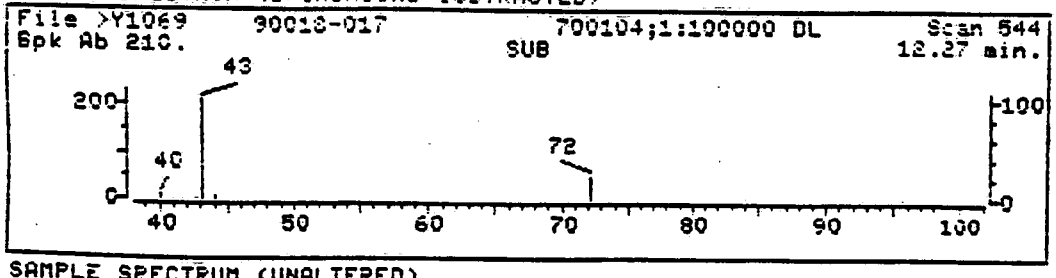
Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 6
Compound Name: Ethanol
Scan Number: 169
Retention Time: 4.48 min.
Quant Ion: 46.0
Area: 2082
Concentration: 13433.50 UG/L
q-value: 73

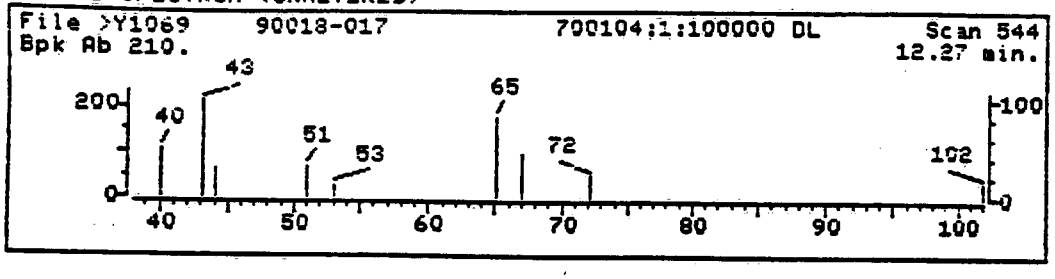
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



Data File: >Y1069::D2
Name: 90018-017
Misc: 700104;1:100000 DL
Quant Time: 900314 15:00
Injected at: 900311 16:27

Quant Output File: ^Y1069::D1

Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 16
Compound Name: 2-Butanone
Scan Number: 544
Retention Time: 12.27 min.
Quant Ion: 72.0
Area: 364
Concentration: 66.54 UG/L
q-value: 94

QUANT REPORT

Operator ID: EJK
Output File: ^Y1070::D1
Data File: >Y1070::D2
Name: 90018-017
Misc: 700104;1:50000 DL

Quant Rev: 6
Quant Time: 900314 15:02
Injected at: 900311 17:06
Dilution Factor: 1.00000

ID File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

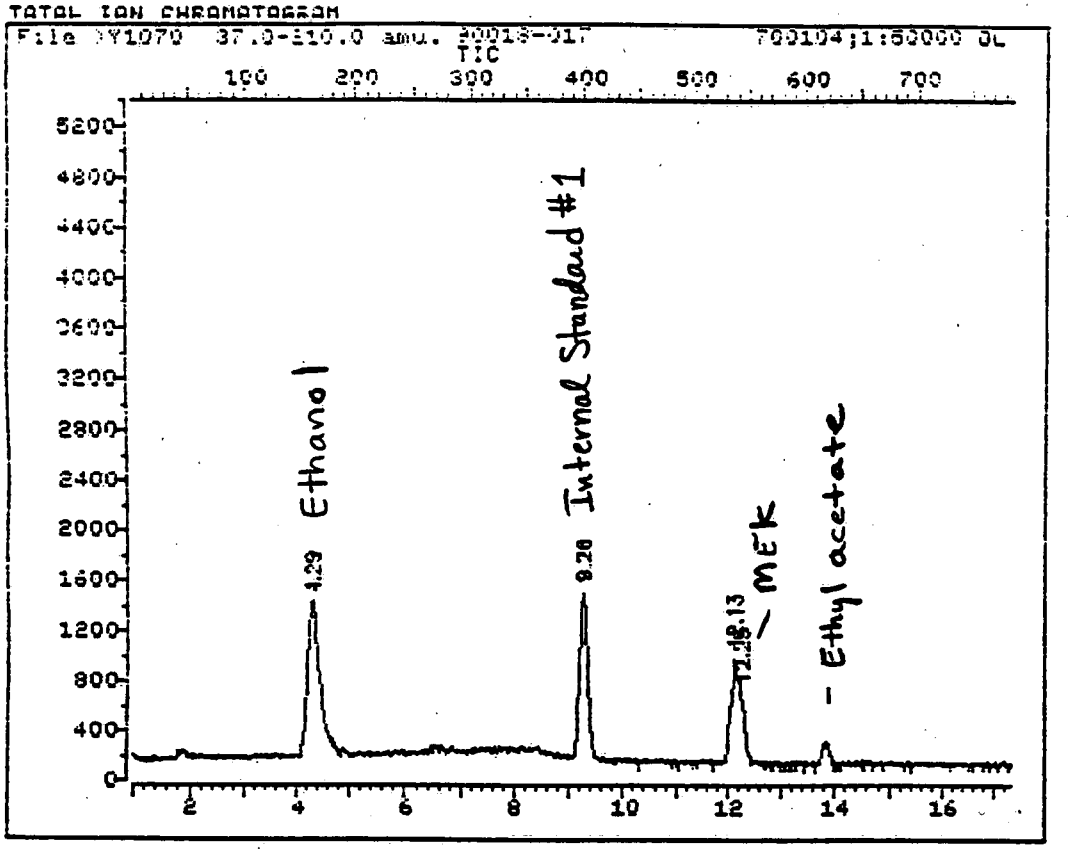
	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.26	128.0	2289	50.00	UG/L	89
6)	Ethanol	4.29	46.0	4356	64291.02	UG/L	69
13)	1,2-Dichloroethane-d4 (surr.)	12.13	65.0	3248	44.98	UG/L	92
16)	2-Butanone	12.25	72.0	579	242.11	UG/L	97
17)	*1,4-Difluorobenzene	19.69	114.0	8784	50.00	UG/L	87
30)	*Chlorobenzene-d5	24.52	117.0	6874	50.00	UG/L	99
36)	Toluene-d8 (surr.)	23.31	98.0	7565	50.94	UG/L	88
41)	p-Bromofluorobenzene (surr.)	28.18	95.0	5218	49.29	UG/L	86

* Compound is ISTD

Methyl Hydrate Purge and Trap Data Package

1:50,000 Dilution

TOTAL ION CHROMATOGRAM



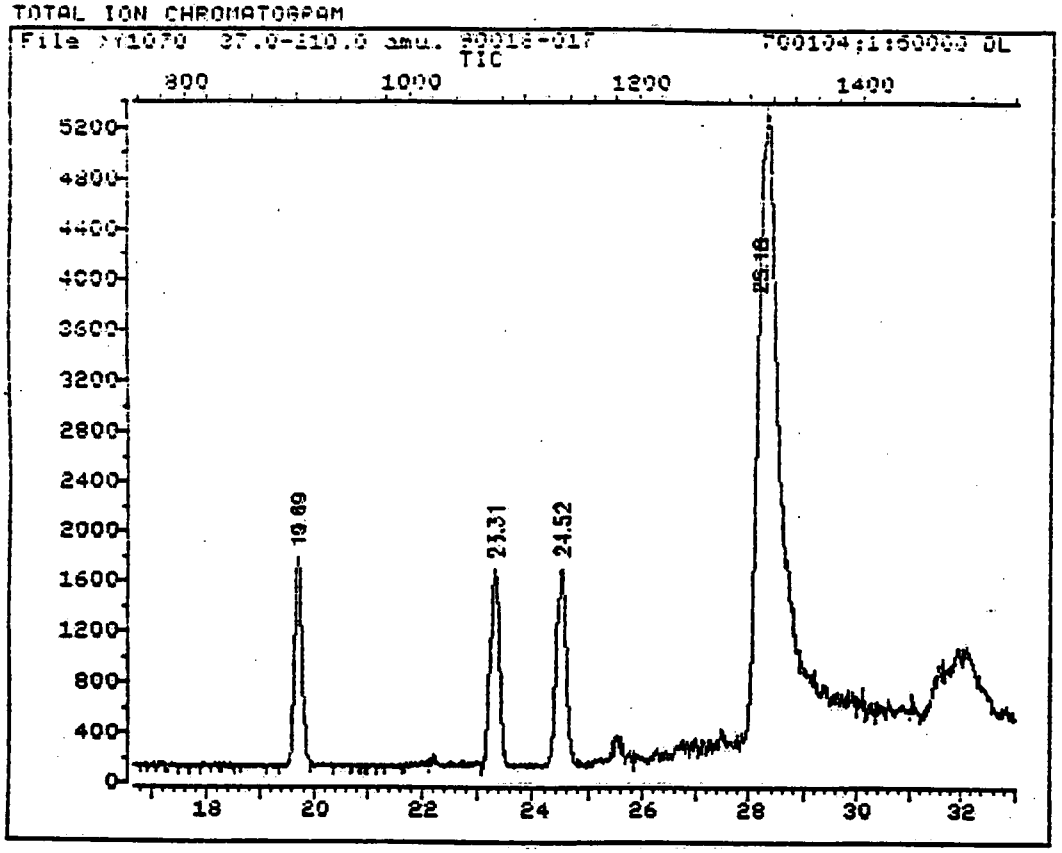
Data File: >Y1070::D2 Quant Output File: ^Y1070::D1
Name: 90018-017
Misc: 700104;1:50000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900314 15:02
Injected at: 900311 17:06

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



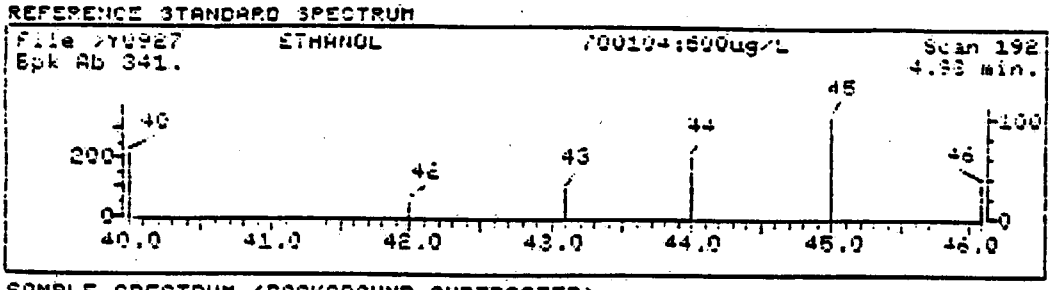
Data File: >Y1070::D2 Quant Output File: ^Y1070::D1
Name: 90018-017
Misc: 700104;1:50000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

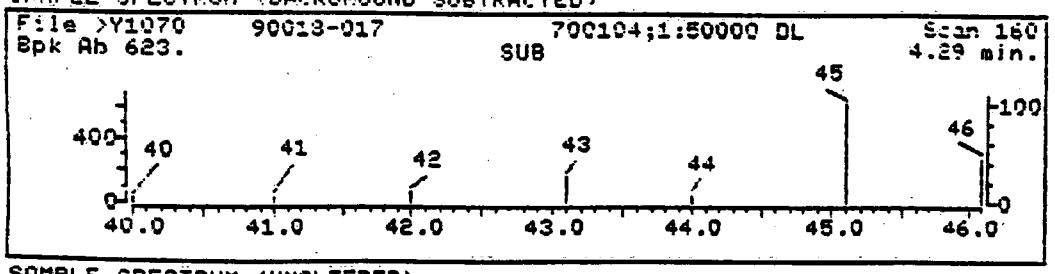
Operator ID: EJK
Quant Time: 900314 15:02
Injected at: 900311 17:06

TIC page 2 of 2

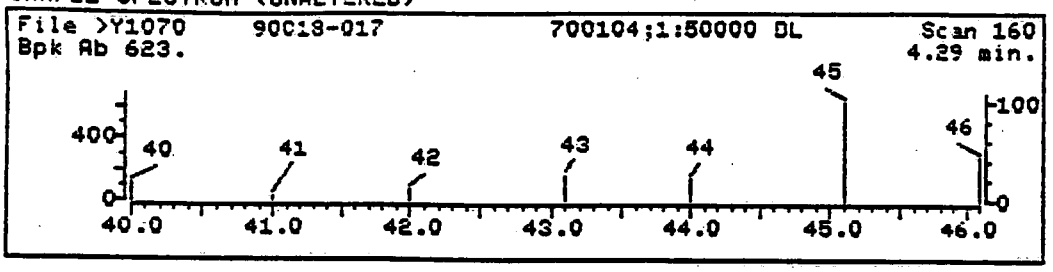
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



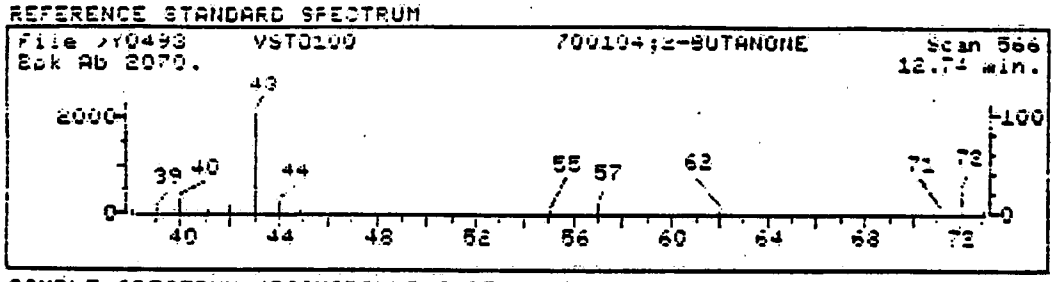
Data File: >Y1070::D2
Name: 90018-017
Misc: 700104:1:50000 DL
Quant Time: 900314 15:02
Injected at: 900311 17:06

Quant Output File: ^Y1070::D1

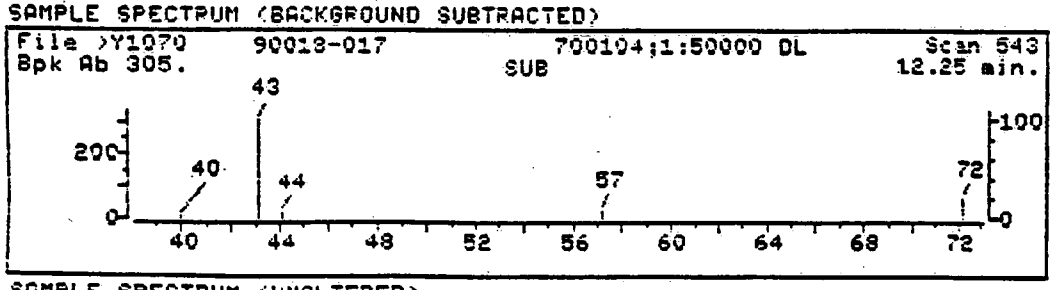
Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 6
Compound Name: Ethanol
Scan Number: 160
Retention Time: 4.29 min.
Quant Ion: 46.0
Area: 4356
Concentration: 64291.02 UG/L
q-value: 69

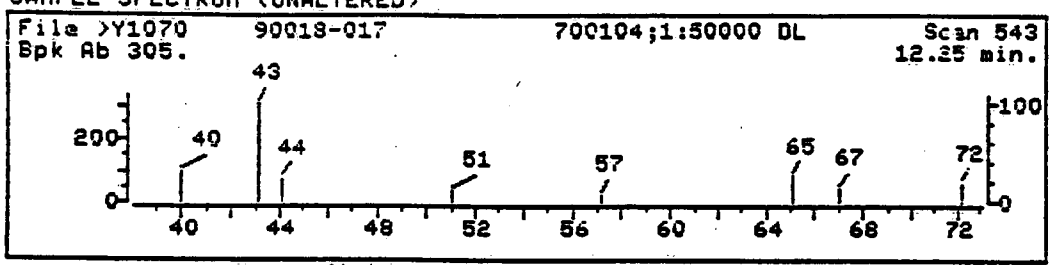
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



Data File: >Y1070::D2
Name: 90018-017
Misc: 700104;1:50000 DL
Quant Time: 900314 15:02
Injected at: 900311 17:06

Quant Output File: ^Y1070::D1

Quant ID File: I_YET0::D2
Last Calibration: 900312 05:57

Compound No: 16
Compound Name: 2-Butanone
Scan Number: 543
Retention Time: 12.25 min.
Quant Ion: 72.0
Area: 579
Concentration: 242.11 UG/L
q-value: 97

QUANT REPORT

Operator ID: EJK
Output File: ^Y1071::D1
Data File: >Y1071::D2
Name: 90018-017
Misc: 700104; 1:10000 DL

Quant Rev: 6
Quant Time: 900314 15:04
Injected at: 900311 17:46
Dilution Factor: 1.00000

ID File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

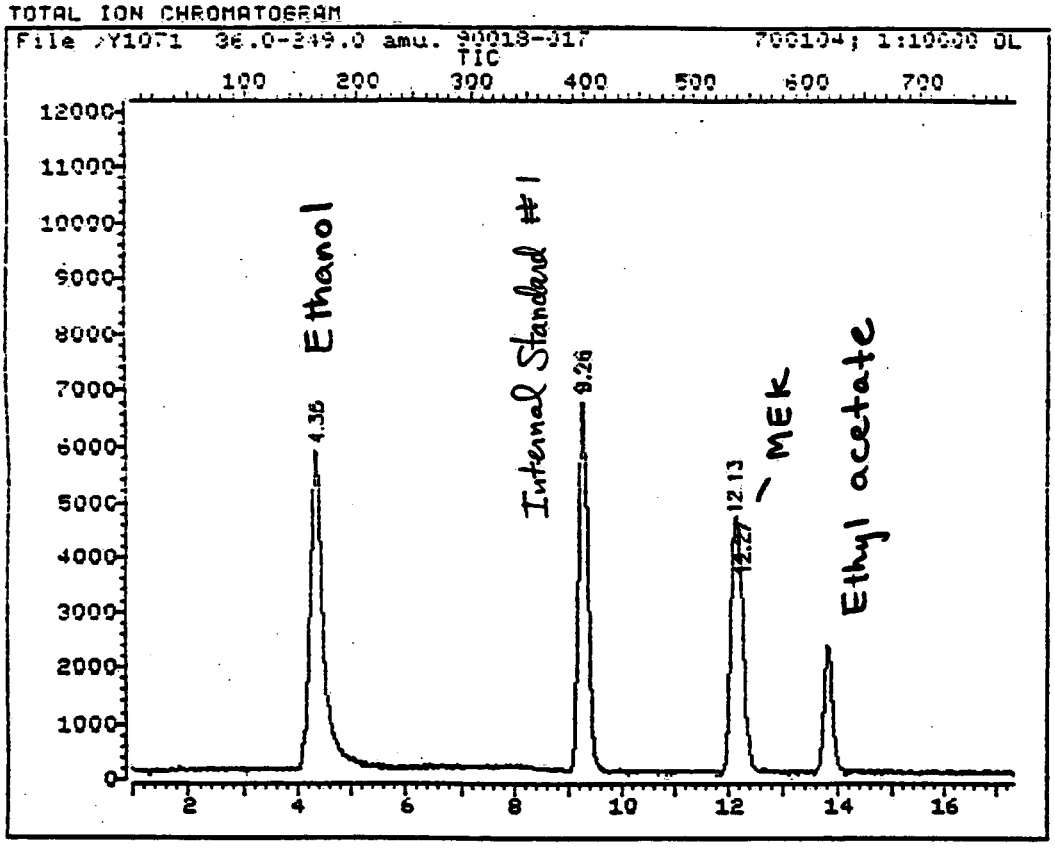
	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.26	128.0	11442	50.00	UG/L	91
6)	Ethanol	4.35	46.0	22242	65671.98	UG/L	70
15)	1,2-Dichloroethane-d4 (surr.)	12.13	65.0	16483	45.67	UG/L	92
16)	2-Butanone	12.27	72.0	4349	363.81	UG/L	98
17)	*1,4-Difluorobenzene	19.67	114.0	37043	50.00	UG/L	93
30)	*Chlorobenzene-d5	24.50	117.0	30368	50.00	UG/L	94
36)	Toluene-d8 (surr.)	23.31	98.0	33108	50.47	UG/L	91
41)	p-Bromofluorobenzene (surr.)	28.16	95.0	24082	51.49	UG/L	88

* Compound is ISTD

Methyl Hydrate Purge and Trap Data Package

1: 10,000 Dilution

TOTAL ION CHROMATOGRAM



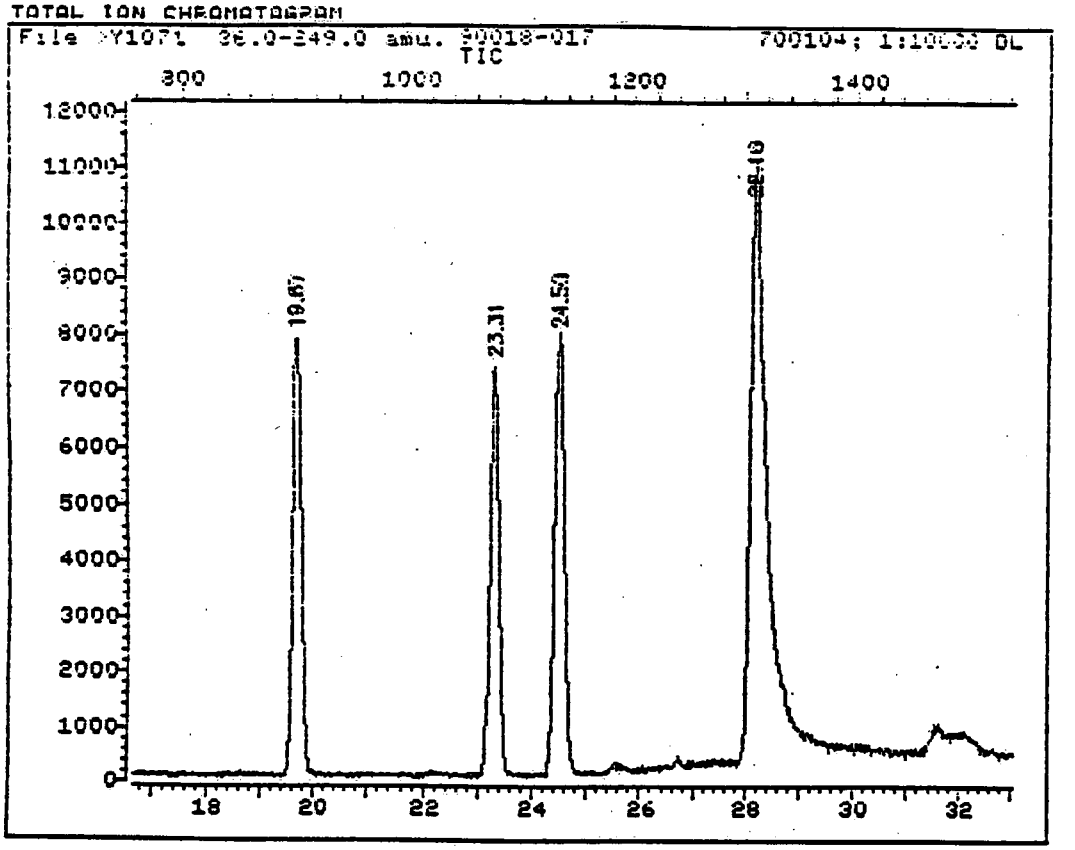
Data File: >Y1071::D2 Quant Output File: ^Y1071::D1
Name: 90018-017
Misc: 700104: 1:10000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900314 15:04
Injected at: 900311 17:46

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



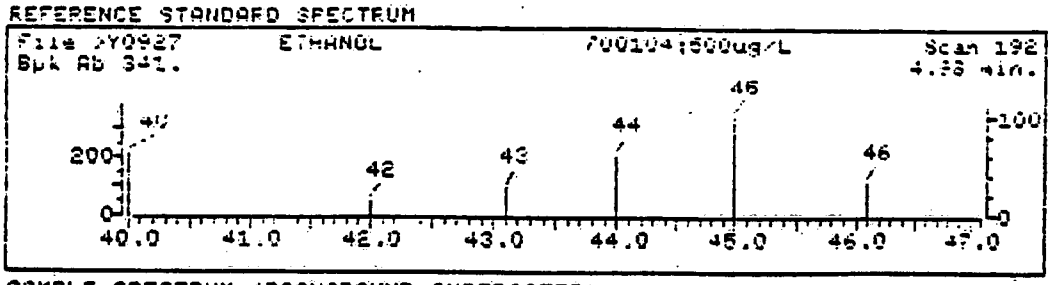
Data File: >Y1071::D2 Quant Output File: ^Y1071::D1
Name: 90018-017
Misc: 700104; 1:10000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

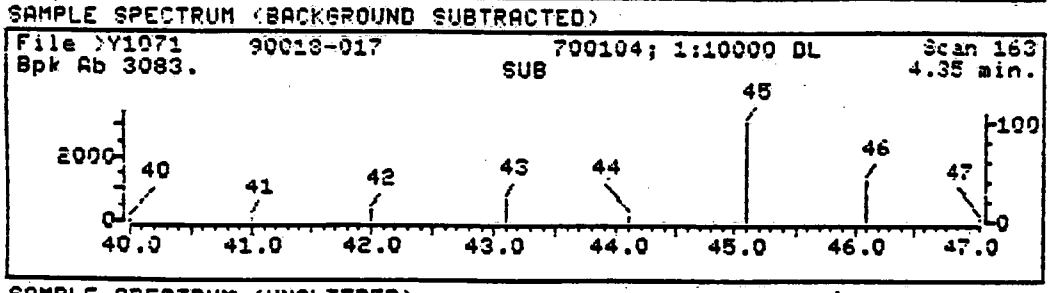
Operator ID: EJK
Quant Time: 900314 15:04
Injected at: 900311 17:46

TIC page 2 of 2

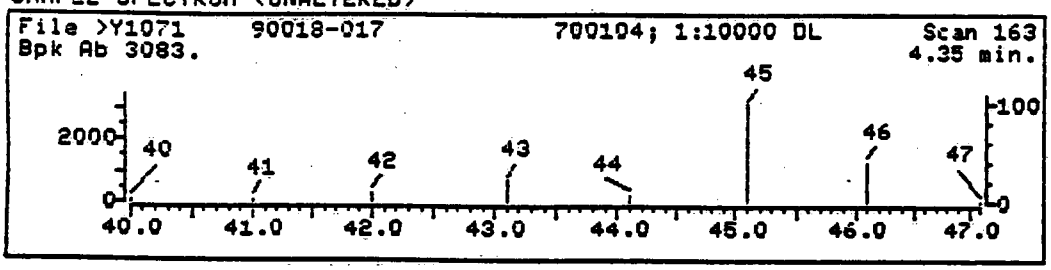
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



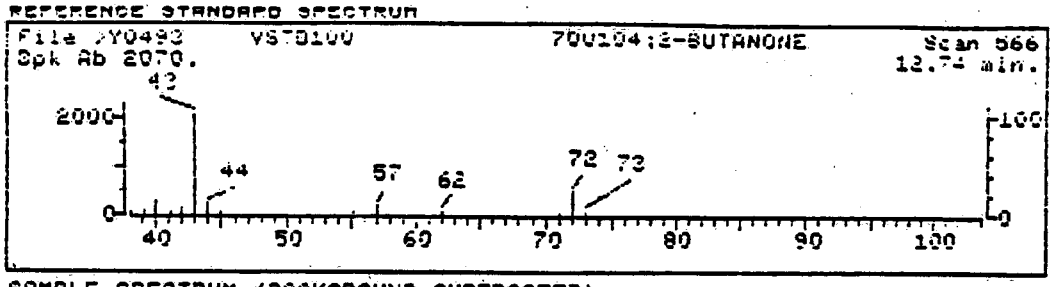
Data File: >Y1071::D2
Name: 90018-017
Misc: 700104; 1:10000 DL
Quant Time: 900314 15:04
Injected at: 900311 17:46

Quant Output File: ^Y1071::D1

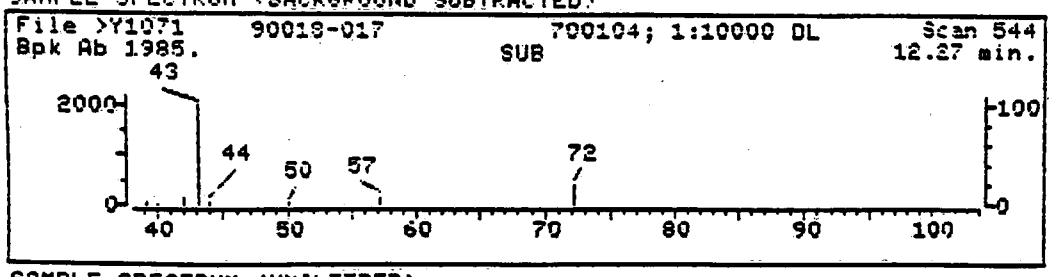
Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 6
Compound Name: Ethanol
Scan Number: 163
Retention Time: 4.35 min.
Quant Ion: 46.0
Area: 22242
Concentration: 65671.98 UG/L
q-value: 70

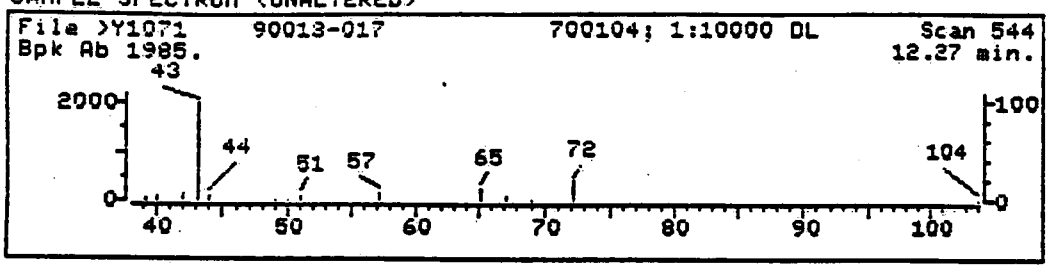
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



Data File: >Y1071::D2
Name: 90018-017
Misc: 700104; 1:10000 DL
Quant Time: 900314 15:04
Injected at: 900311 17:46

Quant Output File: ^Y1071::D1

Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 16
Compound Name: 2-Butanone
Scan Number: 544
Retention Time: 12.27 min.
Quant Ion: 72.0
Area: 4349
Concentration: 363.81 UG/L
q-value: 98

QUANT REPORT

Operator ID: EJK
Output File: ^Y1072::D1
Data File: >Y1072::D2
Name: 90018-017
Misc: 700104:1:5000 DL

Quant Rev: 6
Quant Time: 900314 15:06
Injected at: 900311 18:26
Dilution Factor: 1.00000

ID File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

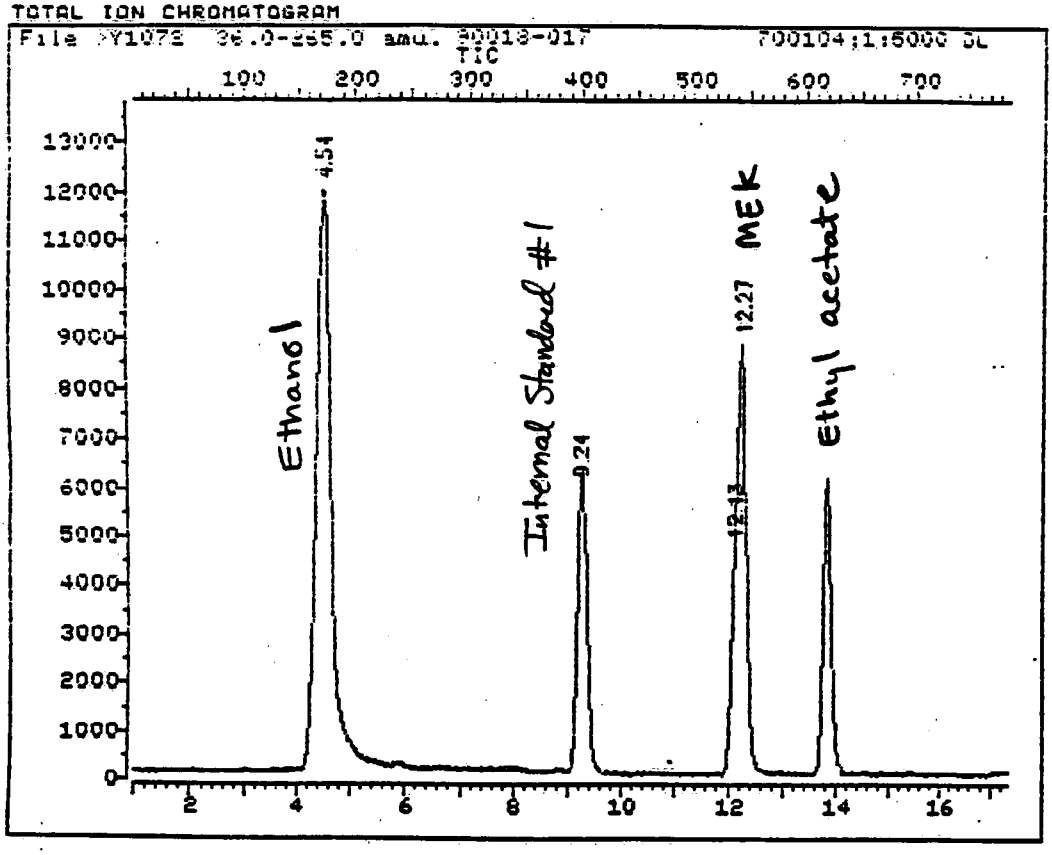
	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.24	128.0	10708	50.00	UG/L	99
6)	Ethanol	4.54	46.0	51851	163590.1	UG/L	70
15)	1,2-Dichloroethane-d4 (surr.)	12.13	65.0	15828	46.86	UG/L	91
16)	2-Butanone	12.27	72.0	11621	1038.78	UG/L	98
17)	*1,4-Difluorobenzene	19.67	114.0	35937	50.00	UG/L	92
30)	*Chlorobenzene-d5	24.48	117.0	28593	50.00	UG/L	96
36)	Toluene-d8 (surr.)	23.29	98.0	31301	50.67	UG/L	96
41)	p-Bromofluorobenzene (surr.)	28.14	95.0	23325	52.97	UG/L	83

* Compound is ISTD

Methyl Hydrate Purge and Trap Data Package

1:5,000 Dilution

TOTAL ION CHROMATOGRAM



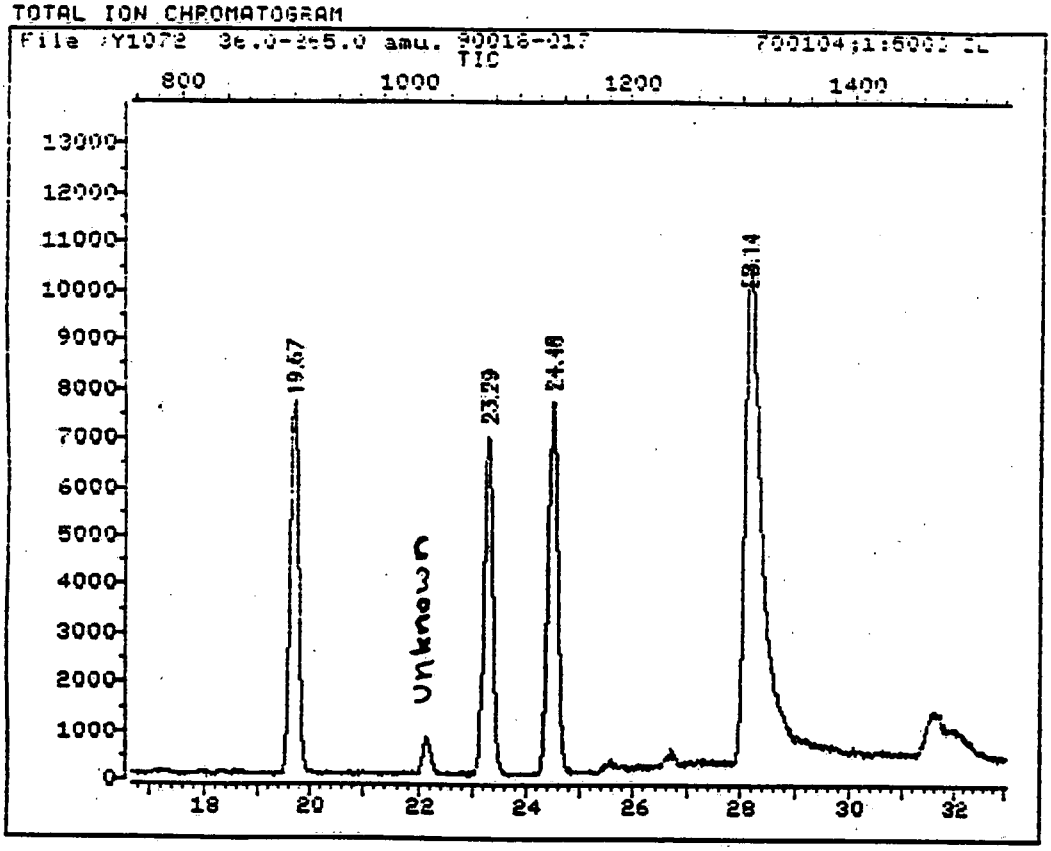
Data File: >Y1072::D2 Quant Output File: ^Y1072::D1
Name: 90018-017
Misc: 700104:1:5000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

Operator ID: EJK
Quant Time: 900314 15:06
Injected at: 900311 18:26

TIC page 1 of 2

TOTAL ION CHROMATOGRAM



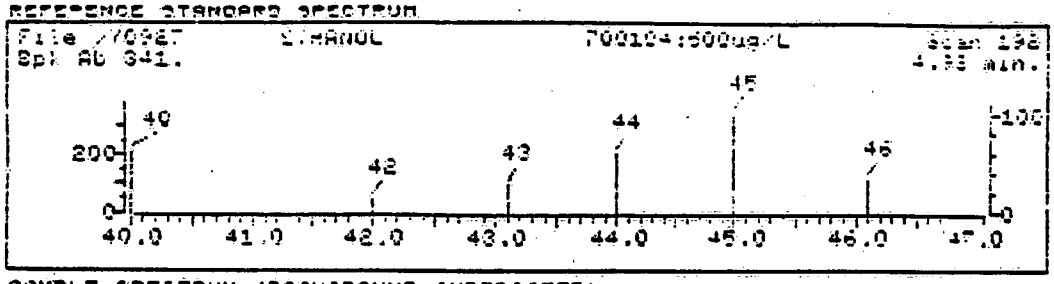
Data File: >Y1072::D2 Quant Output File: ^Y1072::D1
Name: 90018-017
Misc: 700104:1:5000 DL

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900312 05:57

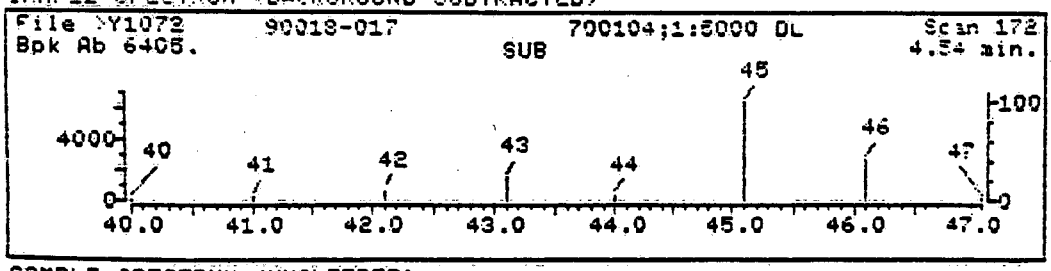
Operator ID: EJK
Quant Time: 900314 15:06
Injected at: 900311 18:26

TIC page 2 of 2

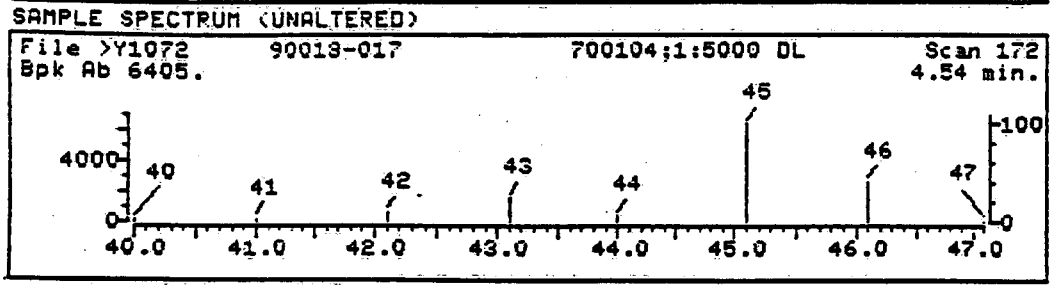
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



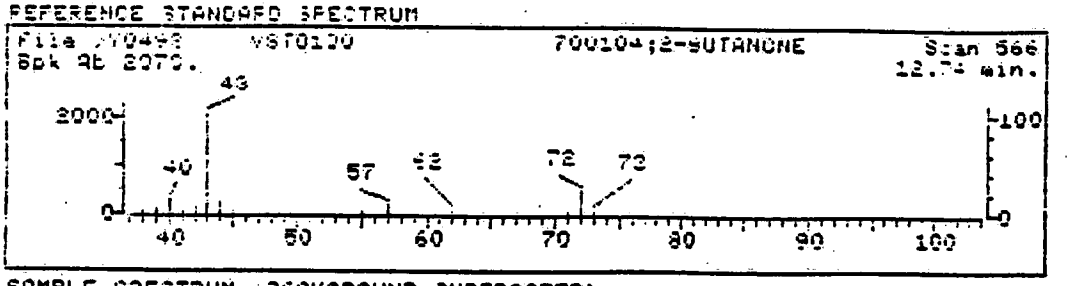
Data File: >Y1072::D2
Name: 90018-017
Misc: 700104;1:5000 DL
Quant Time: 900314 15:06
Injected at: 900311 18:26

Quant Output File: ^Y1072::D1

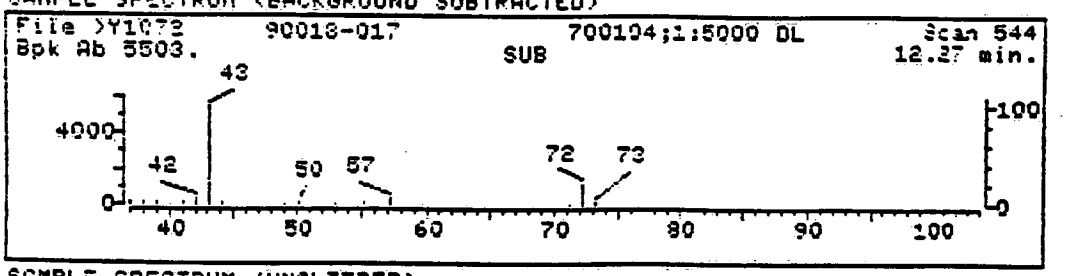
Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 6
Compound Name: Ethanol
Scan Number: 172
Retention Time: 4.54 min.
Quant Ion: 46.0
Area: 51851
Concentration: 163590.1 UG/L
q-value: 70

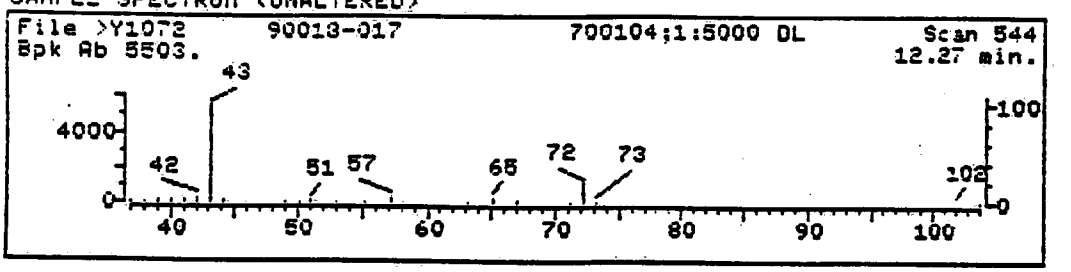
REFERENCE STANDARD SPECTRUM



SAMPLE SPECTRUM (BACKGROUND SUBTRACTED)



SAMPLE SPECTRUM (UNALTERED)



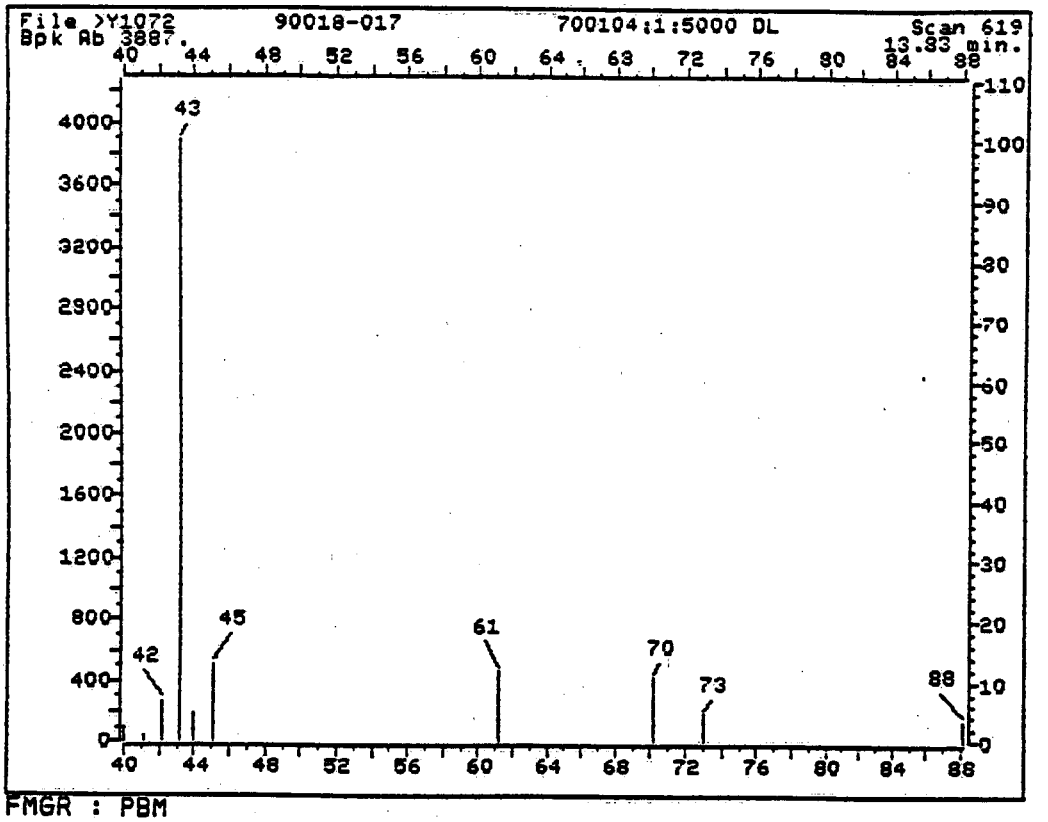
Data File: >Y1072::D2
Name: 90018-017
Misc: 700104:1:5000 DL
Quant Time: 900314 15:06
Injected at: 900311 18:26

Quant Output File: ^Y1072::D1

Quant ID File: I_YETO::D2
Last Calibration: 900312 05:57

Compound No: 16
Compound Name: 2-Butanone
Scan Number: 544
Retention Time: 12.27 min.
Quant Ion: 72.0
Area: 11621
Concentration: 1038.78 UG/L
q-value: 98

Mass Spectra of unidentified peaks in >Y1072 (1:5000 methyl hydrate purge)

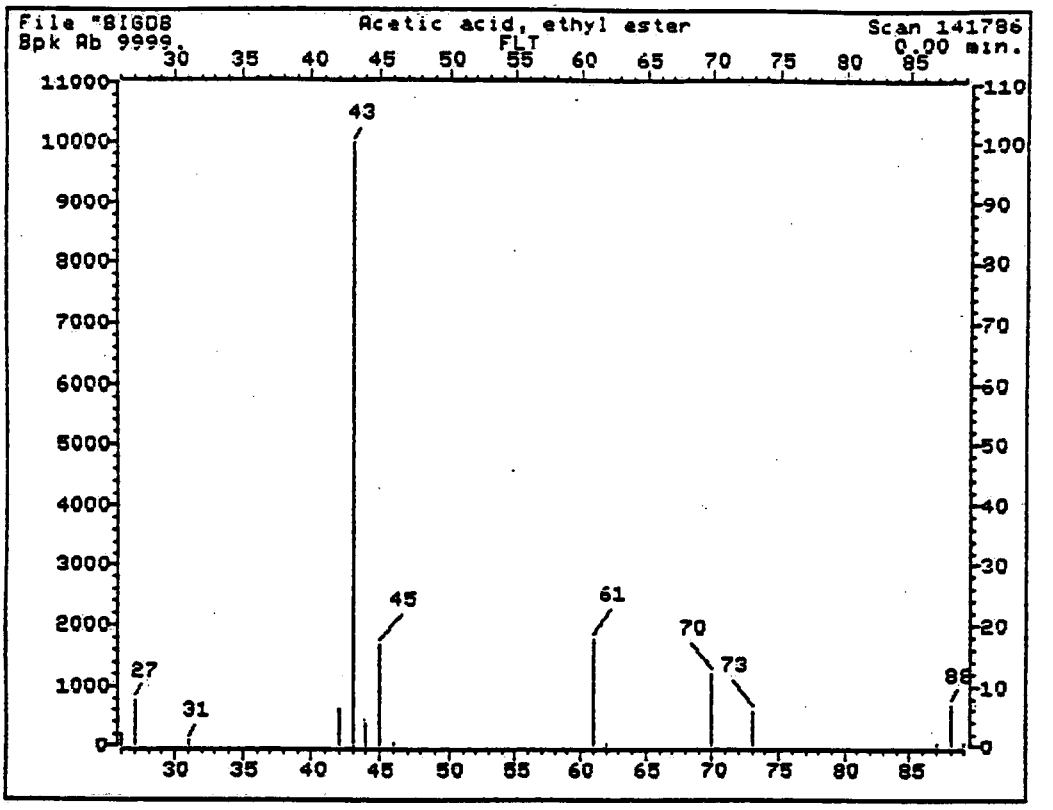


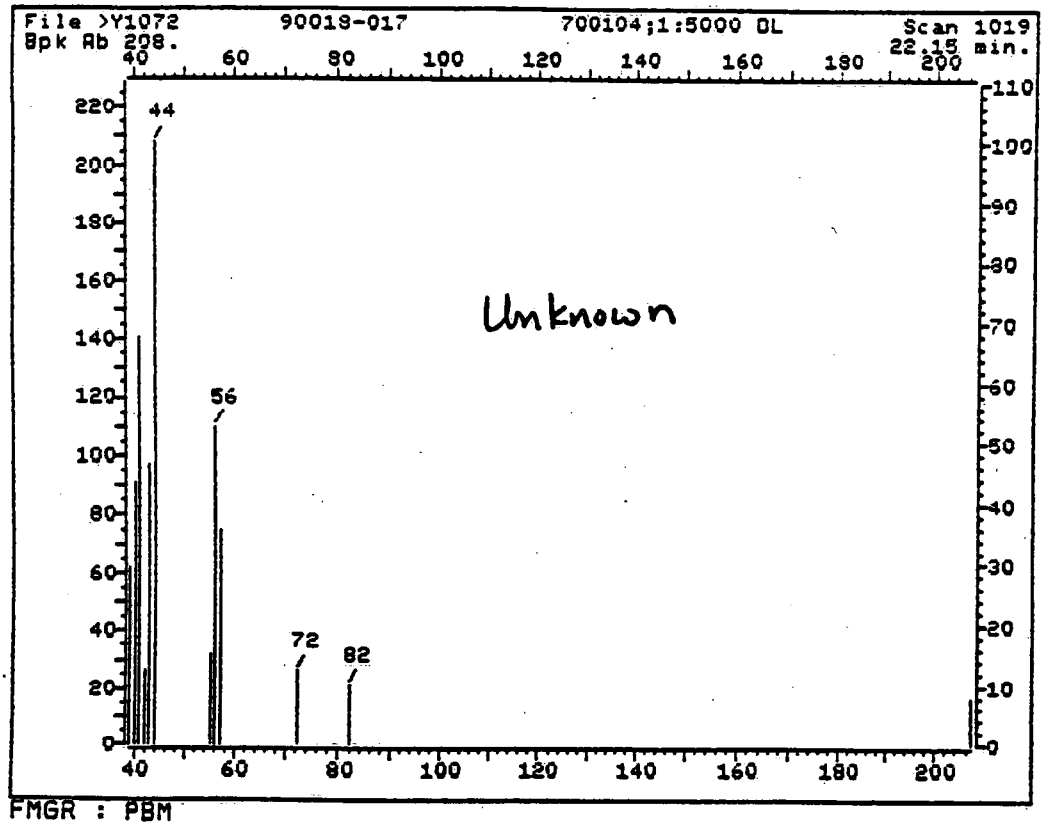
1.	Acetic acid, ethyl ester	88	C4H8O2
2.	Acetic acid, ethyl ester	88	C4H8O2
3.	Acetic acid, ethyl ester	88	C4H8O2
4.	Acetic acid, ethyl ester	88	C4H8O2
5.	3-(4,5-DICHLORO-2-CYANO-3,6-DIHYDROXY-1-PHENYL) INDO	318	C15H8Cl2N2O2
6.	Acetic acid, ethyl ester	88	C4H8O2
7.	Propanoic acid, 2-oxo-	88	C3H4O3
8.	Acetic acid, ethyl ester	88	C4H8O2
9.	Propanoic acid, 2-oxo-	88	C3H4O3
10.	Acetic acid, ethyl ester	88	C4H8O2
11.	Acetic acid, ethyl ester	88	C4H8O2
12.	Acetic acid, ethyl ester	88	C4H8O2
13.	Acetic acid, ethyl ester	88	C4H8O2

Sample file: >Y1072 Spectrum #: 619
Search speed: 1 Tilting option: N No. of ion ranges searched: 44

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	83*	141786	4341	*BIGDB	39	30	1	0	100	5	57	22
2.	83*	141786	4336	*BIGDB	43	34	1	0	89	5	57	25
3.	83*	141786	4338	*BIGDB	44	36	1	0	90	3	57	26
4.	78	141786	4342	*BIGDB	38	45	2	0	91	3	55	13
5.	78	0	4320	*BIGDB	41	34	2	0	74	3	55	14
6.	76*	141786	4337	*BIGDB	38	41	1	0	88	7	45	21
7.	52*	127173	660	*BIGDB	22	58	2	0	68	20	20	13
8.	52*	141786	4343	*BIGDB	25	24	1	0	70	16	20	14
9.	42*	127173	11	*BIGDB	21	55	2	0	83	24	17	17

13. 20* 141786 4340 *BIGDB 31 46 1 0 37 51 5 17

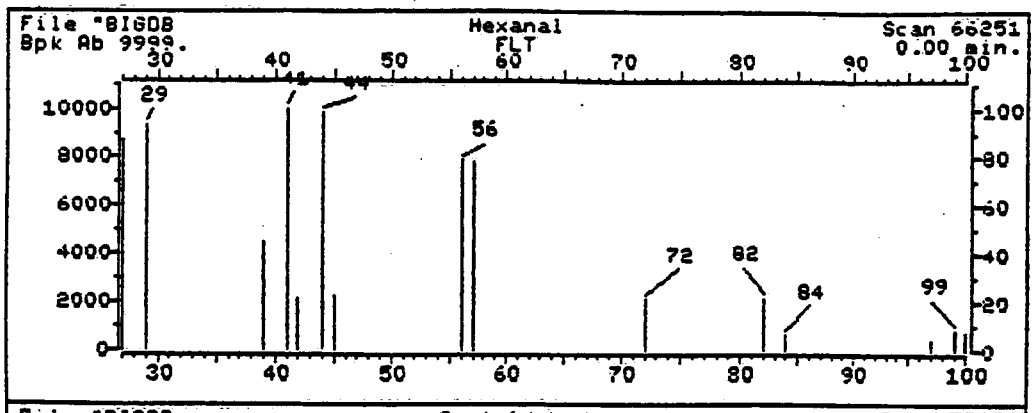


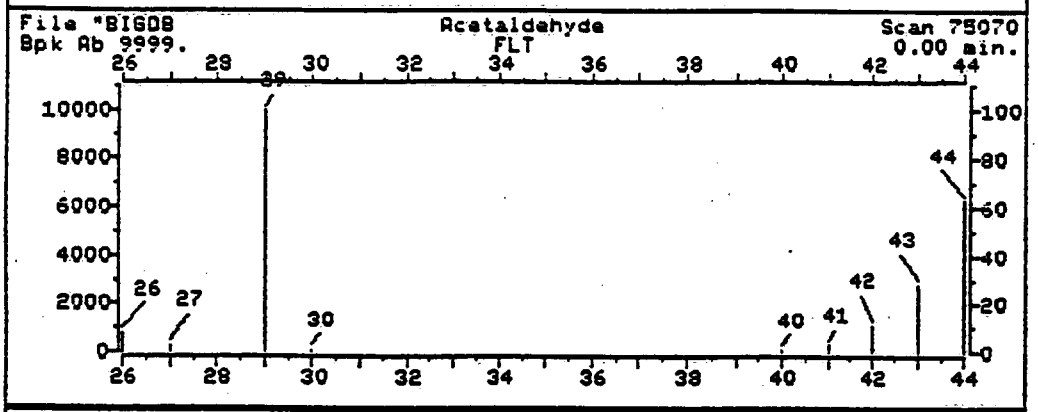


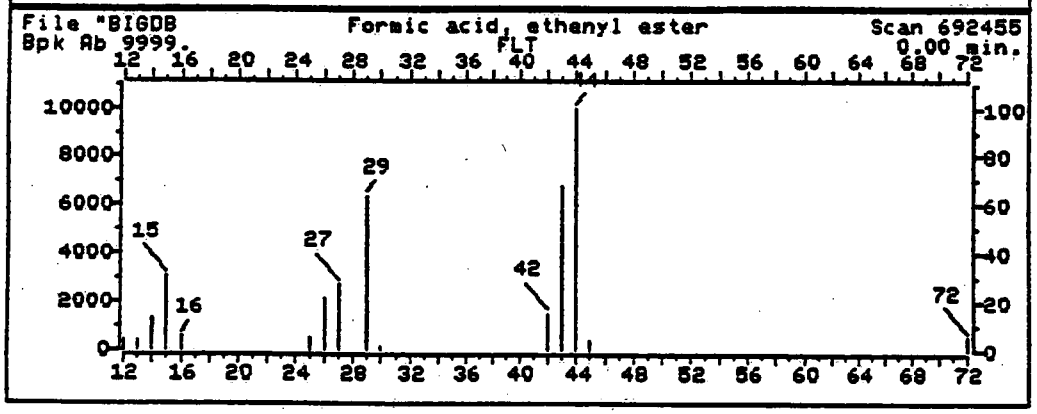
1. Hexanal 100 C6H12O
2. Acetaldehyde 44 C2H4O
3. Acetaldehyde 44 C2H4O
4. Acetaldehyde 44 C2H4O
5. Formic acid, ethenyl ester 72 C3H4O2

Sample file: >Y1072 Spectrum #: 1019
Search speed: 1 Tilting option: N No. of ion ranges searched: 43

	Prob.	CAS #	CON #	ROOT	K	DK	#FLG	TILT	%	CON	C_I	R_IV
1.	30	66251	2203	*BIGDB	35	40	1	0	64	32	12	13
2.	20*	75070	549	*BIGDB	20	37	1	0	83	53	5	14
3.	20*	75070	556	*BIGDB	20	60	1	0	81	53	5	14
4.	20*	75070	552	*BIGDB	20	63	1	0	103	54	5	14
5.	20*	692455	498	*BIGDB	20	73	1	0	68	54	5	14


File "BIGDB
Bpk Ab 9999.
Hexanal
FLT
Scan 66251
0.00 min.
29
41
44
56
72
82
84
99


File "BIGDB
Bpk Ab 9999.
Acetaldehyde
FLT
Scan 75070
0.00 min.
26
27
30
39
40
41
42
43
44


File "BIGDB
Bpk Ab 9999.
Formic acid, ethenyl ester
FLT
Scan 692455
0.00 min.
15
16
27
29
42
44
72

APPENDIX D

ETHANOL STANDARDS

APPENDIX D

ETHANOL STANDARDS

5000 ppb Standard
10000 ppb Standard
20000 ppb Standard

5000 ppb Ethanol Standard

QUANT REPORT

Operator ID: EJK
Output File: ^Y1058::D2
Data File: >Y1058::D2
Name: Ethanol-5000 ppb
Misc: 700104; Methyl Hydrate Study

Quant Rev: 6 Quant Time: 900511 11:0[illegible]
Injected at: 900511 08:5[illegible]
Dilution Factor: 1.00000

ID File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.34	128.0	15824	50.00	UG/L	94
6)	Ethanol	4.56	46.0	2116	5000 ~~208.67~~	UG/L CR 3/19/90	74
15)	1,2-Dichloroethane-d4 (surr.)	12.21	65.0	21136	45.67	UG/L	89
17)	*1,4-Difluorobenzene	19.82	114.0	52967	50.00	UG/L	95
18)	1,1,1-Trichloroethane	13.52	97.0	1117	1.38	UG/L	97
30)	*Chlorobenzene-d5	24.64	117.0	41151	50.00	UG/L	97
36)	Toluene-d8 (surr.)	23.44	98.0	45607	49.35	UG/L	96
41)	p-Bromofluorobenzene (surr.)	28.33	95.0	31036	50.90	UG/L	87

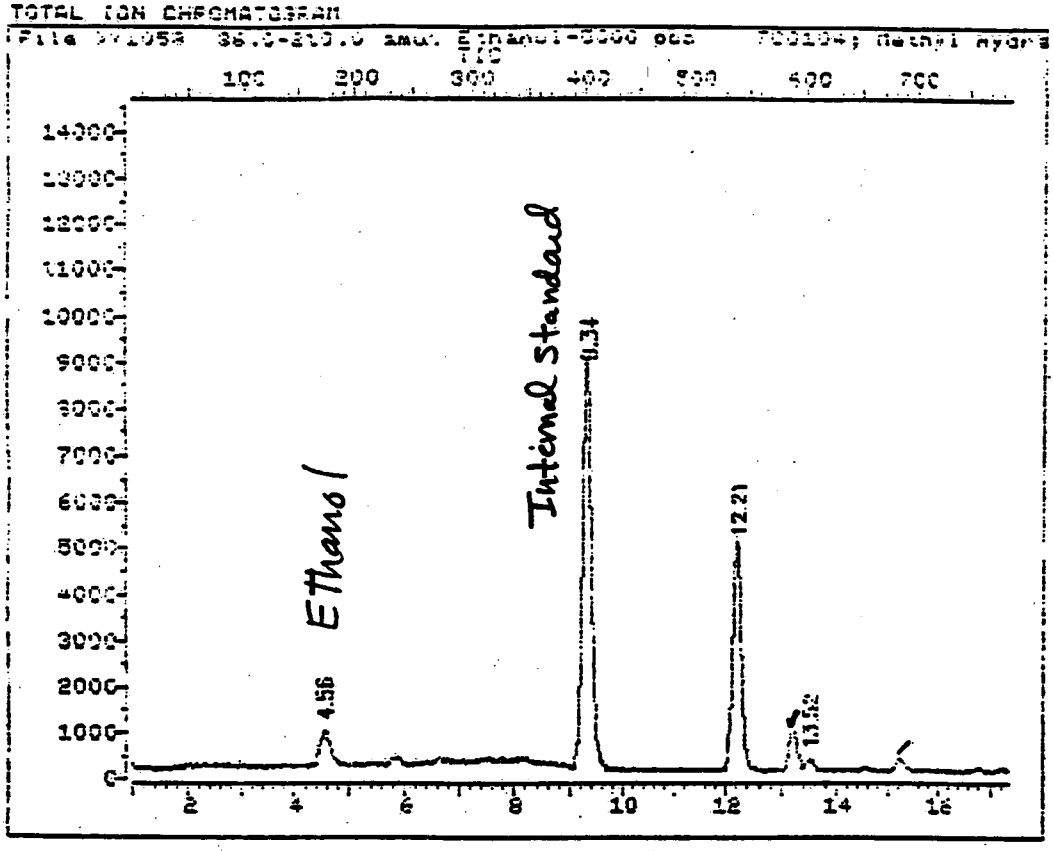
* Compound is ISTD

$$\text{Relative Response Factor} = \frac{\text{Area Ethanol}}{\text{Area Internal Standard \#1}} \times \frac{\text{Concentration Internal Standard}}{\text{Concentration of Ethanol}}$$

$$= \frac{2116}{15824} \times \frac{50\ \mu g/L}{5000\ \mu g/L}$$

$$= 0.00134$$

TOTAL ION CHROMATOGRAM

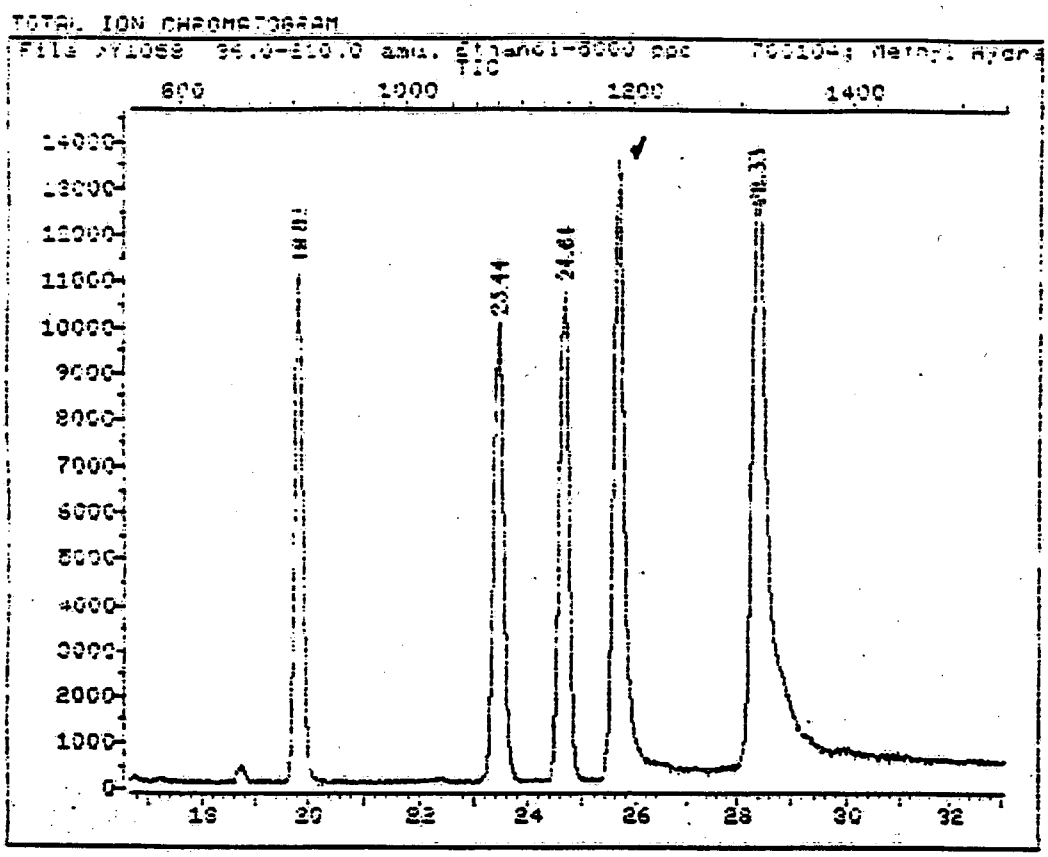


Data File: >Y1058::D2 Quant Output File: ^Y1058::D2
Name: Ethanol-5000 ppb
Misc: 700104: Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:04
Injected at: 900311 08:53

TIC page 1 of 2



Data File: >Y1058::D2 Quant Output File: ^Y1058::D2
Name: Ethanol-5000 ppb
Misc: 700104: Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:04
Injected at: 900311 08:53

TIC page 2 of 2

10,000 ppb Ethanol Standard

QUANT REPORT

Operator ID: EJK
Output File: ^Y1059::D2
Data File: >Y1059::D2
Name: Ethanol-10000 ppb
Misc: 700104: Methyl Hydrate Study

Quant Rev: 6
Quant Time: 900311 11:06
Injected at: 900311 09:35
Dilution Factor: 1.00000

ID File: I_YETC::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

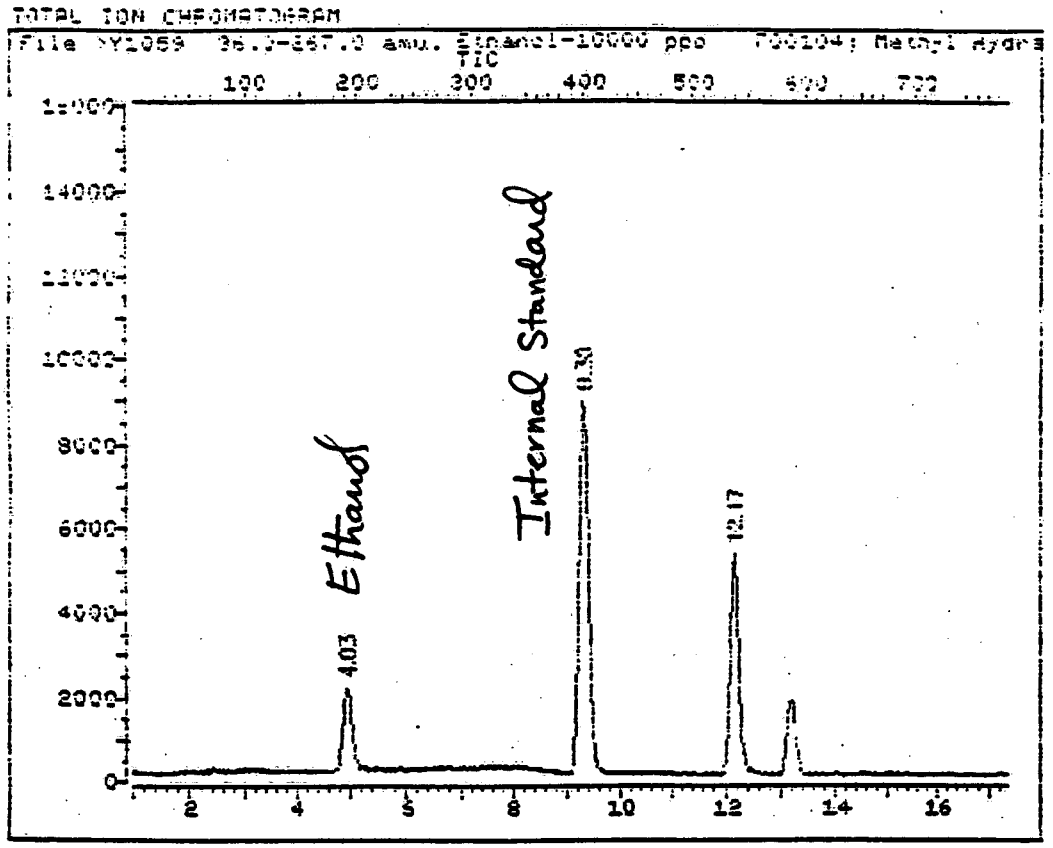
	Compound	R.T.	Q ion	Area	Conc	Units	Q
1)	*Bromochloromethane	9.30	128.0	15332	10,000 50.00	UG/L cr	96
6)	Ethanol	4.93	46.0	4618	~~677.24~~	UG/L	68
15)	1,2-Dichloroethane-d4 (surr.)	12.17	65.0	21499	45.85	UG/L 3/14/90	87
17)	*1,4-Difluorobenzene	19.78	114.0	51817	50.00	UG/L	90
30)	*Chlorobenzene-d5	24.60	117.0	40196	50.00	UG/L	92
36)	Toluene-d8 (surr.)	23.40	98.0	43527	48.20	UG/L	97
41)	p-Bromofluorobenzene (surr.)	28.31	95.0	31221	52.42	UG/L	86

* Compound is ISTD

$$\text{Relative Response Factor} = \frac{\text{Area Ethanol}}{\text{Area Internal Standard \#1}} \times \frac{\text{Concentration Internal Standard}}{\text{Concentration Ethanol}}$$

$$= \frac{4618}{15332} \times \frac{50\ \text{ug/L}}{10{,}000\ \text{ug/L}}$$

$$= 0.00151$$

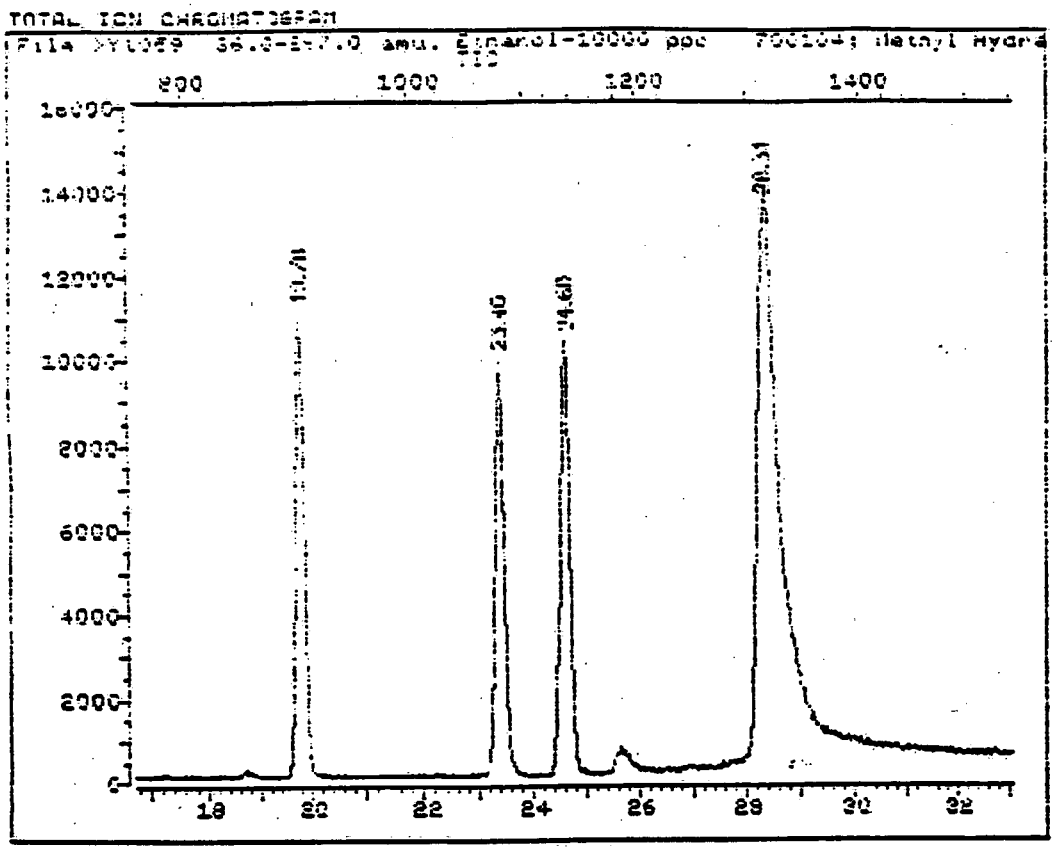


Data File: >Y1059::D2 Quant Output File: ^Y1059::D2
Name: Ethanol-10000 ppb
Misc: 700104: Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:06
Injected at: 900311 09:33

TIC page 1 of 2



Data File: >Y1059::D2 Quant Output File: ^Y1059::D2
Name: Ethanol-10000 ppb
Misc: 700104: Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:06
Injected at: 900311 09:33

TIC page 2 of 2

20,000 ppb Ethanol Standard

QUANT REPORT

Operator ID: EJK Quant Rev: 6 Quant Time: 900311 11:08
Output File: >Y1060::D2 Injected at: 900311 10:13
Data File: >Y1060::D2 Dilution Factor: 1.00000
Name: Ethanol-20000 ppb
Misc: 700104; Methyl Hydrate Study

ID File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

	Compound	R.T.	Q ion	Area	Conc	Units	q
1)	*Bromochloromethane	9.31	128.0	14761	50.00	UG/L	99
6)	Ethanol	5.62	46.0	9381	20,000 ~~1428.96~~	UG/L	76
15)	1,2-Dichloroethane-d4 (surr.)	12.18	65.0	20216	44.78	UG/L	96
17)	*1,4-Difluorobenzene	19.75	114.0	48664	50.00	UG/L	91
30)	*Chlorobenzene-d5	24.57	117.0	39851	50.00	UG/L	94
36)	Toluene-d8 (surr.)	23.36	98.0	42747	47.74	UG/L	91
41)	p-Bromofluorobenzene (surr.)	28.27	95.0	29550	50.05	UG/L	78

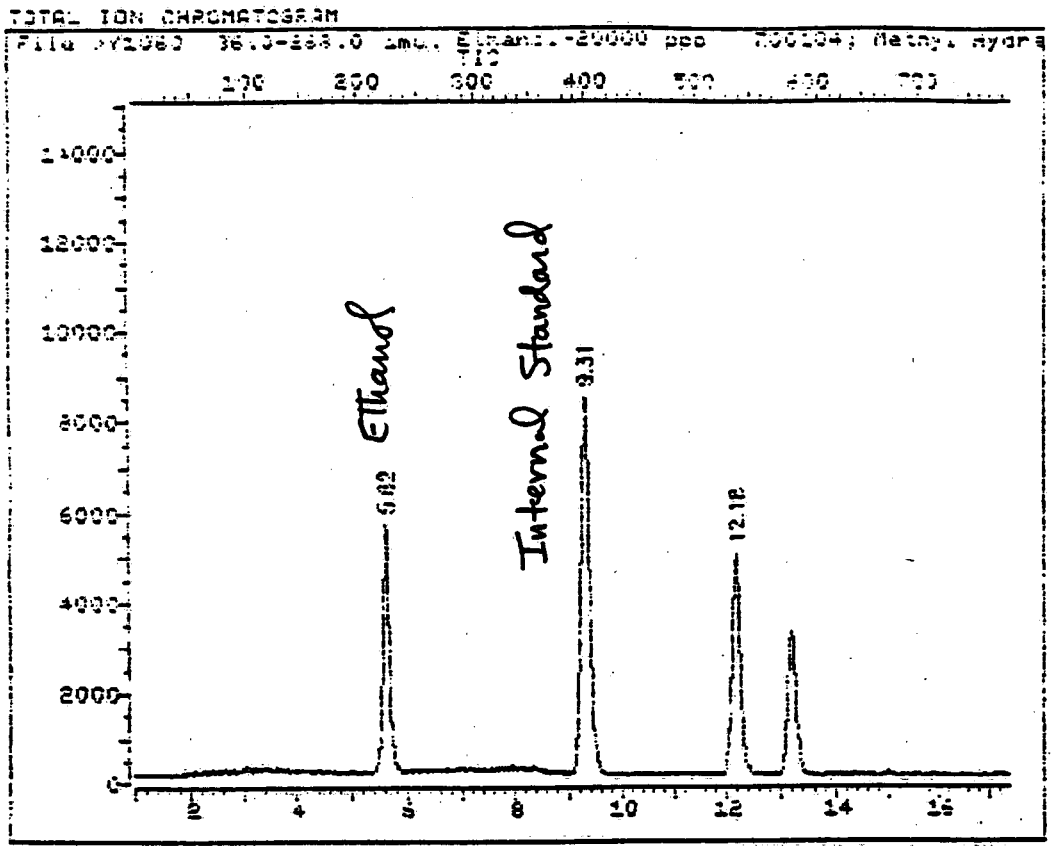
CR 3/19/90

* Compound is ISTD

$$\text{Relative Response Factor} = \frac{\text{Area Ethanol}}{\text{Area Internal Standard \#1}} \times \frac{\text{Concentration Internal Standard}}{\text{Concentration Ethanol}}$$

$$= \frac{9381}{14761} \times \frac{50\ \mu g/L}{20000\ \mu g/L}$$

$$= 0.00159$$

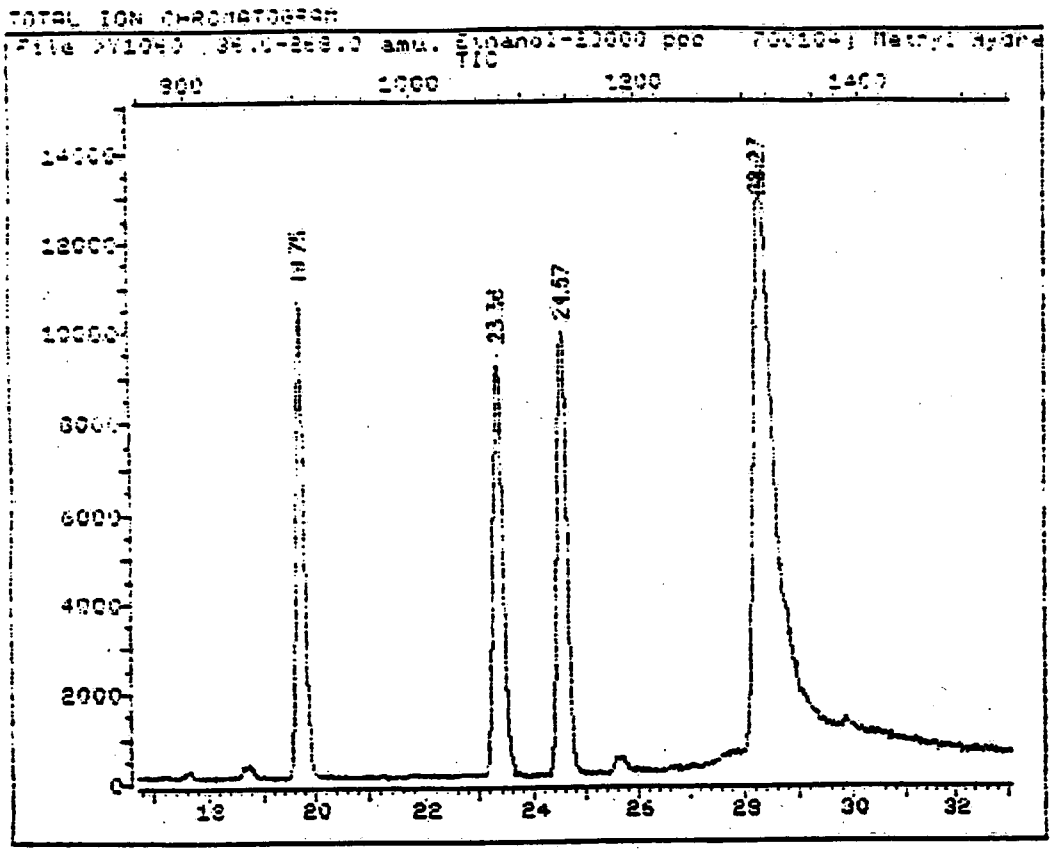


Data File: >Y1060::D2 Quant Output File: ^Y1060::D2
Name: Ethanol-20000 ppb
Misc: 700104; Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:08
Injected at: 900311 10:13

TIC page 1 of 2



Data File: >Y1060::D2 Quant Output File: ^Y1060::D2
Name: Ethanol-20000 ppb
Misc: 700104: Methyl Hydrate Study

Id File: I_YETO::D2
Title: TARGET COMPOUND LIST VOA COMPOUNDS IN WATER
Last Calibration: 900221 15:06

Operator ID: EJK
Quant Time: 900311 11:08
Injected at: 900311 10:13

TIC page 2 of 2

APPENDIX E

DATA VALIDATION GROUNDWATER SUMMARY TABLES FOR VOCs SCANGB

VOLATILE ORGANIC COMPOUNDS
WATER SAMPLING--ROUND 1
SUFFOLK COUNTY AIRPORT
FIRE TRAINING AREA
PHASE II SITE CHARACTERIZATION

LOCATION		1	1	2	3	1	1
DEPTH		0-0.5'	1.5-2.0'	X	X	X	X
DATE		4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87
ECJ POINT		JMW101AX01	JMW101BX01	JMW102XX01	JMW103XX01	JDUP1XXX01	JDUP2XXX01
CC SAMPLE		130705	130717	130697	130707	130696	130692
VOLATILE ORGANIC COMPOS (ug/l)	DET. LIMIT						
BENZENE	5				13		
BROMOFORM	5						
CARBON TETRACHLORIDE	5						
CHLOROBENZENE	5						
DIBROMOCHLOROMETHANE	5						
CHLOROETHANE	10						
2-CHLOROETHYLVINYLETHER	10						
CHLOROFORM	5						
BROMODICHLOROMETHANE	5						
1,1-DICHLOROETHANE	5						5.8
1,2-DICHLOROETHANE	5						
1,1-DICHLOROETHENE	5						
1,2-DICHLOROPROPANE	5						
CIS-1,3-DICHLOROPROPENE	5						
ETHYLBENZENE	5				2.1J		3.5J
BROMOMETHANE	10						
CHLOROMETHANE	10						
METHYLENE CHLORIDE	5		3.5J				4.6J
1,1,2,2-TETRACHLOROETHANE	5						
TETRACHLOROETHENE	5			3.8J		1.0J	
TOLUENE	5				36		
TRANS-1,2-DICHLOROETHENE	5						
STYRENE	5						
ACETONE	10		15		18		
2-BUTANONE	10	18		82		28	
CARBON DISULFIDE	5						
2-HEXANONE	10						
4-METHYL-2-PENTANONE	10						
VINYL ACETATE	10						
XYLENES (TOTAL)	5				34		

NOTE:
X IN DEPTH COLUMN INDICATED A SAMPLE BLANK TAKEN.
JTB INDICATES A TRIP BLANK SAMPLE TAKEN.

LOCATION		4	5	6	7	7	7
DEPTH		X	X	X	0-0.5'	1.5-2.0'	3.0-3.5'
DATE		4-30-87	4-29-87	4-29-87	4-30-87	4-30-87	4-30-87
EQ POINT		JMW104XX01	JMW105XX01	JMW106XX01	JMW107AX01	JMW107BX01	JMW107CX01
CC SAMPLE		131386	130714	130699	130701	130703	130698
VOLATILE ORGANIC COMPDS (ug/l)	DET. LIMIT						
BENZENE	5						
BROMOFORM	5						
CARBON TETRACHLORIDE	5						
CHLOROBENZENE	5						
DIBROMOCHLOROMETHANE	5						
CHLOROETHANE	10						
2-CHLOROETHYLVINYLETHER	10						
CHLOROFORM	5						
BROMODICHLOROMETHANE	5						
1,1-DICHLOROETHANE	5			5.8			
1,2-DICHLOROETHANE	5						
1,1-DICHLOROETHENE	5						
1,2-DICHLOROPROPANE	5						
CIS-1,3-DICHLOROPROPENE	5						
ETHYLBENZENE	5			3.4J			
BROMOMETHANE	10						
CHLOROMETHANE	10						
METHYLENE CHLORIDE	5						
1,1,2,2-TETRACHLOROETHANE	5						
TETRACHLOROETHENE	5						
TOLUENE	5						
TRANS-1,2-DICHLOROETHENE	5						
STYRENE	5						
ACETONE	10						
2-BUTANONE	10				65	56000	
CARBON DISULFIDE	5						
2-HEXANONE	10						
4-METHYL-2-PENTANONE	10						
VINYL ACETATE	10						
XYLENES (TOTAL)	5						

NOTE:
X IN DEPTH COLUMN INDICATED A SAMPLE BLANK TAKEN.
JTB INDICATES A TRIP BLANK SAMPLE TAKEN.

LOCATION		1	2	1	2	1	2
DEPTH		X	X	X	X	X	X
DATE		4-30-87	4-30-87	4-29-87	4-30-87	4-29-87	4-30-87
ECJ POINT		JREP1XXXX01	JREP2XXXX01	JSB1XXXX01	JSB2XXXX01	JTB1XXXX01	JTB2XXXX01
CC SAMPLE		130704	130709	130706	131387	130686	130687
VOLATILE ORGANIC COMPDS (ug/l)	DET. LIMIT						
BENZENE	5						
BROMOFORM	5						
CARBON TETRACHLORIDE	5						
CHLOROBENZENE	5						
DIBROMOCHLOROMETHANE	5						
CHLOROETHANE	10						
2-CHLOROETHYLVINYLETHER	10						
CHLOROFORM	5			16			
BROMODICHLOROMETHANE	5						
1,1-DICHLOROETHANE	5						
1,2-DICHLOROETHANE	5						
1,1-DICHLOROETHENE	5						
1,2-DICHLOROPROPANE	5						
CIS-1,3-DICHLOROPROPENE	5						
ETHYLBENZENE	5						
BROMOMETHANE	10						
CHLOROMETHANE	10						
METHYLENE CHLORIDE	5					4.6J	4.5J
1,1,2,2-TETRACHLOROETHANE	5						
TETRACHLOROETHENE	5						
TOLUENE	5						
TRANS-1,2-DICHLOROETHENE	5						
STYRENE	5						
ACETONE	10				10		
2-BUTANONE	10						
CARBON DISULFIDE	5						
2-HEXANONE	10						
4-METHYL-2-PENTANONE	10						
VINYL ACETATE	10						
XYLENES (TOTAL)	5						

NOTE:
X IN DEPTH COLUMN INDICATED A SAMPLE BLANK TAKEN.
JTB INDICATES A TRIP BLANK SAMPLE TAKEN.

WASVOAHIT

ORGANIC/INORGANIC COMPOUNDS AND HYDROCARBONS
WATER SAMPLING ROUND 1
SUFFOLK COUNTY AIRPORT
FIRE TRAINING AREA
PHASE II SITE CHARACTERIZATION

LOCATION		JMW101A	JMW101B	JMW102	JMW103	JMW103	JDUP1	JDUP1	JDUP2	JMW106	JMW107A
DATE SAMPLED		4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-30-87
DEPTH		0-0.5'	1.5-2.0'	X	X	X	X	X	X	X	0-0.5'
EC/ POINT		JMW101AX01	JMW101BX01	JMW102XX01	JMW103XX01	JMW103XX01	JDUP1XXX01	JDUP1XXX01	JDUP2XXX01	JMW106XX01	JMW107AX01
COMPUCHEM NO.		130705	130717	130697	130707	130764	130696	130772	130692	130699	130701
VOLATILE ORGANIC COMPOUNDS (ug/l)	DETECTION LIMIT										
DILUTION FACTOR		1	1	1	1	1	1	1	1	1	1
BENZENE	5				13						

WASVOAHIT

ORGANIC/INORGANIC COMPOUNDS AND HYDROCARBONS
WATER SAMPLING ROUND 1
SUFFOLK COUNTY AIRPORT
FIRE TRAINING AREA
PHASE II SITE CHARACTERIZATION

LOCATION		JMW101A	JMW101B	JMW102	JMW103	JMW103	JDUP1	JDUP1	JDUP2	JMW106	JMW107A
DATE SAMPLED		4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-30-87
DEPTH		0-0.5'	1.5-2.0'	X	X	X	X	X	X	X	0-0.5'
EC/ POINT		JMW101AX01	JMW101BX01	JMW102XX01	JMW103XX01	JMW103XX01	JDUP1XXX01	JDUP1XXX01	JDUP2XXX01	JMW106XX01	JMW107AX01
COMPUCHEM NO.		130705	130717	130697	130707	130764	130696	130772	130692	130699	130701
VOLATILE ORGANIC COMPOUNDS (ug/l)	DETECTION LIMIT										
DILUTION FACTOR		1	1	1	1	1	1	1	1	1	1
BENZENE	5				13						
1,1-DICHLOROETHANE	5								5.8	5.8	
TOLUENE	5				36						
ACETONE	10		15		18						
2-BUTANONE	10	18		82			28				65
XYLENES (TOTAL)	5				34						
CHLOROFORM	5										
SEMI-VOLATILE COMPOUNDS (ug/l)											
DILUTIONFACTOR		1	1	1	1	1	1	1	1	1	1
BIS-(2-ETHYLHEXYL)PHTHALATE	10	37									
INORGANIC COMPOUND (ug/l)											
LEAD	5					(2.8)					
HYDROCARBONS (mg/l)											
PETROLEUM HYDROCARBON	1							1.1			

WASVOAHIT

LOCATION		JMW107B	JSB1	JSB2	JREP2	JFB1
DATE SAMPLED		4-30-87	4-29-87	4-30-87	4-30-87	4-30-87
DEPTH		1.5-2.0'	X	X	X	X
EQ POINT		JMW107BX01	JSB1XXXX01	JSB2XXXX01	JREP2XXX01	JFB1XXXX01
COMPUCHEM NO.		130703	130706	131387	130765	130760
VOLATILE ORGANIC COMPOUNDS (ug/l)	DETECTION LIMIT					
DILUTION FACTOR		500	1	1	1	1
BENZENE	5					
1,1-DICHLOROETHANE	5					
TOLUENE	5					
ACETONE	10			10		
2-BUTANONE	10	56000				
XYLENES (TOTAL)	5					
CHLOROFORM	5		16			
SEMI-VOLATILE COMPOUNDS (ug/l)						
DILUTIONFACTOR		1	1	1	1	1
BIS-(2-ETHYLHEXYL)PHTHALATE	10					
INORGANIC COMPOUND (mg/kg)						
LEAD	5				(2.3)	(2.6)
HYDROCARBONS (mg/l)						
PETROLEUM HYDROCARBON	1					

NOTE:
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK TAKEN.
JTB INDICATES A TRIP BLANK SAMPLE TAKEN.

WAVORHIT

VOLATILE AND SEMIVOLATILE ORGANIC COMPOUNDS
WATER SAMPLES ROUND 1
SUFFOLK COUNTY AIRPORT
FIRE TRAINING AREA
PHASE II SITE CHARACTERIZATION

LOCATION		JMW101A	JMW101B	JMW102	JMW103	JDUP1	JDUP2	JMW106	JMW107A	JMW107B	JSB1	JSB2
DATE SAMPLED		4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-29-87	4-30-87	4-30-87	4-29-87	4-30-87
DEPTH		0-0.5'	1.5-2.0'	X	X	X	X	X	0-0.5'	1.5-2.0'	X	X
ECJ POINT		JMW101AX01	JMW101BX01	JMW102XX01	JMW103XX01	JDUP1XXX01	JDUP2XXX01	JMW106XX01	JMW107AX01	JMW107BX01	JSB1XXXX01	JSB2XXXX01
COMPUCHEM NO.		130705	130717	130697	130707	130696	130692	130699	130701	130703	130706	131337
	DETECTION LIMIT											
VOLATILE ORGANIC COMPOS (ug/l)												
BENZENE	5				13							
1,1-DICHLOROETHANE	5						5.8	5.8				
TOLUENE	5				36							
ACETONE	10		15		18							10
2-BUTANONE	10	18		82		28			65	56000		
XYLENES (TOTAL)	5				34							
CHLOROFORM	5										16	
SEMIVOLATILE ORGANIC COMPOS (ug/l)												
BIS (2-ETHYLHEXYL)PHTHALATE	10	37										

NOTE:
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK TAKEN.
JTB INDICATES A TRIP BLANK SAMPLE TAKEN.

WR02.WK1

ORGANIC/INORGANIC COMPOUNDS AND HYDROCARBONS
WATER SAMPLING-ROUND 2
SUFFOLK COUNTY AIRPORT
FIRE TRAINING AREA
PHASE II SITE CHARACTERIZATION

SAMPLE POINT		JSB1	JDUP2	JDUP2	JDUP1	JREP2	JREP2	JREP1	JREP1	JMW107C	JMW107C	JMW107B
EU SAMPLE NO.		JSB1XXXX02	JDUP2XXXX02	JDUP2XXXX02	JDUP1XXXX02	JREP2XXXX02	JREP2XXXX02	JREP1XXXX02	JREP1XXXX02	JMW107CX02	JMW107CX02	JMW107BX02
CMPUCHEM NO.		140352	140360	140372	140361	140362	140376	140363	140377	140364	140378	140451
DATE SAMPLED		7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87	7-8-87
DEPTH		X	X	X	X	X	X	X	X	2.0-3.0'	2.0-3.0'	1.0-2.0'
VOLATILE ORGANIC COMPDS (ug/l)	DETECTION LIMIT											
DILUTION FACTOR		1	1		1	1		1		1		100
METHYLENE CHLORIDE	5	3.5JB	1.4JB		3.1JB	1.2JB				1.4JB		
ACETONE	10											
2-BUTANONE	10		19			23		15				14,000
1,1,1-TRICHLOROETHANE	5					3.6J						
TOLUENE	5				26							
BENZENE	5				5.7							
ETHYL BENZENE	5					2.2J						
TETRACHLOROETHENE	5											
2-CHLOROETHYL VINYL ETHER	10											
CHLOROFORM	5											
TOTAL XYLENES	5				33							
SEMIVOLATILE ORGANIC COMPDS(ug/l)												
DILUTION FACTOR		2	2		2	2		2		2		2
BIS (2-ETHYLHEXYL)PHTHALATE	10		3.6J		2.0J	5.8J		15J		2.4J		52
NAPHTHALENE	10					4.8J						
2-METHYLNAPHTHALENE	10					4.4J						
PENTACHLOROPHENOL	50											
INORGANIC COMPOUNDS (ug/l)												
LEAD	5			BDL			BDL		BDL		BDL	
HYDROCARBONS (mg/l)												
PETROLEUM HYDROCARBON	1											

NOTE
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK TAKEN.

WAR02.WK1

SAMPLE POINT		JWW107B	JWW107A	JWW107A	JWW106	JWW106	JWW104	JWW104	JWW105	JWW105	JWW103	JWW103
ECJ SAMPLE NO.		JWW107BX02	JWW107AX02	JWW107AX02	JWW106XX02	JWW106XX02	JWW104XX02	JWW104XX02	JWW105XX02	JWW105XX02	JWW103XX02	JWW103XX02
COMPUCHEM NO.		140469	140450	140486	140365	140379	140366	140381	140367	140380	140368	140382
DATE SAMPLED		7-9-87	7-8-87	7-9-87	7-8-87	7-8-97	7-9-87	7-9-87	7-8-87	7-8-87	7-9-87	7-9-87
DEPTH		1.0-2.0'	0-0.5'	0-0.5'	X	X	X	X	X	X	X	X
	DETECTION LIMIT											
VOLATILE ORGANIC COMPDS (ug/l)												
DILUTION FACTOR			1		1		1		1		1	
METHYLENE CHLORIDE	5		3.5JB		2.8JB		2.0JB				5.9B	
ACETONE	10		14				4.0JB				5.3JB	
2-BUTANONE	10		24		30		18					
1,1,1-TRICHLOROETHANE	5				3.5J							
TOLUENE	5										12	
BENZENE	5										3.1J	
ETHYL BENZENE	5				2.5J						2.9J	
TETRACHLOROETHENE	5											
2-CHLOROETHYL VINYL ETHER	10											
CHLOROFORM	5											
TOTAL XYLENES	5				2.3J						16	
SEMIVOLATILE ORGANIC COMPDS(ug/l)												
DILUTION FACTOR			2		2		2		2		2	
BIS (2-ETHYLHEXYL)PHTHALATE	10				12J		10J		34		4.4J	
NAPHTHALENE	10				2.6J							
2-METHYLNAPHTHALENE	10				2.4J							
PENTACHLOROPHENOL	50											
INORGANIC COMPOUNDS (ug/l)												
LEAD	5	BDL		BDL		BDL		BDL		BDL		BDL
HYDROCARBONS (mg/l)												
PETROLEUM HYDROCARBON	1											

NOTE
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK

HAR02.WK1

SAMPLE POINT		JWH102	JWH202	JWH101B	JWH201B	JWH101A	JUCT	JP3	SB-1	JTB2	JTB1	JWH101A
EPA SAMPLE NO.		JWH102X002	JWH202X002	JWH101BX02	JWH201BX02	JWH101AX02	JUCTRNKX02	JP3XXXXX02	SB-1	JTB2XXXX02	JTB1XXXX02	JWH101AX02
COMPUCHEM NO.		140369	140383	140370	140384	140371	140452	140453	140663	140457	140400	140385
DATE SAMPLED		7-9-87	7-9-87	7-9-87	7-9-87	7-9-87	7-9-87	7-9-87	7-8-87	7-9-87	7-8-87	7-9-87
DEPTH		X	X	1.0-2.0'	1.0-2.0'	0-0.5'	X	X	X	X	X	0-0.5'
VOLATILE ORGANIC COMPDS (ug/l)	DETECTION LIMIT											
DILUTION FACTOR		1		7.69		2.38	1	1	1	1	1	
METHYLENE CHLORIDE	5	4.7JB		37JB		8.7JB			3.1JB	3.2JB	5.8B	
ACETONE	10	2.2JB		51JB		26			26	23	24	
2-BUTANONE	10	9.0J		1,400		7.8J		31	7.8J			
1,1,1-TRICHLOROETHANE	5											
TOLUENE	5											
BENZENE	5											
ETHYL BENZENE	5							2.3J				
TETRACHLOROETHENE	5	3.1J										
2-CHLOROETHYL VINYL ETHER	10			55J								
CHLOROFORM	5										1.0J	
TOTAL XYLENES	5											
SEMIVOLATILE ORGANIC COMPDS (ug/l)												
DILUTION FACTOR		2		2		2	2	2	2	NR	NR	
BIS (2-ETHYLHEXYL)PHTHALATE	10	2.6J		4.6J			3.6J	2.4J				
NAPHTHALENE	10							2.6J				
2-METHYLNAPHTHALENE	10											
PENTACHLOROPHENOL	50						2.4J					
INORGANIC COMPOUNDS (ug/l)												
LEAD	5		BDL		BDL							BDL
HYDROCARBONS (mg/l)												
PETROLEUM HYDROCARBON	1											

NOTE
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK

WAR02.WK1

SAMPLE POINT		JUCT	JP3	JFB1	JBB1	JHH107B	JHH107A	JUCT	JP3
ECJ SAMPLE NO.		JUCTA03X02	JP30000X02	JFB10000X02	JBB1	JHH107BX02	JHH107AX02	JUCTA03X02	JP30000X02
COMPUCHEM NO.		140470	140472	140386	140664	140464	140462	140465	140466
DATE SAMPLED		7-9-87	7-9-87	7-8-87	7-8-87	7-9-87	7-9-87	7-9-87	7-9-87
DEPTH		X	X	X	X	2.0-3.0'	0-0.5'	X	X
VOLATILE ORGANIC COMPDS (ug/L)	DETECTION LIMIT								
DILUTION FACTOR									
METHYLENE CHLORIDE	5								
ACETONE	10								
2-BUTANONE	10								
1,1,1-TRICHLOROETHANE	5								
TOLUENE	5								
BENZENE	5								
ETHYL BENZENE	5								
TETRACHLOROETHENE	5								
2-CHLOROETHYL VINYL ETHER	10								
CHLOROFORM	5								
TOTAL XYLENES	5								
SEMIVOLATILE ORGANIC COMPDS(ug/L)									
DILUTION FACTOR									
BIS (2-ETHYLHEXYL)PHTHALATE	10								
NAPHTHALENE	10								
2-METHYLNAPHTHALENE	10								
PENTACHLOROPHENOL	50								
INORGANIC COMPOUNDS (ug/L)									
LEAD	5	BDL	BDL	BDL					
HYDROCARBONS (ug/L)									
PETROLEUM HYDROCARBON	1					BDL	BDL	BDL	BDL	BDL

NOTE
X IN DEPTH COLUMN INDICATES A SAMPLE BLANK

SUFFOLK COUNTY AIRPORT

TENTATIVE IDENTIFIED COMPOUNDS

ROUND 1

****

(all values in ppb)

TENTATIVE IDENTIFIED COMPOUNDS	RM101A	RM101B	RM102	RM103	RM104	RM105	RM106	RM107A	RM107B	RM107C	DUP1	DUP2	REP1	REP2
ACETICACIDETHYLESTER									1250 J					
ETHANOL	11 J		17 J					32 J	17000J		10 J			
IN-INDEN-1-ONE,2,3-DIHYDRO-				13 J										

SUFFOLK COUNTY AIRPORT

TENTATIVE IDENTIFIED COMPOUNDS

ROUND 2

****

(all values in ppb)

TENTATIVE IDENTIFIED COMPOUNDS	RM101A	RM101B	RM102	RM103	RM104	RM105	RM106	RM107A	RM107B	RM107C	DUP1	DUP2	REP1	REP2	P3
ACETICACIDETHYLESTER	12 J	96 J							950 J						
ETHANOL	140 J	220 J			12 J		19 J	18 J	2000 J		16 J		23 J	9 J	27 J

J - ESTIMATED VALUE

B - VALUE FOUND IN METHOD BLANK

JB - REPORTED VALUE FOUND IN METHOD BLANK BELOW CONTRACT REQUIRED DETECTION LIMIT (CRDL)

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 3 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		SCGW14XXXX03XX	SCGW22XXXX03XX	SCGW10XXXX03XX	SCGW9XXXXX03XX	SCGW11XXXX03XX	SCGW00XXXX03XX	SCGW23XXXX03XX	SCGW24XXXX03XX
LAB NUMBER:		244475	244476	244477	244478	244479	244480	244484	244485
DATE SAMPLED:		02/08/89	02/08/89	02/08/89	02/08/89	02/08/89	02/08/89	02/08/89	02/08/89
DATE ANALYZED:		02/10/89	02/10/89	02/10/89	02/10/89	02/09/89	02/10/89	02/10/89	02/10/89
ANALYTE	CRQL								
Acetone		-	-	-	-	-	-	-	-
1,1,1,-Trichloroethane		35	-	-	-	-	-	-	-
Tetrachloroethene		-	6	-	-	-	-	-	-
2-Butanone		2600 DJ	160 J	5700 DJ	14 J	380 DJ	140 J	R	10 J
Toluene		5	-	-	-	-	8	-	-
Ethylbenzene		13	-	-	-	-	7	-	-
Xylenes (Total)		140	-	-	-	-	34	-	-
Ethanol		880	71	1900	19	130	62	-	10
Ethyl acetate		160	11	350	-	22	5	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 3 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		SCGW101AXX03DX	SCGW101AXX03XX	SCGW101BXX03XX	SCGW102XXX03XX	SCGW103XXX03DX	SCGW103XXX03XX	SCGW104XXX03XX	SCGW105XXX03XX
LAB NUMBER:		244468	244467	244473	244466	244465	244464	244463	244462
DATE SAMPLED:		02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89
DATE ANALYZED:		02/14/89	02/14/89	02/14/89	02/13/89	02/13/89	02/13/89	02/12/89	02/10/89
ANALYTE	CRQL								
Acetone		-	-	-	-	-	-	-	-
1,1,1,-Trichloroethane		-	-	-	-	-	-	-	-
Tetrachloroethene		-	-	-	-	-	-	-	-
2-Butanone		320 J	320 J	R	94 J	38 J	24 J	150 J	460 DJ
Toluene		-	-	-	-	-	-	-	-
Ethylbenzene		-	-	-	-	-	-	-	-
Xylenes (Total)		-	-	-	-	-	-	-	-
Ethanol		900	1100	30	61	26	21	220	750
Ethyl acetate		10	10	-	4	-	-	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 3 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		SCGW106XXX03XX	SCGW107AXX03XX	SCGW107BXX03XX	SCGW107CXX03XX	SCGWP1XXXX03XX	SCGWP2XXXX03XX	SCGWP3XXXX03XX	SCGWP4XXXX03XX
LAB NUMBER:		244454	244459	244461	244460	244472RE	244471	244453	244474
DATE SAMPLED:		02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89	02/07/89
DATE ANALYZED:		02/14/89	02/09/89	02/09/89	02/12/89	02/14/89	02/14/89	02/09/89	02/14/89
ANALYTE	CRQL								
Acetone		-	-	300 J	-	-	-	-	-
1,1,1,-Trichloroethane		-	-	-	-	-	-	-	-
Tetrachloroethene		-	-	-	-	-	-	-	-
2-Butanone		40 J	830 JD	53000 DJ	150 J	13000 J	26 J	170 J	190 J
Toluene		-	-	-	-	-	-	-	-
Ethylbenzene		-	-	-	-	-	-	-	-
Xylenes (Total)		-	-	-	-	-	-	-	-
Ethanol		37	770	33000	95	6500	35	140	120
Ethyl acetate		-	36	3800	7	600	-	7	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 3 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		SCMS1XXXXX03XX	SCMSD1XXXX03XX	SCFB1XXXXX03XX	SCBS1XXXXX03XX	SCBT1XXXXX03XX	SCBS2XXXXX03XX
LAB NUMBER:		244469	244470	244486	244458	244452	248802
DATE SAMPLED:		02/07/89	02/07/89	02/08/89	02/07/89	02/07/89	03/07/89
DATE ANALYZED:		02/12/89	02/14/89	02/09/89	02/09/89	02/09/89	03/08/89
ANALYTE	CRQL						
Acetone		-	-	-	-	-	14
1,1,1,-Trichloroethane		-	-	-	-	-	-
Tetrachloroethene		-	-	-	-	-	-
2-Butanone		320 J	330 J	23	-	-	-
Toluene		-	-	-	-	-	-
Ethylbenzene		-	-	-	-	-	-
Xylenes (Total)		-	-	-	-	-	-
Ethanol		940	1100	6	-	-	-
Ethyl acetate		14	13	-	-	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 4 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		MW-101A	MW-101B	MW-102	MW-106	MW-107A	MW-107B	MW-107C	MW-201
LAB NUMBER:		308911	308927	308928	308936	308915	308916	308917	308937
DATE SAMPLED:		12/12/89	12/13/89	12/13/89	12/13/89	12/12/89	12/12/89	12/12/89	12/14/89
DATE ANALYZED:		12/18/89	12/20/89	12/20/89	12/20/89	12/18/89	12/19/89	12/19/89	12/20/89
ANALYTE	CRQL								
Methylene Chloride	5	-	22	-	-	-	-	-	-
Acetone	10	-	-	-	-	-	-	-	-
2-Butanone	10	-	-	-	-	10	4300 JD	R	-
Benzene	5	-	-	-	-	-	-	-	-
Toluene	5	-	-	-	-	-	-	-	-
Ethylbenzene	5	-	-	-	-	-	-	-	-
Xylene (Total)	5	-	-	-	-	-	-	-	-
Ethanol		15	-	-	-	-	720	-	-
Ethyl Acetate		-	-	-	-	-	160	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 4 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		MW-202	MW-202D	MW-203	MW-204	P-1	P-2	P-3	P-4
LAB NUMBER:		308912	308913	308905	308914	308923	308924	308925	308926
DATE SAMPLED:		12/12/89	12/12/89	12/12/89	12/12/89	12/13/89	12/13/89	12/13/89	12/13/89
DATE ANALYZED:		12/18/89	12/18/89	12/18/89	12/18/89	12/20/89	12/20/89	12/20/89	12/20/89
ANALYTE	CRQL								
Methylene Chloride	5	-	-	-	-	-	-	-	-
Acetone	10	-	-	-	-	-	-	-	-
2-Butanone	10	-	-	-	-	-	-	-	-
Benzene	5	-	-	-	-	-	-	-	-
Toluene	5	-	-	-	-	-	-	-	-
Ethylbenzene	5	-	-	-	-	-	-	-	-
Xylene (Total)	5	-	-	-	-	-	-	-	-
Ethanol		52	-	-	-	-	-	-	-
Ethyl Acetate		-	-	-	-	-	-	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 4 Volatile Aqueous Analysis(ug/L).

SAMPLE LOCATION:		SB-1	SB-2	TB-1	TB-2	MW-103	MW-104	MW-105	MW-105D
LAB NUMBER:		308910	308922	308909	308921	308929	308933	308934	308935
DATE SAMPLED:		12/12/89	12/13/89	12/12/89	12/13/89	12/13/89	12/13/89	12/13/89	12/13/89
DATE ANALYZED:		12/18/89	12/20/89	12/18/89	12/20/89	12/19/89	12/19/89	12/19/89	12/19/89
ANALYTE	CRQL								
Methylene Chloride	5	-	-	-	-	-	-	-	-
Acetone	10	21	-	-	-	-	11 J	-	-
2-Butanone	10	-	-	-	-	-	-	-	-
Benzene	5	-	-	-	-	5	-	-	-
Toluene	5	-	-	-	-	34	-	-	-
Ethylbenzene	5	-	-	-	-	10	-	-	-
Xylene (Total)	5	-	-	-	-	68	-	-	-
Ethanol		-	-	-	-	-	-	-	-
Ethyl Acetate		-	-	-	-	-	-	-	-

Validation Qualifiers: J = Indicates values are estimated because all quality assurance criteria were not met during analysis.

D = Indicates compound sample required dilution to bring detected value within calibration range of method.

R = Indicates that data is not usable because quality control criteria were not met.

Summary of Target Compounds,
Ethanol, and Ethyl Acetate
Detected in Round 5 Volatile Aqueous Analysis (ug/L).

SAMPLE LOCATION:		07MW107AXX05XX	07MW107BX105XX	07MW107BX205XX	07MW107BX305XX	07MW107CXX05XX
LAB NUMBER:		63486	63487	63488	63489	63490
DATE SAMPLED:		10/03/91	10/03/91	10/03/91	10/03/91	10/03/91
DATE ANALYZED:		10/09/91	10/09/91	10/10/91	10/09/91	10/10/91
ANALYTE	CRQL					
Acetone		12	610	24	-	-
1,1,1,-Trichloroethane		-	-	-	-	-
Tetrachloroethene		-	-	-	-	-
2-Butanone		-	1600	-	-	-
Toluene		-	-	-	-	-
Ethylbenzene		-	-	-	-	-
Xylenes (Total)		-	-	-	-	-
Ethanol		-	4400	-	-	-
Ethyl acetate		-	900	-	-	-