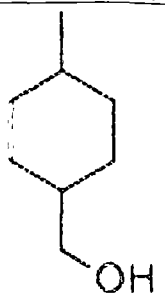
Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
Crude MCHM	4-methylcyclohexane methanol	68 to 89%	100-49-2	128.21	180-202°C
	4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158 25	?°C
	methyl 4-methylcyclohexanecarboxylate	5%	51181-40-9	156.22	191.7 °C
	dimethyl 1,4-cyclohexanedicarboxylate	1%	94-60-0	200 23	132 °C (technical grade)
	methanol	1%	67-56-1	32.04	64.7 °C
	1,4-cyclohexanedimethanol	1-2%	105-08-8	144.21	283 °C
DOWANOL™ DIPPH Glycol Ether	Dipropylene glycol phenyl ether or (methyl-2-phenoxyethoxy)propanol	>60%	51730-94-0	210.27	280 °C
	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152 19	242 7 °C

* Eric Weber, ORD/NERL/ERD, 2/4/2014

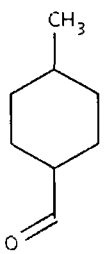
** source dependent

Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
4-methylcyclohexanemethanol	68 to 89%	100-49-2	128 21	180-202°C



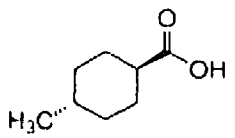
NOTE: The following information has not been peer-reviewed nor does it represent the views of the Agency.

Oxidation of primary alcohol ➔ 4-methyl cyclohexane -1-carbaldehyde (Fig 1) CAS RN: 33242-79-4 Formula· C8H14O MW· 126 19, B.P · 202-205 °C.



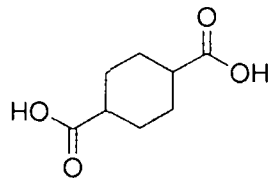
(Fig 1)

Further oxidation of an aldehyde yields a carboxylic acid A stepwise oxidation (as opposed to oxidation of methyl group and opening of the ring)might result in 4-Methyl-1-cyclohexanecarboxylic acid (Fig 2). CAS No.: 13064-83-0 (Fig 2). Formula: CH3C6H10CO2H. MW. 142 20 A powder in pure form. This compound is a napthenic acid (NA) and has been used to study biodegradation kinetics of NAs NAs in the oil refinery business refer to naturally occurring complex mixtures of alkyl-substituted cycloaliphatic carboxylic acids that concentrate in the tailings from extraction of oil from tar sands. The most interesting thing I read with respect to the NAs was one study that found different biodegradation rates between cis- and trans- isomers (Canadian Water Resources Journal, Biodegradation Kinetics of Geometric Isomers of Model Naphthenic Acids in Athabasca River Water J V Headley , K.M Peru , S. Tanapat & G. Putz, Published online· 23 Jan 2013, http.//www tandfonline com/doi/abs/10 4296/cwrj2701025)



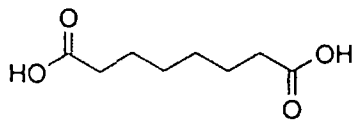
(Fig 2)

If KMnO4 did not open the cyclohexane ring to yield monocarboxylic acids or a dicarboxylic acid you might in theory get 1,4 cyclohexanedicarboxylic acid (Fig 3), CAS No 1076-97-7, a compound with very low water solubility unless deprotonated at more basic pH resulting in a soluble carboxylate



(Fig 3)

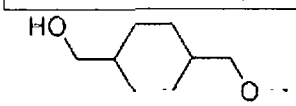
Alkaline KMnO4 would likely open the cyclohexane ring to give a dicarboxylic acid the octanedioic acid (Fig 4) or perhaps smaller acids such as acetic or oxalic acid. Smaller carboxylic acids are formic (C=1), acetic (C=2), propranoic (C=3) and dicarboxylic acids oxalic (C=2), malonic (C=3) succinic (C=4) up to C=5 are soluble in water



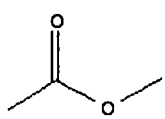
(Fig 4)

In general, open chain carboxylic acids might be the ultimate products of alkaline KMnO4 oxidation of MCHM. KMnO4 prefers to oxidize double bonds so MCHM may not have been oxidized at all by KMnO4 in river water treatment Chlorination may not be sufficient to make carboxylic acids but small soluble carboxylic acids, produced by KMnO4 or free radicals, that make it to chlorination could be halogenated Depending on pH before the chlorination step, the larger dicarboxylic acids may be removed as precipitates

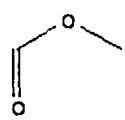
Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP
4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158.25	?^{o}C



In theory, oxidation of primary alcohol and ether groups might result in small open chain carboxylic acids and perhaps acetates such as methyl acetate (Fig 5) or methyl formate (Fig 6) I would trust the QSAR predictions more on this one



(Fig 5)



(Fig 6)

Some EPA Methods

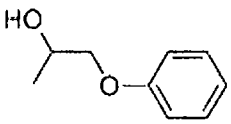
EPA 556 1 DETERMINATION OF CARBONYL COMPOUNDS IN DRINKING WATER BY FAST GAS CHROMATOGRAPHY, 1999 A place to start to detect aldehydes and ketones

EPA 522 DETERMINATION OF 1,4-DIOXANE IN DRINKING WATER BY SOLID PHASE EXTRACTION (SPE) AND GAS CHROMATOGRAPHY/MASS SPECTROMETRY (GC/MS) WITH SELECTED ION MONITORING (SIM), 2008 A place to start for ethers

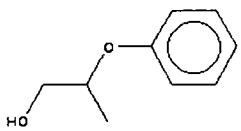
EPA Method 611—Haloethers.

Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
DOWANOL™ DiPPH Glycol Ether	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152 19	242.7 °C

PPh



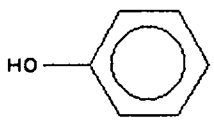
secondary alcohol, major isomer, CAS No.: 770-35-4



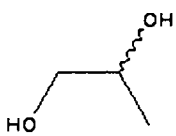
primary alcohol, the minor isomer, CAS No.: 4169-04-4

The EPA's EPIWIN/APO model is reported to estimate atmospheric photodegradation half-life of PPh at 3.45 hrs based on 12 hours of sunlight and avg OH radical concentration of 1 5E6 OH/cm^3 Free radical oxidation might result in phenol (Fig and propylene glycol (I attempted writing out the free radical reaction and terminated it there) I also found literature indicating that acidic KMnO4 could oxidize phenyl glycol ether to phenol and carboxylic acids Another source indicated propylene glycol (Fig 8) oxidation to oxalic (Fig 9) and carbonic acids (Fig 10)

Phenol (Fig 7) Formula: C6H6O. Molecular weight· 94 1112 CAS No · 108-95-2



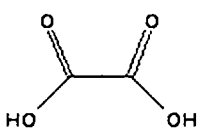
(Fig 7)



(Fig 8)

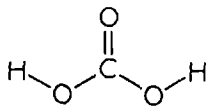
Propylene glycol (Fig 8) CAS No. 57-55-6 Formula· C3H8O2. Molecular weight 76 0944

Oxalic acid (Fig 9) CAS No 144-62-7 Molecular weight 90.03



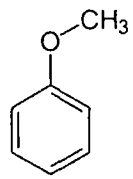
(Fig 9)

Carbonic acid (Fig 10)·



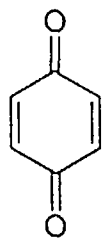
(Fig 10)

Biological methylation of phenol to anisole (Fig 11) is reported in the literature Anisole (methoxy benzene) CAS No.: 100-66-3 Formula· C7H8O. Molecular weight. 108.1378 Article on halogenated anisoles in the environment Fresenius J Anal Chem (2001) 371 598–606, "Halogenated methyl-phenyl ethers (anisoles) in the environment Determination of vapor pressures, aqueous solubilities, Henry's law constants, and gas/water- (Kgw), n-octanol/water- (Kow) and gas/n-octanol (Kgo) partition coefficients "



(Fig 11)

Oxidation of phenol with KMnO4 is reported to produce benzoquinones (Fig 12)



(Fig 12)

I found one article that reported using PPh as a model compound for chlorination. Environ Sci Technol. 2004, 38, 4019-4025, "Transformation of Aromatic Ether and Amine-Containing Pharmaceuticals during Chlorine Disinfection." Researchers looked at chlorination of pharmaceuticals using PPh (1-phenoxy-2-propanol) as a model compound Used RP-HPLC , 30%HEPES buffer/70%acetonitrile and UV detection at 275 The point might be that if PPh survives drinking water pre-treatment, it may halogenate.

Effect of Biodegradation on MCHM Released to the Elk River, West Virginia

Concept Proposal by Michelle M. Lorah, Charles Walker, and Doug Chambers

U.S. Geological Survey

As a result of the estimated 10,000-gallon spill of crude 4-methylcyclohexanemethanol (MCHM) that drained from a storage tank and entered the Elk River in West Virginia in January 2014, information on the environmental fate of this chemical mixture is critically needed. Little appears to be known about the transport properties and degradation reactions of MCHM, despite its common use as a frothing agent to clean coal and subsequent release to the environment in wash water The relatively low solubility of MCHM in water and the lipophilic nature of this compound, as suggested by its chemical structure, indicate that sorption of MCHM to soils and sediment beneath the storage tank and in the bottom sediments of the Elk River could slow its transport and complete flushing from the area impacted by the spill. Slow release of MCHM from dissolution of pools of the compound and sorbed material could provide a long-term source of contaminants to water. For many organic compounds, biodegradation reactions are the primary mechanism for attenuation and potential complete destruction of the contaminant in soils, groundwater, and bottom sediments. Alternatively, biodegradation sometimes produces intermediate compounds that are more soluble and toxic than the parent compound (i.e production of vinyl chloride from incomplete degradation of trichloroethylene). Defining biodegradation processes and products, therefore, is important to provide an understanding of the fate and toxicity of the MCHM released in this spill and at coal washing facilities. We propose to evaluate the biodegradation of crude MCHM and pure MCHM in laboratory microcosms using sediment exposed to crude MCHM at the spill site by the Elk River, West Virginia.

Freedom_0006097_0007

MCHM is a saturated alicyclic primary alcohol with a methyl (CH_3) and hydroxymethyl (CH_2OH) group on the cyclohexane ring, which can give *cis* and *trans* isomers depending on the positions of these groups. The relative amounts of the isomers and other components in crude MCHM commercial mixtures can vary with supplier. Eastman lists MCHM as consisting of 68-89 percent MCHM, 4-10 percent water, 5 percent methyl 4-methylcyclohexanecarboxylate, 1 percent dimethyl 1,4-cyclohexanedicarboxylate, 1-2 percent 1,4-cyclohexanedimethanol, and 1 percent methanol (Material Safety Data Sheet, Eastman Chemical Company, 2011). Only one limited study of biodegradation of MCHM is known, completed by Eastman Kodak Company of crude MCHM using a standard 28-day carbon dioxide (CO_2) evolution test and laboratory-prepared water that was inoculated with activated sludge microorganisms previously unexposed to MCHM (Beglinger, 1997). The crude MCHM was classified as "not readily biodegradable" according to the test protocol because less than 60 percent biodegradation was measured within 10 days. Substantial CO_2 evolution was measured, however, after a 9-day lag period and indicated 53-54 percent degradation within the 28-day test period. If microorganisms used in this test had been previously exposed to MCHM, the lag period before degradation may not have occurred. Degradation products besides CO_2 were not measured, nor the relative amount of MCHM degradation compared to other components of the crude mixture. Recent controversy over reports of possible formaldehyde generation from crude MCHM released in the West Virginia spill demonstrate the need to evaluate both pure MCHM and the crude mixture.

Although alicyclic hydrocarbons are substantial components of petroleum mixtures, and thus are common contaminants, relatively few studies of their biodegradation under aerobic and anaerobic conditions have been reported (Rios-Hernandez et al., 2003). Based on the chemical structure of MCHM, it is likely that the primary alcohol is oxidized to corresponding aldehydes

and carboxylic acid, producing intermediates such as 4-methylcyclohexanecarboxylic acid, which is a naphthenic acid. Naphthenic acids are natural components of hydrocarbon deposits and their environmental fate and toxicity have been reviewed recently because they are major contaminants in extraction water from oil sands and other petroleum deposits (Headley and McMartin, 2004). Naphthenic acids generally are considered weakly biodegradable, although both aerobic and anaerobic cultures of native microbial communities from oil sands tailings water have been shown to be capable of degrading a range of these compounds (Headley and McMartin, 2004). Alkylsuccinate derivatives, in addition to carboxylic acid compounds, also have been identified as metabolites under sulfate-reducing conditions in a study that used ethylcyclopentane as a model alicyclic hydrocarbon (Rios-Hernandez et al., 2003).

We propose to characterize the biodegradation processes, rates, and metabolites using site water and sediment with native microbial communities potentially acclimated to crude MCHM from exposure at the Elk River spill site to the MCHM. Replicate microcosms would be prepared in the laboratory under a range of redox conditions, amended with crude MCHM, and monitored for loss of MCHM and production and removal of metabolites. Sterile controls also would be prepared to measure potential loss due to abiotic processes such as sorption. Samples collected from the site would be analyzed for metabolites observed in the laboratory to confirm their potential importance on environmental fate of MCHM Microcosm preparation and analysis would be performed in the USGS Maryland-Delaware-DC research laboratory. A GC/MS with purge and trap and a GC/FID are available in this laboratory for analyses. Additional analytical support could be obtained from the USGS National Water Quality Laboratory for metabolite identification Collection of samples for laboratory testing and confirmation analyses would be performed the USGS West Virginia Water Science Center.

Freedom_0006097_0009

References Cited

Beglinger, J.M., 1997, Determination of ready biodegradability (biotic degradation) using the CO_2 evolution test (modified Sturm), Study No. EN-113-872790-1: Eastman Chemical Company, Rochester, NY, 41 p. Accessed on February 12, 2014 at http://www.eastman com/Pages/Eastman-Crude-MCHM-Studies.aspx.

Headley, J.V , and McMartin, D.W., 2004, A Review of the Occurrence and Fate of Naphthenic Acids in Aquatic Environments· Journal of Environmental Science and Health Part A—Toxic/Hazardous Substances & Environmental Engineering, vol A39, no. 8, pp. 1989–2010.

Rios-Hernandex, L.A., Gieg, L.M., and Suflita, J.M., 2003, Biodegradation of an alicyclic hydrocarbon by a sulfate-reducing enrichment from a gas condensate-contaminated aquifer· Applied and Environmental Microbiology, v 69, no. 1, p. 434-443.

Speijers, G.J.A., and Renwick, A. Alicyclic Primary Alcohols, Aldehydes, Acids, and Related Esters, WHO Food Additive Series: 50 INCHEM: International Programme on Chemical Safety. Accessed on February 12, 2014 at http.//www inchem.org/documents/jecfa/jecmono/v50je10 htm.

Warner, Sue

From: Warner, Sue
Sent: Thursday, April 10, 2014 9 31 AM
To: Gundersen, Jennifer, Graybill, Eric, Molnar, Adam, Zawodny, Peggy, Poff, Kevin, Nguyen, Hoang
Cc: Caporale, Cynthia
Subject: RE Request for Review WV TAP project results

The main breakdown products of MCHM are excepted to be:

4-methyl cyclohexane-1-carbaldehyde
4-methyl-1-cyclohexanecarboxylic acid
1,4 cyclohexanedicarboxylic acid

Ex. 5 - Deliberative

The following may also be seen, but may also be present from other sources. octanedioic acid, acetic acid, oxalic acid, formic acid, propanoic acid, malonic acid, succinic acid, chlorinated carboxylic acids, methyl acetate, methyl formate

The main breakdown products of PPH are expected to be.

Phenol
Propylene glycol
Halogenated PPH

Ex. 5 - Deliberative

The following may also be seen, but may also be present from other sources: oxalic acid, carbonic acid, carboxylic acids, chlorinated carboxylic acids, anisole (methoxy benzene) and benzoquinones

-----Original Message-----
From: Warner, Sue
Sent· Tuesday, April 08, 2014 3 42 PM
To. Gundersen, Jennifer, Graybill, Eric, Molnar, Adam; Zawodny, Peggy, Poff, Kevin, Nguyen, Hoang
Cc· Caporale, Cynthia
Subject· RE Request for Review WV TAP project results

We will meet on Thursday at 10·00 in E201.

-----Original Message-----
From· Gundersen, Jennifer
Sent: Tuesday, April 08, 2014 8 32 AM
To. Warner, Sue, Graybill, Eric; Molnar, Adam; Zawodny, Peggy; Poff, Kevin, Nguyen, Hoang
Cc: Caporale, Cynthia
Subject. RE· Request for Review. WV TAP project results

I can do Thu at 10

-----Original Message-----
From Warner, Sue
Sent. Monday, April 07, 2014 2·36 PM
To: Graybill, Eric, Molnar, Adam; Zawodny, Peggy; Poff, Kevin, Gundersen, Jennifer, Nguyen, Hoang
Cc: Caporale, Cynthia
Subject RE. Request for Review WV TAP project results

Can we meet sometime this week? How about Wednesday or Thursday morning at 10 00?

Attached is some information on the breakdown products

-----Original Message-----
From. Caporale, Cynthia
Sent. Monday, April 07, 2014 2.18 PM
To: Warner, Sue; Graybill, Eric, Molnar, Adam, Zawodny, Peggy, Poff, Kevin, Gundersen, Jennifer, Nguyen, Hoang
Subject: Request for Review· WV TAP project results
Importance: High

All,

Since this data has information on TICs and there is still an interest in confirming the potential breakdown products of MCHM/PPH post-treatment, the File 6 needs to be reviewed. The goal is to review the individual TICs and determine if the tentative identification indicates a source material (those compounds on the MSDS for crude material) or if it could be a potential breakdown product

With this much data, I would like each of you to review a portion of the results so as not to have the entire task on one person. Please meet and decide how to divide up the results (e g , each review 50-60 pages) and provide a proposed completion date Sue and Kevin have some extensive information on the potential breakdown products based on previous conference calls so work with them if you need this background. The outcome of this review should be a report that highlights what was reviewed, by whom, what TICs were determined to be present, and the tentative classification (source material, breakdown product, other).

This is an unusual request for us so please let me know if further clarification or discussion is needed. Our Water Protection Division is very much interested in what you determine.

I'm suggesting a 2-week turnaround time but if after you meet as a group you determine you need more time please let me know

Thank you to Sue who did the leg work on this and found the type of information we have been searching for these past few months!

Cindy

-----Original Message-----
From: Warner, Sue
Sent: Monday, April 07, 2014 10.49 AM
To Caporale, Cynthia, Graybill, Eric; Molnar, Adam; Zawodny, Peggy; Poff, Kevin, Gundersen, Jennifer
Subject: RE: WV TAP project results

I have reviewed the files and found that File 1 has a few TICs , presented as text only File 4 has 265 pages of TICs, presented as text only File 6 has 398 pages of TIC spectra for us to look at We should look for breakdown products in these TICs

-----Original Message-----
From: McCann, Mark
Sent· Monday, April 07, 2014 8 45 AM
To. Gundersen, Jennifer
Cc Caporale, Cynthia, Warner, Sue; Graybill, Eric, Molnar, Adam, Zawodny, Peggy; Poff, Kevin

Freedom_0006097_0012

Ex. 5 - Deliberative

Breakdown products

Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
Crude MCHM	4-methylcyclohexane methanol	68 to 89%	100-49-2	128 21	180-202°C
	4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158 25	?°C
	methyl 4-methylcyclohexanecarboxylate	5%	51181-40-9	156.22	191.7 °C
	dimethyl 1,4-cyclohexanedicarboxylate	1%	94-60-0	200 23	132 °C (technical grade)
	methanol	1%	67-56-1	32 04	64 7 °C
	1,4-cyclohexanedimethanol	1-2%	105-08-8	144 21	283 °C
DOWANOL™ DIPPH Glycol Ether	Dipropylene glycol phenyl ether or (methyl-2-phenoxyethoxy)propanol	>60%	51730-94-0	210 27	280 °C
	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152.19	242.7 °C

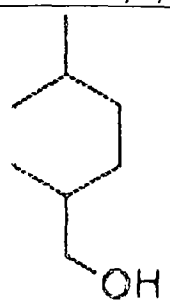
* Eric Weber, ORD/NERL/ERD, 2/4/2014

** source dependent

acids
aldehydes
acetic acid
oxalic acid
propanoic acid
malonic "
succinic "
} & chlorinated versions
methyl acetate or formate

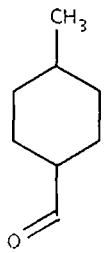
chlorinated PPH
benzoquinone
phenol
propylene glycol
carbonic acid
anisole

Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
4-methylcyclohexanemethanol	68 to 89%	100-49-2	128 21	180-202°C



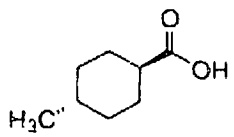
NOTE: The following information has not been peer-reviewed nor does it represent the views of the Agency.

Oxidation of primary alcohol ➔ 4-methyl cyclohexane -1-carbaldehyde (Fig 1) CAS RN· 33242-79-4 Formula. C8H14O MW· 126.19, B P. · 202-205 °C.



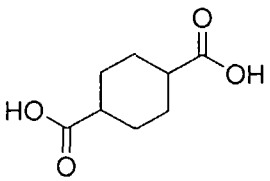
(Fig 1)

Further oxidation of an aldehyde yields a carboxylic acid A stepwise oxidation (as opposed to oxidation of methyl group and opening of the ring)might result in 4-Methyl-1-cyclohexanecarboxylic acid (Fig 2) CAS No.: 13064-83-0 (Fig 2) Formula. CH3C6H10CO2H MW: 142 20. A powder in pure form. This compound is a napthenic acid (NA) and has been used to study biodegradation kinetics of NAs NAs in the oil refinery business refer to naturally occurring complex mixtures of alkyl-substituted cycloaliphatic carboxylic acids that concentrate in the tailings from extraction of oil from tar sands. The most interesting thing I read with respect to the NAs was one study that found different biodegradation rates between cis- and trans- isomers (Canadian Water Resources Journal, Biodegradation Kinetics of Geometric Isomers of Model Naphthenic Acids in Athabasca River Water J V. Headley , K.M Peru , S Tanapat & G Putz, Published online· 23 Jan 2013,
http //www tandfonline.com/doi/abs/10.4296/cwrj2701025)



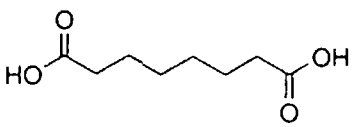
(Fig 2)

If KMnO4 did not open the cyclohexane ring to yield monocarboxylic acids or a dicarboxylic acid you might in theory get 1,4 cyclohexanedicarboxylic acid (Fig 3), CAS No 1076-97-7, a compound with very low water solubility unless deprotonated at more basic pH resulting in a soluble carboxylate.



(Fig 3)

Alkaline KMnO4 would likely open the cyclohexane ring to give a dicarboxylic acid the octanedioic acid (Fig 4) or perhaps smaller acids such as acetic or oxalic acid. Smaller carboxylic acids are formic (C=1), acetic (C=2), propranoic (C=3) and dicarboxylic acids oxalic (C=2), malonic (C=3) succinic (C=4) up to C=5 are soluble in water

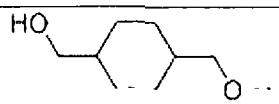


(Fig 4)

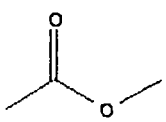
In general, open chain carboxylic acids might be the ultimate products of alkaline KMnO4 oxidation of MCHM. KMnO4 prefers to oxidize double bonds so MCHM may not have been oxidized at all by KMnO4 in river water treatment. Chlorination may not be sufficient to make carboxylic acids but small soluble carboxylic acids, produced by KMnO4 or free radicals, that make it to chlorination could be halogenated Depending on pH before the chlorination step, the larger dicarboxylic acids may be removed as precipitates

Small chlorinated carboxylic acids

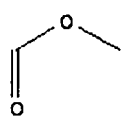
Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP
4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158.25	?°C



In theory, oxidation of primary alcohol and ether groups might result in small open chain carboxylic acids and perhaps acetates such as methyl acetate (Fig 5) or methyl formate (Fig 6). I would trust the QSAR predictions more on this one



(Fig 5)



(Fig 6)

Some EPA Methods

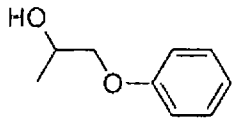
EPA 556.1 DETERMINATION OF CARBONYL COMPOUNDS IN DRINKING WATER BY FAST GAS CHROMATOGRAPHY, 1999 A place to start to detect aldehydes and ketones.

EPA 522 DETERMINATION OF 1,4-DIOXANE IN DRINKING WATER BY SOLID PHASE EXTRACTION (SPE) AND GAS CHROMATOGRAPHY/MASS SPECTROMETRY (GC/MS) WITH SELECTED ION MONITORING (SIM), 2008. A place to start for ethers

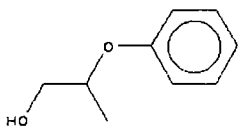
EPA Method 611—Haloethers

Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
DOWANOL™ DiPPH Glycol Ether	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152 19	242 7 ^{O}C

PPh



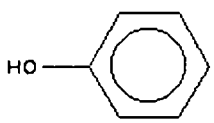
secondary alcohol, major isomer, CAS No · 770-35-4



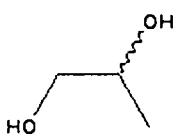
primary alcohol, the minor isomer, CAS No.· 4169-04-4

The EPA's EPIWIN/APO model is reported to estimate atmospheric photodegradation half-life of PPh at 3.45 hrs based on 12 hours of sunlight and avg OH radical concentration of 1 5E6 OH/cm^3. Free radical oxidation might result in phenol (Fig and propylene glycol (I attempted writing out the free radical reaction and terminated it there.) I also found literature indicating that acidic KMnO4 could oxidize phenyl glycol ether to phenol and carboxylic acids Another source indicated propylene glycol (Fig 8) oxidation to oxalic (Fig 9) and carbonic acids (Fig 10).

Phenol (Fig 7) Formula. C6H6O. Molecular weight 94 1112 CAS No · 108-95-2



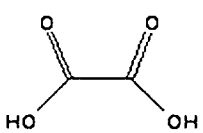
(Fig 7)



(Fig 8)

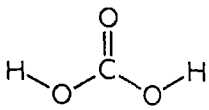
Propylene glycol (Fig 8). CAS No.. 57-55-6. Formula: C3H8O2. Molecular weight 76.0944

Oxalic acid (Fig 9) CAS No 144-62-7 Molecular weight 90 03



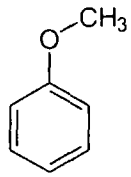
(Fig 9)

Carbonic acid (Fig 10)·



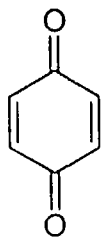
(Fig 10)

Biological methylation of phenol to anisole (Fig 11) is reported in the literature Anisole (methoxy benzene) CAS No 100-66-3. Formula· C7H8O Molecular weight. 108 1378. Article on halogenated anisoles in the environment Fresenius J Anal Chem (2001) 371 .598–606, "Halogenated methyl-phenyl ethers (anisoles) in the environment Determination of vapor pressures, aqueous solubilities, Henry's law constants, and gas/water- (Kgw), n-octanol/water- (Kow) and gas/n-octanol (Kgo) partition coefficients "



(Fig 11)

Oxidation of phenol with KMnO4 is reported to produce benzoquinones (Fig 12)



(Fig 12)

I found one article that reported using PPh as a model compound for chlorination. Environ Sci Technol. 2004, 38, 4019-4025, "Transformation of Aromatic Ether and Amine-Containing Pharmaceuticals during Chlorine Disinfection." Researchers looked at chlorination of pharmaceuticals using PPh (1-phenoxy-2-propanol) as a model compound Used RP-HPLC , 30%HEPES buffer/70%acetonitrile and UV detection at 275 The point might be that if PPh survives drinking water pre-treatment, it may halogenate.

#1

1F

SEMIVOLATILE ORGANICS ANALYSIS DATA SHEET
TENTATIVELY IDENTIFIED COMPOUNDS

EPA SAMPLE NO
WVL01

Lab Name ___Lancaster Laboratories___ Contract _____
Lab Code LANCAS Case No _____ SAS No _____ SDG No _____
Matrix (soil/water) WATER Lab Sample ID 7390454
Sample wt/vol 1042 (g/mL) mL Lab File ID dc0066 d
Level (low/med) LOW Date Received 03/12/14
% Moisture Decanted (Y/N) Date Extracted 03/13/14
Concentrated Extract Volume 1000 (uL) Date Analyzed 03/13/14
Injection Volume 1 (uL) Dilution Factor 1
GPC Cleanup N pH Extraction Sepf

CONCENTRATION UNITS
Number TICs found 14 (ug/L or ug/Kg) ug/L

	CAS NUMBER	COMPOUND NAME	RT	EST CONC	Q
1	75-27-4	Methane, bromodichloro-	1 583	9	J
2	1985-88-2	1,1-Dimethyl-3-chloropropano	2 151	250	J
3	507-45-9	Butane, 2,3-dichloro-2-methy	3 367	22	J
4	2419-74-1	2-Butanol, 1,4-dichloro-	3 623	4	J
5	124-18-5	Decane	3 892	2	BJ
6	6321-14-8	2-Hexanone, 3-hydroxy-3,5-di	4 253	7	J
7	0-00-0	O-CHLOROPHENOL-D4	5 640	8	J
8	124-18-5	Decane	5 792	1	J
9	17639-93-9	Propanoic acid, 2-chloro-, m	6 409	11	J
10	541-02-6	Cyclopentasiloxane, decameth	7 290	6	J
11	1528-23-0	endo-4-Oxatricyclo[5 2 1 0(2	7 715	3	J
12	392-71-2	2,6-Dichloro-4-fluorophenol	8 047	6	J
13	21031-46-9	3-Butenenitrile, 3-chloro-	8 076	6	J
14	0-00-0	2,4,6-TRICHLOROPHENOL-D2	9 539	8	J
15					
16	SVOCTIC	Total SVOC TICs		320	J
17					
18					
19					
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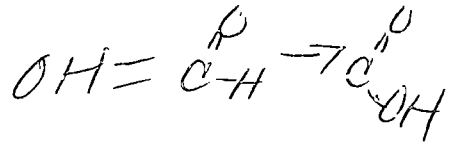
30					

page 1 of 1

FORM I SV-1

words



4-methyl cyclohexane carboxylic acid

1F

SEMIVOLATILE ORGANICS ANALYSIS DATA SHEET
TENTATIVELY IDENTIFIED COMPOUNDS

EPA SAMPLE NO
WVL02

Lab Name Lancaster Laboratories Contract
Lab Code LANCAS Case No SAS No SDG No
Matrix (soil/water) WATER Lab Sample ID 7390455
Sample wt/vol 1051 (g/mL) mL Lab File ID dc0067 d
Level (low/med) LOW Date Received 03/12/14
% Moisture Decanted (Y/N) Date Extracted 03/13/14
Concentrated Extract Volume 1000 (uL) Date Analyzed 03/13/14
Injection Volume 1 (uL) Dilution Factor 1
GPC Cleanup N pH Extraction Sepf

CONCENTRATION UNITS
Number TICs found 9 (ug/L or ug/Kg) ug/L

	CAS NUMBER	COMPOUND NAME	RT	EST CONC	Q
1	75-27-4	Methane, bromodichloro-	1 578	9	J
2	1985-88-2	1,1-Dimethyl-3-chloropropano	3 146	230	J
3	507-45-9	Butane, 2,3-dichloro-2-methy	3 367	16	J
4	994-05-8	Butane, 2-methoxy-2-methyl-	3 554	7	J
5	2419-74-1	2-Butanol, 1,4-dichloro-	3 623	4	J
6	74421-00-4	Butane, 2,3-dimethoxy-2-meth	3 892	1	J
7	541-35-5	Butanamide	4 253	9	J
8	124-18-5	Decane	5 792	6	BJ
9	541-02-6	Cyclopentasiloxane, decameth	7 290	5	J
10					
11	SVOCTIC	Total SVOC TICs		250	J
12					
13					
14					
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1F

SEMIVOLATILE ORGANICS ANALYSIS DATA SHEET
TENTATIVELY IDENTIFIED COMPOUNDS

EPA SAMPLE NO
WVL07

Lab Name Lancaster Laboratories Contract
Lab Code LANCAS Case No SAS No SDG No
Matrix (soil/water) WATER Lab Sample ID 7390457
Sample wt/vol 1050 (g/mL) mL Lab File ID dc0069 d
Level (low/med) LOW Date Received 03/12/14
% Moisture Decanted (Y/N) Date Extracted 03/13/14
Concentrated Extract Volume 1000 (uL) Date Analyzed 03/13/14
Injection Volume 1 (uL) Dilution Factor 1
GPC Cleanup N pH Extraction Sepf

CONCENTRATION UNITS
Number TICs found 15 (ug/L or ug/Kg) ug/L

	CAS NUMBER	COMPOUND NAME	RT	EST CONC	Q
1	75-27-4	Methane, bromodichloro-	1 583	6	J
2	17773-64-7	1-Butene, 2-chloro-3-methyl-	1 723	1	J
3	1985-88-2	1,1-Dimethyl-3-chloropropano	3 157	270	J
4	507-45-9	Butane, 2,3-dichloro-2-methy	3 373	26	J
5	2419-74-1	2-Butanol, 1,4-dichloro-	3 623	4	J
6	74421-00-4	Butane, 2,3-dimethoxy-2-meth	3 892	2	J
7	2588-77-4	2-Methyl-3-bromo-2-butanol	4 253	7	J
8	0-00-0	O-CHLOROPHENOL-D4	5 640	8	J
9	124-18-5	Decane	5 792	2	BJ
10	17639-93-9	Propanoic acid, 2-chloro-, m	6 409	11	J
11	541-02-6	Cyclopentasiloxane, decameth	7 290	8	J
12	498-66-8	2-Norbornene	7 715	3	J
13	392-71-2	2,6-Dichloro-4-fluorophenol	8 047	6	J
14	21031-46-9	3-Butenenitrile, 3-chloro-	8 076	5	J
15	0-00-0	2,4,6-TRICHLOROPHENOL-D2	9 539	10	J
16					
17	SVOCTIC	Total SVOC TICs		350	J
18					
19					
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page 1 of 1

FORM I SV-1

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Ex. 5 - Deliberative

File :H:\5S021714\02171415.D
Operator : RM
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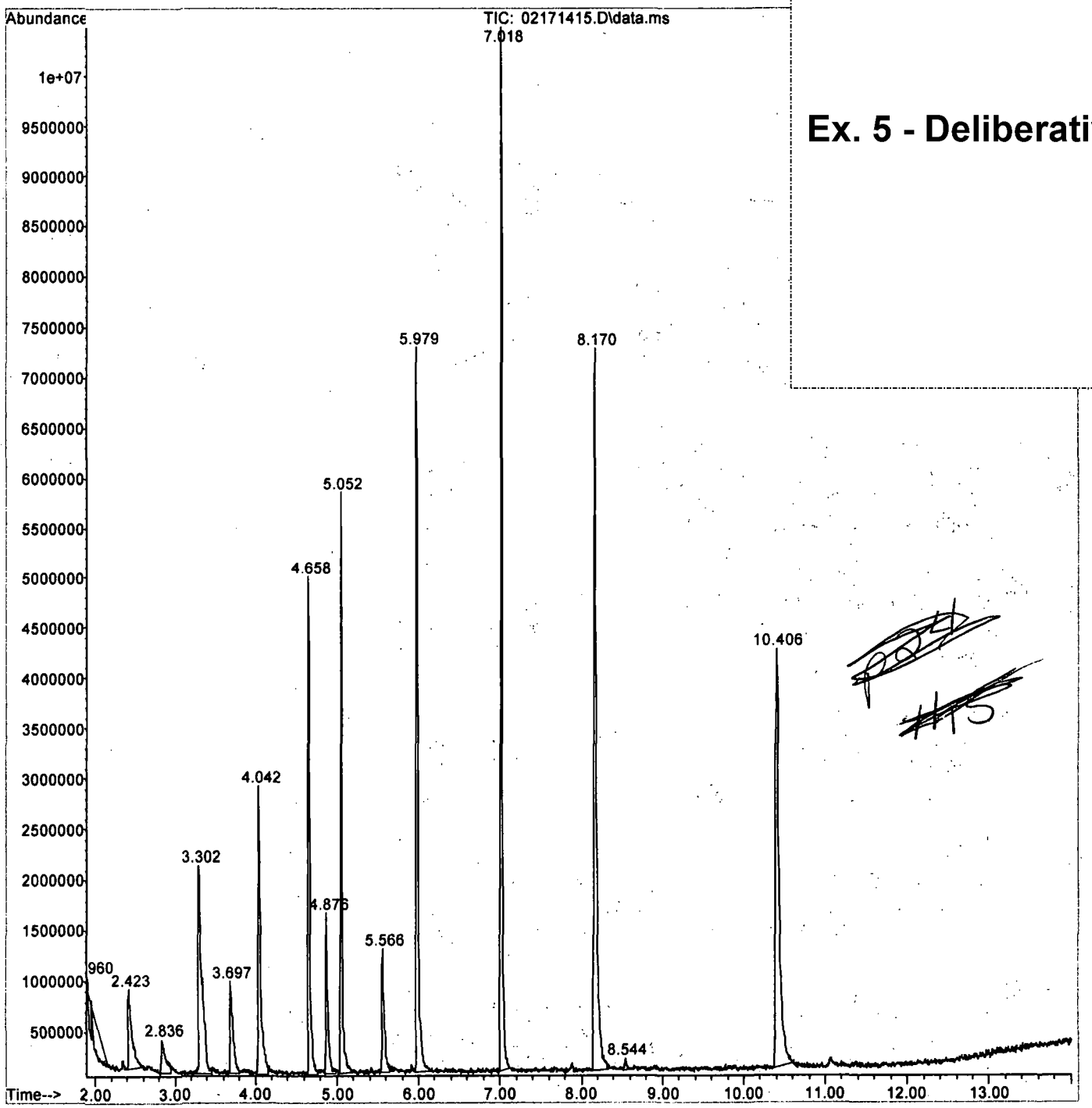
Instrument : SVMS5
Sample Name: 1402552-02A
Misc Info : 1X 14ACW - 55804
Vial Number: 14



Ex. 5 - Deliberative

Library Search Report

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Acq On : 17 Feb 2014 9:30 pm
Operator : RM
Sample : 1402552-02A
Misc : 1X 14ACW - 55804
ALS Vial : 14 Sample Multiplier: 1

Search Libraries: H:\NIST11.L Minimum Quality: 0

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

Pk#	RT	Area%	Library/ID	Ref#	CAS#	Qual
1	1.962	-3.53	H:\NIST11.L			
			Methane, bromodichloro-	32801	000075-27-4	42
			Ethane, 1,1,2,2-tetrachloro-	35232	000079-34-5	37
			Trichloromethane	8988	000067-66-3	37
2	2.426	2.95	H:\NIST11.L			
			1,1-Dimethyl-3-chloropropanol	9768	001985-88-2	72
			Butanamide	1862	000541-35-5	47
			Acetic acid, 3-methoxy-2-butyl ester	21966	1000151-29-7	47
3	2.837	1.31	H:\NIST11.L			
			Phenol, 2-fluoro-	6349	000367-12-4	72
			Phenol, 4-fluoro-	6350	000371-41-5	72
			1,3-Benzodioxol-2-one	16119	002171-74-6	37
4	3.301	7.22	H:\NIST11.L			
			1,2-Dichlorobenzene-D4	24120	002199-69-1	50
			1,4-Dichlorobenzene-D4	24121	003855-82-1	40
			Benzene, 1,2,3,4-tetrafluoro-	24220	000551-62-2	35
5	3.695	2.75	H:\NIST11.L			
			Nitrobenzene-D5	12062	004165-60-0	91
			Nitrobenzene-D5	12063	004165-60-0	47
			Butyramide, 2-cyano-2-ethyl-	18269	018705-38-9	17
6	4.042	6.98	H:\NIST11.L			
			Naphthalene-D8	15661	001146-65-2	94
			Naphthalene-D8	15662	001146-65-2	91
			Tricyclo[4.4.0.0(2,8)]decane	15759	049700-59-6	45
7	4.659	8.04	H:\NIST11.L			
			1,1'-Biphenyl, 2-fluoro-	39867	000321-60-8	94
			1,1'-Biphenyl, 2-fluoro-	39868	000321-60-8	91
			1,1'-Biphenyl, 2-fluoro-	39865	000321-60-8	91

Freedom_0006097_0026

Library Search Report

Data Path : H:\5S021714\
Data File : 02171415.D
Acq On : 17 Feb 2014 9:30 pm
Operator : RM
Sample : 1402552-02A
Misc : 1X 14ACW - 55804
ALS Vial : 14 Sample Multiplier: 1

Search Libraries: H:\NIST11.L Minimum Quality: 0

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

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			Benzenamine, 4-chloro-N,N-diethyl-	47884	002873-89-4	93
			o-Chloro-N,N-diethylaniline	47879	019372-80-6	91
			3-Chloro-2,6-diethylaniline	47880	067330-62-5	80
9	5.052	9.37	H:\NIST11.L			
			Acenaphthene-d10	33726	015067-26-2	90
			3,6-Dimethyloxazolo(5,4-c)pyridazi n-4-amine	34104	1000244-73-9	27
			1,2,3,4,5,8-Hexahydroisoquinoline, 1-[3-hydroxybenzyl]-6-methoxy-	120220	1000126-16-5	25
10	5.563	2.70	H:\NIST11.L			
			Phenol, 2,4,6-tribromo-	168020	000118-79-6	99
			Phenol, 2,3,5-tribromo-	168018	057383-81-0	99
			Phenol, 2,4,6-tribromo-	168021	000118-79-6	99
11	5.981	12.61	H:\NIST11.L			
			Anthracene-D10-	51751	001719-06-8	97
			Anthracene-D10-	51750	001719-06-8	94
			Phenanthrene-D10	51752	001517-22-2	93
12	7.020	14.79	H:\NIST11.L			
			p-Terphenyl-d14	97569	001718-51-0	98
			1H-1,3-Benzimidazole-5,6-dicarboni trile, 1-phenyl-	97497	1000351-16-9	72
			4-Benzylbiphenyl	97592	000613-42-3	72
13	8.172	16.93	H:\NIST11.L			
			Chrysene-D12	94357	001719-03-5	96
			4-Hydroxy-5-methoxy-2-methyl-1,10-phenanthroline	93879	093533-14-3	58
			9,10-Anthracenedione, 1,4-dihydroxy-	93971	000081-64-1	53
14	8.542	0.22	H:\NIST11.L			

Freedom_0006097_0027

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Data File : 02171415.D
Acq On : 17 Feb 2014 9:30 pm
Operator : RM
Sample : 1402552-02A
Misc : 1X 14ACW - 55804
ALS Vial : 14 Sample Multiplier: 1

Search Libraries: H:\NIST11.L Minimum Quality: 0

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

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			ydroxy-6-(trifluoromethyl)-			
			7-Benzhydrylidene-2,3-diaza-bicycl	124482	079593-46-7	14
			o[2.2.1]hept-2-ene, N-oxide			
			2-Methylphenanthro[3,4-d][1,3]oxaz	101514	098033-24-0	11
			ol-10-ol			
15	10.405	14.45	H:\NIST11.L			
			Perylene-D12	114295	001520-96-3	95
			3,4-Dibromobenzaldehyde	112716	074003-55-7	58
			Benzamide, N-[(1,5-dimethyl-1H-pyr	113778	1000337-83-3	53
			rol-2-yl)methyl]-2,6-difluoro-			

Freedom_0006097_0028

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Acquired : 19-FEB-2014 13:56
Instrument : HP19760.i
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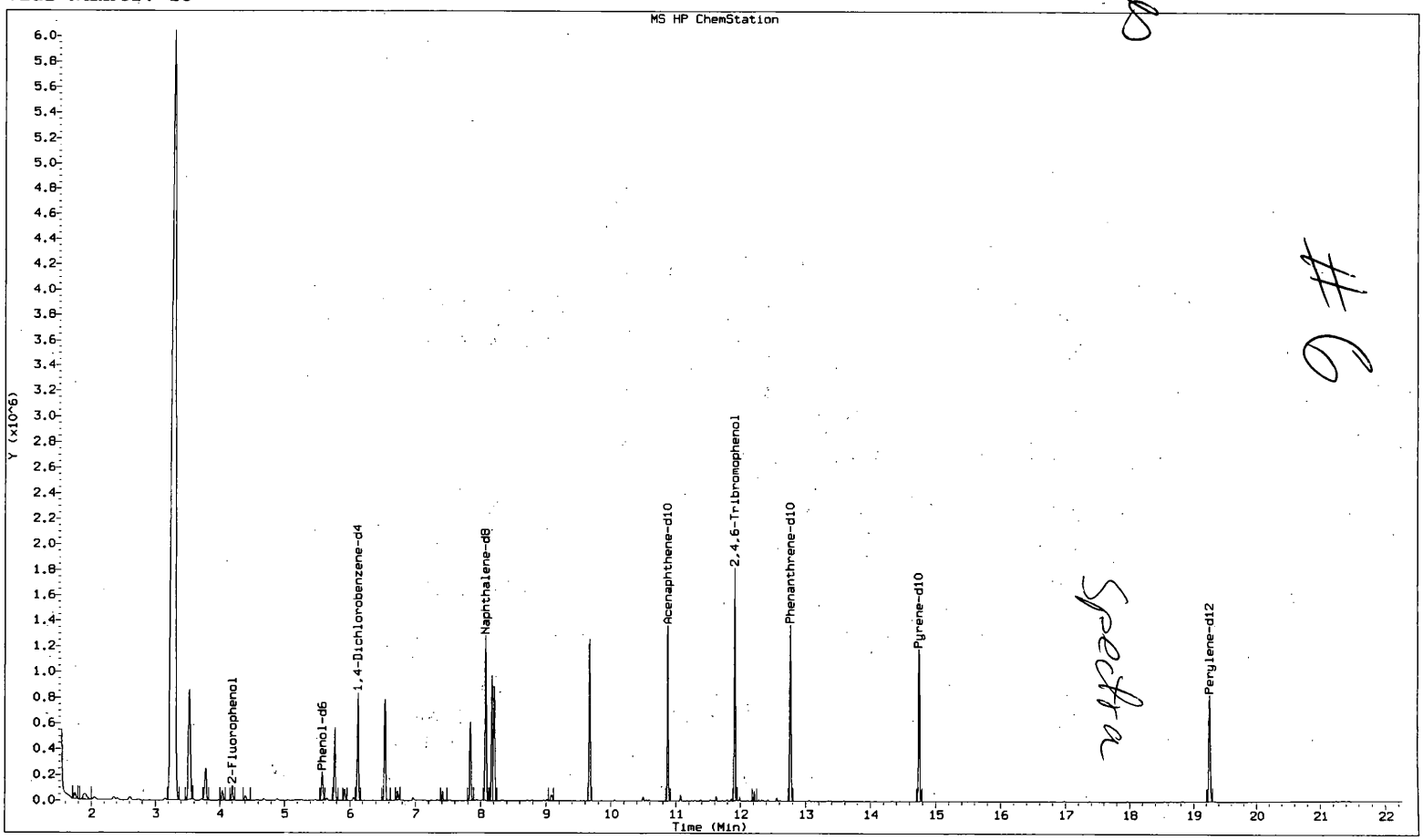
Misc Info : 14049WAA;WL13166;;1055;1000;0;db0806;13166;
Vial Number: 15



Spectra

#6

Lancaster Labs

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Operator : jmg00346 Inst ID: HP19760.i
Smp Info : SSKC1;7365697;1;0;SAMPLE;;;
Misc Info : 14049WAA;WL13166;;1055;1000;0;db0806;13166;
Comment : Max. number of TICs to report is 50, 18 TICs were found initially.
Method : /chem/HP19760.i/14feb19.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 15:13 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 15
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1055.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.124	1170806	10.000
* 48 Naphthalene-d8	8.077	1807783	10.000
* 83 Acenaphthene-d10	10.880	1555968	10.000
* 120 Phenanthrene-d10	12.769	1556656	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-					CAS #: 75-27-4		
1.747	96108	0.82086852	0.77807	90	NIST05a.l	31325	21
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.892	173428	1.48126962	1.40404	93	NIST05a.l	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.309	24805514	211.866855	200.82166	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.530	1675331	14.3091984	13.56322	90	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.781	460394	3.93227973	3.72727	32	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.043	125772	1.07423472	1.01823	40	NIST05a.l	13998	21
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.399	62127	0.53063190	0.50296	74	NIST05a.l	33655	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.774	801743	6.84778014	6.49078	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.926	121738	1.03977510	0.98556	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.538	1143167	9.76392948	9.25490	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans- (1)					CAS #: 13937-49-3		
6.730	95584	0.81639541	0.77383	83	WILEY275.l	19674	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.412	89394	0.49449662	0.46871	91	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.843	756467	4.18449992	3.96635	47	NIST05a.l	13652	48
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.170	1112745	6.15530174	5.83440	43	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.205	1077741	5.96167328	5.65087	50	NIST05a.l	3933	48

Target compound.
Do not report.
ajs00193 03/01/2014

Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc					CAS #: 63506-25-2		
9.079	82297	0.45523953	0.43150	72	WILEY275.1	109601	48
Sulfur monochloride					CAS #: 10025-67-9		
9.674	1521394	9.77779576	9.26805	38	NIST05a.1	14872	83
Benzene, (1-methyldecyl)-					CAS #: 4536-88-3		
12.209	66826	0.42928907	0.40690	93	NIST05a.1	80019	120

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

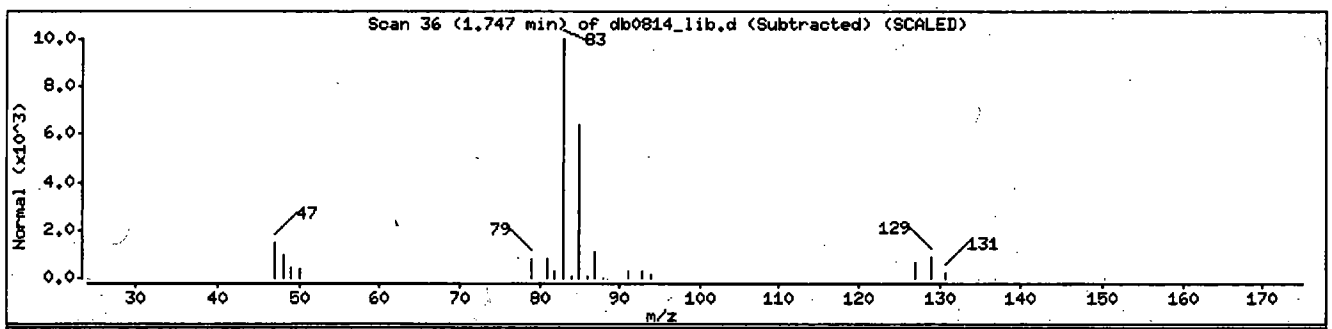
Volume Injected (uL): 1.0

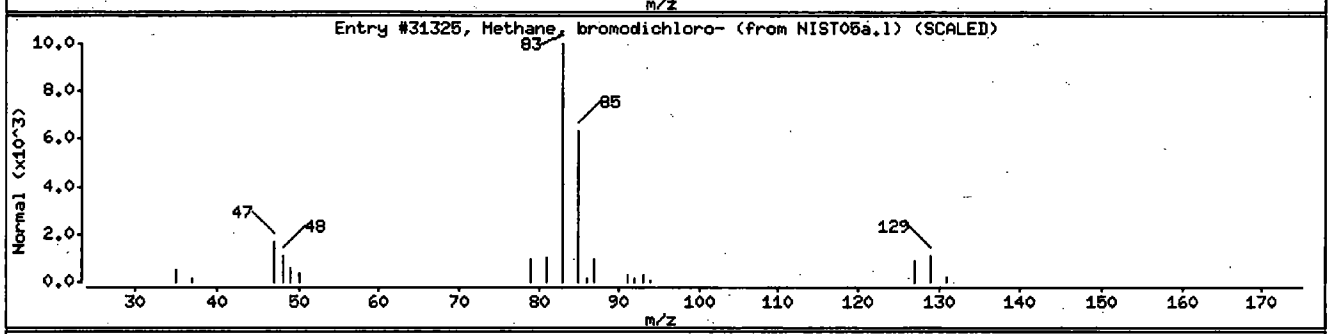
Operator: jmg00346

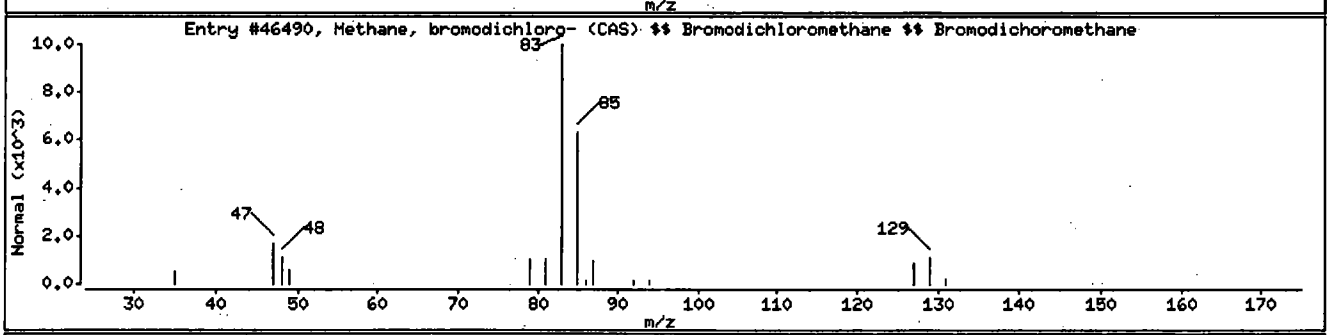
Column phase: J&W DB-5MS

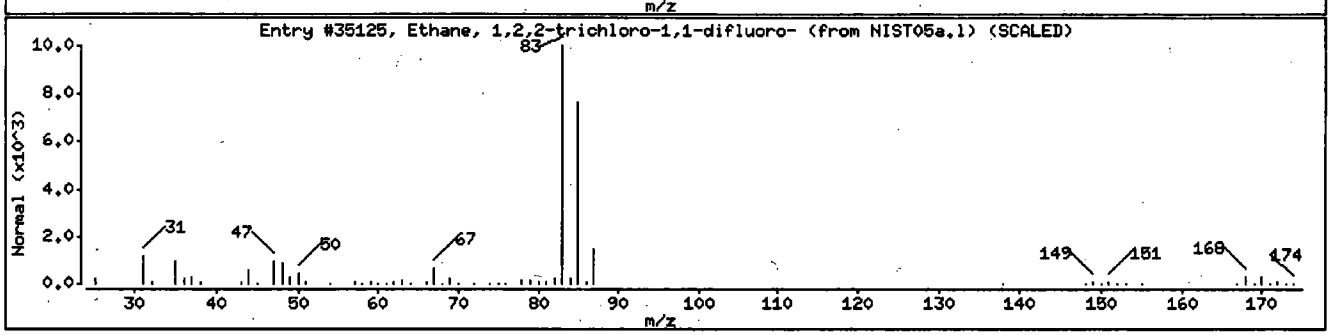
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

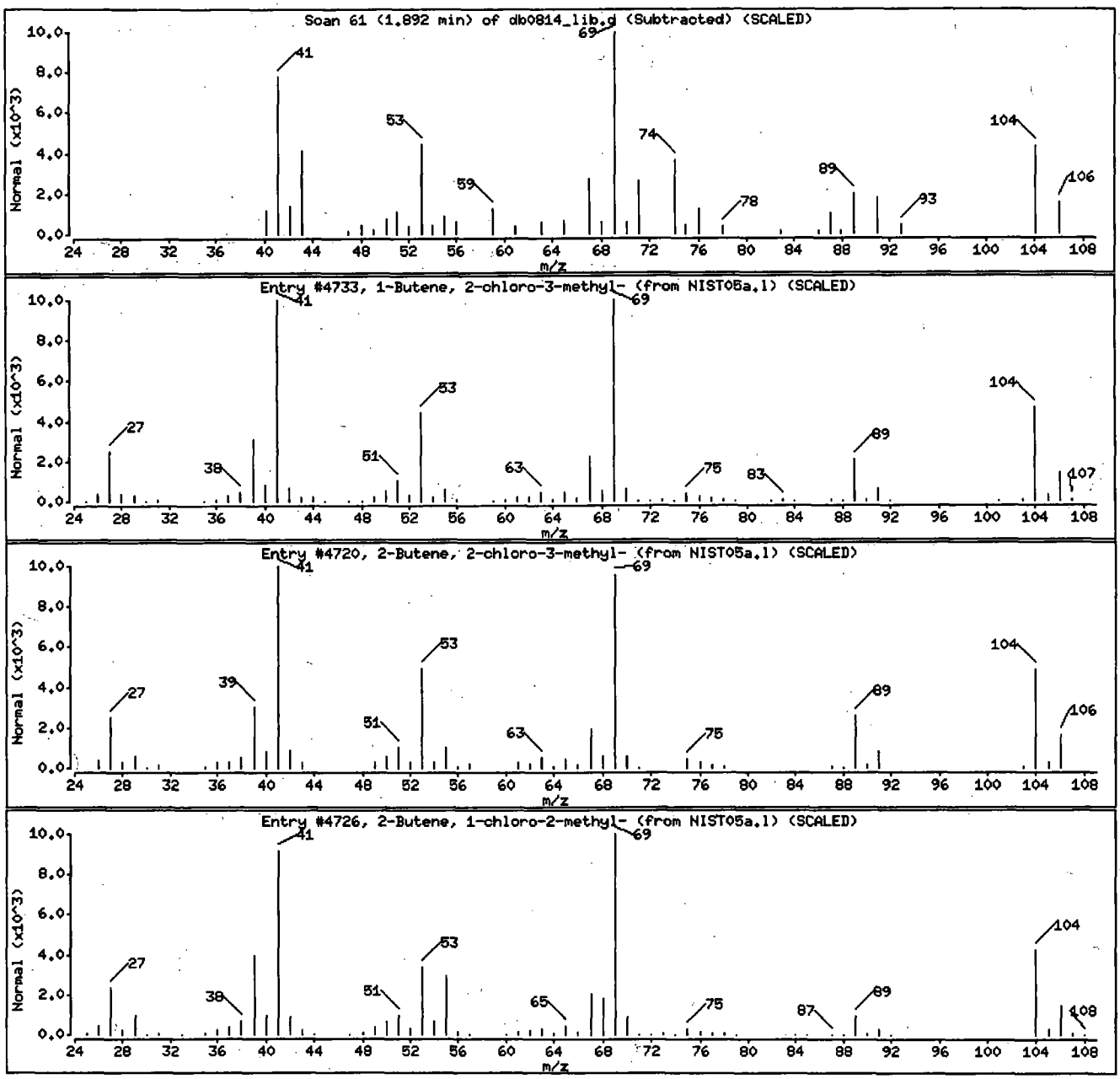
Client ID: SSKC1 Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	93	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	81	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4726	72	C5H9Cl	104



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

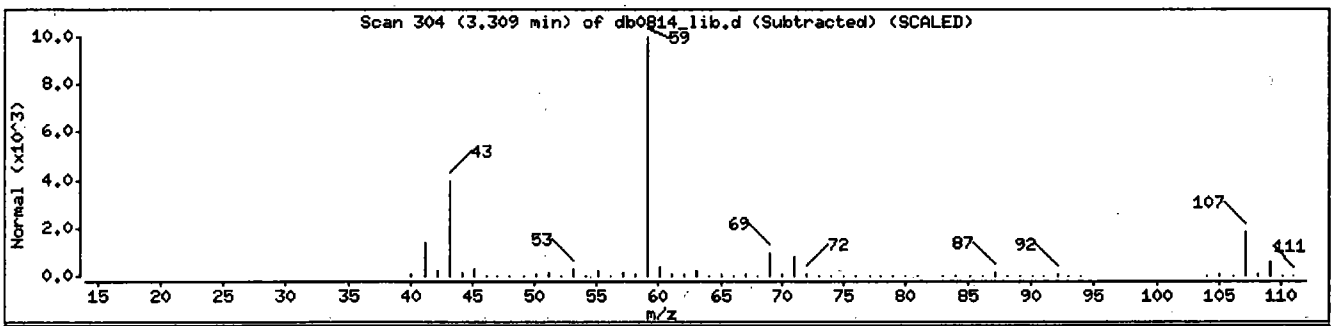
Volume Injected (uL): 1.0

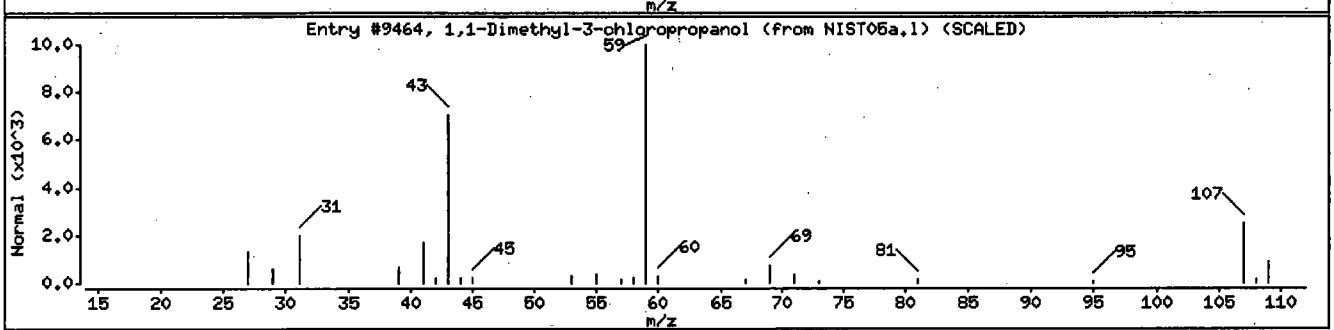
Operator: jmg00346

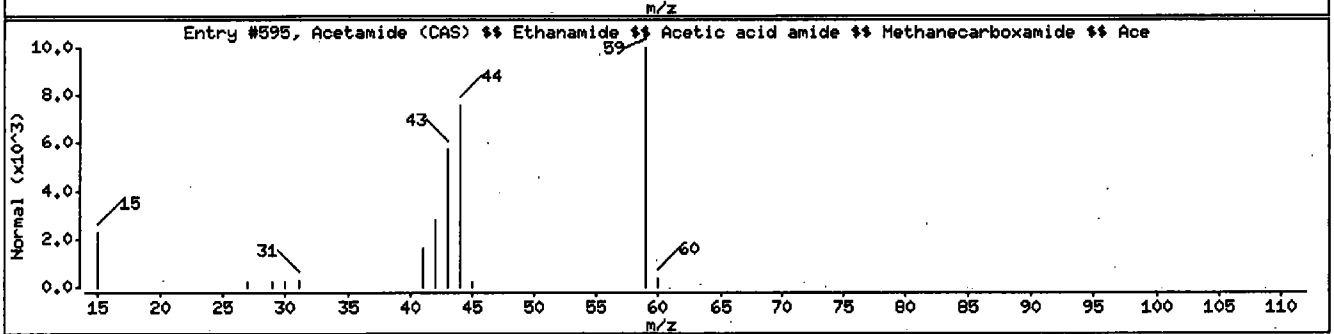
Column phase: J&W DB-5MS

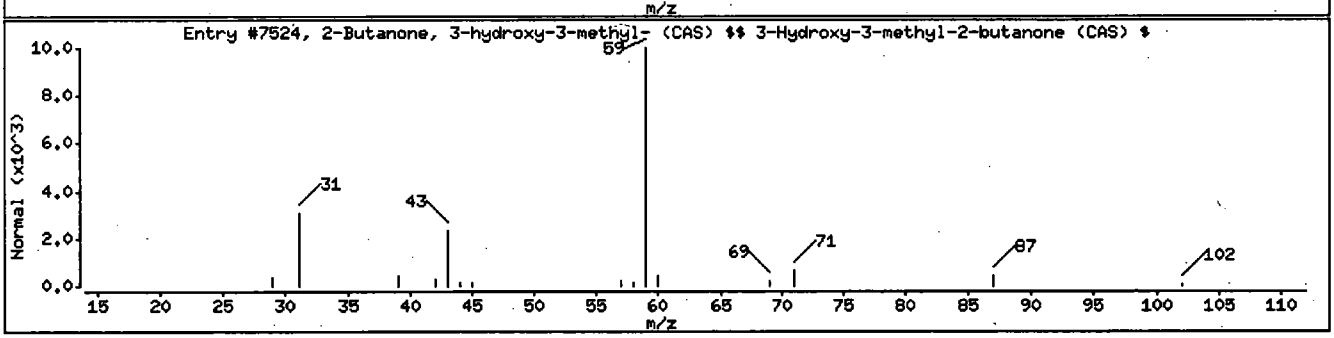
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102





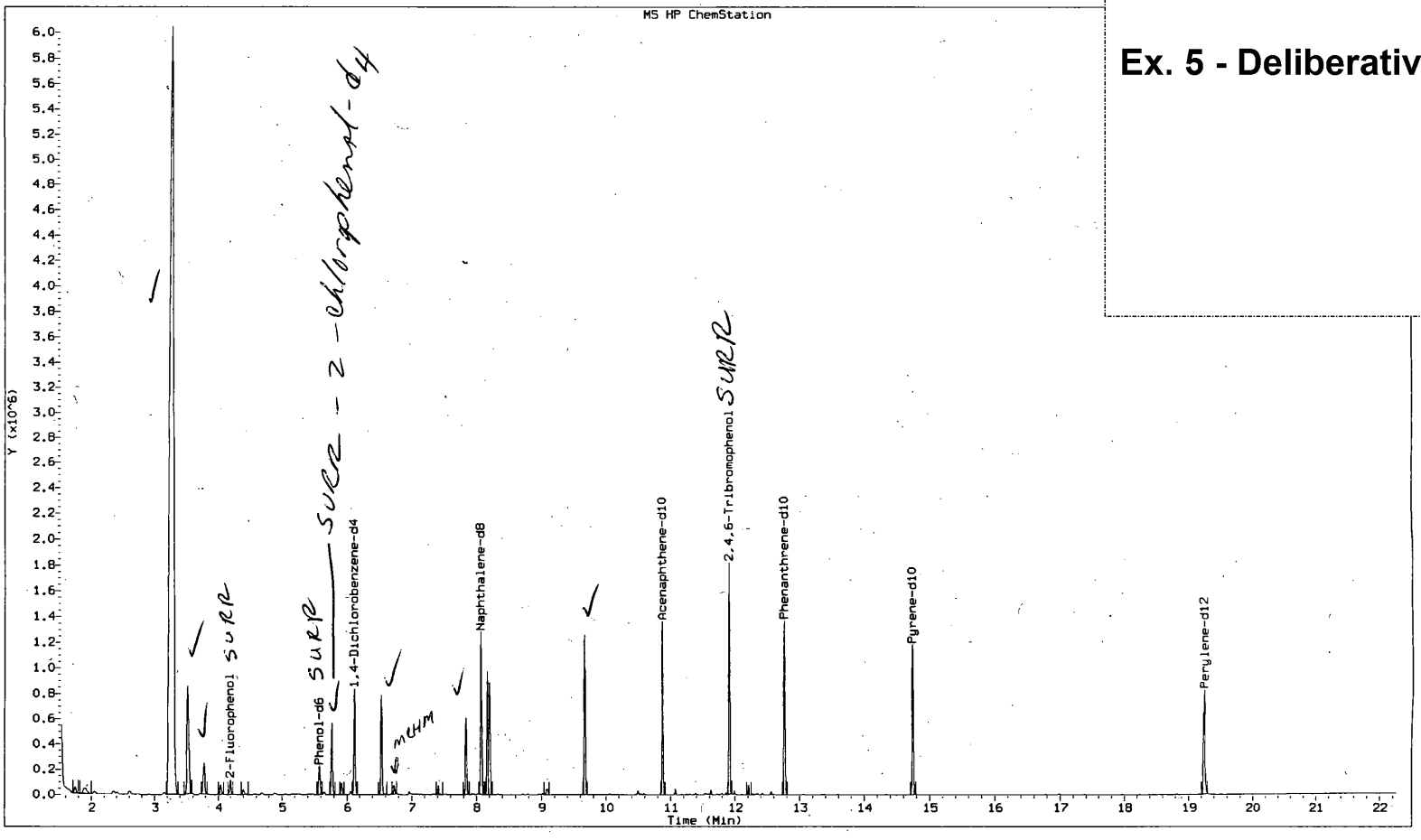




Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

#1

File : /chem/HP19760.i/14feb19.b/db0814_lib.d
Operator : jmg00346
Acquired : 19-FEB-2014 13:56
Instrument : HP19760.i
Sample Name: SSKC1/7365697;1;0;SAMPLE;;;
Misc Info : 14049WAA;WL13166;;1055;1000;0;db0806;13166;
Vial Number: 15



Ex. 5 - Deliberative

Lancaster Labs

Data file : /chem/HP19760.i/14feb19.b/db0814_lib.d
Lab Smp Id: 7365697 Client Smp ID: SSKC1
Inj Date : 19-FEB-2014 13:56
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : SSKC1;7365697;1;0;SAMPLE;;;
Misc Info : 14049WAA;WL13166;;1055;1000;0;db0806;13166;
Comment : Max. number of TICs to report is 50, 18 TICs were found initially.
Method : /chem/HP19760.i/14feb19.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 15:13 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 15
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1055.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.124	1170806	10.000
* 48 Naphthalene-d8	8.077	1807783	10.000
* 83 Acenaphthene-d10	10.880	1555968	10.000
* 120 Phenanthrene-d10	12.769	1556656	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #

Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.747	96108	0.82086852	0.77807	90	NIST05a.l	31325	21
1-Butene, 2-chloro-3-methyl-				CAS #: 17773-64-7			
1.892	173428	1.48126962	1.40404	93	NIST05a.l	4733	21(ML)
1,1-Dimethyl-3-chloropropanol				CAS #: 1985-88-2			
3.309	24805514	211.866855	200.82166	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-				CAS #: 507-45-9			
3.530	1675331	14.3091984	13.56322	90	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-				CAS #: 2419-74-1			
3.781	460394	3.93227973	3.72727	32	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-				CAS #: 74421-00-4			
4.043	125772	1.07423472	1.01823	40	NIST05a.l	13998	21
2-Methyl-3-bromo-2-butanol				CAS #: 2588-77-4			
4.399	62127	0.53063190	0.50296	74	NIST05a.l	33655	21
O-CHLOROPHENOL-D4 SURR				CAS #: 0-00-0			
5.774	801743	6.84778014	6.49078	91	WILEY275.l	18902	21
Decane				CAS #: 124-18-5			
5.926	121738	1.03977510	0.98556	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester				CAS #: 17639-93-9			
6.538	1143167	9.76392948	9.25490	38	NIST05a.l	9448	21
MCHM Cyclohexanemethanol, 4-methyl-, trans-				CAS #: 3937-49-3			
6.730	95584	0.81639541	0.77383	83	WILEY275.l	19674	21
Cyclopentasiloxane, decamethyl-				CAS #: 541-02-6			
7.412	89394	0.49449662	0.46871	91	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy				CAS #: 77-73-6			
7.843	756467	4.18449992	3.96635	47	NIST05a.l	13652	48
2,6-Dichloro-4-fluorophenol SURR - not a match				CAS #: 392-71-2			
8.170	1112745	6.15530174	5.83440	43	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-				CAS #: 21031-46-9			
8.205	1077741	5.96167328	5.65087	50	NIST05a.l	3933	48

largest peak

Target compound.
Do not report.
ajs00193 03/01/2014

They report the TIC, no matter the quality - not good

Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc				CAS #: 63506-25-2			
9.079	82297	0.45523953	0.43150	72	WILEY275.1	109601	48
Sulfur monochloride				CAS #: 10025-67-9			
9.674	1521394	9.77779576	9.26805	38	NIST05a.1	14872	83
Benzene, (1-methyldecyl)-				CAS #: 4536-88-3			
12.209	66826	0.42928907	0.40690	93	NIST05a.1	80019	120

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

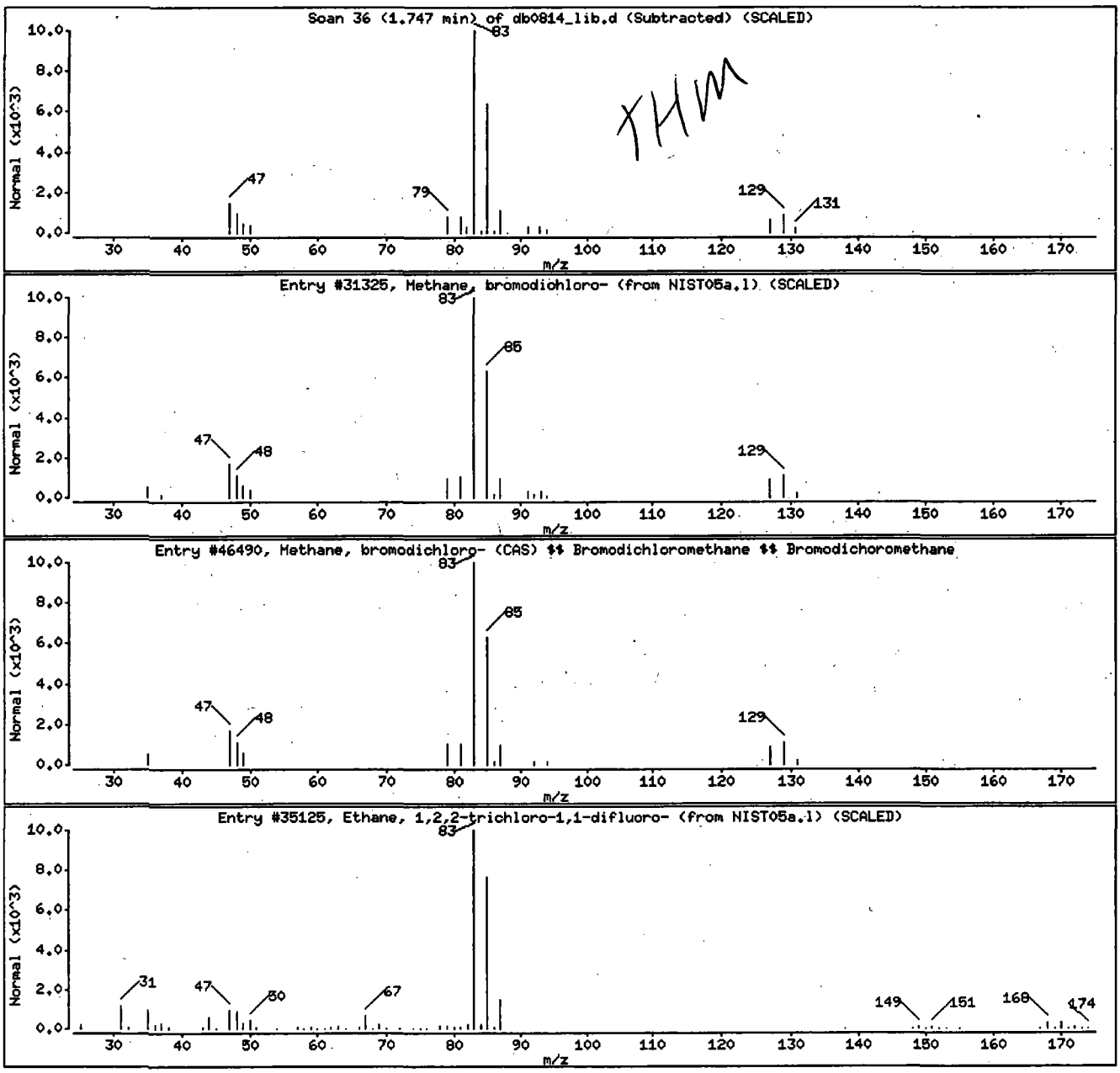
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

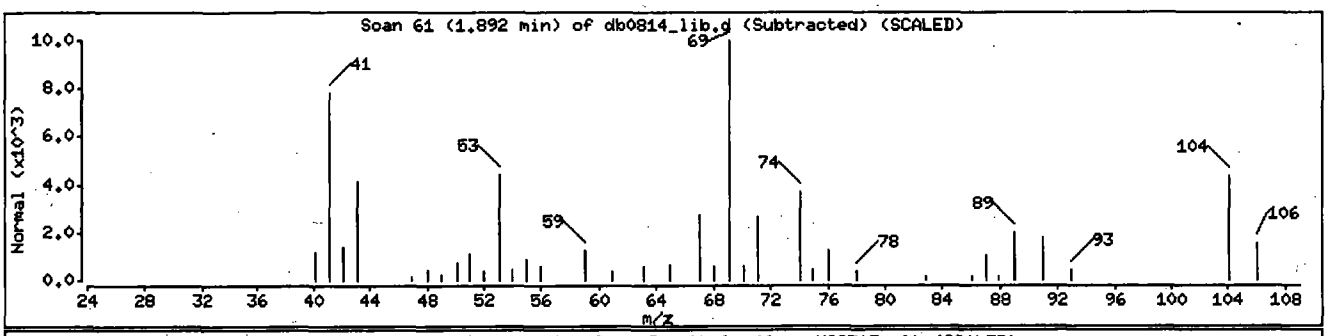
Volume Injected (uL): 1.0

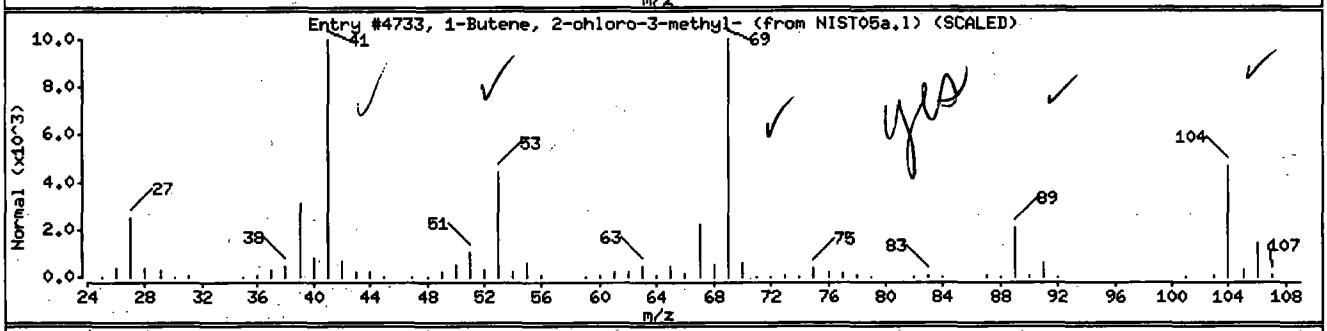
Operator: jmg00346

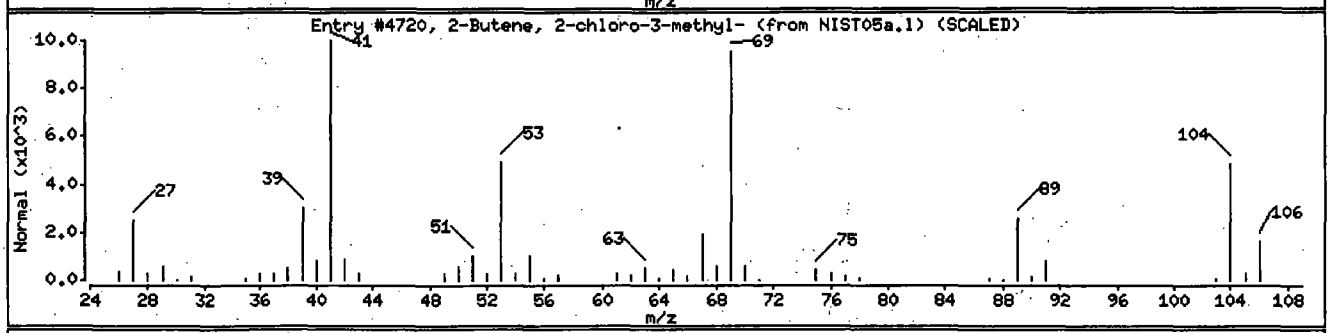
Column phase: J&W DB-5MS

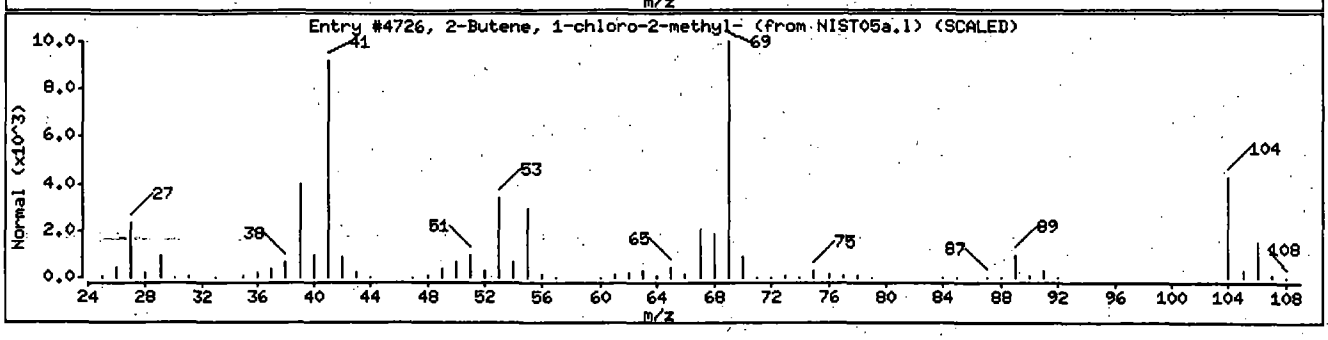
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	93	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	81	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4726	72	C5H9Cl	104









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

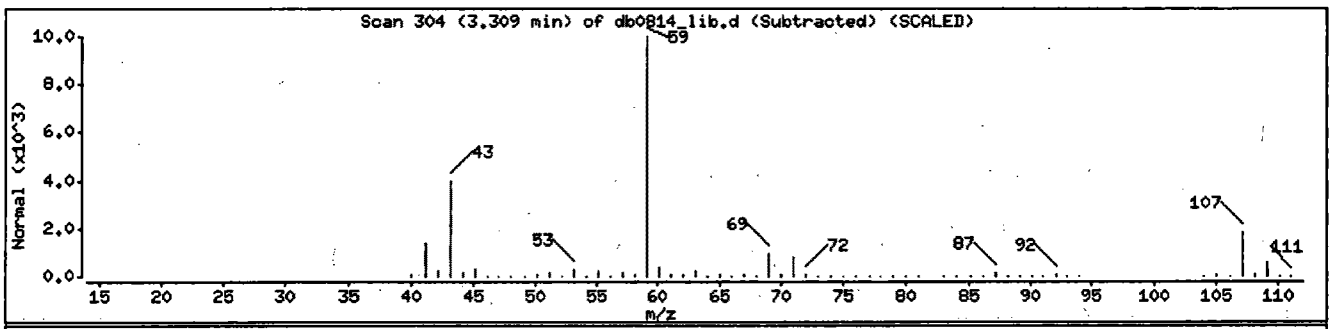
Client ID: SSKC1 Instrument: HP19760.i

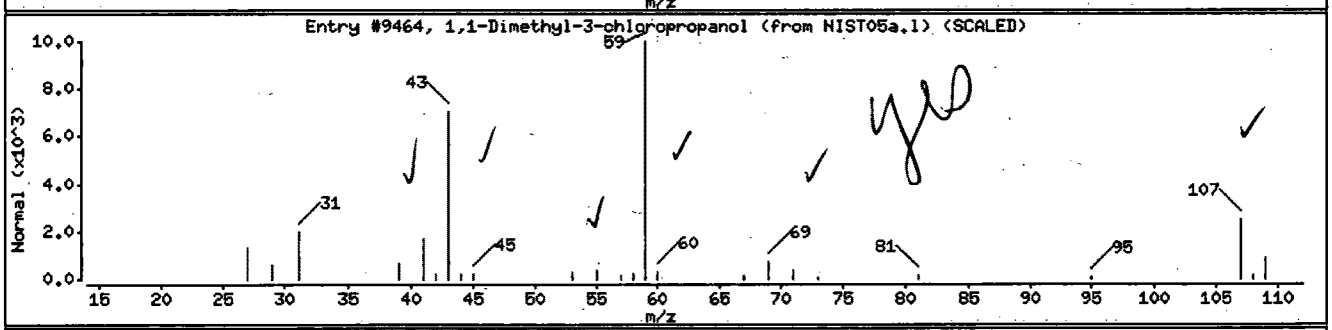
Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

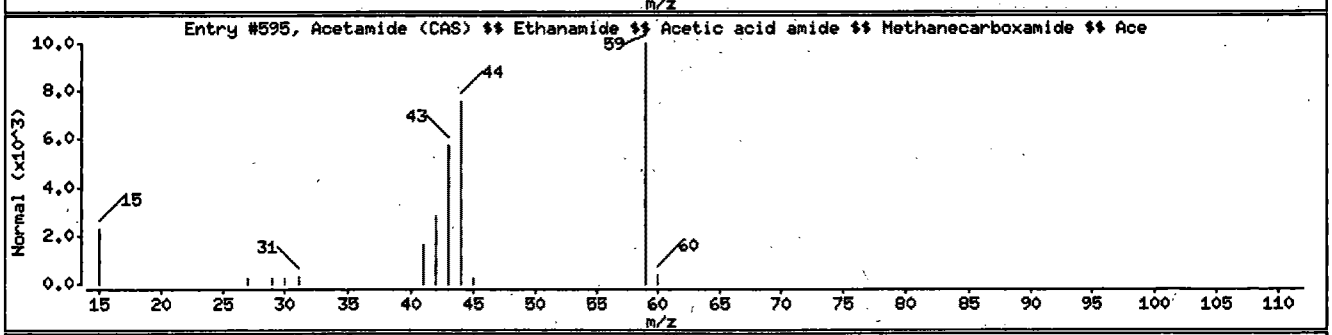
Volume Injected (uL): 1.0 Operator: jmg00346

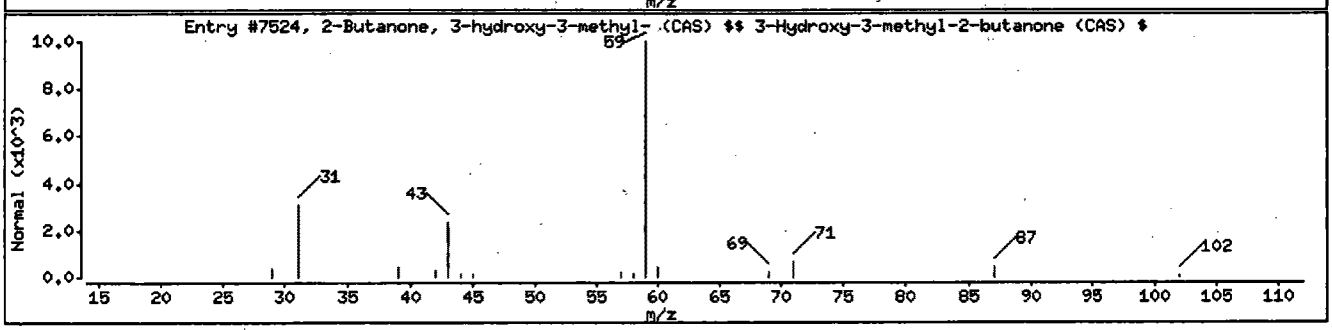
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

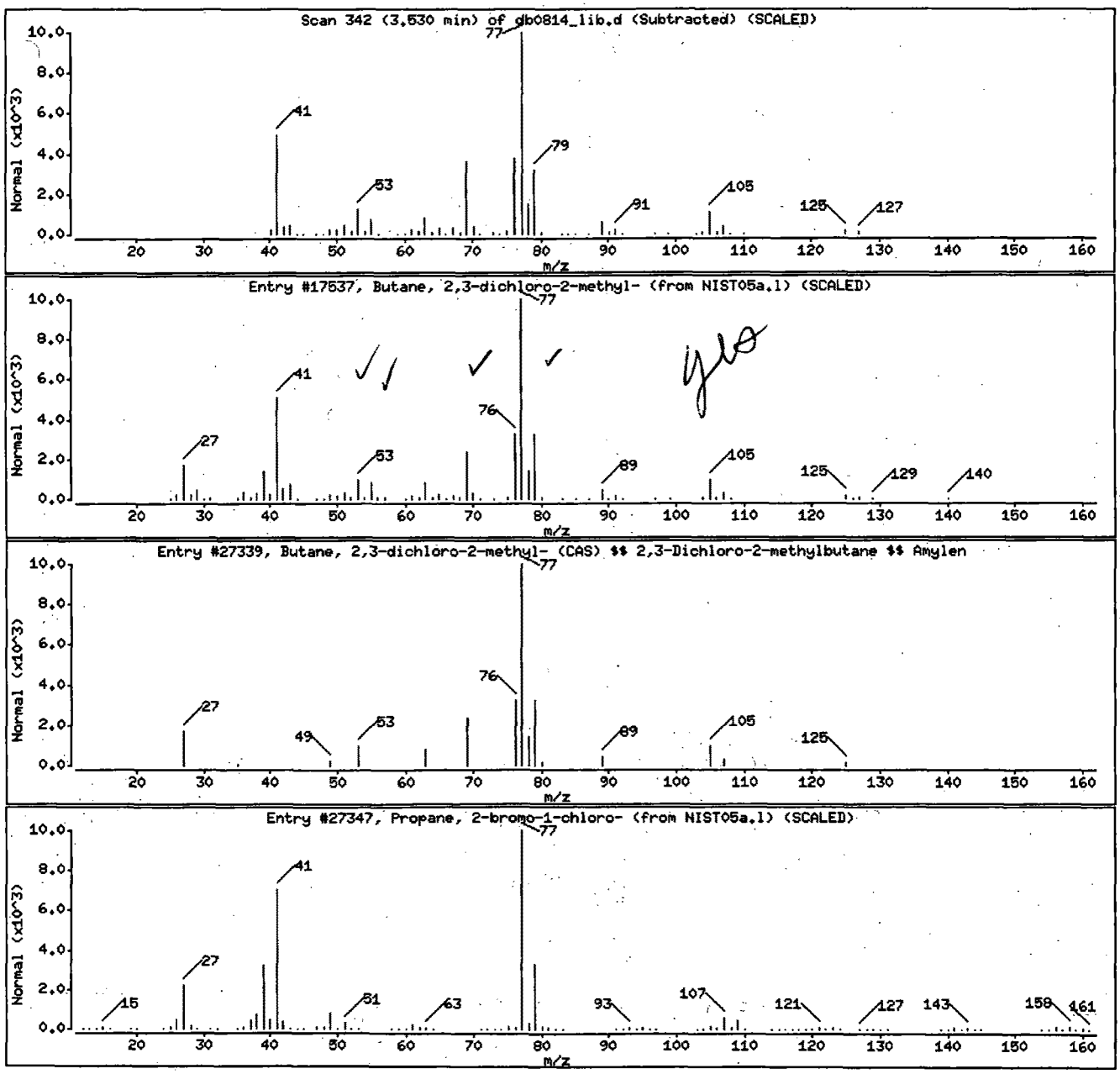
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	90	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	38	C3H6BrCl	156



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

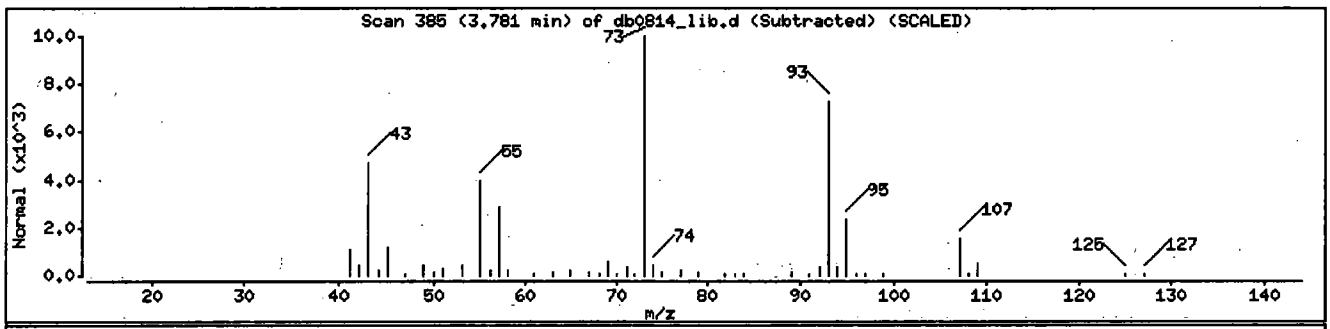
Volume Injected (uL): 1.0

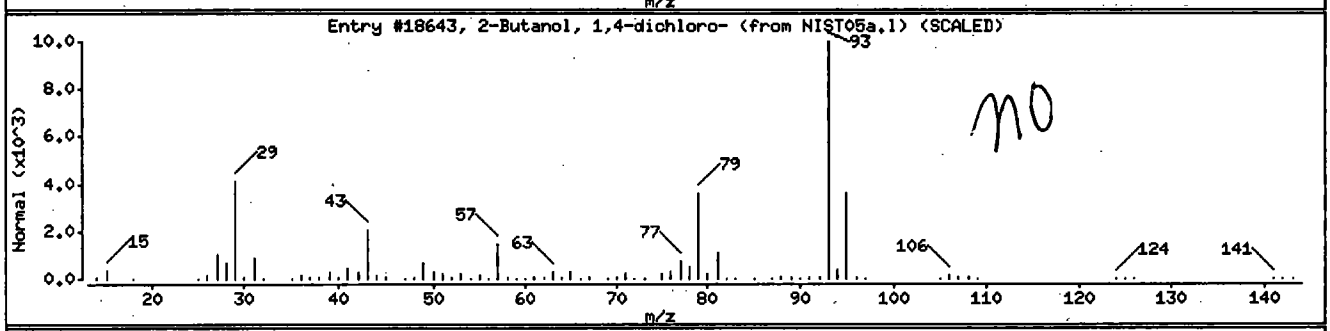
Operator: jmg00346

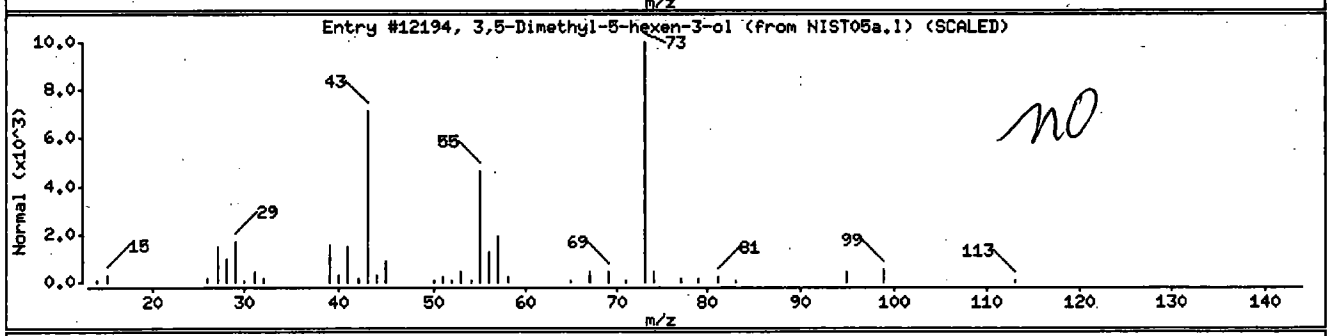
Column phase: J&W DB-5MS

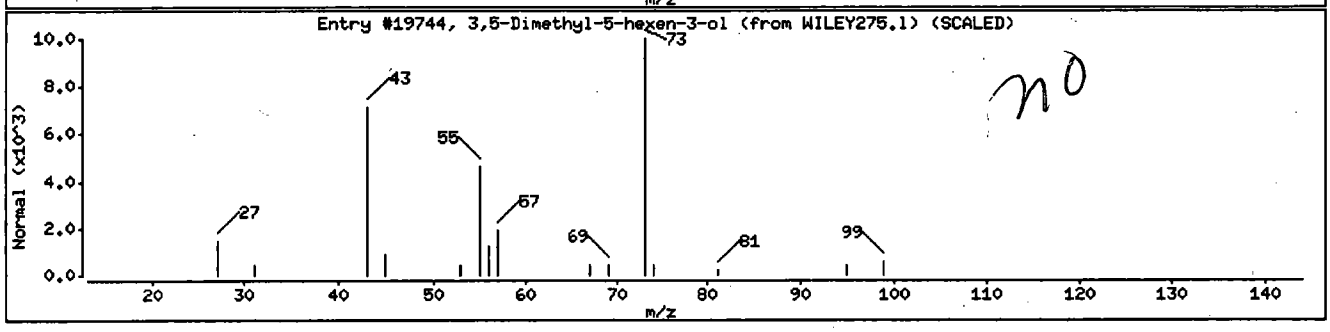
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	NO 32	C4H8Cl2O	142
3,5-Dimethyl-5-hexen-3-ol	1569-46-6	NIST05a.l	12194	12	C8H16O	128
3,5-Dimethyl-5-hexen-3-ol	0-00-0	WILEY275.l	19744	12	C8H16O	128









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

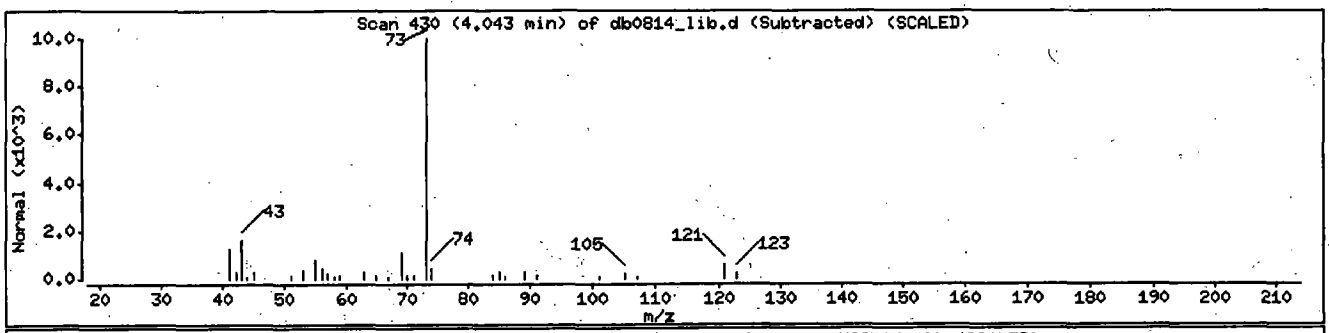
Client ID: SSKC1 Instrument: HP19760.i

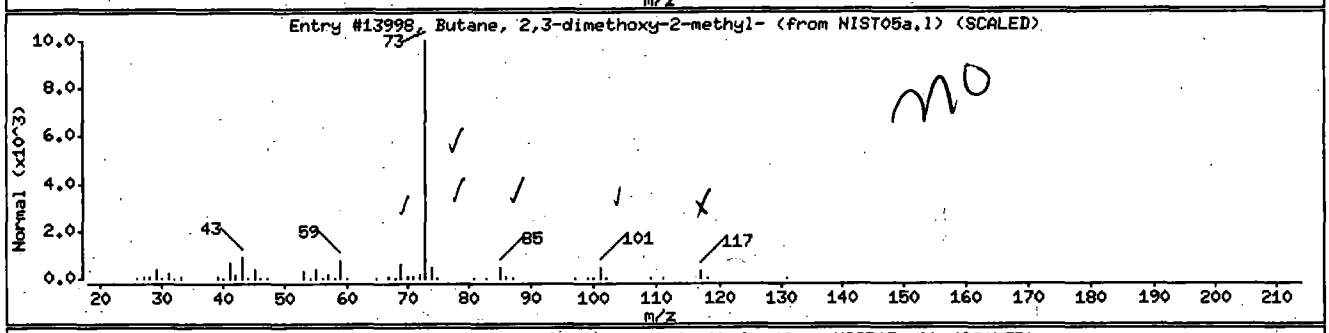
Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

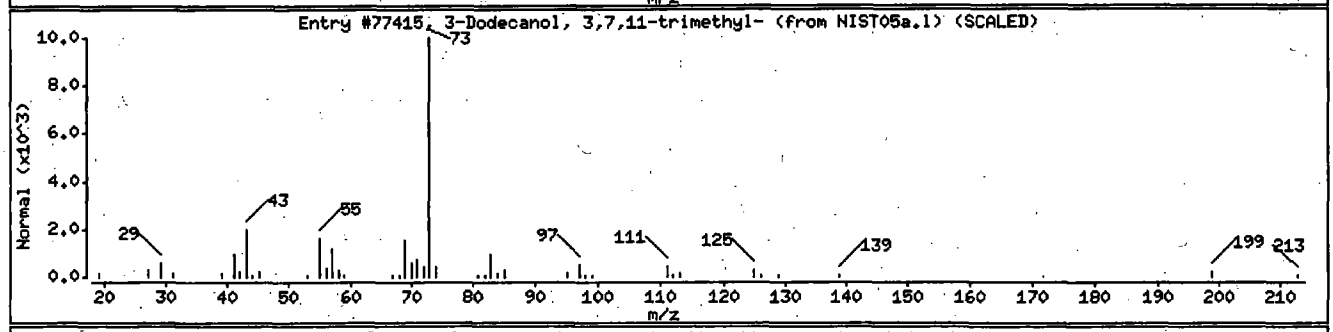
Volume Injected (uL): 1.0 Operator: jmg00346

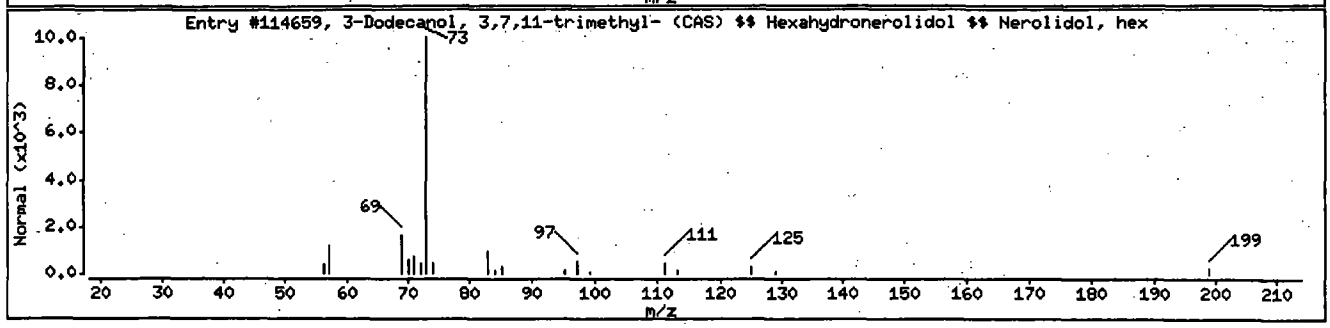
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	LOW 40	C7H16O2	132
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	38	C15H32O	228
3-Dodecanol, 3,7,11-trimethyl- (CAS) $$	7278-65-1	WILEY275.l	114659	38	C15H32O	228









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

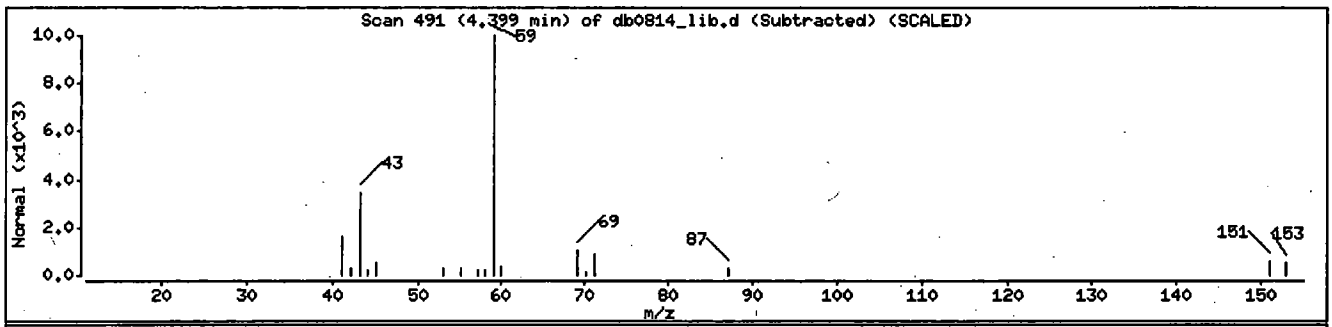
Client ID: SSKC1 Instrument: HP19760.i

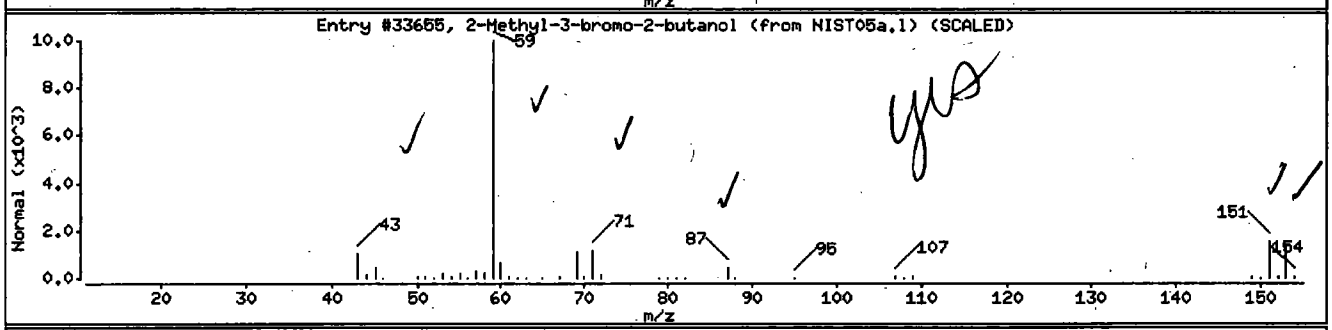
Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

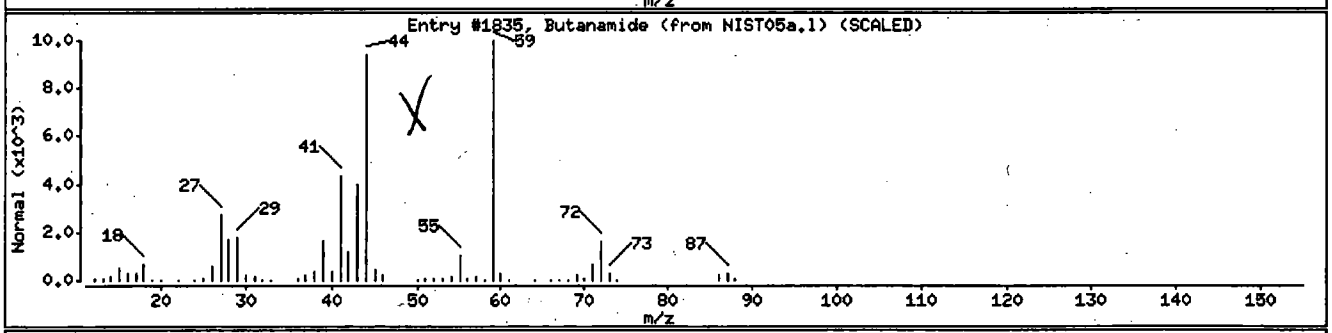
Volume Injected (uL): 1.0 Operator: jmg00346

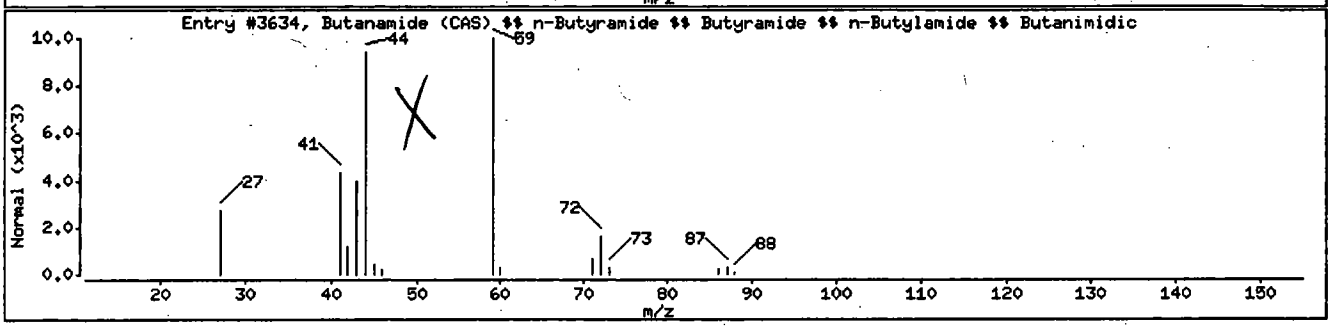
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	74	C5H11BrO	166
Butanamide	541-35-5	NIST05a.l	1835	64	C4H9NO	87
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3634	64	C4H9NO	87









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

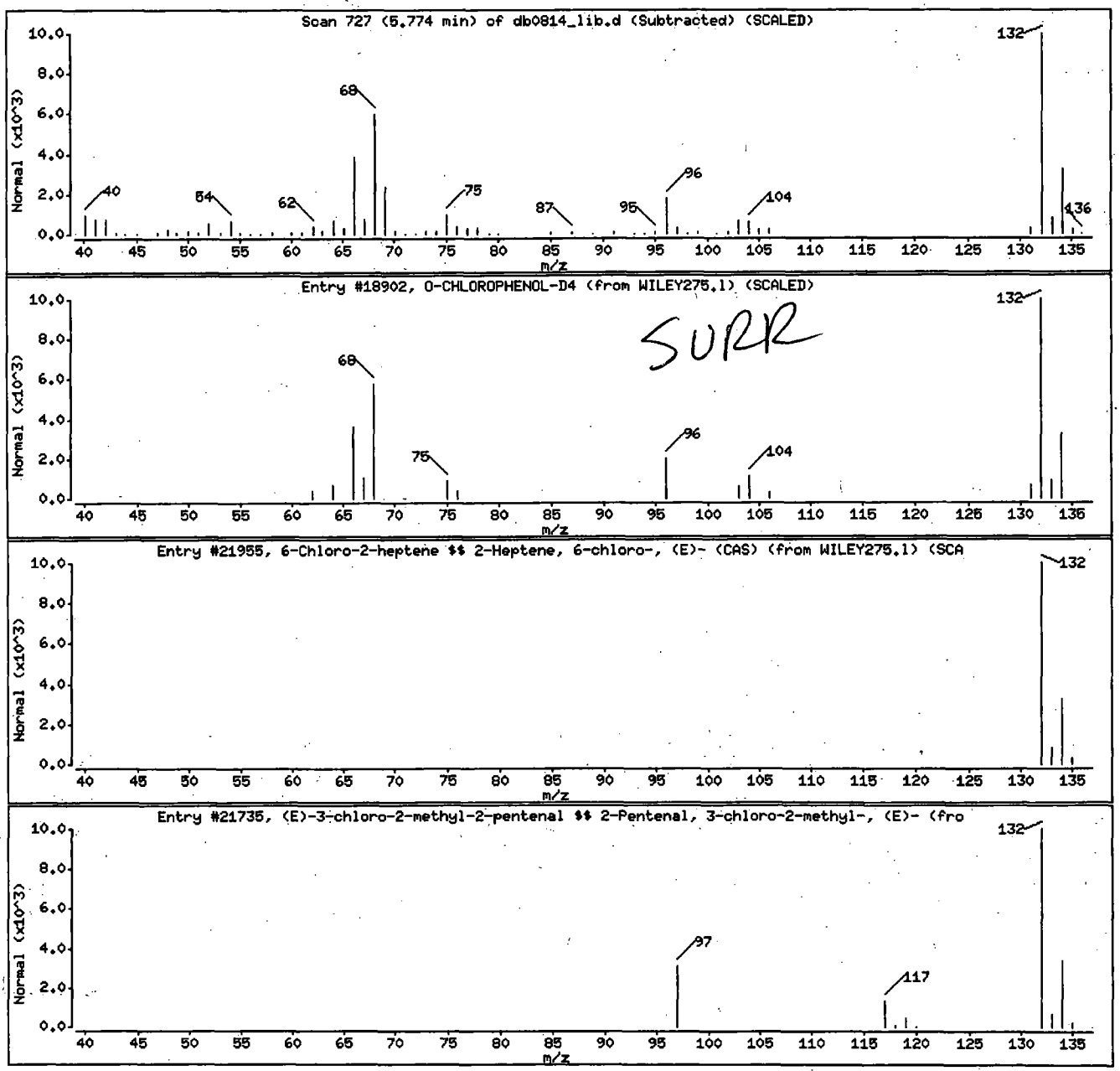
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

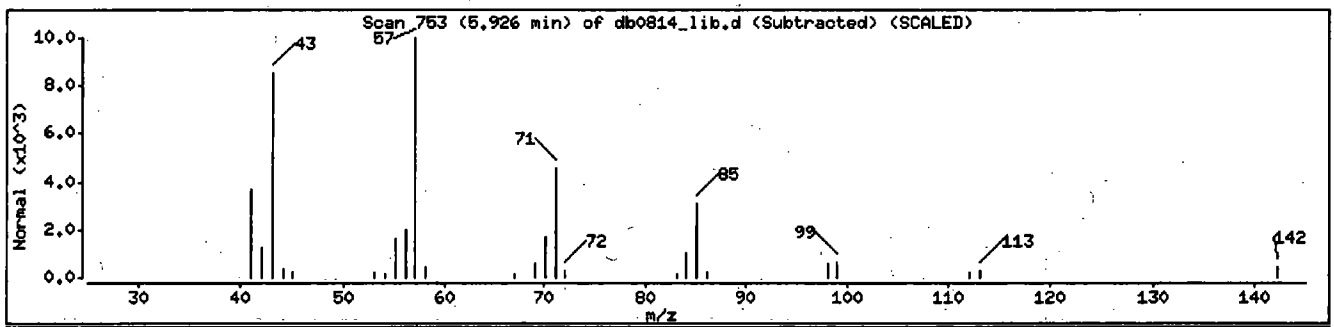
Volume Injected (uL): 1.0

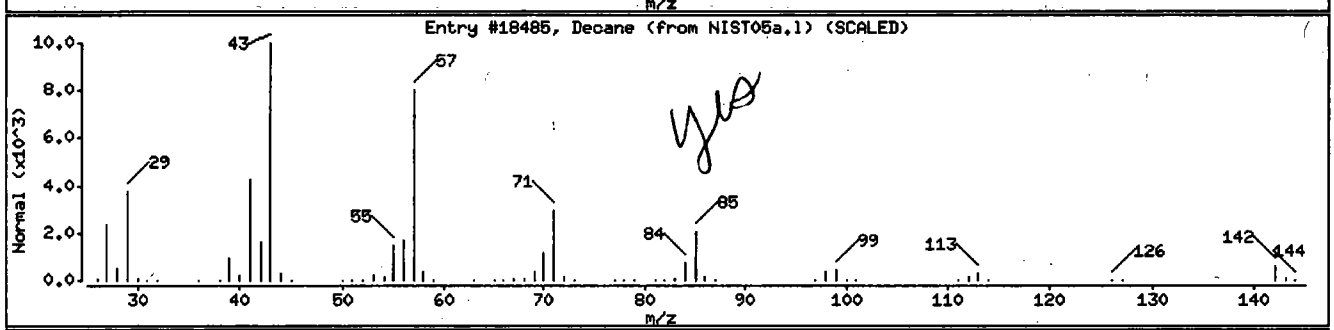
Operator: jmg00346

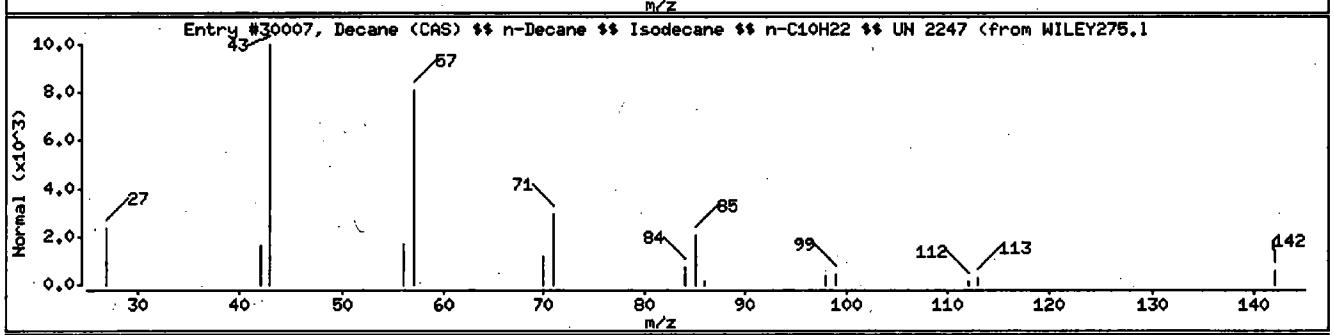
Column phase: J&W DB-5MS

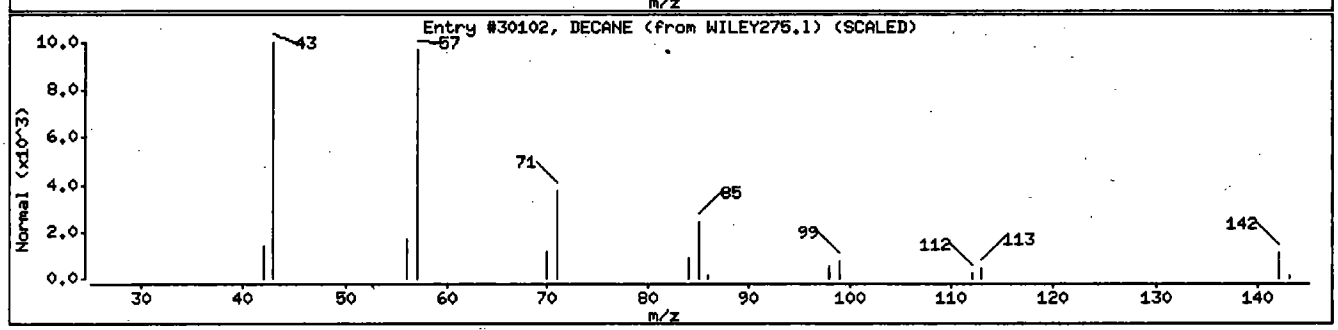
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	96	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	90	C10H22	142









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

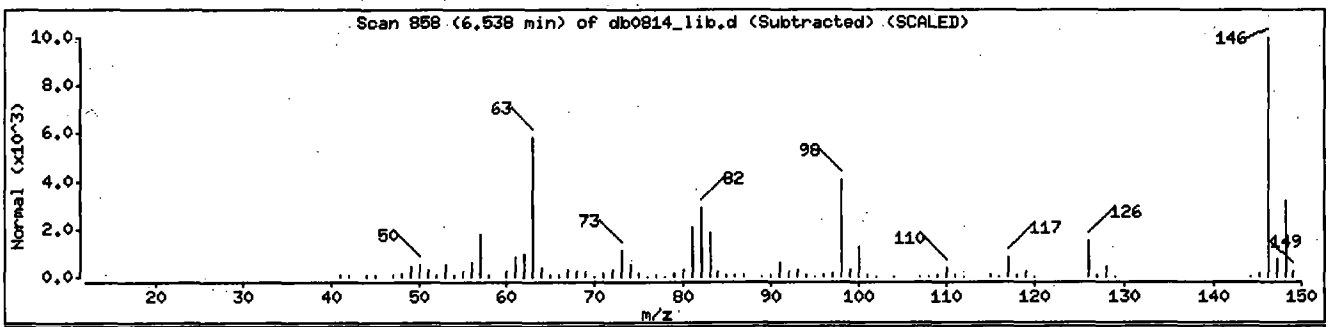
Volume Injected (uL): 1.0

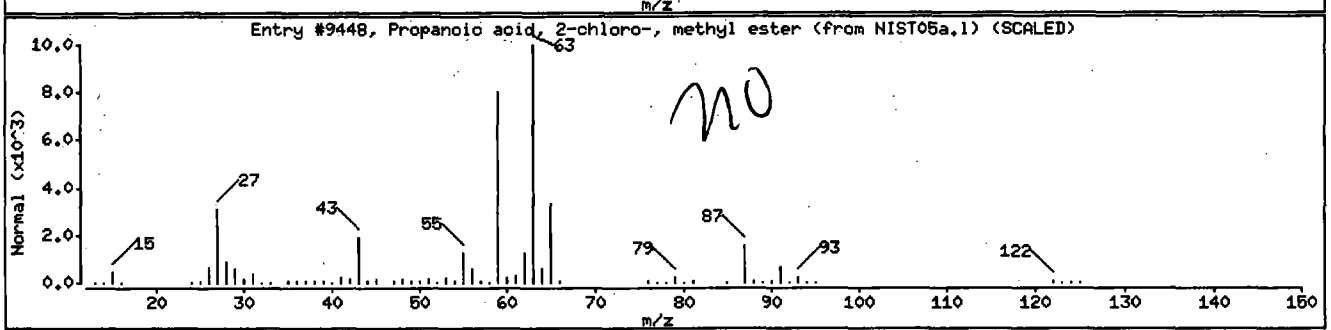
Operator: jmg00346

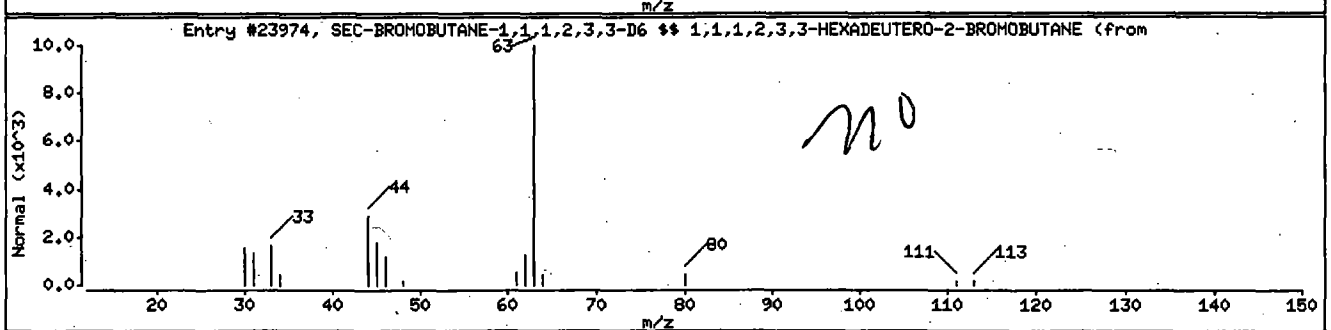
Column phase: J&W DB-5MS

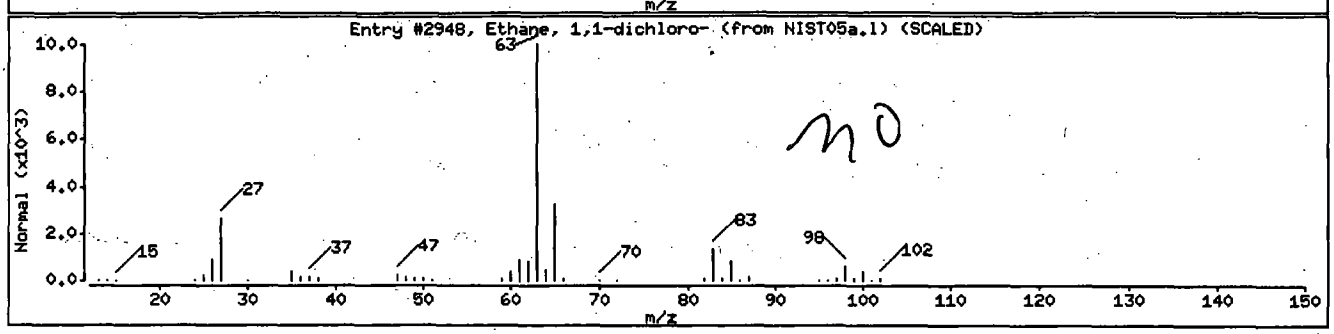
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	23	C2H4Cl2	98



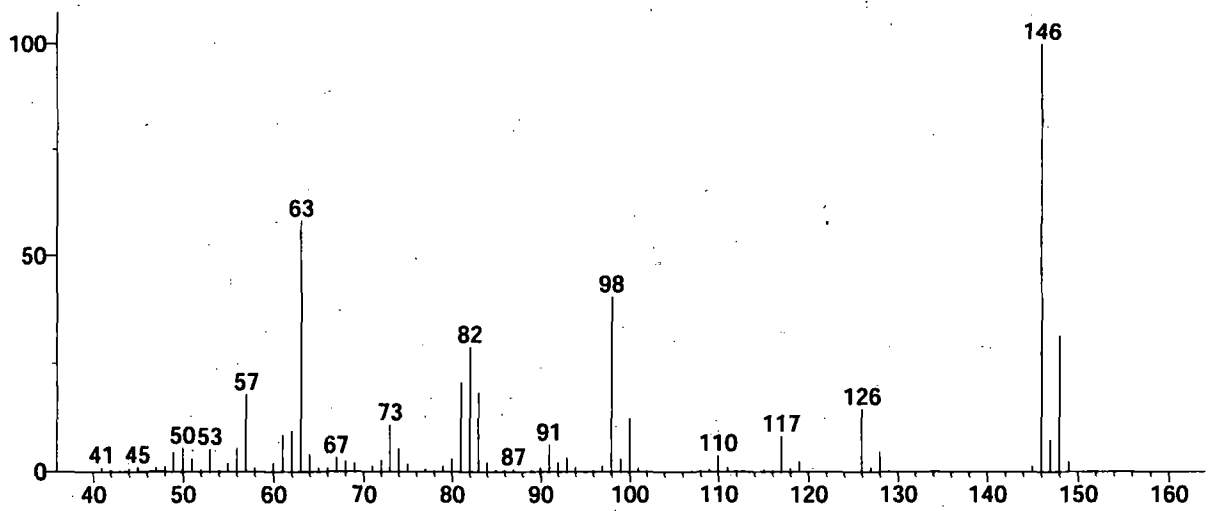






Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Unknown; InLib=484



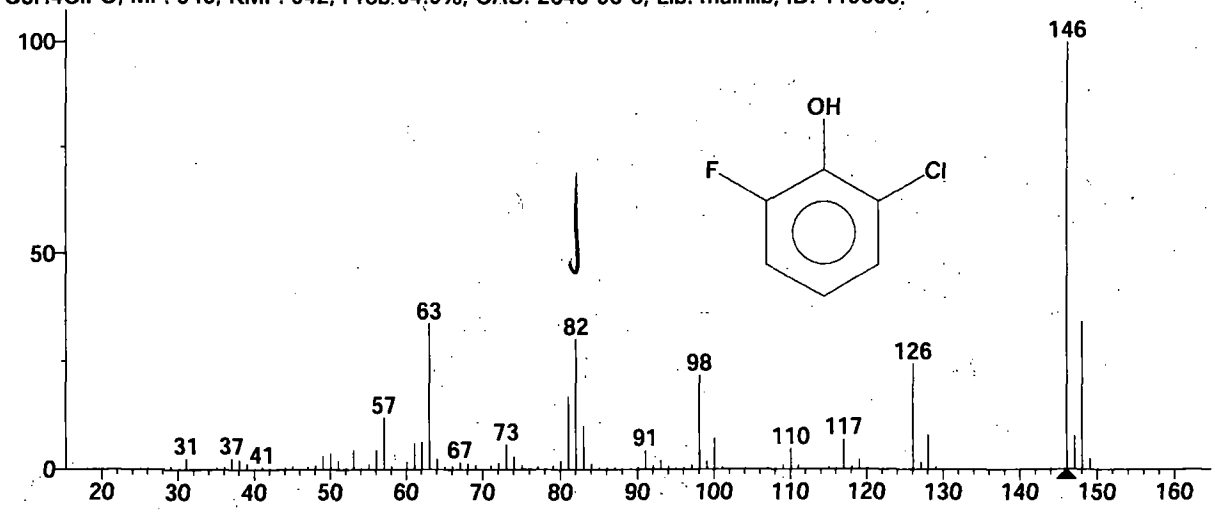
(Text File) Scan 858 (6.538 min): DB0814.D\data.ms

Name: Scan 858 (6.538 min): DB0814.D\data.ms
MW: N/A ID#: 23 DB: Text File
Comment: SSKC1;7365697;1;0;SAMPLE;;;
10 largest peaks:
146 999 | 63 580 | 98 403 | 148 314 | 82 287 | 81 206 | 83 181 | 57 177 | 126 144 | 100 123 |
Synonyms:
no synonyms.

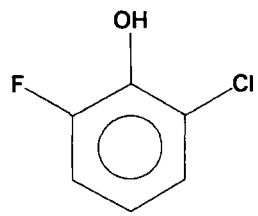
Ex. 5 - Deliberative

Ex. 5 - Deliberative

Hit 1 : 2-Chloro-6-fluorophenol
C6H4ClFO; MF: 940; RMF: 942; Prob.94.9%; CAS: 2040-90-6; Lib: mainlib; ID: 119096.



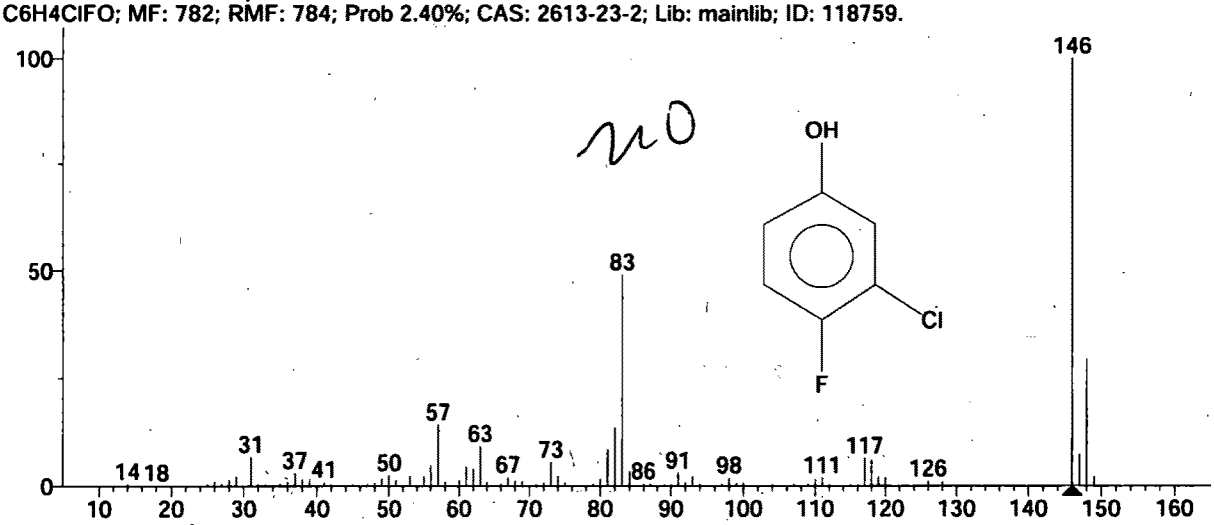
(mainlib) 2-Chloro-6-fluorophenol



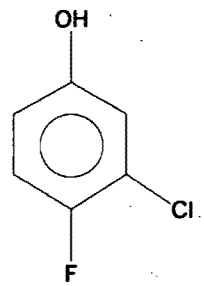
Name: 2-Chloro-6-fluorophenol
Formula: C_6H_4ClFO
MW: 146 Exact Mass: 145.99347 CAS#: 2040-90-6 NIST#: 352540 ID#: 119096 DB: mainlib
Other DBs: None
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
146 999 | 148 342 | 63 338 | 82 302 | 126 244 | 98 217 | 81 169 | 57 120 | 83 101 | 128 80 |
Synonyms:
no synonyms.

Freedom_0006097_0051

Hit 2 : 3-Chloro-4-fluorophenol
C6H4ClFO; MF: 782; RMF: 784; Prob 2.40%; CAS: 2613-23-2; Lib: mainlib; ID: 118759.

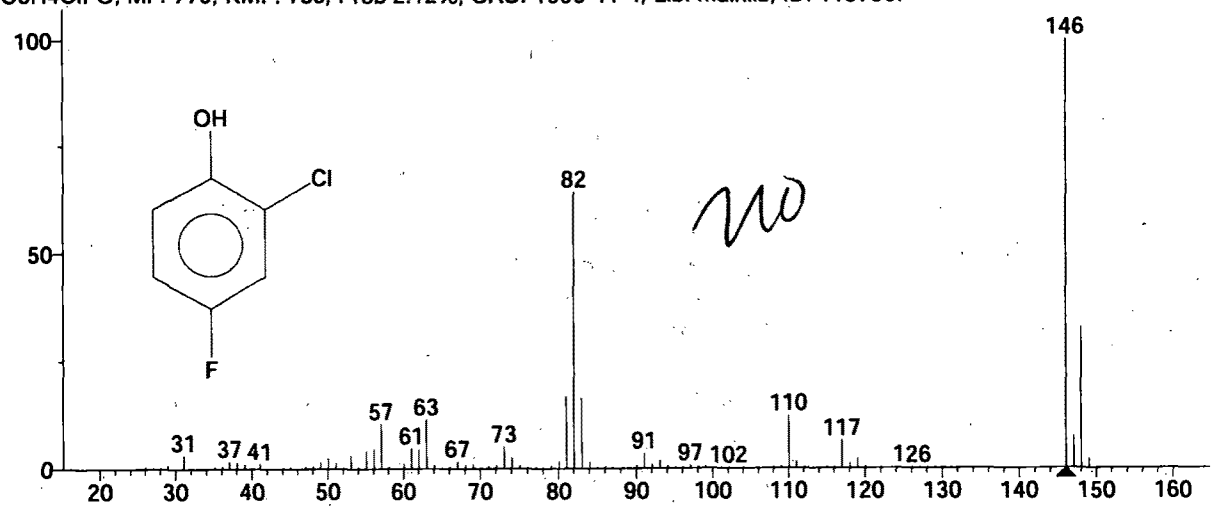


(mainlib) 3-Chloro-4-fluorophenol

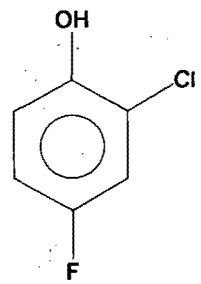


Name: 3-Chloro-4-fluorophenol
Formula: C_6H_4ClFO
MW: 146 Exact Mass: 145.99347 CAS#: 2613-23-2 NIST#: 343611 ID#: 118759 DB: mainlib
Other DBs: Fine, EINECS
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
146 999 | 83 489 | 148 293 | 57 141 | 82 134 | 63 91 | 81 85 | 147 74 | 31 67 | 117 64 |
Synonyms:
1.Phenol, 3-chloro-4-fluoro-

Hit 3 : 2-Chloro-4-fluorophenol
C6H4ClFO; MF: 779; RMF: 780; Prob 2.12%; CAS: 1996-41-4; Lib: mainlib; ID: 118756.



(mainlib) 2-Chloro-4-fluorophenol



Name: 2-Chloro-4-fluorophenol
Formula: C_6H_4ClFO
MW: 146 Exact Mass: 145.99347 CAS#: 1996-41-4 NIST#: 373451 ID#: 118756 DB: mainlib
Other DBs: Fine, NIH, EINECS, IRDB
Contributor: NIST Mass Spectrometry Data Center, 2009
10 largest peaks:
146 999 | 82 641 | 148 326 | 81 166 | 83 163 | 110 121 | 63 112 | 57 103 | 147 73 | 117 64 |
Synonyms:
1.Phenol, 2-chloro-4-fluoro-

Freedom_0006097_0053

Target compound, do not report. AJS00193 03/01/2014

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

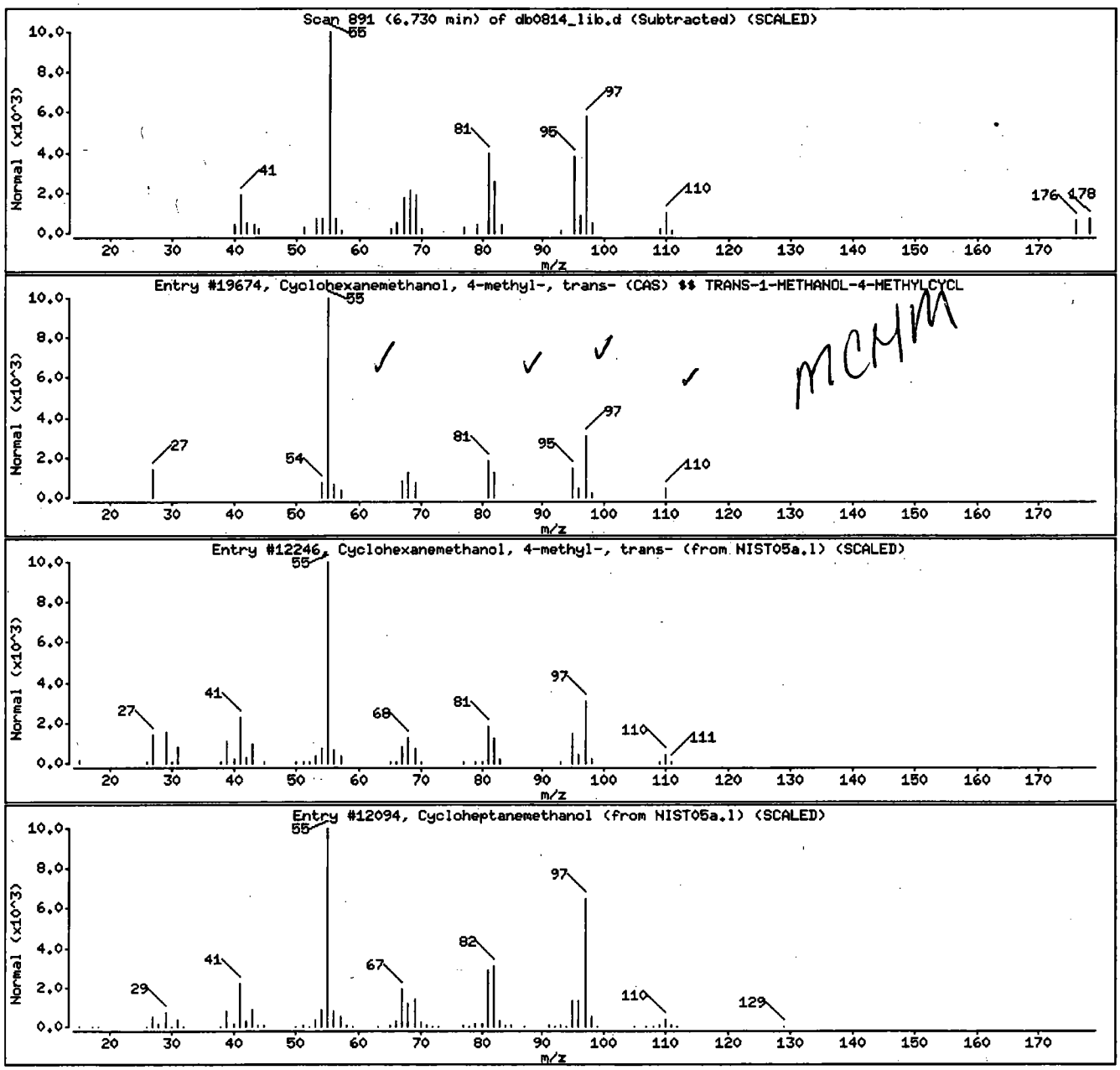
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	83	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	64	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12094	47	C8H16O	128



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

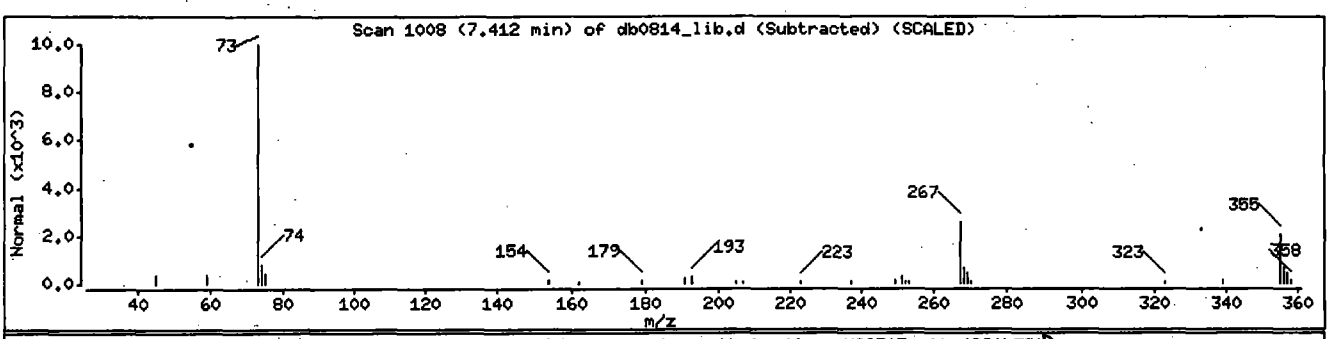
Volume Injected (uL): 1.0

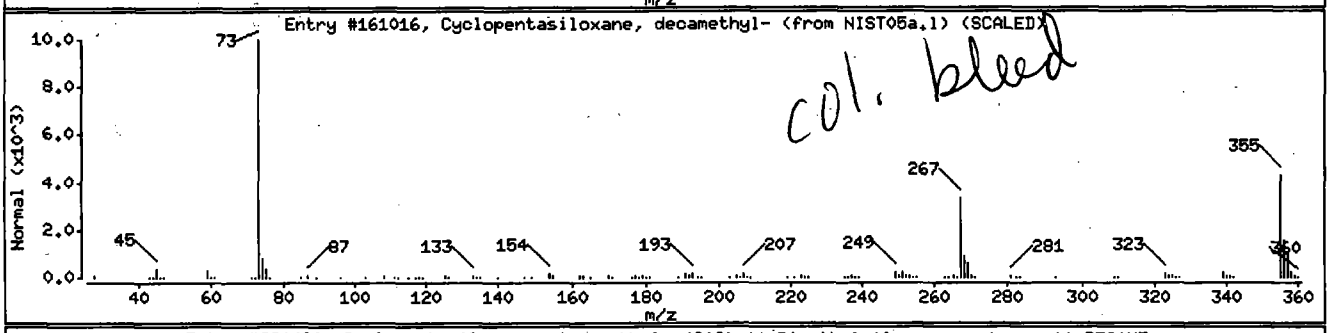
Operator: jmg00346

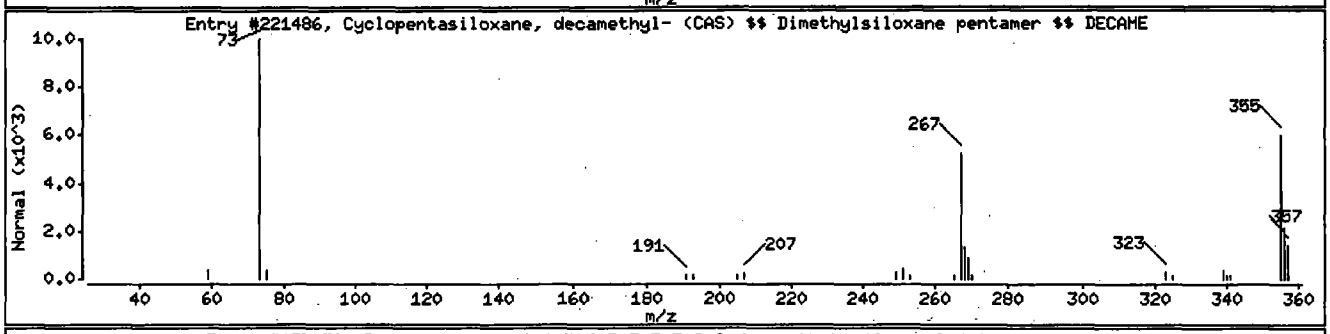
Column phase: J&W DB-5MS

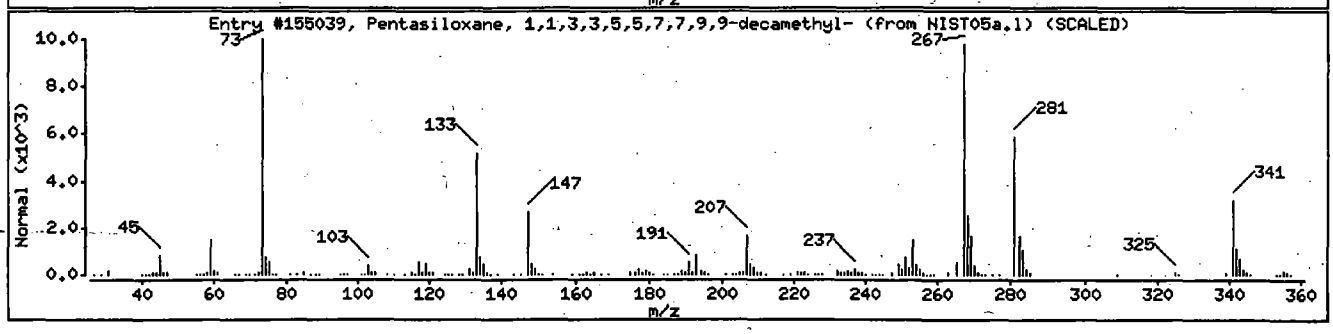
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	91	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decam	995-83-5	NIST05a.l	155039	38	C10H32O4Si5	356









Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

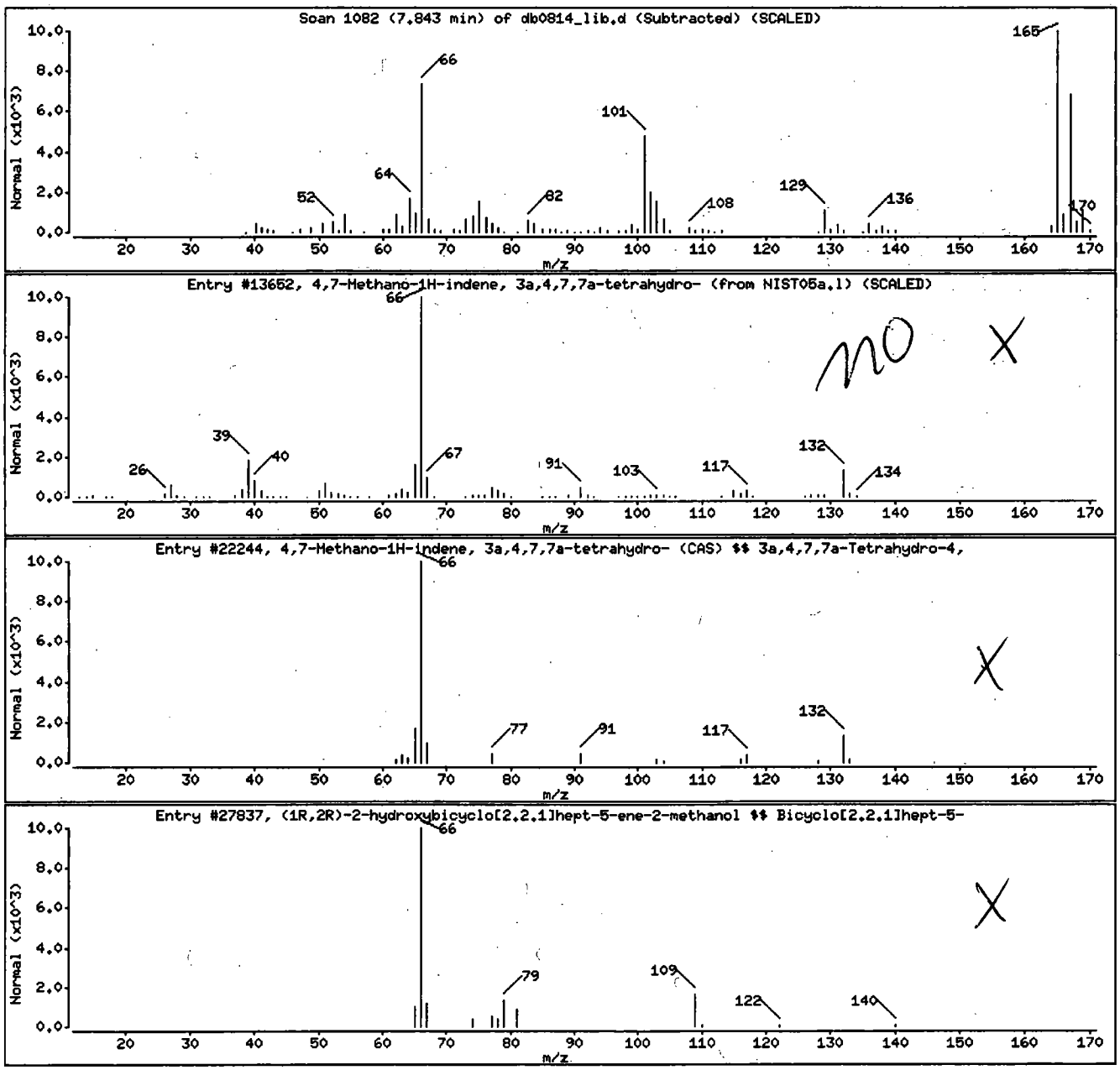
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

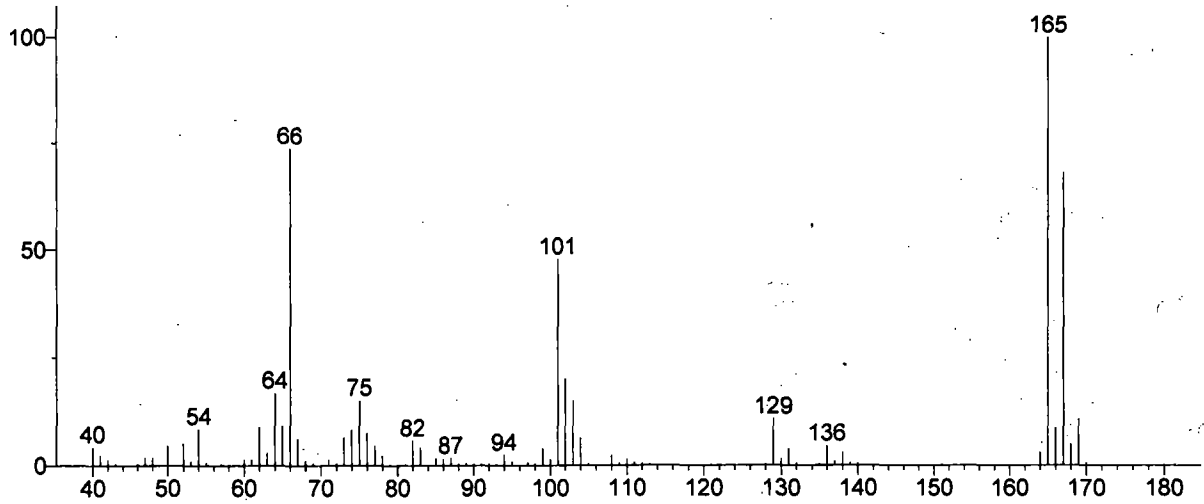
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	47	C10H12	132
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22244	47	C10H12	132
(1R,2R)-2-hydroxybicyclo[2.2.1]hept-5-en	116697-44-0	WILEY275.l	27837	47	C8H12O2	140



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

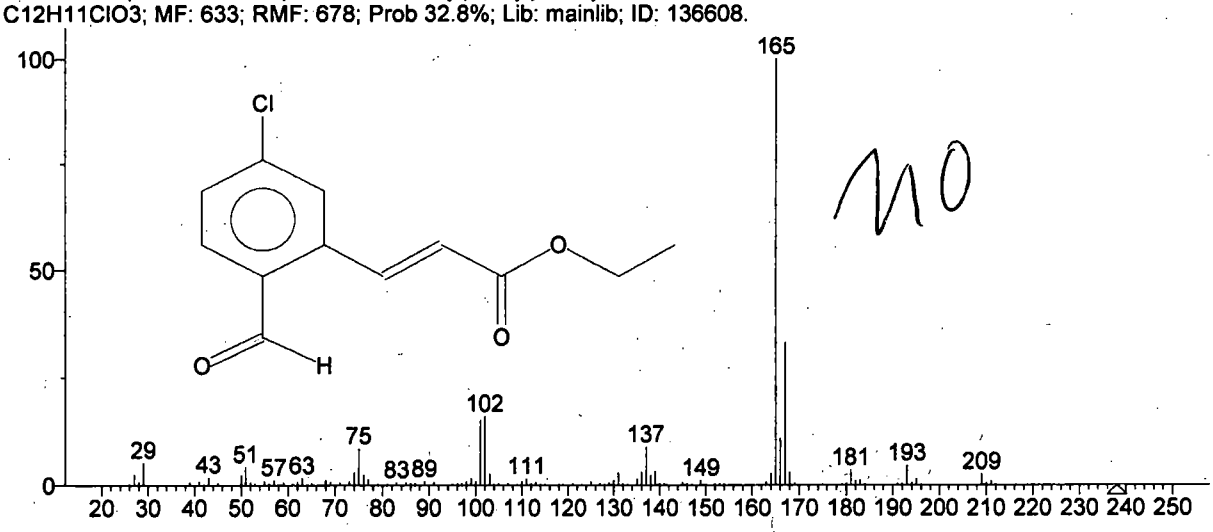
Unknown; InLib=-1163



(Text File) Scan 1082 (7.843 min): DB0814.D\data.ms

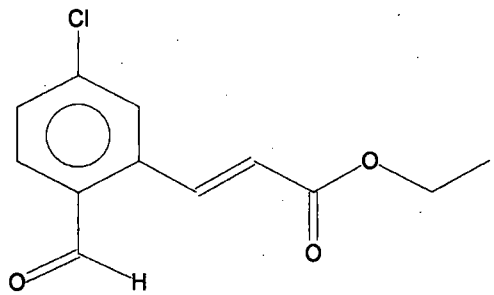
Name: Scan 1082 (7.843 min): DB0814.D\data.ms
MW: N/A ID#: 24 DB: Text File
Comment: SSKC1;7365697;1;0;SAMPLE;;;
10 largest peaks:
165 999 | 66 737 | 167 681 | 101 476 | 102 200 | 64 167 | 75 150 | 103 150 | 129 108 | 169 108 |
Synonyms:
no synonyms.

Hit 1 : 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester
C12H11ClO3; MF: 633; RMF: 678; Prob 32.8%; Lib: mainlib; ID: 136608.



110

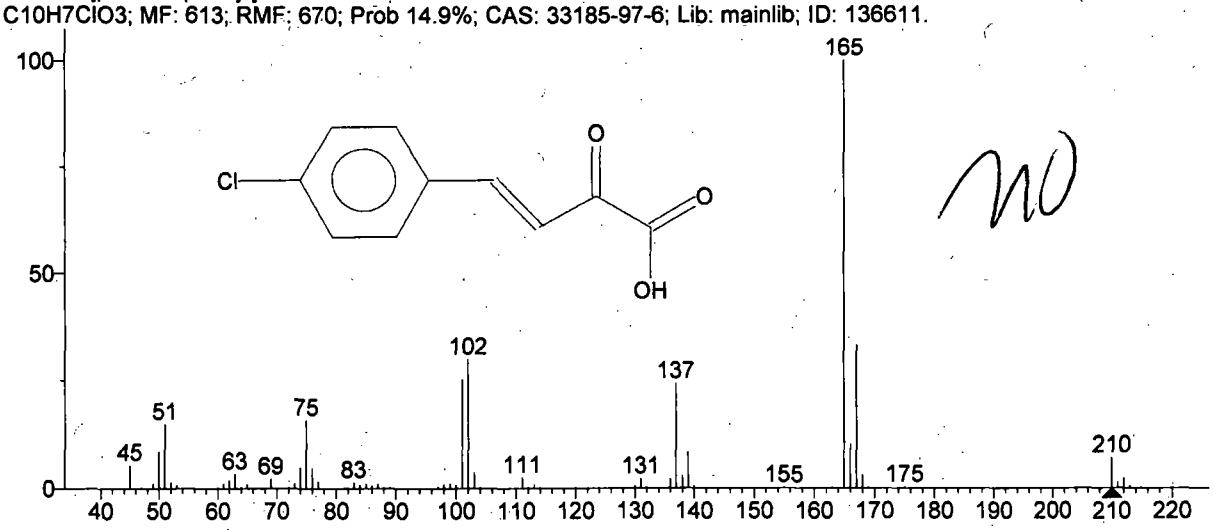
(mainlib) 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester



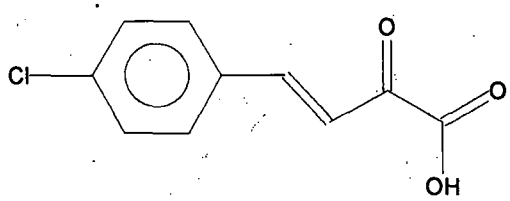
Name: 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester
Formula: $C_{12}H_{11}ClO_3$
MW: 238 Exact Mass: 238.039672 NIST#: 196814 ID#: 136608 DB: mainlib
Contributor: Chemical Concepts
10 largest peaks:
165 999 | 167 330 | 102 159 | 101 150 | 166 108 | 137 88 | 75 85 | 29 52 | 193 45 | 51 42 |
Synonyms:
1.Ethyl (2E)-3-(5-chloro-2-formylphenyl)-2-propenoate #

Freedom_0006097_0058

Hit 2 : 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid
C10H7ClO3; MF: 613; RMF: 670; Prob 14.9%; CAS: 33185-97-6; Lib: mainlib; ID: 136611.



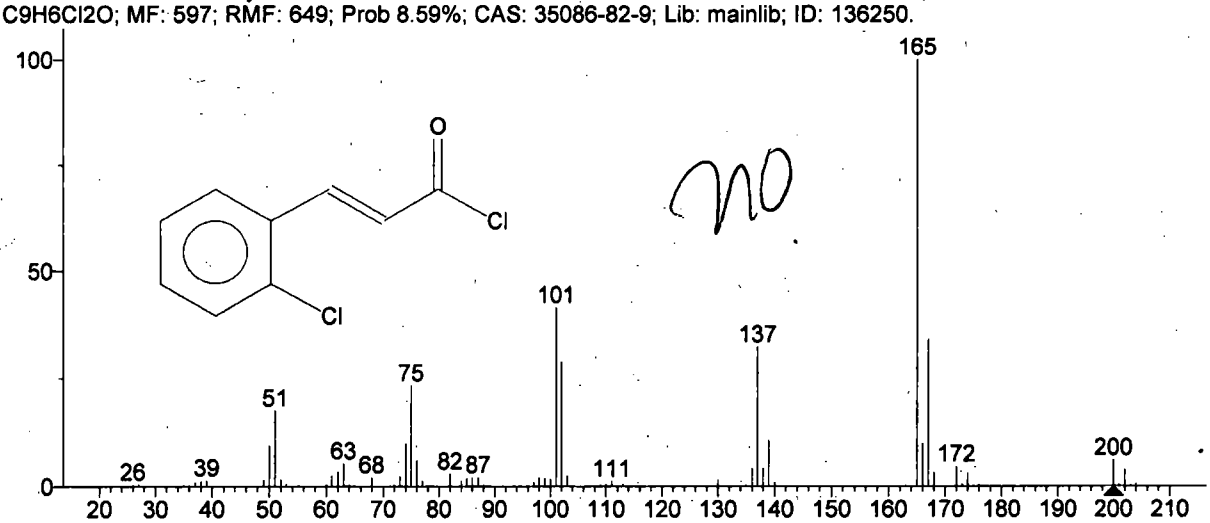
(mainlib) 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid



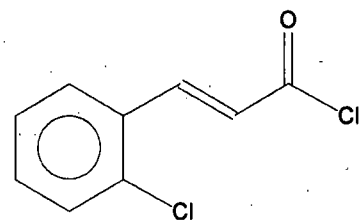
Name: 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid
Formula: $C_{10}H_7ClO_3$
MW: 210 Exact Mass: 210.008371 CAS#: 33185-97-6 NIST#: 255898 ID#: 136611 DB: mainlib
Other DBs: None
Contributor: Div. of Experiment Therapeutics WRAIR, WRAMC, Washington DC 20307
10 largest peaks:
165 999 | 167 332 | 102 298 | 101 252 | 137 241 | 75 158 | 51 148 | 166 101 | 50 85 | 139 82 |
Synonyms:
1.(3E)-4-(4-Chlorophenyl)-2-oxo-3-butenoic acid #

Freedom_0006097_0059

Hit 3 : 2-Chlorocinnamoyl chloride
C9H6Cl2O; MF: 597; RMF: 649; Prob 8.59%; CAS: 35086-82-9; Lib: mainlib; ID: 136250.



(mainlib) 2-Chlorocinnamoyl chloride



Name: 2-Chlorocinnamoyl chloride
Formula: $C_9H_6Cl_2O$
MW: 200 Exact Mass: 199.97957 CAS#: 35086-82-9 NIST#: 341179 ID#: 136250 DB: mainlib
Other DBs: None
Contributor: NIST Mass Spectrometry Data Center
10 largest peaks:
165 999 | 101 414 | 167 340 | 137 322 | 102 288 | 75 232 | 51 174 | 139 106 | 74 98 | 166 98 |
Synonyms:
no synonyms.

Freedom_0006097_0060

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

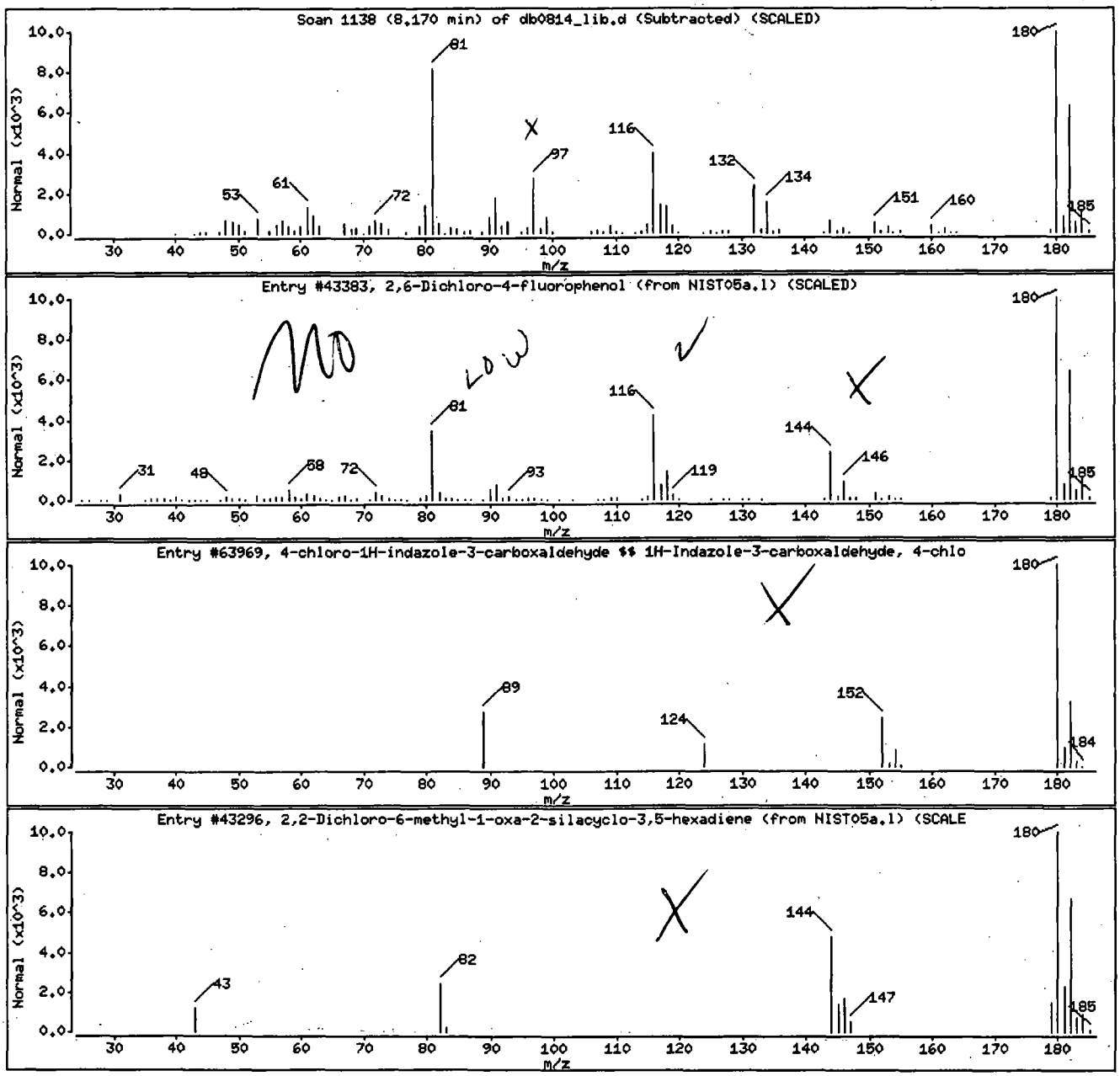
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	43	C6H3Cl2FO	180
4-chloro-1H-indazole-3-carboxaldehyde $$	102735-85-3	WILEY275.l	63969	25	C8H5ClN2O	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	22	C5H6Cl2OSi	180



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

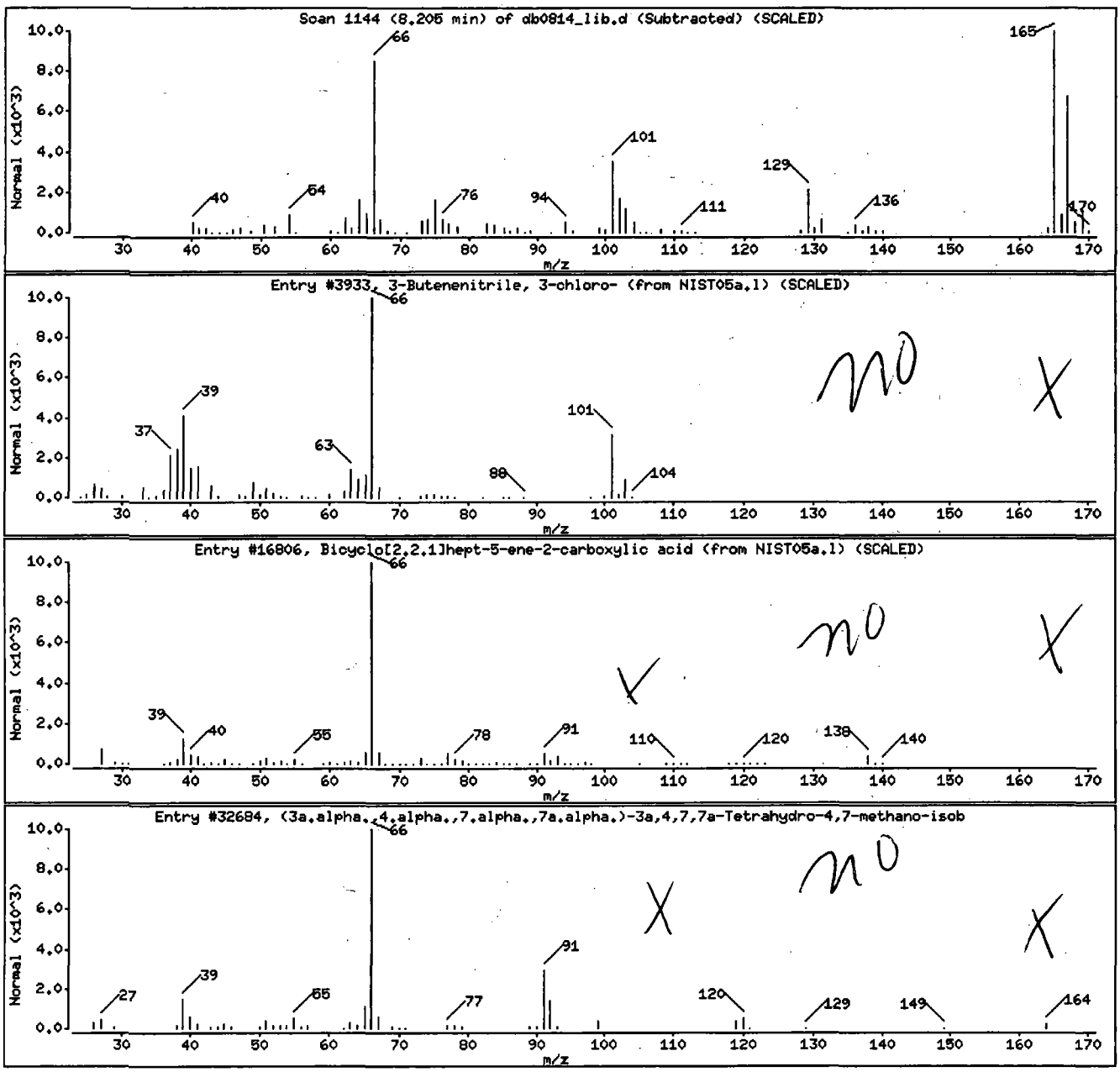
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

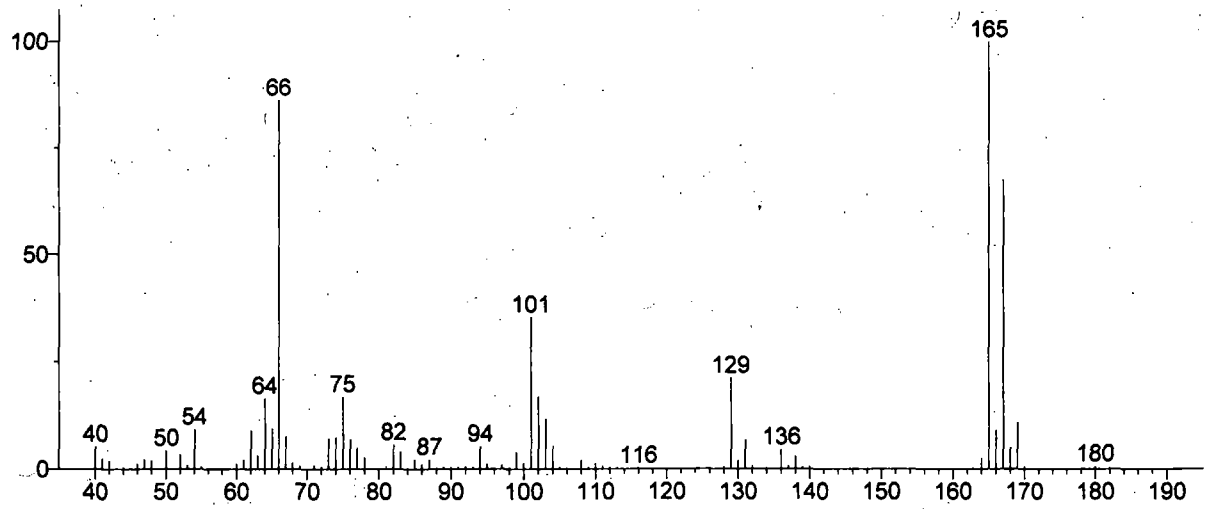
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138
(3a.alpha.,4.alpha.,7.alpha.,7a.alpha.)-	129-64-6	NIST05a.l	32684	47	C9H8O3	164



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

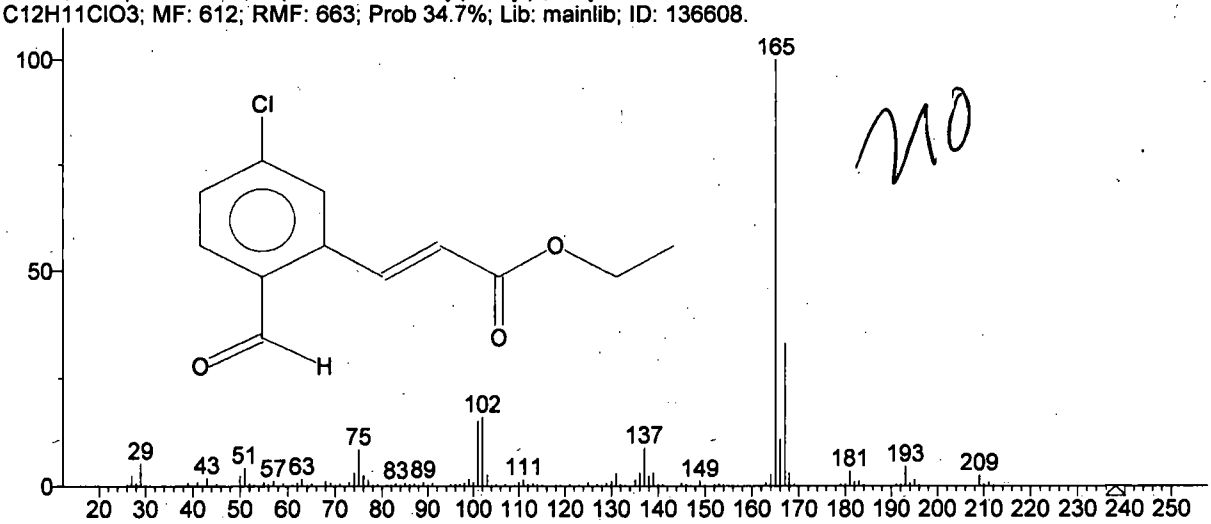
Unknown; InLib=-1187



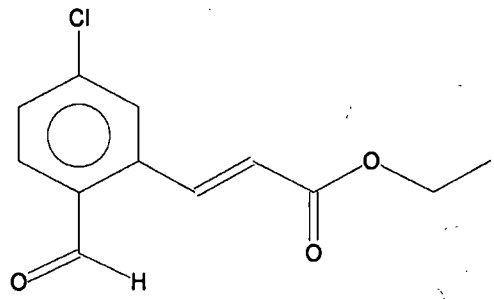
(Text File) Scan 1144 (8.205 min): DB0814.D\data.ms

Name: Scan 1144 (8.205 min): DB0814.D\data.ms
MW: N/A ID#: 26 DB: Text File
Comment: SSKC1;7365697;1;0;SAMPLE;;;
10 largest peaks:
165 999 | 66 860 | 167 673 | 101 351 | 129 210 | 75 167 | 102 167 | 64 163 | 103 116 | 169 108 |
Synonyms:
no synonyms.

Hit 1 : 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester
C12H11ClO3; MF: 612; RMF: 663; Prob 34.7%; Lib: mainlib; ID: 136608.

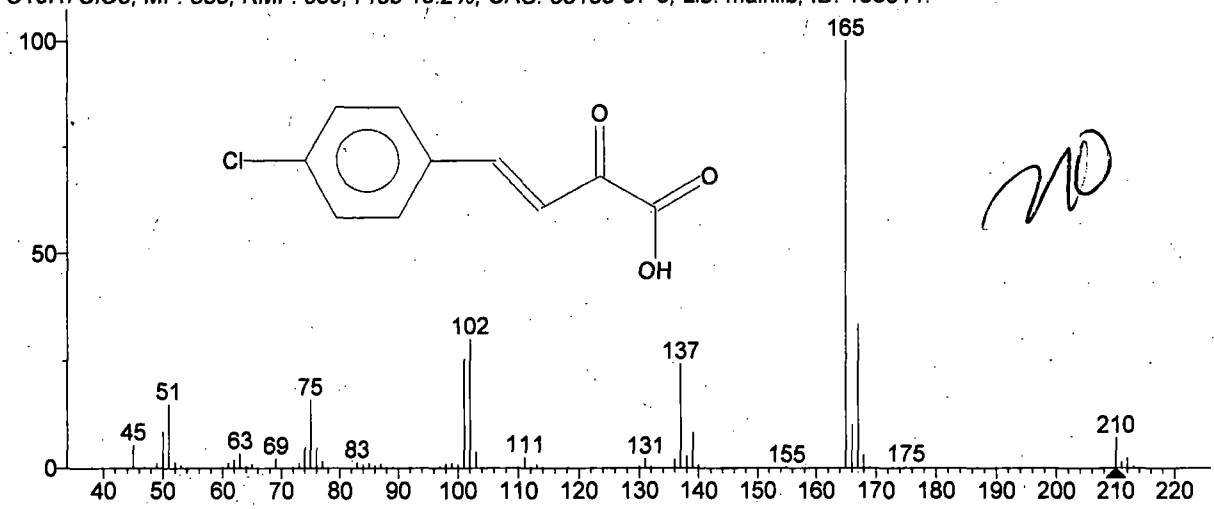


(mainlib) 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester

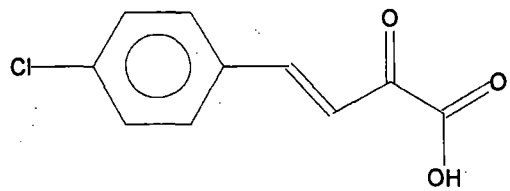


Name: 2-Propenoic acid, 3-(5-chloro-2-formylphenyl)-, ethyl ester
Formula: $C_{12}H_{11}ClO_3$
MW: 238 Exact Mass: 238.039672 NIST#: 196814 ID#: 136608 DB: mainlib
Contributor: Chemical Concepts
10 largest peaks:
165 999 | 167 330 | 102 159 | 101 150 | 166 108 | 137 88 | 75 85 | 29 52 | 193 45 | 51 42 |
Synonyms:
1.Ethyl (2E)-3-(5-chloro-2-formylphenyl)-2-propenoate #

Hit 2 : 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid
C10H7ClO3; MF: 585; RMF: 650; Prob 10.2%; CAS: 33185-97-6; Lib: mainlib; ID: 136611.

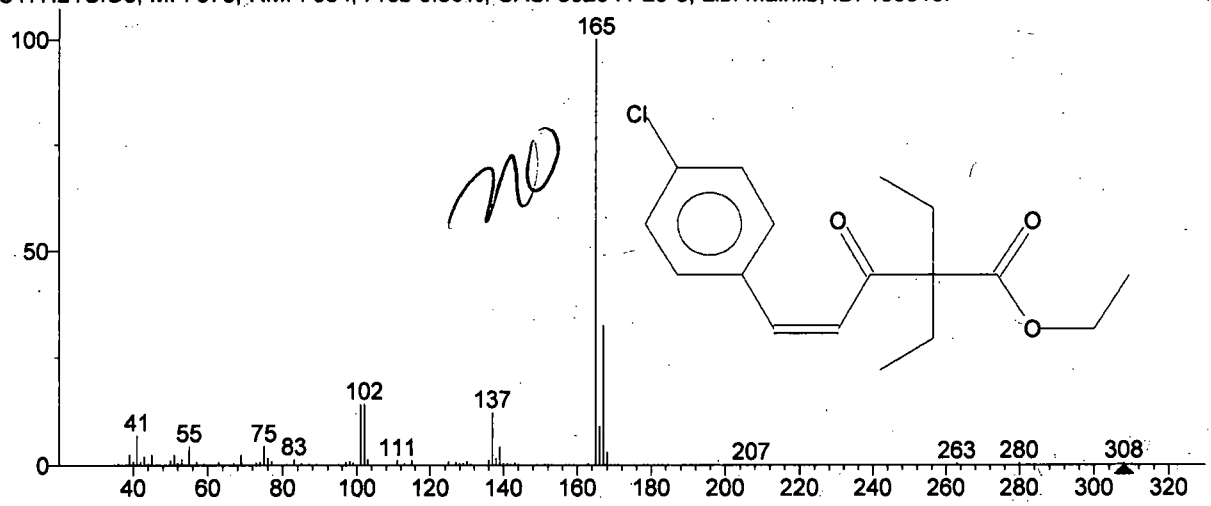


(mainlib) 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid

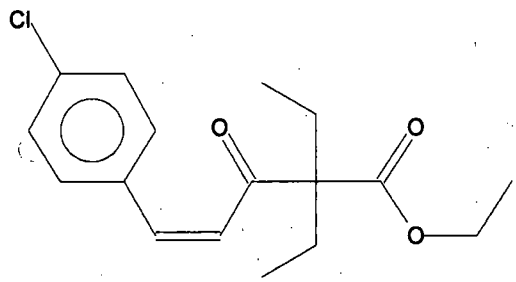


Name: 4-[p-Chlorophenyl]-2-oxo-3-butenoic acid
Formula: $C_{10}H_7ClO_3$
MW: 210 Exact Mass: 210.008371 CAS#: 33185-97-6 NIST#: 255898 ID#: 136611 DB: mainlib
Other DBs: None
Contributor: Div. of Experiment Therapeutics WRAIR, WRAMC, Washington DC 20307
10 largest peaks:
165 999 | 167 332 | 102 298 | 101 252 | 137 241 | 75 158 | 51 148 | 166 101 | 50 85 | 139 82 |
Synonyms:
1.(3E)-4-(4-Chlorophenyl)-2-oxo-3-butenoic acid #

Hit 3 : 4-Pentenoic acid, 5-(4-chlorophenyl)-2,2-diethyl-3-oxo-, ethyl ester
C17H21ClO3; MF: 573; RMF: 634; Prob 6.80%; CAS: 302941-29-3; Lib: mainlib; ID: 136610.



(mainlib) 4-Pentenoic acid, 5-(4-chlorophenyl)-2,2-diethyl-3-oxo-, ethyl ester



Name: 4-Pentenoic acid, 5-(4-chlorophenyl)-2,2-diethyl-3-oxo-, ethyl ester
Formula: $C_{17}H_{21}ClO_3$
MW: 308 Exact Mass: 308.117922 CAS#: 302941-29-3 NIST#: 271528 ID#: 136610 DB: mainlib
Other DBs: None
Contributor: A.A.Kutin, Moscow, Russia
10 largest peaks:
165 999 | 167 324 | 102 141 | 101 139 | 137 122 | 166 90 | 41 68 | 55 43 | 75 43 | 139 42 |
Synonyms:
1.Ethyl (4Z)-5-(4-chlorophenyl)-2,2-diethyl-3-oxo-4-pentenoate #

Freedom_0006097_0066

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

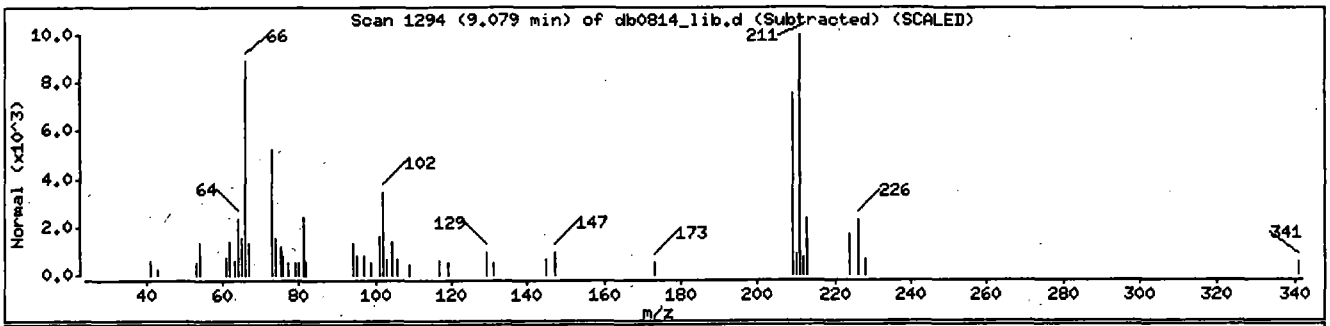
Client ID: SSKC1 Instrument: HP19760.i

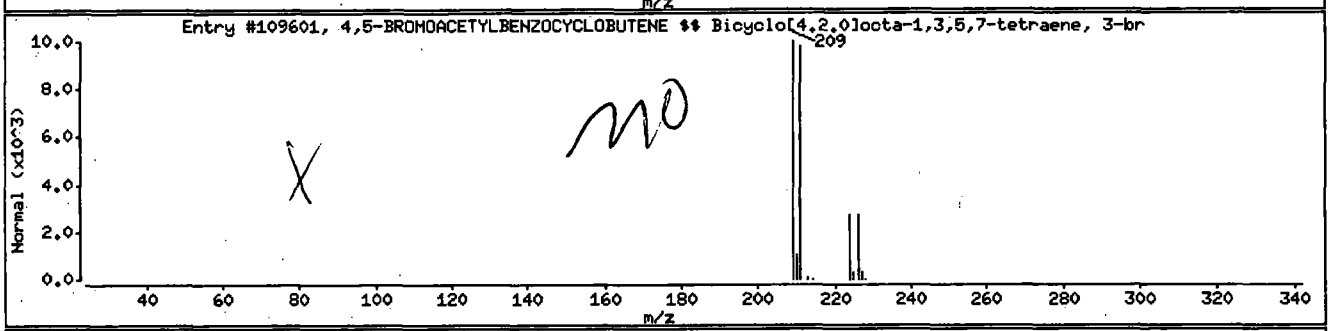
Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

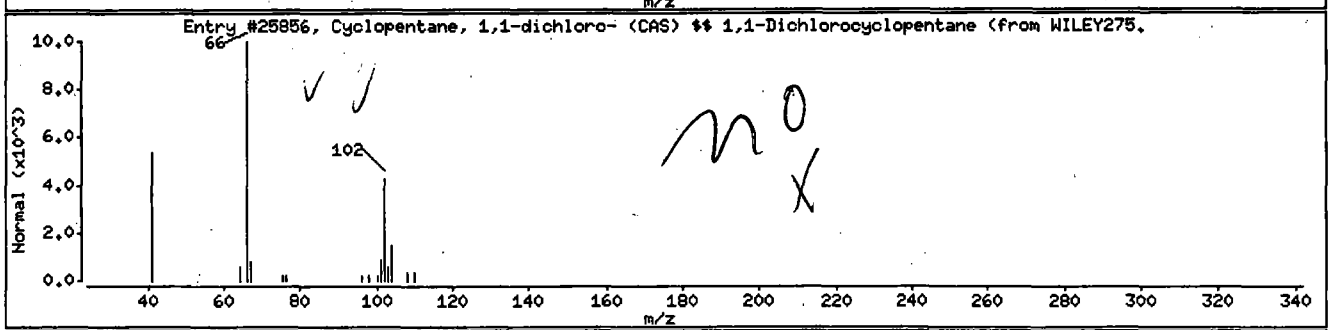
Volume Injected (uL): 1.0 Operator: jmg00346

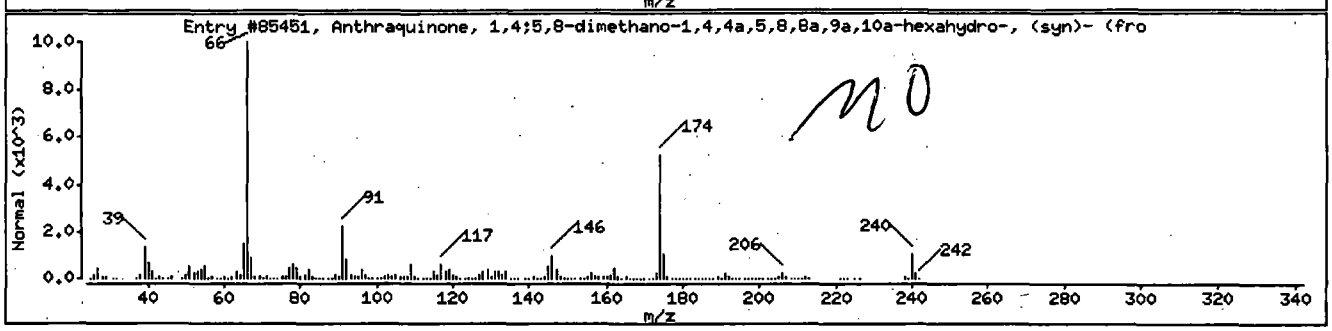
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63506-25-2	WILEY275.l	109601	72	C10H9BrO	224
Cyclopentane, 1,1-dichloro- (CAS) $$ 1,1	31038-06-9	WILEY275.l	25856	37	C5H8Cl2	138
Anthraquinone, 1,4;5,8-dimethano-1,4,4a,	1000210-97-9	NIST05a.l	85451	32	C16H16O2	240



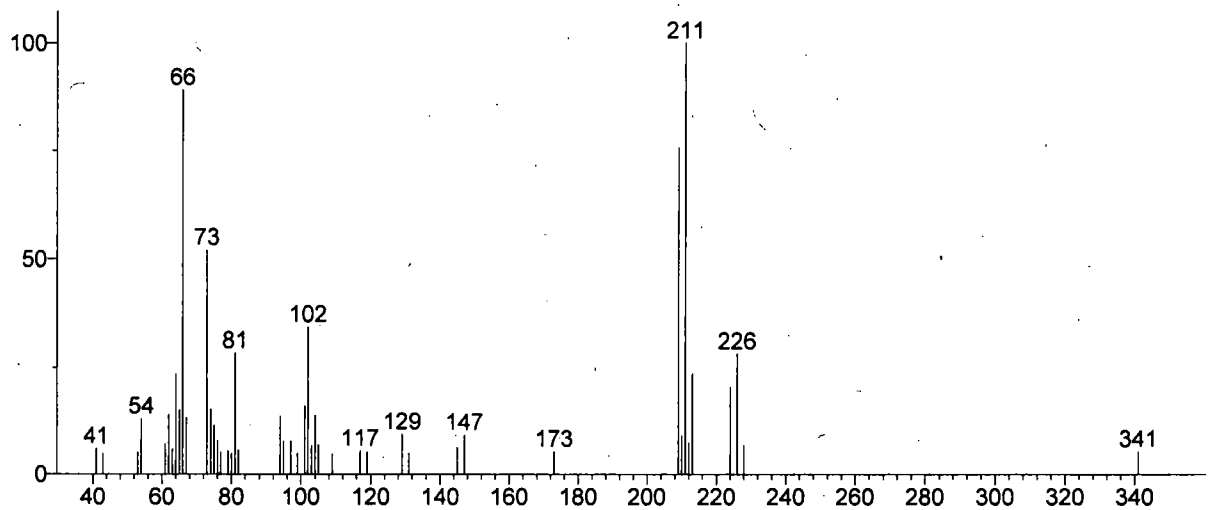






Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

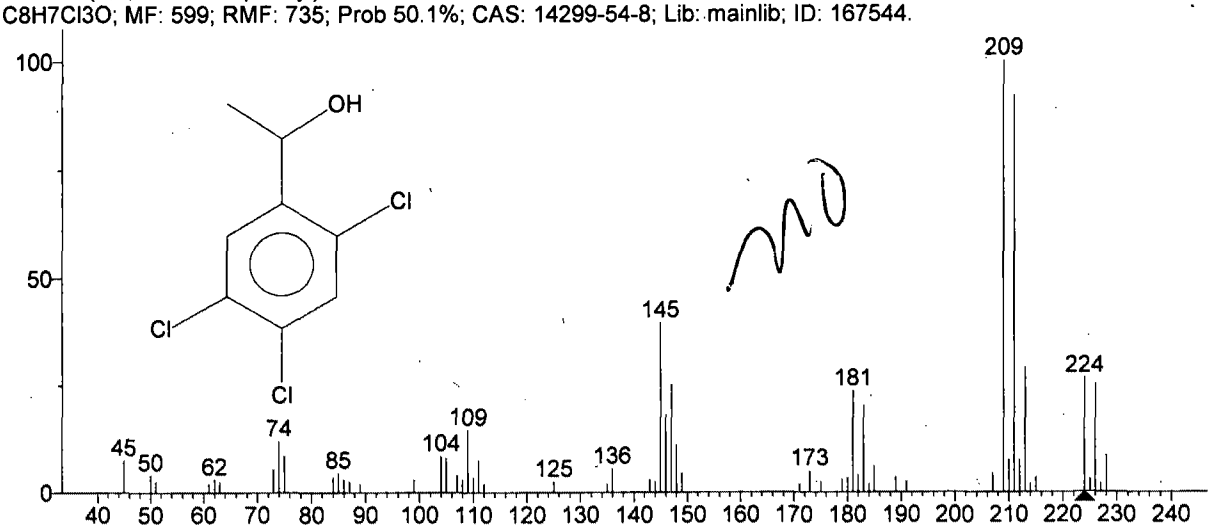
Unknown; InLib=-1296



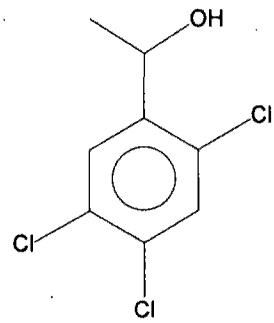
(Text File) Scan 1294 (9.079 min): DB0814.D\data.ms

Name: Scan 1294 (9.079 min): DB0814.D\data.ms
MW: N/A ID#: 27 DB: Text File
Comment: SSKC1;7365697;1;0;SAMPLE;;;
10 largest peaks:
211 999 | 66 889 | 209 757 | 73 519 | 102 343 | 81 283 | 226 281 | 64 235 | 213 235 | 224 203 |
Synonyms:
no synonyms.

Hit 1 : 1-(2,4,5-Trichlorophenyl)ethanol
C8H7Cl3O; MF: 599; RMF: 735; Prob 50.1%; CAS: 14299-54-8; Lib: mainlib; ID: 167544.



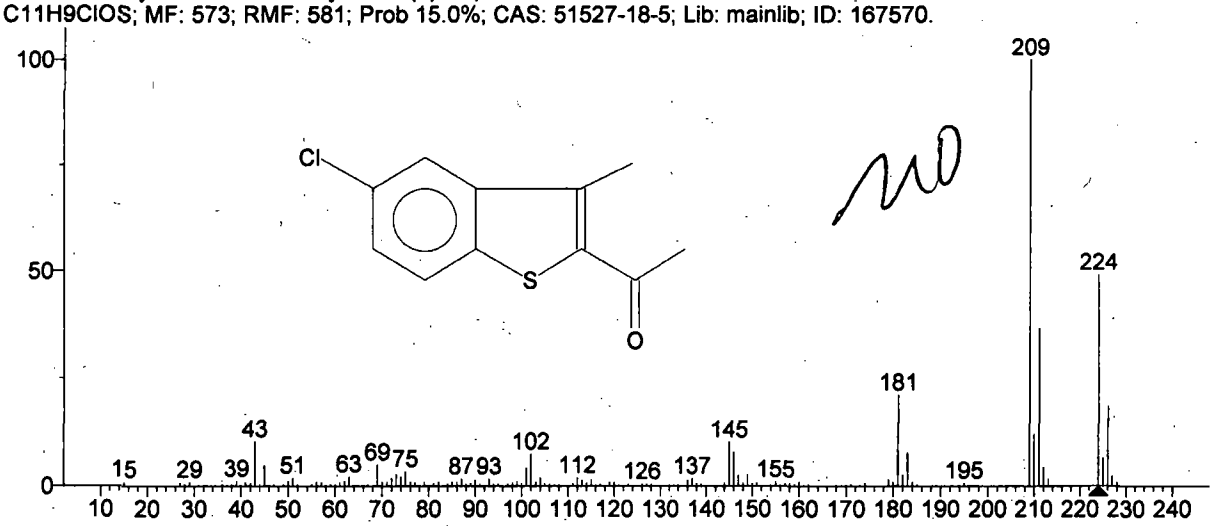
(mainlib) 1-(2,4,5-Trichlorophenyl)ethanol



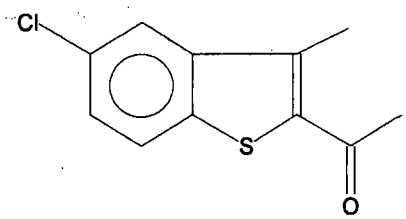
Name: 1-(2,4,5-Trichlorophenyl)ethanol
Formula: $C_8H_7Cl_3O$
MW: 224 Exact Mass: 223.956248 CAS#: 14299-54-8 NIST#: 117274 ID#: 167544 DB: mainlib
Other DBs: None
Contributor: FDA, Los Angeles District Laboratory
10 largest peaks:
209 999 | 211 919 | 145 395 | 213 290 | 224 265 | 147 250 | 226 250 | 181 235 | 183 200 | 146 180 |
Synonyms:
no synonyms.

Freedom_0006097_0069

Hit 2 : 2-Acetyl-5-chloro-3-methylbenzo(b)thiophene
C11H9ClOS; MF: 573; RMF: 581; Prob 15.0%; CAS: 51527-18-5; Lib: mainlib; ID: 167570.

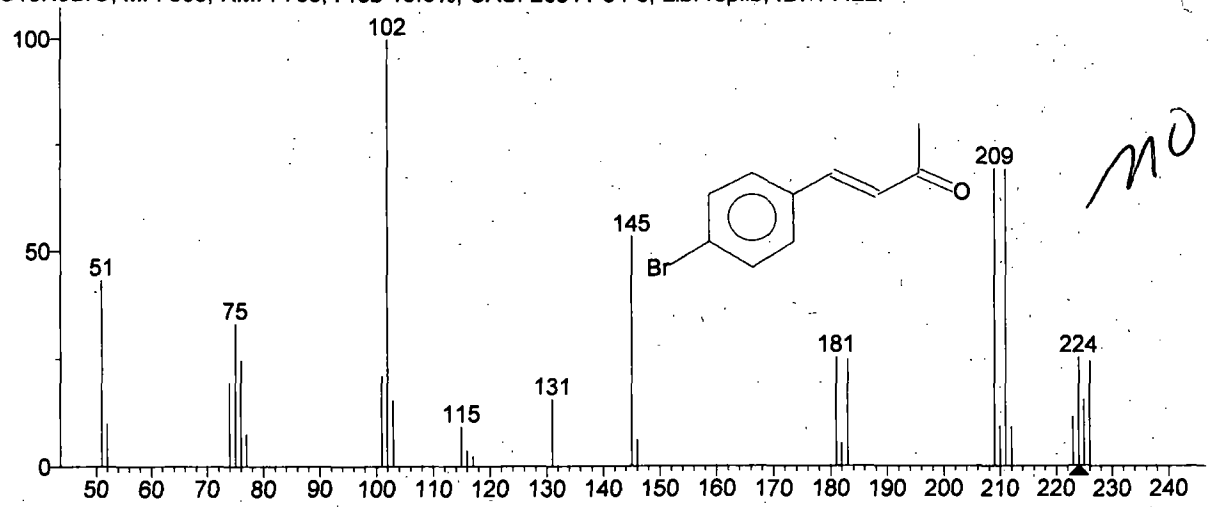


(mainlib) 2-Acetyl-5-chloro-3-methylbenzo(b)thiophene



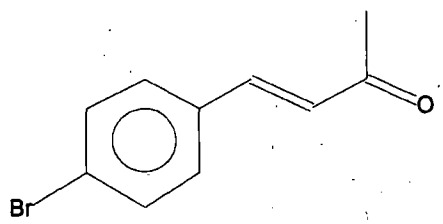
Name: 2-Acetyl-5-chloro-3-methylbenzo(b)thiophene
Formula: $C_{11}H_9ClOS$
MW: 224 Exact Mass: 224.006264 CAS#: 51527-18-5 NIST#: 234642 ID#: 167570 DB: mainlib
Other DBs: None
Contributor: Japan AIST/NIMC Database- Spectrum MS-IW-2761
10 largest peaks:
209 999 | 224 491 | 211 366 | 181 211 | 226 184 | 210 119 | 43 103 | 145 101 | 146 78 | 183 76 |
Synonyms:
1.1-(5-Chloro-3-methyl-1-benzothien-2-yl)ethanone #

Hit 3 : 3-Buten-2-one 4-[p-bromophenyl]-
C10H9BrO; MF: 563; RMF: 733; Prob 10.6%; CAS: 20511-04-0; Lib: replib; ID: 14422.



no

(replib) 3-Buten-2-one 4-[p-bromophenyl]-



Name: 3-Buten-2-one 4-[p-bromophenyl]-
Formula: $C_{10}H_9BrO$
MW: 224 Exact Mass: 223.983677 CAS#: 20511-04-0 NIST#: 145195 ID#: 14422 DB: replib
Other DBs: None
Contributor: ASES Database, Dalian Institute, P.R. China
10 largest peaks:
102 999 | 209 693 | 211 692 | 145 535 | 51 431 | 75 330 | 181 253 | 224 253 | 183 247 | 76 244 |
Synonyms:
1.4-Bromo-benzalacetone
2.(3E)-4-(4-Bromophenyl)-3-buten-2-one #

Freedom_0006097_0071

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

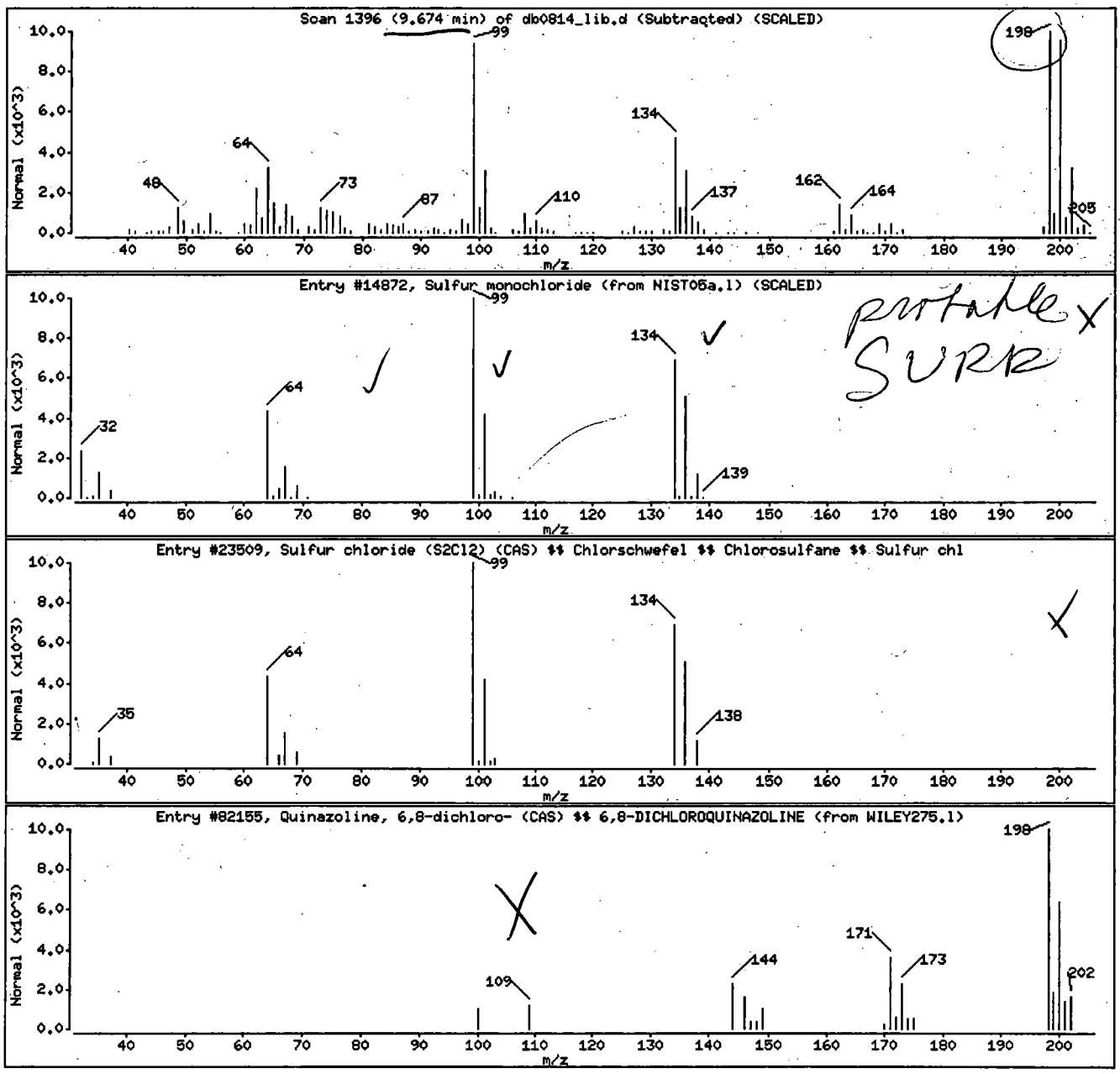
Client ID: SSKC1 Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

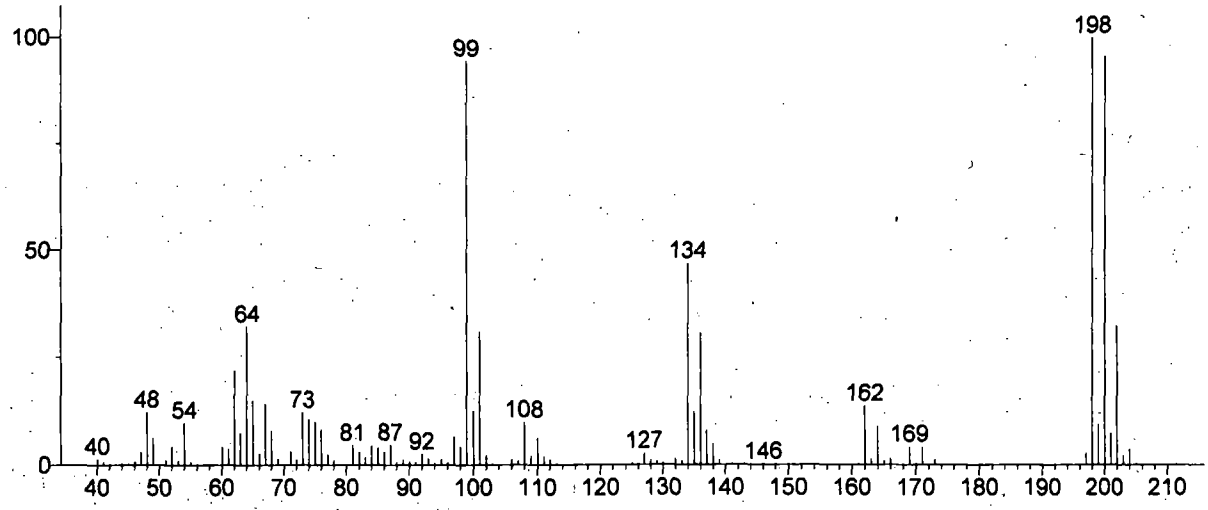
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Sulfur chloride (S2Cl2) (CAS) $$ Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134
Quinazoline, 6,8-dichloro- (CAS) $$ 6,8-	17227-49-6	WILEY275.l	82155	38	C8H4Cl2N2	198



Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

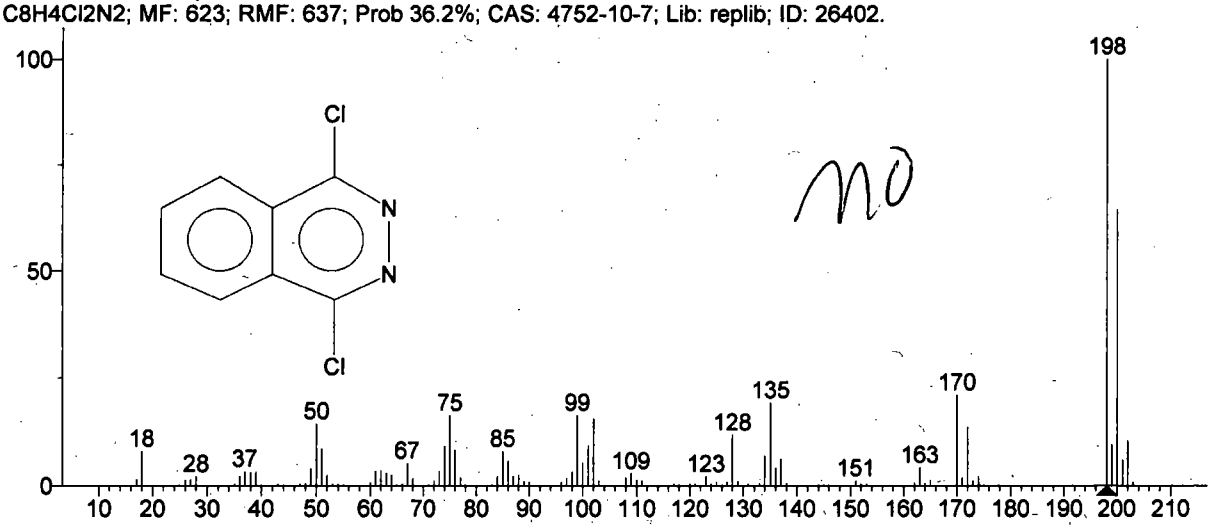
Unknown; InLib=-1008



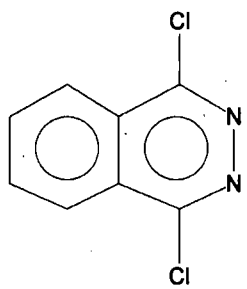
(Text File) Scan 1396 (9.674 min): DB0814.D\data.ms

Name: Scan 1396 (9.674 min): DB0814.D\data.ms
MW: N/A ID#: 28 DB: Text File
Comment: SSKC1;7365697;1;0;SAMPLE;;;
10 largest peaks:
198 999 | 200 955 | 99 943 | 134 469 | 202 324 | 64 321 | 101 307 | 136 306 | 62 218 | 65 149 |
Synonyms:
no synonyms.

Hit 1 : 1,4-Dichlorophthalazine
C8H4Cl2N2; MF: 623; RMF: 637; Prob 36.2%; CAS: 4752-10-7; Lib: replib; ID: 26402.



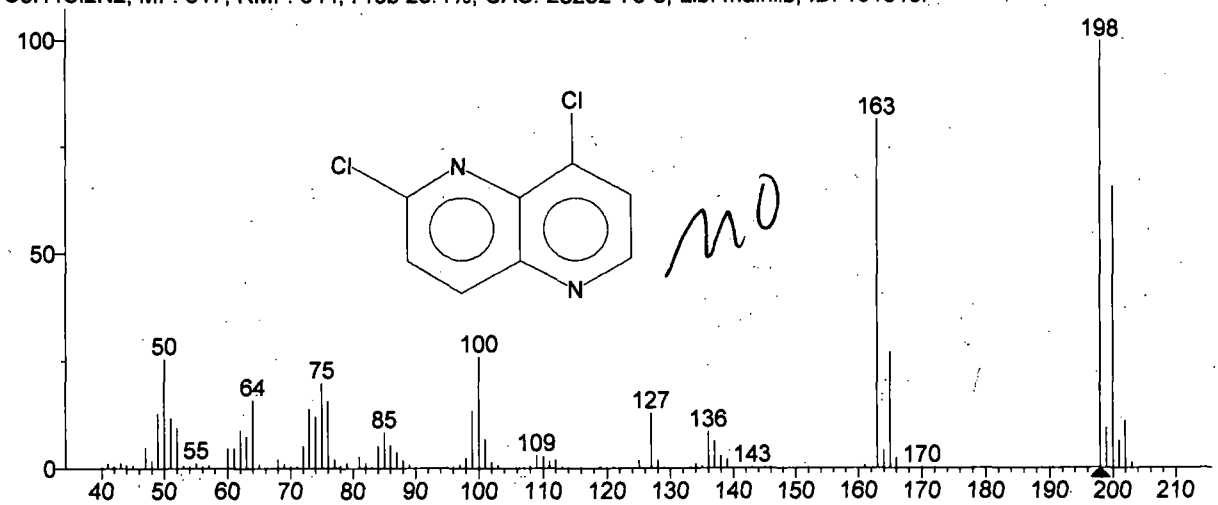
(replib) 1,4-Dichlorophthalazine



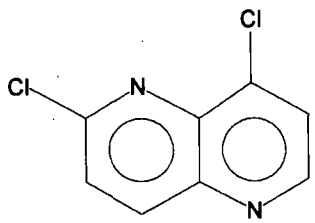
Name: 1,4-Dichlorophthalazine
Formula: $C_8H_4Cl_2N_2$
MW: 198 Exact Mass: 197.975154 CAS#: 4752-10-7 NIST#: 239011 ID#: 26402 DB: replib
Other DBs: Fine, HODOC, EINECS
Contributor: Japan AIST/NIMC Database- Spectrum MS-NW-8054
10 largest peaks:
198 999 | 200 642 | 170 210 | 135 191 | 99 163 | 75 162 | 102 154 | 50 143 | 172 136 | 128 117 |
Synonyms:
1.Phthalazine, 1,4-dichloro-

Freedom_0006097_0074

Hit 2 : 1,5-Naphthyridine, 2,8-dichloro-
C8H4Cl2N2; MF: 617; RMF: 644; Prob 28.4%; CAS: 28252-76-8; Lib: mainlib; ID: 161510.



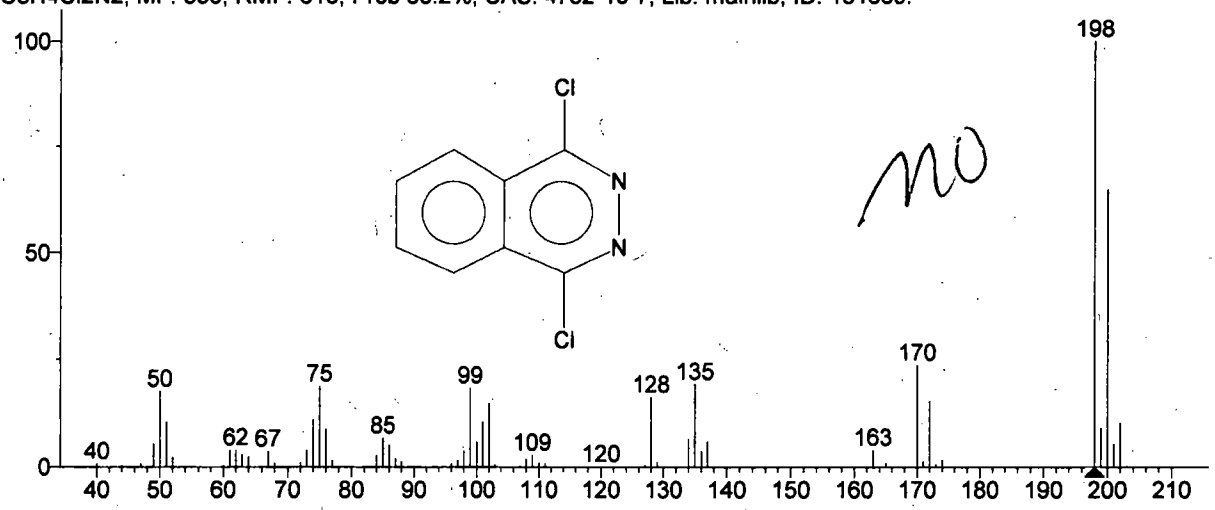
(mainlib) 1,5-Naphthyridine, 2,8-dichloro-



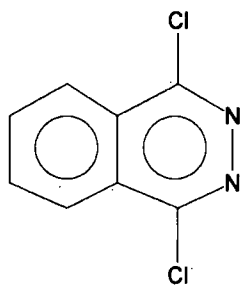
Name: 1,5-Naphthyridine, 2,8-dichloro-
Formula: $C_8H_4Cl_2N_2$
MW: 198 Exact Mass: 197.975154 CAS#: 28252-76-8 NIST#: 214645 ID#: 161510 DB: mainlib
Other DBs: None
Contributor: Div. of Experiment Therapeutics WRAIR, WRAMC, Washington DC 20307
10 largest peaks:
198 999 | 163 813 | 200 658 | 165 269 | 100 257 | 50 253 | 75 197 | 64 158 | 76 154 | 73 137 |
Synonyms:
1.4,6-Dichloro-1,5-naphthyridine
2.2,8-Dichloro[1,5]naphthyridine #

Freedom_0006097_0075

Hit 3 : 1,4-Dichlorophthalazine
C8H4Cl2N2; MF: 589; RMF: 616; Prob 36.2%; CAS: 4752-10-7; Lib: mainlib; ID: 161669.



(mainlib) 1,4-Dichlorophthalazine



Name: 1,4-Dichlorophthalazine
Formula: $C_8H_4Cl_2N_2$
MW: 198 Exact Mass: 197.975154 CAS#: 4752-10-7 NIST#: 92309 ID#: 161669 DB: mainlib
Other DBs: Fine, HODOC, EINECS
Contributor: J.E. WILKINSON S-CUBED, SAN DIEGO, CA.
10 largest peaks:
198 999 | 200 646 | 170 236 | 135 192 | 75 186 | 99 183 | 50 175 | 128 162 | 172 152 | 102 148 |
Synonyms:
1.Phthalazine, 1,4-dichloro-

Freedom_0006097_0076

Data File: /chem/HP19760.i/14feb19.b/db0814_lib.d

Date : 19-FEB-2014 13:56

Client ID: SSKC1

Instrument: HP19760.i

Sample Info: SSKC1;7365697;1;0;SAMPLE;;;

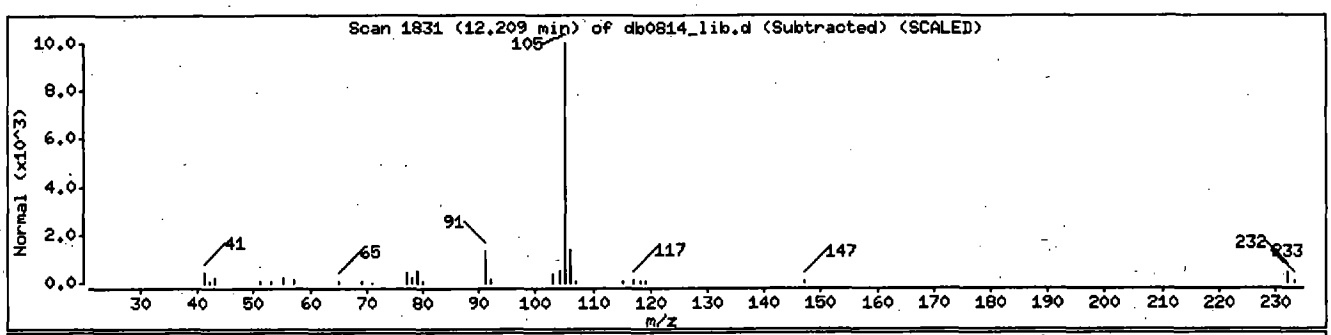
Volume Injected (uL): 1.0

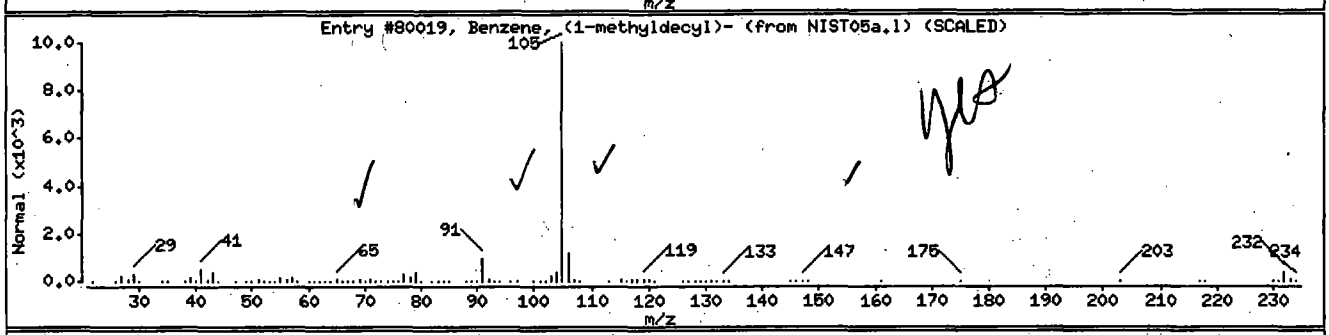
Operator: jmg00346

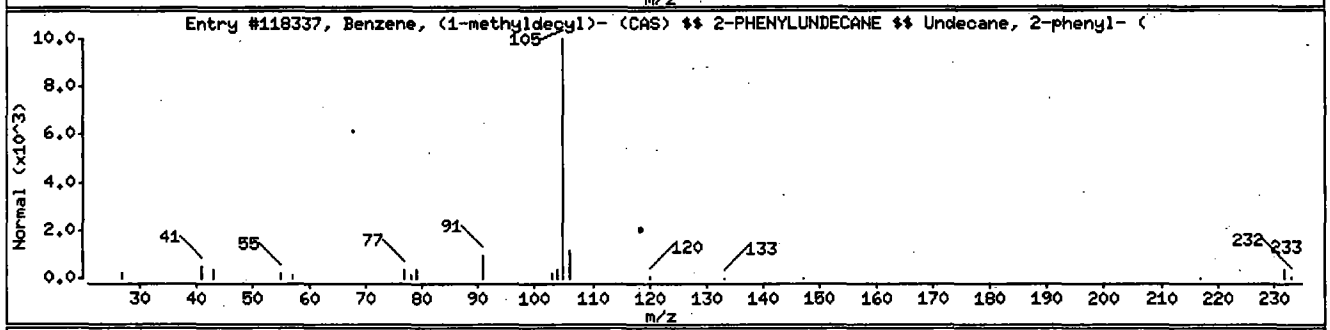
Column phase: J&W DB-5MS

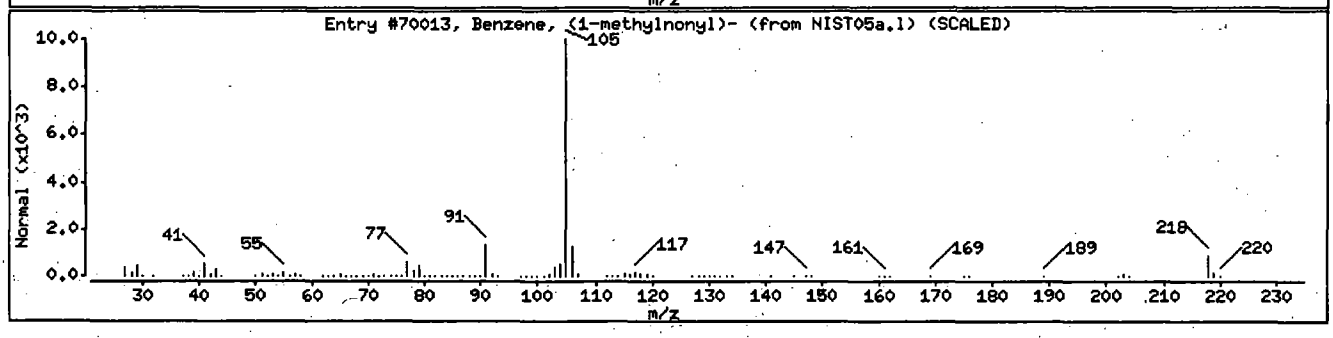
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Benzene, (1-methyldecyl)-	4536-88-3	NIST05a.l	80019	93	C17H28	232
Benzene, (1-methyldecyl)- (CAS) $$ 2-PHE	4536-88-3	WILEY275.l	118337	87	C17H28	232
Benzene, (1-methylnonyl)-	4537-13-7	NIST05a.l	70013	72	C16H26	218





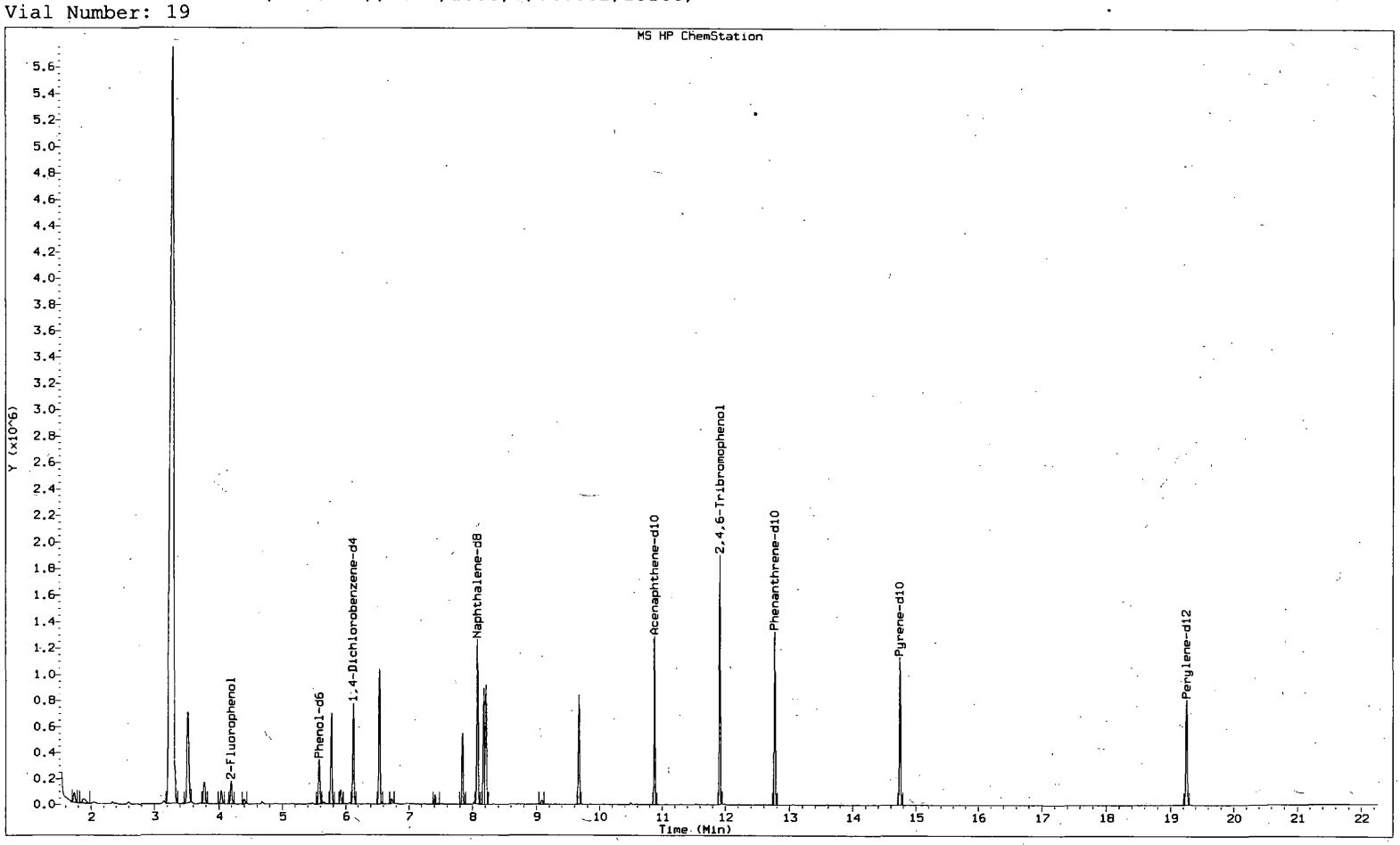




Digitally signed by Andrew J. Strebel on 03/01/2014 at 16:12.
Target 3.5 esignature user ID: ajs00193

#2

File : /chem/HP19760.i/14feb19.b/db0818_lib.d
Operator : jmg00346
Acquired : 19-FEB-2014 15:44
Instrument : HP19760.i
Sample Name: SSKH1;7365701;1;0;SAMPLE;;;
Misc Info : 14049WAB;WL13166;;1041;1000;0;db0802;13166;
Vial Number: 19



Lancaster Labs

Data file : /chem/HP19760.i/14feb19.b/db0818_lib.d
Lab Smp Id: 7365701 Client Smp ID: SSKH1
Inj Date : 19-FEB-2014 15:44
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : SSKH1;7365701;1;0;SAMPLE;;;
Misc Info : 14049WAB;WL13166;;1041;1000;0;db0802;13166;
Comment : Max. number of TICs to report is 50, 17 TICs were found initially.
Method : /chem/HP19760.i/14feb19.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 15:13 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 19
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1041.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.124	1153572	10.000
* 48 Naphthalene-d8	8.077	1819980	10.000
* 83 Acenaphthene-d10	10.880	1540355	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.735	142223	1.23289088	1.18433	91	NIST05a.1	31325	21

Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.887	133567	1.15785671	1.11225	70	NIST05a.l	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.297	21337305	184.967171	177.68220	74	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.519	1478899	12.8201692	12.31524	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.775	313533	2.71792934	2.61088	25	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.037	184670	1.60085058	1.53780	9	NIST05a.l	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.399	62663	0.54320479	0.52181	74	NIST05a.l	33655	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.774	1022262	8.86170284	8.51268	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.920	153897	1.33409213	1.28154	96	NIST05a.l	18488	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.538	1504496	13.0420542	12.52839	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.730	56832	0.49266207	0.47325	64	NIST05a.l	12246	21)
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.412	91354	0.50194912	0.48217	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.844	685480	3.76641687	3.61807	27	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.170	1035941	5.69204216	5.46785	90	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.205	1099470	6.04110810	5.80317	50	NIST05a.l	3933	48
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc					CAS #: 63506-25-2		
9.079	58807	0.32312010	0.31039	80	WILEY275.l	109601	48

Target compound.
Do not report.
ajs00193 03/01/2014

Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d
Report Date: 01-Mar-2014 17:03

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
====	====	==========	==========	====	=======	=========	======
Sulfur monochloride				CAS #: 10025-67-9			
9.668	966197	6.27255774	6.02551	38	NIST05a.l	14872	83

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

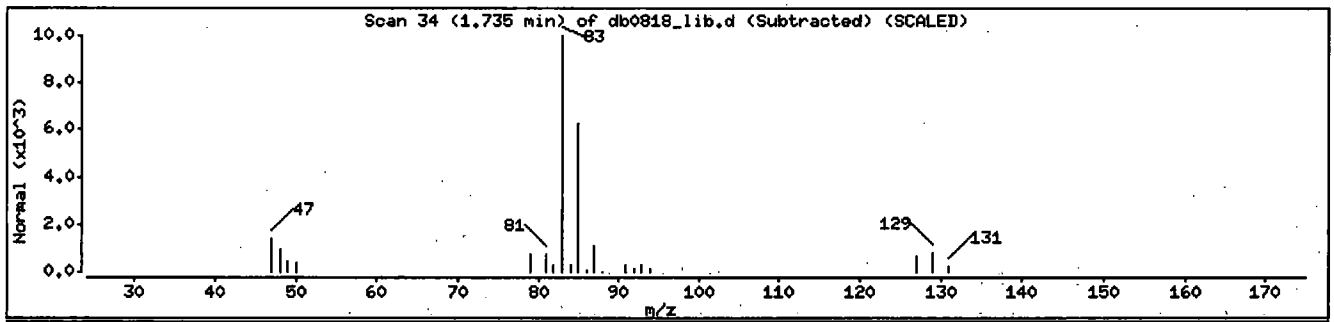
Volume Injected (uL): 1.0

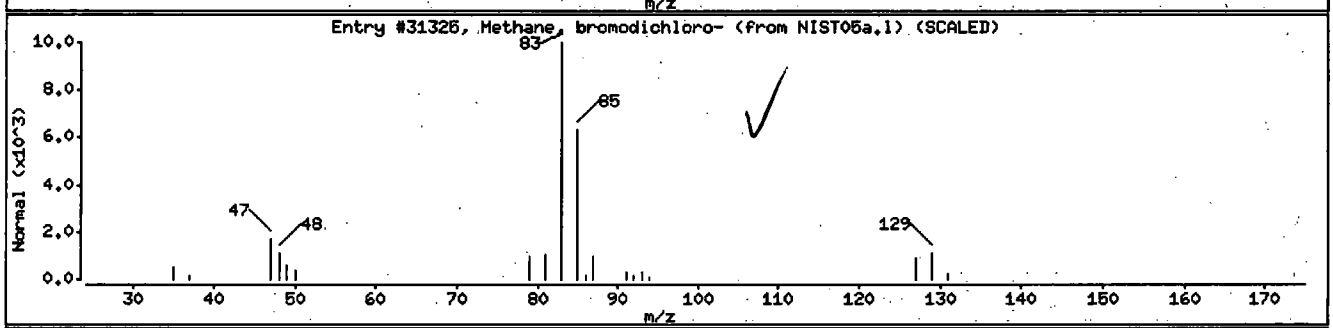
Operator: jmg00346

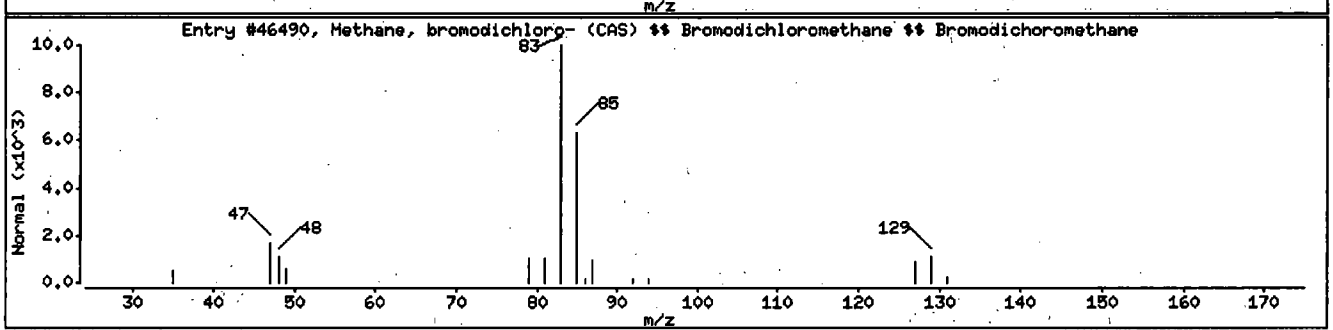
Column phase: J&W DB-5MS

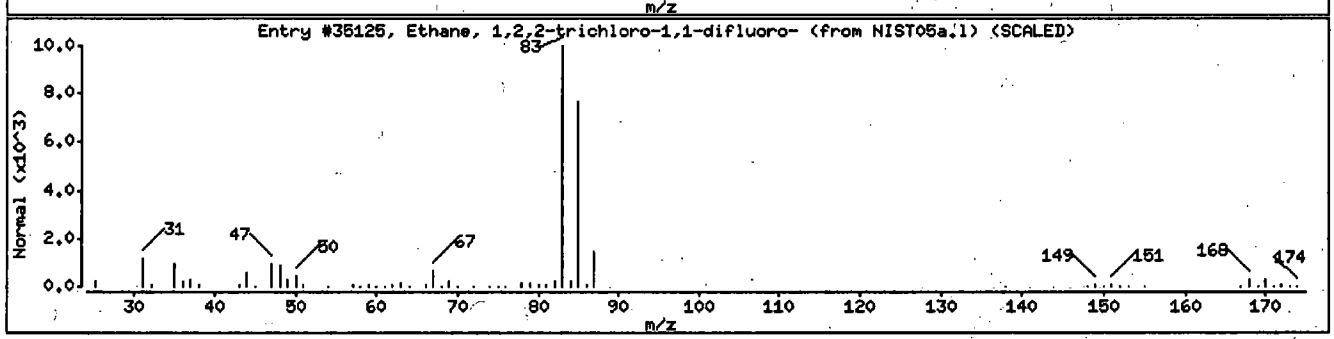
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	91	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	91	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

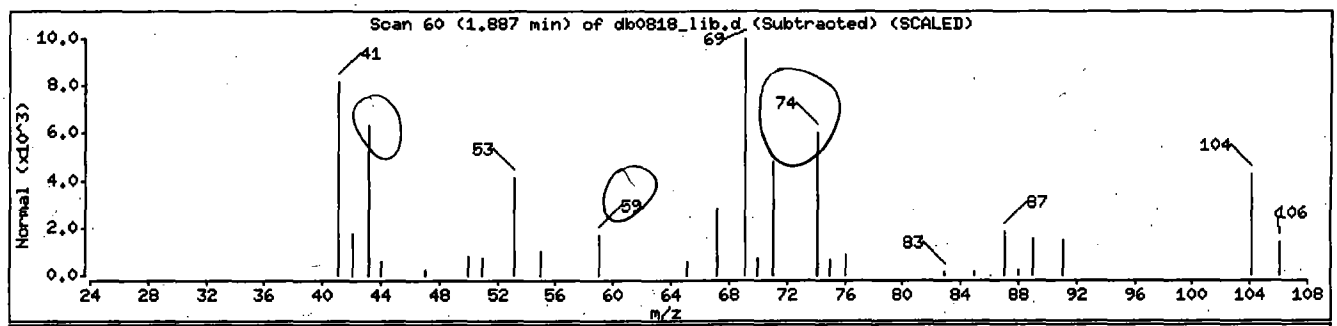
Volume Injected (uL): 1.0

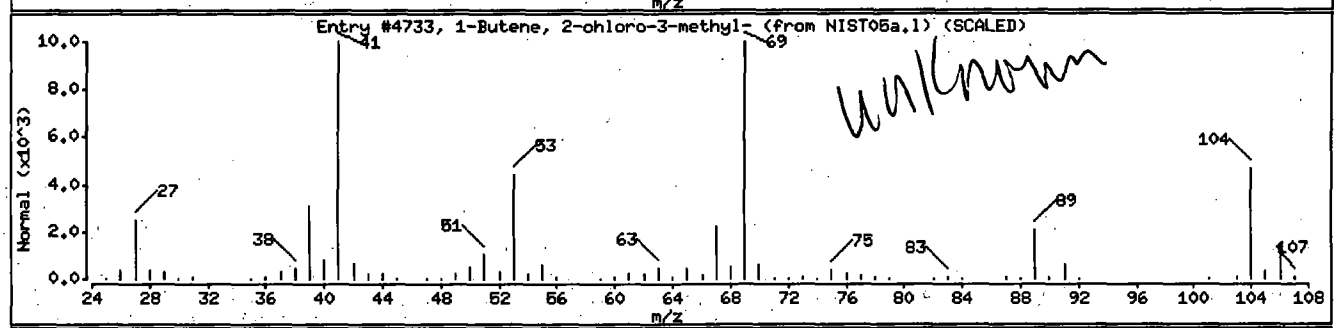
Operator: jmg00346

Column phase: J&W DB-5MS

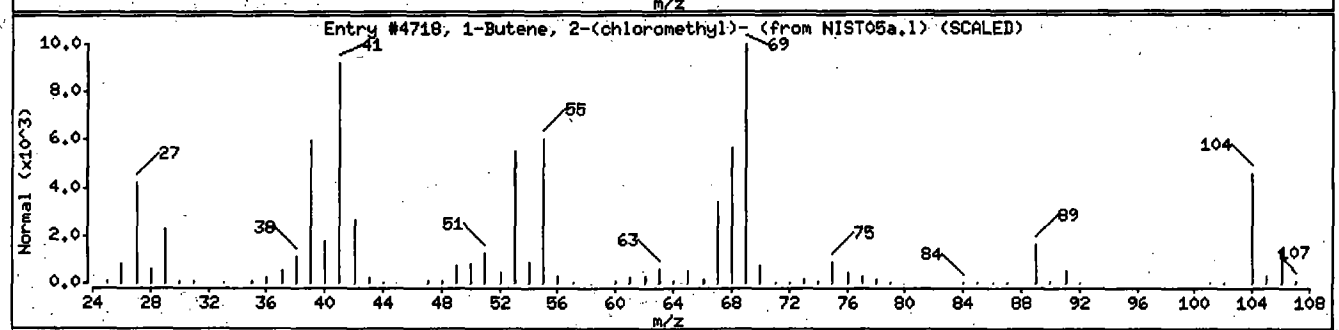
Column diameter: 0.18

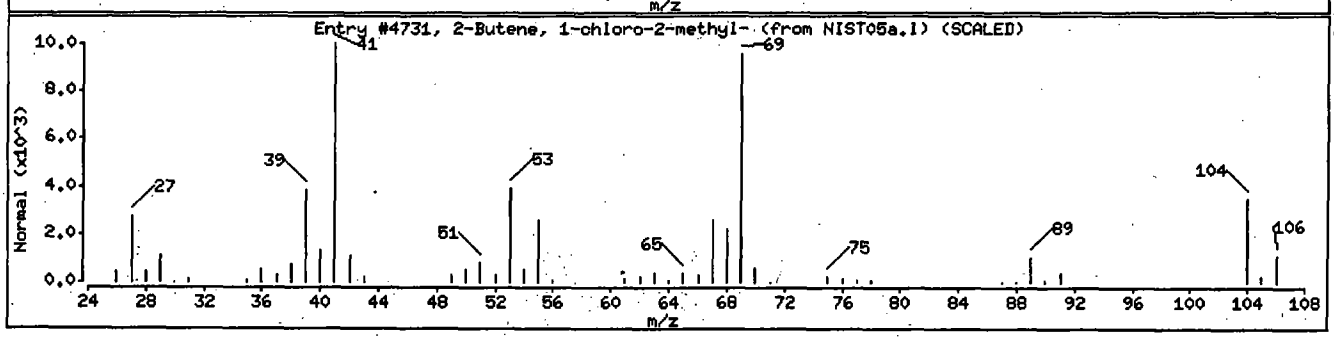
Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	70	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4718	68	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4731	64	C5H9Cl	104





unknown





Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

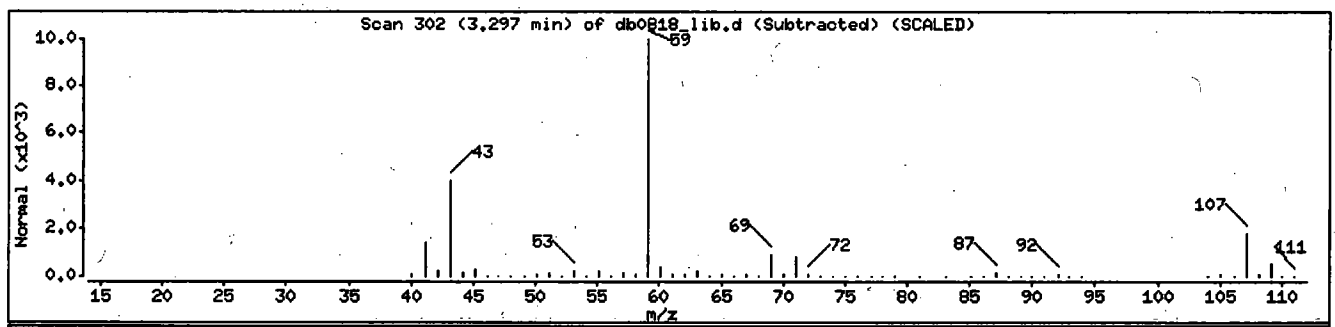
Volume Injected (uL): 1.0

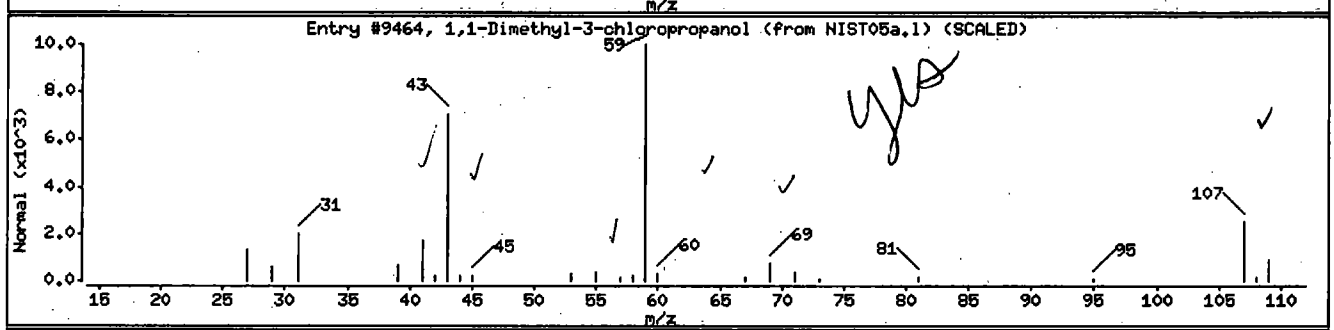
Operator: jmg00346

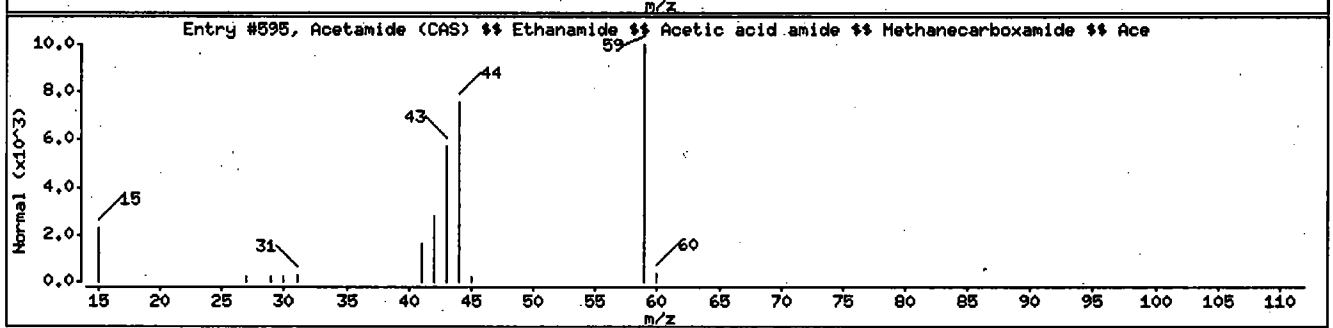
Column phase: J&W DB-5MS

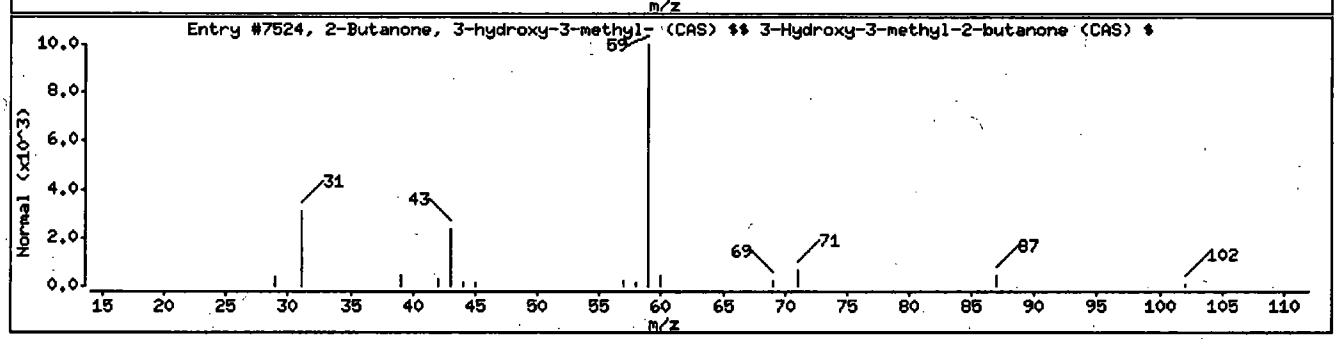
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	74	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

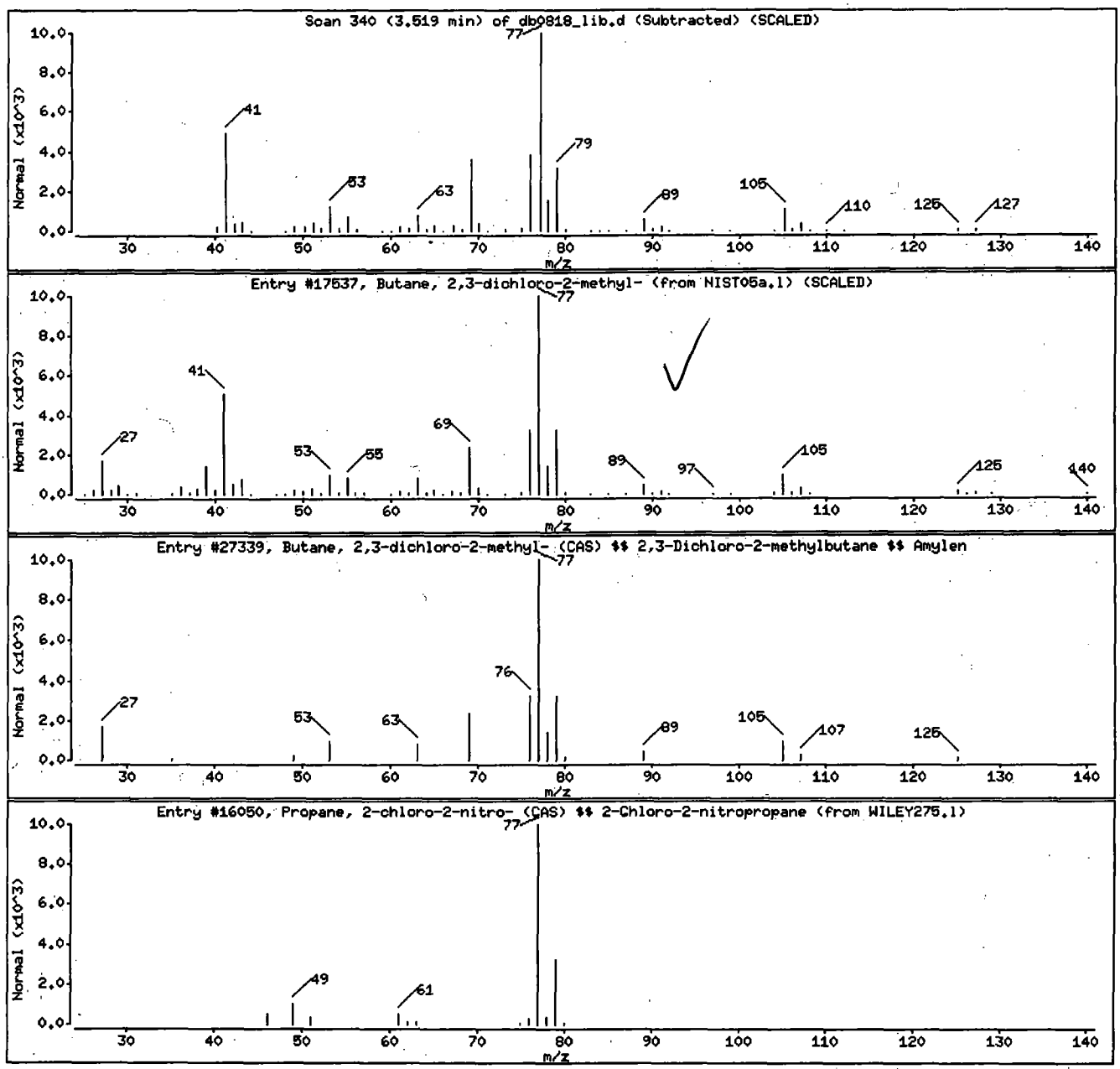
Client ID: SSKH1 Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123



Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

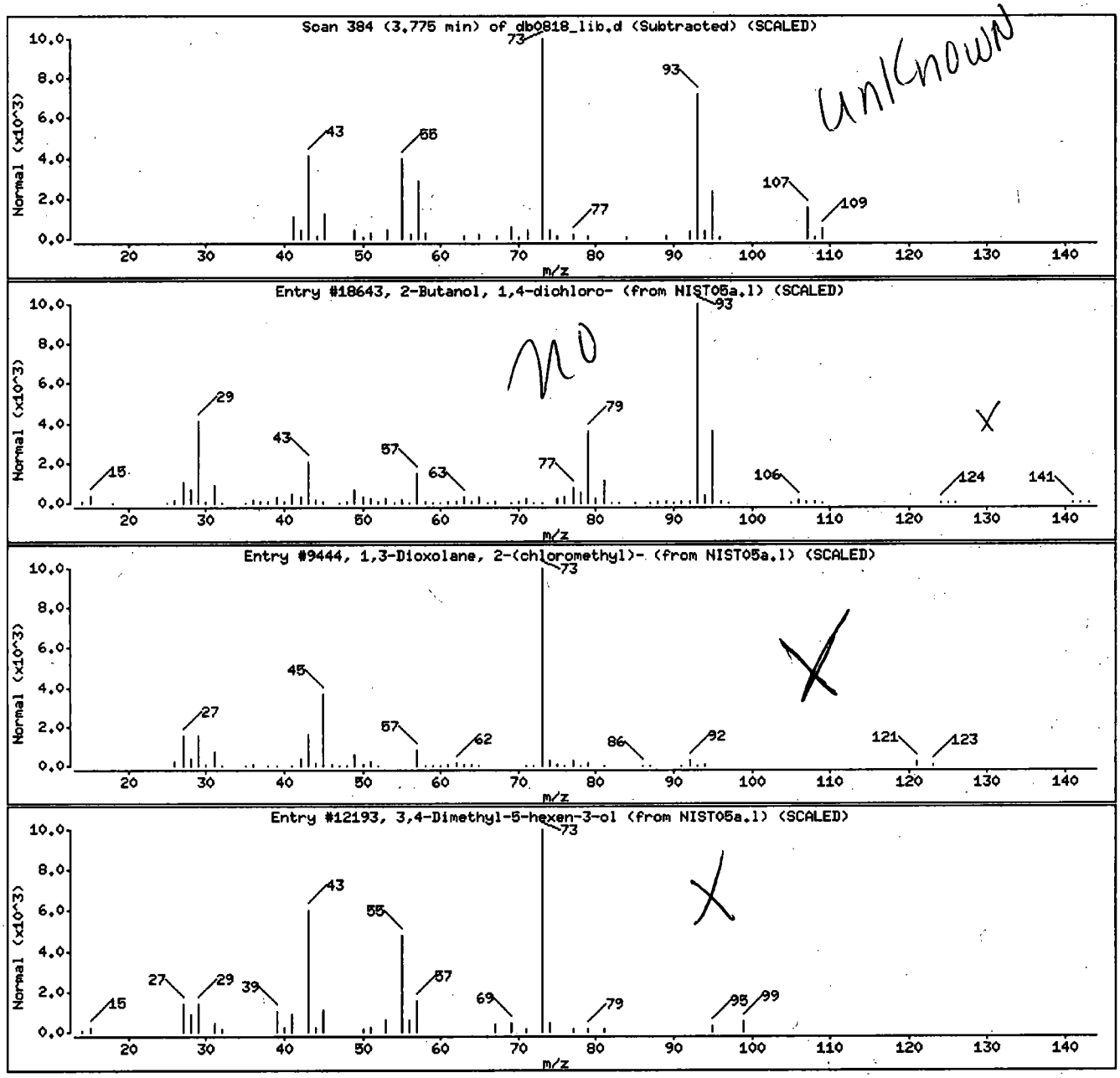
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	25	C4H8Cl2O	142
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9444	10	C4H7ClO2	122
3,4-Dimethyl-5-hexen-3-ol	1569-45-5	NIST05a.l	12193	10	C8H16O	128



Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0

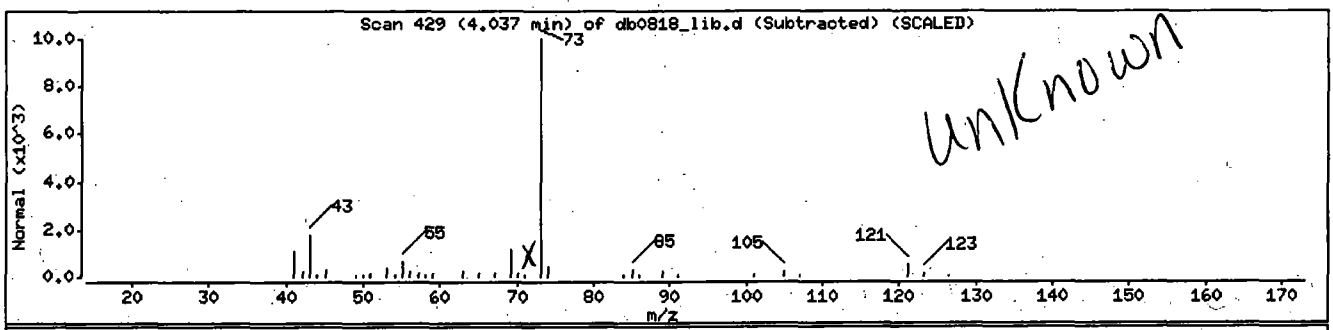
Operator: jmg00346

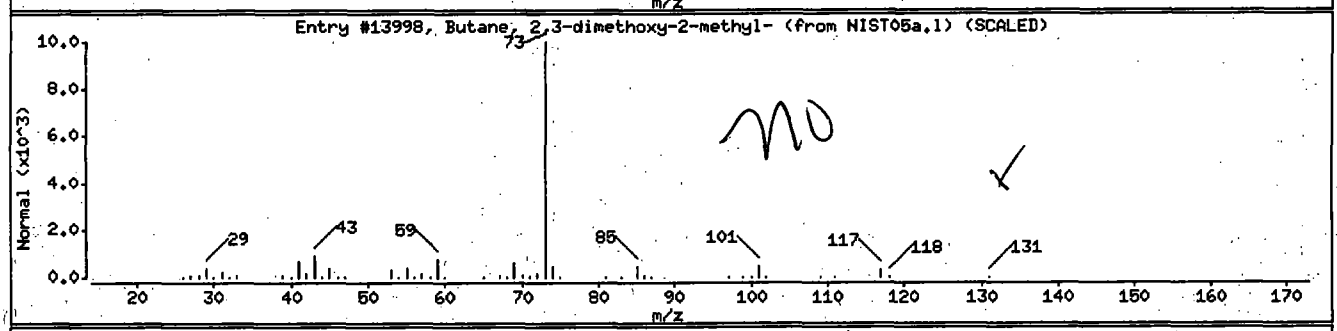
Column phase: J&W DB-5MS

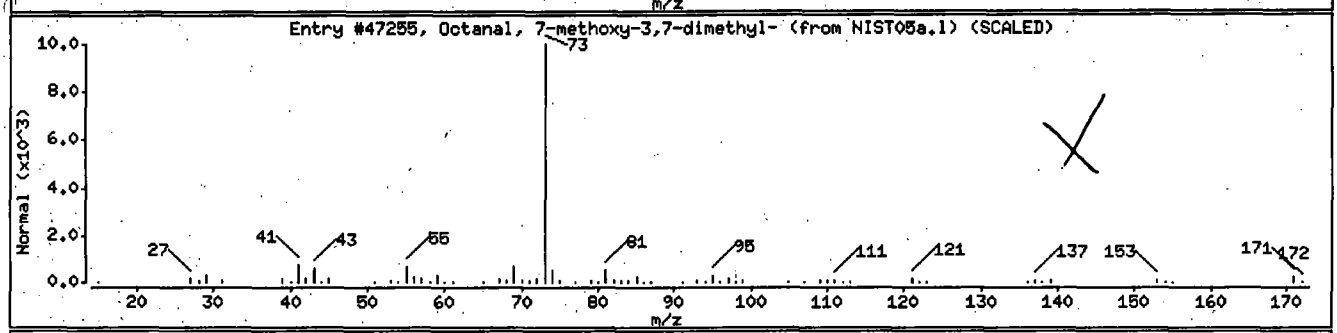
Column diameter: 0.18

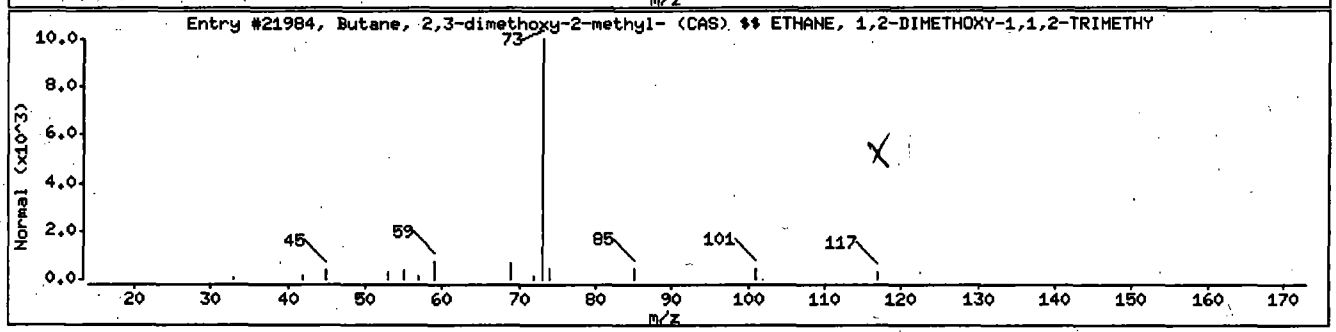
Printed low me first

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	9	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	45	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

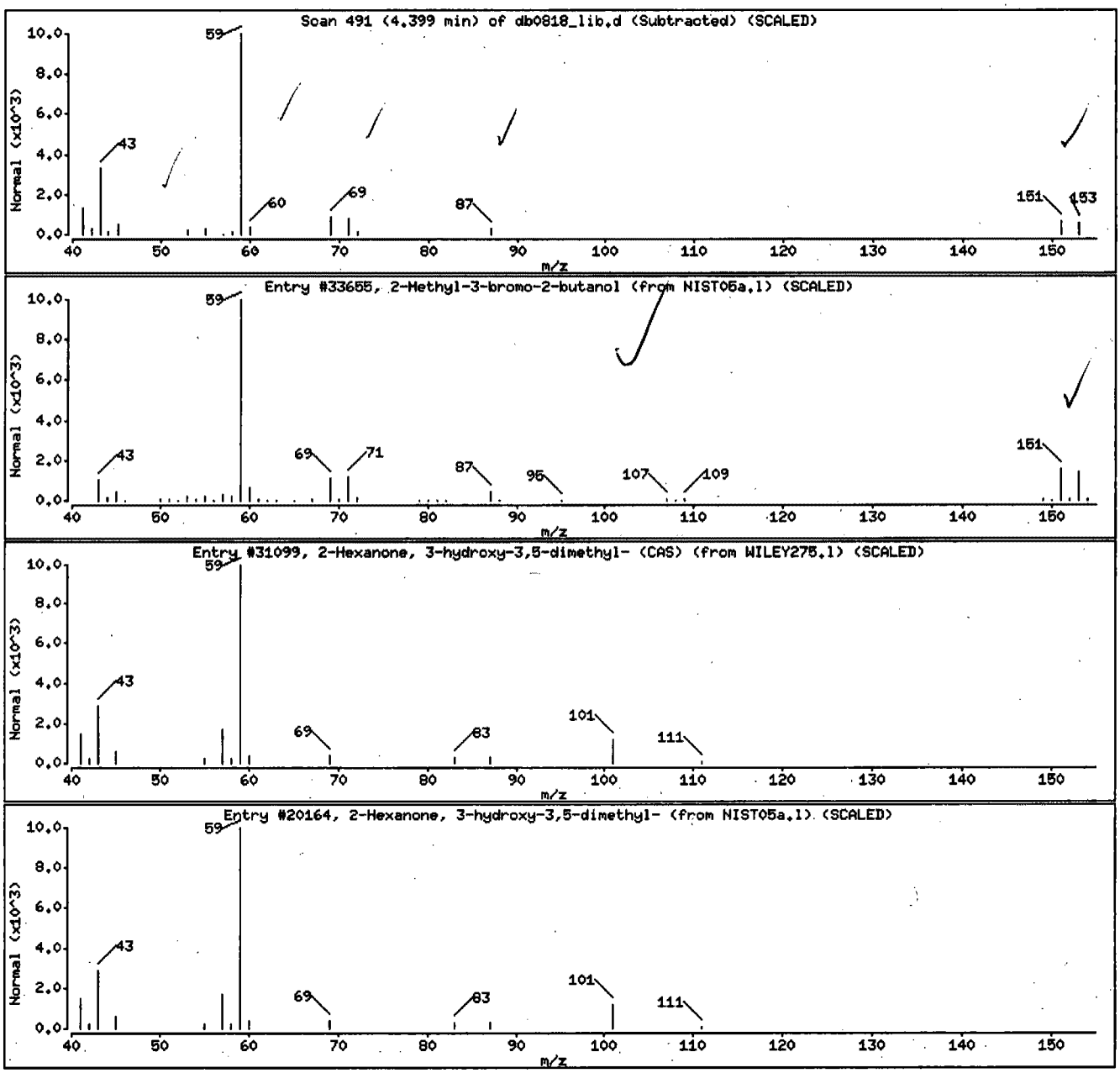
Client ID: SSKH1 Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	74	C5H11BrO	166
2-Hexanone, 3-hydroxy-3,5-dimethyl- (CAS	6321-14-8	WILEY275.l	31099	72	C8H16O2	144
2-Hexanone, 3-hydroxy-3,5-dimethyl-	6321-14-8	NIST05a.l	20164	64	C8H16O2	144



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

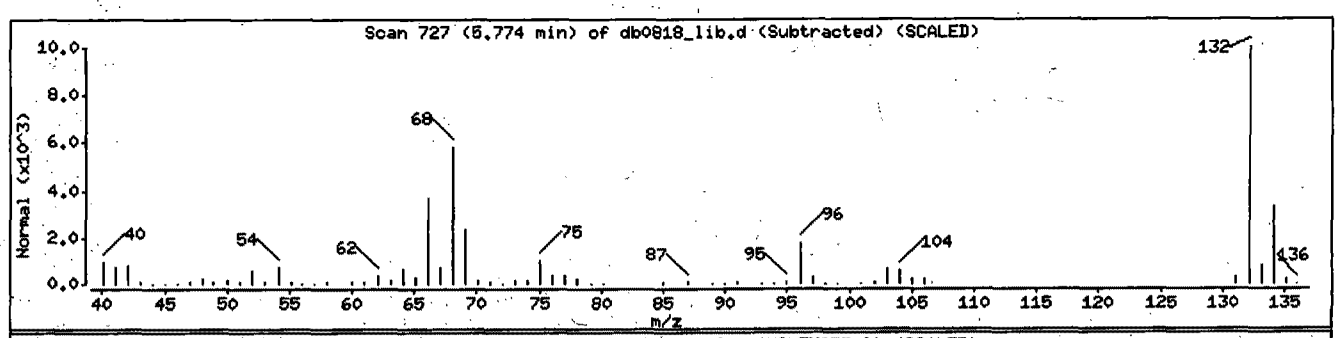
Client ID: SSKH1 Instrument: HP19760.i

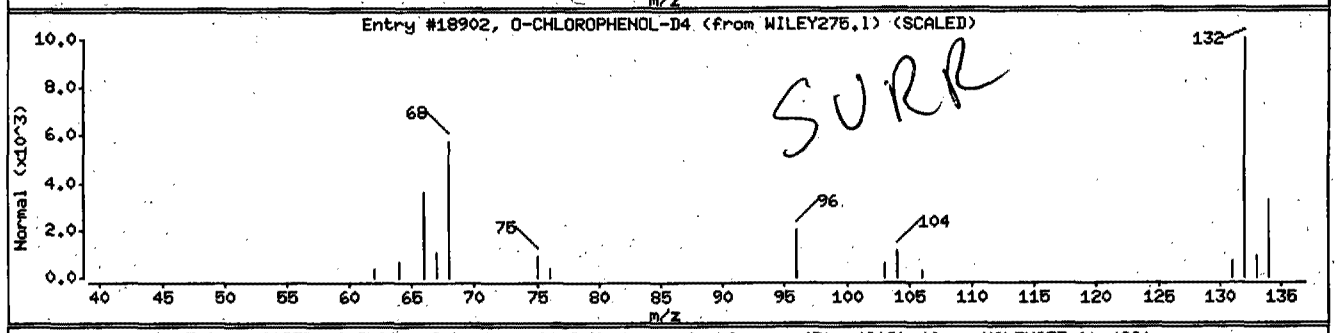
Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

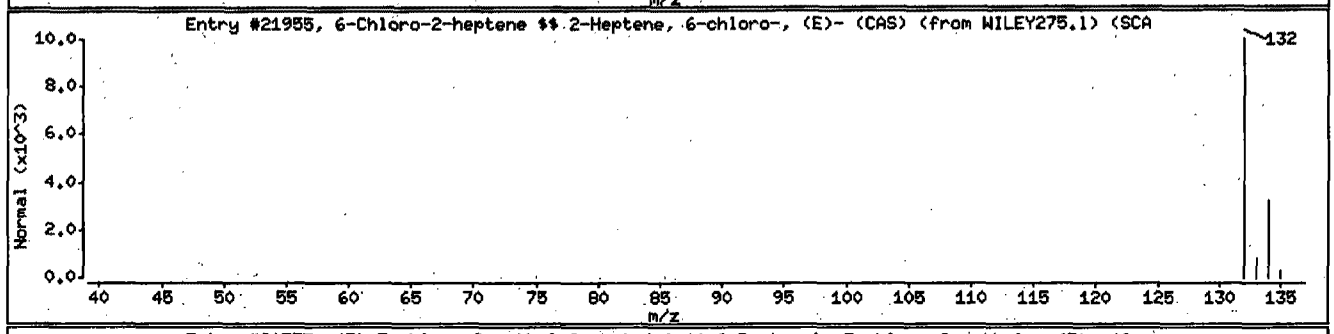
Volume Injected (uL): 1.0 Operator: jmg00346

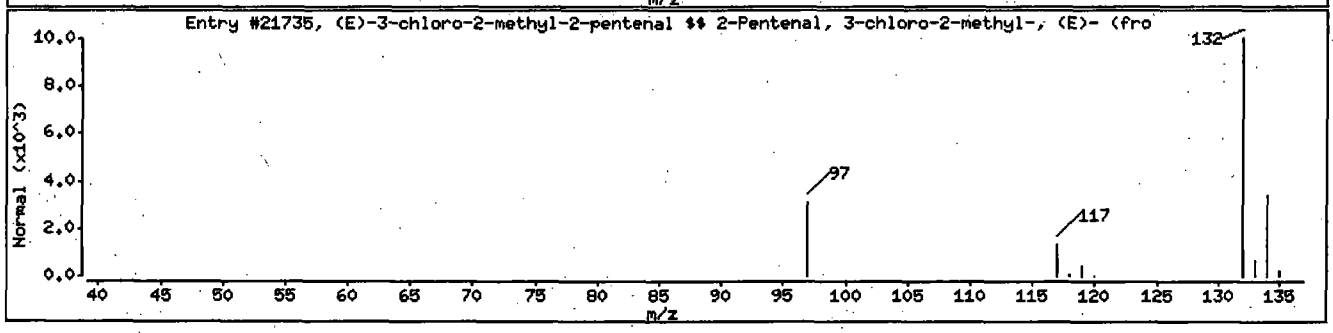
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.l	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.l	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.l	21735	78	C6H9ClO	132









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

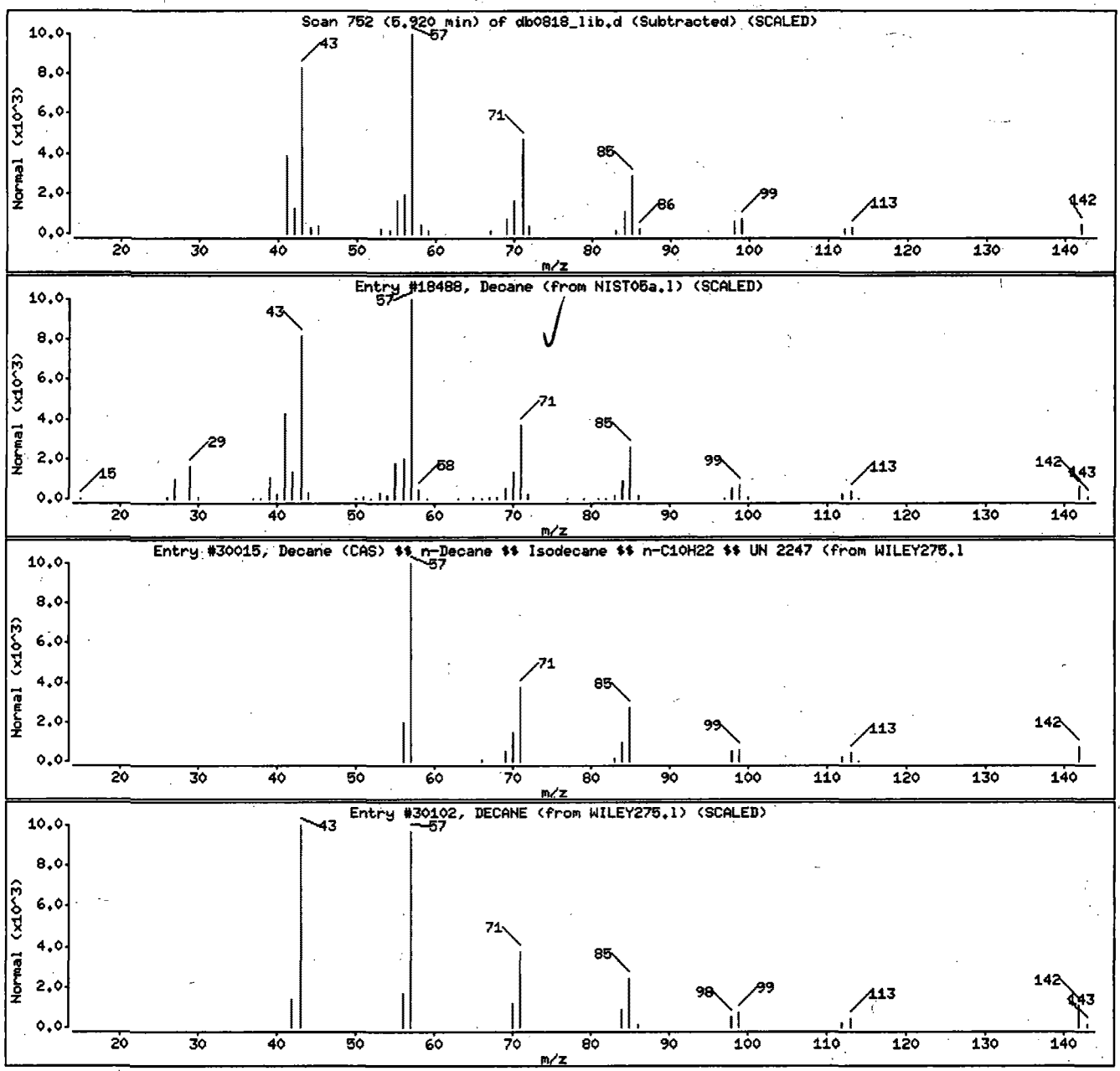
Client ID: SSKH1 Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18488	96	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30015	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

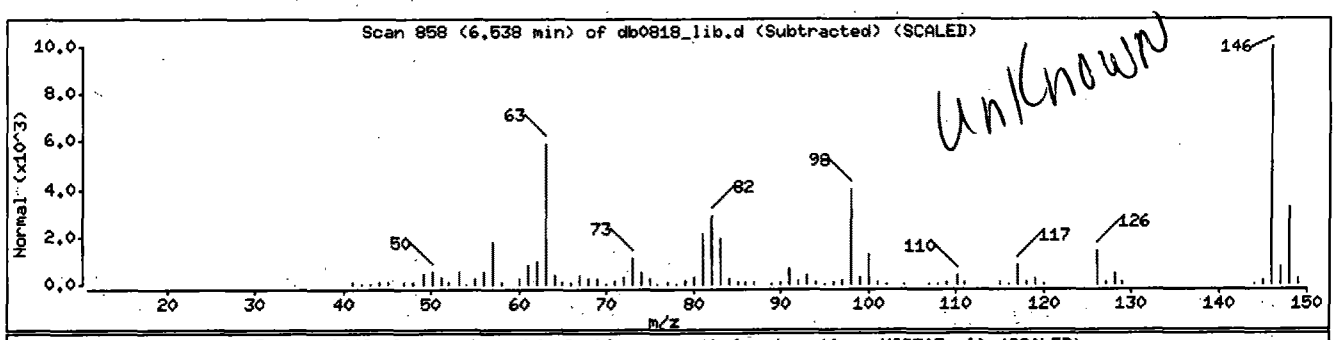
Client ID: SSKH1 Instrument: HP19760.i

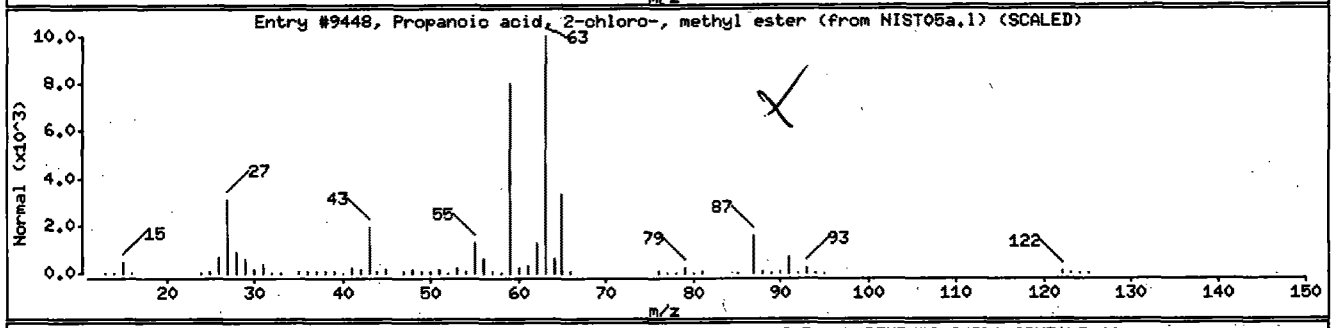
Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

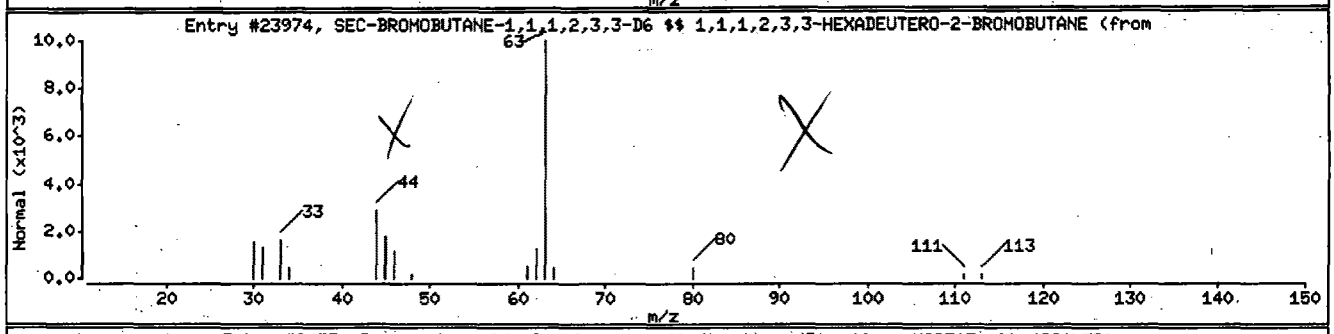
Volume Injected (uL): 1.0 Operator: jmg00346

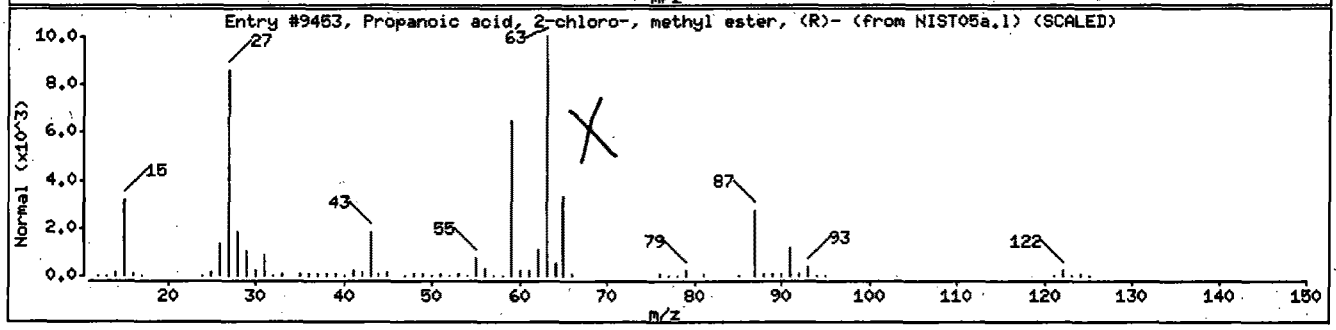
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Propanoic acid, 2-chloro-, methyl ester,	77287-29-7	NIST05a.l	9453	23	C4H7ClO2	122









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Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

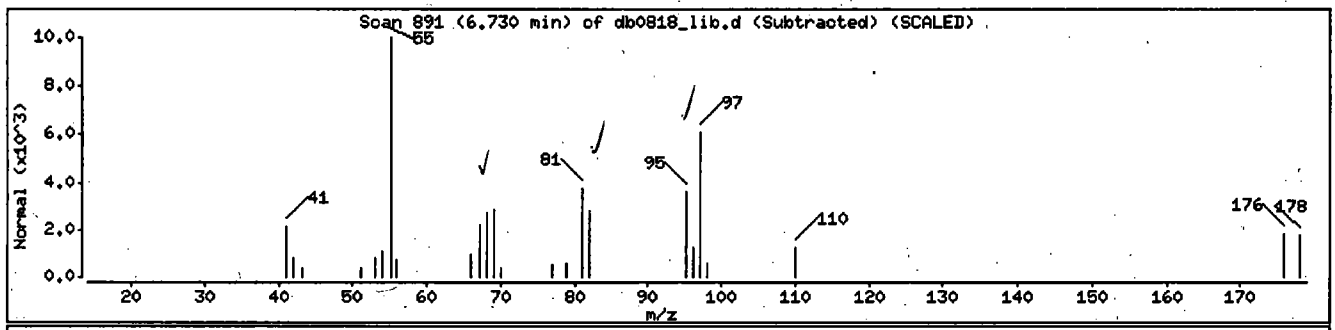
Volume Injected (uL): 1.0

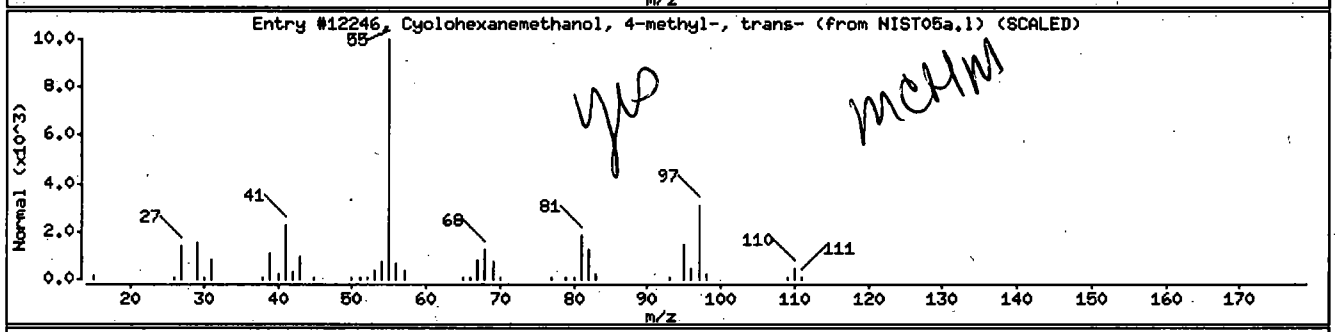
Operator: jmg00346

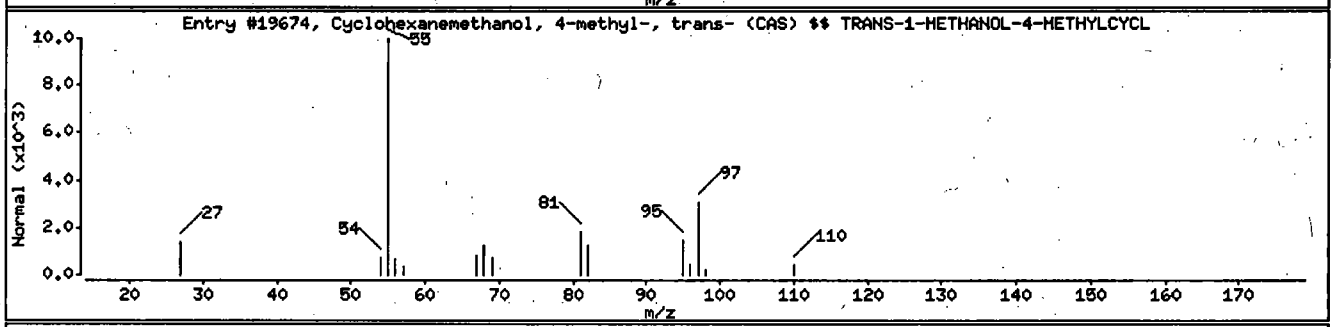
Column phase: J&W DB-5MS

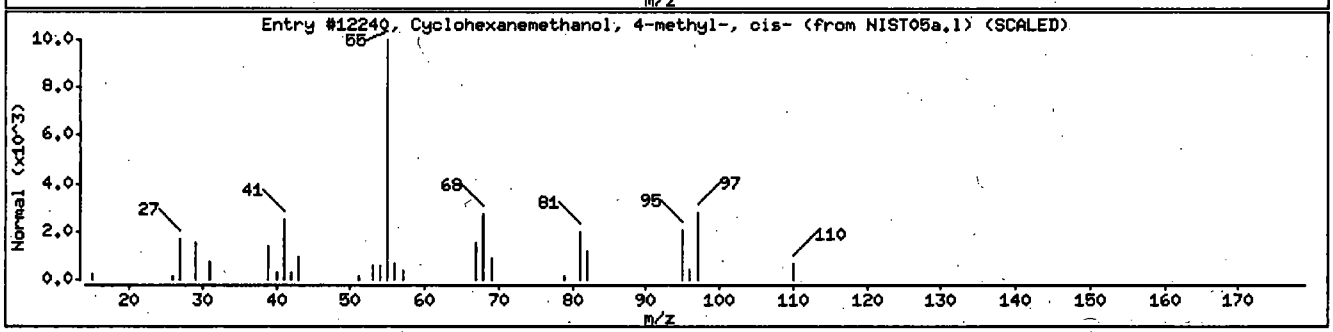
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	64	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	64	C8H16O	128
Cyclohexanemethanol, 4-methyl-, cis-	3937-48-2	NIST05a.l	12240	59	C8H16O	128









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

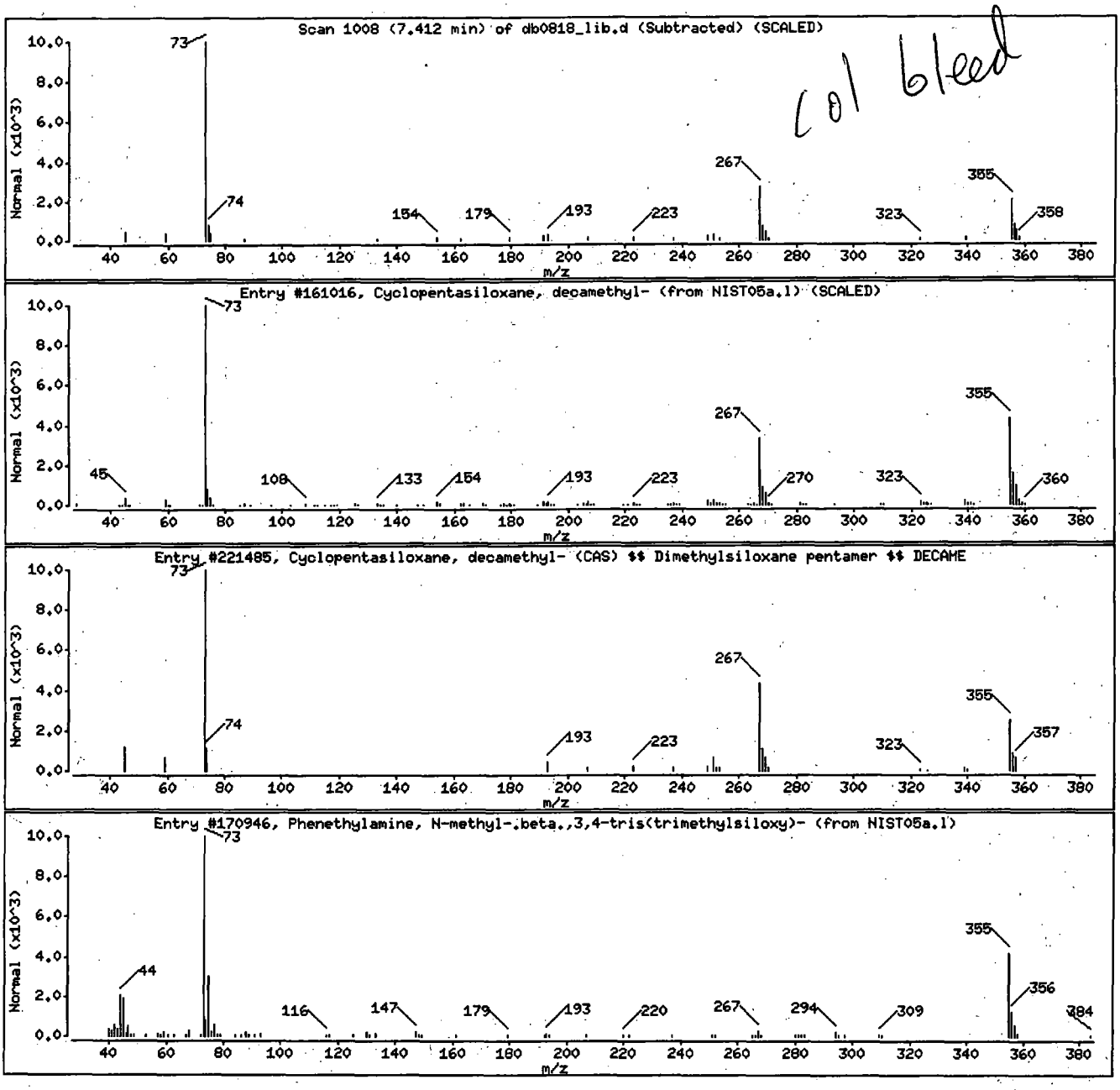
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	83	C10H30O5Si5	370
Phenethylamine, N-methyl-.beta.,3,4-tris	10538-85-9	NIST05a.l	170946	47	C18H37NO3Si3	399



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Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

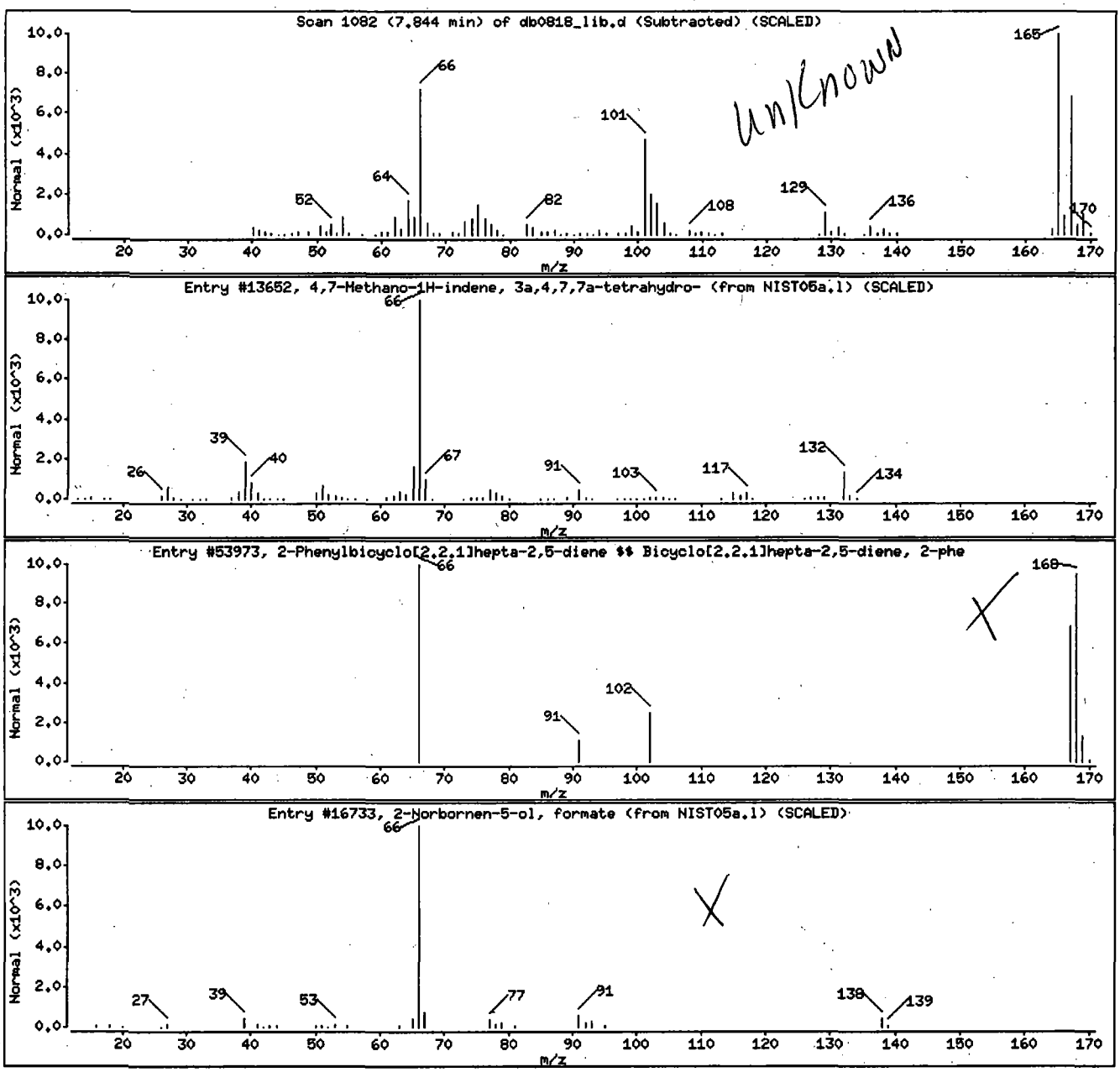
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	27	C10H12	132
2-Phenylbicyclo[2.2.1]hepta-2,5-diene $$	74437-39-1	WILEY275.l	53973	38	C13H12	168
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	30	C8H10O2	138



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

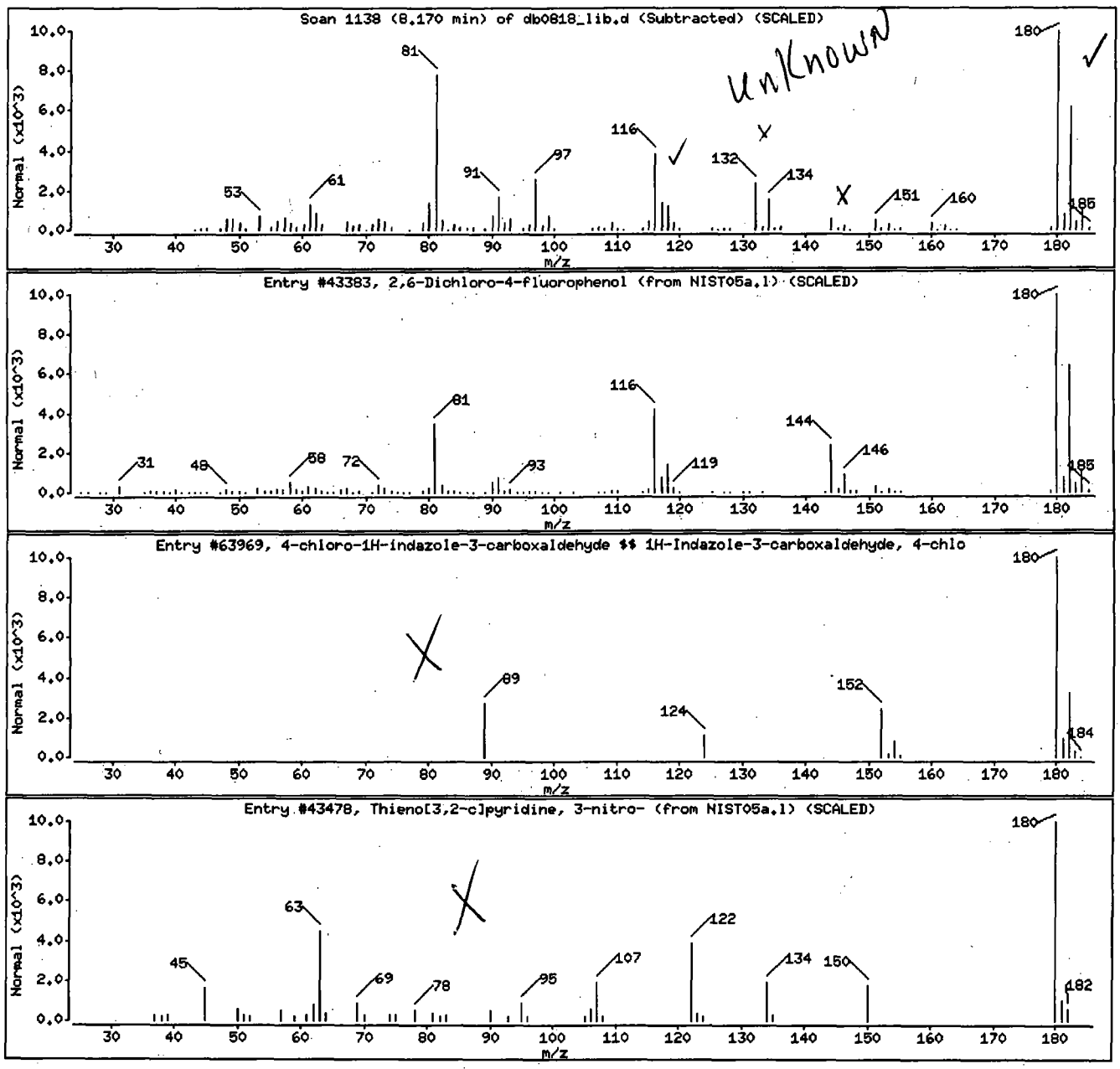
Client ID: SSKH1 Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	90	C6H3Cl2FO	180
4-chloro-1H-indazole-3-carboxaldehyde $$	102735-85-3	WILEY275.l	63969	16	C8H5ClN2O	180
Thieno[3,2-c]pyridine, 3-nitro-	28783-05-3	NIST05a.l	43478	14	C7H4N2O2S	180



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Data File: /chem/HP19760.i/14feb19.b/db0818_lib.d

Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

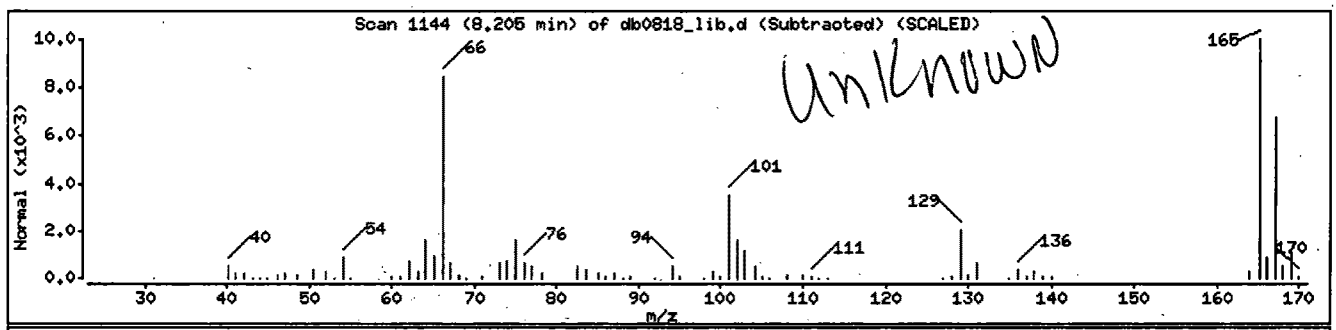
Volume Injected (uL): 1.0

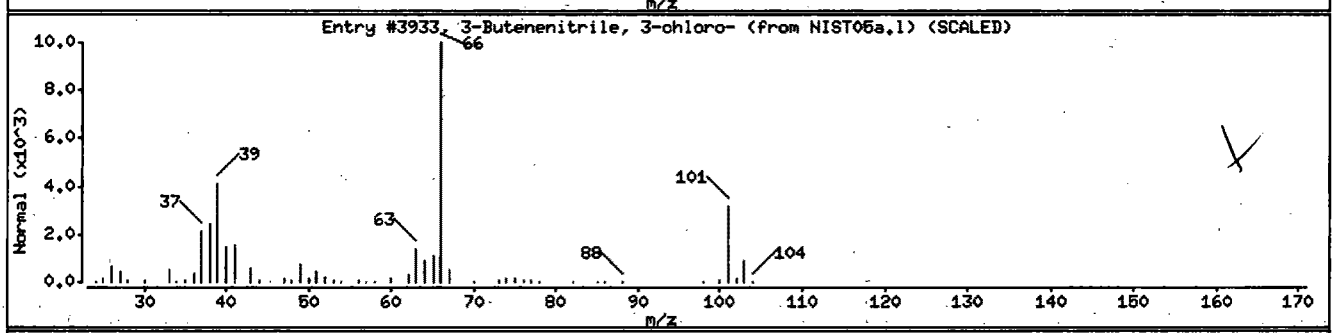
Operator: jmg00346

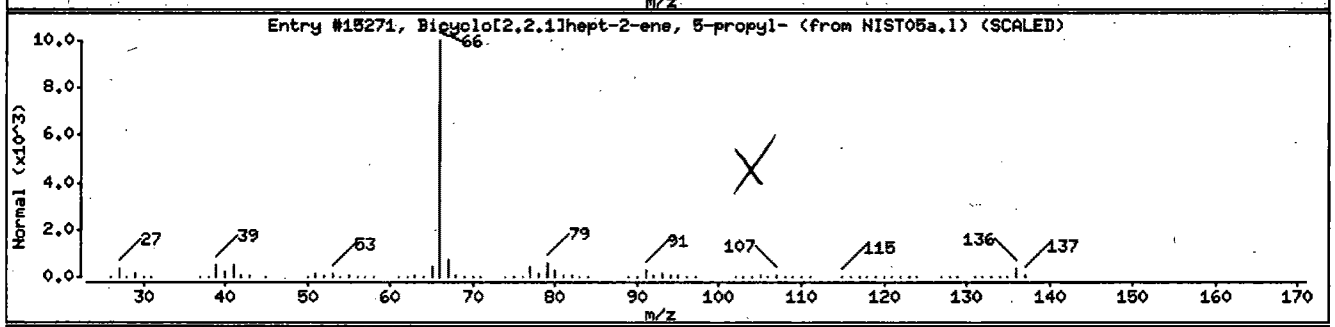
Column phase: J&W DB-5MS

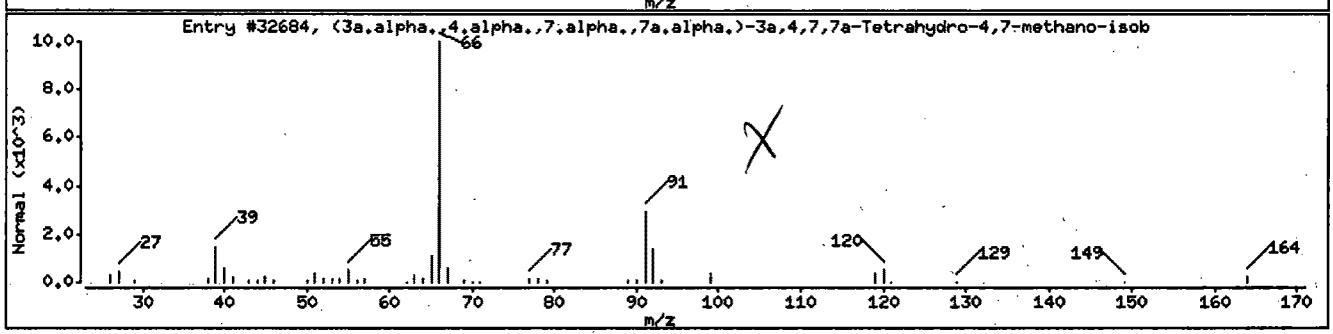
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136
(3a.alpha.,4.alpha.,7.alpha.,7a.alpha.)-	129-64-6	NIST05a.l	32684	47	C9H8O3	164









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Date : 19-FEB-2014 15:44

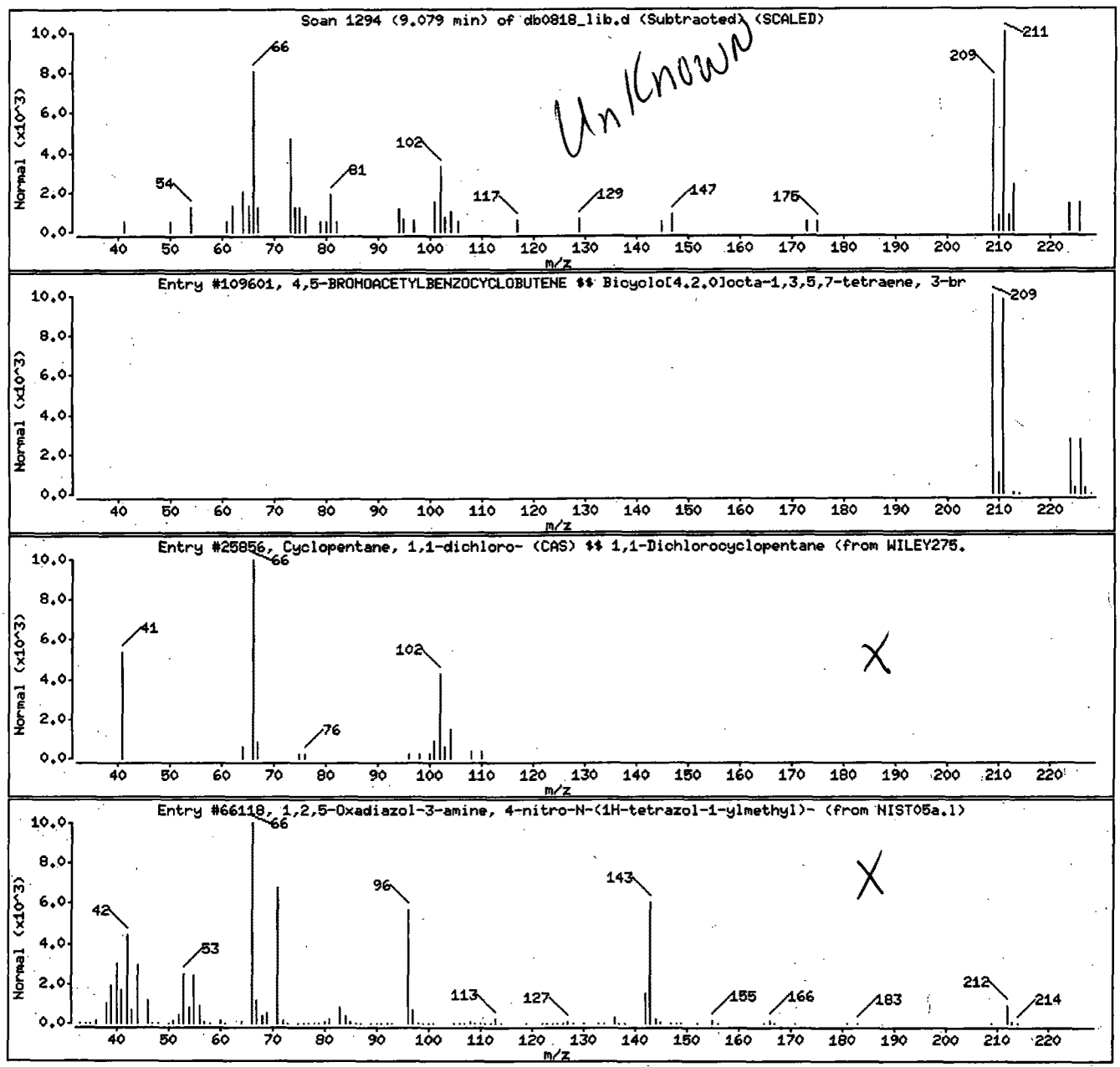
Client ID: SSKH1 Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63506-25-2	WILEY275.l	109601	80	C10H9BrO	224
Cyclopentane, 1,1-dichloro- (CAS) $$ 1,1	31038-06-9	WILEY275.l	25856	43	C5H8Cl2	138
1,2,5-Oxadiazol-3-amine, 4-nitro-N-(1H-t	1000277-41-1	NIST05a.l	66118	32	C4H4N8O3	212



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Date : 19-FEB-2014 15:44

Client ID: SSKH1

Instrument: HP19760.i

Sample Info: SSKH1;7365701;1;0;SAMPLE;;;

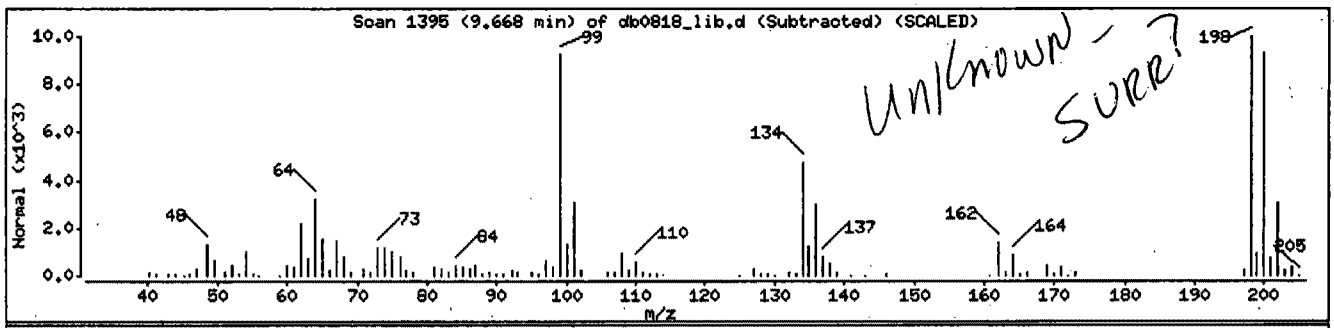
Volume Injected (uL): 1.0

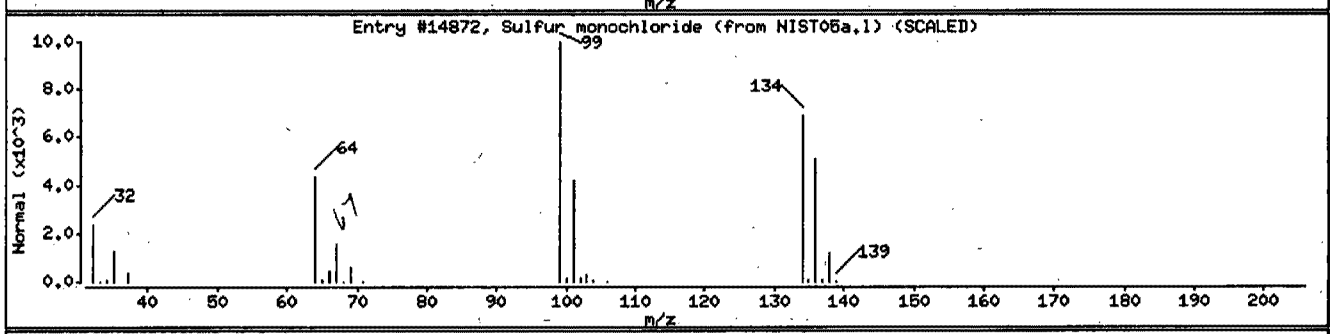
Operator: jmg00346

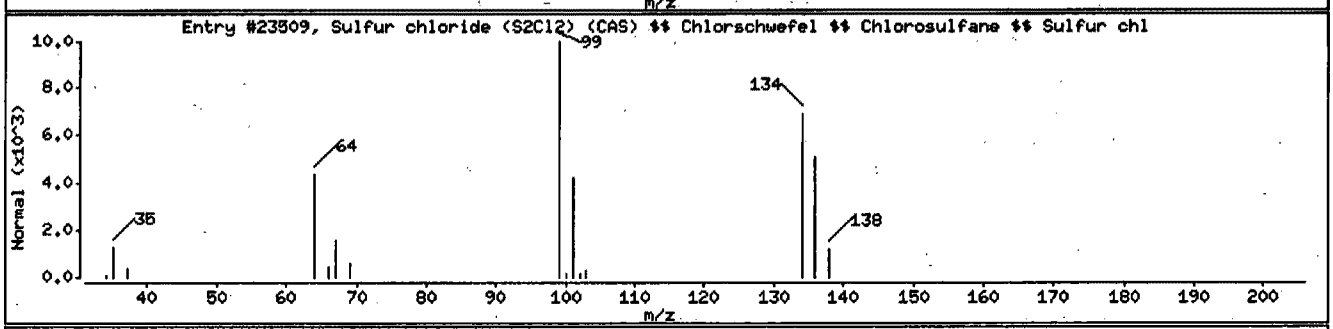
Column phase: J&W DB-5MS

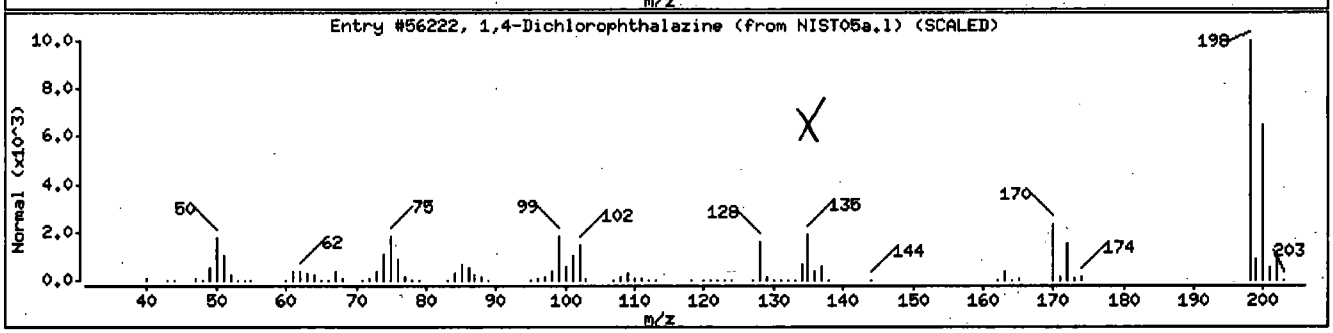
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Sulfur chloride (S2Cl2) (CAS) ** Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	35	C8H4Cl2N2	198



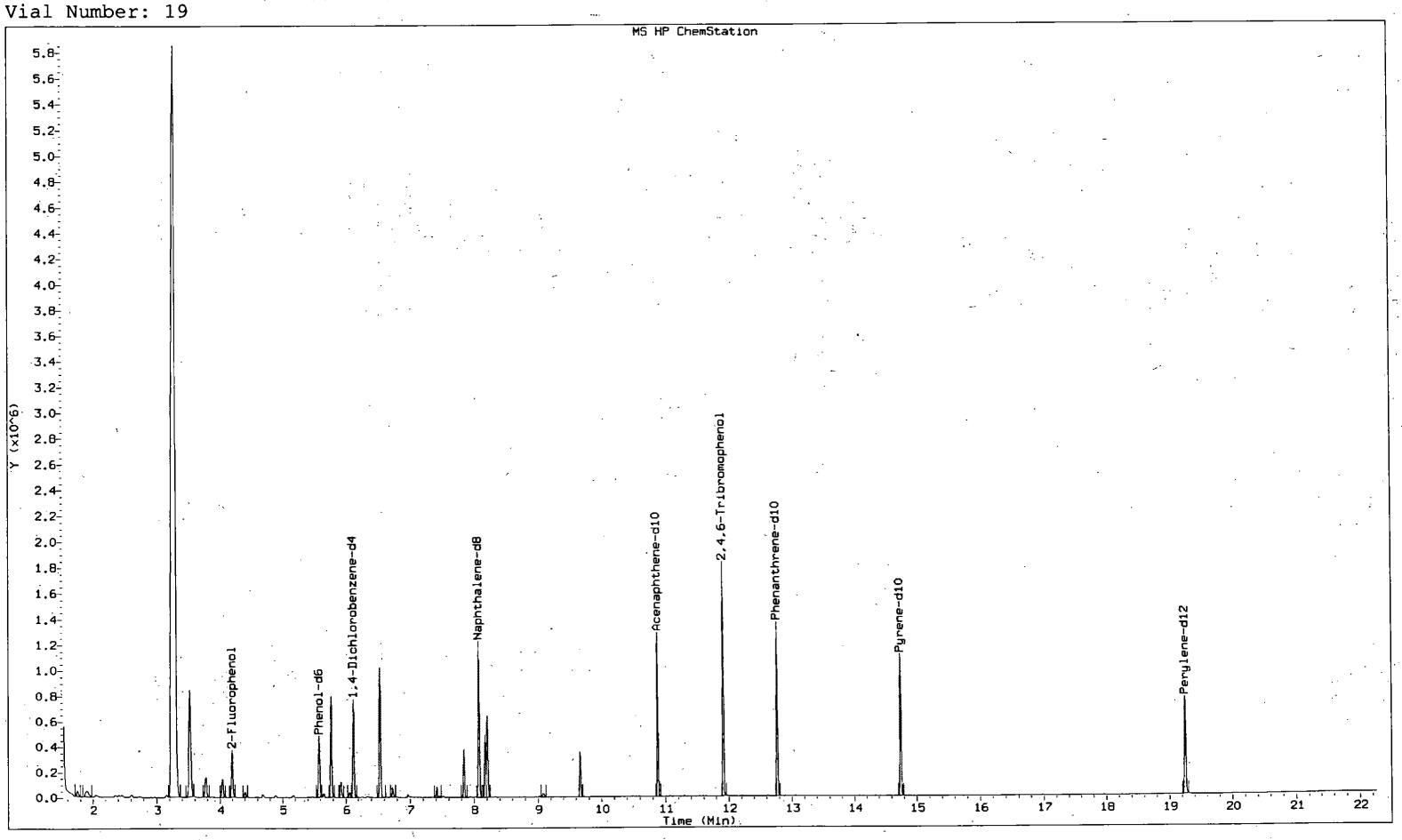






Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:05.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb18a.b/db0778_lib.d
Operator : ceb05247
Acquired : 19-FEB-2014 04:57
Instrument : HP19760.i
Sample Name: H2011;7365713;1;0;SAMPLE;;;
Misc Info : 14049WAC;wva;;1052;1000;0;db0774;13166;
Vial Number: 19



Lancaster Labs

Data file : /chem/HP19760.i/14feb18a.b/db0778_lib.d
Lab Smp Id: 7365713 Client Smp ID: H2011
Inj Date : 19-FEB-2014 04:57
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H2011;7365713;1;0;SAMPLE;;;
Misc Info : 14049WAC;wva;;1052;1000;0;db0774;13166;
Comment : Max. number of TICs to report is 50, 18 TICs were found initially.
Method : /chem/HP19760.i/14feb18a.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 17:17 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 19
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1052.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.124	1111961	10.000
* 48 Naphthalene-d8	8.077	1723017	10.000
* 83 Acenaphthene-d10	10.880	1479740	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.747	88678	0.79749207	0.75807	90	NIST05a.l	31325	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.904	177702	1.59809896	1.51910	55	NIST05a.l	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.303	22733525	204.445220	194.33956	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.524	1643307	14.7784471	14.04795	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.775	316889	2.84982133	2.70895	37	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.043	254690	2.29046045	2.17724	38	NIST05a.l	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.399	67206	0.60439187	0.57451	64	NIST05a.l	33655	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.774	1122809	10.0975503	9.59843	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.926	189286	1.70226675	1.61812	95	NIST05a.l	18485	21
Oxirane, ethenyl-					CAS #: 930-22-3		
6.060	51432	0.46253173	0.43966	7	NIST05a.l	525	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.538	1468319	13.2047619	12.55205	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.730	109111	0.98124682	0.93274	59	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.412	110494	0.64128111	0.60958	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.843	470895	2.73296619	2.59787	27	NIST05a.l	13656	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.170	566263	3.28646343	3.12401	87	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.205	760481	4.41365729	4.19549	50	NIST05a.l	3933	48

Target compound.
Do not report.
ajs00193 03/01/2014

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc					CAS #: 63506-25-2		
9.079	49118	0.28506924	0.27097	80	WILEY275.1	109601	48(ML)
Sulfur monochloride					CAS #: 10025-67-9		
9.668	403303	2.72549977	2.59077	38	NIST05a.1	14872	83(L)

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

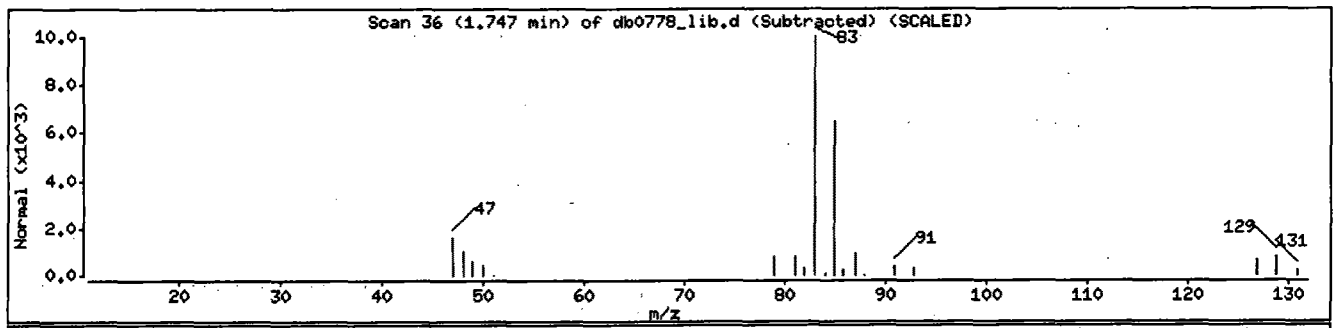
Volume Injected (uL): 1.0

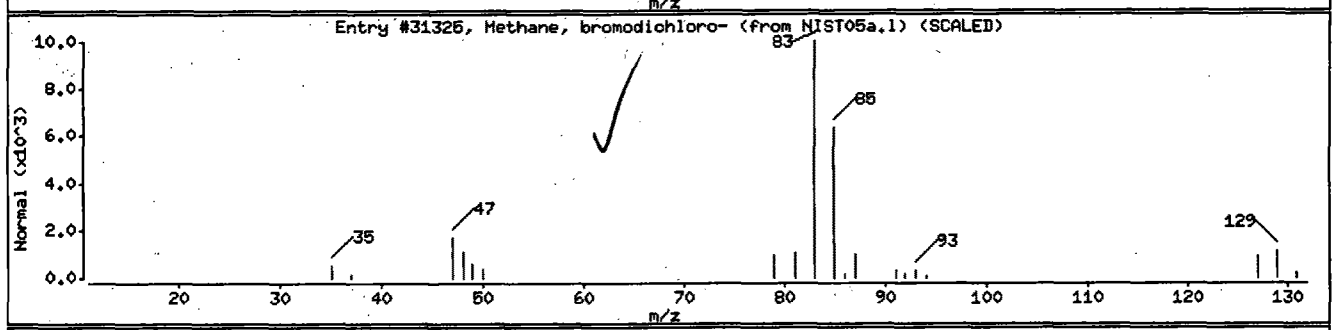
Operator: ceb05247

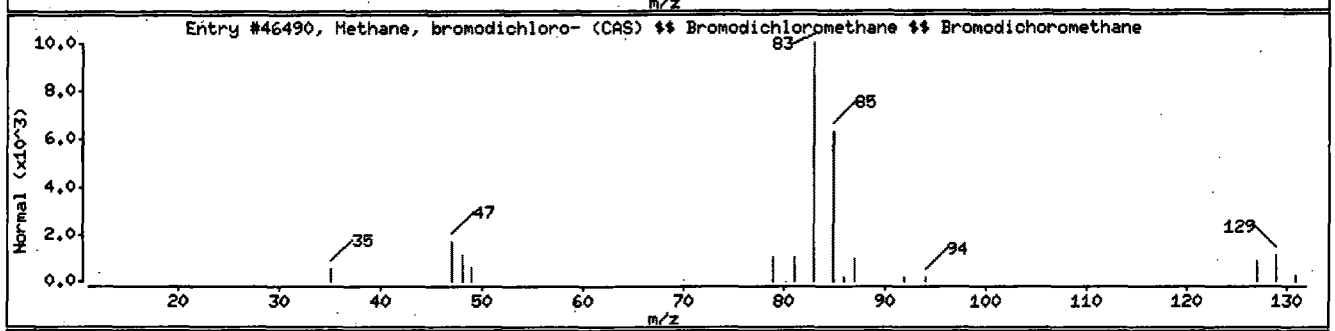
Column phase: J&W DB-5MS

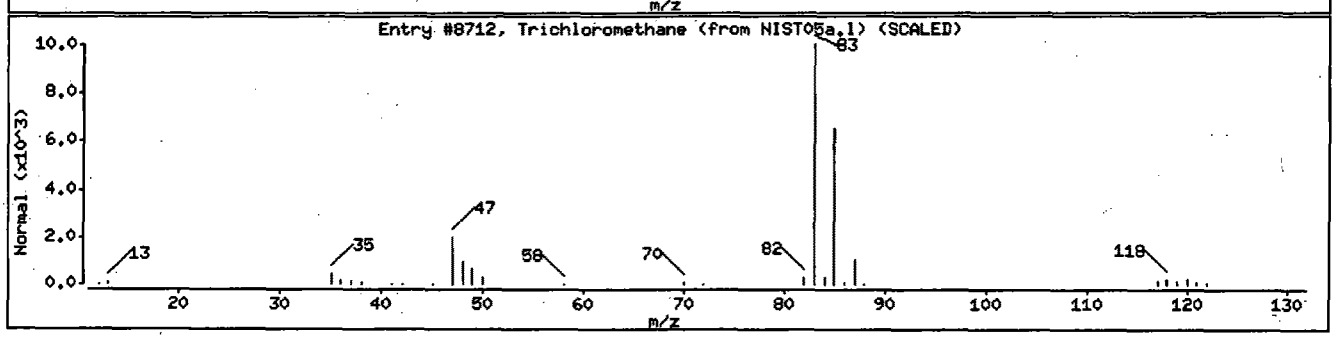
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









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Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

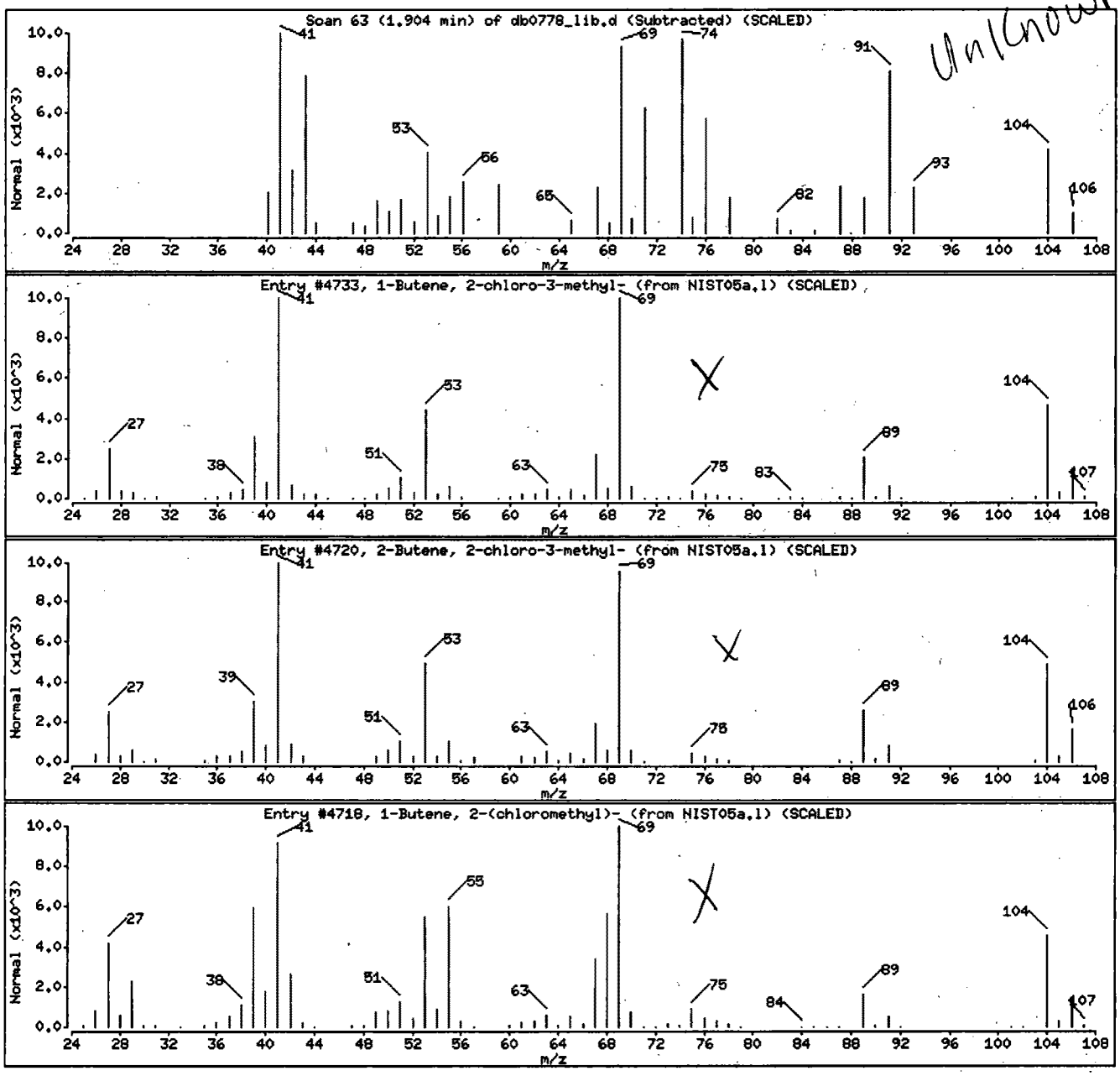
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	56	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	46	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4718	46	C5H9Cl	104



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Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

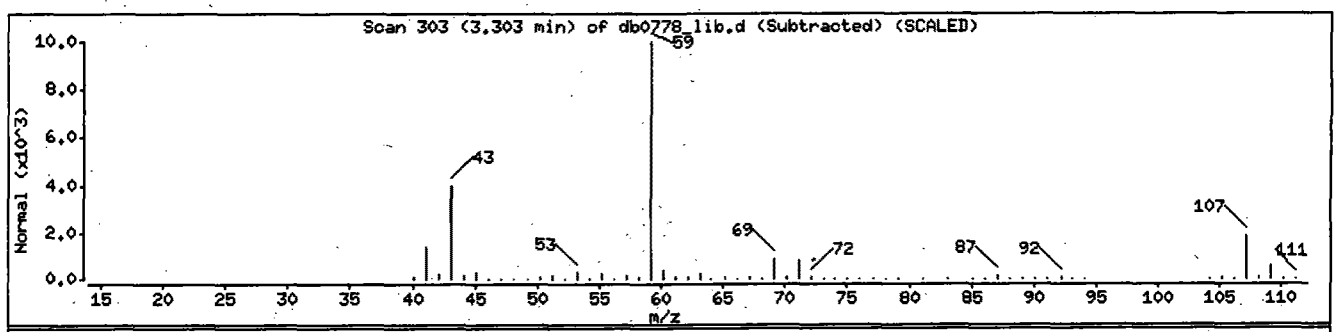
Volume Injected (uL): 1.0

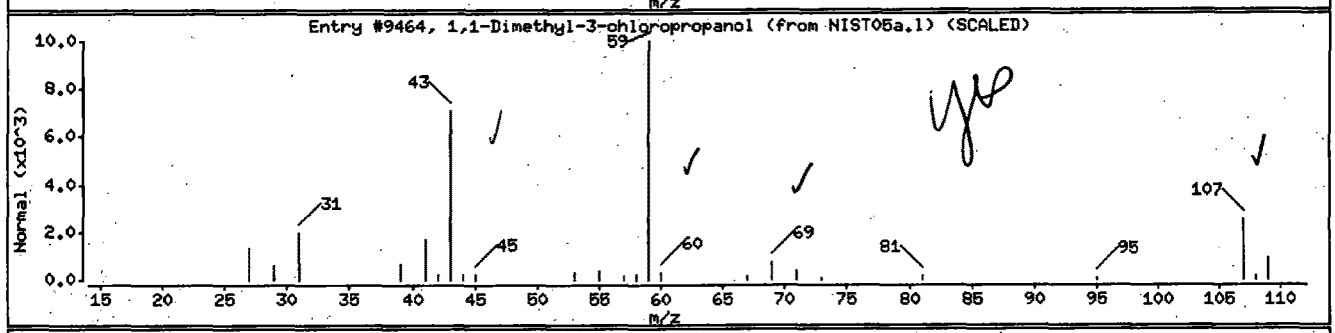
Operator: ceb05247

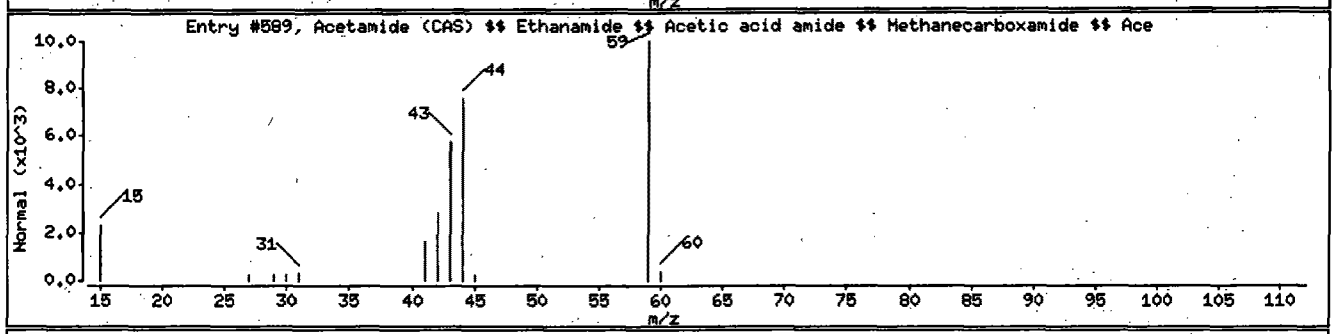
Column phase: J&W DB-5MS

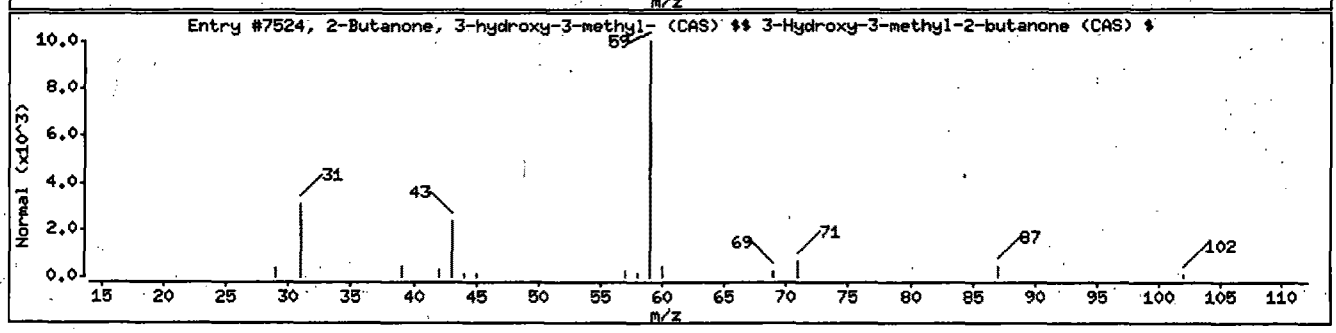
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









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Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

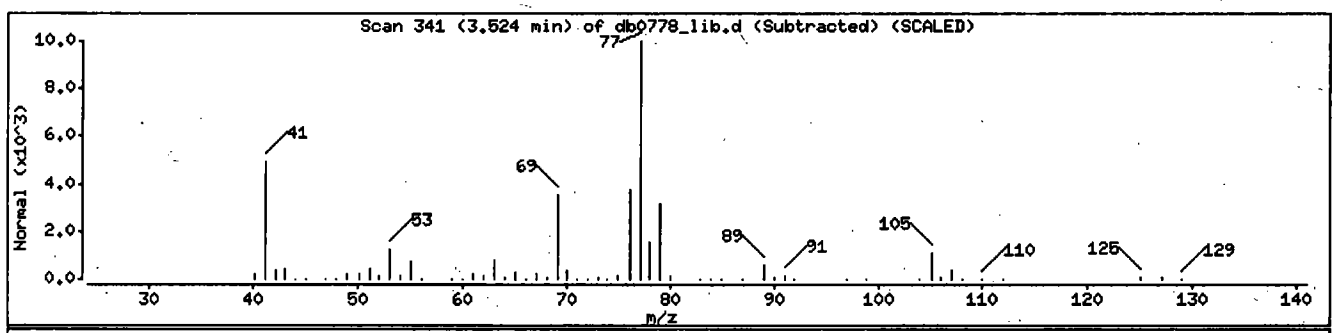
Volume Injected (uL): 1.0

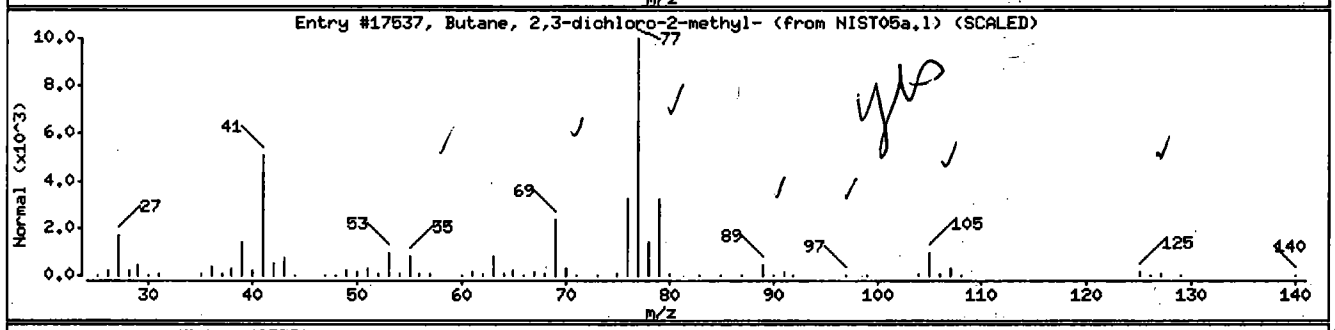
Operator: ceb05247

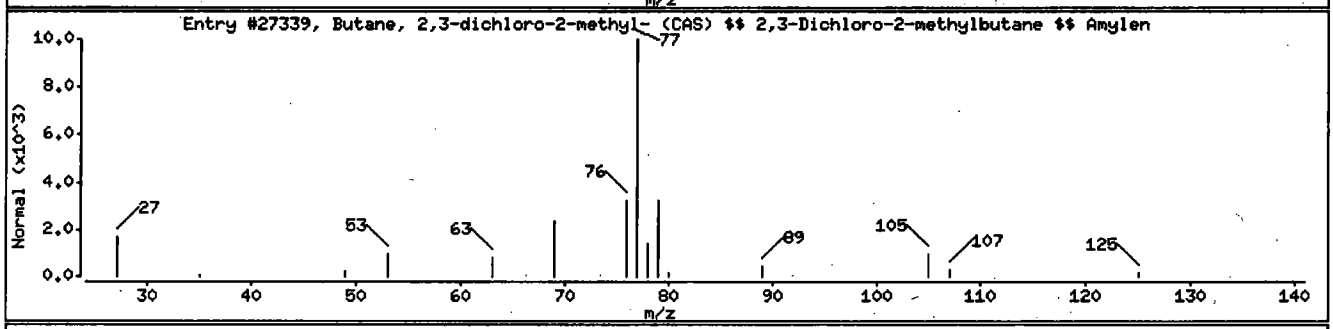
Column phase: J&W DB-5MS

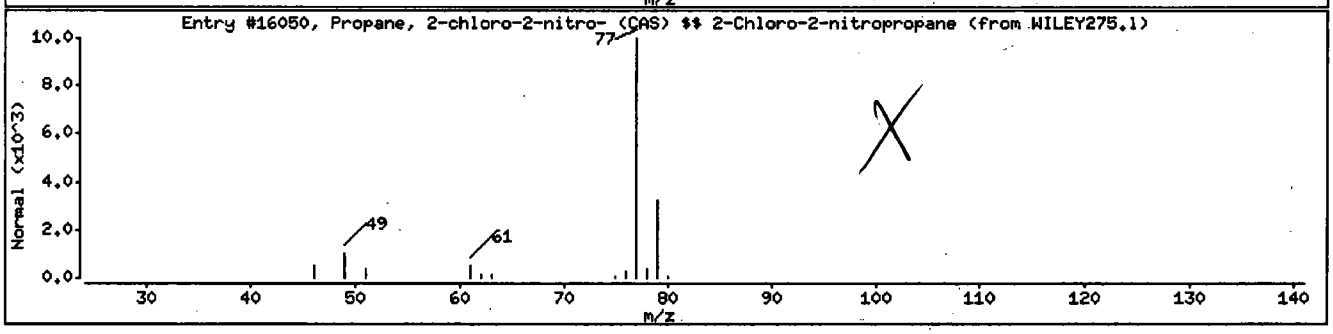
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









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Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

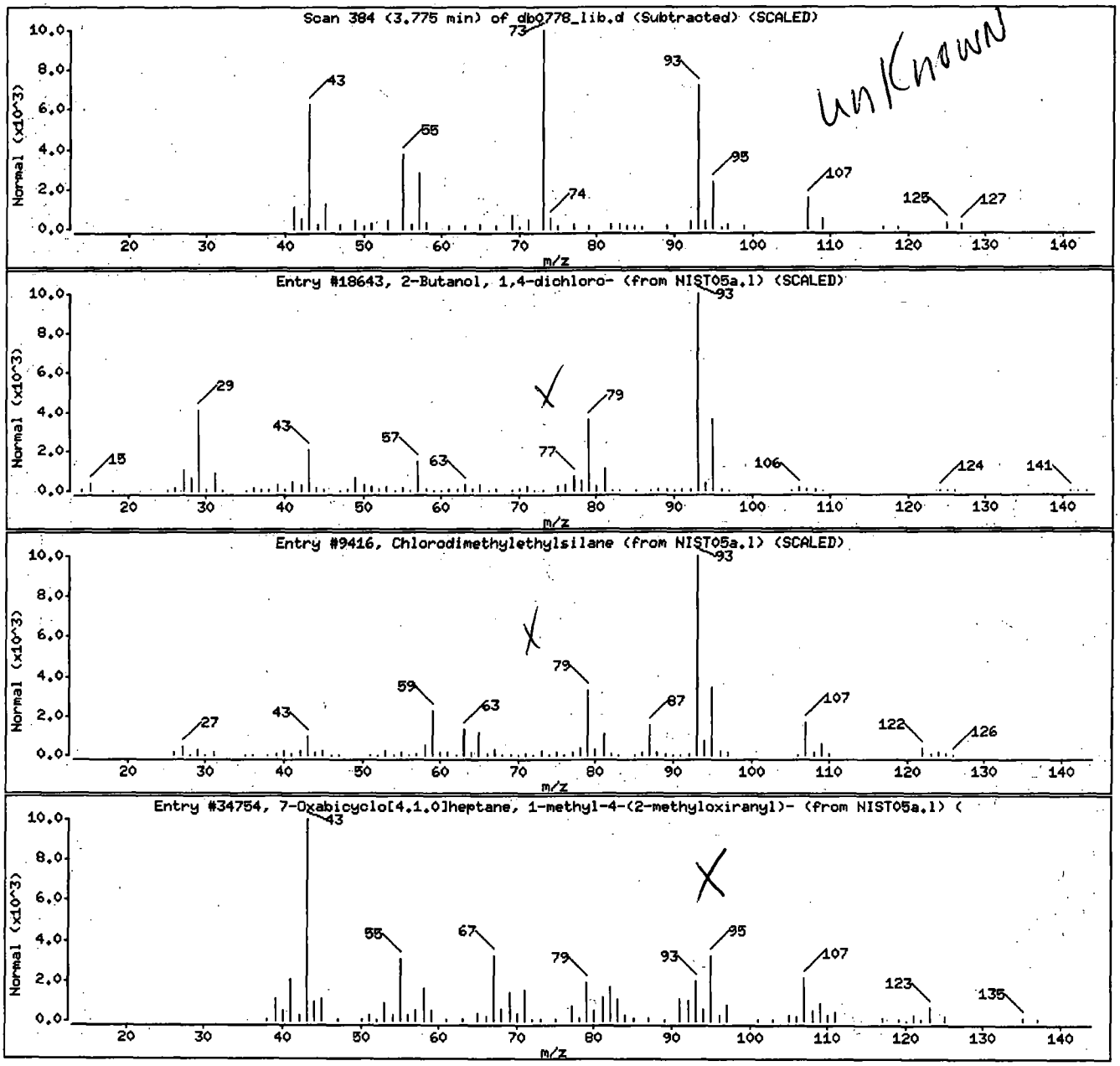
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	37	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	NIST05a.l	34754	12	C10H16O2	168



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Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

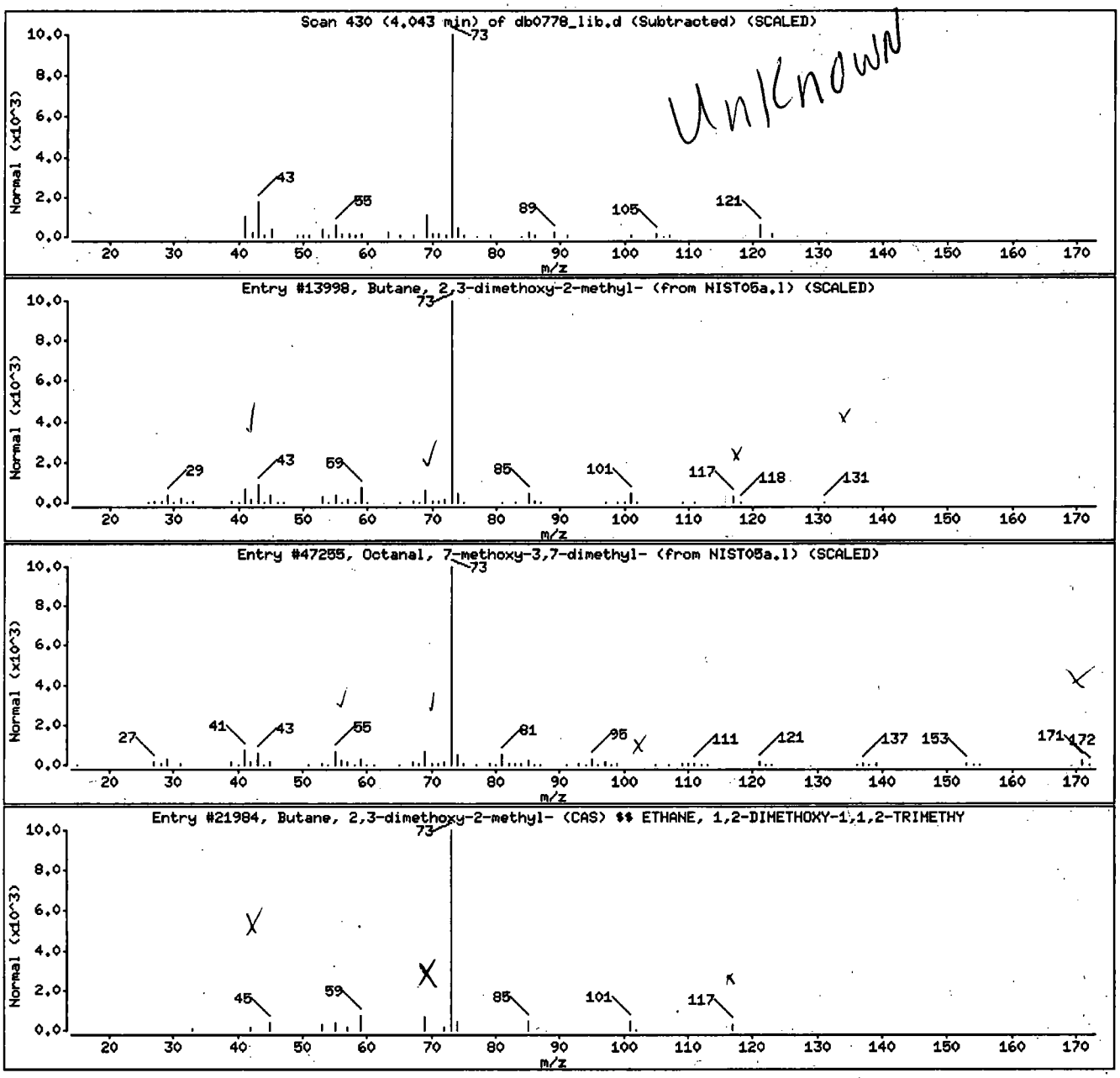
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	38	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	38	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132



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Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

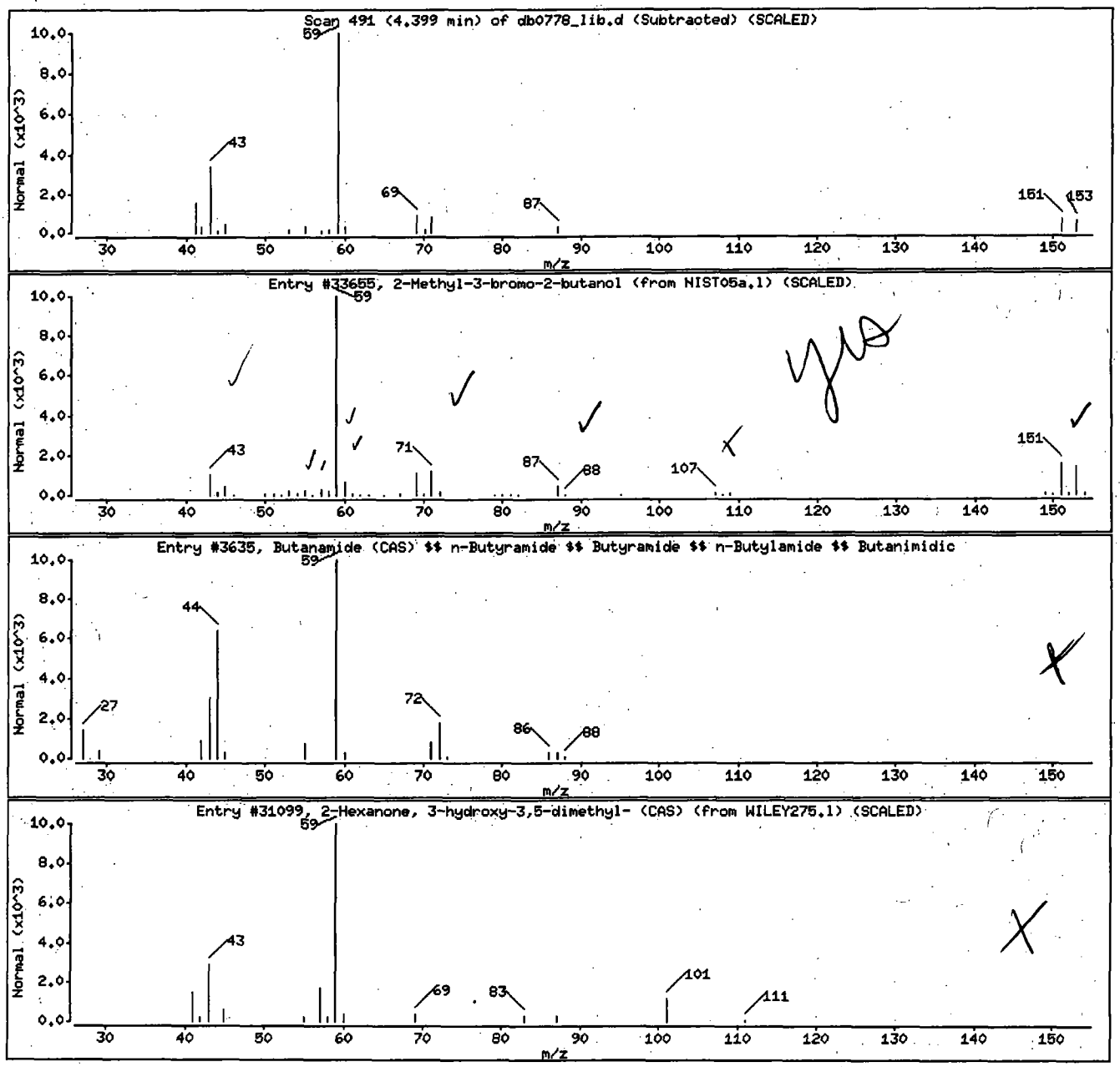
Volume Injected (uL): 1.0

Operator: oeb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	64	C5H11BrO	166
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3635	64	C4H9NO	87
2-Hexanone, 3-hydroxy-3,5-dimethyl- (CAS	6321-14-8	WILEY275.l	31099	50	C8H16O2	144



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Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

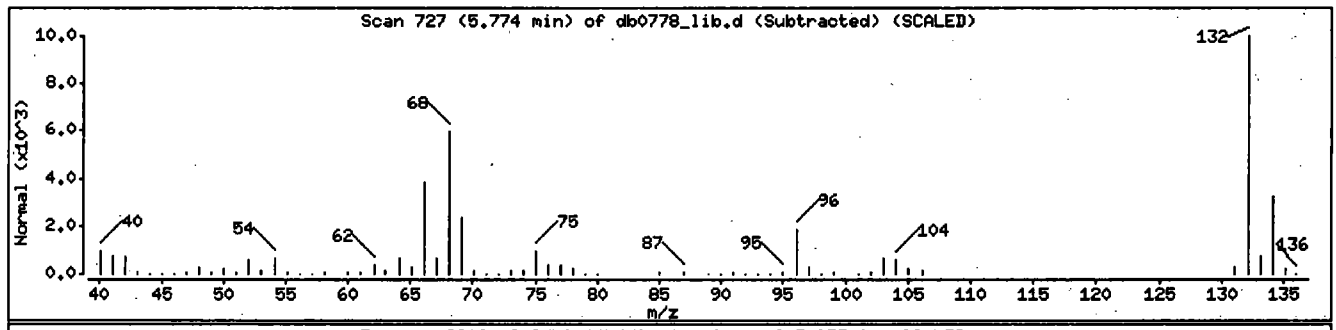
Volume Injected (uL): 1.0

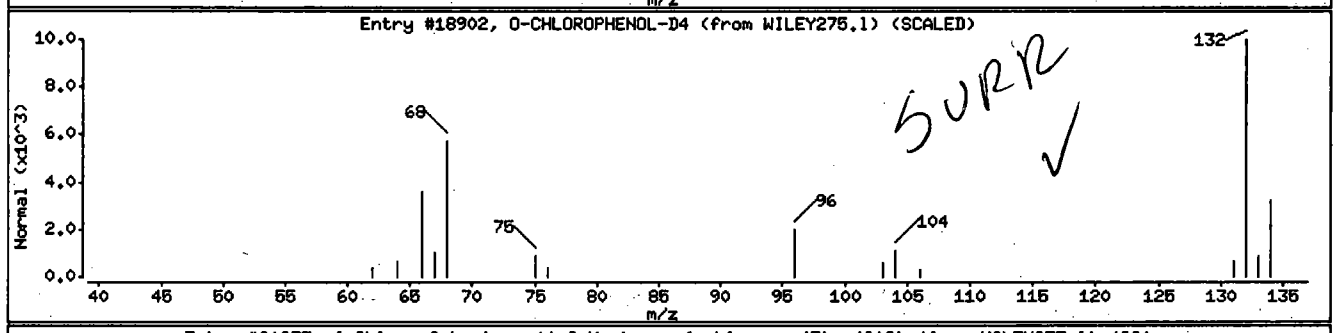
Operator: ceb05247

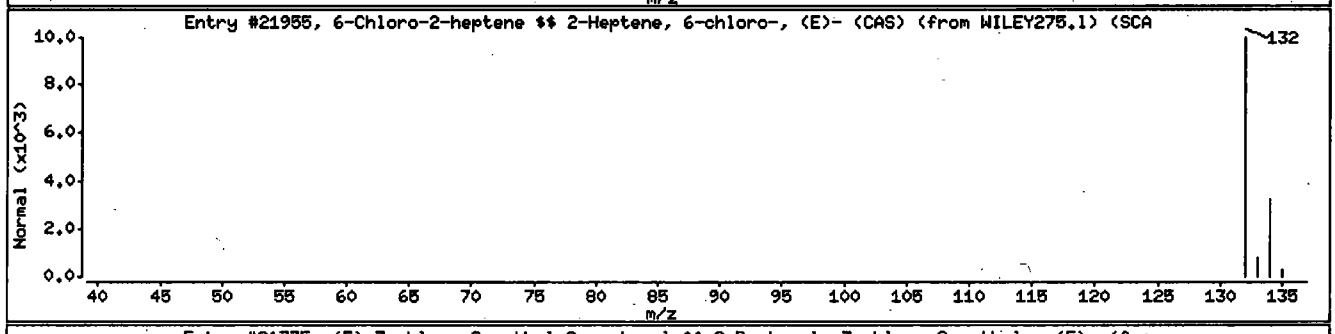
Column phase: J&W DB-5MS

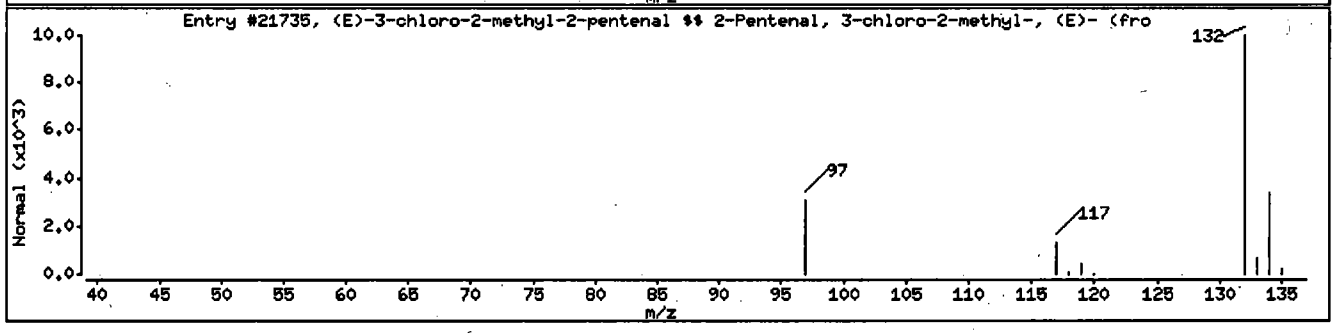
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132









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Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

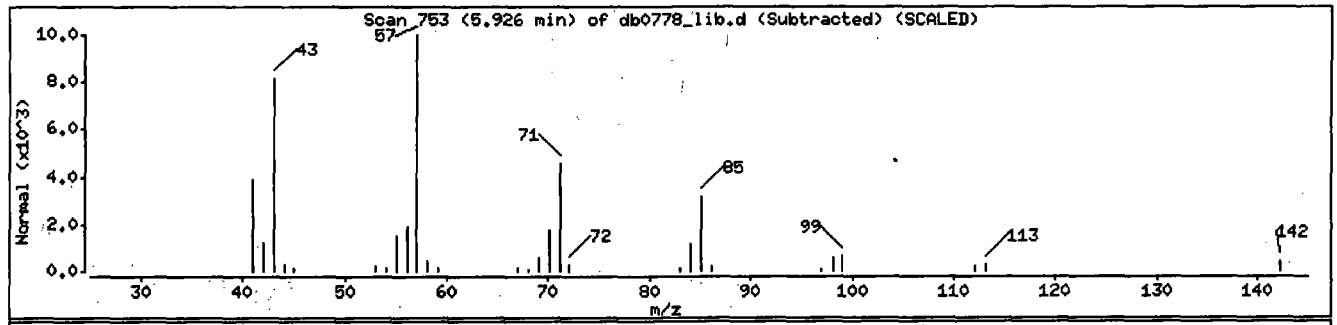
Volume Injected (uL): 1.0

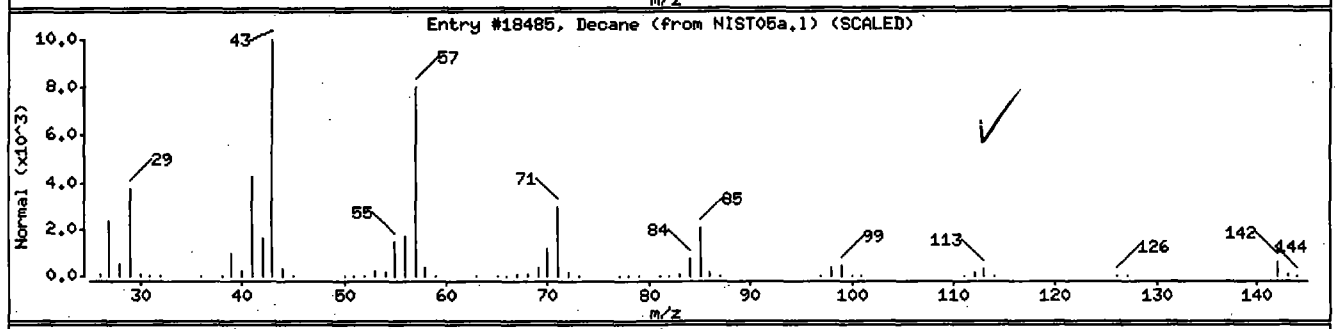
Operator: ceb05247

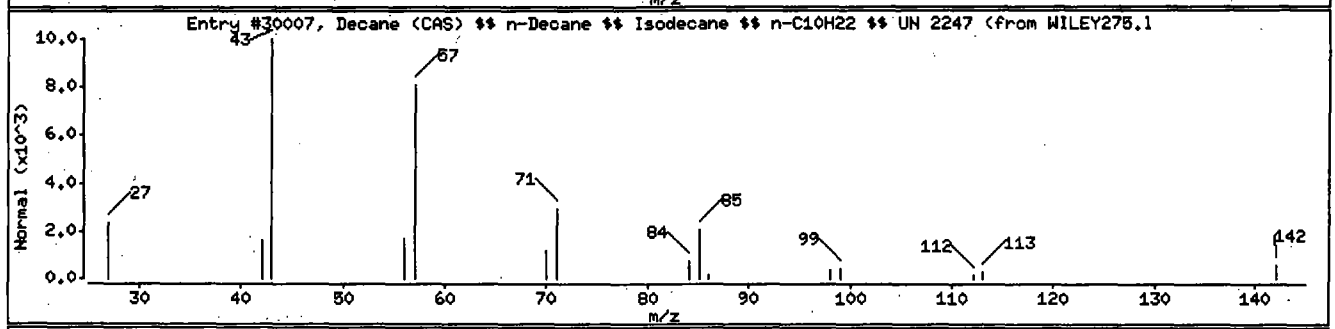
Column phase: J&W DB-5MS

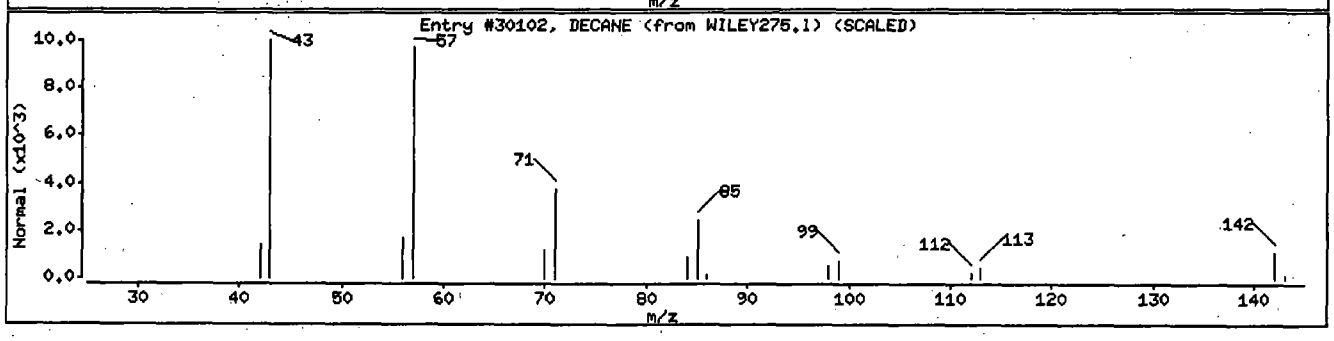
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

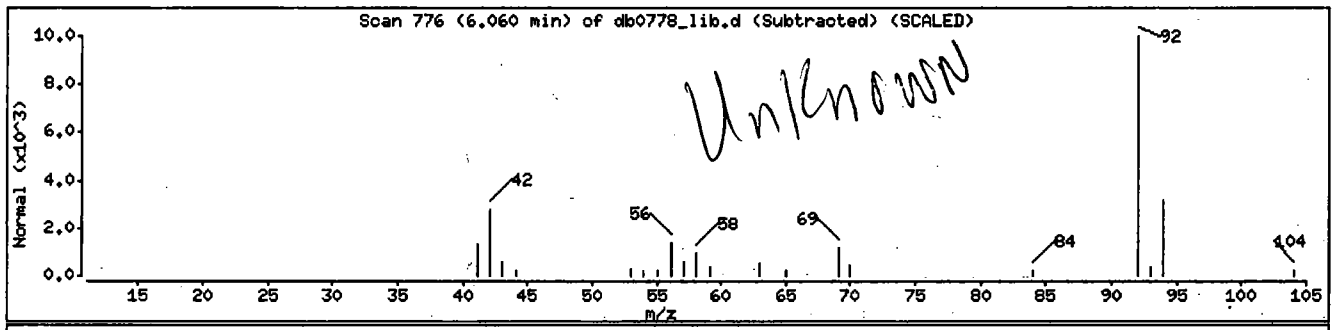
Volume Injected (uL): 1.0

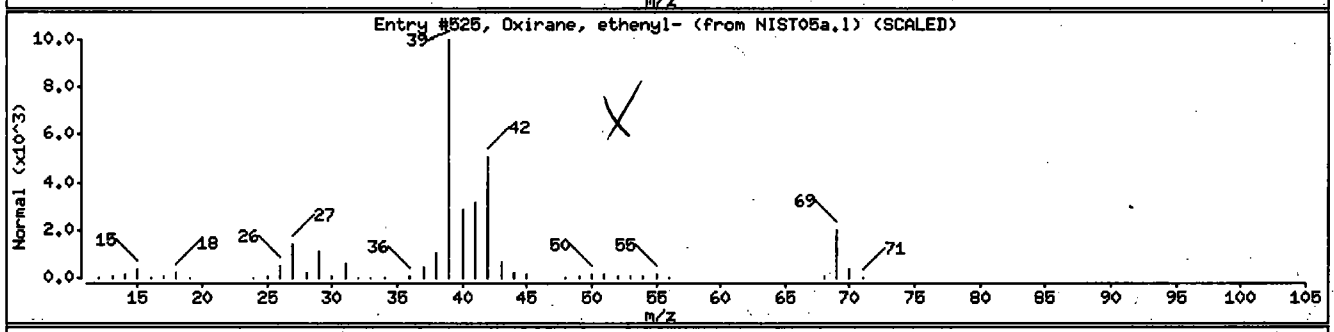
Operator: ceb05247

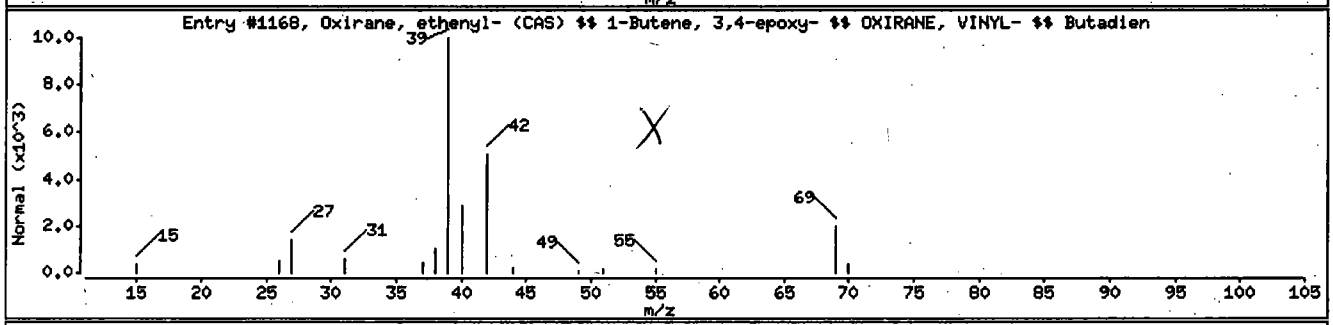
Column phase: J&W DB-5MS

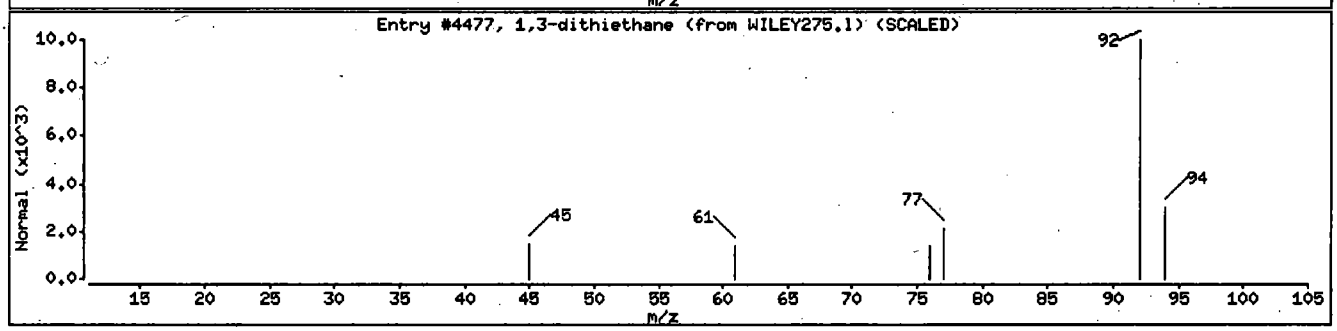
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Oxirane, ethenyl-	930-22-3	NIST05a.l	525	7	C4H6O	70
Oxirane, ethenyl- (CAS) $$ 1-Butene, 3,4	930-22-3	WILEY275.l	1168	7	C4H6O	70
1,3-dithiethane	0-00-0	WILEY275.l	4477	5	C2H4S2	92









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

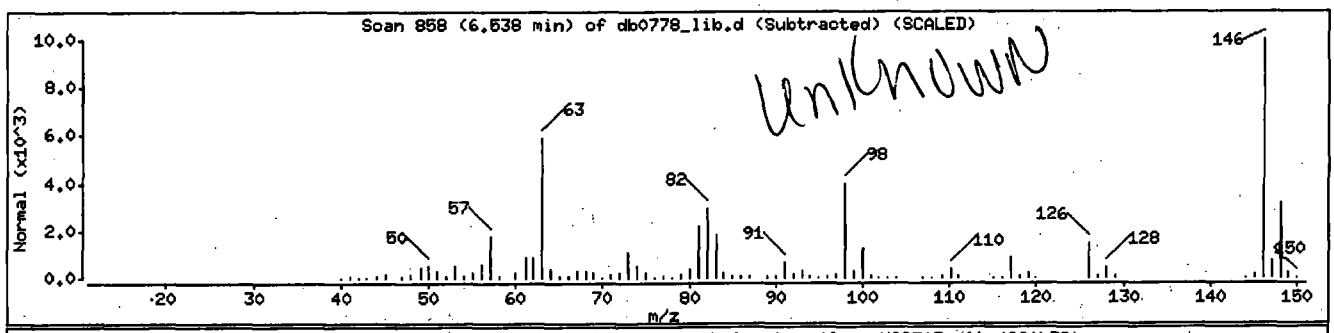
Volume Injected (uL): 1.0

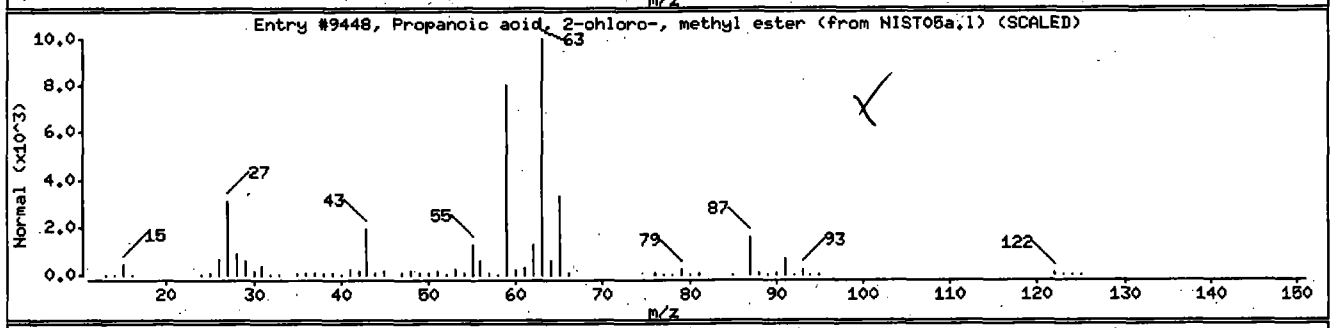
Operator: ceb05247

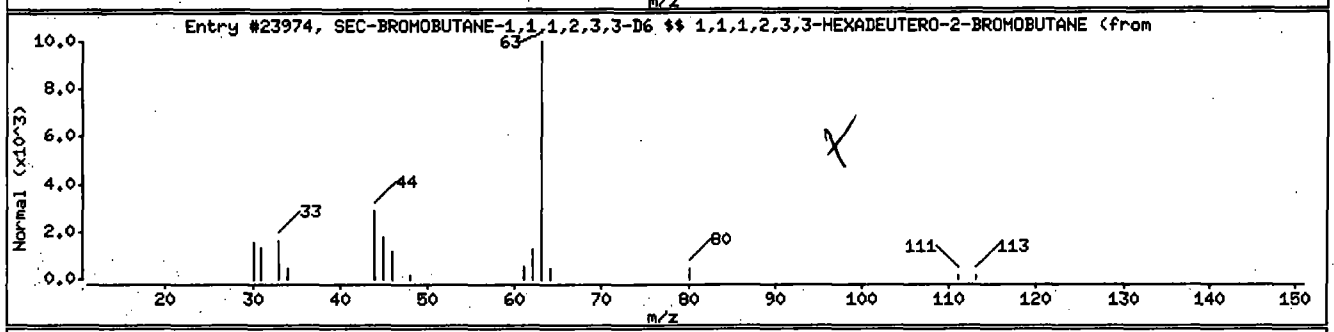
Column phase: J&W DB-5MS

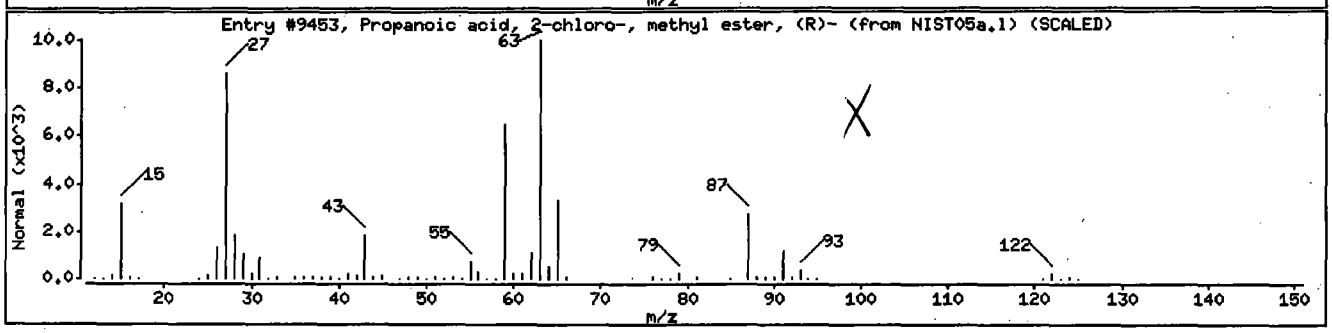
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Propanoic acid, 2-chloro-, methyl ester,	77287-29-7	NIST05a.l	9453	23	C4H7ClO2	122









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

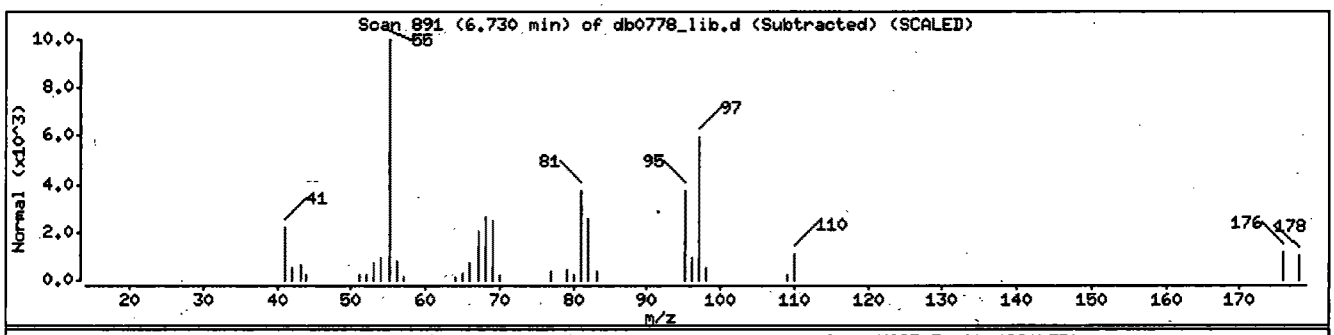
Volume Injected (uL): 1.0

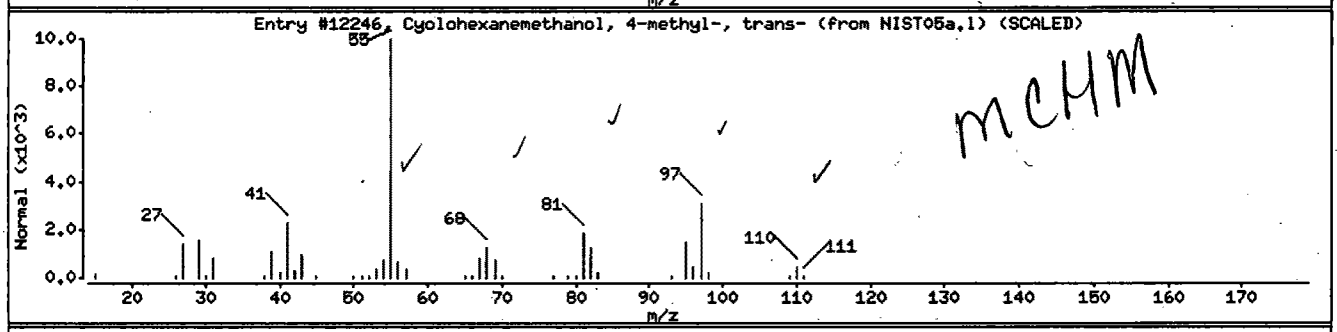
Operator: ceb05247

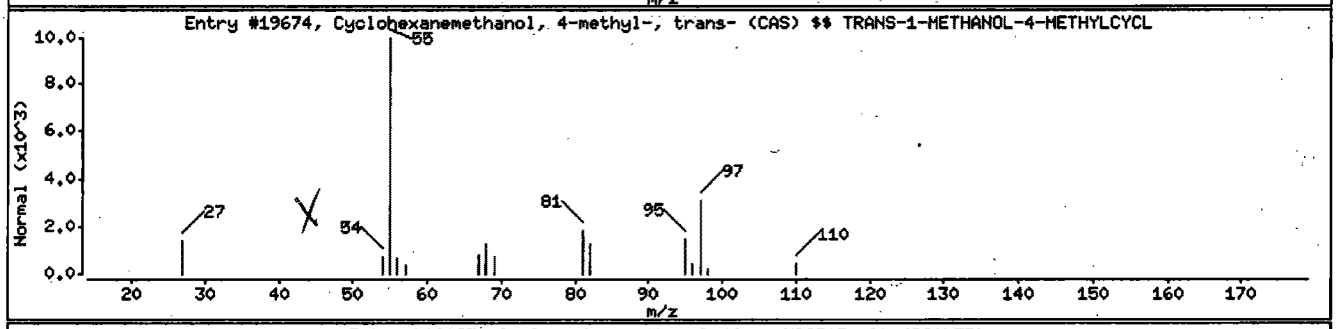
Column phase: J&W DB-5MS

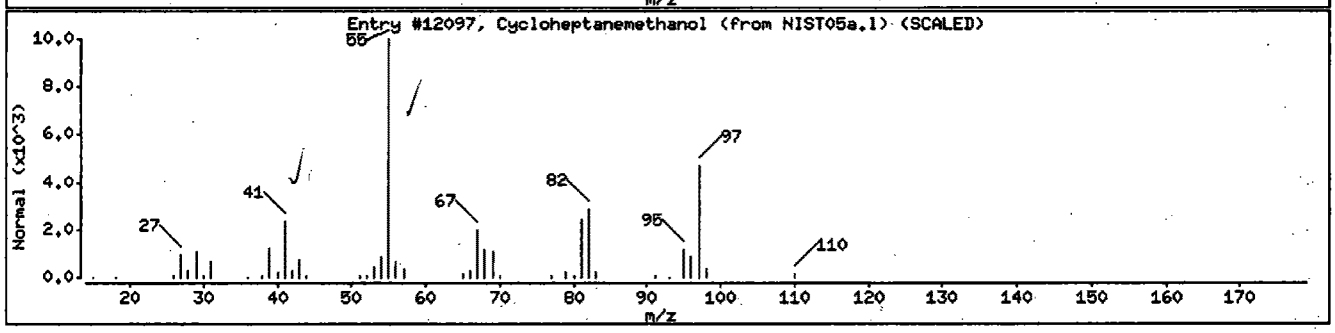
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	59	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	59	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12097	53	C8H16O	128









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

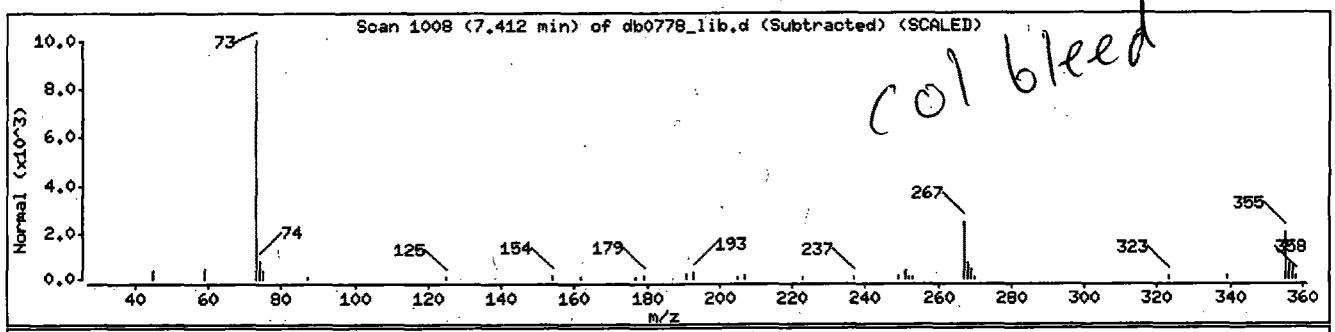
Volume Injected (uL): 1.0

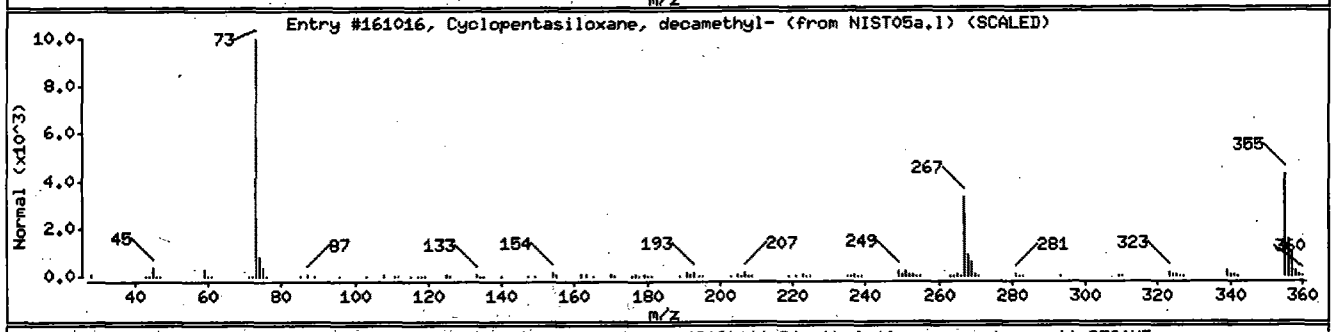
Operator: ceb05247

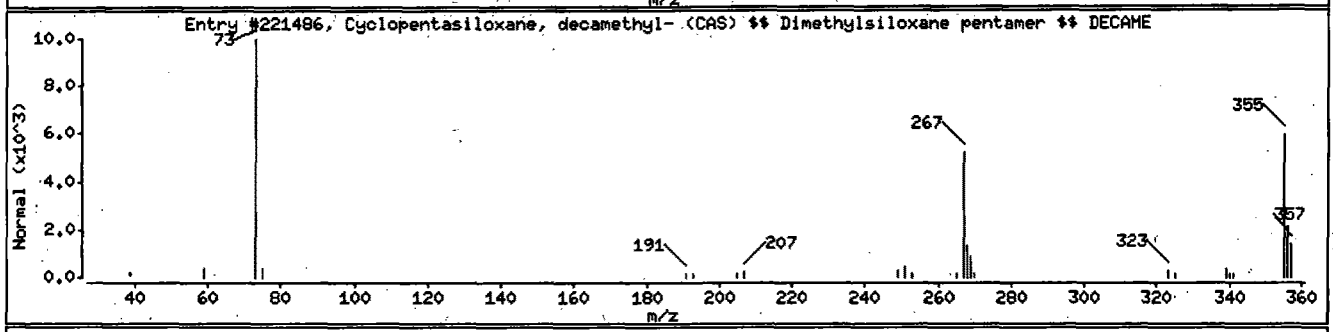
Column phase: J&W DB-5MS

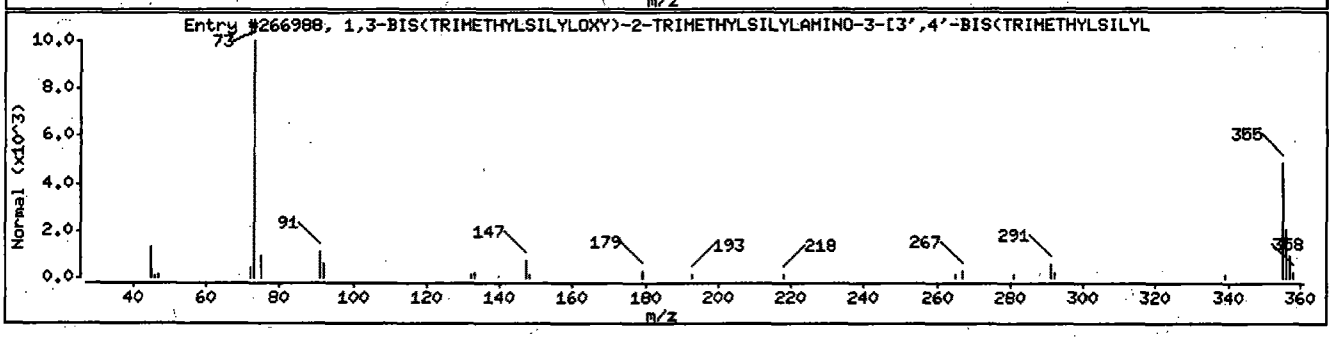
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
1,3-BIS(TRIMETHYLSILYLOXY)-2-TRIMETHYLSI	0-00-0	WILEY275.l	266988	38	C24H51NO5Si5	573









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

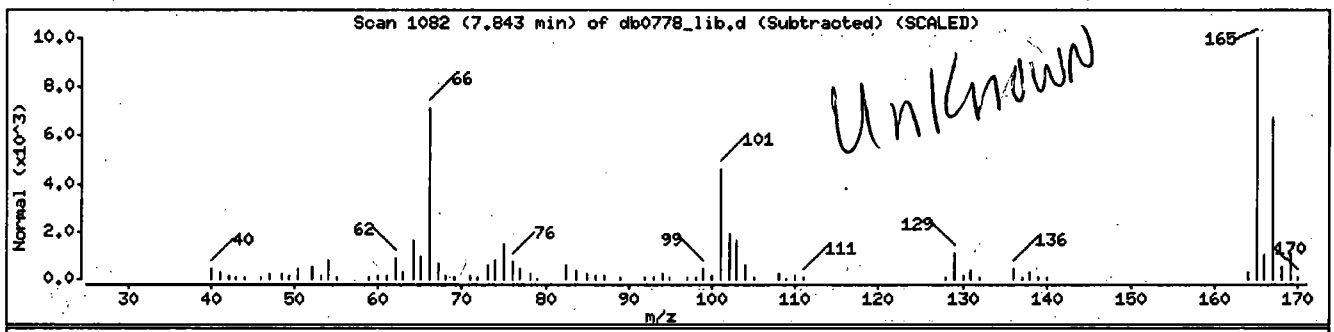
Volume Injected (uL): 1.0

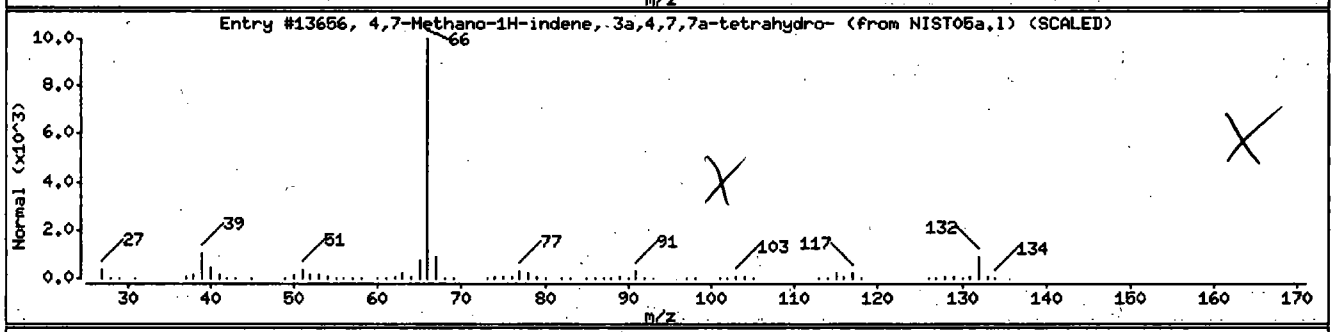
Operator: ceb05247

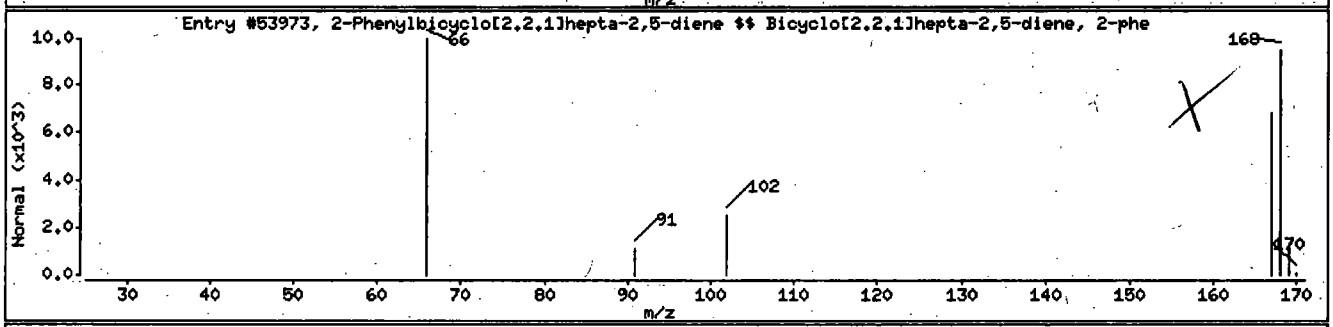
Column phase: J&W DB-5MS

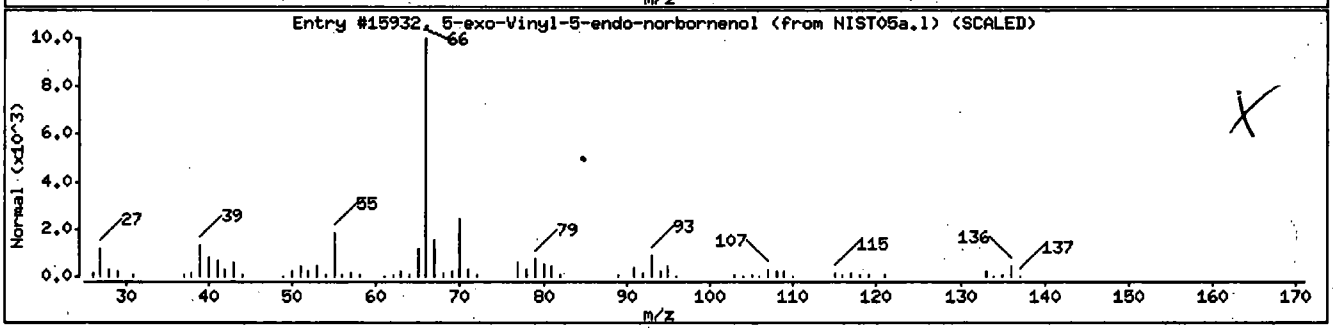
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13656	27	C10H12	132
2-Phenylbicyclo[2.2.1]hepta-2,5-diene $$	74437-39-1	WILEY275.l	53973	38	C13H12	168
5-exo-Vinyl-5-endo-norbornenol	37165-54-1	NIST05a.l	15932	27	C9H12O	136









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

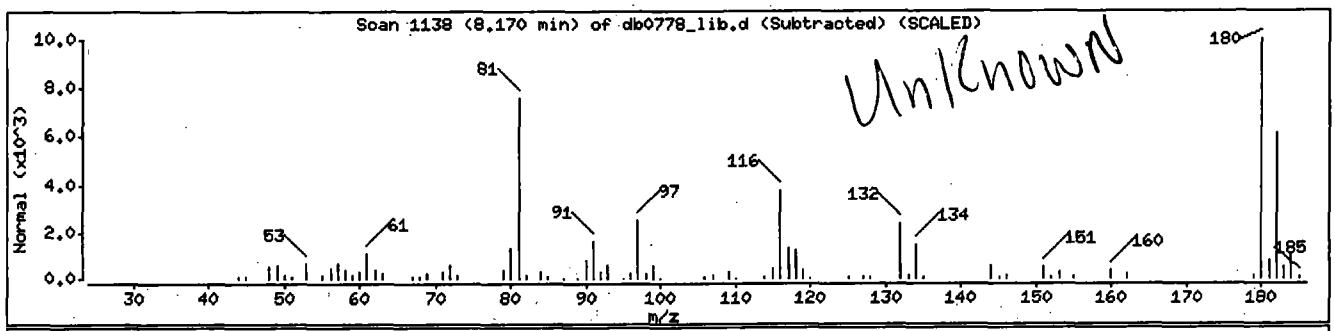
Volume Injected (uL): 1.0

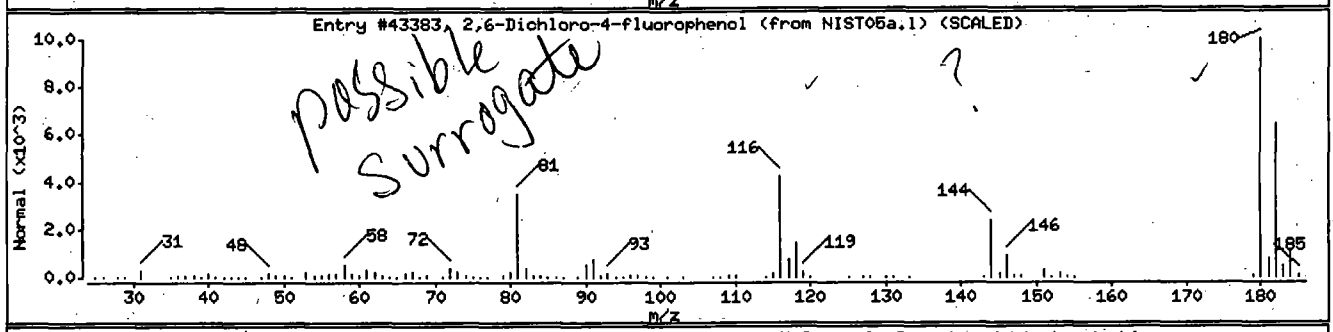
Operator: ceb05247

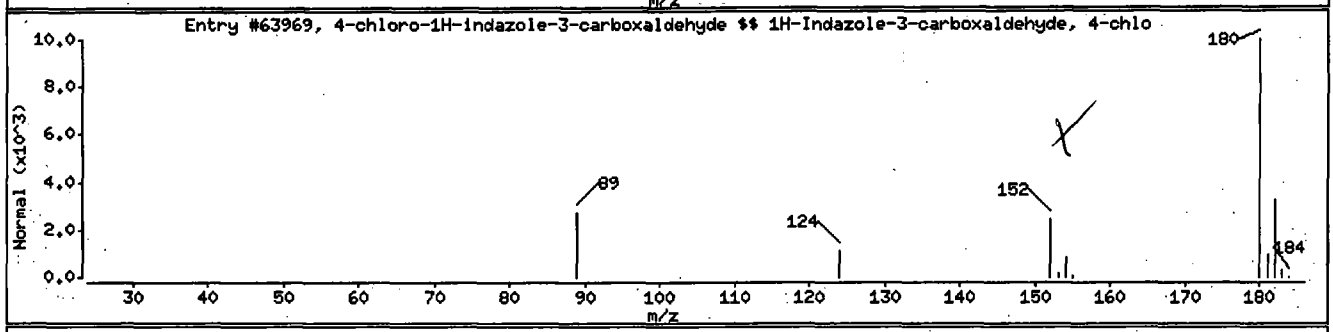
Column phase: J&W DB-5MS

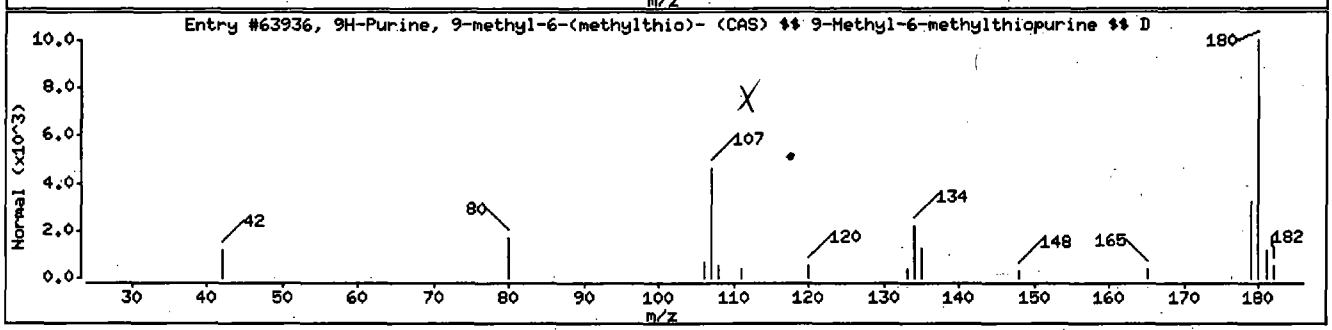
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	87	C6H3Cl2FO	180
4-chloro-1H-indazole-3-carboxaldehyde $$	102735-85-3	WILEY275.l	63969	25	C8H5ClN2O	180
9H-Purine, 9-methyl-6-(methylthio)- (CAS	1127-75-9	WILEY275.l	63936	14	C7H8N4S	180









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

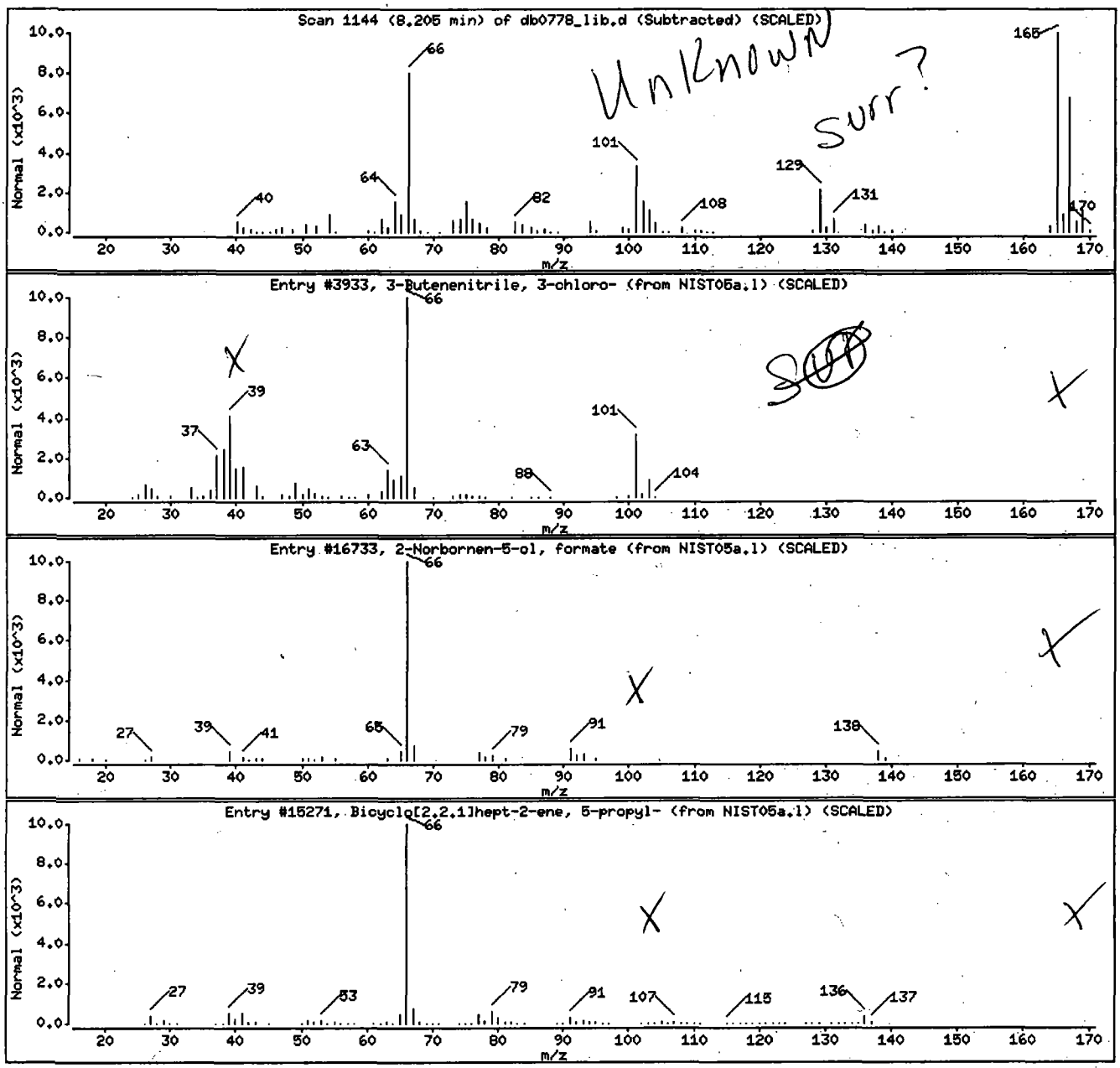
Client ID: H2011 Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	49	C8H10O2	138
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136



Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

Client ID: H2011

Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

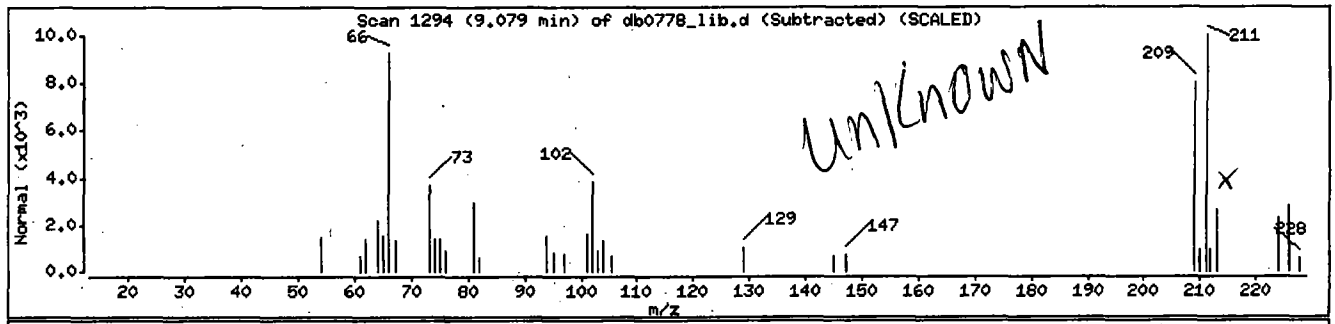
Volume Injected (uL): 1.0

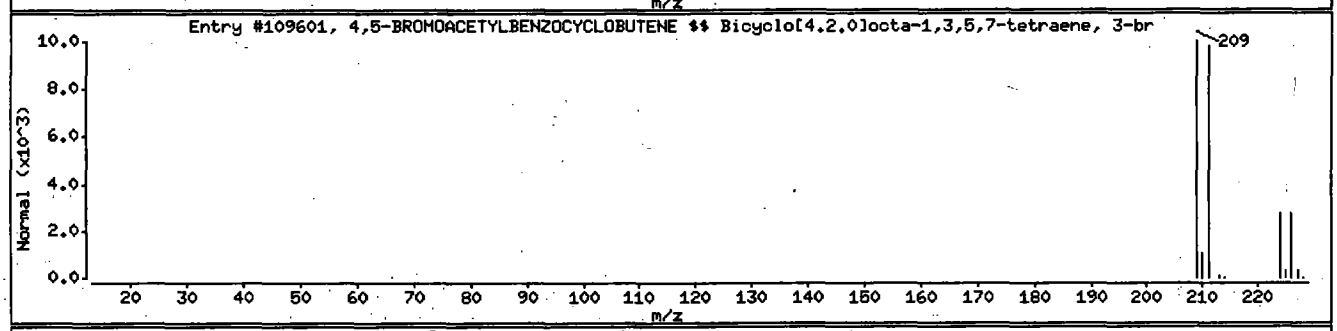
Operator: ceb05247

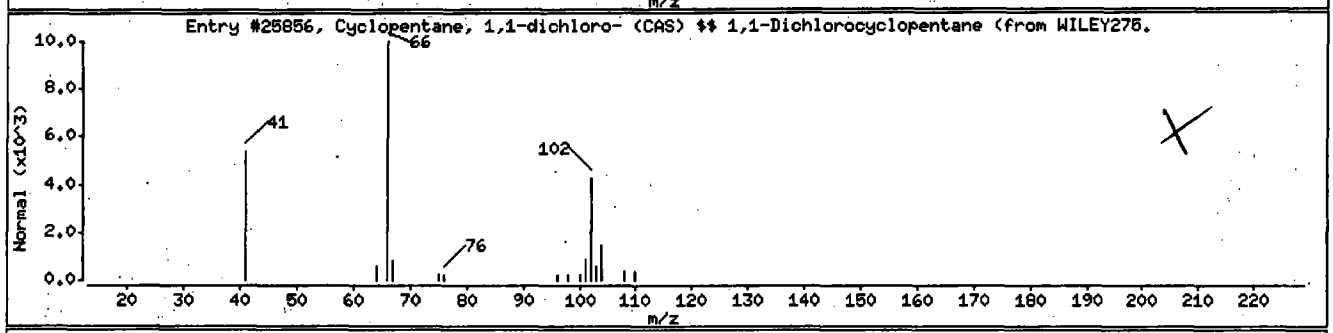
Column phase: J&W DB-5MS

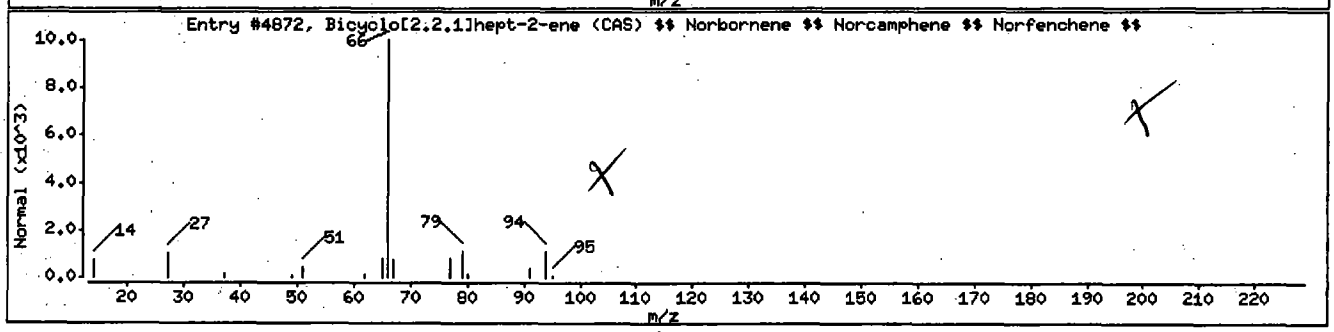
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63506-25-2	WILEY275.l	109601	80	C10H9BrO	224
Cyclopentane, 1,1-dichloro- (CAS) $$ 1,1	31038-06-9	WILEY275.l	25856	43	C5H8Cl2	138
Bicyclo[2.2.1]hept-2-ene (CAS) $$ Norbor	498-66-8	WILEY275.l	4872	32	C7H10	94









Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb18a.b/db0778_lib.d

Date : 19-FEB-2014 04:57

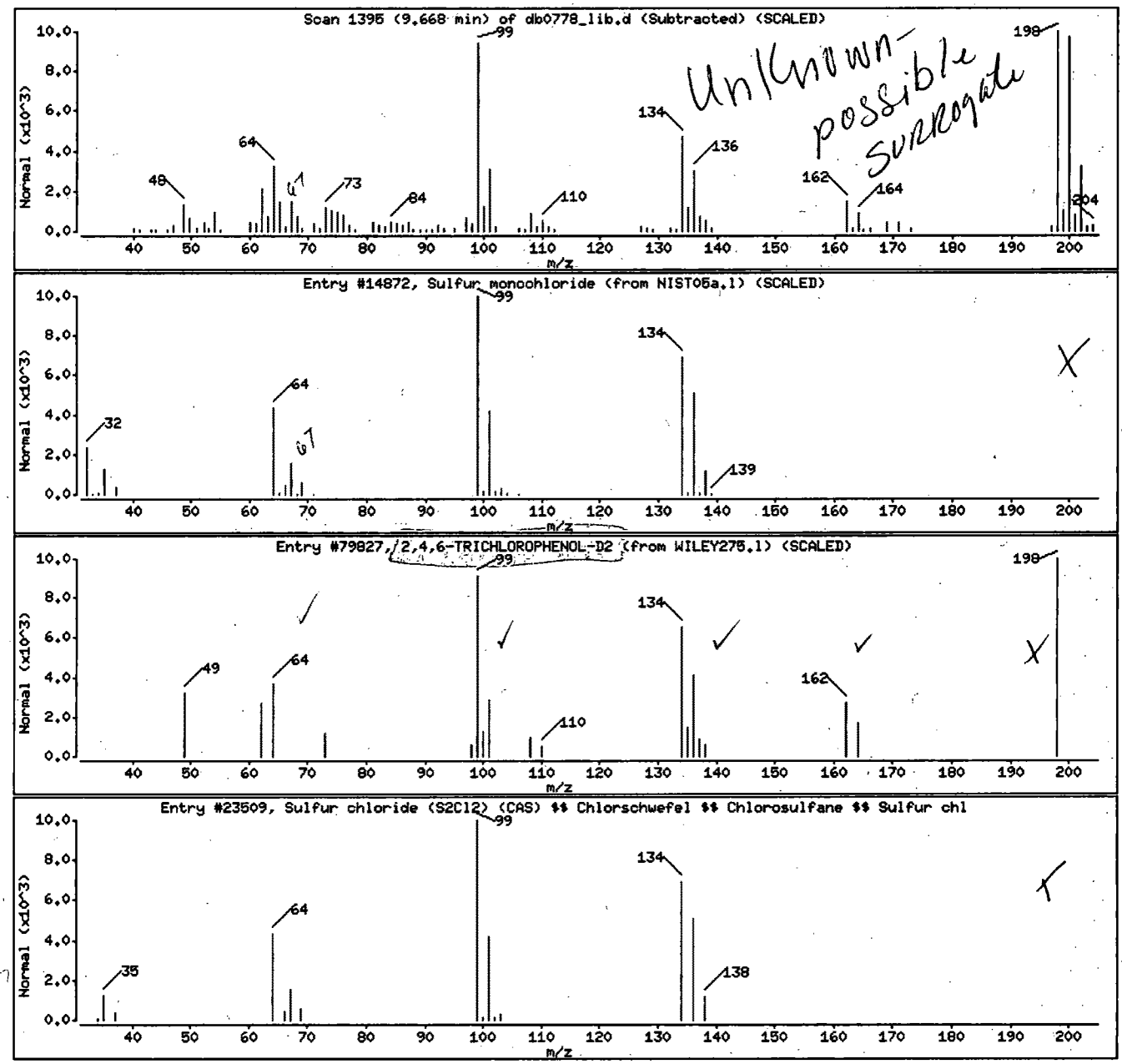
Client ID: H2011 | Instrument: HP19760.i

Sample Info: H2011;7365713;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 | Operator: ceb05247

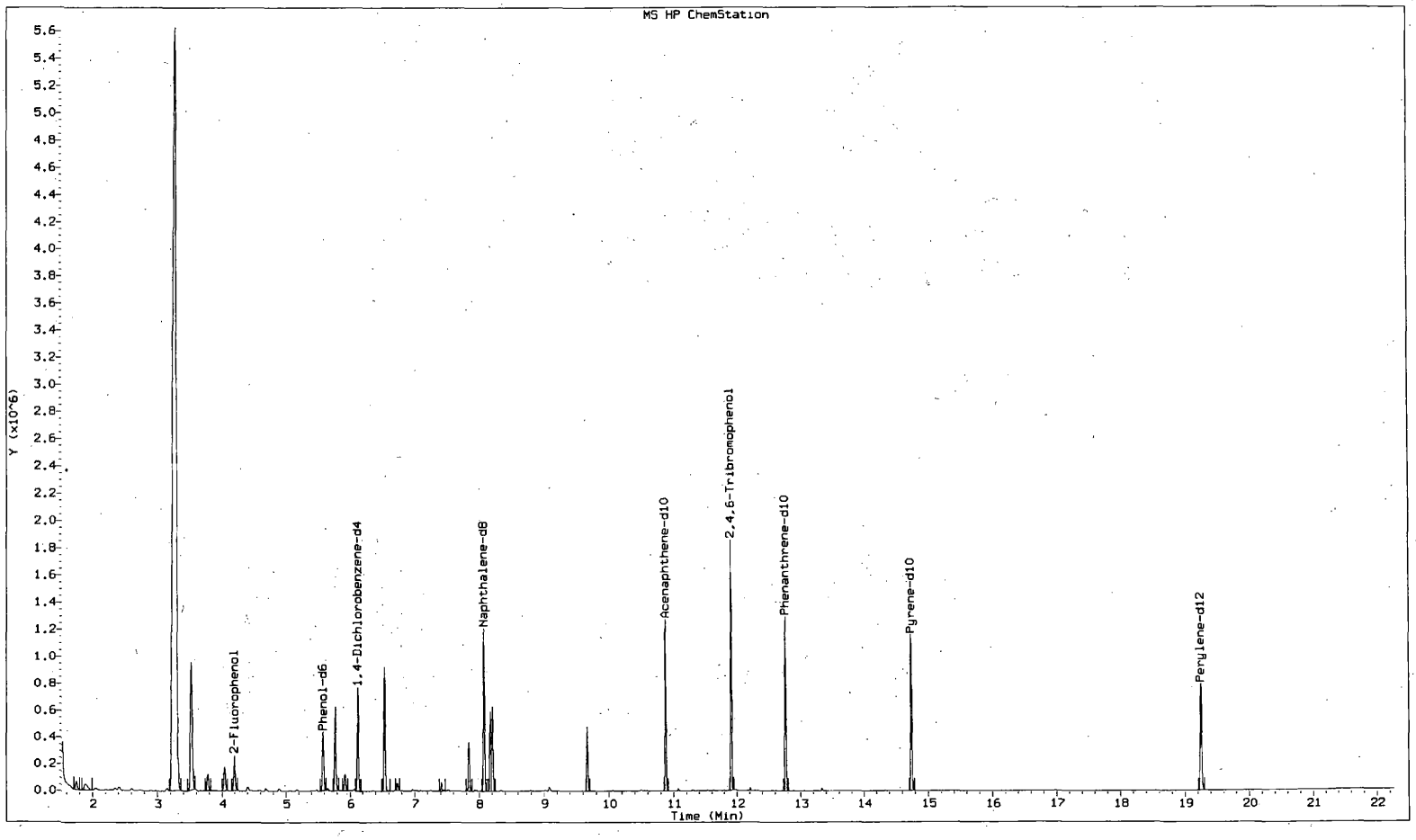
Column phase: J&W DB-5MS | Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	46	C6HD2Cl3O	198
Sulfur chloride (S2Cl2) (CAS) $$ Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134



Digitally signed by Andrew J. Strebel on 03/01/2014 at 17:50.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb19a.b/db0843_lib.d
Operator : ceb05247
Acquired : 20-FEB-2014 02:39
Instrument : HP19760.i
Sample Name: H2021;7365717;1;0;SAMPLE;;;
Misc Info : 14049WAD;WL13166;;1051;1000;0;db0832;13166;
Vial Number: 14



Lancaster Labs

Data file : /chem/HP19760.i/14feb19a.b/db0843_lib.d
Lab Smp Id: 7365717 Client Smp ID: H2021
Inj Date : 20-FEB-2014 02:39
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H2021;7365717;1;0;SAMPLE;;;
Misc Info : 14049WAD;WL13166;;1051;1000;0;db0832;13166;
Comment : Max. number of TICs to report is 50, 15 TICs were found initially.
Method : /chem/HP19760.i/14feb19a.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 20:28 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 14
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1051.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.124	1093059	10.000
* 48 Naphthalene-d8	8.077	1677517	10.000
* 83 Acenaphthene-d10	10.880	1474884	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.747	120326	1.10081688	1.04739	90	NIST05a.1	31323	21

Digitally signed by Andrew J. Strebel on 03/01/2014 at 20:37.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.892	164546	1.50536674	1.43231	93	NIST05a.l	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.297	20460805	187.188377	178.10502	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.524	1902846	17.4084353	16.56368	90	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.781	231622	2.11902680	2.01620	9	NIST05a.l	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.043	314597	2.87813015	2.73846	39	NIST05a.l	13998	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.774	940476	8.60406510	8.18655	94	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.926	176076	1.61085577	1.53268	94	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.538	1328821	12.1568965	11.56698	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.730	81249	0.74331595	0.70724	64	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl- (CAS) $$					CAS #: 541-02-6		
7.412	83408	0.49721342	0.47308	83	WILEY275.l	221485	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.843	452926	2.69997954	2.56896	27	NIST05a.l	13656	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.170	679185	4.04875113	3.85228	90	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.205	756841	4.51166899	4.29273	50	NIST05a.l	3933	48
Sulfur monochloride					CAS #: 10025-67-9		
9.668	546168	3.70312410	3.52342	38	NIST05a.l	14872	83(L)

Target compound.
Do not report.
ajs00193 03/01/2014

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/01/2014 at 20:37.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19a.b/db0843_lib.d

Date : 20-FEB-2014 02:39

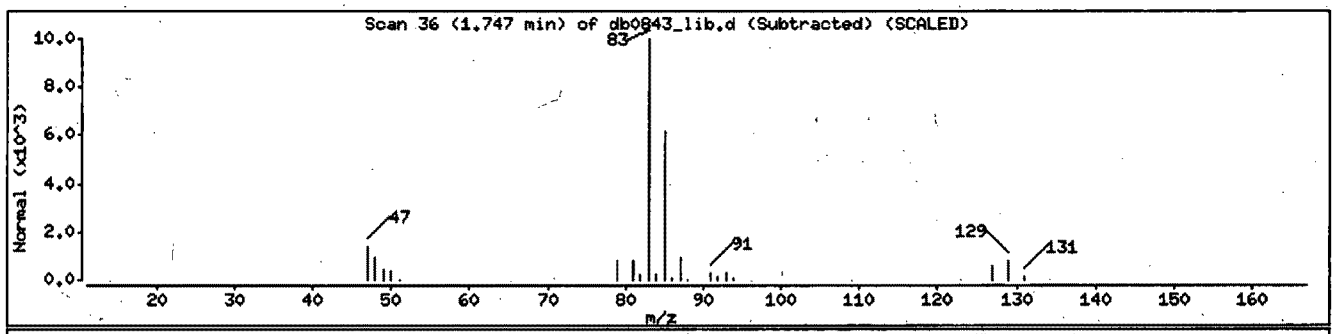
Client ID: H2021 Instrument: HP19760.i

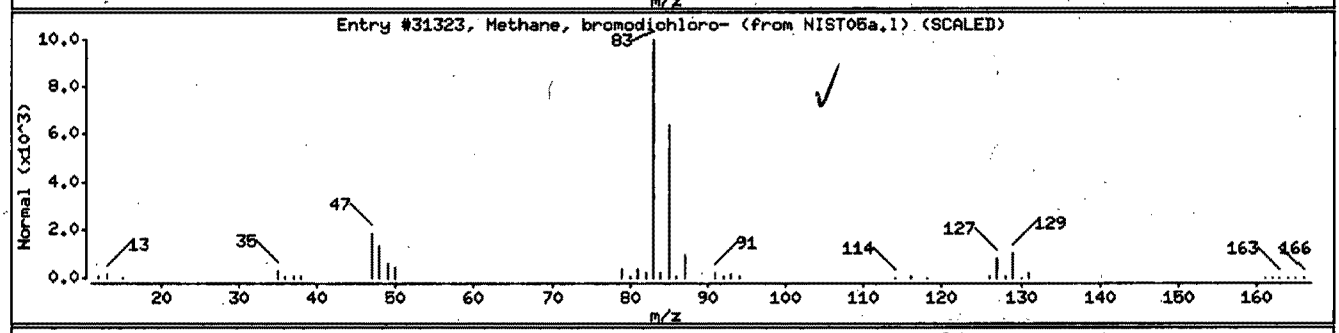
Sample Info: H2021;7366717;1;0;SAMPLE;;;

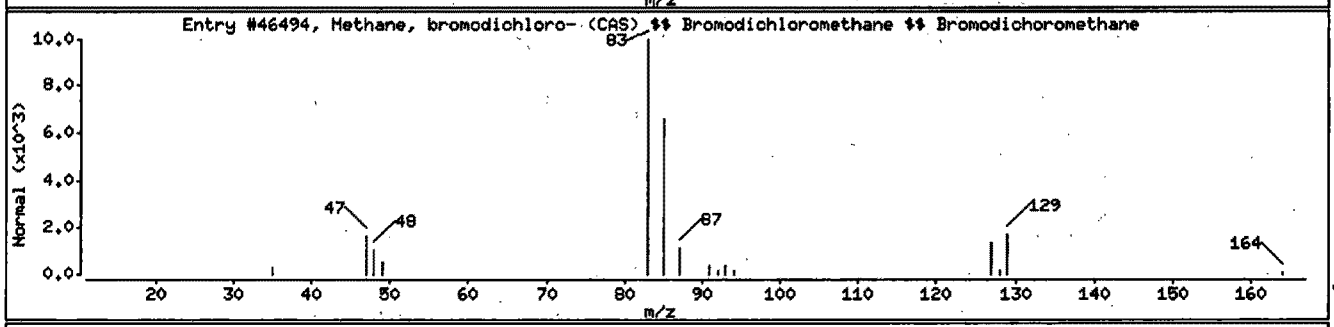
Volume Injected (uL): 1.0 Operator: oeb05247

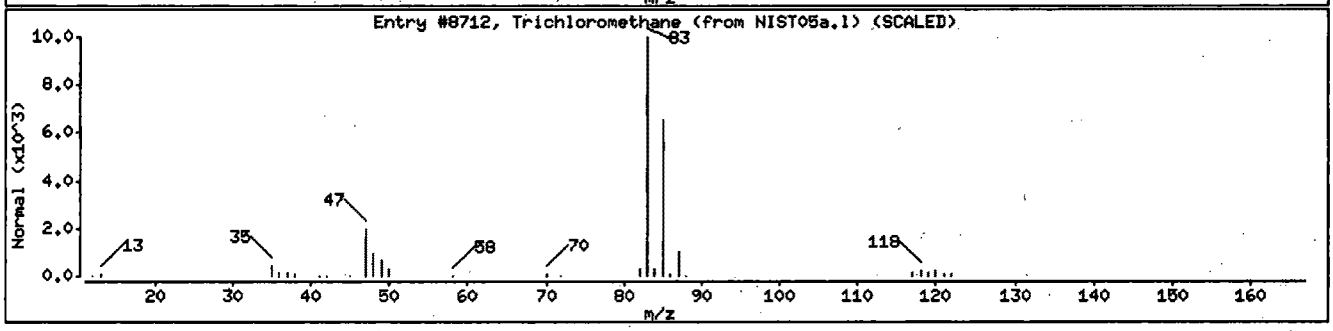
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46494	83	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









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Data File: /chem/HP19760.i/14feb19a.b/db0843_lib.d

Date : 20-FEB-2014 02:39

Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

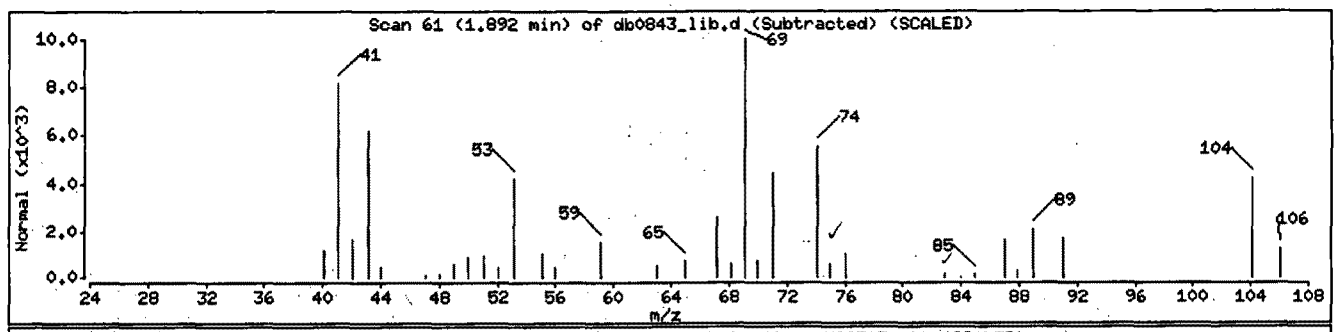
Volume Injected (uL): 1.0

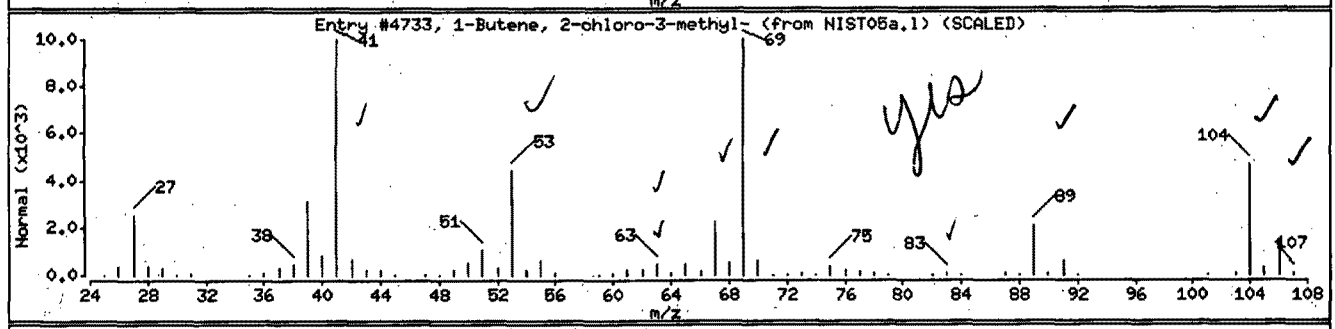
Operator: ceb05247

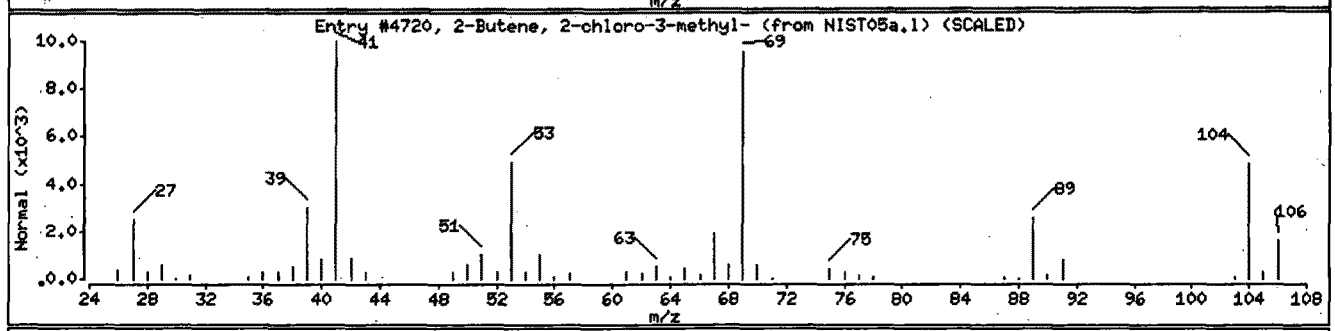
Column phase: J&W DB-5MS

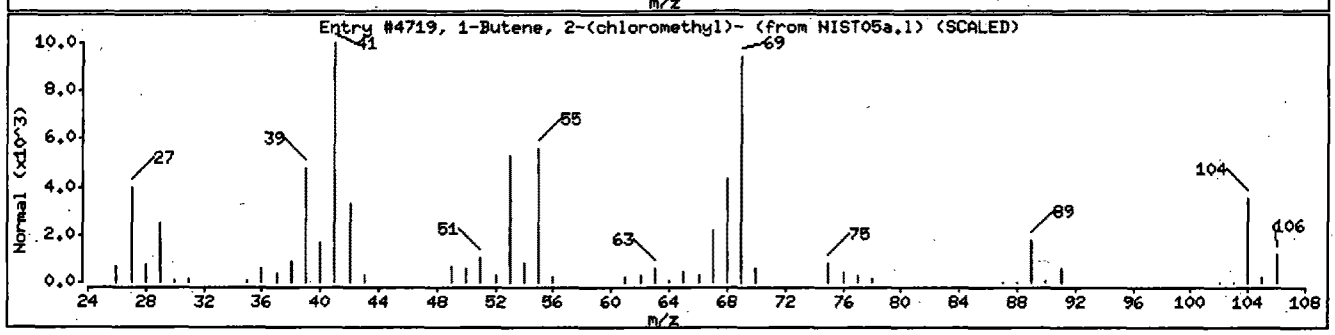
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	93	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	76	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4719	68	C5H9Cl	104









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Date : 20-FEB-2014 02:39

Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

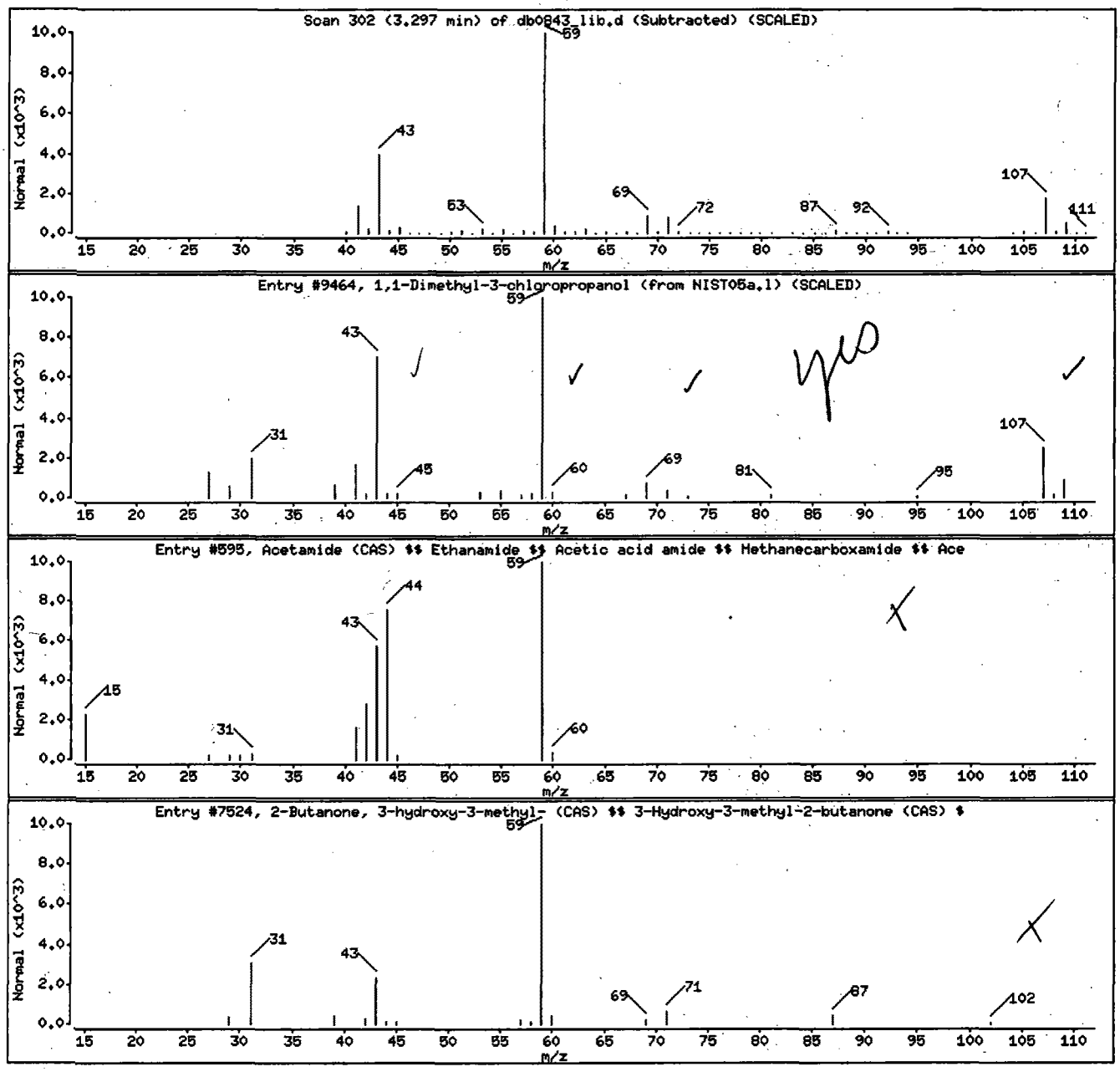
Volume Injected (uL): 1.0

Operator: oeb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102



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Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7366717;1;0;SAMPLE;;;

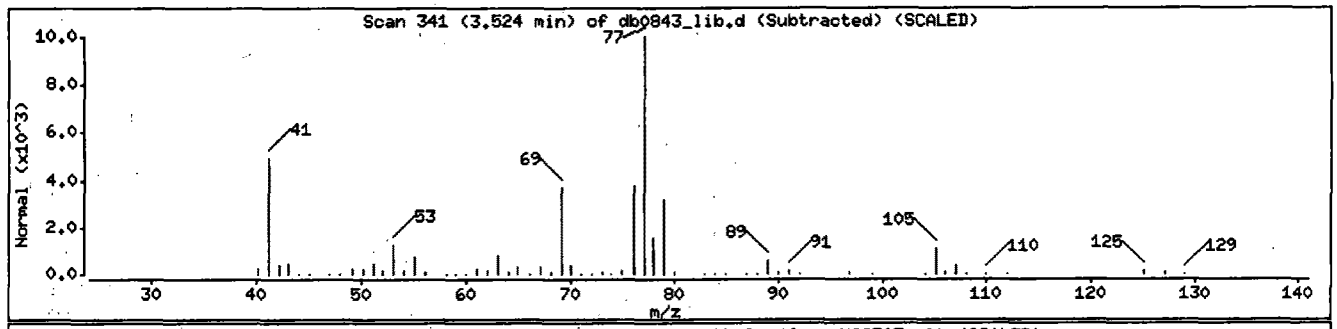
Volume Injected (uL): 1.0

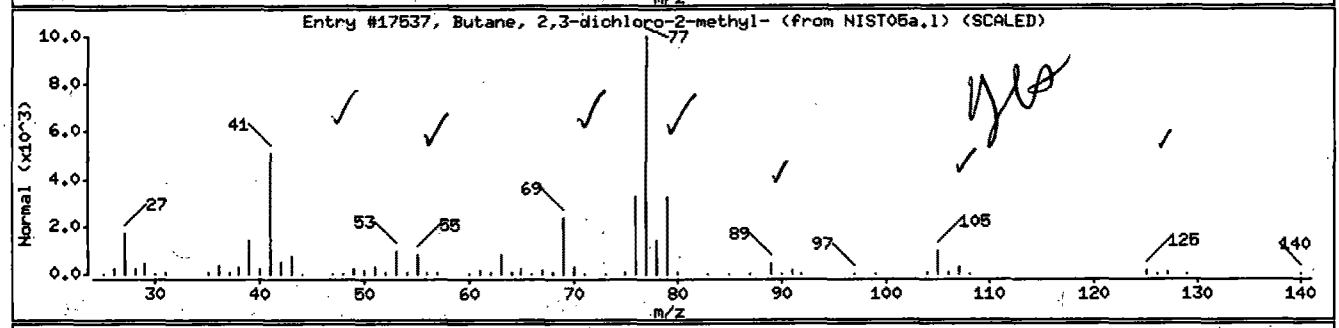
Operator: ceb05247

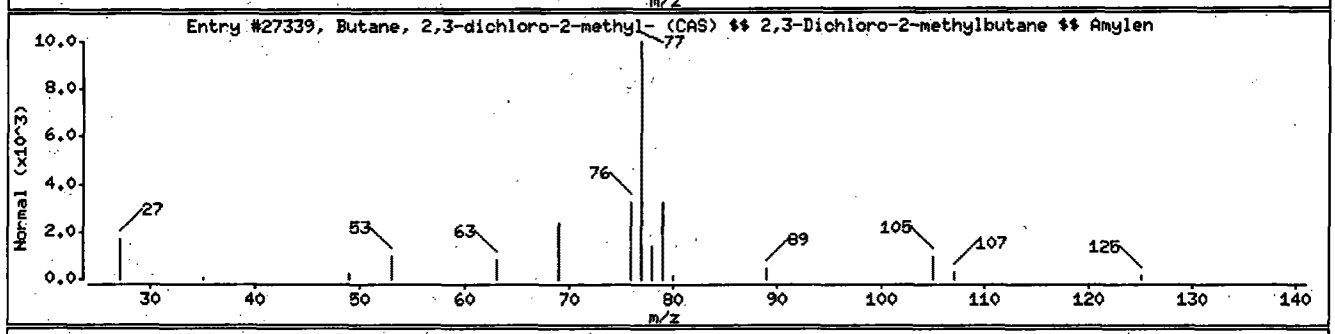
Column phase: J&W DB-5MS

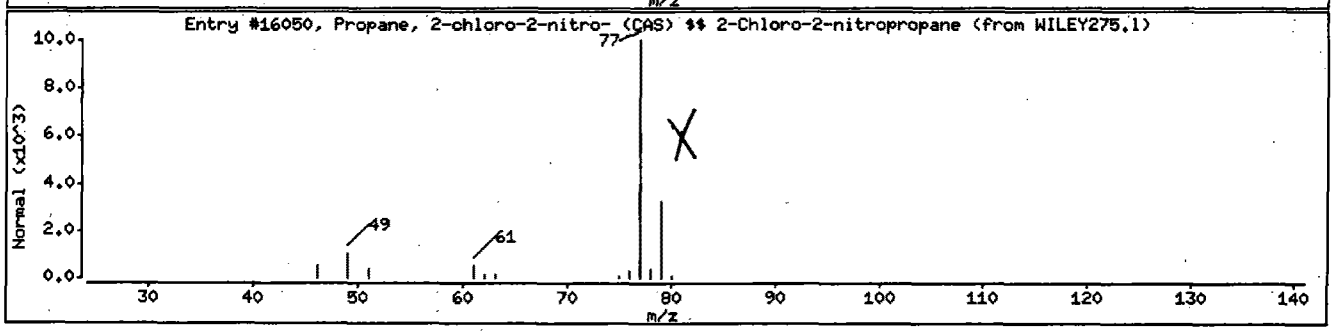
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	90	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	90	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









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Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

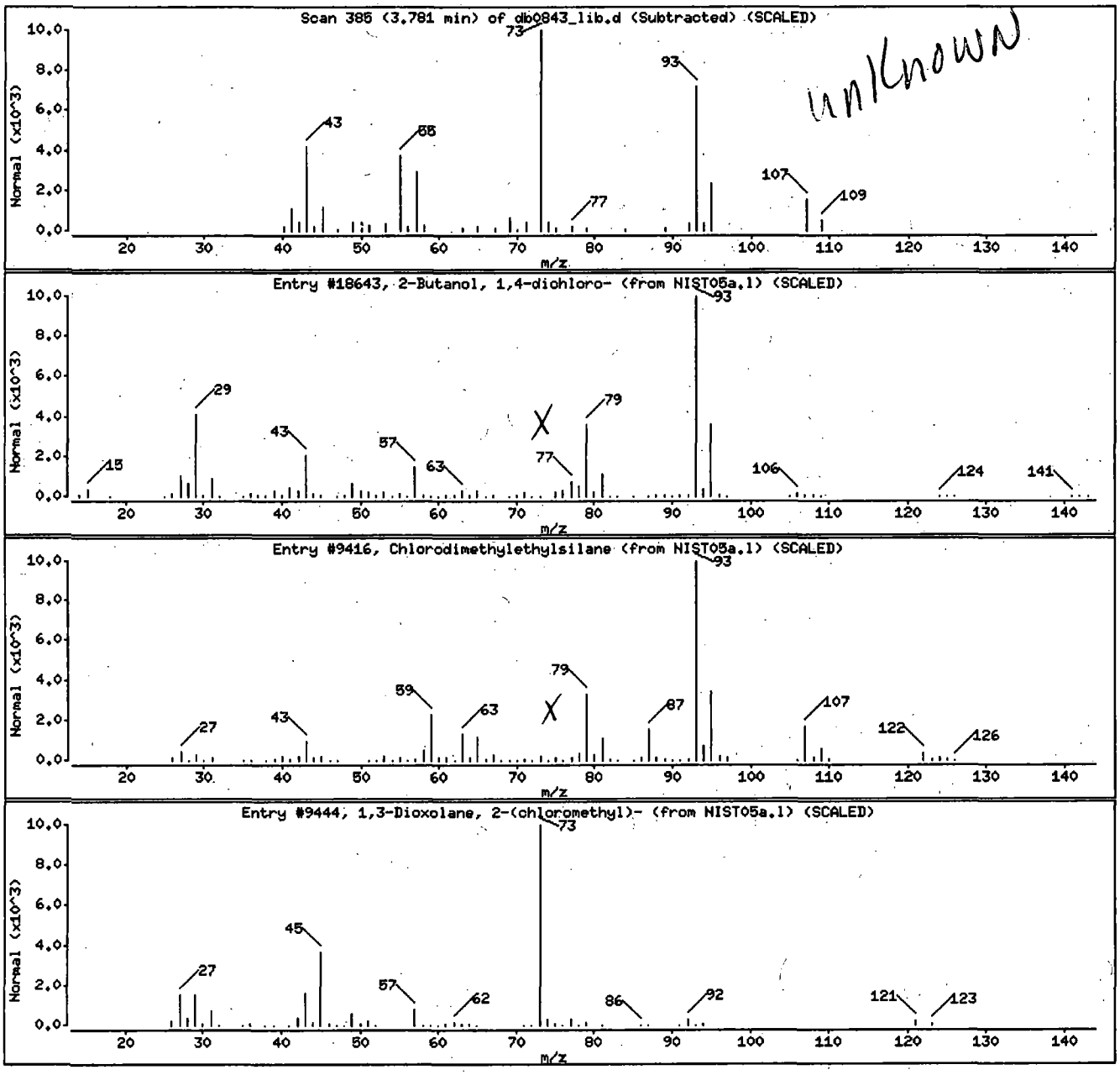
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	9	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9444	10	C4H7ClO2	122



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Sample Info: H2021;7365717;1;0;SAMPLE;;;

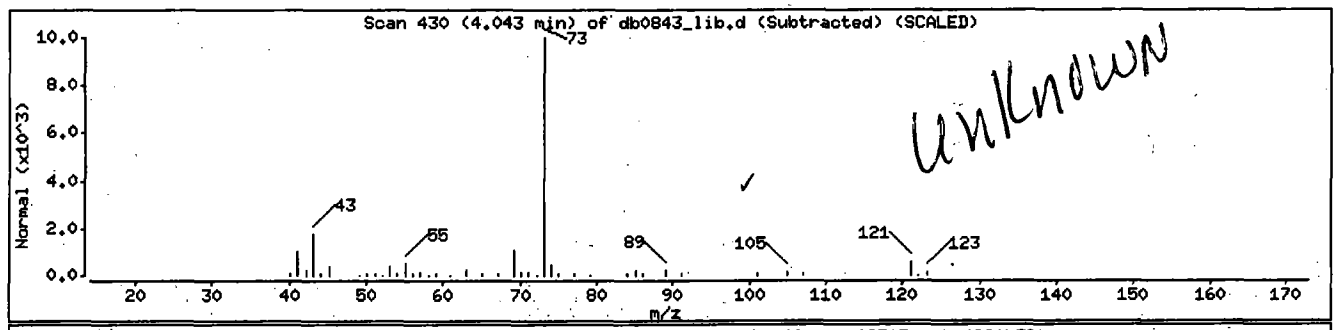
Volume Injected (uL): 1.0

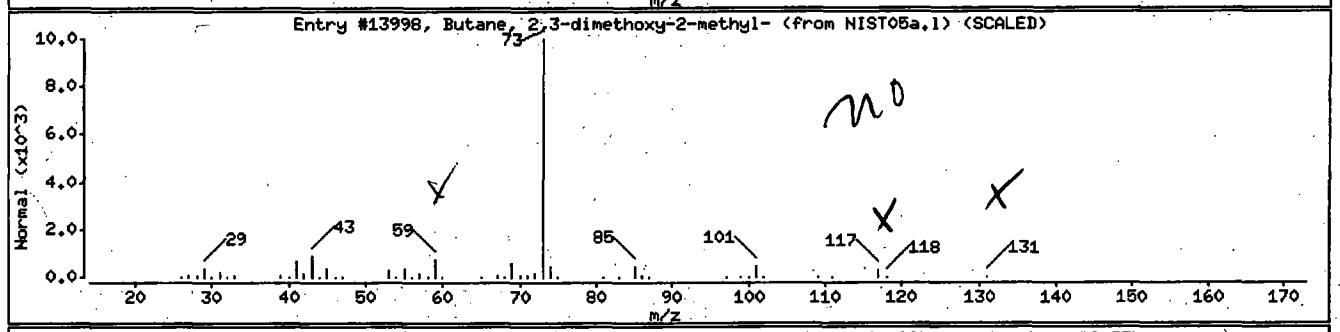
Operator: oeb05247

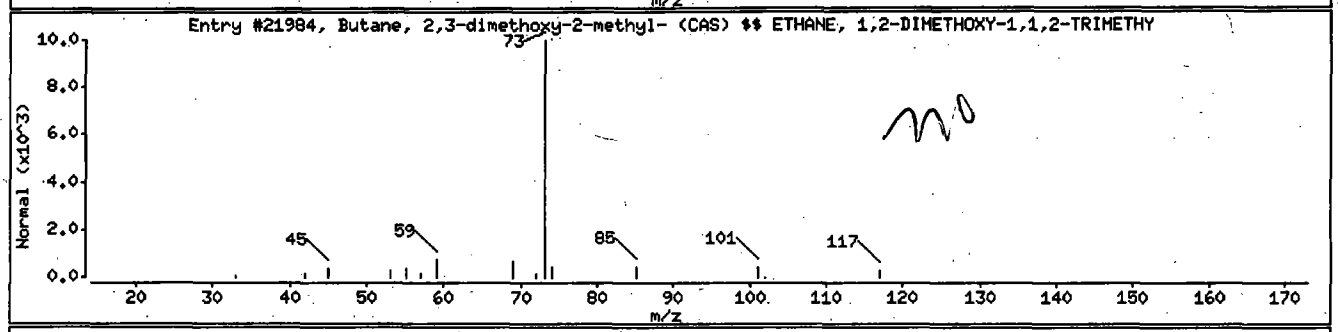
Column phase: J&W DB-5MS

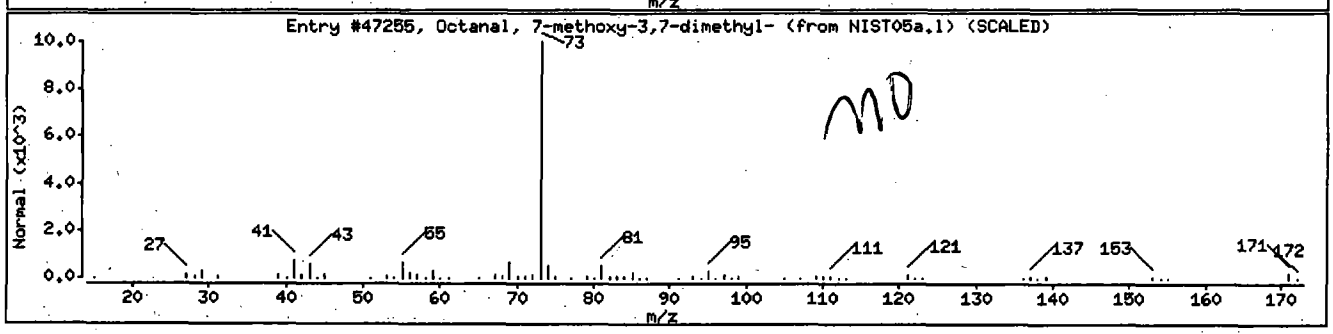
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	39	C7H16O2	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	39	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	36	C11H22O2	186









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Date : 20-FEB-2014 02:39

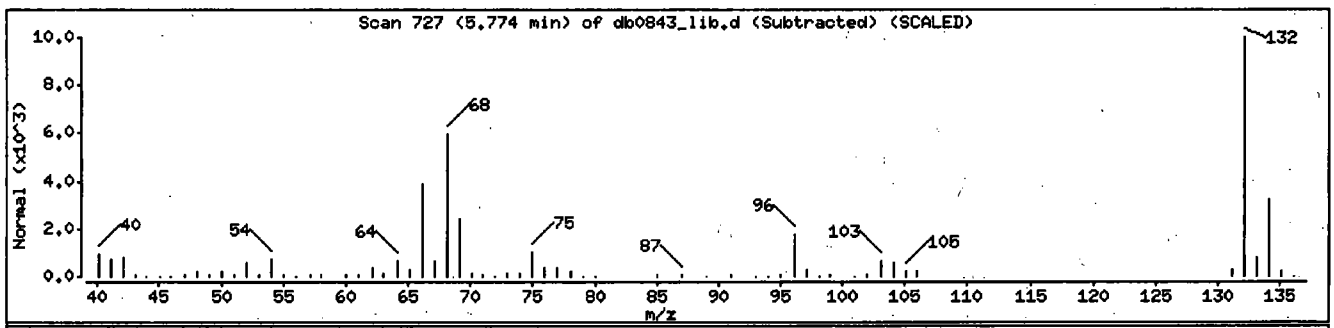
Client ID: H2021 | Instrument: HP19760.i

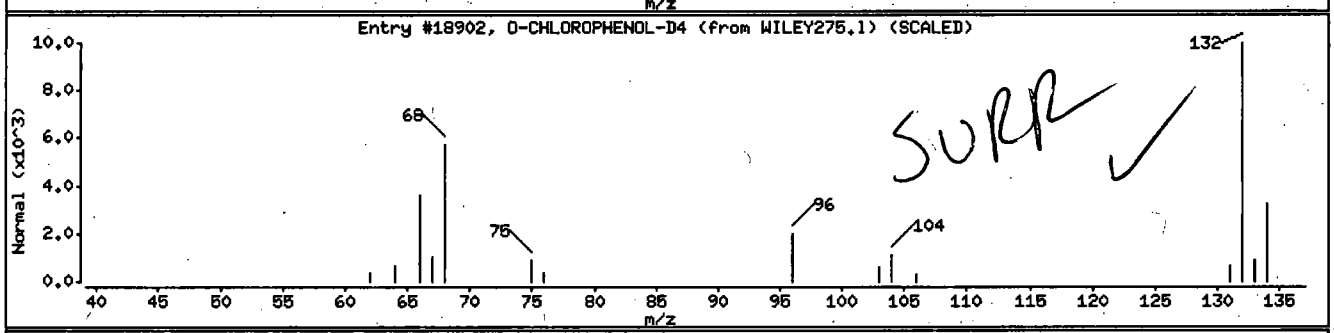
Sample Info: H2021;7365717;1;0;SAMPLE;;;

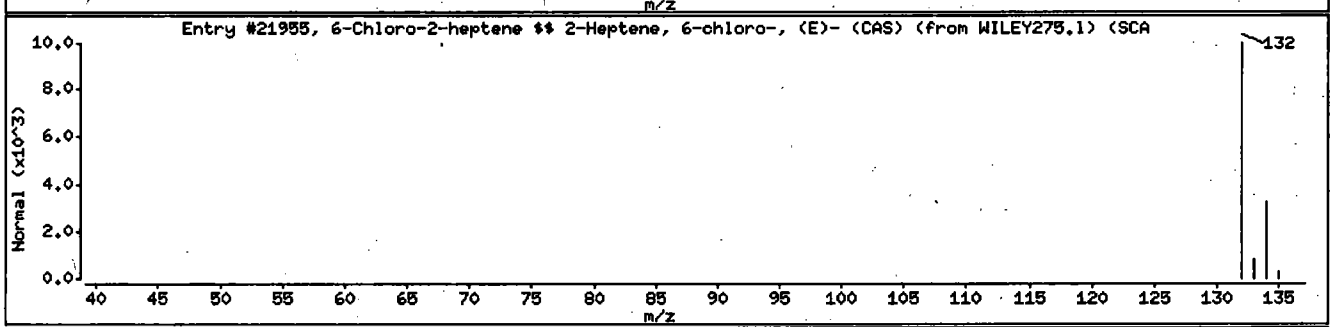
Volume Injected (uL): 1.0 | Operator: oeb05247

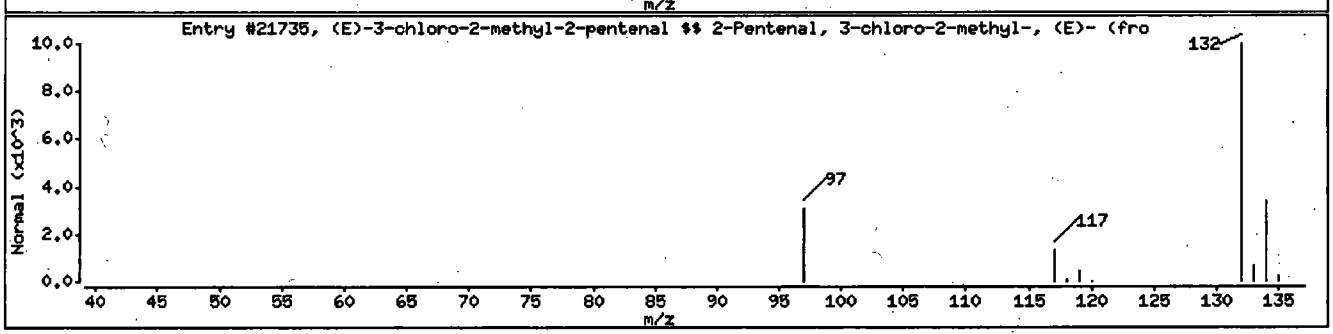
Column phase: J&W DB-5MS | Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	94	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132









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Date : 20-FEB-2014 02:39

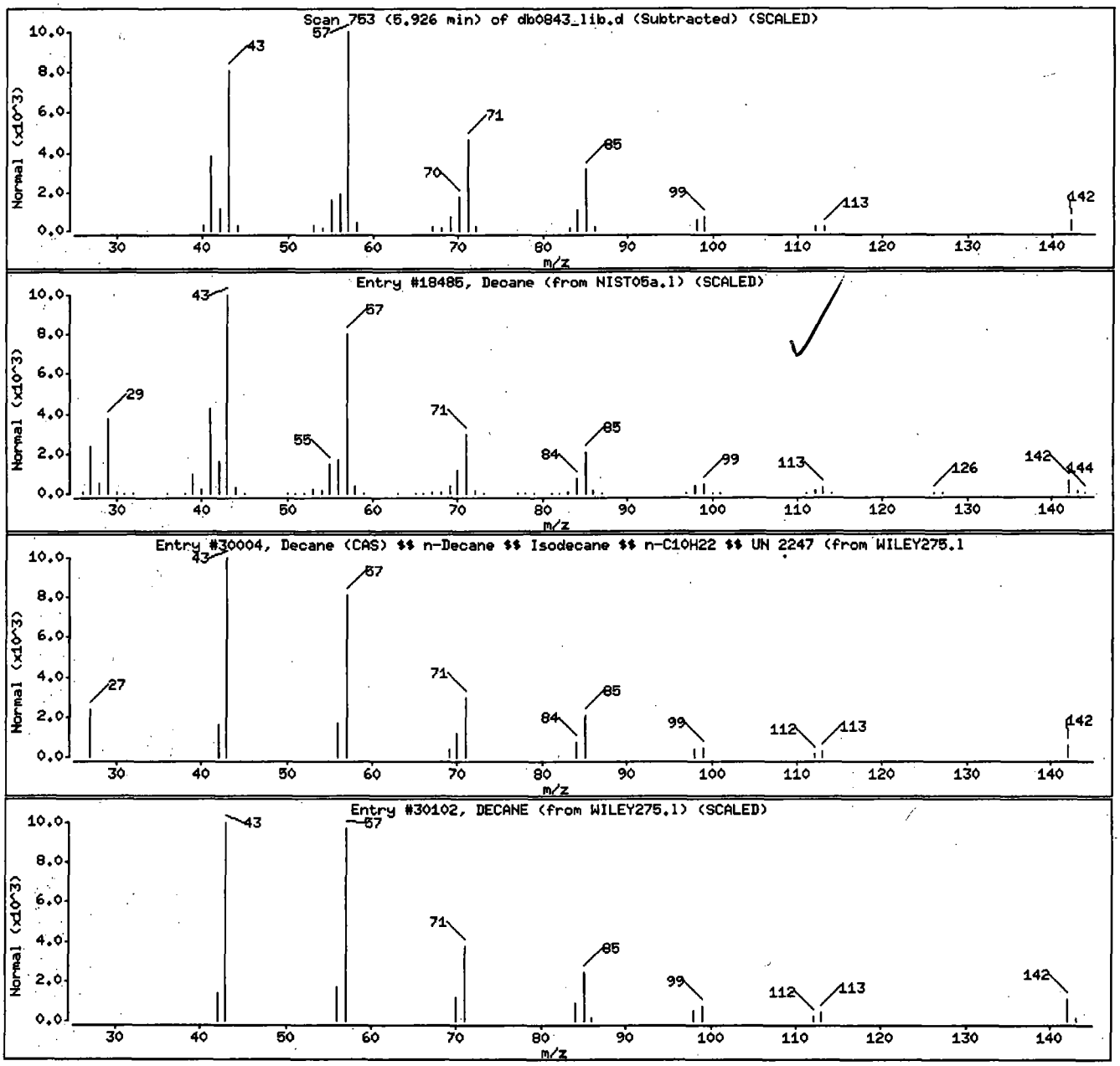
Client ID: H2021 Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	94	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	94	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142



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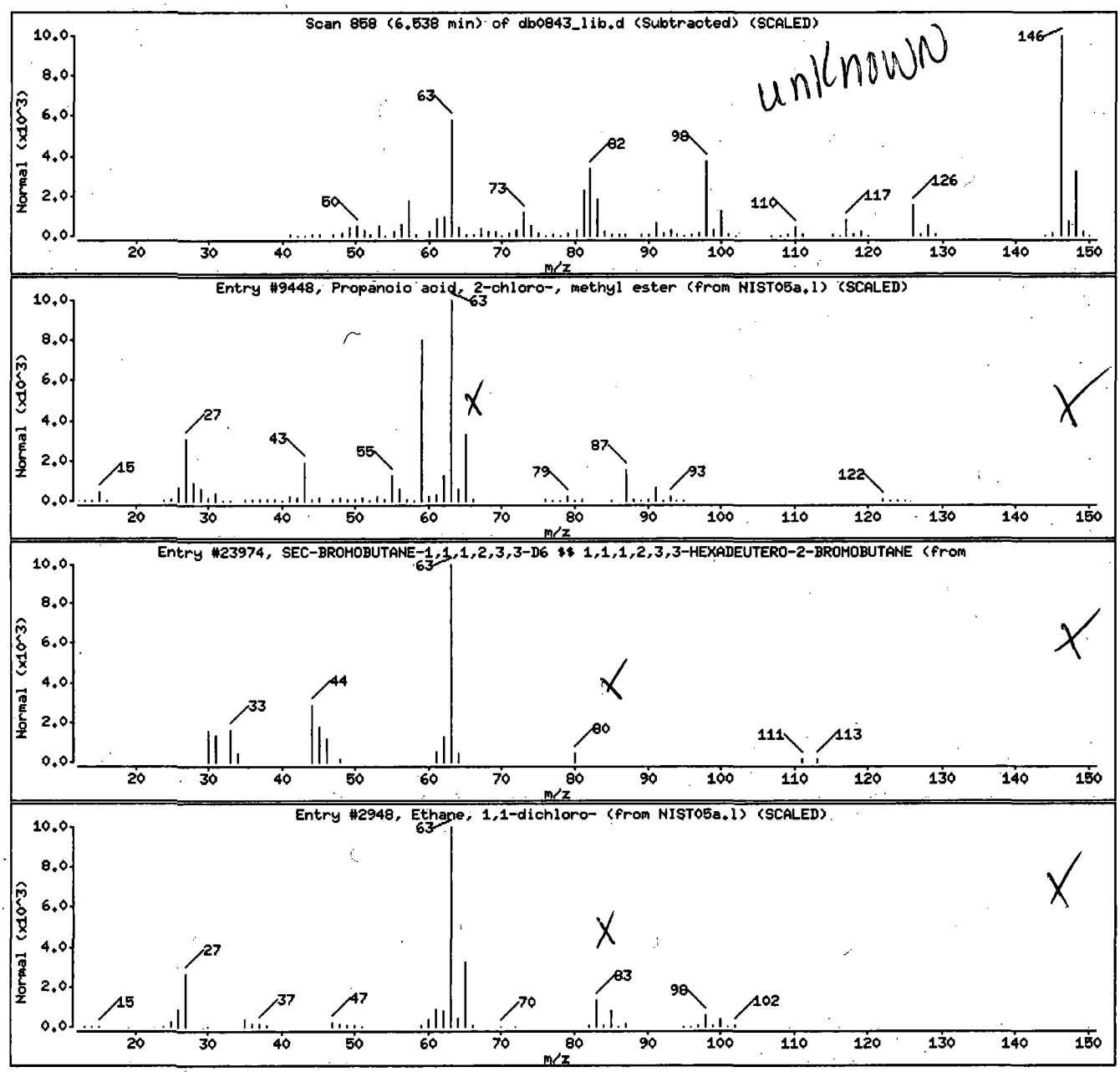
Client ID: H2021 Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,2,3,3-D6 ** 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	25	C2H4Cl2	98



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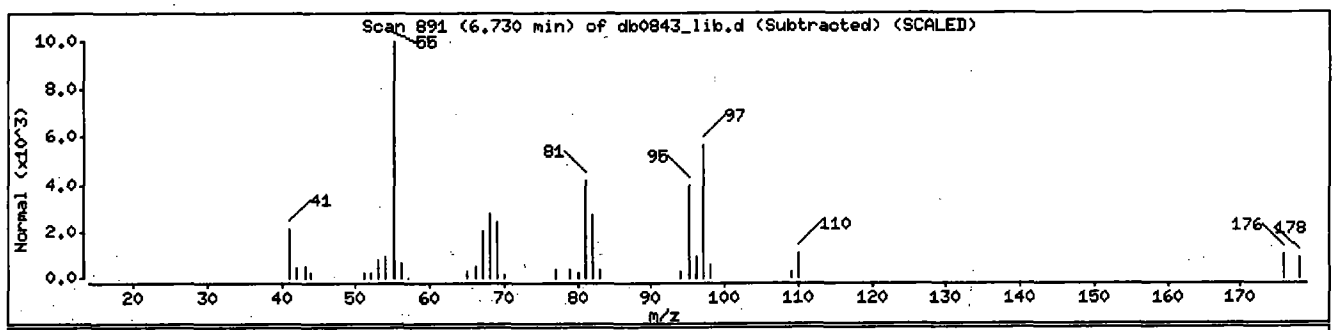
Client ID: H2021 Instrument: HP19760.i

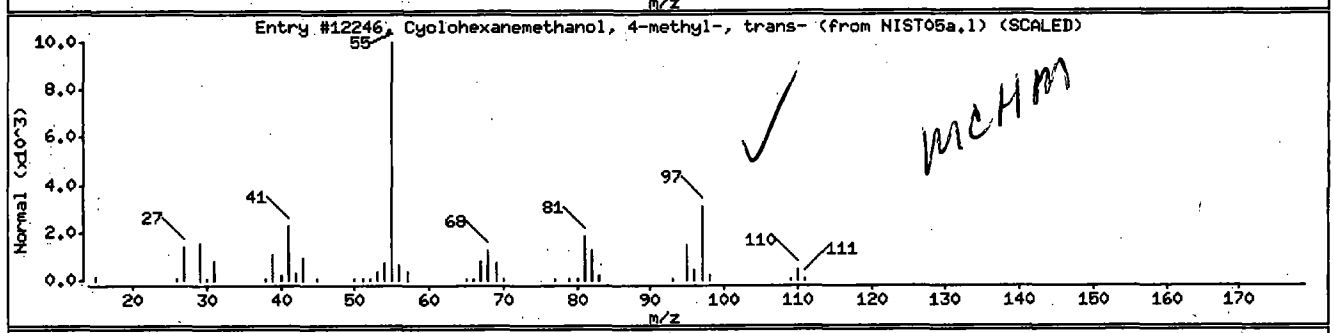
Sample Info: H2021;7365717;1;0;SAMPLE;;;

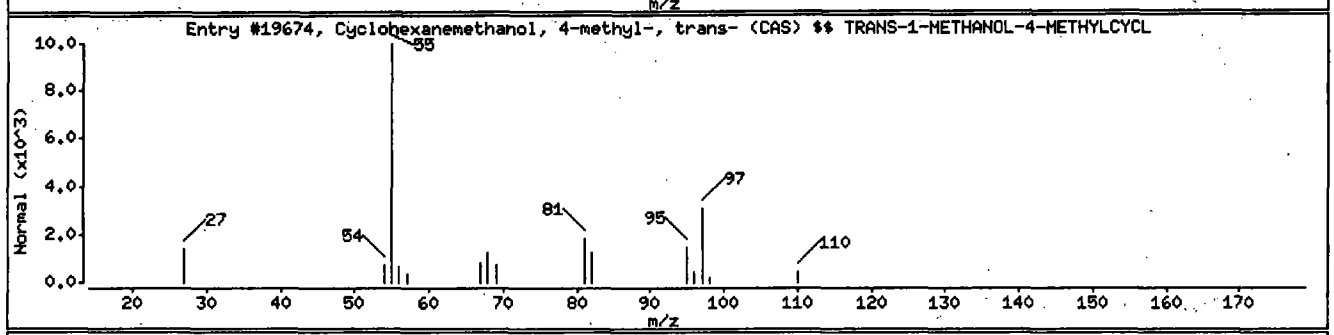
Volume Injected (uL): 1.0 Operator: ceb05247

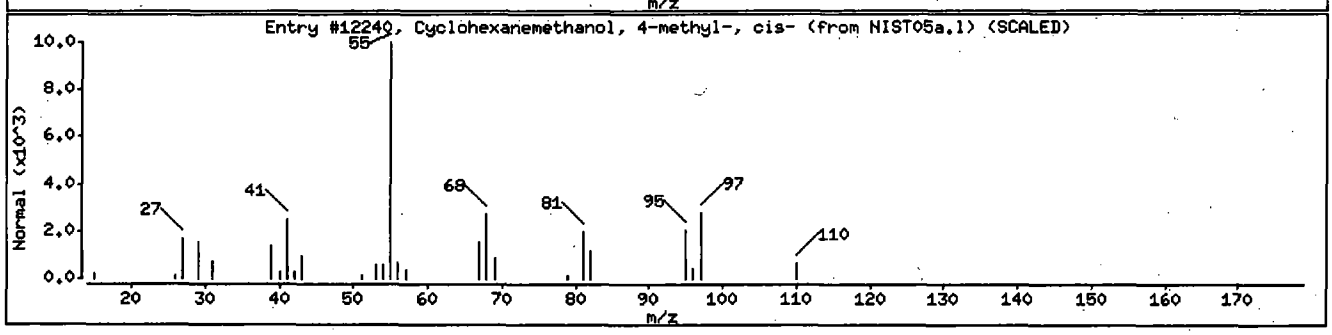
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	64	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	64	C8H16O	128
Cyclohexanemethanol, 4-methyl-, cis-	3937-48-2	NIST05a.l	12240	56	C8H16O	128









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Sample Info: H2021;7365717;1;0;SAMPLE;;;

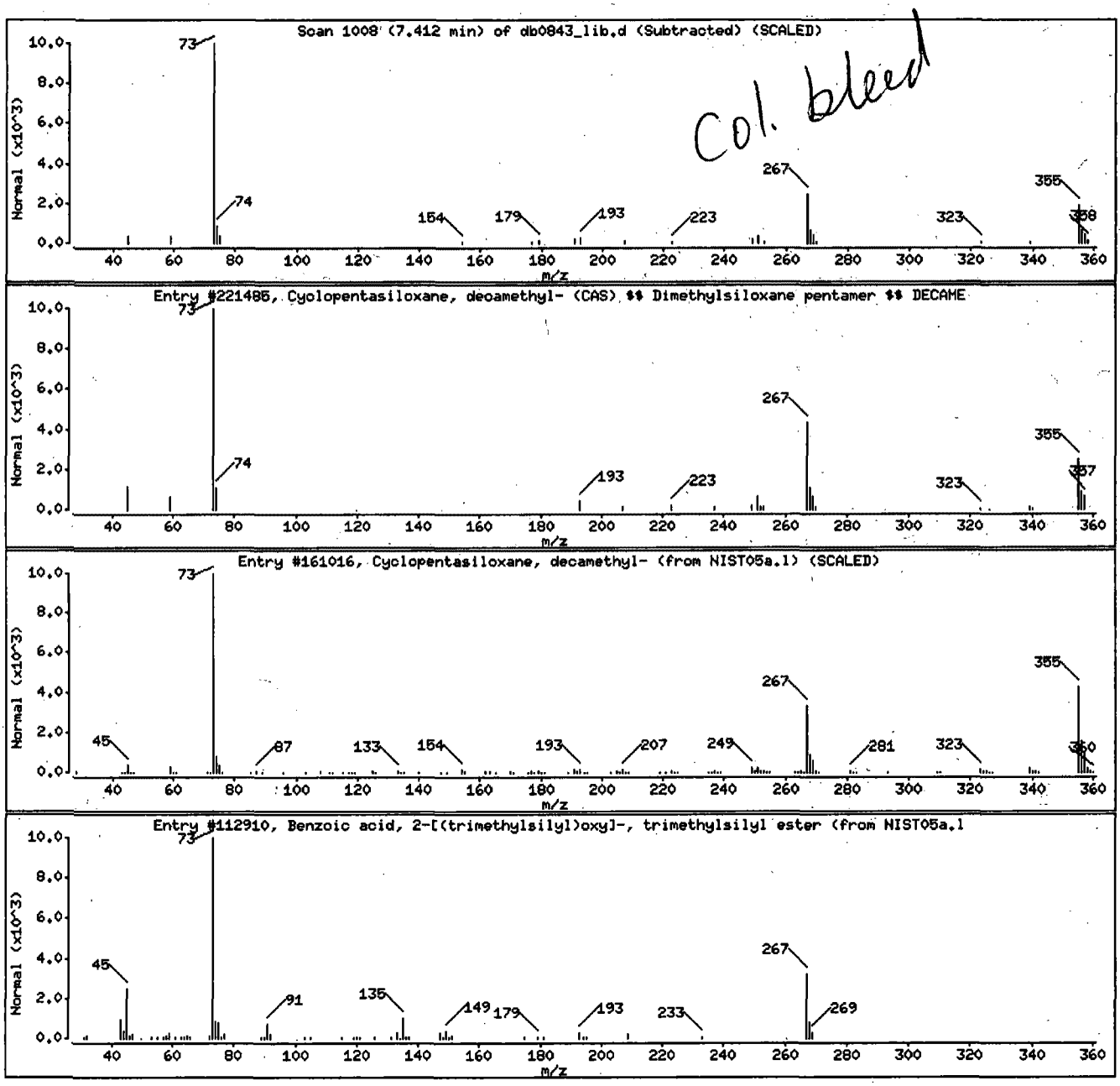
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	83	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	78	C10H30O5Si5	370
Benzoic acid, 2-[(trimethylsilyl)oxy]-,	3789-85-3	NIST05a.l	112910	38	C13H22O3Si2	282



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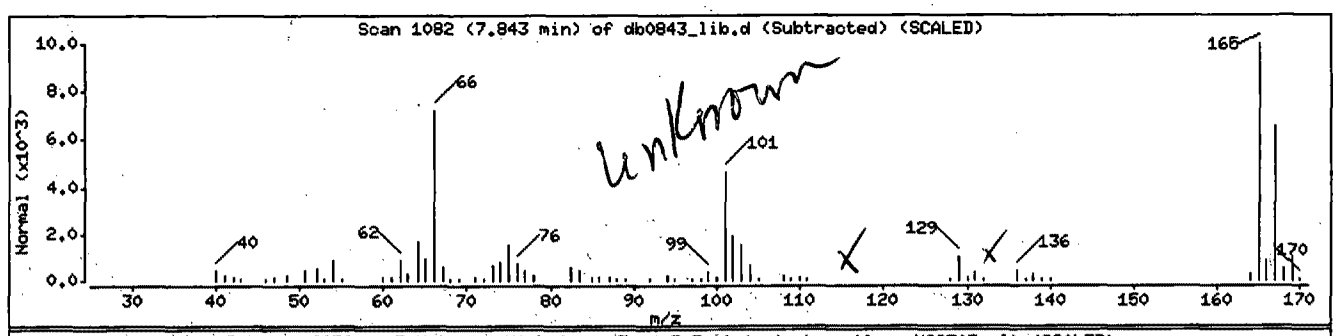
Volume Injected (uL): 1.0

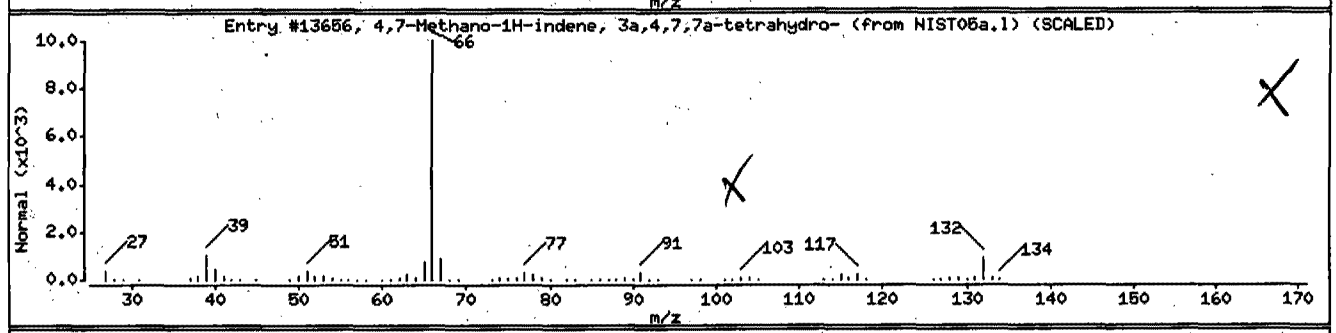
Operator: ceb05247

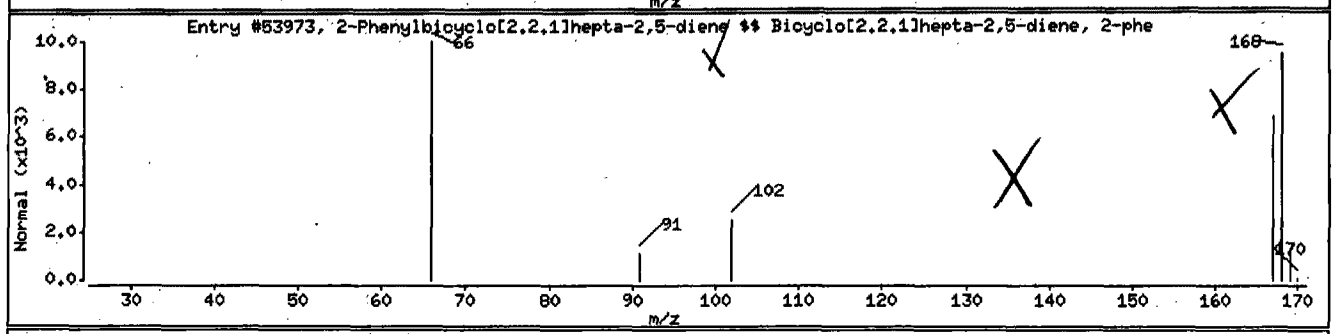
Column phase: J&W DB-5MS

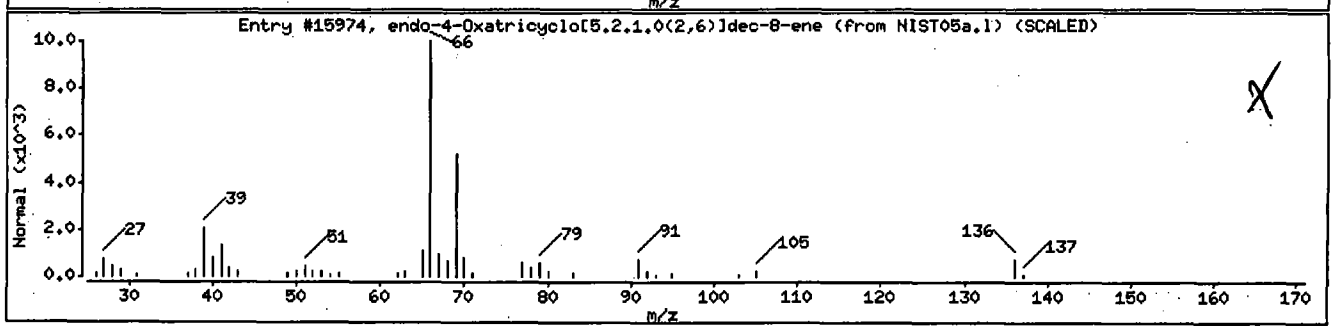
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13656	27	C10H12	132
2-Phenylbicyclo[2.2.1]hepta-2,5-diene $$	74437-39-1	WILEY275.l	53973	38	C13H12	168
endo-4-Oxatricyclo[5.2.1.0(2,6)]deo-8-en	1528-23-0	NIST05a.l	15974	30	C9H12O	136









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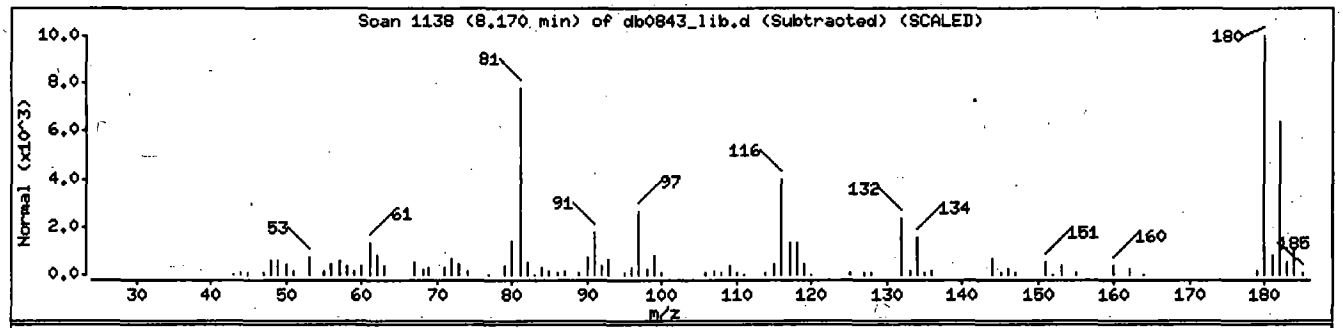
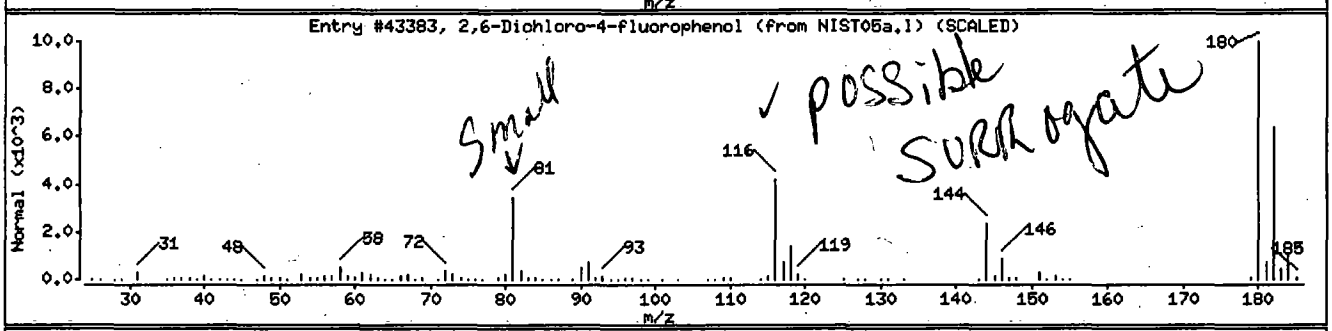
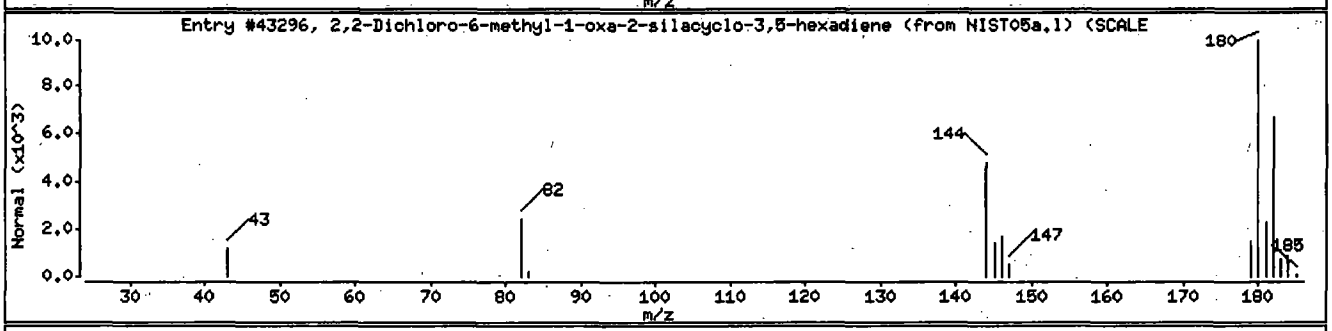
Volume Injected (uL): 1.0 Operator: ceb05247

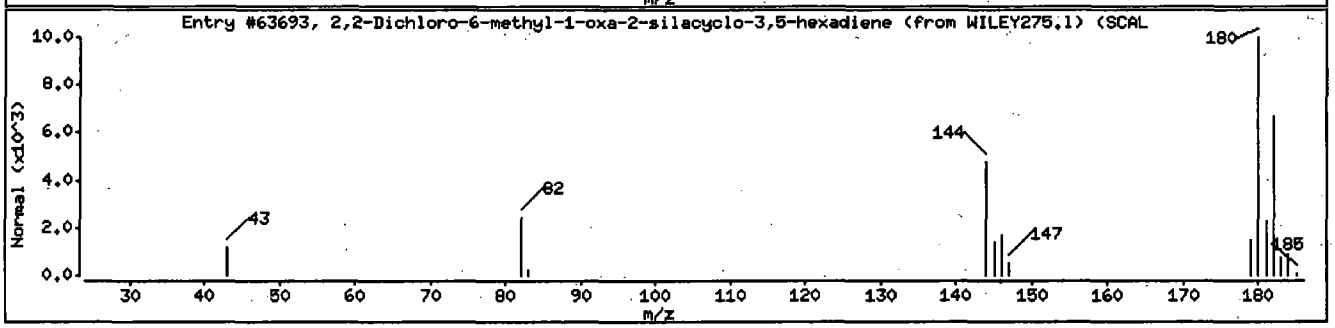
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	90	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	27	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	27	C5H6Cl2OSi	180









Digitally signed by Andrew J. Strebel on 03/01/2014 at 20:37.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19a.b/db0843_lib.d

Date : 20-FEB-2014 02:39

Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

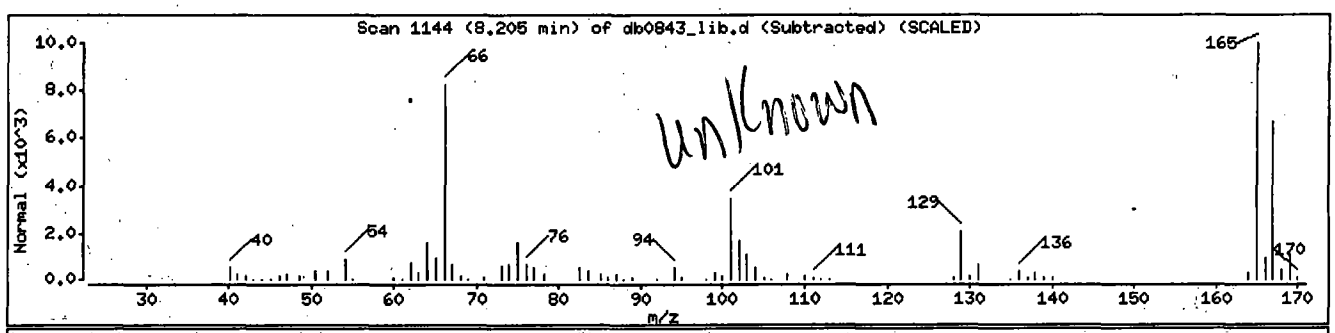
Volume Injected (uL): 1.0

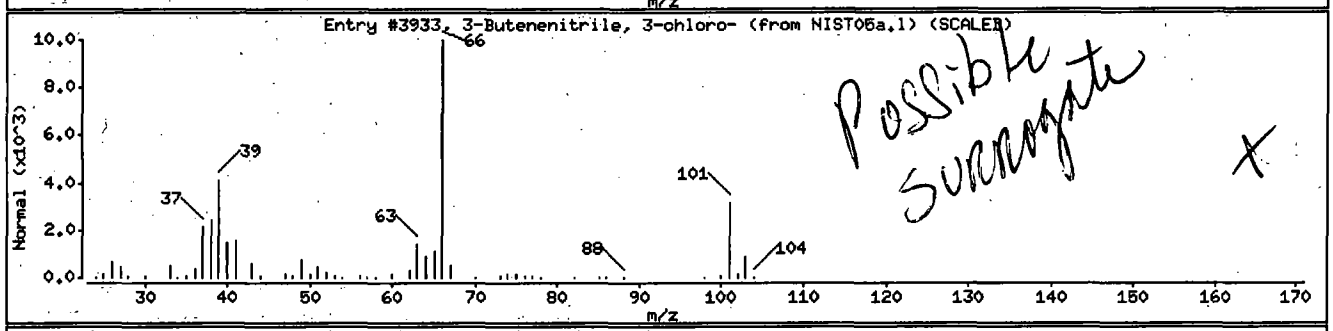
Operator: ceb05247

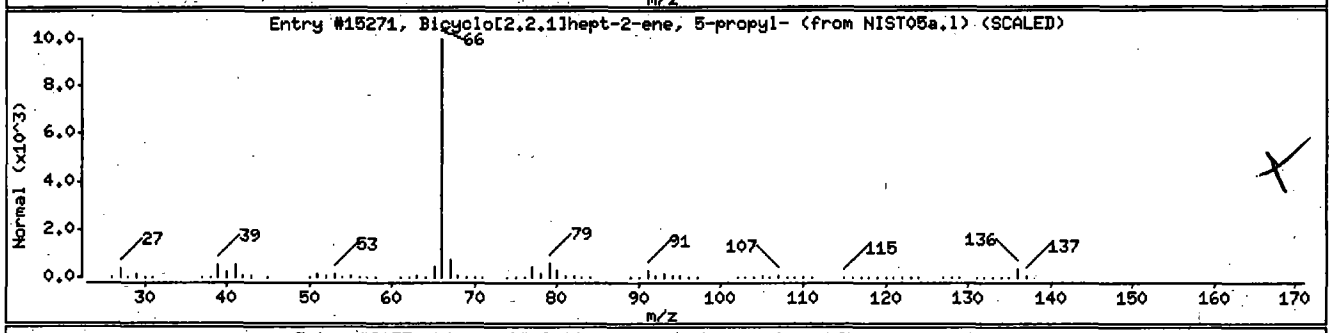
Column phase: J&W DB-5MS

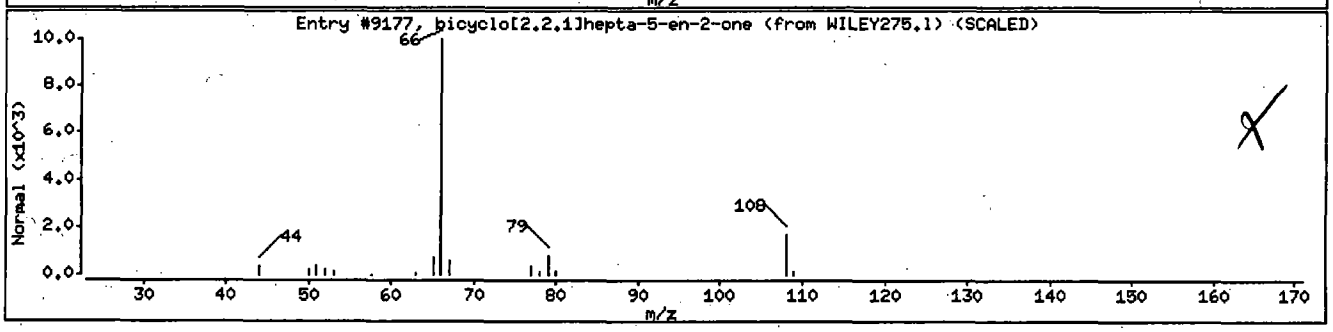
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136
bicyclo[2.2.1]hepta-5-en-2-one	0-00-0	WILEY275.l	9177	49	C7H8O	108









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb19a.b/db0843_lib.d

Date : 20-FEB-2014 02:39

Client ID: H2021

Instrument: HP19760.i

Sample Info: H2021;7365717;1;0;SAMPLE;;;

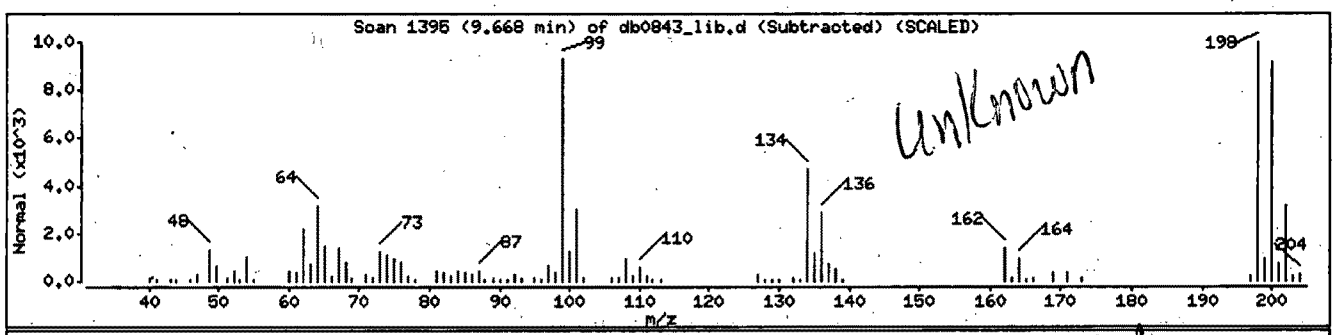
Volume Injected (uL): 1.0

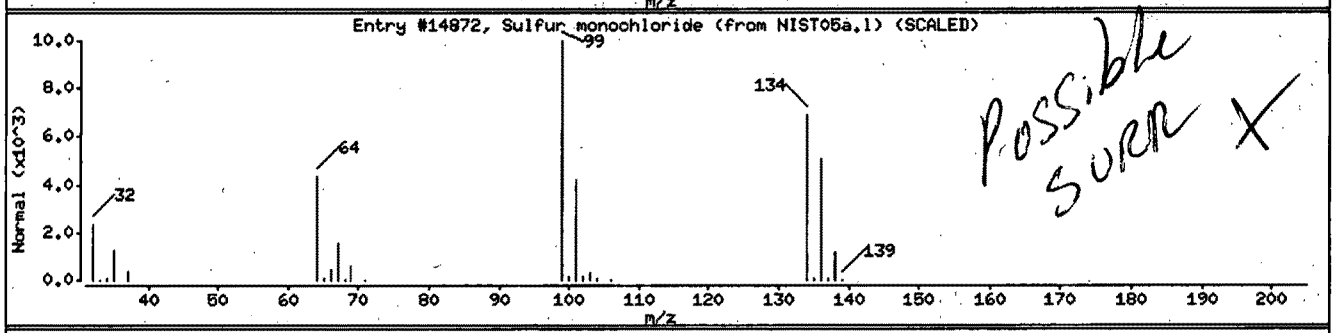
Operator: ceb05247

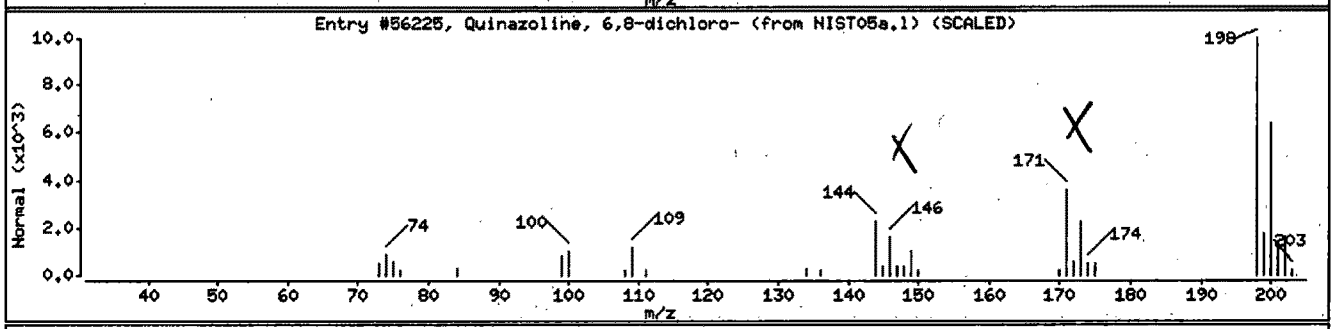
Column phase: J&W DB-5MS

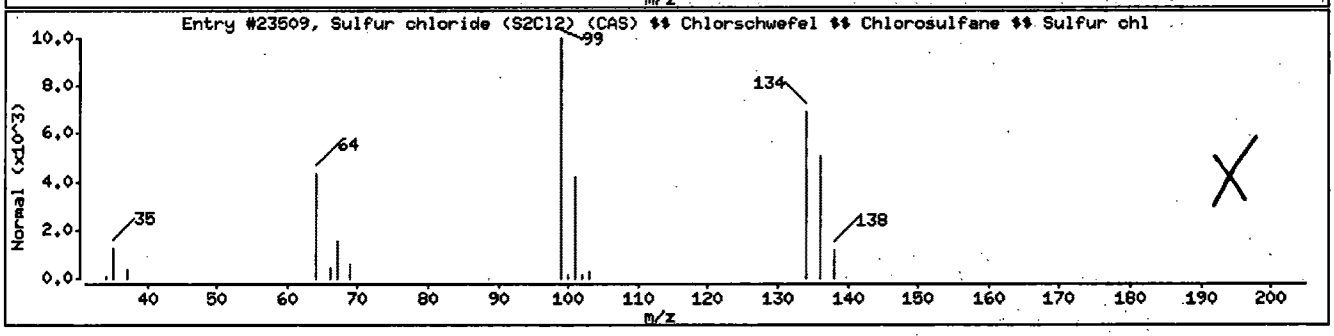
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Quinazoline, 6,8-dichloro-	17227-49-5	NIST05a.l	56225	38	C8H4Cl2N2	198
Sulfur chloride (S2Cl2) (CAS) $$ Chlorso	10025-67-9	WILEY275.l	23509	38	Cl2S2	134



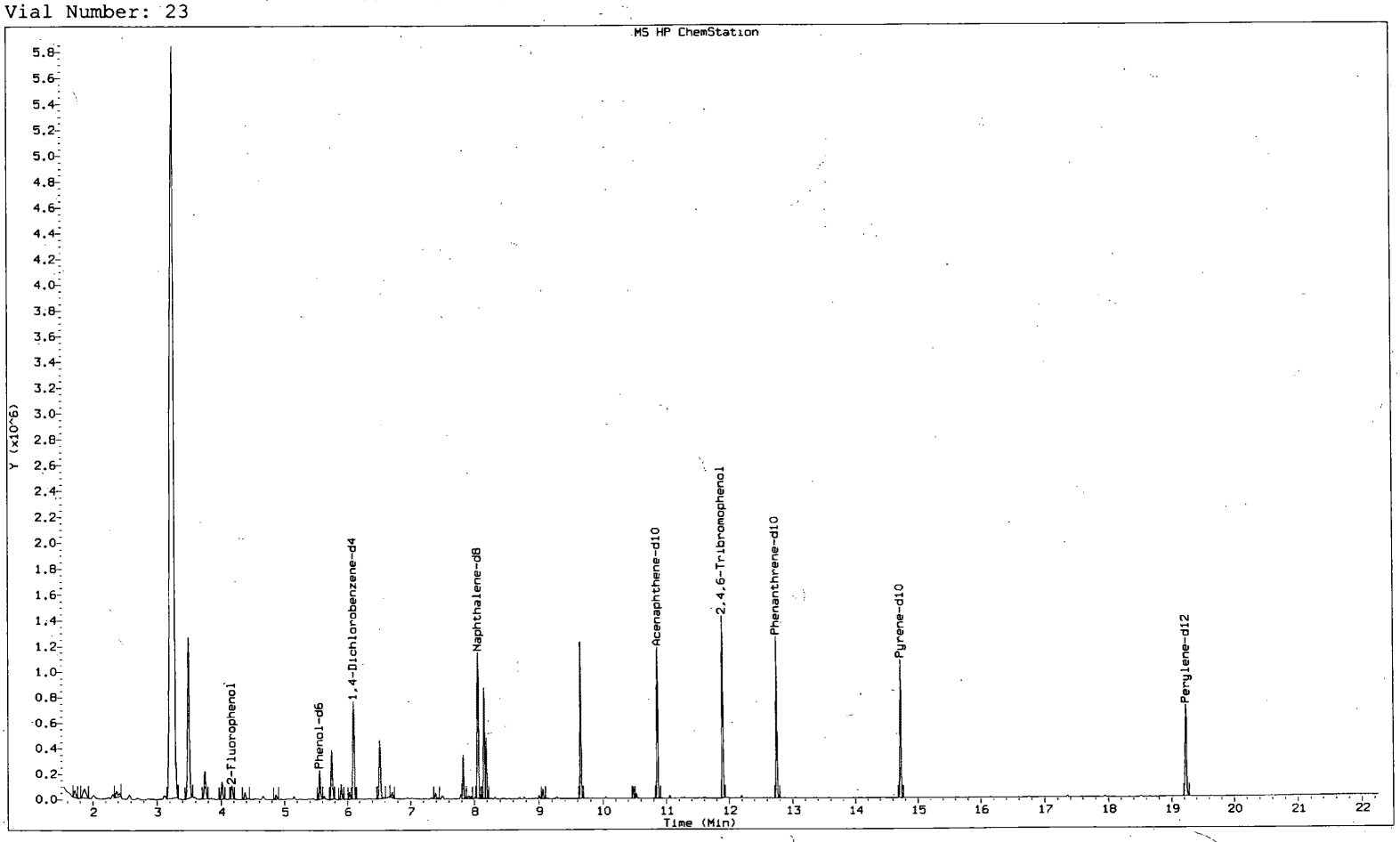






Digitally signed by Andrew J. Strebel on 03/01/2014 at 20:37.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb20.b/db0892_lib.d
Operator : jmg00346
Acquired : 20-FEB-2014 16:13
Instrument : HP19760.i
Sample Name: H3011;7366650;1;0;SAMPLE;;;
Misc Info : 14050WAA;WL13166;;1050;1000;0;db0872;13166;
Vial Number: 23



Lancaster Labs

Data file : /chem/HP19760.i/14feb20.b/db0892_lib.d
Lab Smp Id: 7366650 Client Smp ID: H3011
Inj Date : 20-FEB-2014 16:13
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H3011;7366650;1;0;SAMPLE;;;
Misc Info : 14050WAA;WL13166;;1050;1000;0;db0872;13166;
Comment : Max. number of TICs to report is 50, 22 TICs were found initially.
Method : /chem/HP19760.i/14feb20.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 20:47 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 23
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1050.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	1066791	10.000
* 48 Naphthalene-d8	8.059	1567695	10.000
* 83 Acenaphthene-d10	10.863	1410153	10.000

	CONCENTRATIONS				QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.717	103036	0.96585336	0.91986	83	NIST05a.l	31323	21

Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.869	240039	2.25010293	2.14295	64	NIST05a.l	4733	21(L)
Methane, dichloronitro-					CAS #: 7119-89-3		
2.370	118785	1.11347492	1.06045	43	NIST05a.l	12675	21
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.280	23173890	217.229733	206.88546	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.495	2449498	22.9613460	21.86794	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.752	411697	3.85920339	3.67543	23	NIST05a.l	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.014	243467	2.28223222	2.17355	38	NIST05a.l	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.375	103009	0.96559935	0.91961	38	NIST05a.l	33655	21(L)
Ethane, 1,1,2,2-tetrachloro- (CAS) $$ 1,					CAS #: 79-34-5		
4.865	60364	0.56584207	0.53889	95	WILEY275.l	50253	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.751	569402	5.33751616	5.08334	91	WILEY275.l	18902	21
Decane (CAS) $$ n-Decane $$ Isodecane $$					CAS #: 124-18-5		
5.902	176290	1.65252559	1.57383	94	WILEY275.l	30012	21
Oxirane, ethenyl-					CAS #: 930-22-3		
6.036	79331	0.74363637	0.70822	7	NIST05a.l	526	21(L)
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.514	723425	6.78130956	6.45839	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.713	80417	0.75382313	0.71792	32	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.395	65279	0.41639949	0.39657	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	440560	2.81024214	2.67642	27	NIST05a.l	13652	48(L)

Target compound.
Do not report.
ajs00193 03/01/2014

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1H-Pyrazole, 1-methyl- (CAS) $$ 1-Methyl					CAS #: 930-36-9		
7.913	57685	0.36796168	0.35043	53	WILEY275.1	2324	48
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.152	1003257	6.39956803	6.09482	43	NIST05a.1	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	601393	3.83615737	3.65348	50	NIST05a.1	3933	48
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc					CAS #: 63506-25-2		
9.062	99773	0.63643018	0.60612	78	WILEY275.1	109601	48(L)
Sulfur monochloride					CAS #: 10025-67-9		
9.650	1540074	10.9213238	10.40126	38	NIST05a.1	14872	83
2-bromo-7,7-dichlorocyclo[4.1.0]heptan					CAS #: 113035-97-5		
10.478	96348	0.68324377	0.65070	91	WILEY275.1	127158	83

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

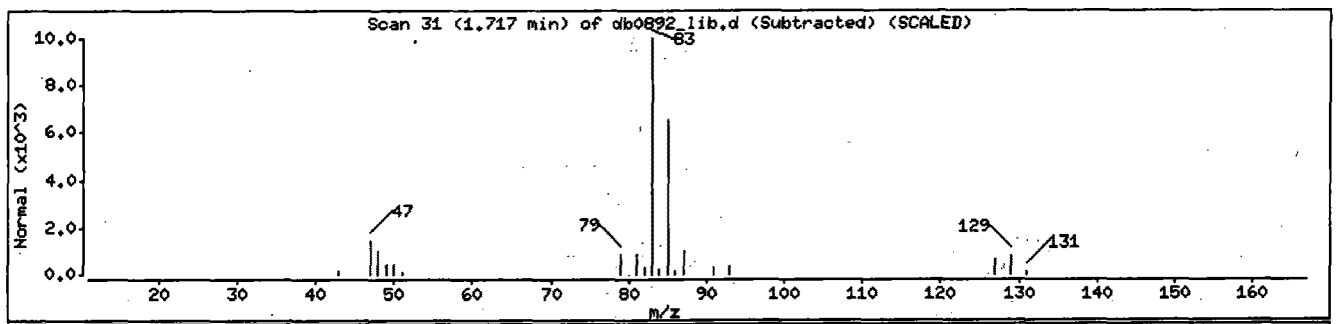
Volume Injected (uL): 1.0

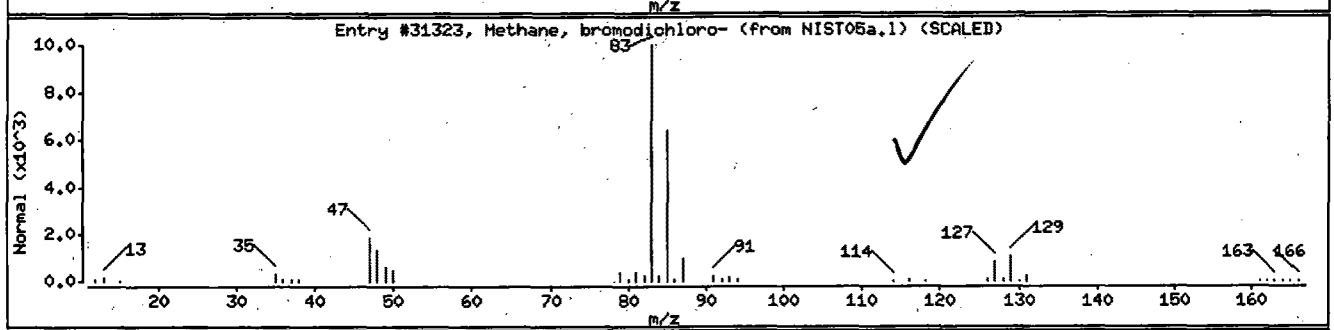
Operator: jmg00346

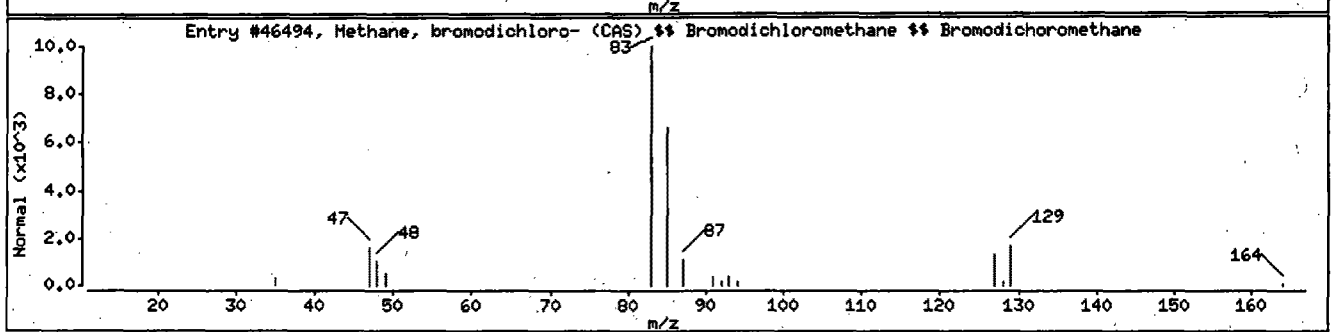
Column phase: J&W DB-5MS

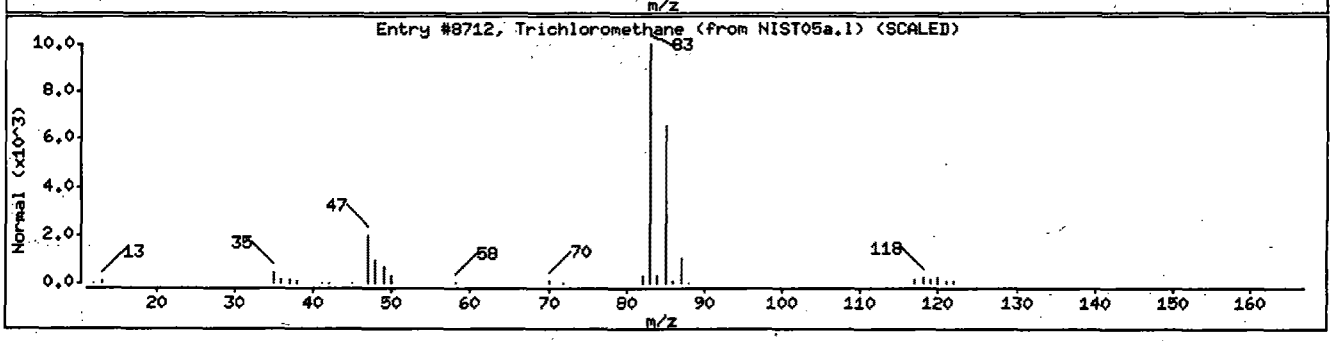
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	83	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46494	83	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

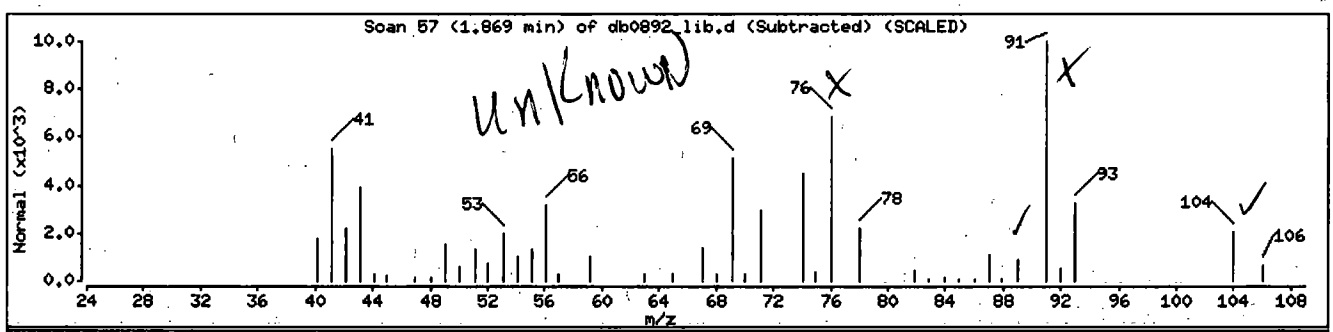
Volume Injected (uL): 1.0

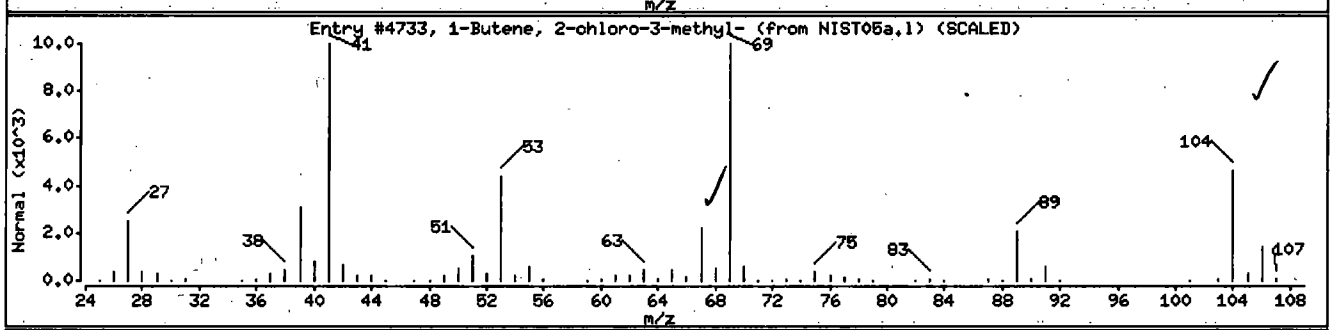
Operator: jmg00346

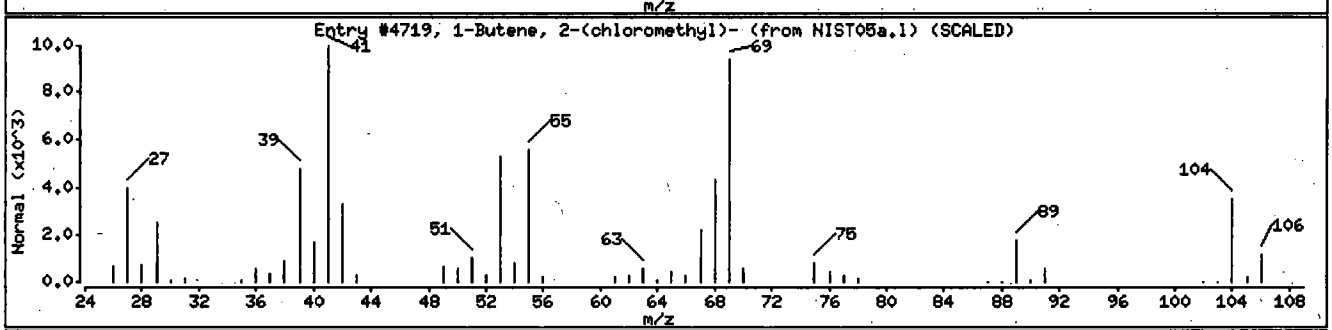
Column phase: J&W DB-5MS

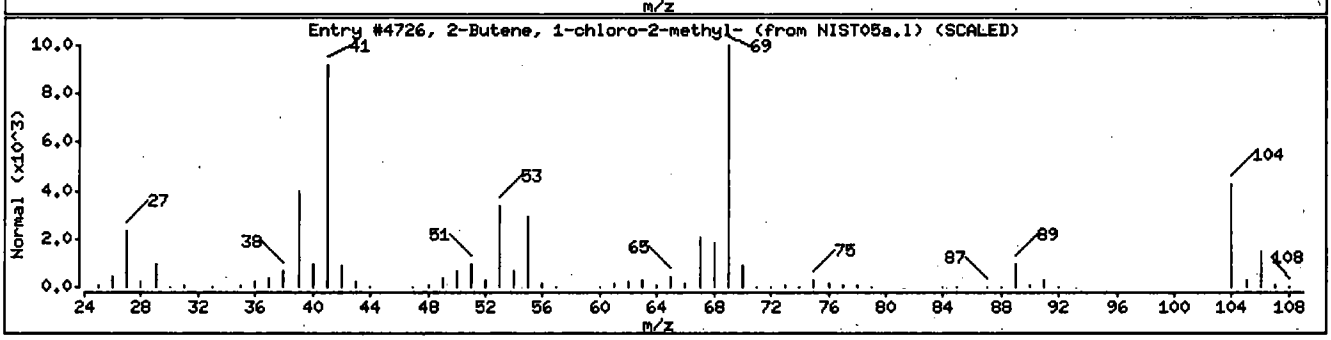
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	64	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4719	64	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4726	53	C5H9Cl	104









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

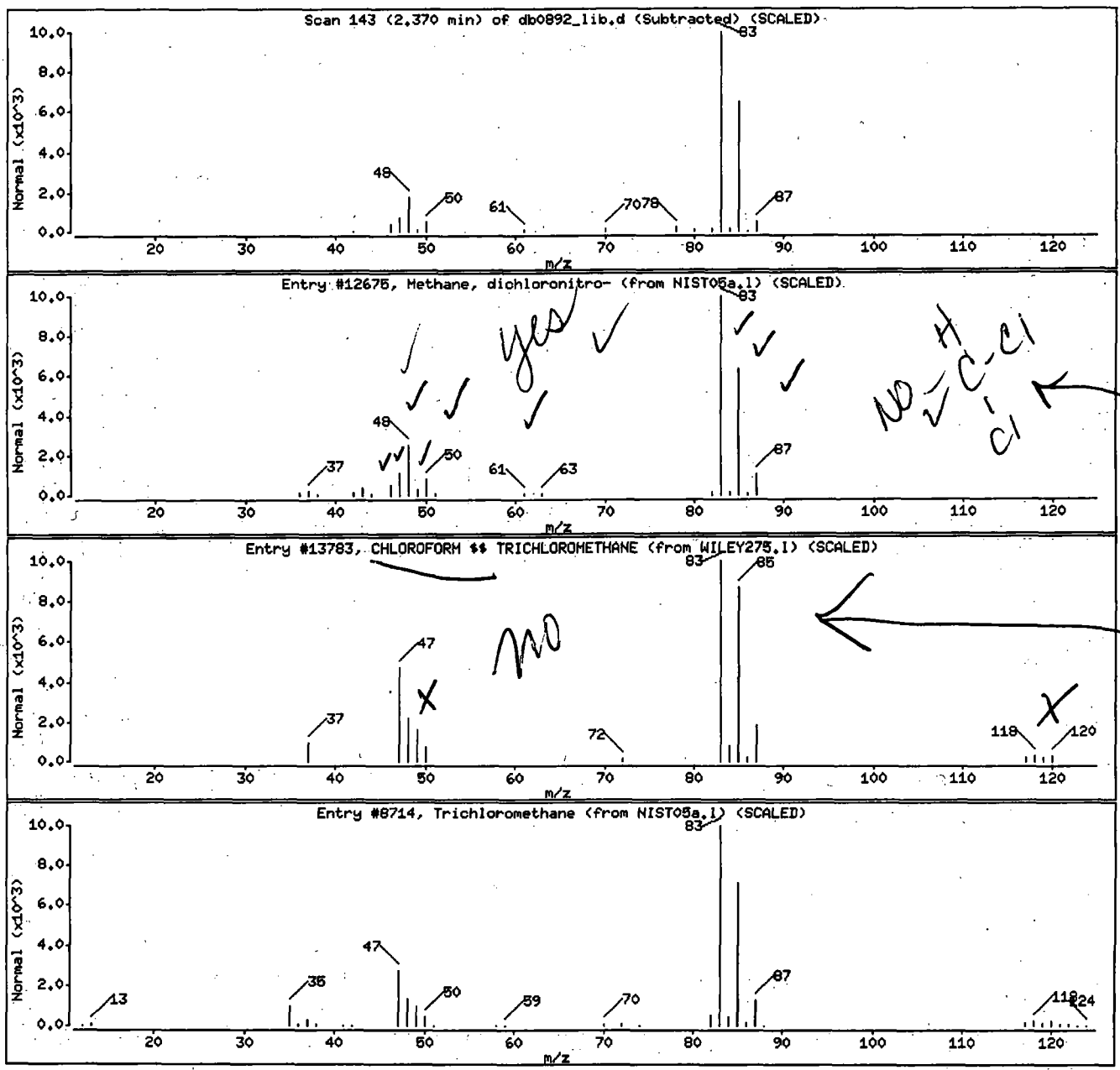
Client ID: H3011 Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, dichloronitro-	7119-89-3	NIST05a.l	12675	43	CHCl2NO2	129
CHLOROFORM $$ TRICHLOROMETHANE	67-66-3	WILEY275.l	13783	40	CHCl3	118
Trichloromethane	67-66-3	NIST05a.l	8714	9	CHCl3	118



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

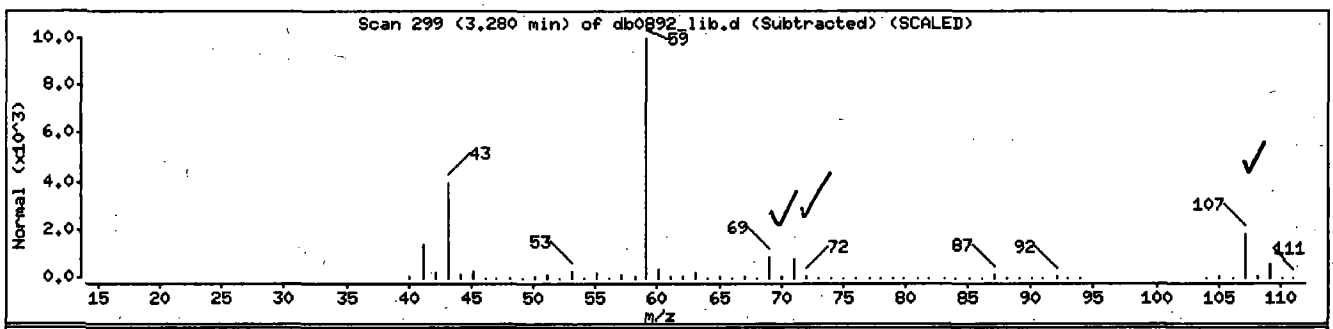
Volume Injected (uL): 1.0

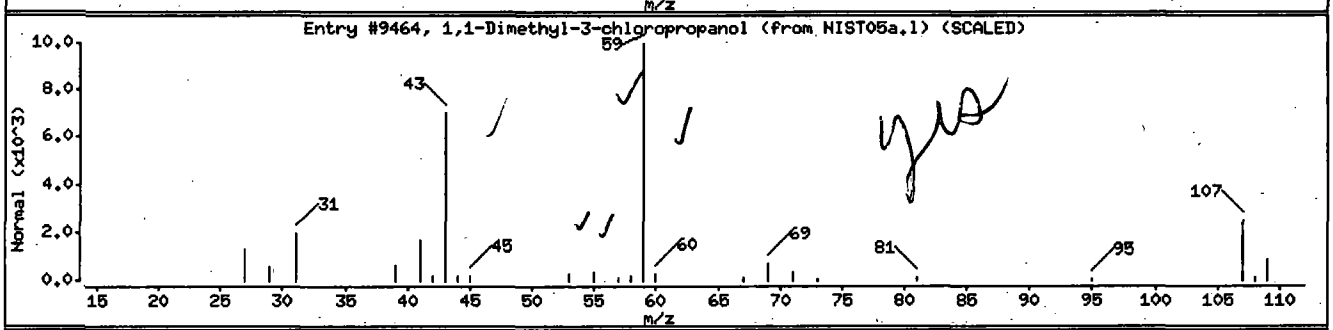
Operator: jmg00346

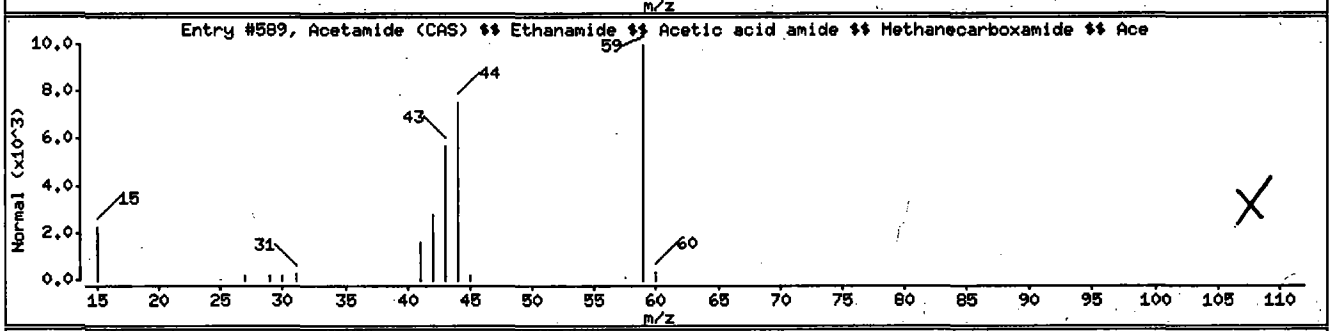
Column phase: J&W DB-5MS

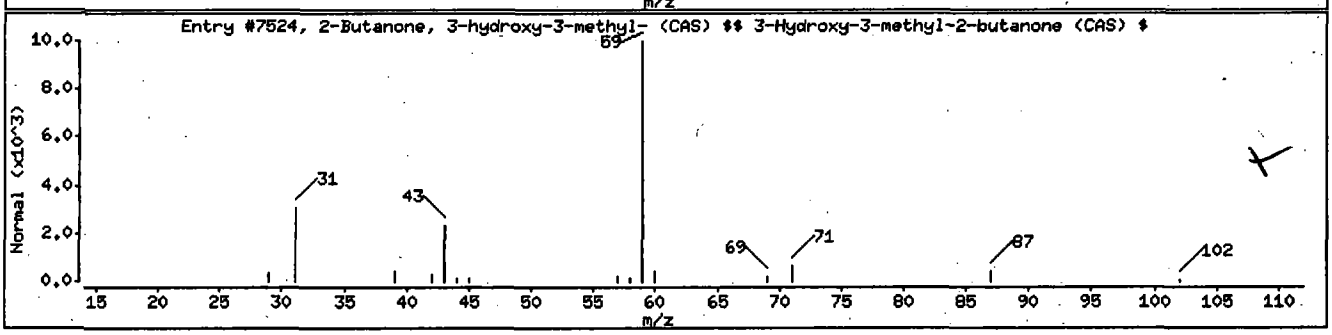
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10:
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

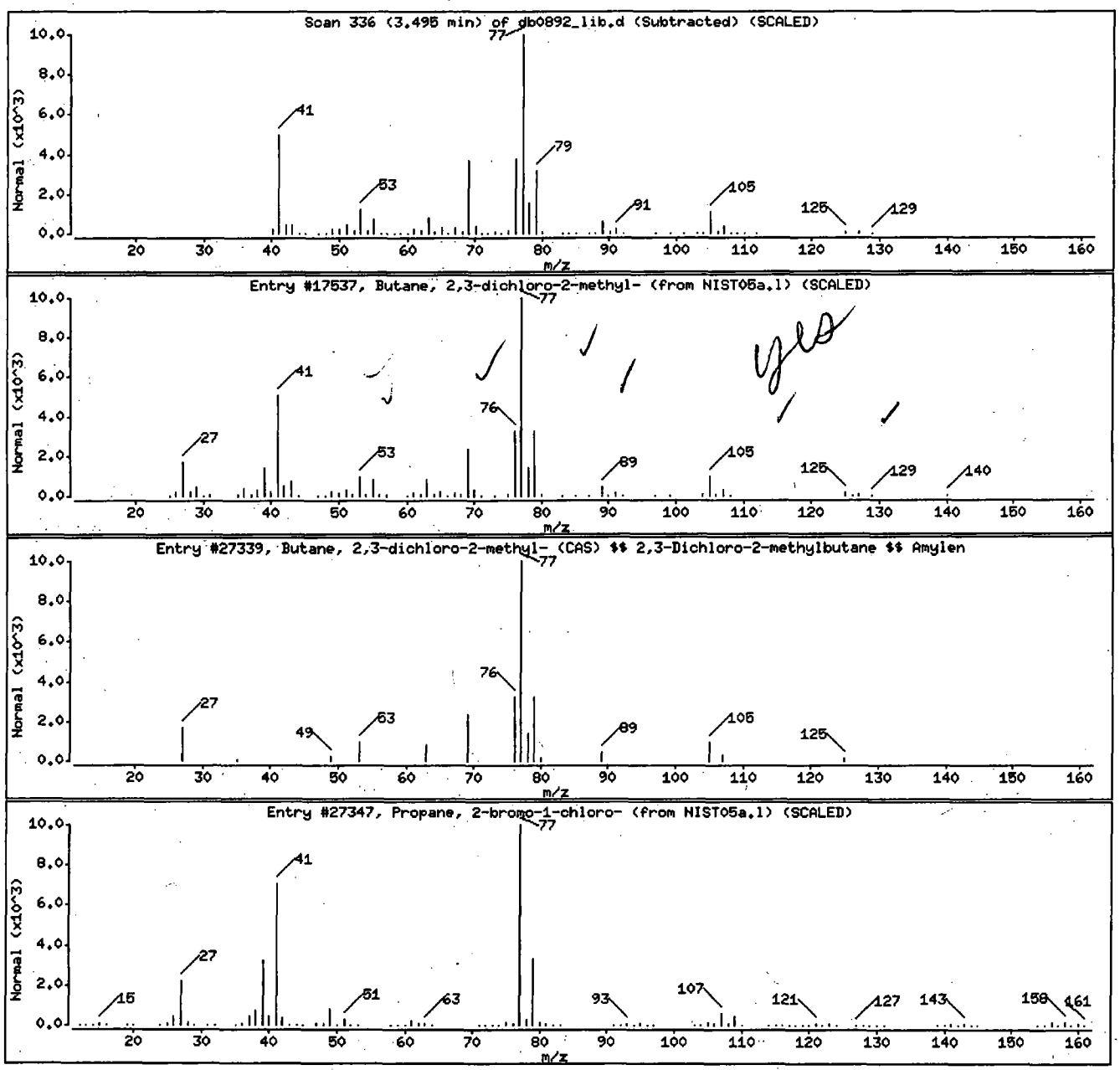
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	40	C3H6BrCl	156



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

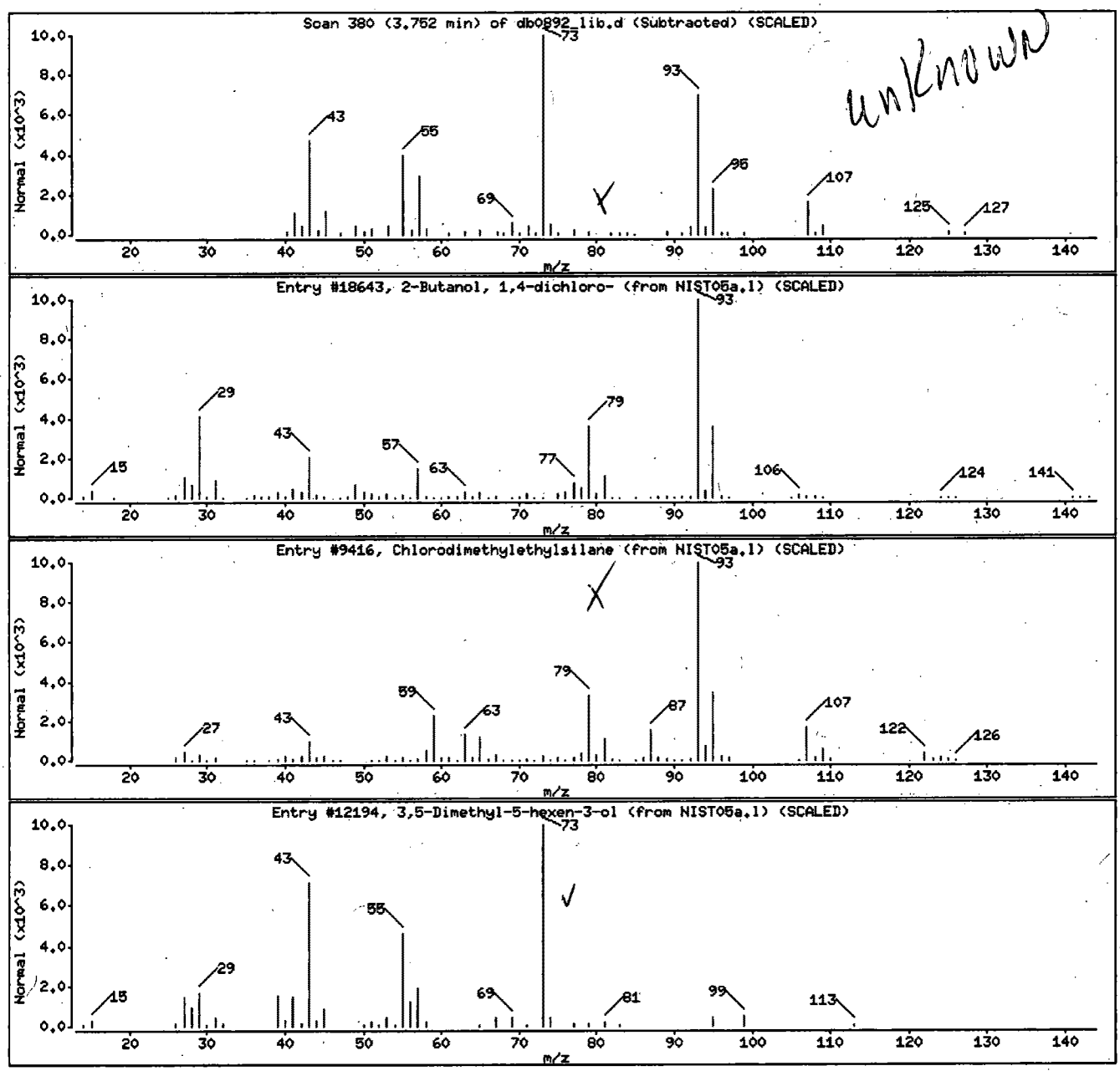
Client ID: H3011 | Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 | Operator: jmg00346

Column phase: J&W DB-5MS | Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	23	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	28	C4H11ClSi	122
3,5-Dimethyl-5-hexen-3-ol	1569-46-6	NIST05a.l	12194	12	C8H16O	128



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

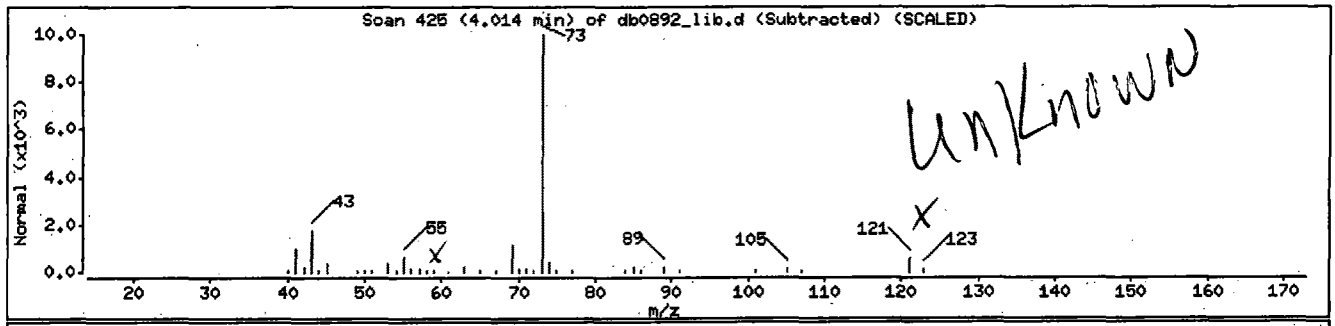
Volume Injected (uL): 1.0

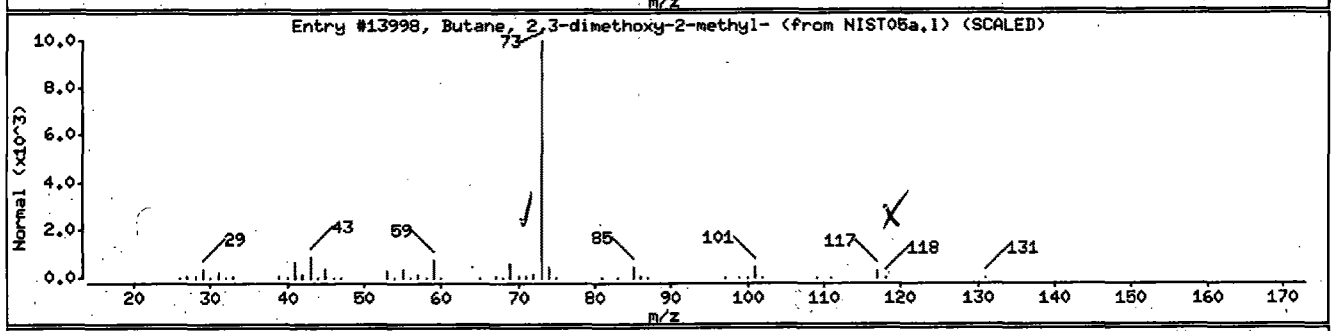
Operator: jmg00346

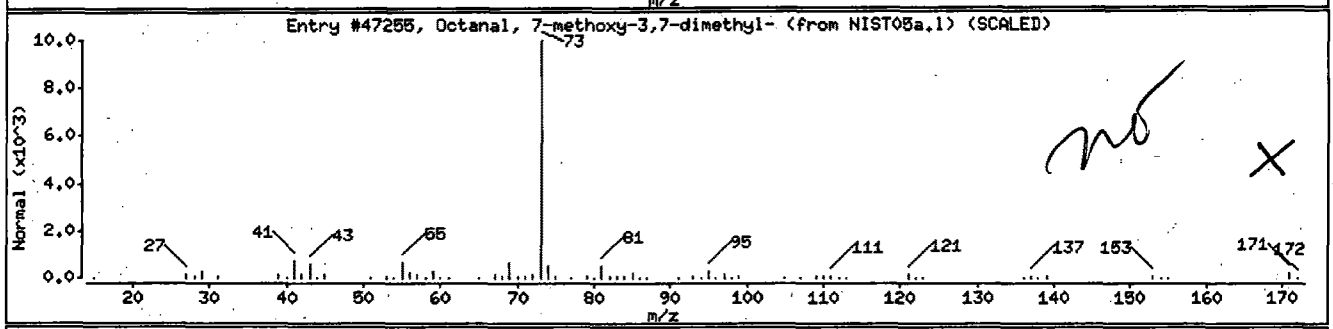
Column phase: J&W DB-5MS

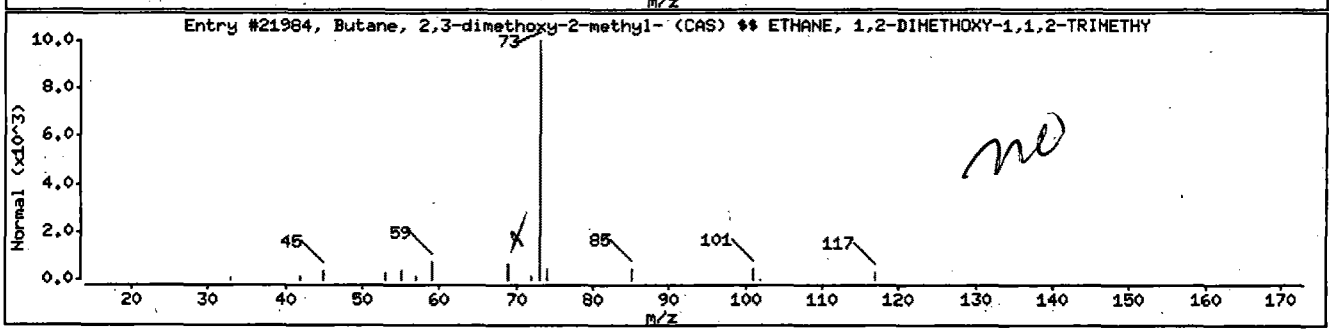
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	38	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	38	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) **	74421-00-4	WILEY275.l	21984	38	C7H16O2	132









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

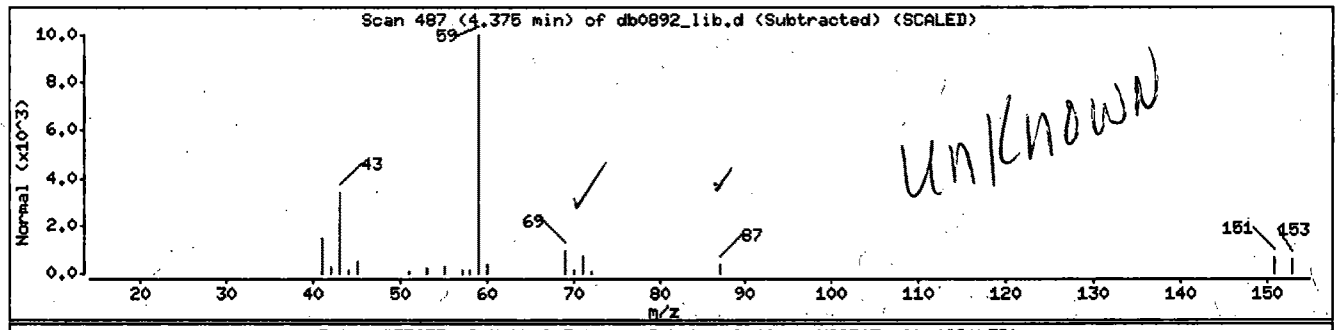
Client ID: H3011 Instrument: HP19760.i

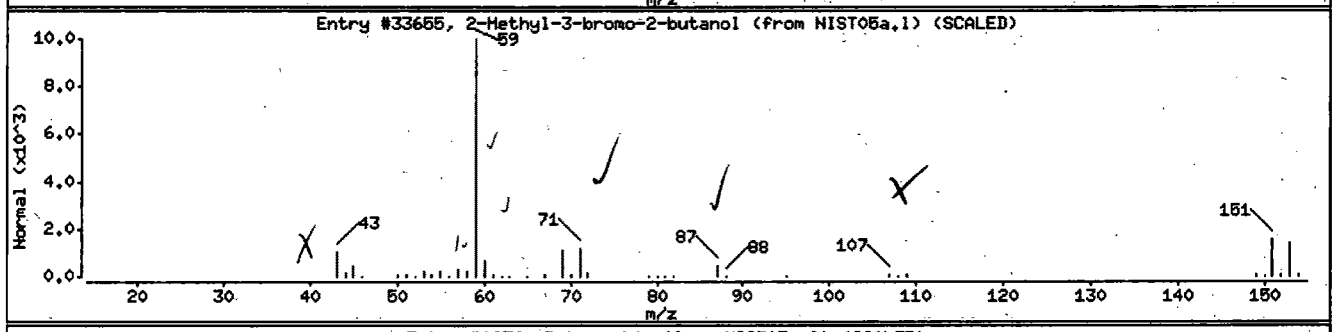
Sample Info: H3011;7366650;1;0;SAMPLE;;;

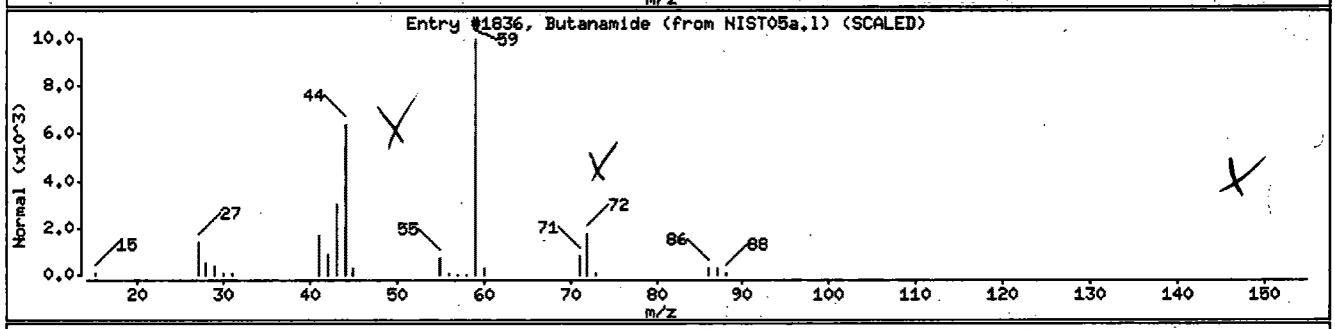
Volume Injected (uL): 1.0 Operator: jmg00346

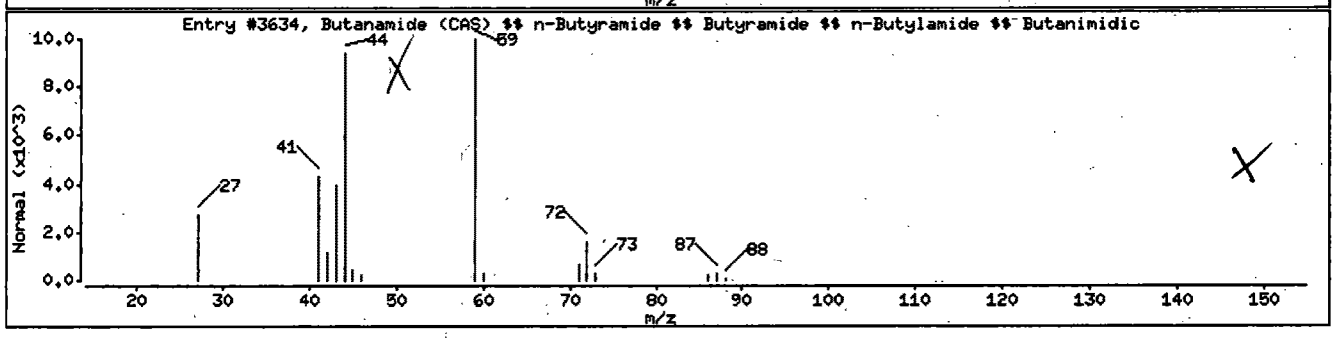
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	38	C5H11BrO	166
Butanamide	541-35-5	NIST05a.l	1836	64	C4H9NO	87
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3634	64	C4H9NO	87









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Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

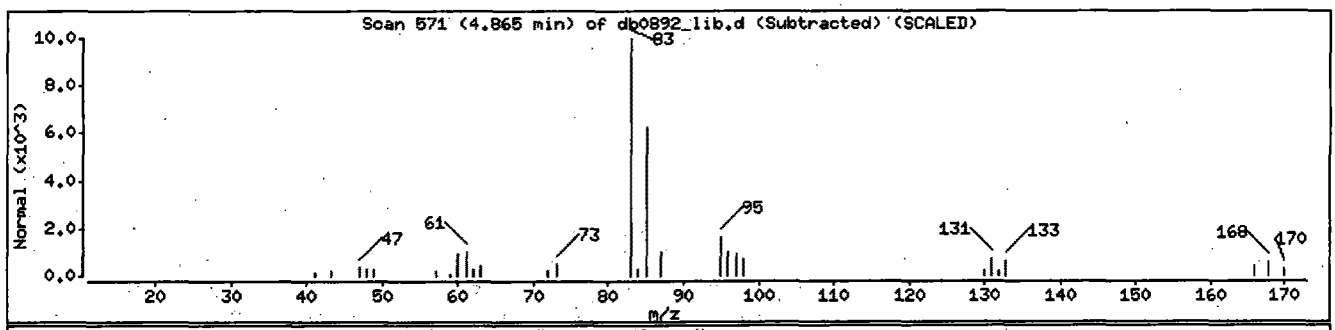
Volume Injected (uL): 1.0

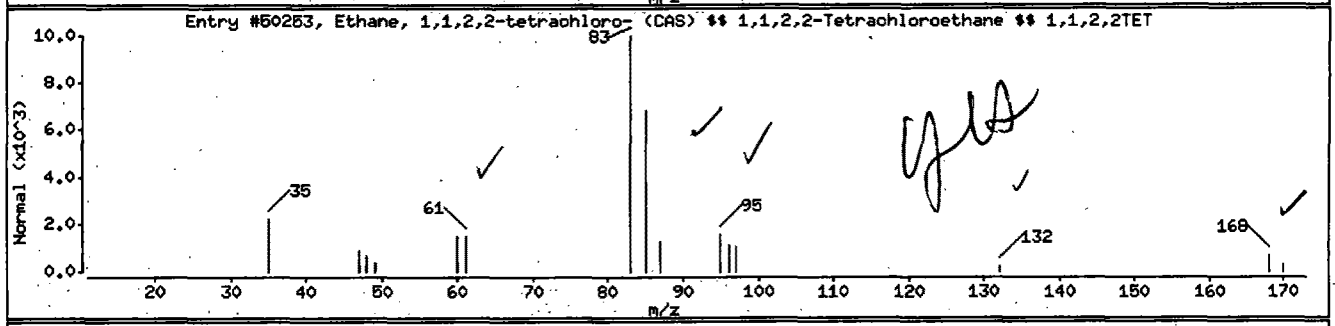
Operator: jmg00346

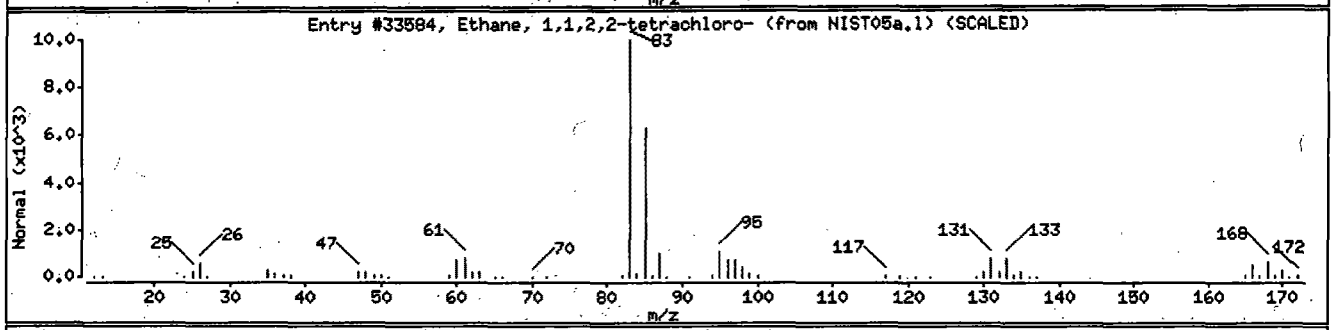
Column phase: J&W DB-5MS

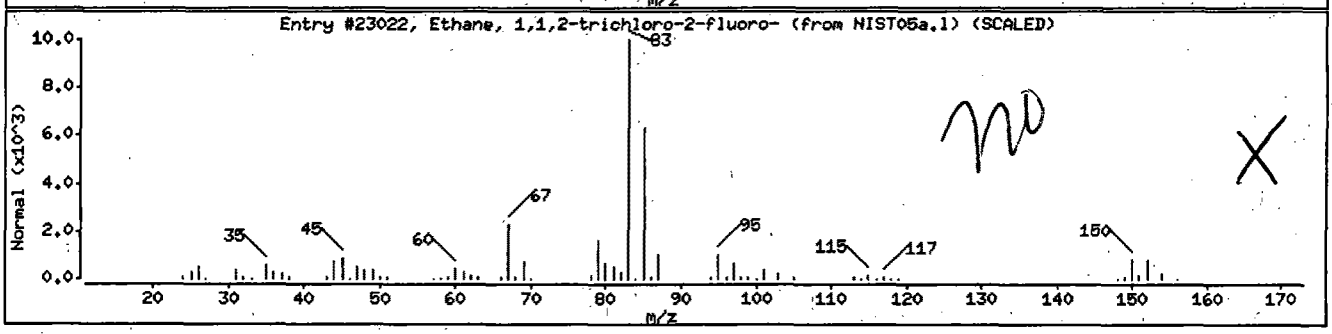
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Ethane, 1,1,2,2-tetrachloro- (CAS) $$ 1,	79-34-5	WILEY275.l	50253	95	C2H2Cl4	166
Ethane, 1,1,2,2-tetrachloro-	79-34-5	NIST05a.l	33584	94	C2H2Cl4	166
Ethane, 1,1,2-trichloro-2-fluoro-	359-28-4	NIST05a.l	23022	64	C2H2Cl3F	150









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Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

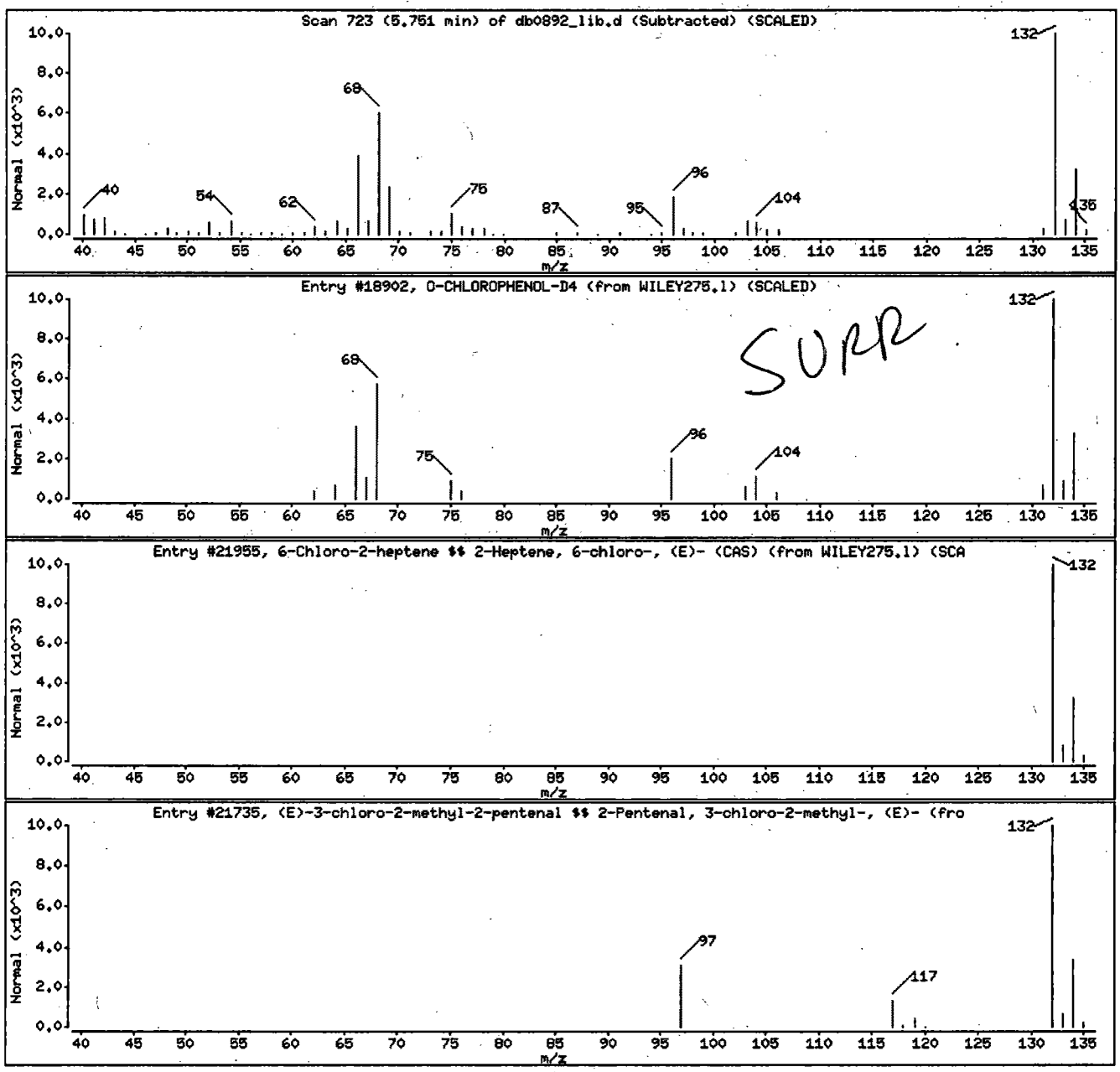
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

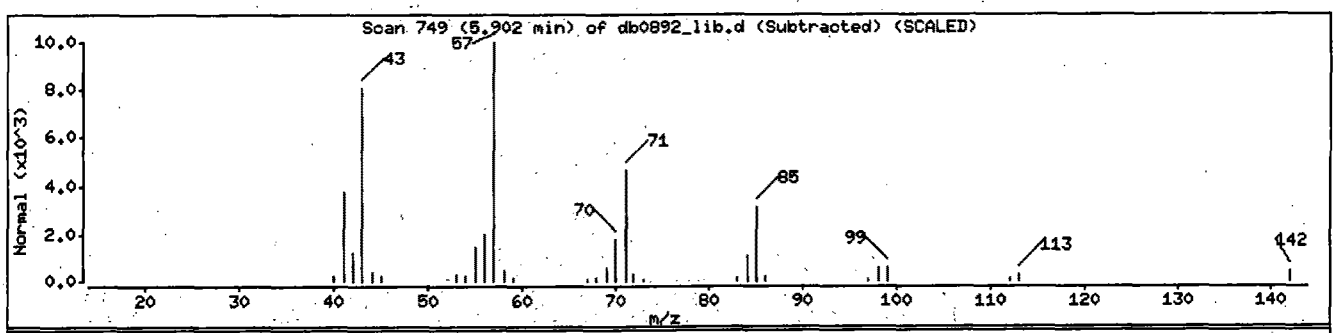
Client ID: H3011 Instrument: HP19760.i

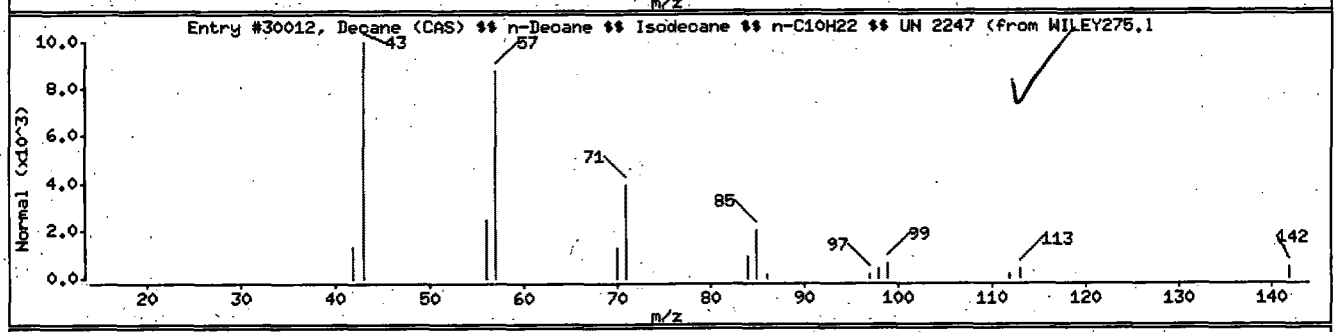
Sample Info: H3011;7366650;1;0;SAMPLE;;;

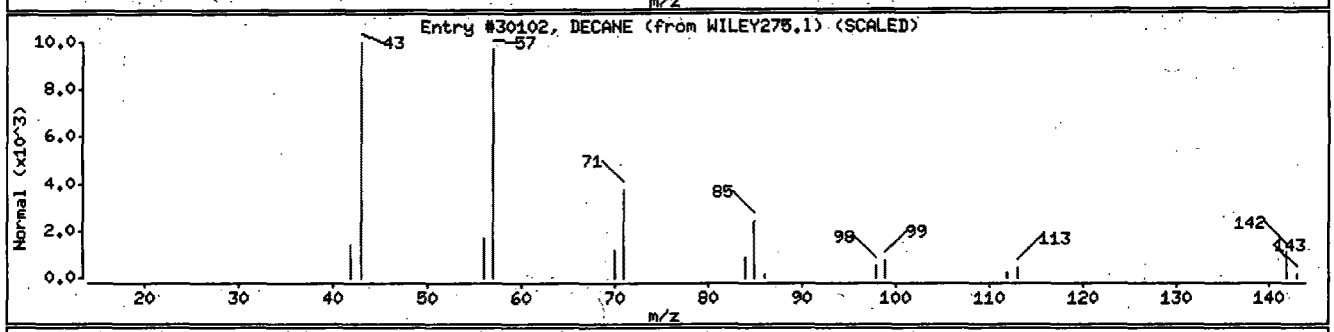
Volume Injected (uL): 1.0 Operator: jmg00346

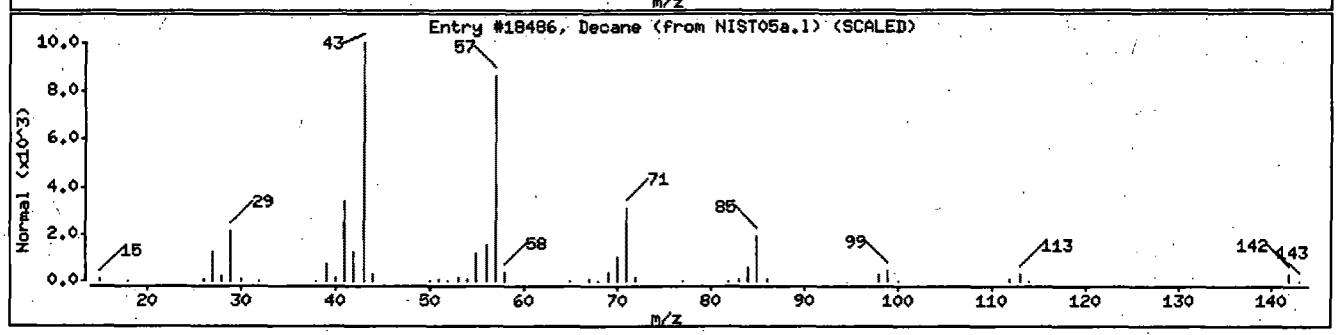
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.1	30012	94	C10H22	142
DECANE	0-00-0	WILEY275.1	30102	91	C10H22	142
Decane	124-18-5	NIST05a.1	18486	87	C10H22	142









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Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

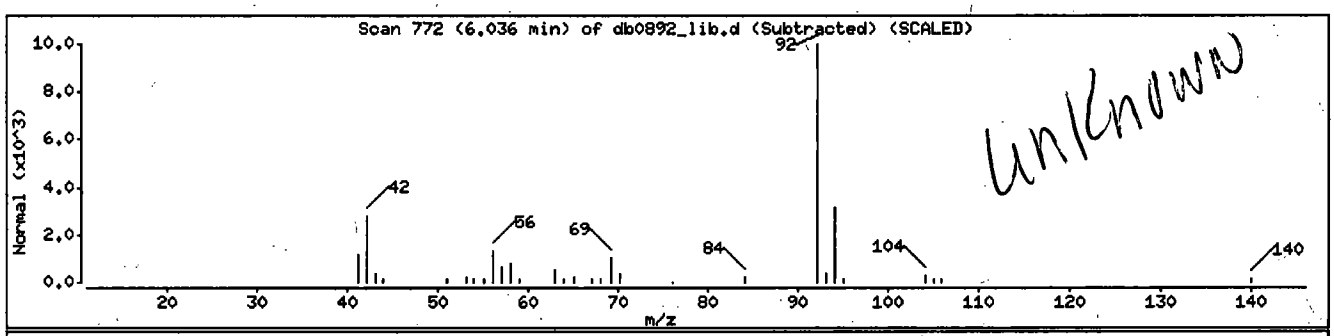
Volume Injected (uL): 1.0

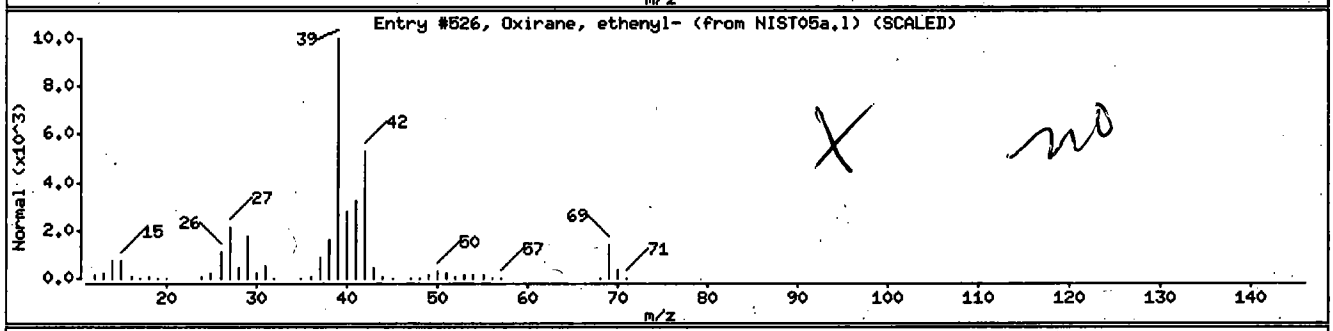
Operator: jmg00346

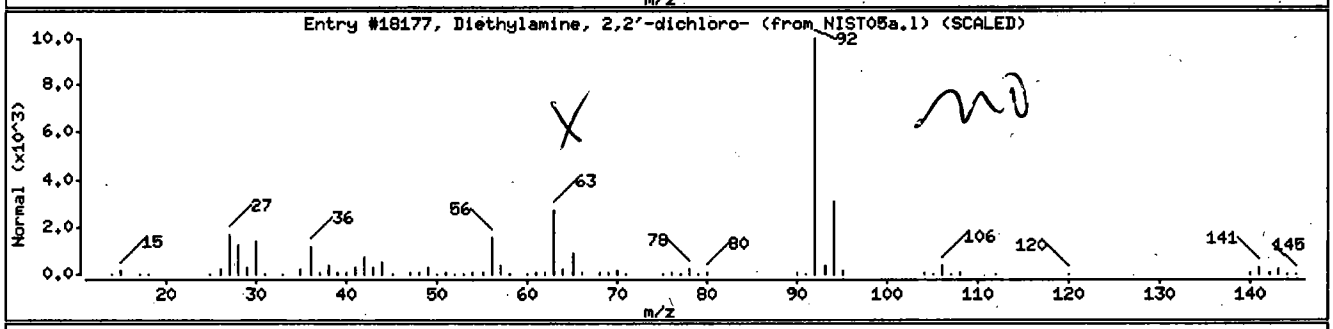
Column phase: J&W DB-5MS

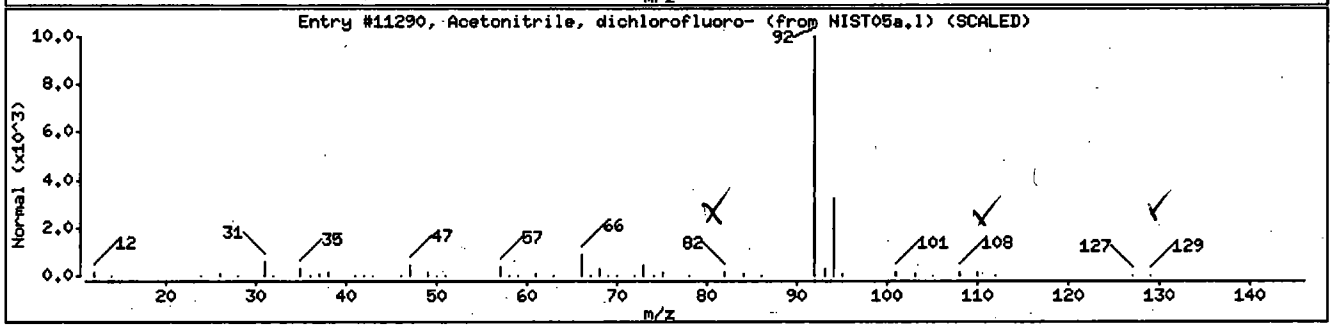
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Oxirane, ethenyl-	930-22-3	NIST05a.l	526	7	C4H6O	70
Diethylamine, 2,2'-dichloro-	334-22-5	NIST05a.l	18177	38	C4H9Cl2N	141
Acetonitrile, dichlorofluoro-	353-82-2	NIST05a.l	11290	9	C2Cl2FN	127









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

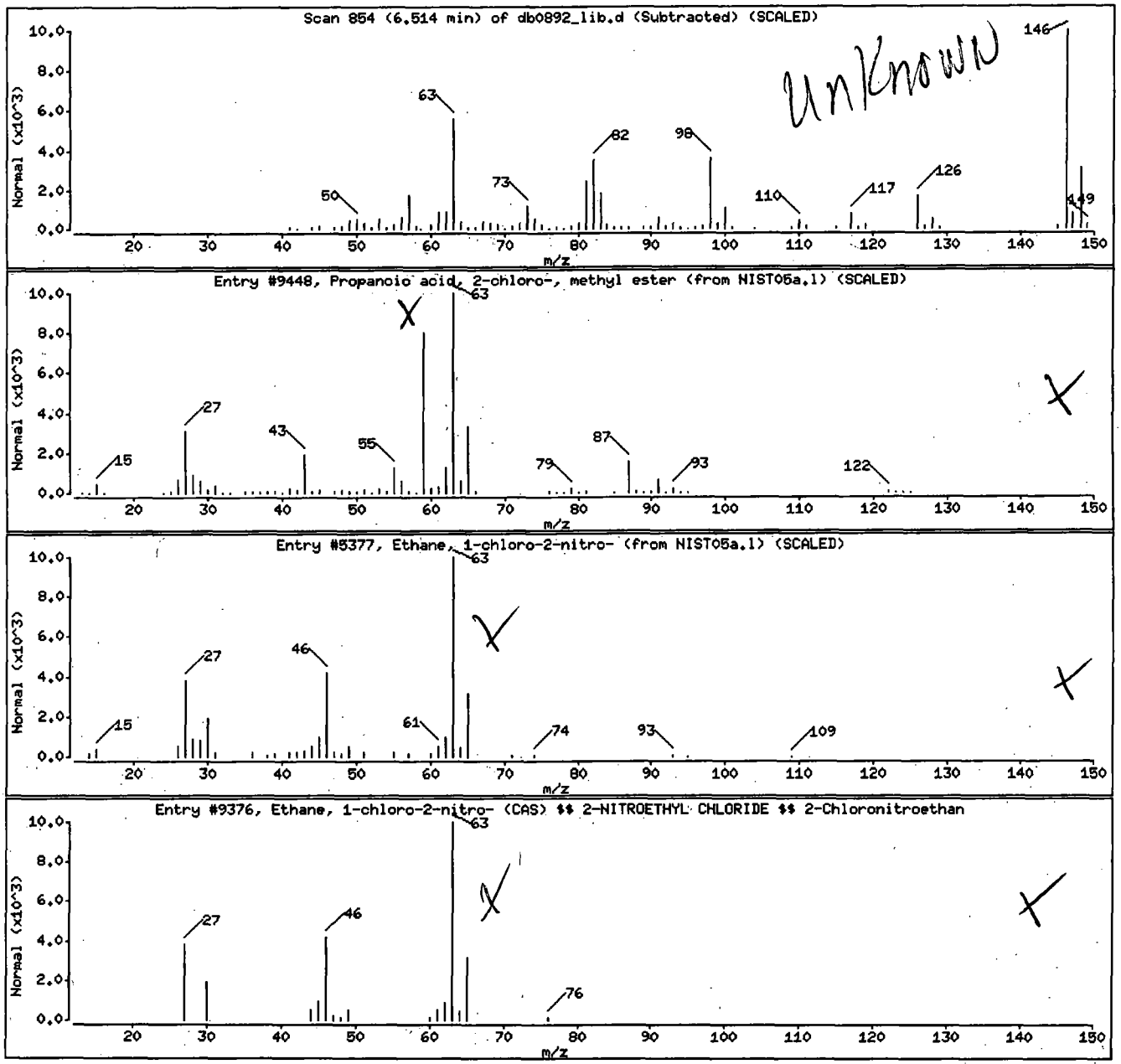
Client ID: H3011 Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
Ethane, 1-chloro-2-nitro-	625-47-8	NIST05a.l	5377	37	C2H4ClNO2	109
Ethane, 1-chloro-2-nitro- (CAS) $$ 2-NIT	625-47-8	WILEY275.l	9376	37	C2H4ClNO2	109



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Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/01/2014

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

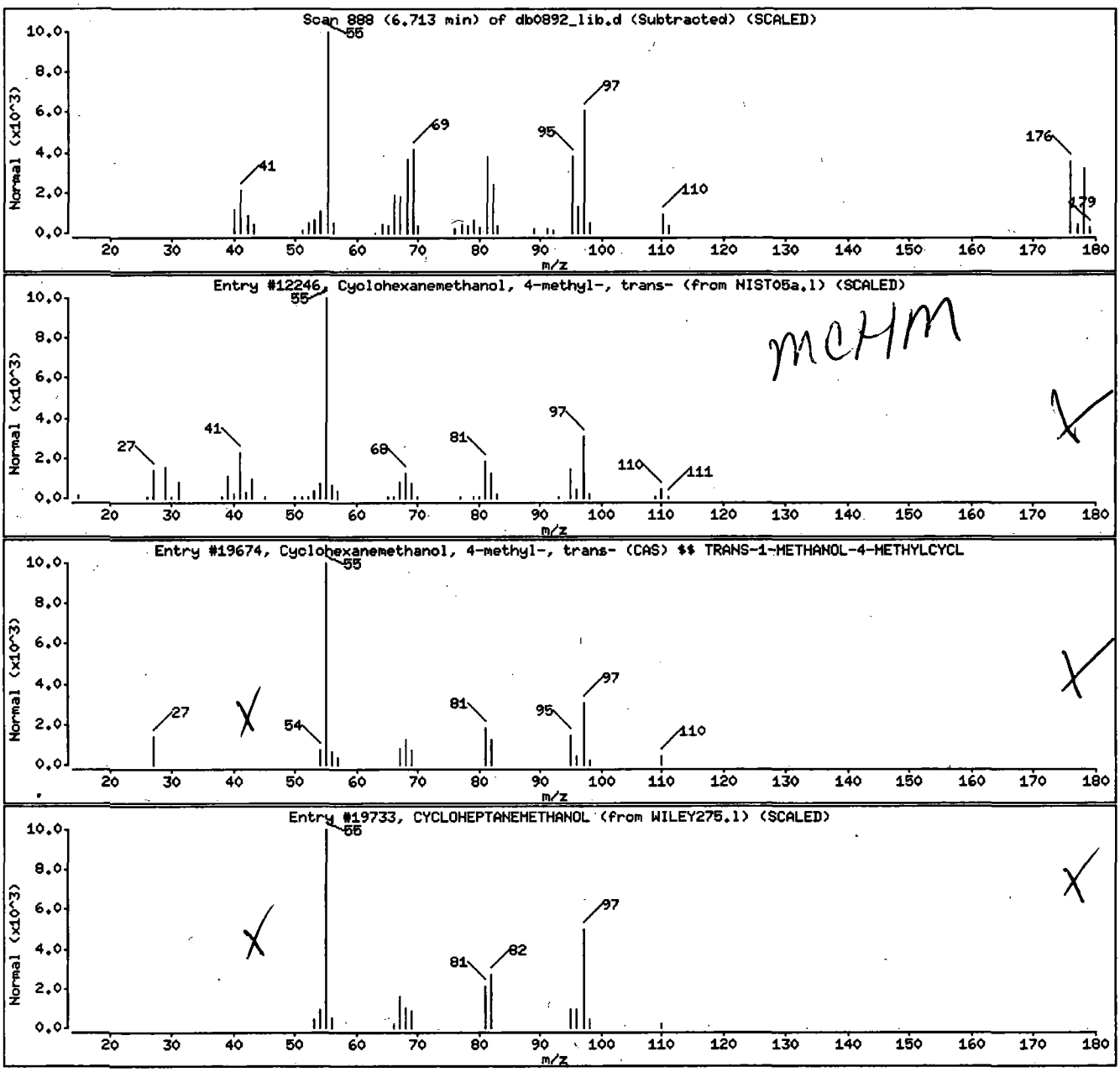
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	32	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	32	C8H16O	128
CYCLOHEPTANEMETHANOL	0-00-0	WILEY275.l	19733	27	C8H16O	128



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Target 3.5 esignature user ID: ajs00193

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Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

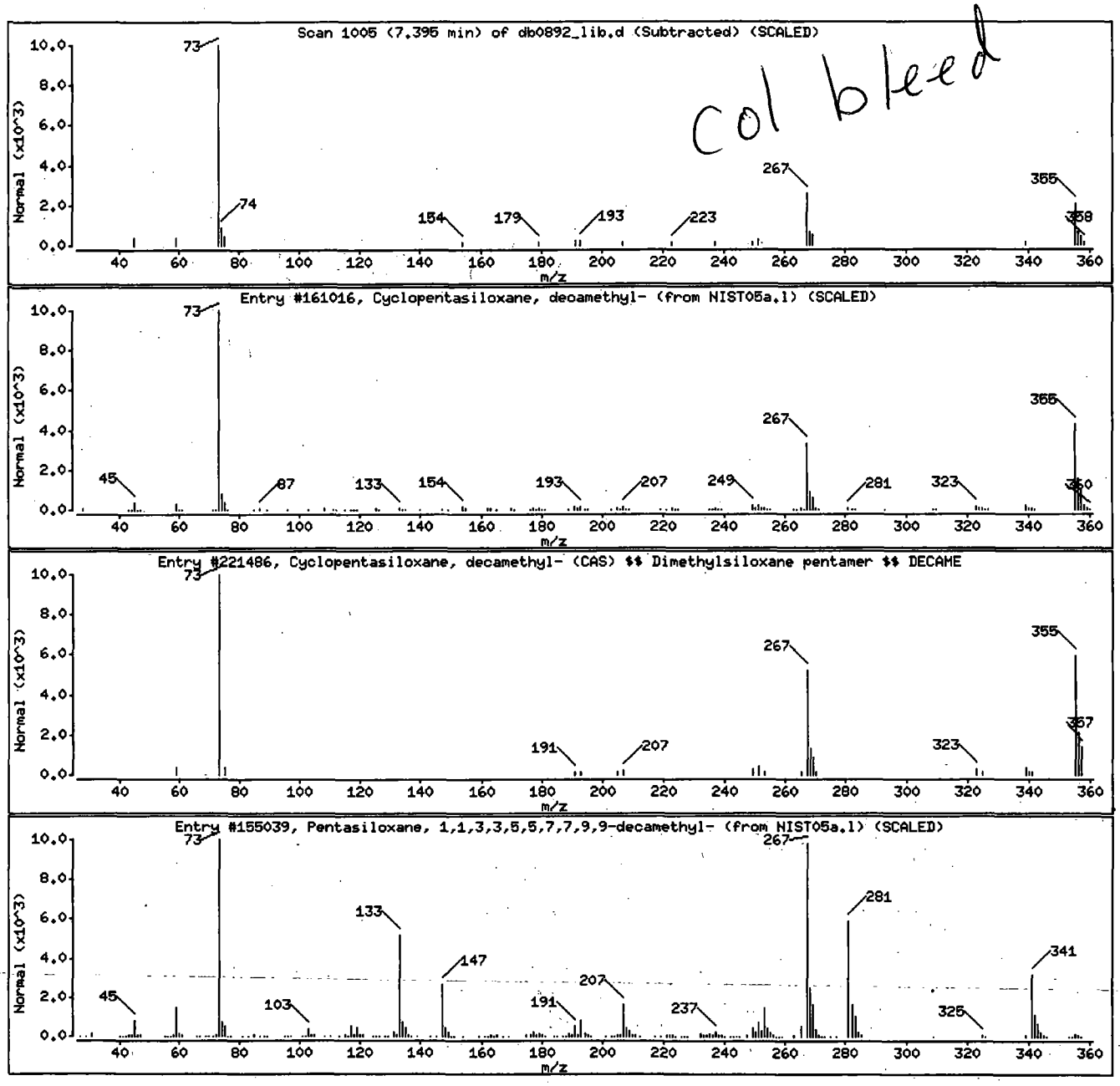
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	72	C10H30O5Si5	370
Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decam	995-83-5	NIST05a.l	155039	38	C10H32O4Si5	356



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Date : 20-FEB-2014 16:13

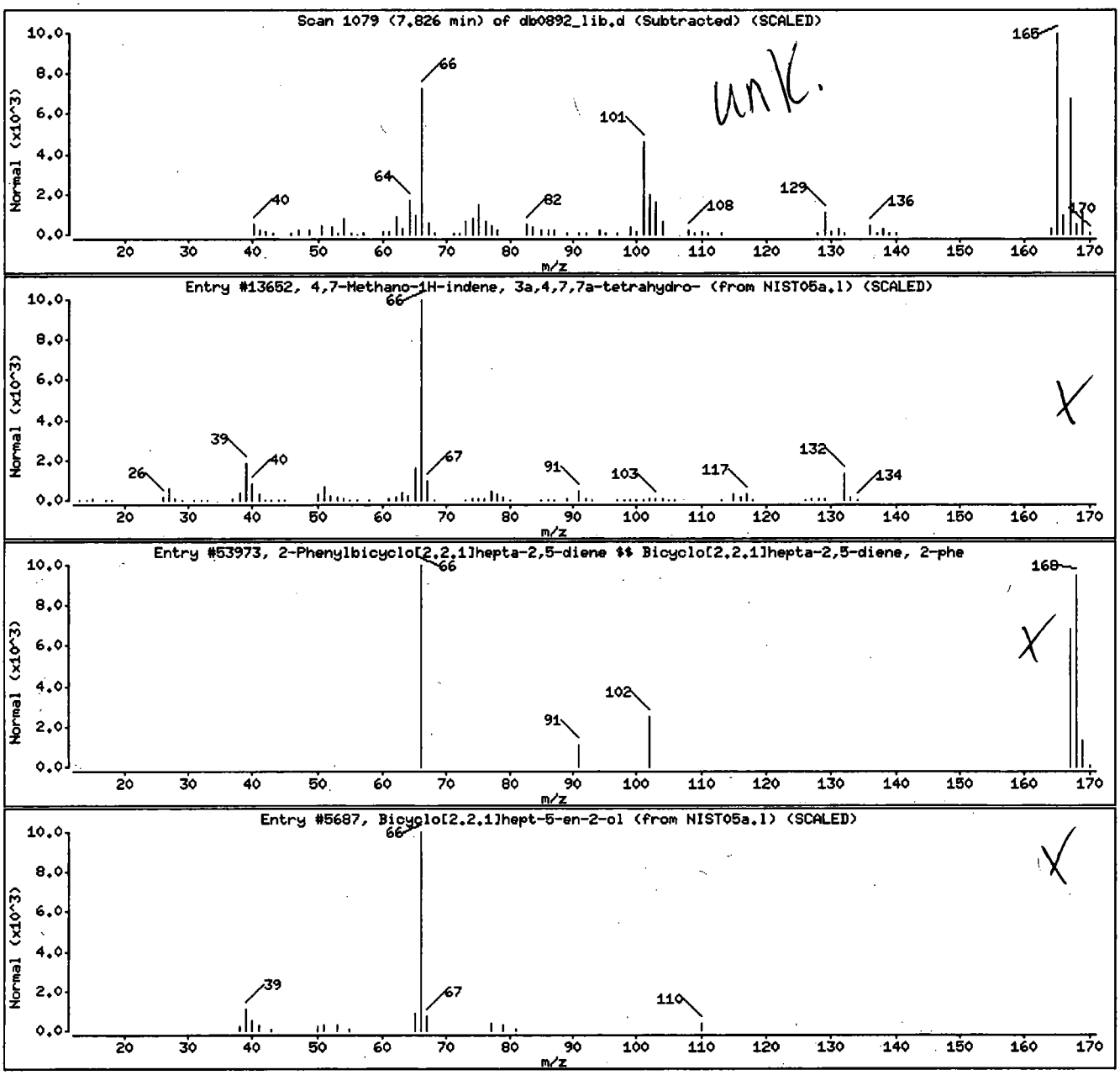
Client ID: H3011 Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	27	C10H12	132
2-Phenylbicyclo[2.2.1]hepta-2,5-diene $$	74437-39-1	WILEY275.l	53973	38	C13H12	168
Bicyclo[2.2.1]hept-5-en-2-ol	13080-90-5	NIST05a.l	5687	30	C7H10O	110



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Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

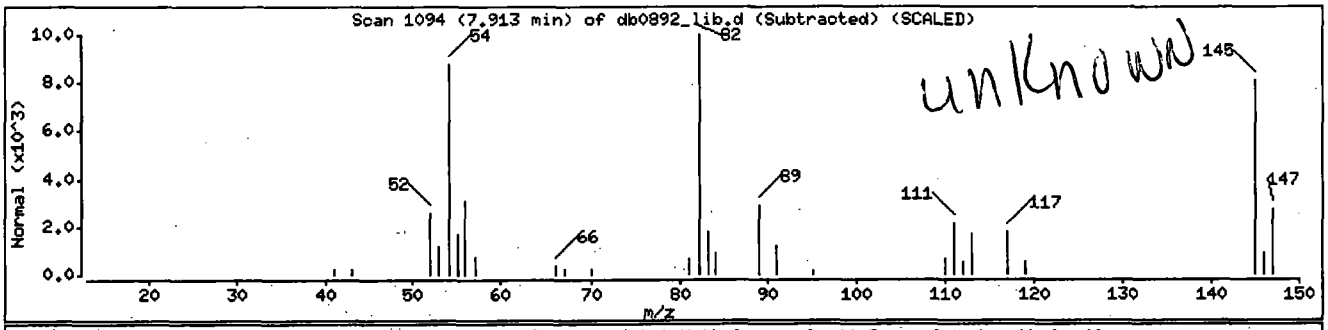
Volume Injected (uL): 1.0

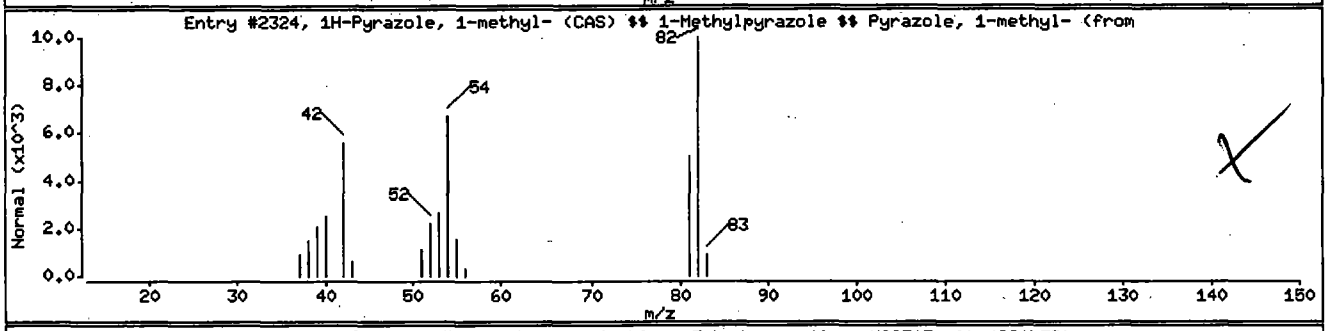
Operator: jmg00346

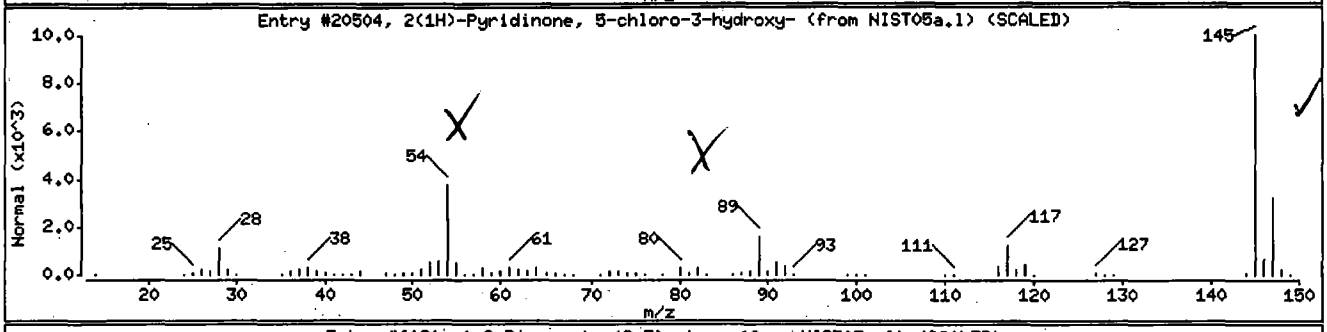
Column phase: J&W DB-5MS

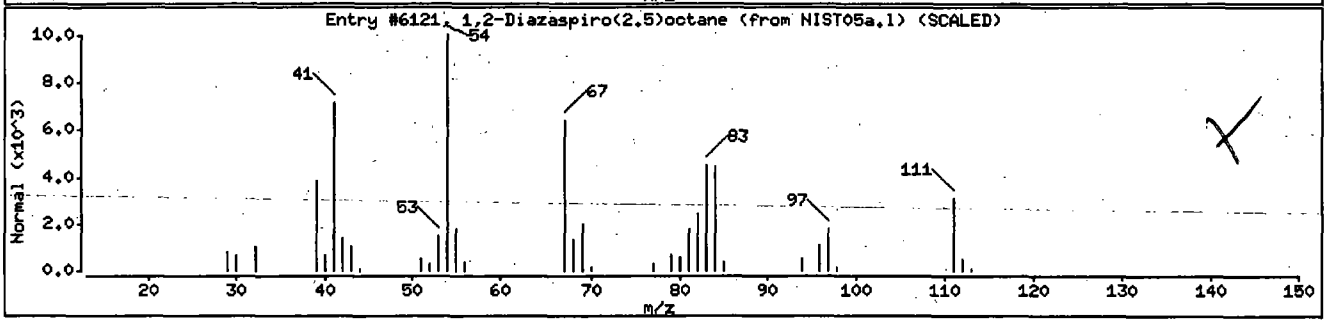
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1H-Pyrazole, 1-methyl- (CAS) $$ 1-Methyl	930-36-9	WILEY275.l	2324	53	C4H6N2	82
2(1H)-Pyridinone, 5-chloro-3-hydroxy-	53233-89-9	NIST05a.l	20504	52	C5H4ClNO2	145
1,2-Diazaspiro(2,5)octane	185-79-5	NIST05a.l	6121	38	C6H12N2	112









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Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

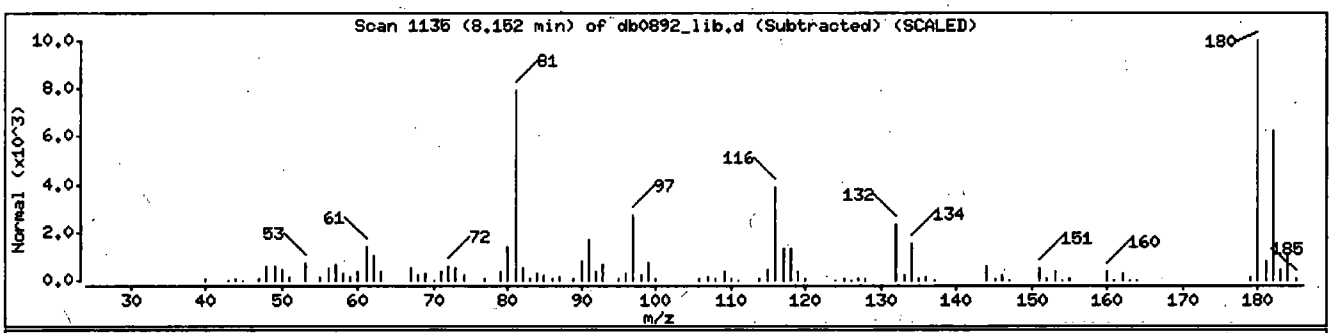
Volume Injected (uL): 1.0

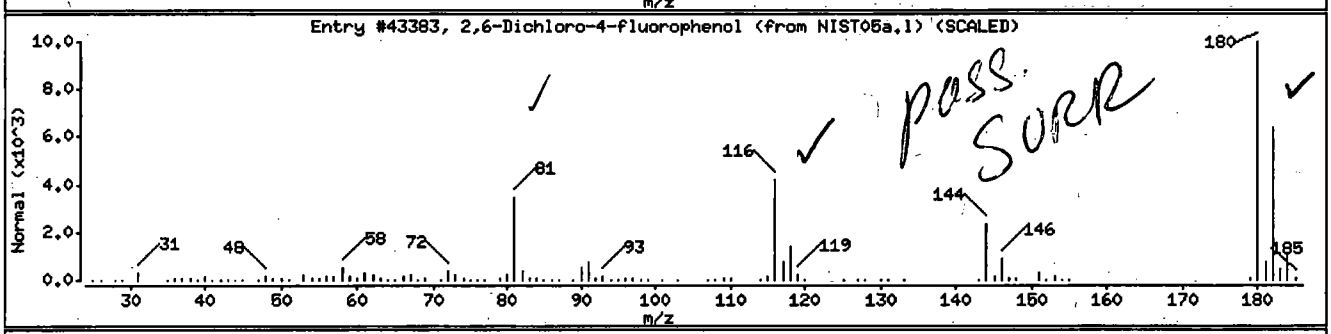
Operator: jmg00346

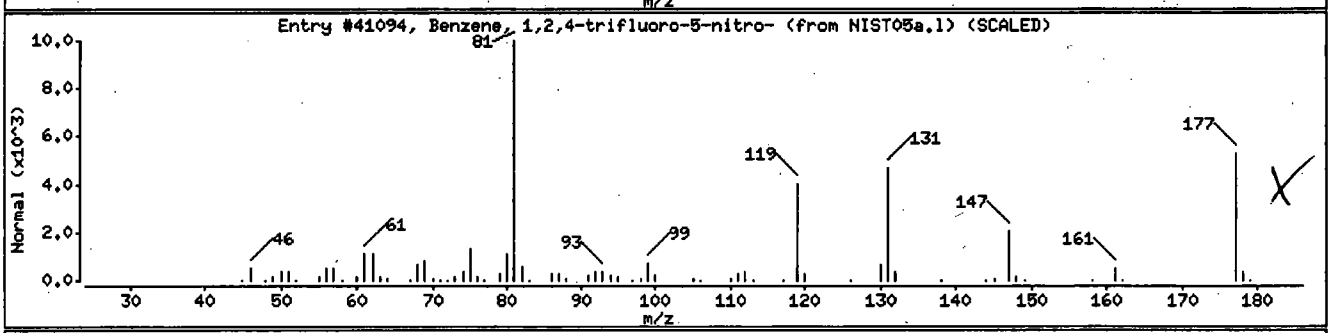
Column phase: J&W DB-5MS

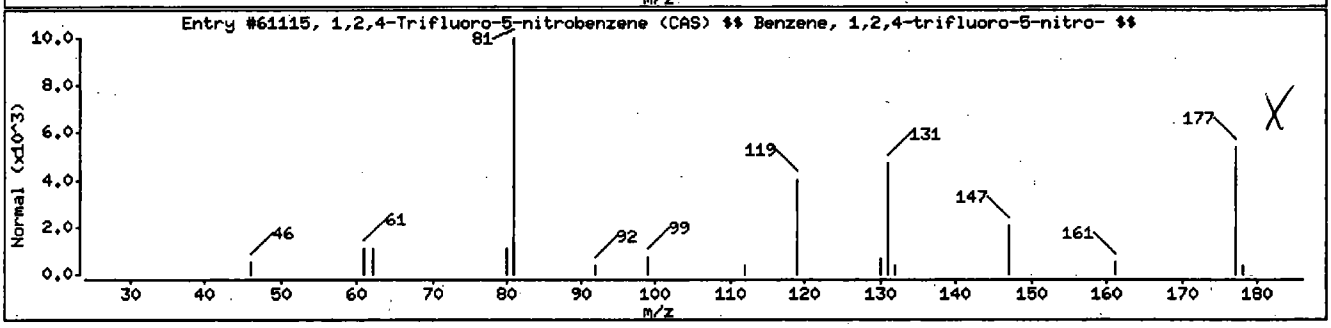
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	43	C6H3Cl2FO	180
Benzene, 1,2,4-trifluoro-5-nitro-	2105-61-5	NIST05a.l	41094	12	C6H2F3NO2	177
1,2,4-Trifluoro-5-nitrobenzene (CAS) $$	2105-61-5	WILEY275.l	61115	12	C6H2F3NO2	177









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

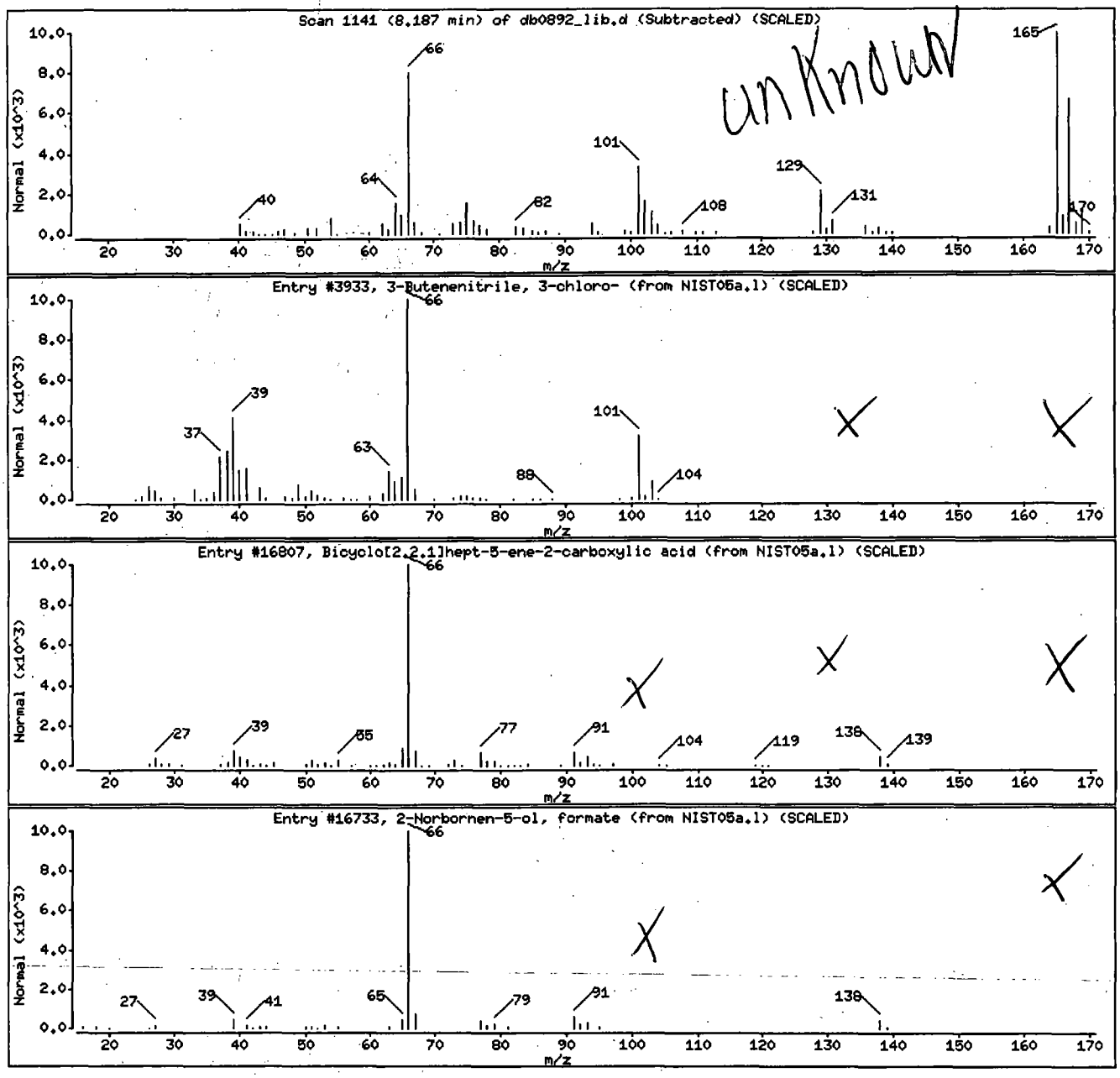
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16807	47	C8H10O2	138
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	47	C8H10O2	138



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

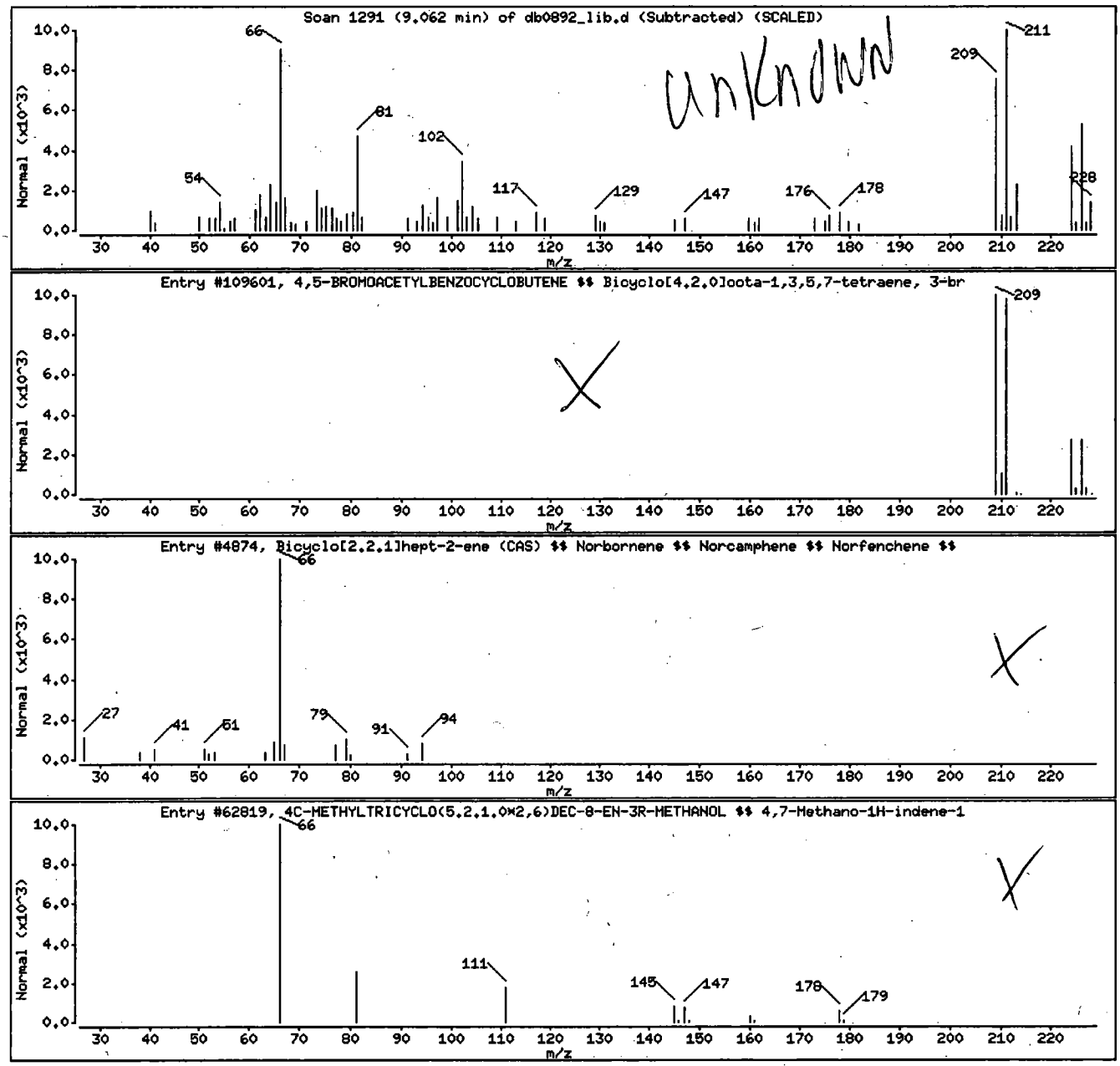
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63506-25-2	WILEY275.l	109601	78	C10H9BrO	224
Bicyclo[2.2.1]hept-2-ene (CAS) $$ Norbor	498-66-8	WILEY275.l	4874	43	C7H10	94
4C-METHYLTRICYCLO(5.2.1.0X2,6)DEC-8-EN-3	68304-00-7	WILEY275.l	62819	43	C12H18O	178



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

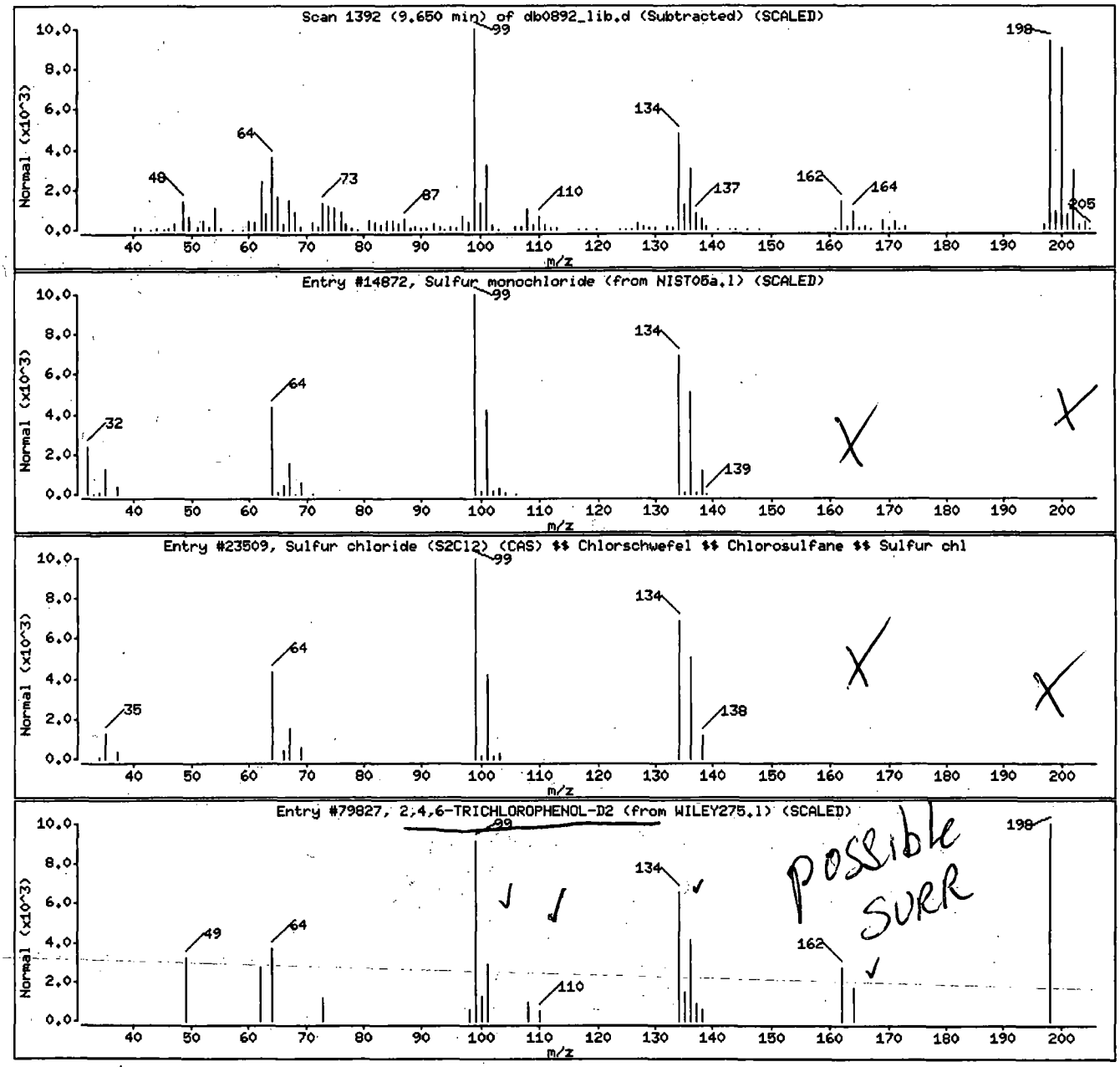
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Sulfur chloride (S2Cl2) (CAS) $$ Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	38	C6HD2Cl3O	198



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0892_lib.d

Date : 20-FEB-2014 16:13

Client ID: H3011

Instrument: HP19760.i

Sample Info: H3011;7366650;1;0;SAMPLE;;;

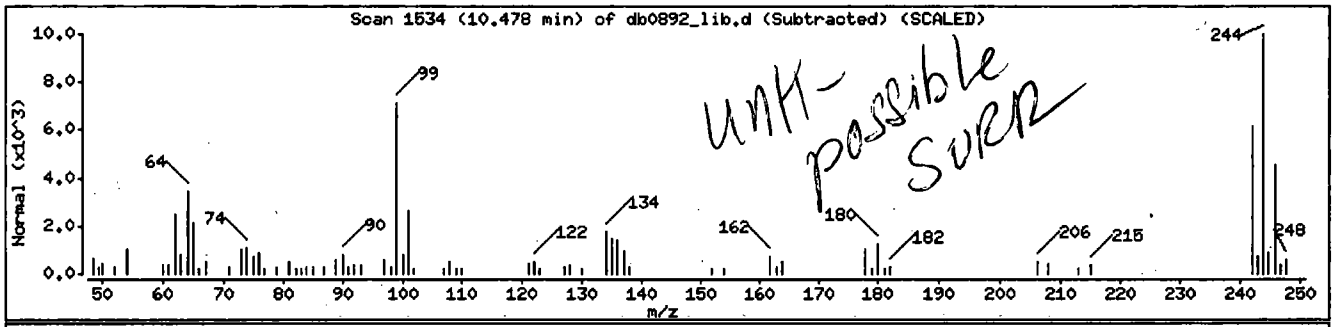
Volume Injected (uL): 1.0

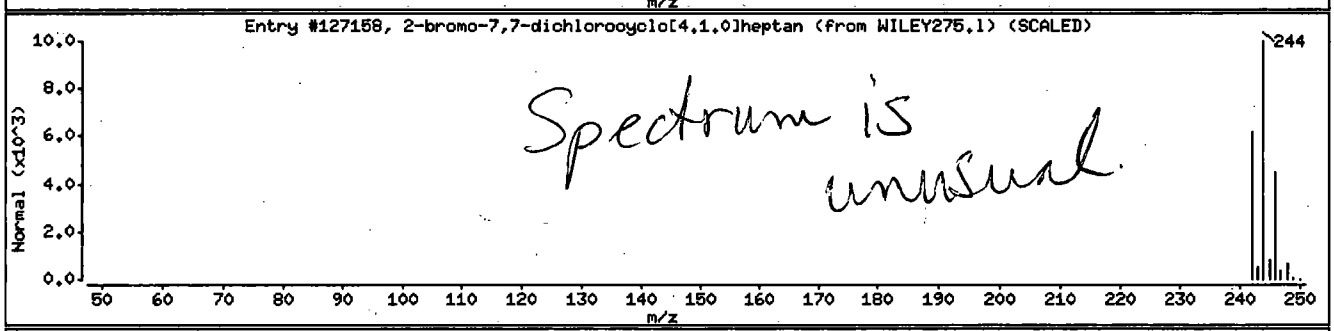
Operator: jmg00346

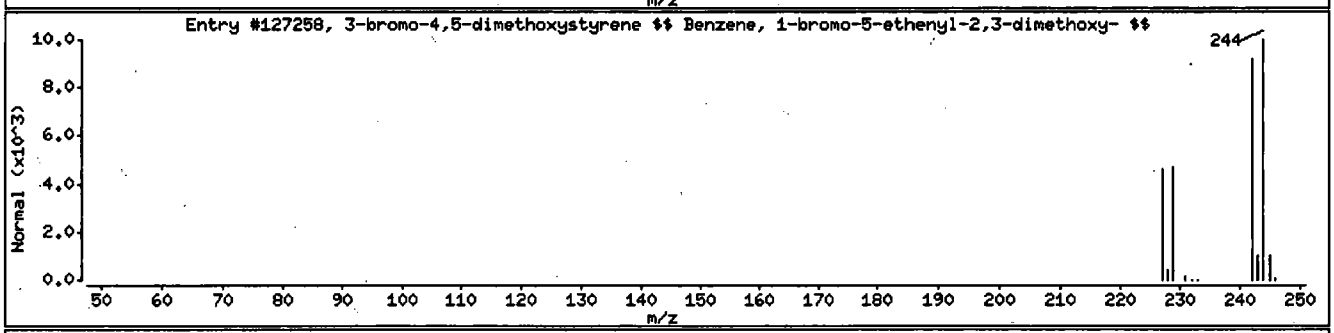
Column phase: J&W DB-5MS

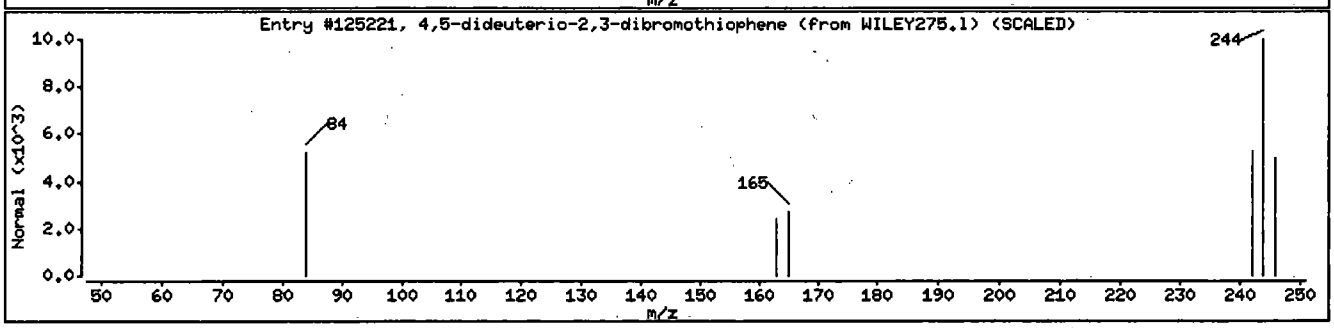
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-bromo-7,7-dichlorocyclo[4.1.0]heptan	113035-97-5	WILEY275.l	127158	91	C7H9BrCl2	242
3-bromo-4,5-dimethoxystyrene $$ Benzene,	5293-42-5	WILEY275.l	127258	58	C10H11BrO2	242
4,5-dideuterio-2,3-dibromothiophene	137040-63-2	WILEY275.l	125221	53	C4D2Br2S	242



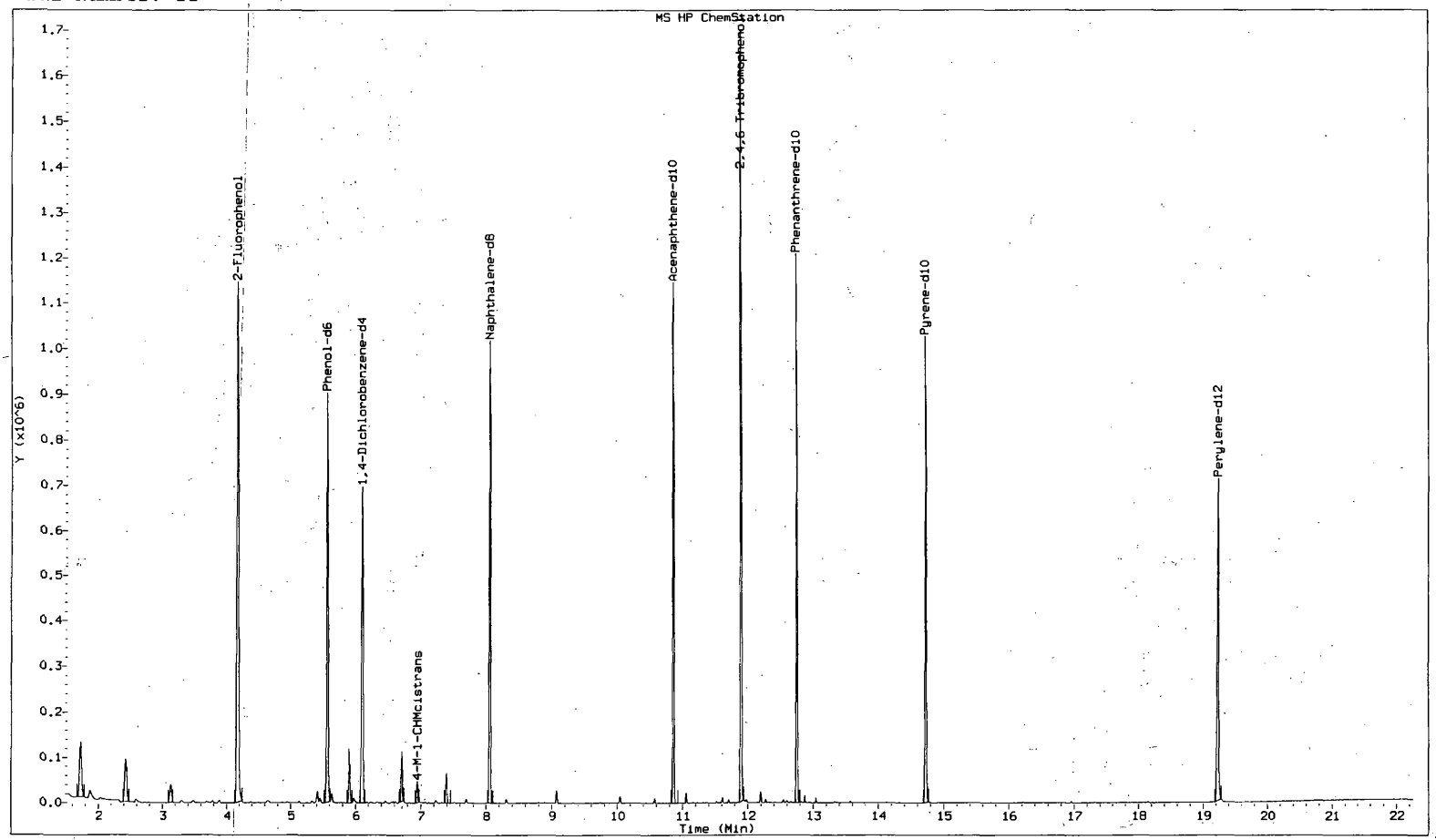






Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:10.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb20a.b/db0910_lib.d
Operator : ceb05247
Acquired : 21-FEB-2014 00:28
Instrument : HP19760.i
Sample Name: H3021;7366654;1;0;SAMPLE;;;
Misc Info : 14050WAB;WL13166;;1040;1000;0;db0902;13166;
Vial Number: 11



Lancaster Labs

Data file : /chem/HP19760.i/14feb20a.b/db0910_lib.d
Lab Smp Id: 7366654 Client Smp ID: H3021
Inj Date : 21-FEB-2014 00:28
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H3021;7366654;1;0;SAMPLE;;;
Misc Info : 14050WAB;WL13166;;1040;1000;0;db0902;13166;
Comment : Max. number of TICs to report is 50, 6 TICs were found initially.
Method : /chem/HP19760.i/14feb20a.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 21:20 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 11
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1040.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	979613	10.000
* 48 Naphthalene-d8	8.059	1265819	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.729	267465	2.73030720	2.62529	91	NIST05a.1	31325	21
2,2-dimethoxybutane				CAS #: 0-00-0			
2.423	215781	2.20271317	2.11799	74	WILEY275.1	14183	21

Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Methane, dibromochloro- (CAS) $$ Methane					CAS #: 124-48-1		
3.128	80382	0.82054775	0.78898	98	WILEY275.1	90360	21
Decane					CAS #: 124-18-5		
5.903	167545	1.71031898	1.64453	91	NIST05a.1	18488	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.707	134909	1.37717069	1.32420	83	NIST05a.1	12246	21
Cyclopentasiloxane, decamethyl- (CAS) $$					CAS #: 541-02-6		
7.395	77844	0.61497322	0.59132	87	WILEY275.1	221485	48

Target compound.
Do not report.
ajs00193 03/02/2014

Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

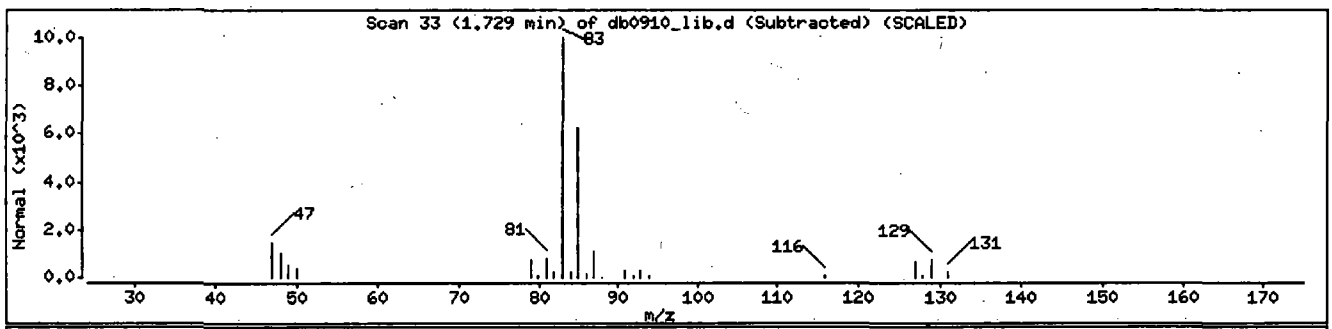
Client ID: H3021 Instrument: HP19760.i

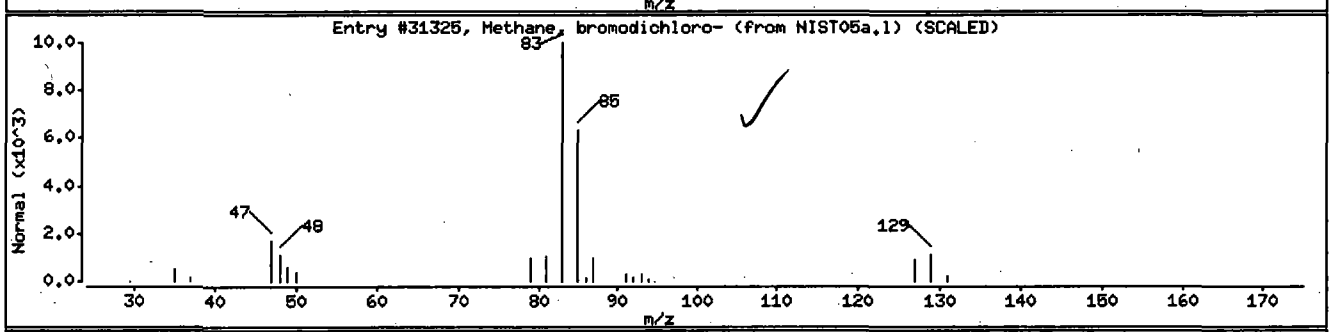
Sample Info: H3021;7366654;1;0;SAMPLE;;;

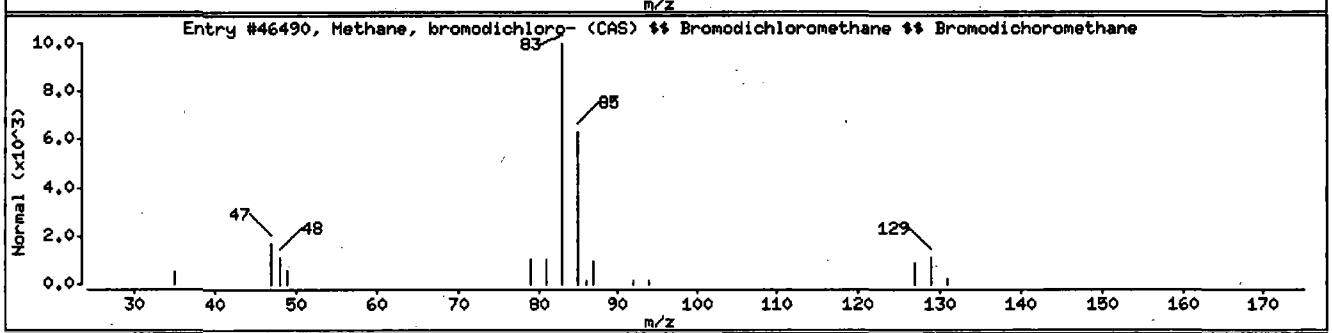
Volume Injected (uL): 1.0 Operator: ceb05247

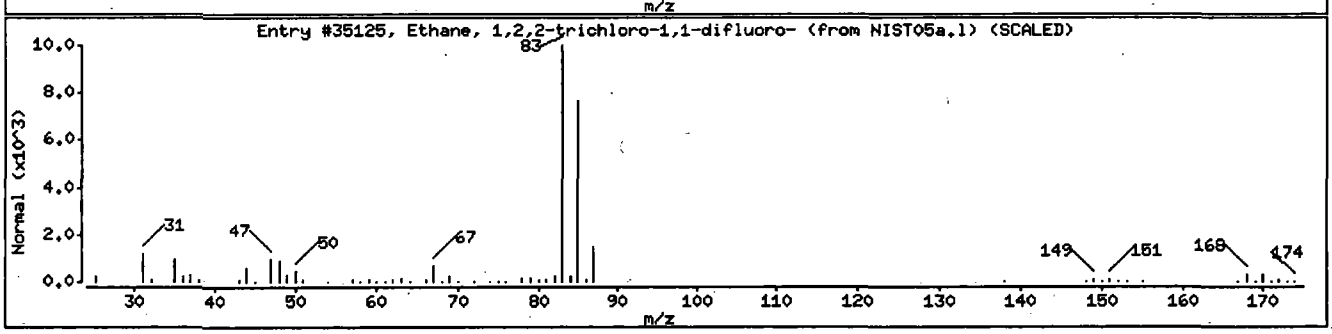
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	91	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	91	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

Client ID: H3021

Instrument: HP19760.i

Sample Info: H3021;7366654;1;0;SAMPLE;;;

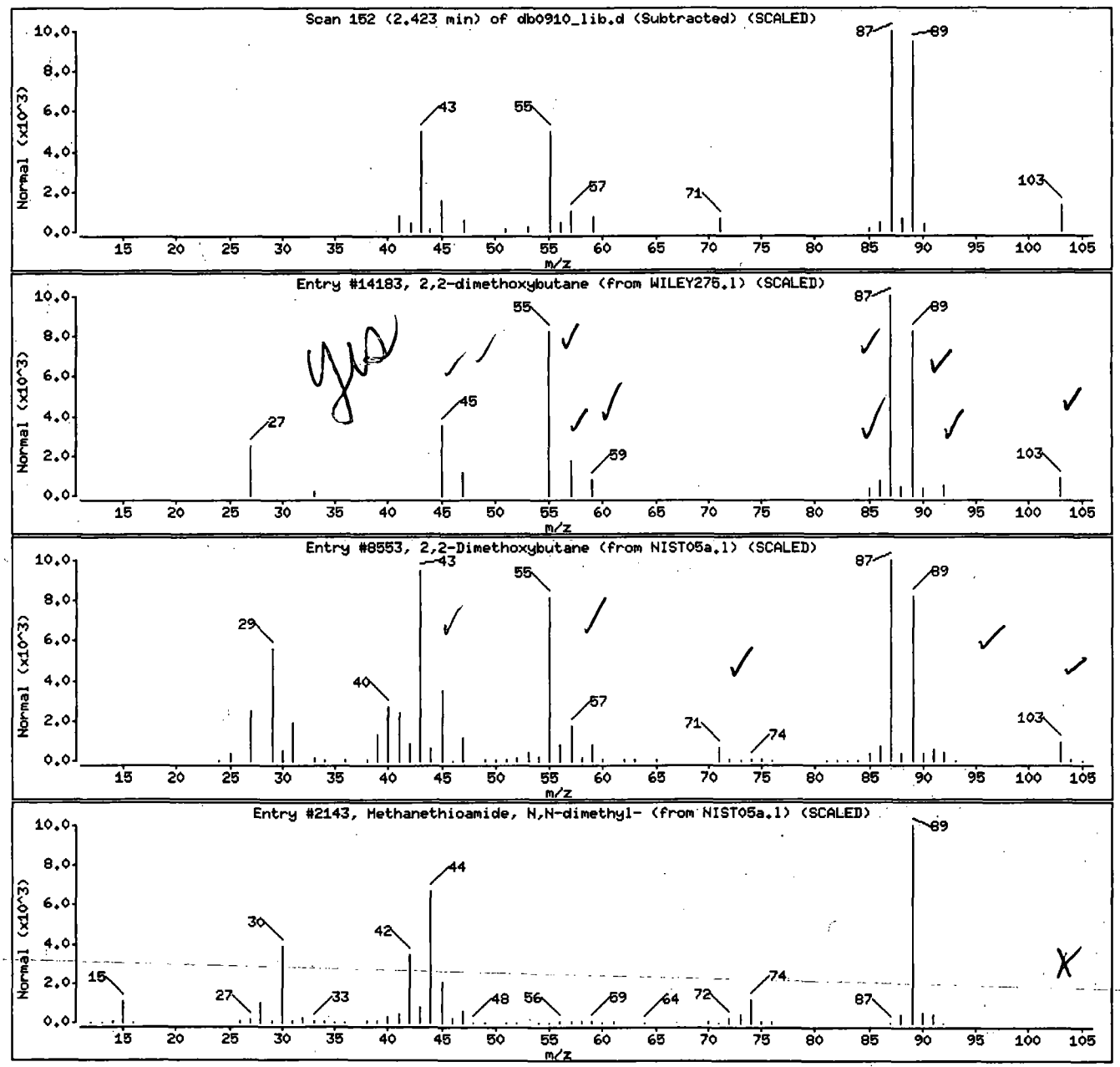
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,2-dimethoxybutane	0-00-0	WILEY275.l	14183	74	C6H1402	118
2,2-Dimethoxybutane	3453-99-4	NIST05a.l	8553	64	C6H1402	118
Methanethioamide, N,N-dimethyl-	758-16-7	NIST05a.l	2143	42	C3H7NS	89



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

Client ID: H3021

Instrument: HP19760.i

Sample Info: H3021;7366654;1;0;SAMPLE;;;

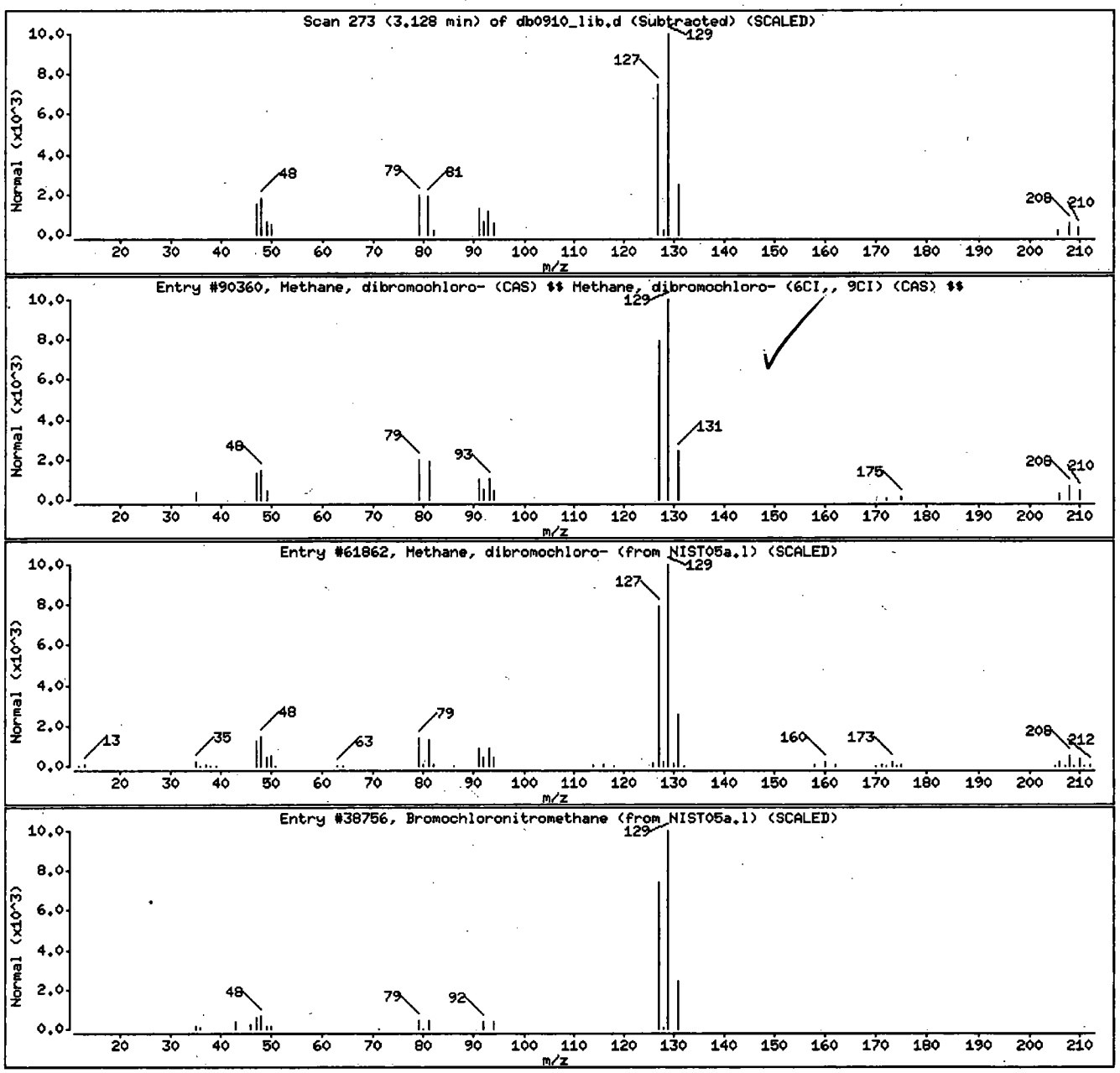
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, dibromochloro- (CAS) $$ Methane	124-48-1	WILEY275.l	90360	98	CHBr2Cl	206
Methane, dibromochloro-	124-48-1	NIST05a.l	61862	96	CHBr2Cl	206
Bromochloronitromethane	135531-25-8	NIST05a.l	38756	50	CHBrClNO2	173



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

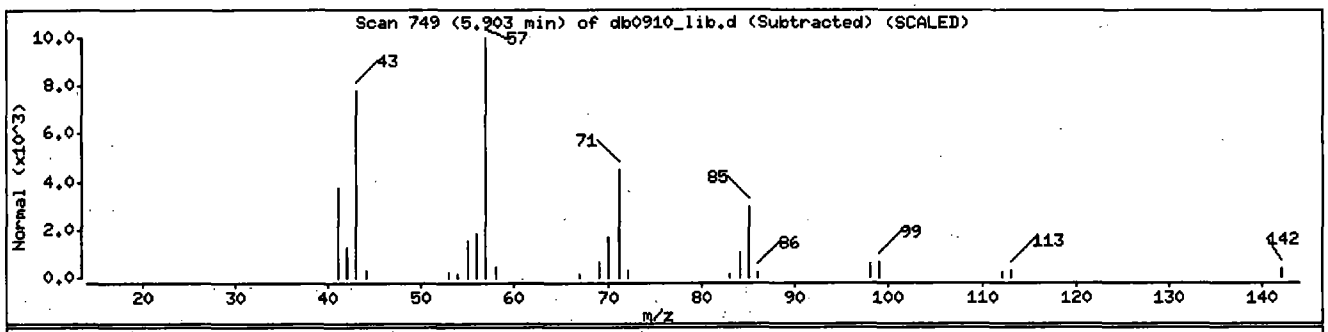
Client ID: H3021 Instrument: HP19760.i

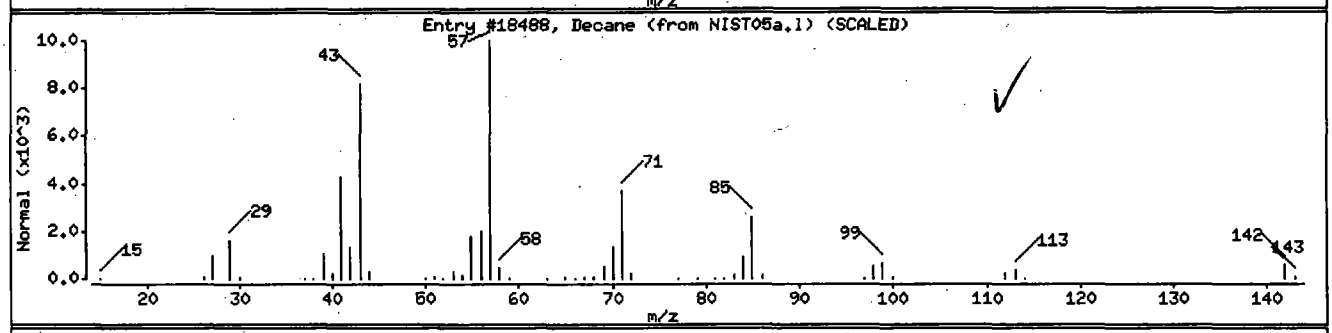
Sample Info: H3021;7366654;1;0;SAMPLE;;;

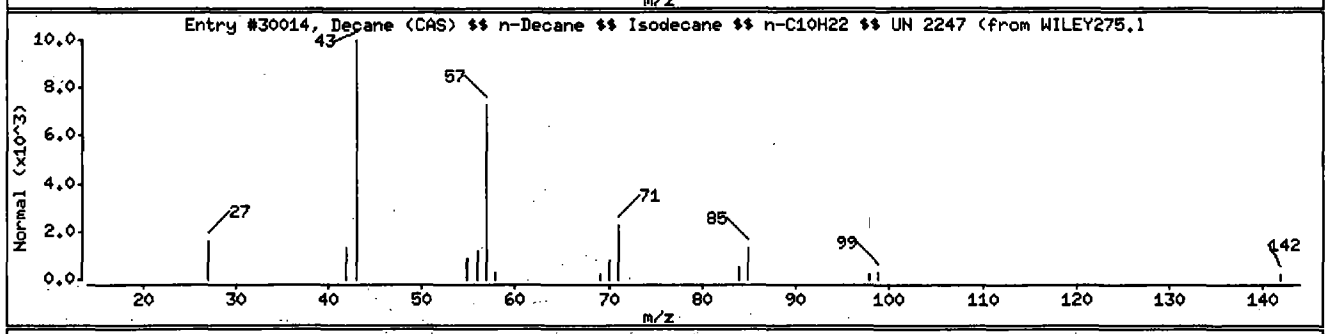
Volume Injected (uL): 1.0 Operator: ceb05247

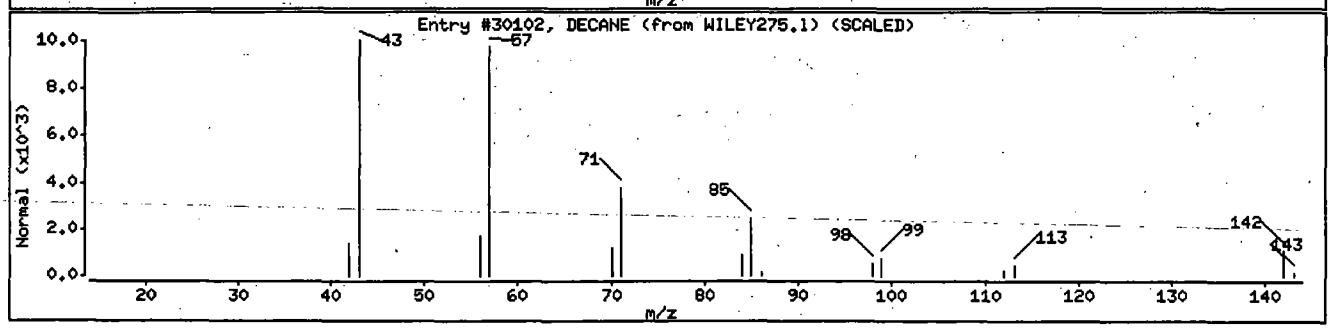
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18488	91	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30014	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

Client ID: H3021

Instrument: HP19760.i

Sample Info: H3021;7366654;1;0;SAMPLE;;;

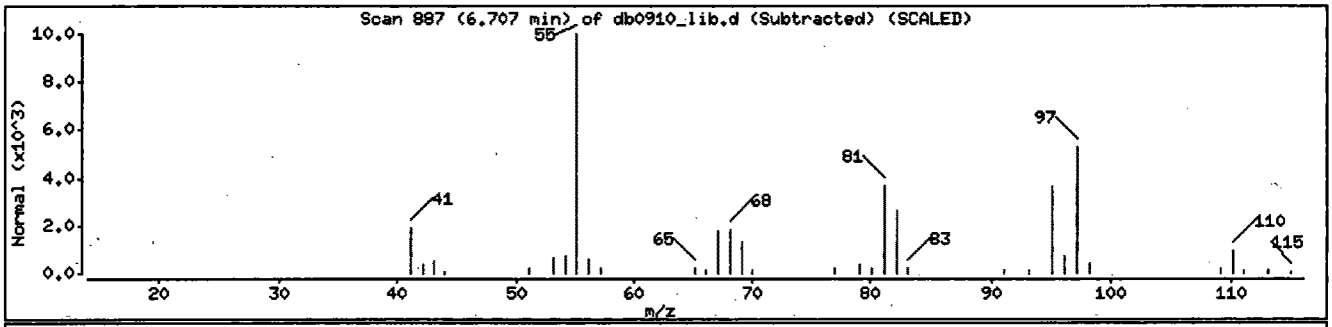
Volume Injected (uL): 1.0

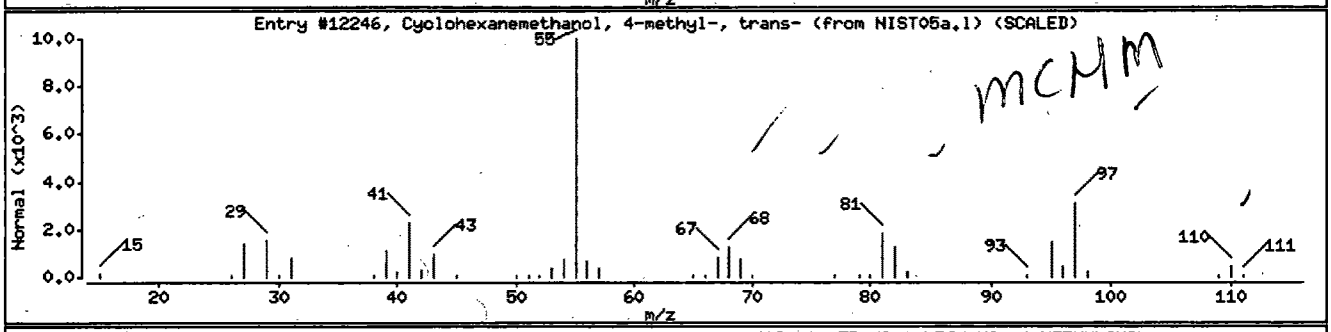
Operator: ceb05247

Column phase: J&W DB-5HS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	83	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	83	C8H16O	128
Cyclohexanemethanol, 2-methyl- (CAS) $$	2105-40-0	WILEY275.l	19672	64	C8H16O	128





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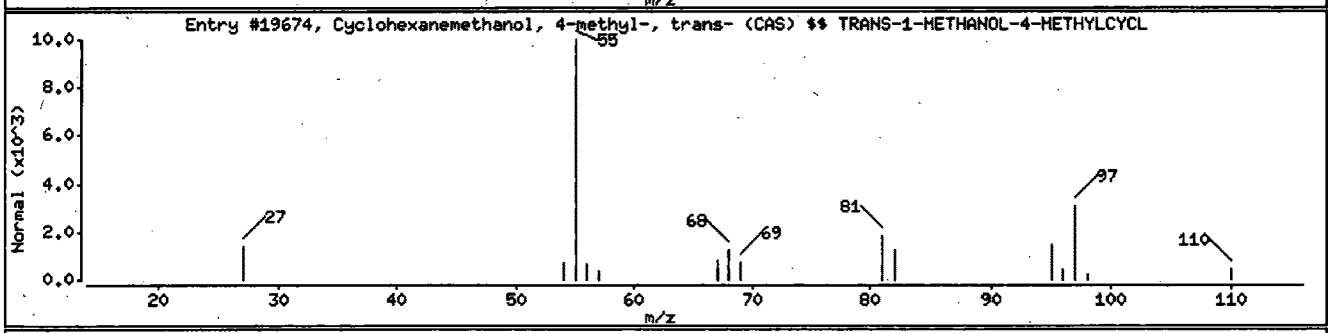
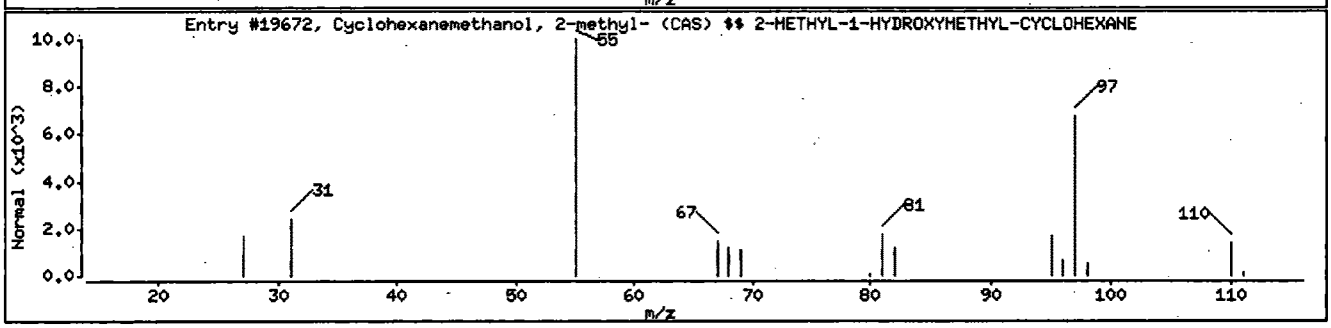




Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20a.b/db0910_lib.d

Date : 21-FEB-2014 00:28

Client ID: H3021

Instrument: HP19760.i

Sample Info: H3021;7366654;1;0;SAMPLE;;;

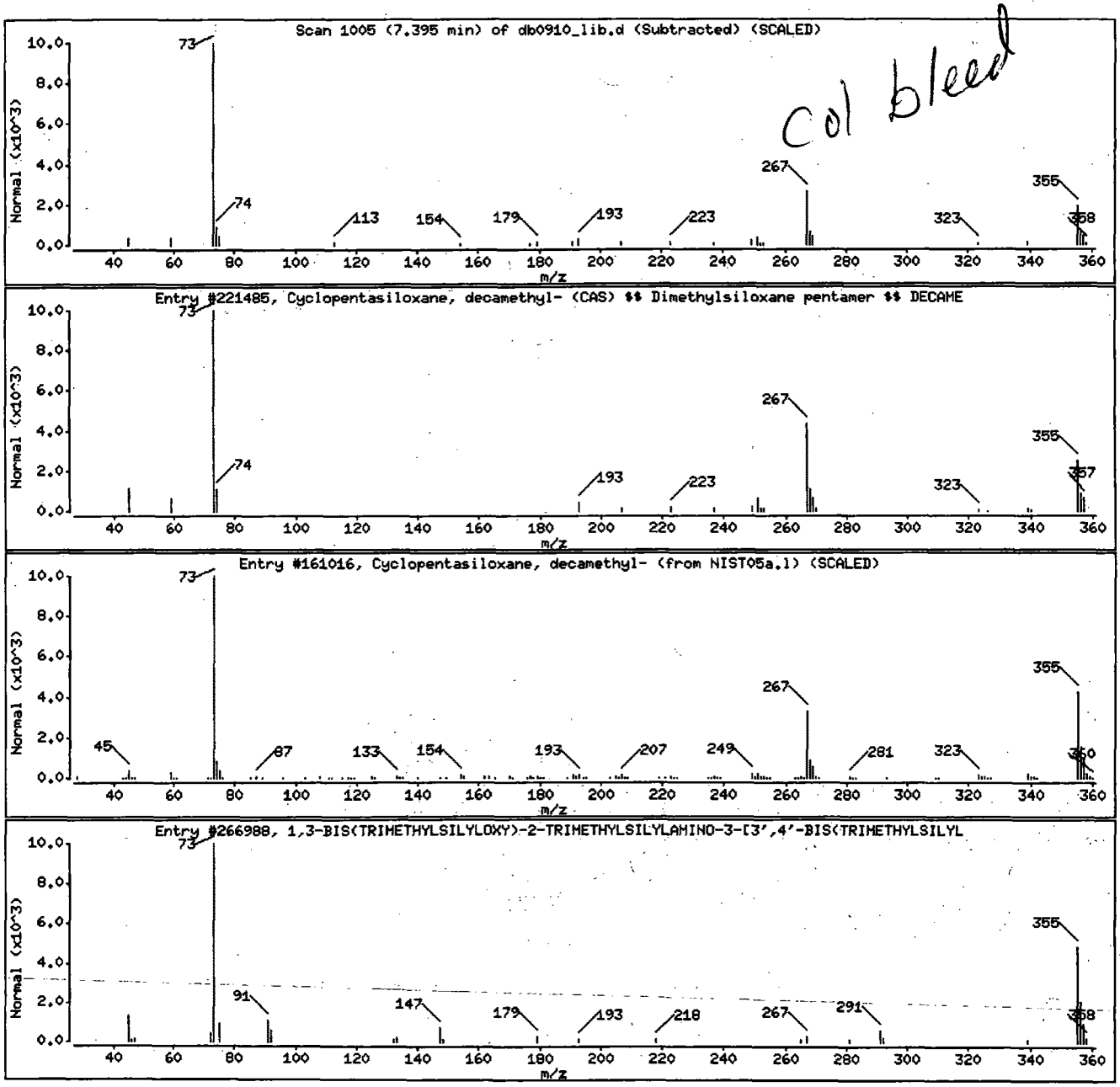
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

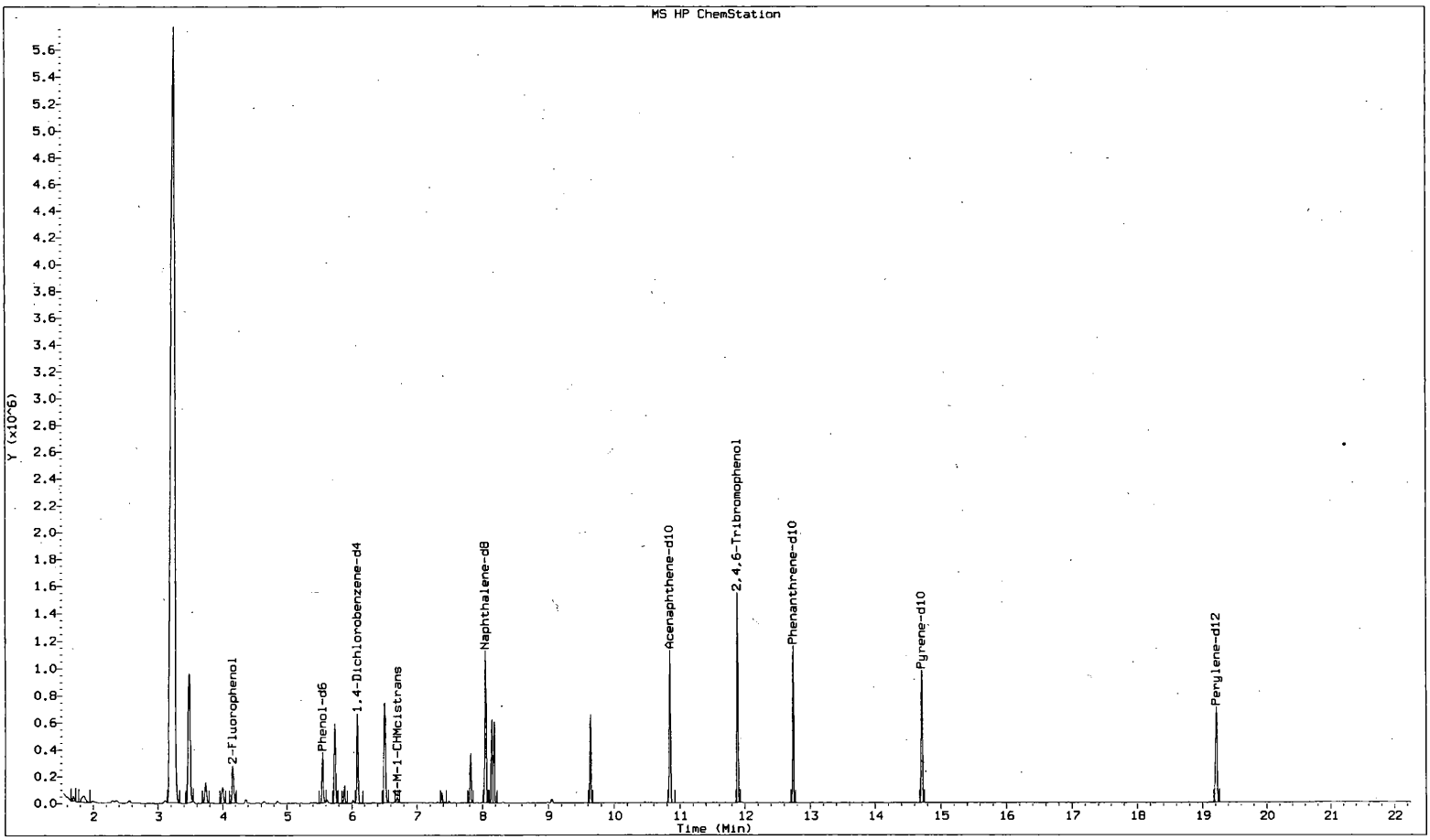
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	87	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	83	C10H30O5Si5	370
1,3-BIS(TRIMETHYLSILYLOXY)-2-TRIMETHYLSI	0-00-0	WILEY275.l	266988	38	C24H51NO5Si6	673



Digitally signed by Andrew J. Strebel on 03/01/2014 at 21:24.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb23.b/db1042_lib.d
Operator : ceb05247
Acquired : 24-FEB-2014 02:20
Instrument : HP19760.i
Sample Name: H4011;7370723;1;0;SAMPLE;;;
Misc Info : 14052WAN;WL13463;;1051;1000;0;db1026;13166;
Vial Number: 22



Lancaster Labs

Data file : /chem/HP19760.i/14feb23.b/db1042_lib.d
Lab Smp Id: 7370723 Client Smp ID: H4011
Inj Date : 24-FEB-2014 02:20
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H4011;7370723;1;0;SAMPLE;;;
Misc Info : 14052WAN;WL13463;;1051;1000;0;db1026;13166;
Comment : Max. number of TICs to report is 50, 14 TICs were found initially.
Method : /chem/HP19760.i/14feb23.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 12:40 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 22
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1051.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.089	967725	10.000
* 48 Naphthalene-d8	8.042	1466976	10.000
* 83 Acenaphthene-d10	10.845	1286098	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.694	66653	0.68875634	0.65533	90	NIST05a.1	31325	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.846	202588	2.09344443	1.99185	50	NIST05a.1	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.262	23112033	238.828465	227.23926	74	NIST05a.1	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.484	2075668	21.4489364	20.40812	83	NIST05a.1	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.734	313480	3.23934918	3.08215	25	NIST05a.1	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.002	225336	2.32850970	2.21551	38	NIST05a.1	13998	21(L)
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.739	873501	9.02633179	8.58832	89	WILEY275.1	18902	21
Decane (CAS) $$ n-Decane $$ Isodecane $$					CAS #: 124-18-5		
5.891	186933	1.93167332	1.83793	91	WILEY275.1	30015	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.509	1204615	12.4479044	11.84386	35	NIST05a.1	9448	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.377	104653	0.71339175	0.67877	90	NIST05a.1	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.814	462611	3.15349842	3.00047	43	NIST05a.1	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.141	744165	5.07278266	4.82662	87	NIST05a.1	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.170	733044	4.99697124	4.75449	50	NIST05a.1	3933	48
Sulfur monochloride					CAS #: 10025-67-9		
9.639	749797	5.83001326	5.54711	38	NIST05a.1	14872	83(L)

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

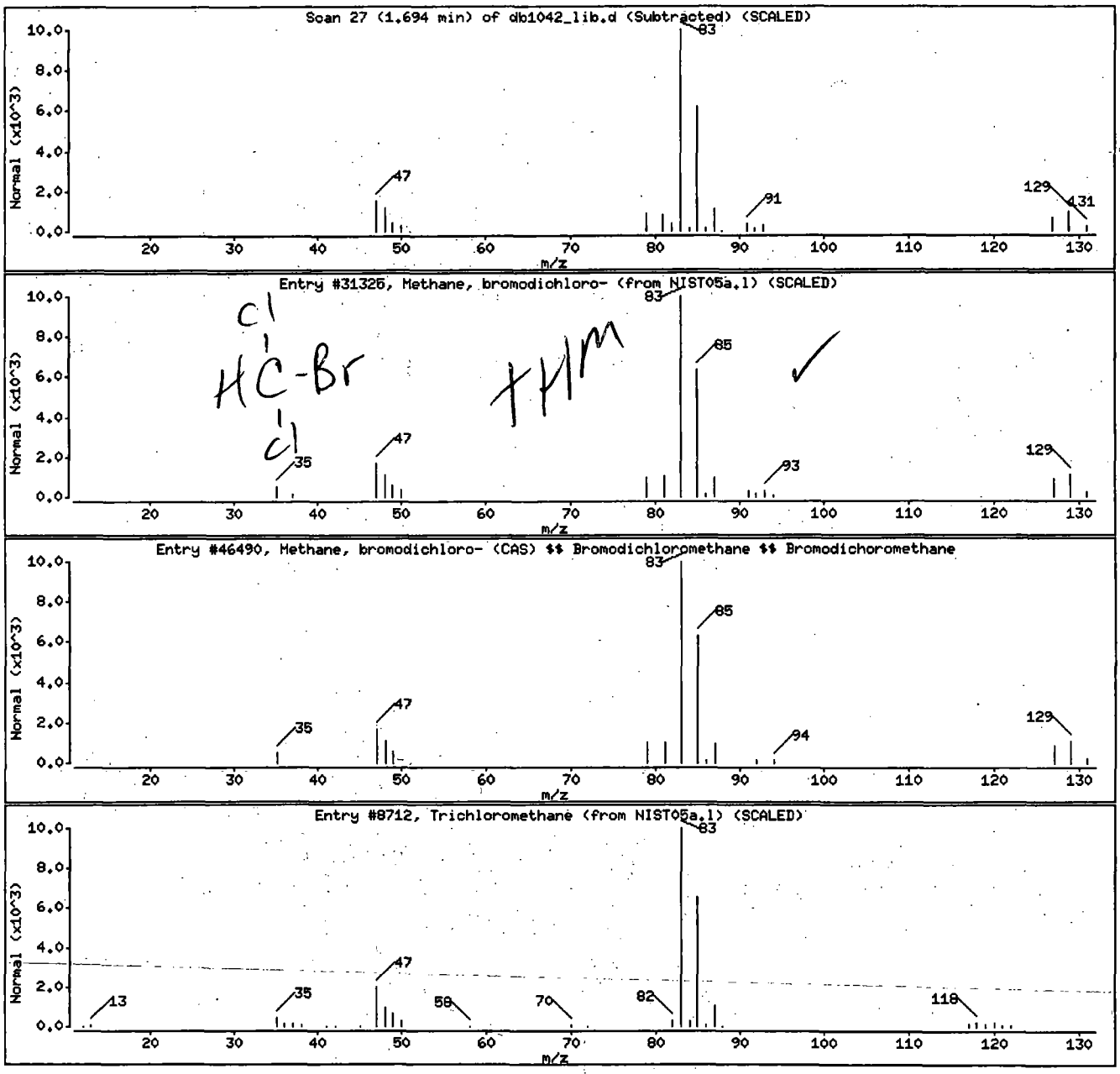
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	72	CHCl3	118



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

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Sample Info: H4011;7370723;1;0;SAMPLE;;;

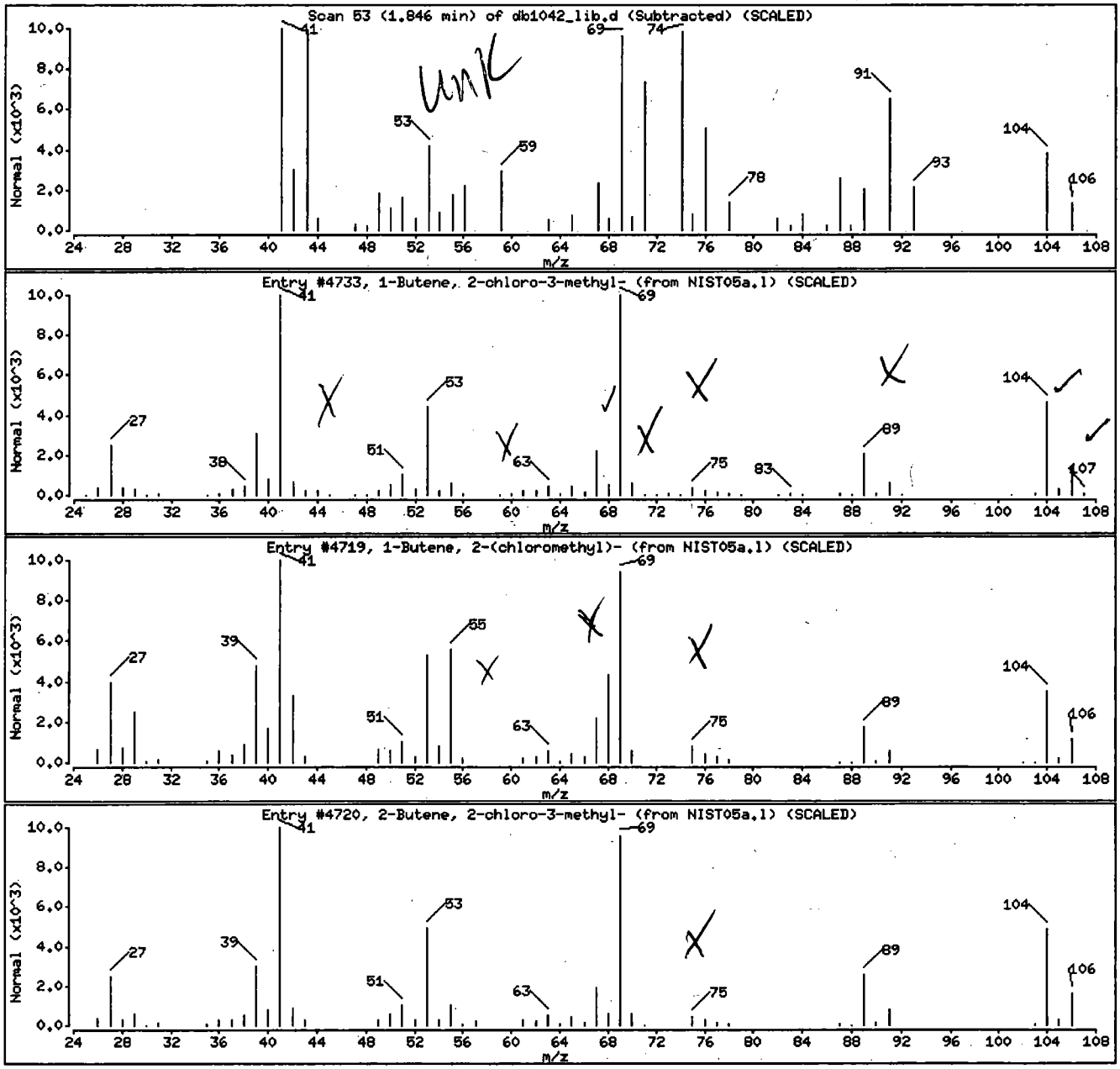
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	60	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4719	55	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	45	C5H9Cl	104



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Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

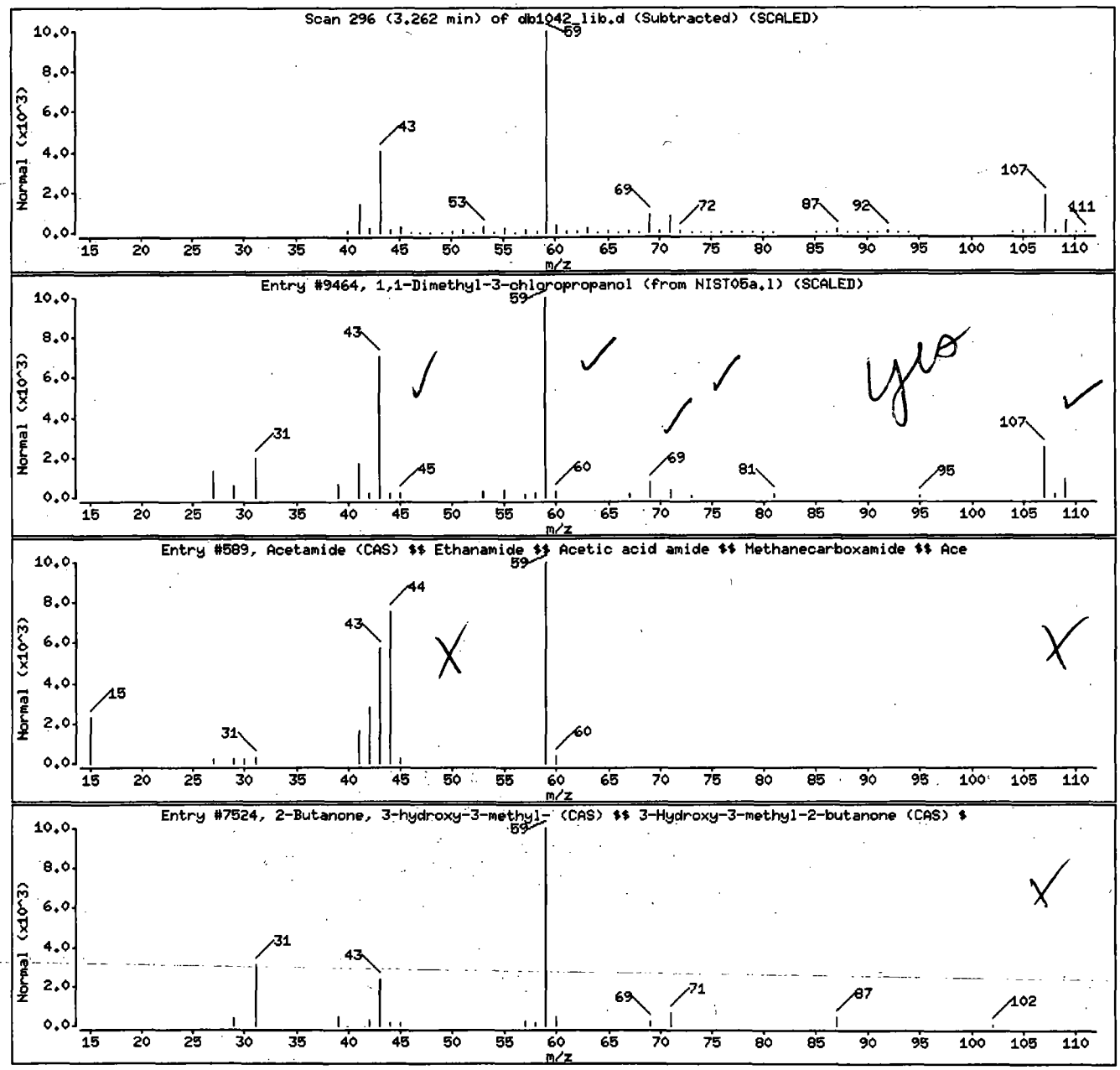
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	74	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102



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Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

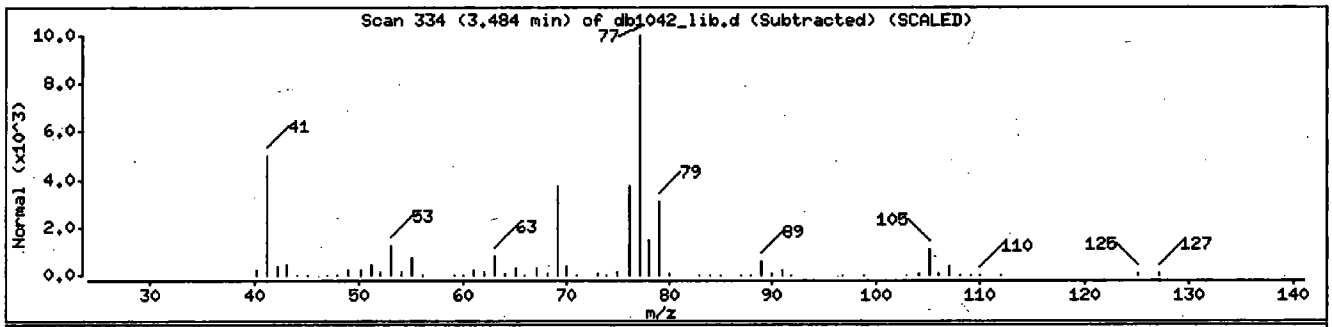
Volume Injected (uL): 1.0

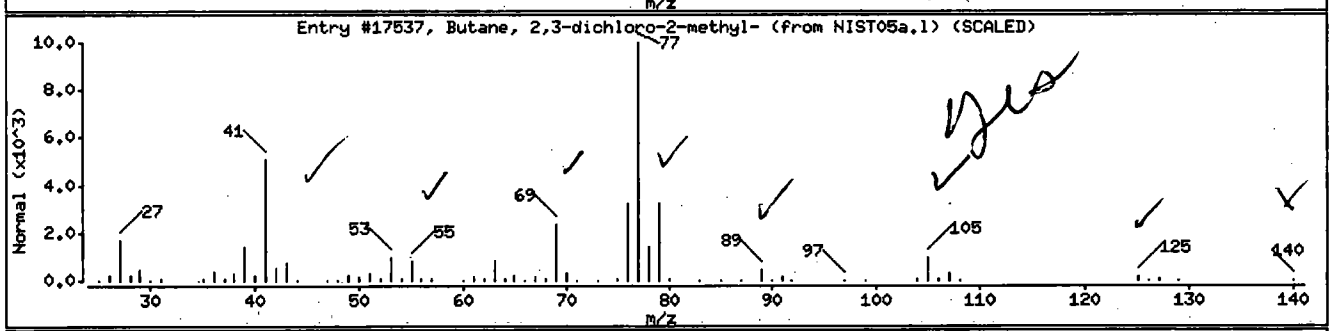
Operator: ceb05247

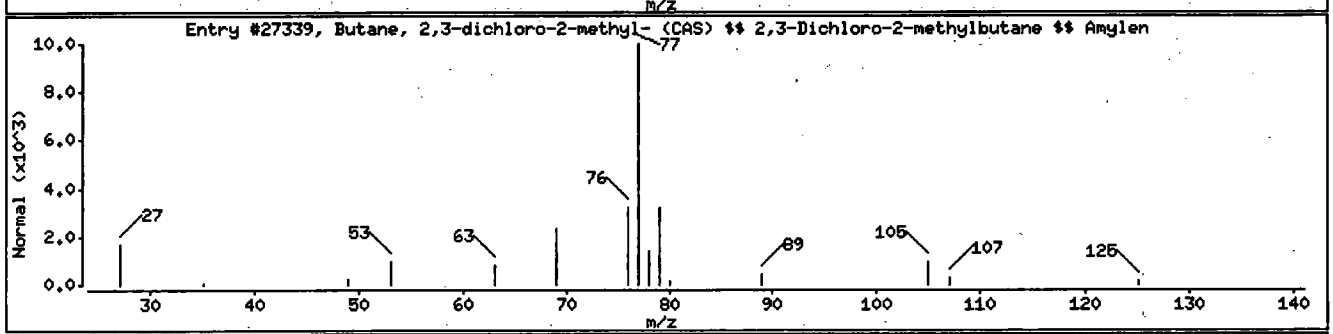
Column phase: J&W DB-5MS

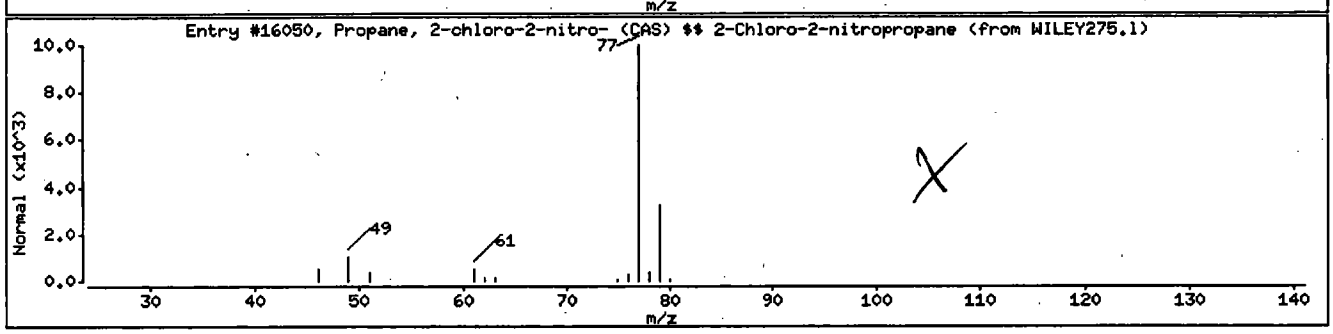
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-46-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









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Target 3.5 esignature user ID: ajs00193

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Date : 24-FEB-2014 02:20

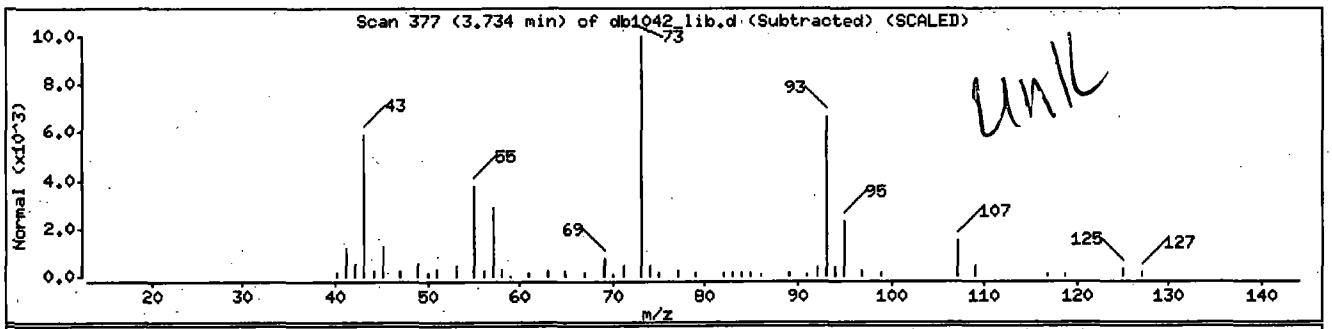
Client ID: H4011 Instrument: HP19760.i

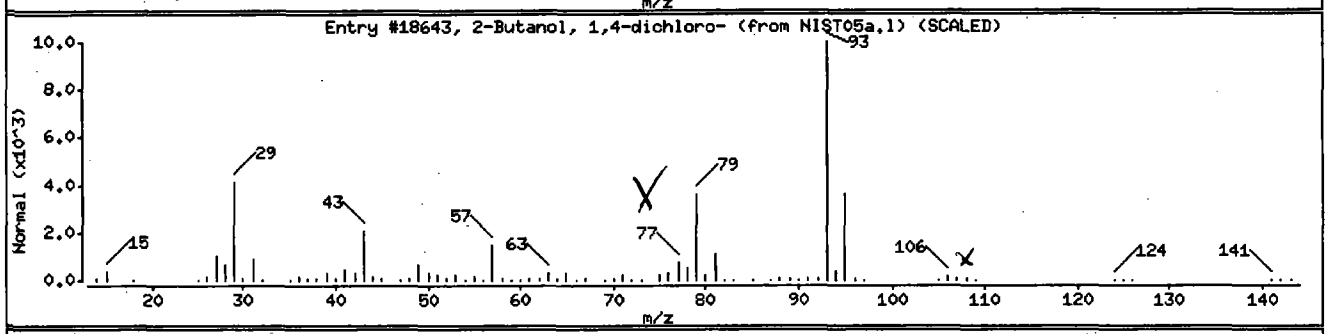
Sample Info: H4011;7370723;1;0;SAMPLE;;;

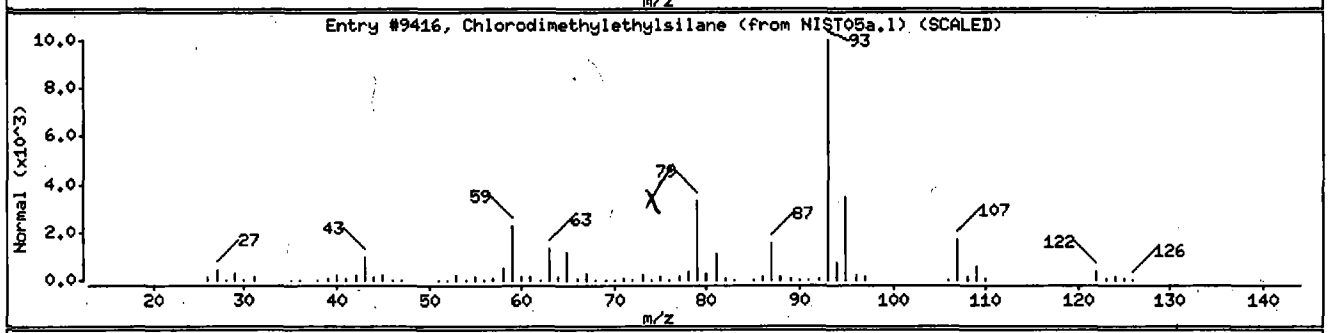
Volume Injected (uL): 1.0 Operator: ceb05247

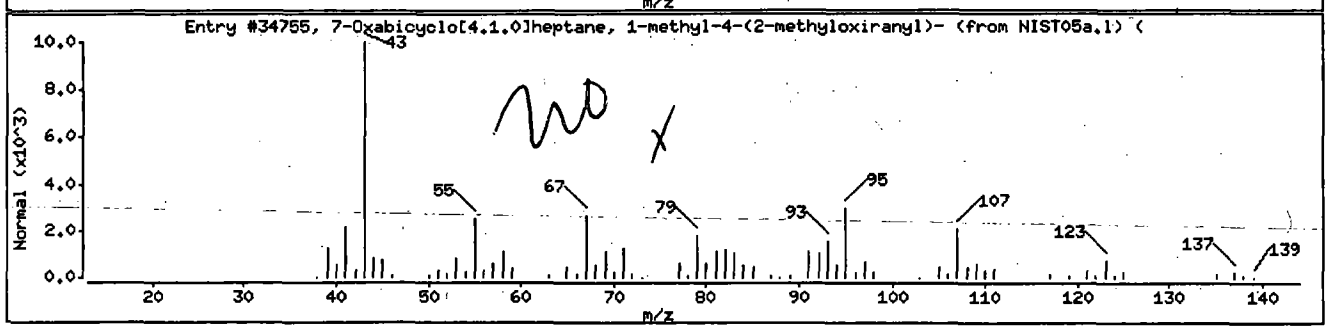
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	25	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	NIST05a.l	34755	12	C10H16O2	168









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Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

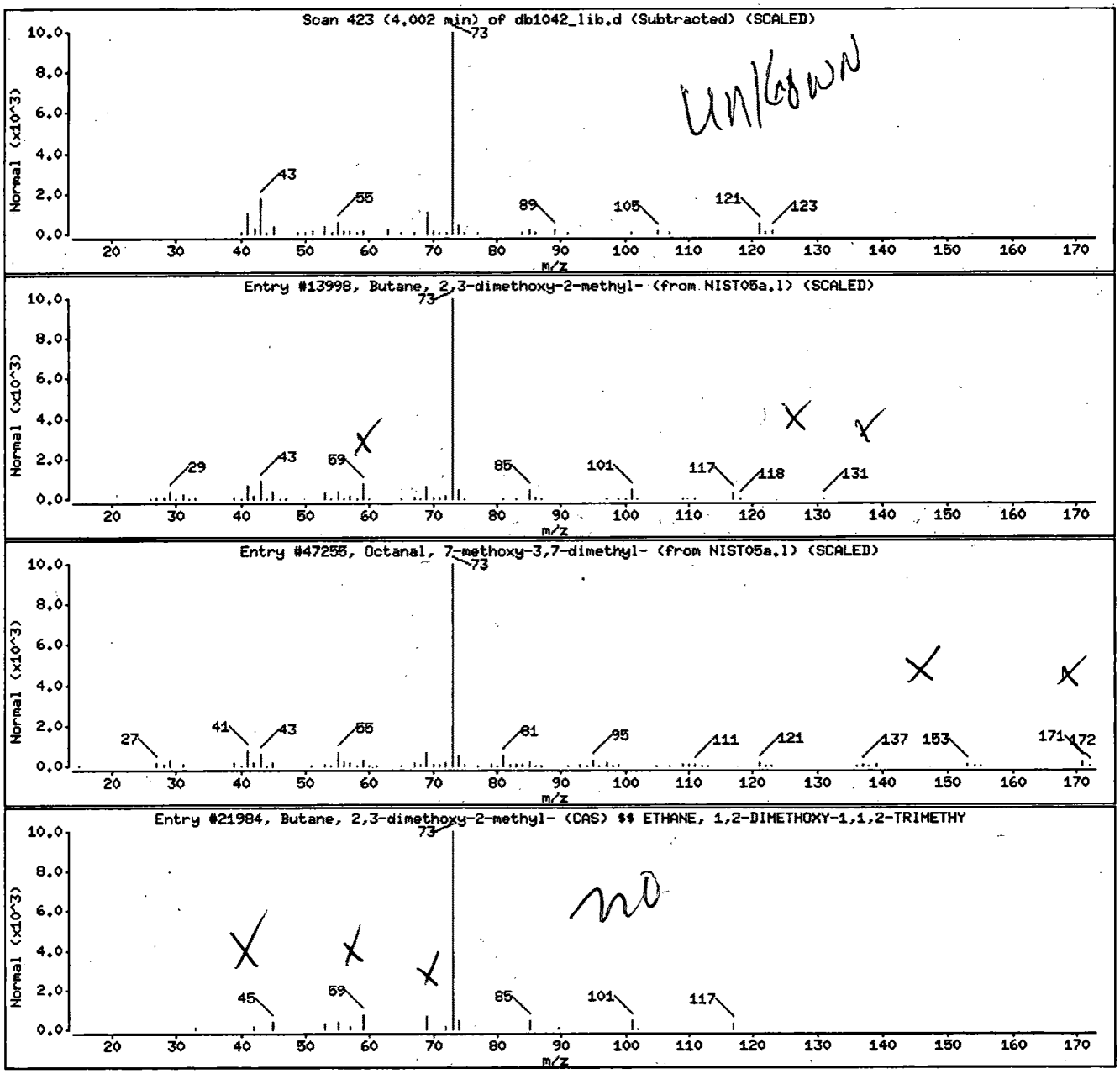
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	38	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	42	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132



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Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

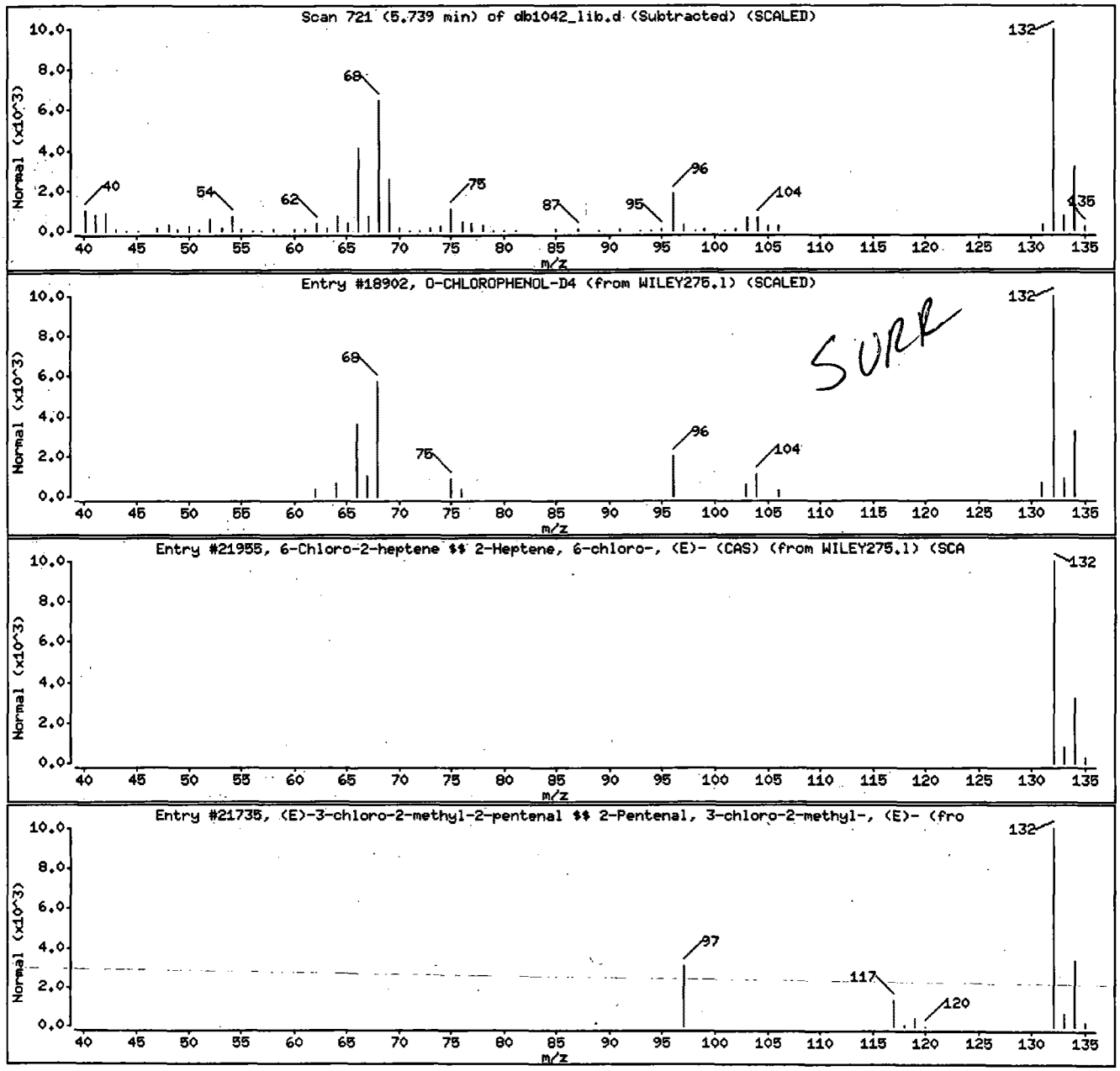
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.l	18902	89	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.l	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.l	21735	78	C6H9ClO	132



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Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

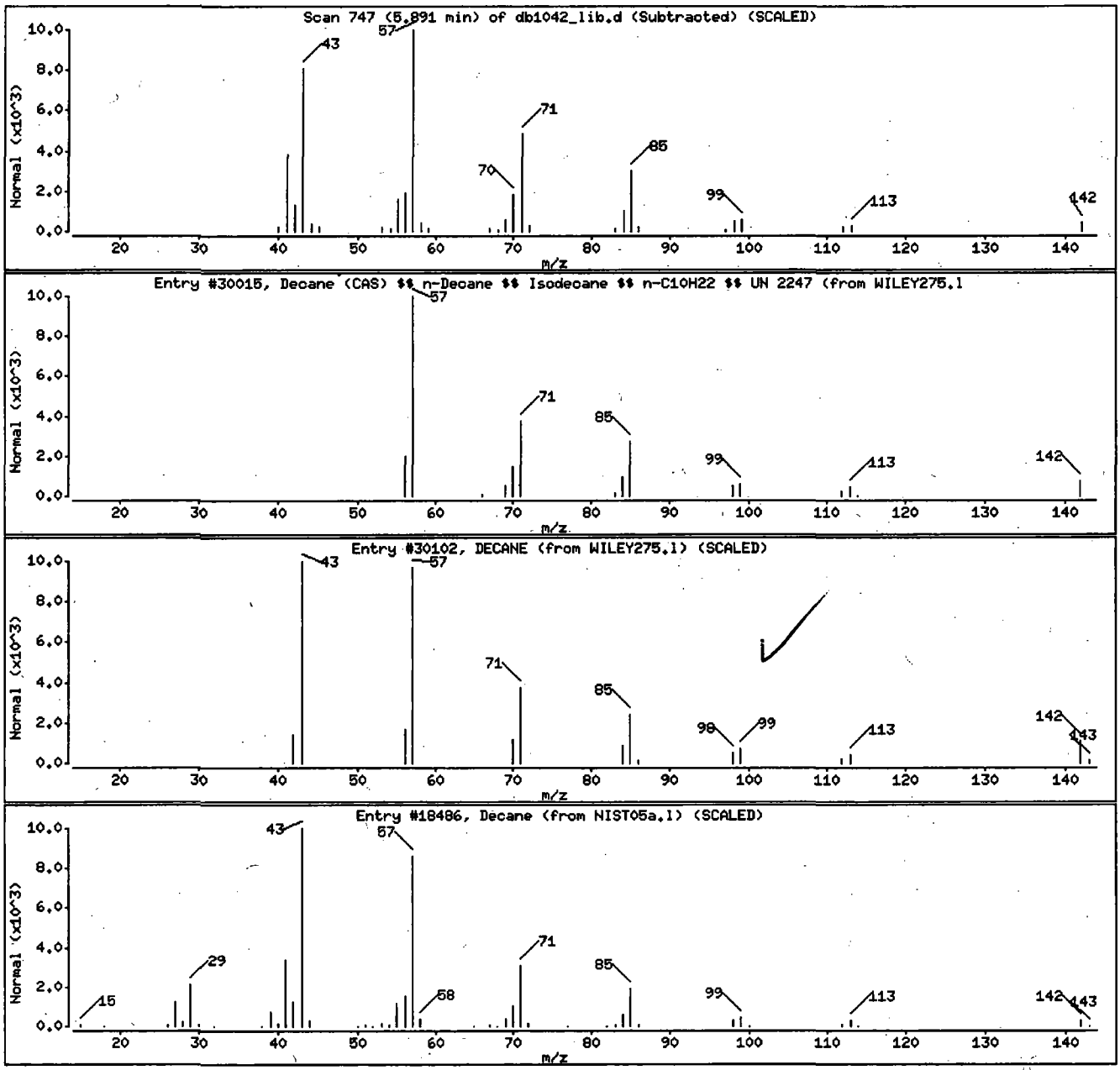
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30015	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142
Decane	124-18-5	NIST05a.l	18486	87	C10H22	142



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

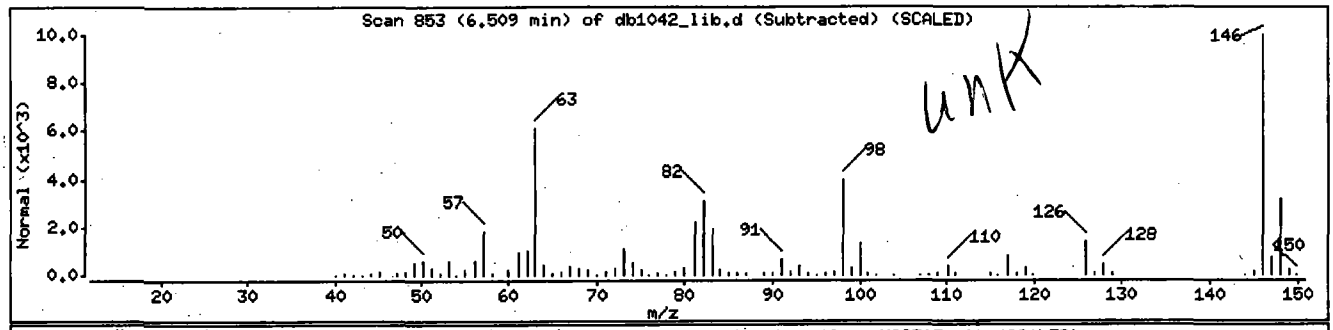
Volume Injected (uL): 1.0

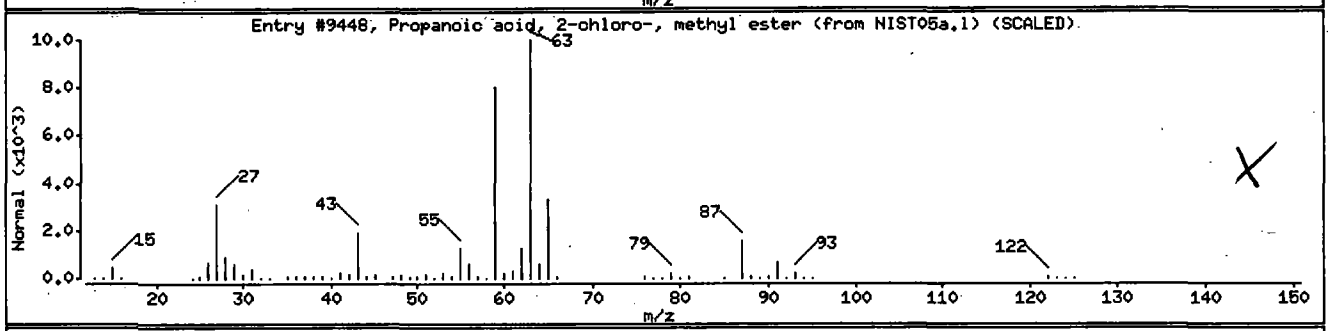
Operator: oeb05247

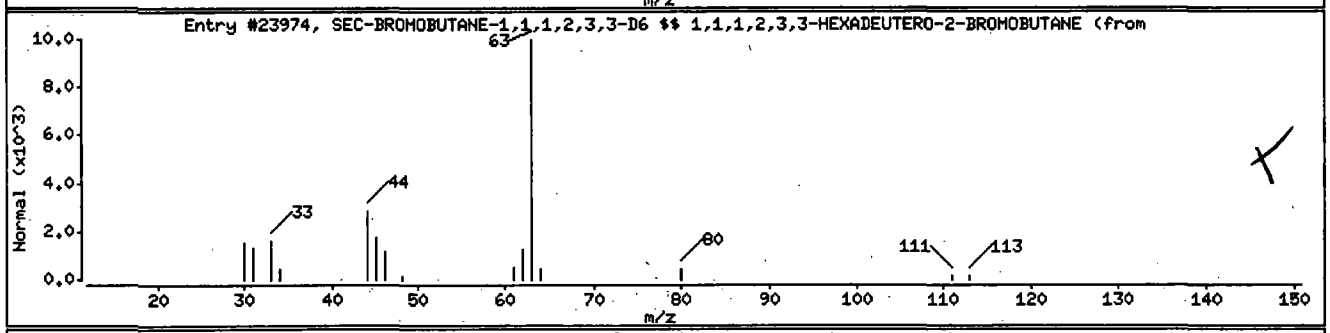
Column phase: J&W DB-5MS

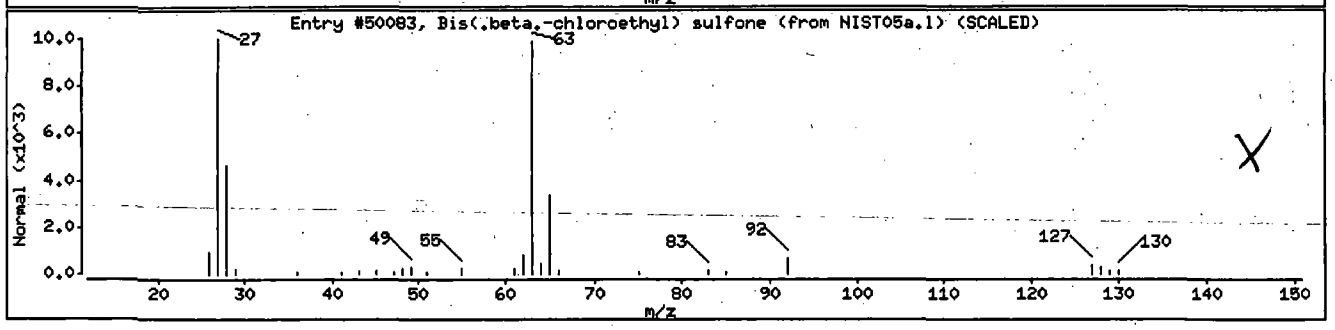
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	26	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	23	C4H8Cl2O2S	190









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Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

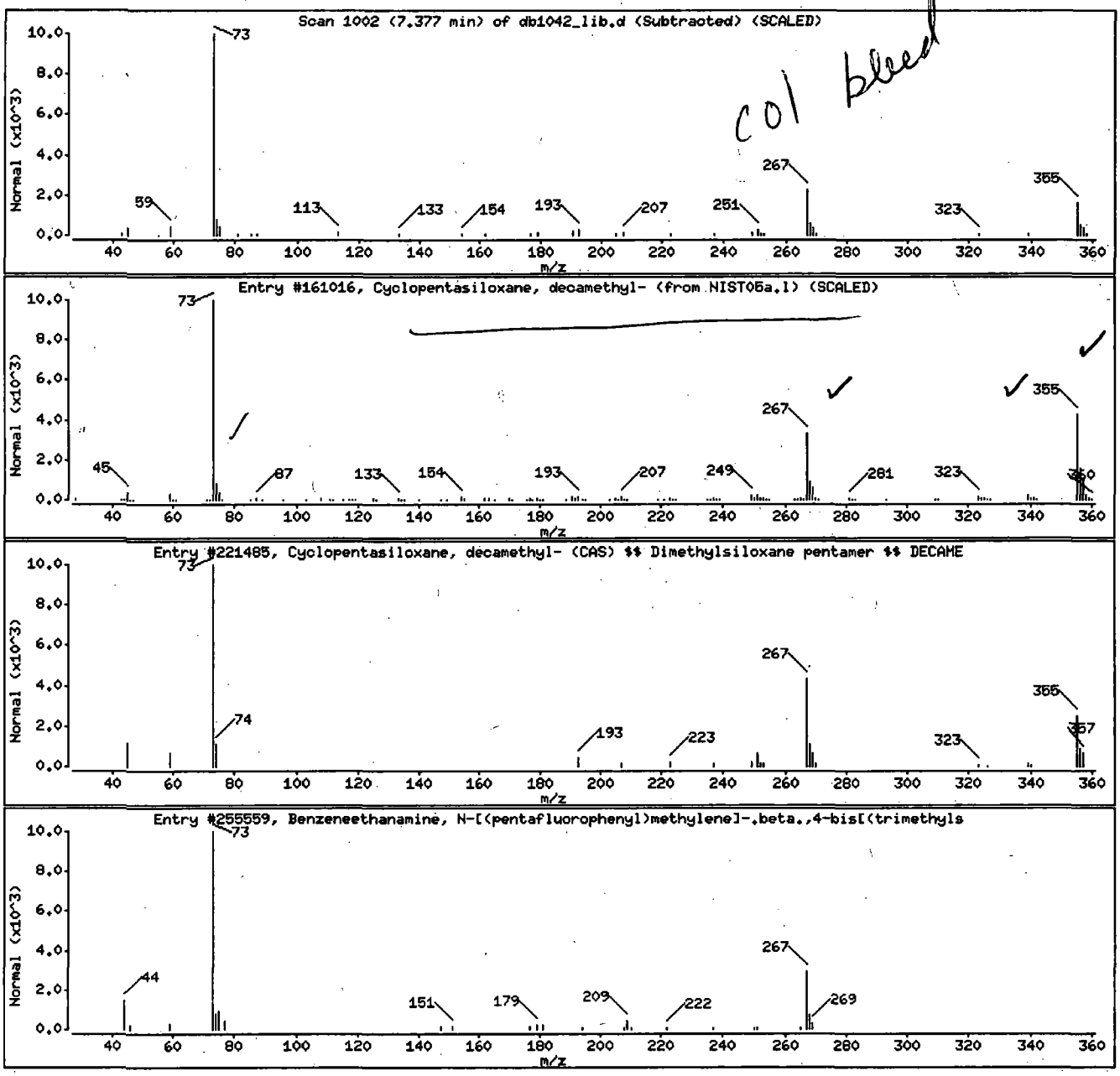
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	80	C10H30O5Si5	370
Benzeneethanamine, N-[(pentafluorophenyl	55429-85-1	WILEY275.l	255559	40	C21H26F5NO2Si2	475



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Date : 24-FEB-2014 02:20

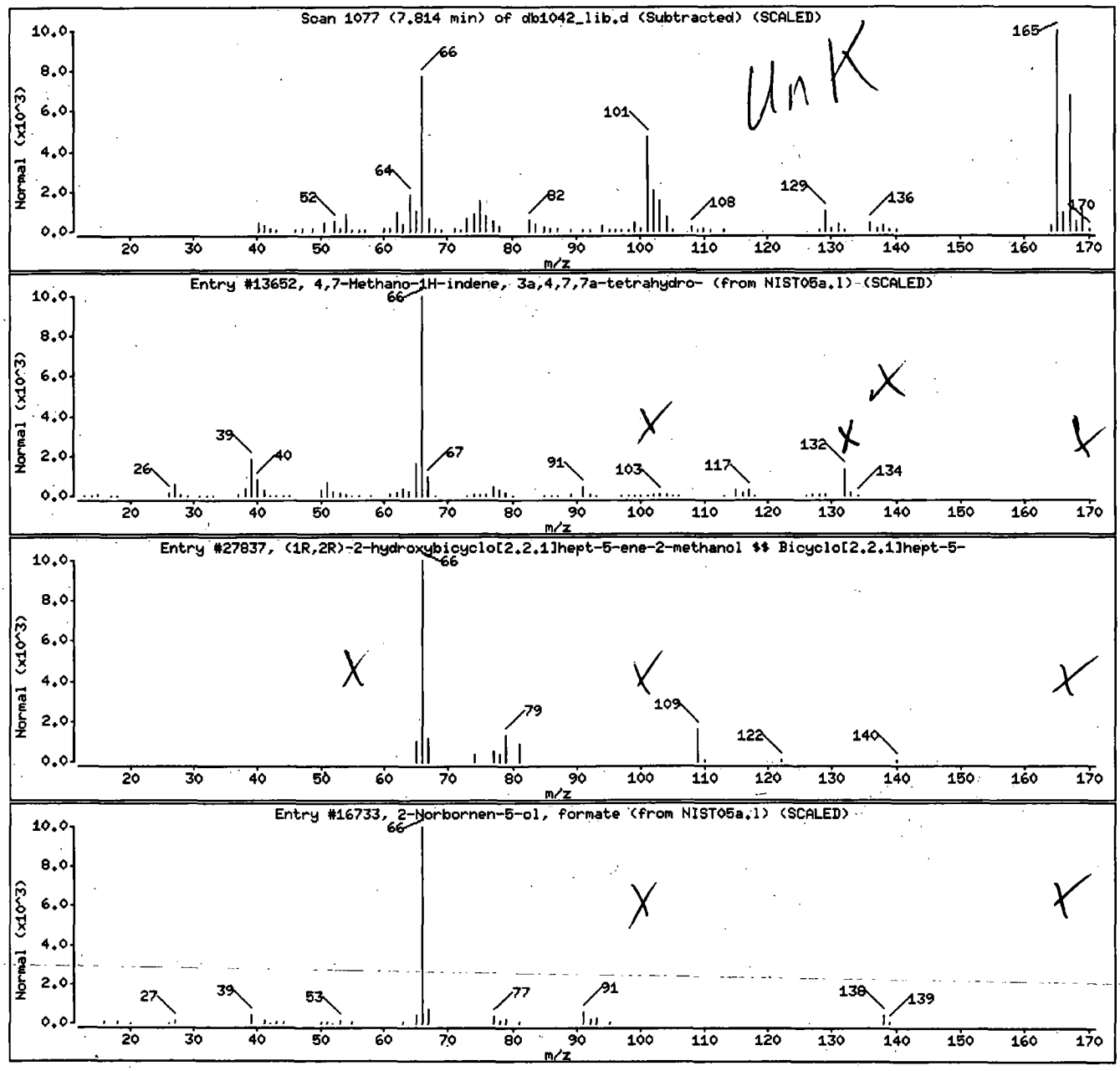
Client ID: H4011 Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	47	C10H12	132
(1R,2R)-2-hydroxybicyclo[2.2.1]hept-5-en	116697-44-0	WILEY275.l	27837	47	C8H12O2	140
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H10O2	138



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

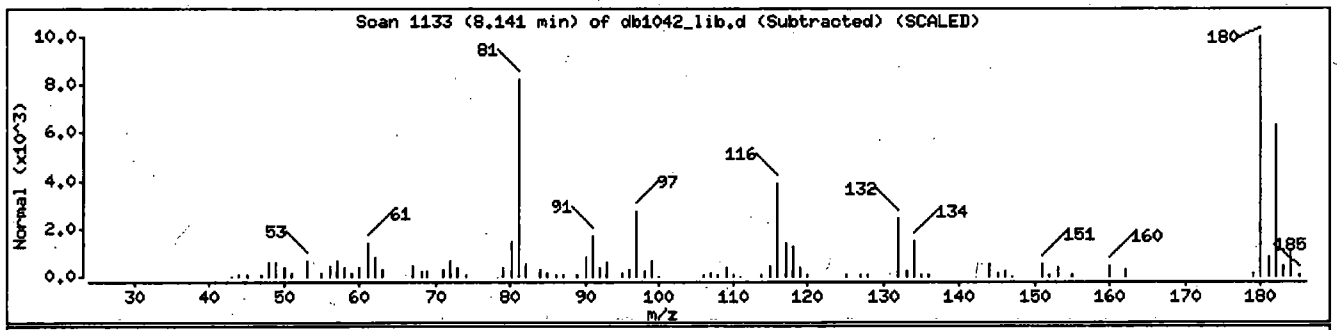
Volume Injected (uL): 1.0

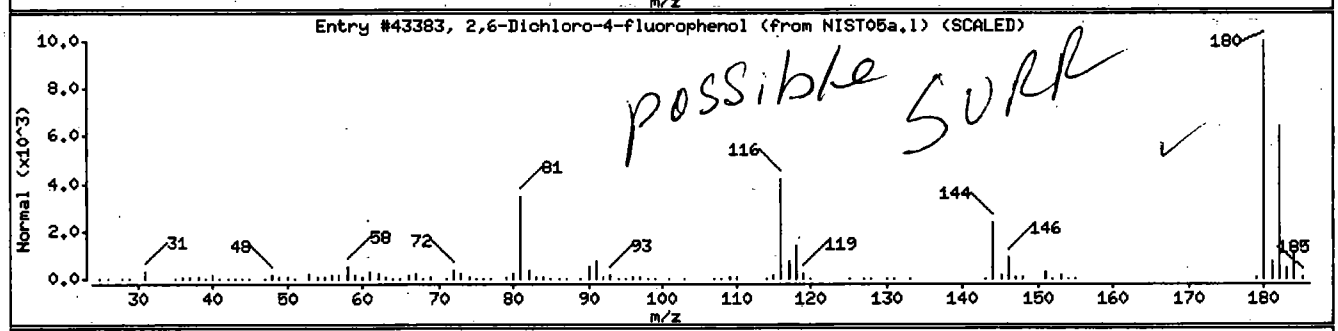
Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	87	C6H3Cl2FO	180
2-Fluoro-5-hydroxybenzotrifluoride	61721-07-1	NIST05a.l	43467	14	C7H4F4O	180
Benzene, 1,2,4-trichloro- (CAS) $$ 1,2,4	120-82-1	WILEY275.l	63743	12	C6H3Cl3	180





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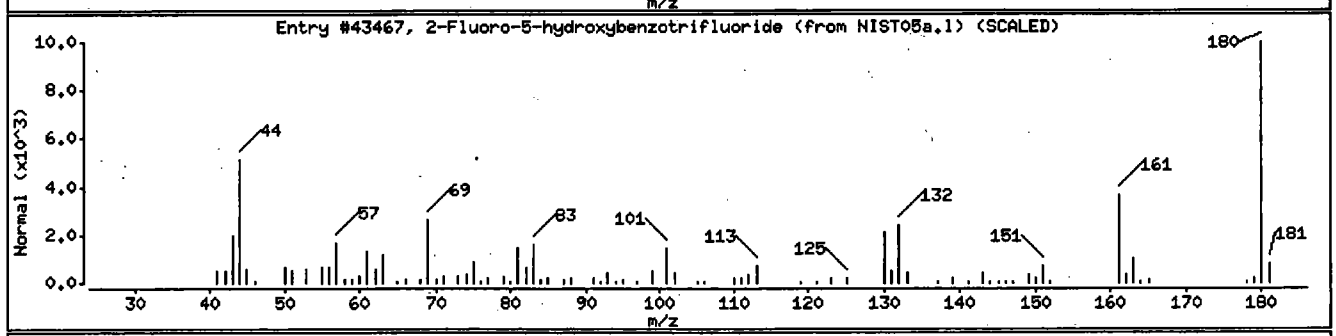

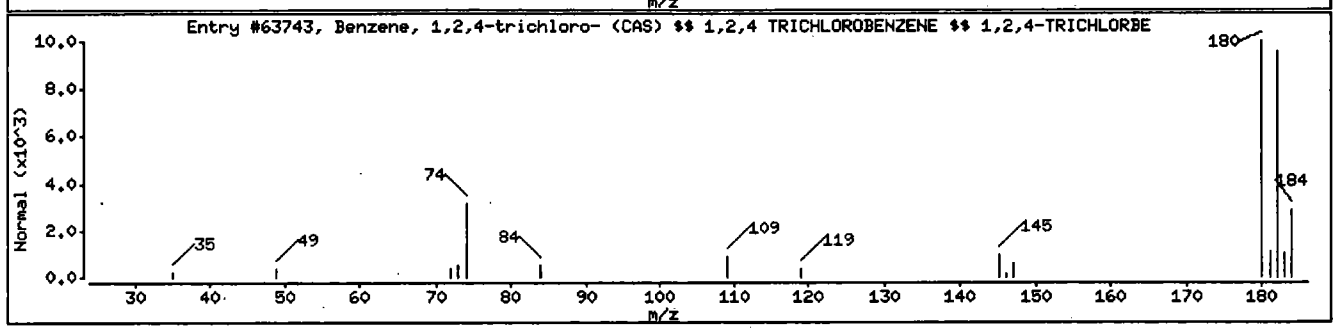

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

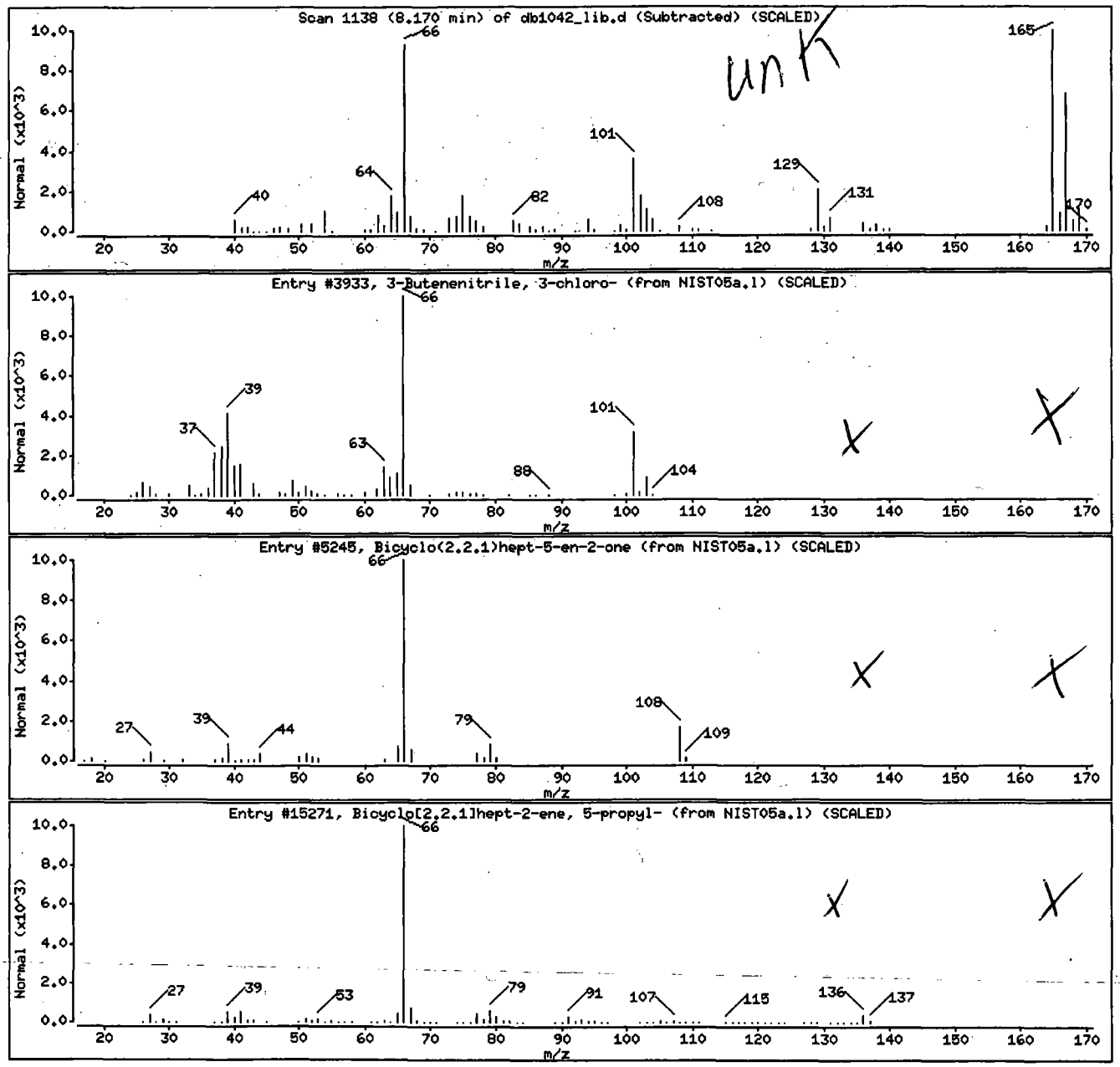
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo(2.2.1)hept-5-en-2-one	694-98-4	NIST05a.l	5245	49	C7H8O	108
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136



Digitally signed by Andrew J. Strebel on 03/02/2014 at 12:48.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1042_lib.d

Date : 24-FEB-2014 02:20

Client ID: H4011

Instrument: HP19760.i

Sample Info: H4011;7370723;1;0;SAMPLE;;;

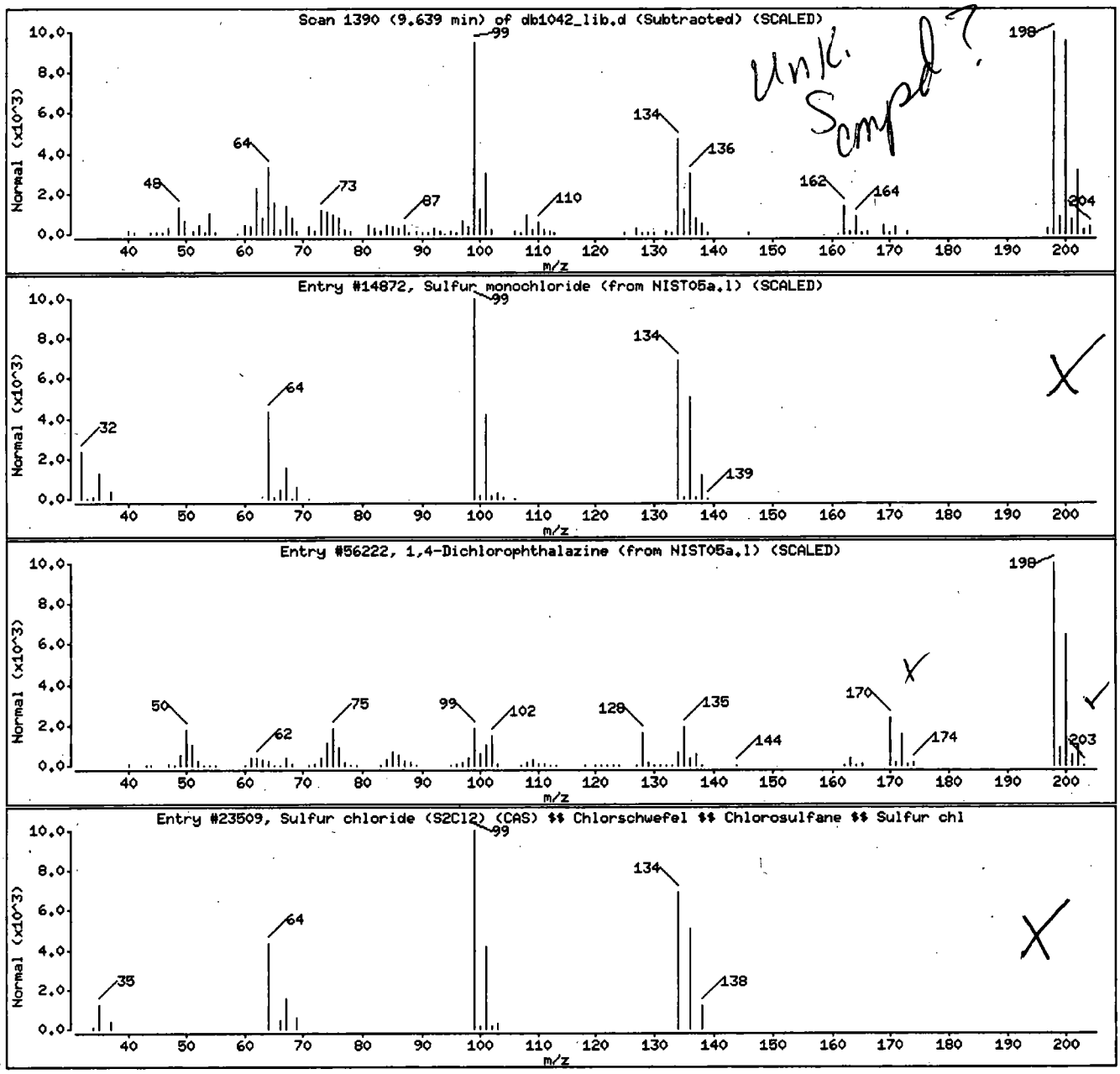
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

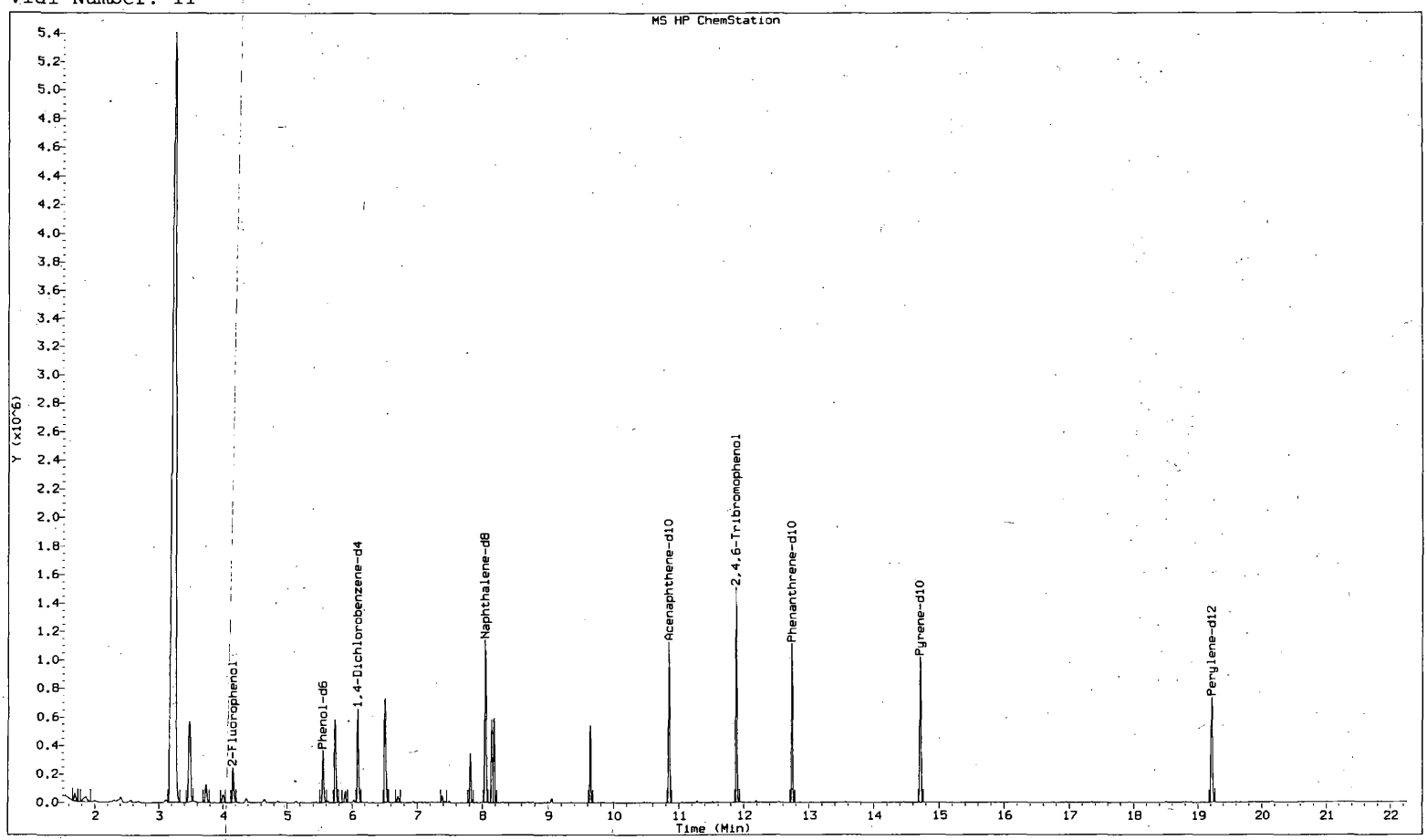
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	38	C8H4Cl2N2	198
Sulfur chloride (S2Cl2) (CAS) $$ Chlorso	10025-67-9	WILEY275.l	23509	38	Cl2S2	134



Digitally signed by Andrew J. Strebel on 03/02/2014 at 12:48.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb23.b/db1030_lib.d
Operator : ceb05247
Acquired : 23-FEB-2014 21:24
Instrument : HP19760.i
Sample Name: H4021;7370727;1;0;SAMPLE;;;
Misc Info : 14052WAM;WL13463;;1041;1000;0;db1022;13166;
Vial Number: 11



Lancaster Labs

Data file : /chem/HP19760.i/14feb23.b/db1030_lib.d
Lab Smp Id: 7370727 Client Smp ID: H4021
Inj Date : 23-FEB-2014 21:24
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H4021;7370727;1;0;SAMPLE;;;
Misc Info : 14052WAM;WL13463;;1041;1000;0;db1022;13166;
Comment : Max. number of TICs to report is 50, 15 TICs were found initially.
Method : /chem/HP19760.i/14feb23.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 12:40 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 11
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1041.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.089	956957	10.000
* 48 Naphthalene-d8	8.042	1463667	10.000
* 83 Acenaphthene-d10	10.845	1281918	10.000

CONCENTRATIONS					QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.689	108581	1.13464431	1.08995	90	NIST05a.1	31323	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.858	142943	1.49372238	1.43489	25	NIST05a.1	4733	21(ML)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.251	20590728	215.168688	206.69422	83	NIST05a.1	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.478	1194156	12.4786742	11.98719	83	NIST05a.1	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.734	242104	2.52993190	2.43029	25	NIST05a.1	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
3.997	101682	1.06255828	1.02070	38	NIST05a.1	13998	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.739	851518	8.89817582	8.54771	89	WILEY275.1	18902	21
Decane					CAS #: 124-18-5		
5.891	113699	1.18813407	1.14133	95	NIST05a.1	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.509	1157521	12.0958436	11.61944	35	NIST05a.1	9448	21
Cyclohexanemethanol, 4-methyl-, cis-					CAS #: 3937-48-2		
6.701	66475	0.69464585	0.66728	53	NIST05a.1	12240	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.383	63620	0.43465956	0.41754	90	NIST05a.1	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.814	437114	2.98643214	2.86881	43	NIST05a.1	13656	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.141	674718	4.60977631	4.42821	46	NIST05a.1	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.170	709032	4.84421741	4.65342	50	NIST05a.1	3933	48
Sulfur monochloride					CAS #: 10025-67-9		
9.639	616881	4.81216957	4.62264	38	NIST05a.1	14872	83(L)

Target compound.
Do not report.
ajs00193 03/02/2014

QC Flag Legend

M - Compound response manually integrated.
L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

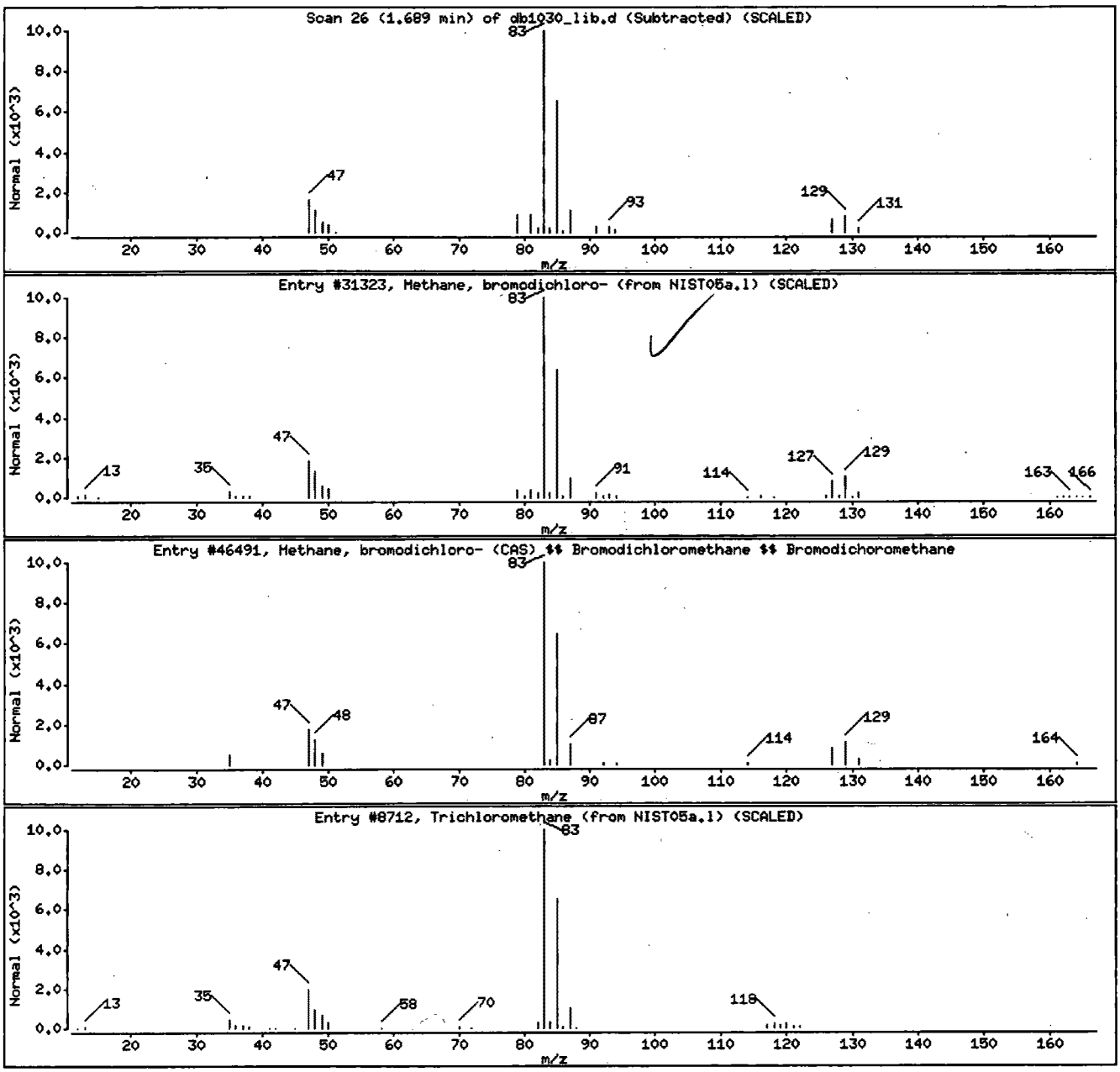
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46491	90	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

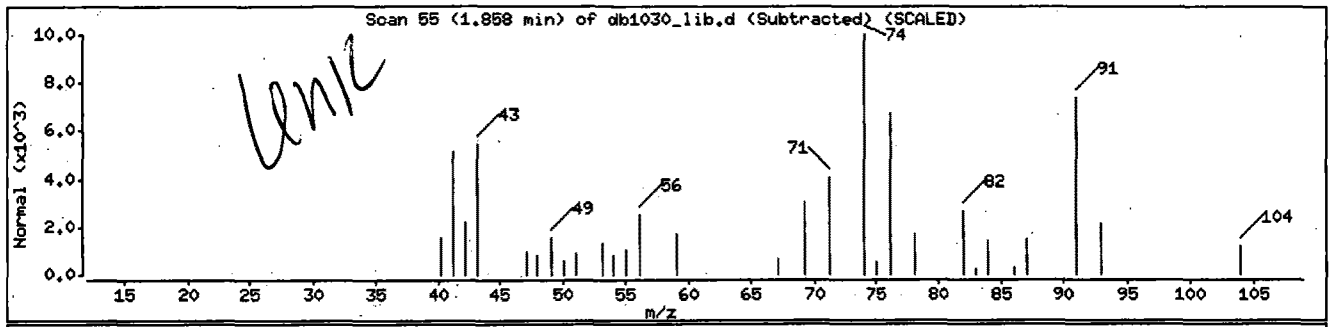
Volume Injected (uL): 1.0

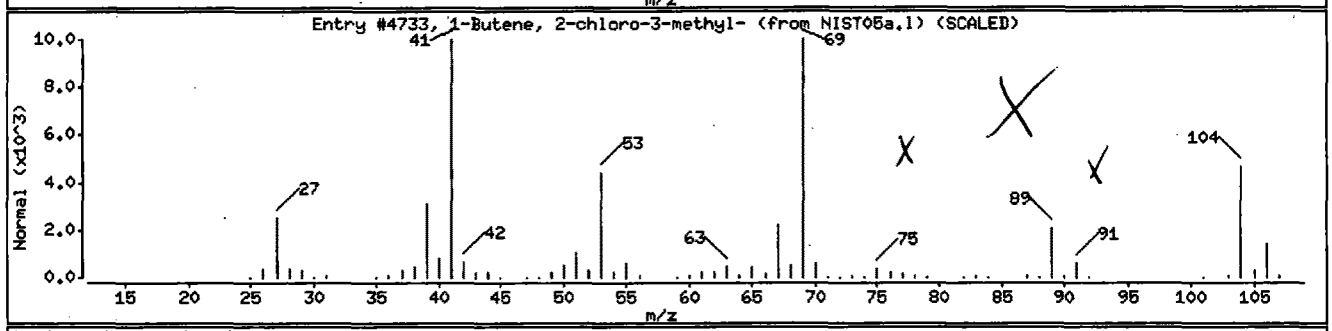
Operator: ceb05247

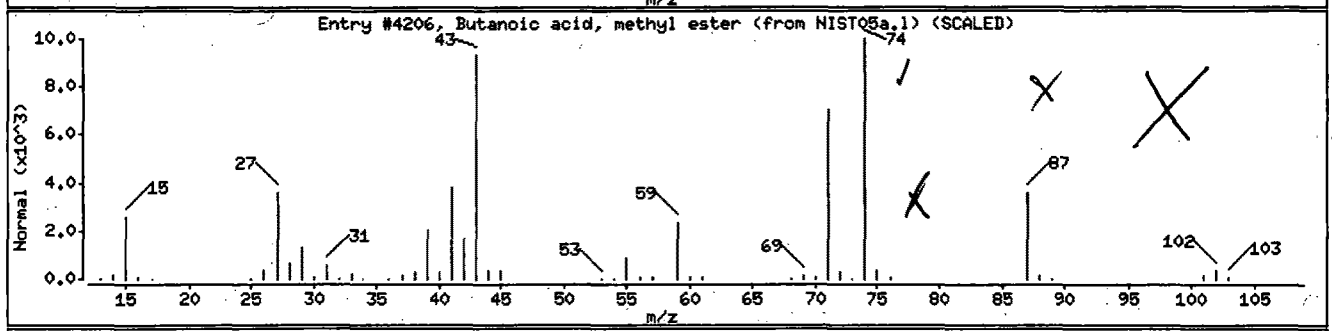
Column phase: J&W DB-5MS

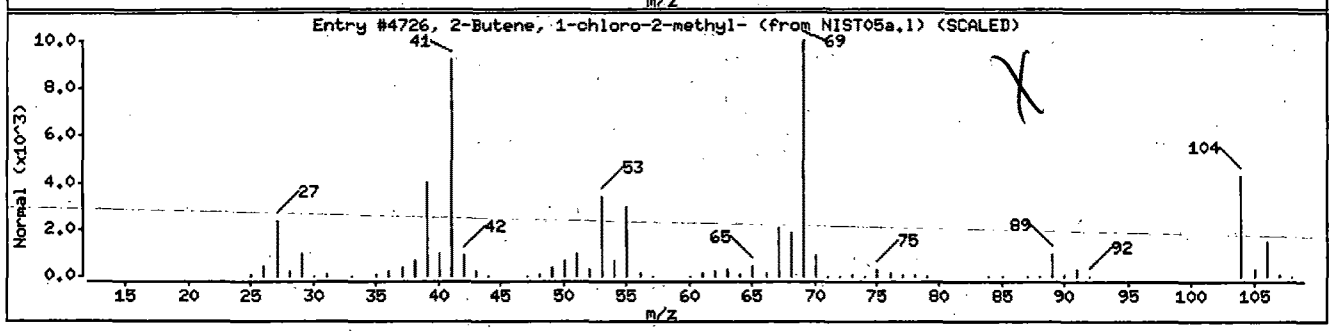
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	25	C5H9Cl	104
Butanoic acid, methyl ester	623-42-7	NIST05a.l	4206	47	C5H10O2	102
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4726	15	C5H9Cl	104









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

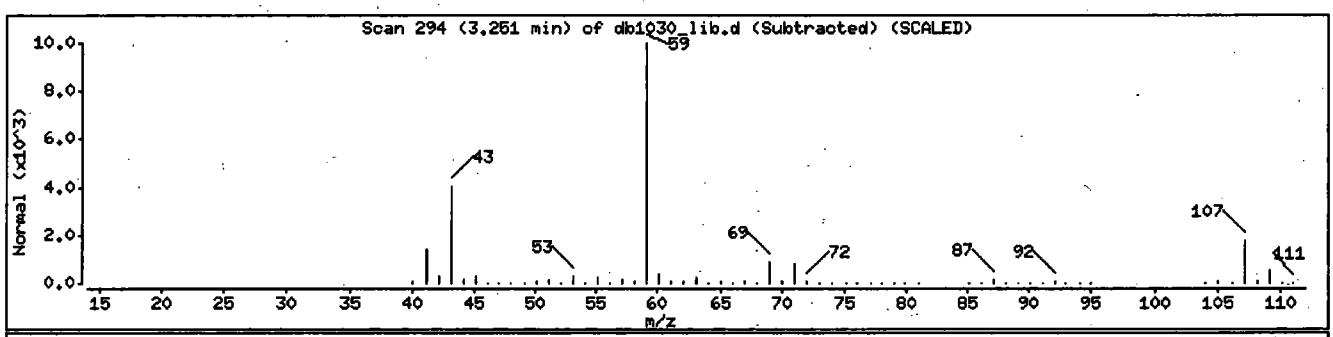
Volume Injected (uL): 1.0

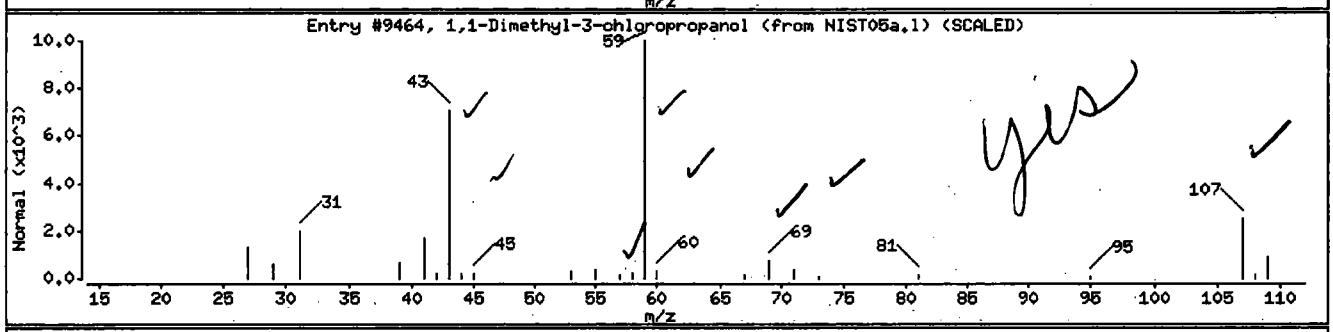
Operator: oeb05247

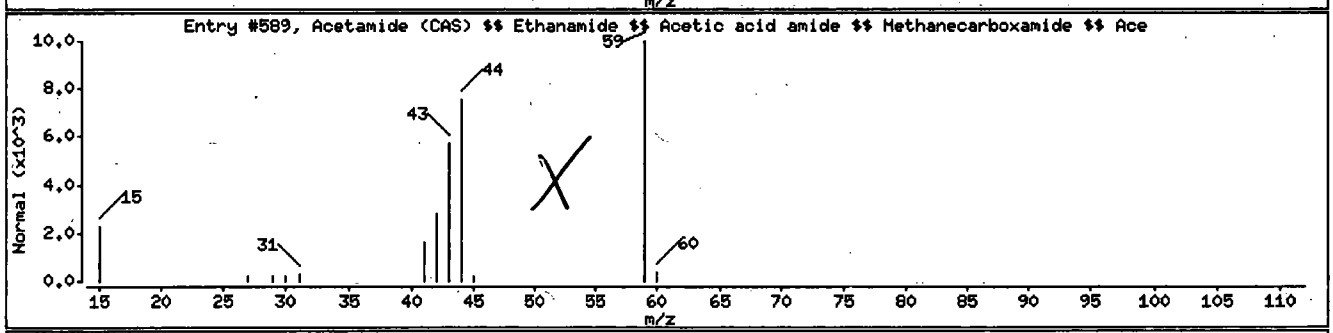
Column phase: J&W DB-5MS

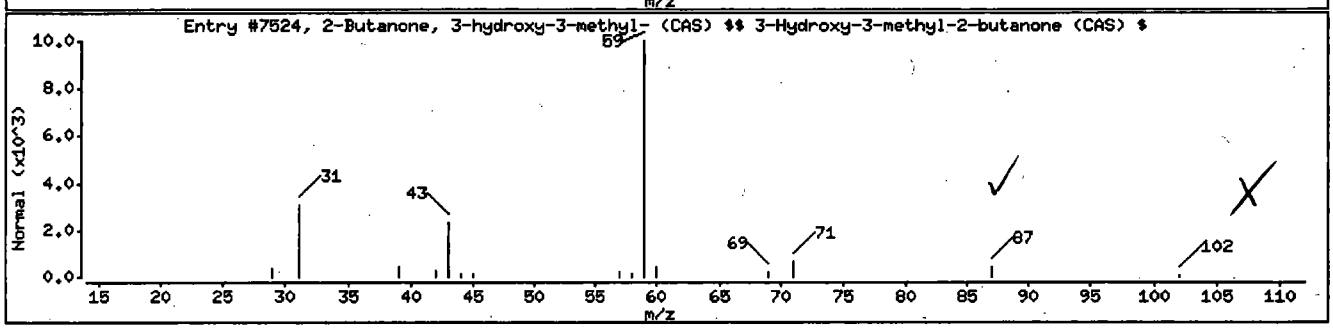
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

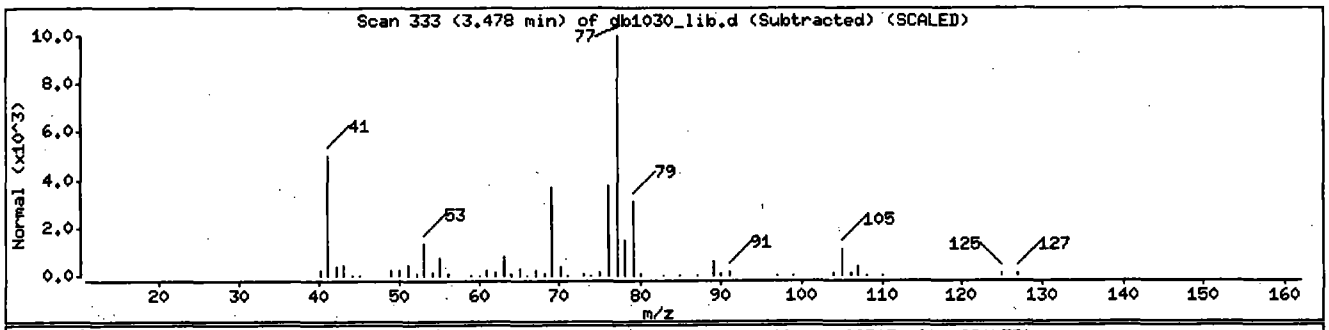
Volume Injected (uL): 1.0

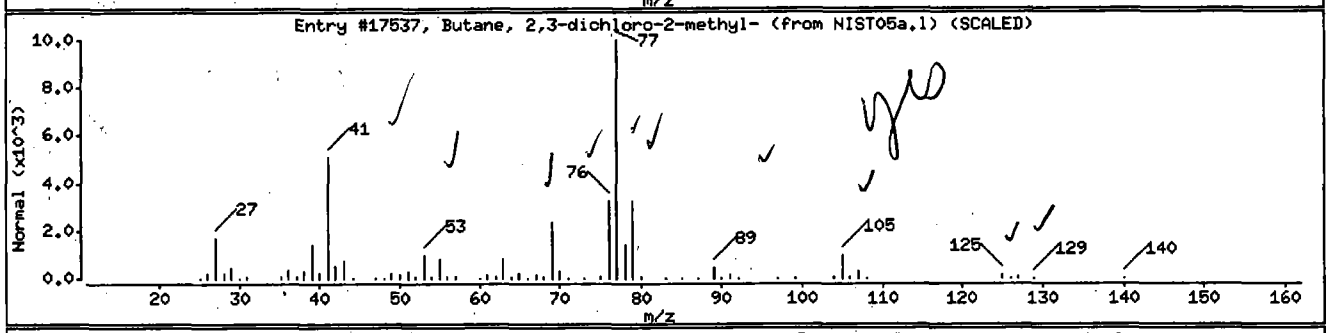
Operator: ceb05247

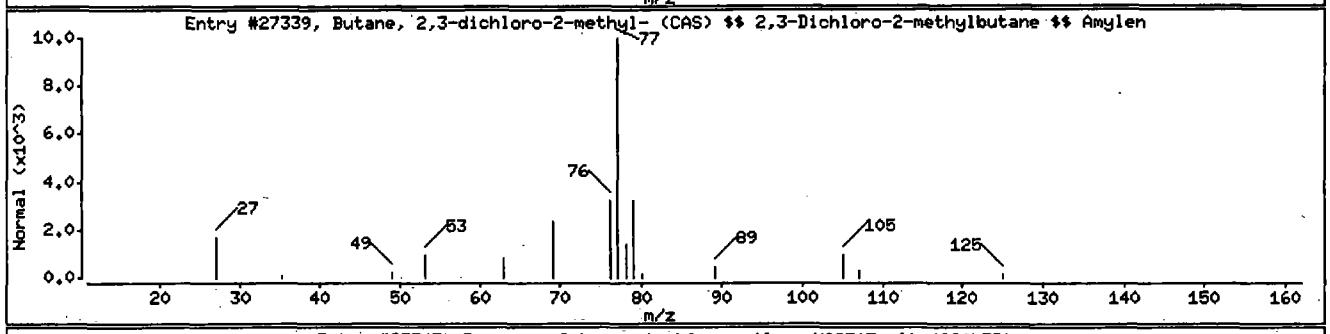
Column phase: J&W DB-5MS

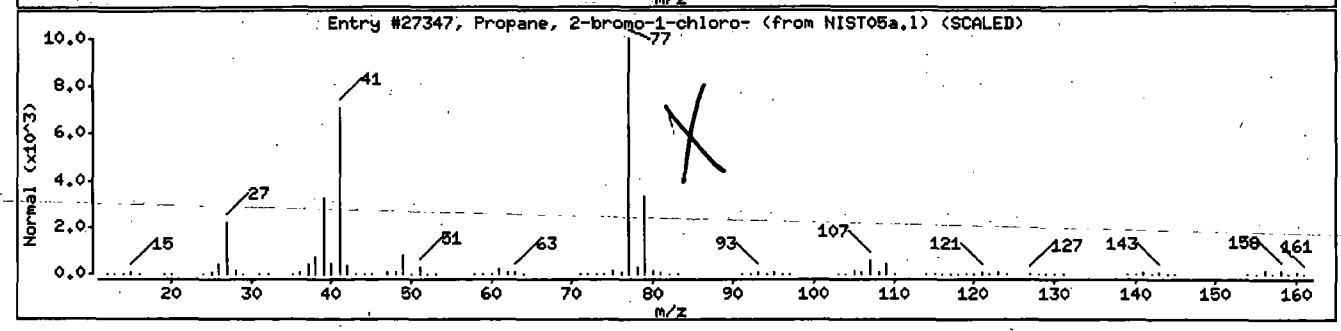
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	59	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	50	C3H6BrCl	156









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

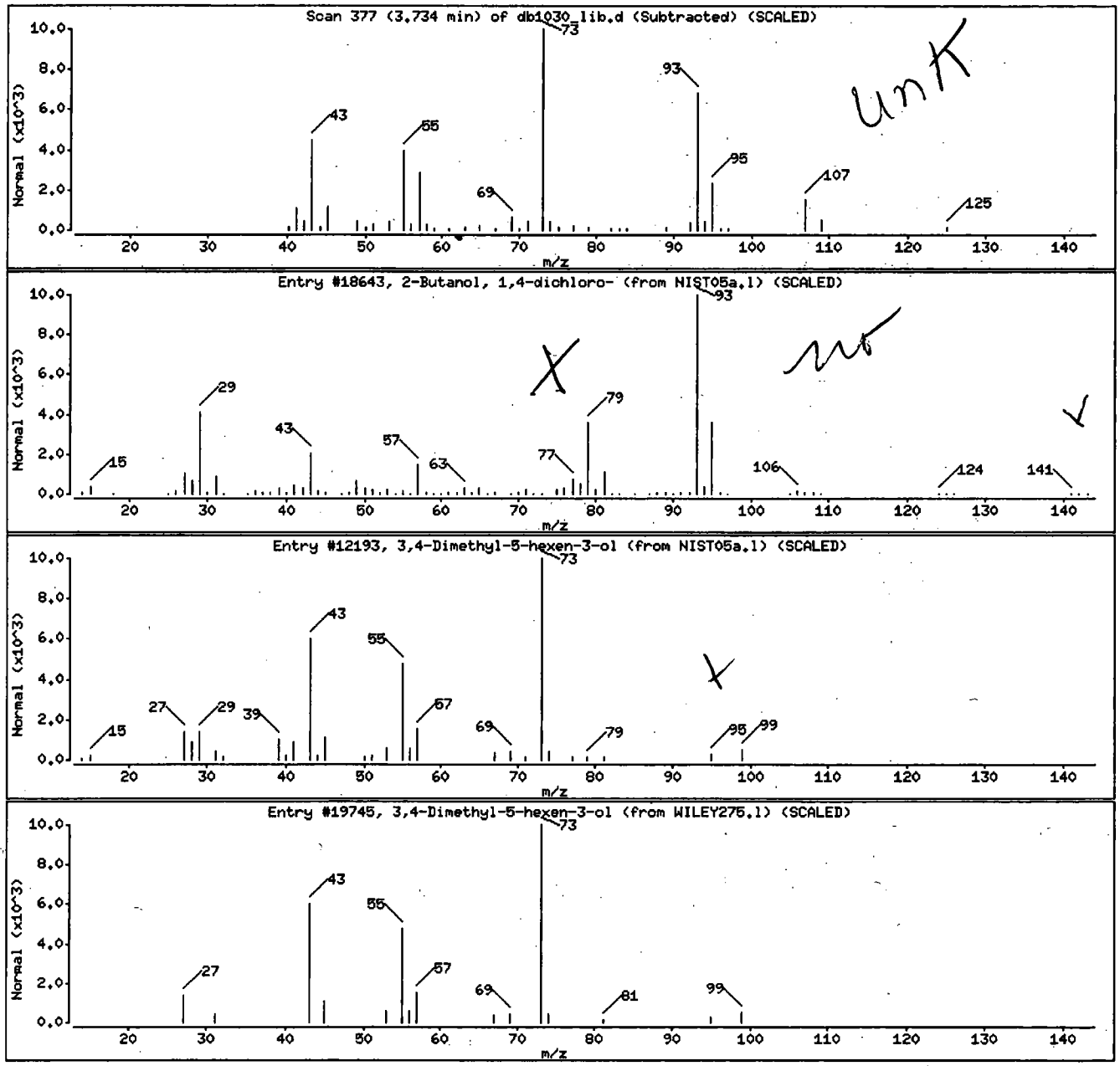
Volume Injected (uL): 1.0

Operator: ceb06247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	26	C4H8Cl2O	142
3,4-Dimethyl-5-hexen-3-ol	1569-45-5	NIST05a.l	12193	10	C8H16O	128
3,4-Dimethyl-5-hexen-3-ol	0-00-0	WILEY275.l	19745	10	C8H16O	128



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

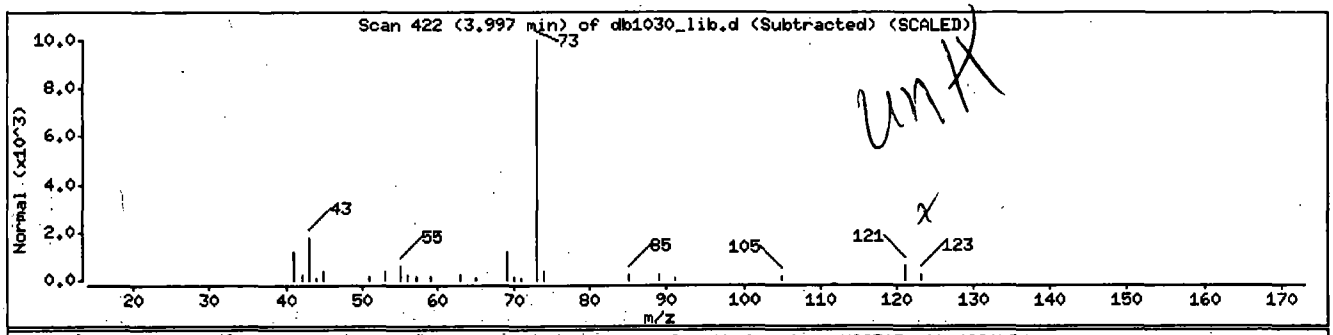
Volume Injected (uL): 1.0

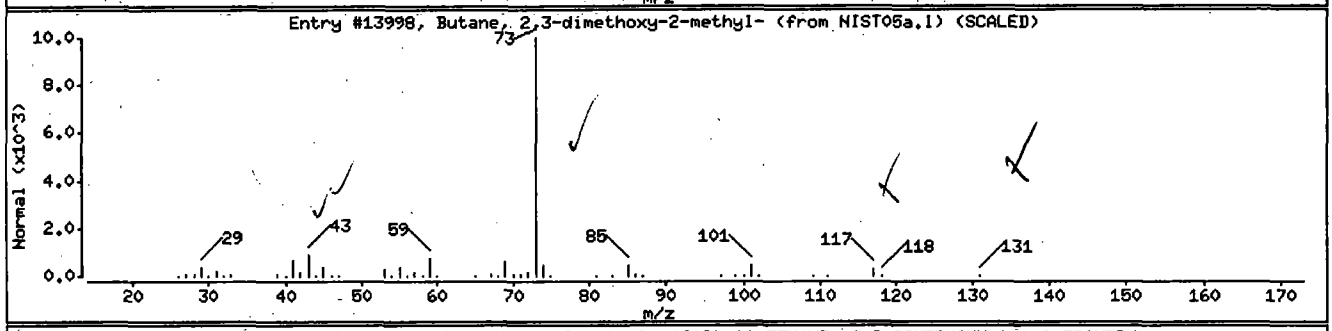
Operator: ceb05247

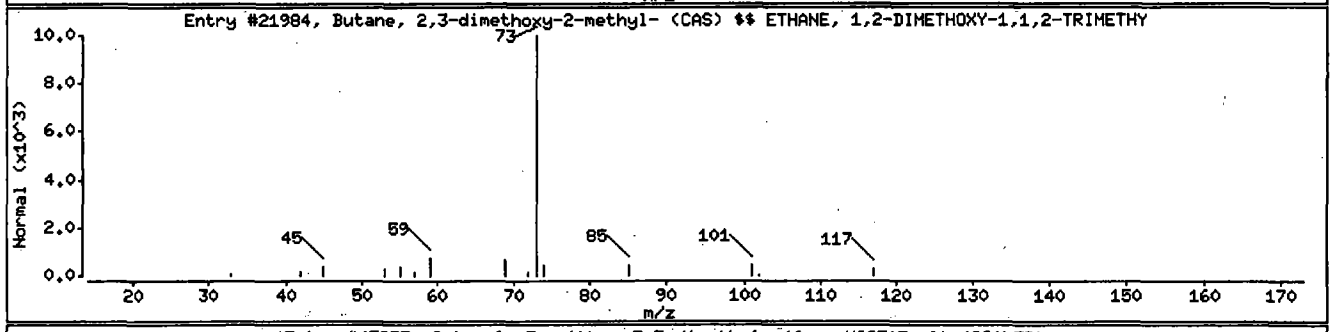
Column phase: J&W DB-5MS

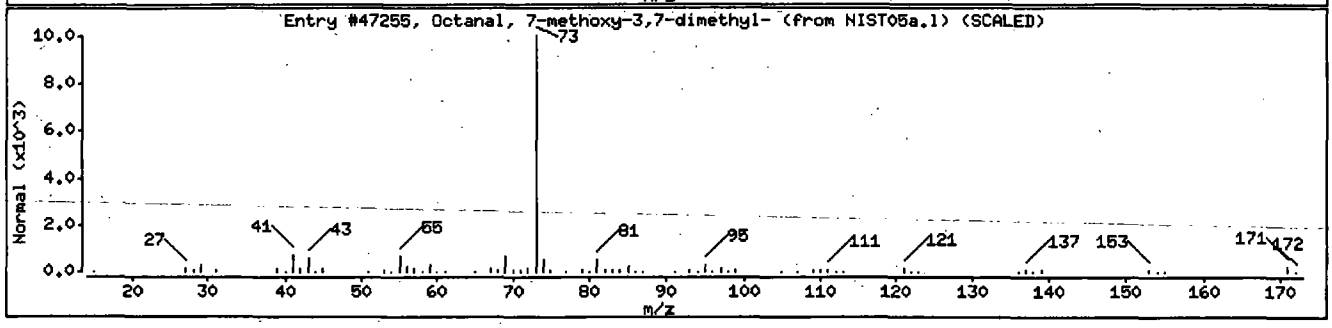
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	38	C7H1602	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H1602	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	33	C11H2202	186









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

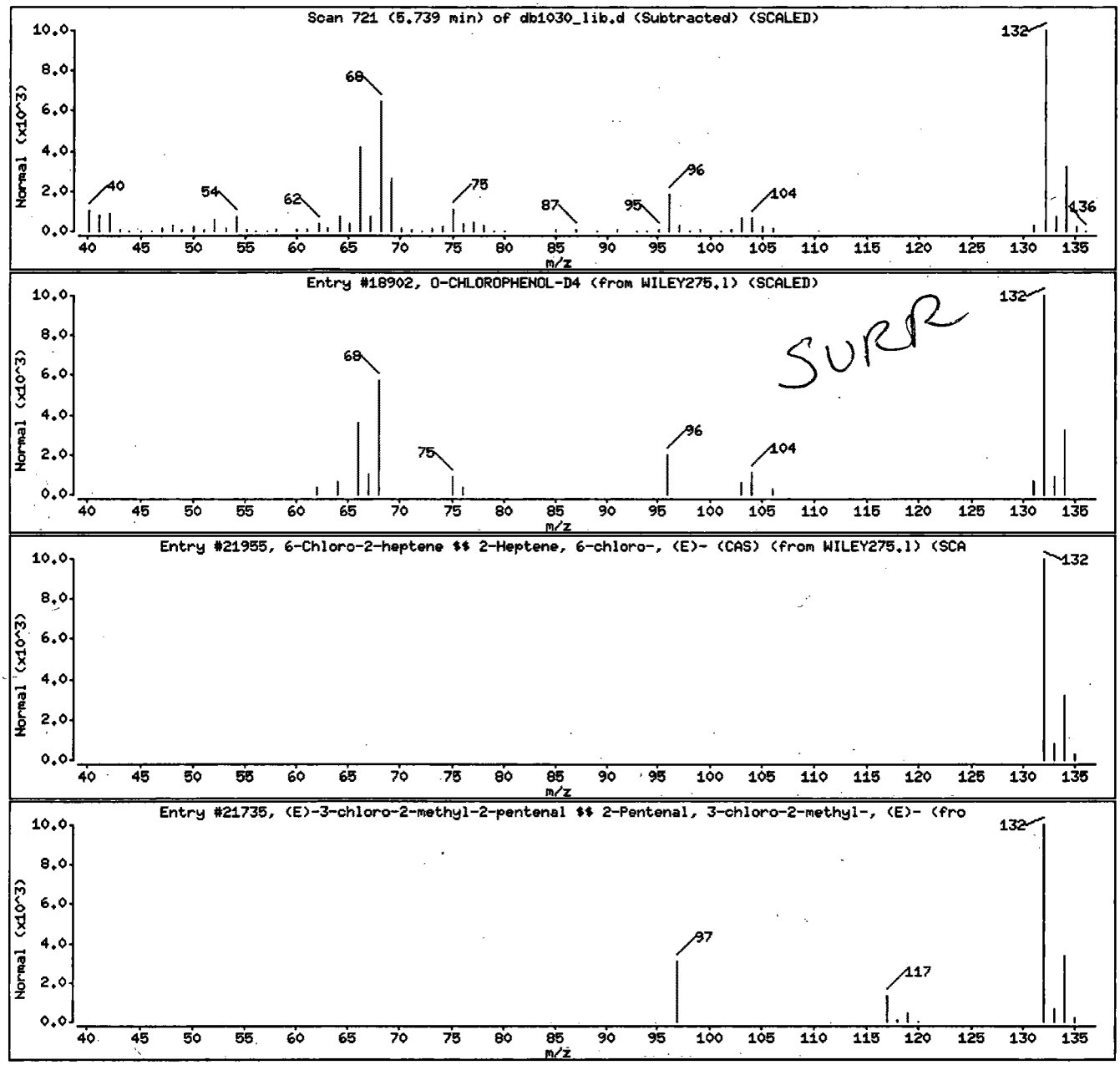
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5HS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	89	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

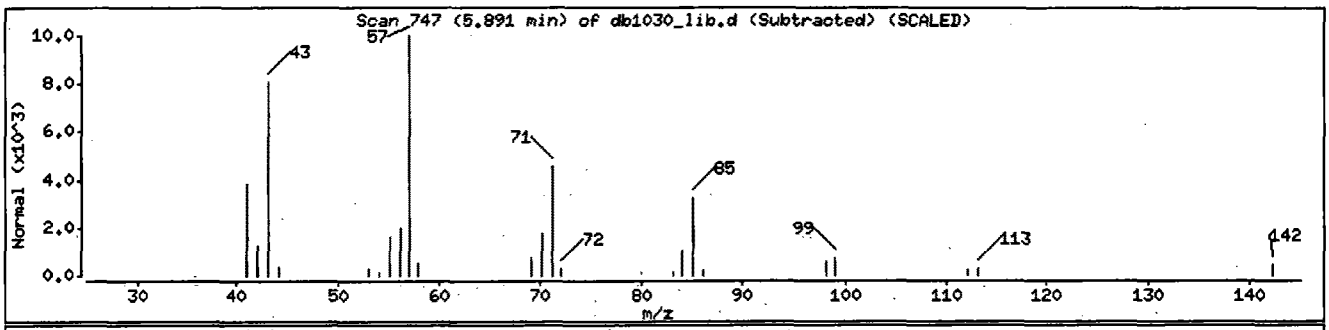
Client ID: H4021 Instrument: HP19760.i

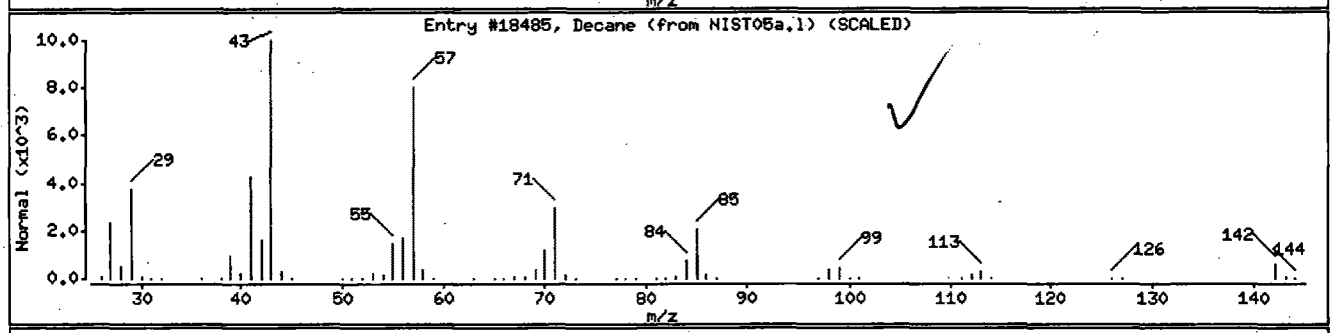
Sample Info: H4021;7370727;1;0;SAMPLE;;;

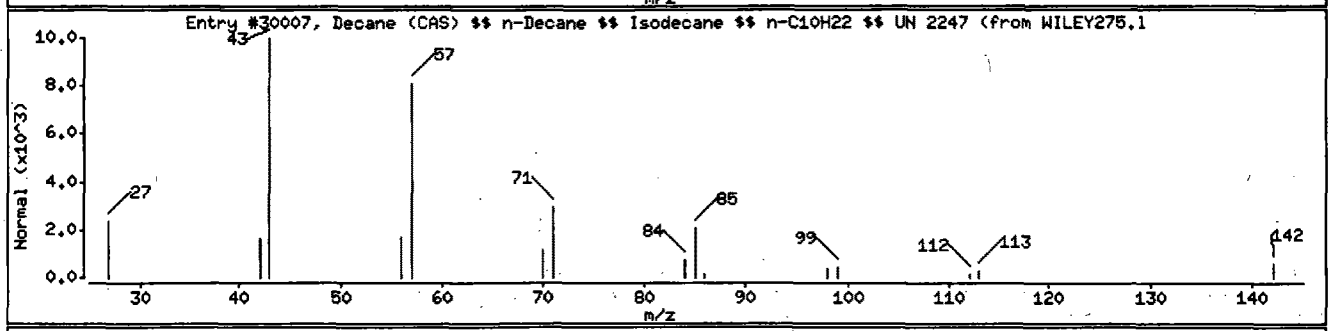
Volume Injected (uL): 1.0 Operator: ceb05247

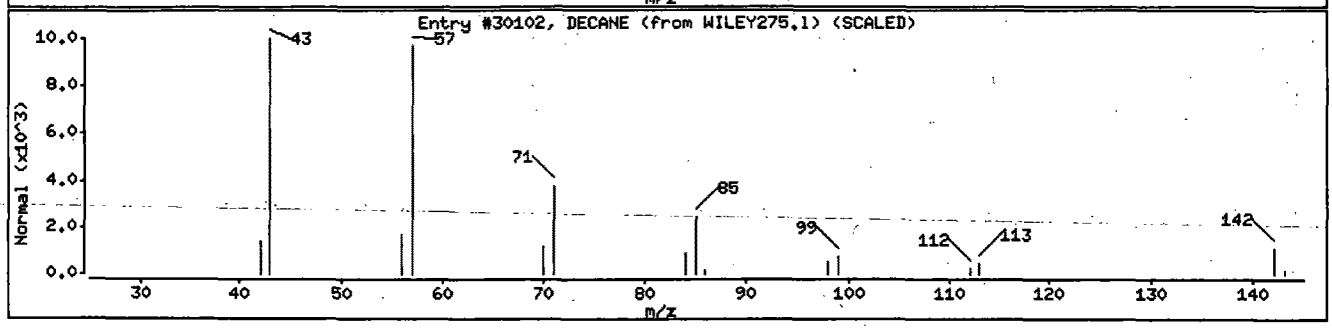
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

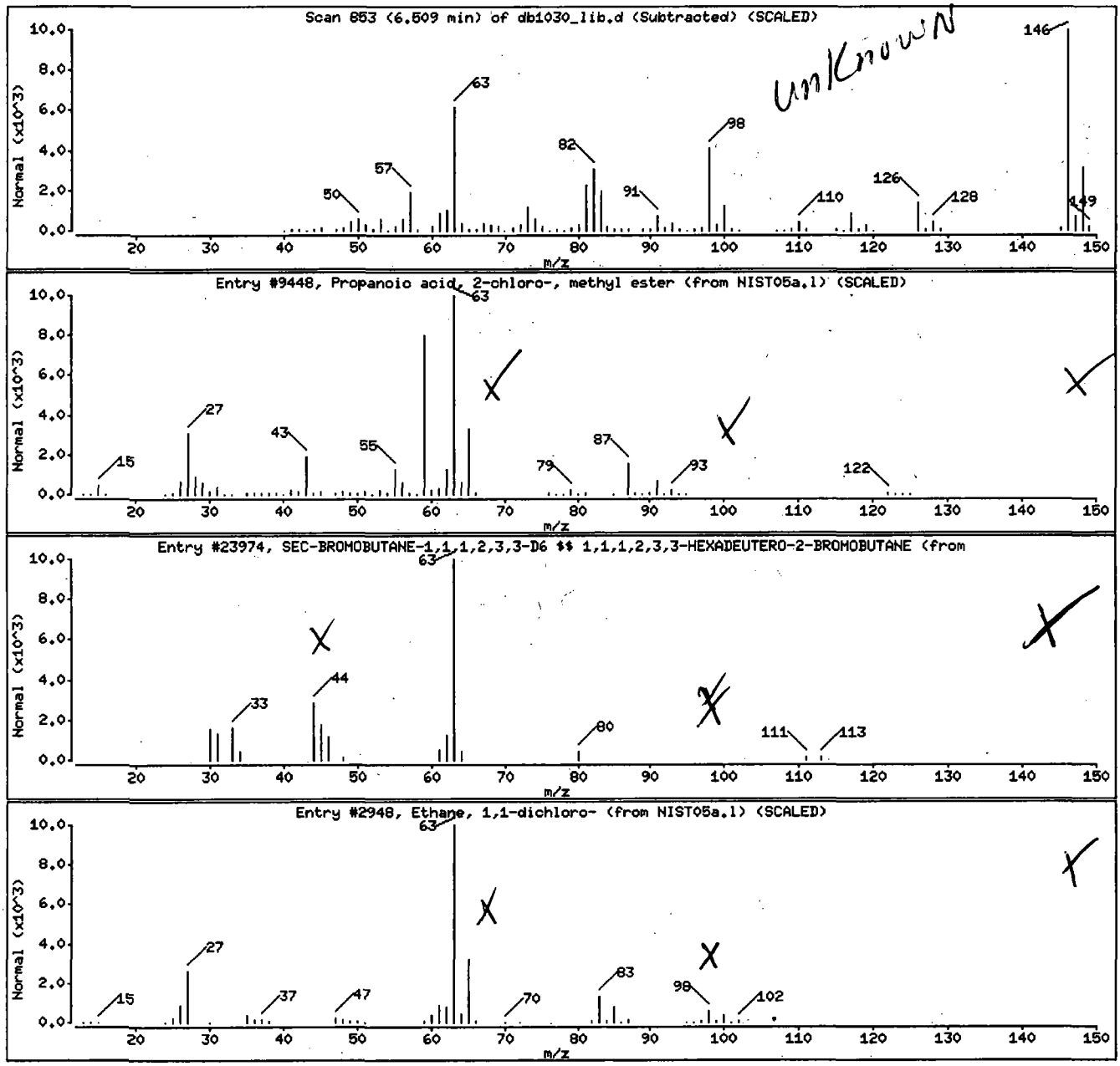
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	36	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	23	C2H4Cl2	98



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

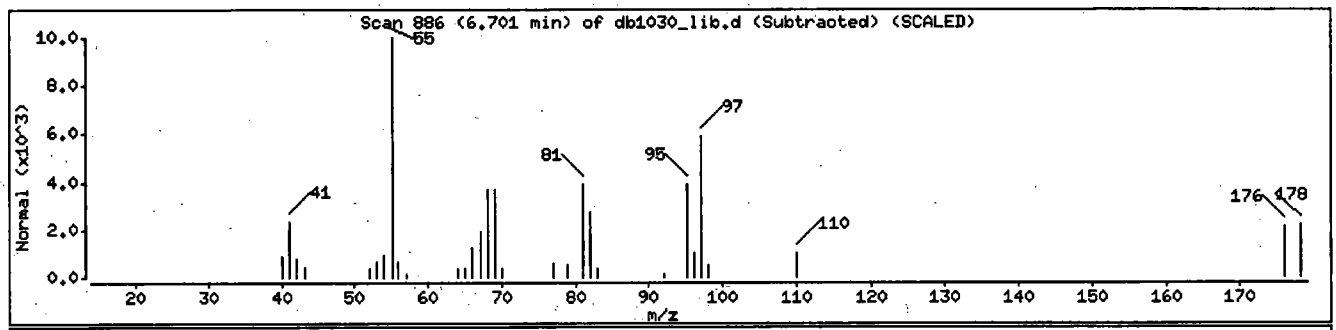
Volume Injected (uL): 1.0

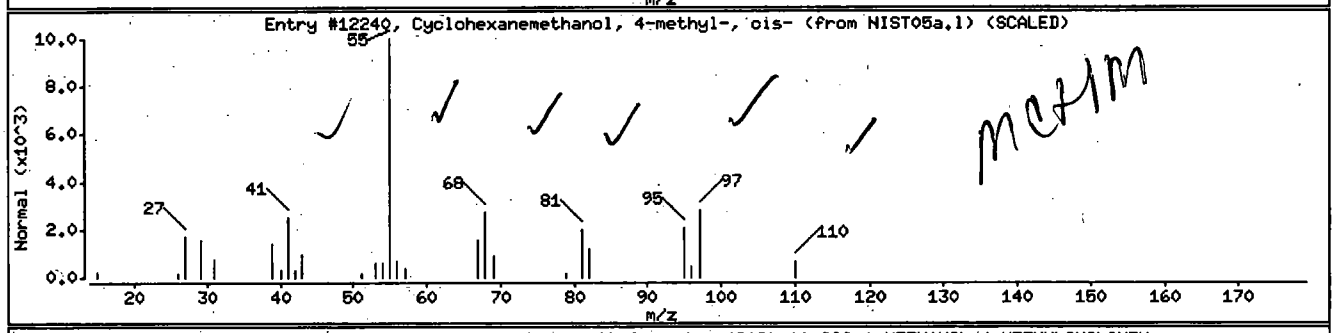
Operator: ceb05247

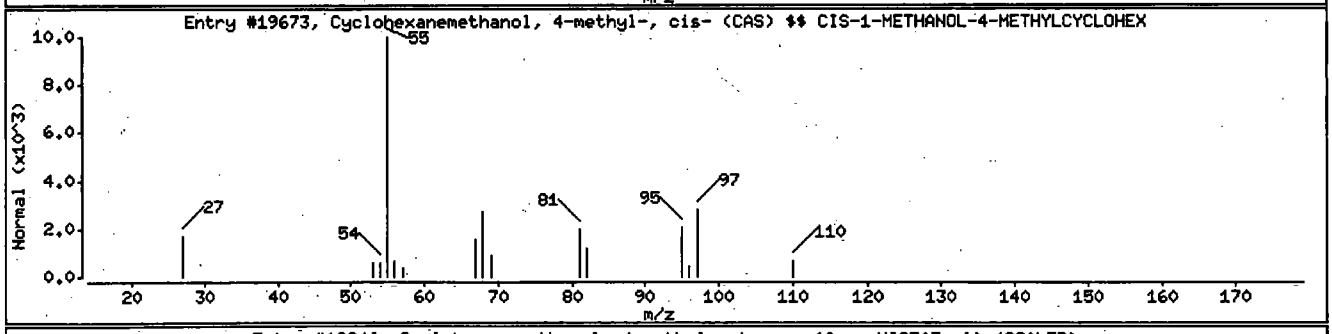
Column phase: J&W DB-5MS

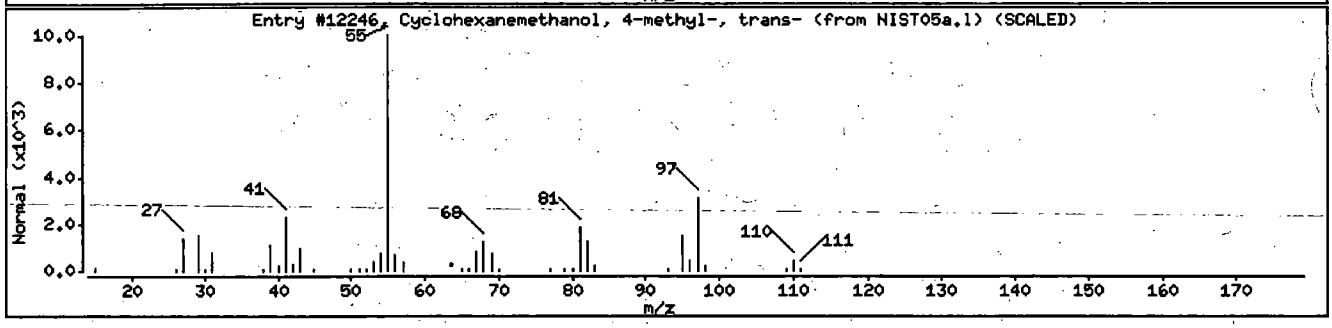
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, cis-	3937-48-2	NIST05a.l	12240	53	C8H16O	128
Cyclohexanemethanol, 4-methyl-, cis- (CA	3937-48-2	WILEY275.l	19673	53	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	50	C8H16O	128









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

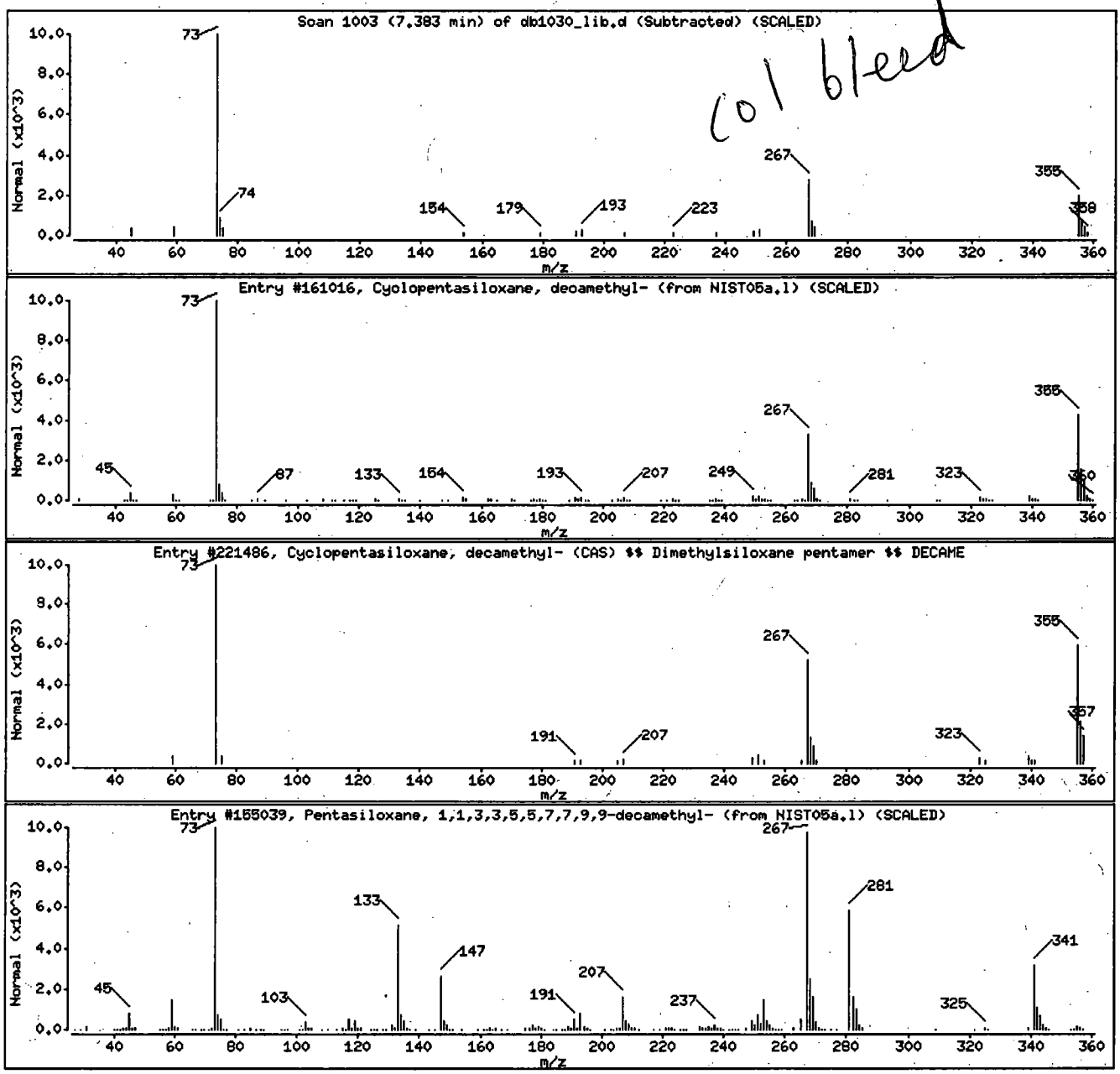
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	72	C10H30O5Si5	370
Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decam	995-83-5	NIST05a.l	155039	38	C10H32O4Si5	356



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

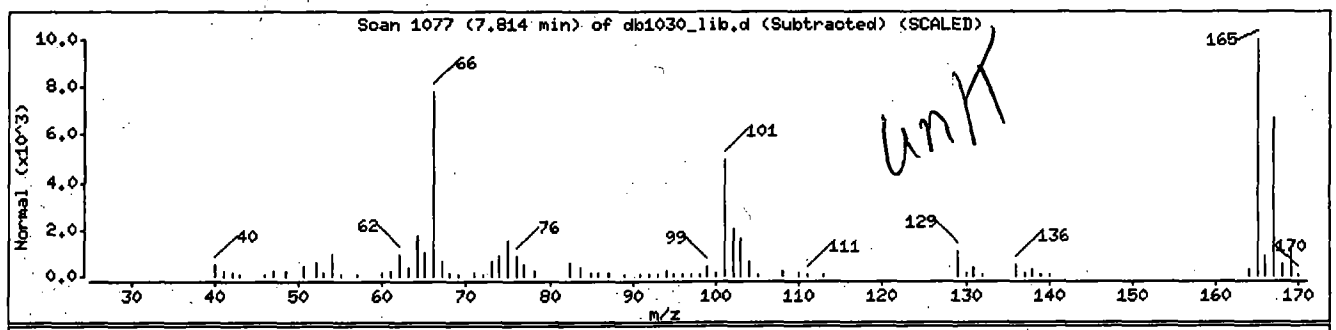
Volume Injected (uL): 1.0

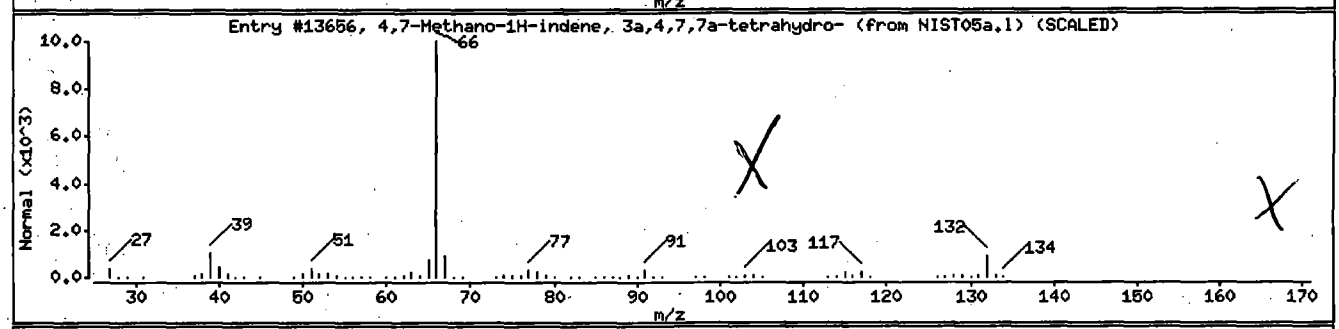
Operator: ceb05247

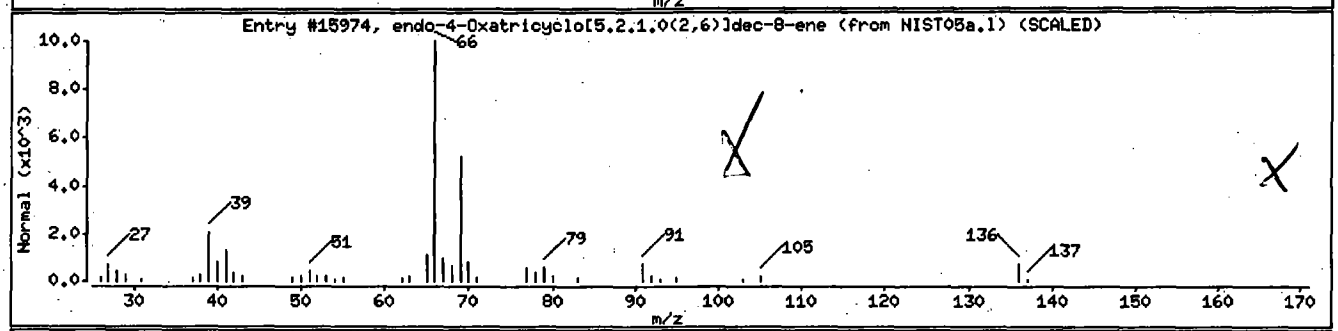
Column phase: J&W DB-5MS

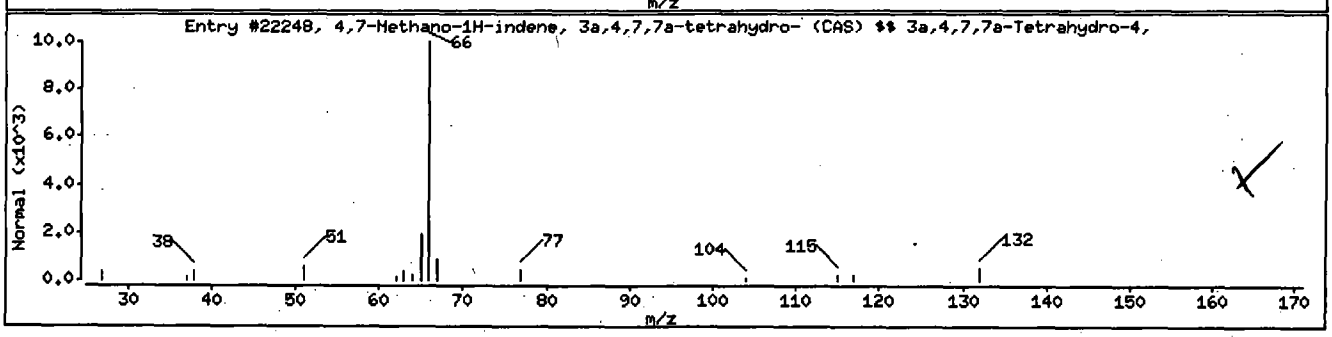
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13656	43	C10H12	132
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	46	C9H12O	136
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22248	46	C10H12	132









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

Client ID: H4021

Instrument: HP19760.i

Sample Info: H4021;7370727;1;0;SAMPLE;;;

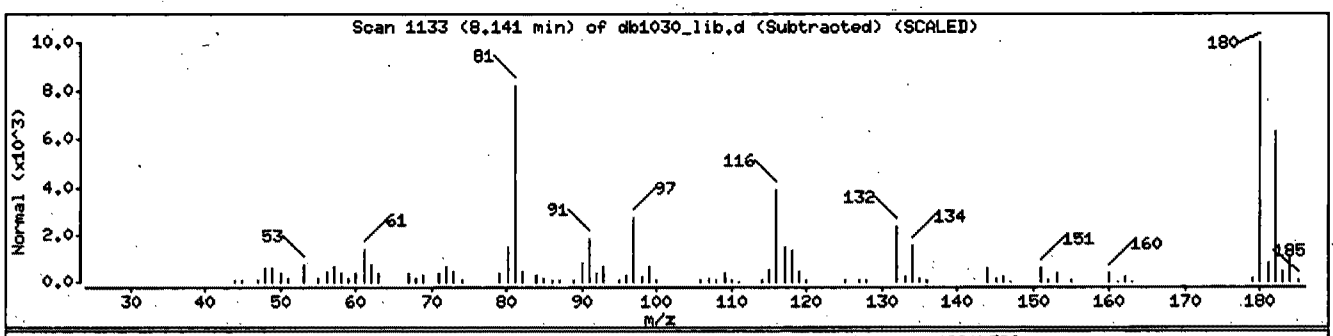
Volume Injected (uL): 1.0

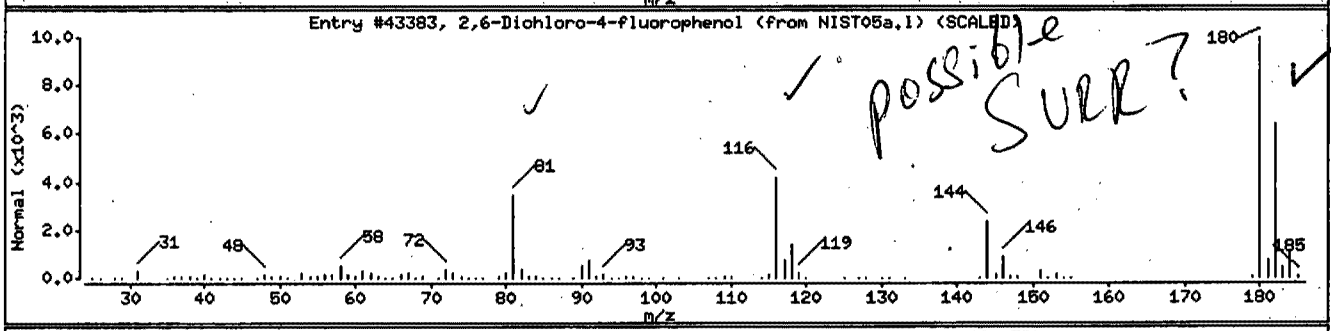
Operator: ceb05247

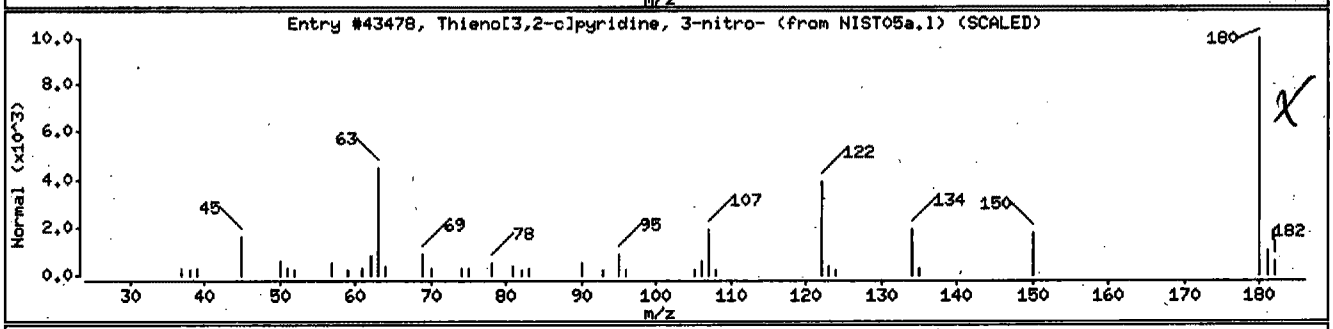
Column phase: J&W DB-5MS

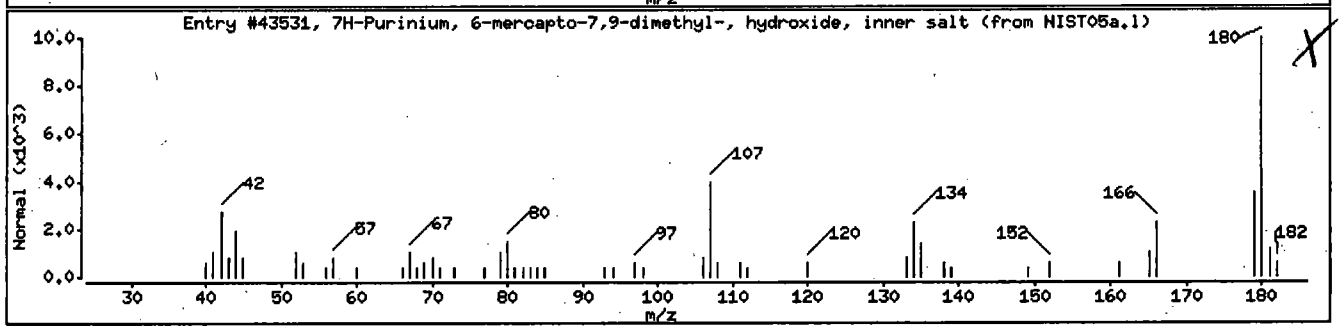
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	46	C6H3Cl2FO	180
Thieno[3,2-c]pyridine, 3-nitro-	28783-05-3	NIST05a.l	43478	14	C7H4N2O2S	180
7H-Purinium, 6-mercapto-7,9-dimethyl-, h	5752-11-4	NIST05a.l	43531	14	C7H8N4S	180









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

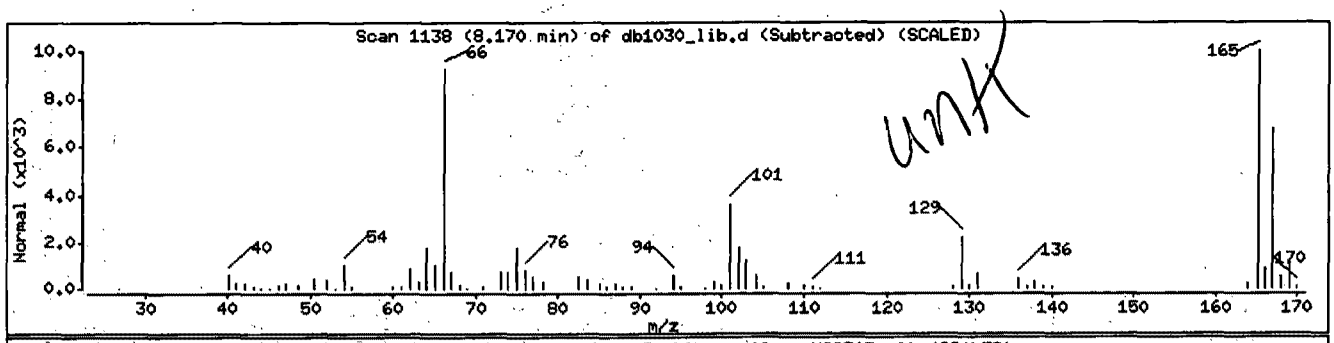
Client ID: H4021 Instrument: HP19760.i

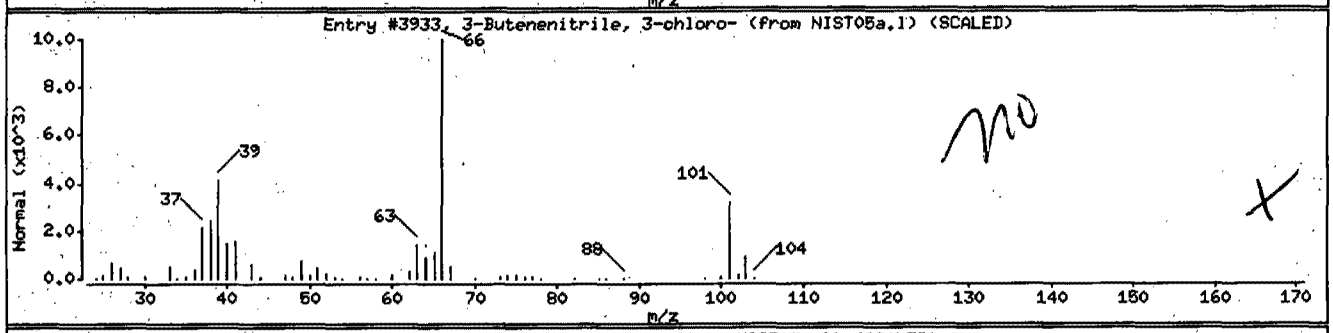
Sample Info: H4021;7370727;1;0;SAMPLE;;;

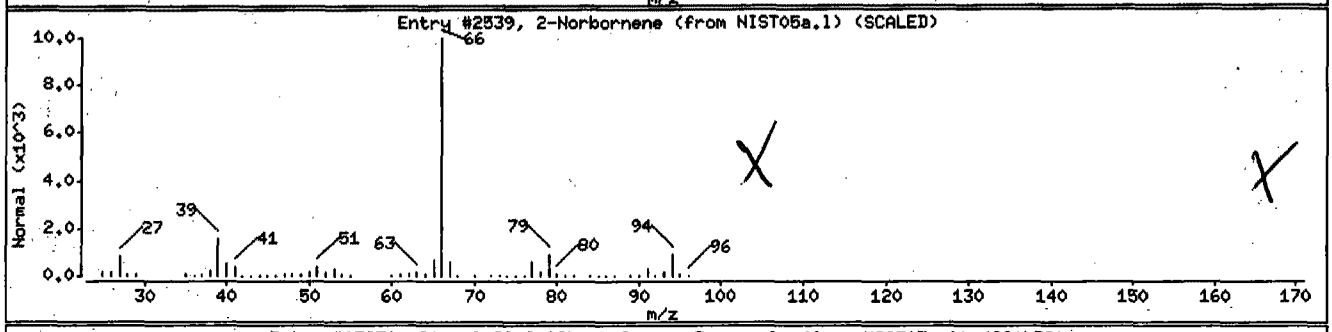
Volume Injected (uL): 1.0 Operator: ceb05247

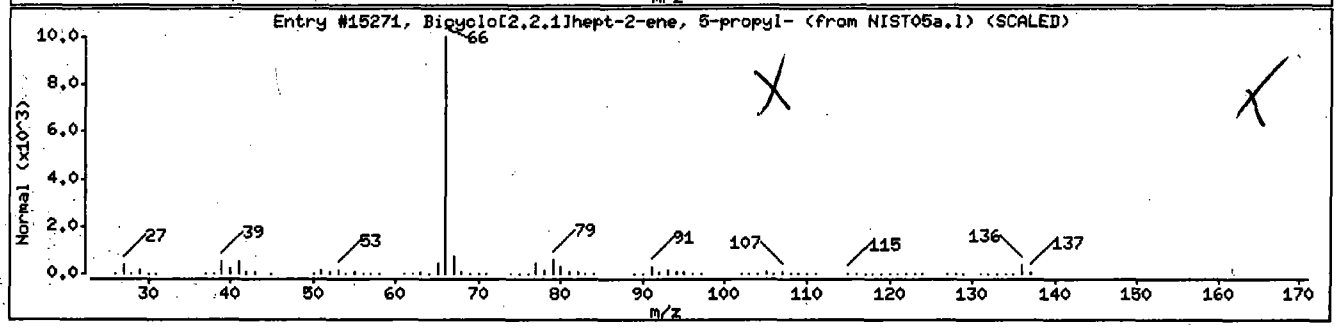
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
2-Norbornene	498-66-8	NIST05a.l	2539	49	C7H10	94
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16.	136









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb23.b/db1030_lib.d

Date : 23-FEB-2014 21:24

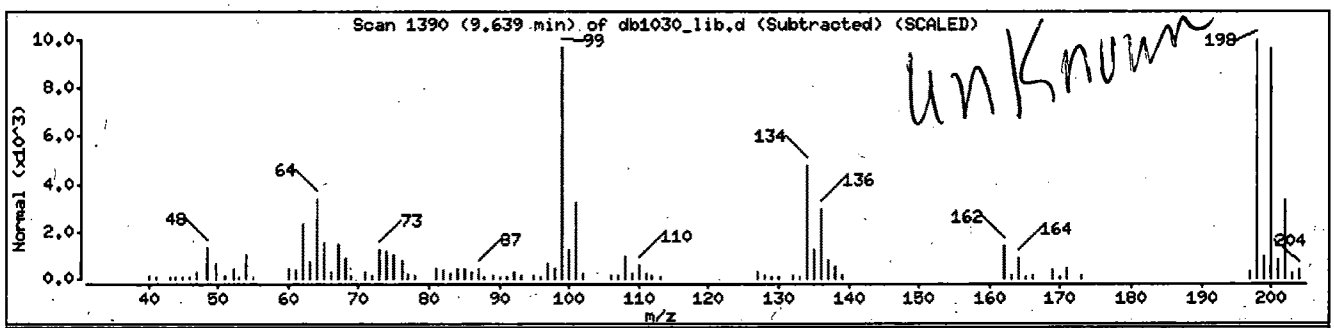
Client ID: H4021 | Instrument: HP19760.i

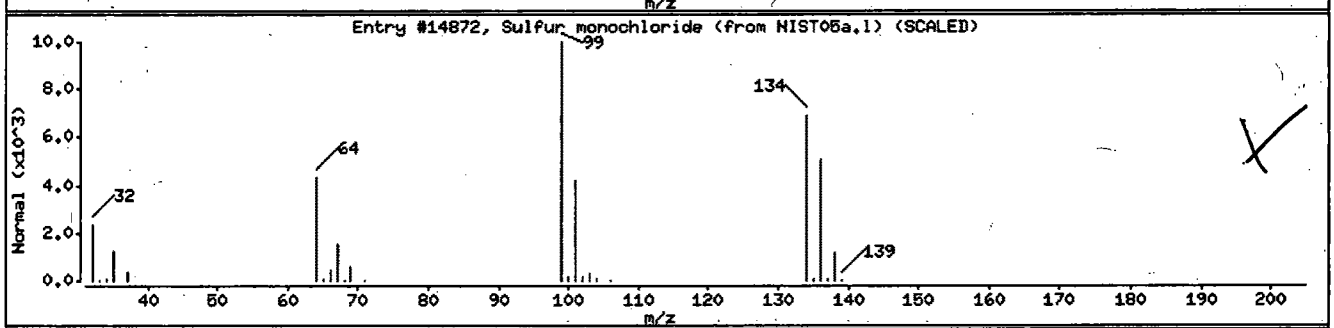
Sample Info: H4021;7370727;1;0;SAMPLE;;;

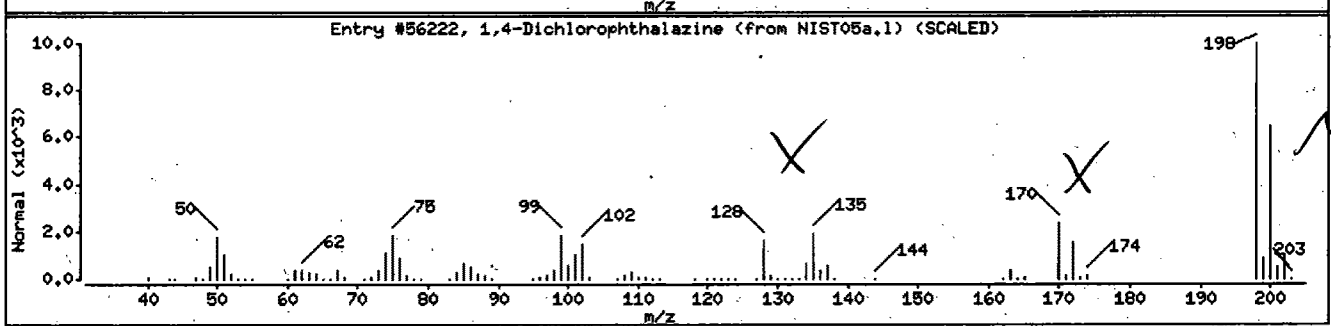
Volume Injected (uL): 1.0 | Operator: ceb05247

Column phase: J&W DB-5MS | Column diameter: 0.18

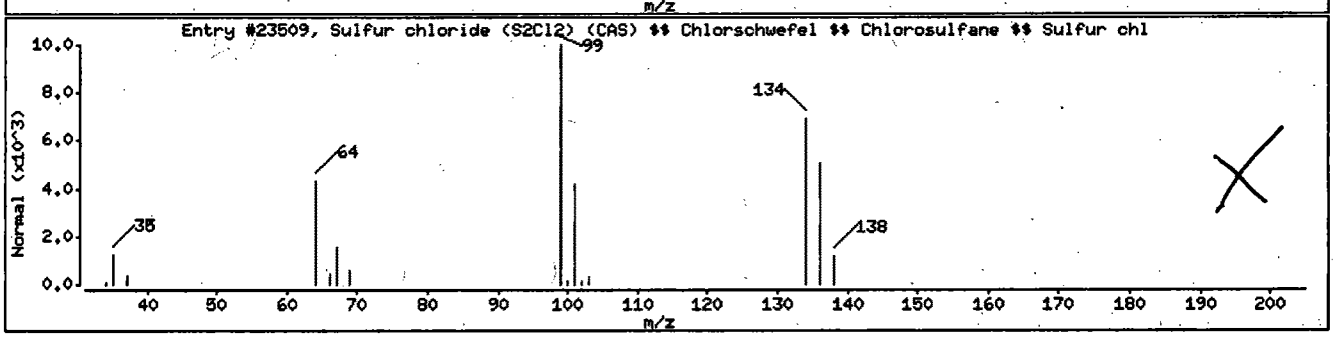
Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	C12S2	134
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	38	C8H4C12N2	198
Sulfur chloride (S2Cl2) (CAS) $$ Chlorso	10025-67-9	WILEY275.l	23509	38	C12S2	134





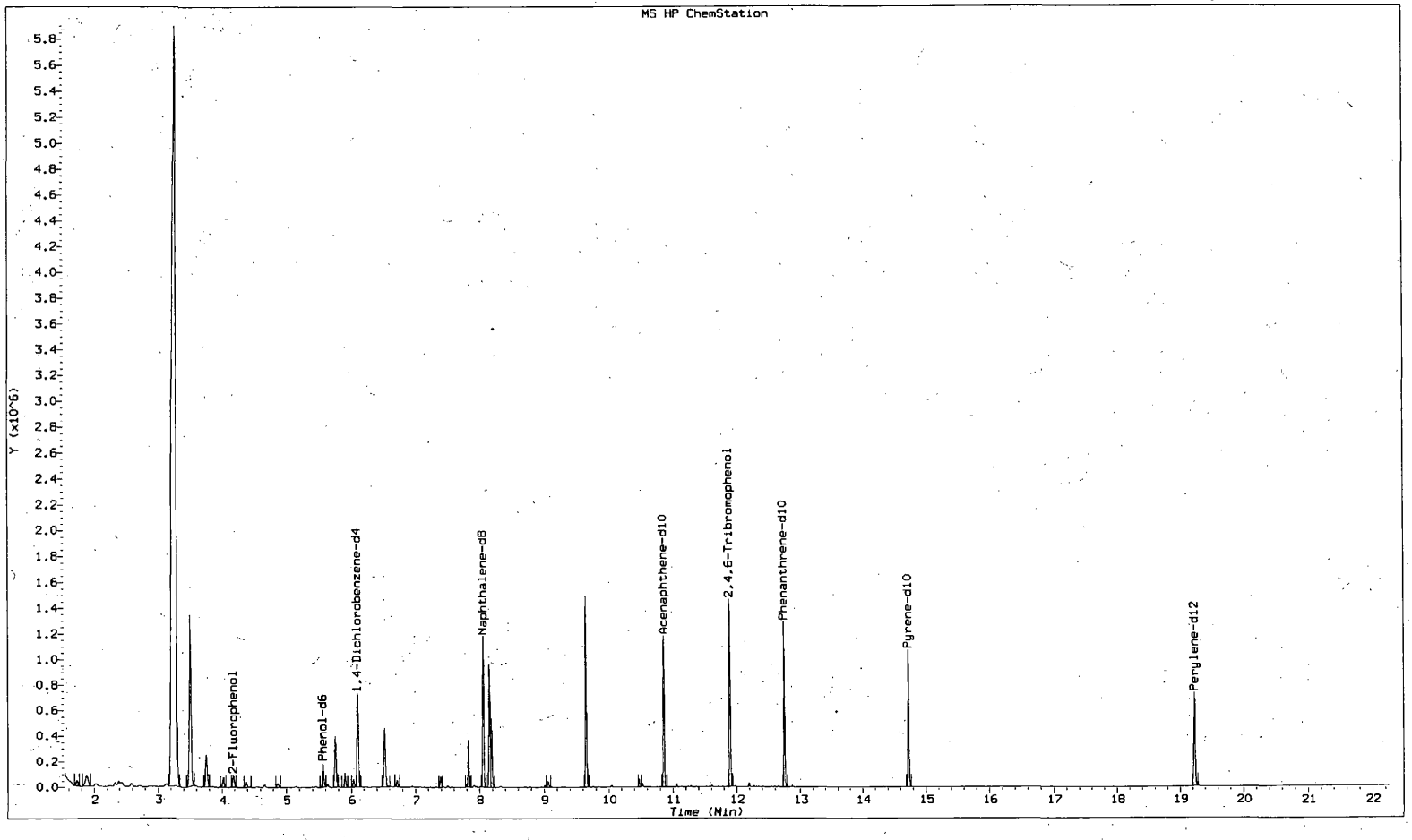


ratio off



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:01.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb21.b/db0975_lib.d
Operator : jmg00346
Acquired : 21-FEB-2014 16:44
Instrument : HP19760.i
Sample Name: H5011;7366665;1;0;SAMPLE;;;
Misc Info : 14050WAC;WL13166;;1051;1000;0;db0952;13166;
Vial Number: 26



Lancaster Labs

Data file : /chem/HP19760.i/14feb21.b/db0975_lib.d
Lab Smp Id: 7366665 Client Smp ID: H5011
Inj Date : 21-FEB-2014 16:44
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H5011;7366665;1;0;SAMPLE;;;
Misc Info : 14050WAC;WL13166;;1051;1000;0;db0952;13166;
Comment : Max. number of TICs to report is 50, 20 TICs were found initially.
Method : /chem/HP19760.i/14feb21.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 13:10 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 26
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1051.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.107	1057146	10.000
* 48 Naphthalene-d8	8.059	1547480	10.000
* 83 Acenaphthene-d10	10.863	1395333	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.729	81871	0.77445266	0.73687	90	NIST05a.l	31323	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.881	270957	2.56310221	2.43872	92	NIST05a.l	4733	21(L)
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.285	24224804	229.152839	218.03314	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.507	2583967	24.4428598	23.25676	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.758	475715	4.49999221	4.28162	38	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.020	135819	1.28476984	1.22242	28	NIST05a.l	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.381	81634	0.77220929	0.73473	74	NIST05a.l	33655	21
Ethane, 1,1,2,2-tetrachloro-					CAS #: 79-34-5		
4.865	52354	0.49523828	0.47120	94	NIST05a.l	33584	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.757	570038	5.39223745	5.13057	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.903	168572	1.59459408	1.51721	95	NIST05a.l	18488	21
Diethylamine, 2,2'-dichloro-					CAS #: 334-22-5		
6.037	85858	0.81216622	0.77275	38	NIST05a.l	18177	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.520	740338	7.00317497	6.66334	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.713	81199	0.76809933	0.73082	53	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.395	95947	0.62002333	0.58993	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	458467	2.96266800	2.81890	43	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.152	1133635	7.32568257	6.97020	86	NIST05a.l	43383	48

Target compound.
Do not Report.
ajs00193 03/02/2014

Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	665173	4.29842649	4.08984	40	NIST05a.1	3933	48(L)
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc					CAS #: 63506-25-2		
9.062	66585	0.43027905	0.40939	80	WILEY275.1	109601	48(L)
Sulfur monochloride					CAS #: 10025-67-9		
9.656	1798008	12.8858617	12.26057	27	NIST05a.1	14872	83(L)
2-bromo-7,7-dichlorocyclo[4.1.0]heptan					CAS #: 113035-97-5		
10.478	65846	0.47190113	0.44900	91	WILEY275.1	127158	83

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

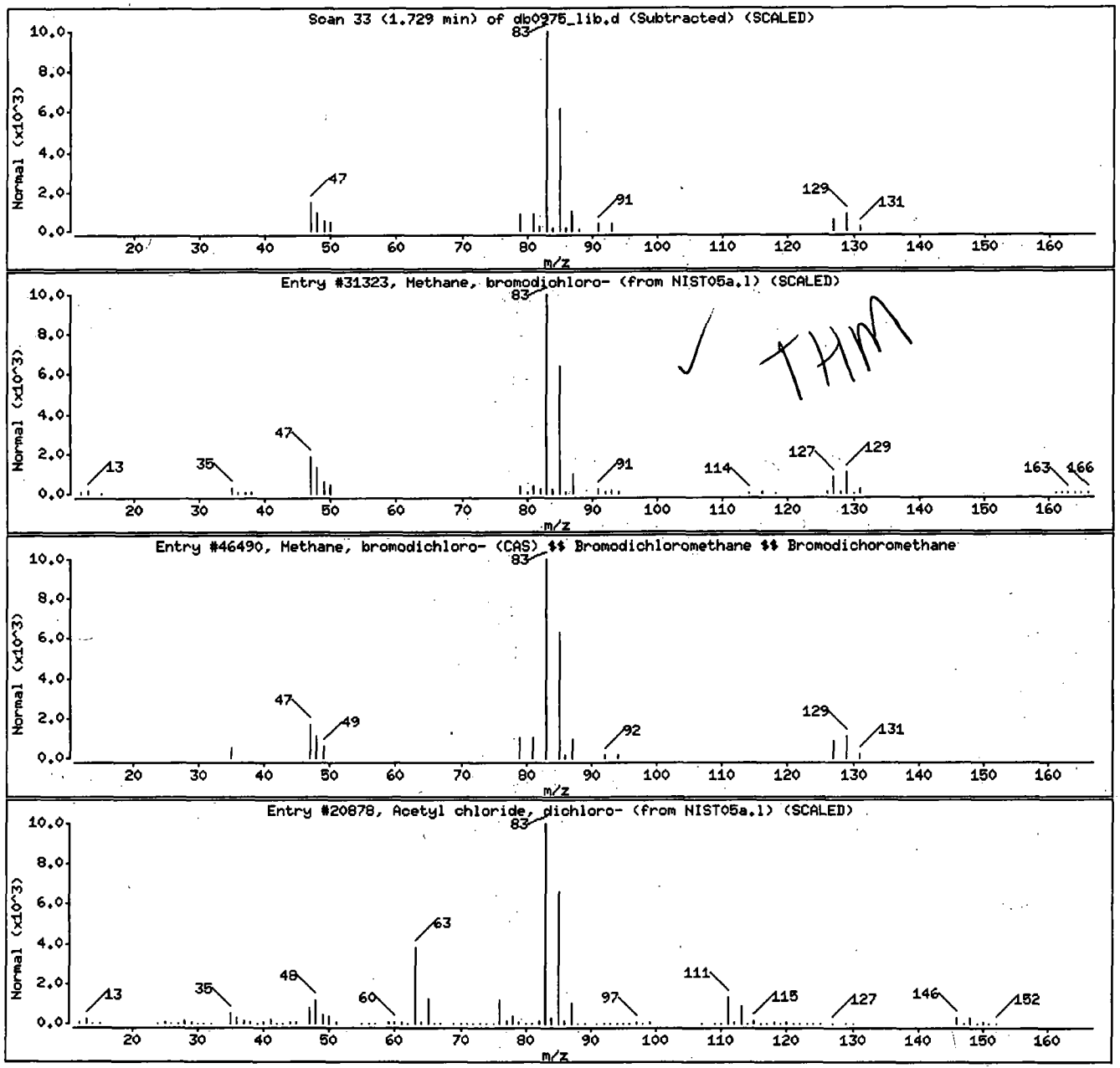
Client ID: H5011 Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Acetyl chloride, dichloro-	79-36-7	NIST05a.l	20878	78	C2HCl3O	146



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

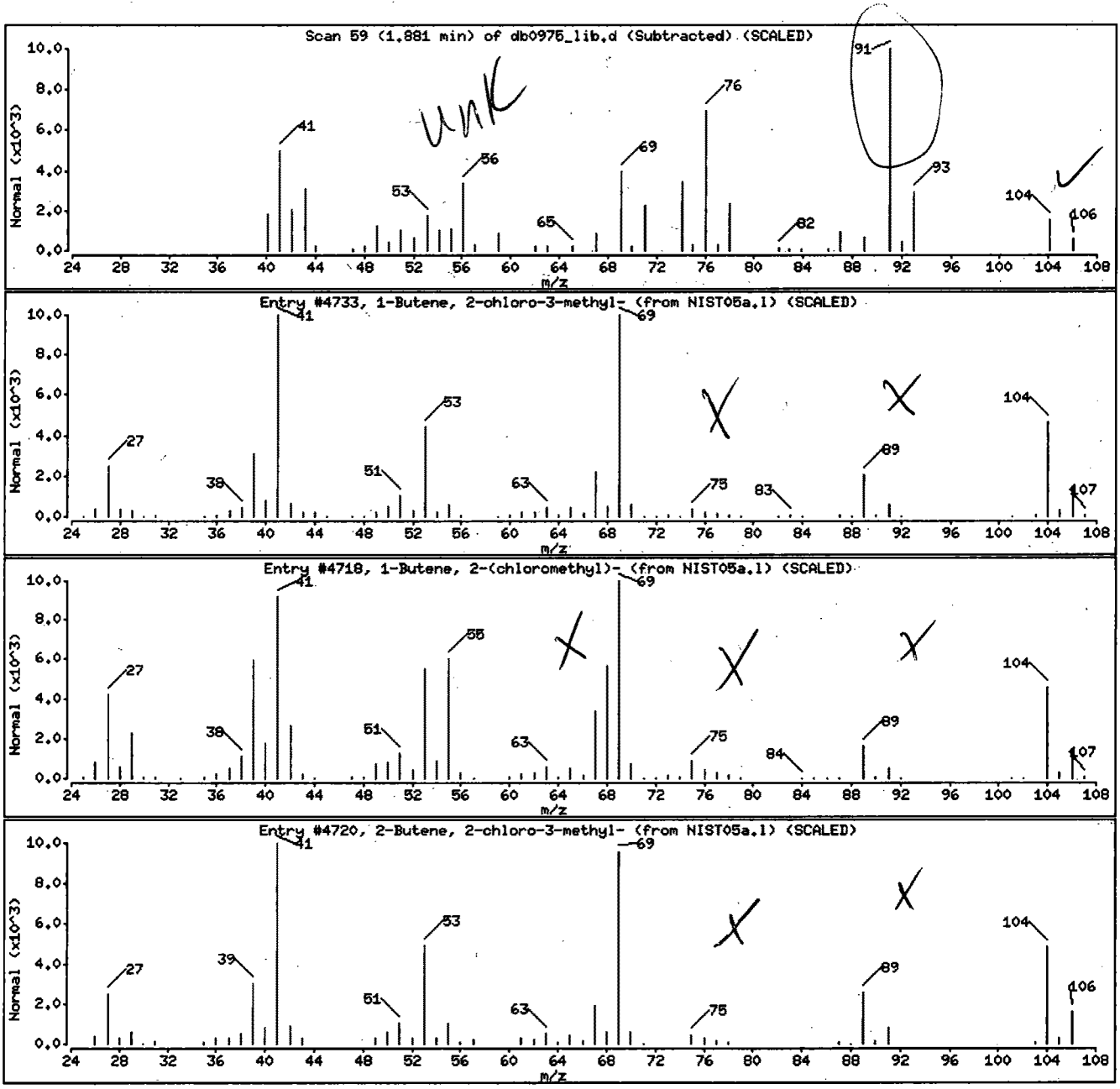
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	92	C5H9Cl	104
1-Butene, 2-(chloromethyl)-	23010-02-8	NIST05a.l	4718	76	C5H9Cl	104
2-Butene, 2-chloro-3-methyl-	17773-65-8	NIST05a.l	4720	70	C5H9Cl	104



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

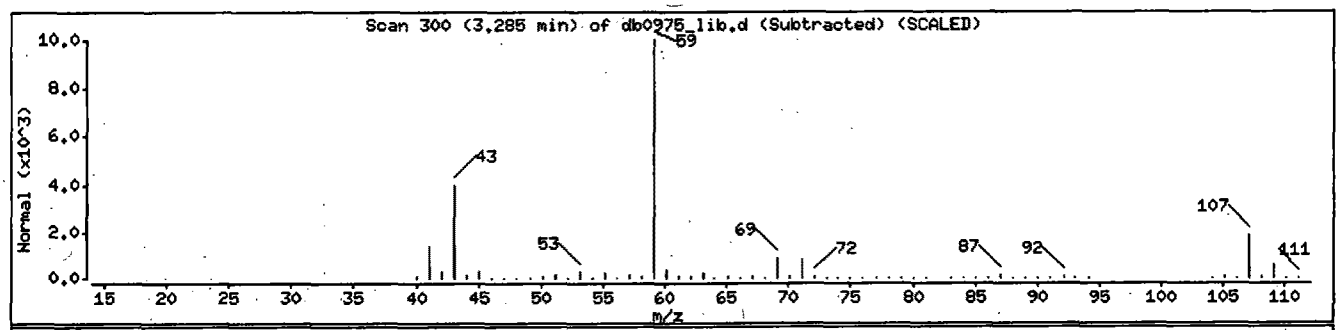
Volume Injected (uL): 1.0

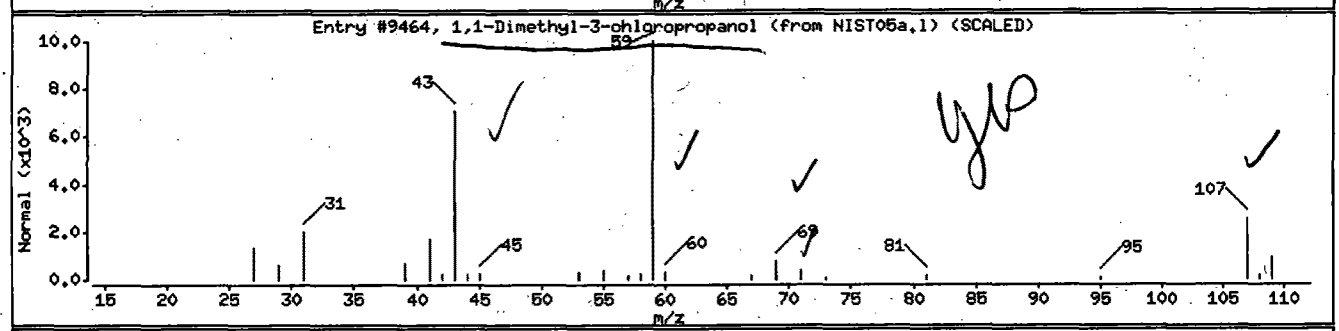
Operator: jmg00346

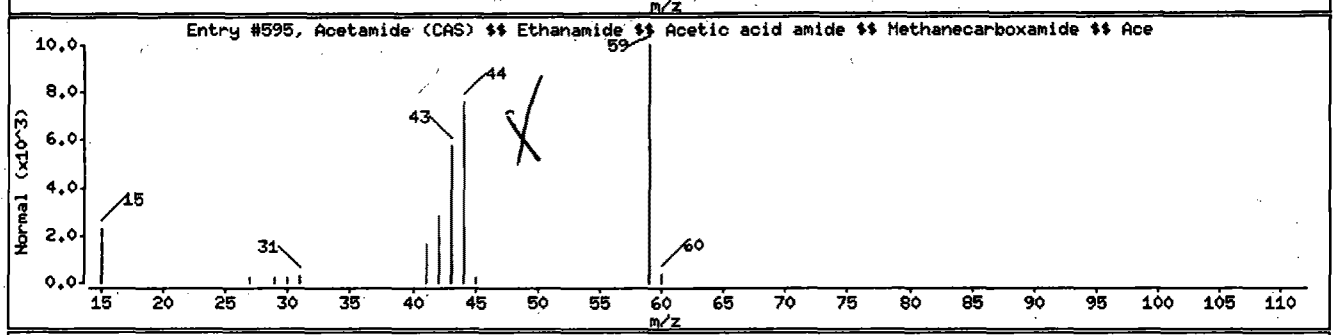
Column phase: J&W DB-5MS

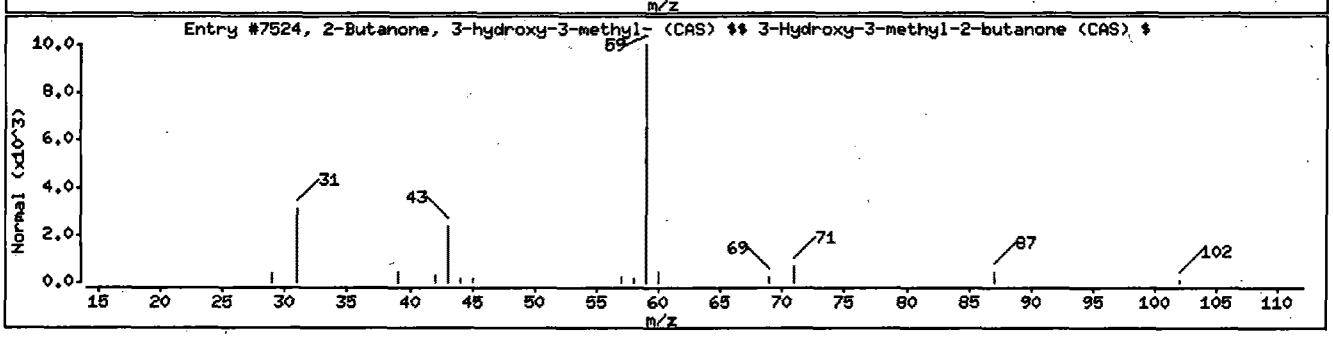
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

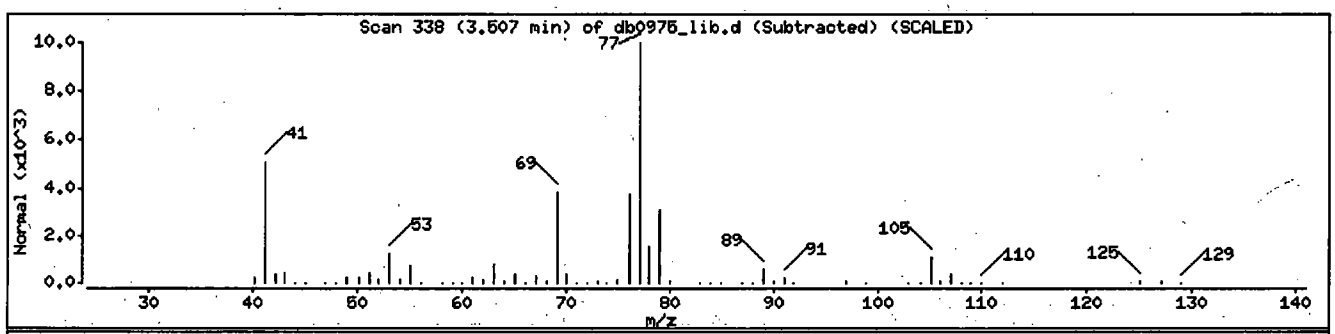
Volume Injected (uL): 1.0

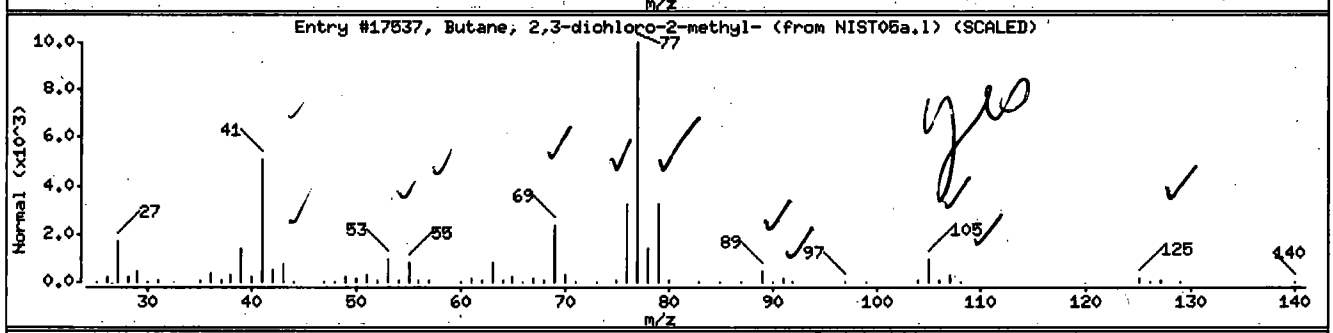
Operator: jmg00346

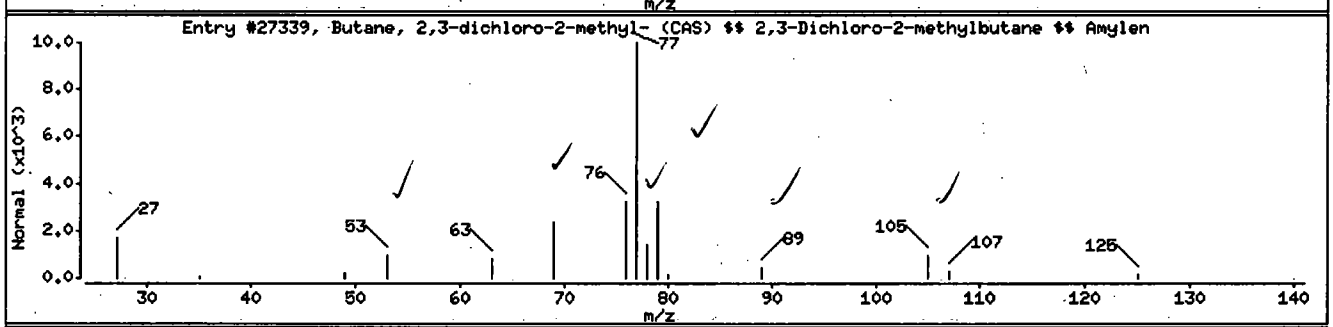
Column phase: J&W DB-5MS

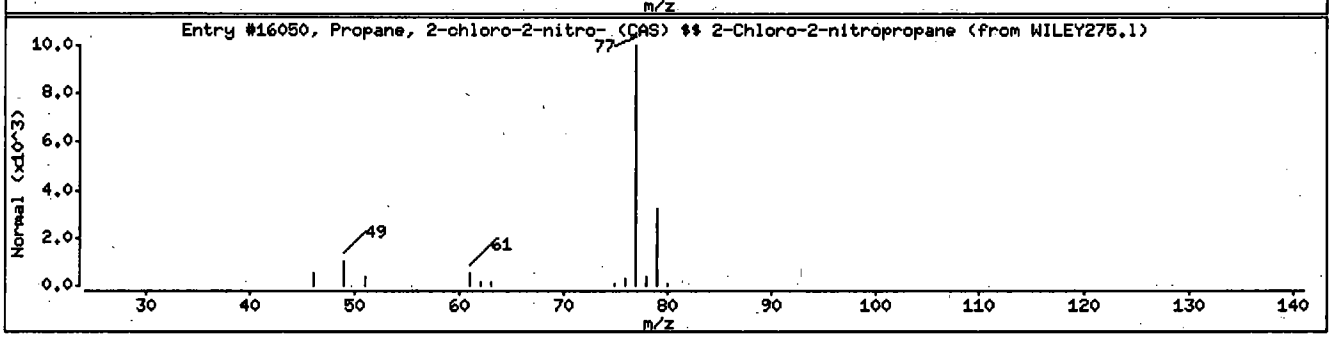
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	74	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









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Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

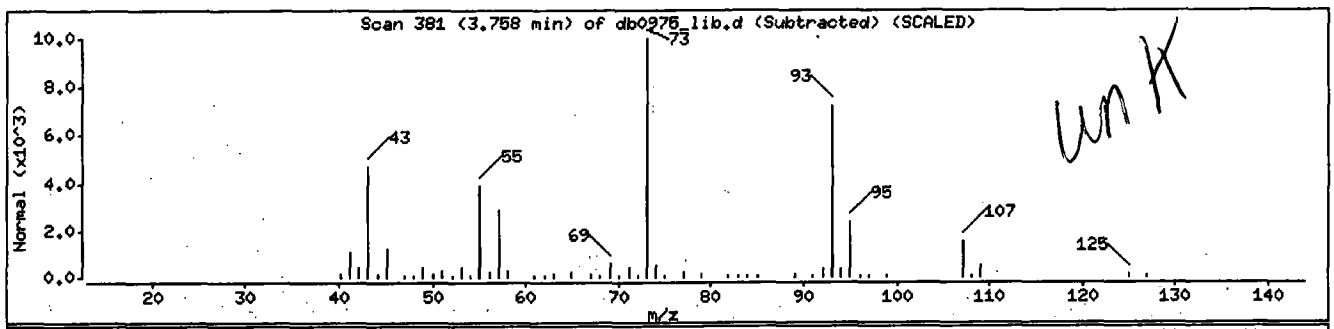
Volume Injected (uL): 1.0

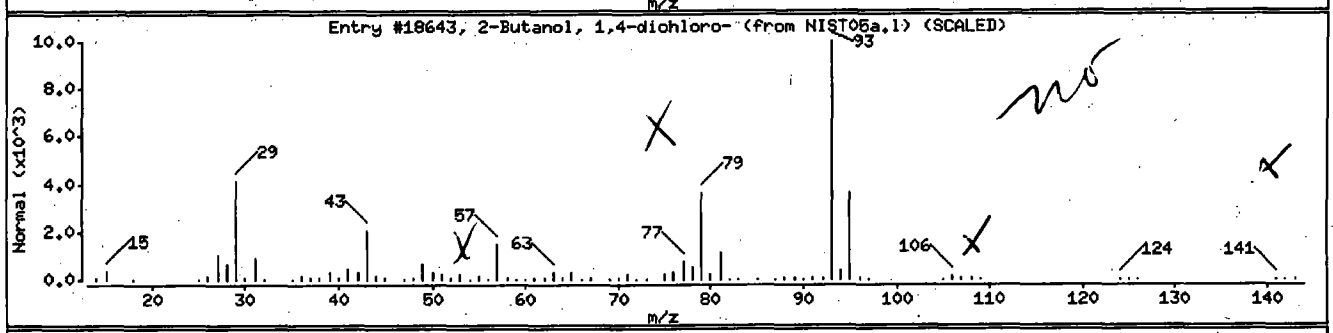
Operator: jmg00346

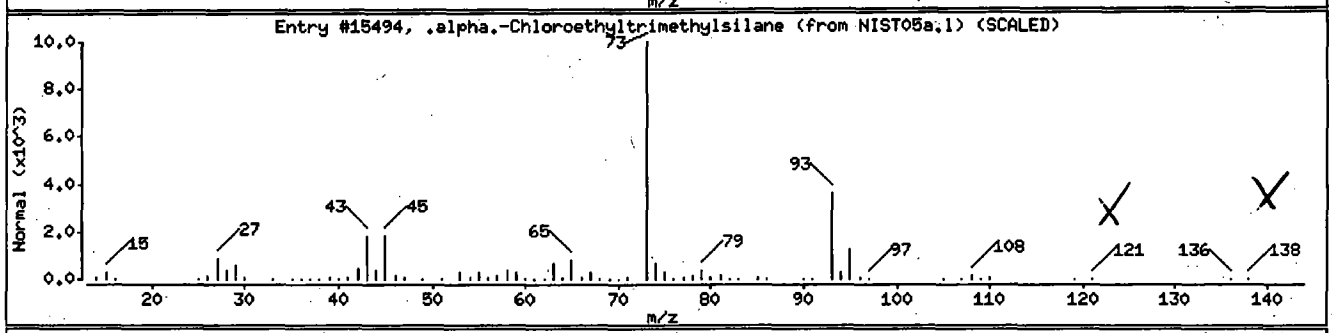
Column phase: J&W DB-5MS

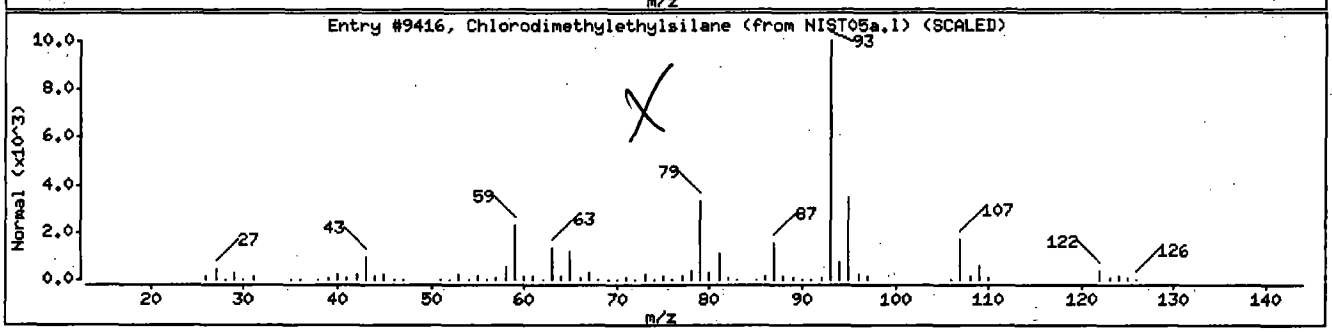
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	38	C4H8Cl2O	142
.alpha.-Chloroethyltrimethylsilane	7787-87-3	NIST05a.l	15494	33	C5H13ClSi	136
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122









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Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

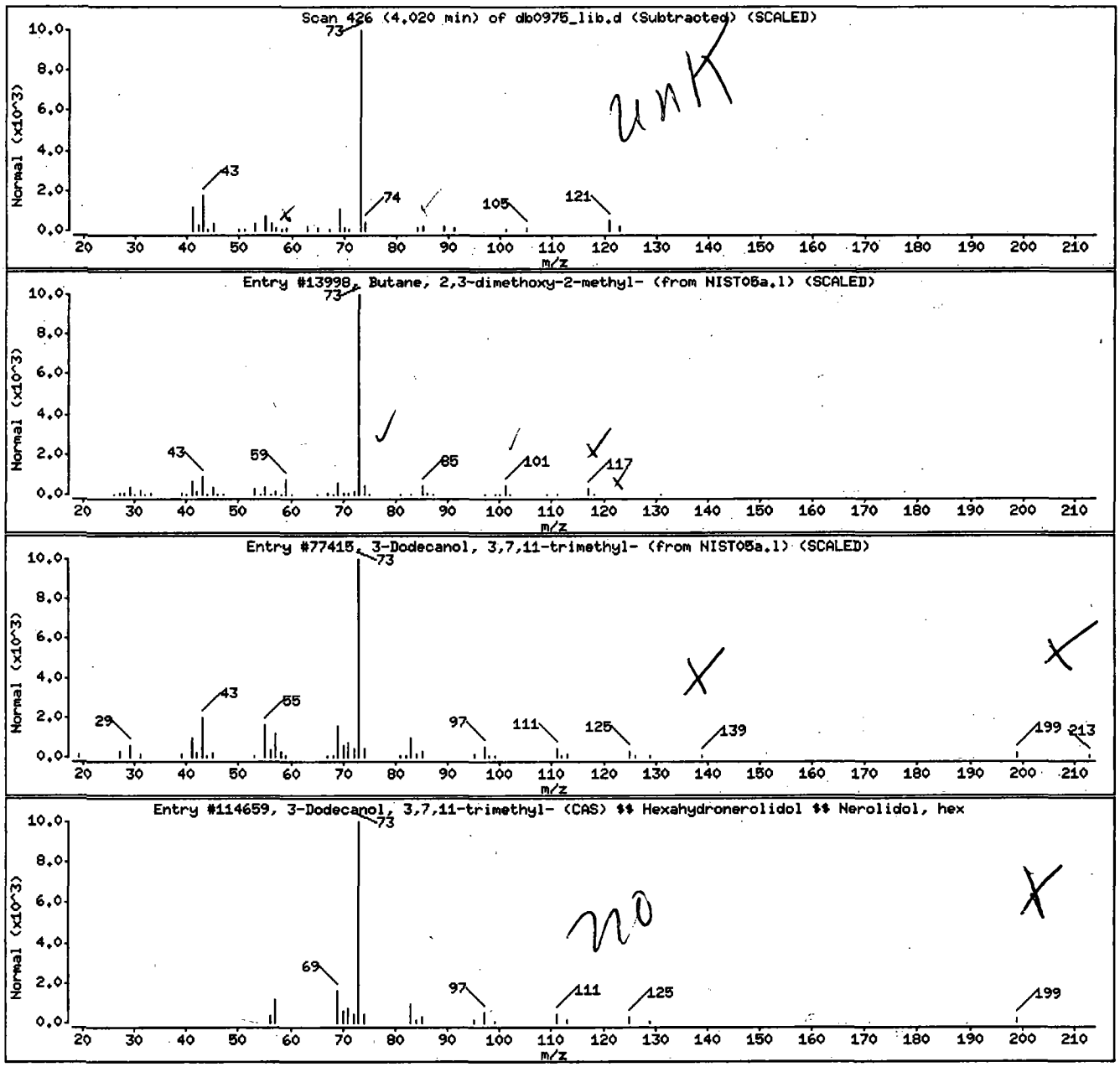
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	28	C7H16O2	132
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	38	C15H32O	228
3-Dodecanol, 3,7,11-trimethyl- (CAS) $$	7278-65-1	WILEY275.l	114659	38	C15H32O	228



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Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

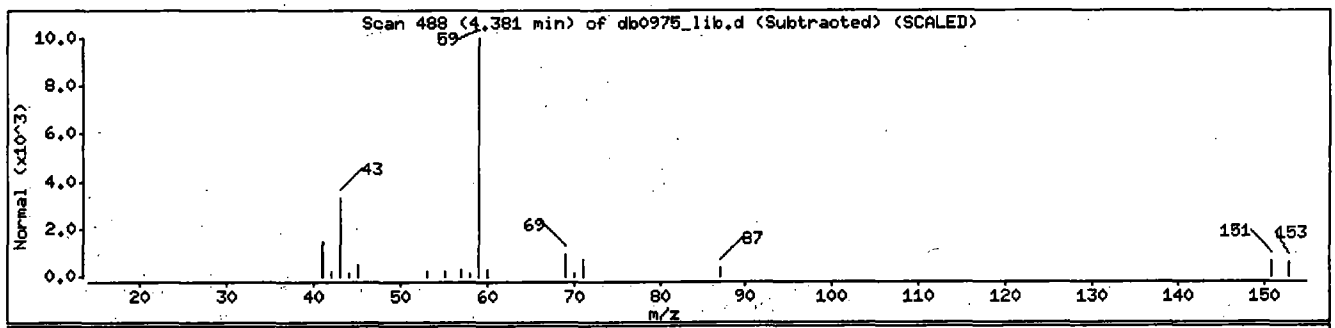
Volume Injected (uL): 1.0

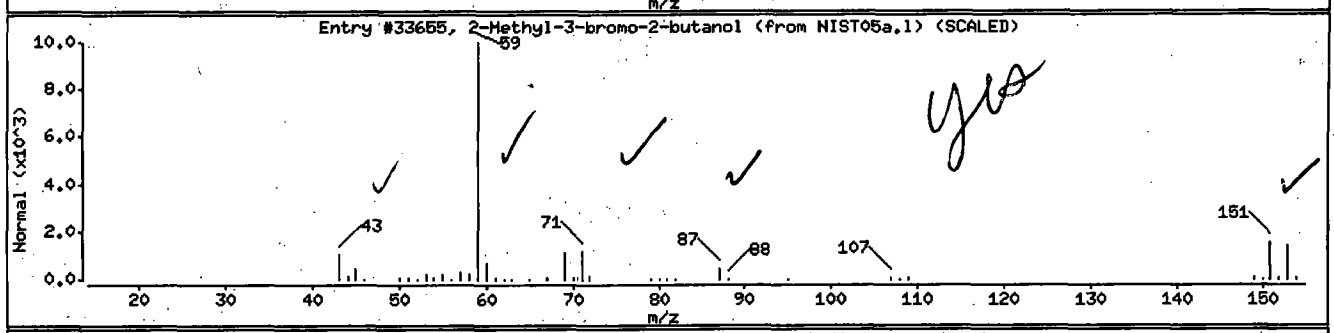
Operator: jmg00346

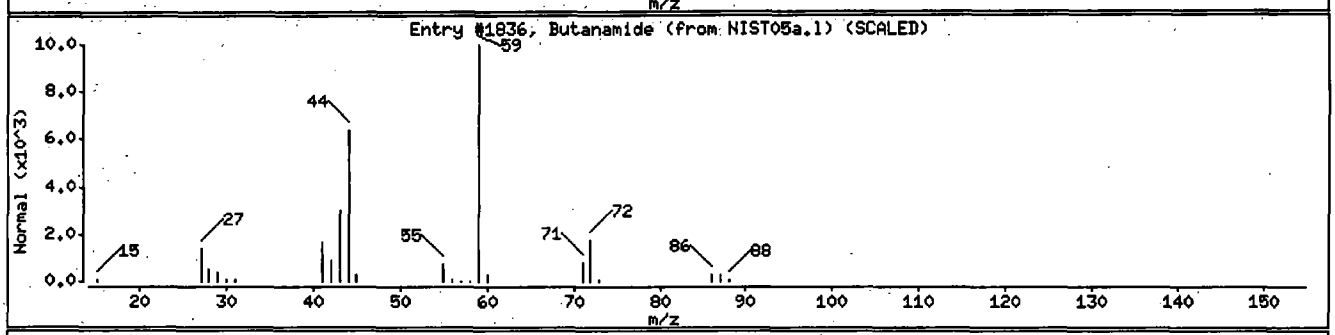
Column phase: J&W DB-5MS

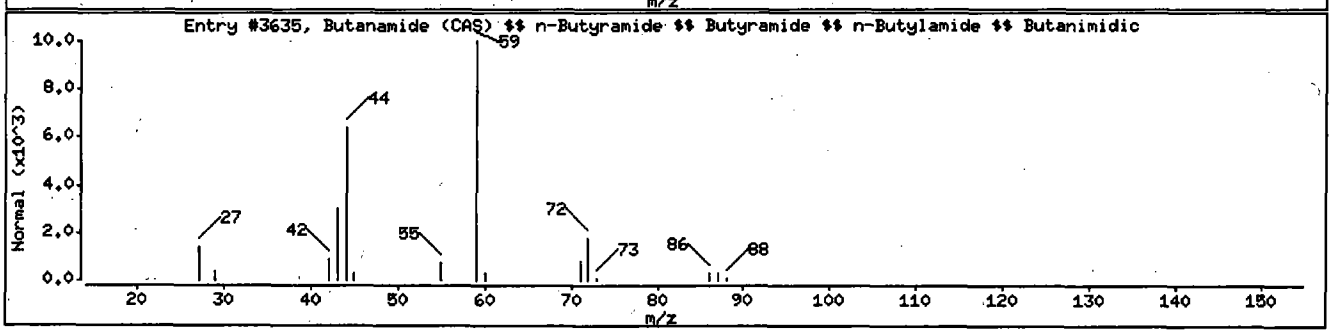
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	74	C5H11BrO	166
Butanamide	541-35-5	NIST05a.l	1836	64	C4H9NO	87
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3635	64	C4H9NO	87









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

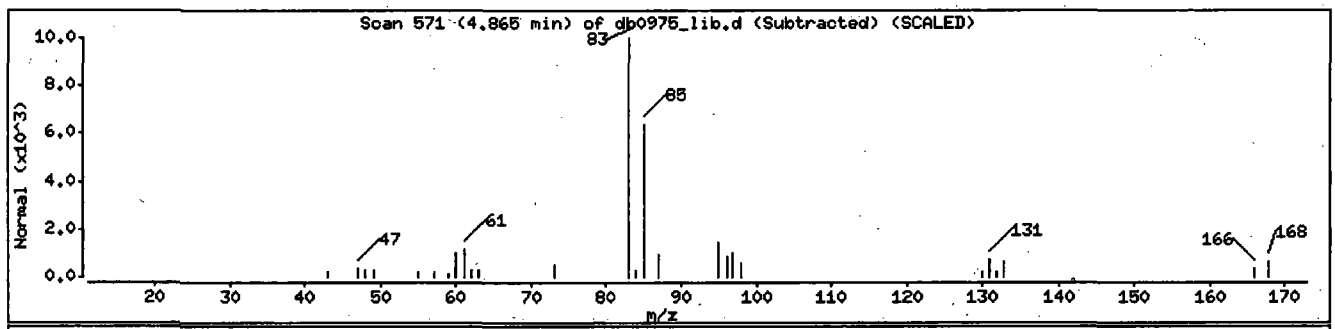
Volume Injected (uL): 1.0

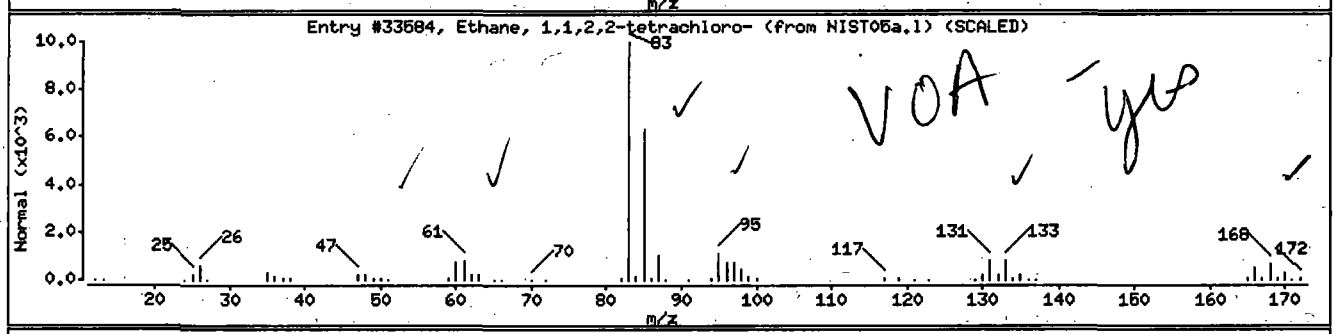
Operator: jmg00346

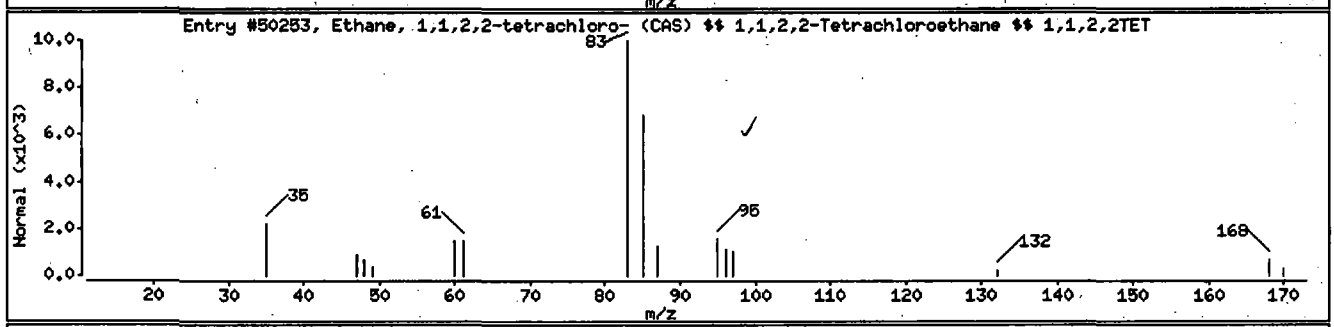
Column phase: J&W DB-5MS

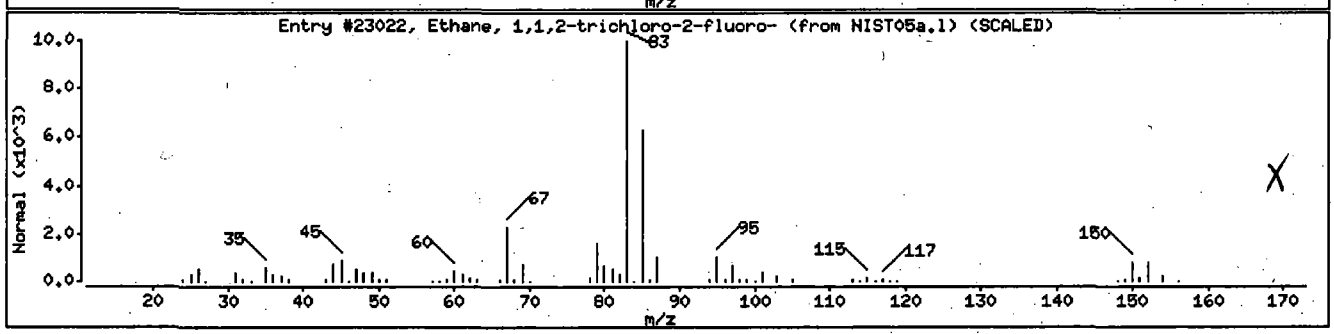
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Ethane, 1,1,2,2-tetrachloro-	79-34-5	NIST05a.l	33684	94	C2H2Cl4	166
Ethane, 1,1,2,2-tetrachloro- (CAS) $$ 1,	79-34-5	WILEY275.l	50253	94	C2H2Cl4	166
Ethane, 1,1,2-trichloro-2-fluoro-	359-28-4	NIST05a.l	23022	64	C2H2Cl3F	150









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Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

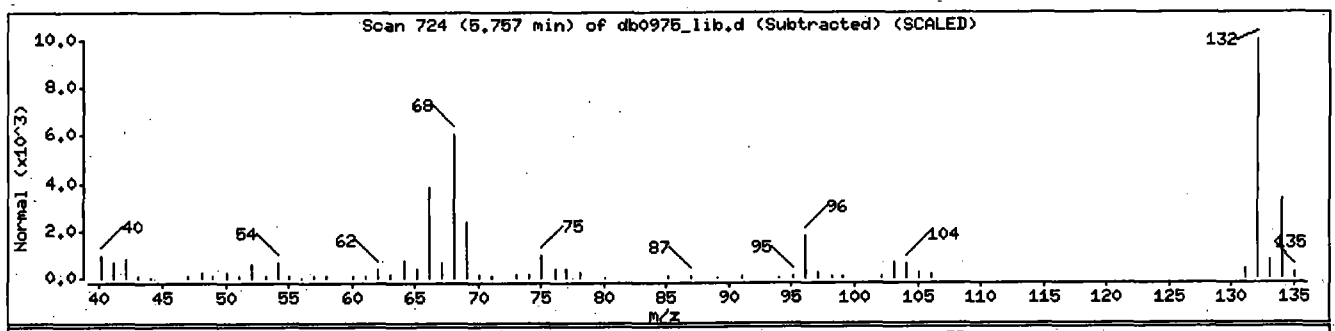
Volume Injected (uL): 1.0

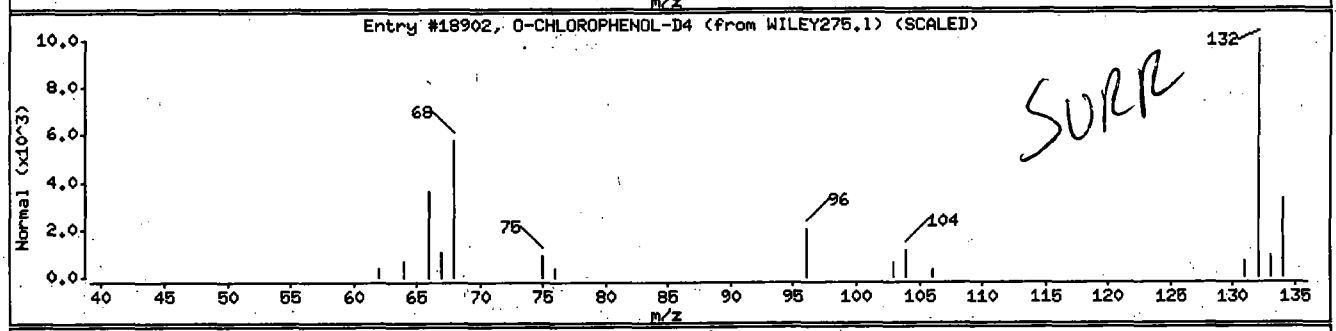
Operator: jmg00346

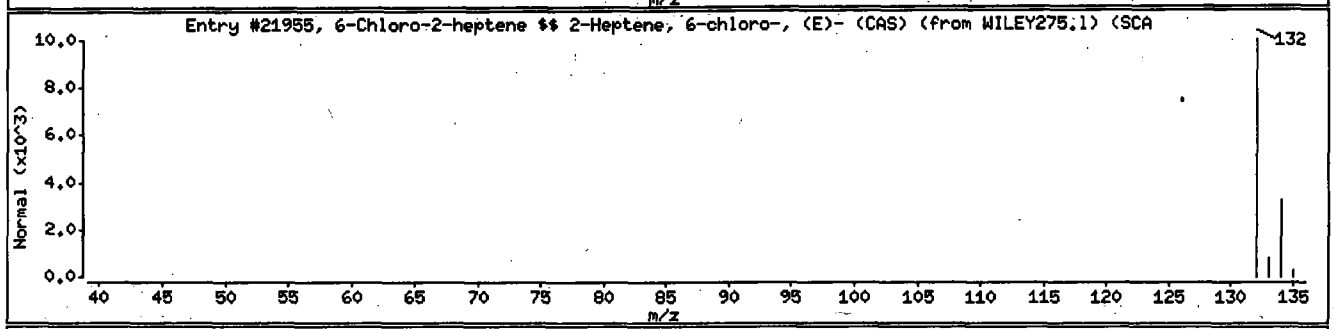
Column phase: J&W DB-5MS

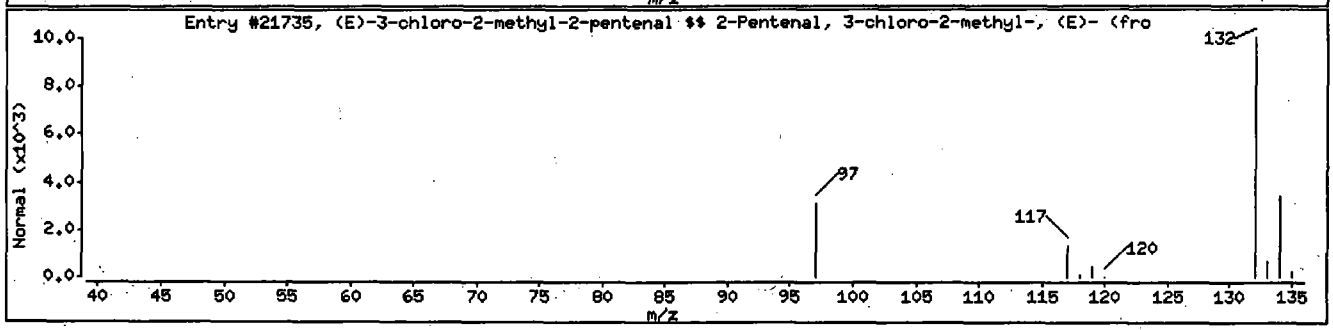
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.l	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.l	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.l	21735	72	C6H9ClO	132









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;736666;1;0;SAMPLE;;;

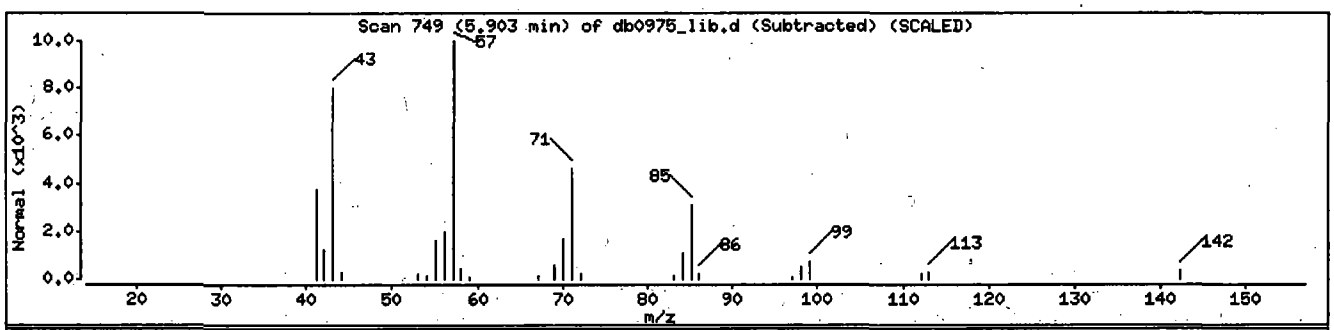
Volume Injected (uL): 1.0

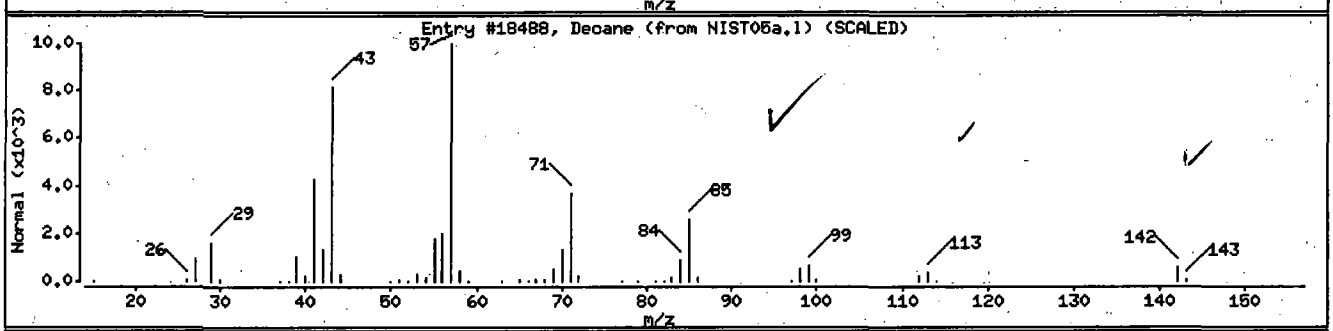
Operator: jmg00346

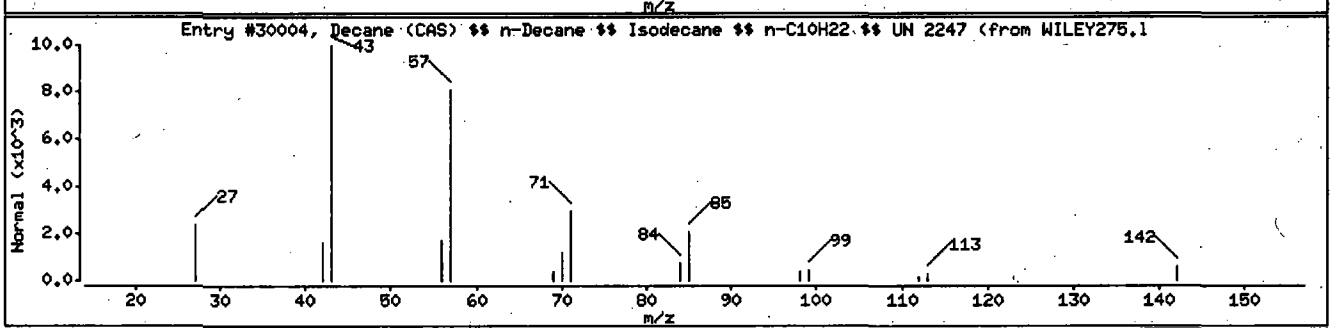
Column phase: J&W DB-5MS

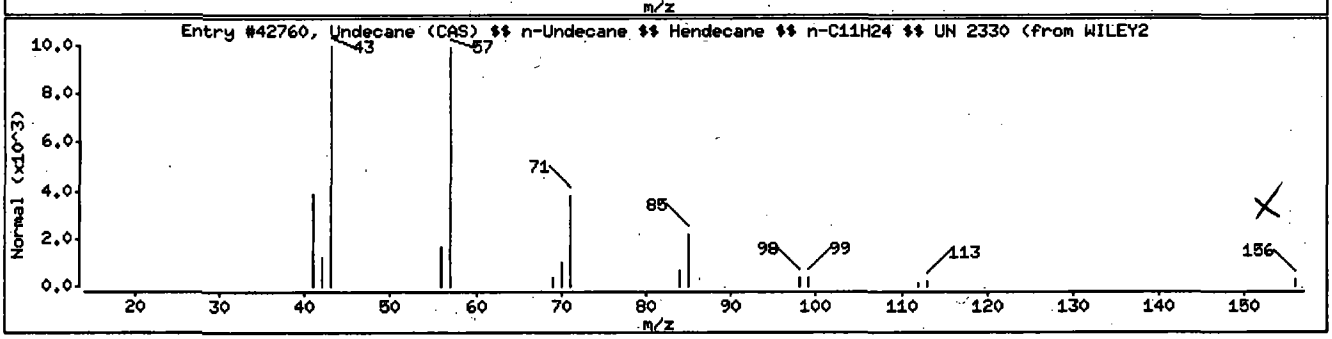
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18488	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	95	C10H22	142
Undecane (CAS) $$ n-Undecane $$ Hendecan	1120-21-4	WILEY275.l	42760	80	C11H24	156









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Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

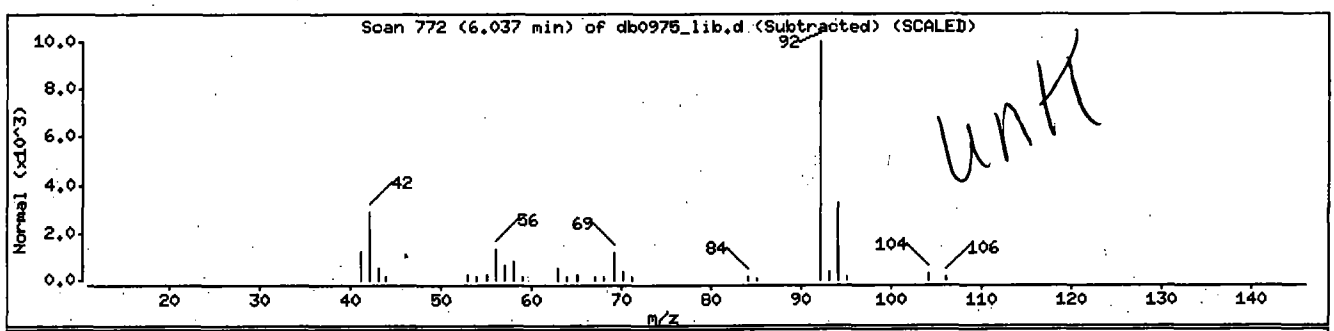
Volume Injected (uL): 1.0

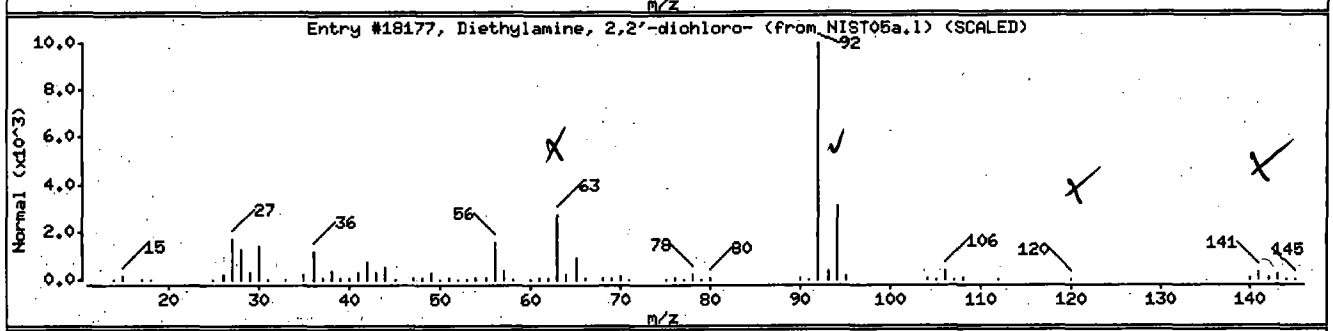
Operator: jmg00346

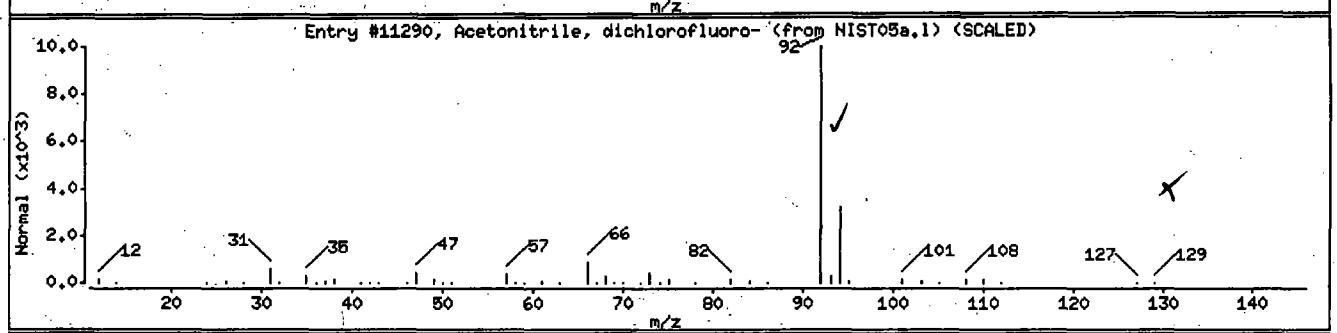
Column phase: J&W DB-5MS

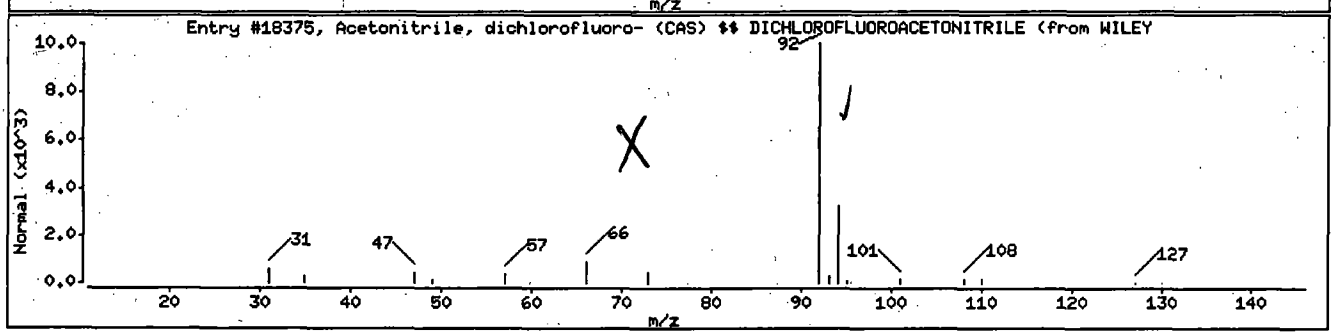
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Diethylamine, 2,2'-dichloro-	334-22-5	NIST05a.l	18177	38	C4H9Cl2N	141
Acetonitrile, dichlorofluoro-	353-82-2	NIST05a.l	11290	9	C2Cl2FN	127
Acetonitrile, dichlorofluoro- (CAS) $$ D	353-82-2	WILEY275.l	18375	9	C2Cl2FN	127









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

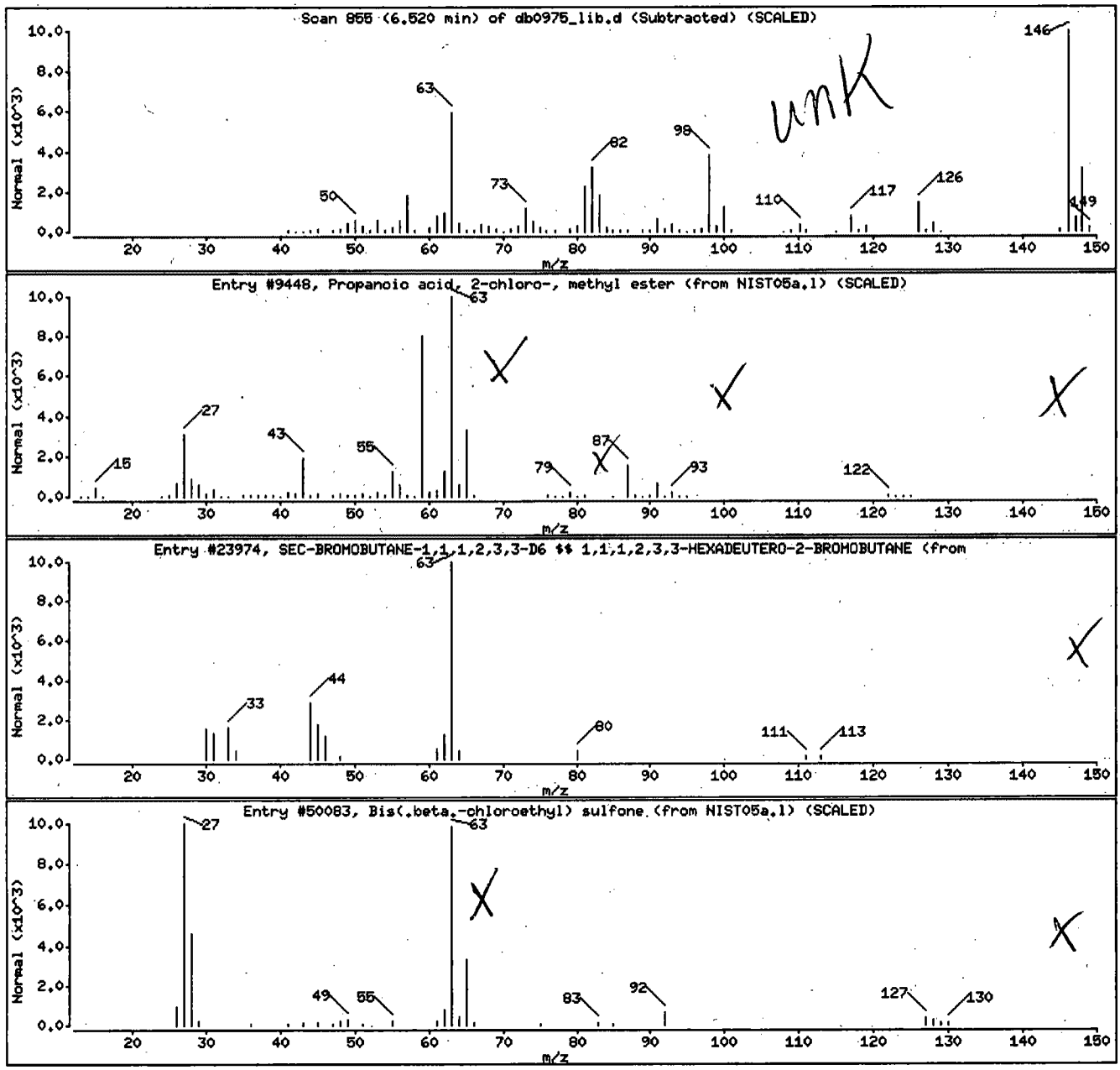
Client ID: H5011 Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 ** 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	23	C4H8Cl2O2S	190



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

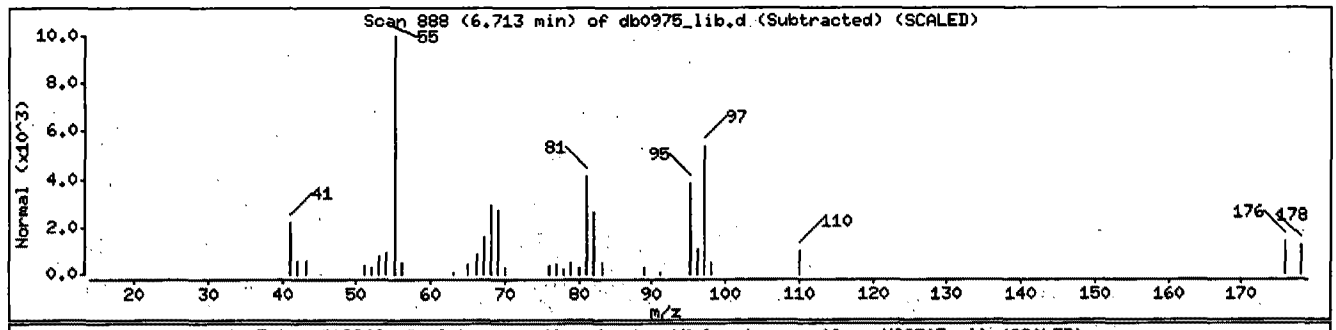
Client ID: H5011 Instrument: HP19760.i

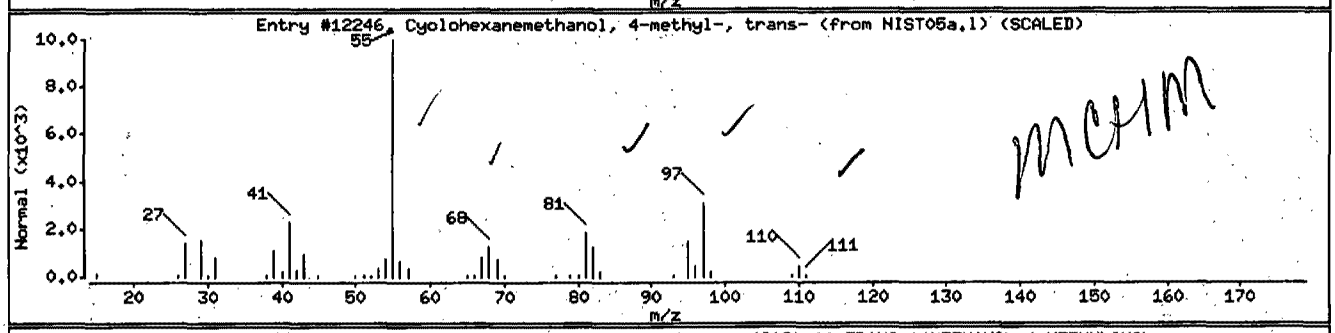
Sample Info: H5011;7366665;1;0;SAMPLE;;;

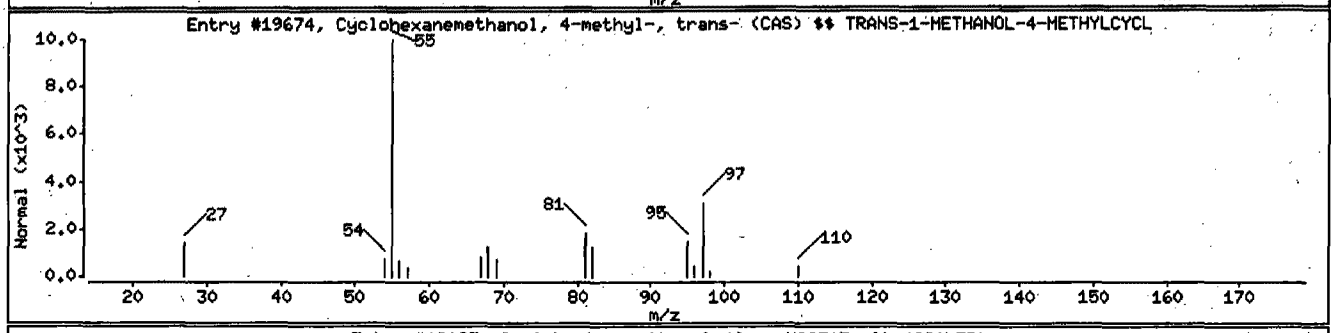
Volume Injected (uL): 1.0 Operator: jmg00346

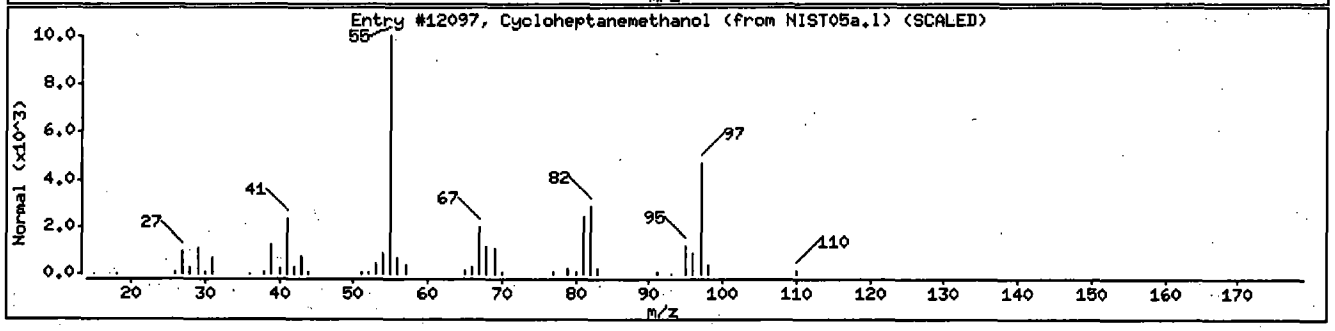
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	53	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	53	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12097	50	C8H16O	128









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

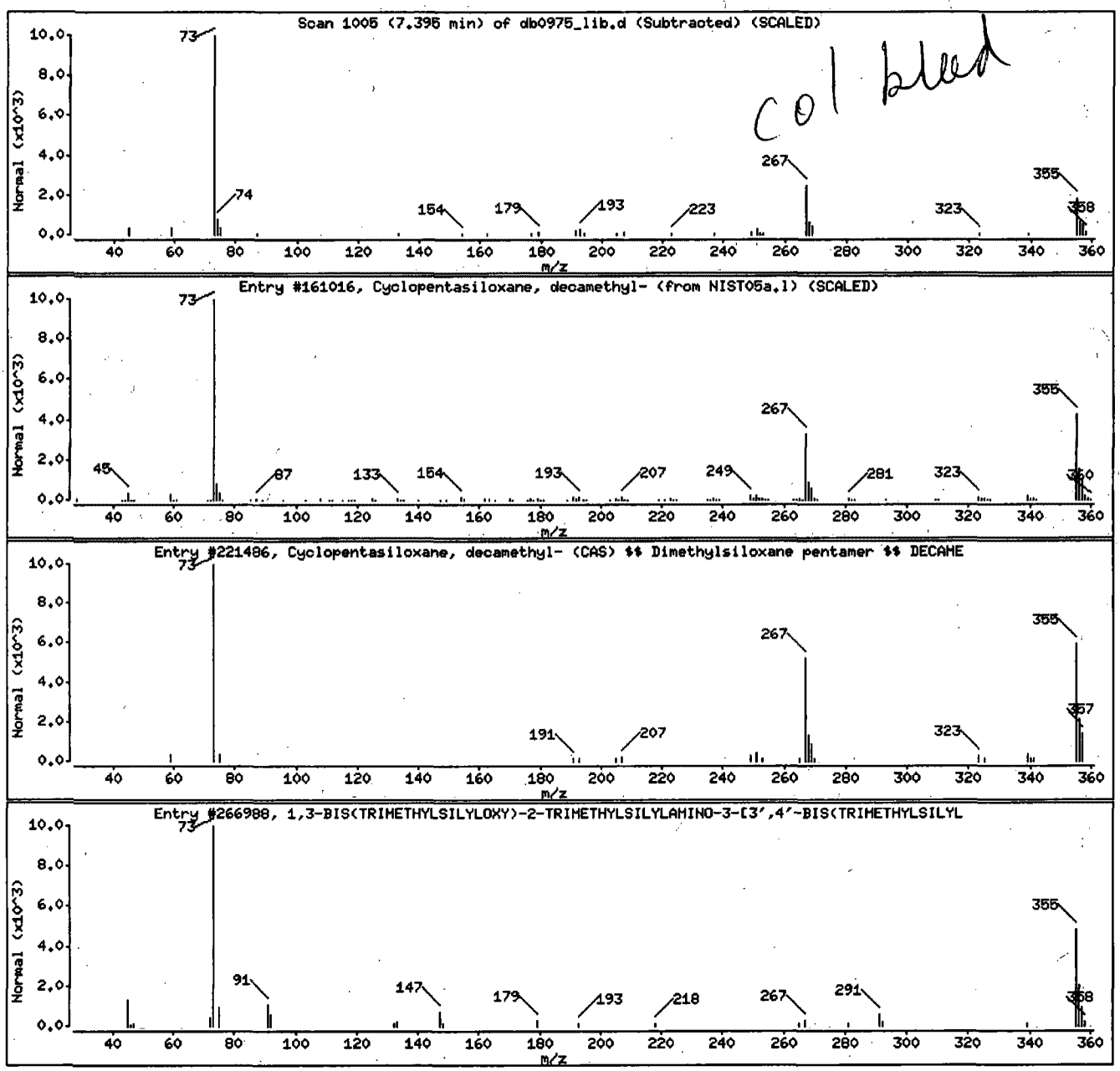
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	83	C10H30O5Si5	370
1,3-BIS(TRIMETHYLSILYLOXY)-2-TRIMETHYLSI	0-00-0	WILEY275.l	266988	43	C24H61NO6Si6	573



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

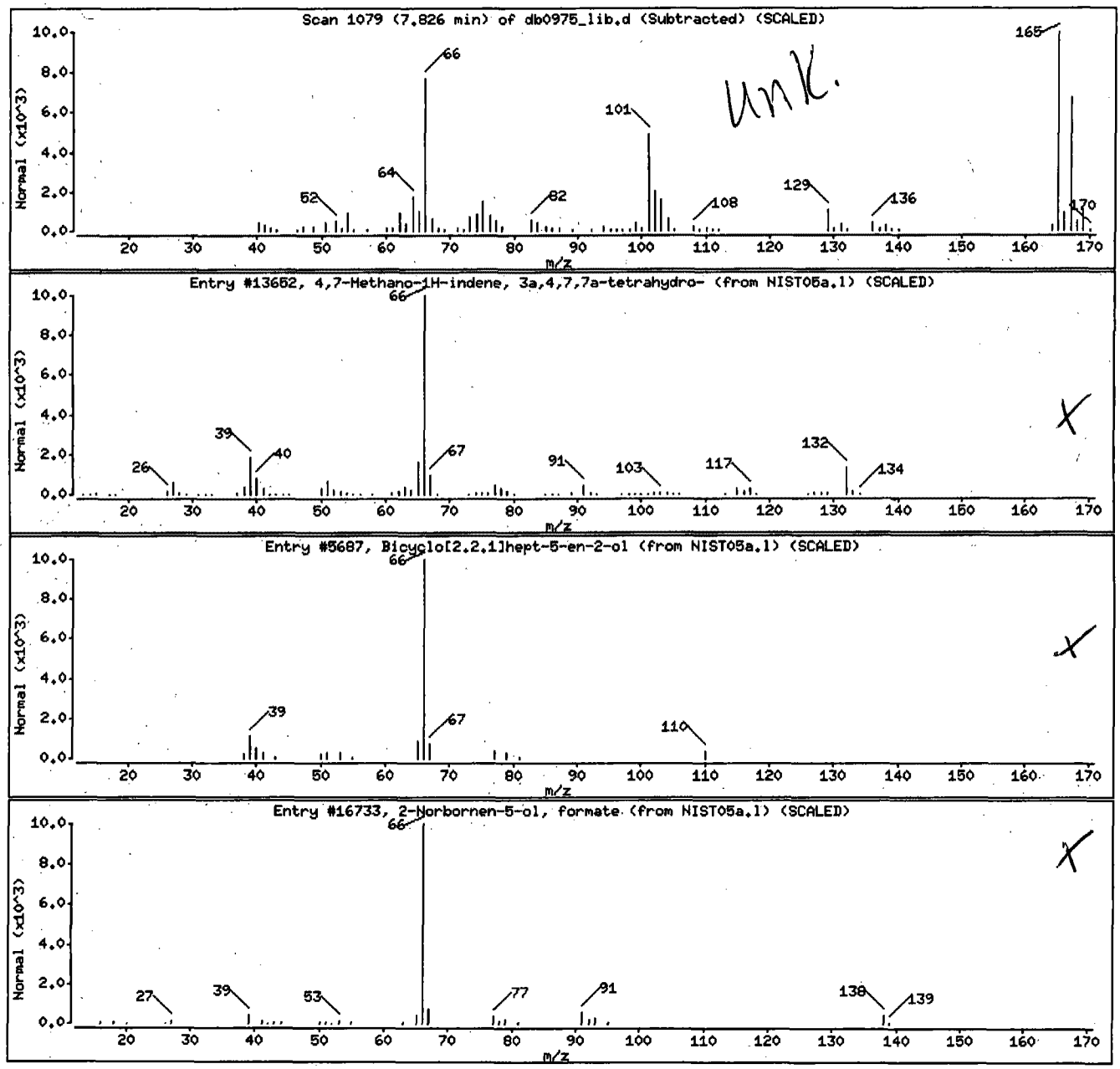
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	43	C10H12	132
Bicyclo[2.2.1]hept-5-en-2-ol	13080-90-5	NIST05a.l	5687	46	C7H10O	110
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H10O2	138



Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

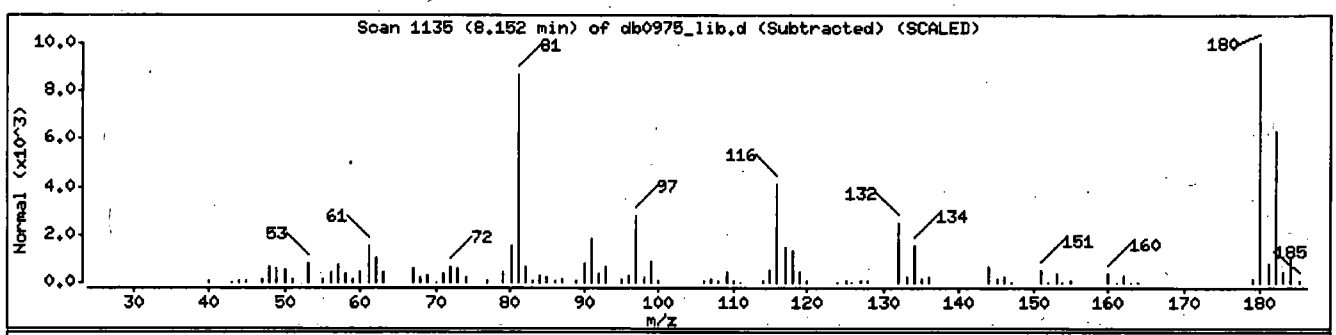
Client ID: H5011 Instrument: HP19760.i

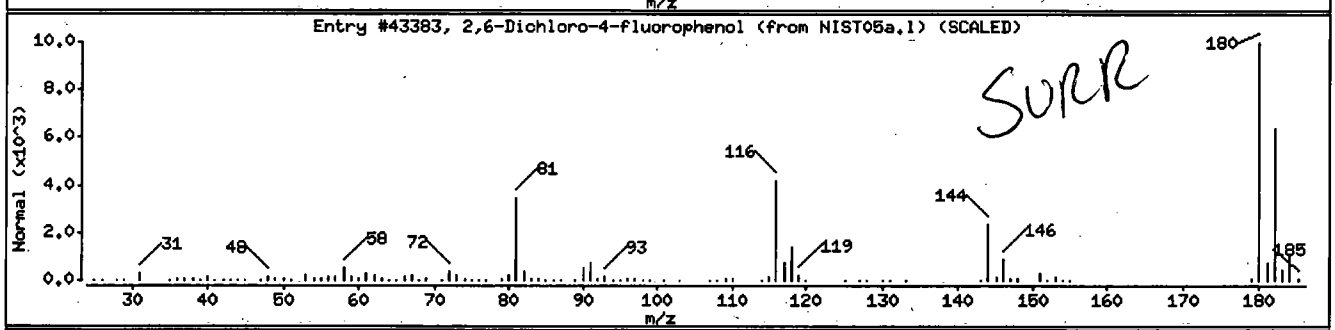
Sample Info: H5011;7366665;1;0;SAMPLE;;;

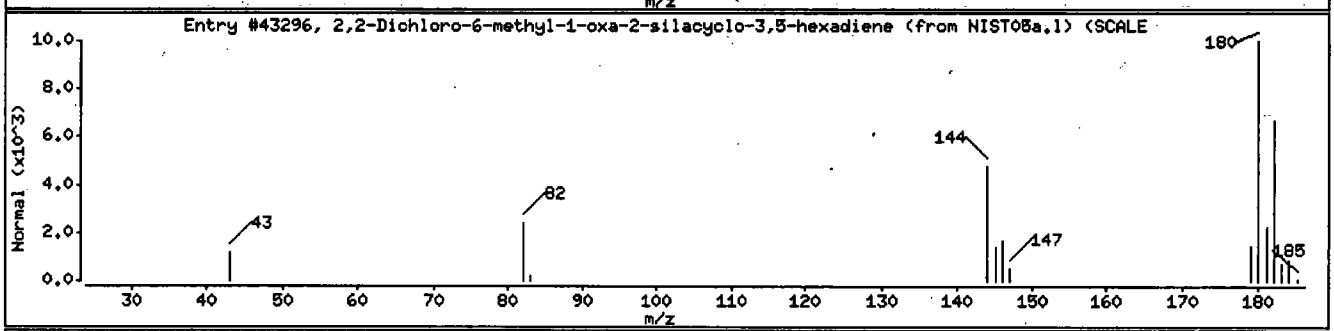
Volume Injected (uL): 1.0 Operator: jmg00346

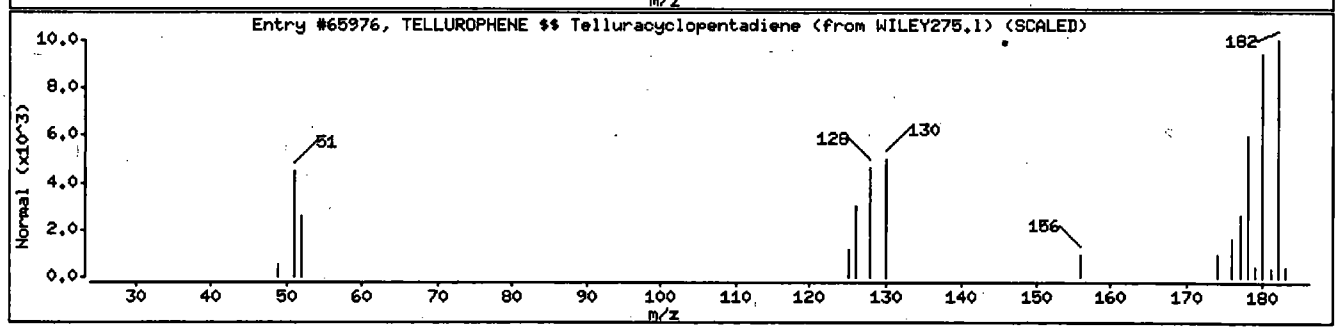
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	86	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	12	C5H6Cl2OSi	180
TELLUROPHENE $$ Telluracyclopentadiene	288-08-4	WILEY275.l	65976	11	C4H4Te	182









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

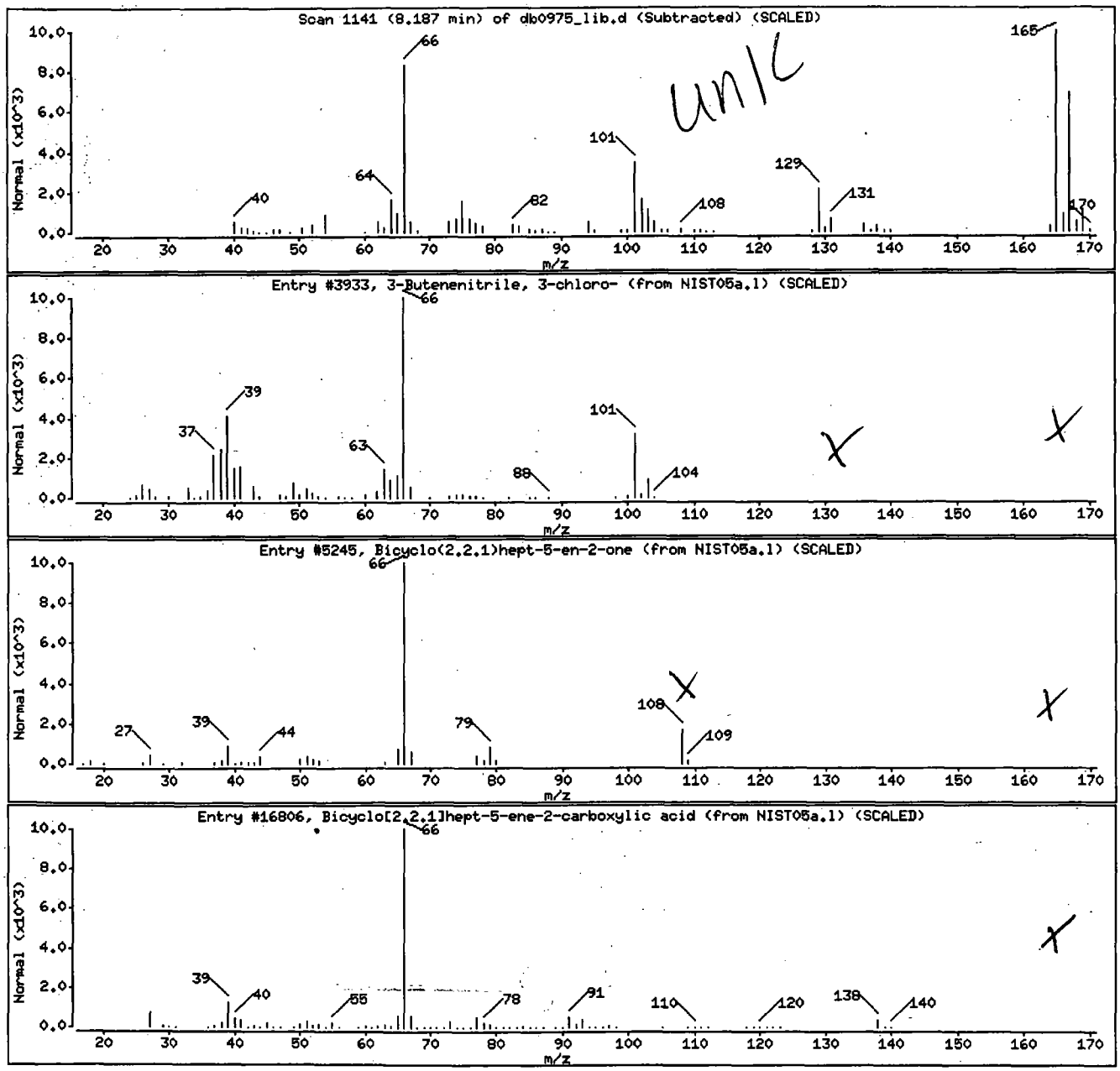
Client ID: H5011 Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	40	C4H4ClN	101
Bicyclo(2.2.1)hept-5-en-2-one	694-98-4	NIST05a.l	5245	49	C7H8O	108
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

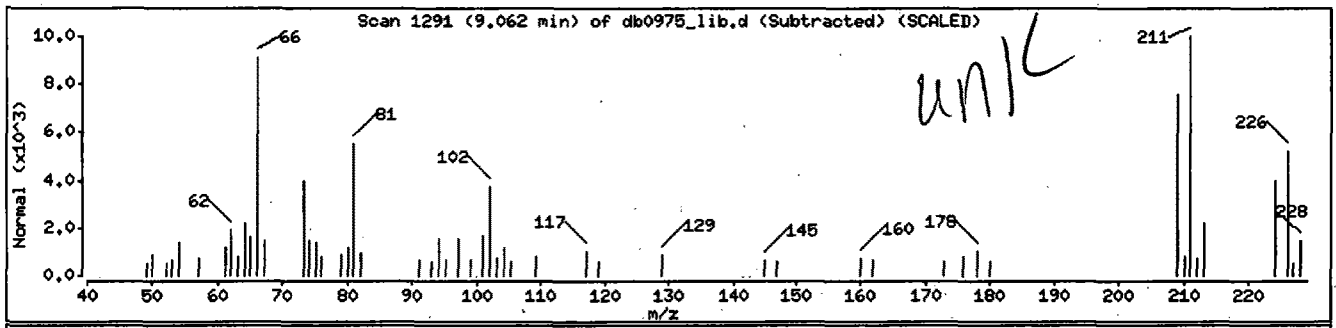
Volume Injected (uL): 1.0

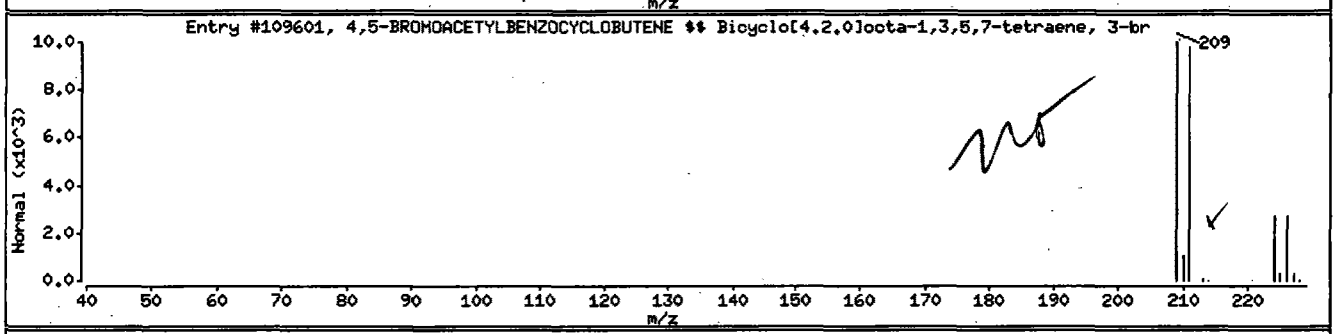
Operator: jmg00346

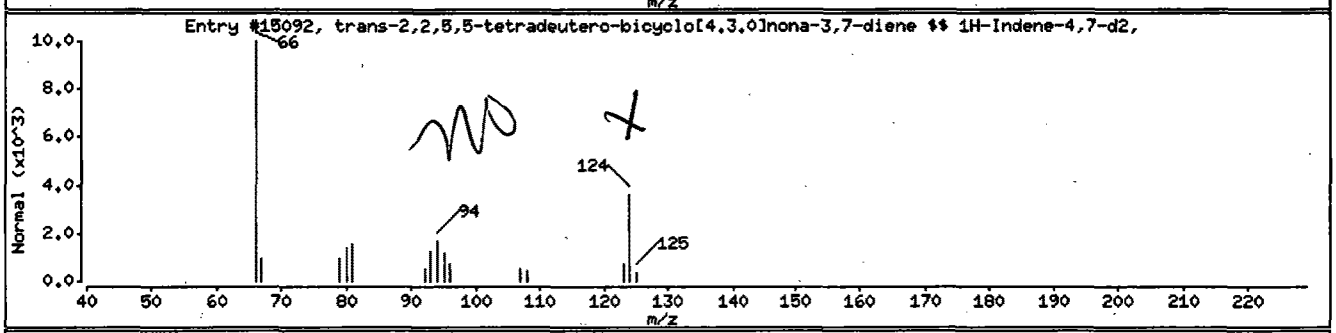
Column phase: J&W DB-5MS

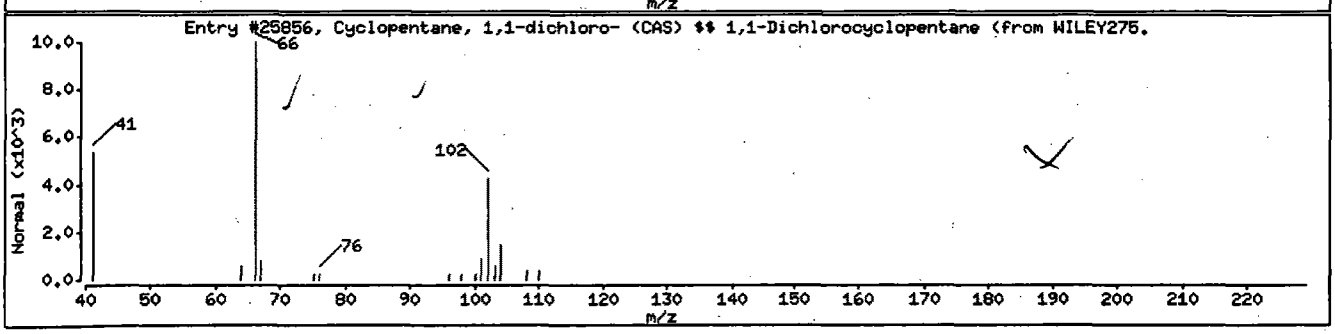
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63606-26-2	WILEY275.l	109601	80	C10H9BrO	224
trans-2,2,5,5-tetradeutero-bicyclo[4.3.0	98042-55-8	WILEY275.l	15092	43	C9H8D4	124
Cyclopentane, 1,1-dichloro- (CAS) $$ 1,1	31038-06-9	WILEY275.l	25856	43	C5H8Cl12	138









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

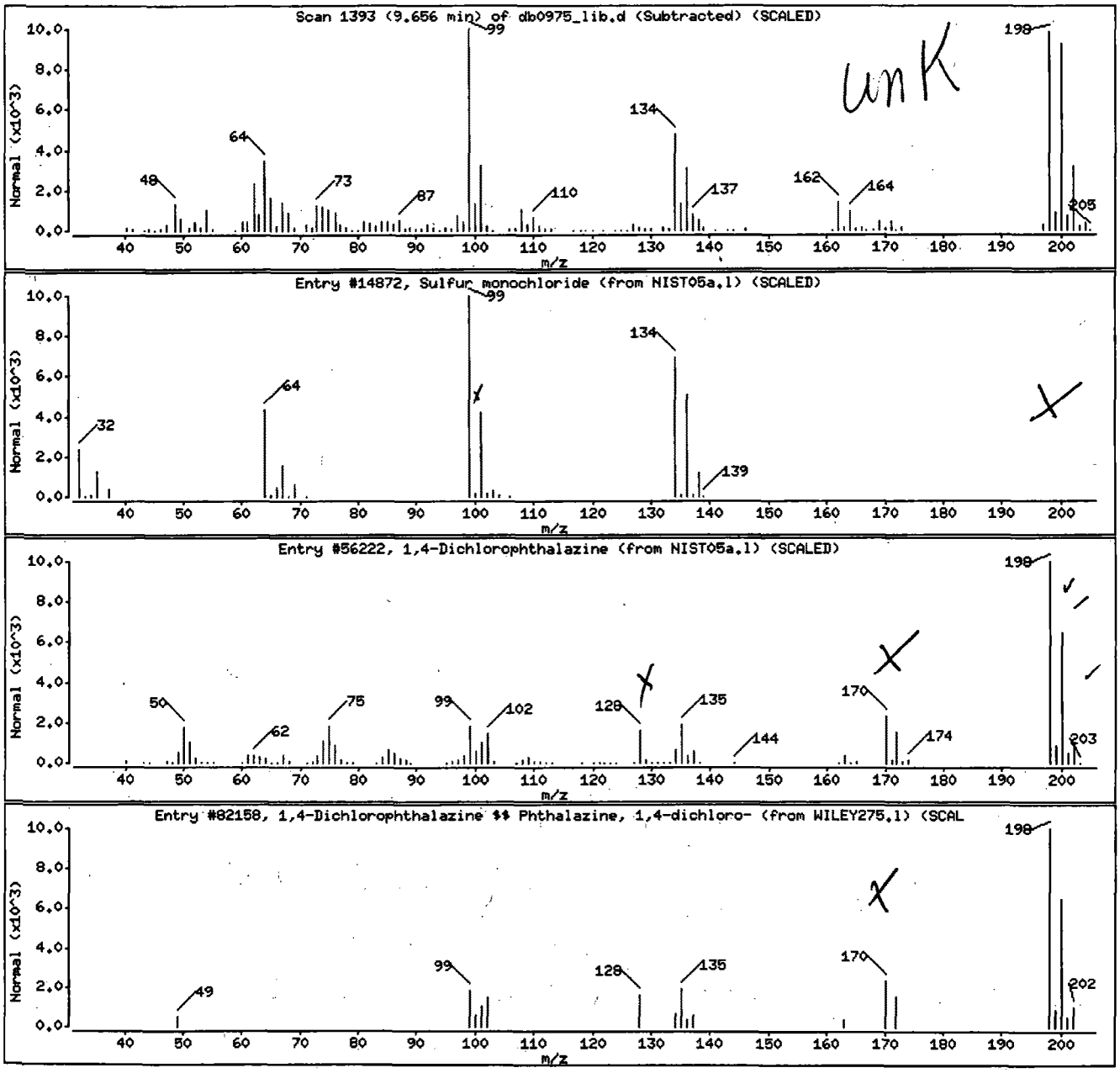
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	27	Cl2S2	134
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	38	C8H4Cl2N2	198
1,4-Dichlorophthalazine $$ Phthalazine,	4752-10-7	WILEY275.l	82158	35	C8H4Cl2N2	198



ratios OK

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0975_lib.d

Date : 21-FEB-2014 16:44

Client ID: H5011

Instrument: HP19760.i

Sample Info: H5011;7366665;1;0;SAMPLE;;;

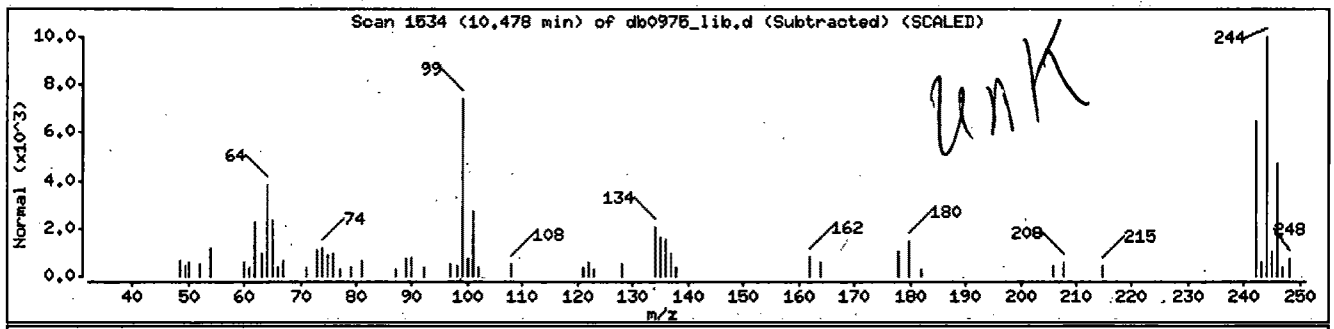
Volume Injected (uL): 1.0

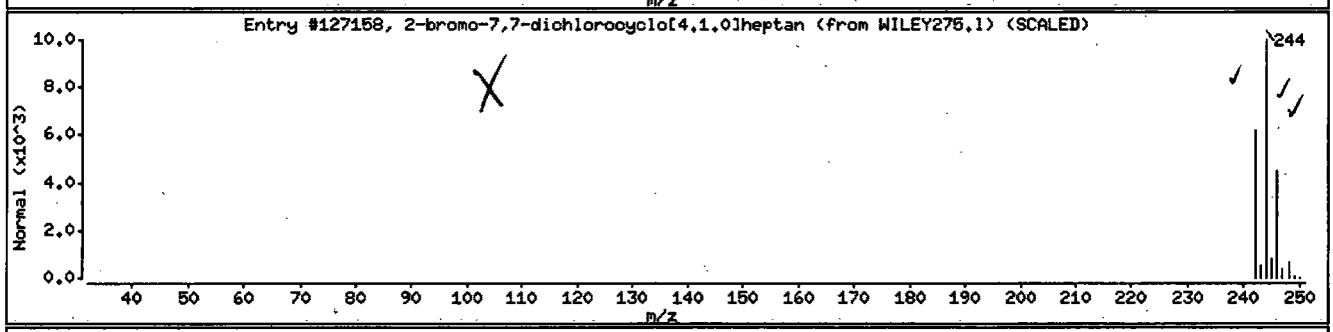
Operator: jmg00346

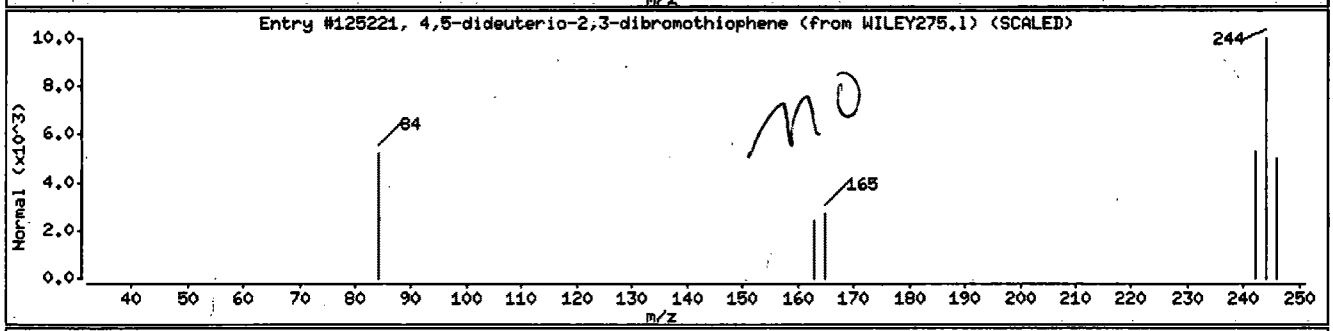
Column phase: J&W DB-5MS

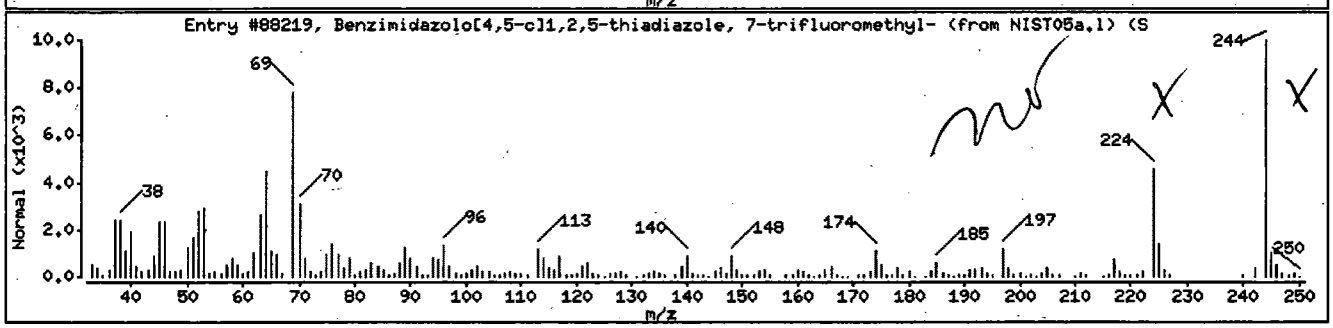
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-bromo-7,7-dichlorocyclo[4.1.0]heptan	113035-97-5	WILEY275.l	127158	91	C7H9BrCl2	242
4,5-dideuterio-2,3-dibromothiophene	137040-63-2	WILEY275.l	125221	37	C4D2Br2S	242
Benzimidazolo[4,5-c]1,2,5-thiadiazole, 7	39592-72-8	NIST05a.l	88219	17	C8H3F3N4S	244



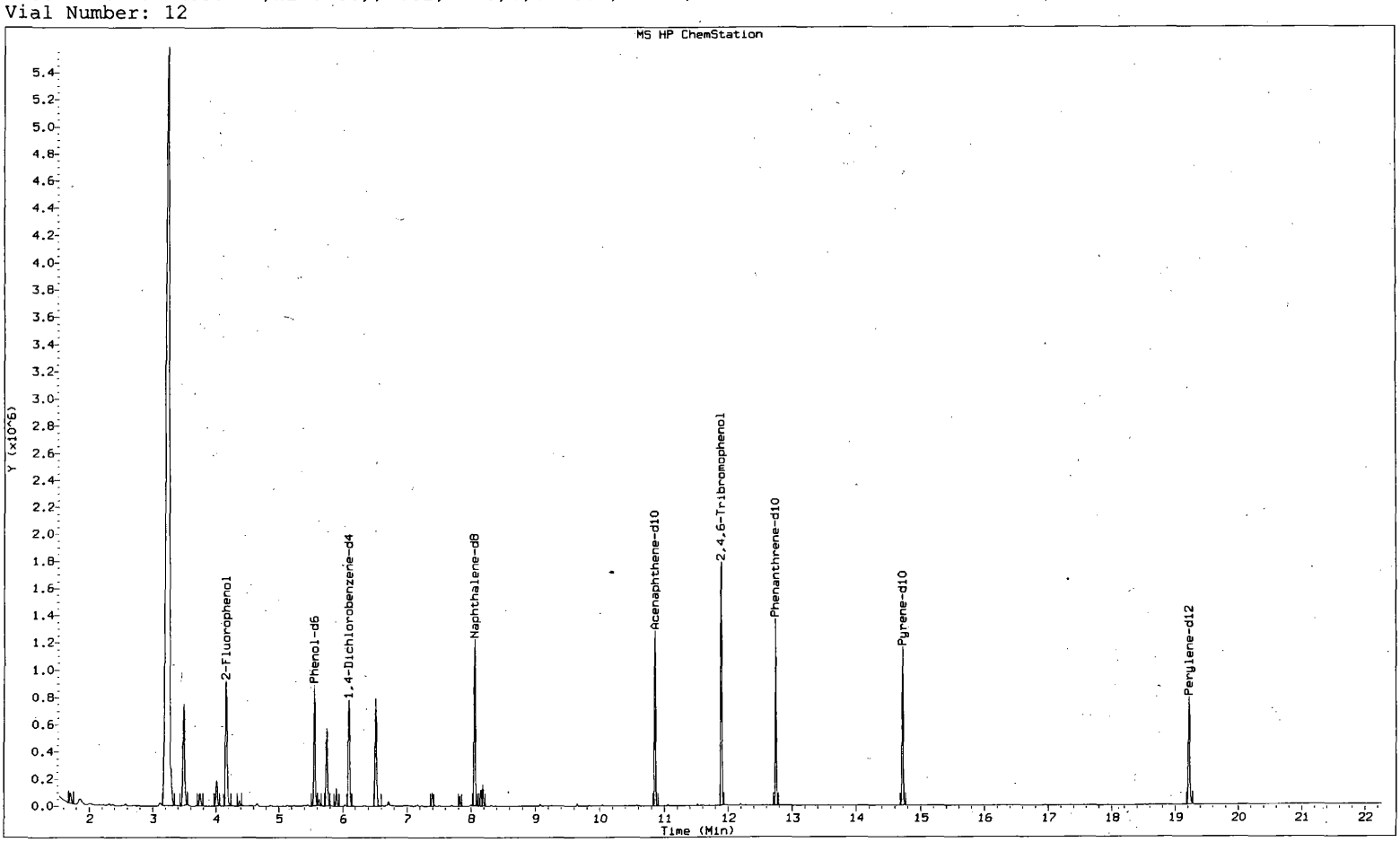






Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:26.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb20.b/db0881_lib.d
Operator : jmg00346
Acquired : 20-FEB-2014 11:18
Instrument : HP19760.i
Sample Name: H5021;7366669;1;0;SAMPLE;;;
Misc Info : 14050WAD;WL13166;;1052;1000;0;db0837;13166;
Vial Number: 12



Lancaster Labs

Data file : /chem/HP19760.i/14feb20.b/db0881_lib.d
Lab Smp Id: 7366669 Client Smp ID: H5021
Inj Date : 20-FEB-2014 11:18
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H5021;7366669;1;0;SAMPLE;;;
Misc Info : 14050WAD;WL13166;;1052;1000;0;db0837;13166;
Comment : Max. number of TICs to report is 50, 14 TICs were found initially.
Method : /chem/HP19760.i/14feb20.b/8270_WVA_lib.m
Meth Date : 01-Mar-2014 20:47 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 12
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1052.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	1118043	10.000
* 48 Naphthalene-d8	8.059	1581889	10.000

	CONCENTRATIONS				QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.706	149223	1.33468325	1.26871	91	NIST05a.1	31325	21
1,1-Dimethyl-3-chloropropanol				CAS #: 1985-88-2			
3.268	20615004	184.384640	175.27057	83	NIST05a.1	9464	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:43.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.495	1466076	13.1128699	12.46470	78	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.746	172664	1.54434419	1.46800	33	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.014	336144	3.00654217	2.85792	36	NIST05a.l	13998	21
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.375	62017	0.55469563	0.52727	9	NIST05a.l	33655	21(L)
Cyclotetrasiloxane, octamethyl-					CAS #: 556-67-2		
5.634	59983	0.53649970	0.50998	91	NIST05a.l	122480	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.751	838425	7.49903443	7.12835	94	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.903	192209	1.71915777	1.63418	94	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.515	1191113	10.6535497	10.12694	38	NIST05a.l	9448	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.395	118116	0.74667813	0.70977	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	82218	0.51974800	0.49405	25	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.152	134302	0.84899858	0.80703	89	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	195666	1.23691424	1.17577	50	NIST05a.l	3933	48

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:43.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0881_lib.d

Date : 20-FEB-2014 11:18

Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

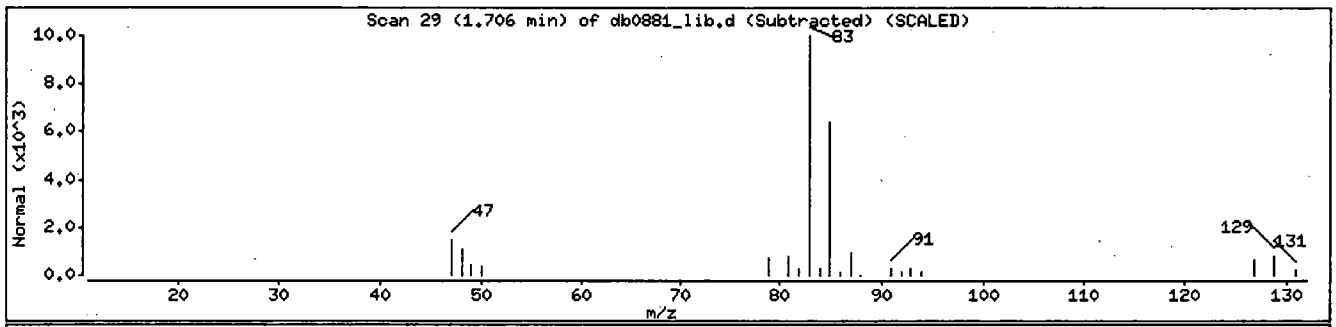
Volume Injected (uL): 1.0

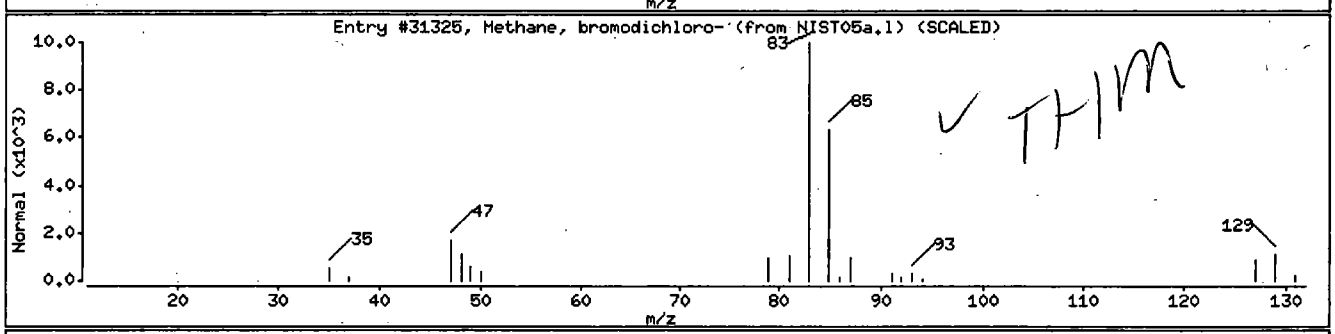
Operator: jmg00346

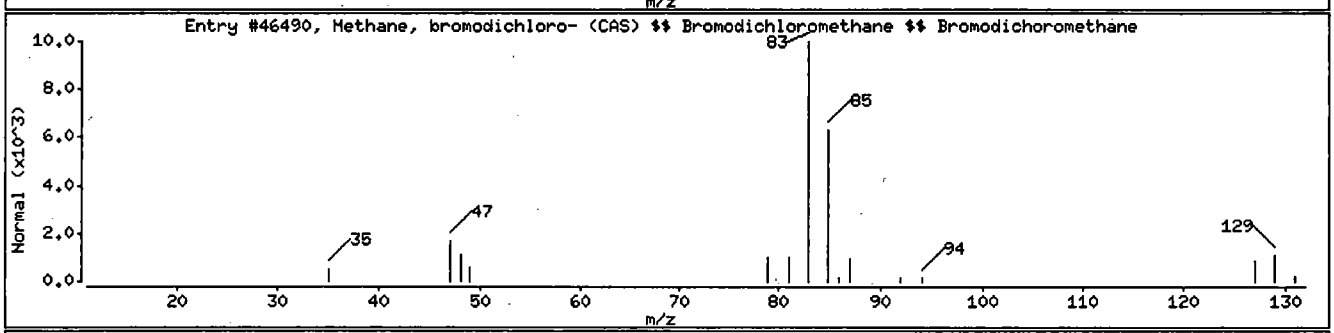
Column phase: J&W DB-5MS

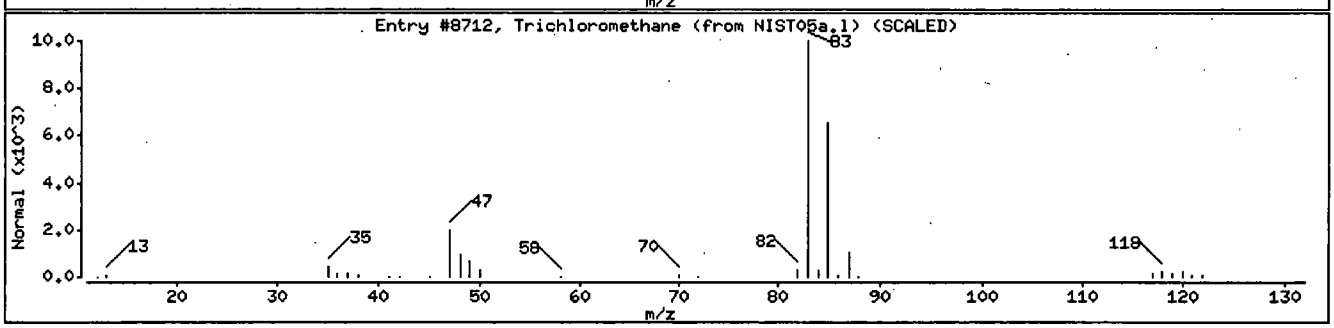
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	91	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	91	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:43.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0881_lib.d

Date : 20-FEB-2014 11:18

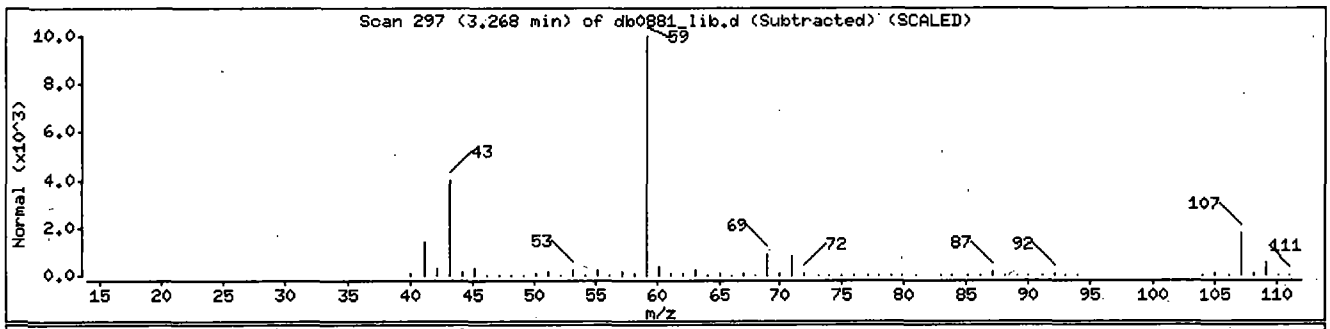
Client ID: H5021 Instrument: HP19760.i

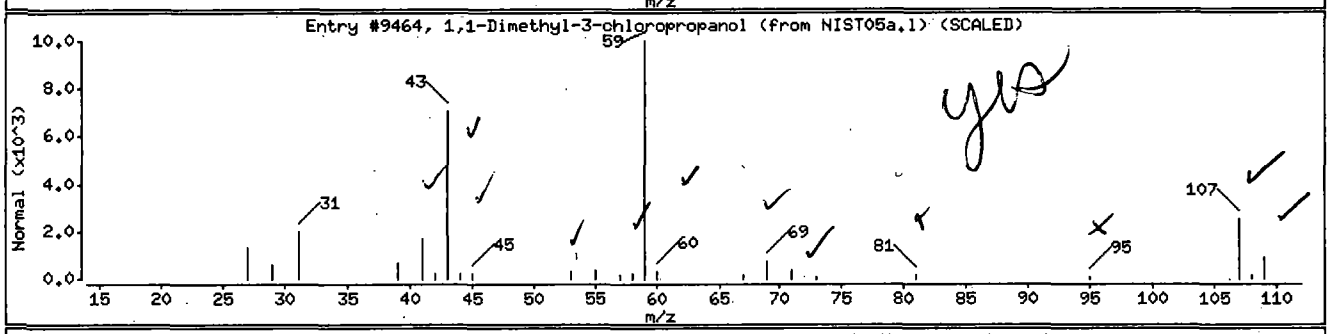
Sample Info: H5021;7366669;1;0;SAMPLE;;;

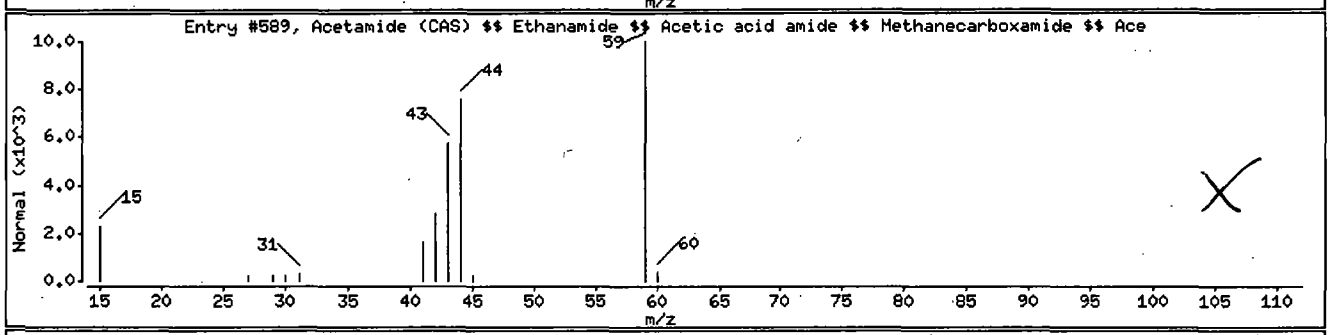
Volume Injected (uL): 1.0 Operator: jmg00346

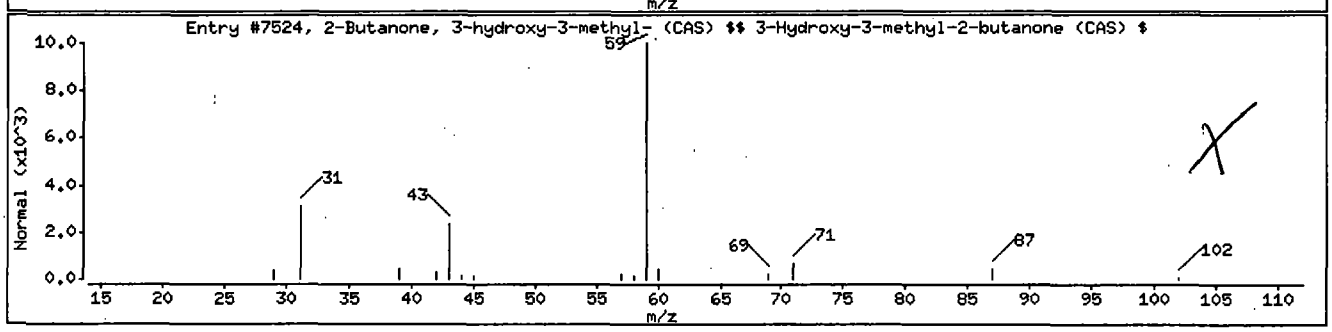
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0881_lib.d

Date : 20-FEB-2014 11:18

Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

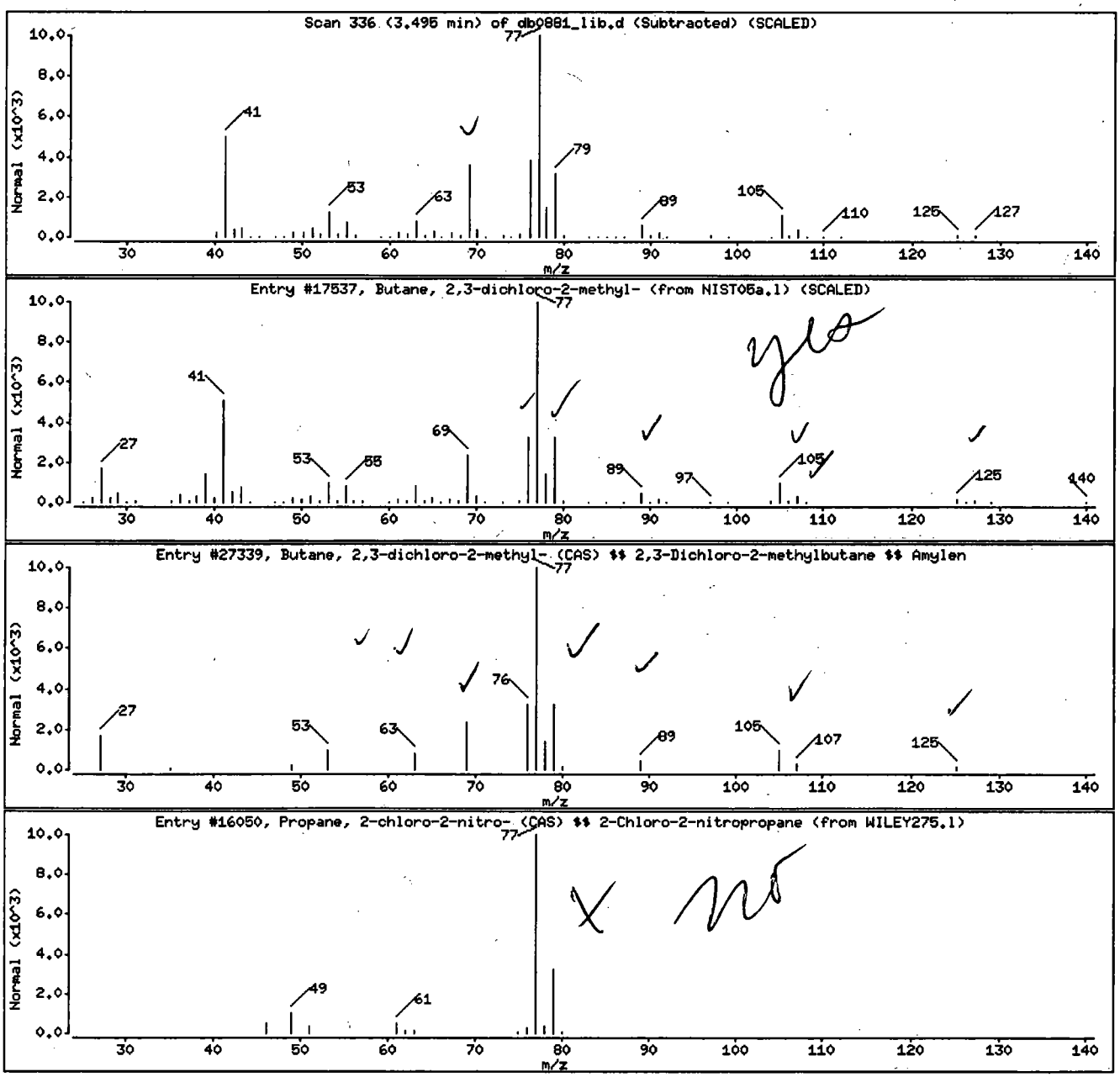
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	78	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	78	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	25	C3H6ClNO2	123



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Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

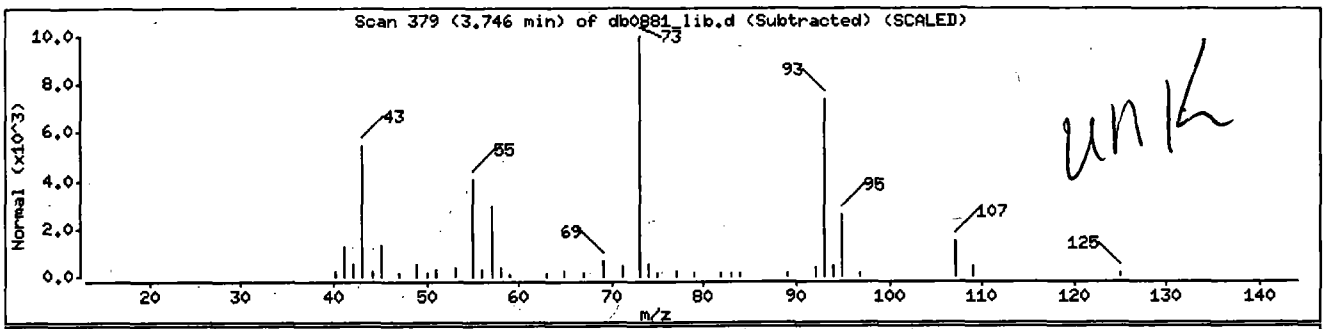
Volume Injected (uL): 1.0

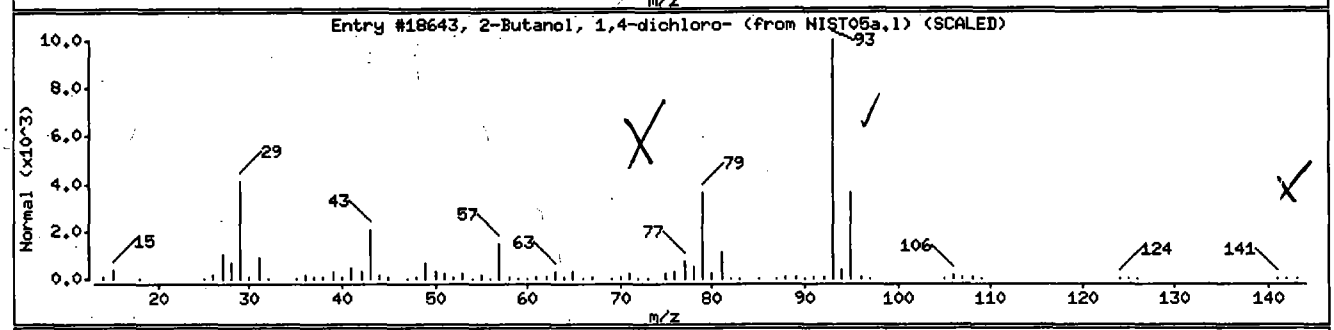
Operator: jmg00346

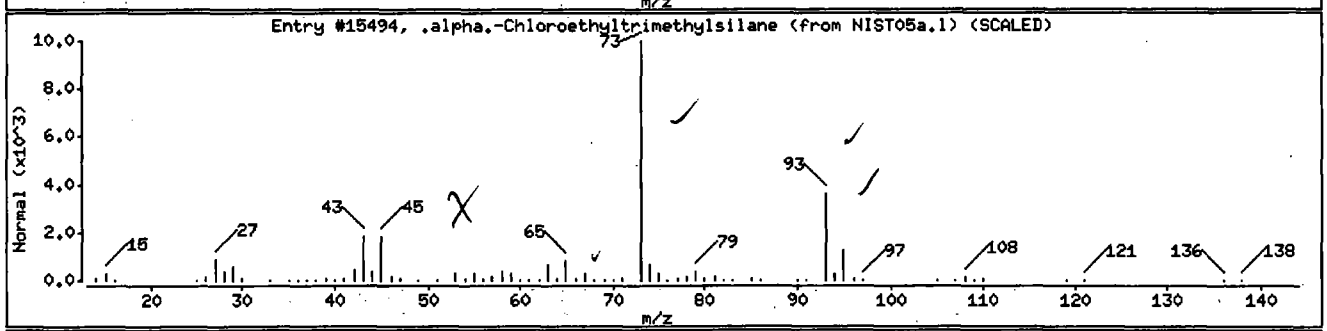
Column phase: J&W DB-5MS

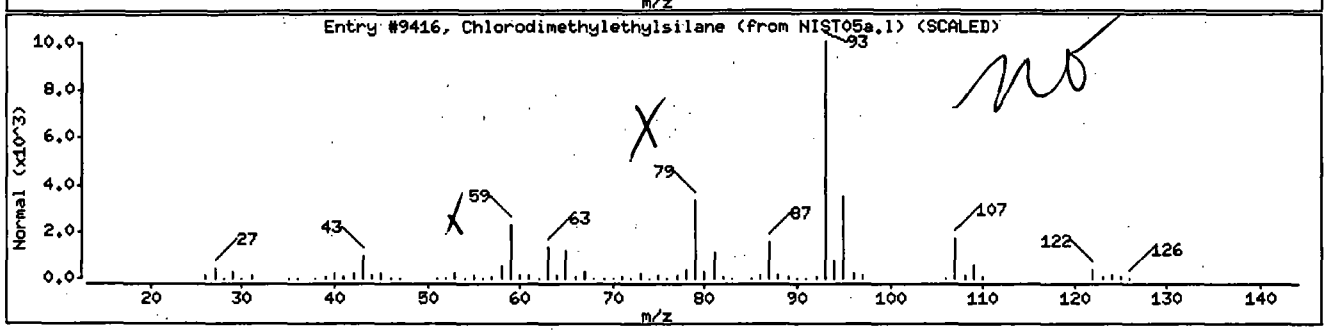
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	33	C4H8Cl2O	142
.alpha.-Chloroethyltrimethylsilane	7787-87-3	NIST05a.l	15494	9	C5H13ClSi	136
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	9	C4H11ClSi	122









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Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

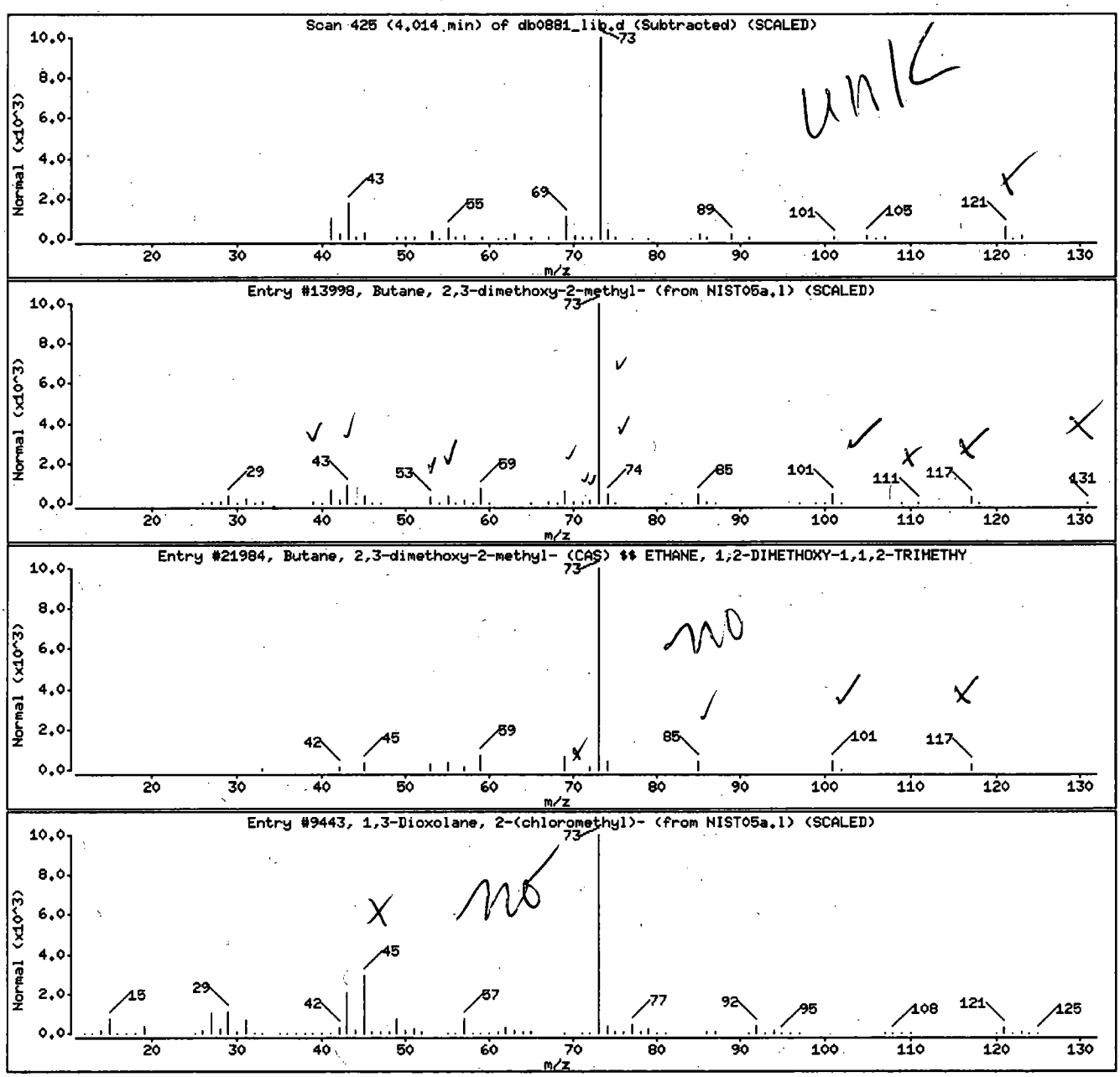
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	36	C7H16O2	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	36	C7H16O2	132
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9443	9	C4H7ClO2	122



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Date : 20-FEB-2014 11:18

Client ID: H5021 Instrument: HP19760.i

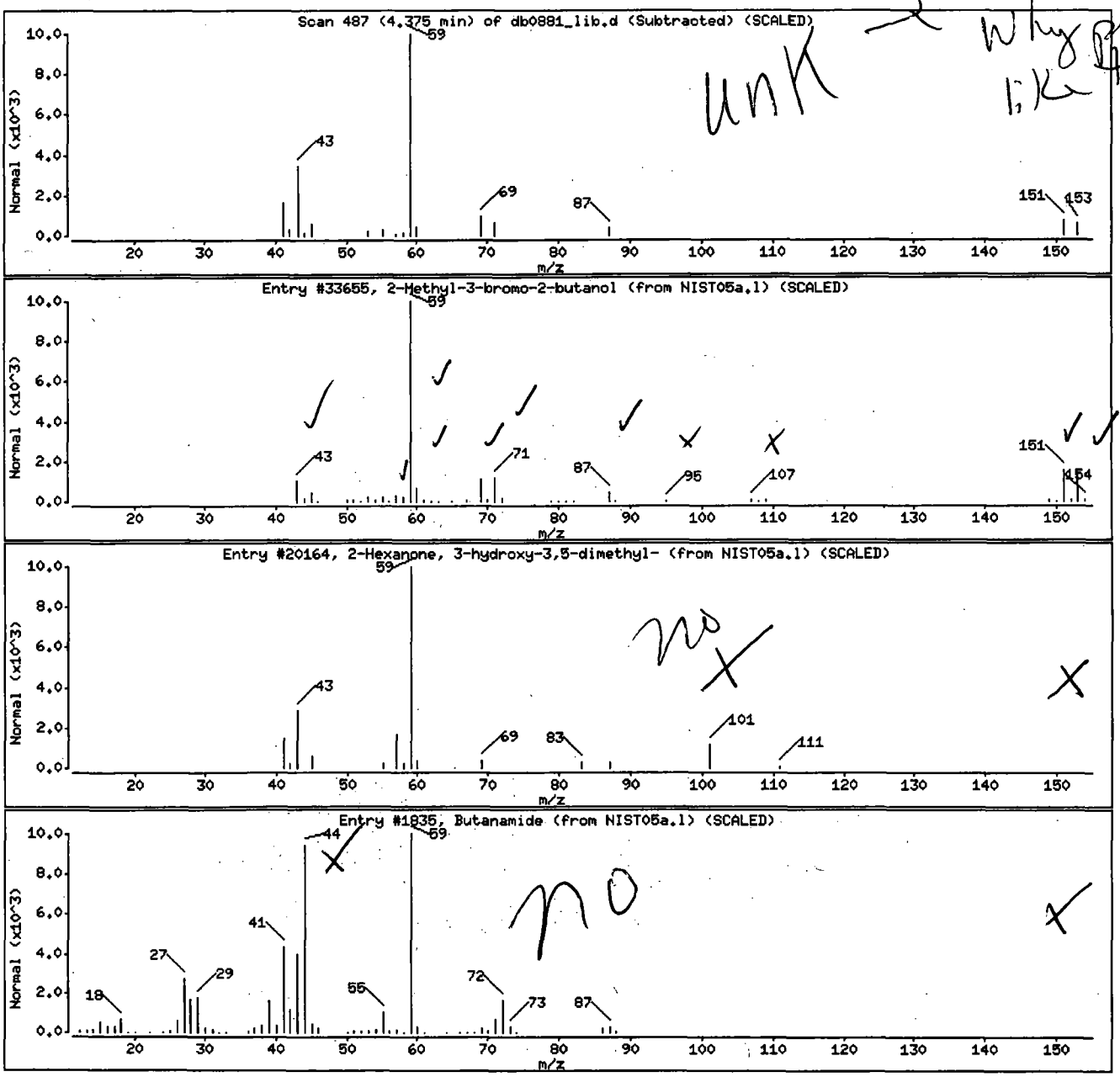
Sample Info: H5021;7366669;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: jmg00346

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	9	C5H11BrO	166
2-Hexanone, 3-hydroxy-3,5-dimethyl-	6321-14-8	NIST05a.l	20164	64	C8H16O2	144
Butanamide	541-35-5	NIST05a.l	1835	64	C4H9NO	87

Why presently like this?



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Date : 20-FEB-2014 11:18

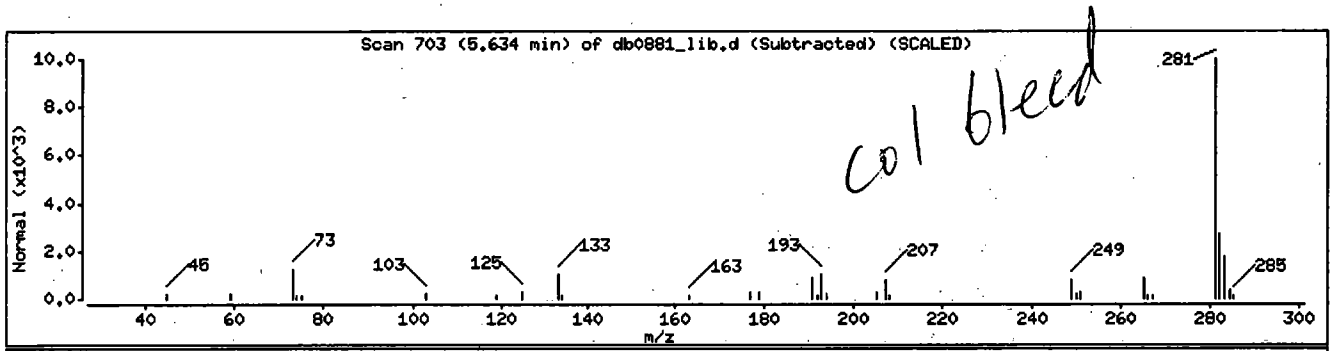
Client ID: H5021 Instrument: HP19760.i

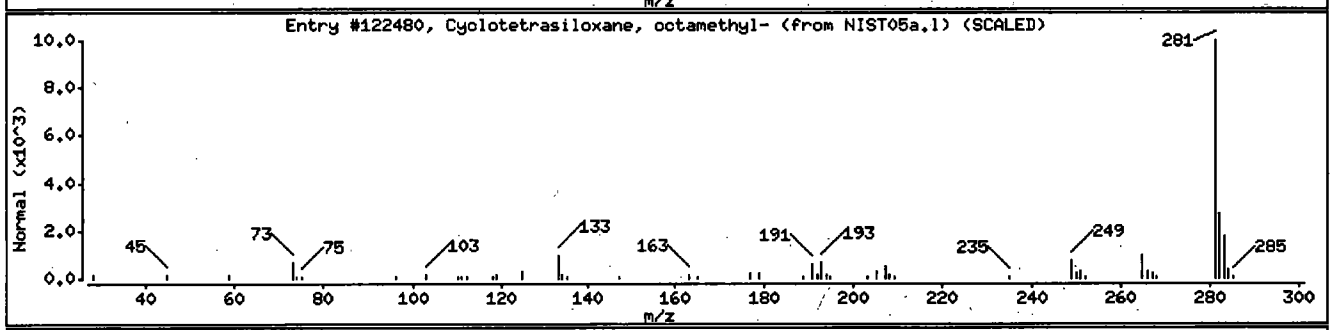
Sample Info: H5021;7366669;1;0;SAMPLE;;;

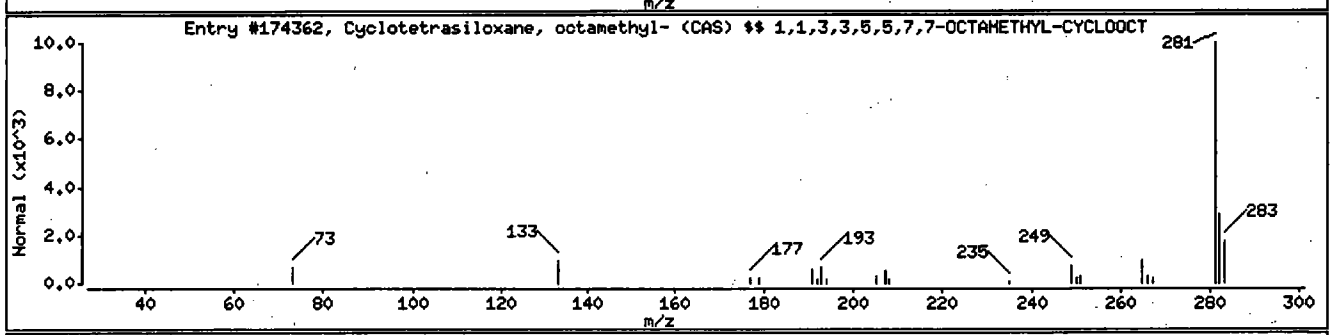
Volume Injected (uL): 1.0 Operator: jmg00346

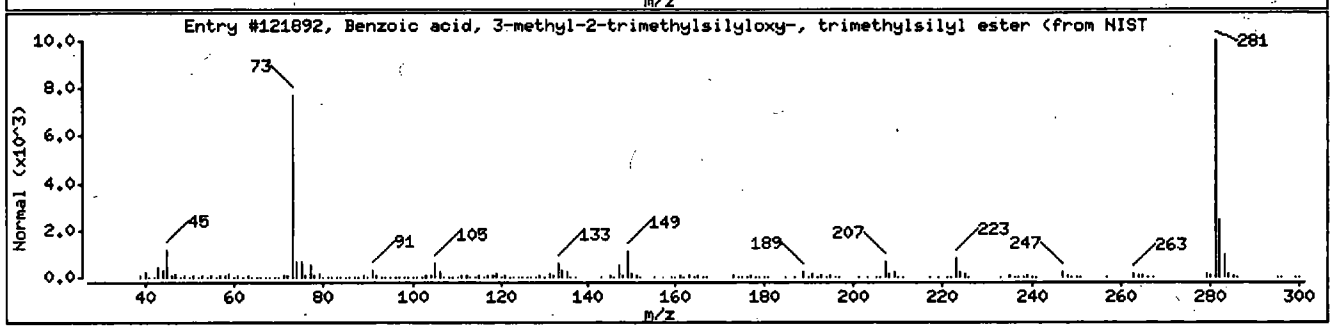
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclotetrasiloxane, octamethyl-	556-67-2	NIST05a.l	122480	91	C8H24O4Si4	296
Cyclotetrasiloxane, octamethyl- (CAS) $$	556-67-2	WILEY275.l	174362	91	C8H24O4Si4	296
Benzoic acid, 3-methyl-2-trimethylsilylo	1000153-57-1	NIST05a.l	121892	59	C14H24O3Si2	296









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Date : 20-FEB-2014 11:18

Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

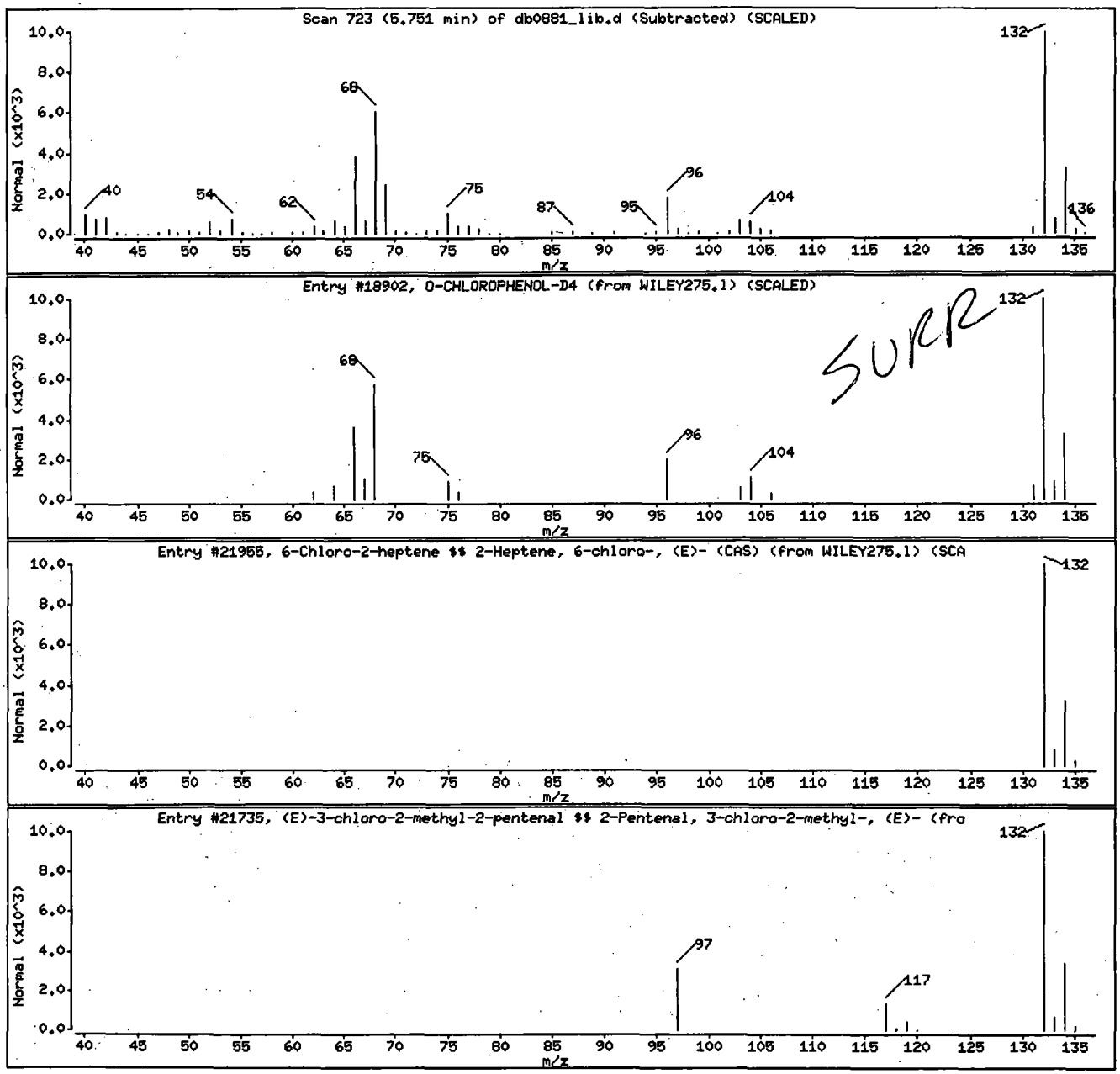
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	94	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31367-76-3	WILEY275.1	21735	78	C6H9ClO	132



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Data File: /chem/HP19760.i/14feb20.b/db0881_lib.d

Date : 20-FEB-2014 11:18

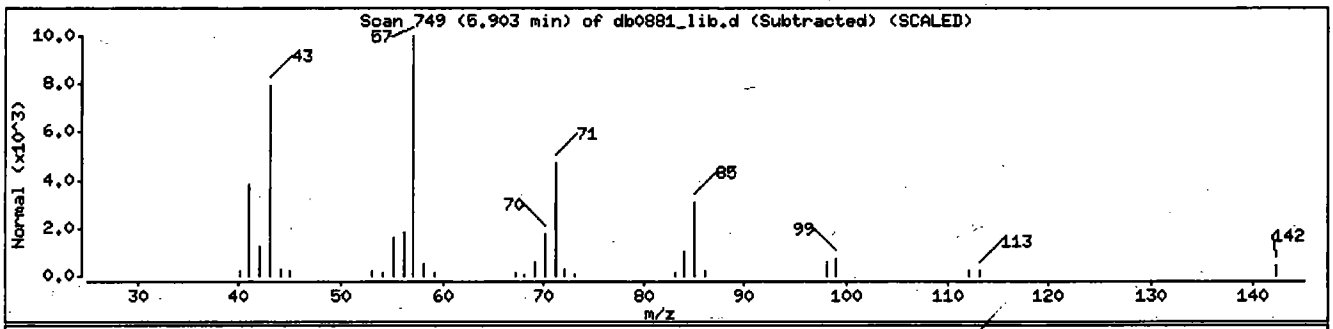
Client ID: H5021 Instrument: HP19760.i

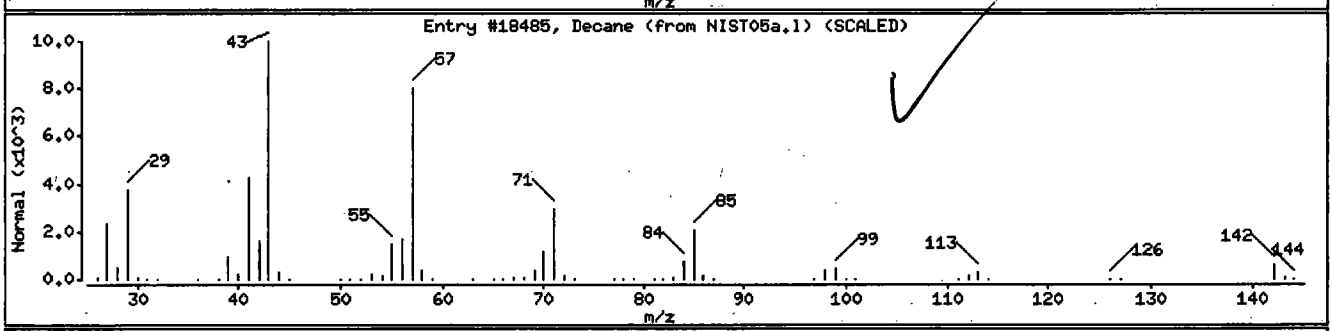
Sample Info: H5021;7366669;1;0;SAMPLE;;;

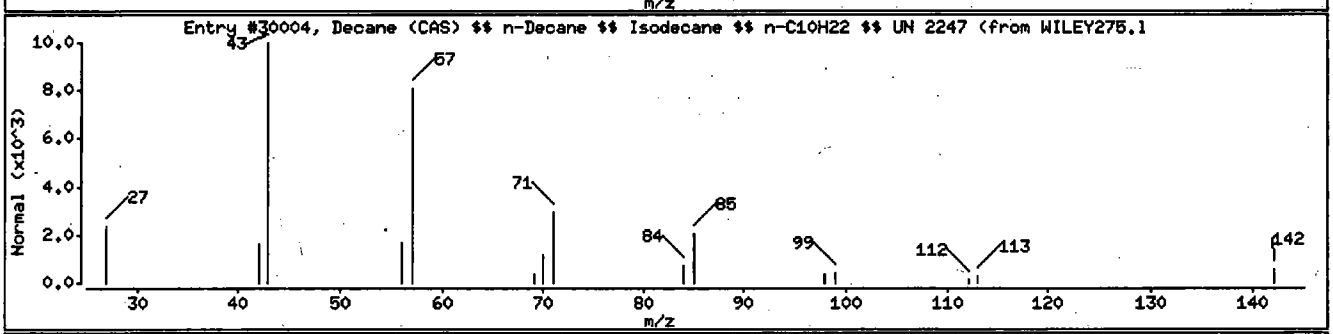
Volume Injected (uL): 1.0 Operator: jmg00346

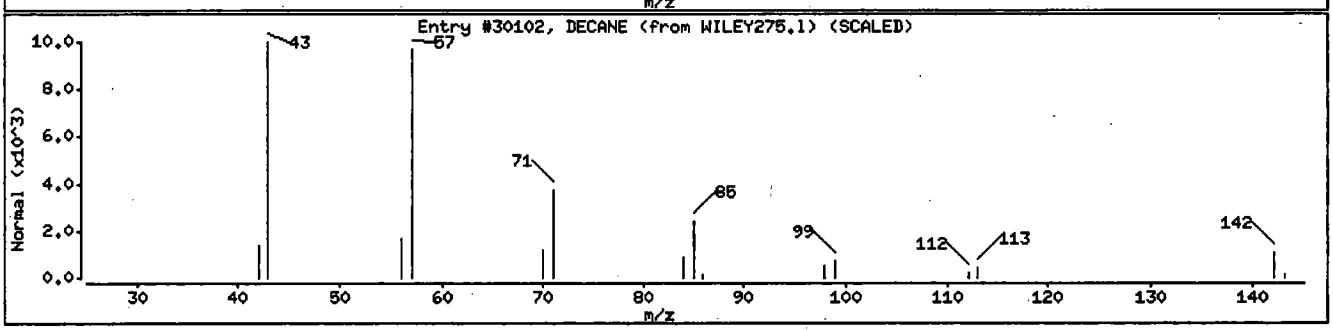
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	94	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	94	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb20.b/db0881_lib.d

Date : 20-FEB-2014 11:18

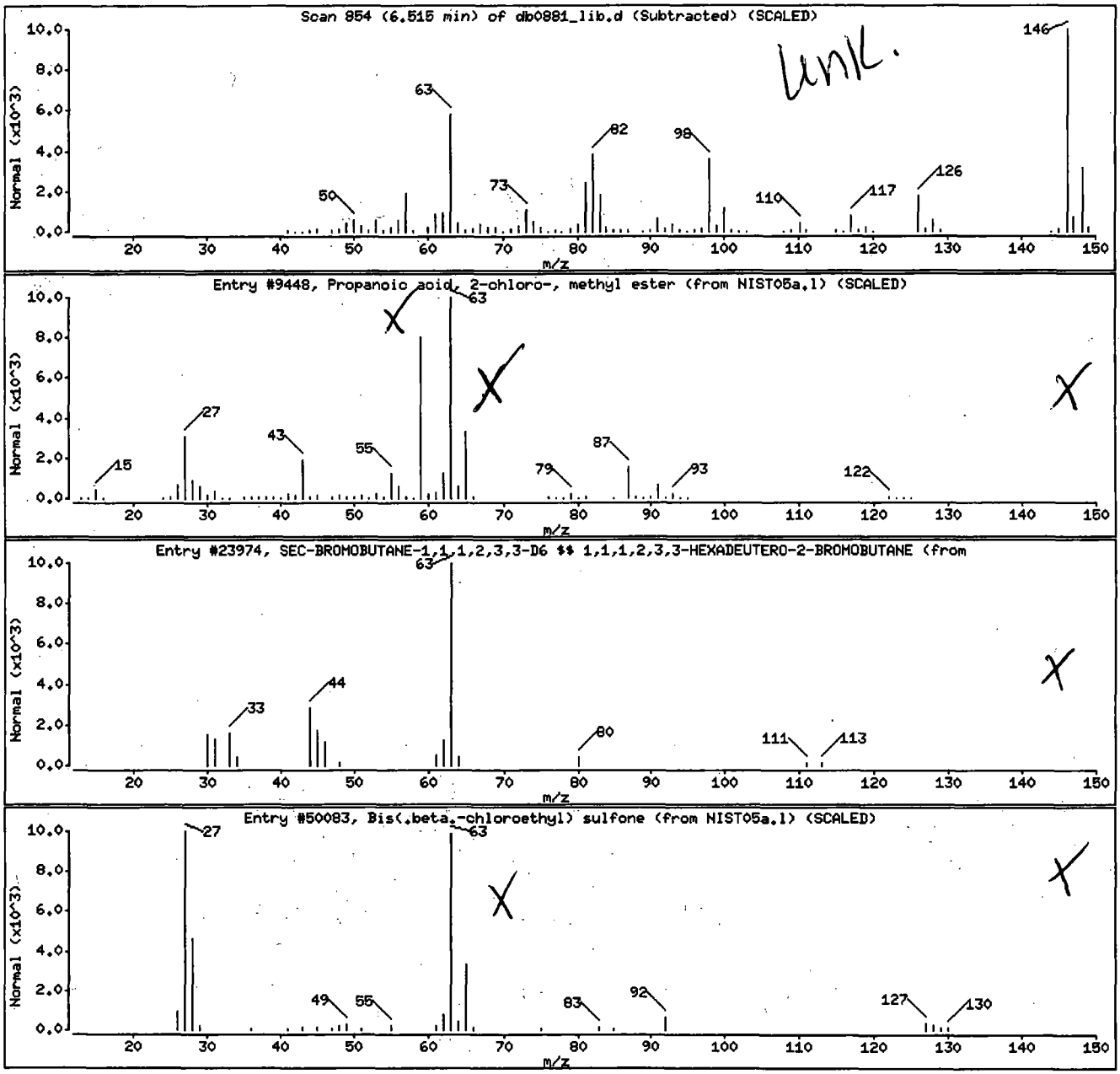
Client ID: H5021 | Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 | Operator: jmg00346

Column phase: J&W DB-5MS | Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	23	C4H8Cl2O2S	190



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Date : 20-FEB-2014 11:18

Client ID: H5021

Instrument: HP19760.i

Sample Info: H5021;736669;1;0;SAMPLE;;;

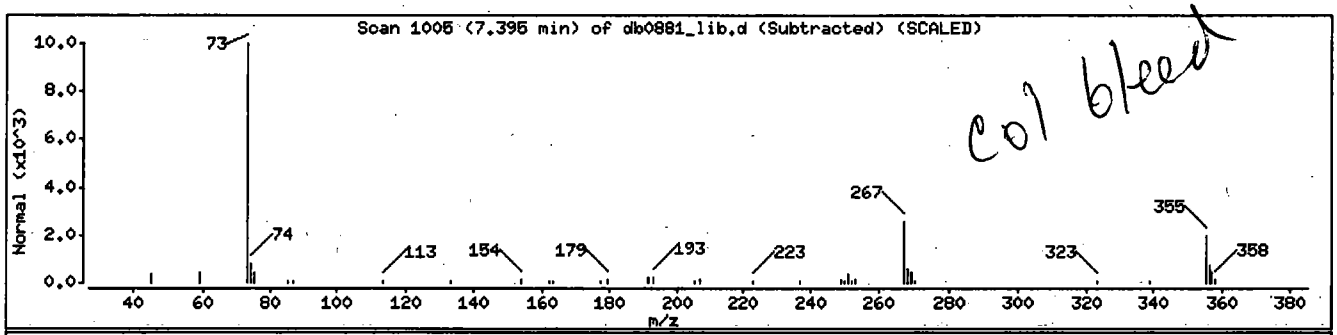
Volume Injected (uL): 1.0

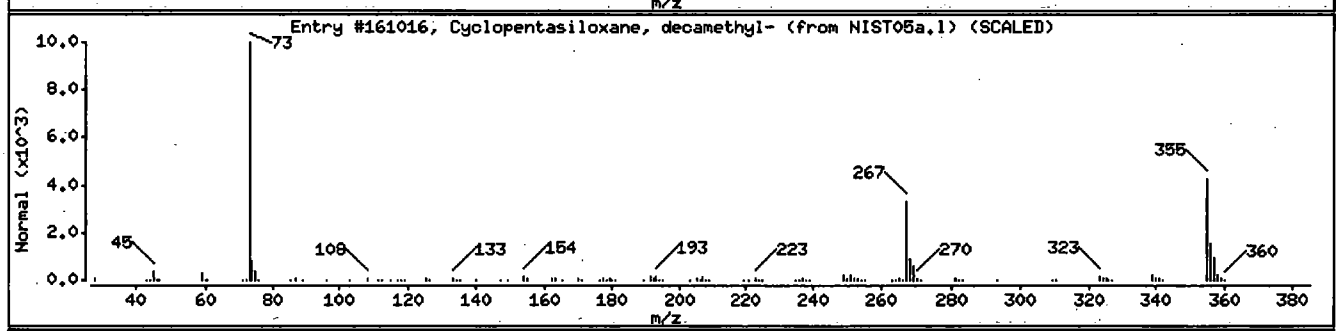
Operator: jmg00346

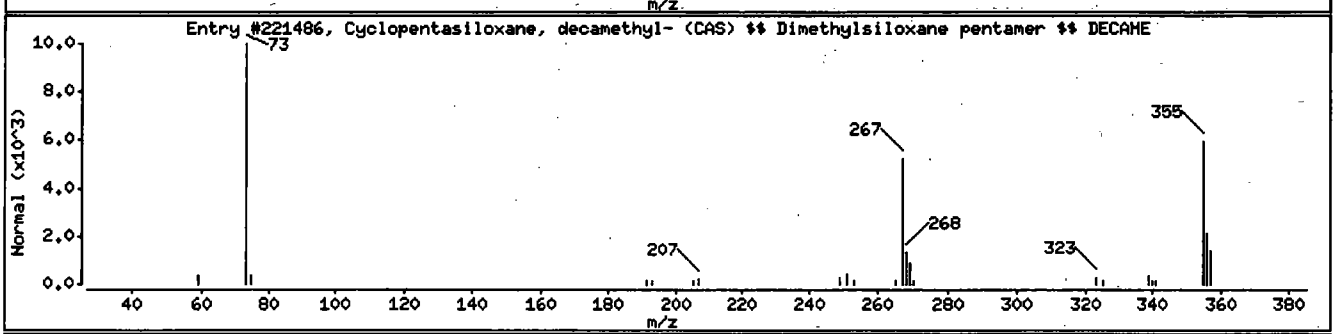
Column phase: J&W DB-5MS

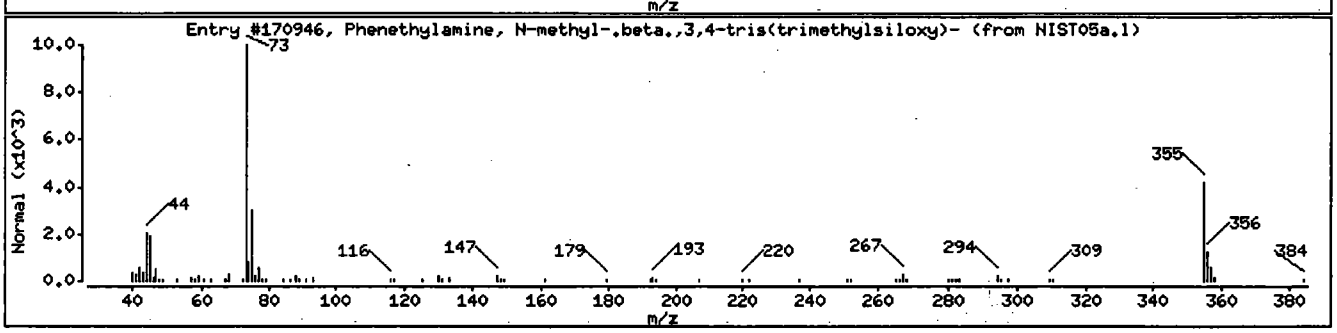
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
Phenethylamine, N-methyl-.beta.,3,4-tris	10538-85-9	NIST05a.l	170946	37	C18H37NO3Si3	399









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Instrument: HP19760.i

Sample Info: H5021;7366669;1;0;SAMPLE;;;

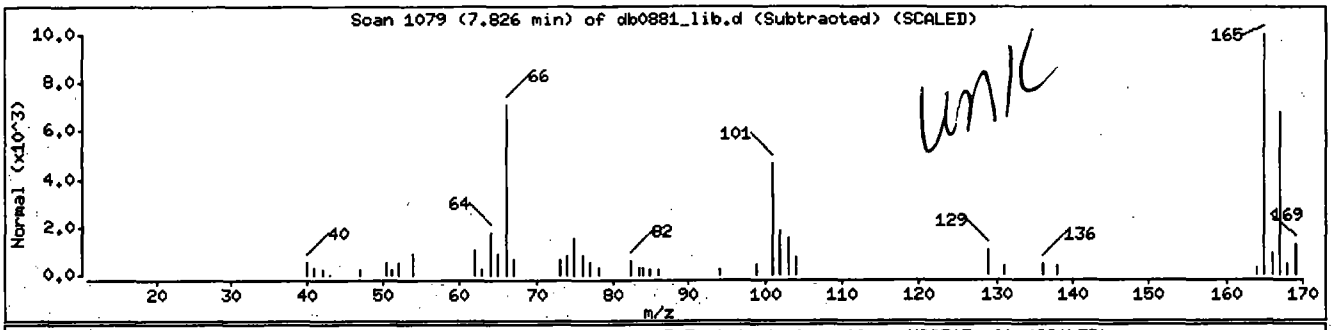
Volume Injected (uL): 1.0

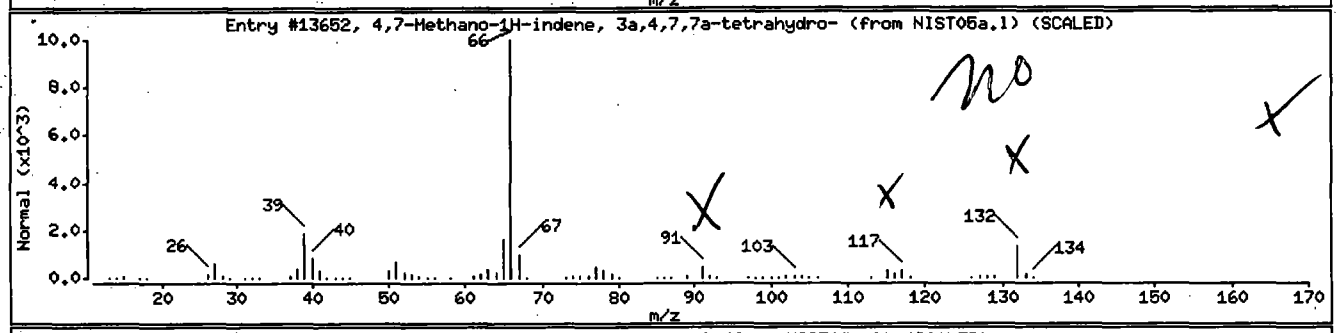
Operator: jmg00346

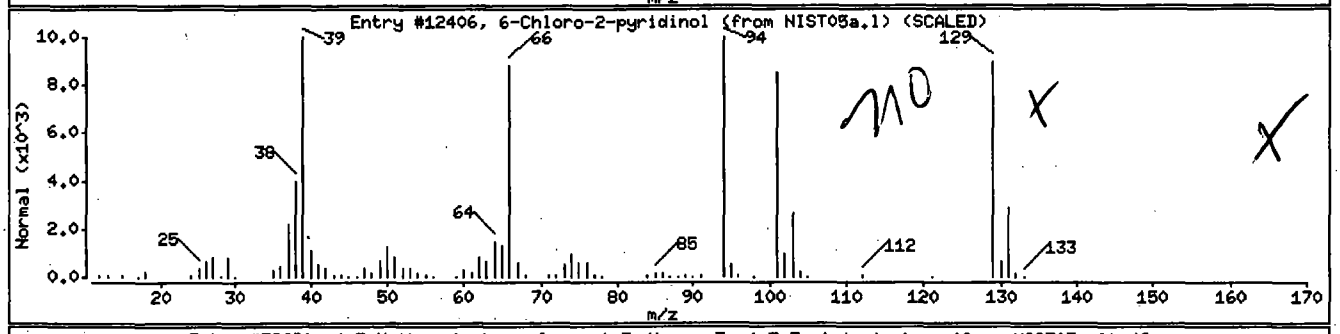
Column phase: J&W DB-5MS

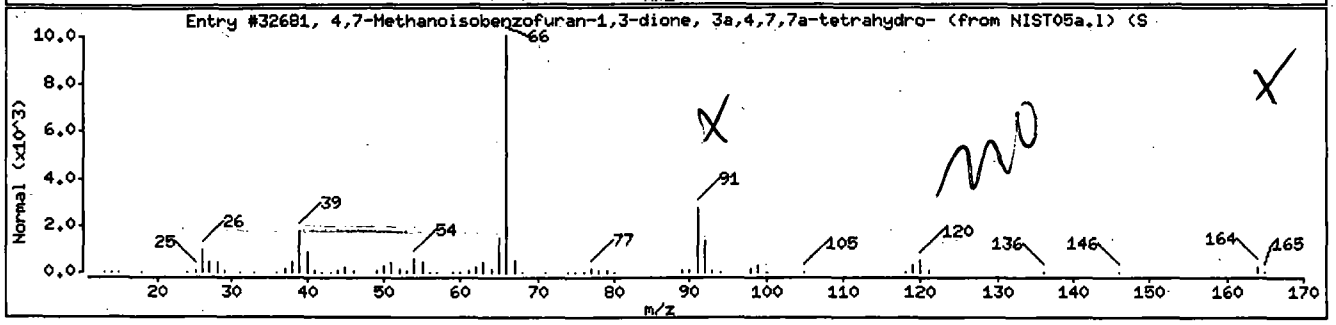
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	25	C10H12	132
6-Chloro-2-pyridinol	16879-02-0	NIST05a.l	12406	50	C5H4ClNO	129
4,7-Methanoisobenzofuran-1,3-dione, 3a,4	826-62-0	NIST05a.l	32681	43	C9H8O3	164









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Sample Info: H5021;7366669;1;0;SAMPLE;;;

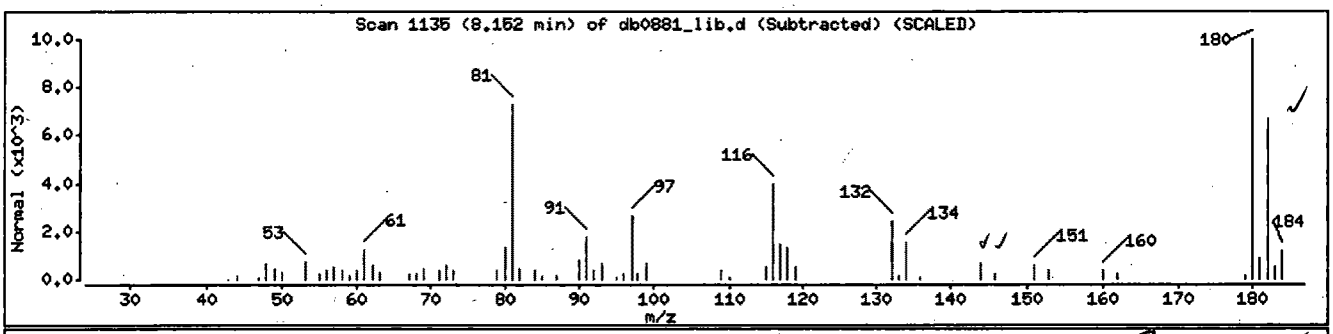
Volume Injected (uL): 1.0

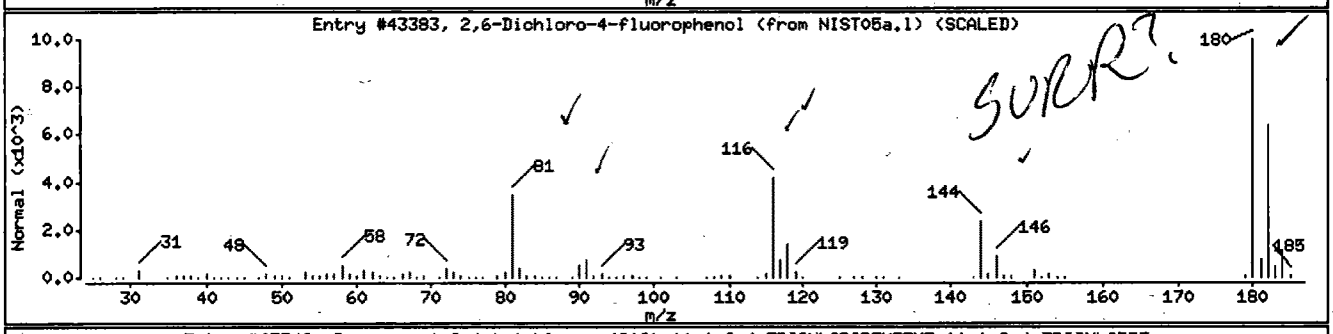
Operator: jmg00346

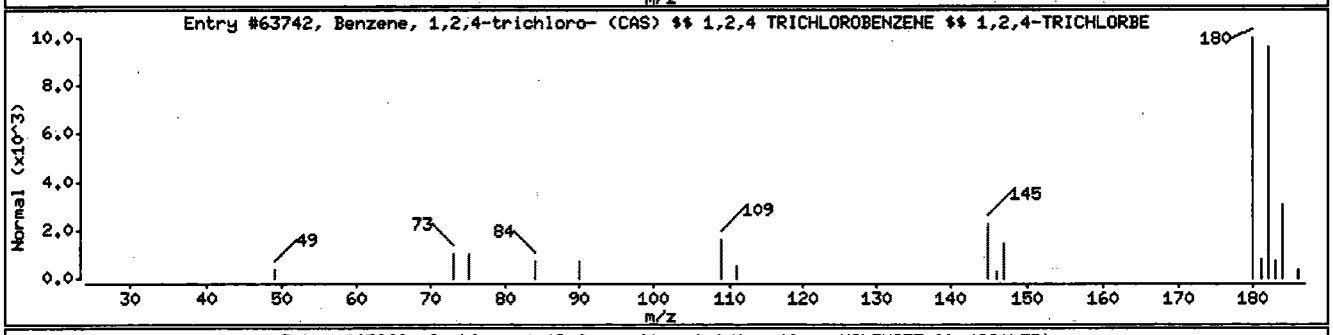
Column phase: J&W DB-5MS

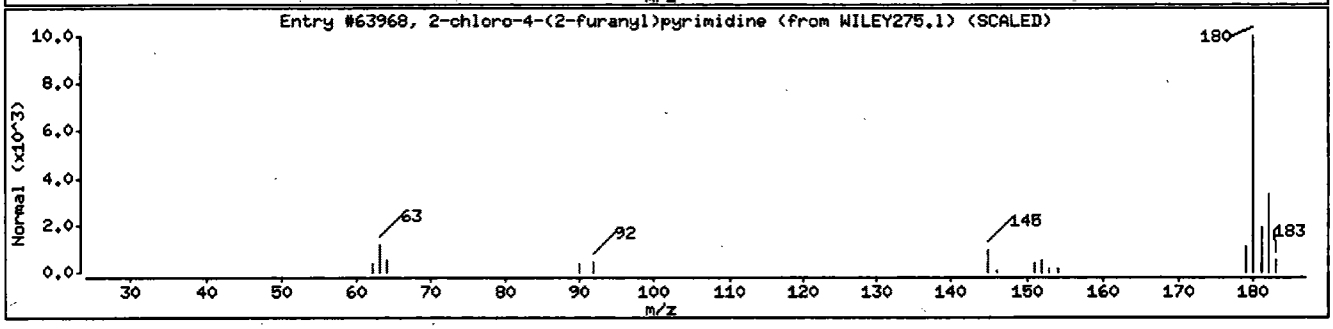
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	89	C6H3Cl2FO	180
Benzene, 1,2,4-trichloro- (CAS) $$ 1,2,4	120-82-1	WILEY275.l	63742	35	C6H3Cl3	180
2-chloro-4-(2-furanyl)pyrimidine	0-00-0	WILEY275.l	63968	27	C8H5ClN2O	180









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Sample Info: H5021;7366669;1;0;SAMPLE;;;

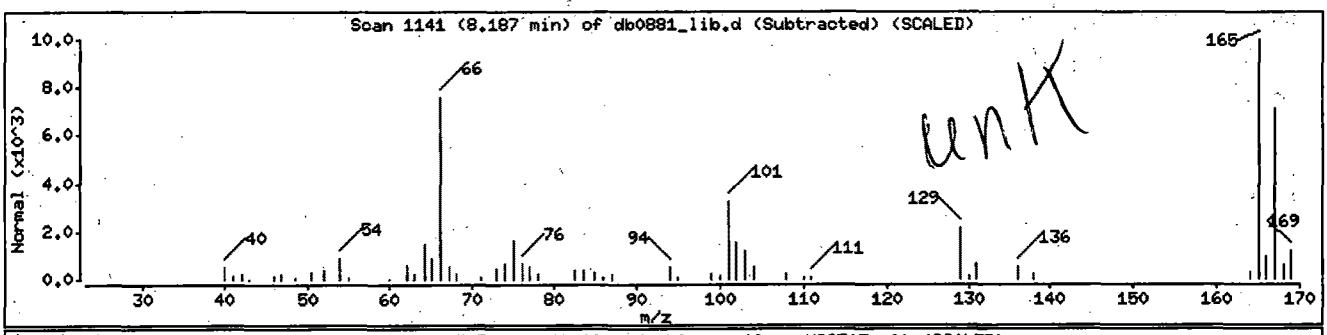
Volume Injected (uL): 1.0

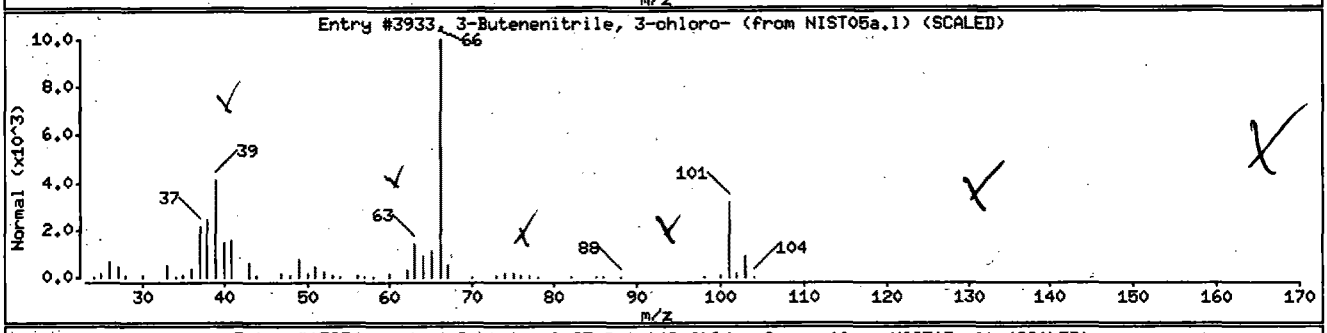
Operator: jmg00346

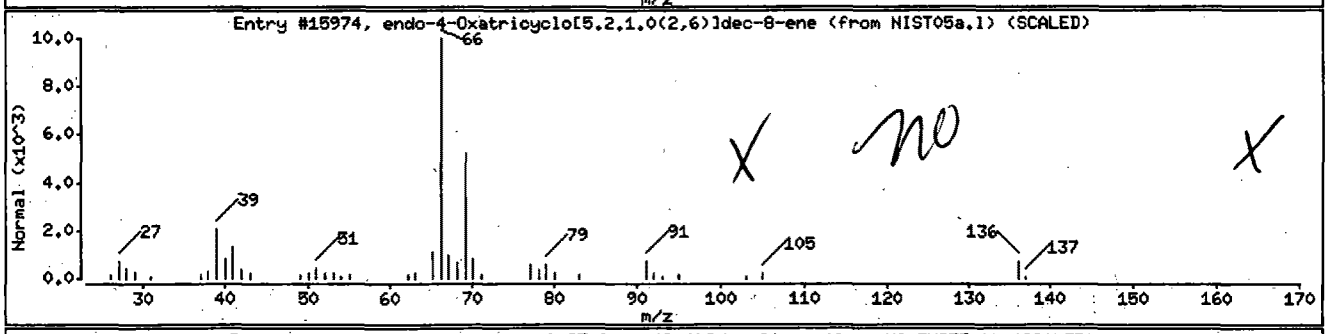
Column phase: J&W DB-5MS

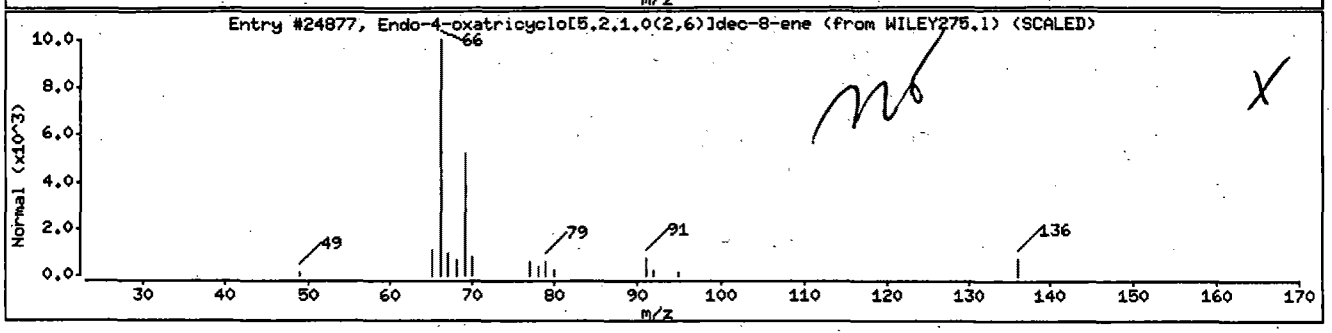
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	49	C9H12O	136
Endo-4-oxatricyclo[5.2.1.0(2,6)]dec-8-en	0-00-0	WILEY275.l	24877	49	C9H12O	136



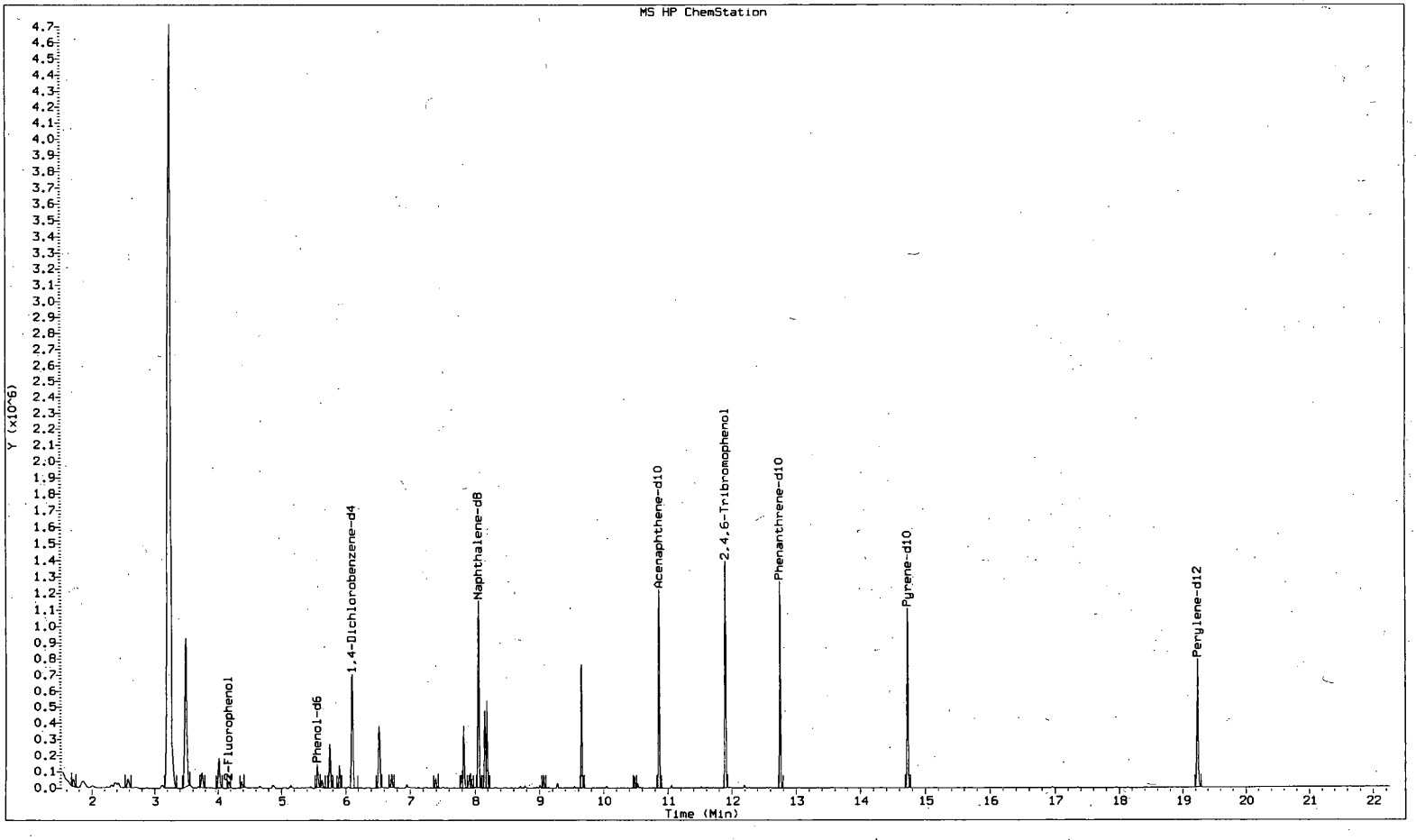






Digitally signed by Andrew J. Strebel on 03/02/2014 at 13:43.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb21a.b/db0988_lib.d
Operator : ceb05247
Acquired : 21-FEB-2014 22:09
Instrument : HP19760.i
Sample Name: H6011;7366680;1;0;SAMPLE;;;
Misc Info : 14050WAF;WL13166;;1051;1000;0;db0956;13166;
Vial Number: 9



Lancaster Labs

Data file : /chem/HP19760.i/14feb21a.b/db0988_lib.d
Lab Smp Id: 7366680 Client Smp ID: H6011
Inj Date : 21-FEB-2014 22:09
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H6011;7366680;1;0;SAMPLE;;;
Misc Info : 14050WAF;WL13166;;1051;1000;0;db0956;13166;
Comment : Max. number of TICs to report is 50, 22 TICs were found initially.
Method : /chem/HP19760.i/14feb21a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:02 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 9
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1051.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.106	1038643	10.000
* 48 Naphthalene-d8	8.059	1528866	10.000
* 83 Acenaphthene-d10	10.863	1380567	10.000

CONCENTRATIONS					QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.706	84398	0.81257613	0.77314	90	NIST05a.l	31325	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Toluene					CAS #: 108-88-3		
2.574	123285	1.18698491	1.12938	93	NIST05a.l	2400	21
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.256	14616465	140.726448	133.89766	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.495	1963065	18.9002741	17.98313	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.752	187221	1.80255099	1.71508	9	NIST05a.l	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.020	332277	3.19914500	3.04390	9	NIST05a.l	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.375	56113	0.54025614	0.51404	33	NIST05a.l	33655	21(L)
Cyclotetrasiloxane, octamethyl-					CAS #: 556-67-2		
5.634	63996	0.61614844	0.58624	91	NIST05a.l	122480	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.757	391189	3.76634451	3.58358	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.908	204417	1.96811503	1.87261	95	NIST05a.l	18488	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.520	604043	5.81569137	5.53348	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.713	119114	1.14682595	1.09117	78	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.394	69571	0.45505216	0.43297	90	NIST05a.l	161016	48
3-Amino-5-chloro-1-methyl-2(1H)-pyrazino					CAS #: 87486-43-9		
7.797	92016	0.60186077	0.57265	16	WILEY275.l	44515	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	497310	3.25280358	3.09496	46	WILEY275.l	22248	48(L)
2(1H)-Pyridinone, 5-chloro-3-hydroxy-					CAS #: 53233-89-9		
7.913	95053	0.62172256	0.59155	74	NIST05a.l	20504	48

Target compound.
Do not report.
ajs00193 03/02/2014

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUANT QUAL	LIBRARY	LIB ENTRY	CPND #
4-AMINO-3-CHLOROBENZENETHIOL				CAS #: 0-00-0			
7.948	60636	0.39660693	0.37736	14	WILEY275.l	44523	48
2,6-Dichloro-4-fluorophenol				CAS #: 392-71-2			
8.158	564931	3.69509418	3.51578	87	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-				CAS #: 21031-46-9			
8.187	660319	4.31900937	4.10942	50	NIST05a.l	3933	48
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc				CAS #: 63506-25-2			
9.061	99260	0.64924041	0.61773	78	WILEY275.l	109601	48
1,4-Dichlorophthalazine				CAS #: 4752-10-7			
9.656	916829	6.64096249	6.31870	38	NIST05a.l	56222	83
2-bromo-7,7-dichlorocyclo[4.1.0]heptan				CAS #: 113035-97-5			
10.478	74730	0.54129835	0.51503	91	WILEY275.l	127158	83

QC Flag Legend

L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

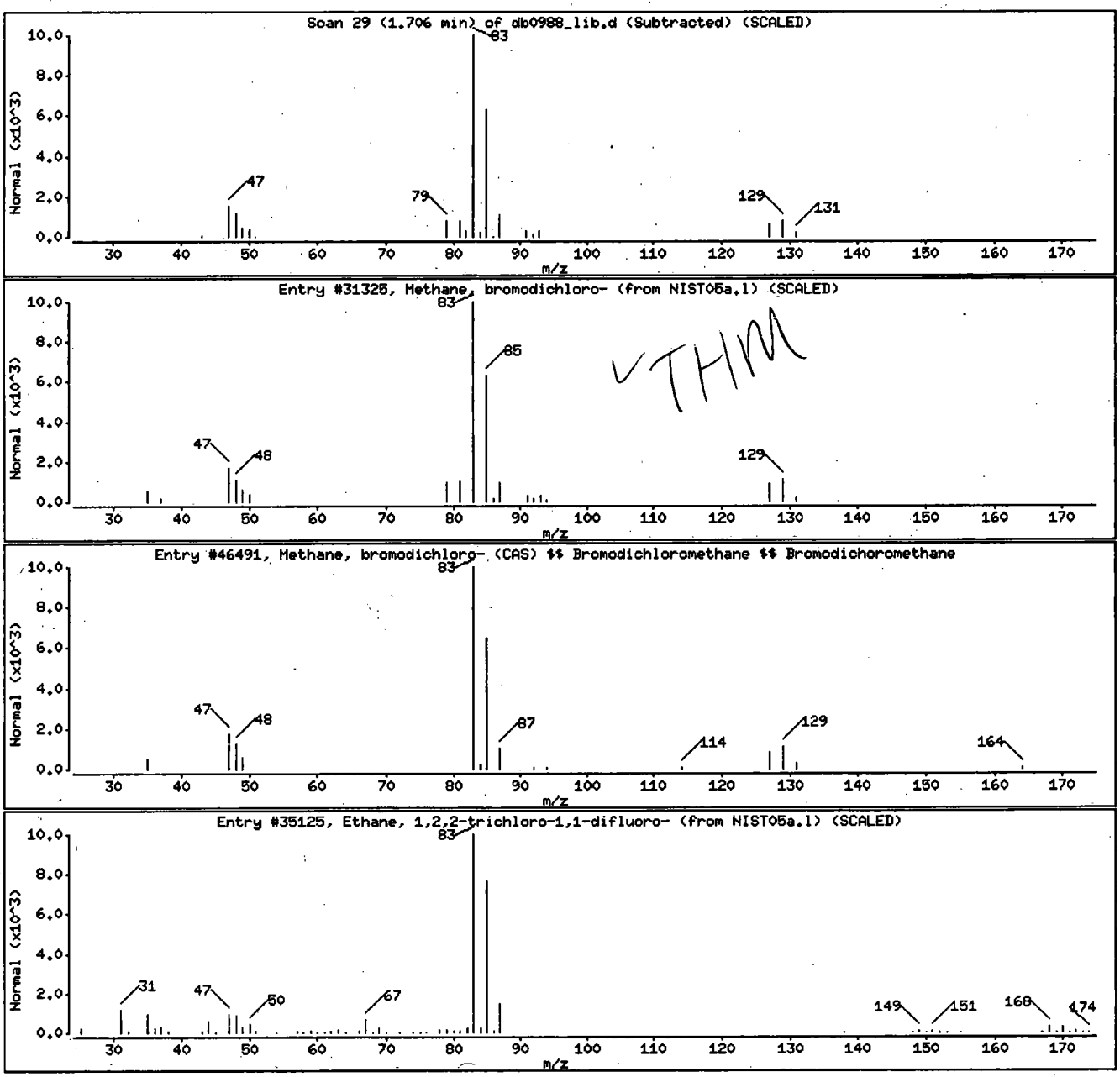
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46491	90	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

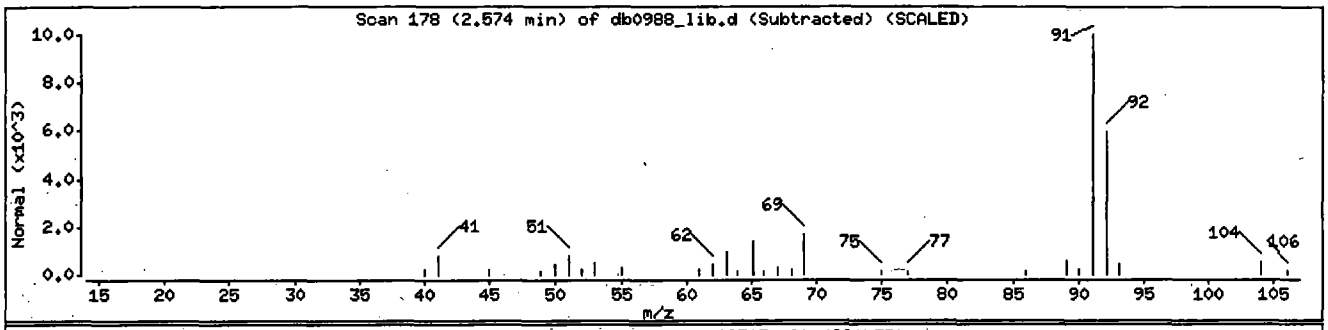
Volume Injected (uL): 1.0

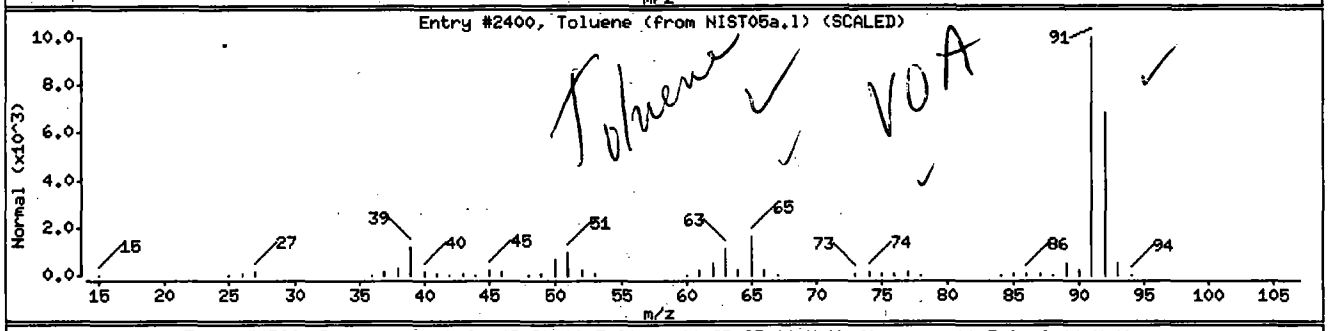
Operator: ceb05247

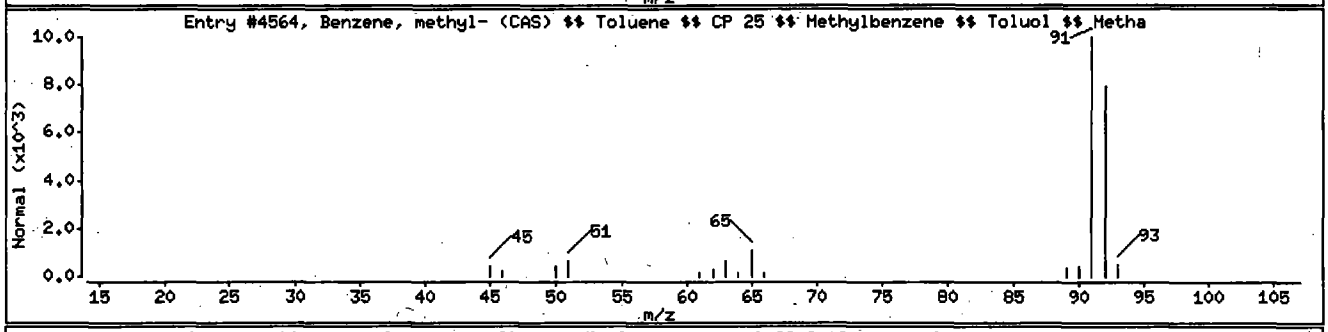
Column phase: J&W DB-5MS

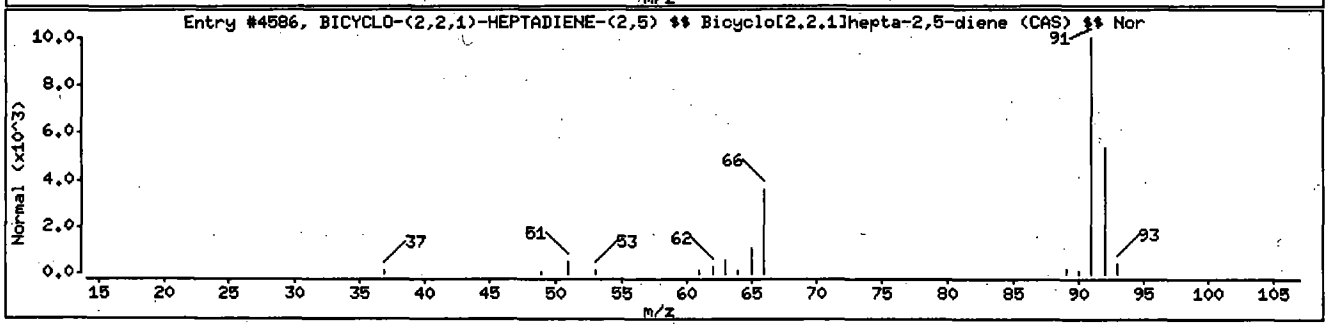
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Toluene	108-88-3	NIST05a.l	2400	93	C7H8	92
Benzene, methyl- (CAS) $$ Toluene $$ CP	108-88-3	WILEY275.l	4564	81	C7H8	92
BICYCLO-(2,2,1)-HEPTADIENE-(2,5) $$ Bicy	121-46-0	WILEY275.l	4586	74	C7H8	92









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

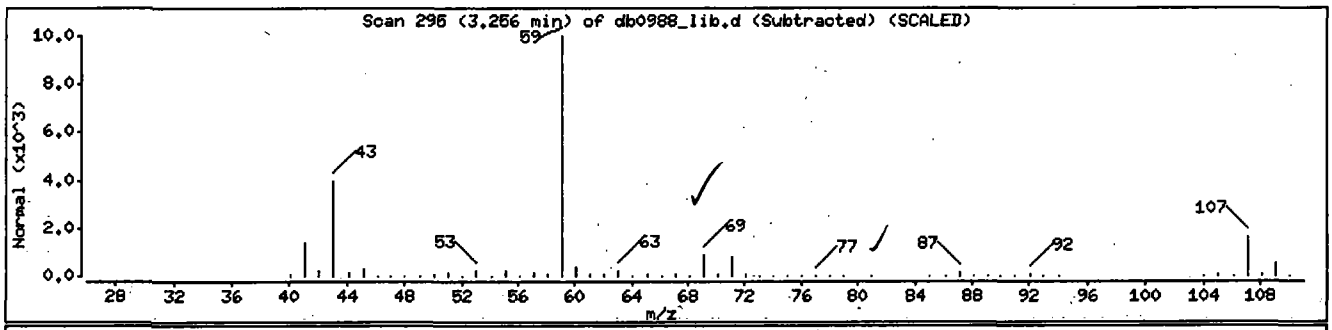
Volume Injected (uL): 1.0

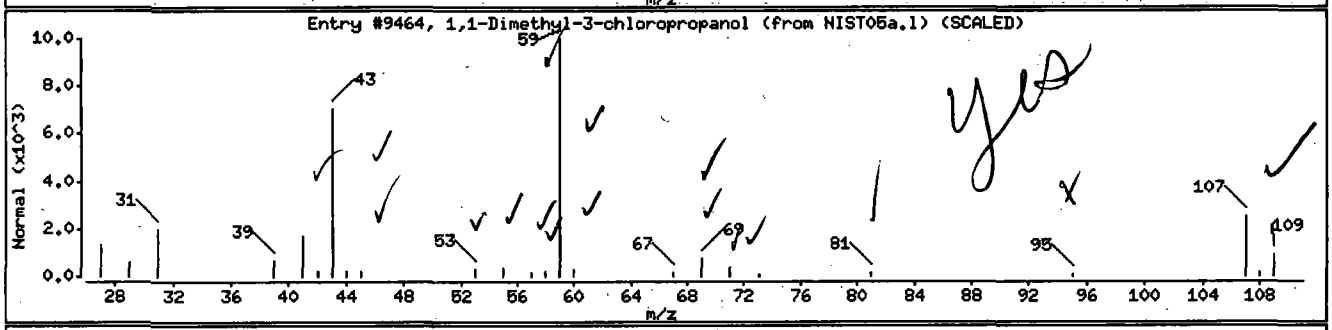
Operator: ceb05247

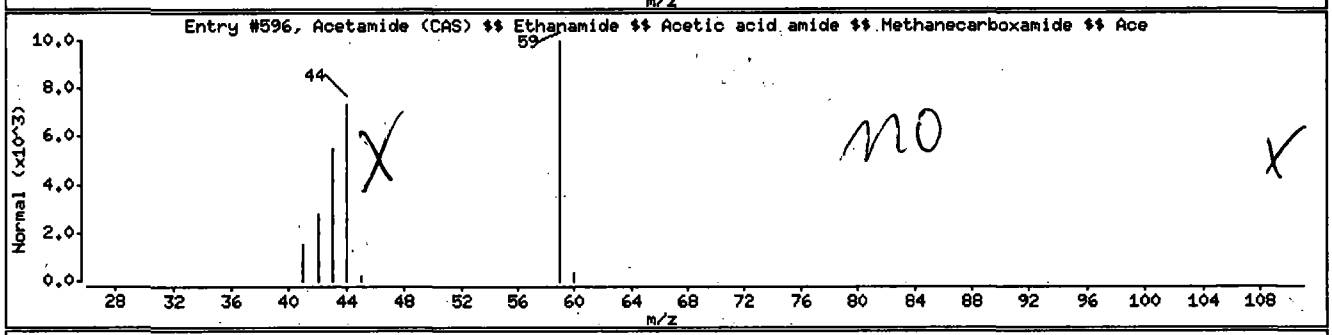
Column phase: J&W DB-5MS

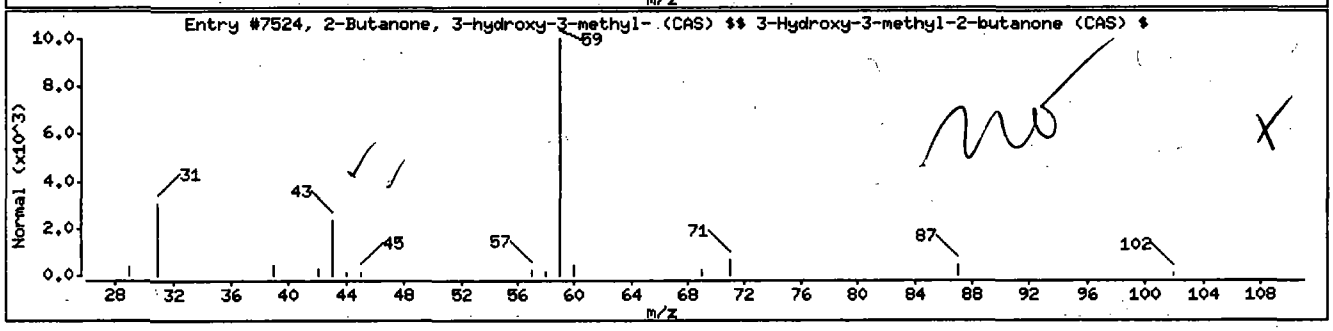
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	596	45	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	42	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

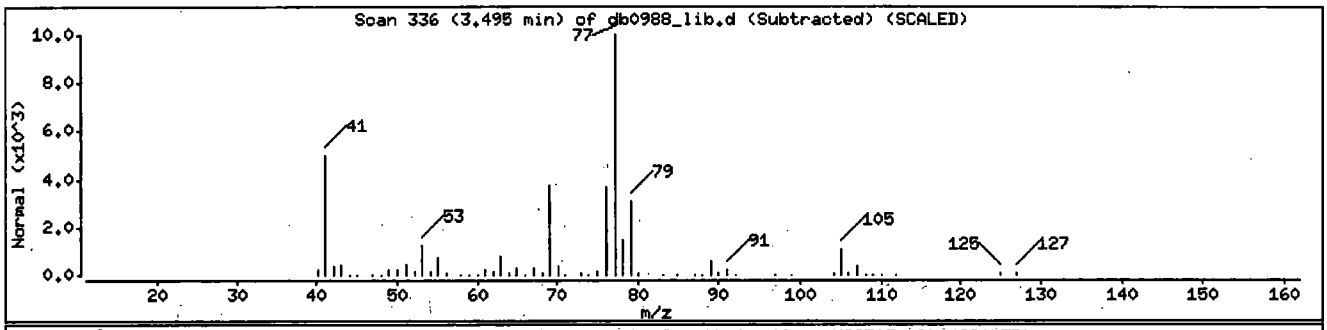
Volume Injected (uL): 1.0

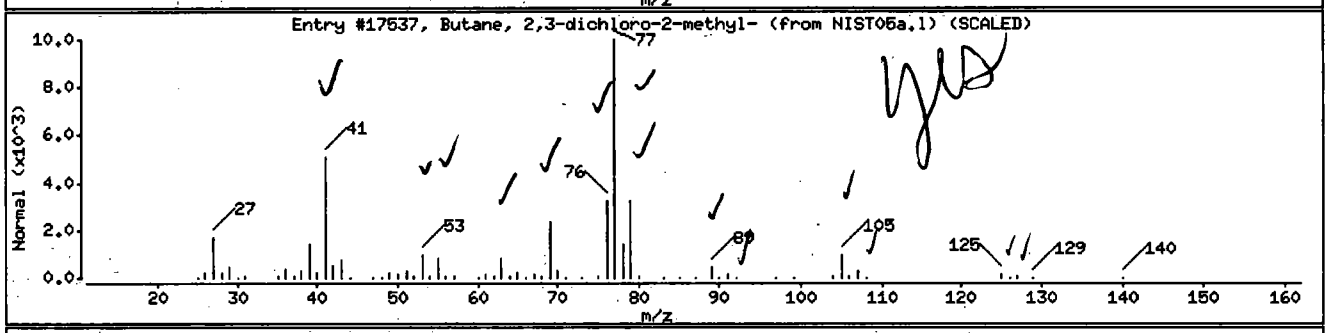
Operator: ceb05247

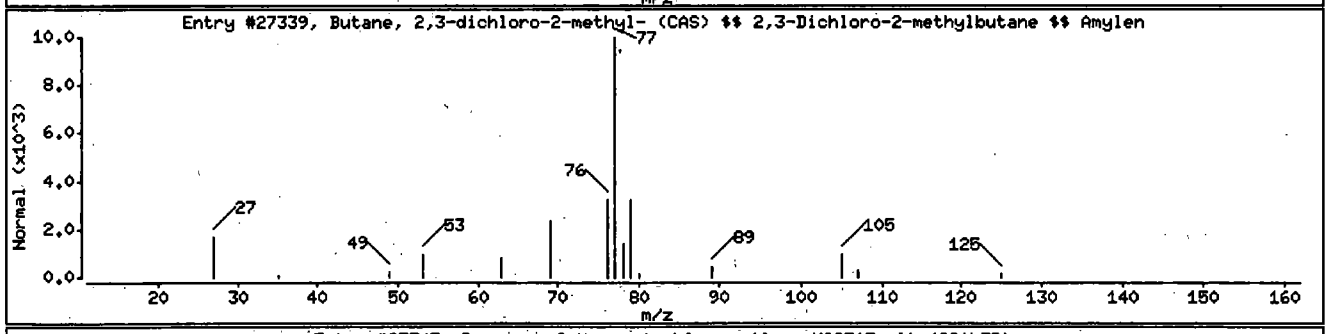
Column phase: J&W DB-5MS

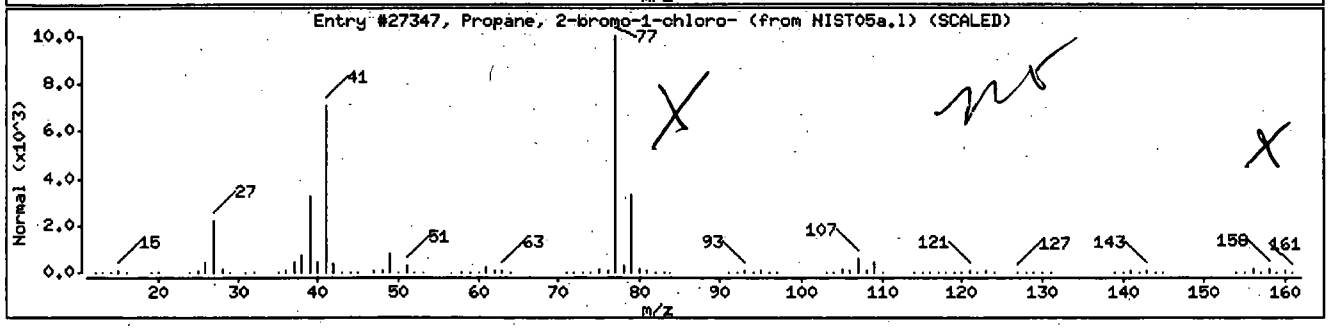
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17637	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	47	C3H6BrCl	156









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14:
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

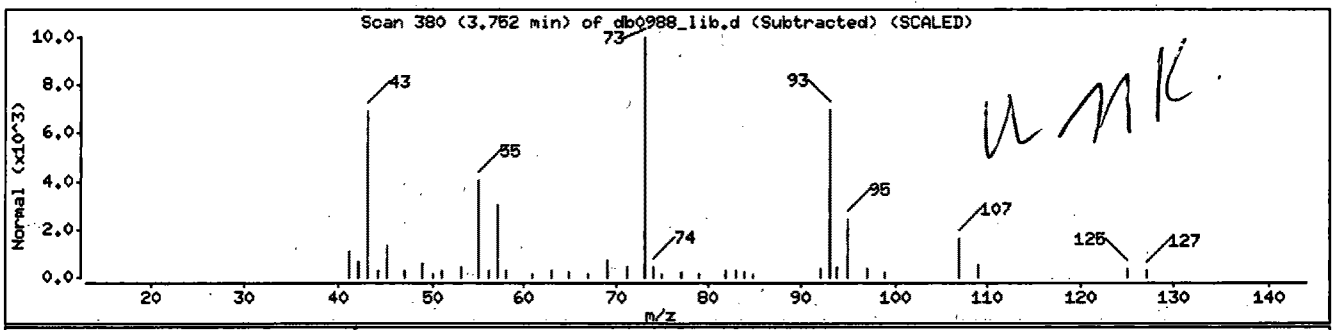
Volume Injected (uL): 1.0

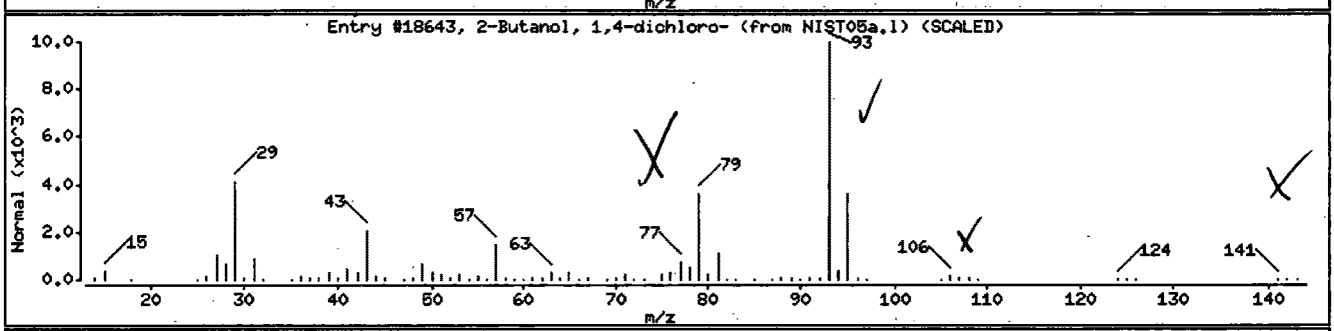
Operator: ceb05247

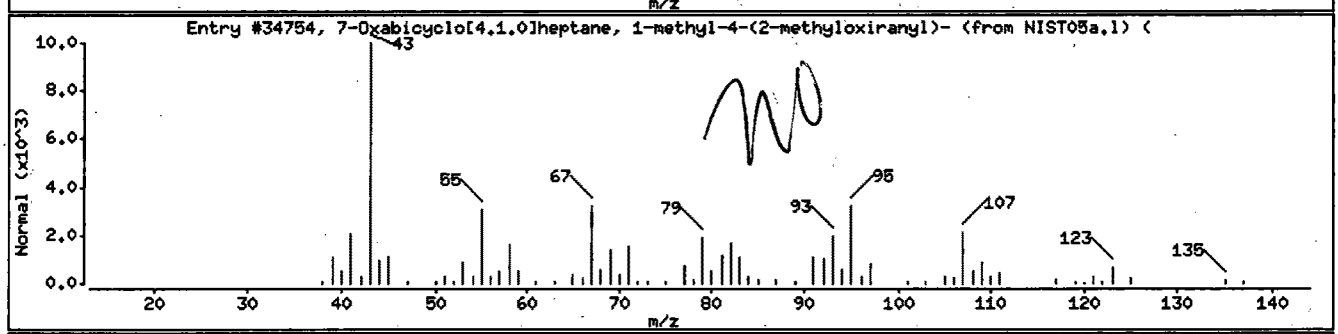
Column phase: J&W DB-5MS

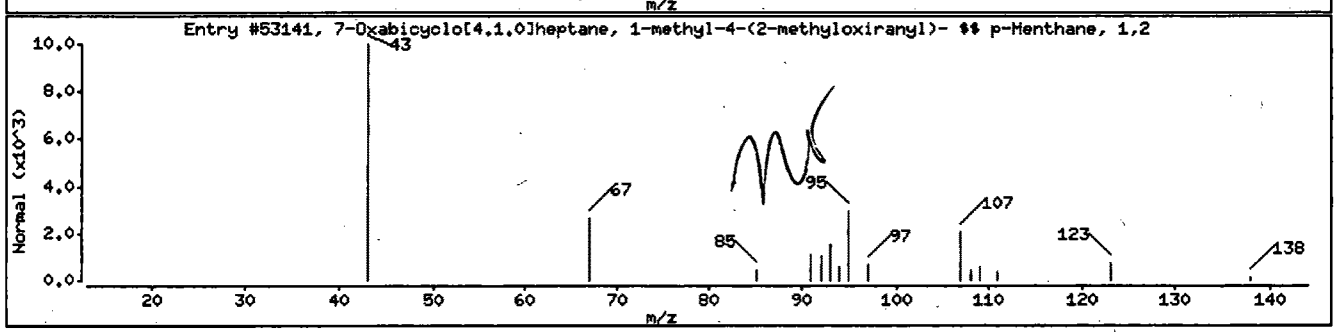
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	9	C4H8Cl2O	142
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	NIST05a.l	34754	12	C10H16O2	168
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	WILEY275.l	53141	12	C10H16O2	168









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

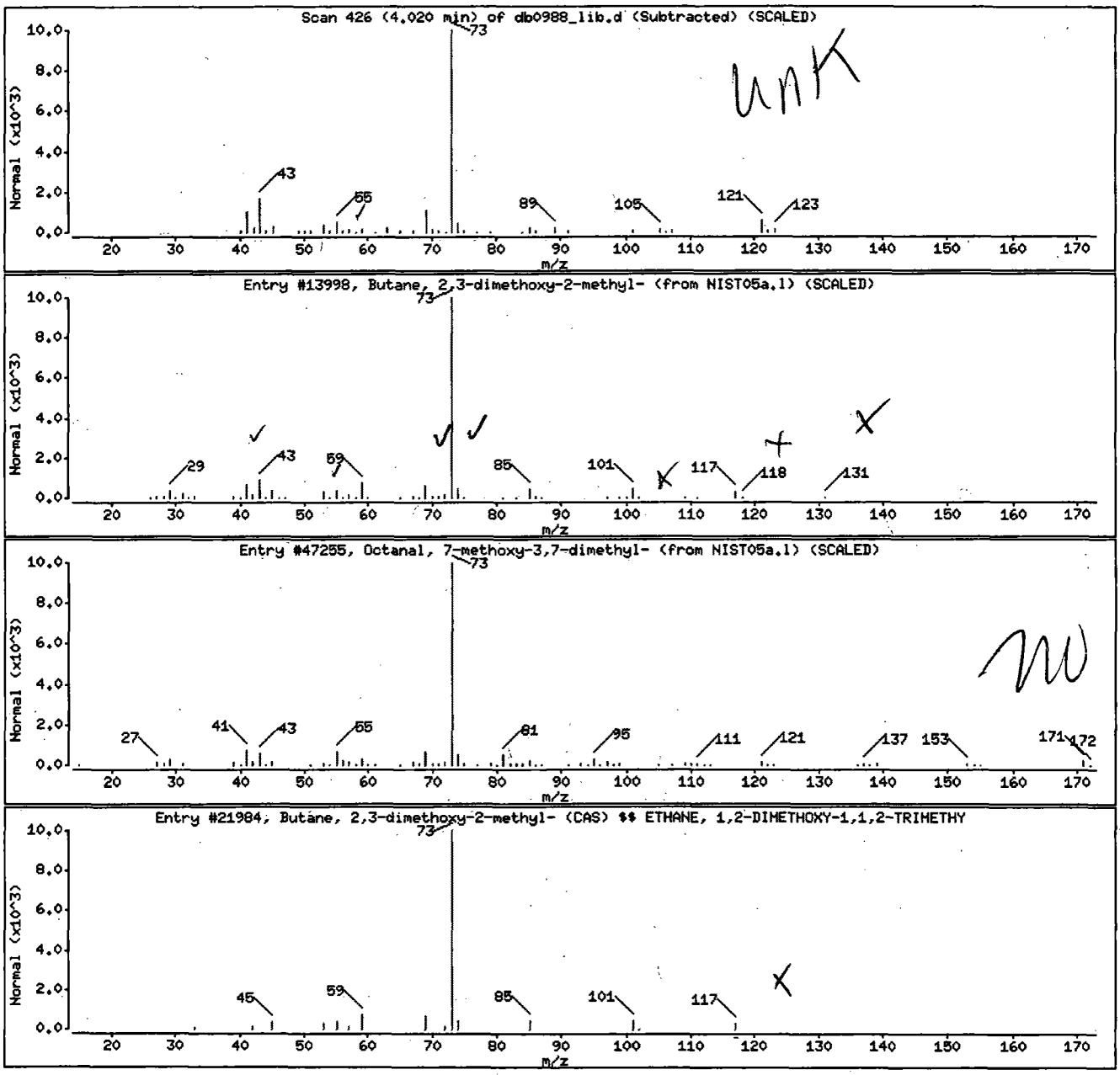
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	9	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	38	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

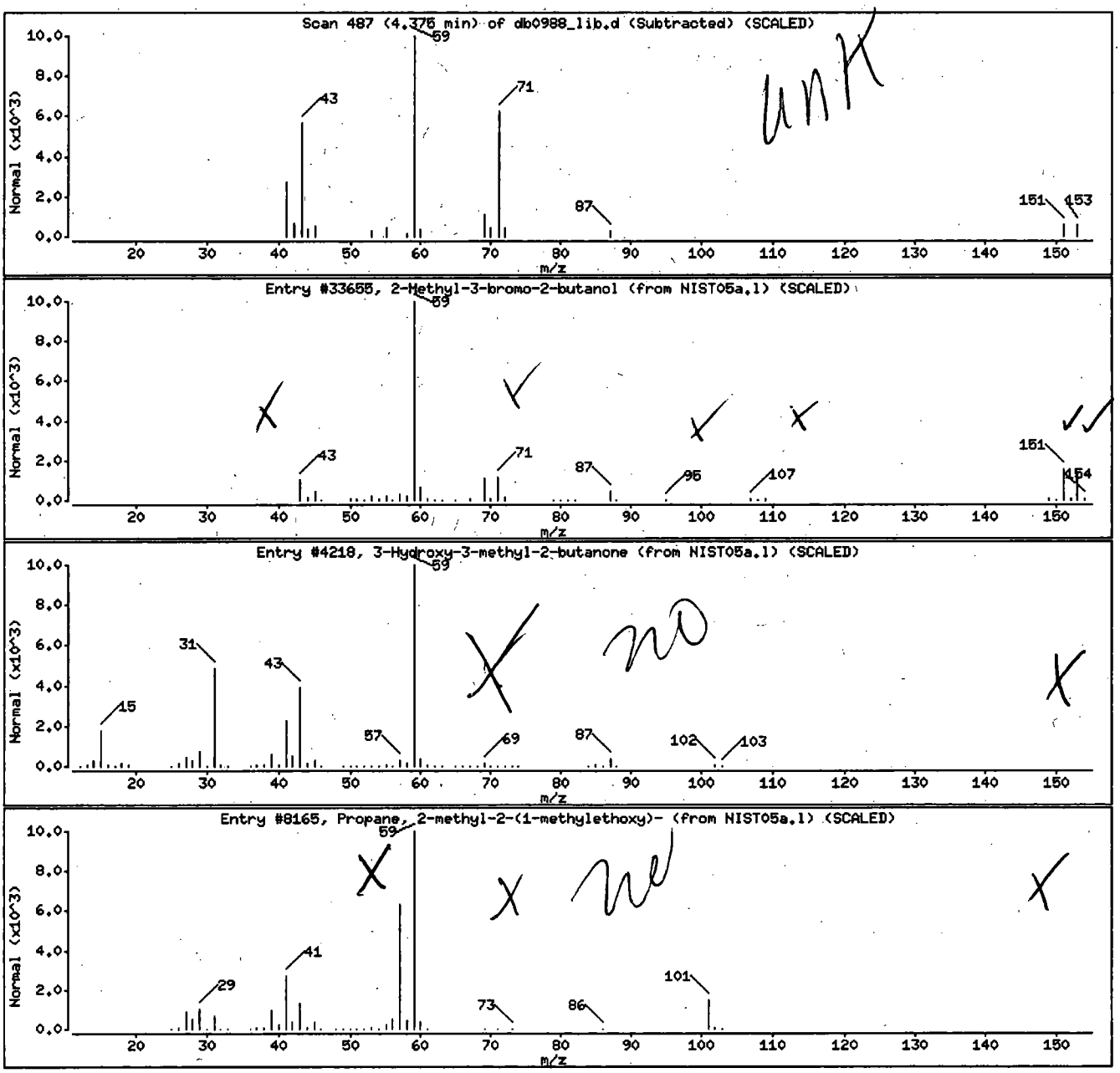
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	37	C5H11BrO	166
3-Hydroxy-3-methyl-2-butanone	115-22-0	NIST05a.l	4218	43	C5H10O2	102
Propane, 2-methyl-2-(1-methylethoxy)-	17348-59-3	NIST05a.l	8165	37	C7H16O	116



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

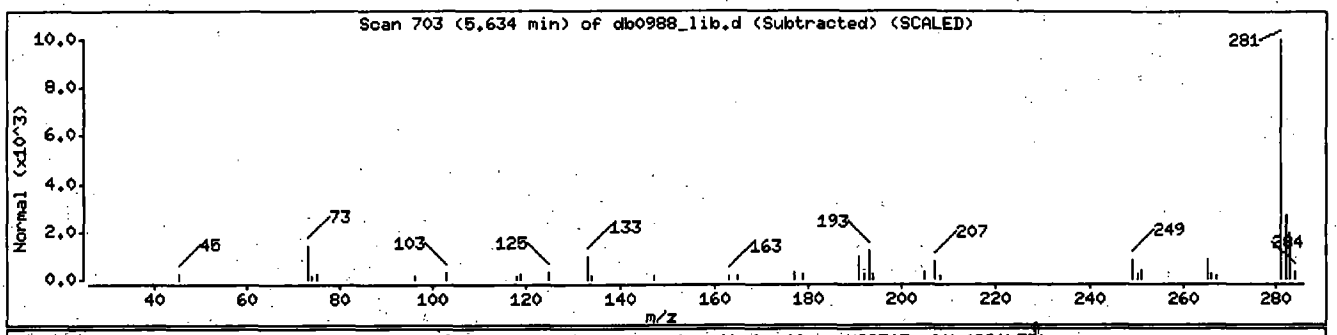
Volume Injected (uL): 1.0

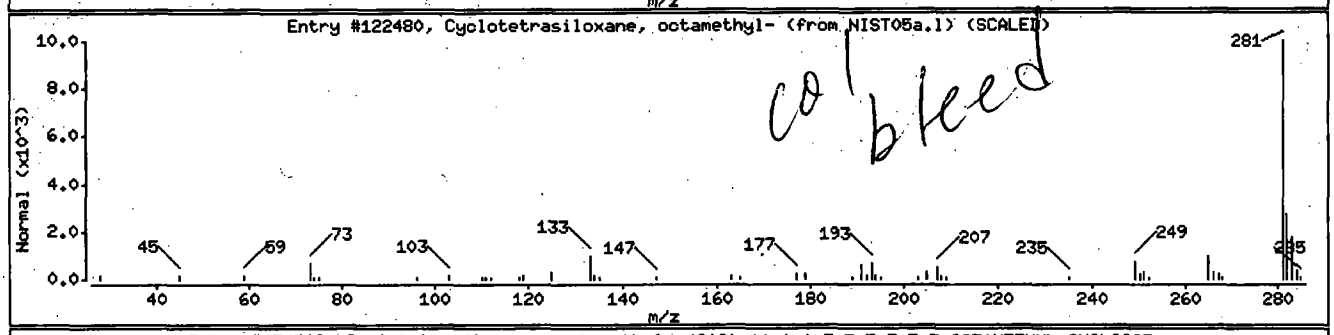
Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclotetrasiloxane, octamethyl-	556-67-2	NIST05a.l	122480	91	C8H24O4Si4	296
Cyclotetrasiloxane, octamethyl- (CAS) $$	556-67-2	WILEY275.l	174362	91	C8H24O4Si4	296
7H-Dibenzo[b,g]carbazole, 7-methyl-	3557-49-1	NIST05a.l	112705	53	C21H15N	281





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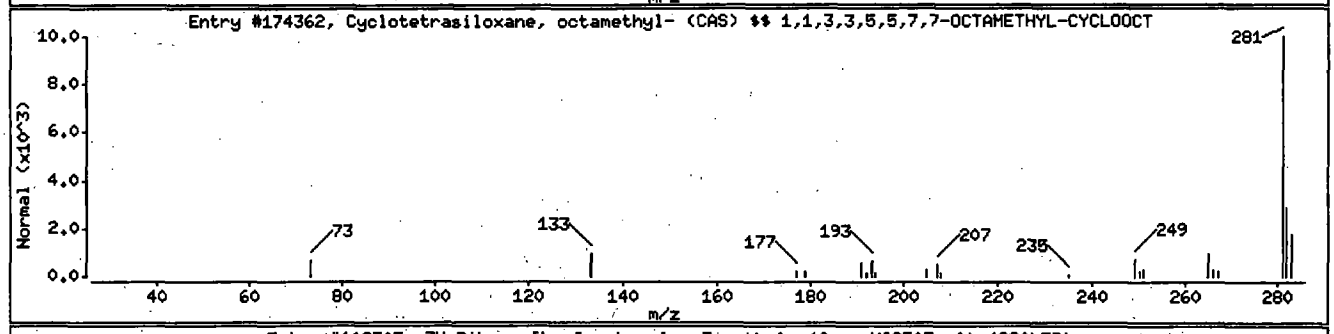

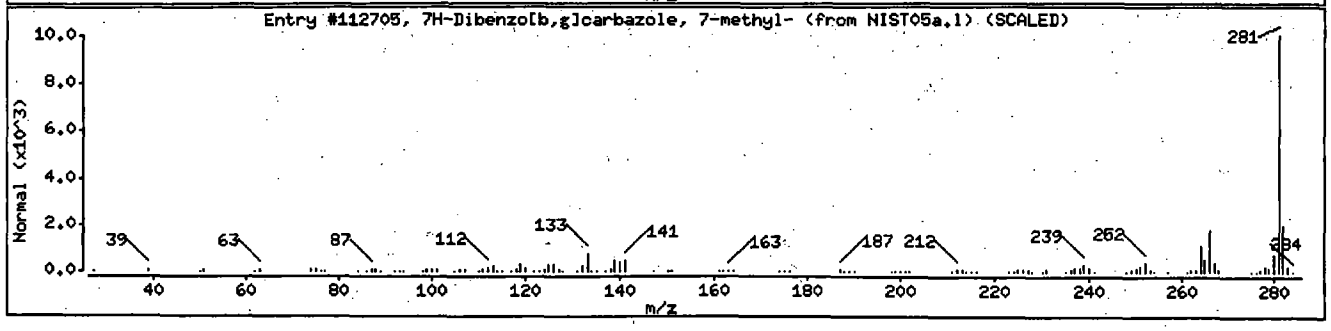

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

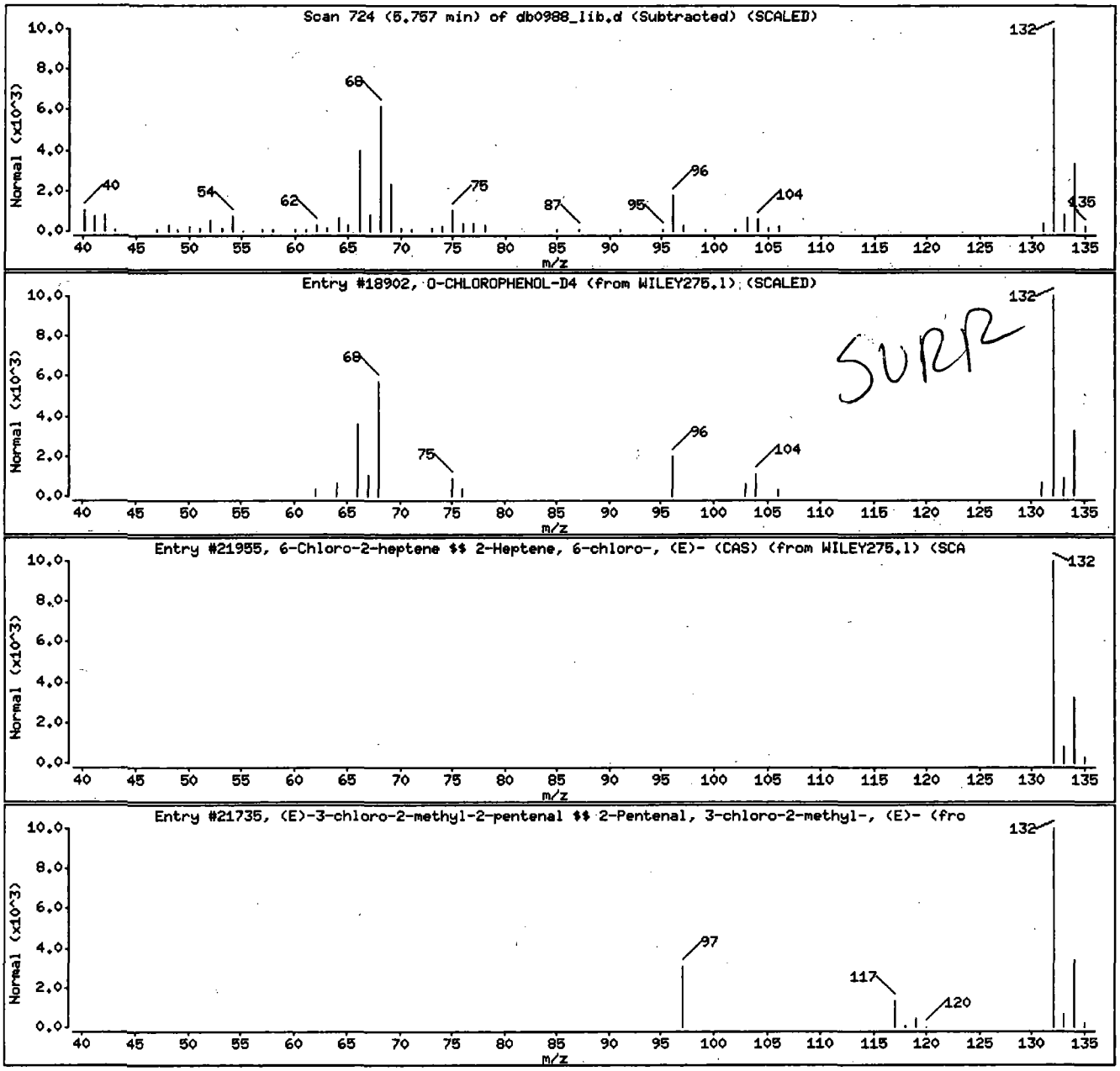
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

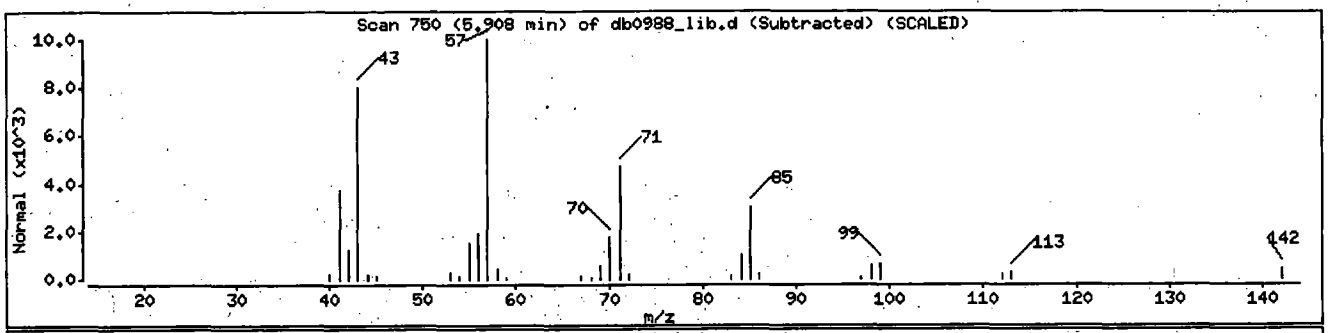
Client ID: H6011 Instrument: HP19760.i

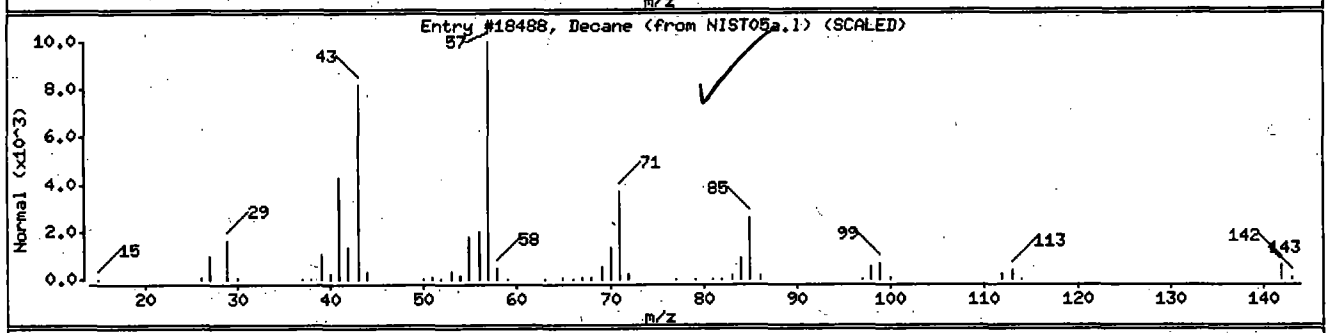
Sample Info: H6011;7366680;1;0;SAMPLE;;;

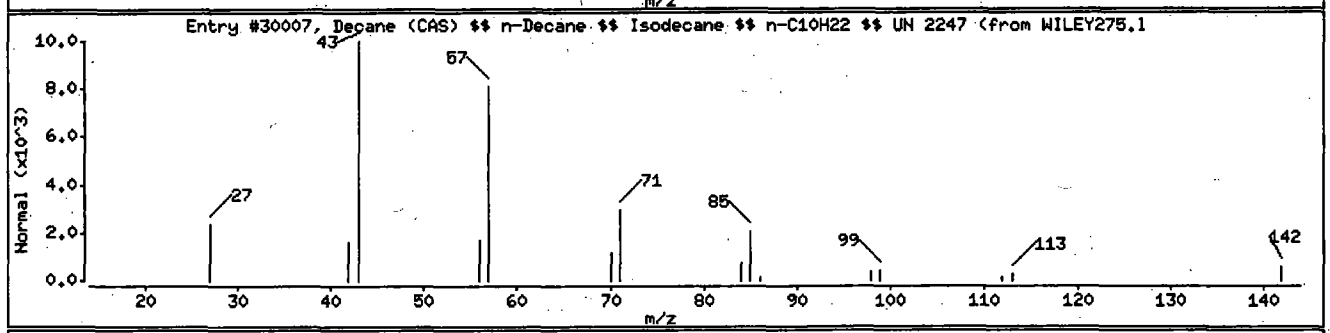
Volume Injected (uL): 1.0 Operator: ceb05247

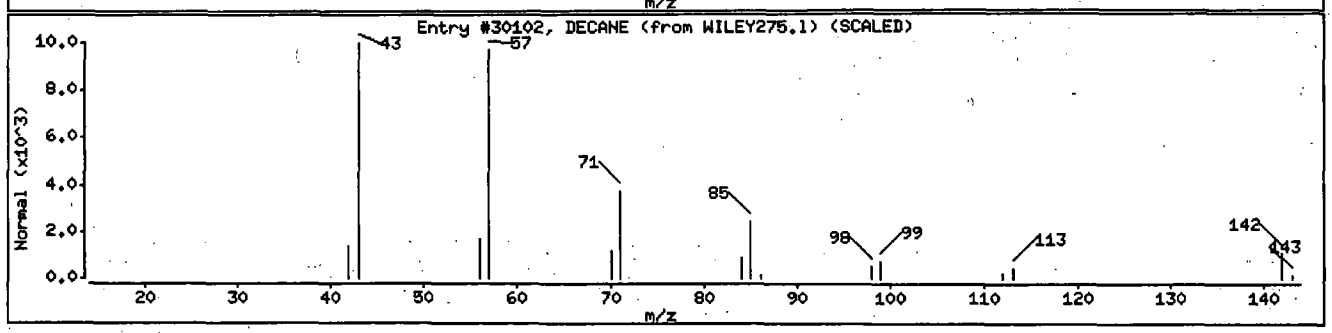
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18488	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Date : 21-FEB-2014 22:09

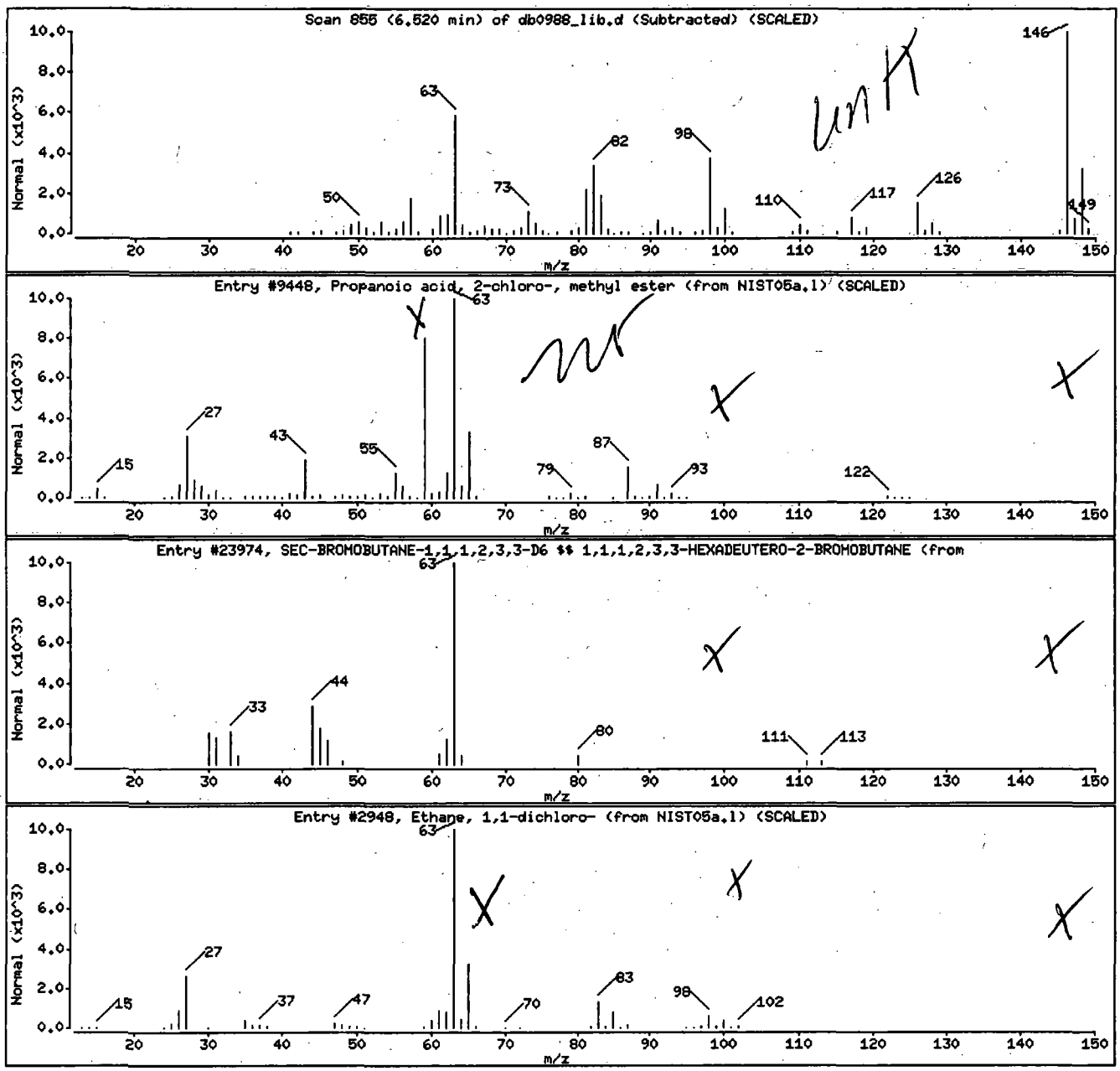
Client ID: H6011 Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	25	C2H4Cl2	98



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

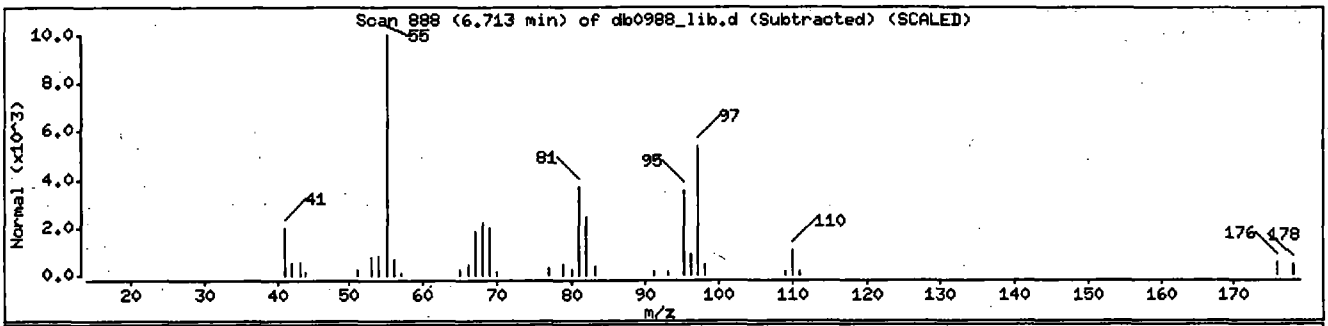
Volume Injected (uL): 1.0

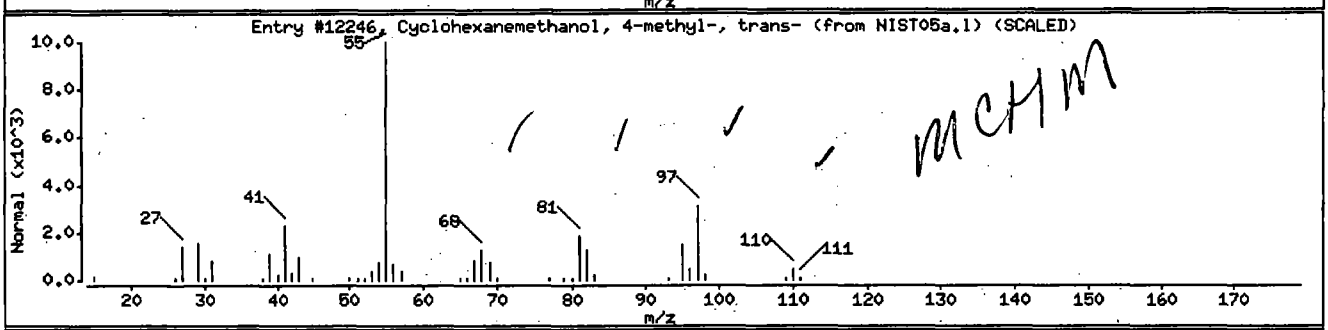
Operator: ceb05247

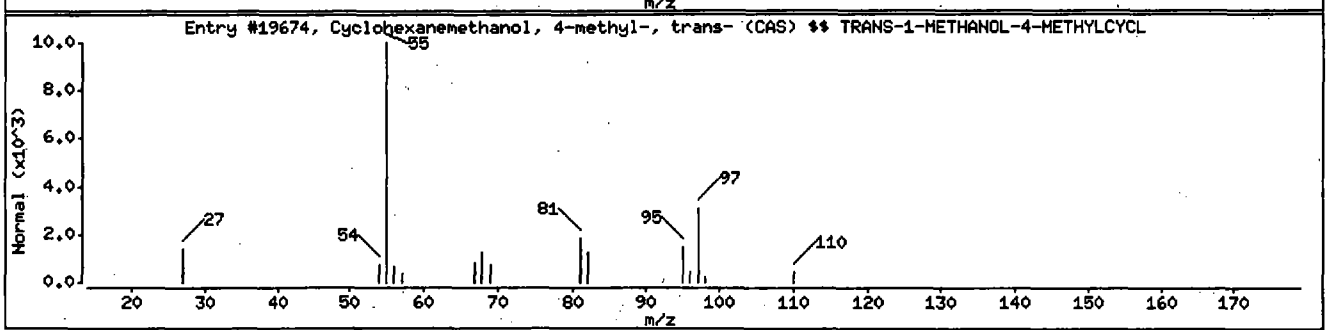
Column phase: J&W DB-5MS

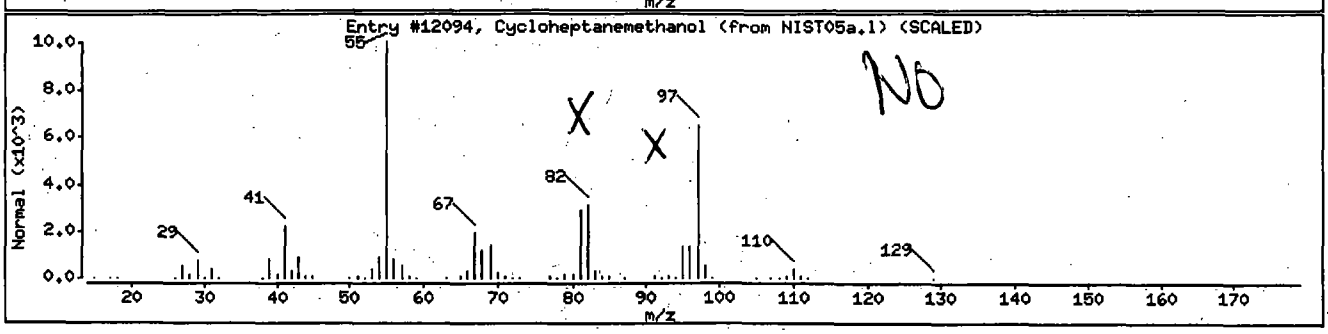
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	78	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	78	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12094	53	C8H16O	128









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Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

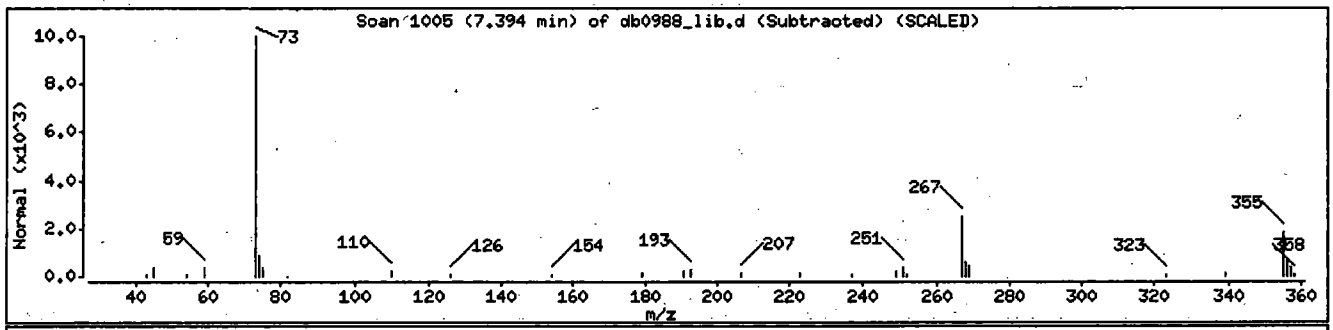
Volume Injected (uL): 1.0

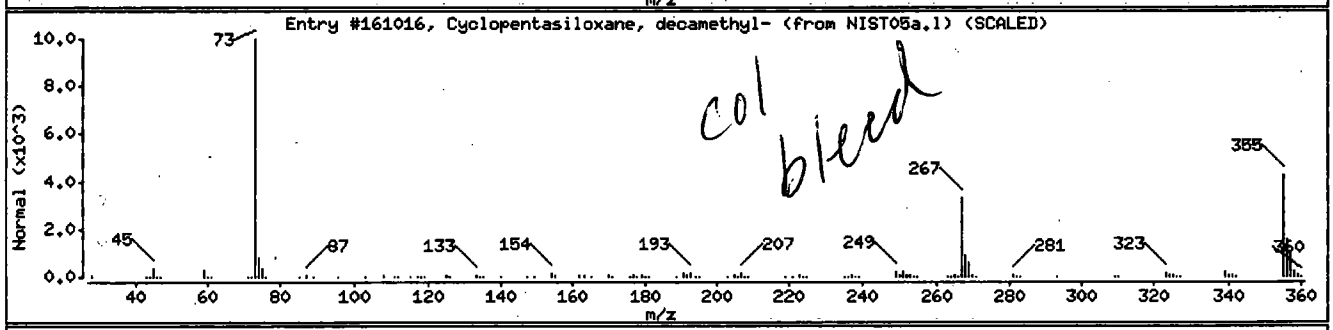
Operator: ceb05247

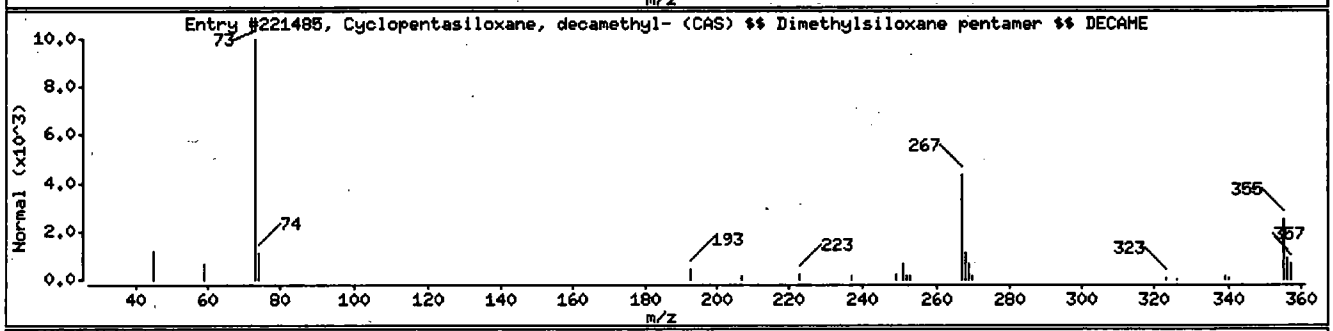
Column phase: J&W DB-5MS

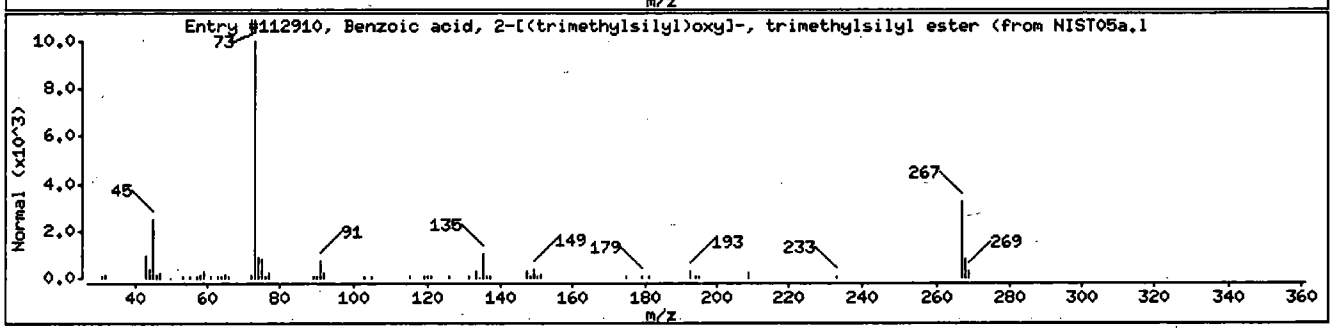
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	87	C10H30O5Si5	370
Benzoic acid, 2-[(trimethylsilyl)oxy]-,	3789-85-3	NIST05a.l	112910	38	C13H22O3Si2	282









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Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

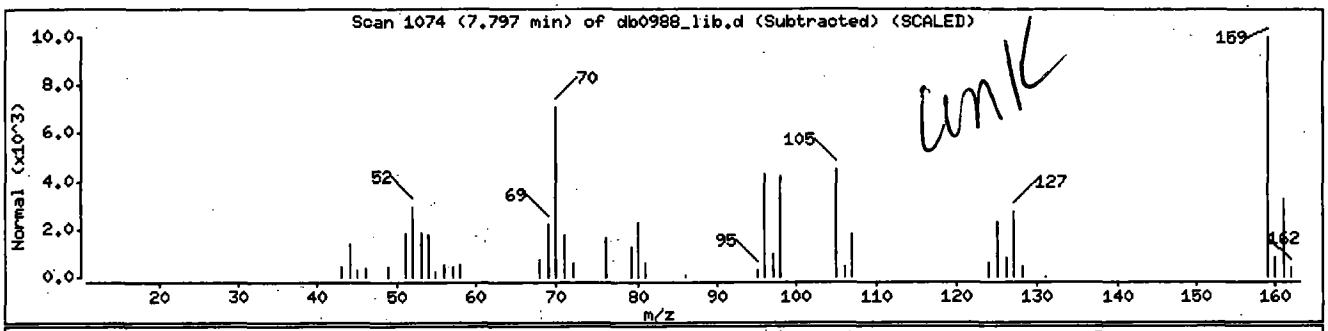
Volume Injected (uL): 1.0

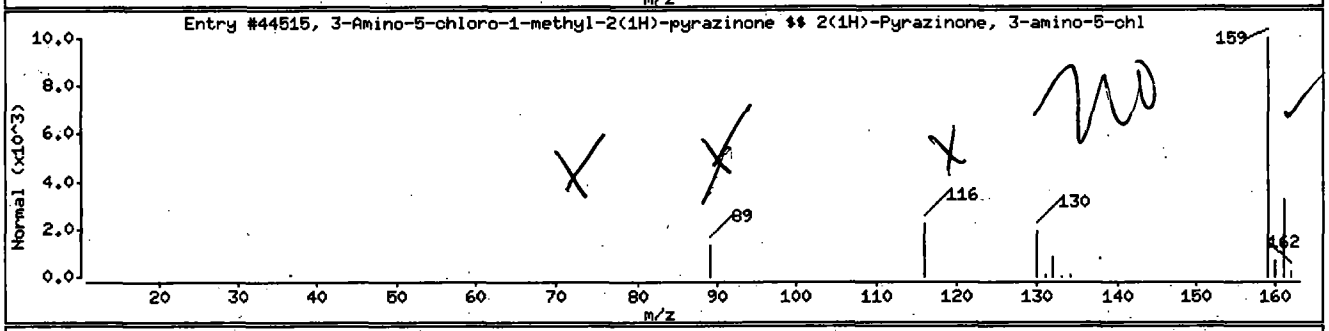
Operator: ceb05247

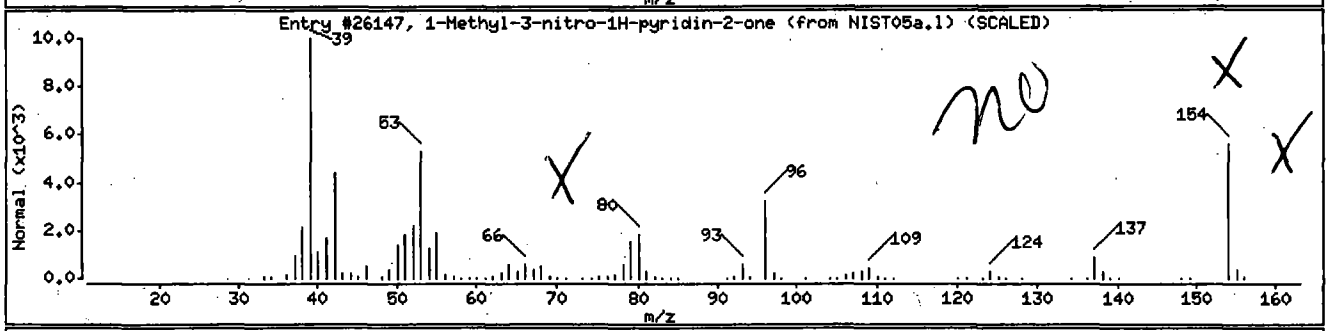
Column phase: J&W DB-5MS

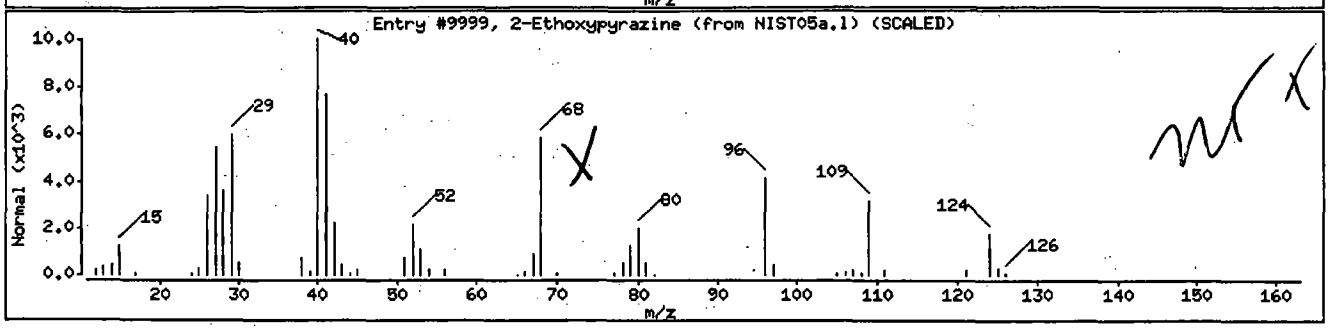
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Amino-5-chloro-1-methyl-2(1H)-pyrazino	87486-43-9	WILEY275.l	44515	16	C5H6ClN3O	159
1-Methyl-3-nitro-1H-pyridin-2-one	32896-91-6	NIST05a.l	26147	10	C6H6N2O3	154
2-Ethoxypyrazine	38028-67-0	NIST05a.l	9999	10	C6H8N2O	124









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Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

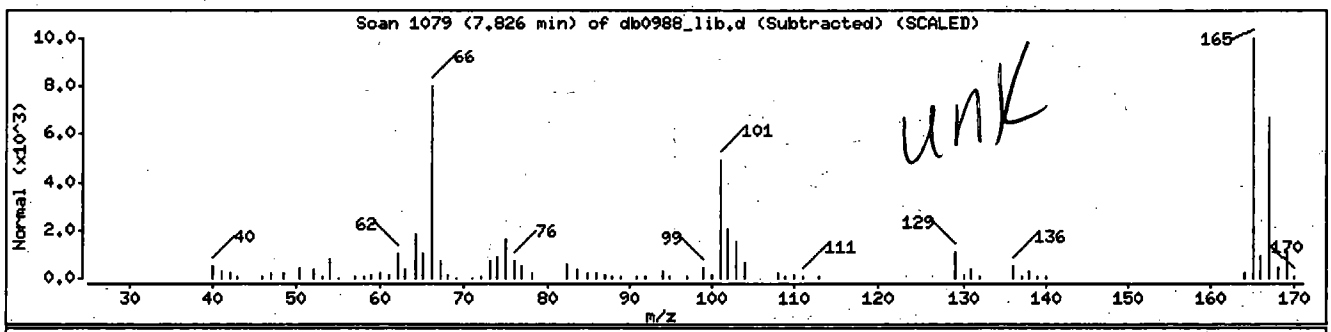
Volume Injected (uL): 1.0

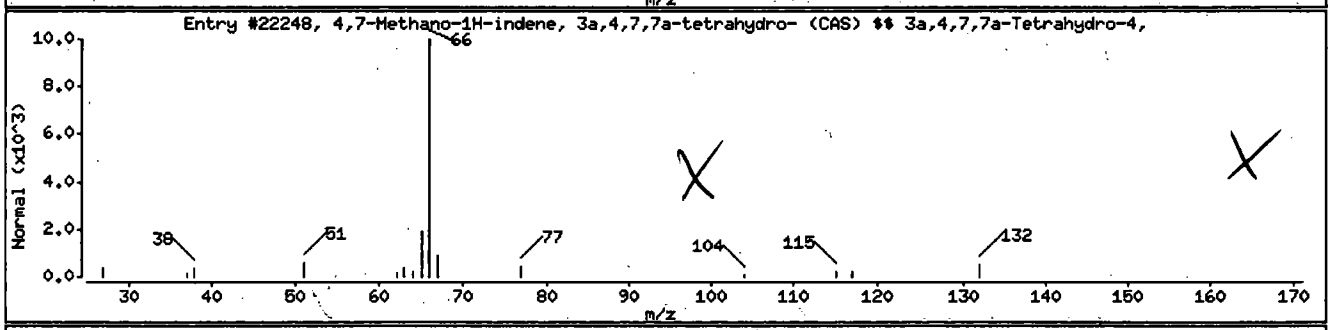
Operator: ceb05247

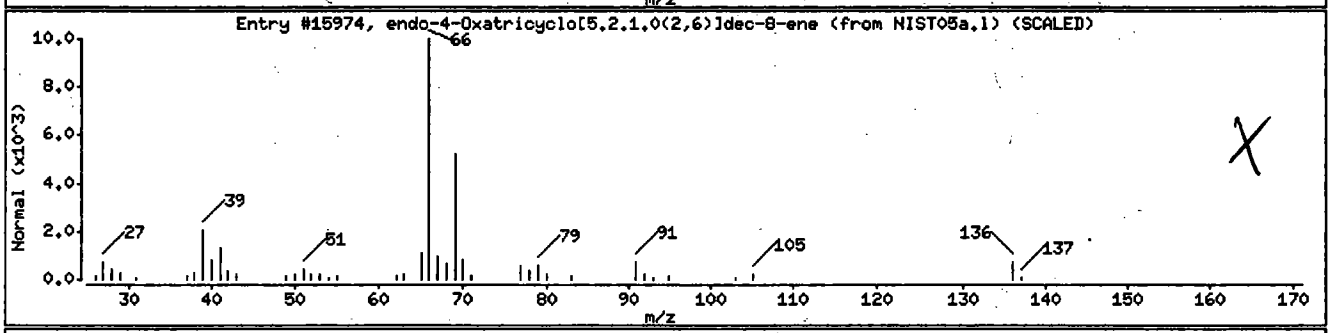
Column phase: J&W DB-5MS

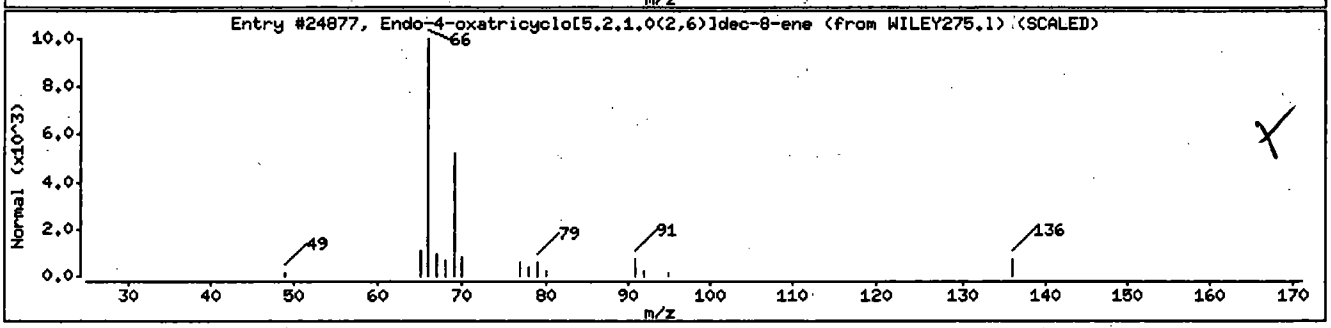
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22248	46	C10H12	132
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	46	C9H12O	136
Endo-4-oxatricyclo[5.2.1.0(2,6)]dec-8-en	0-00-0	WILEY275.l	24877	46	C9H12O	136









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Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

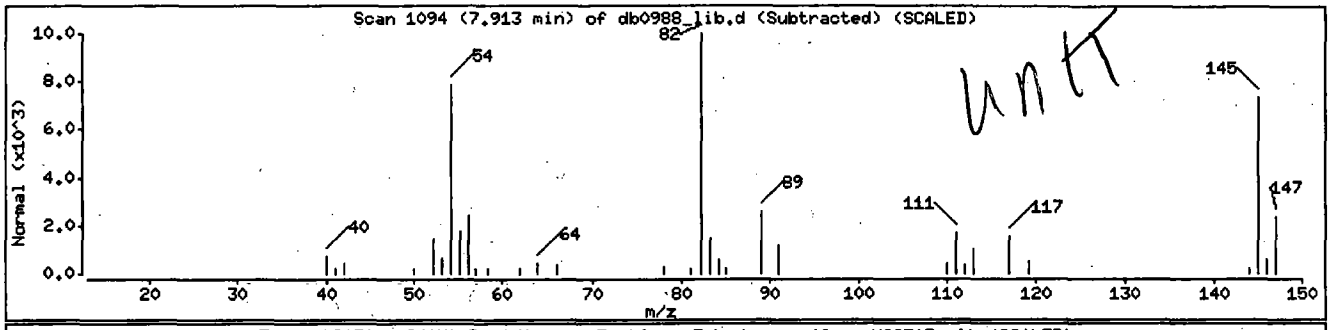
Volume Injected (uL): 1.0

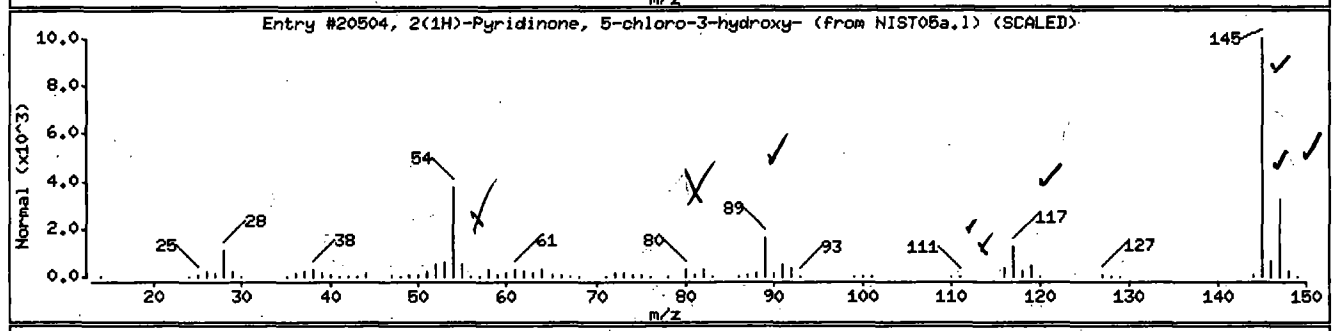
Operator: oeb05247

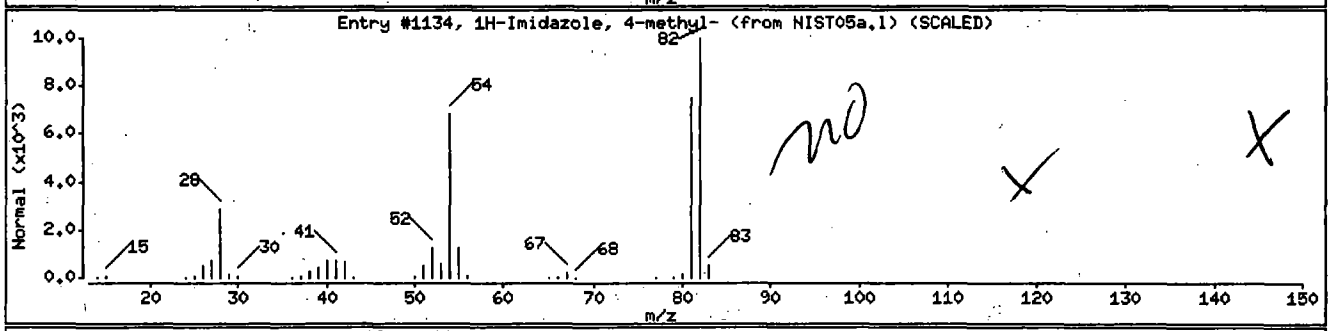
Column phase: J&W DB-5MS

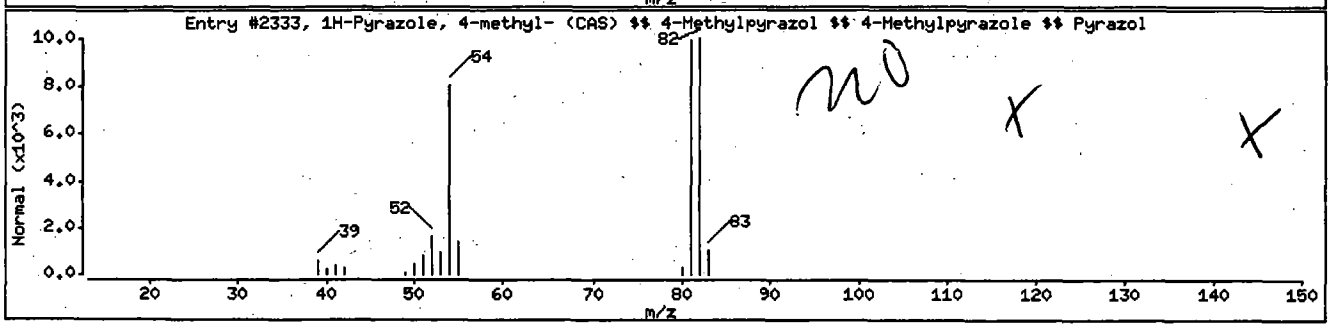
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2(1H)-Pyridinone, 5-chloro-3-hydroxy-	53233-89-9	NIST05a.l	20504	74	C5H4ClNO2	145
1H-Imidazole, 4-methyl-	822-36-6	NIST05a.l	1134	58	C4H6N2	82
1H-Pyrazole, 4-methyl- (CAS) $$ 4-Methyl	7554-65-6	WILEY275.l	2333	53	C4H6N2	82









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Date : 21-FEB-2014 22:09

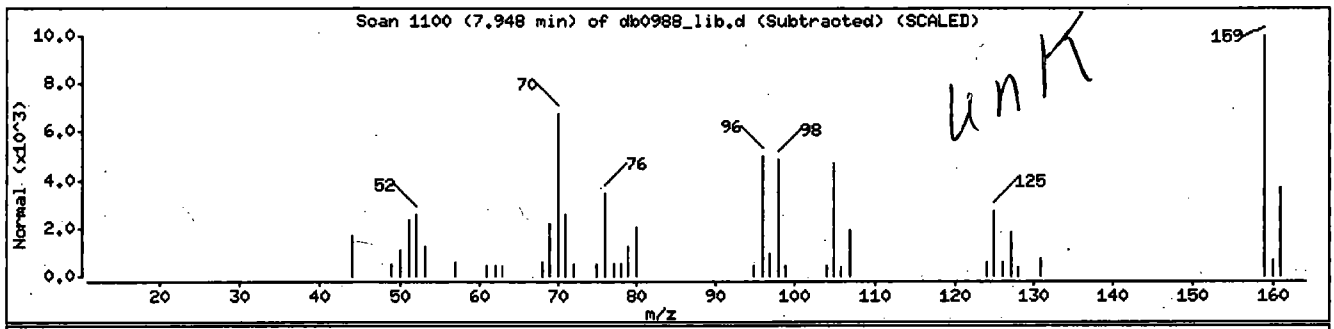
Client ID: H6011 Instrument: HP19760.i

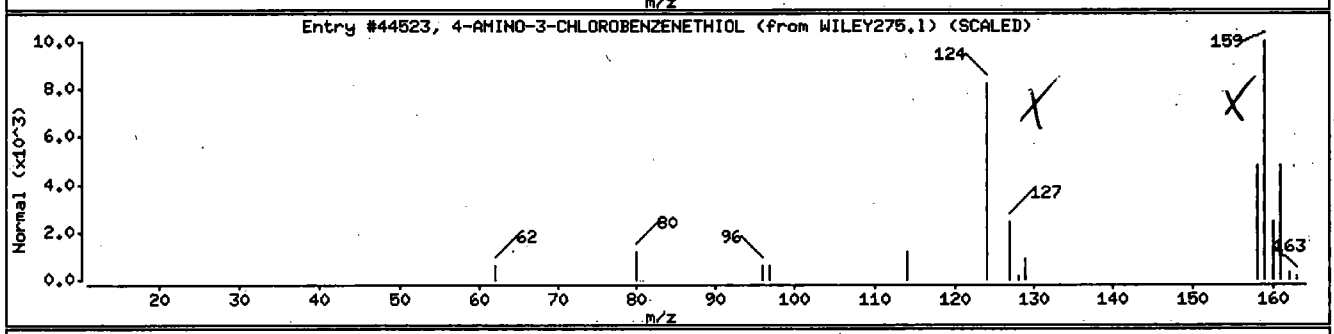
Sample Info: H6011;7366680;1;0;SAMPLE;;;

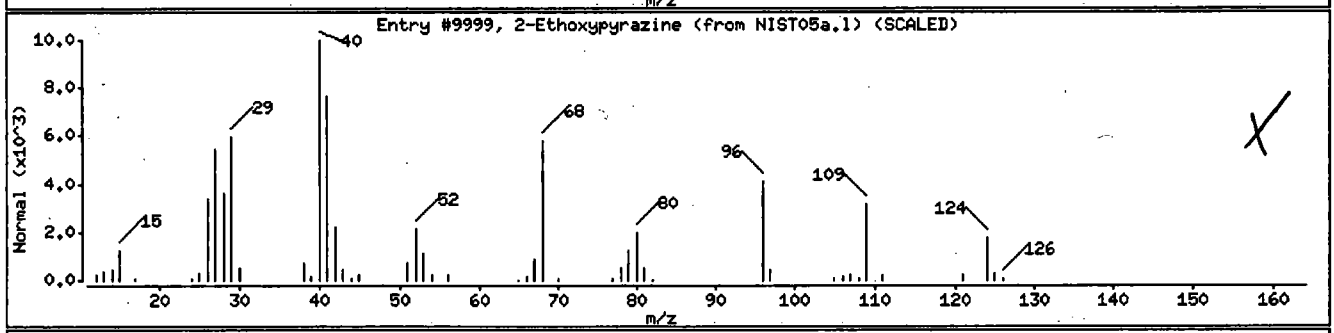
Volume Injected (uL): 1.0 Operator: ceb05247

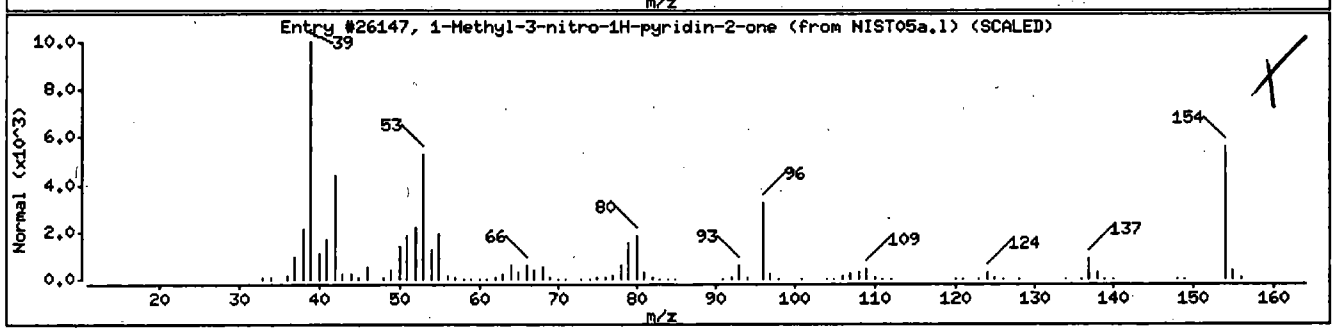
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4-AMINO-3-CHLOROBENZENETHIOL	0-00-0	WILEY275.l	44523	14	C6H6ClNS	159
2-Ethoxypyrazine	38028-67-0	NIST05a.l	9999	12	C6H8N2O	124
1-Methyl-3-nitro-1H-pyridin-2-one	32896-91-6	NIST05a.l	26147	10	C6H6N2O3	154









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Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

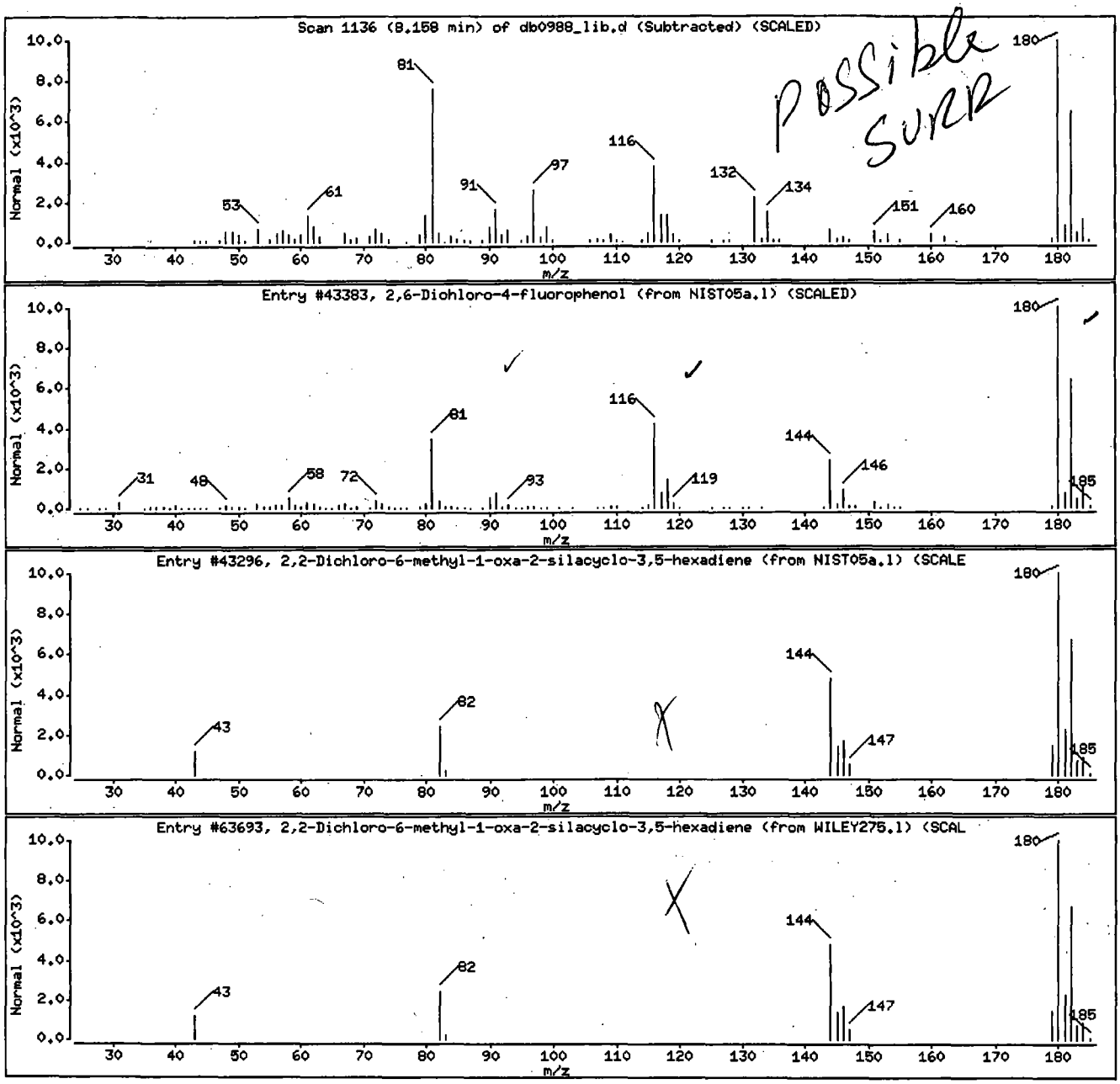
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	87	C6H3C12FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	35	C5H6C12OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	35	C5H6C12OSi	180



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Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

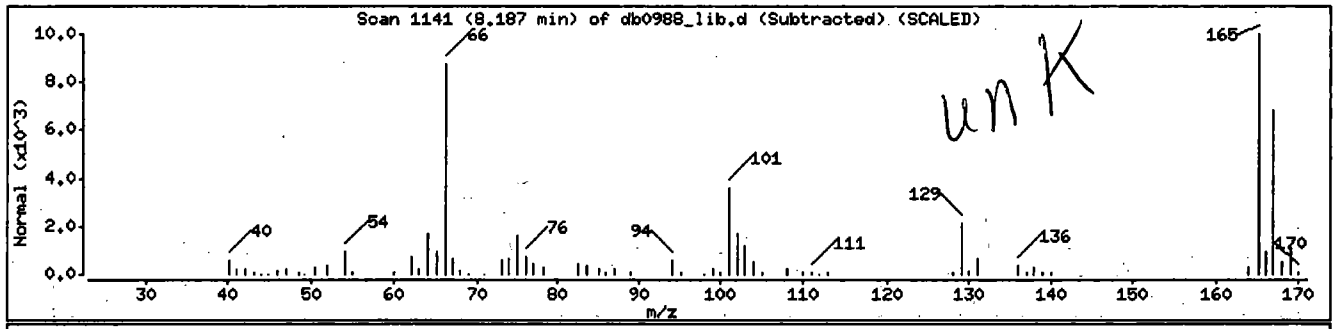
Volume Injected (uL): 1.0

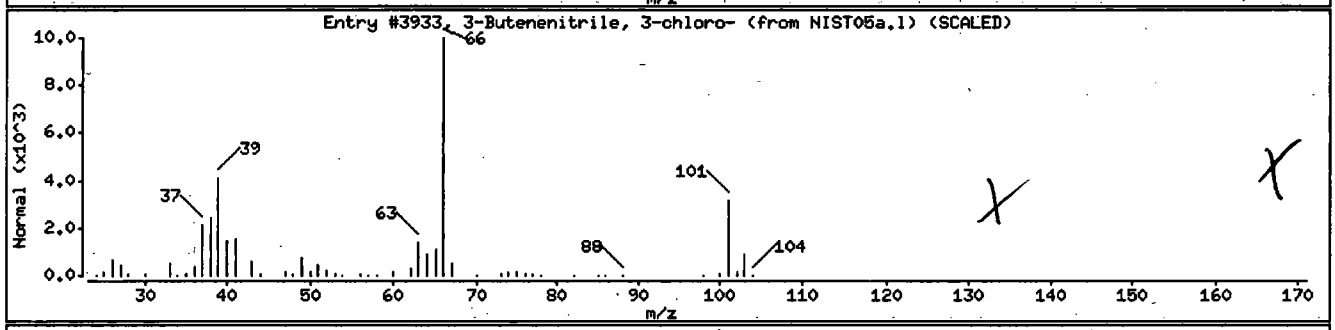
Operator: ceb05247

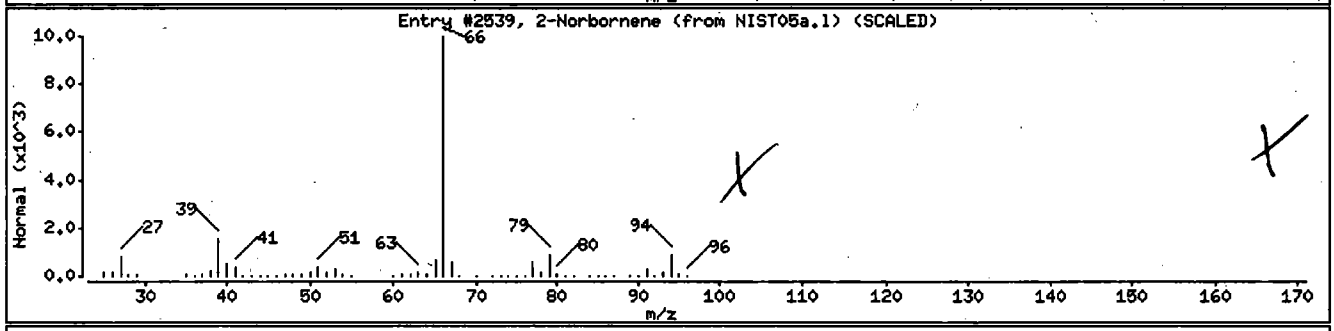
Column phase: J&W DB-5MS

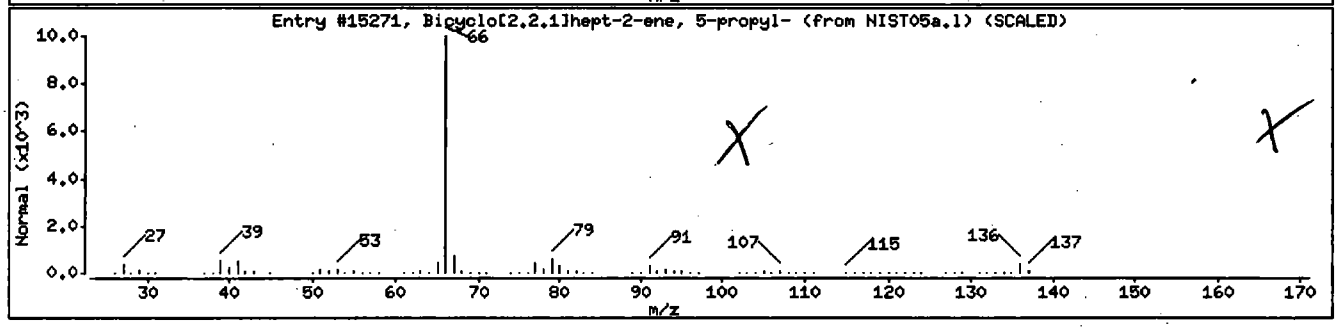
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
2-Norbornene	498-66-8	NIST05a.l	2539	49	C7H10	94
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

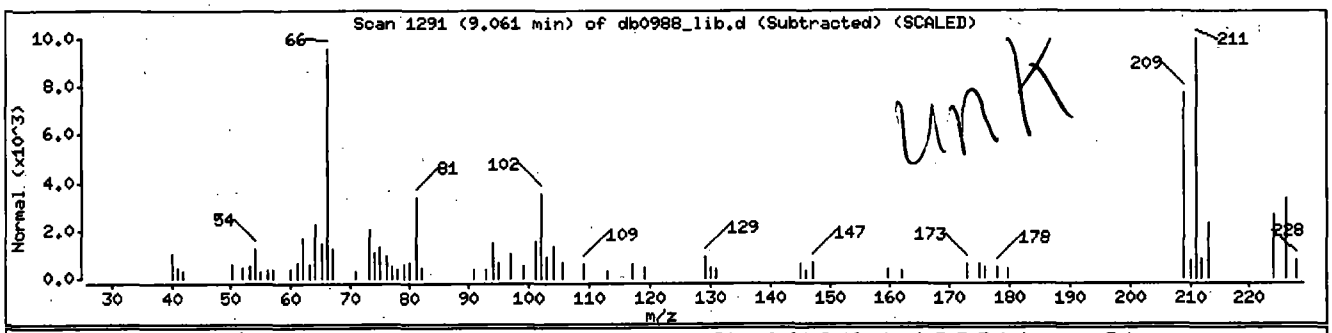
Volume Injected (uL): 1.0

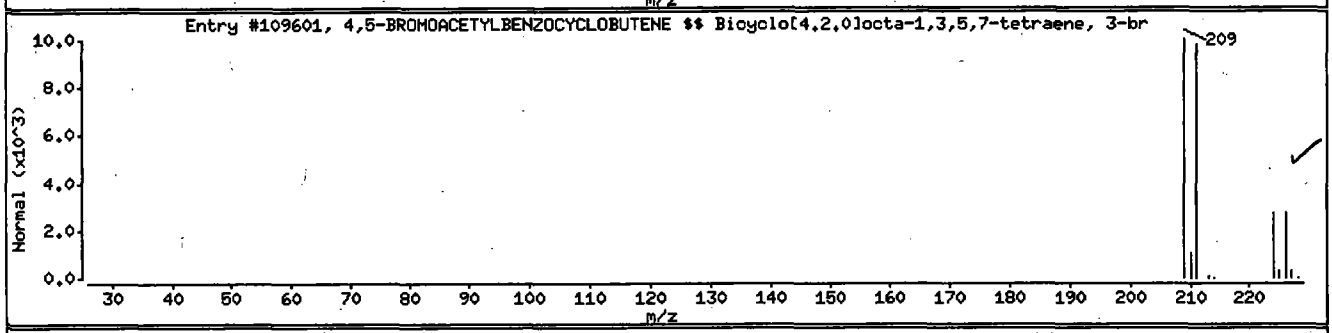
Operator: oeb05247

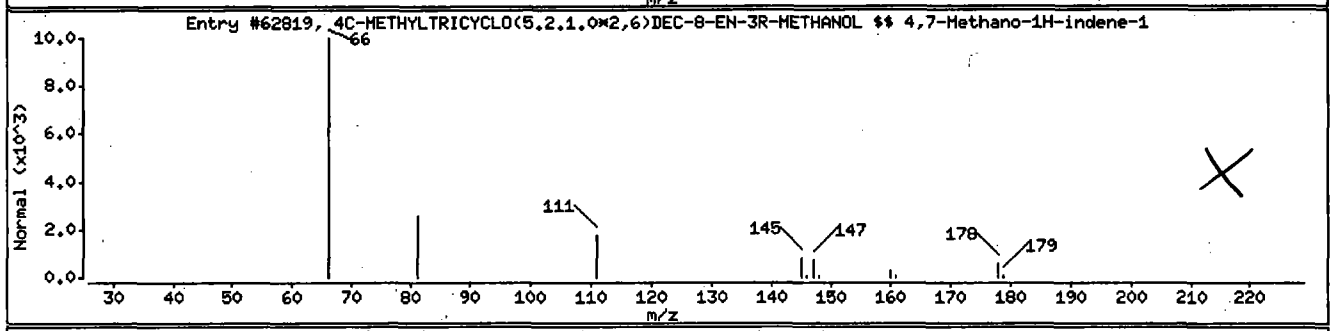
Column phase: J&W DB-5MS

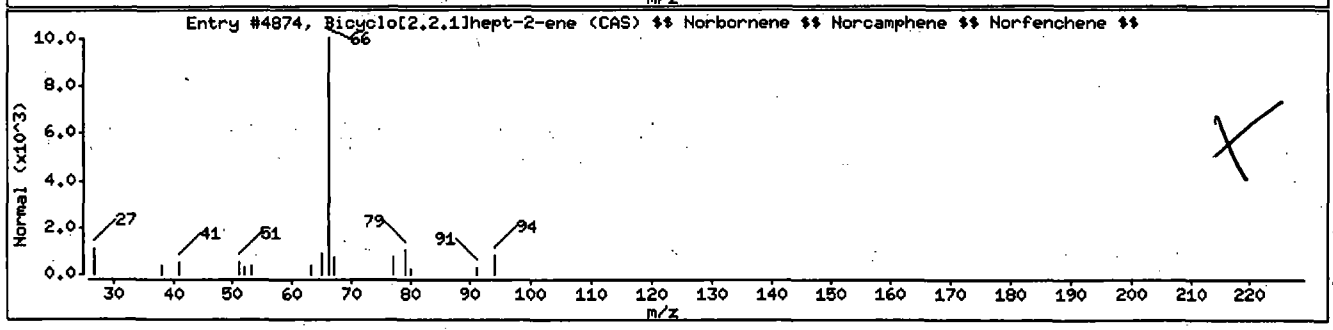
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,5-BROMOACETYLBENZOCYCLOBUTENE $$ Bicyc	63506-25-2	WILEY275.l	109601	78	C10H9BrO	224
4C-METHYLTRICYCLO(5.2.1.0*2,6)DEC-8-EN-3	68304-00-7	WILEY275.l	62819	43	C12H18O	178
Bicyclo[2.2.1]hept-2-ene (CAS) $$ Norbor	498-66-8	WILEY275.l	4874	43	C7H10	94









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

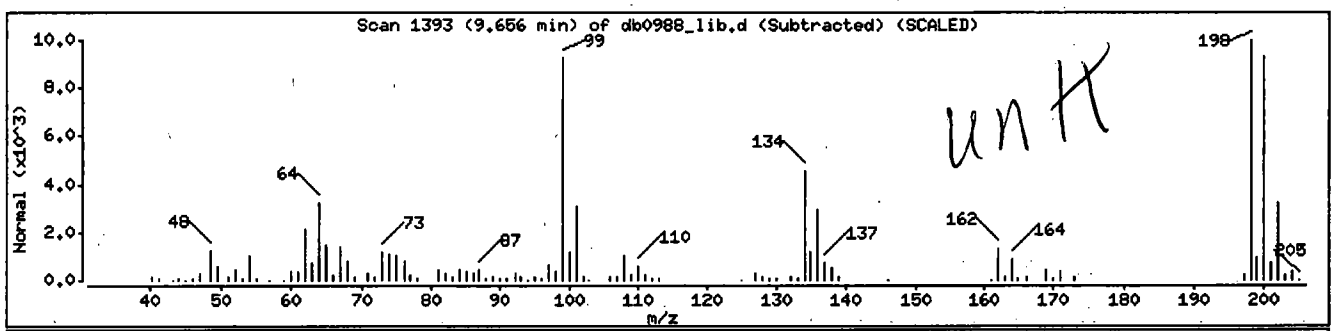
Volume Injected (uL): 1.0

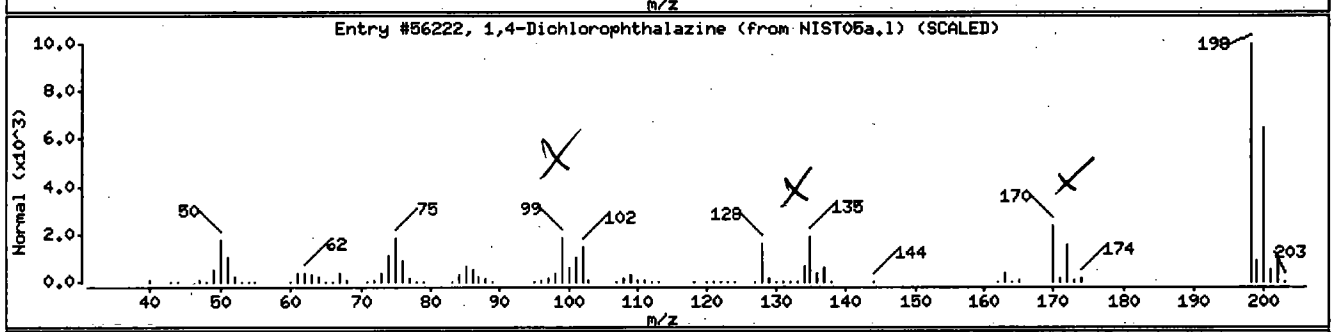
Operator: ceb05247

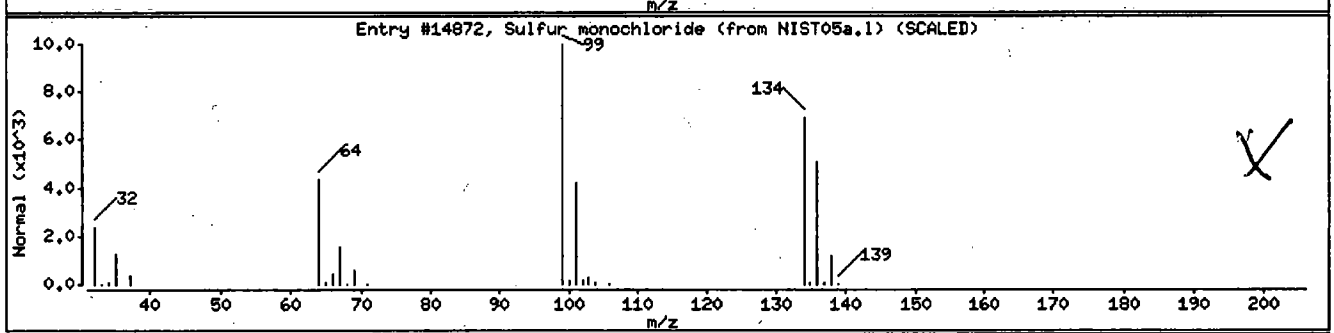
Column phase: J&W DB-5MS

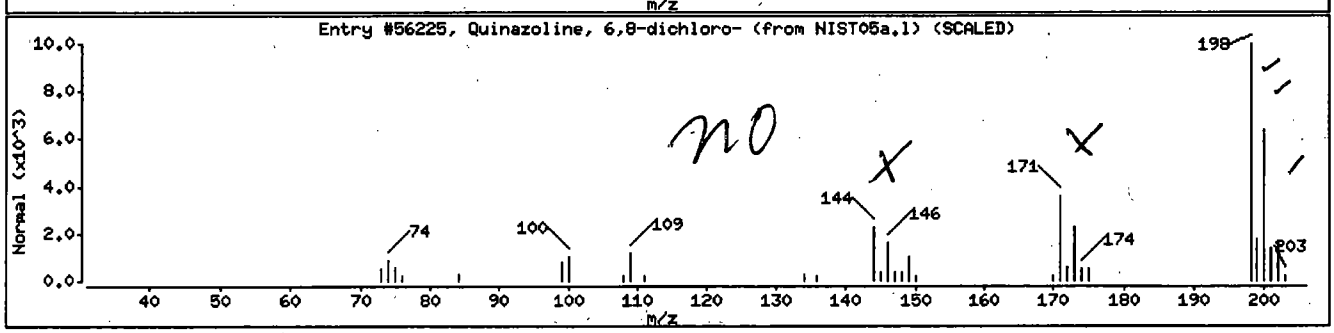
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	38	C8H4Cl2N2	198
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Quinazoline, 6,8-dichloro-	17227-49-5	NIST05a.l	56225	38	C8H4Cl2N2	198









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0988_lib.d

Date : 21-FEB-2014 22:09

Client ID: H6011

Instrument: HP19760.i

Sample Info: H6011;7366680;1;0;SAMPLE;;;

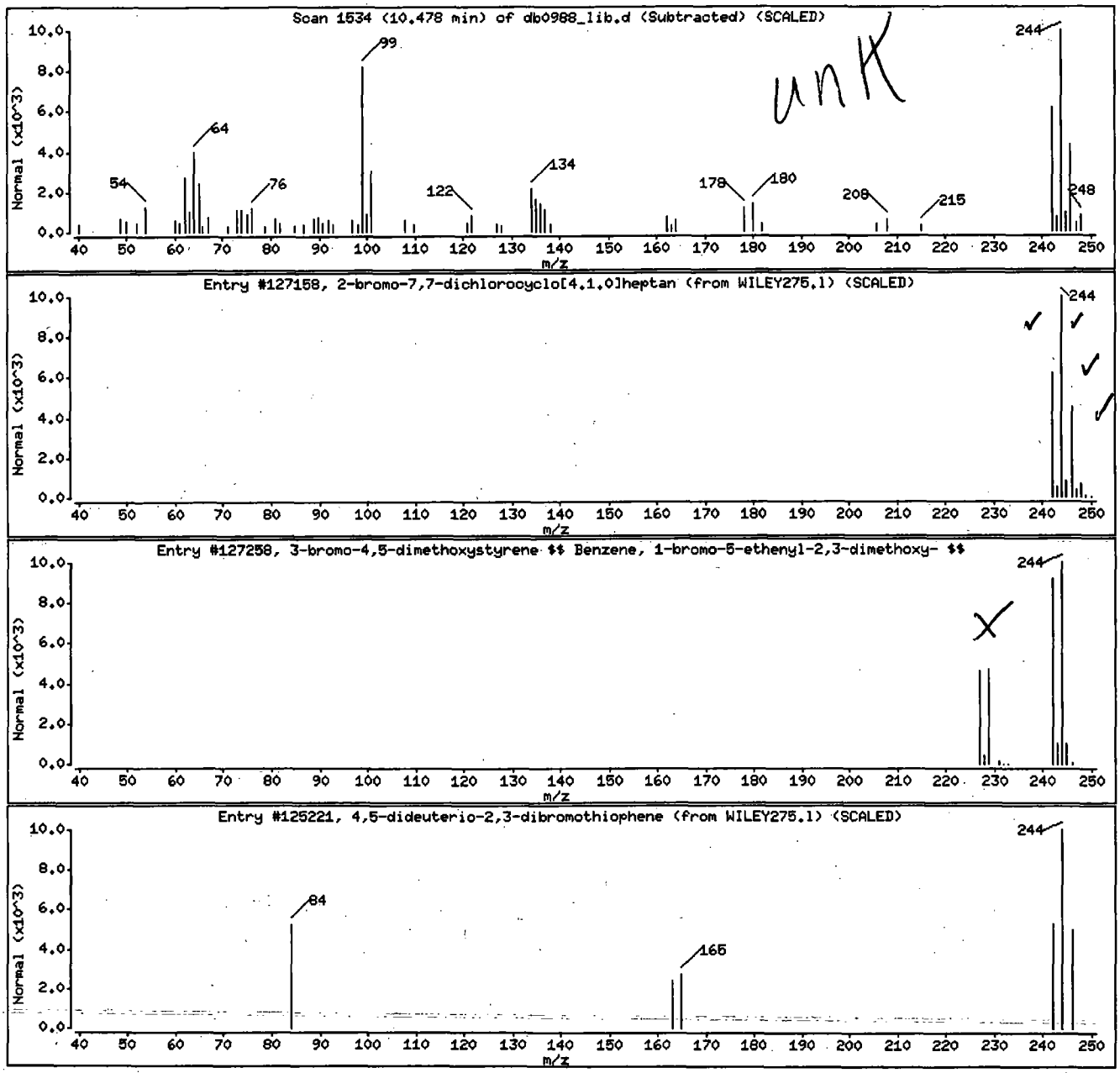
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

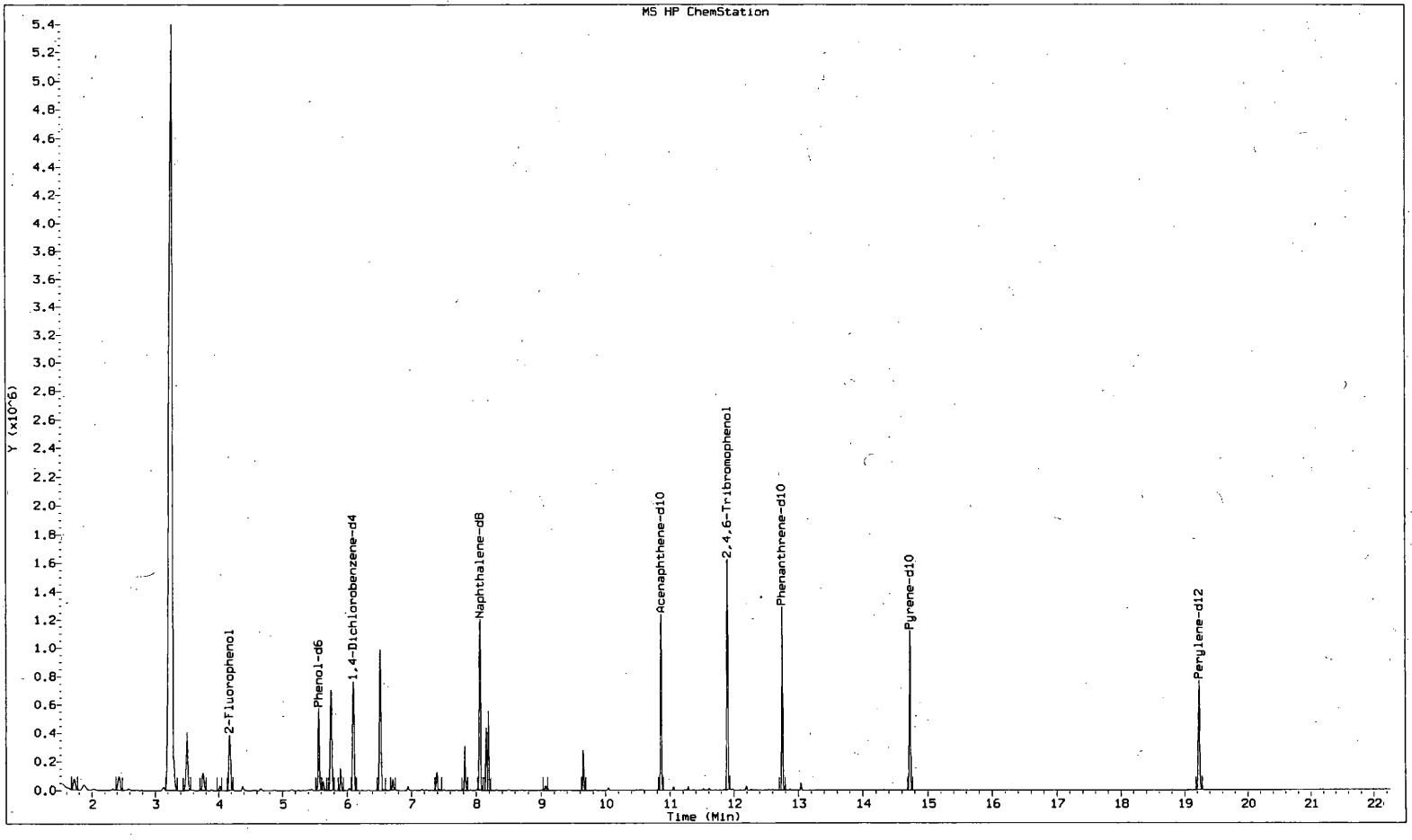
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-bromo-7,7-dichlorocyclo[4.1.0]heptan	113035-97-5	WILEY275.l	127158	91	C7H9BrCl2	242
3-bromo-4,5-dimethoxystyrene $$ Benzene,	5293-42-5	WILEY275.l	127258	64	C10H11BrO2	242
4,5-dideuterio-2,3-dibromothiophene	137040-63-2	WILEY275.l	125221	46	C4D2Br2S	242



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:14.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb21.b/db0964_lib.d
Operator : jmg00346
Acquired : 21-FEB-2014 11:48
Instrument : HP19760.i
Sample Name: H6021;7366684;1;0;SAMPLE;;;
Misc Info : 14050WAE;WL13166;;1046;1000;0;db0906;13166;
Vial Number: 15



Lancaster Labs

Data file : /chem/HP19760.i/14feb21.b/db0964_lib.d
Lab Smp Id: 7366684 Client Smp ID: H6021
Inj Date : 21-FEB-2014 11:48
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H6021;7366684;1;0;SAMPLE;;;
Misc Info : 14050WAE;WL13166;;1046;1000;0;db0906;13166;
Comment : Max. number of TICs to report is 50, 17 TICs were found initially.
Method : /chem/HP19760.i/14feb21.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 13:10 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 15
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1046.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	1081883	10.000
* 48 Naphthalene-d8	8.059	1641472	10.000
* 83 Acenaphthene-d10	10.863	1435846	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.723	163187	1.50836222	1.44202	91	NIST05a.l	31325	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
2,2-Dimethoxybutane					CAS #: 3453-99-4		
2.429	217210	2.00770253	1.91940	74	NIST05a.l	8553	21
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.274	19300895	178.400905	170.55535	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.501	784650	7.25262841	6.93367	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.752	235414	2.17596467	2.08027	23	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.020	50802	0.46957269	0.44892	9	NIST05a.l	13998	21(L)
Cyclotetrasiloxane, octamethyl-					CAS #: 556-67-2		
5.634	82025	0.75817207	0.72482	91	NIST05a.l	122480	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.757	1063873	9.83353105	9.40108	90	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.902	213047	1.96922519	1.88262	91	NIST05a.l	18486	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.520	1517869	14.0298755	13.41288	35	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.713	99232	0.91721758	0.87688	64	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl- (CAS) $$					CAS #: 541-02-6		
7.395	157292	0.95823964	0.91609	90	WILEY275.l	221485	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	375336	2.28657975	2.18602	46	WILEY275.l	22248	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.152	504382	3.07274282	2.93761	90	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	671347	4.08990505	3.91004	40	NIST05a.l	3933	48(L)
Cyclohexasiloxane, dodecamethyl-					CAS #: 540-97-6		
9.073	51103	0.31132267	0.29763	72	NIST05a.l	179153	48

Target compound.
Do not report.
ajs00193 03/02/2014

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Target 3.5 esignature user ID: ajs00193

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
====	====	==========	==========	====	=======	=========	======
Sulfur monochloride				CAS #: 10025-67-9			
9.650	314234	2.18849155	2.09224	38	NIST05a.l	14872	83(L)

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

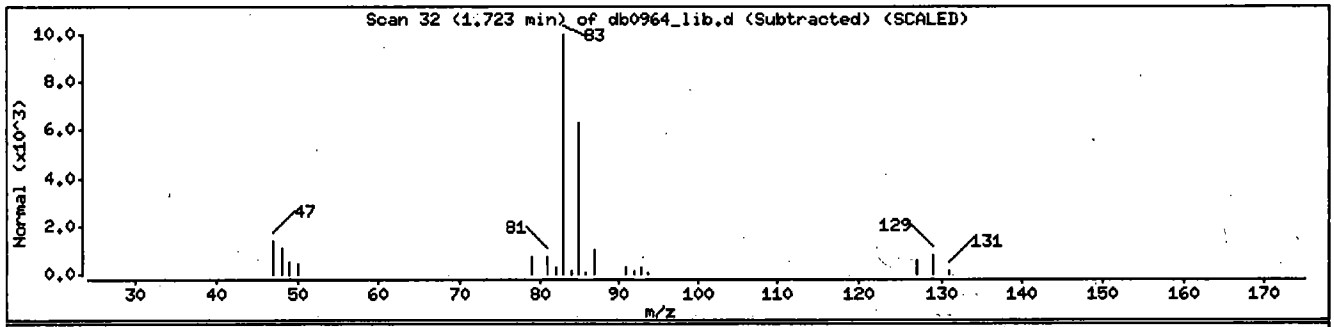
Volume Injected (uL): 1.0

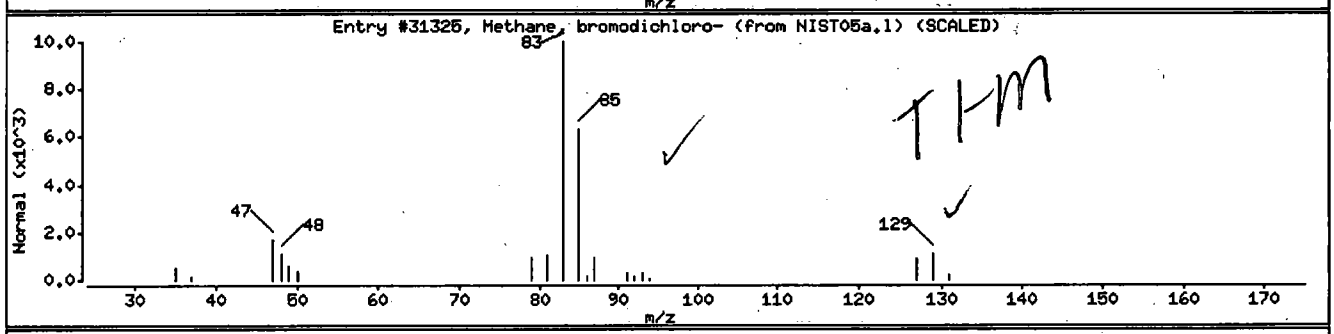
Operator: jmg00346

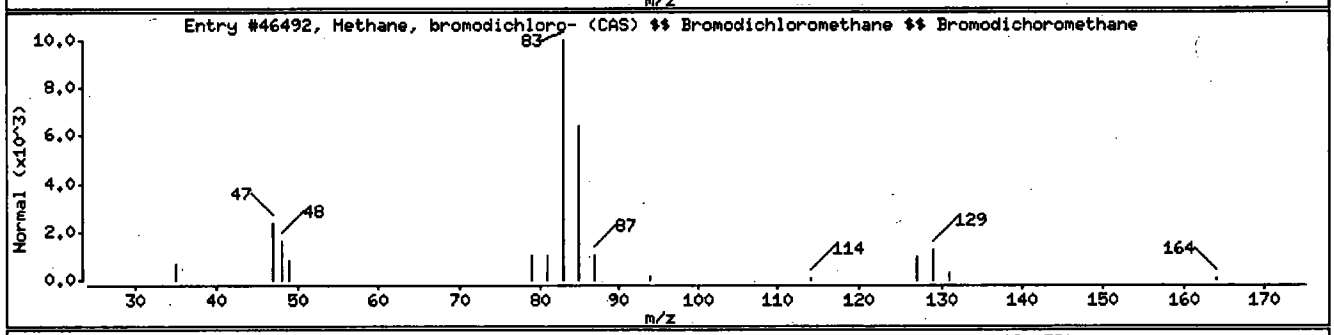
Column phase: J&W DB-5MS

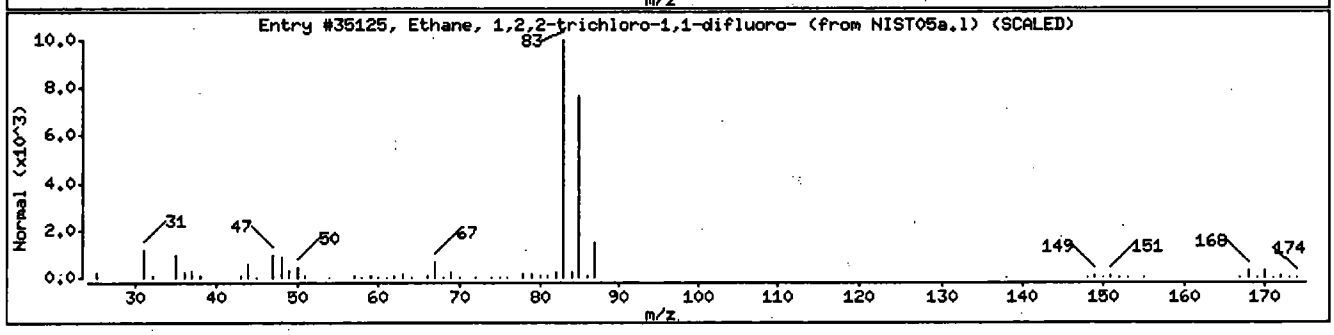
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	91	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46492	83	CHBrCl2	162
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	78	C2HCl3F2	168









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

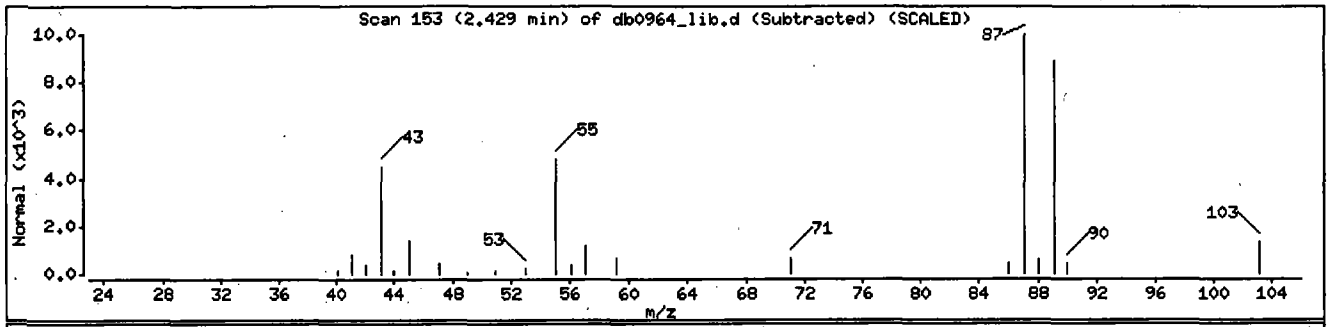
Volume Injected (uL): 1.0

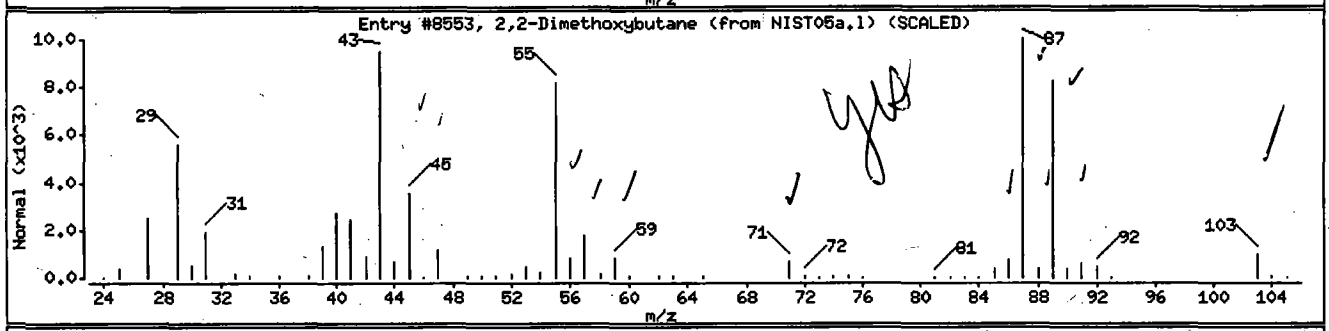
Operator: jmg00346

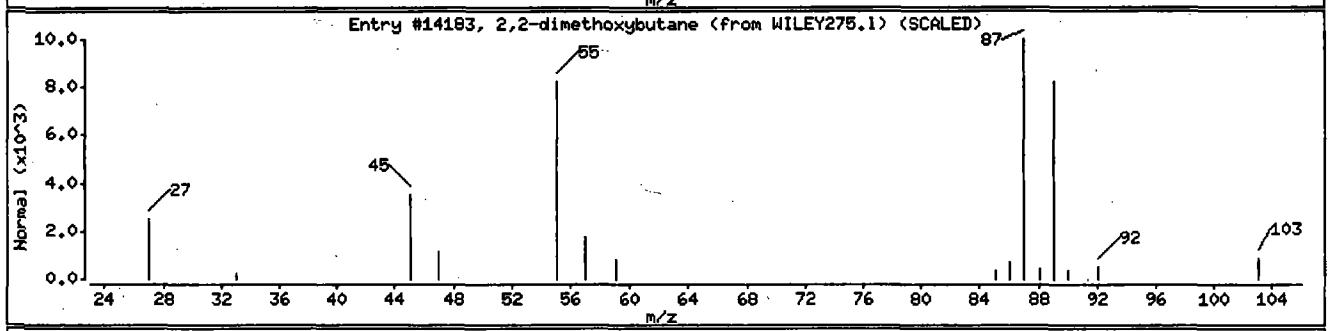
Column phase: J&W DB-5MS

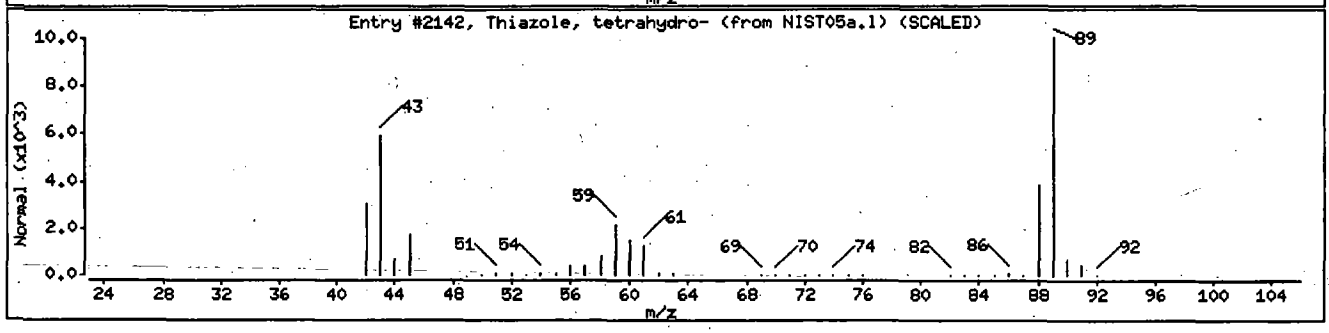
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,2-Dimethoxybutane	3453-99-4	NIST05a.l	8553	74	C6H14O2	118
2,2-dimethoxybutane	0-00-0	WILEY275.l	14183	74	C6H14O2	118
Thiazole, tetrahydro-	504-78-9	NIST05a.l	2142	53	C3H7NS	89









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

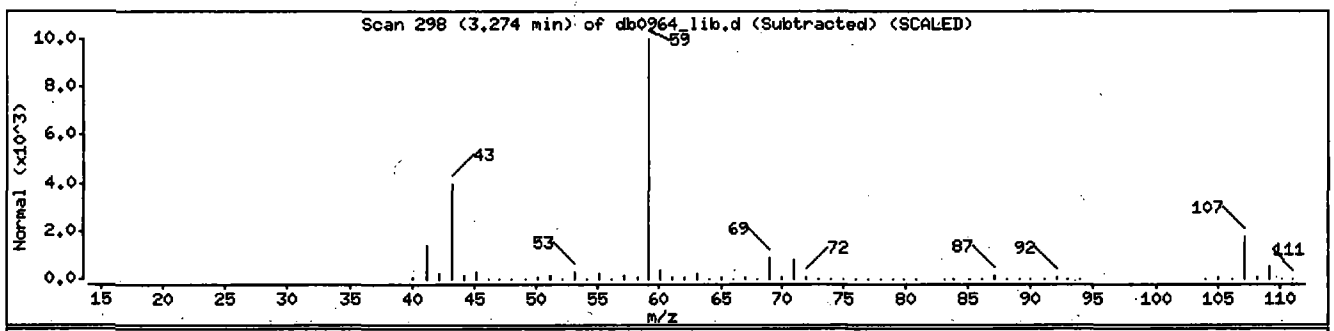
Volume Injected (uL): 1.0

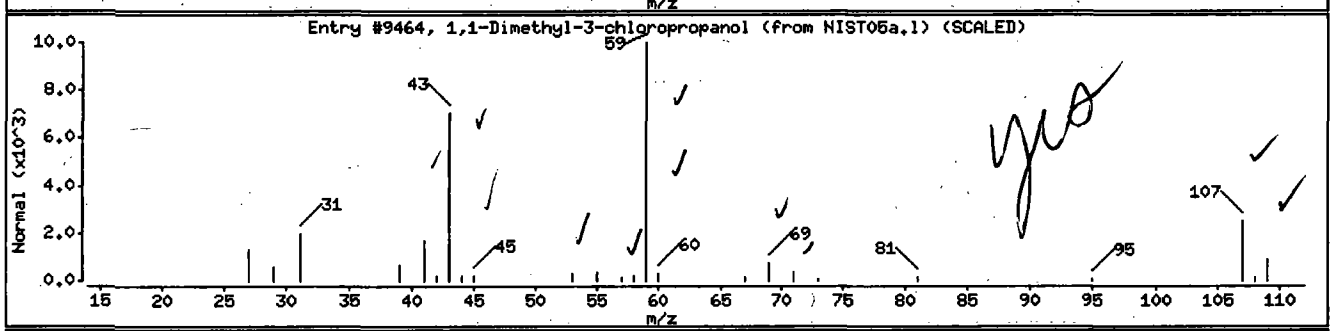
Operator: jmg00346

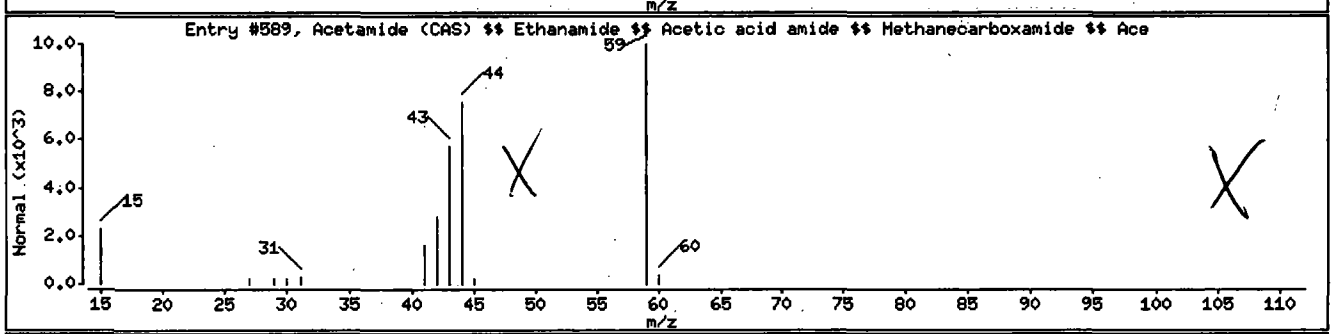
Column phase: J&W DB-5MS

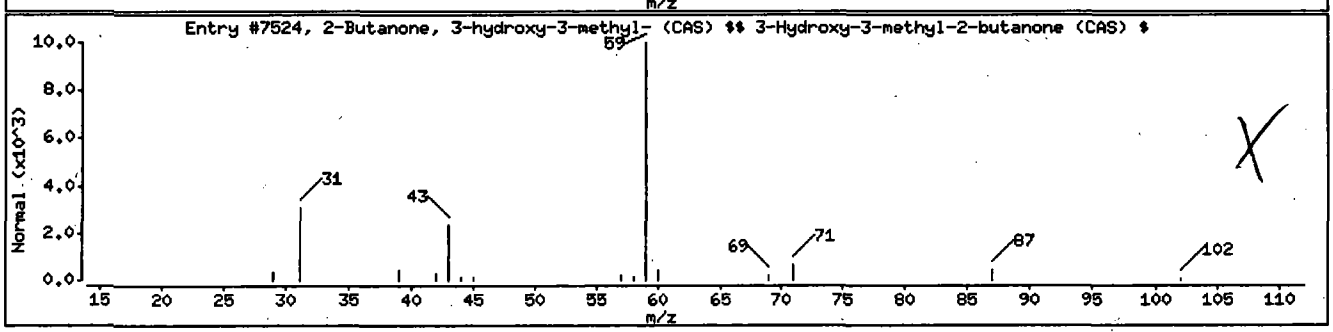
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

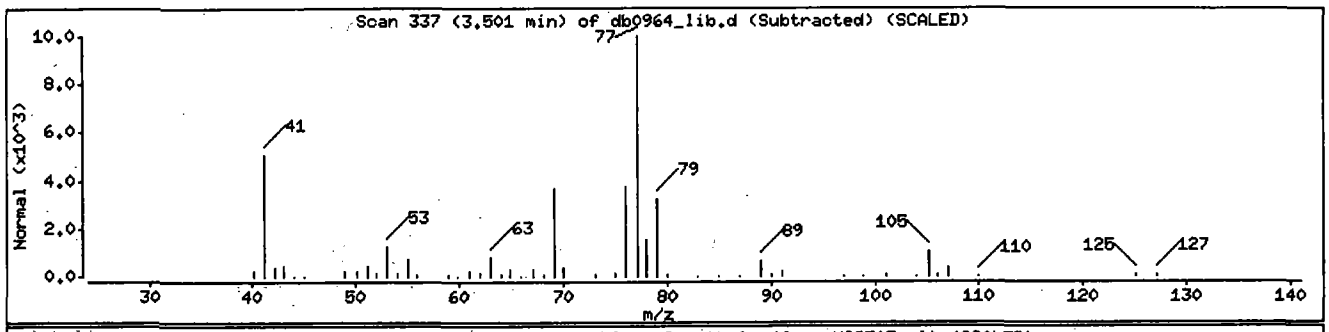
Client ID: H6021 Instrument: HP19760.i

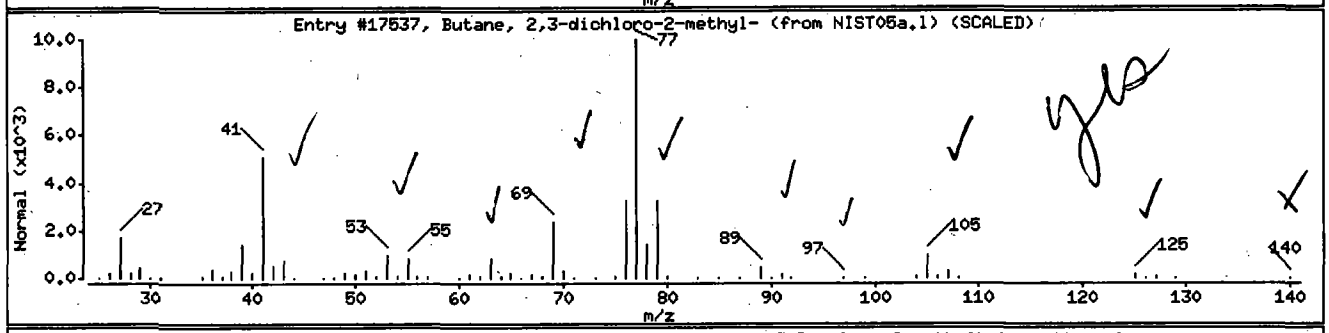
Sample Info: H6021;7366684;1;0;SAMPLE;;;

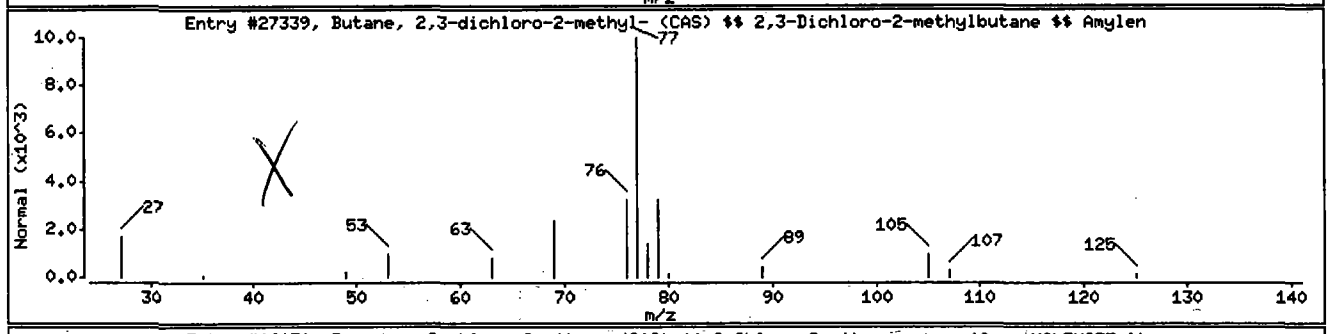
Volume Injected (uL): 1.0 Operator: jmg00346

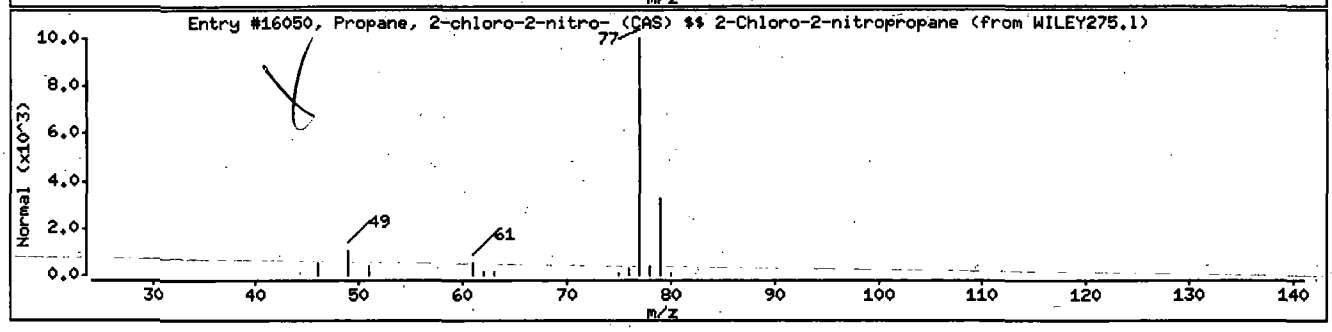
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

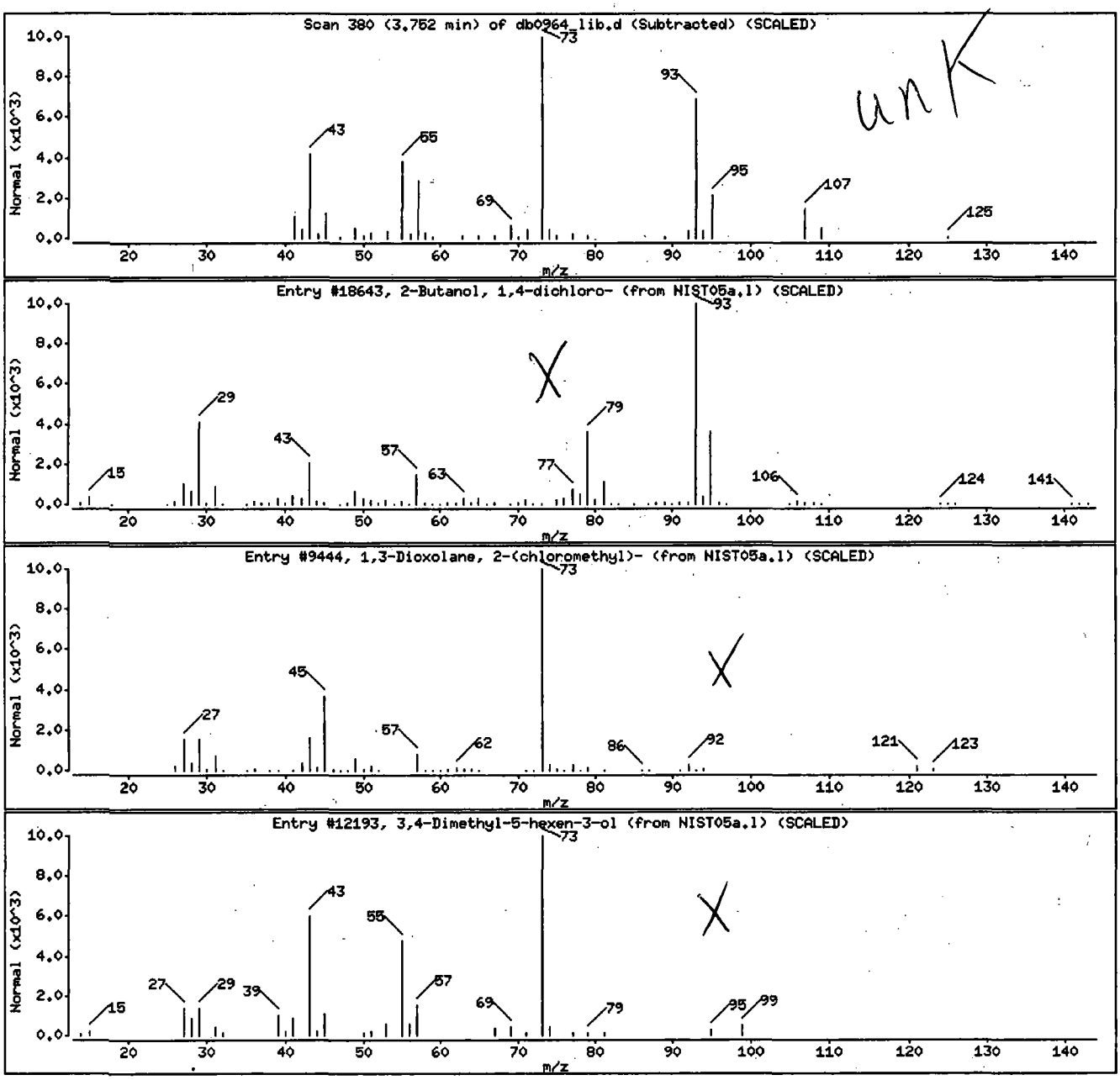
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	23	C4H8Cl2O	142
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9444	10	C4H7ClO2	122
3,4-Dimethyl-5-hexen-3-ol	1569-45-5	NIST05a.l	12193	10	C8H16O	128



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

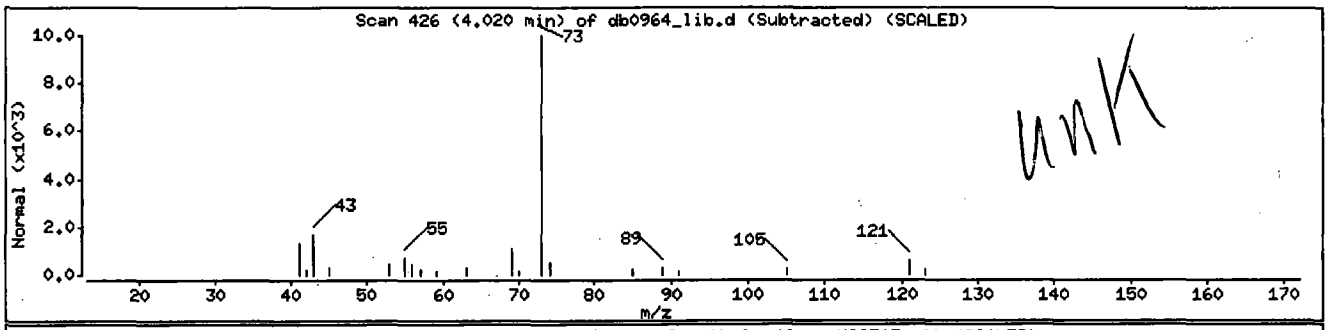
Volume Injected (uL): 1.0

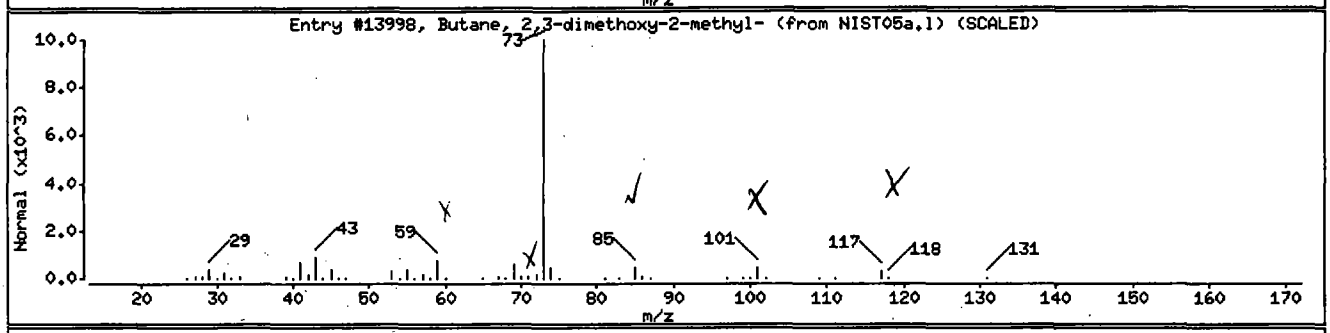
Operator: jmg00346

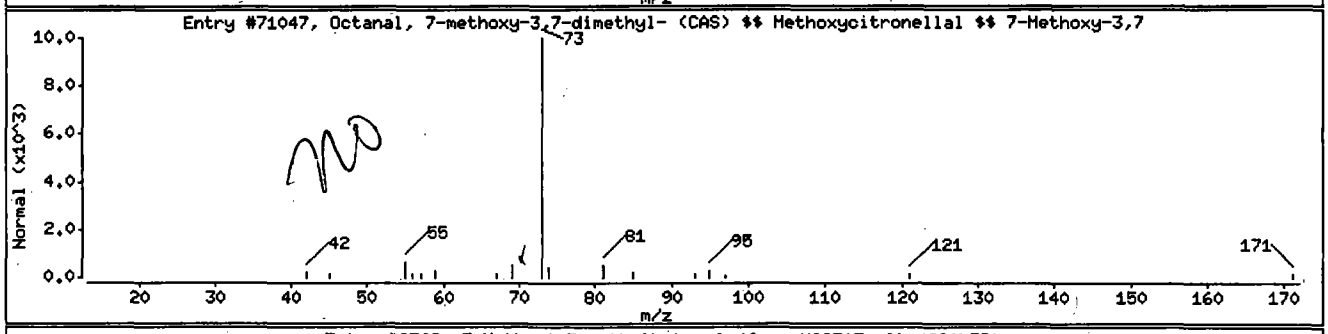
Column phase: J&W DB-5MS

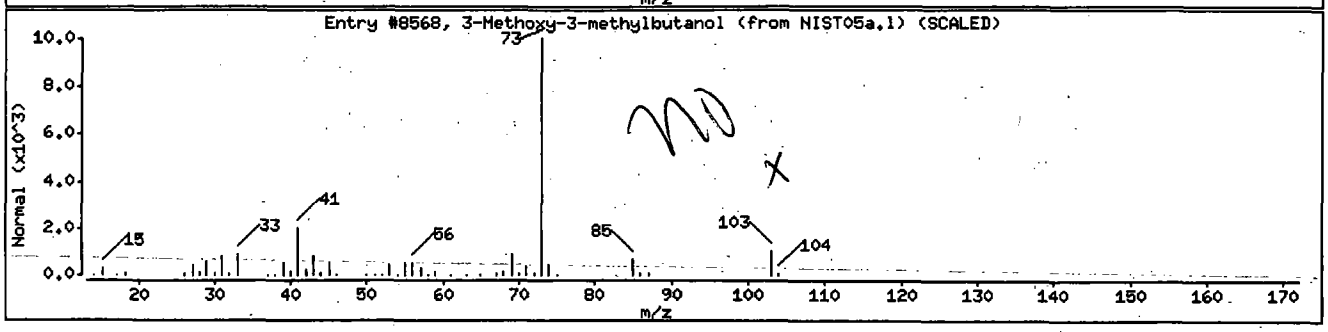
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	9	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl- (CAS) *	3613-30-7	WILEY275.l	71047	50	C11H22O2	186
3-Methoxy-3-methylbutanol	56539-66-3	NIST05a.l	8568	39	C6H14O2	118









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Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

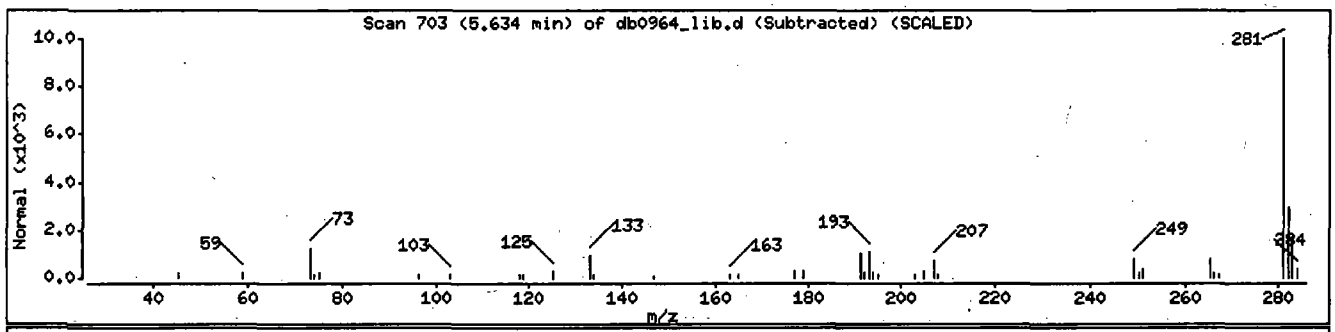
Volume Injected (uL): 1.0

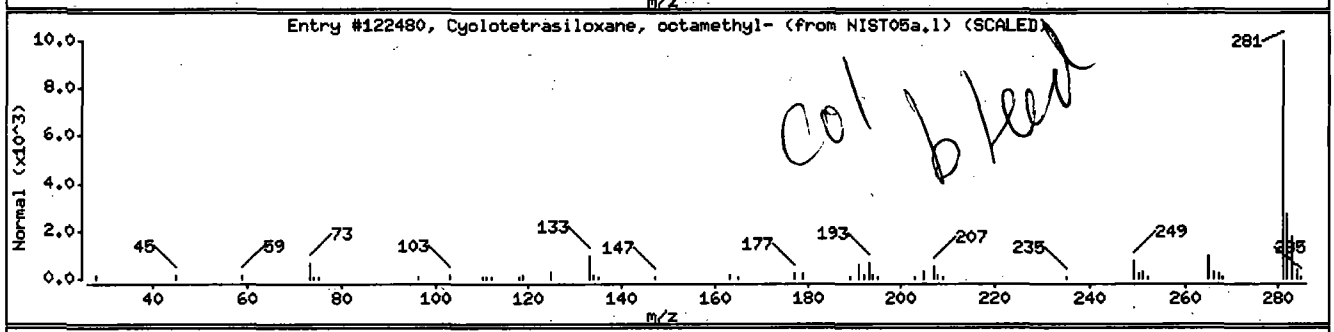
Operator: jmg00346

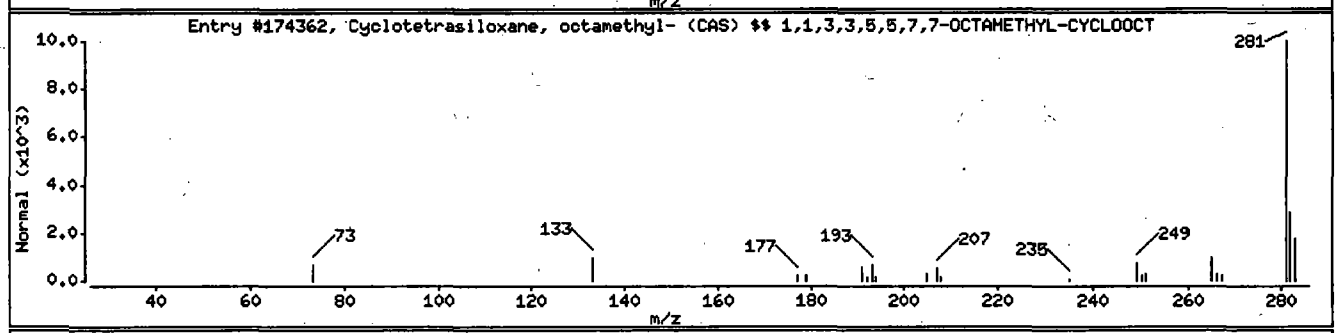
Column phase: J&W DB-5MS

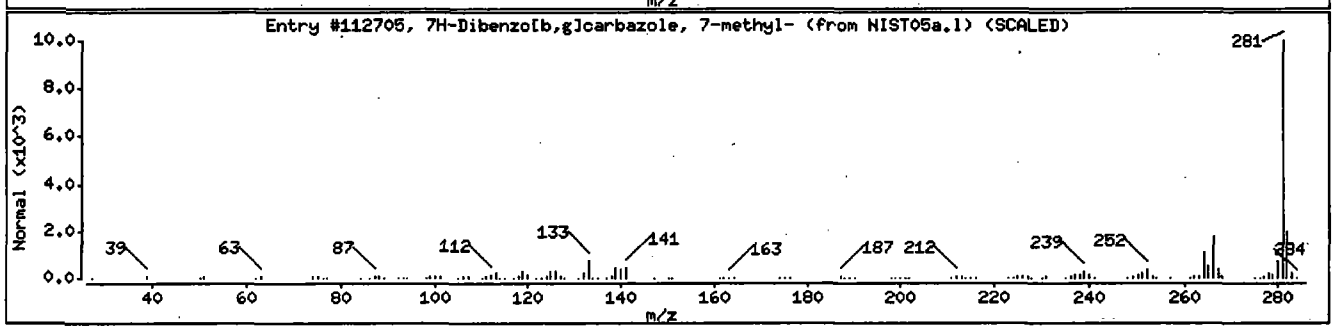
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclotetrasiloxane, octamethyl-	556-67-2	NIST05a.l	122480	91	C8H24O4Si4	296
Cyclotetrasiloxane, octamethyl- (CAS) $$	556-67-2	WILEY275.l	174362	91	C8H24O4Si4	296
7H-Dibenzo[b,g]carbazole, 7-methyl-	3557-49-1	NIST05a.l	112705	59	C21H15N	281









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Target 3.5 esignature user ID: ajs00193

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Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

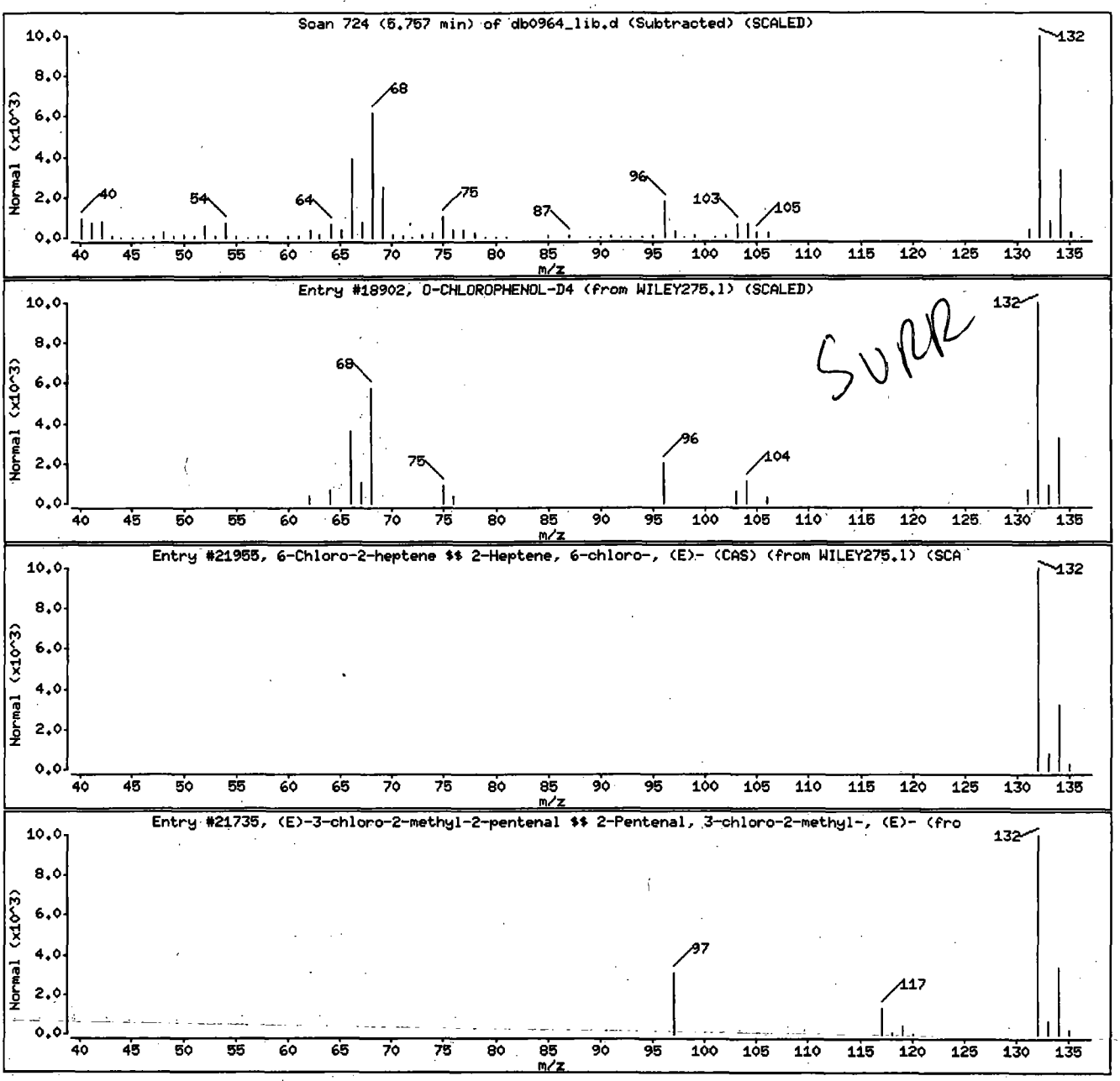
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	90	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132



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Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

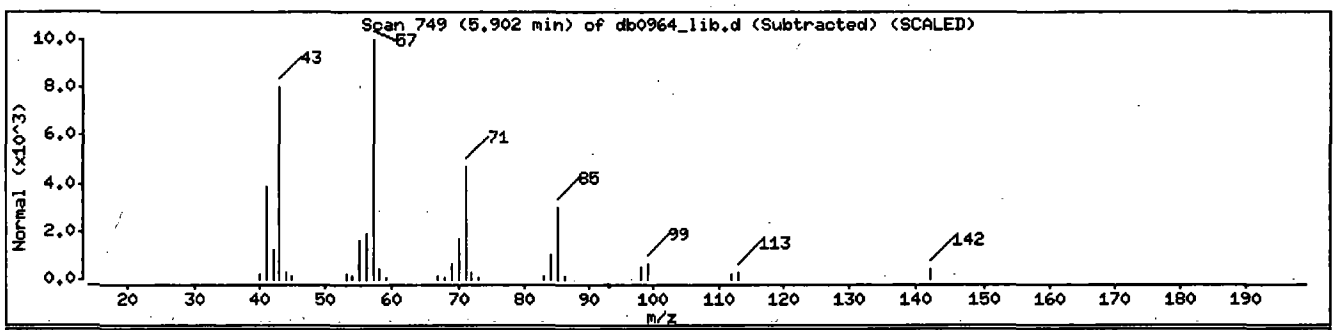
Volume Injected (uL): 1.0

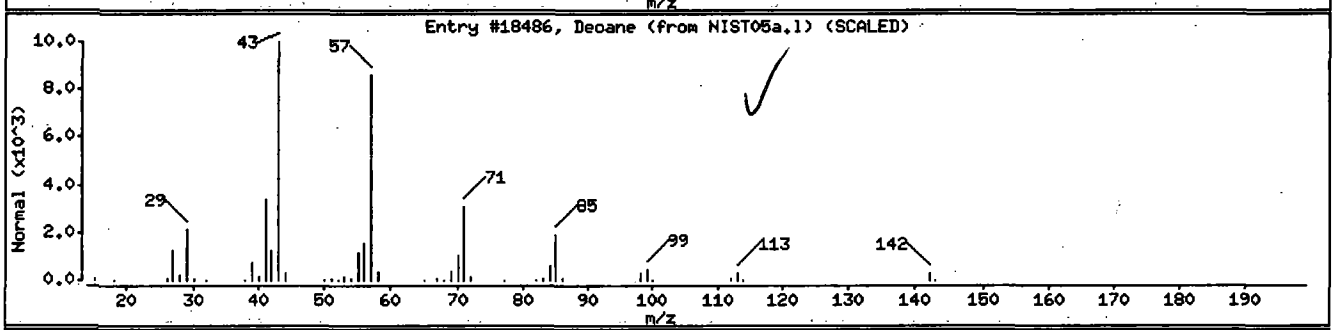
Operator: jmg00346

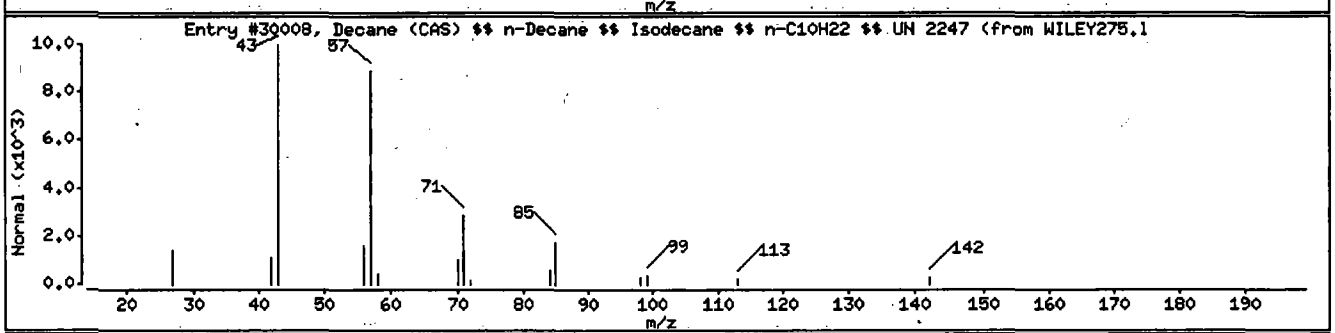
Column phase: J&W DB-5MS

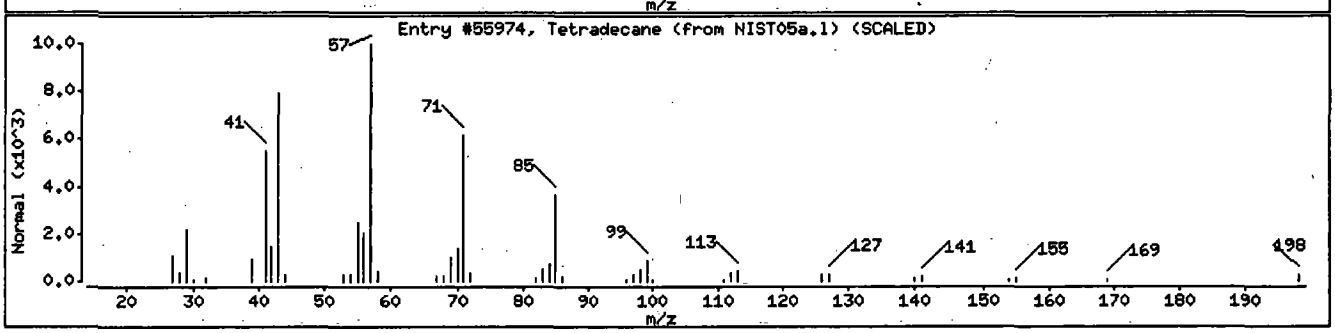
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18486	91	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30008	91	C10H22	142
Tetradecane	629-59-4	NIST05a.l	55974	86	C14H30	198









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

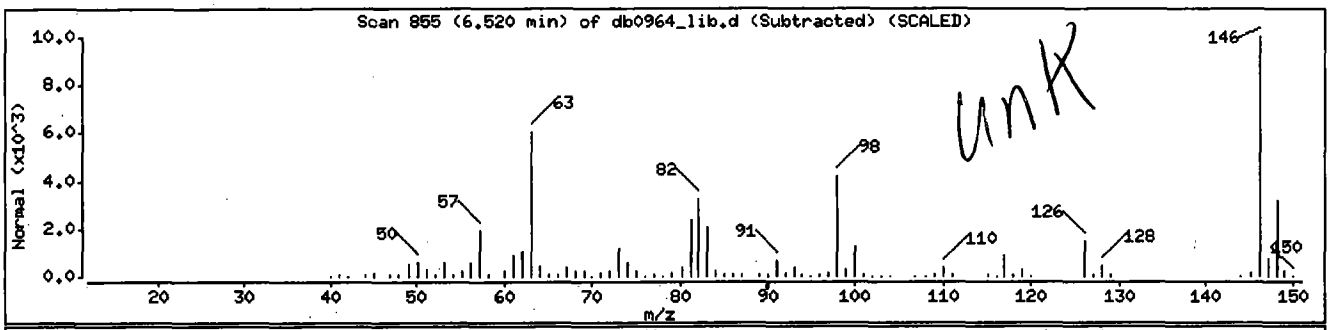
Volume Injected (uL): 1.0

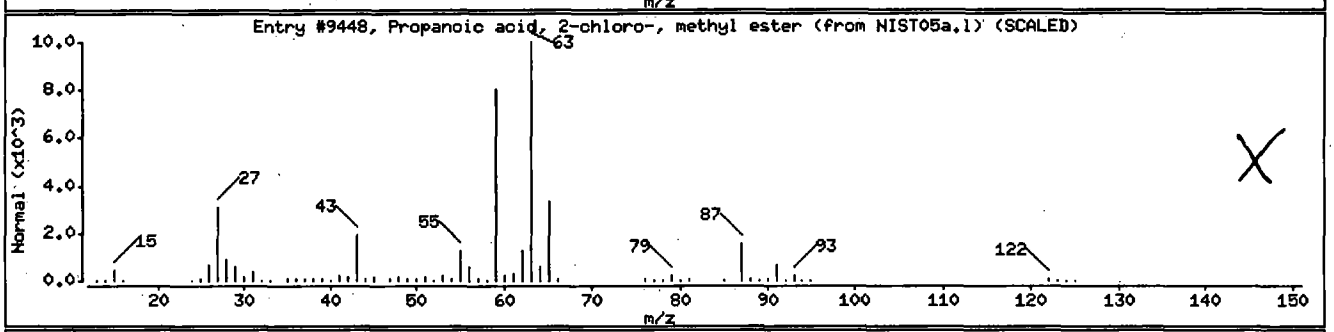
Operator: jmg00346

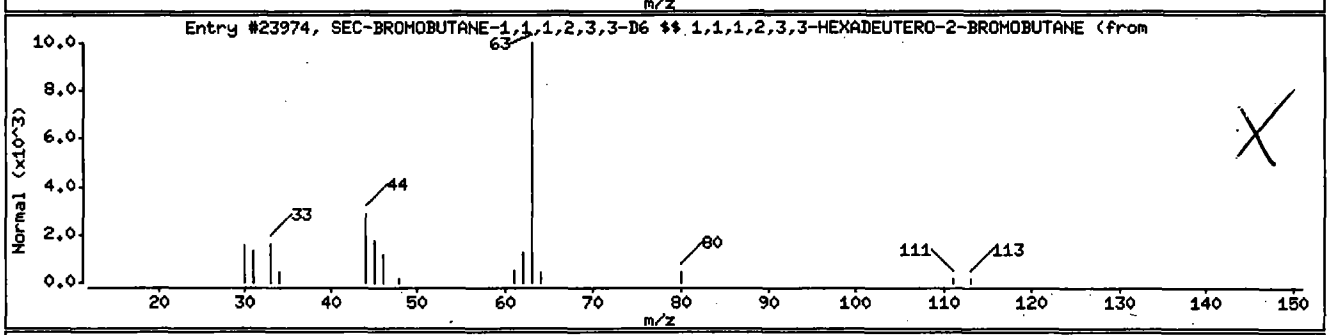
Column phase: J&W DB-5MS

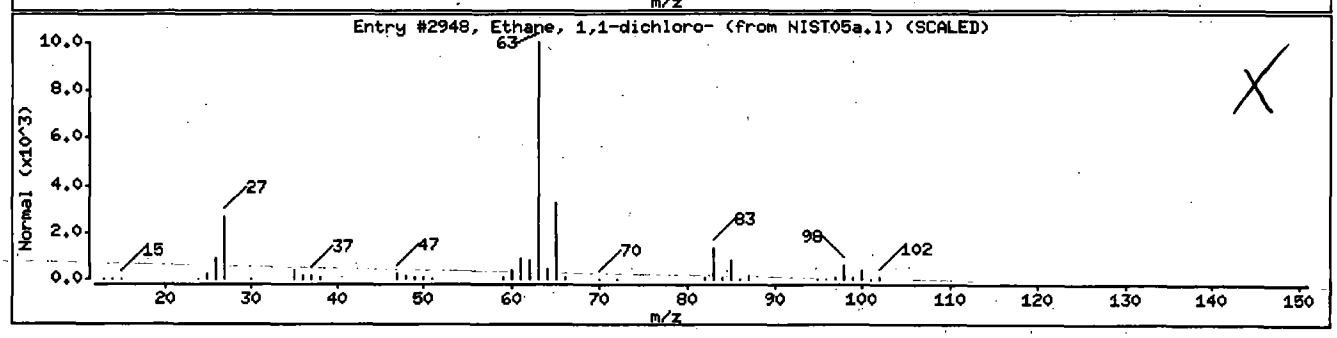
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	23	C2H4Cl2	98









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Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

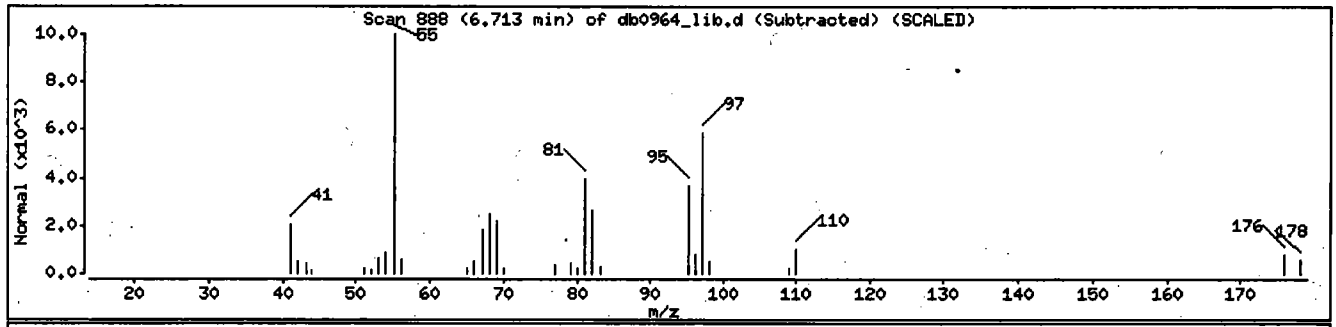
Volume Injected (uL): 1.0

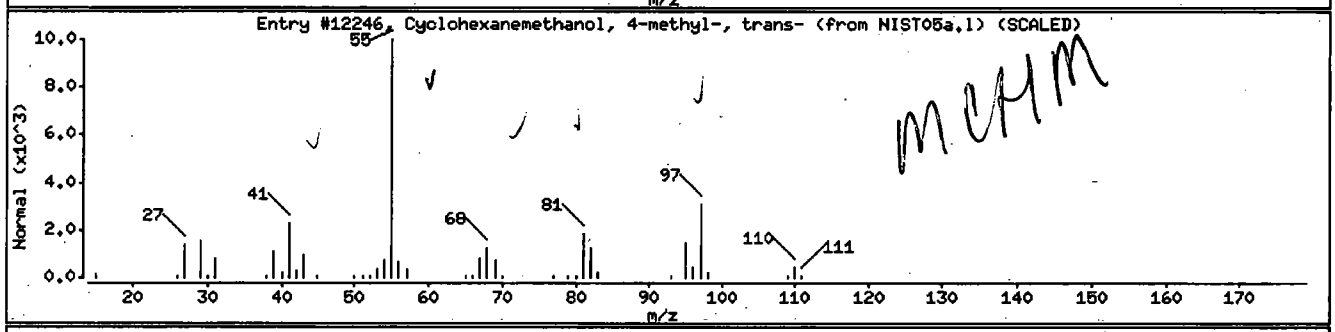
Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	64	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	64	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12094	53	C8H16O	128





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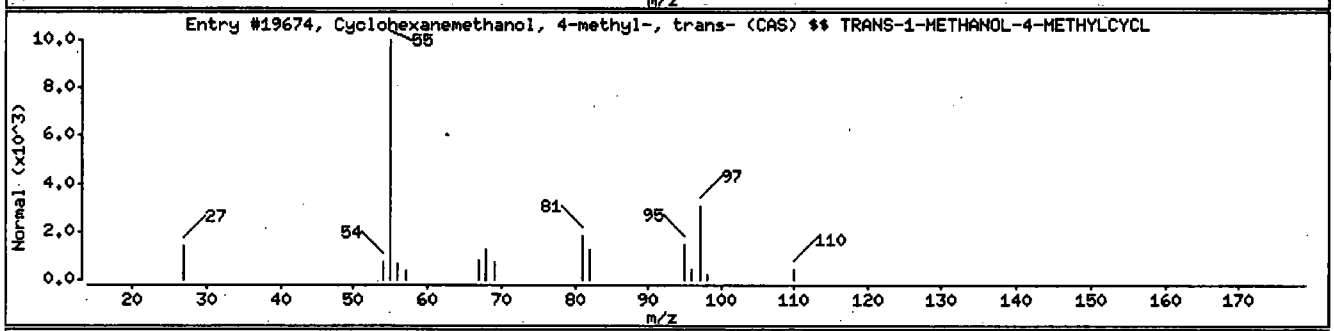

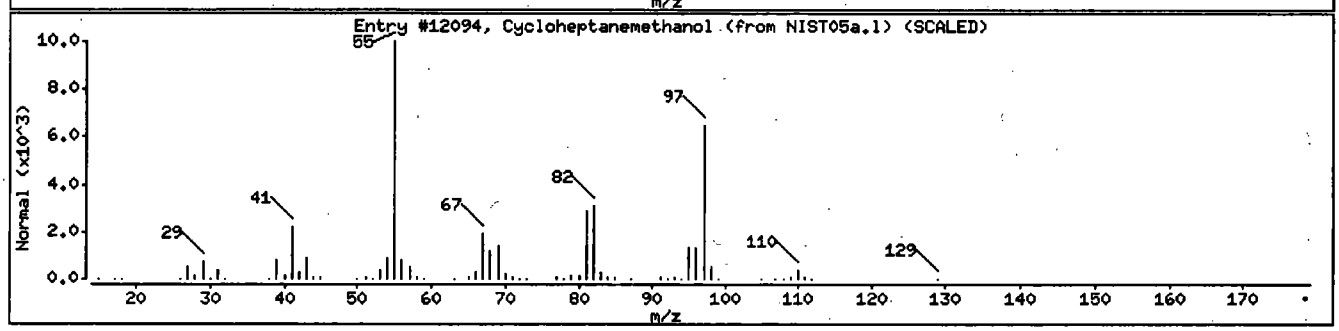

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

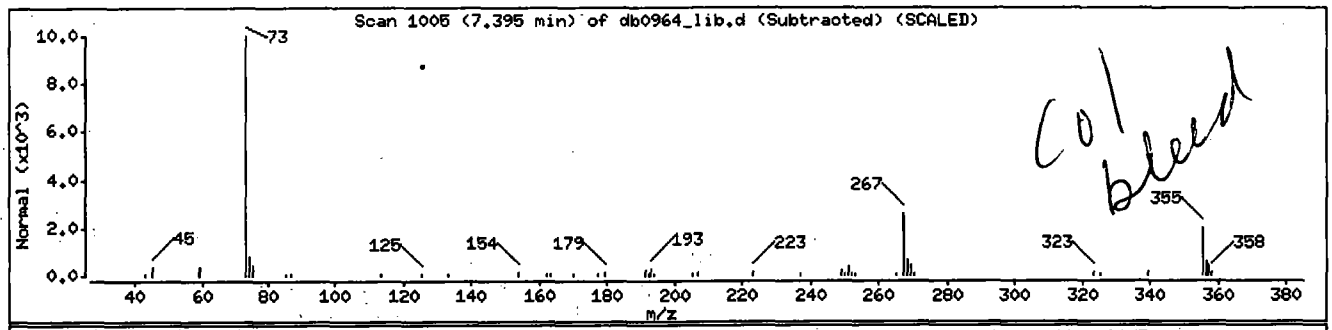
Client ID: H6021 Instrument: HP19760.i

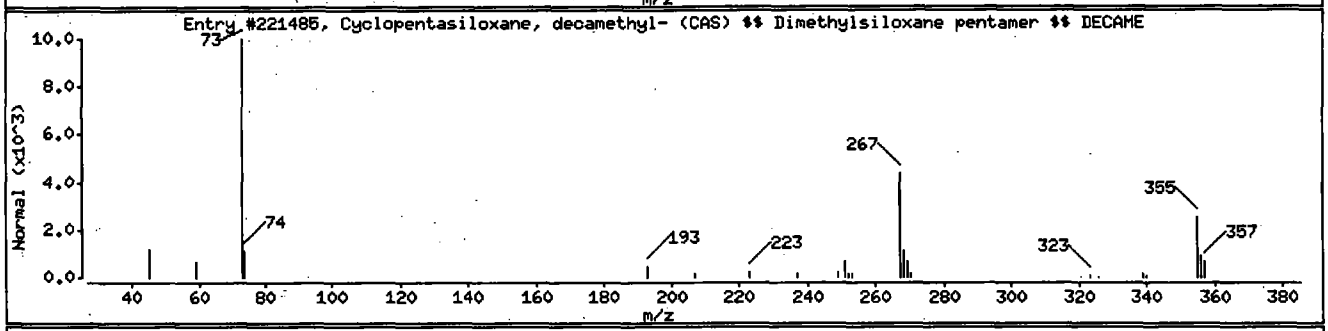
Sample Info: H6021;7366684;1;0;SAMPLE;;;

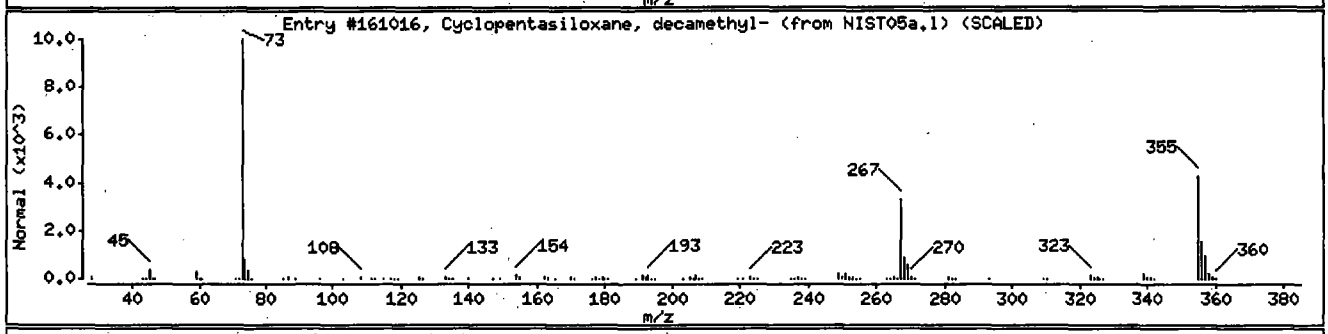
Volume Injected (uL): 1.0 Operator: jmg00346

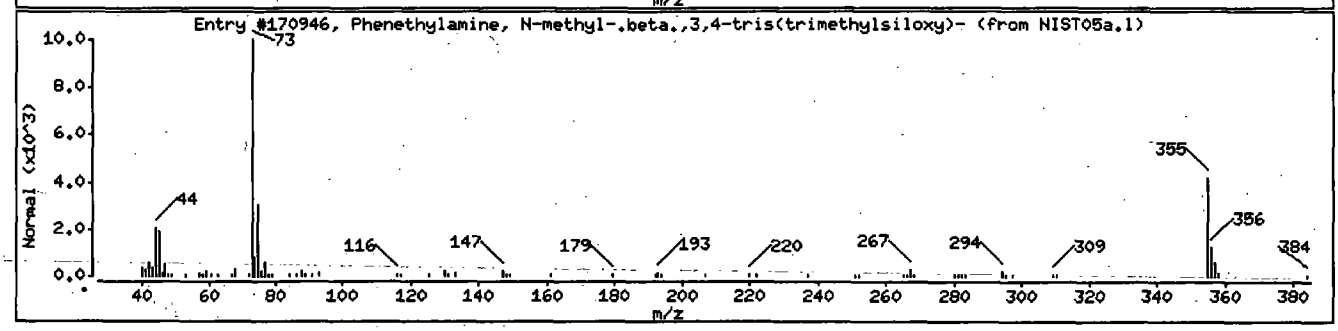
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221485	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	83	C10H30O5Si5	370
Phenethylamine, N-methyl-.beta.,3,4-tris	10538-85-9	NIST05a.l	170946	47	C18H37NO3Si3	399









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Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

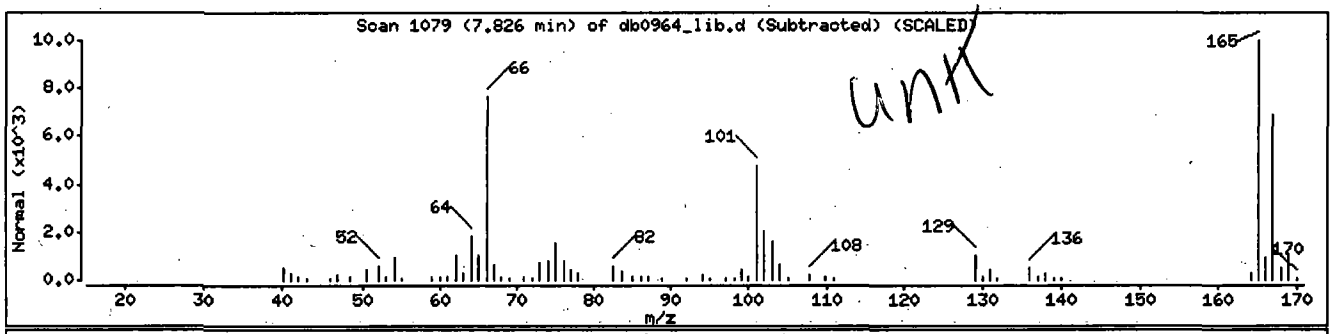
Volume Injected (uL): 1.0

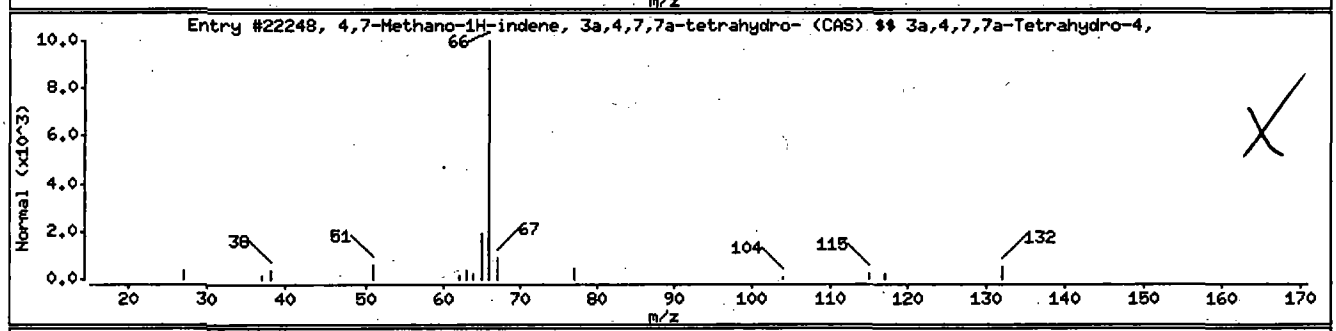
Operator: jmg00346

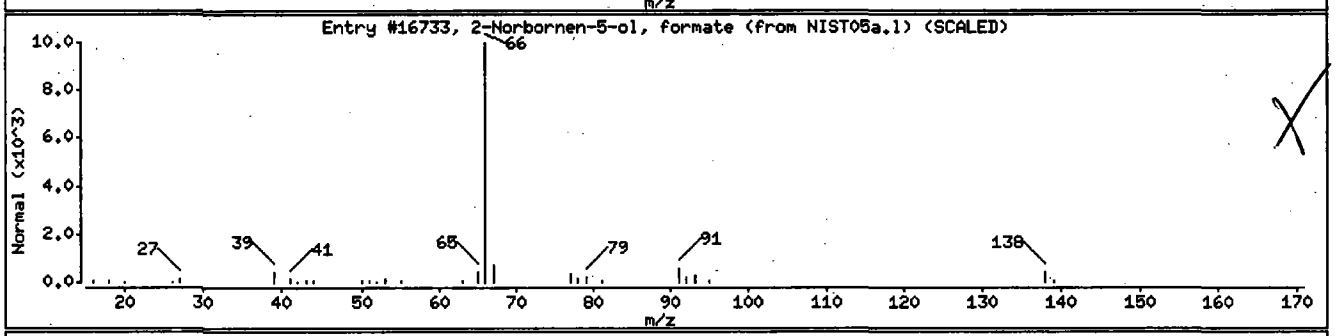
Column phase: J&W DB-5MS

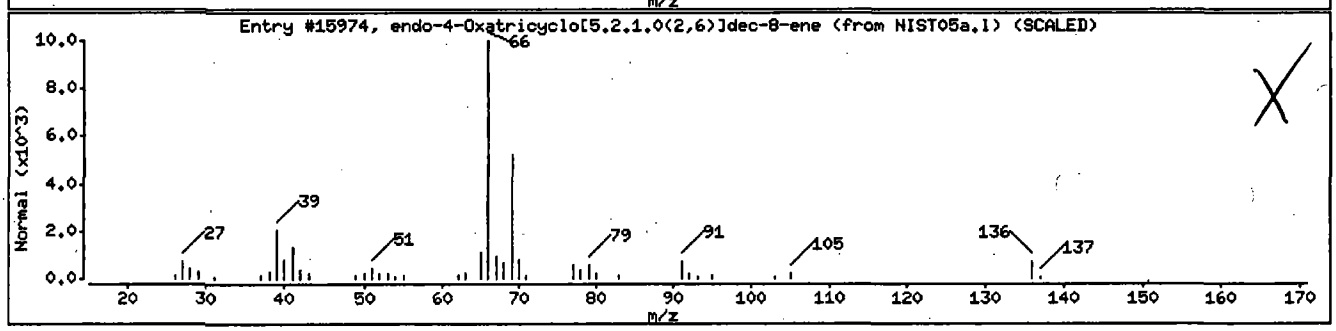
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22248	46	C10H12	132
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H1002	138
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	46	C9H120	136









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

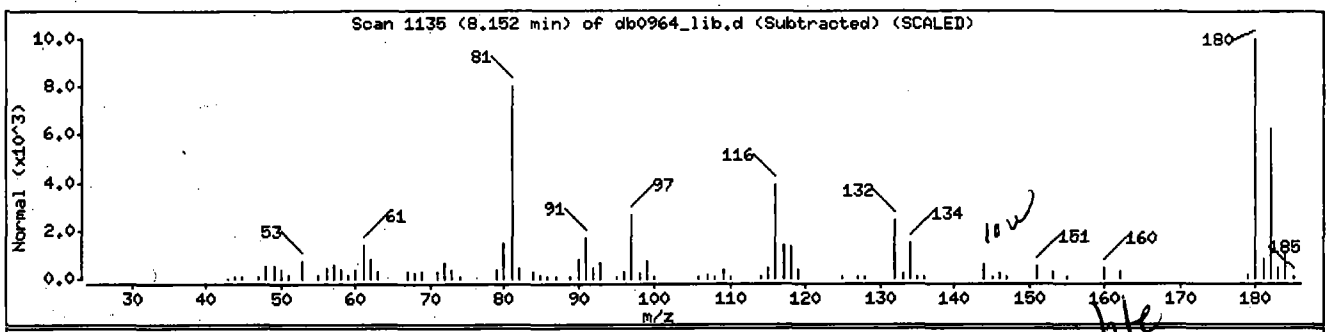
Client ID: H6021 Instrument: HP19760.i

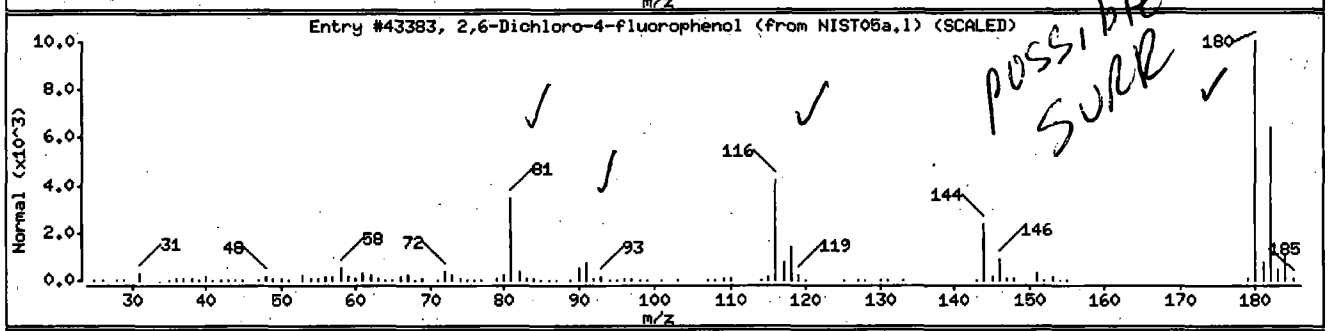
Sample Info: H6021;7366684;1;0;SAMPLE;;;

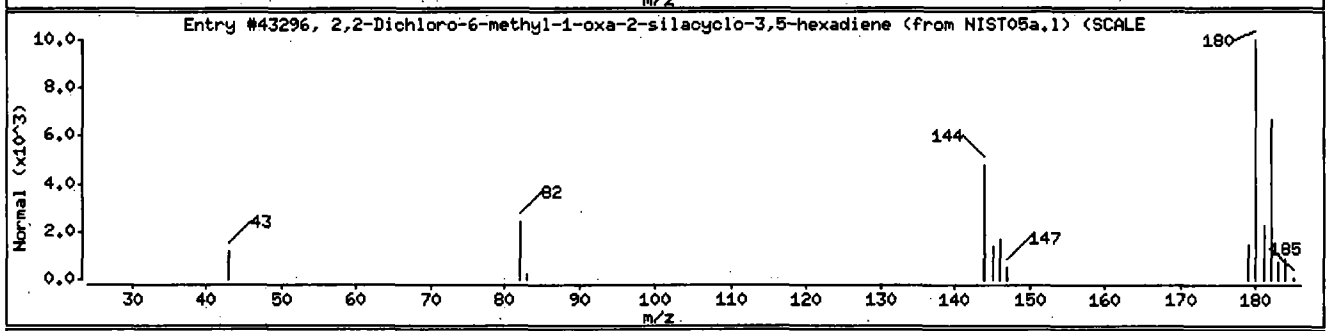
Volume Injected (uL): 1.0 Operator: jmg00346

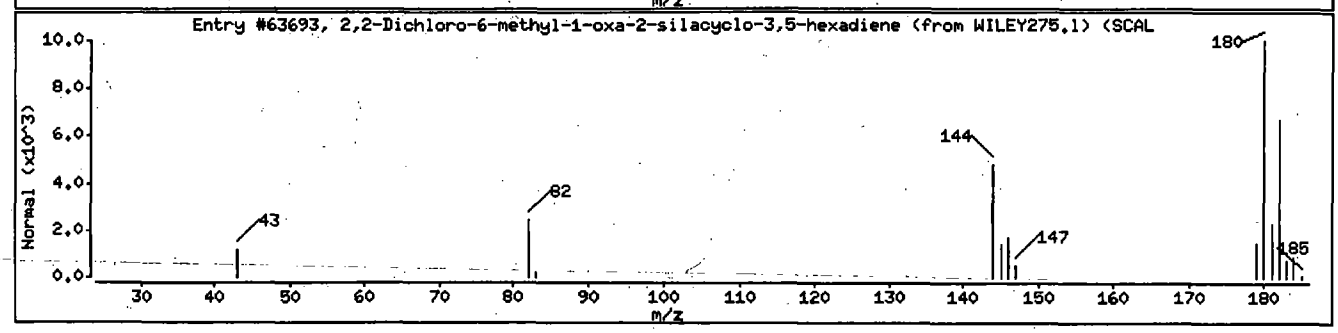
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	90	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	27	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	27	C5H6Cl2OSi	180









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

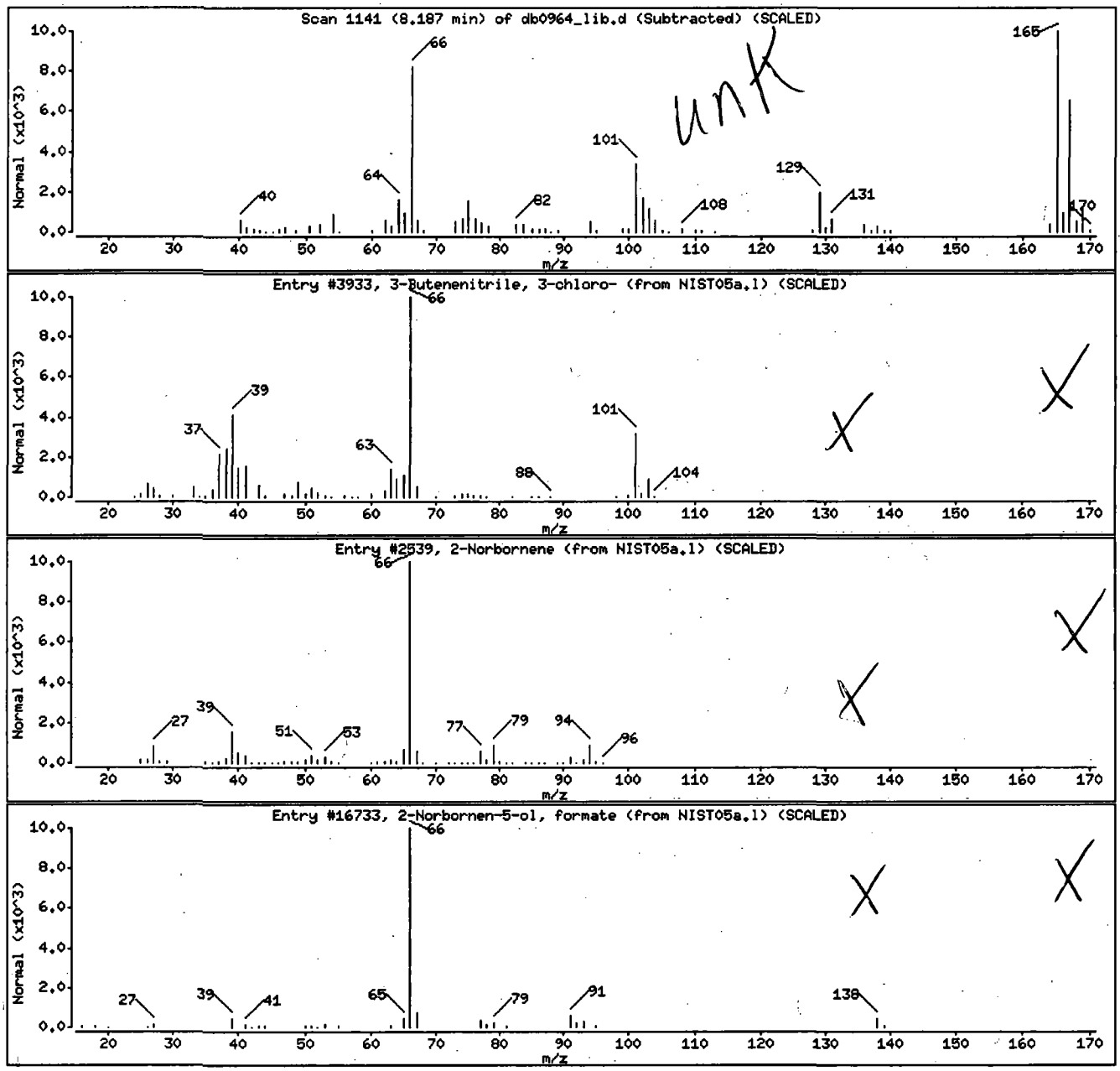
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	40	C4H4ClN	101
2-Norbornene	498-66-8	NIST05a.l	2539	47	C7H10	94
2-Norbornen-5-ol, formate	1000142-76-9	NIST05a.l	16733	47	C8H10O2	138



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Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

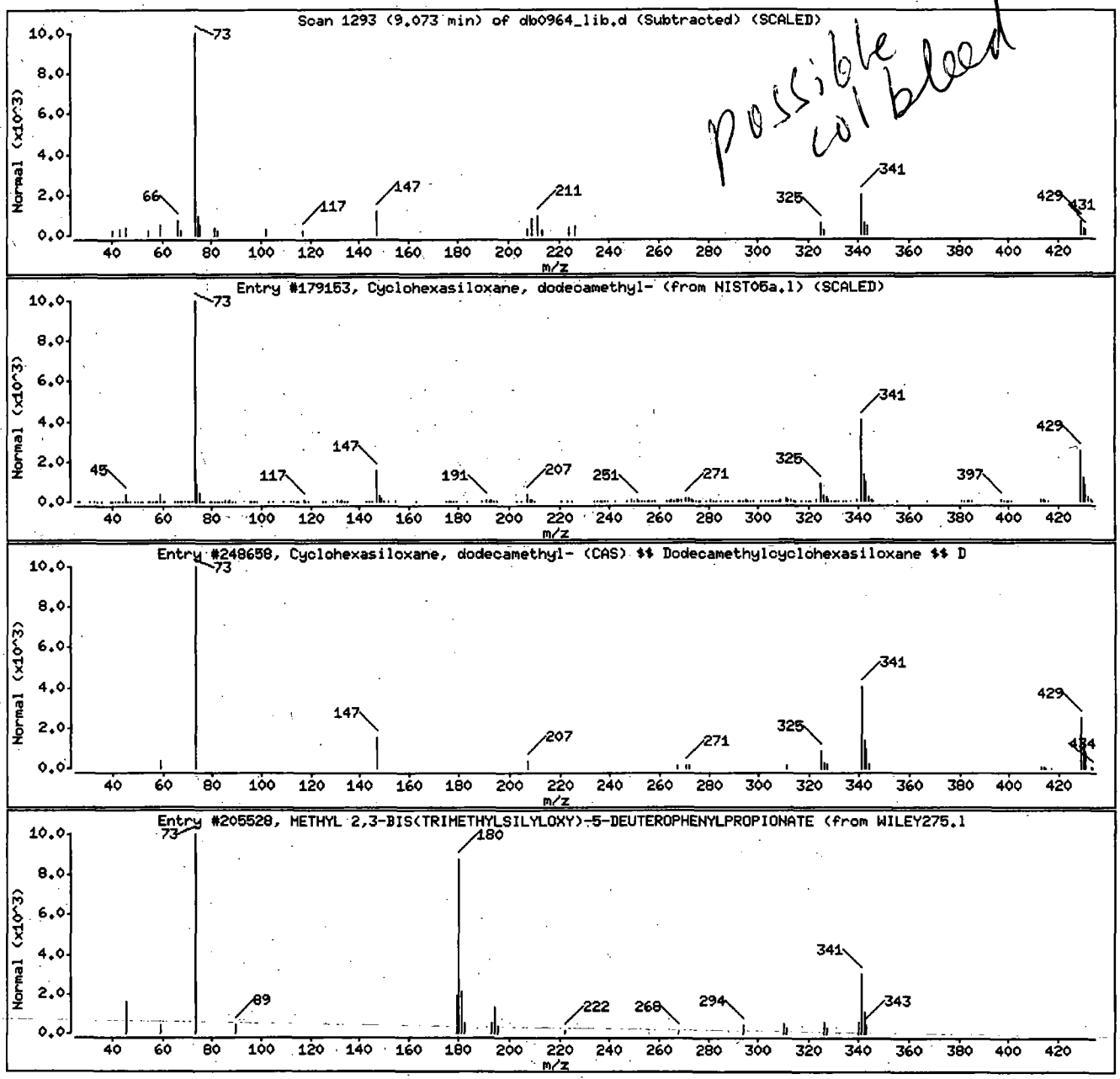
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexasiloxane, dodecamethyl-	540-97-6	NIST05a.l	179153	72	C12H36O6Si6	444
Cyclohexasiloxane, dodecamethyl- (CAS) $	540-97-6	WILEY275.l	248658	72	C12H36O6Si6	444
METHYL 2,3-BIS(TRIMETHYLSILYLOXY)-5-DEUT	0-00-0	WILEY275.l	205528	38	C16H27D04Si2	341



possible col bleed

Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21.b/db0964_lib.d

Date : 21-FEB-2014 11:48

Client ID: H6021

Instrument: HP19760.i

Sample Info: H6021;7366684;1;0;SAMPLE;;;

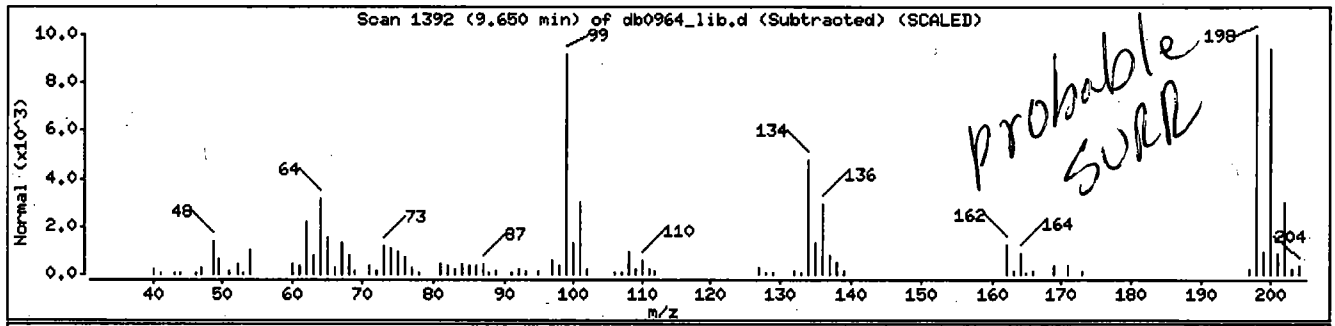
Volume Injected (uL): 1.0

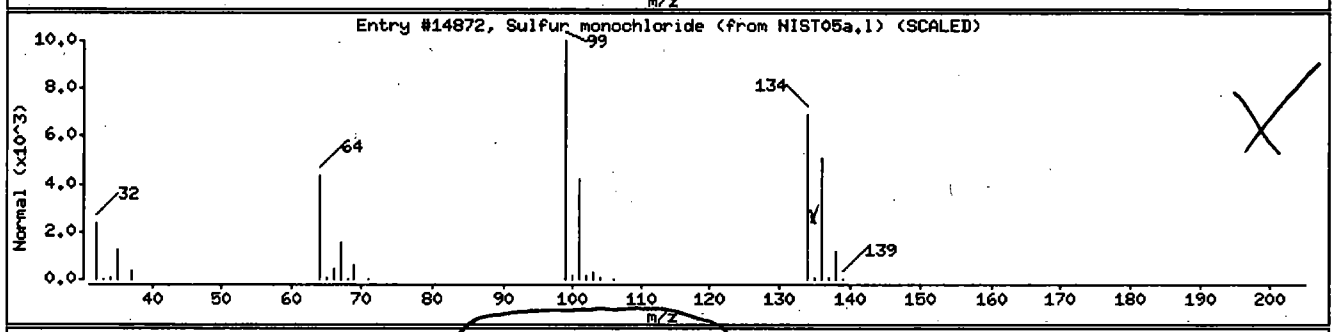
Operator: jmg00346

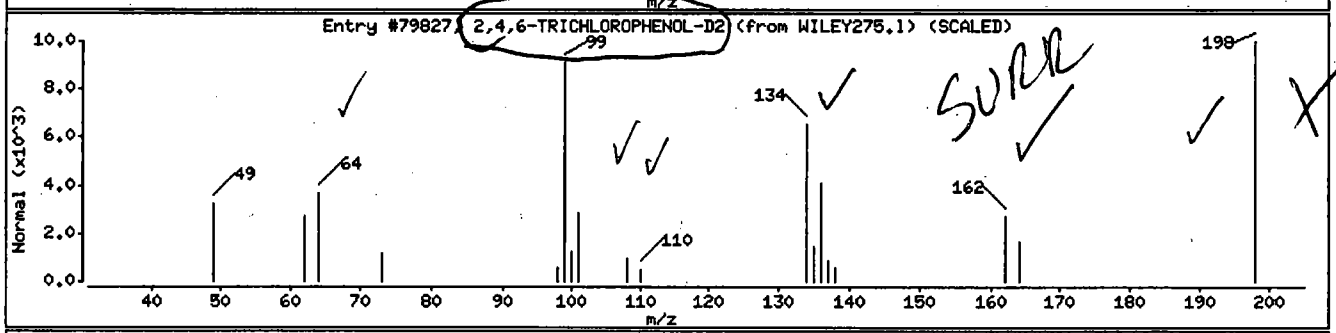
Column phase: J&W DB-5MS

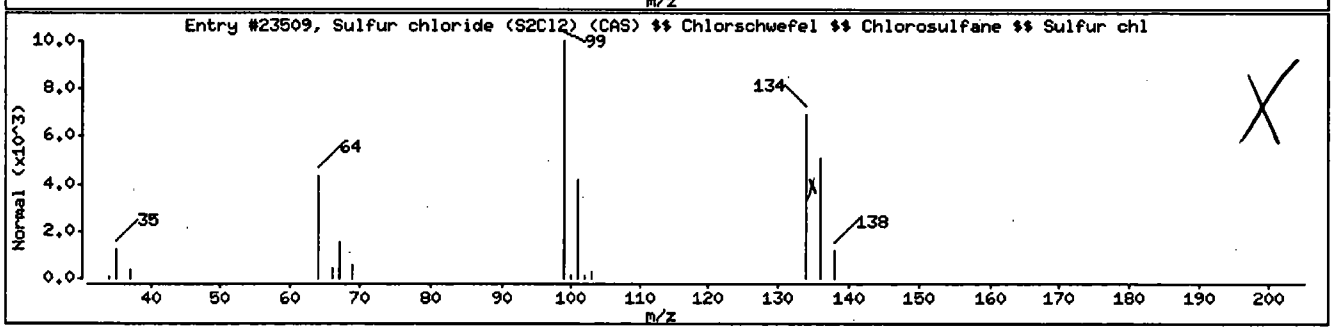
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	64	C6HD2Cl3O	198
Sulfur chloride (S2Cl2) (CAS) $$ Chlorso	10025-67-9	WILEY275.l	23509	38	Cl2S2	134



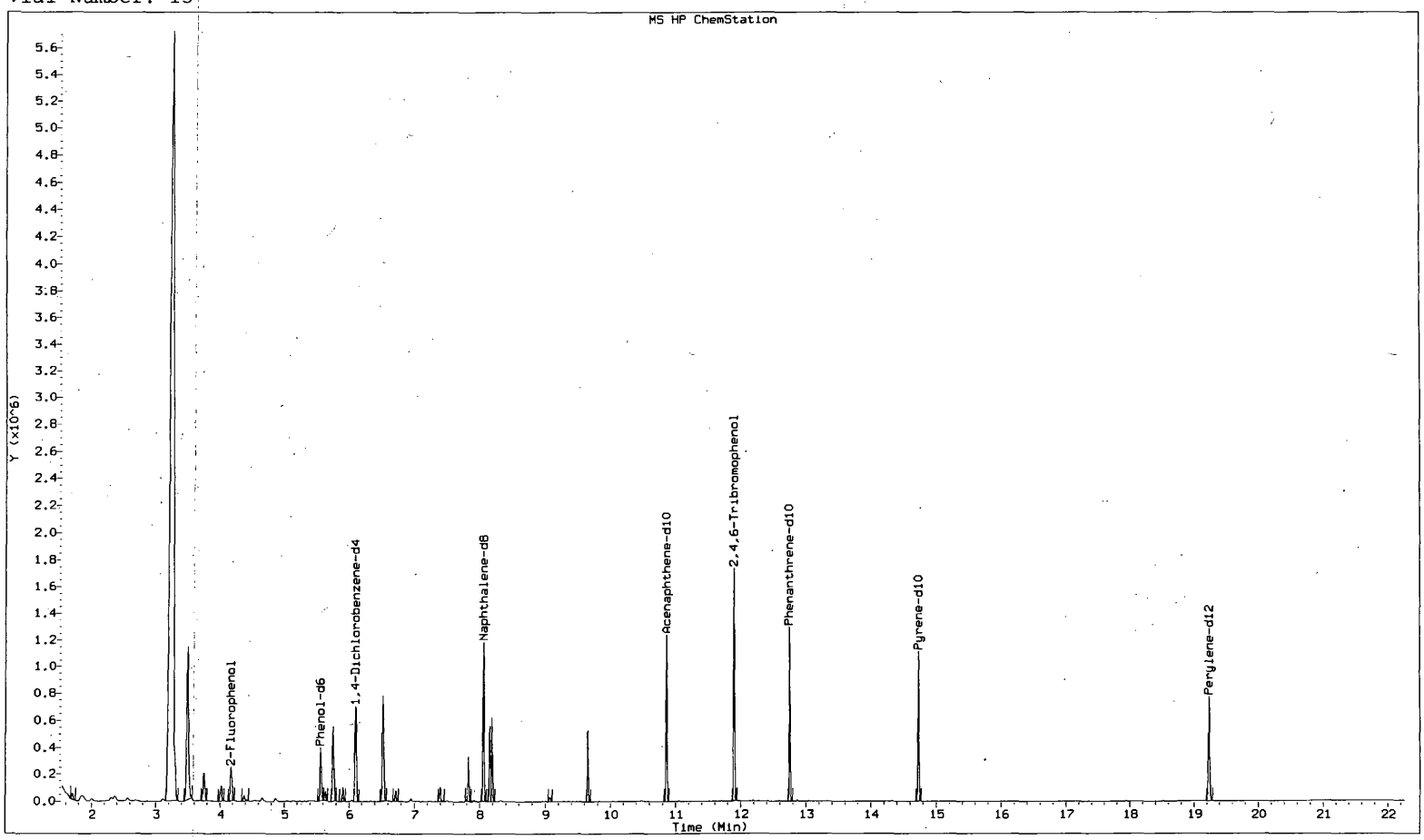






Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:30.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb21a.b/db0992_lib.d
Operator : ceb05247
Acquired : 21-FEB-2014 23:56
Instrument : HP19760.i
Sample Name: H7011;7368054;1;0;SAMPLE;;;
Misc Info : 14050WAL;WL13463;;1062;1000;0;db0960;13166;
Vial Number: 13



Lancaster Labs

Data file : /chem/HP19760.i/14feb21a.b/db0992_lib.d
Lab Smp Id: 7368054 Client Smp ID: H7011
Inj Date : 21-FEB-2014 23:56
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H7011;7368054;1;0;SAMPLE;;;
Misc Info : 14050WAL;WL13463;;1062;1000;0;db0960;13166;
Comment : Max. number of TICs to report is 50, 17 TICs were found initially.
Method : /chem/HP19760.i/14feb21a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:02 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 13
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1062.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	1055676	10.000
* 48 Naphthalene-d8	8.059	1573683	10.000
* 83 Acenaphthene-d10	10.863	1401808	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.700	77241	0.73166841	0.68895	83	NIST05a.l	31323	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.274	22836814	216.323952	203.69487	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.495	2402801	22.7607685	21.43198	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.752	415495	3.93581357	3.70603	25	NIST05a.l	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.014	214820	2.03490222	1.91610	38	NIST05a.l	13998	21
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.375	84983	0.80501080	0.75801	74	NIST05a.l	33655	21
Cyclotetrasiloxane, octamethyl- (CAS) $$					CAS #: 556-67-2		
5.634	91535	0.86707191	0.81645	91	WILEY275.l	174364	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.757	832550	7.88641113	7.42599	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.903	153808	1.45695867	1.37190	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.520	1182169	11.1982153	10.54445	38	NIST05a.l	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.713	114398	1.08365045	1.02038	78	NIST05a.l	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.395	131556	0.83597188	0.78716	91	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	414879	2.63635748	2.48244	43	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.158	654330	4.15795186	3.91520	87	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	757387	4.81282858	4.53185	50	NIST05a.l	3933	48
Cyclohexasiloxane, dodecamethyl-					CAS #: 540-97-6		
9.073	50410	0.32033195	0.30163	58	NIST05a.l	179153	48

Target compound.
Do not report.
ajs00193 03/02/2014

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Target 3.5 esignature user ID: ajs00193

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
====	====	==========	==========	====	=======	=========	======
Sulfur monochloride				CAS #: 10025-67-9			
9.656	638878	4.55752757	4.29145	38	NIST05a.l	14872	83(L)

QC Flag Legend

L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

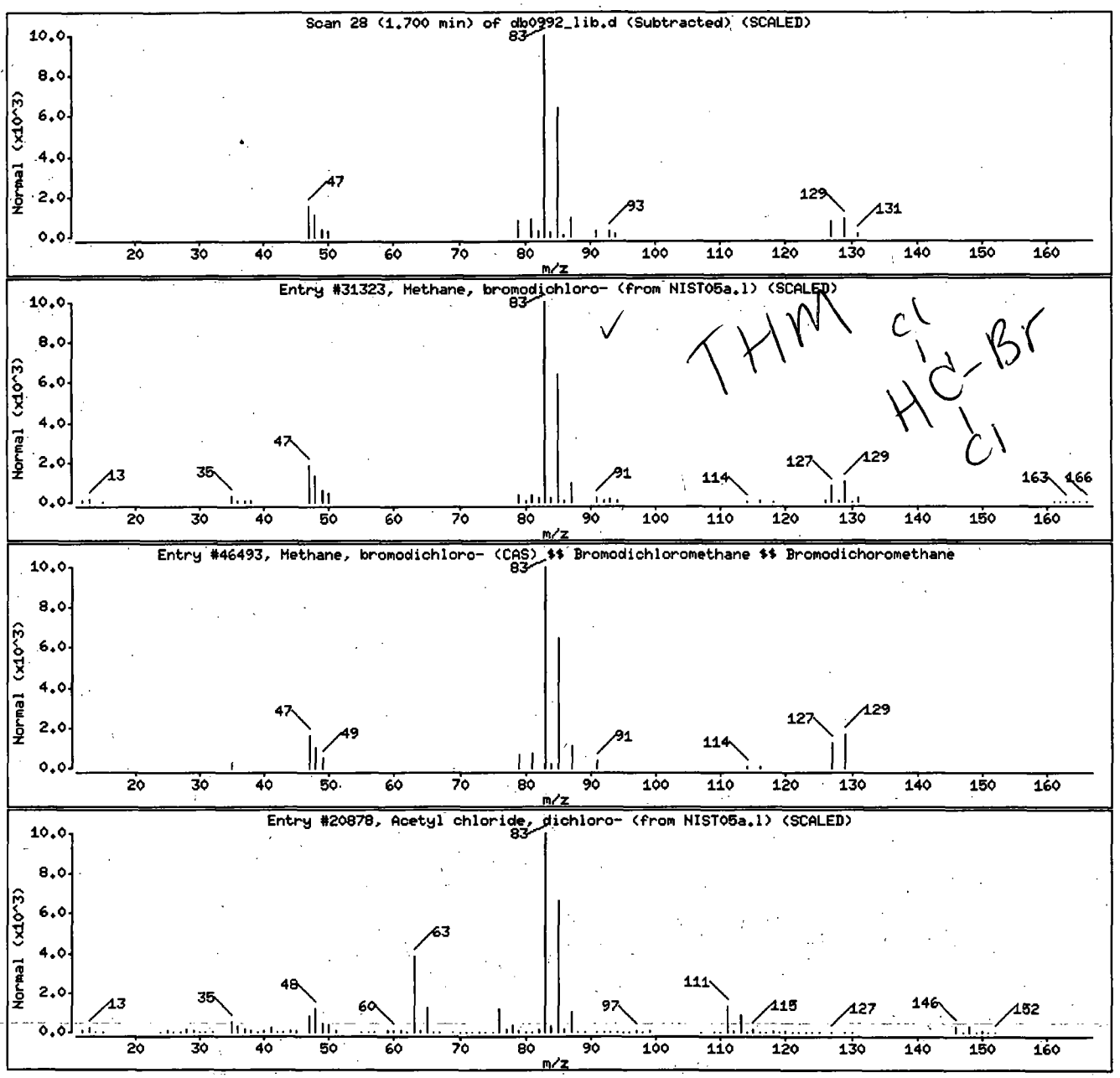
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	83	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46493	83	CHBrCl2	162
Acetyl chloride, dichloro-	79-36-7	NIST05a.l	20878	72	C2HCl3O	146



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

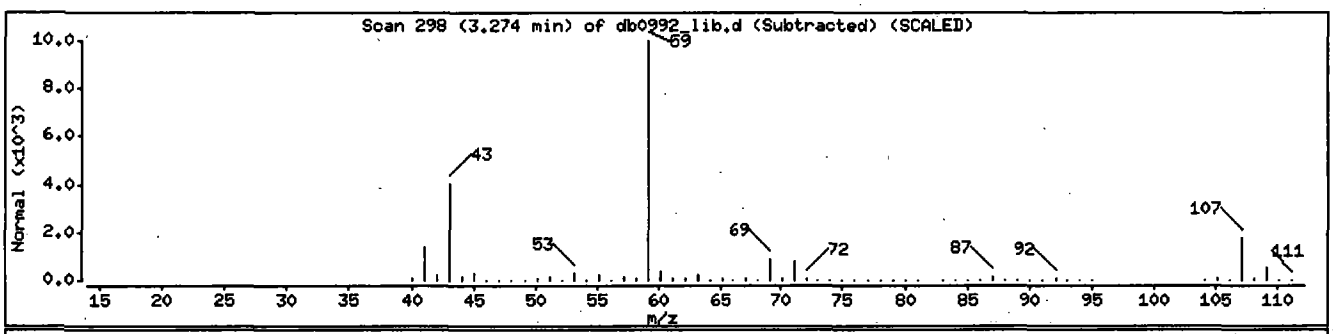
Volume Injected (uL): 1.0

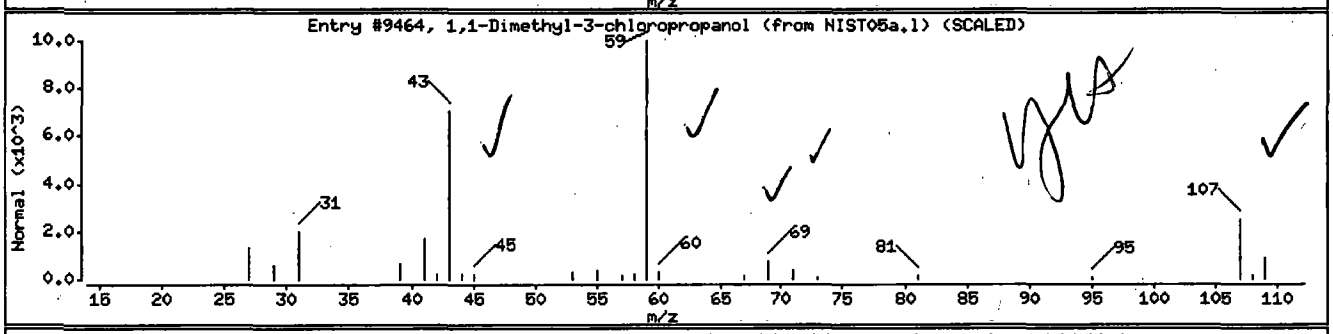
Operator: ceb05247

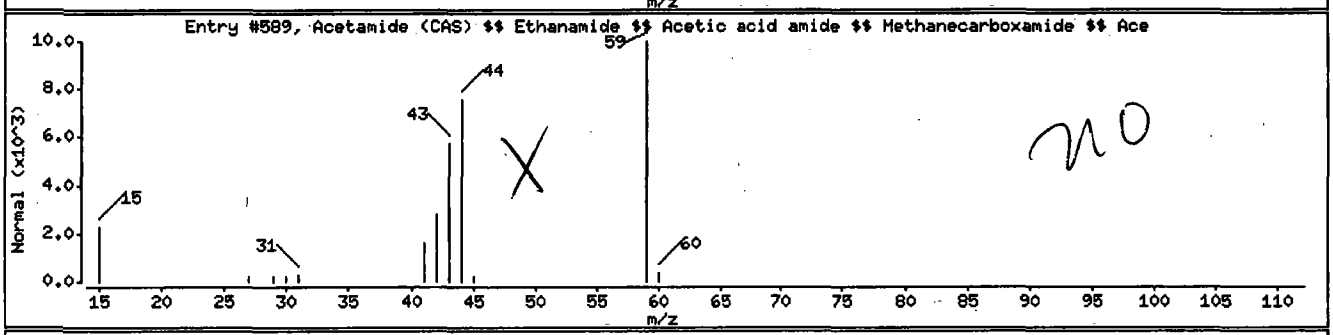
Column phase: J&W DB-5MS

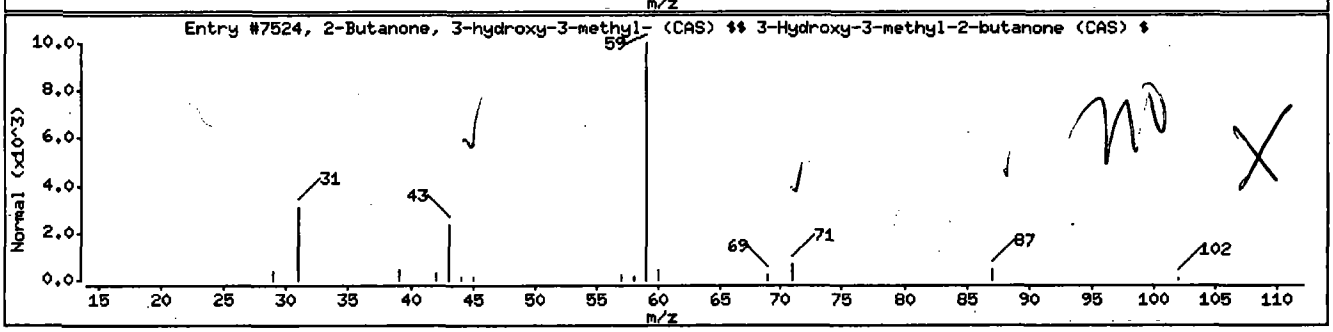
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

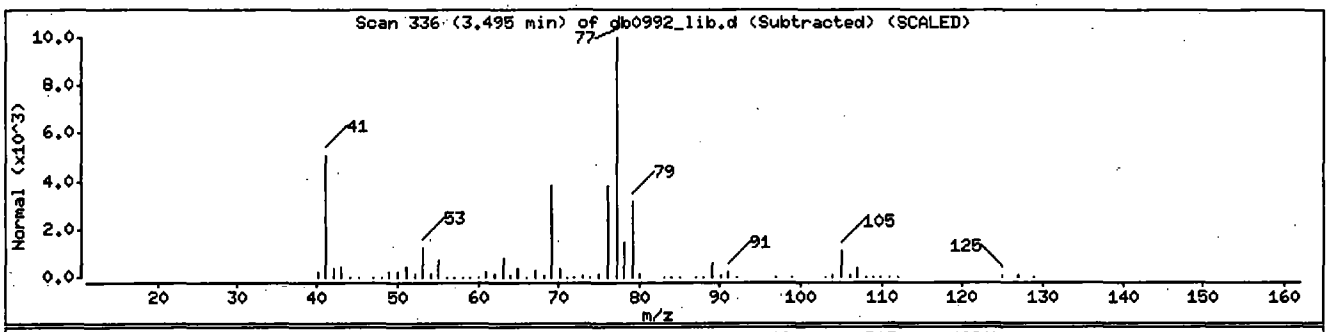
Volume Injected (uL): 1.0

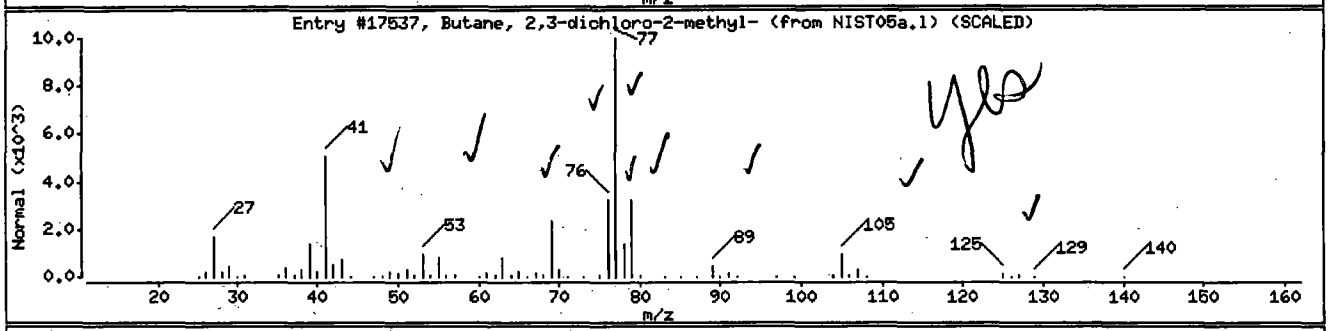
Operator: ceb05247

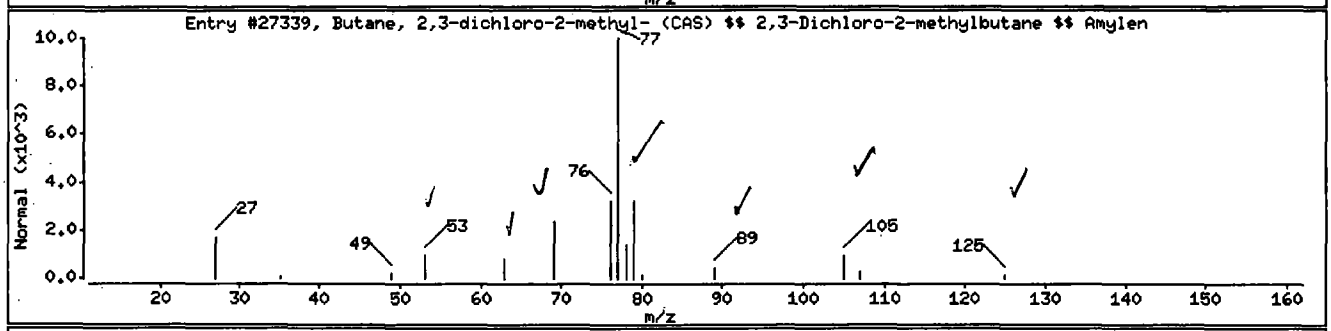
Column phase: J&W DB-5MS

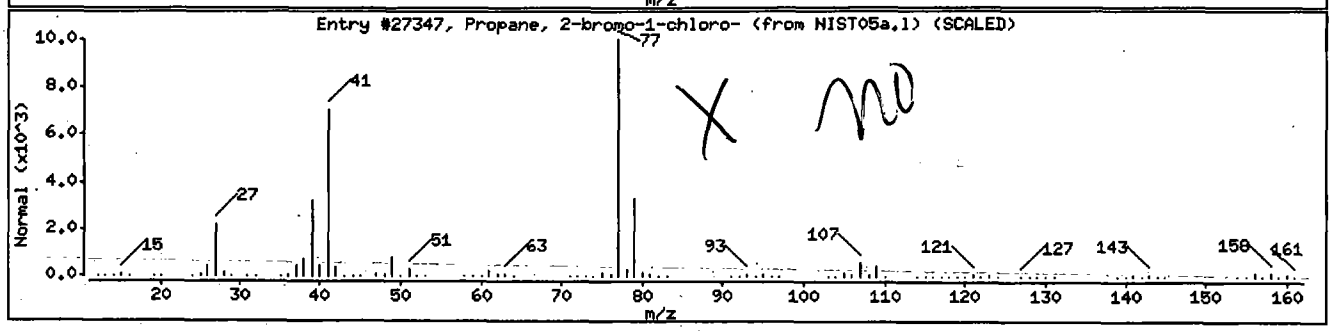
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	40	C3H6BrCl	156









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

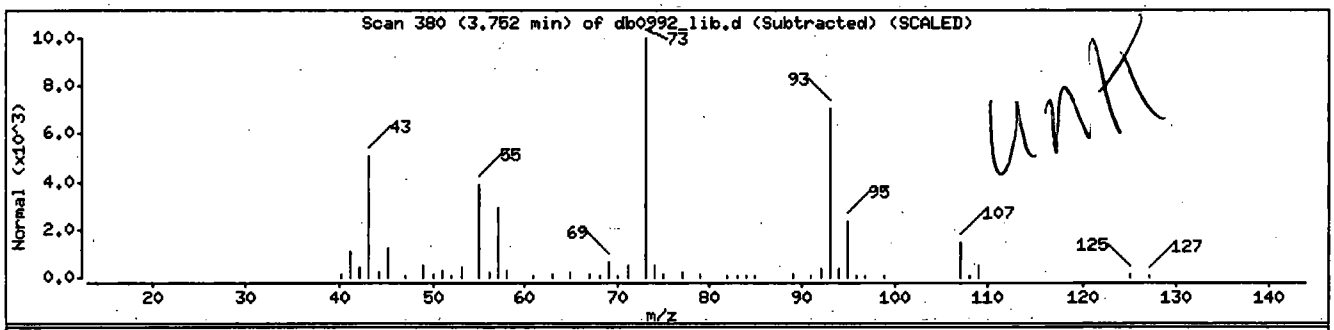
Volume Injected (uL): 1.0

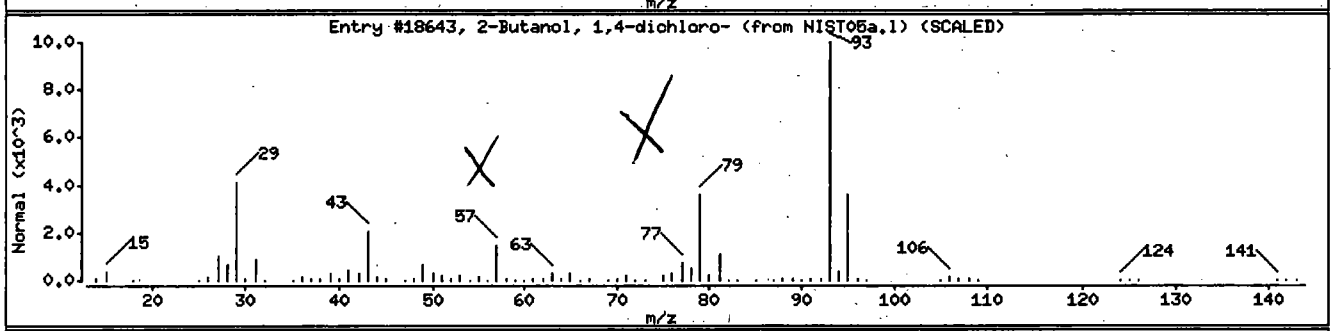
Operator: ceb05247

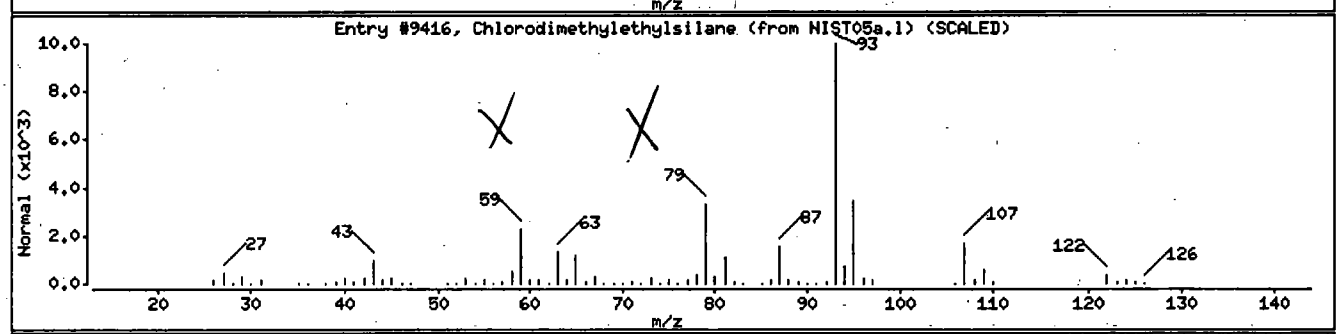
Column phase: J&W DB-5MS

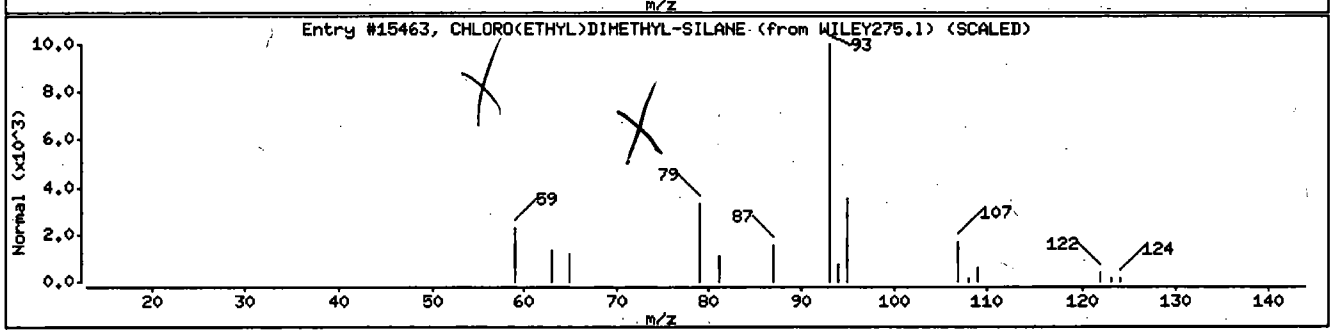
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	26	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122
CHLORO(ETHYL)DIMETHYL-SILANE	0-00-0	WILEY275.l	15463	33	C4H11ClSi	122









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

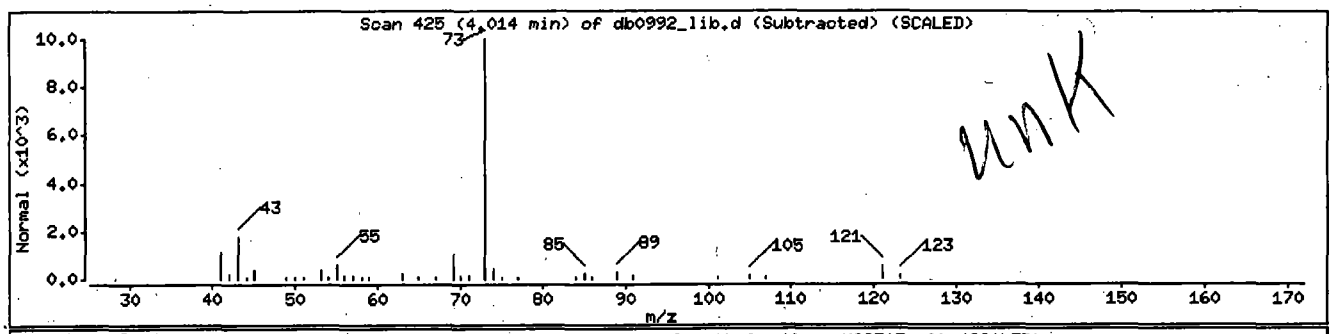
Volume Injected (uL): 1.0

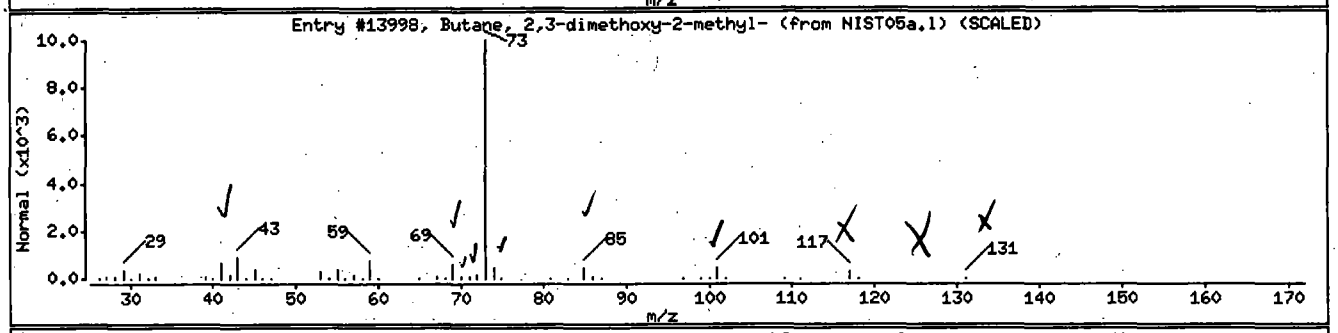
Operator: ceb05247

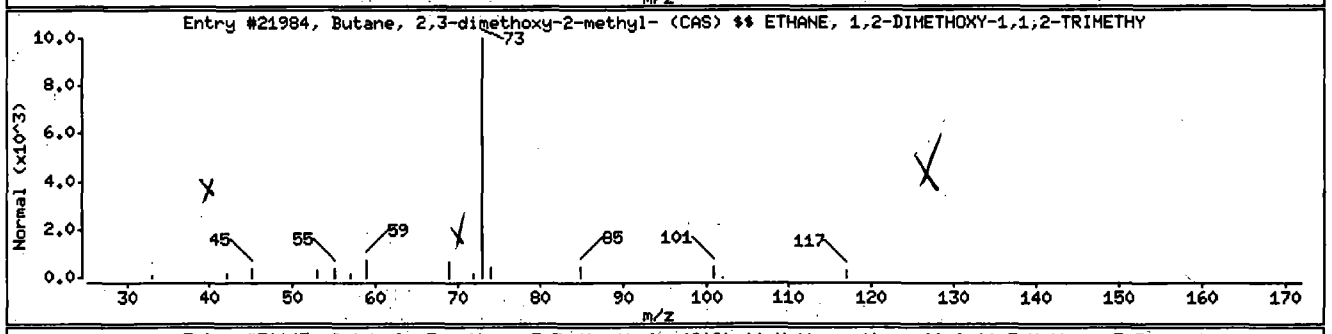
Column phase: J&W DB-5MS

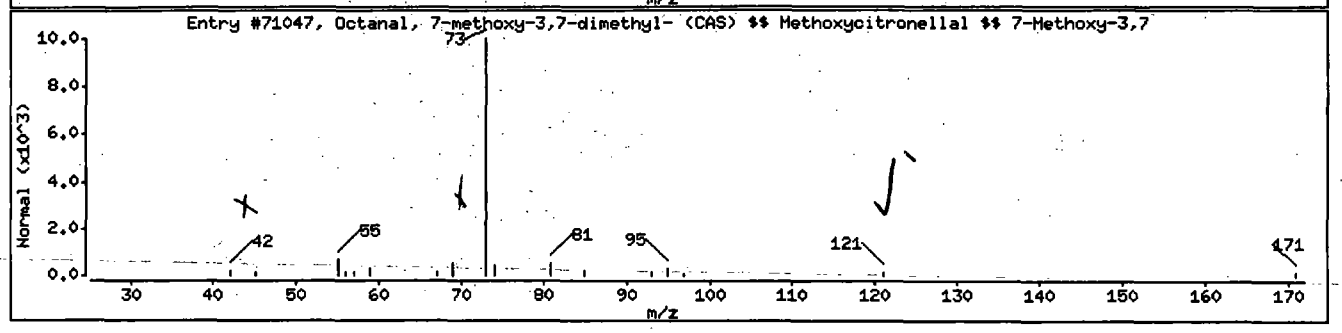
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	38	C7H16O2	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl- (CAS) $	3613-30-7	WILEY275.l	71047	33	C11H22O2	186









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

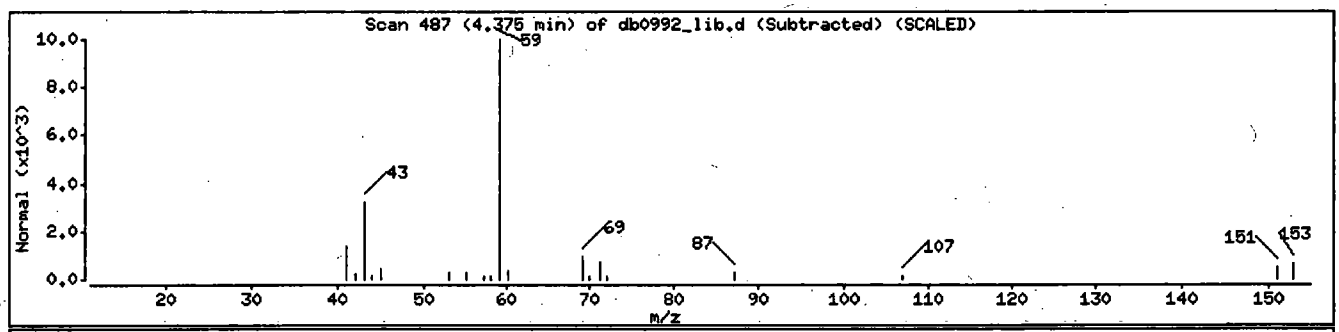
Client ID: H7011 Instrument: HP19760.i

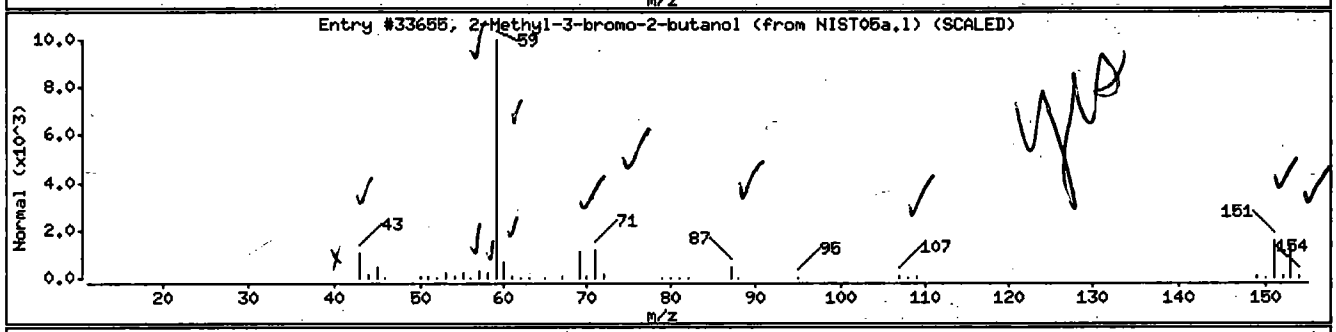
Sample Info: H7011;7368054;1;0;SAMPLE;;;

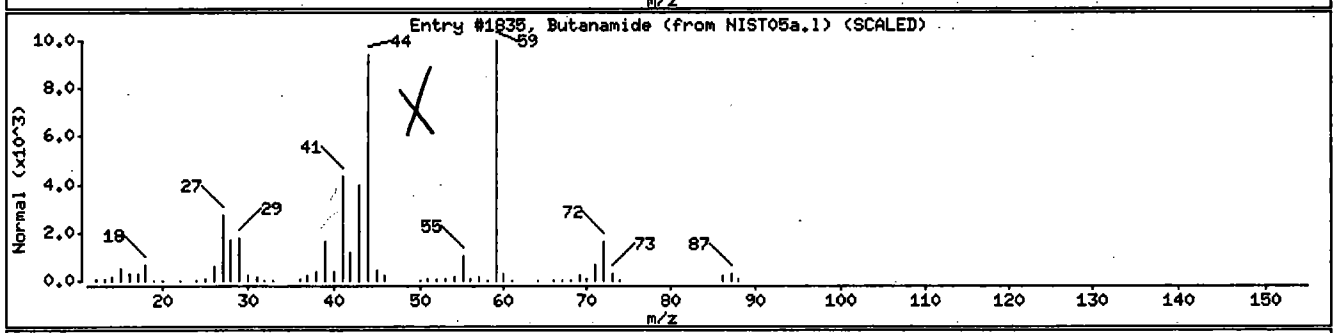
Volume Injected (uL): 1.0 Operator: ceb05247

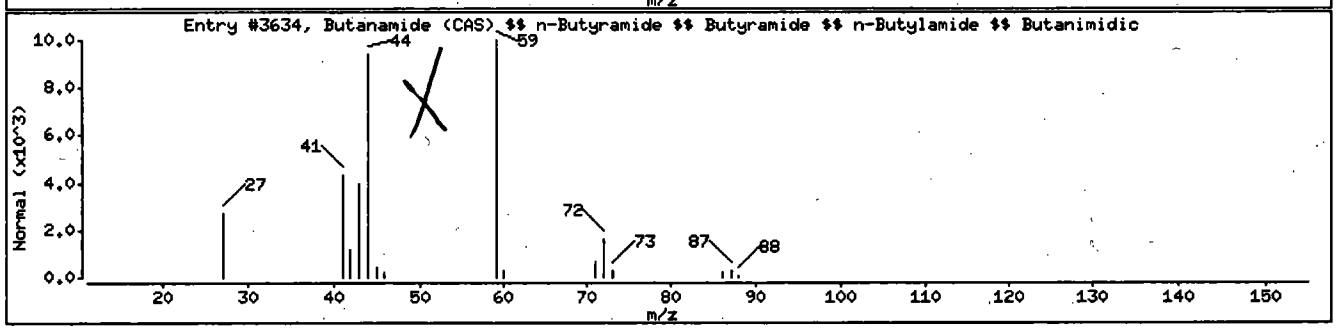
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	74	C5H11BrO	166
Butanamide	541-35-5	NIST05a.l	1835	64	C4H9NO	87
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3634	64	C4H9NO	87









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

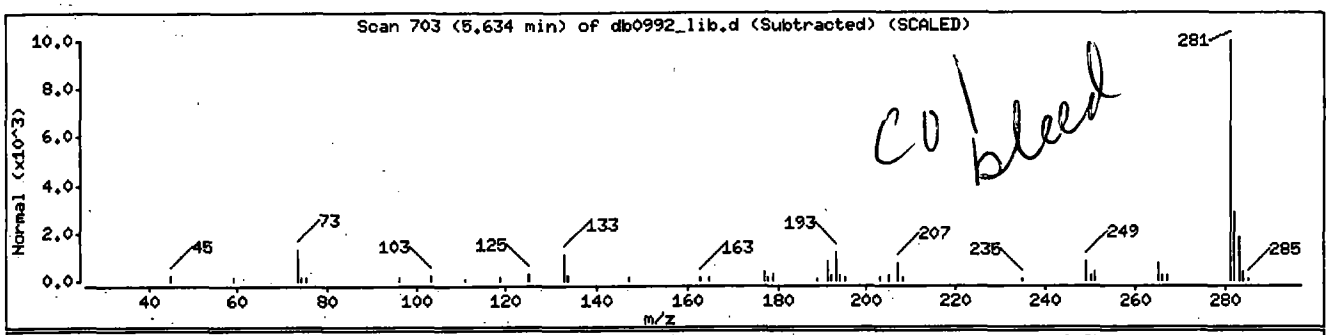
Volume Injected (uL): 1.0

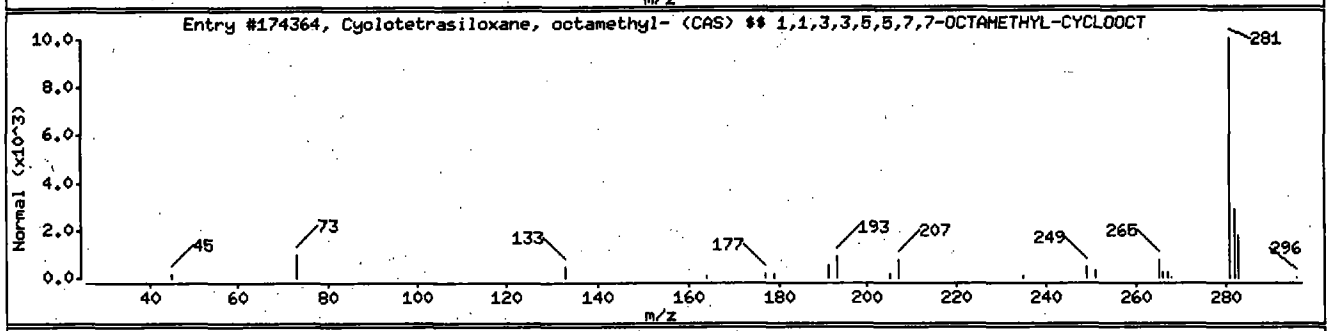
Operator: ceb05247

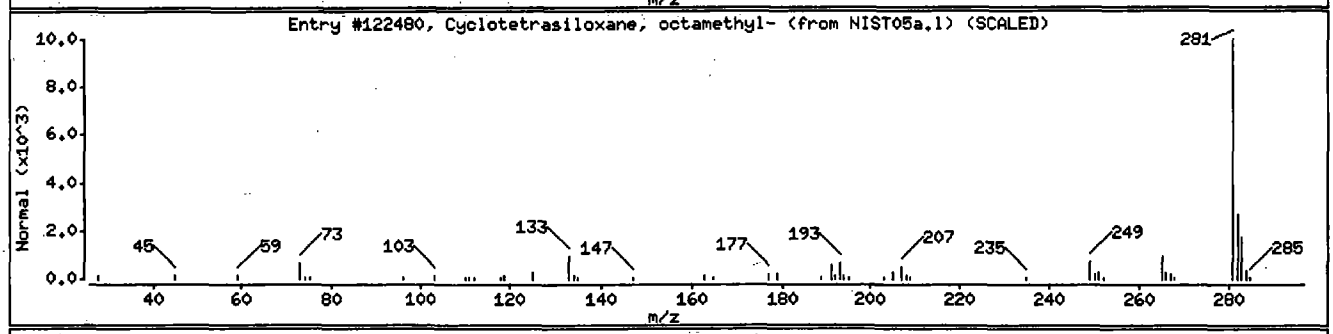
Column phase: J&W DB-5MS

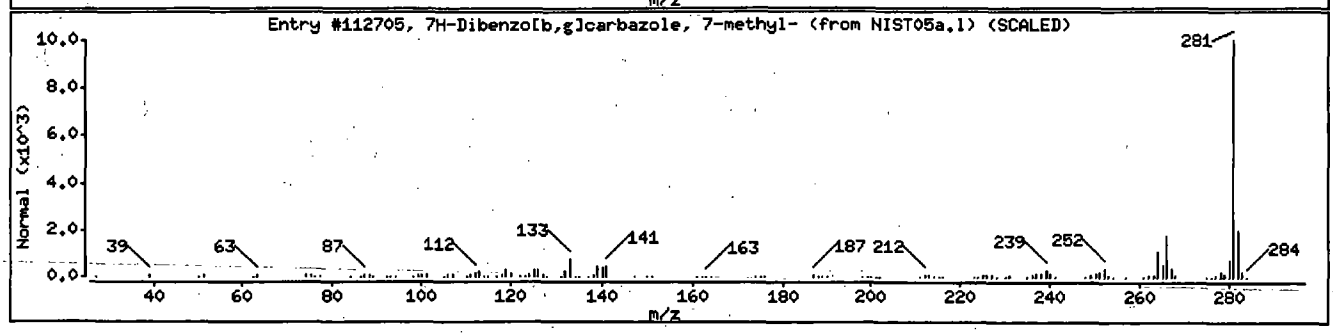
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclotetrasiloxane, octamethyl- (CAS) $$	556-67-2	WILEY275.l	174364	91	C8H24O4Si4	296
Cyclotetrasiloxane, octamethyl-	556-67-2	NIST05a.l	122480	90	C8H24O4Si4	296
7H-Dibenzo[b,g]carbazole, 7-methyl-	3557-49-1	NIST05a.l	112705	59	C21H15N	281









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

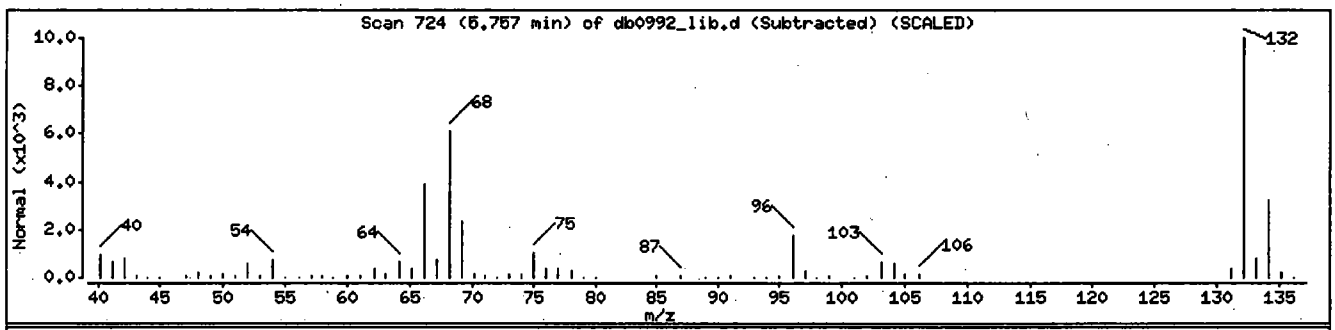
Volume Injected (uL): 1.0

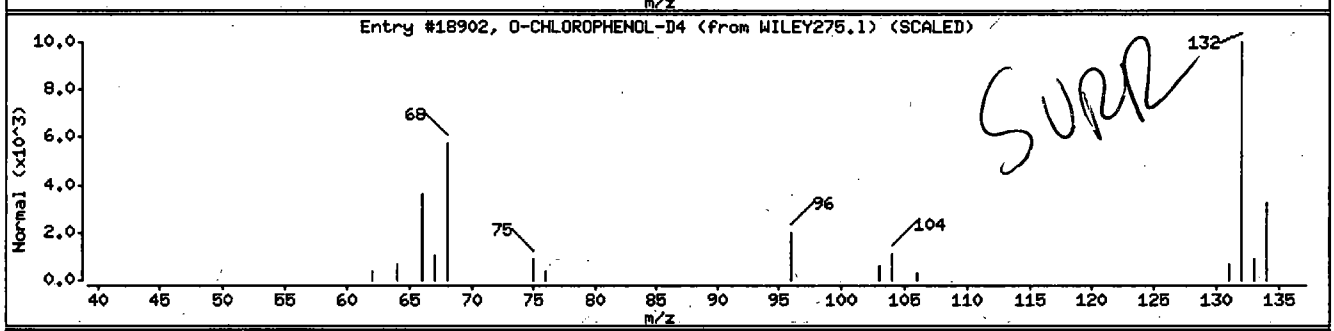
Operator: ceb05247

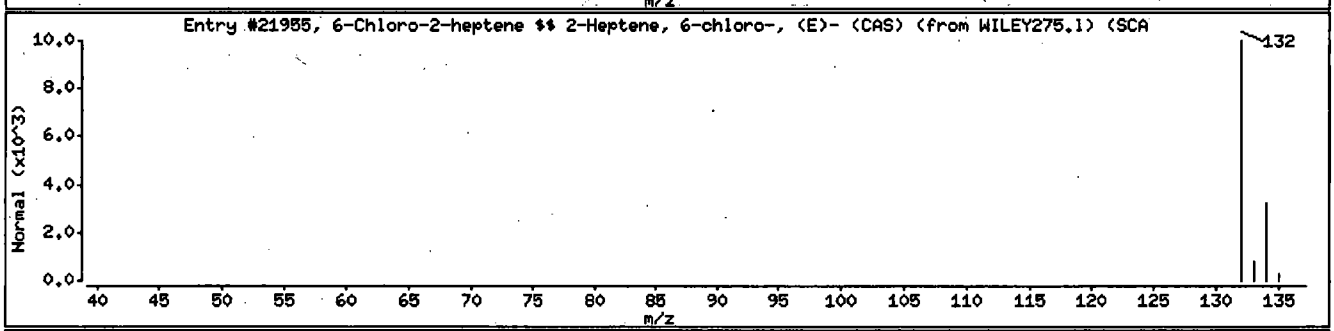
Column phase: J&W DB-5MS

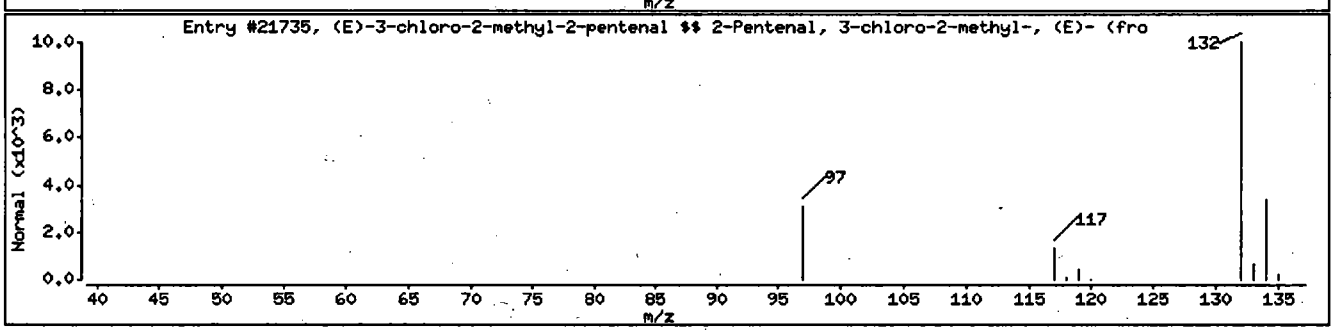
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

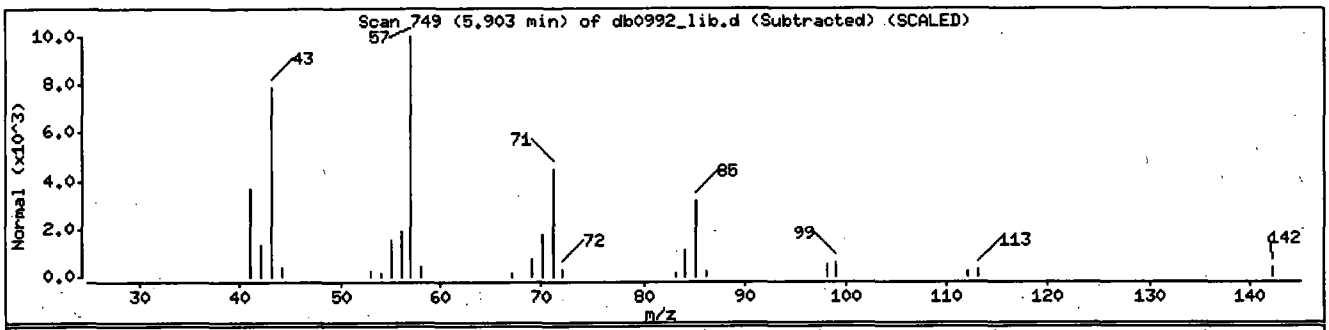
Volume Injected (uL): 1.0

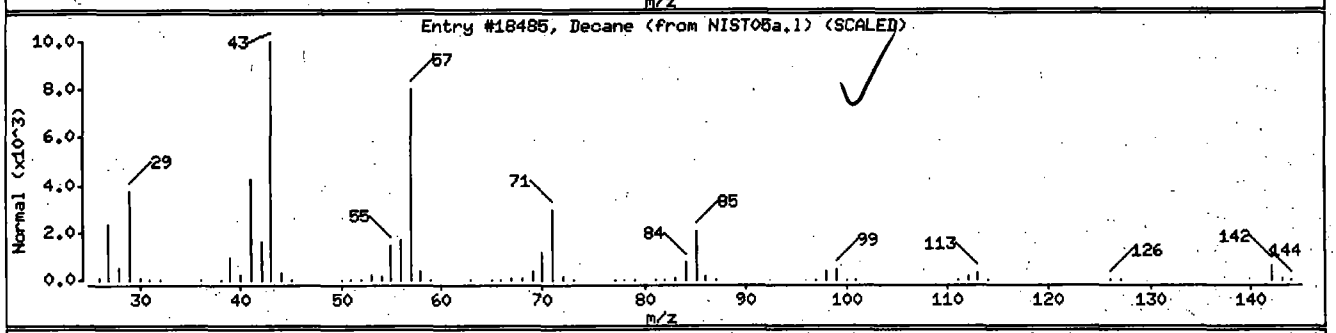
Operator: ceb05247

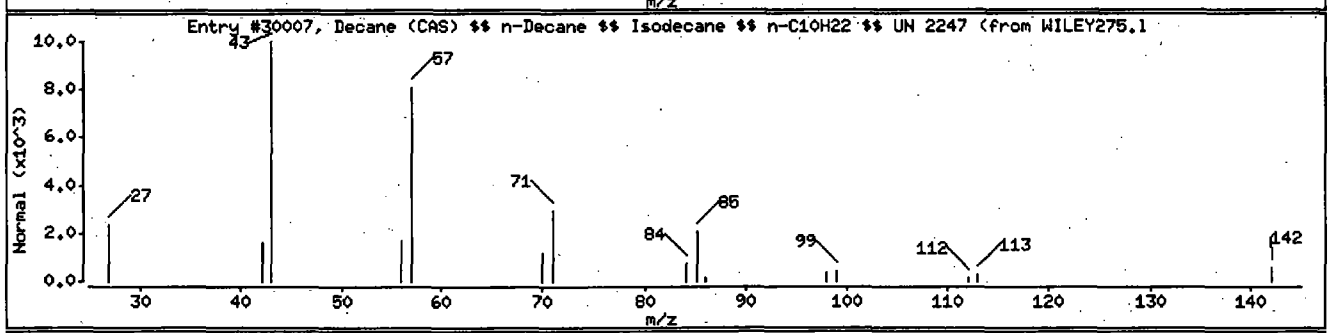
Column phase: J&W DB-5MS

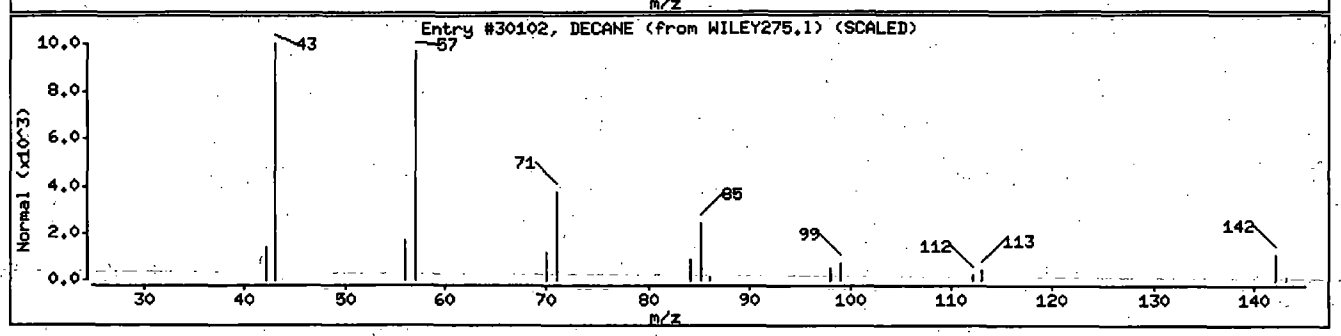
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

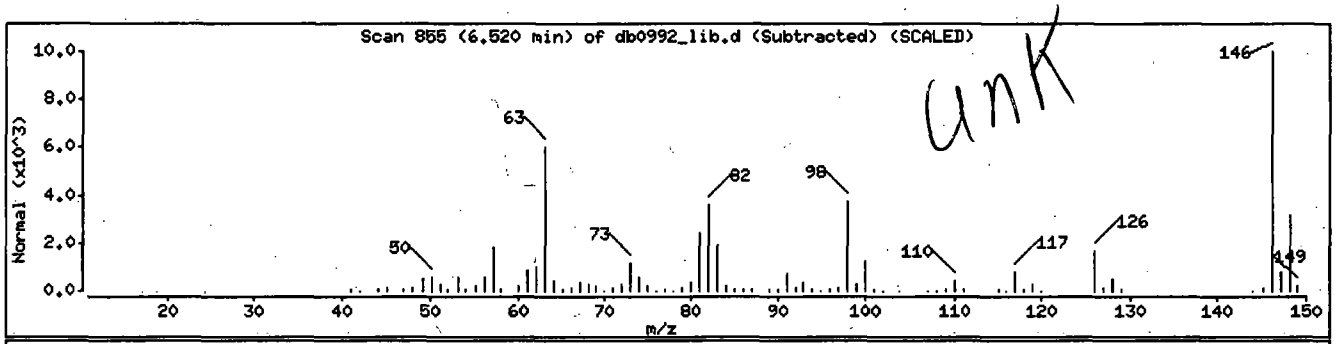
Volume Injected (uL): 1.0

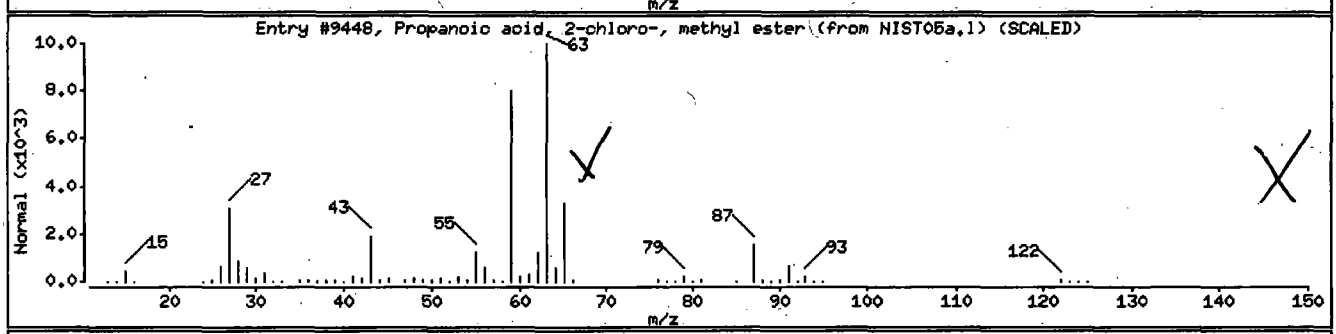
Operator: ceb05247

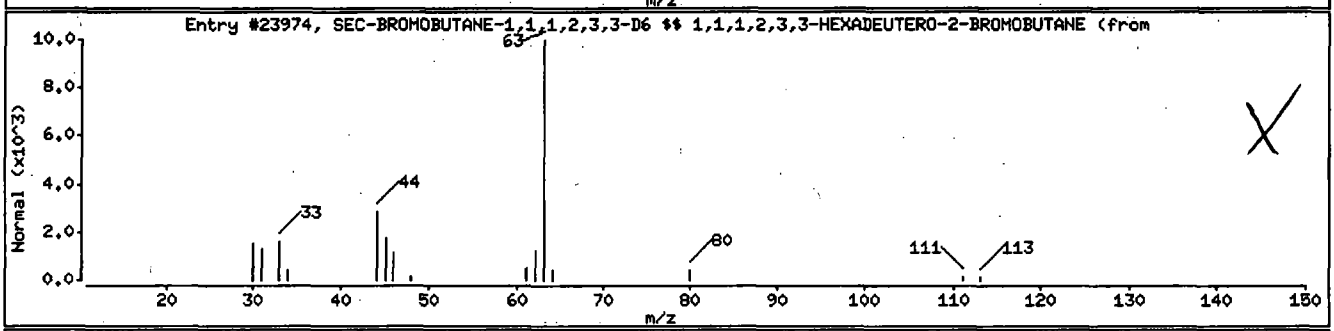
Column phase: J&W DB-5MS

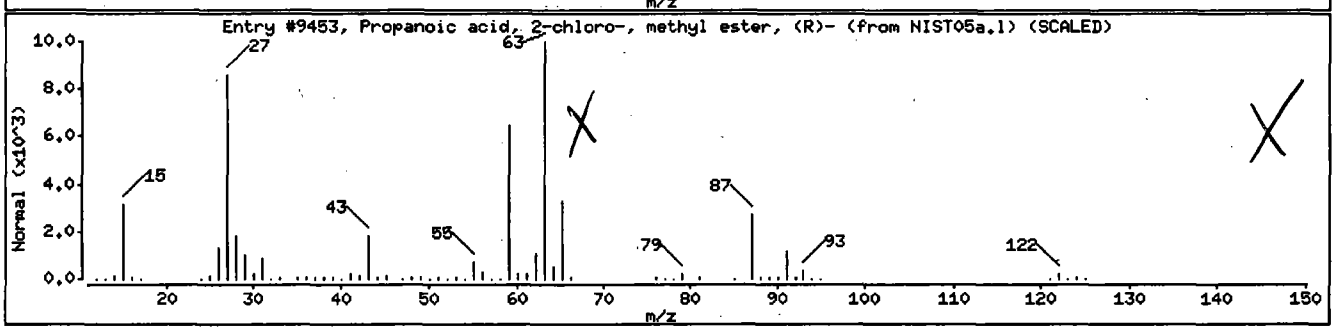
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	39	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Propanoic acid, 2-chloro-, methyl ester,	77287-29-7	NIST05a.l	9453	23	C4H7ClO2	122









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Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

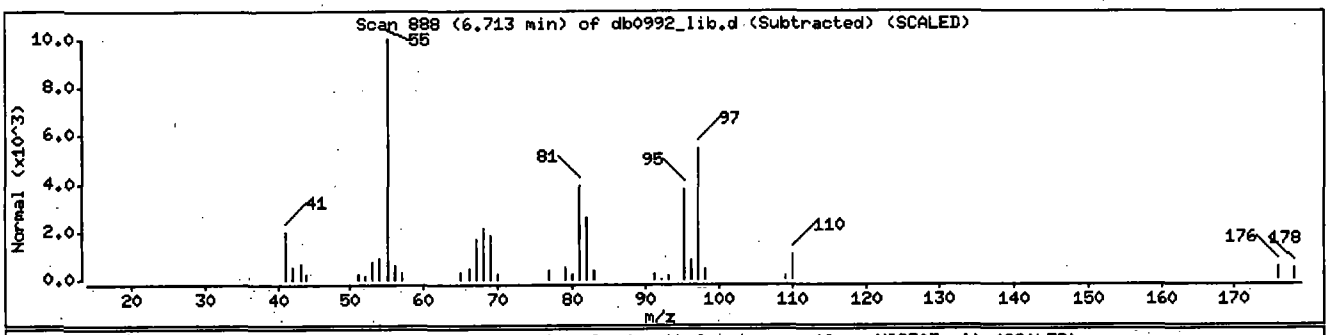
Volume Injected (uL): 1.0

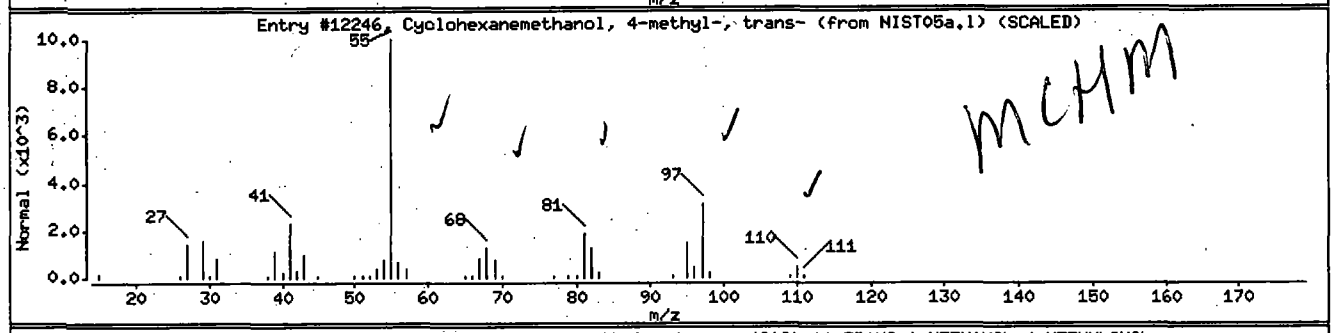
Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	78	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	78	C8H16O	128
Cycloheptanemethanol	4448-75-3	NIST05a.l	12097	50	C8H16O	128





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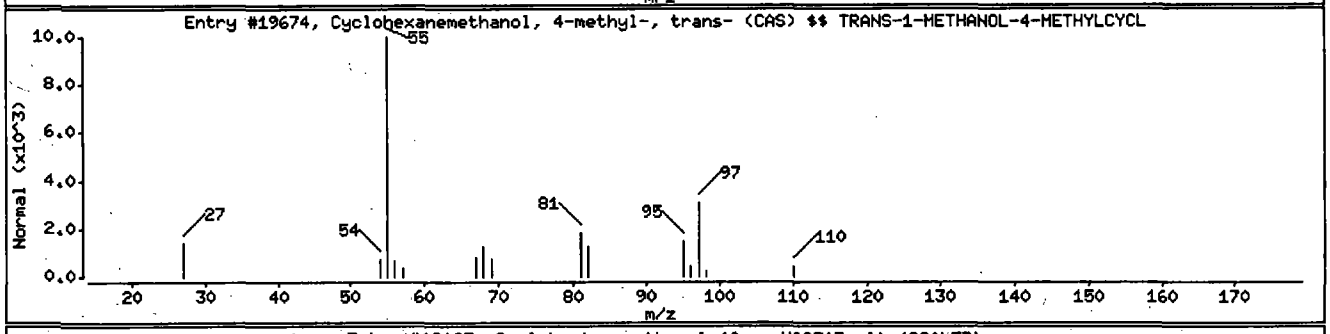

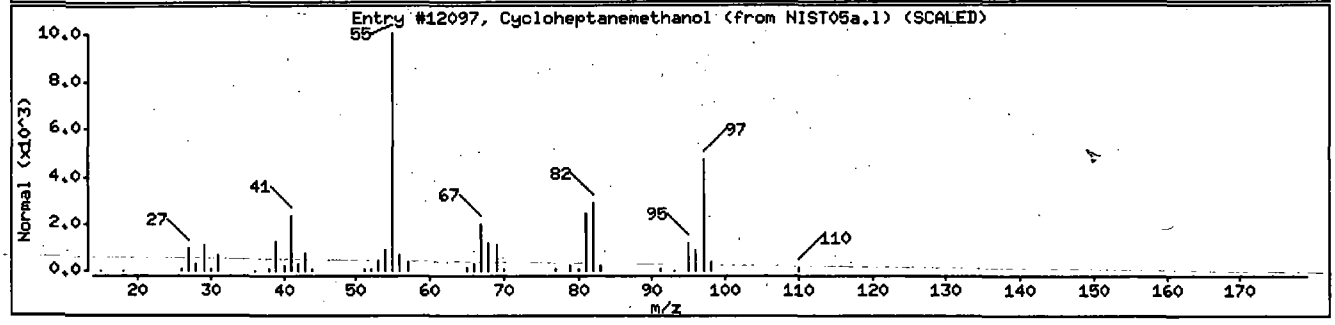

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

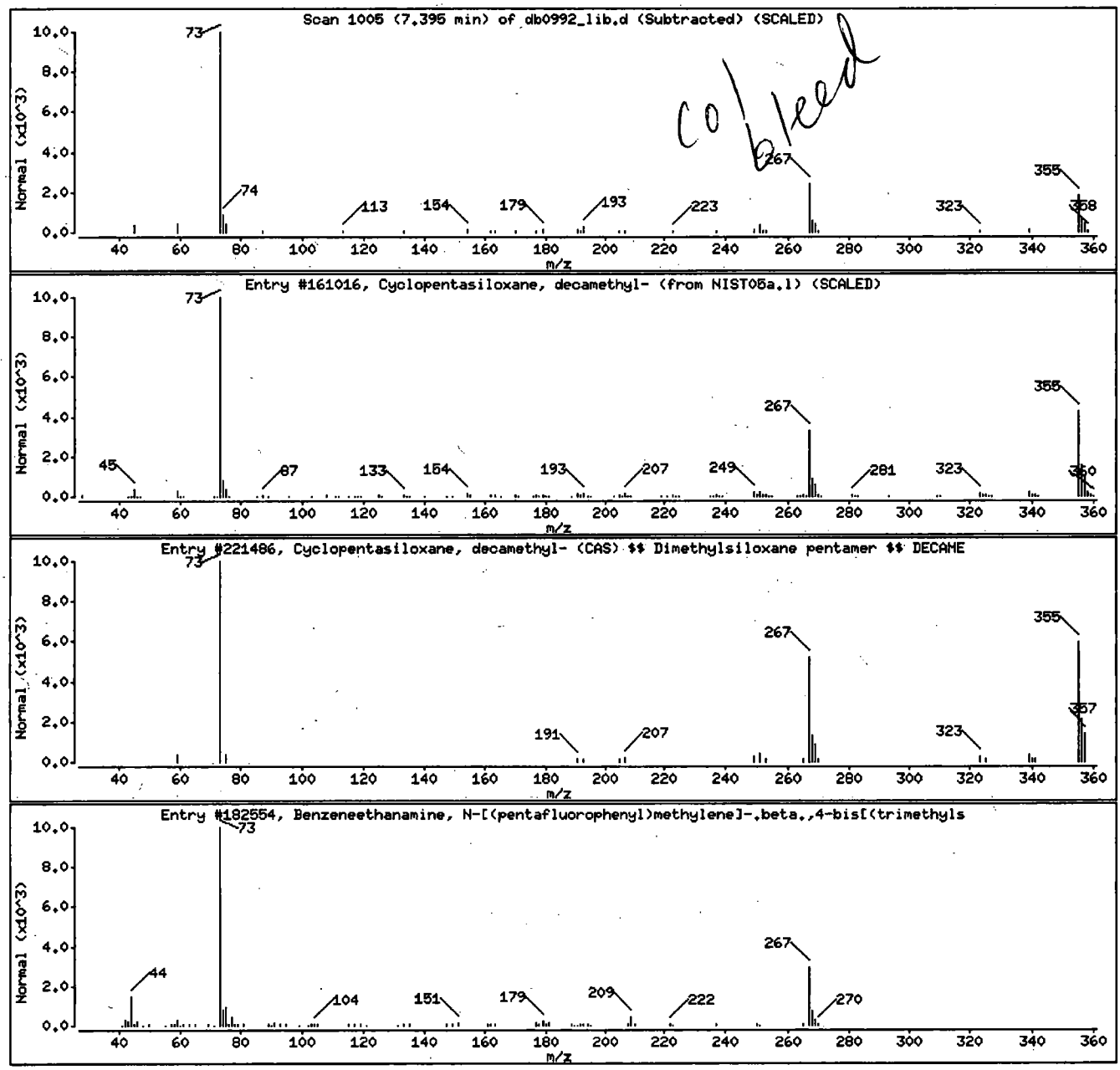
Client ID: H7011 Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	91	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
Benzeneethanamine, N-[(pentafluorophenyl	55429-85-1	NIST05a.l	182554	38	C21H26F5NO2Si	475



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

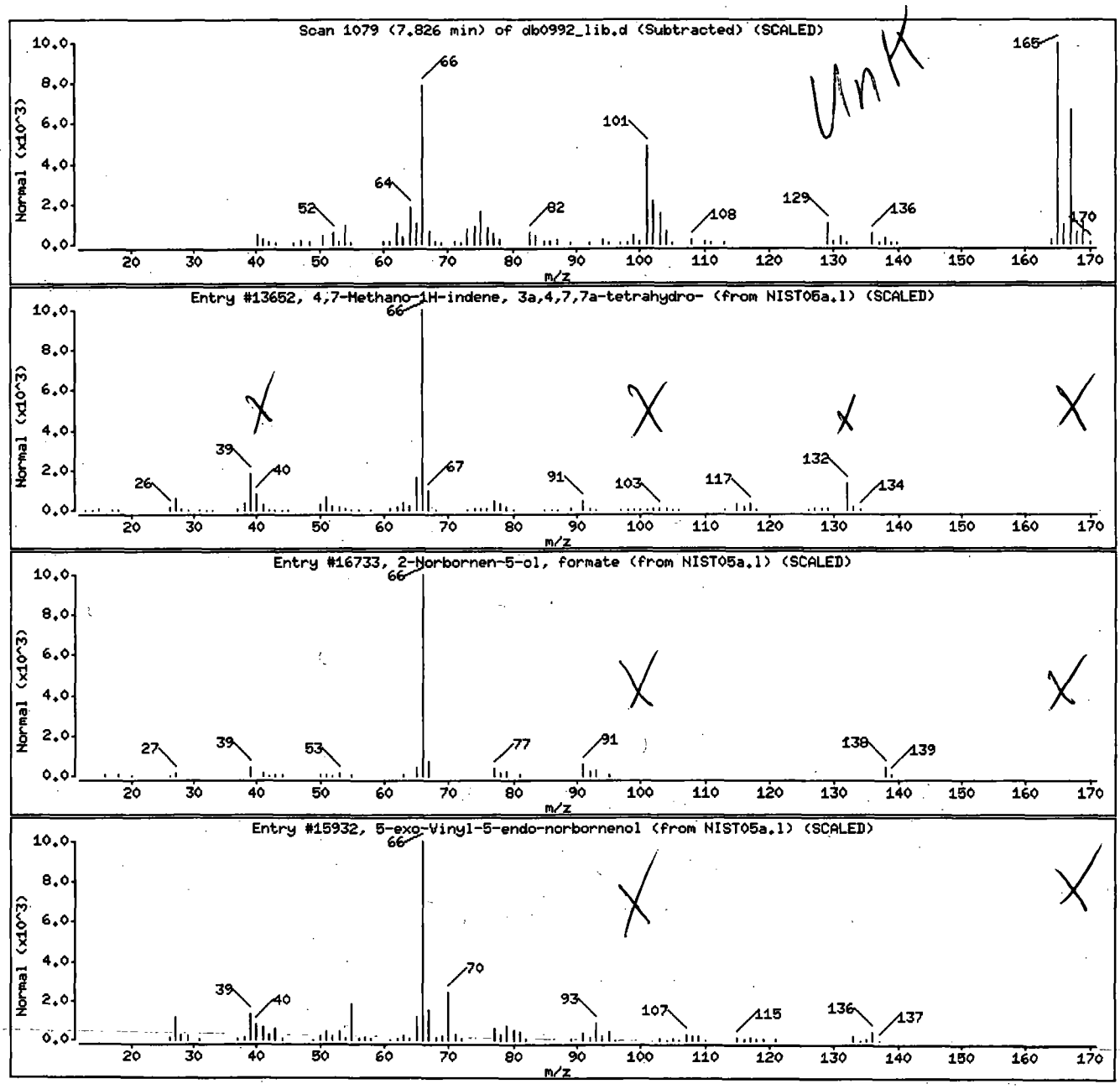
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	43	C10H12	132
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H10O2	138
5-exo-Vinyl-5-endo-norbornenol	37165-54-1	NIST05a.l	15932	43	C9H12O	136



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

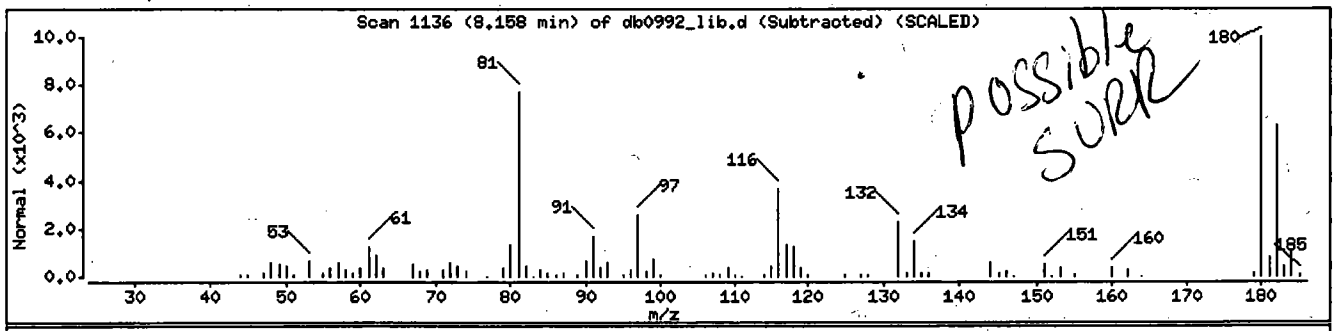
Volume Injected (uL): 1.0

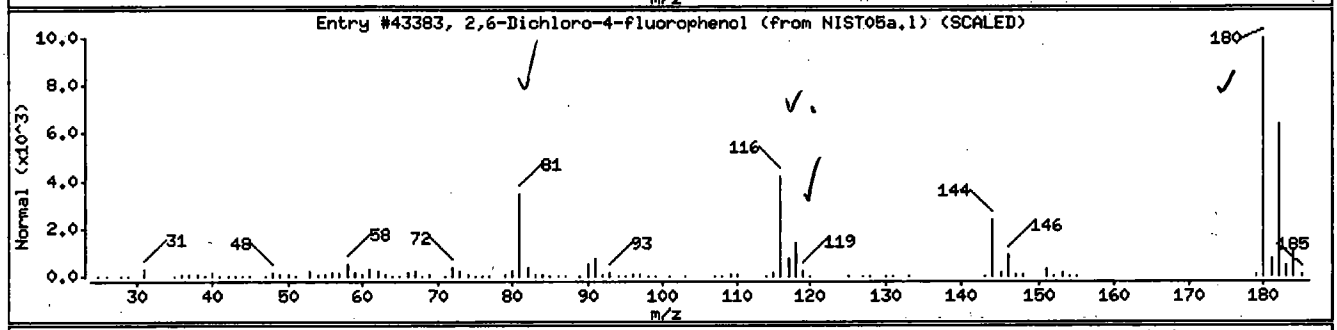
Operator: ceb05247

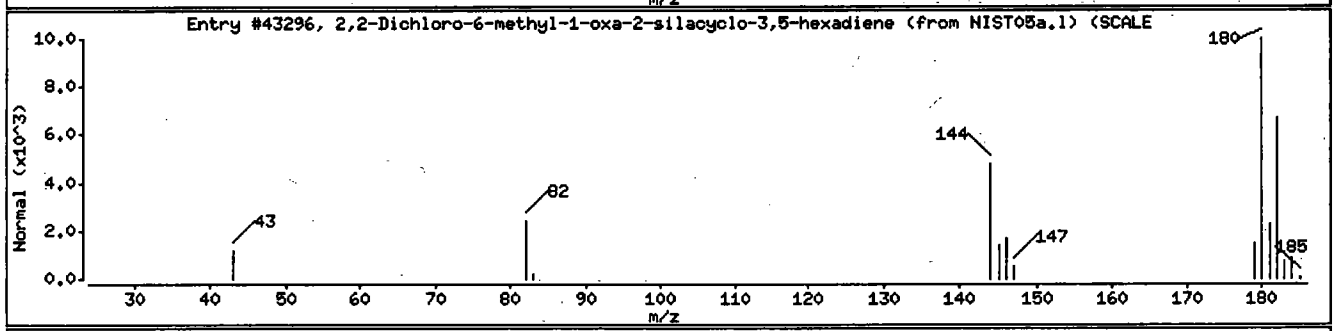
Column phase: J&W DB-5MS

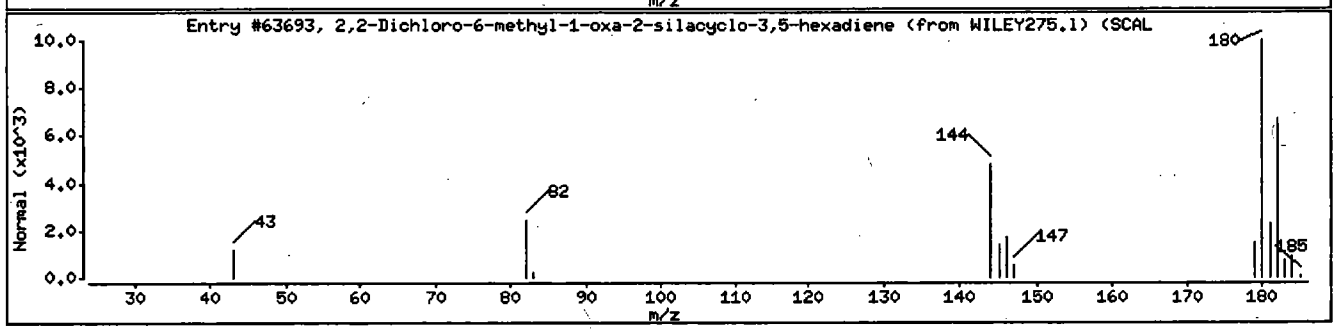
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	87	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	35	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	35	C5H6Cl2OSi	180









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

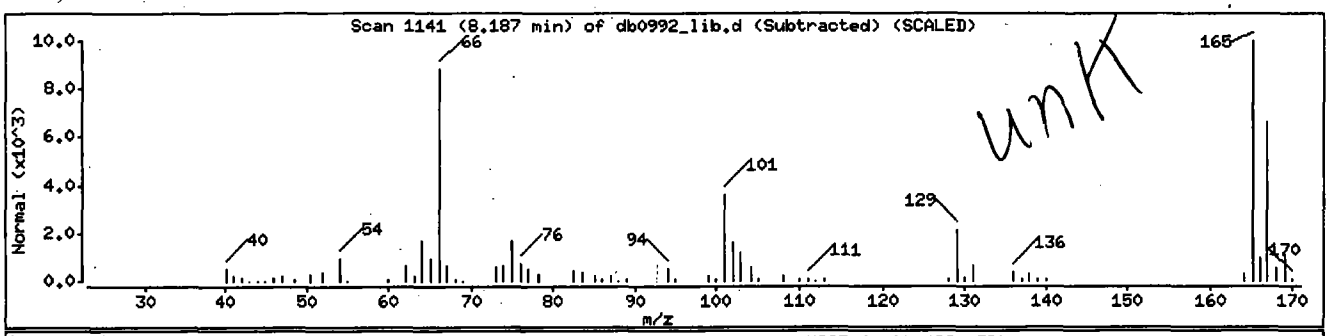
Volume Injected (uL): 1.0

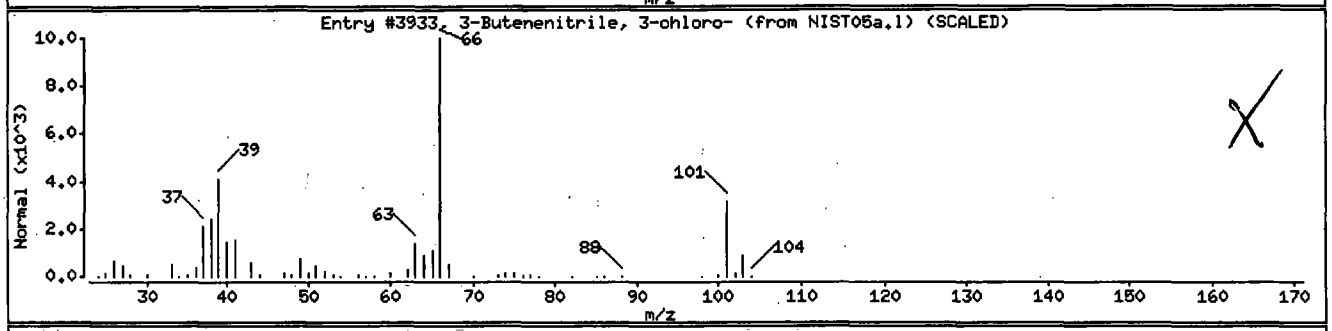
Operator: oeb05247

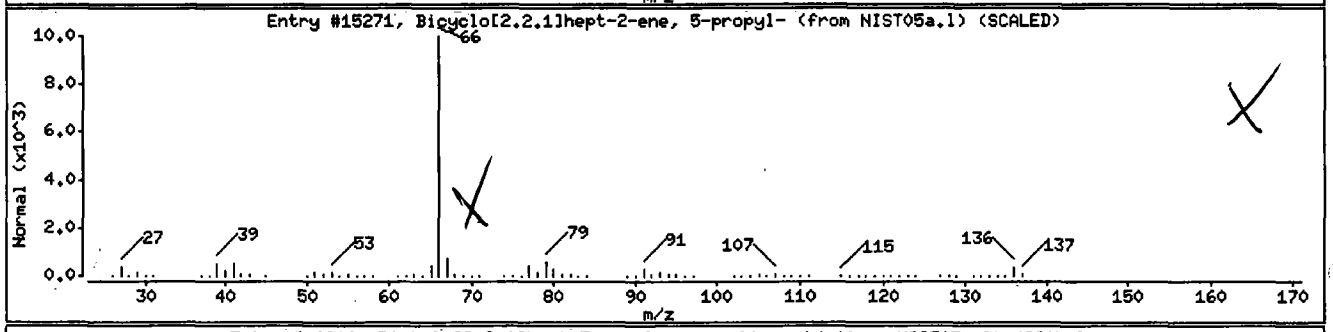
Column phase: J&W DB-5MS

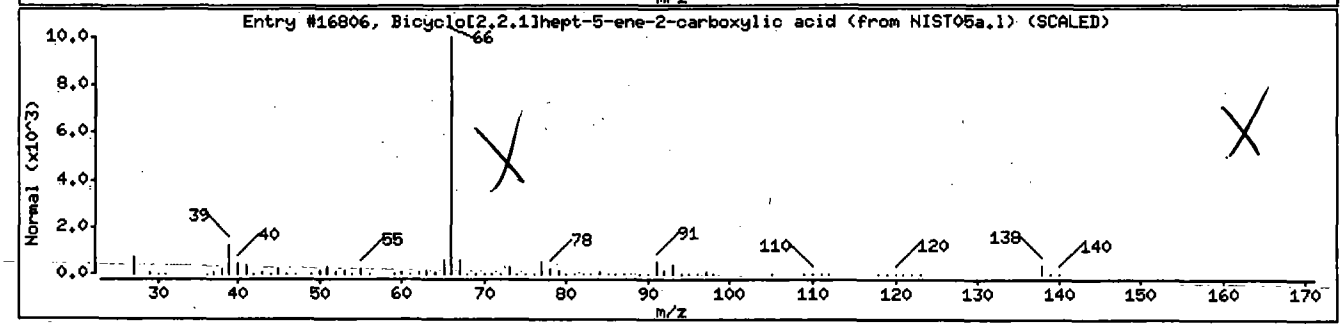
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

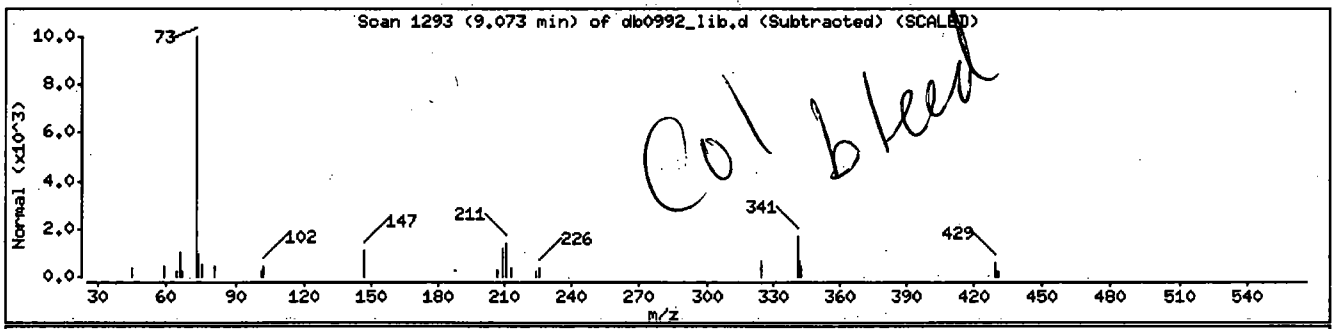
Volume Injected (uL): 1.0

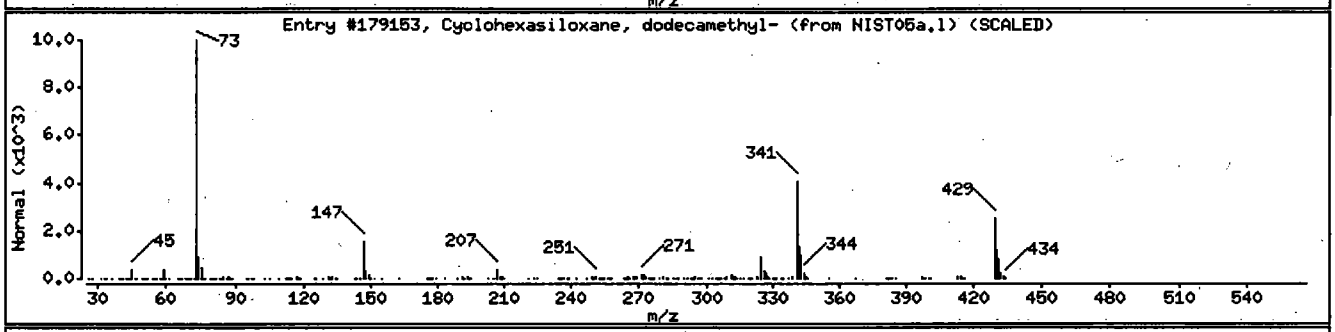
Operator: ceb05247

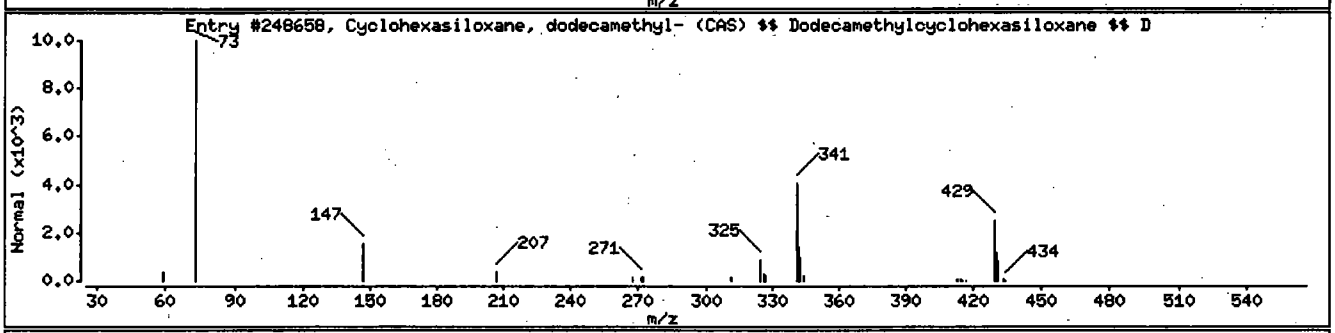
Column phase: J&W DB-5MS

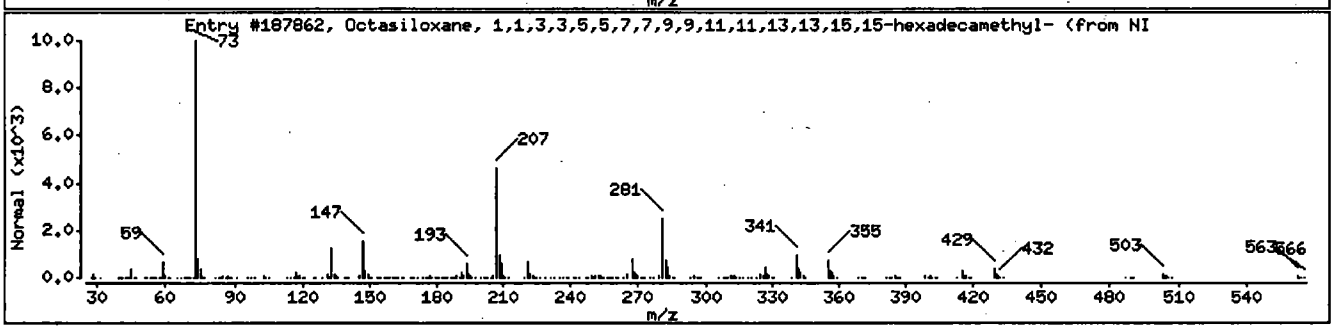
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexasiloxane, dodecamethyl-	540-97-6	NIST05a.l	179153	58	C12H36O6Si6	444
Cyclohexasiloxane, dodecamethyl- (CAS) $	540-97-6	WILEY275.l	248658	58	C12H36O6Si6	444
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,	19095-24-0	NIST05a.l	187862	36	C16H50O7Si8	578









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0992_lib.d

Date : 21-FEB-2014 23:56

Client ID: H7011

Instrument: HP19760.i

Sample Info: H7011;7368054;1;0;SAMPLE;;;

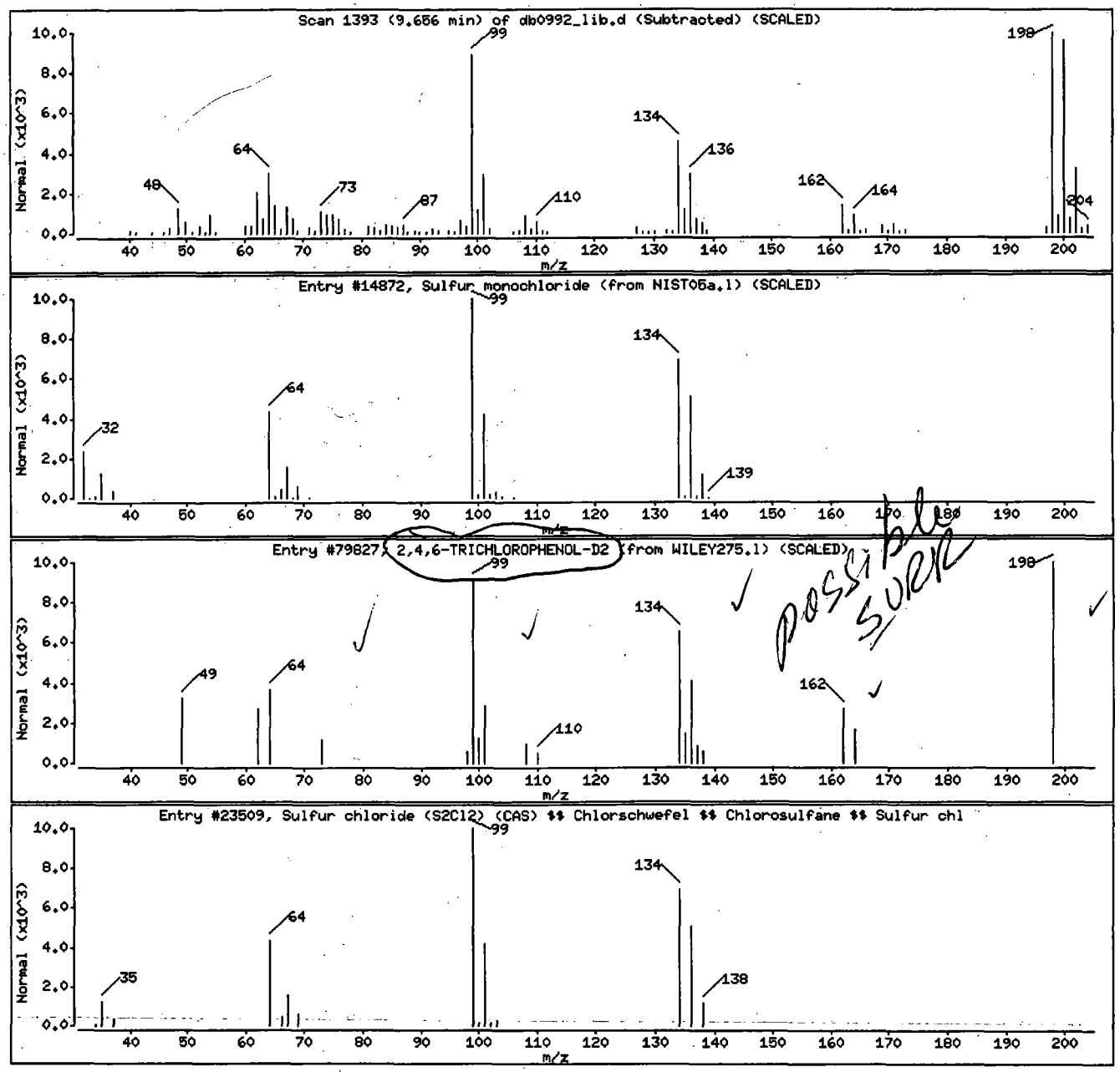
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

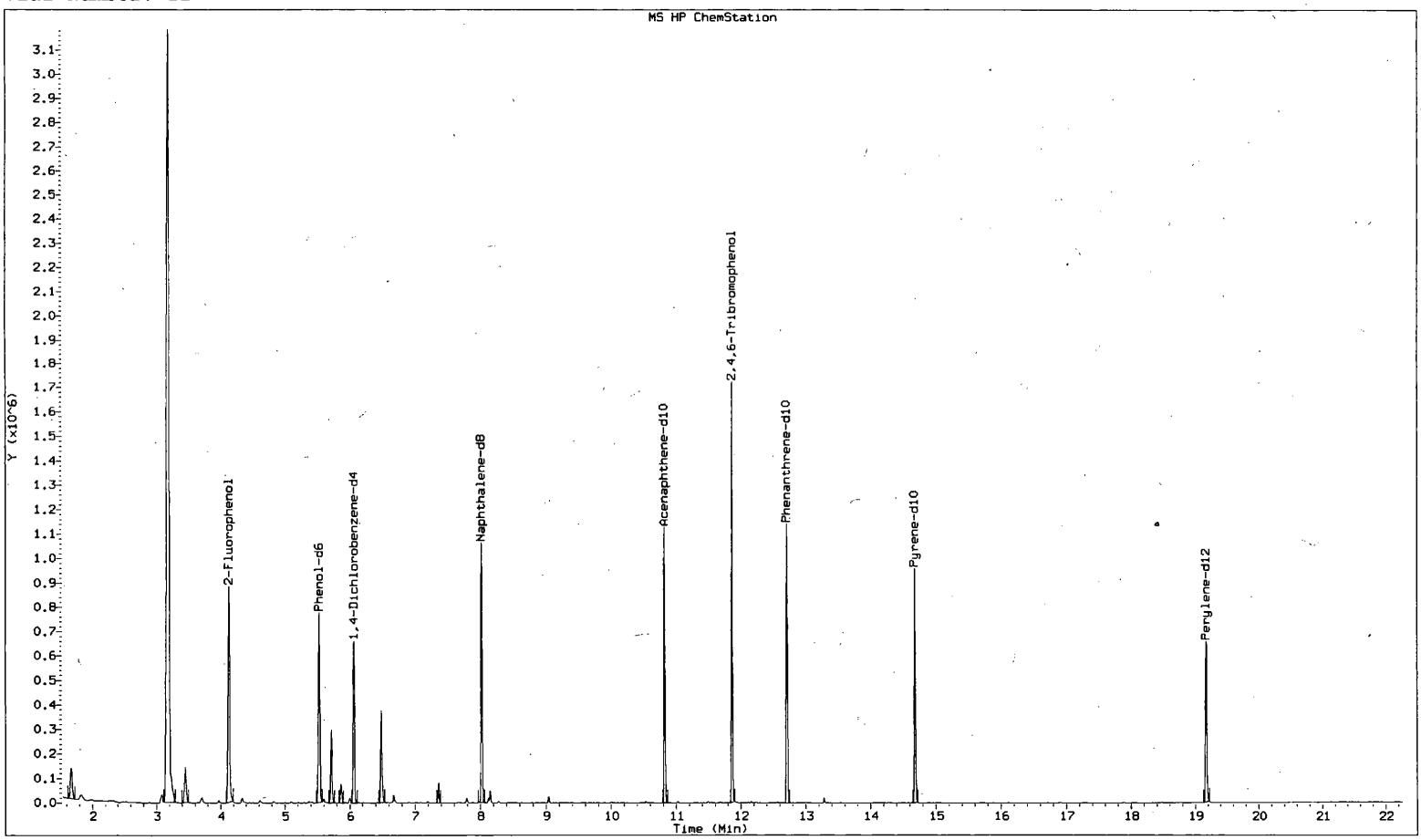
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	C12S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	46	C6HD2Cl3O	198
Sulfur chloride (S2Cl2) (CAS) ** Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134



Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:41.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb24.b/db1060_lib.d
Operator : jmg00346
Acquired : 24-FEB-2014 11:02
Instrument : HP19760.i
Sample Name: H7021;7368058;1;0;SAMPLE;;;
Misc Info : 14050WAM;WL13166;;1045;1000;0;db1056;13166;
Vial Number: 11



Lancaster Labs

Data file : /chem/HP19760.i/14feb24.b/db1060_lib.d
Lab Smp Id: 7368058 Client Smp ID: H7021
Inj Date : 24-FEB-2014 11:02
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H7021;7368058;1;0;SAMPLE;;;
Misc Info : 14050WAM;WL13166;;1045;1000;0;db1056;13166;
Comment : Max. number of TICs to report is 50, 7 TICs were found initially.
Method : /chem/HP19760.i/14feb24.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:47 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 11
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1045.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.066	983201	10.000
* 48 Naphthalene-d8	8.018	1316148	10.000

	CONCENTRATIONS				QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.671	264806	2.69330910	2.57732	90	NIST05a.1	31323	21
1,1-Dimethyl-3-chloropropanol				CAS #: 1985-88-2			
3.186	8042836	81.8025414	78.27994	83	NIST05a.1	9464	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.449	285295	2.90169357	2.77674	83	NIST05a.l	17537	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.716	439495	4.47004008	4.27755	94	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.867	111952	1.13865007	1.08961	94	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.479	606011	6.16365469	5.89823	38	NIST05a.l	9448	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.360	93497	0.71038476	0.67979	91	NIST05a.l	161016	48

Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

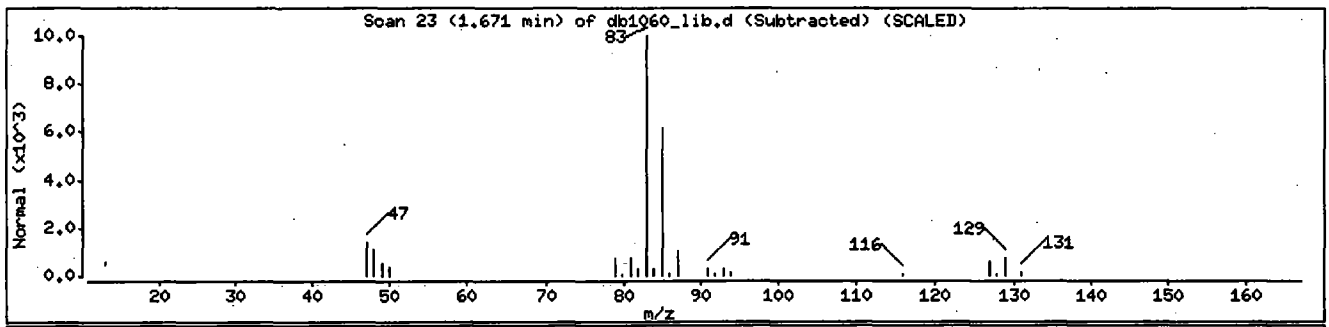
Volume Injected (uL): 1.0

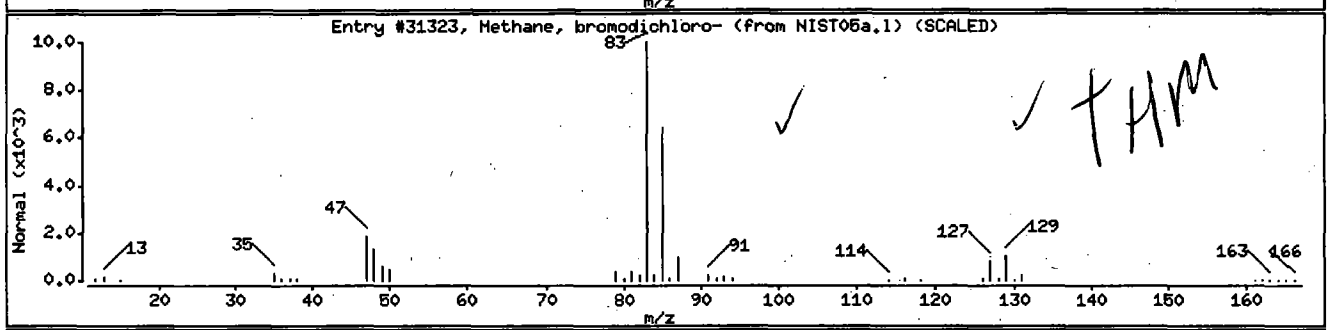
Operator: jmg00346

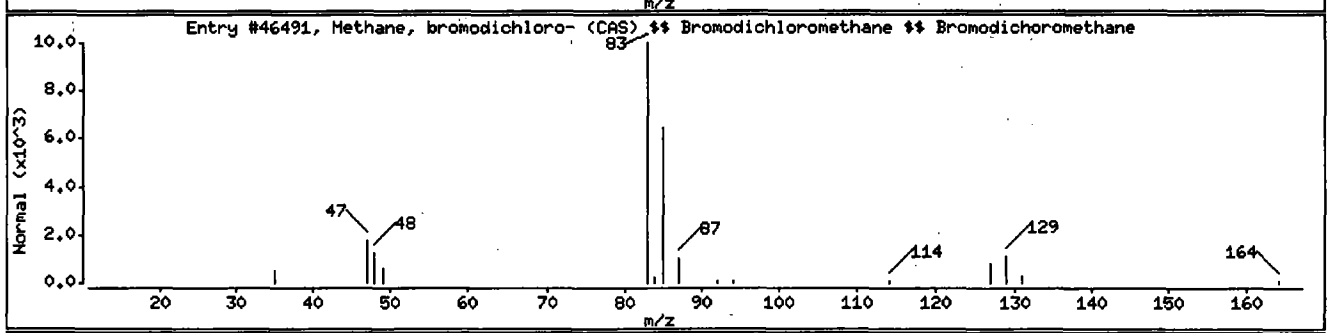
Column phase: J&W DB-5MS

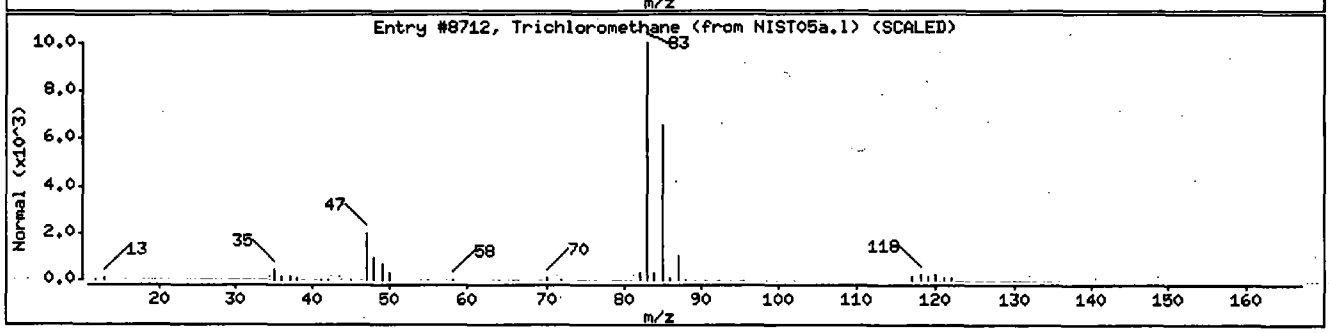
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46491	90	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

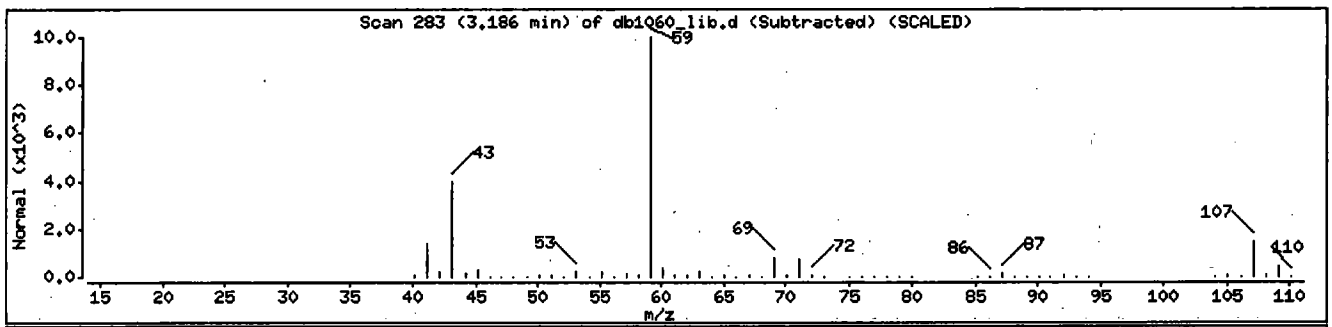
Client ID: H7021 Instrument: HP19760.i

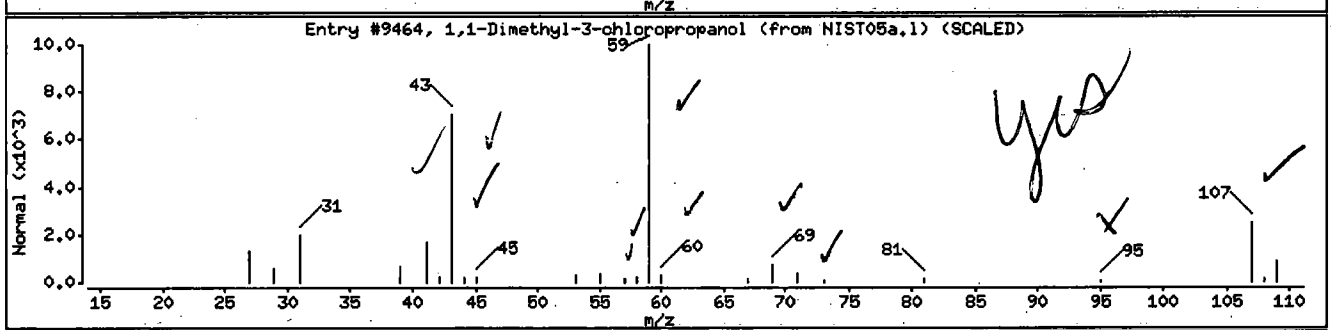
Sample Info: H7021;7368058;1;0;SAMPLE;;;

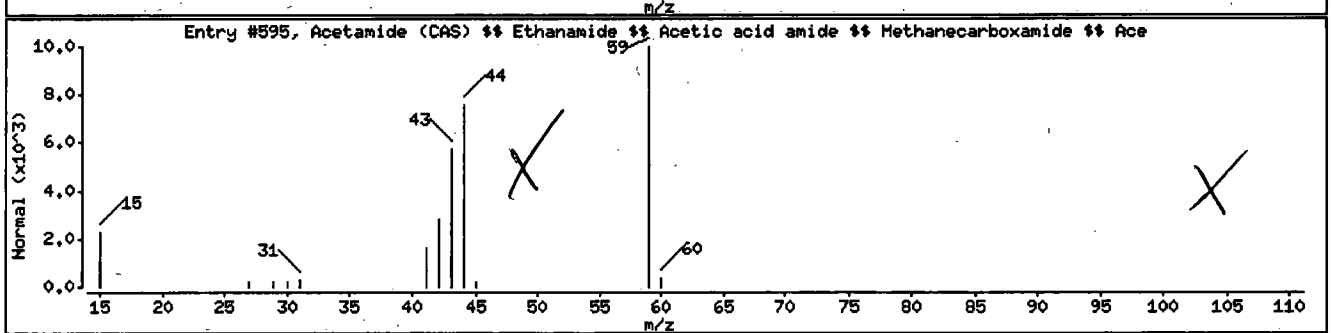
Volume Injected (uL): 1.0 Operator: jmg00346

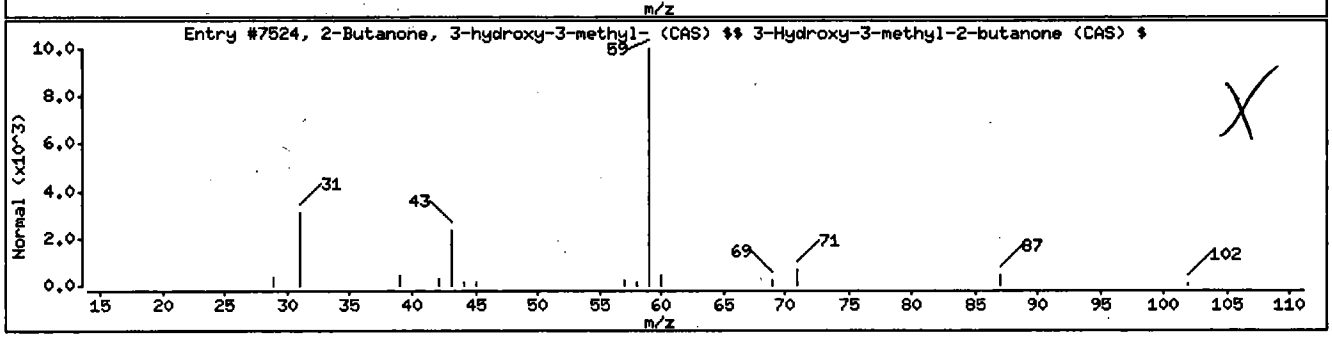
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	45	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	42	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

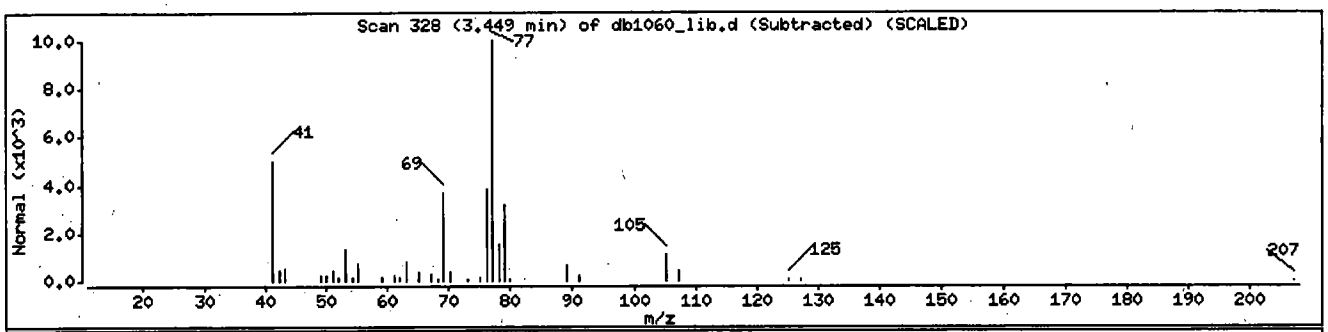
Volume Injected (uL): 1.0

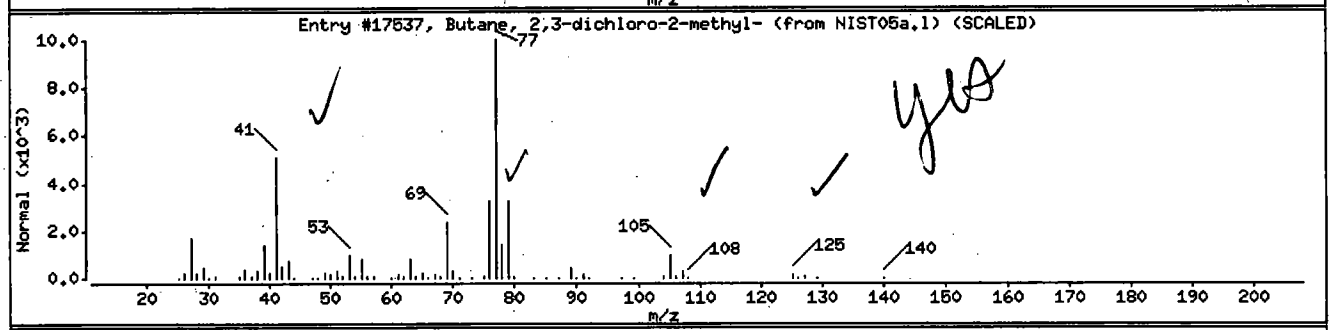
Operator: jmg00346

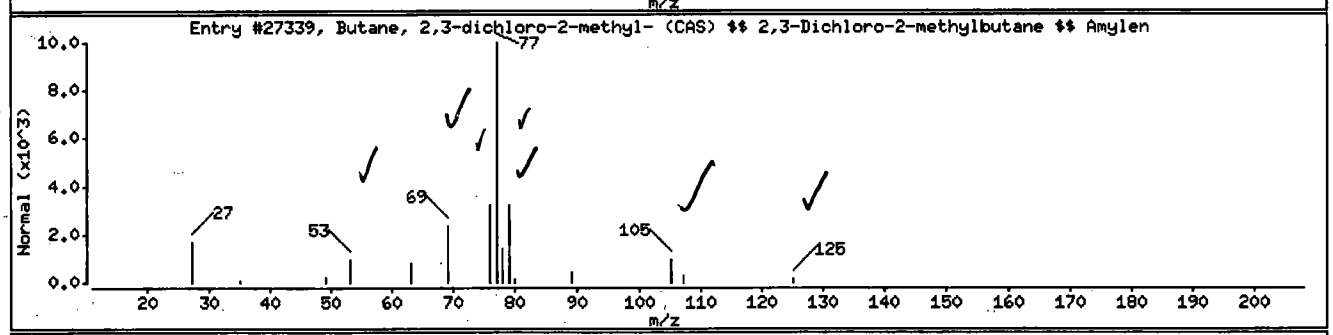
Column phase: J&W DB-5MS

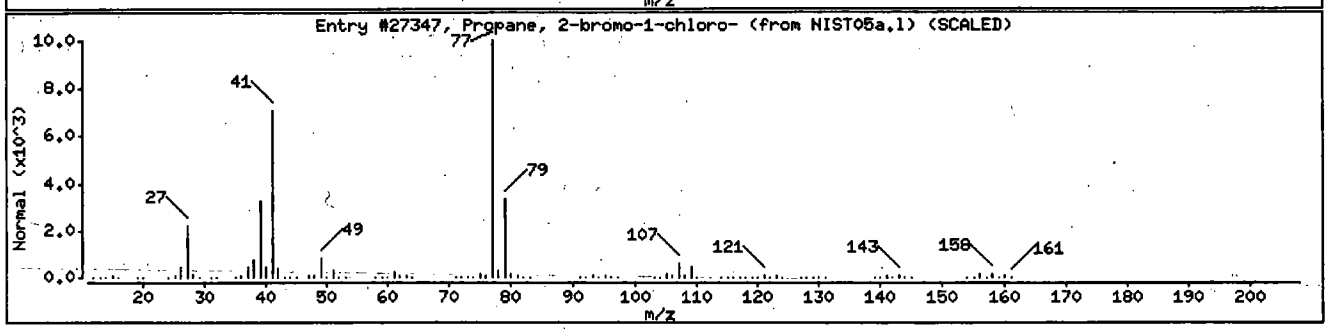
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	74	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	40	C3H6BrCl	156









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

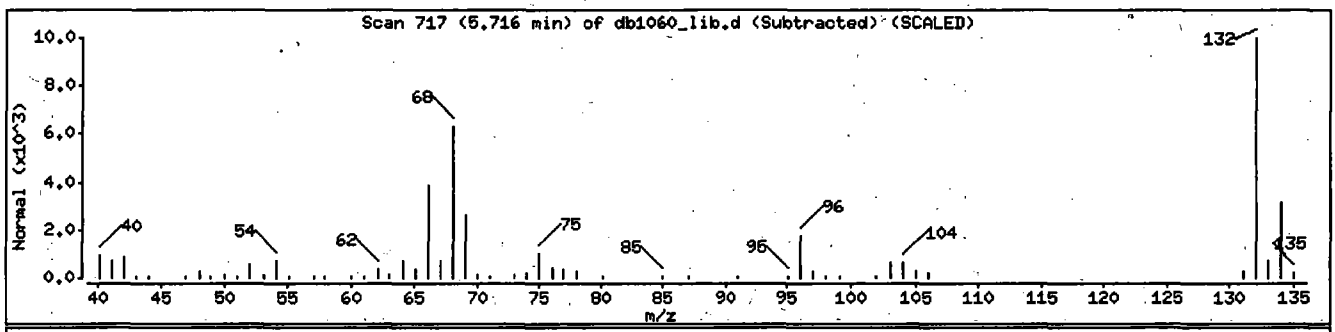
Volume Injected (uL): 1.0

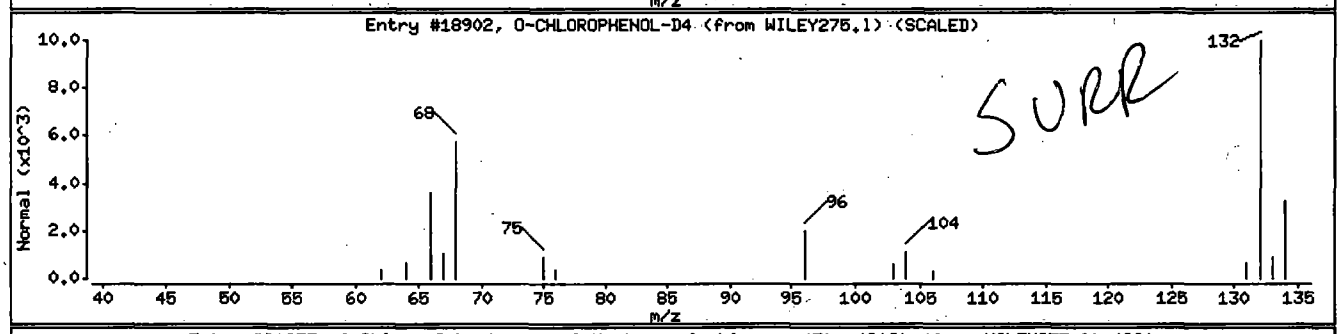
Operator: jmg00346

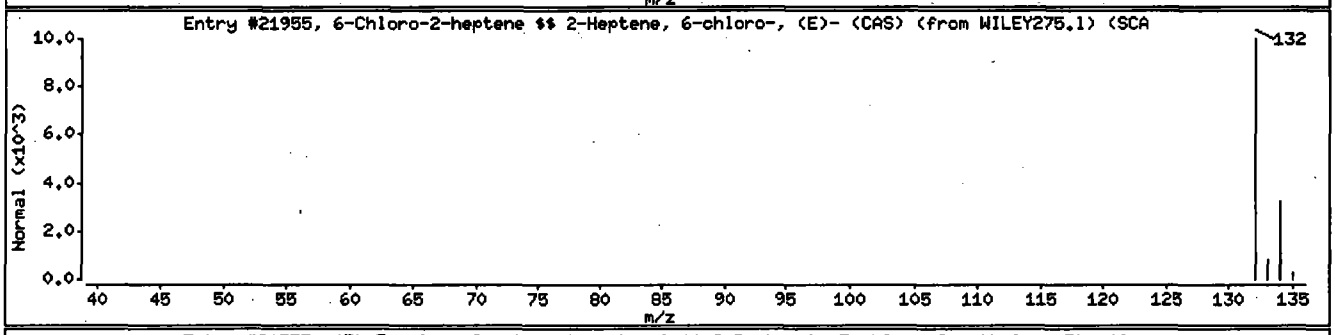
Column phase: J&W DB-5MS

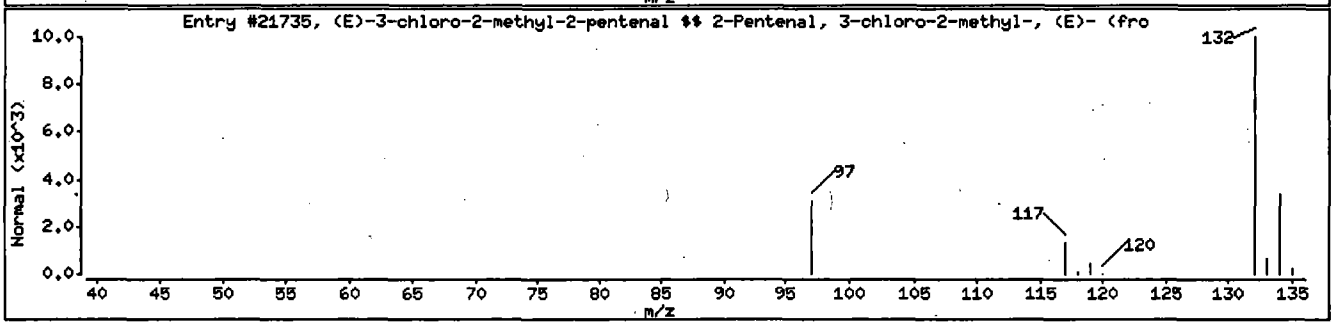
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.l	18902	94	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.l	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.l	21735	78	C6H9ClO	132









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

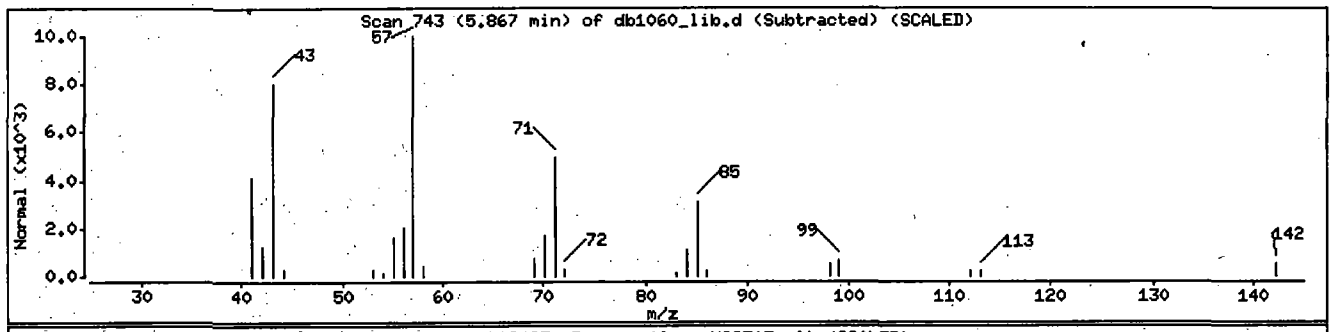
Volume Injected (uL): 1.0

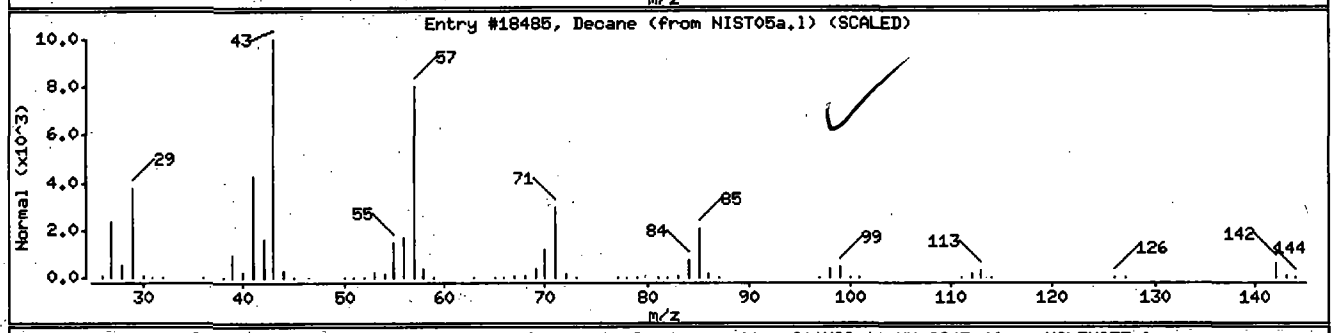
Operator: jmg00346

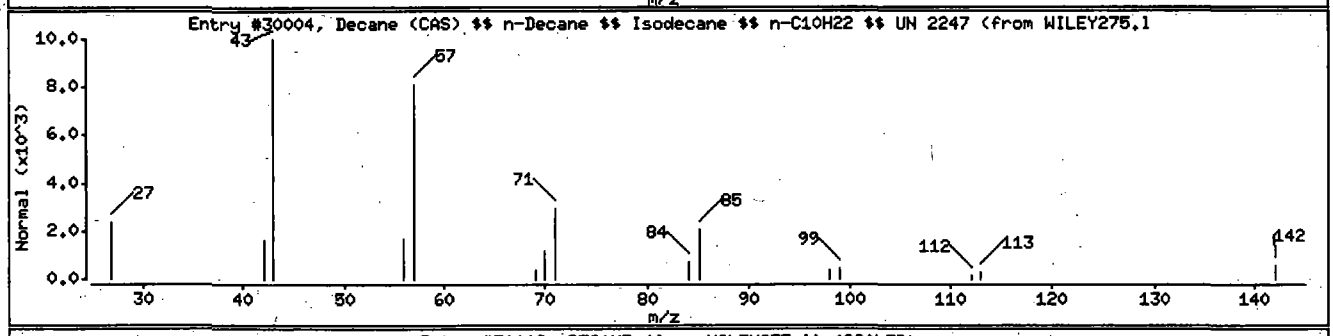
Column phase: J&W DB-5HS

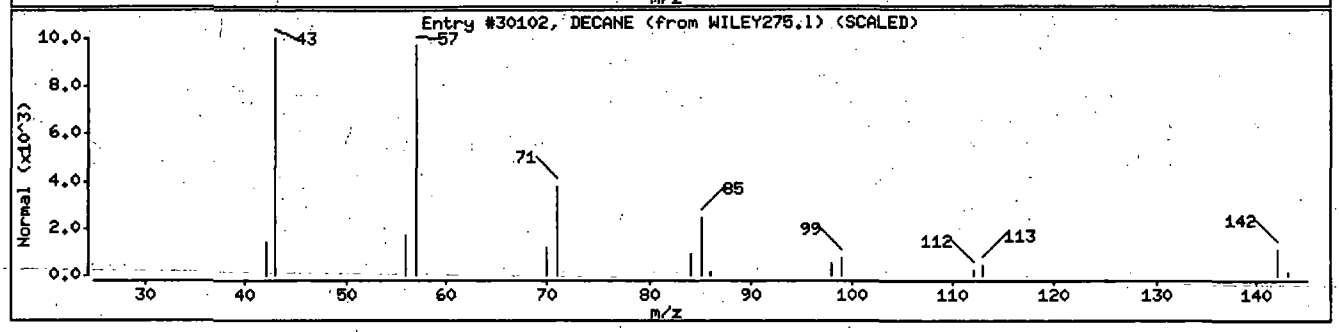
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	94	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	94	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

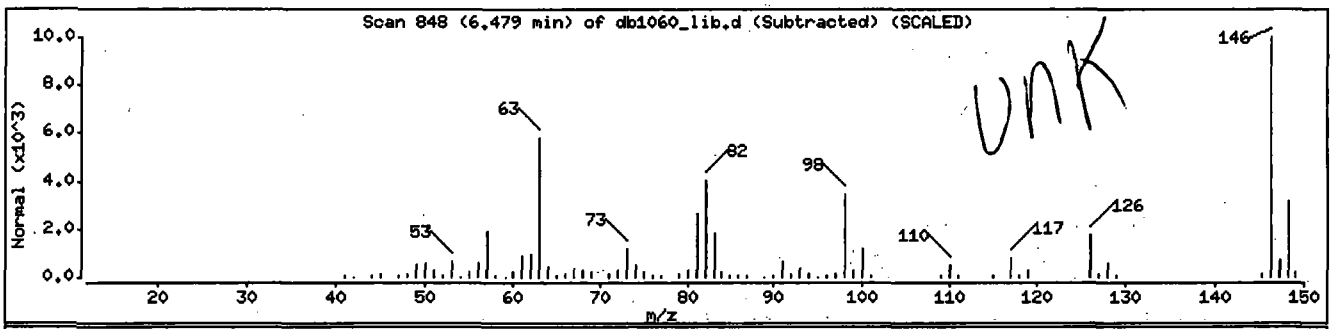
Volume Injected (uL): 1.0

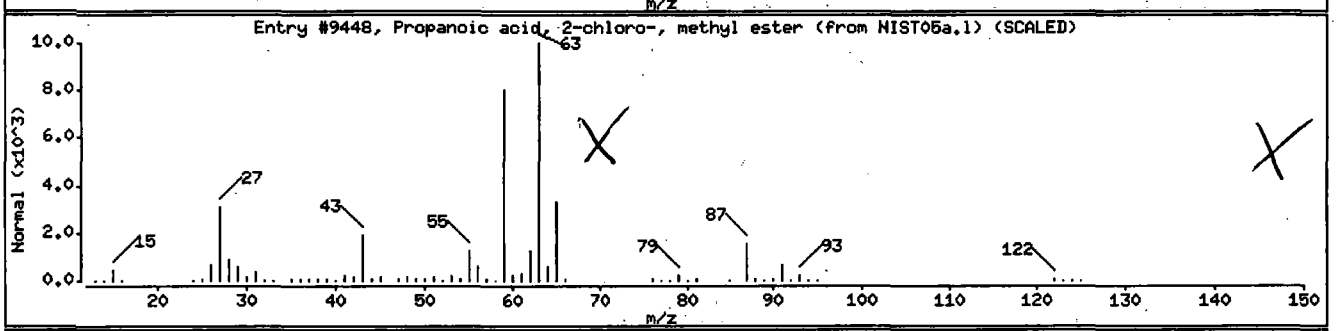
Operator: jmg00346

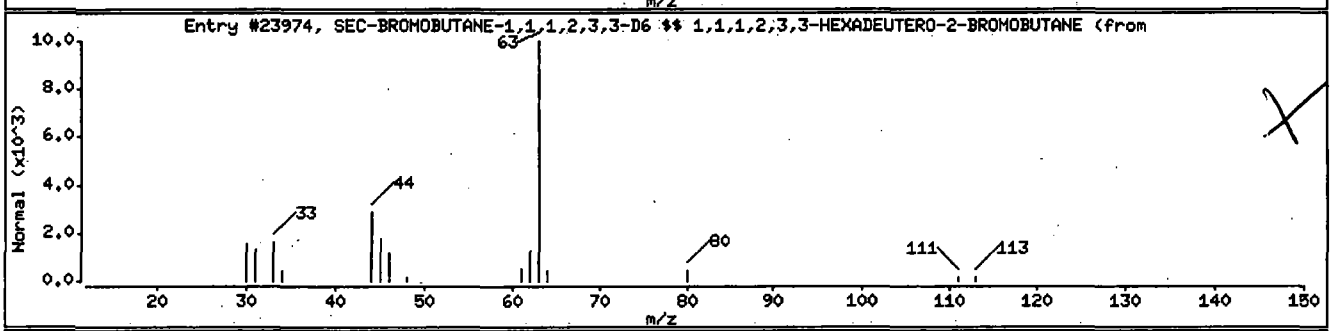
Column phase: J&W DB-5MS

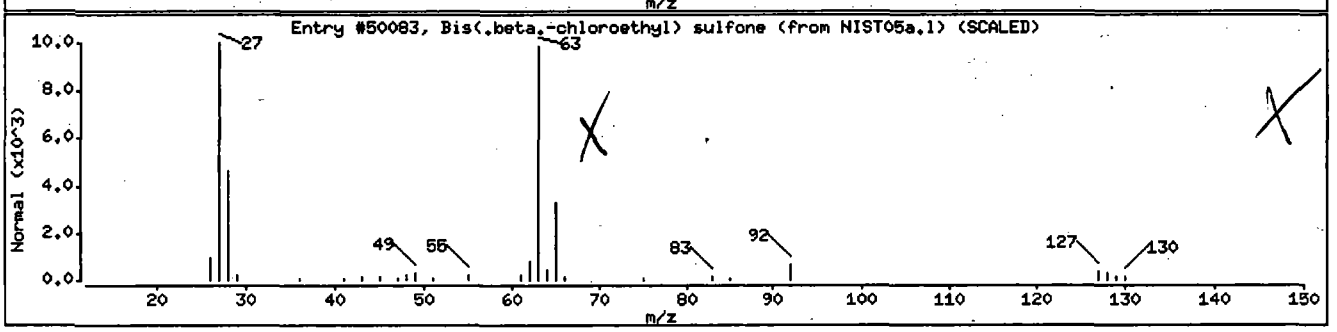
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	32	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	23	C4H8Cl2O2S	190









Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1060_lib.d

Date : 24-FEB-2014 11:02

Client ID: H7021

Instrument: HP19760.i

Sample Info: H7021;7368058;1;0;SAMPLE;;;

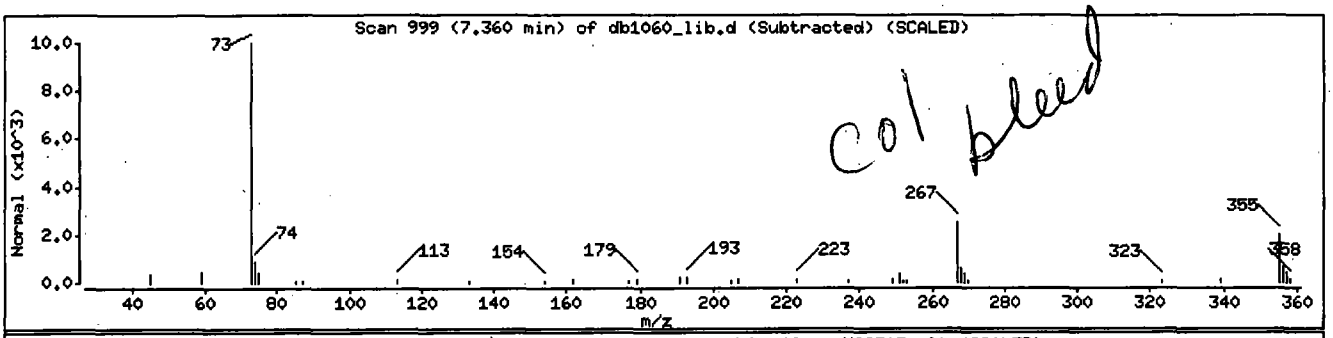
Volume Injected (uL): 1.0

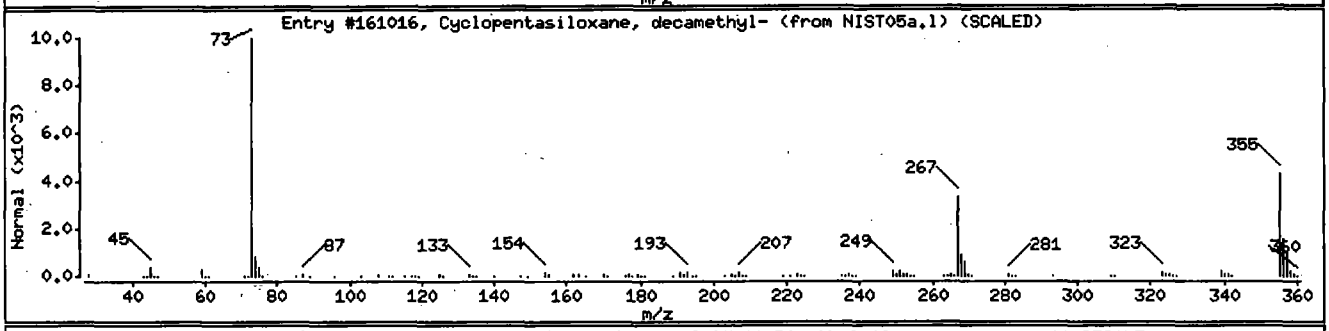
Operator: jmg00346

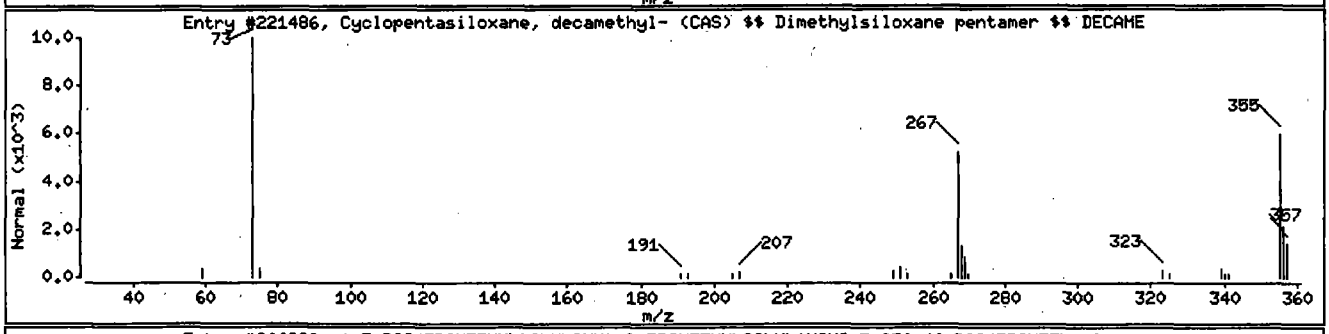
Column phase: J&W DB-5MS

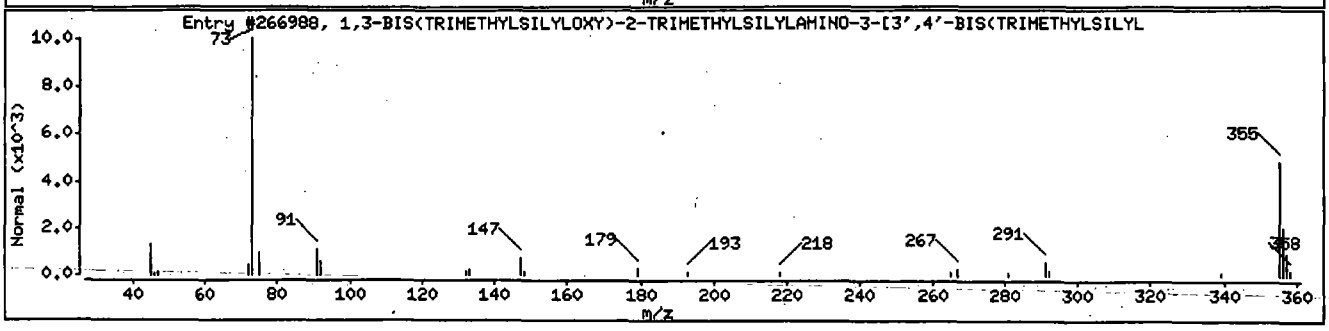
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	91	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
1,3-BIS(TRIMETHYLSILYLOXY)-2-TRIMETHYLSI	0-00-0	WILEY275.l	266988	43	C24H51NO5Si5	573



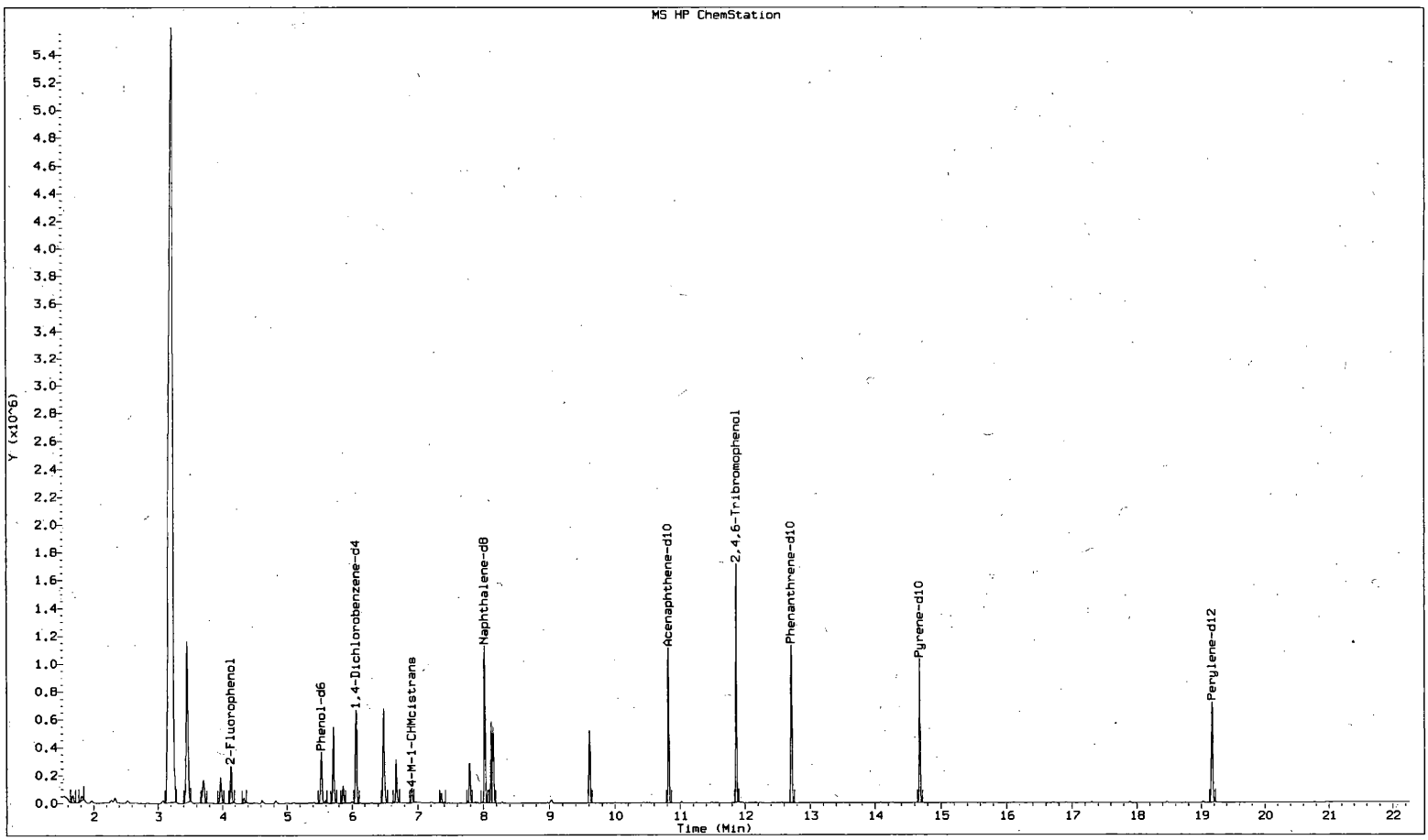






Digitally signed by Andrew J. Strebel on 03/02/2014 at 14:50.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb24a.b/db1095_lib.d
Operator : ceb05247
Acquired : 25-FEB-2014 02:32
Instrument : HP19760.i
Sample Name: H8011;7368069;1;0;SAMPLE;;;
Misc Info : 14050WAN;WL13463;;1049;1000;0;db1082;13166;
Vial Number: 17



Lancaster Labs

Data file : /chem/HP19760.i/14feb24a.b/db1095_lib.d
Lab Smp Id: 7368069 Client Smp ID: H8011
Inj Date : 25-FEB-2014 02:32
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H8011;7368069;1;0;SAMPLE;;;
Misc Info : 14050WAN;WL13463;;1049;1000;0;db1082;13166;
Comment : Max. number of TICs to report is 50, 16 TICs were found initially.
Method : /chem/HP19760.i/14feb24a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:59 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 17
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1049.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.060	967773	10.000
* 48 Naphthalene-d8	8.018	1416408	10.000
* 83 Acenaphthene-d10	10.822	1259788	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.671	99720	1.03040225	0.98227	83	NIST05a.1	31323	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.817	68900	0.71194628	0.67869	89	NIST05a.l	4733	21
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.233	22354527	230.989305	220.19952	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.454	2256933	23.3208889	22.23154	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.705	333811	3.44927072	3.28815	25	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
3.973	327865	3.38782507	3.22957	38	NIST05a.l	13998	21
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.335	55272	0.57112152	0.54444	25	NIST05a.l	33655	21(L)
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.716	797196	8.23742825	7.85264	89	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.867	175267	1.81103556	1.72644	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.479	1109204	11.4614041	10.92602	35	NIST05a.l	9448	21(L)
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 13937-4-3		
6.672	395764	4.08942789	3.89840	53	WILEY275.l	19674	21(L)
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.360	92701	0.65447924	0.62390	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.791	374846	2.64645167	2.52283	43	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.117	616332	4.35137470	4.14811	86	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.146	697252	4.92267817	4.69273	50	NIST05a.l	3933	48
Sulfur monochloride					CAS #: 10025-67-9		
9.609	617141	4.89876973	4.66994	27	NIST05a.l	14872	83(L)

Target compound.
Do not report.
ajs00193 03/02/2014

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
Sulfur monochloride					CAS #: 10025-67-9		
9.650	314234	2.18849155	2.09224	38	NIST05a.l	14872	83(L)

QC Flag Legend

L - Operator selected an alternate library search match.

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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

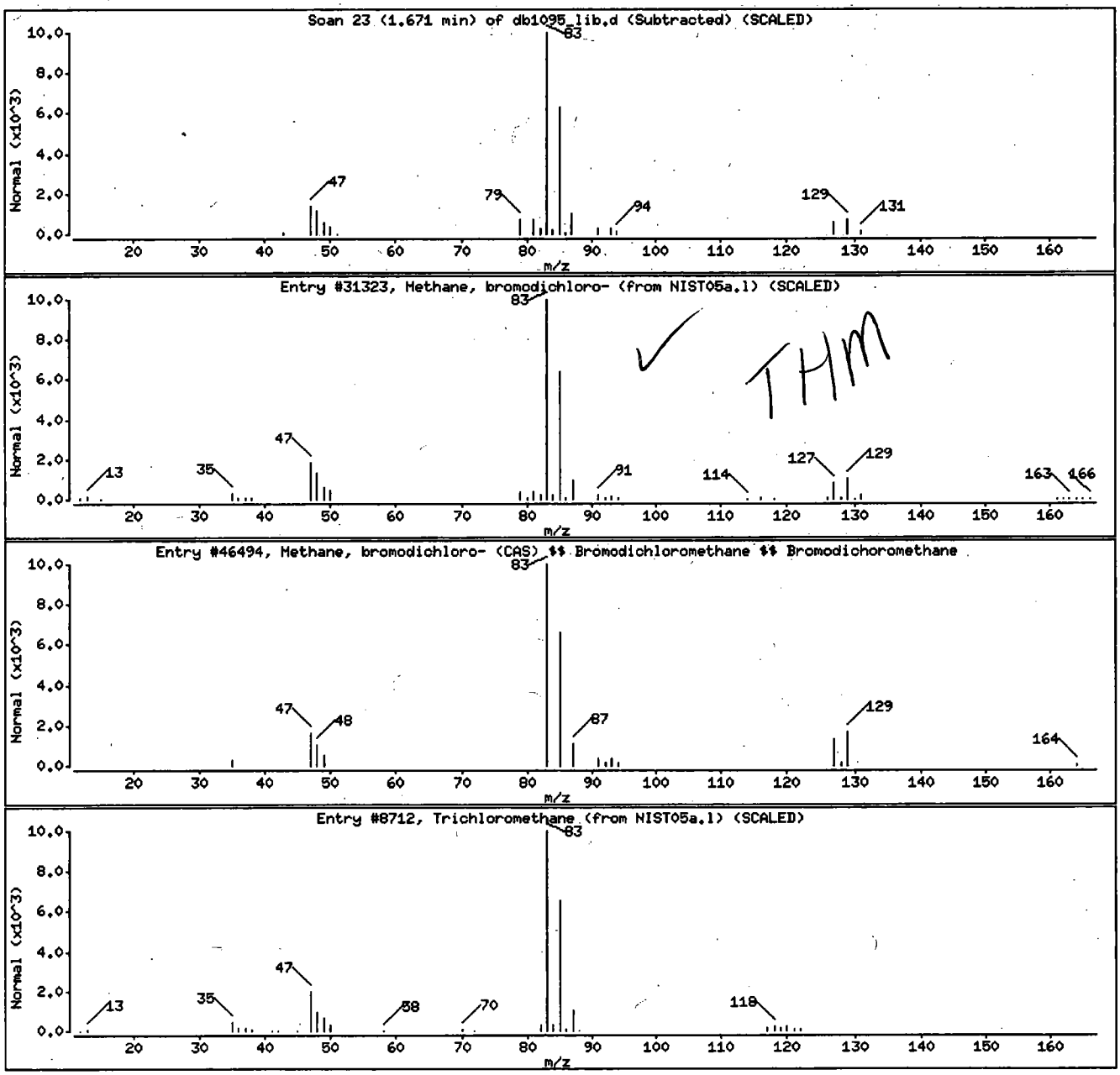
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	83	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46494	83	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

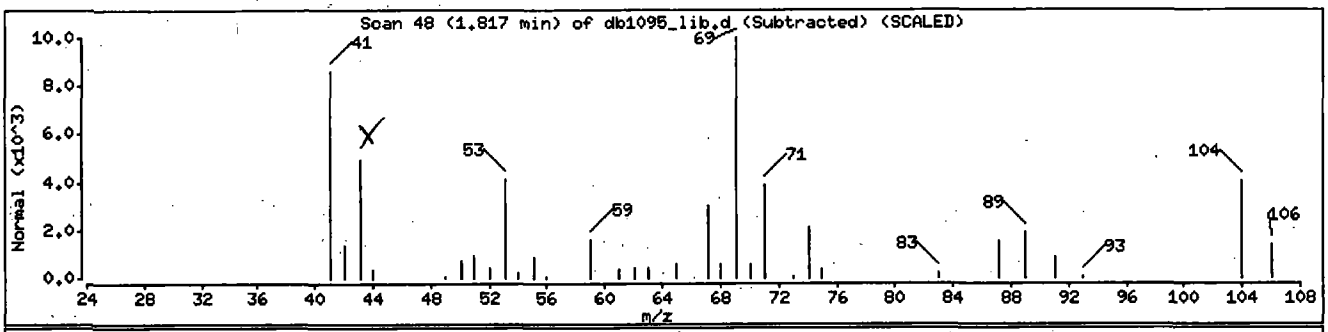
Volume Injected (uL): 1.0

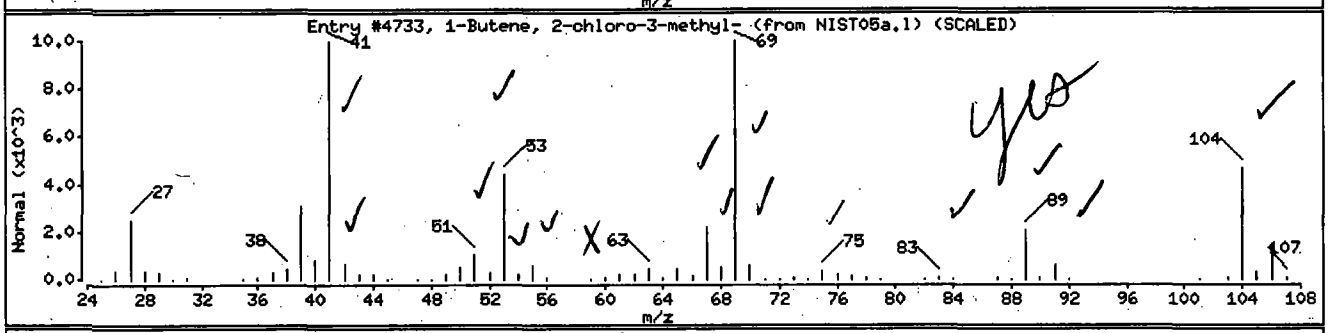
Operator: ceb05247

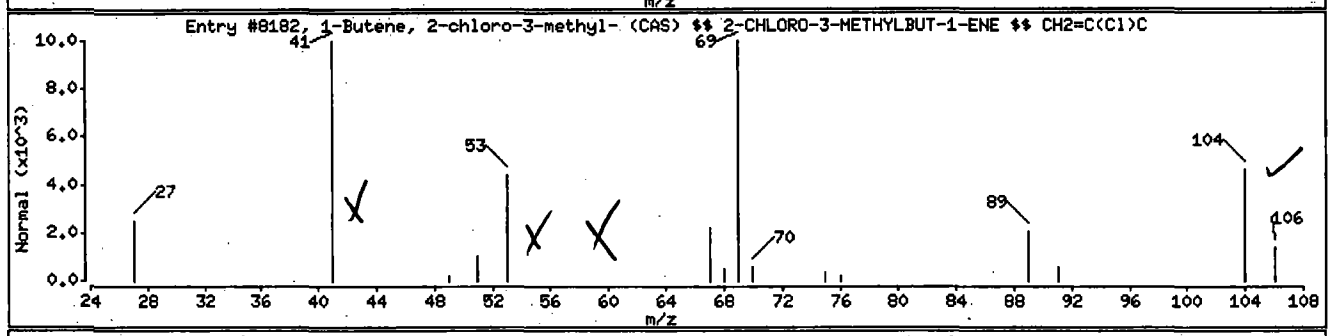
Column phase: J&W DB-5MS

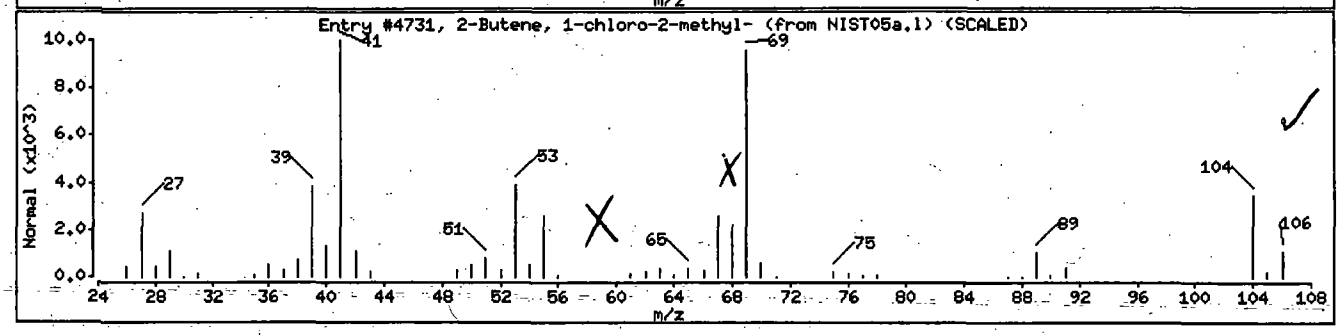
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	89	C5H9Cl	104
1-Butene, 2-chloro-3-methyl- (CAS) $$ 2-	17773-64-7	WILEY275.l	8182	89	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4731	81	C5H9Cl	104









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

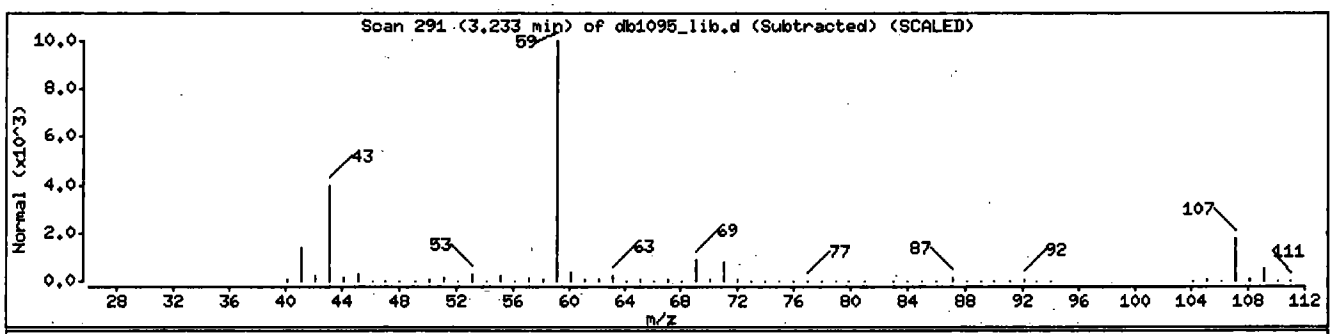
Volume Injected (uL): 1.0

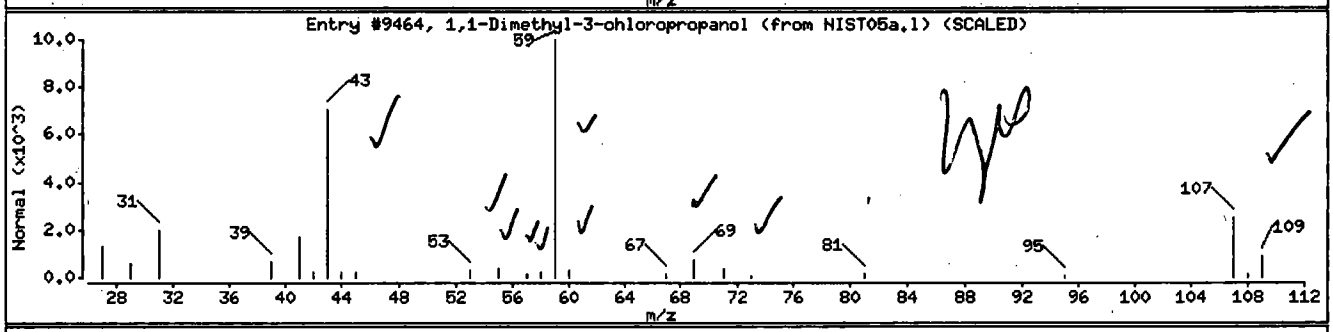
Operator: ceb05247

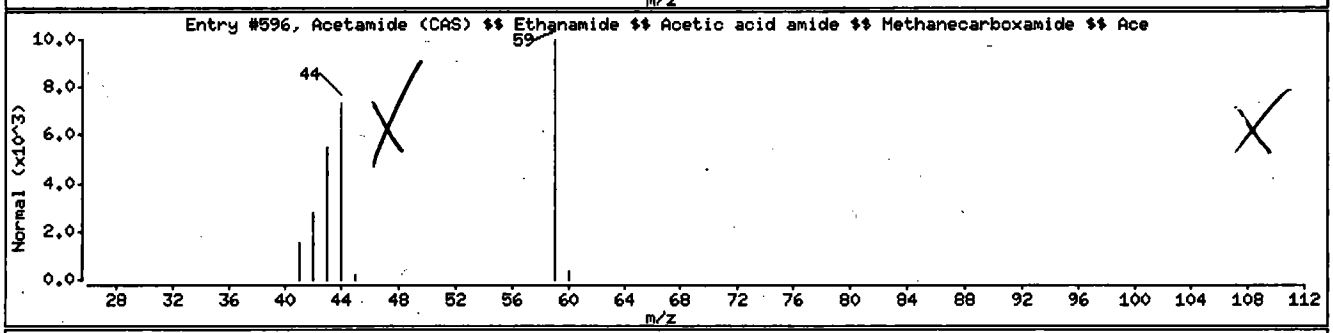
Column phase: J&W DB-5MS

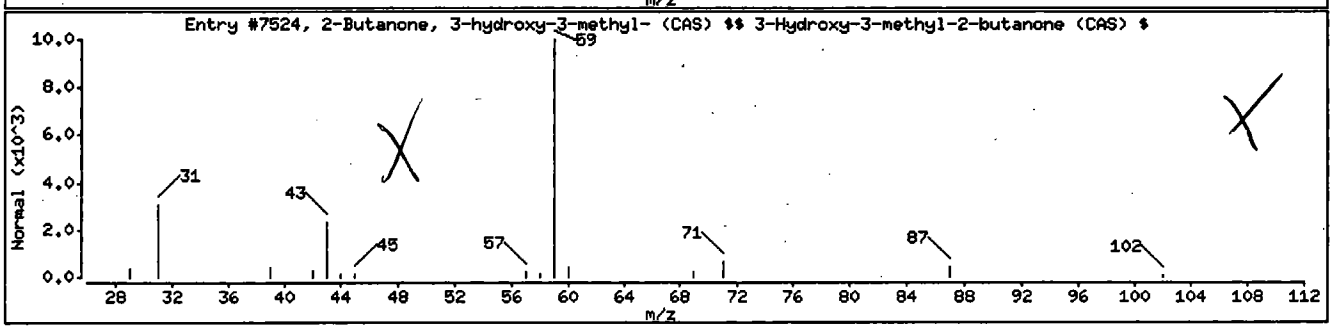
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	596	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

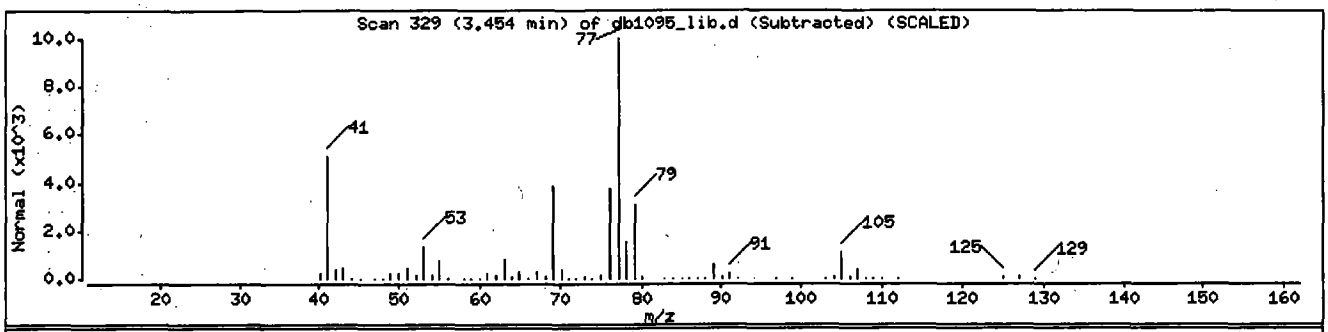
Volume Injected (uL): 1.0

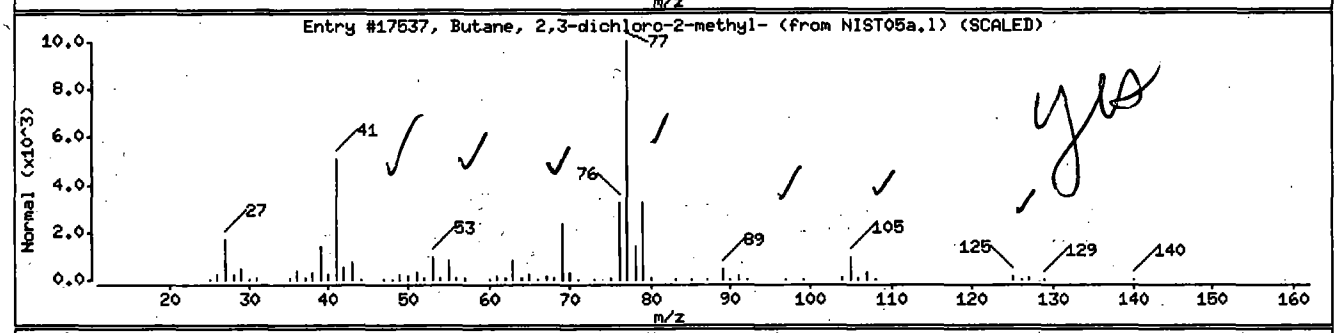
Operator: ceb05247

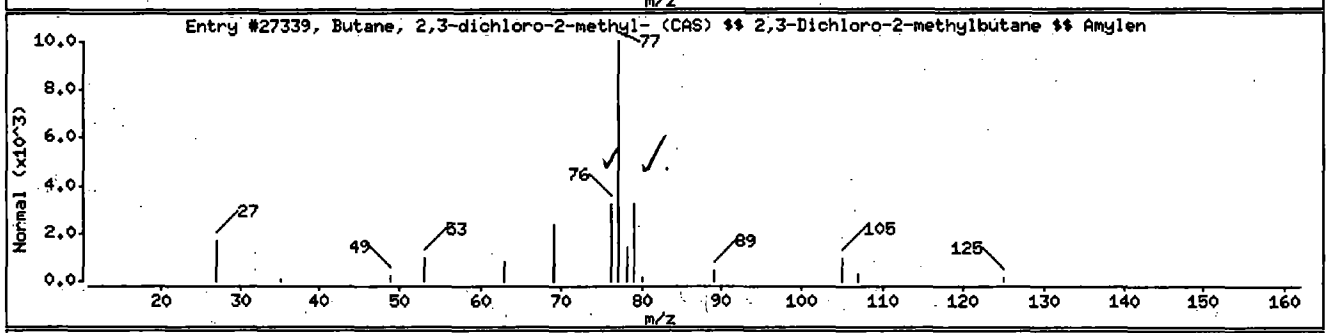
Column phase: J&W DB-5MS

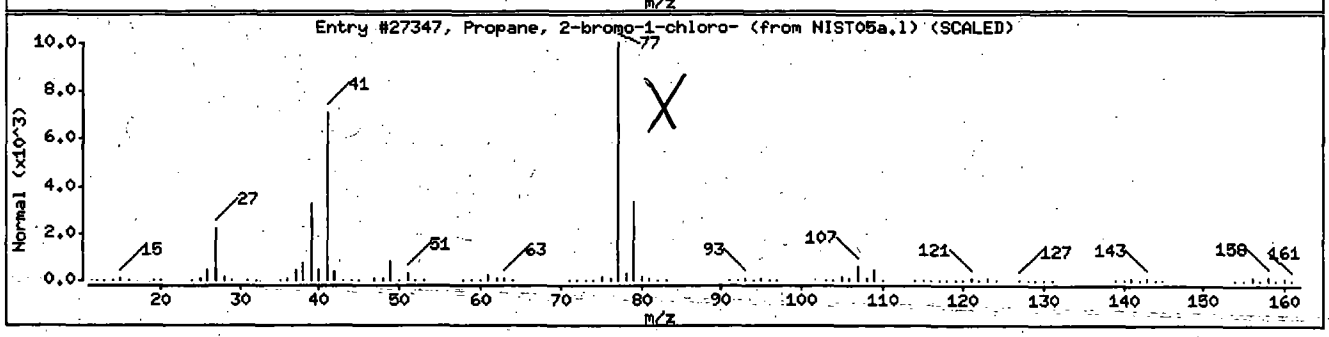
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-bromo-1-chloro-	3017-95-6	NIST05a.l	27347	38	C3H6BrCl	156









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

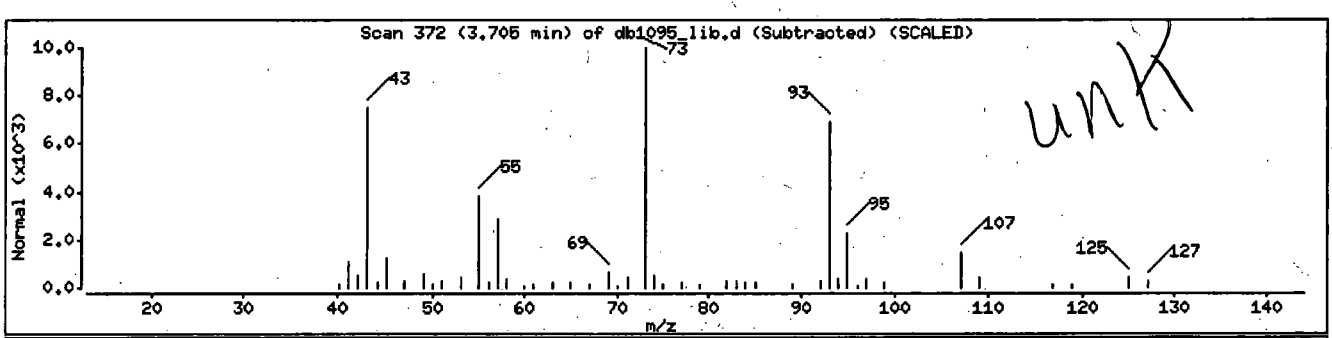
Volume Injected (uL): 1.0

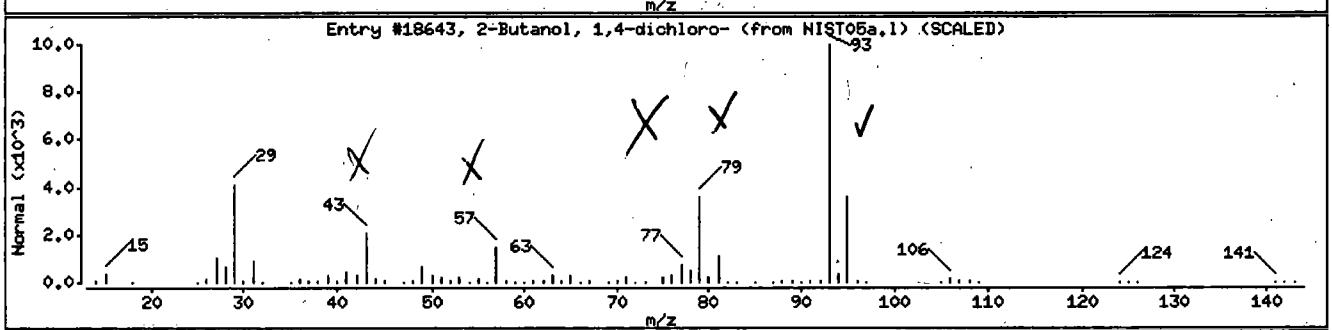
Operator: ceb05247

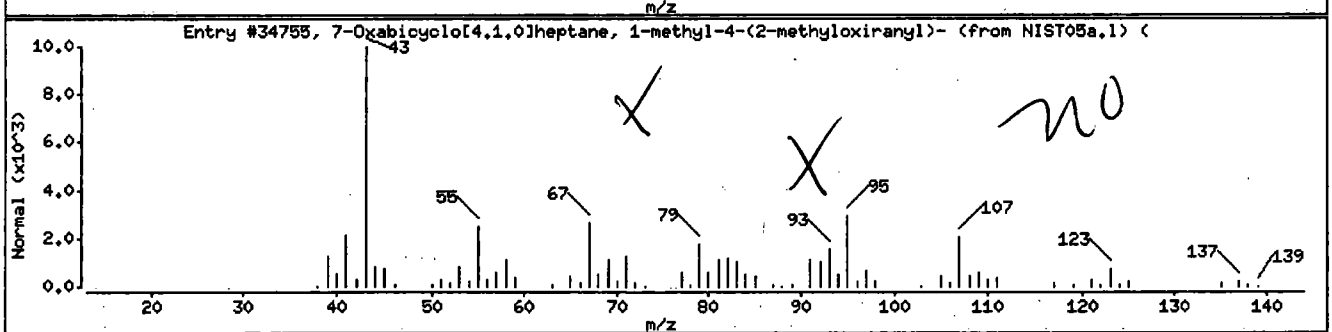
Column phase: J&W DB-5MS

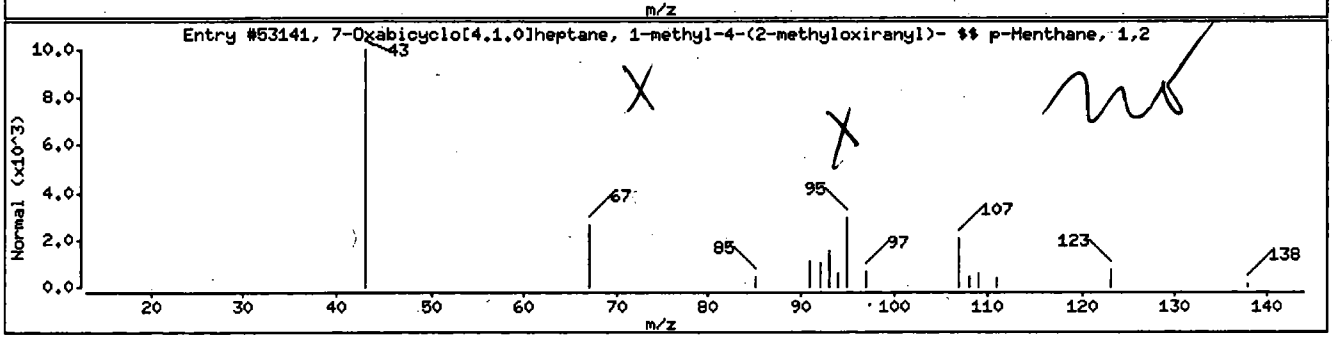
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	25	C4H8Cl2O	142
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	NIST05a.l	34755	16	C10H16O2	168
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(	96-08-2	WILEY275.l	53141	16	C10H16O2	168









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

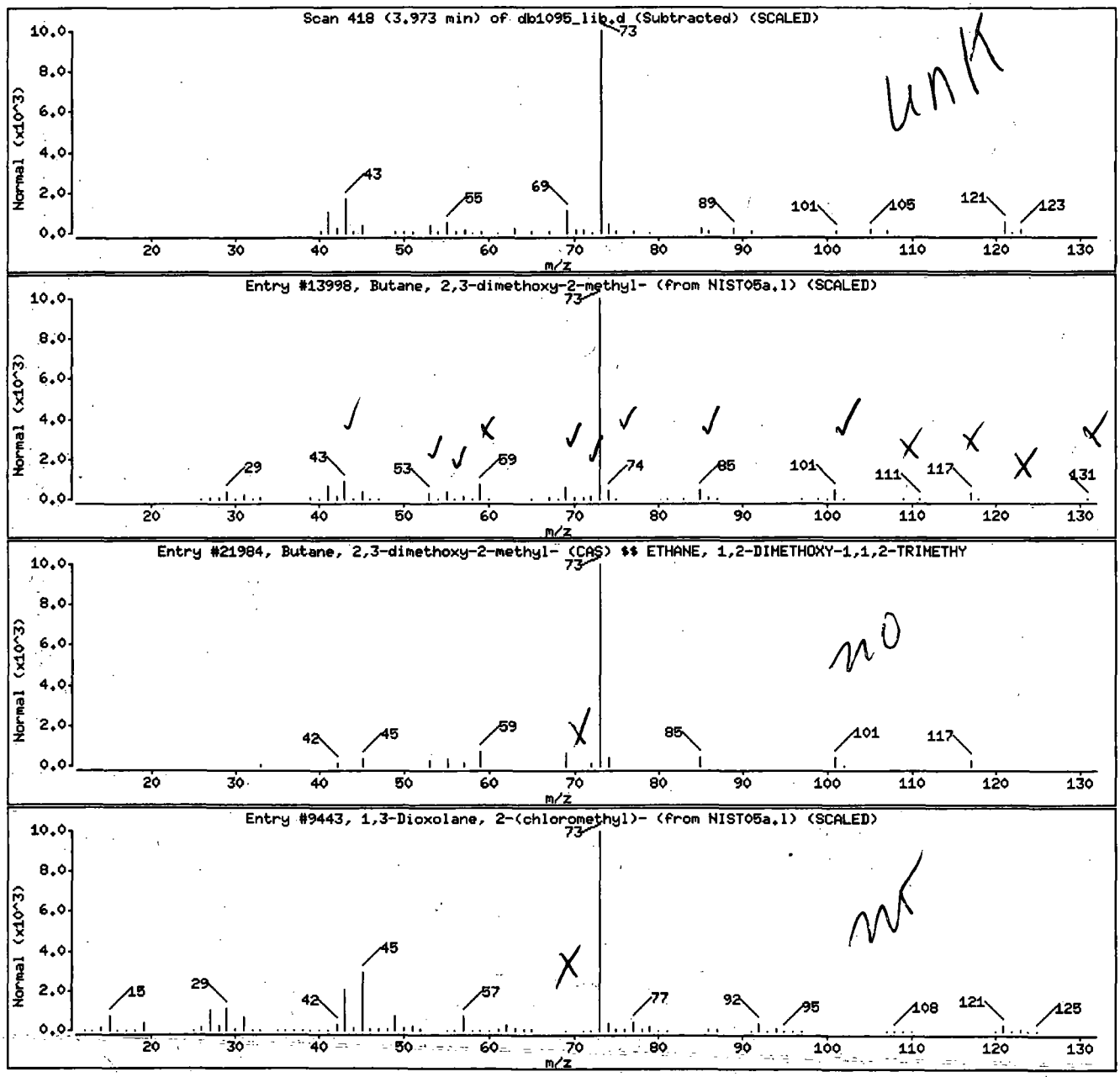
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	48	C7H16O2	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9443	9	C4H7ClO2	122



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

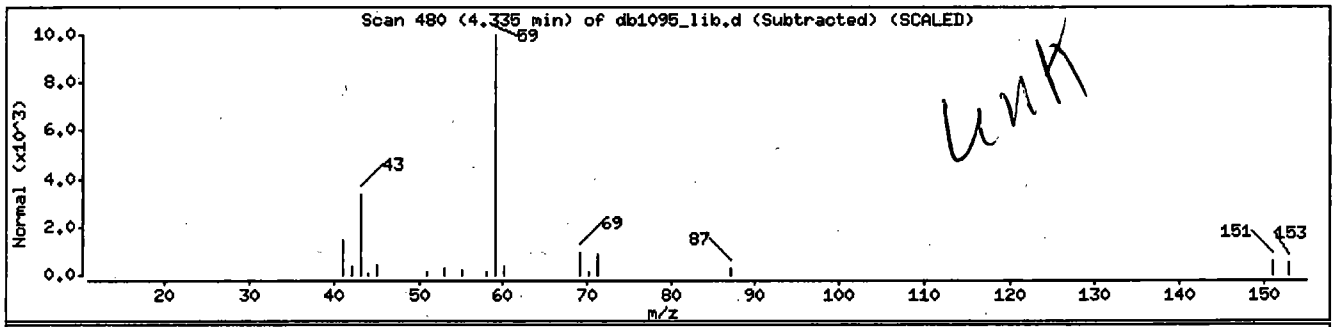
Volume Injected (uL): 1.0

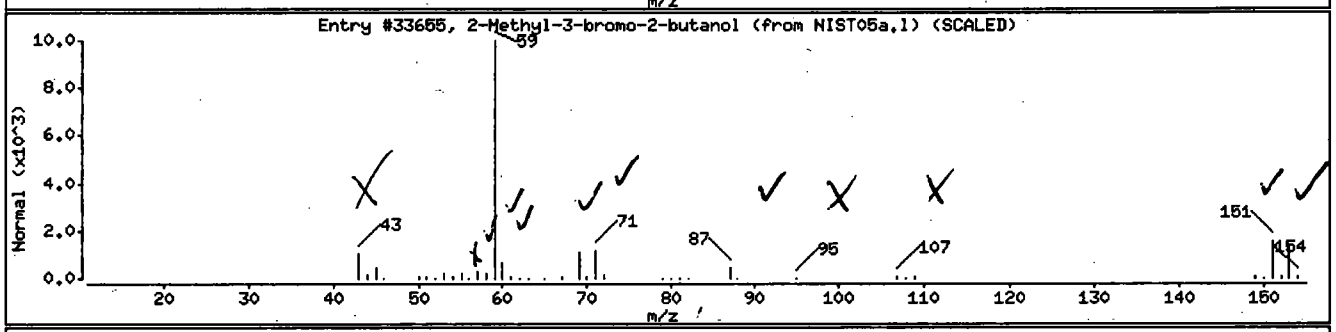
Operator: ceb05247

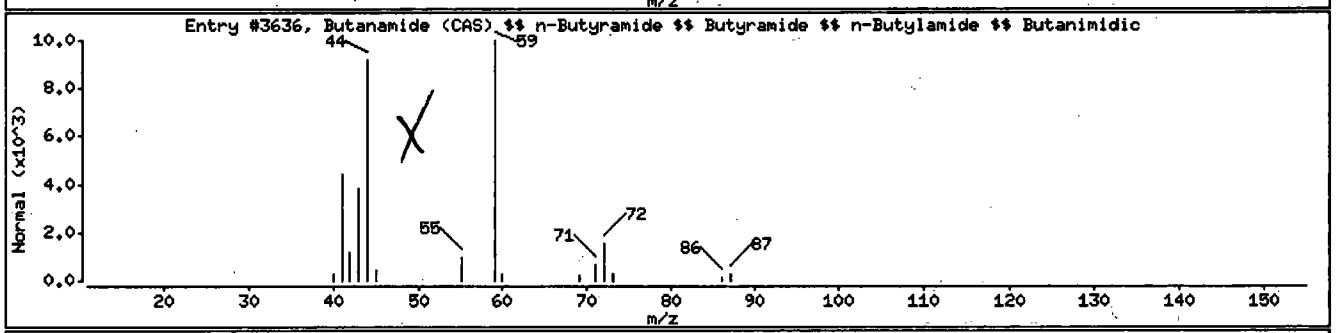
Column phase: J&W DB-5MS

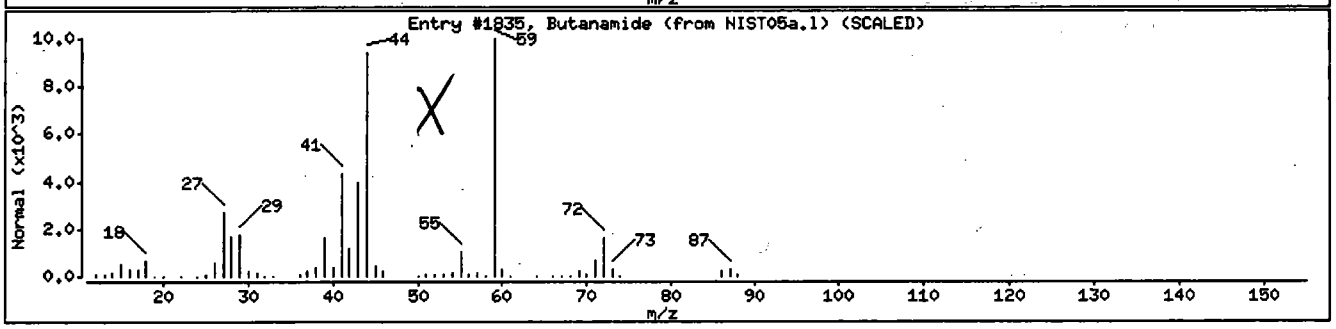
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	25	C5H11BrO	166
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3636	64	C4H9NO	87
Butanamide	541-35-5	NIST05a.l	1835	59	C4H9NO	87









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

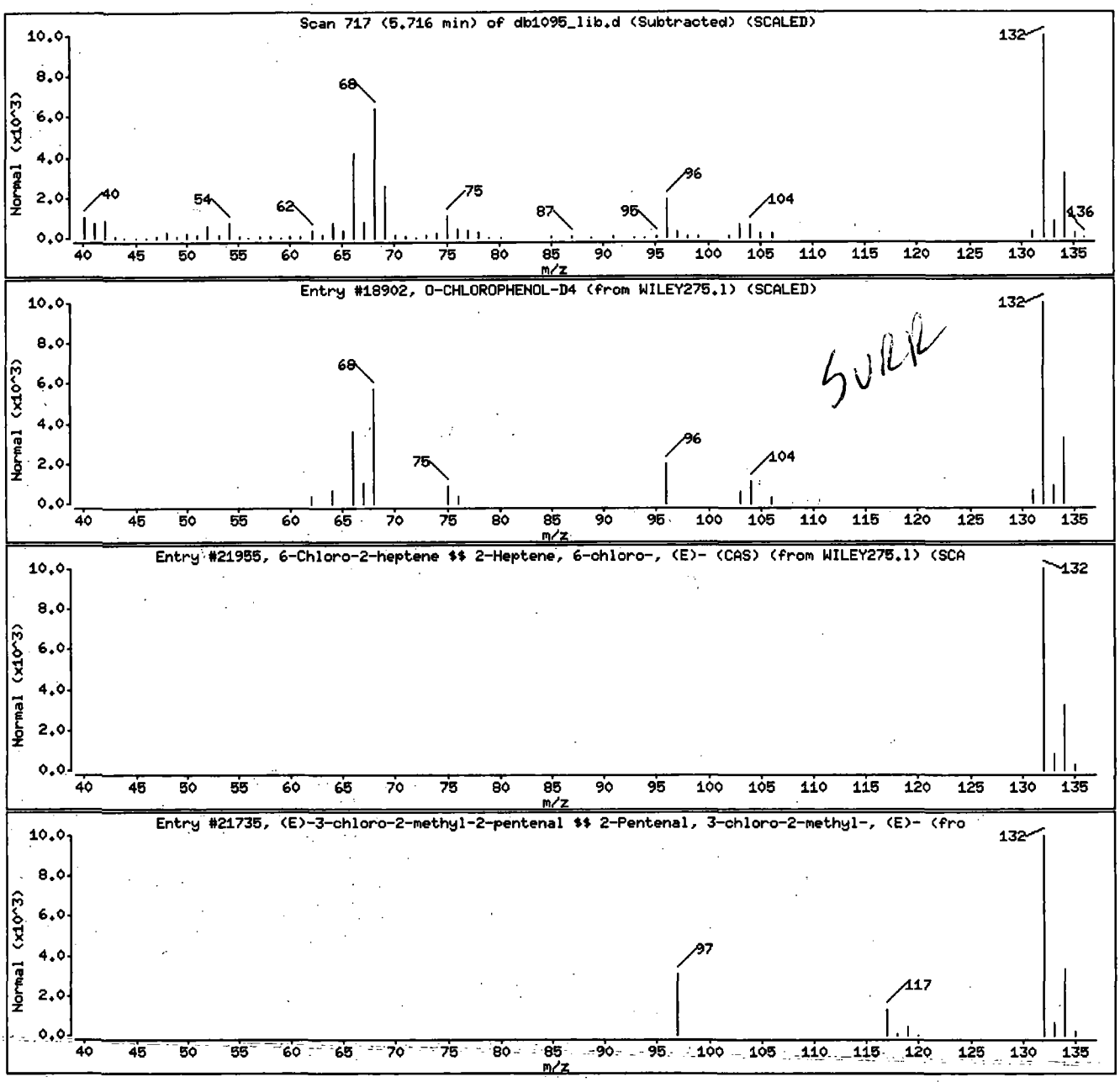
Client ID: H8011 Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	89	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	78	C6H9ClO	132



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

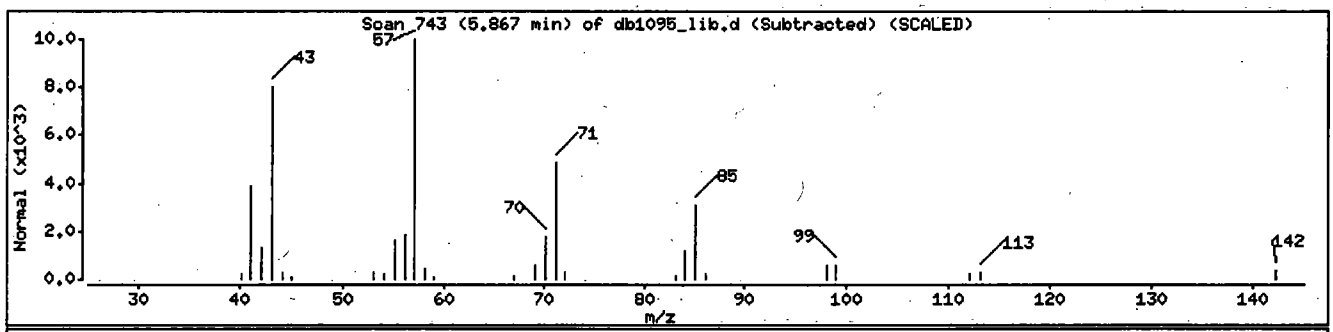
Volume Injected (uL): 1.0

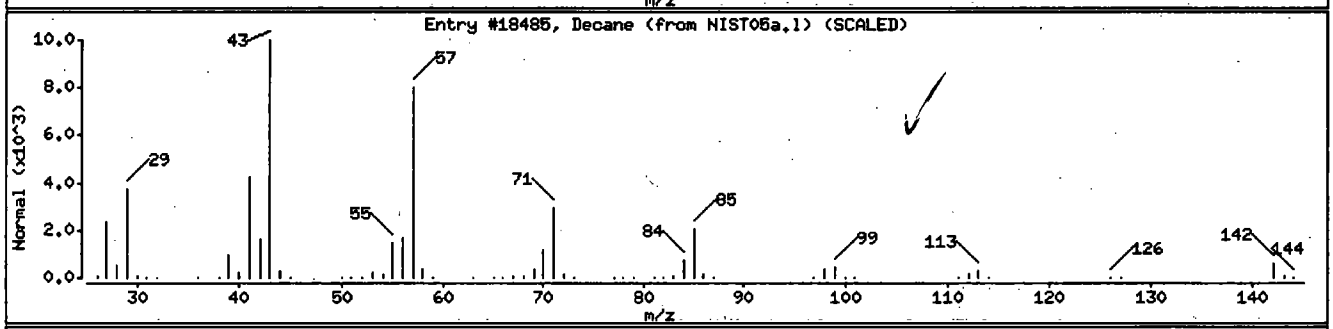
Operator: ceb05247

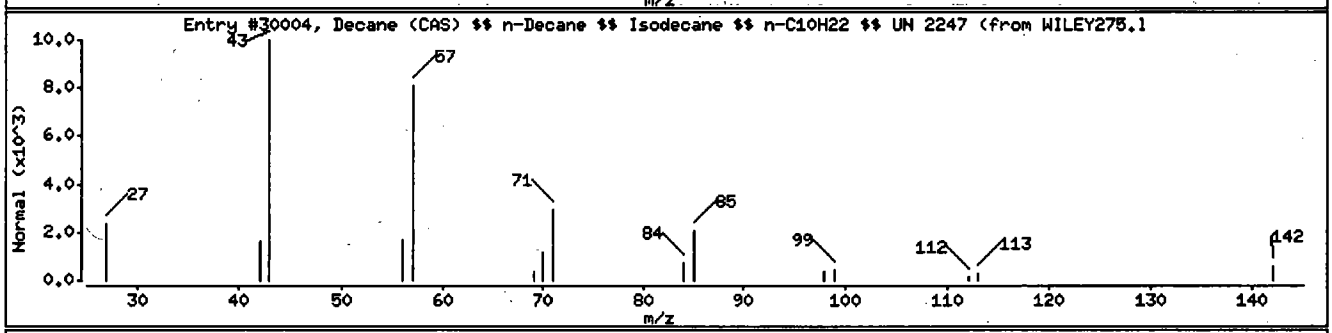
Column phase: J&W DB-5MS

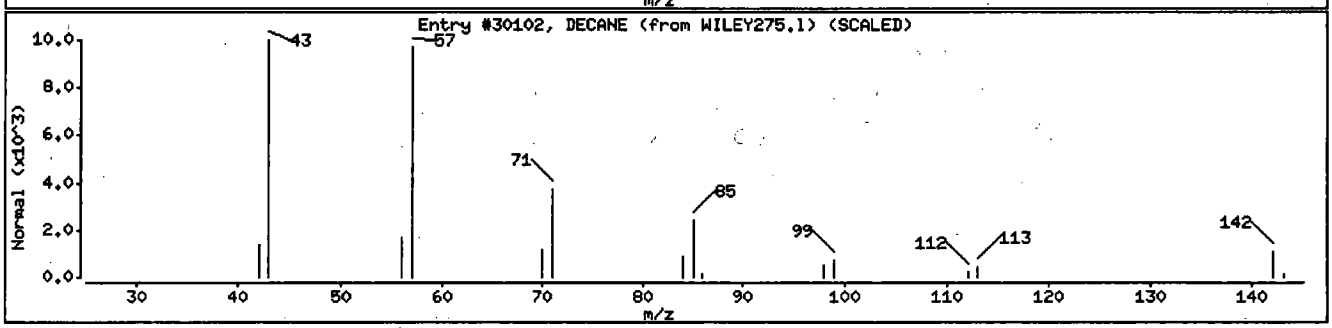
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

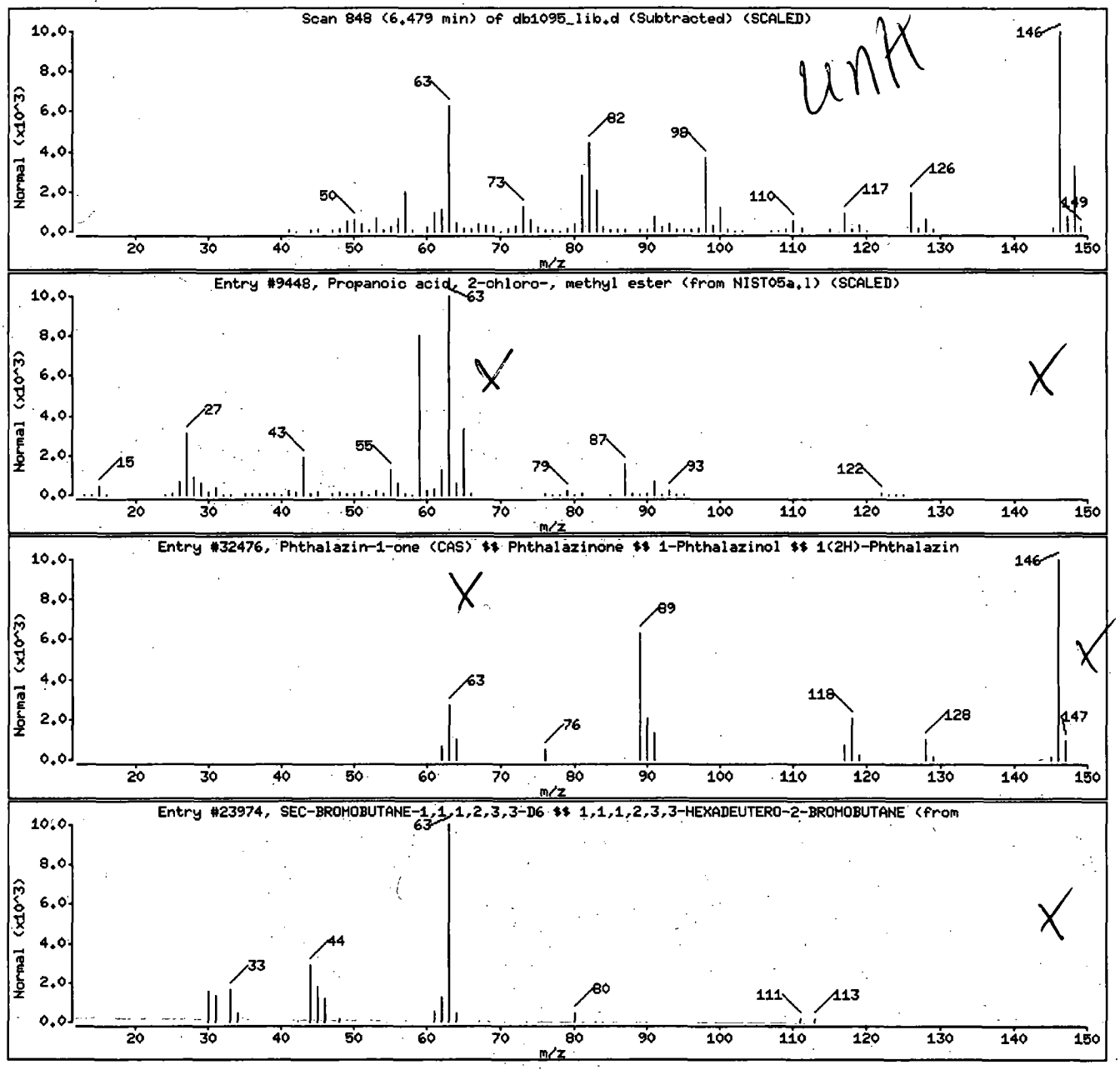
Volume Injected (uL): 1.0

Operator: oeb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
Phthalazin-1-one (CAS) $$ Phthalazinone	119-39-1	WILEY275.l	32476	40	C8H6N2O	146
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

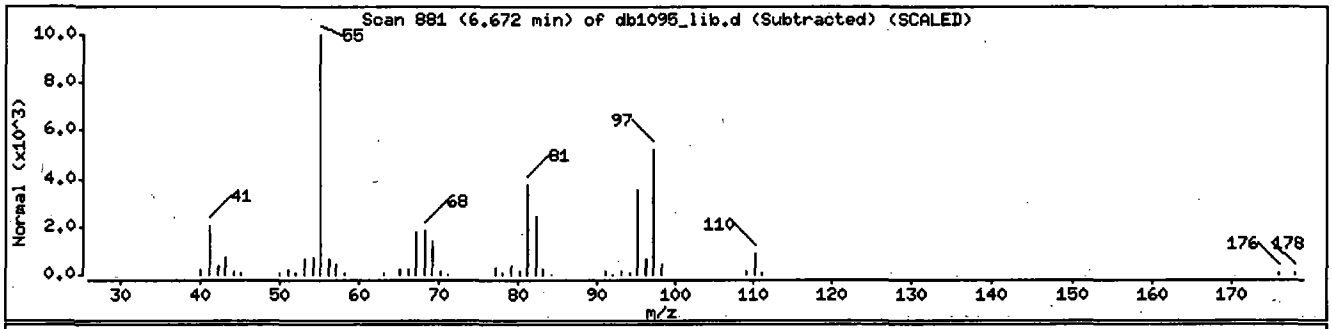
Volume Injected (uL): 1.0

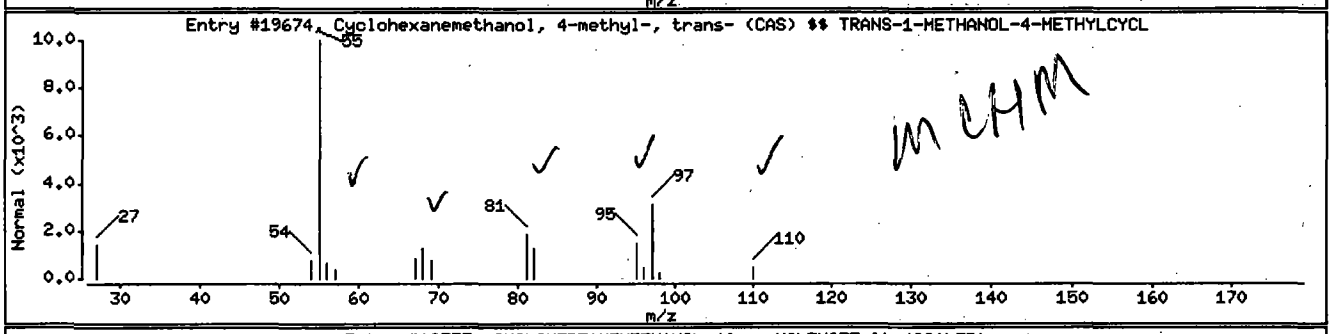
Operator: ceb05247

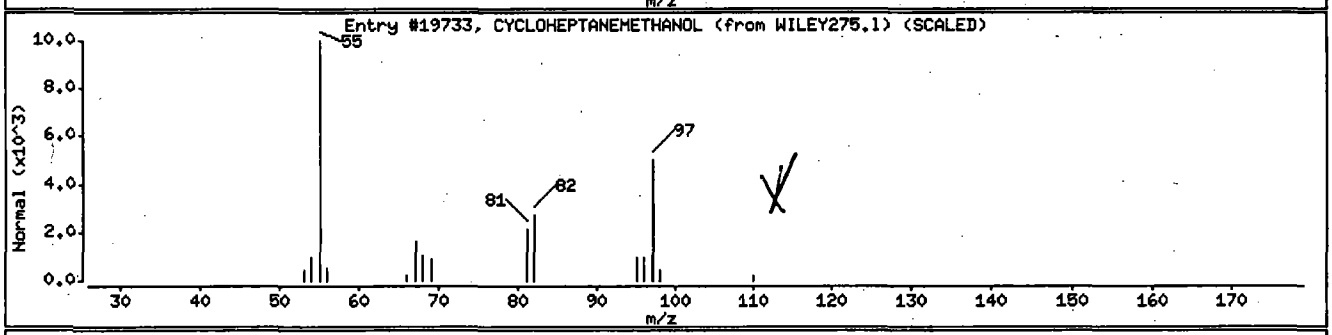
Column phase: J&W DB-5MS

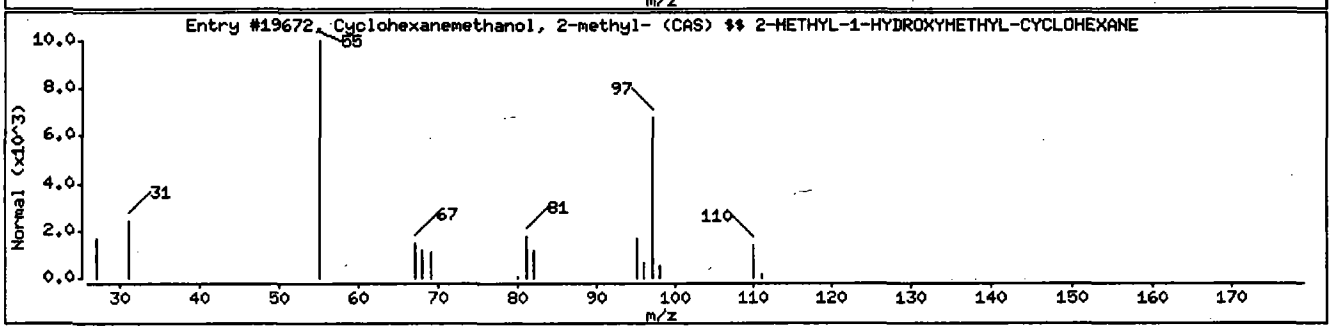
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.1	19674	53	C8H16O	128
CYCLOHEPTANEMETHANOL	0-00-0	WILEY275.1	19733	64	C8H16O	128
Cyclohexanemethanol, 2-methyl- (CAS) $$	2105-40-0	WILEY275.1	19672	56	C8H16O	128









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

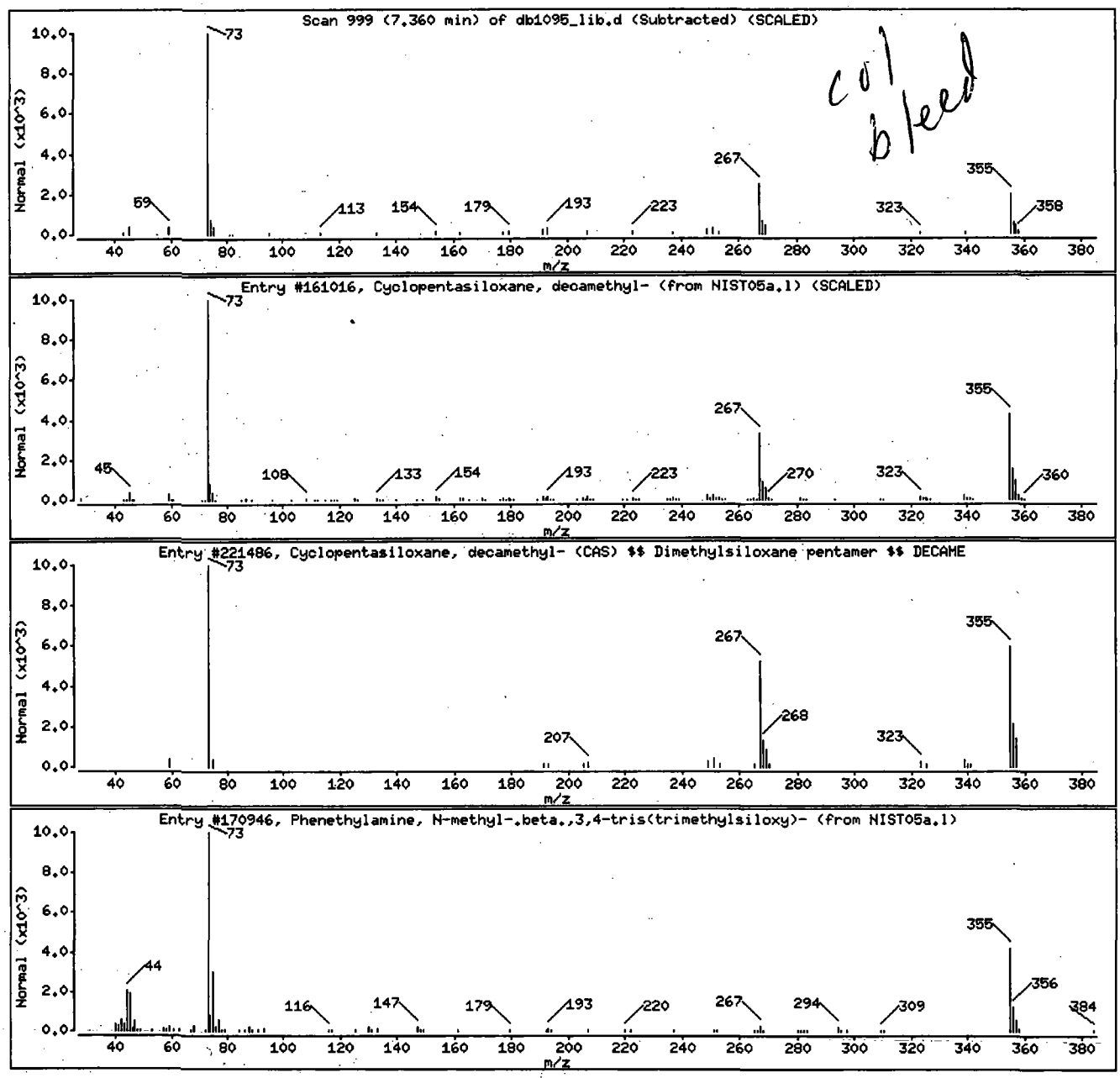
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	72	C10H30O5Si5	370
Phenethylamine, N-methyl-.beta.,3,4-tris	10538-85-9	NIST05a.l	170946	47	C18H37NO3Si3	399



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

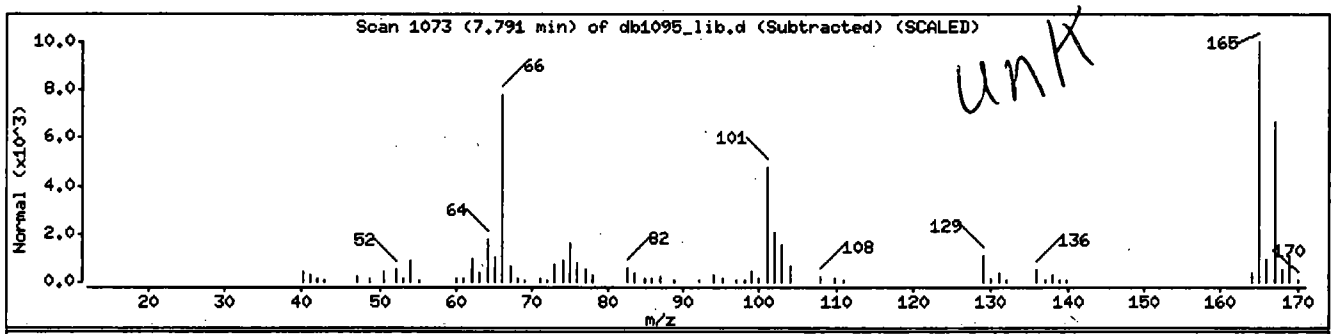
Volume Injected (uL): 1.0

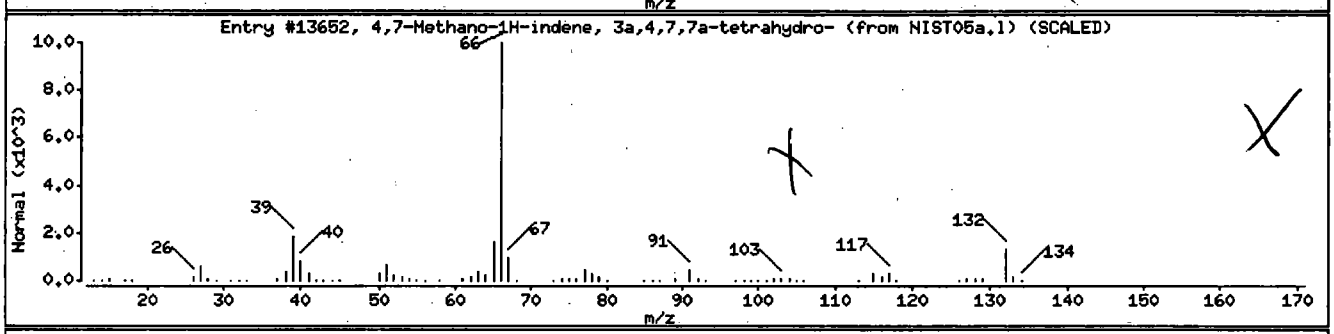
Operator: ceb05247

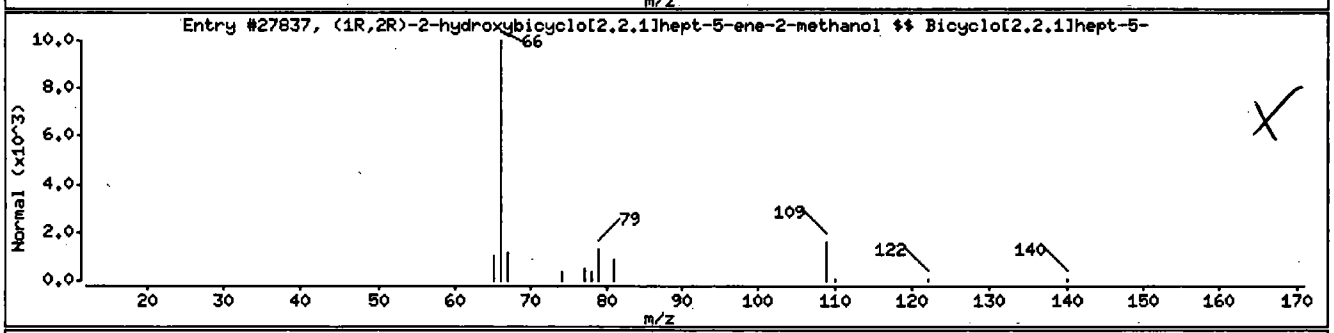
Column phase: J&W DB-5MS

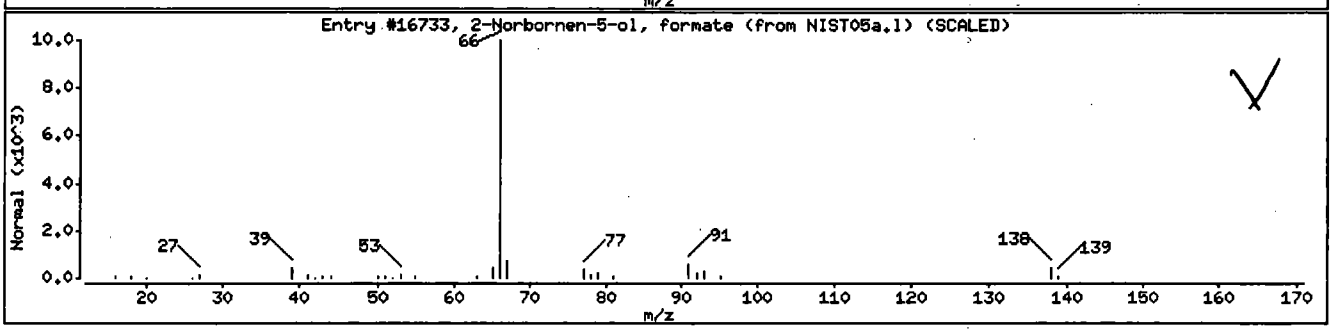
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	43	C10H12	132
(1R,2R)-2-hydroxybicyclo[2.2.1]hept-5-en	116697-44-0	WILEY275.l	27837	47	C8H12O2	140
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H10O2	138









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

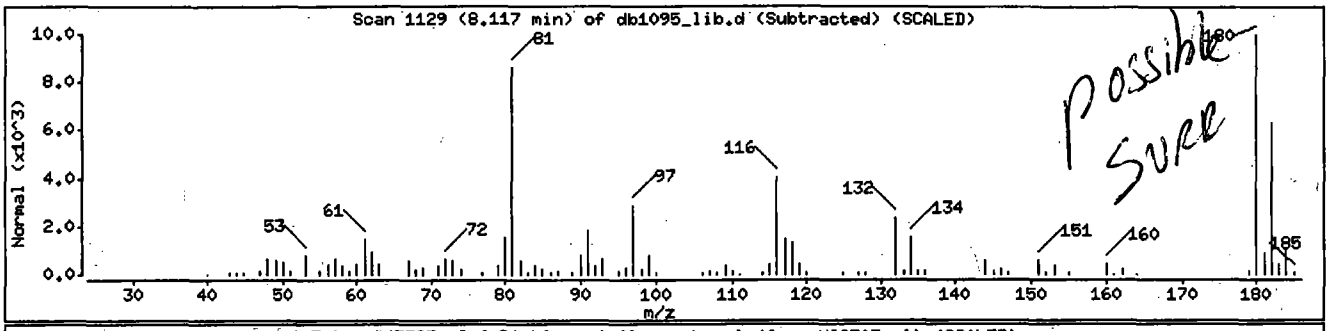
Volume Injected (uL): 1.0

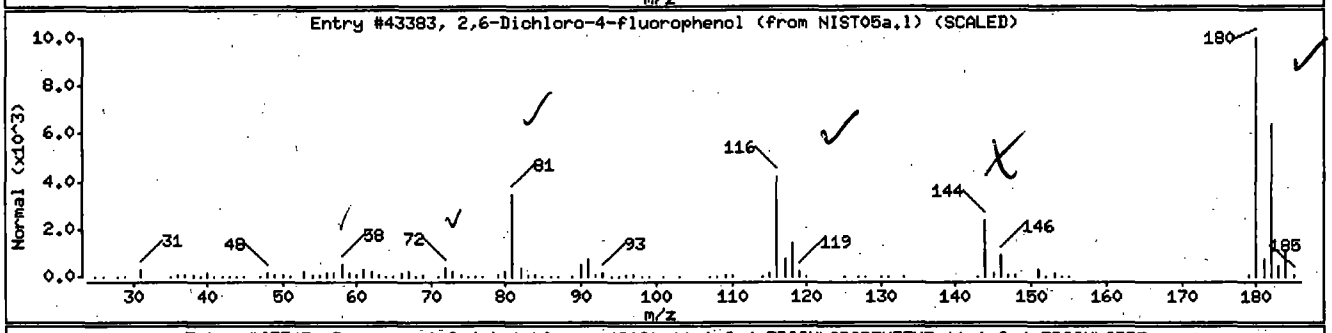
Operator: ceb05247

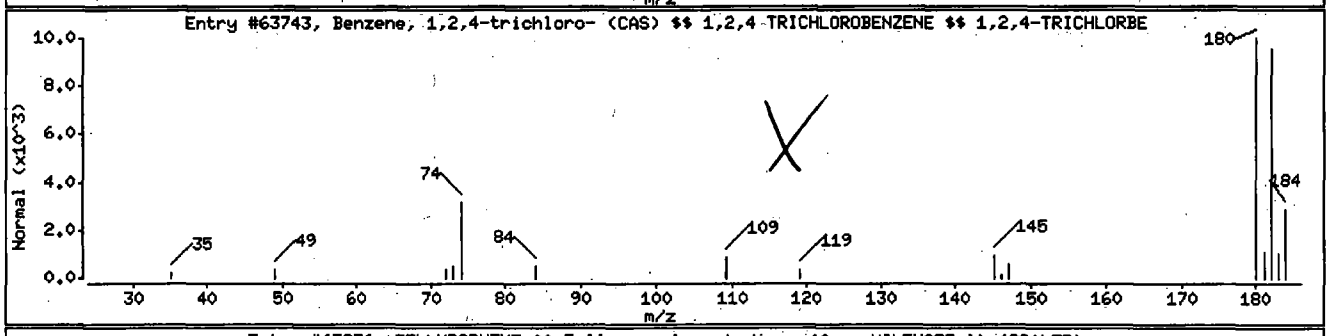
Column phase: J&W DB-5MS

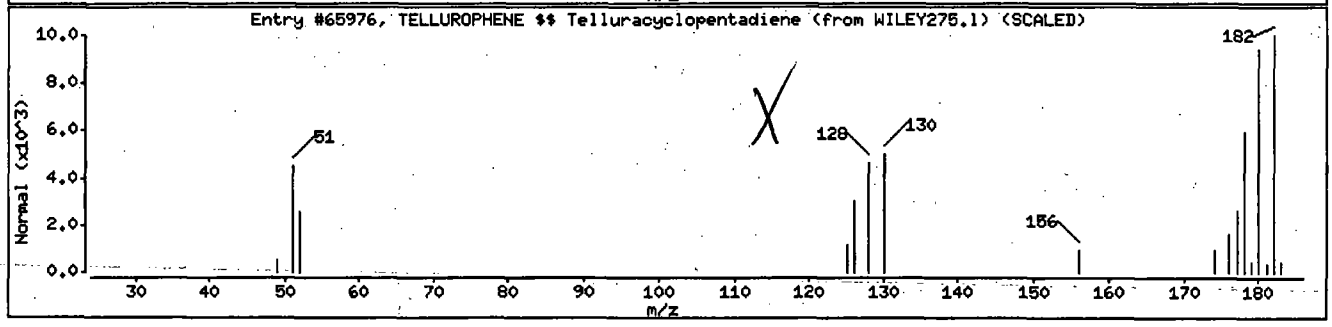
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	86	C6H3C12FO	180
Benzene, 1,2,4-trichloro- (CAS) $$ 1,2,4	120-82-1	WILEY275.l	63743	12	C6H3C13	180
TELLUROPHENE $$ Telluracyclopentadiene	288-08-4	WILEY275.l	65976	11	C4H4Te	182









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

Client ID: H8011

Instrument: HP19760.i

Sample Info: H8011;7368069;1;0;SAMPLE;;;

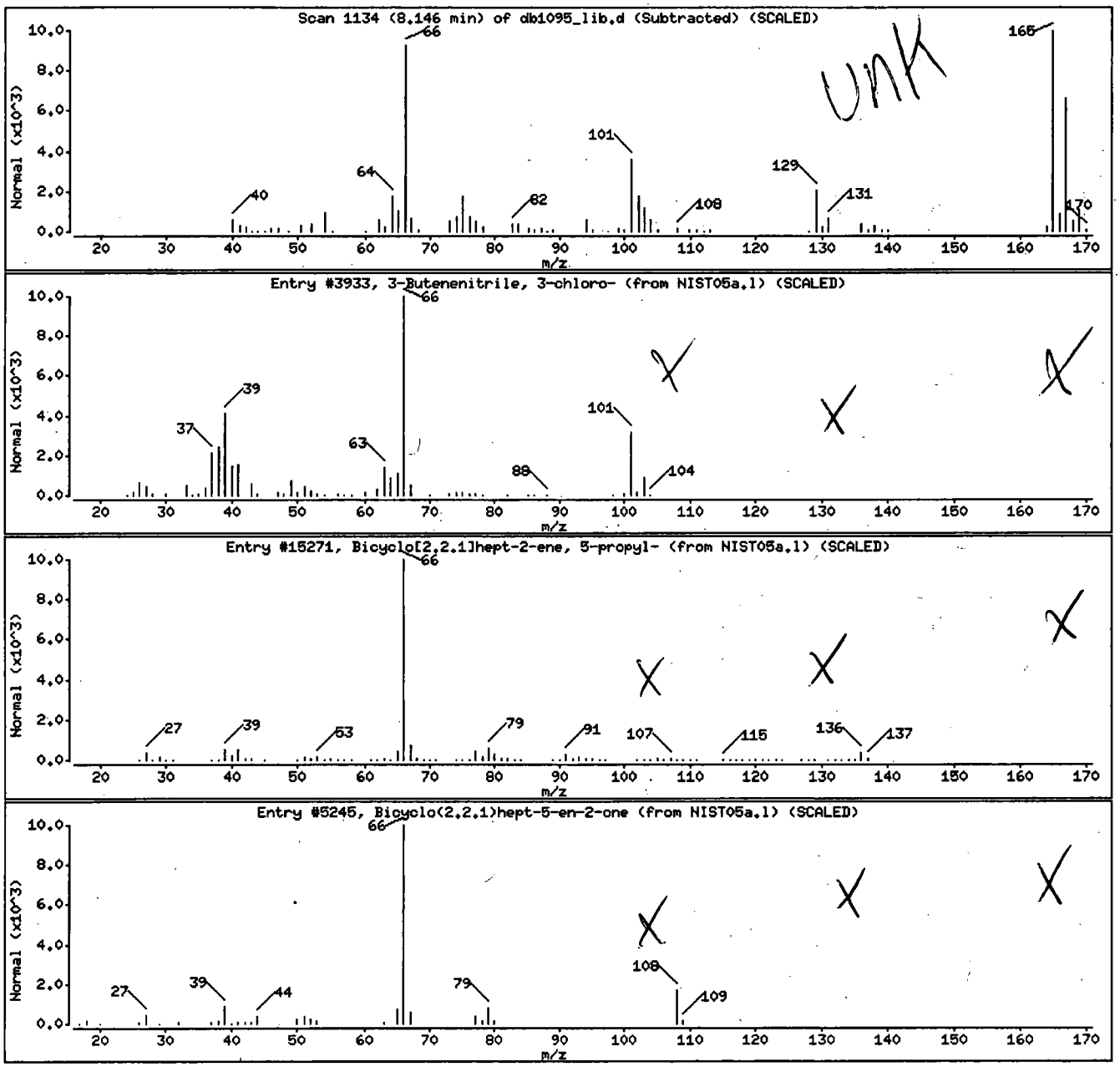
Volume Injected (uL): 1.0

Operator: oeb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136
Bicyclo(2.2.1)hept-5-en-2-one	694-98-4	NIST05a.l	5245	49	C7H8O	108



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1095_lib.d

Date : 25-FEB-2014 02:32

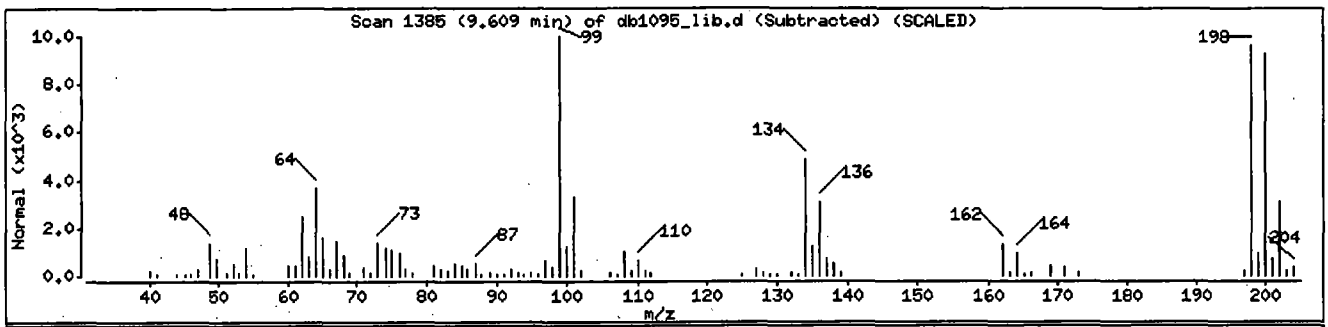
Client ID: H8011 | Instrument: HP19760.i

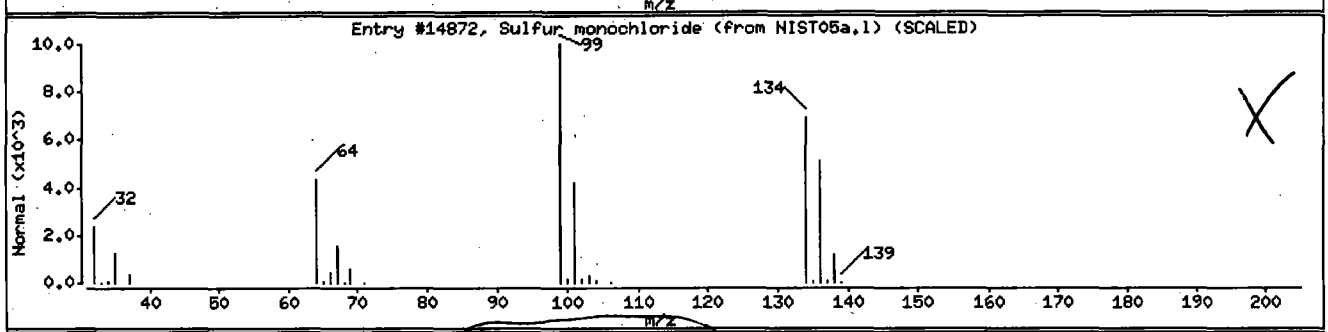
Sample Info: H8011;7368069;1;0;SAMPLE;;;

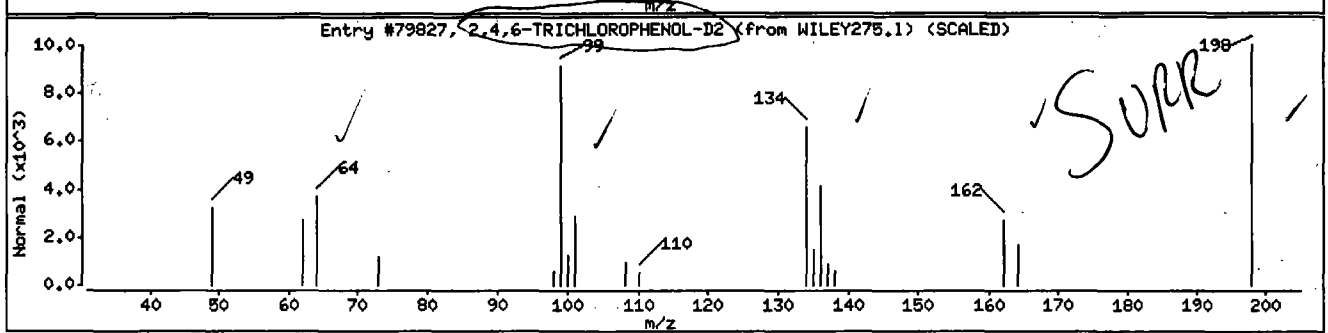
Volume Injected (uL): 1.0 | Operator: ceb05247

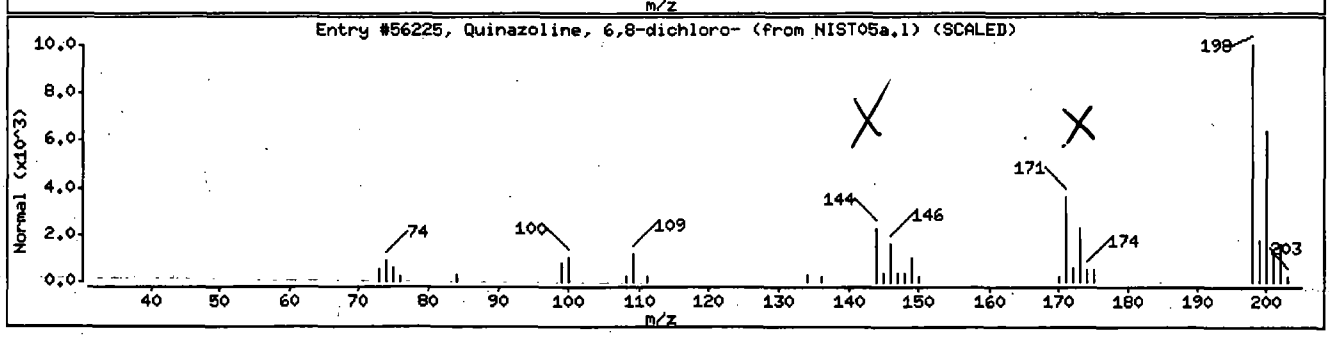
Column phase: J&W DB-5MS | Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	27	C12S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	64	C6HD2Cl3O	198
Quinazoline, 6,8-dichloro-	17227-49-5	NIST05a.l	56225	38	C8H4Cl2N2	198



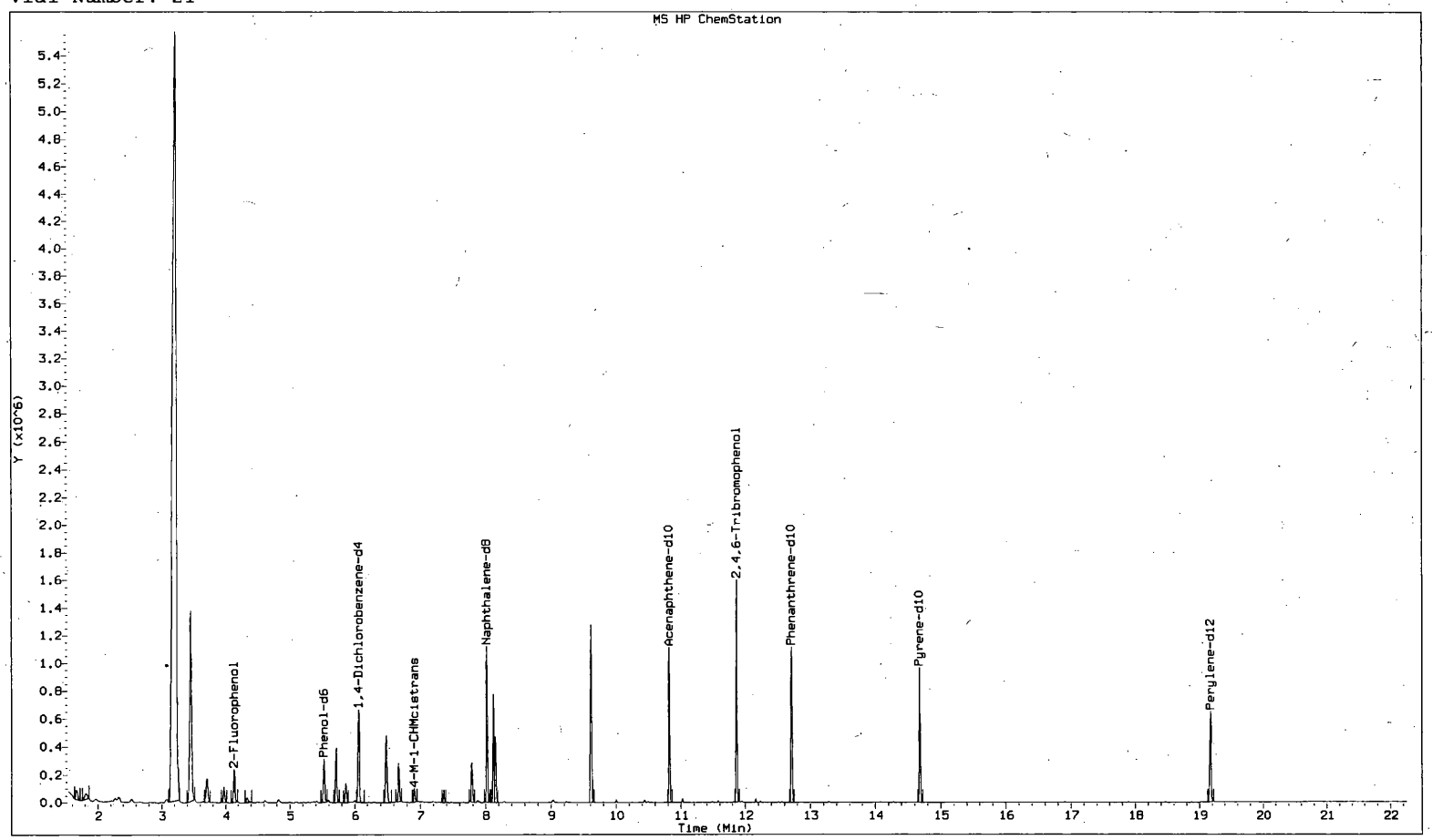






Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:06.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb24.b/db1070_lib.d
Operator : jmg00346
Acquired : 24-FEB-2014 15:30
Instrument : HP19760.i
Sample Name: H8021;7368073;1;0;SAMPLE;;;
Misc Info : 14051WAB;WL13166;;1058;1000;0;db1052;13166;
Vial Number: 21



Lancaster Labs

Data file : /chem/HP19760.i/14feb24.b/db1070_lib.d
Lab Smp Id: 7368073 Client Smp ID: H8021
Inj Date : 24-FEB-2014 15:30
Operator : jmg00346 Inst ID: HP19760.i
Smp Info : H8021;7368073;1;0;SAMPLE;;;
Misc Info : 14051WAB;WL13166;;1058;1000;0;db1052;13166;
Comment : Max. number of TICs to report is 50, 16 TICs were found initially.
Method : /chem/HP19760.i/14feb24.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:47 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 21
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1058.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.060	971016	10.000
* 48 Naphthalene-d8	8.018	1399474	10.000
* 83 Acenaphthene-d10	10.822	1257526	10.000

	CONCENTRATIONS				QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.665	137987	1.42105696	1.34315	91	NIST05a.1	31325	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1-Butene, 2-chloro-3-methyl-					CAS #: 17773-64-7		
1.817	127020	1.30810894	1.23639	62	NIST05a.1	4733	21
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.227	21767664	224.174050	211.88473	83	NIST05a.1	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.454	2853561	29.3873640	27.77633	83	NIST05a.1	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.705	325077	3.34780587	3.16427	37	NIST05a.1	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
3.973	197533	2.03428665	1.92276	36	NIST05a.1	13998	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.335	70823	0.72936800	0.68938	9	NIST05a.1	33655	21(L)
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.716	584210	6.01648400	5.68665	91	WILEY275.1	18902	21
Decane					CAS #: 124-18-5		
5.867	205086	2.11207574	1.99629	91	NIST05a.1	18486	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.479	804287	8.28294332	7.82886	35	NIST05a.1	9448	21
Cyclohexanemethanol, 4-methyl-, trans-					CAS #: 3937-49-3		
6.672	362289	3.73103010	3.52649	83	NIST05a.1	12246	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.360	102754	0.73423357	0.69398	90	NIST05a.1	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.791	369786	2.64231835	2.49746	43	WILEY275.1	22244	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.117	920440	6.57704057	6.21648	86	NIST05a.1	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.146	542317	3.87514939	3.66271	50	NIST05a.1	3933	48
Sulfur monochloride					CAS #: 10025-67-9		
9.615	1486292	11.8191729	11.17124	27	NIST05a.1	14872	83(L)

Target compound.
Do not report.
ajs00193 03/02/2014

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

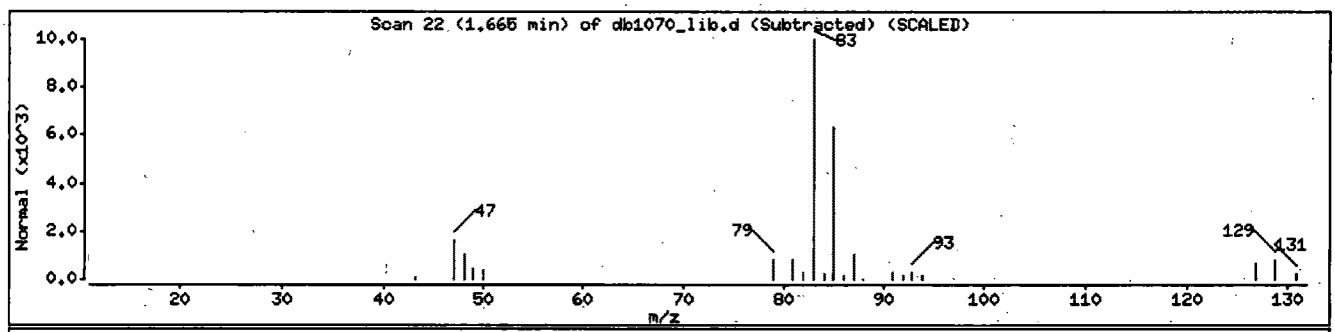
Volume Injected (uL): 1.0

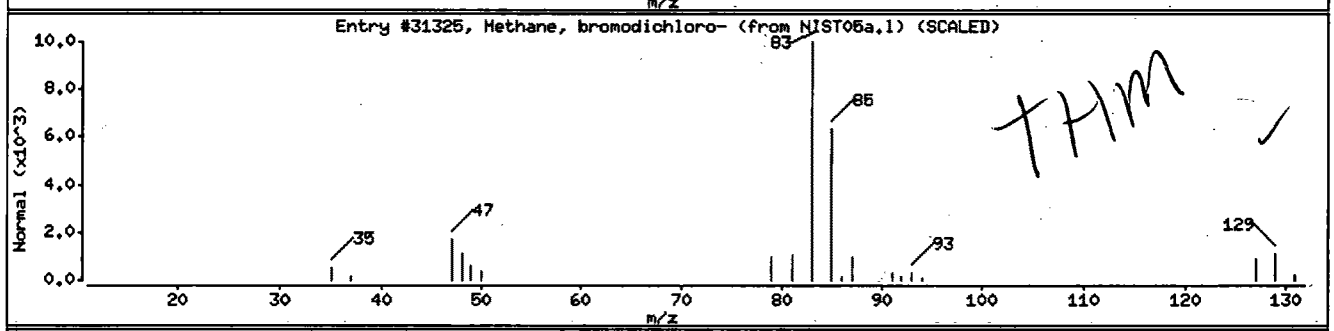
Operator: jmg00346

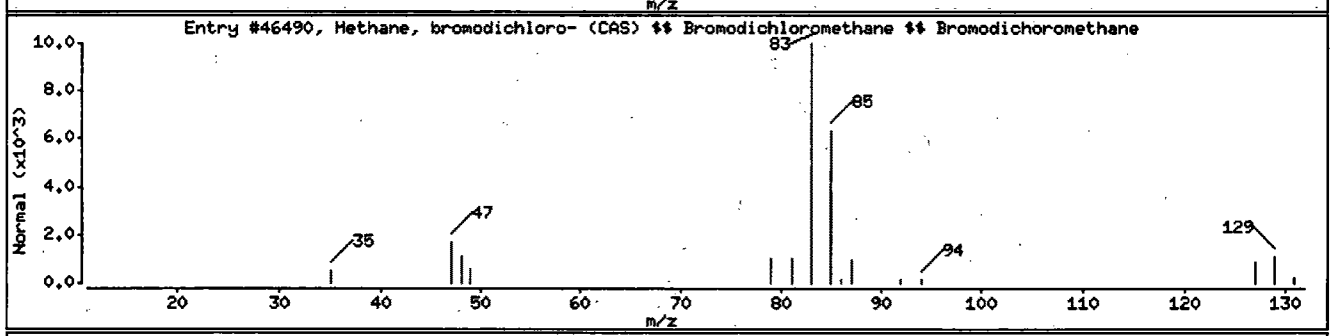
Column phase: J&W DB-5MS

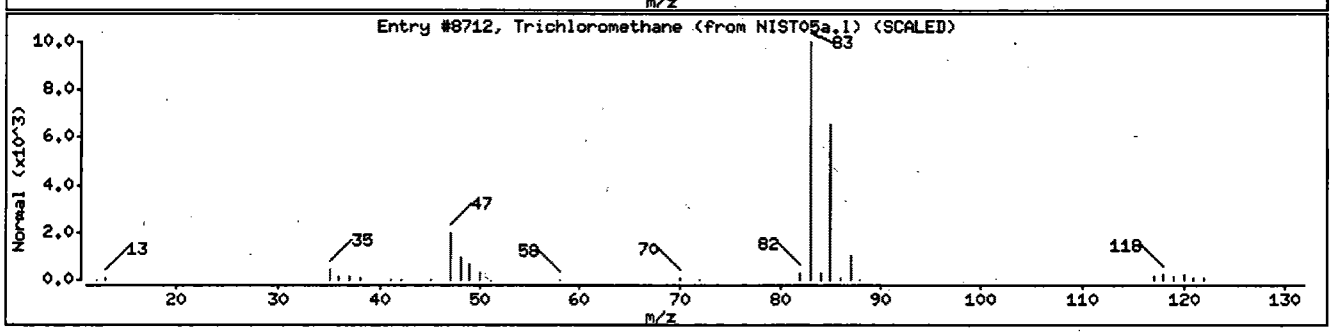
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31325	91	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	91	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 16:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

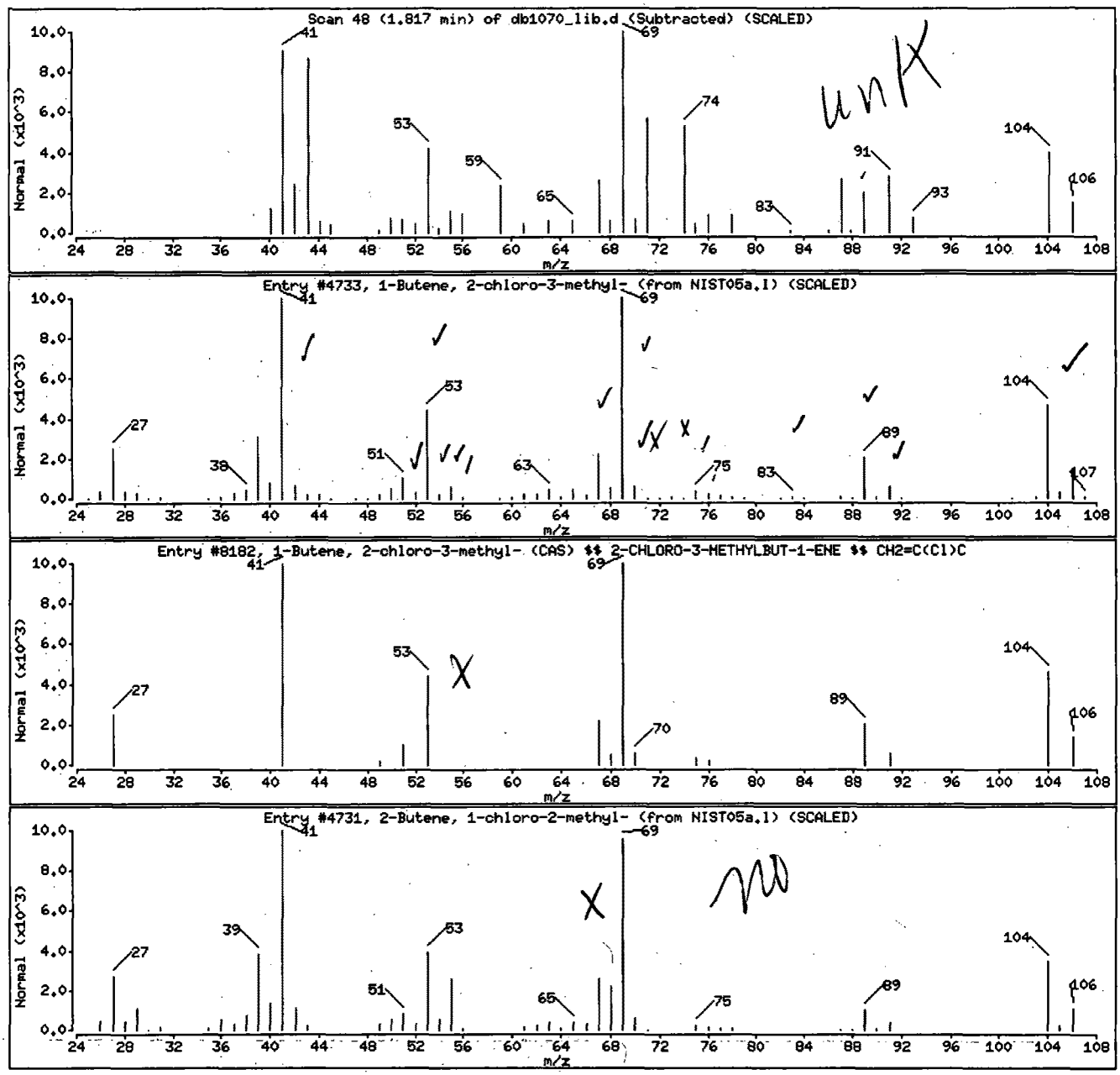
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1-Butene, 2-chloro-3-methyl-	17773-64-7	NIST05a.l	4733	62	C5H9Cl	104
1-Butene, 2-chloro-3-methyl- (CAS) $$ 2-	17773-64-7	WILEY275.l	8182	62	C5H9Cl	104
2-Butene, 1-chloro-2-methyl-	13417-43-1	NIST05a.l	4731	58	C5H9Cl	104



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

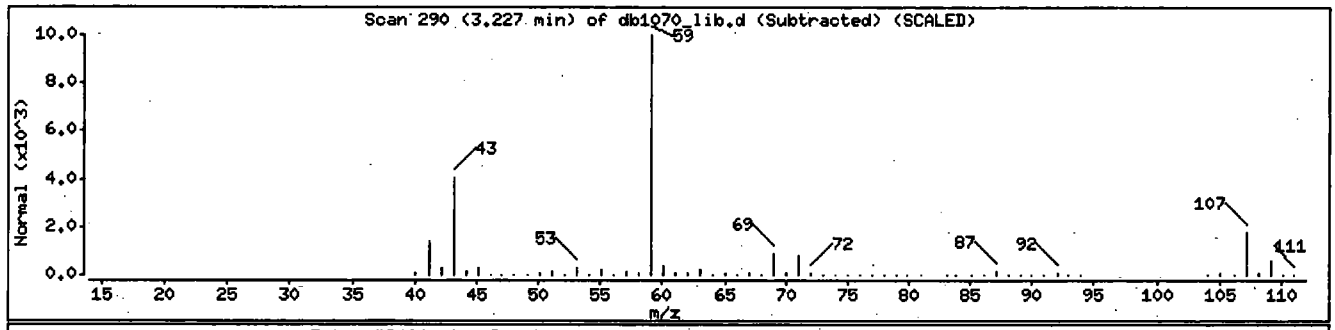
Volume Injected (uL): 1.0

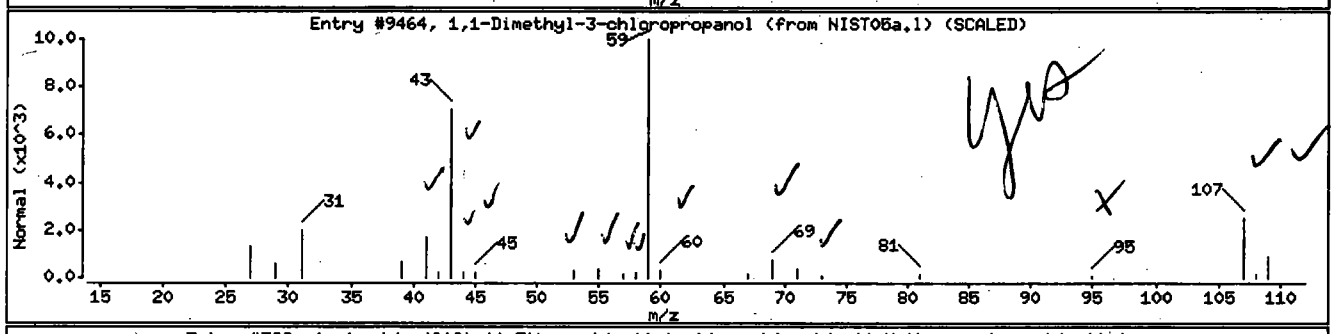
Operator: jmg00346

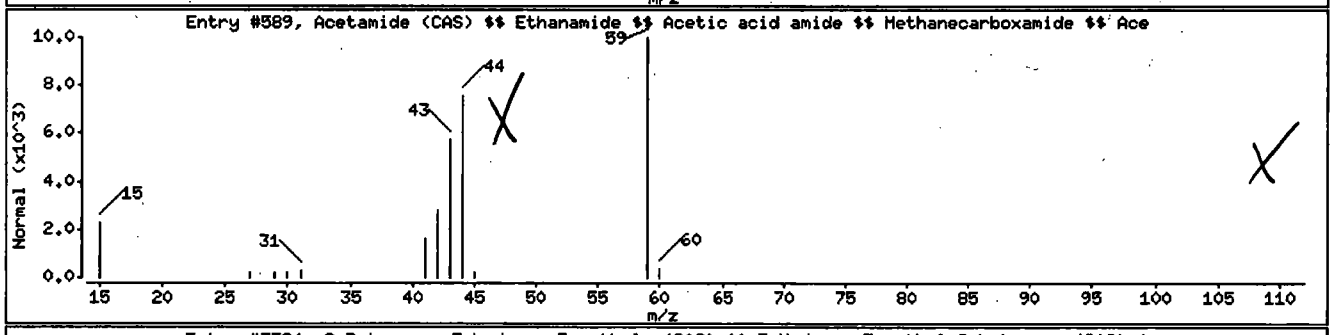
Column phase: J&W DB-5HS

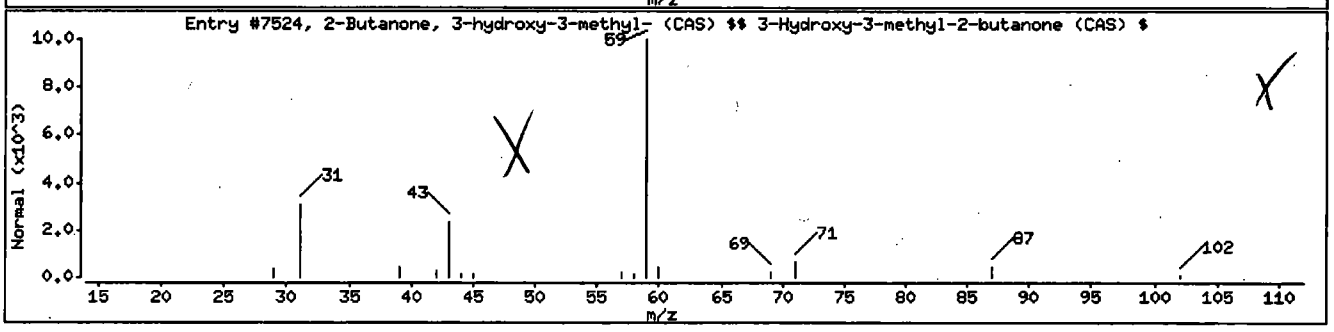
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

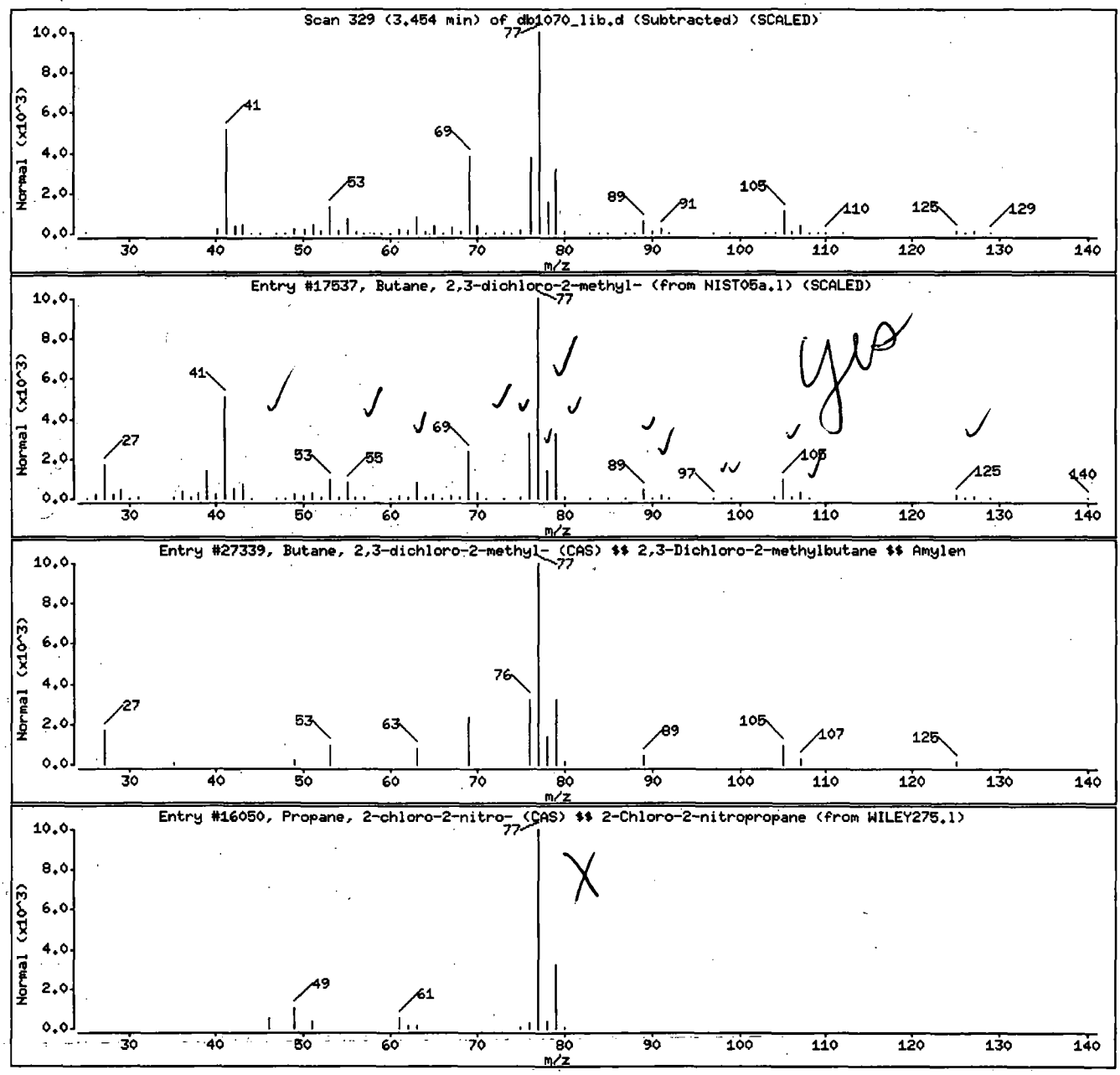
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	28	C3H6ClNO2	123



yes

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

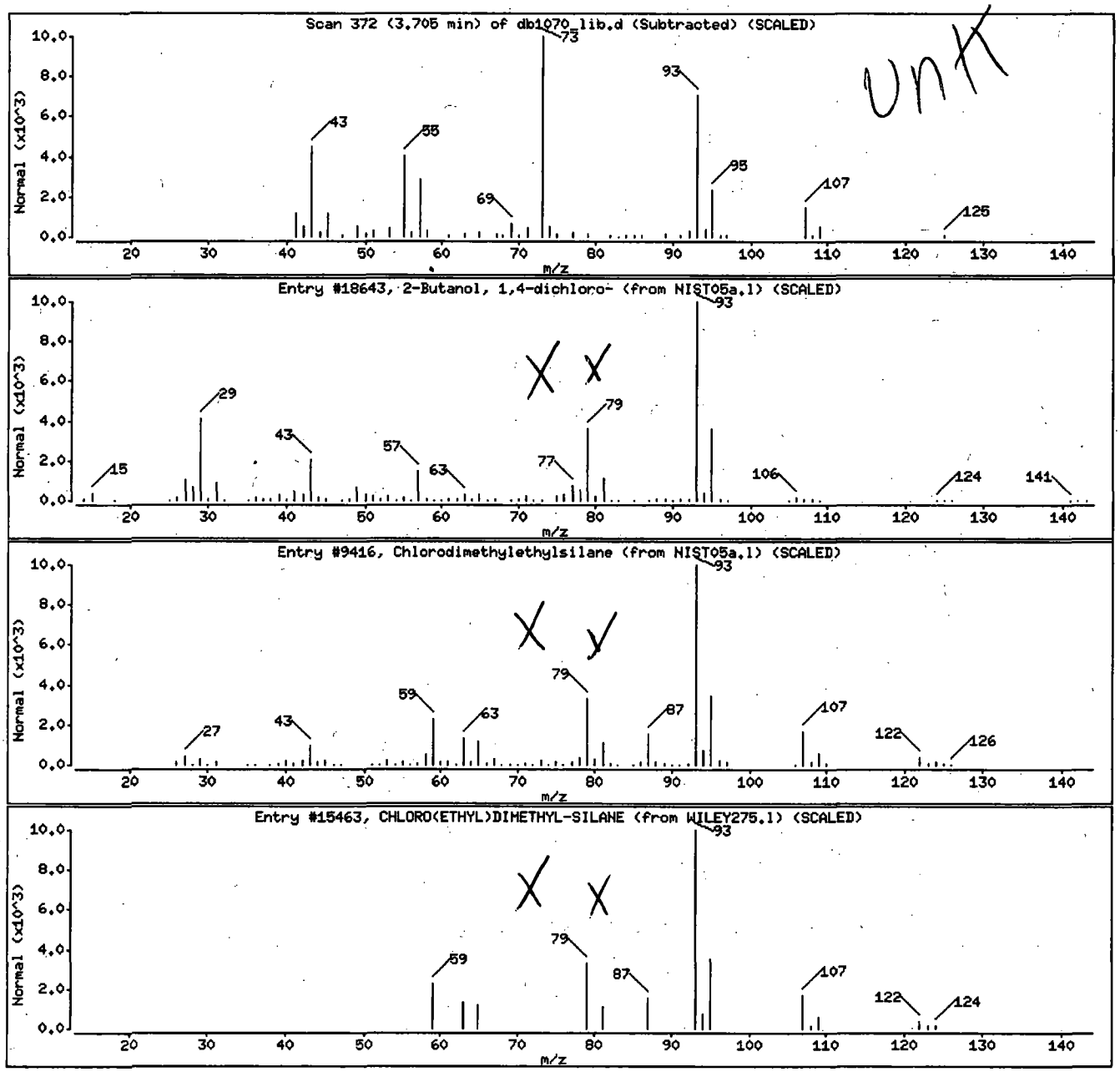
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	37	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	28	C4H11ClSi	122
CHLORO(ETHYL)DIMETHYL-SILANE	0-00-0	WILEY275.l	15463	28	C4H11ClSi	122



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

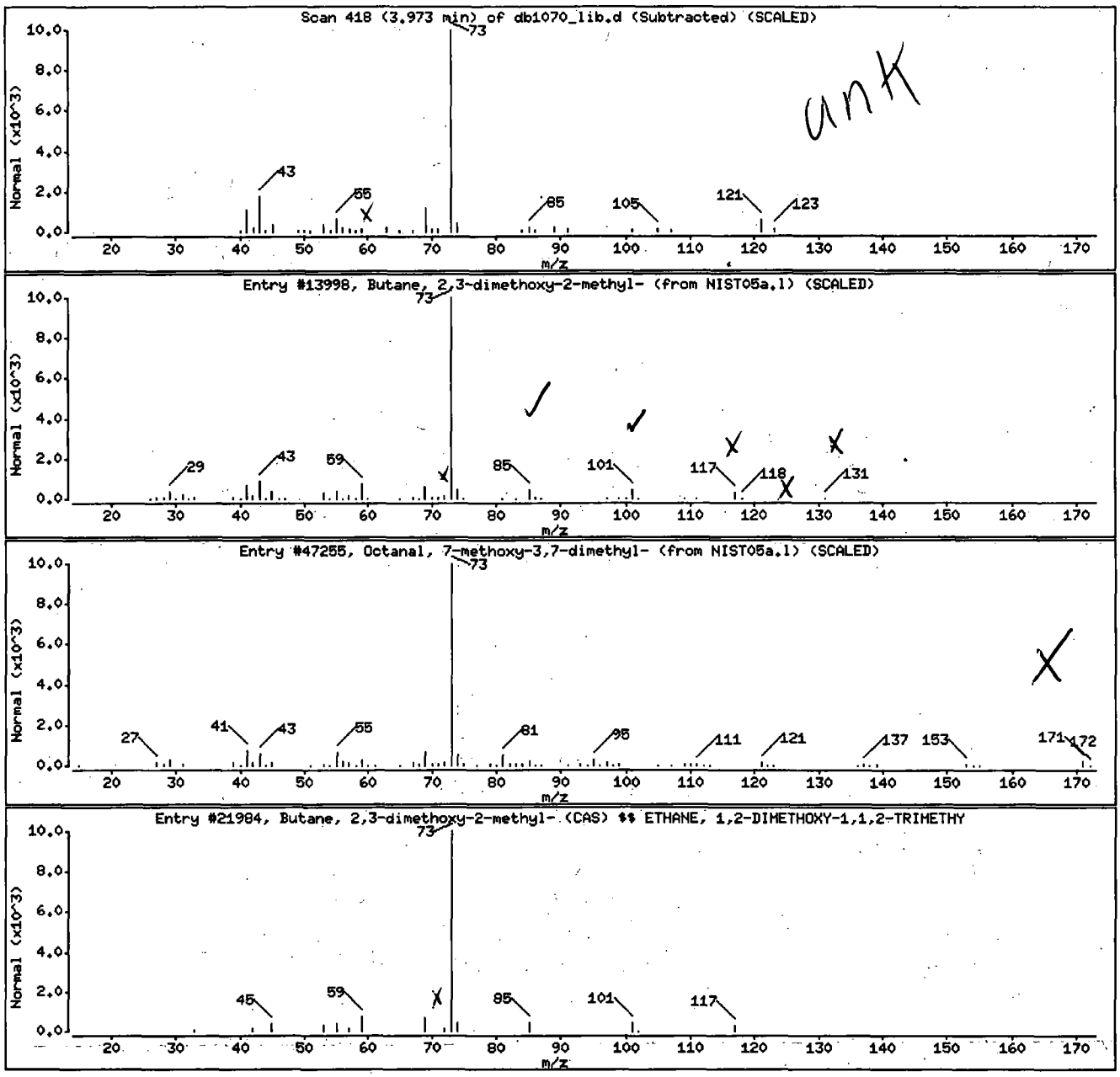
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	36	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	45	C11H22O2	186
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132



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Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

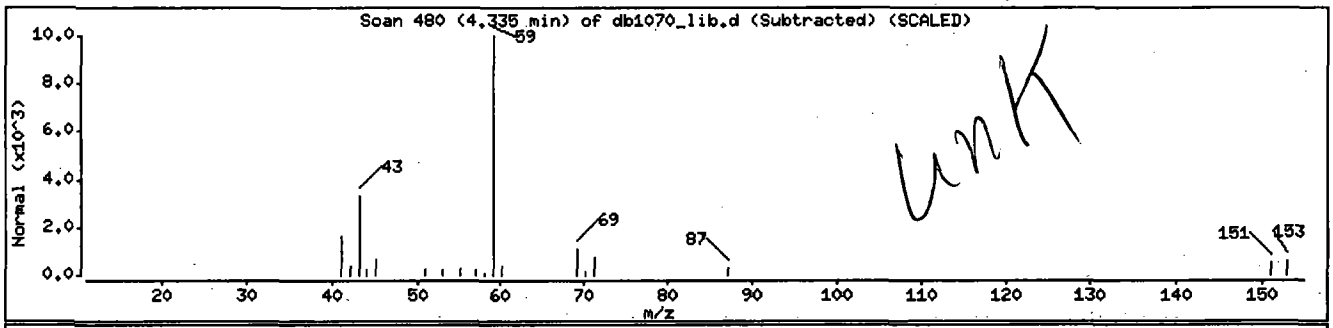
Volume Injected (uL): 1.0

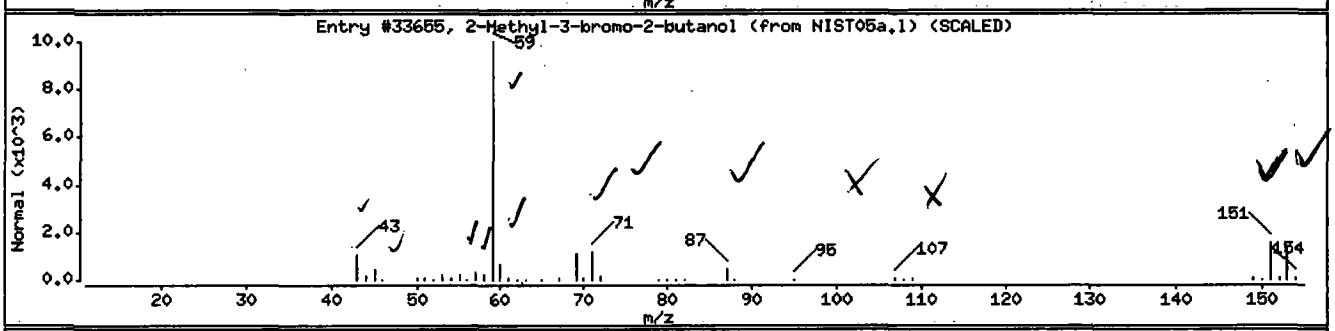
Operator: jmg00346

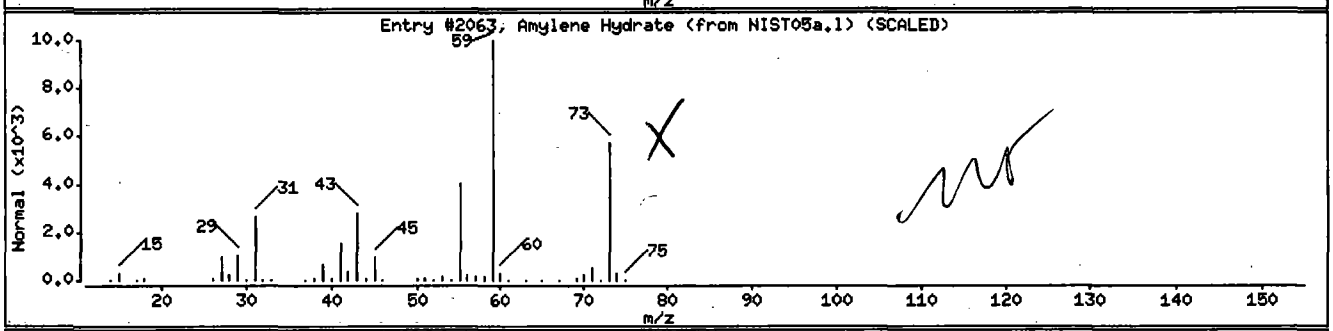
Column phase: J&W DB-5MS

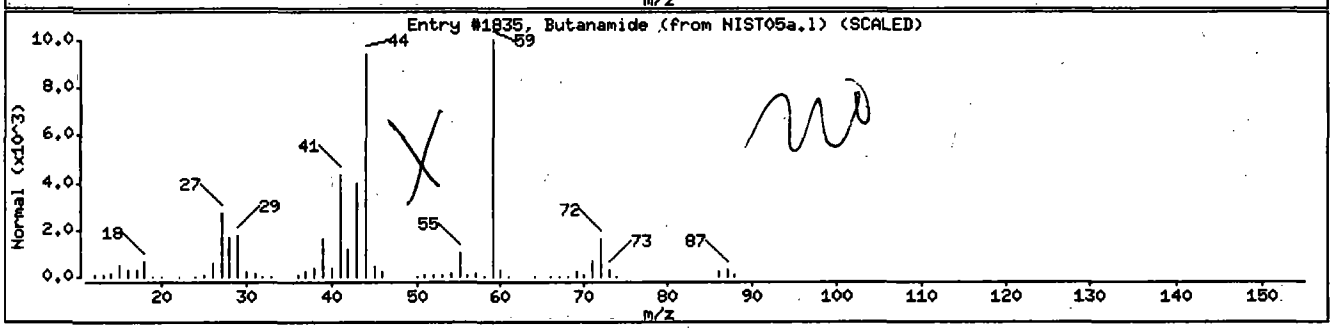
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	9	C5H11BrO	166
Amylene Hydrate	75-85-4	NIST05a.l	2063	64	C5H12O	88
Butanamide	541-35-5	NIST05a.l	1835	59	C4H9NO	87









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Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

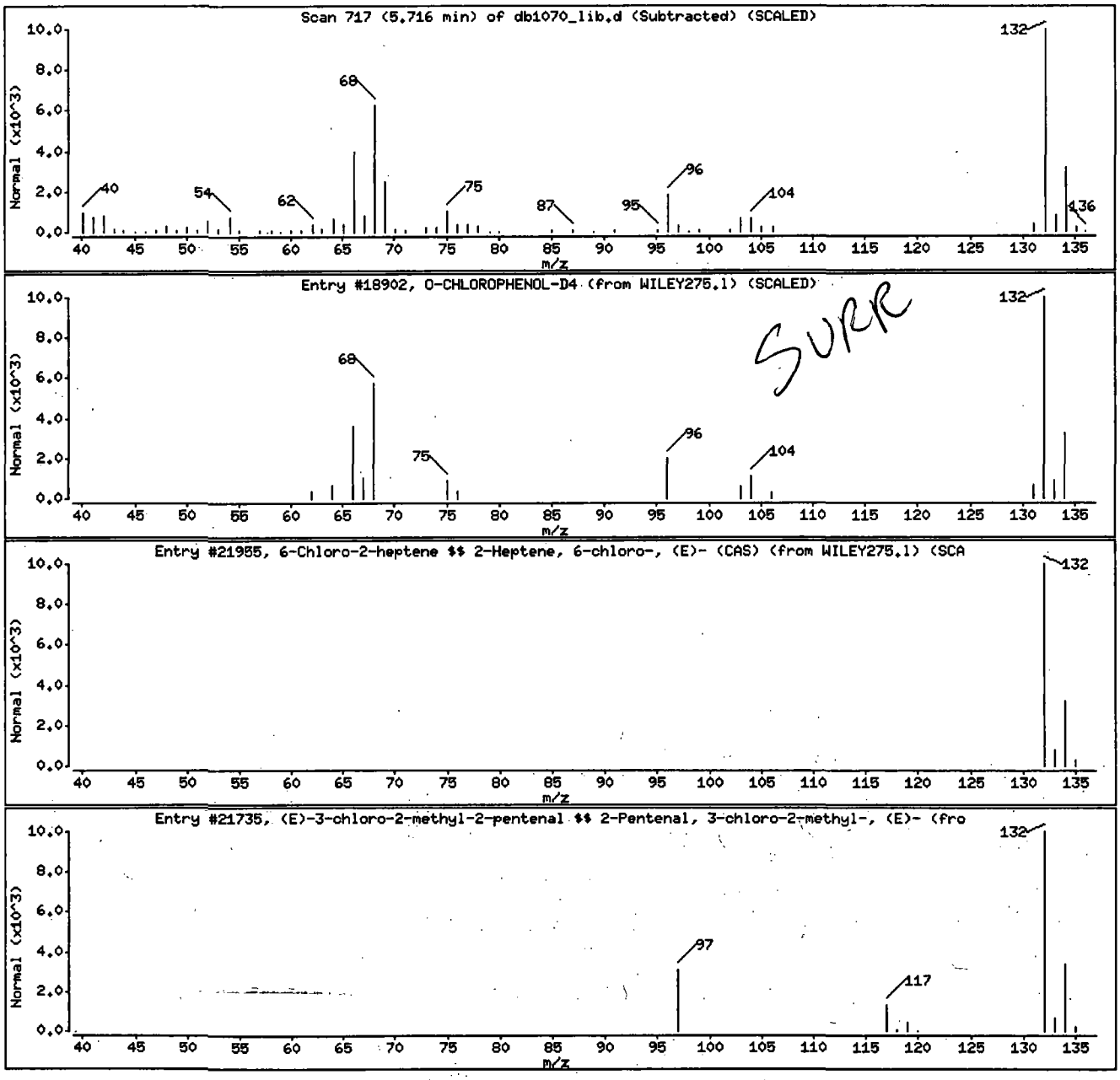
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132



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Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

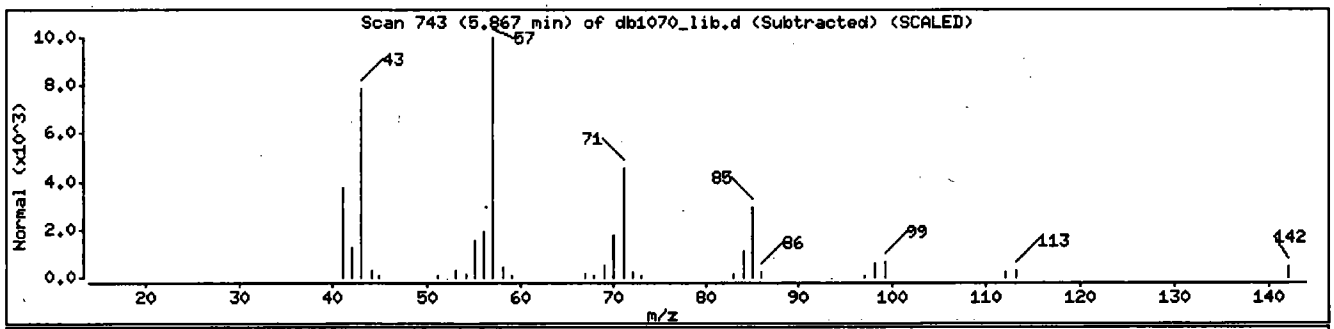
Volume Injected (uL): 1.0

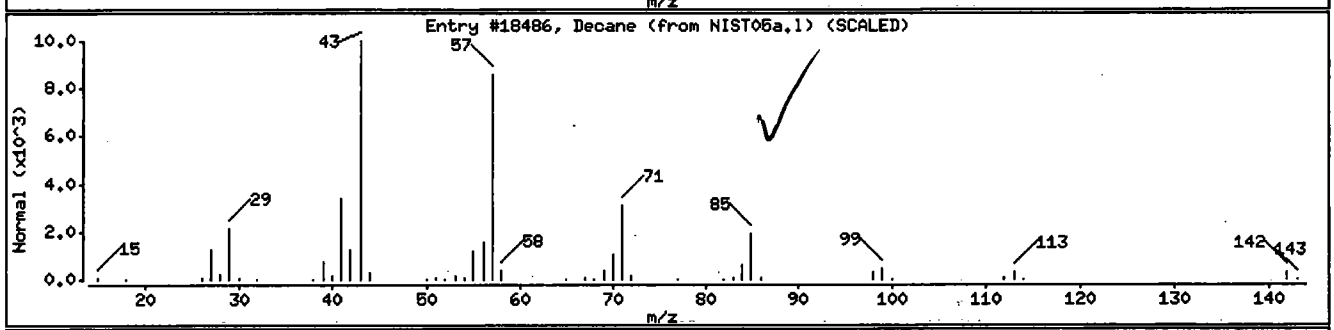
Operator: jmg00346

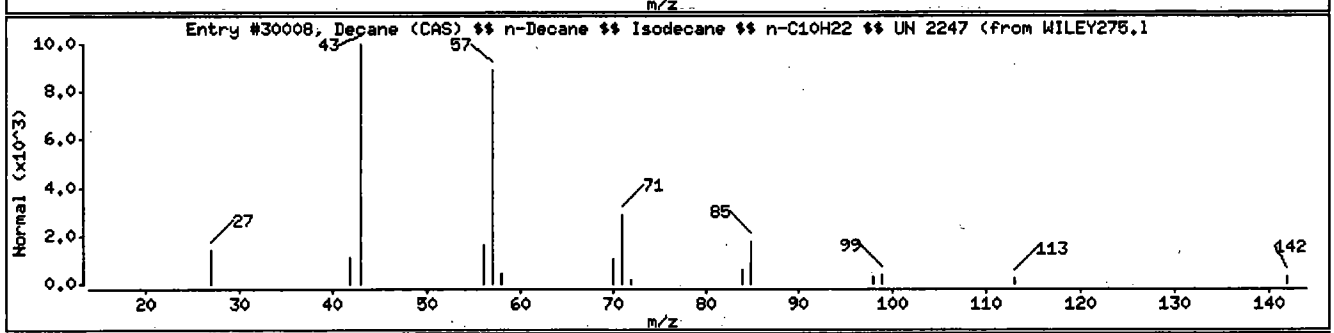
Column phase: J&W DB-5MS

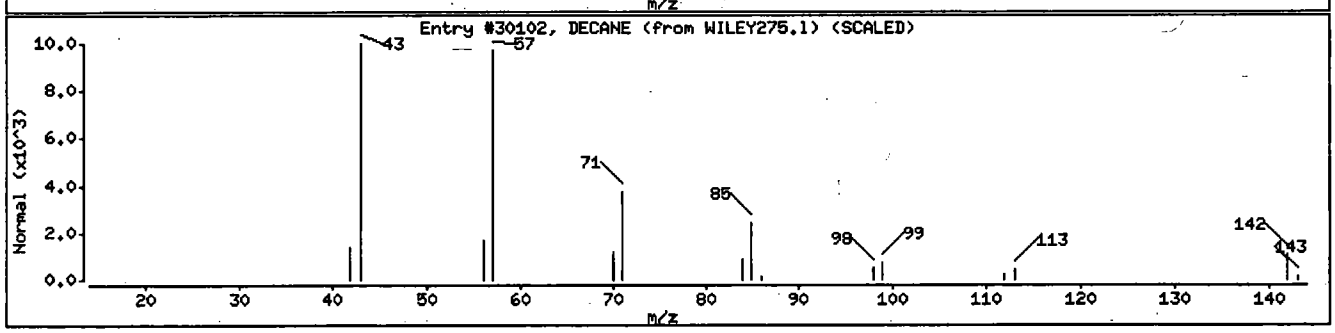
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18486	91	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30008	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

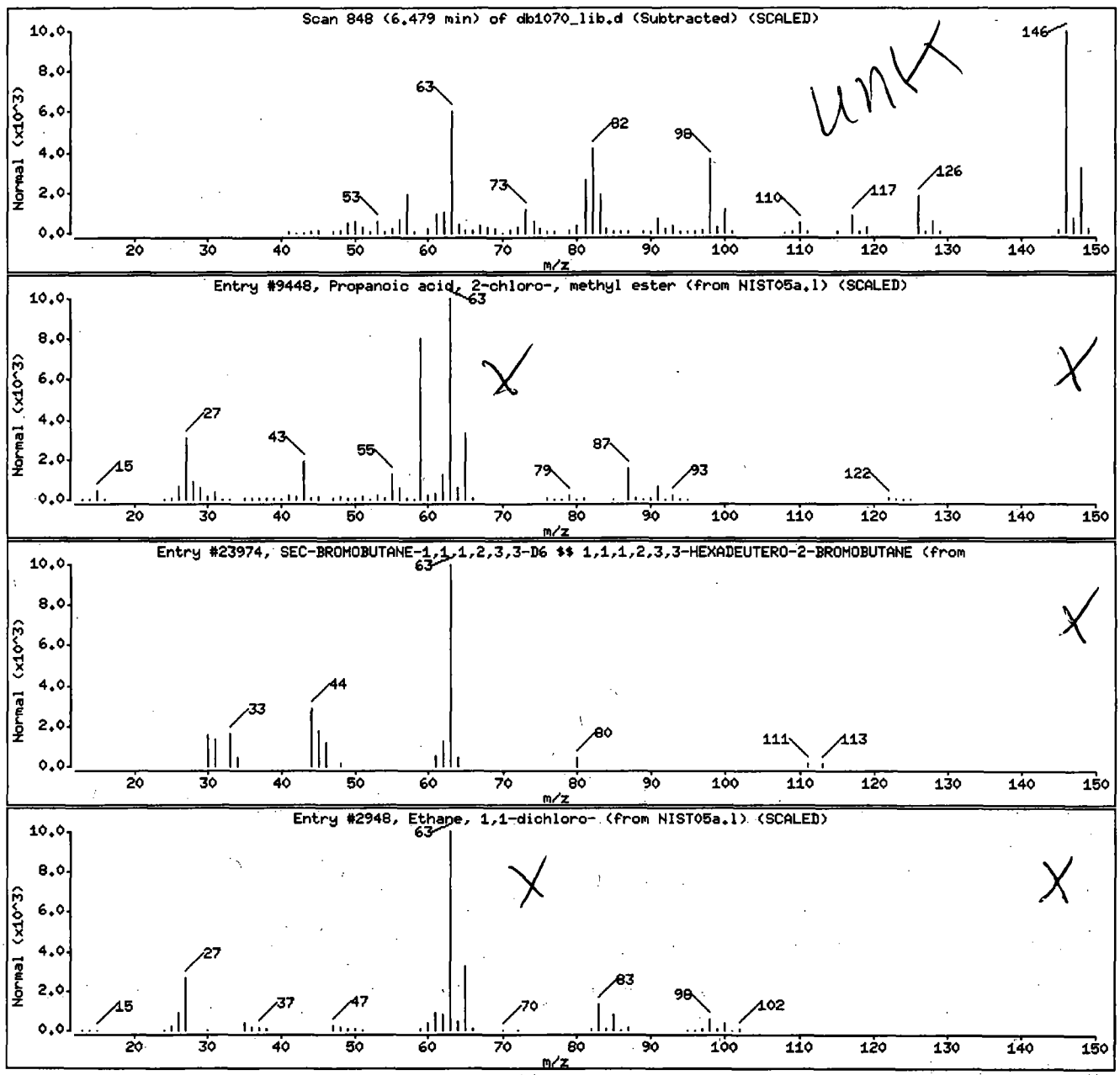
Volume Injected (uL): 1.0

Operator: jmg00346

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	23	C2H4Cl2	98



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Target 3.5 esignature user ID: ajs00193

Target compound, do not report. ajs00193 03/02/2014

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

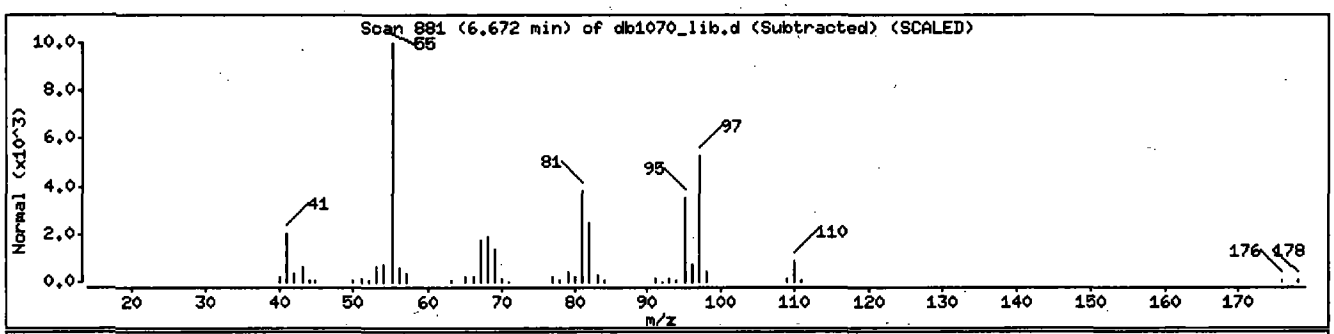
Volume Injected (uL): 1.0

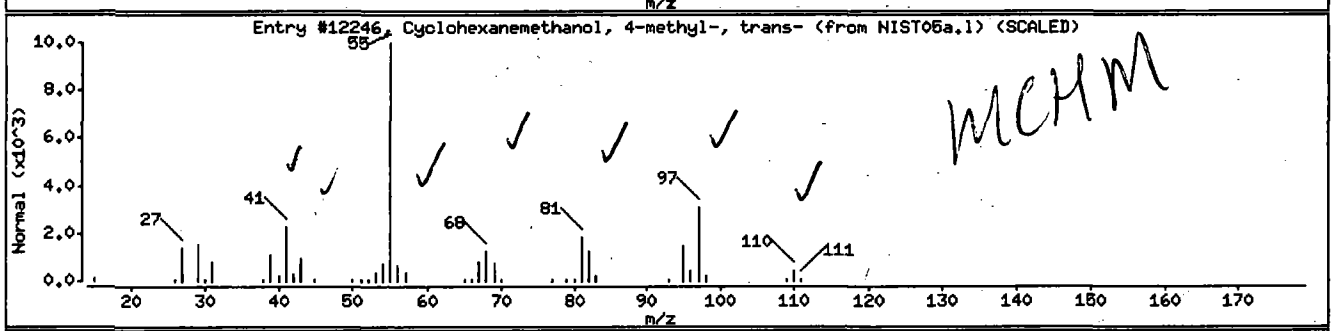
Operator: jmg00346

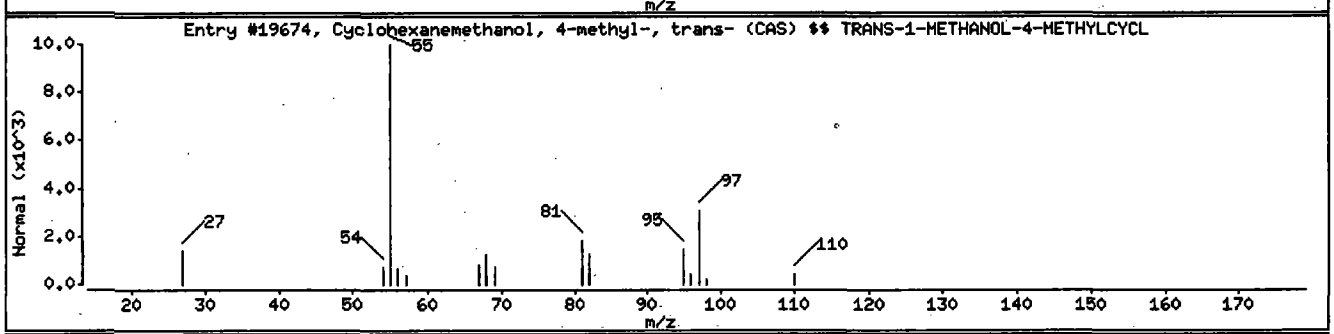
Column phase: J&W DB-5MS

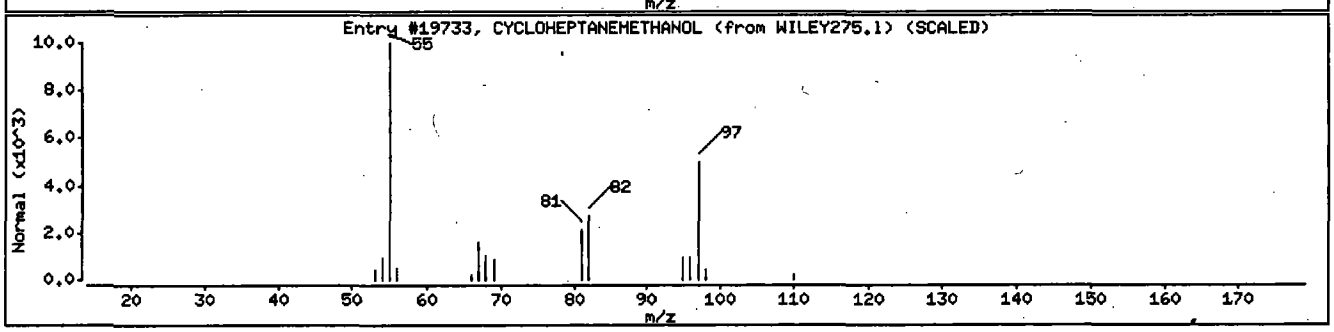
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclohexanemethanol, 4-methyl-, trans-	3937-49-3	NIST05a.l	12246	87	C8H16O	128
Cyclohexanemethanol, 4-methyl-, trans- (	3937-49-3	WILEY275.l	19674	83	C8H16O	128
CYCLOHEPTANEMETHANOL	0-00-0	WILEY275.l	19733	59	C8H16O	128









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Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

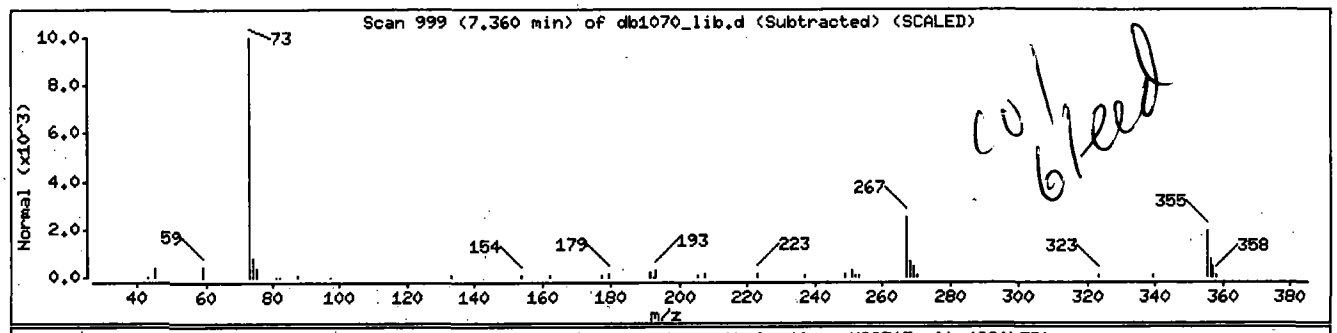
Volume Injected (uL): 1.0

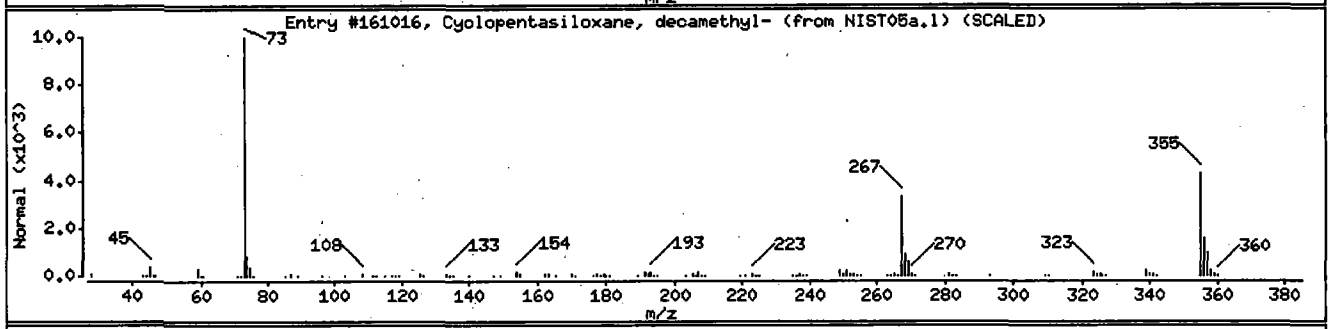
Operator: jmg00346

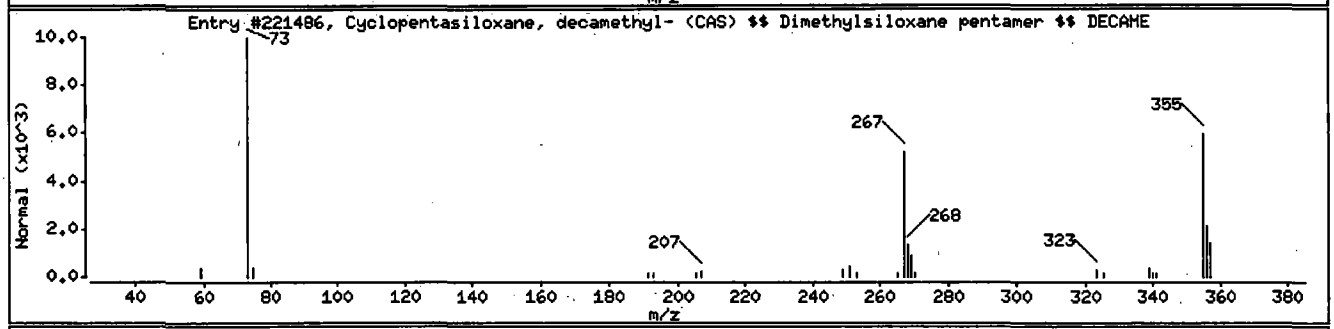
Column phase: J&W DB-5MS

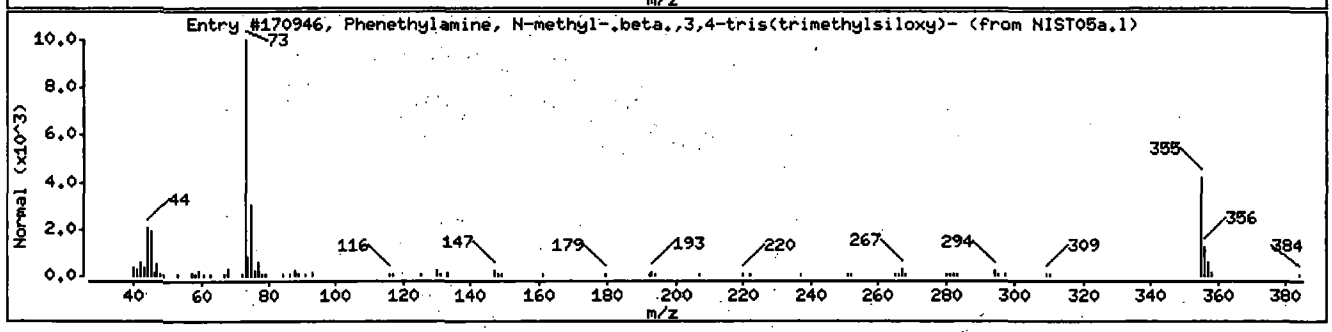
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	90	C10H30O5Si5	370
Phenethylamine, N-methyl-.beta.,3,4-tris	10538-85-9	NIST05a.l	170946	38	C18H37NO3Si3	399









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

Client ID: H8021

Instrument: HP19760.i

Sample Info: H8021;7368073;1;0;SAMPLE;;;

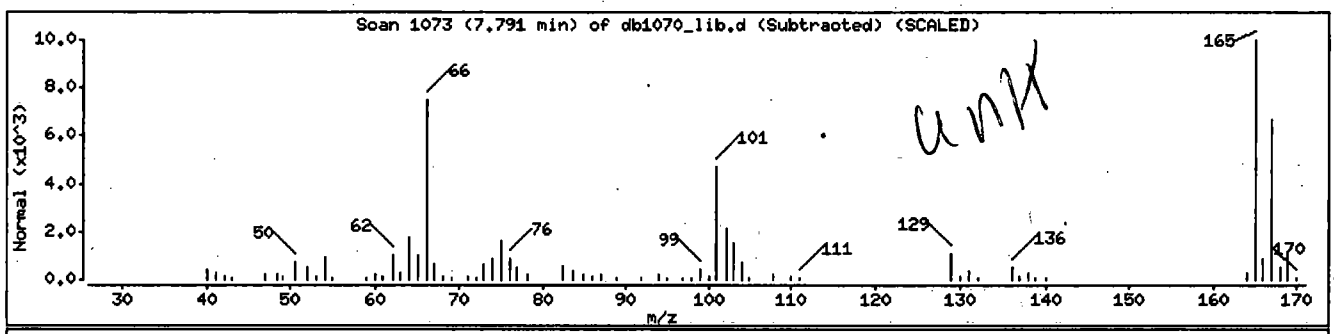
Volume Injected (uL): 1.0

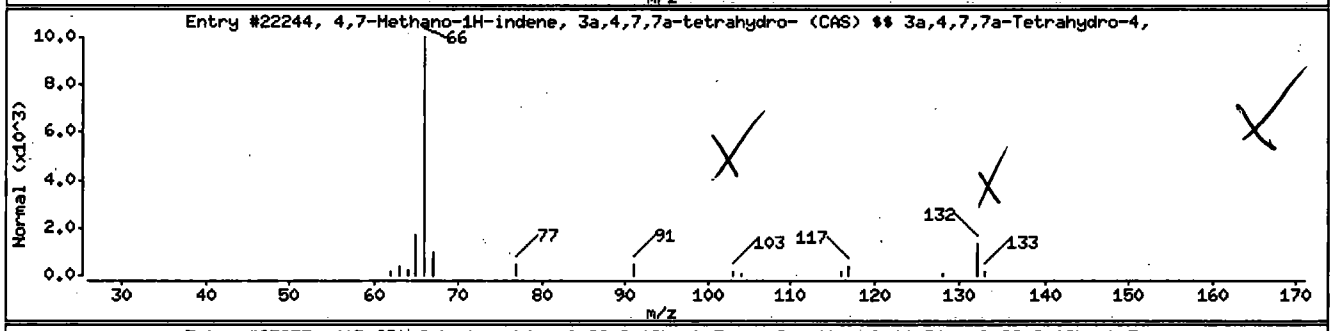
Operator: jmg00346

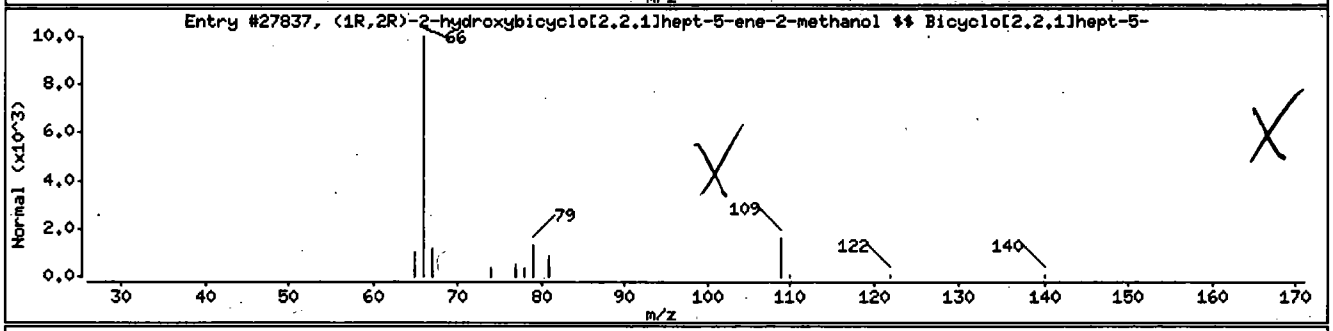
Column phase: J&W DB-5HS

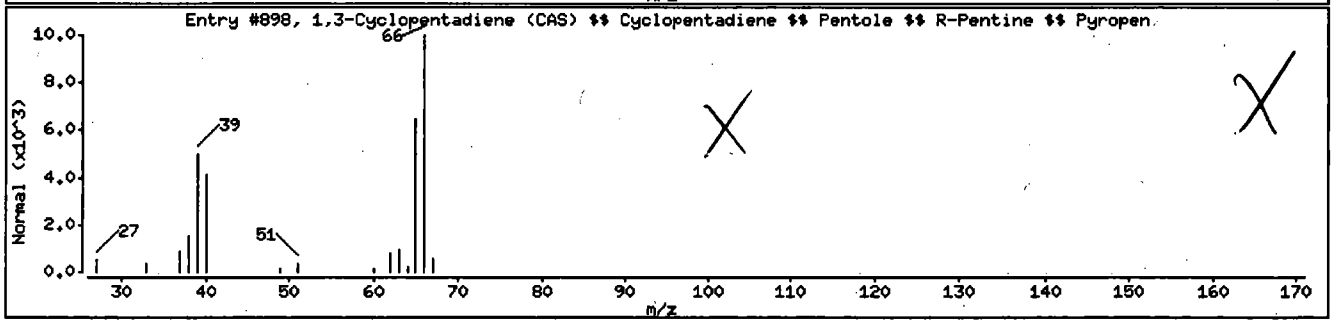
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22244	43	C10H12	132
(1R,2R)-2-hydroxybicyclo[2.2.1]hept-5-en	116697-44-0	WILEY275.l	27837	47	C8H12O2	140
1,3-Cyclopentadiene (CAS) $$ Cyclopentad	542-92-7	WILEY275.l	898	47	C5H6	66









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

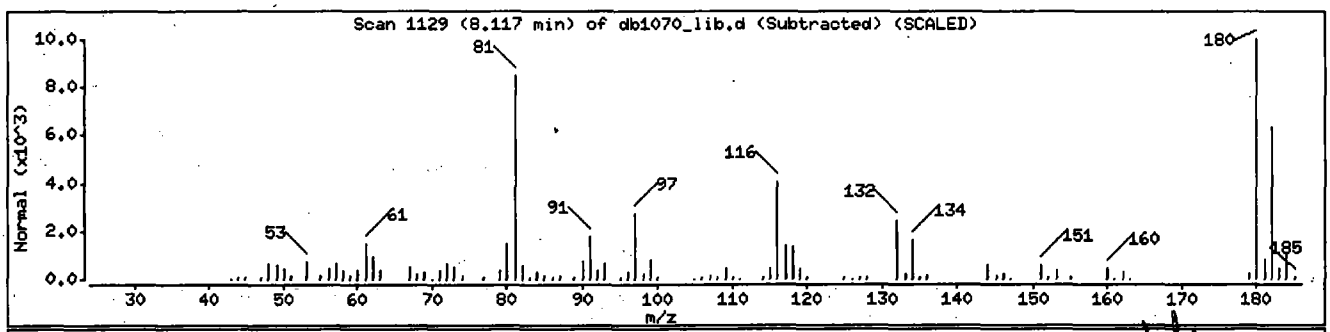
Client ID: H8021 Instrument: HP19760.i

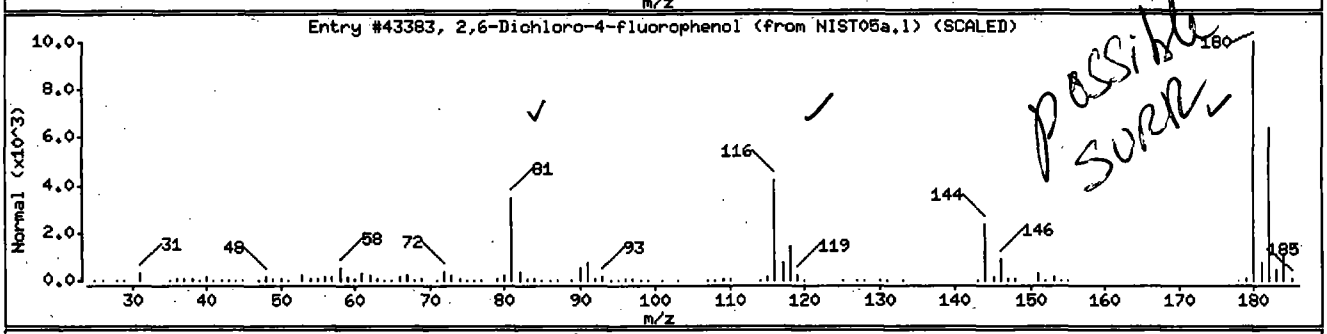
Sample Info: H8021;7368073;1;0;SAMPLE;;;

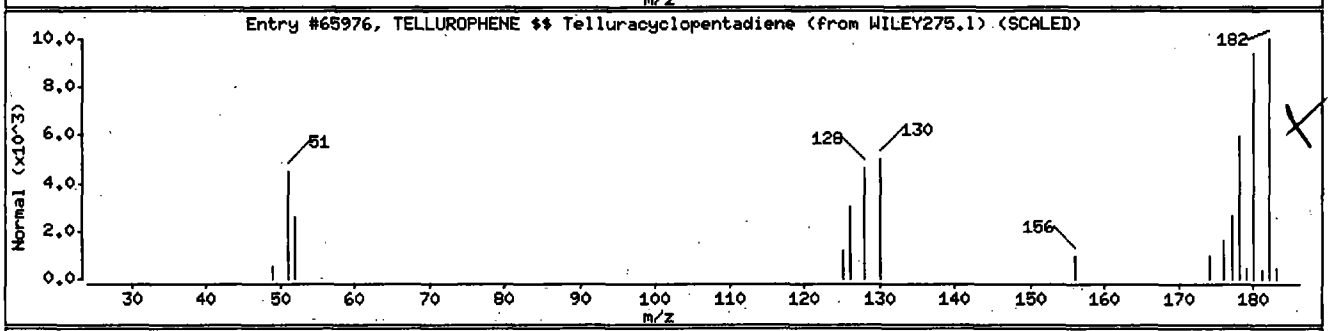
Volume Injected (uL): 1.0 Operator: jmg00346

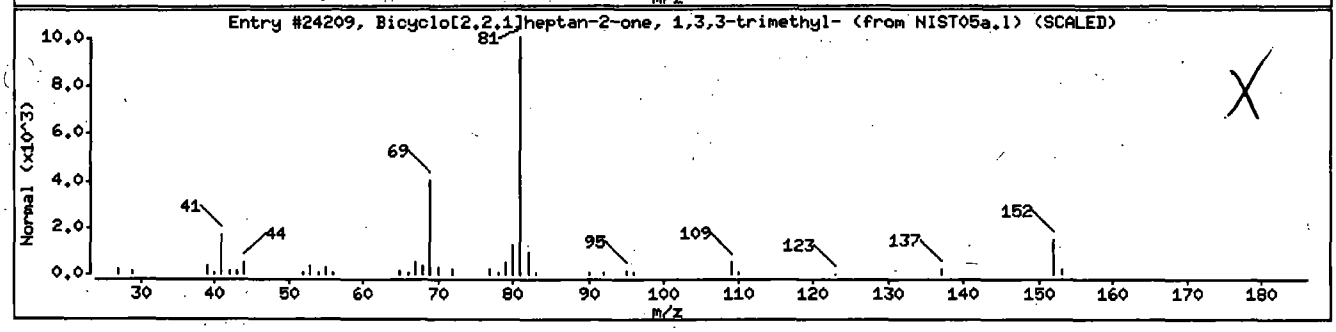
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	86	C6H3Cl2FO	180
TELLUROPHENE $$ Telluracyclopentadiene	288-08-4	WILEY275.l	65976	11	C4H4Te	182
Bicyclo[2.2.1]heptan-2-one, 1,3,3-trimet	1195-79-5	NIST05a.l	24209	10	C10H16O	152









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Date : 24-FEB-2014 15:30

Client ID: H8021

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Sample Info: H8021;7368073;1;0;SAMPLE;;;

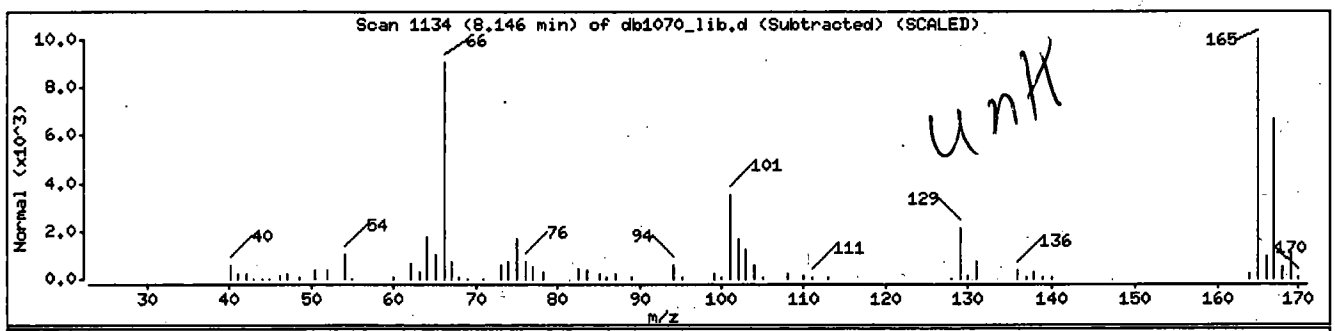
Volume Injected (uL): 1.0

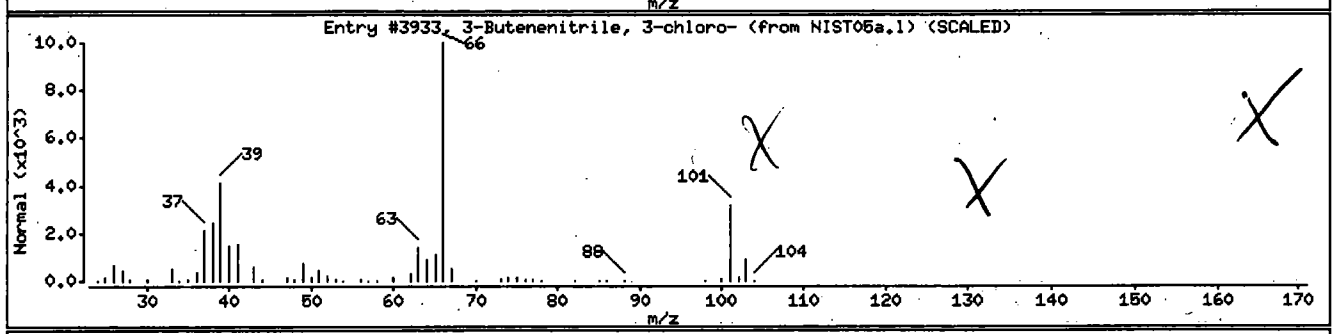
Operator: jmg00346

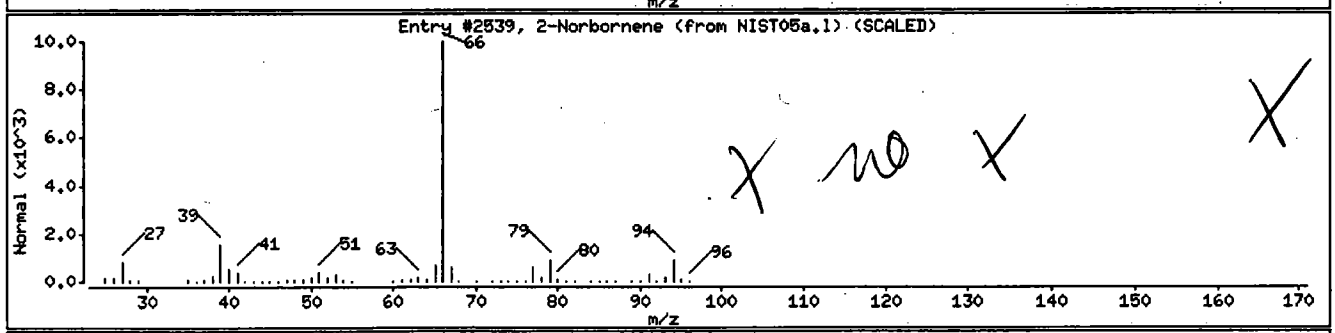
Column phase: J&W DB-5MS

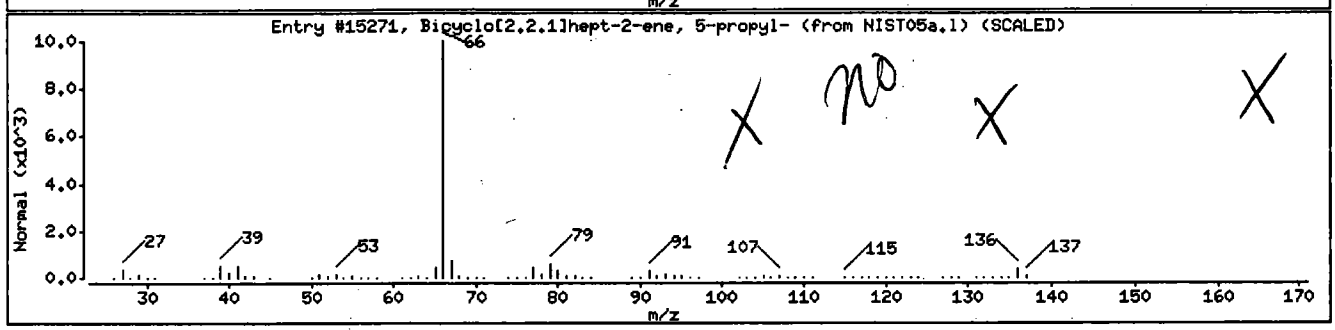
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
2-Norbornene	498-66-8	NIST05a.l	2539	49	C7H10	94
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136









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Data File: /chem/HP19760.i/14feb24.b/db1070_lib.d

Date : 24-FEB-2014 15:30

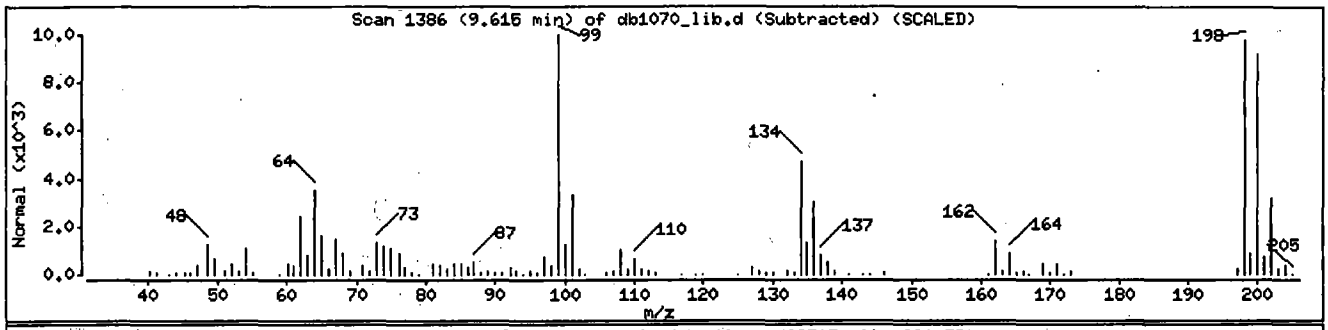
Client ID: H8021 Instrument: HP19760.i

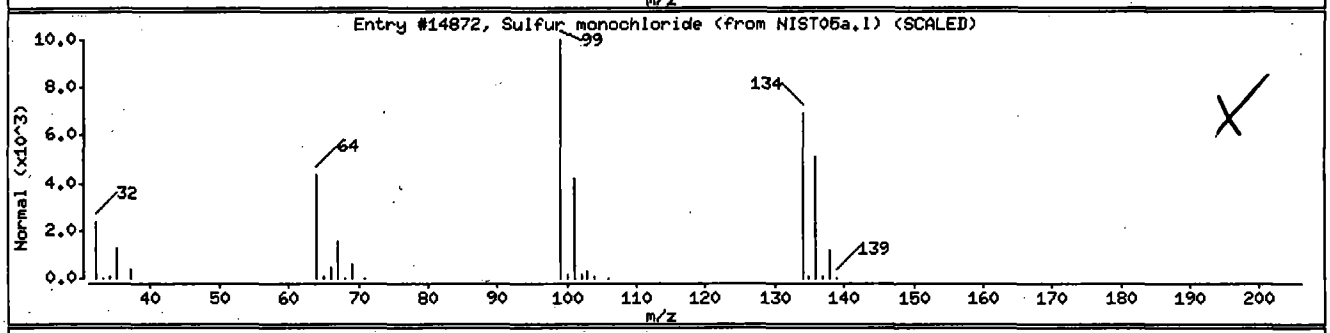
Sample Info: H8021;7368073;1;0;SAMPLE;;;

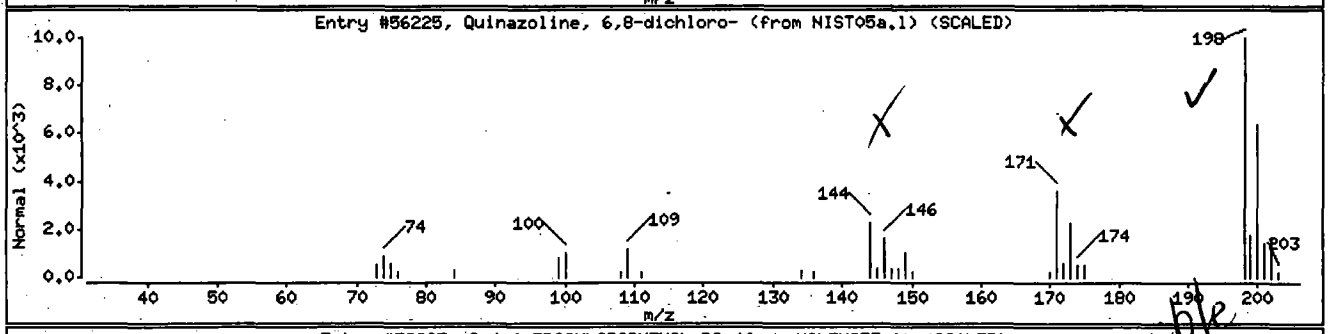
Volume Injected (uL): 1.0 Operator: jmg00346

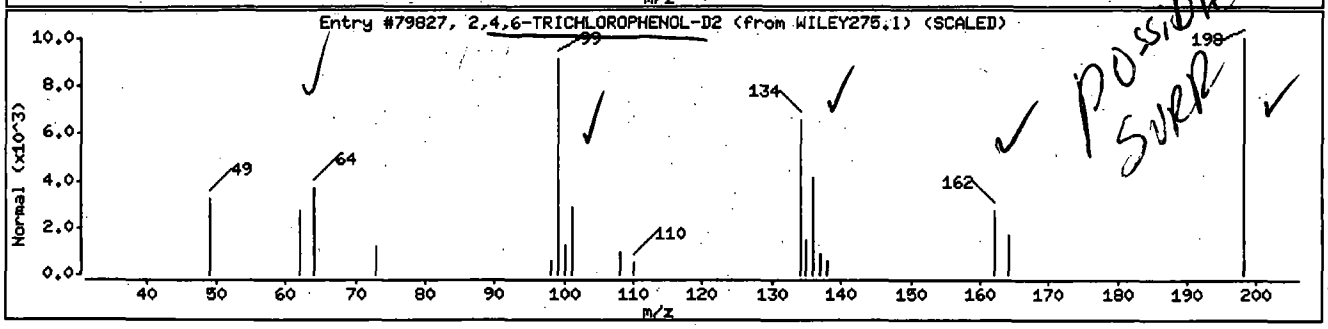
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	27	Cl2S2	134
Quinazoline, 6,8-dichloro-	17227-49-5	NIST05a.l	56225	43	C8H4Cl2N2	198
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	38	C6HD2Cl3O	198



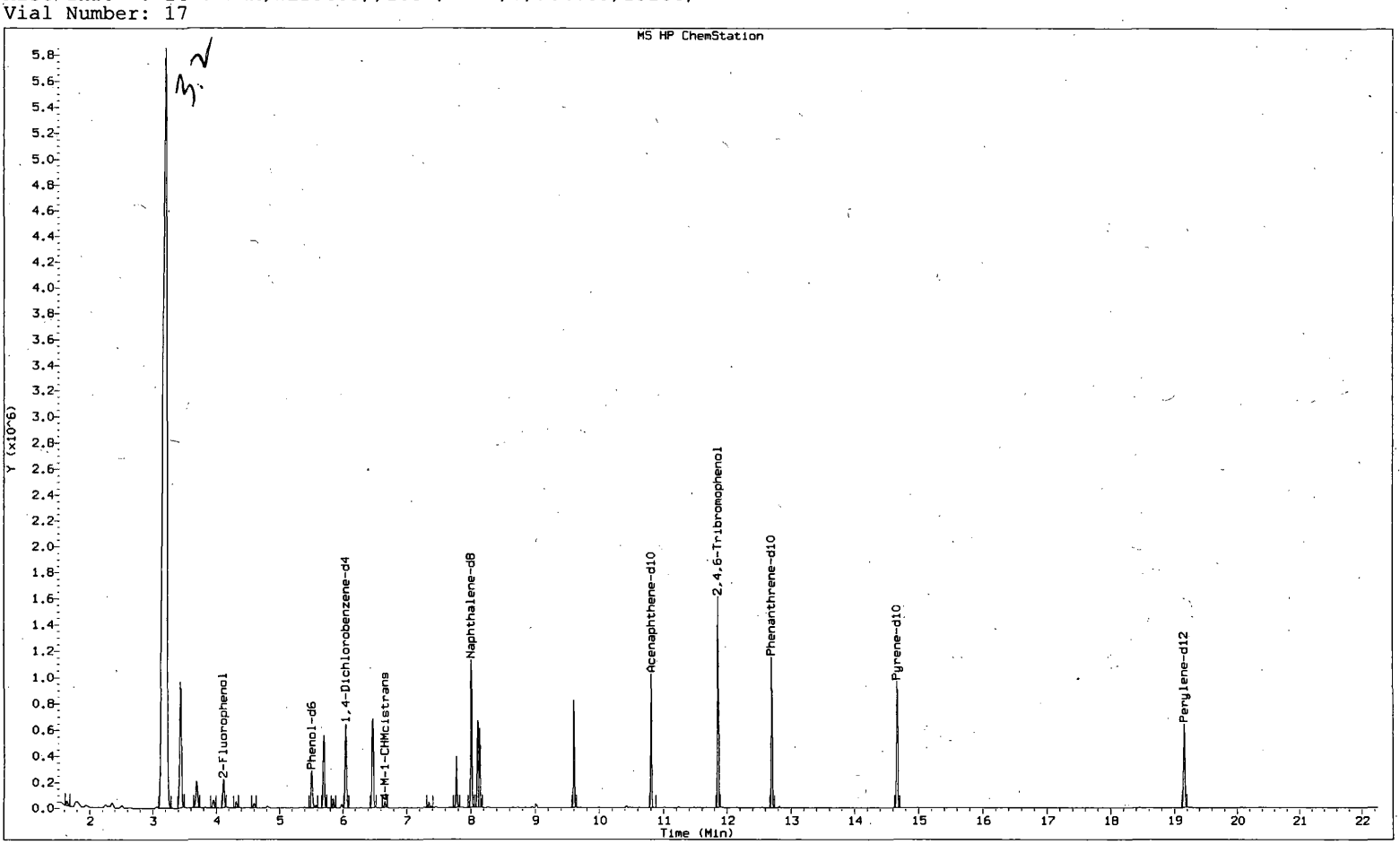






Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:15.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb25a.b/db1176_lib.d
Operator : ceb05247
Acquired : 26-FEB-2014 03:06
Instrument : HP19760.i
Sample Name: H9011;7369302;1;0;SAMPLE;;;
Misc Info : 14051WAM;WL13463;;1058;1000;0;db1168;13166;
Vial Number: 17



Lancaster Labs

Data file : /chem/HP19760.i/14feb25a.b/db1176_lib.d
Lab Smp Id: 7369302 Client Smp ID: H9011
Inj Date : 26-FEB-2014 03:06
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H9011;7369302;1;0;SAMPLE;;;
Misc Info : 14051WAM;WL13463;;1058;1000;0;db1168;13166;
Comment : Max. number of TICs to report is 50, 15 TICs were found initially.
Method : /chem/HP19760.i/14feb25a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 15:23 ajs00193 Quant Type: ISTD
Cal Date : 25-FEB-2014 21:43 Cal File: db1164_lib.d
Als bottle: 17
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1058.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.048	939430	10.000
* 48 Naphthalene-d8	8.001	1420058	10.000
* 83 Acenaphthene-d10	10.810	1234895	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.642	71695	0.76317524	0.72133	83	NIST05a.l	31324	21

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Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.221	25030989	266.448527	251.84170	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.437	1876592	19.9758442	18.88076	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.688	402287	4.28224072	4.04748	37	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$					CAS #: 74421-00-4		
3.956	102132	1.08716678	1.02756	38	WILEY275.l	21984	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.317	76485	0.81415859	0.76952	43	NIST05a.l	33655	21(L)
Butane, 1,3-dichloro-3-methyl-					CAS #: 624-96-4		
4.597	56332	0.59963609	0.56676	36	NIST05a.l	17535	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.698	800016	8.51597166	8.04912	89	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.850	98587	1.04942837	0.99189	94	NIST05a.l	18486	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.468	1101721	11.7275454	11.08463	35	NIST05a.l	9448	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.342	63074	0.44416232	0.41981	90	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.773	503018	3.54223112	3.34804	46	WILEY275.l	22248	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.100	810479	5.70736433	5.39448	86	NIST05a.l	43383	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.135	761441	5.36204212	5.06809	40	NIST05a.l	3933	48(L)
Sulfur monochloride					CAS #: 10025-67-9		
9.598	959521	7.77006370	7.34410	25	NIST05a.l	14872	83(L)

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:28
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

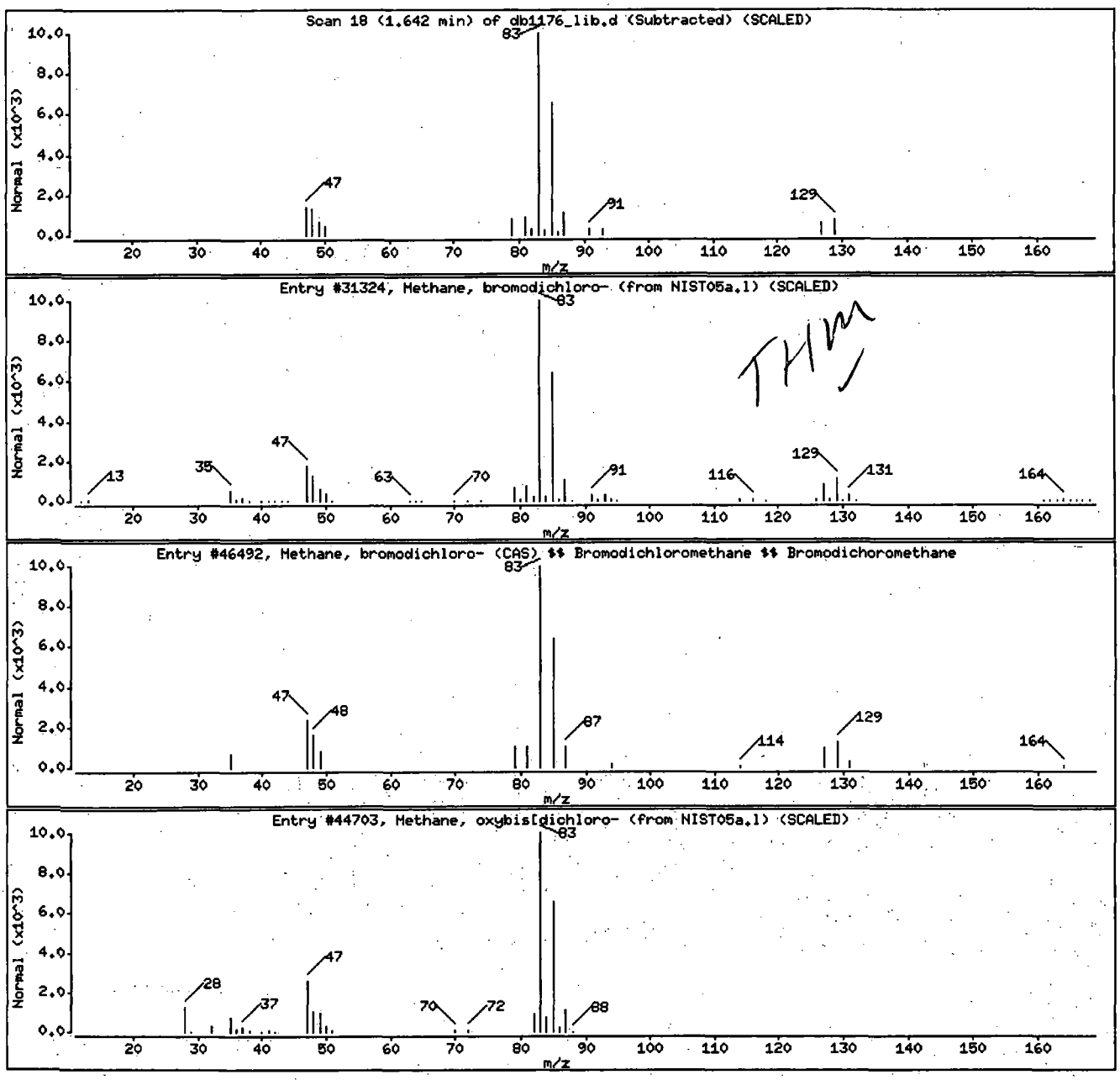
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31324	83	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46492	83	CHBrCl2	162
Methane, oxybis[dichloro-	20524-86-1	NIST05a.l	44703	72	C2H2Cl4O	182



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Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

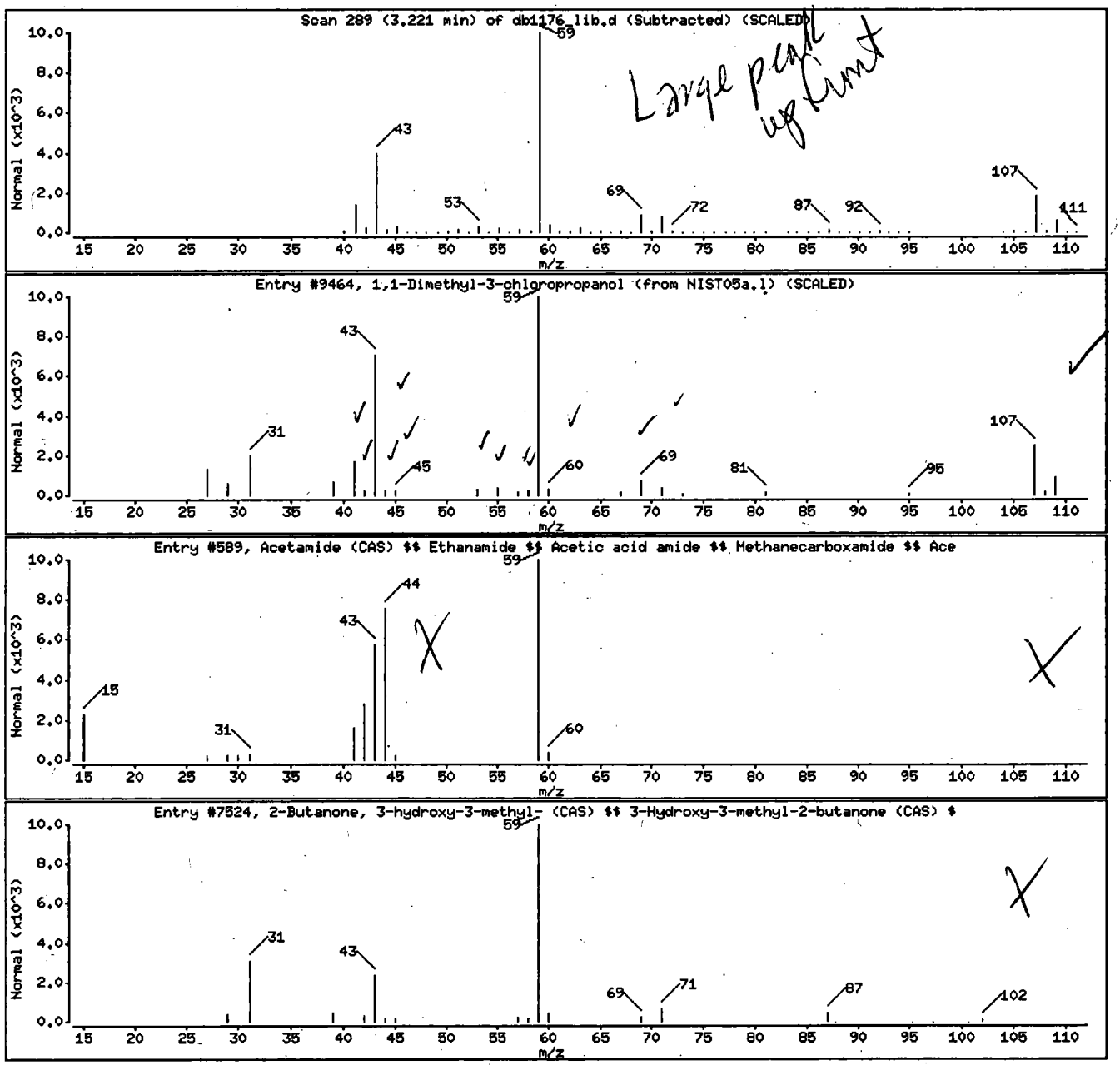
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102



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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

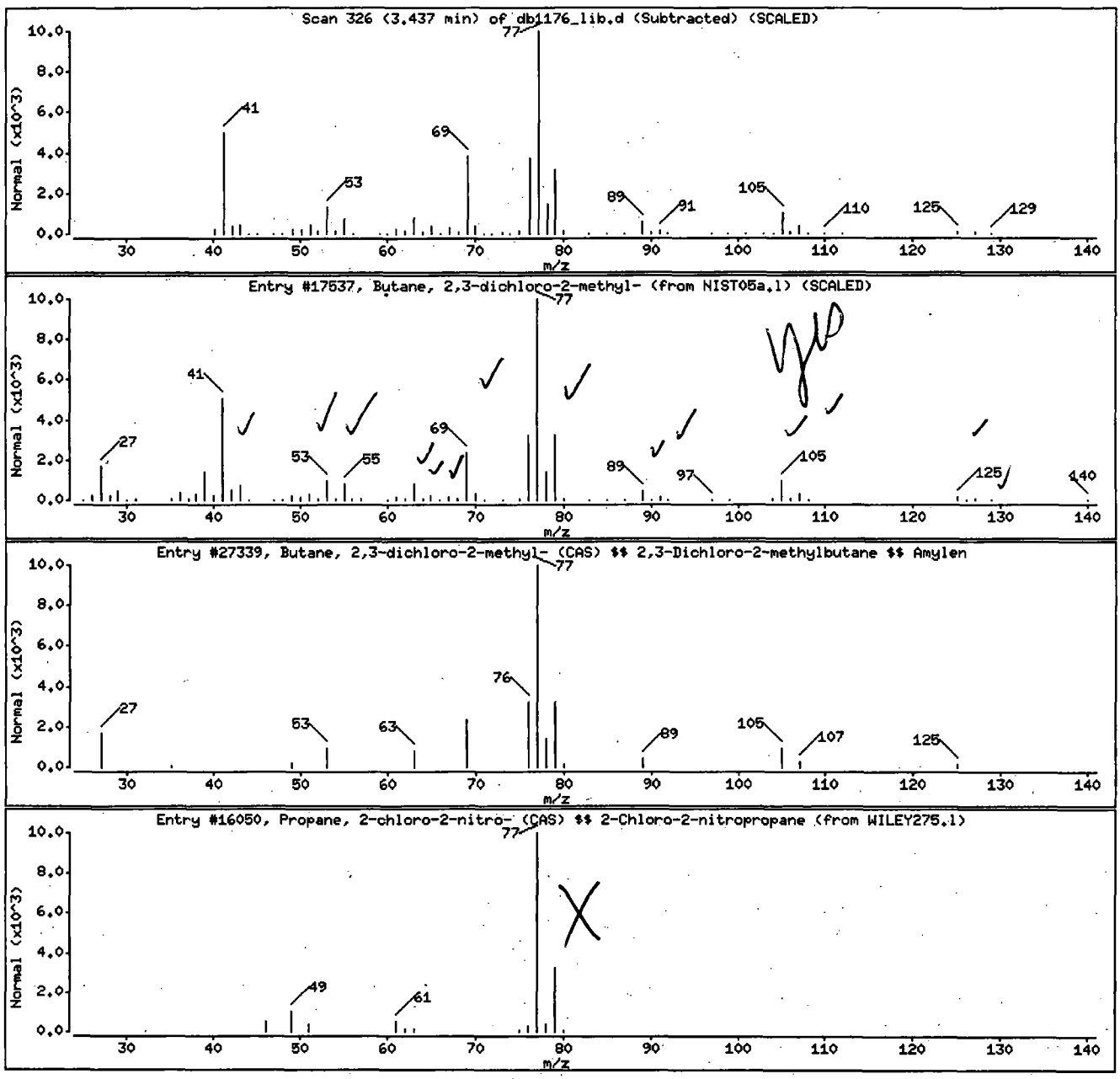
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	28	C3H6ClNO2	123



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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

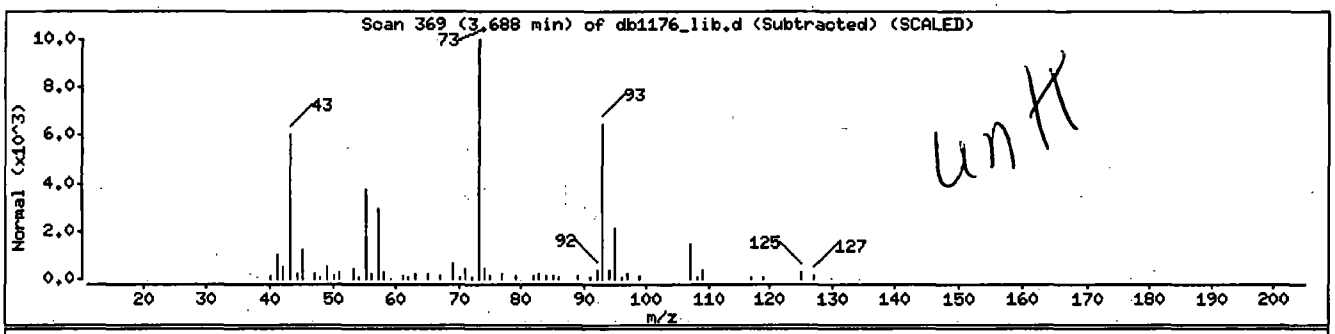
Volume Injected (uL): 1.0

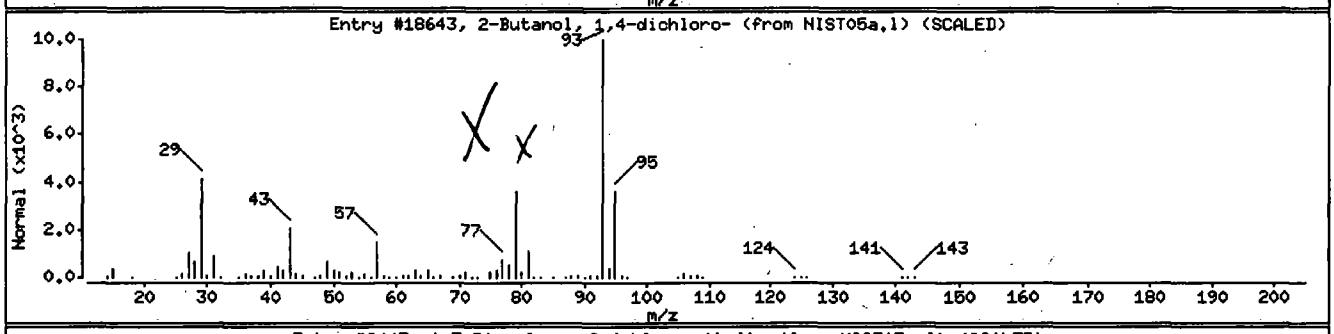
Operator: ceb05247

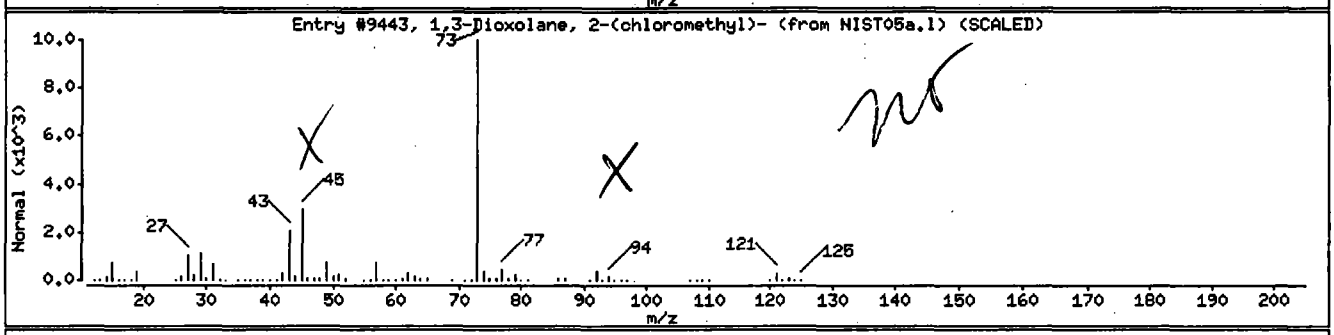
Column phase: J&W DB-5MS

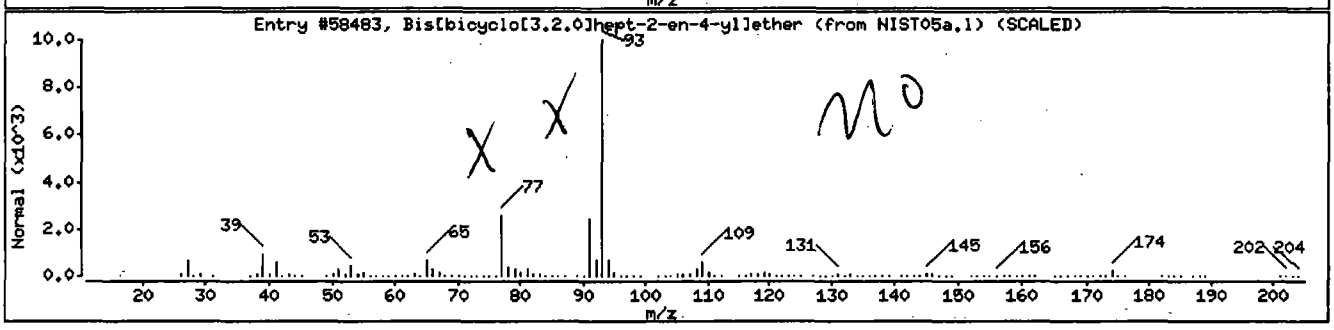
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	37	C4H8Cl2O	142
1,3-Dioxolane, 2-(chloromethyl)-	2568-30-1	NIST05a.l	9443	12	C4H7ClO2	122
Bis[bicyclo[3.2.0]hept-2-en-4-yl]ether	1000153-89-5	NIST05a.l	58483	12	C14H18O	202









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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

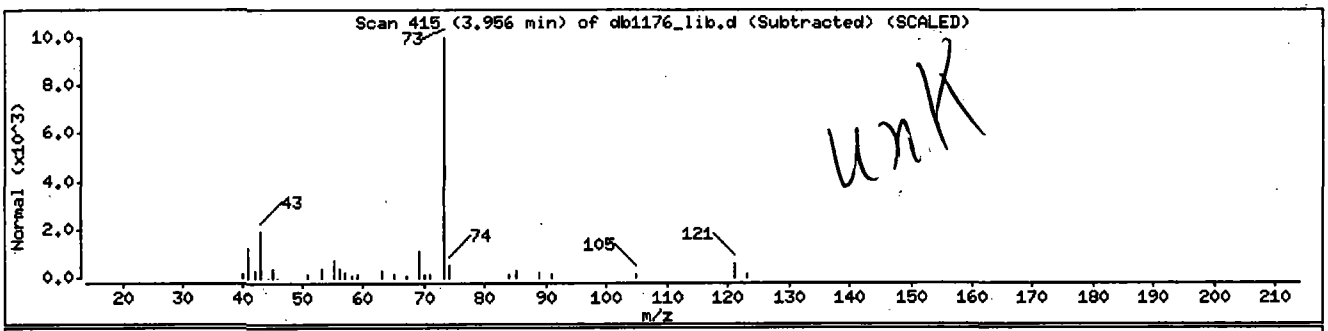
Volume Injected (uL): 1.0

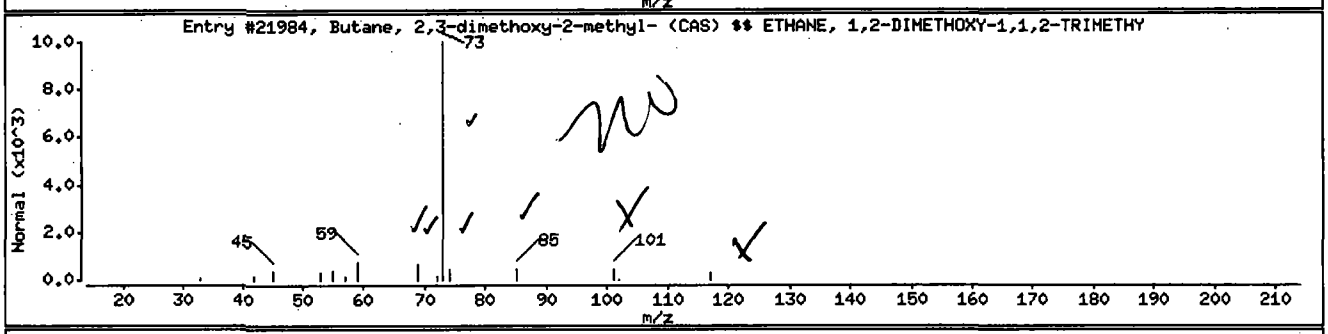
Operator: ceb05247

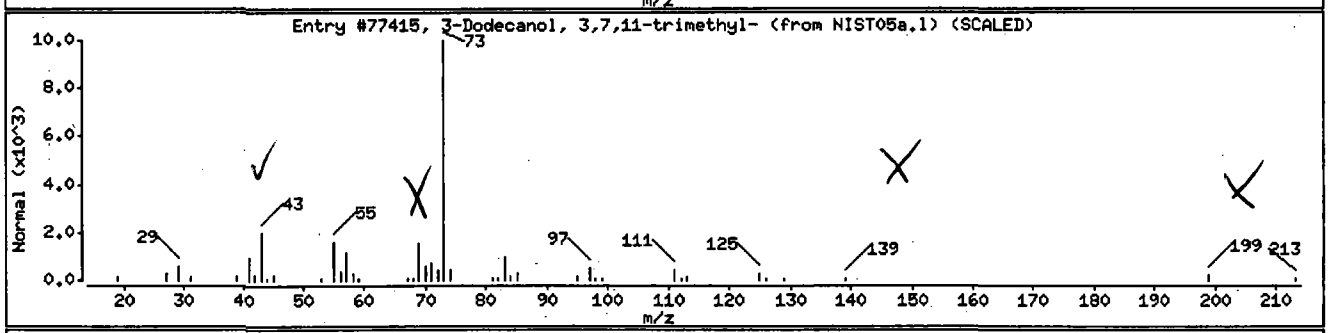
Column phase: J&W DB-5MS

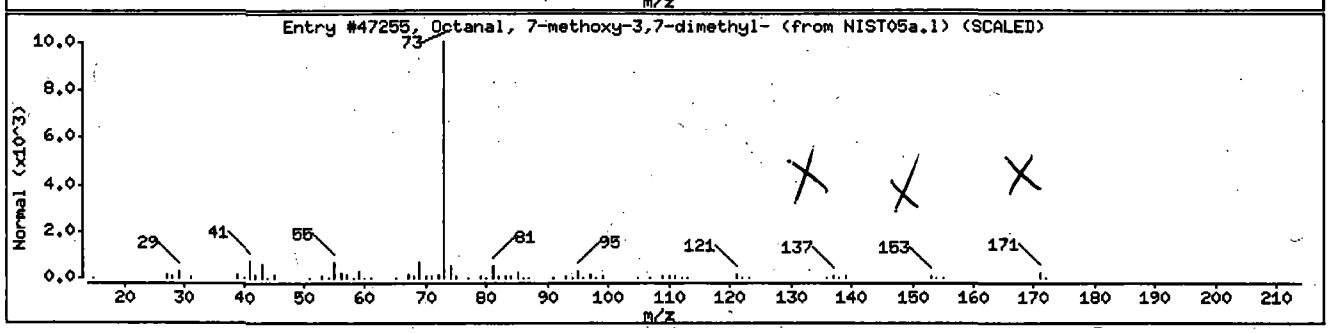
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	38	C15H32O	228
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	38	C11H22O2	186









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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

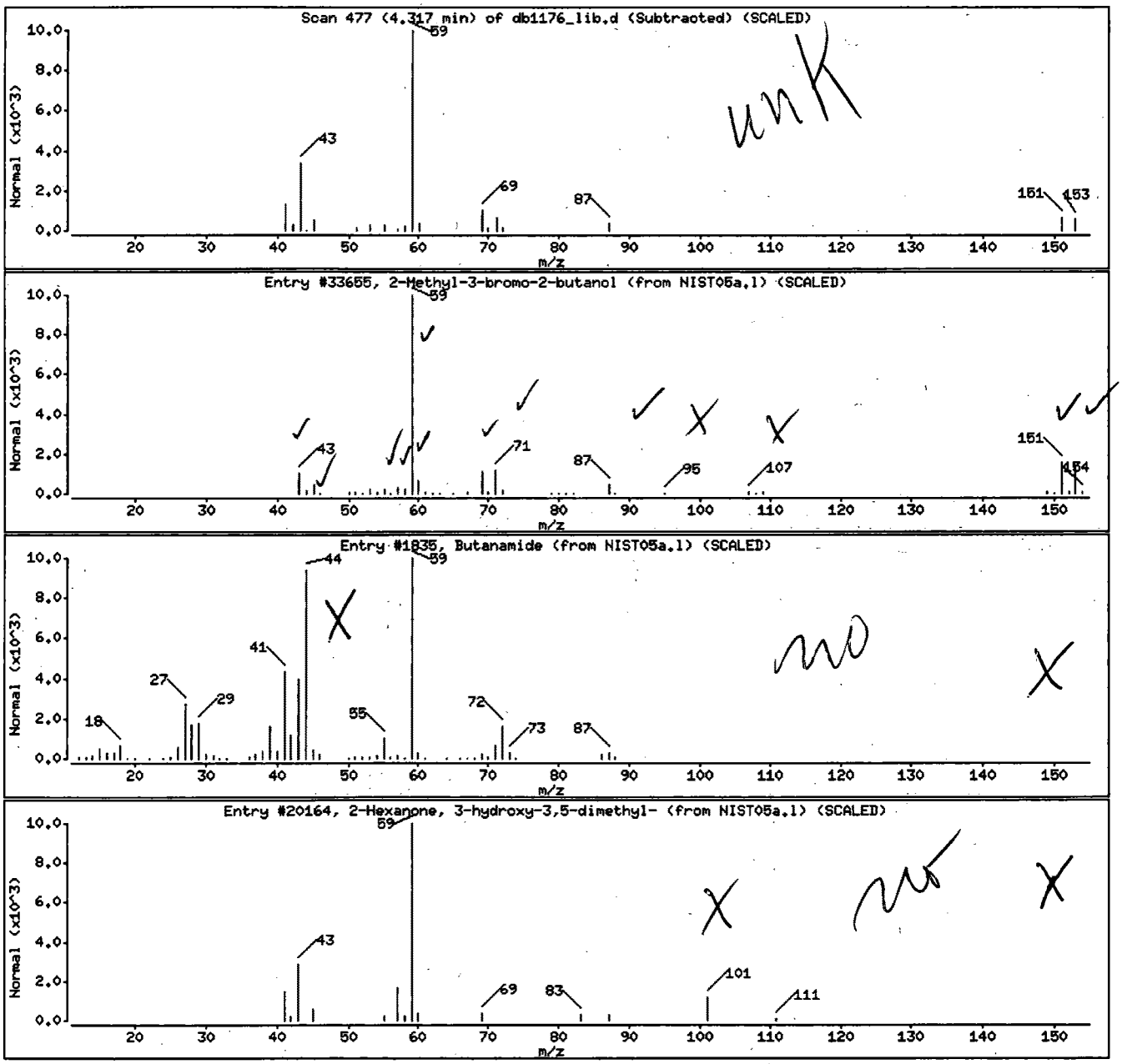
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	43	C6H11BrO	166
Butanamide	541-35-5	NIST05a.l	1835	64	C4H9NO	87
2-Hexanone, 3-hydroxy-3,5-dimethyl-	6321-14-8	NIST05a.l	20164	64	C8H16O2	144



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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

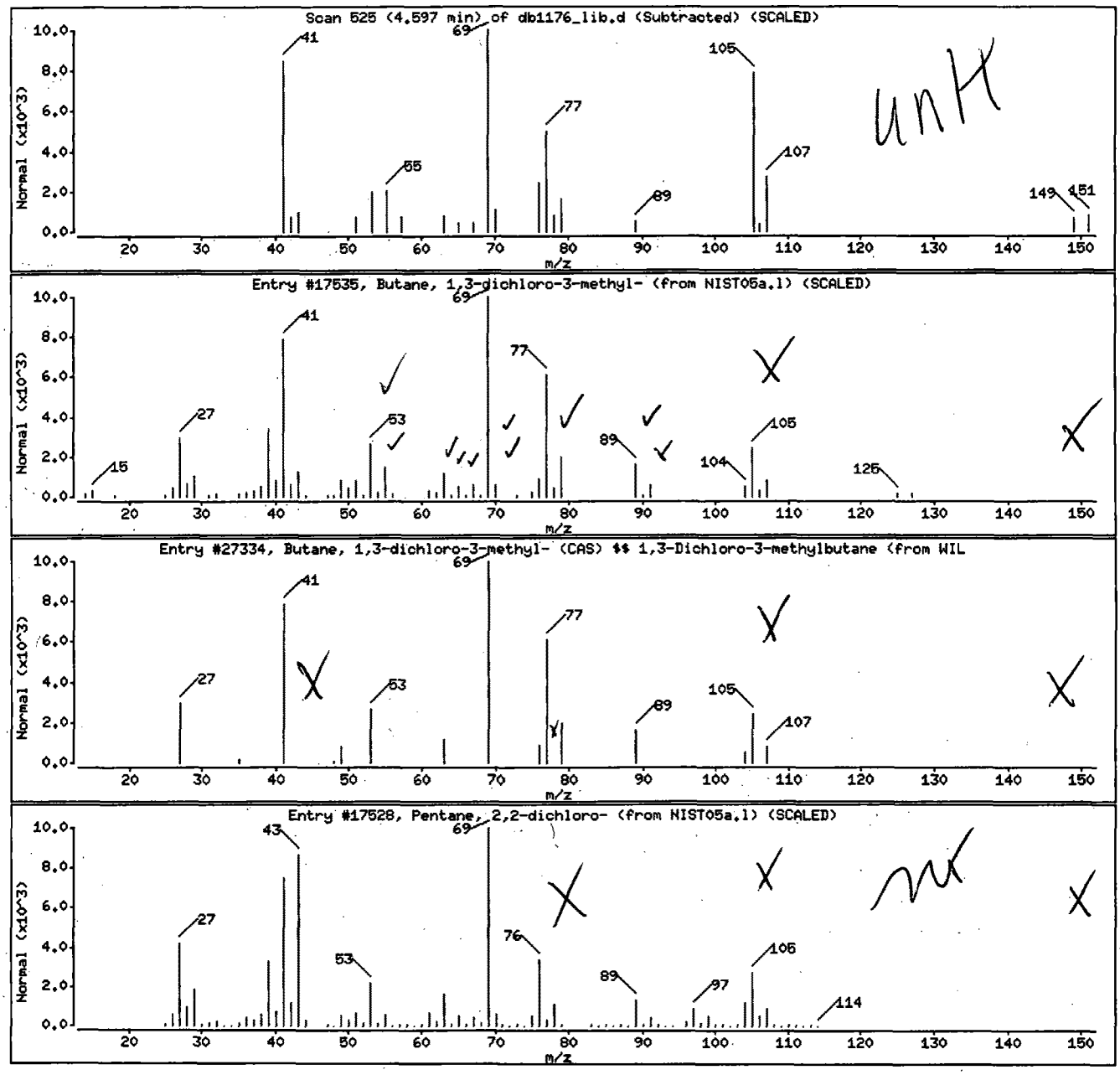
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 1,3-dichloro-3-methyl-	624-96-4	NIST05a.l	17535	36	C5H10Cl2	140
Butane, 1,3-dichloro-3-methyl- (CAS) $$	624-96-4	WILEY275.l	27334	36	C5H10Cl2	140
Pentane, 2,2-dichloro-	34887-14-4	NIST05a.l	17528	33	C5H10Cl2	140



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Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

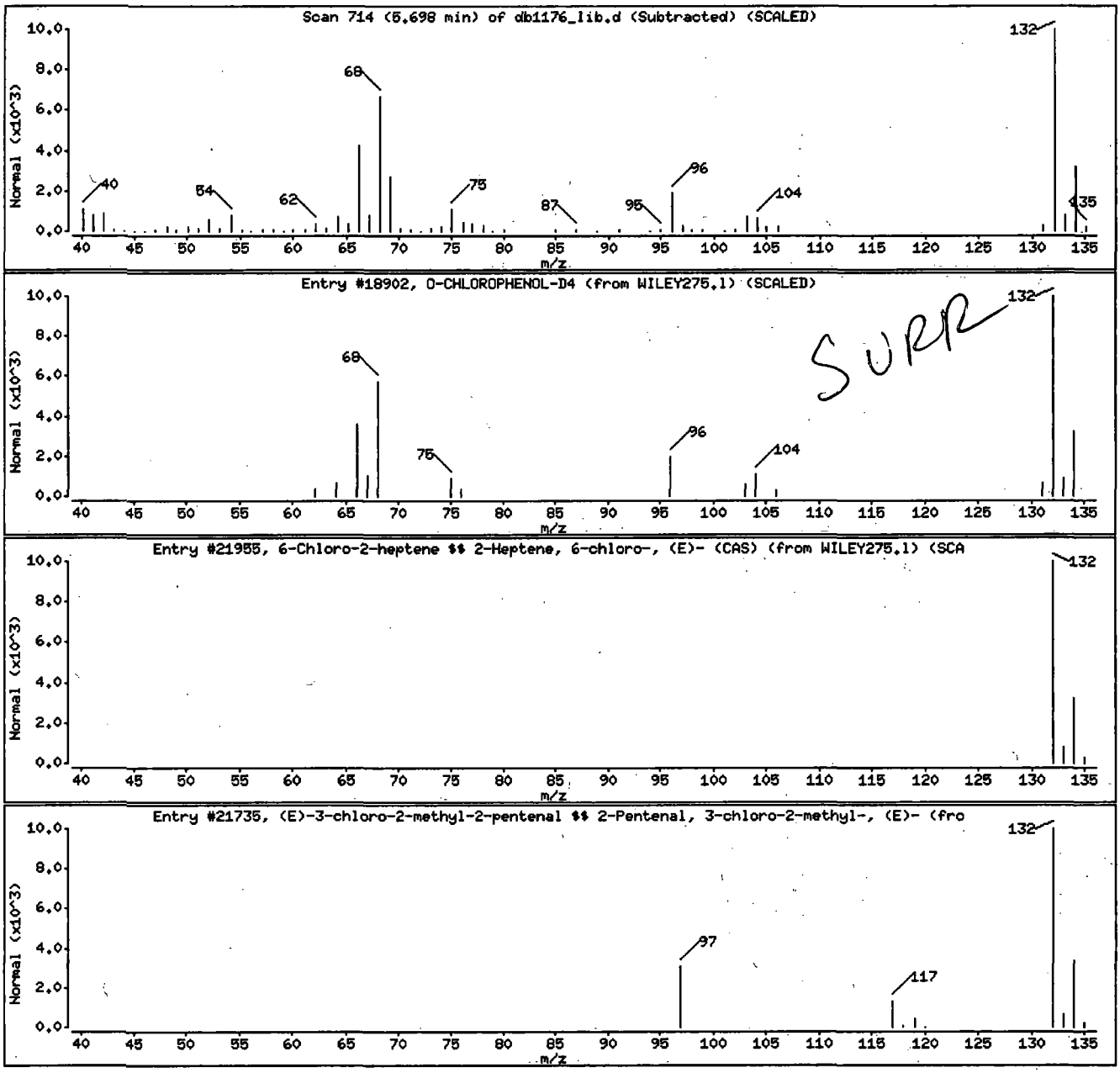
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.l	18902	89	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.l	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.l	21735	78	C6H9ClO	132



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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

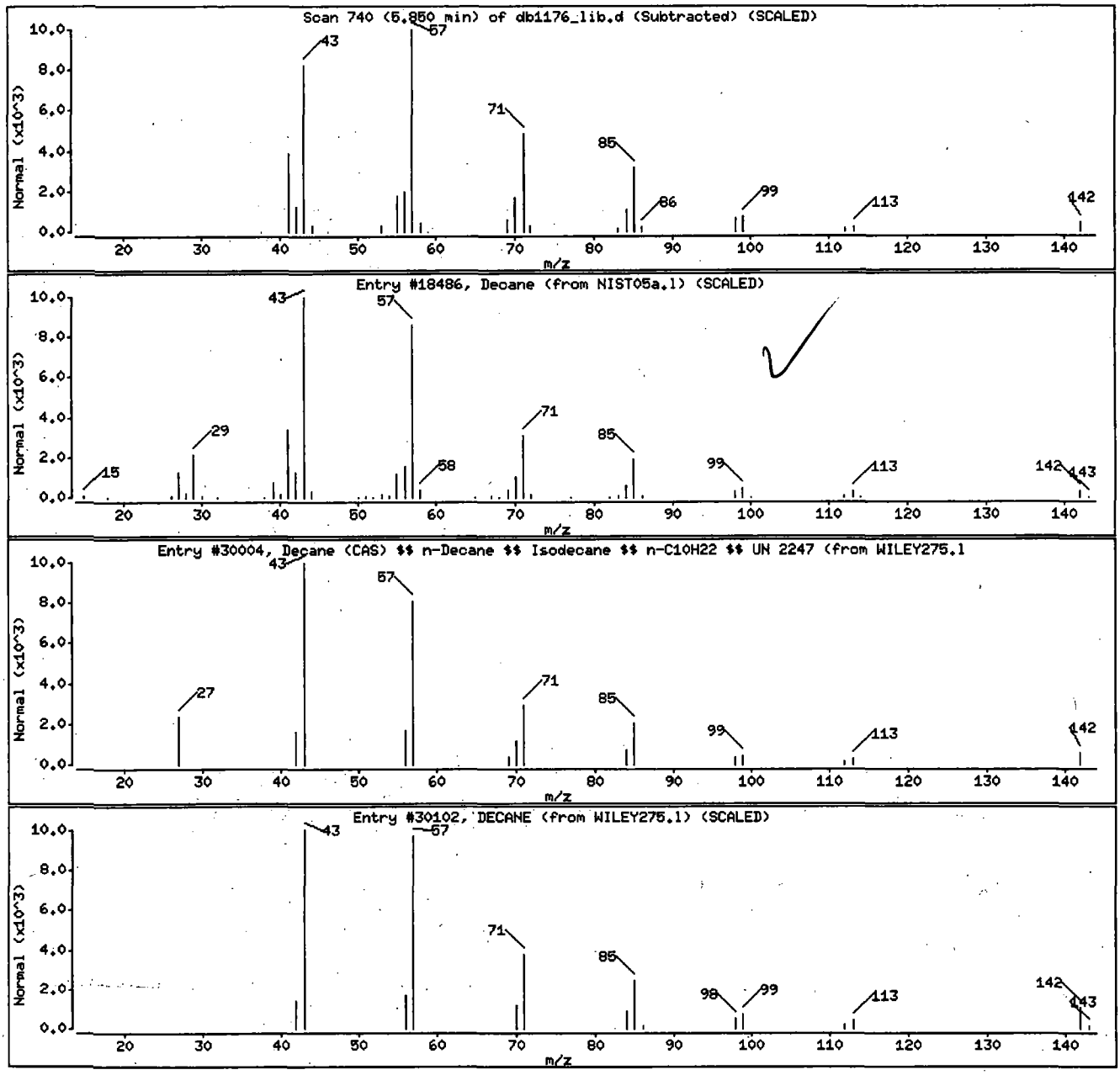
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18486	94	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30004	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142



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Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

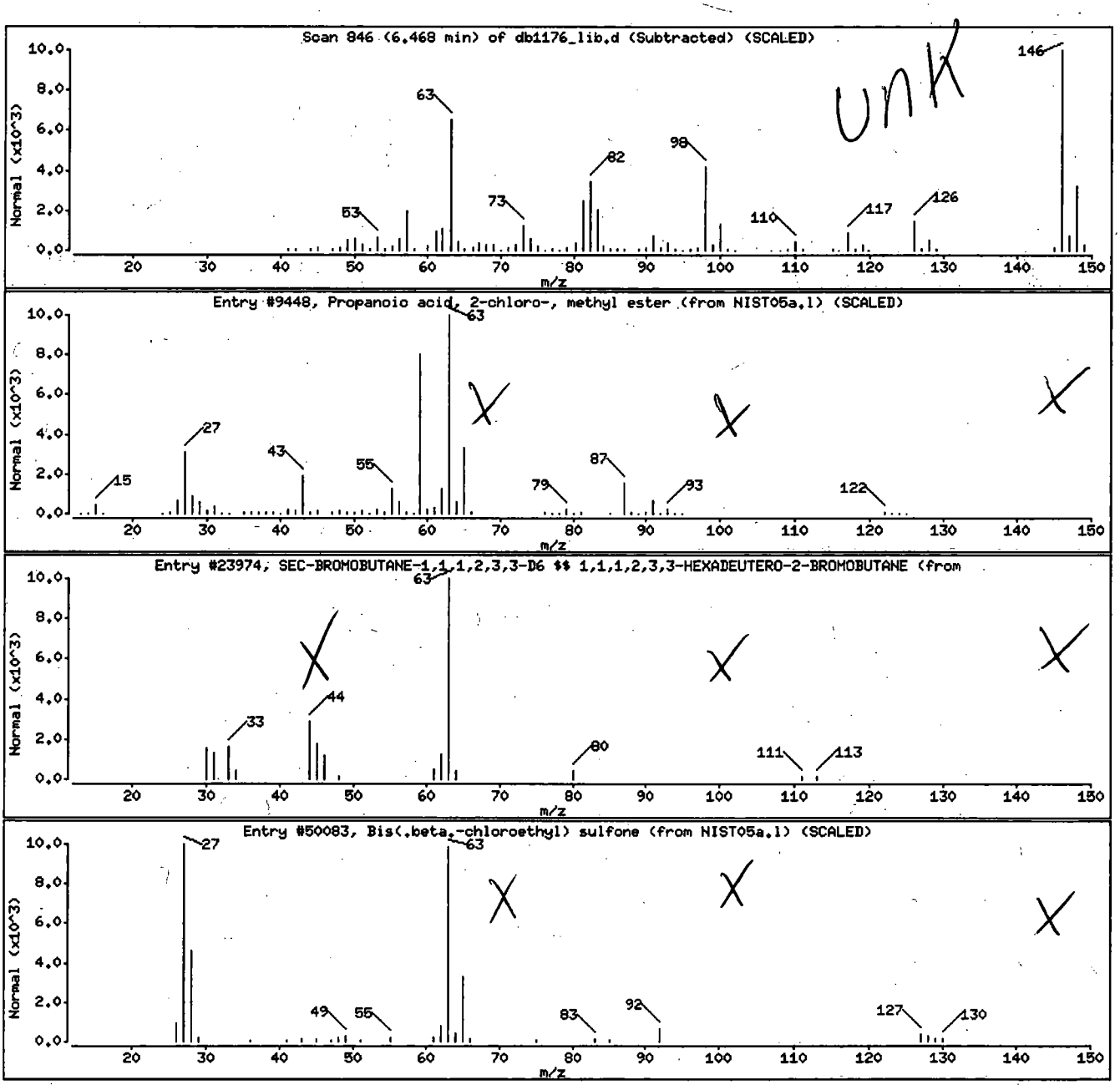
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 ** 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	23	C4H8Cl2O2S	190



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Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

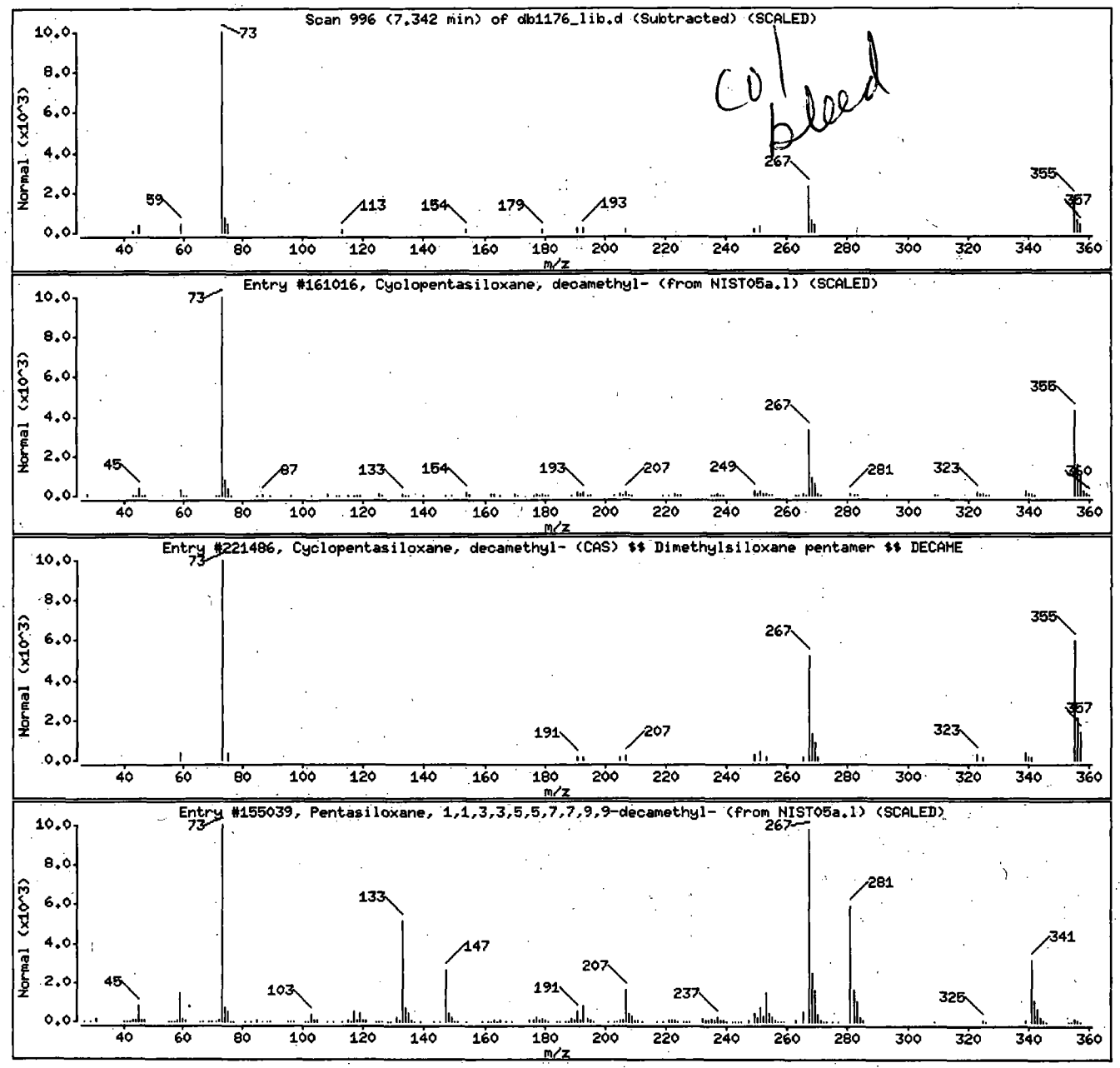
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	90	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	83	C10H30O5Si5	370
Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decam	995-83-5	NIST05a.l	155039	38	C10H32O4Si5	356



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

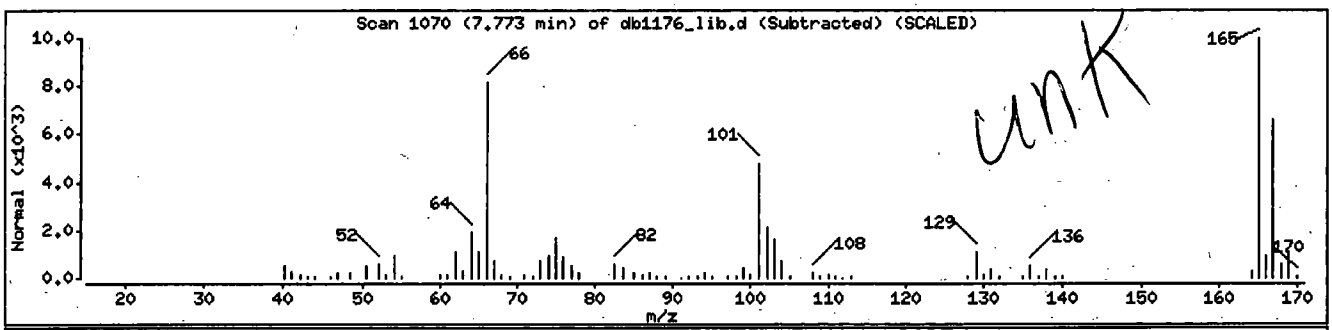
Volume Injected (uL): 1.0

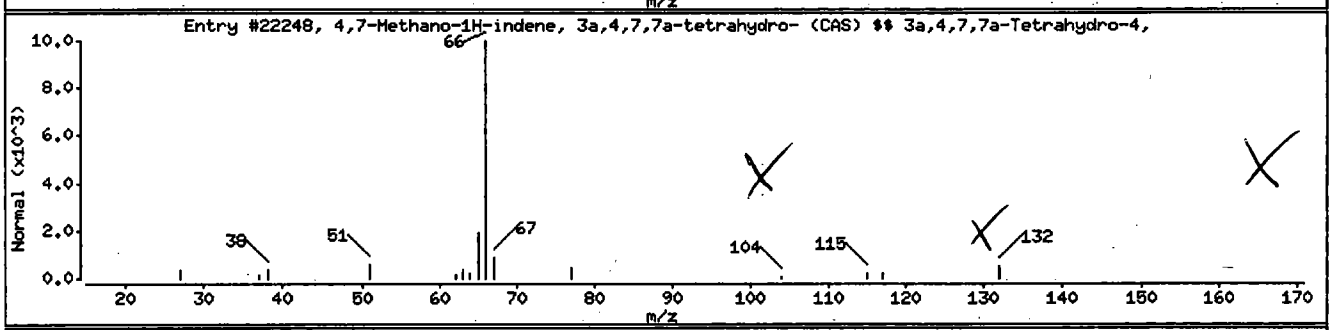
Operator: ceb05247

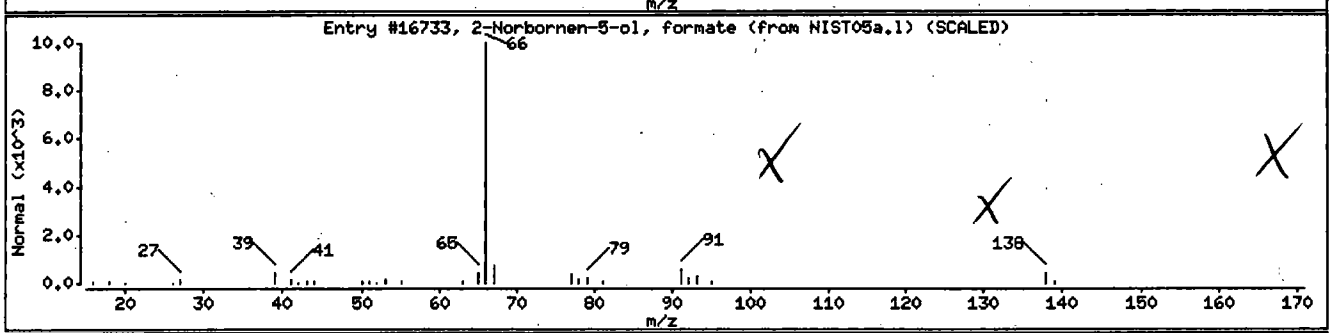
Column phase: J&W DB-5HS

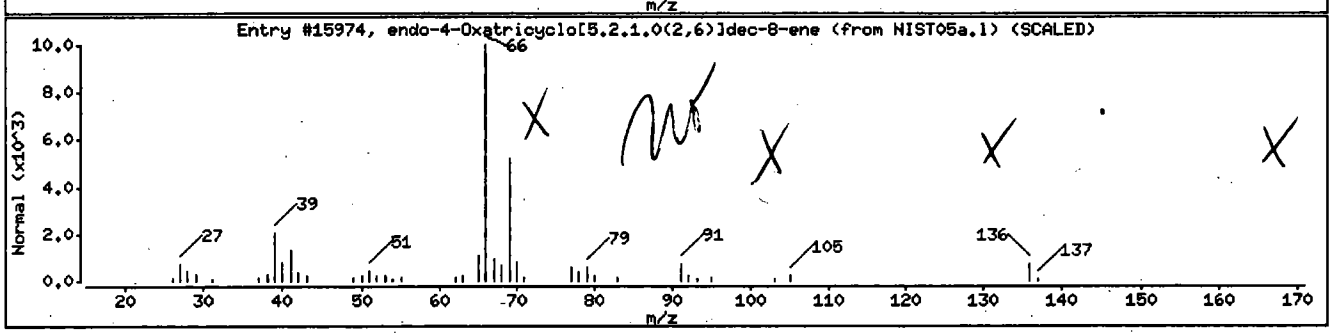
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	WILEY275.l	22248	46	C10H12	132
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H1002	138
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	46	C9H120	136









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:28:
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

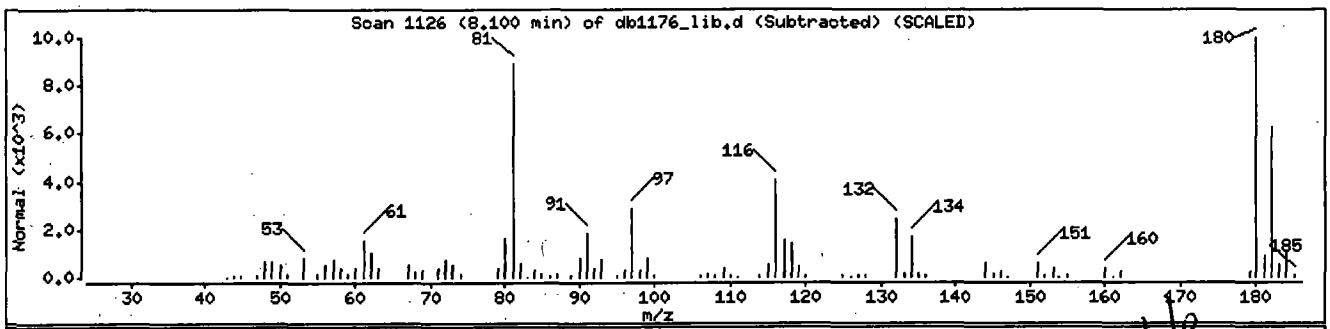
Volume Injected (uL): 1.0

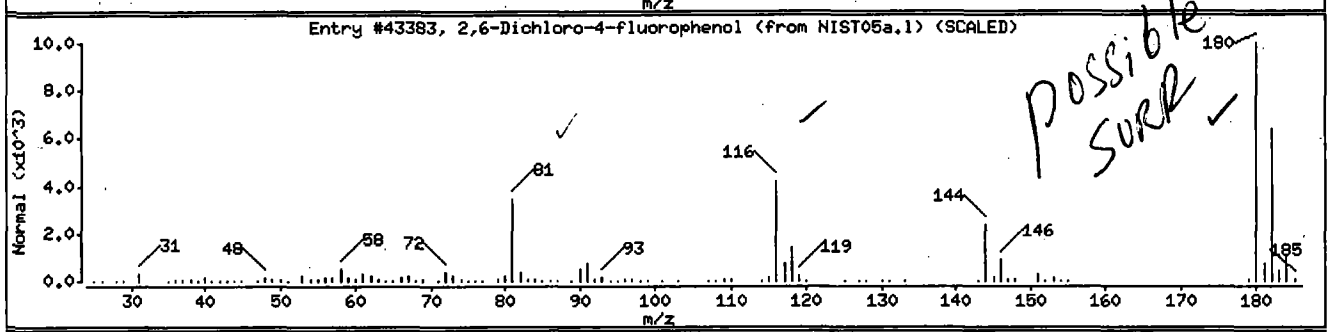
Operator: ceb05247

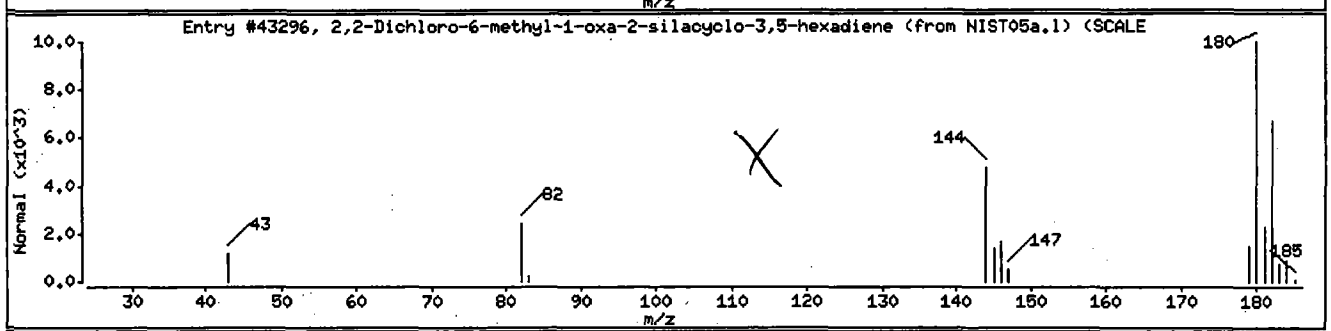
Column phase: J&W DB-5MS

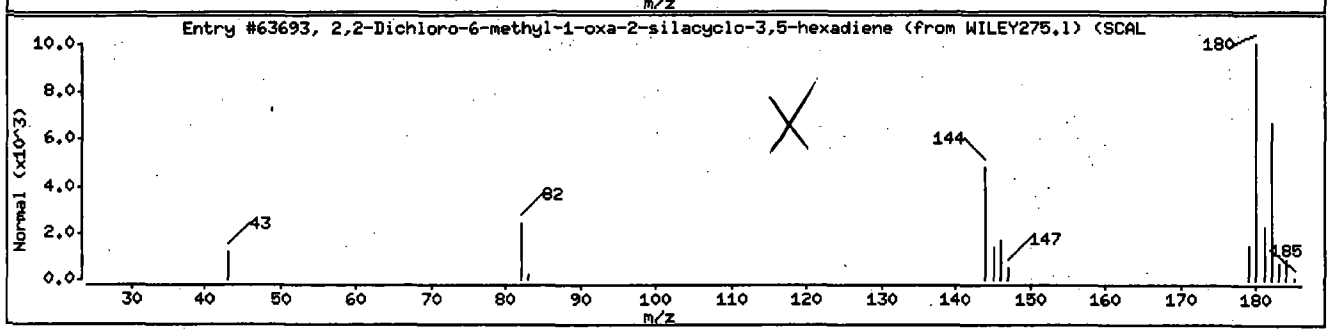
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43383	86	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	12	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	12	C5H6Cl2OSi	180









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:28.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

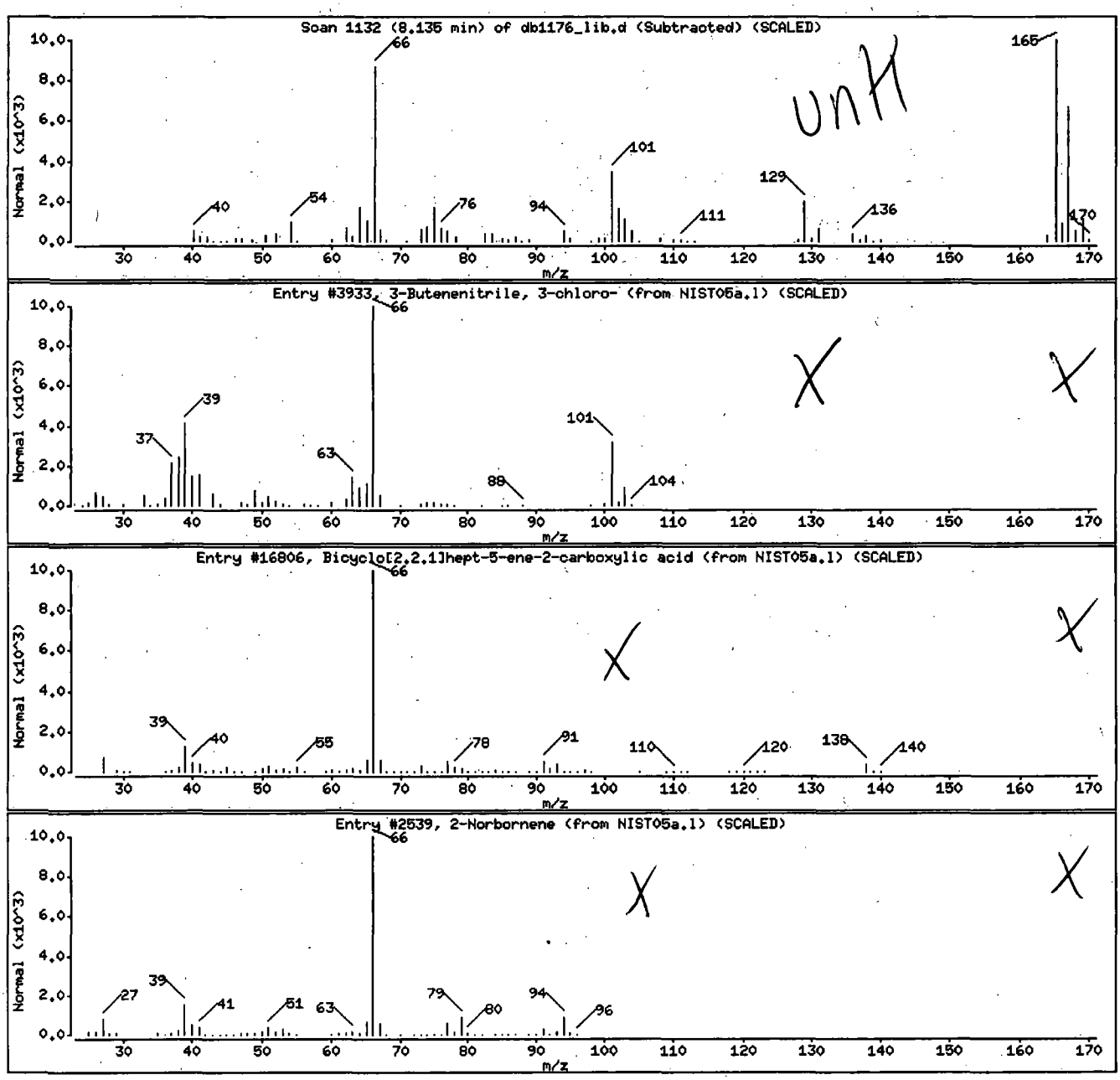
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	40	C4H4ClN	101
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138
2-Norbornene	498-66-8	NIST05a.l	2539	47	C7H10	94



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:28.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1176_lib.d

Date : 26-FEB-2014 03:06

Client ID: H9011

Instrument: HP19760.i

Sample Info: H9011;7369302;1;0;SAMPLE;;;

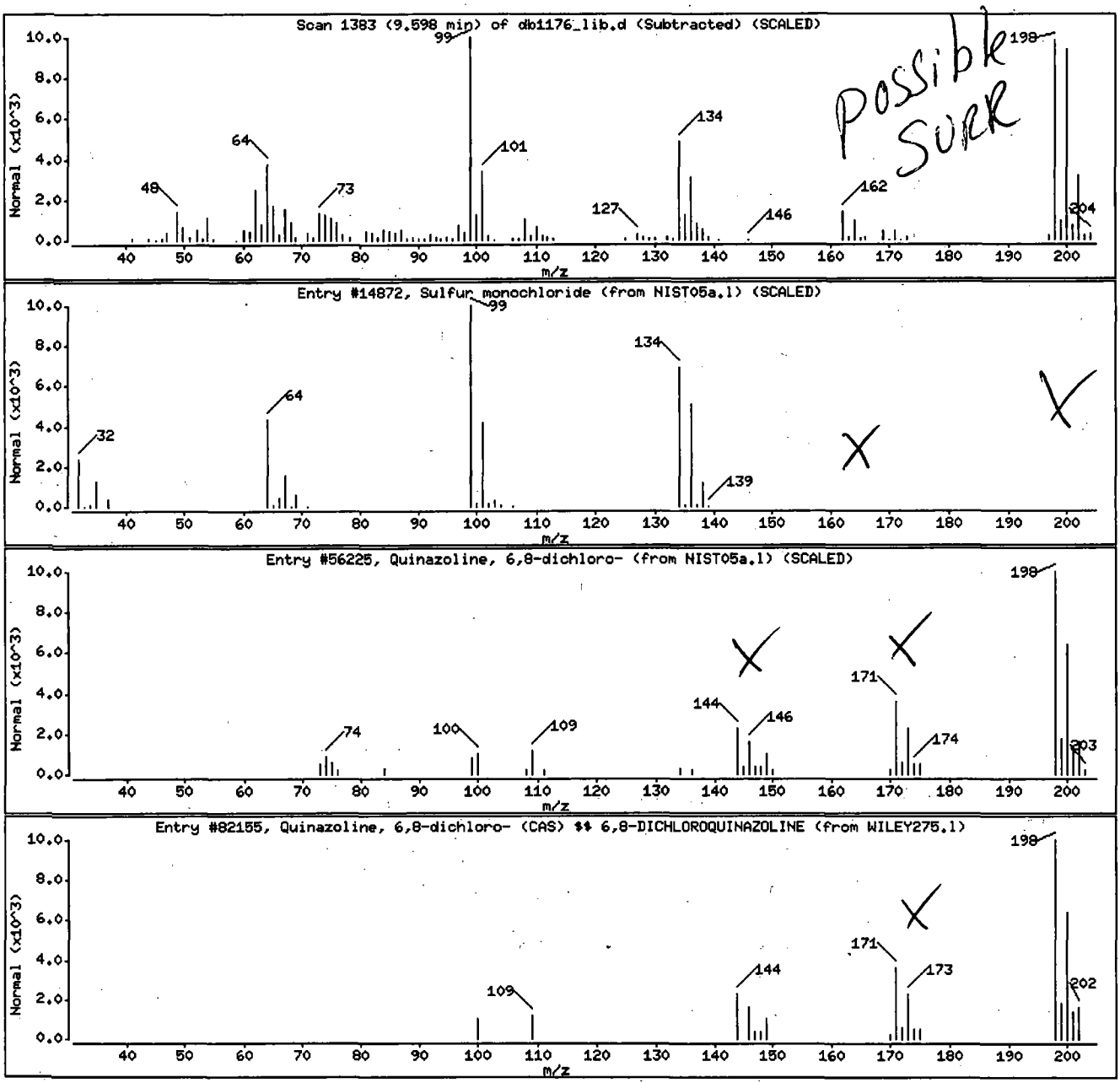
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

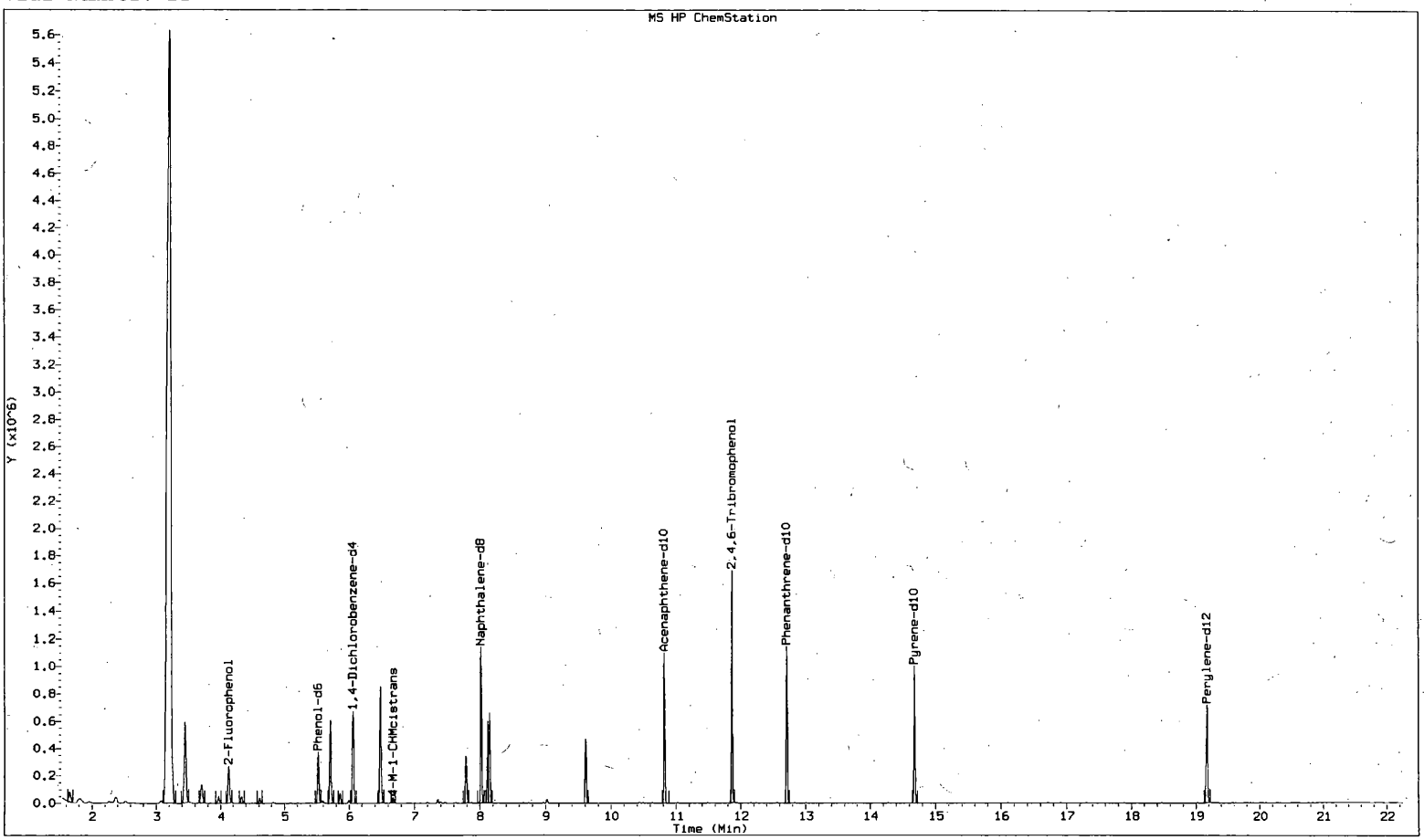
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	25	C12S2	134
Quinazoline, 6,8-dichloro-	17227-49-5	NIST05a.l	56225	43	C8H4C12N2	198
Quinazoline, 6,8-dichloro- (CAS) $$ 6,8-	17227-49-5	WILEY275.l	82155	43	C8H4C12N2	198



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:28.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb24a.b/db1099_lib.d
Operator : ceb05247
Acquired : 25-FEB-2014 04:19
Instrument : HP19760.i
Sample Name: H9021;7369306;1;0;SAMPLE;;;
Misc Info : 14051WAN;WL13463;;1053;1000;0;db1086;13166;
Vial Number: 21



Lancaster Labs

Data file : /chem/HP19760.i/14feb24a.b/db1099_lib.d
Lab Smp Id: 7369306 Client Smp ID: H9021
Inj Date : 25-FEB-2014 04:19
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H9021;7369306;1;0;SAMPLE;;;
Misc Info : 14051WAN;WL13463;;1053;1000;0;db1086;13166;
Comment : Max. number of TICs to report is 50, 14 TICs were found initially.
Method : /chem/HP19760.i/14feb24a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:59 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 21
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1053.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.060	959923	10.000
* 48 Naphthalene-d8	8.018	1460728	10.000
* 83 Acenaphthene-d10	10.822	1269744	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.653	152902	1.59285105	1.51267	90	NIST05a.1	31323	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.227	22777792	237.287530	225.34428	83	NIST05a.1	9464	21
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.449	1216407	12.6719110	12.03410	83	NIST05a.1	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.705	254257	2.64871724	2.51540	23	NIST05a.1	18643	21(L)
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$					CAS #: 74421-00-4		
3.973	90212	0.93977857	0.89247	28	WILEY275.1	21984	21(L)
2-Methyl-3-bromo-2-butanol					CAS #: 2588-77-4		
4.335	81862	0.85280068	0.80987	64	NIST05a.1	33655	21(L)
Butane, 1,3-dichloro-3-methyl-					CAS #: 624-96-4		
4.614	68131	0.70975692	0.67403	42	NIST05a.1	17535	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.716	938477	9.77658167	9.28450	91	WILEY275.1	18902	21
Decane					CAS #: 124-18-5		
5.862	105904	1.10325623	1.04772	96	NIST05a.1	18488	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.480	1348291	14.0458173	13.33885	35	NIST05a.1	9448	21
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.785	455965	3.12148844	2.96437	43	NIST05a.1	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.117	636297	4.35602135	4.13677	53	NIST05a.1	43384	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.147	812724	5.56382337	5.28378	40	NIST05a.1	3933	48(L)
Sulfur monochloride					CAS #: 10025-67-9		
9.610	550036	4.33186828	4.11383	38	NIST05a.1	14872	83

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 28-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

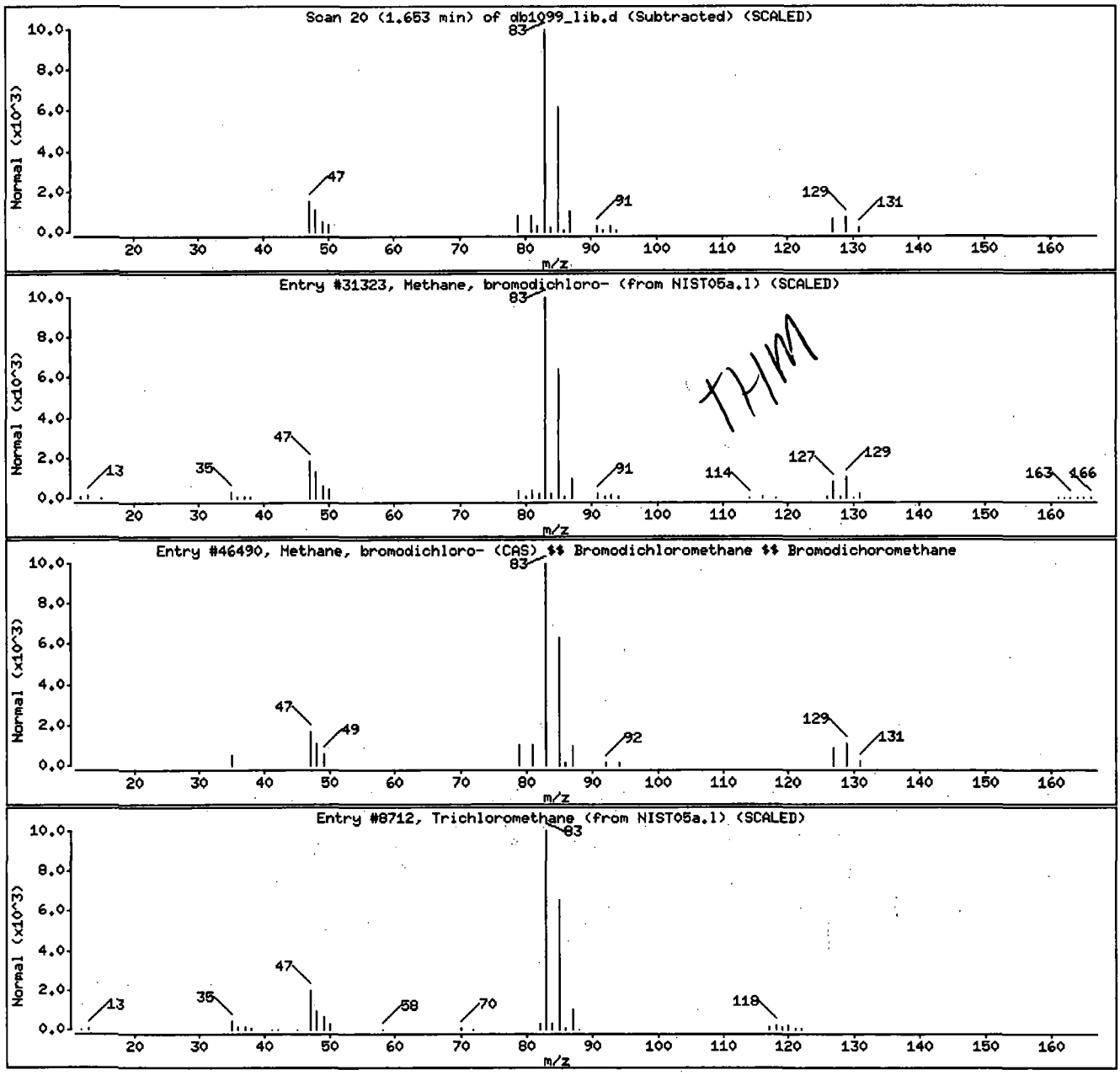
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46490	90	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

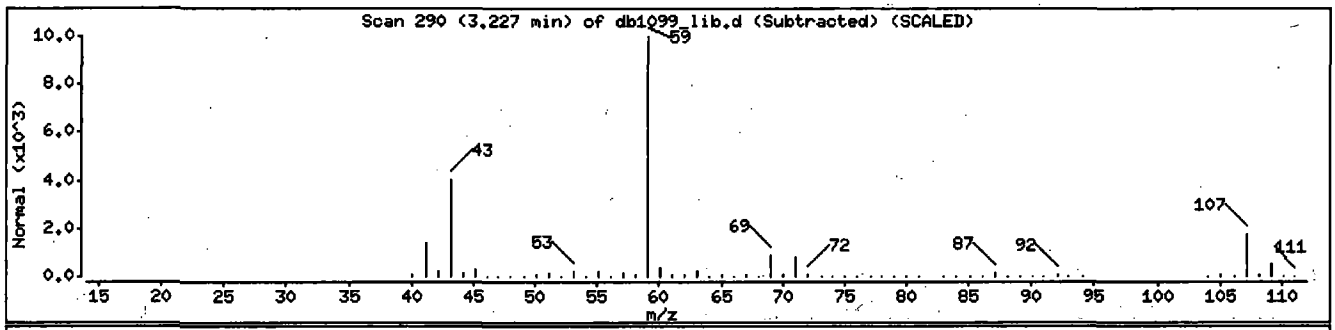
Volume Injected (uL): 1.0

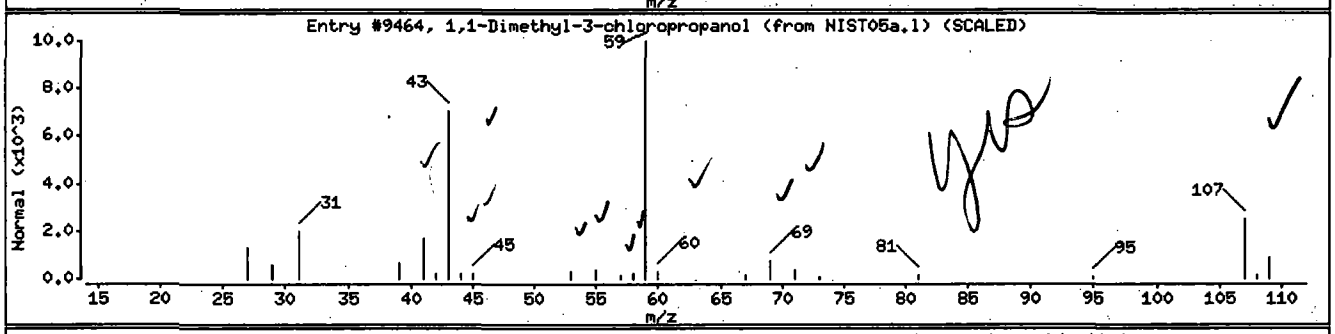
Operator: ceb05247

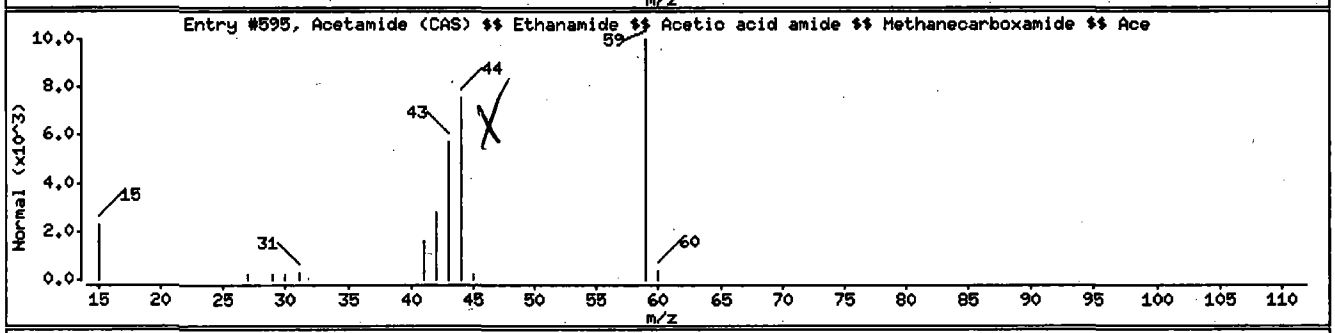
Column phase: J&W DB-5MS

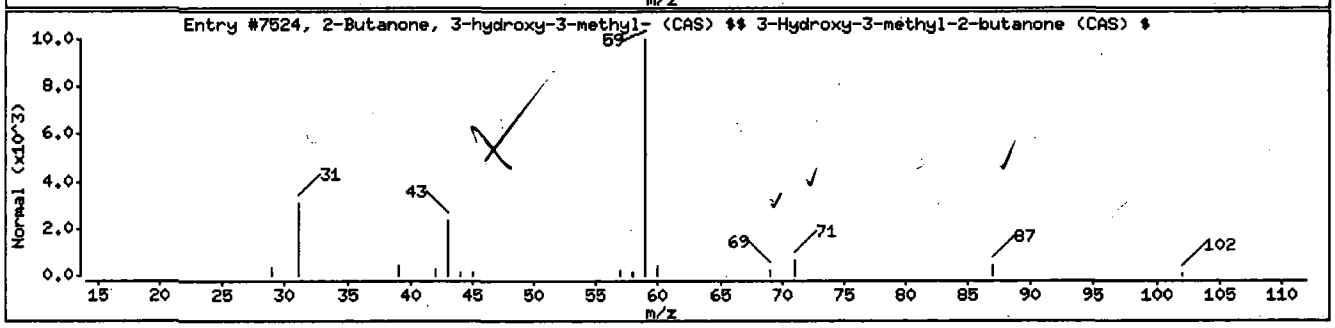
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

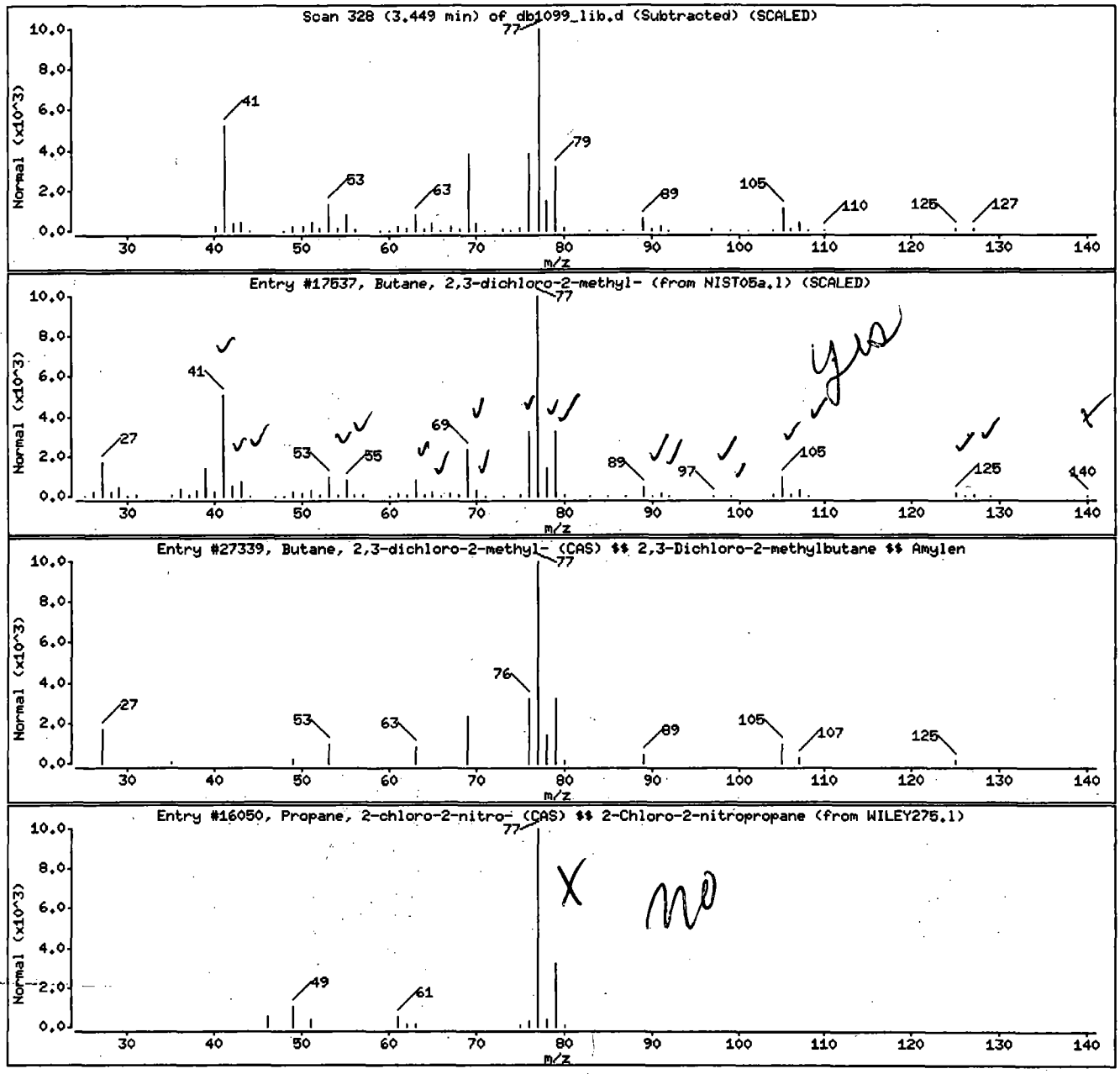
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17637	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	78	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	25	C3H6ClNO2	123



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

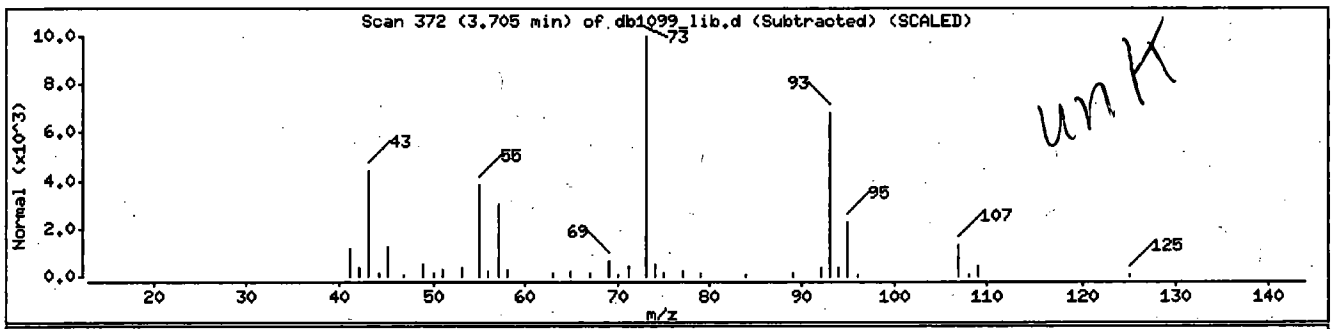
Volume Injected (uL): 1.0

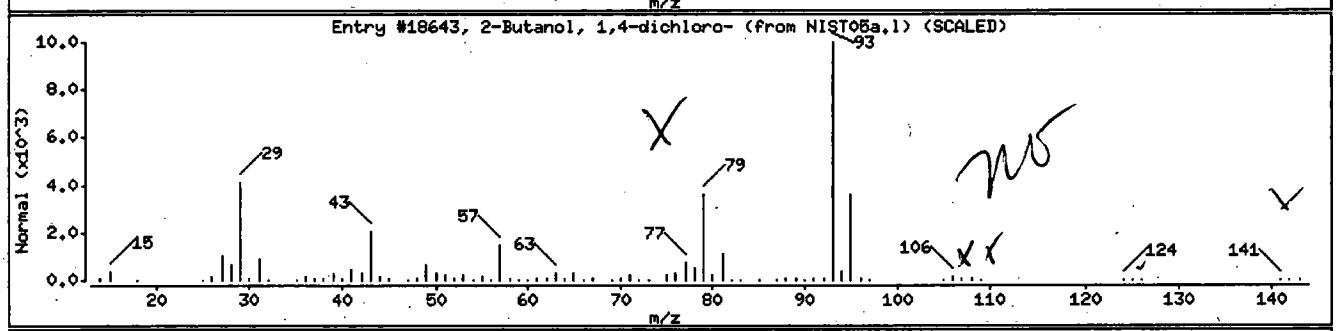
Operator: ceb05247

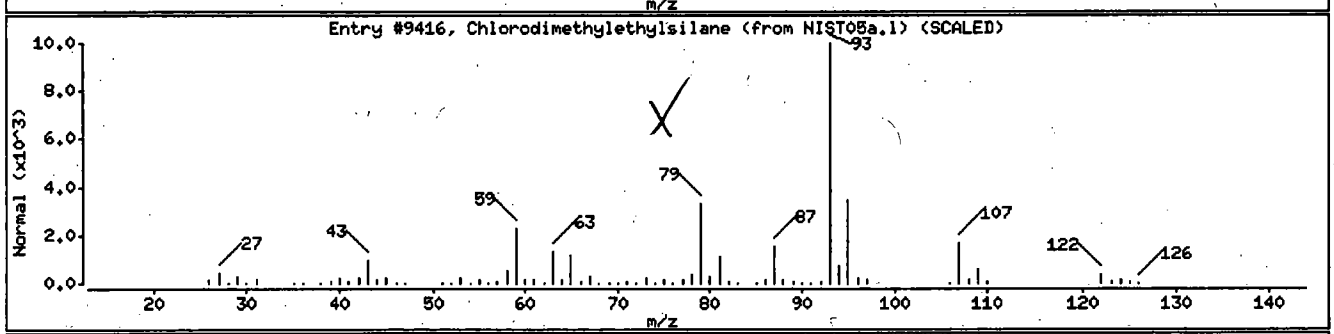
Column phase: J&W DB-5MS

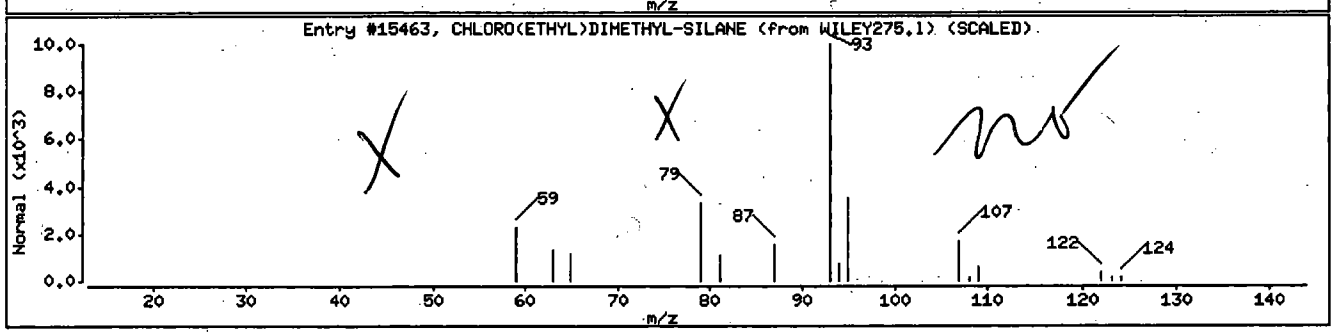
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	23	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	28	C4H11ClSi	122
CHLORO(ETHYL)DIMETHYL-SILANE	0-00-0	WILEY275.l	15463	28	C4H11ClSi	122









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

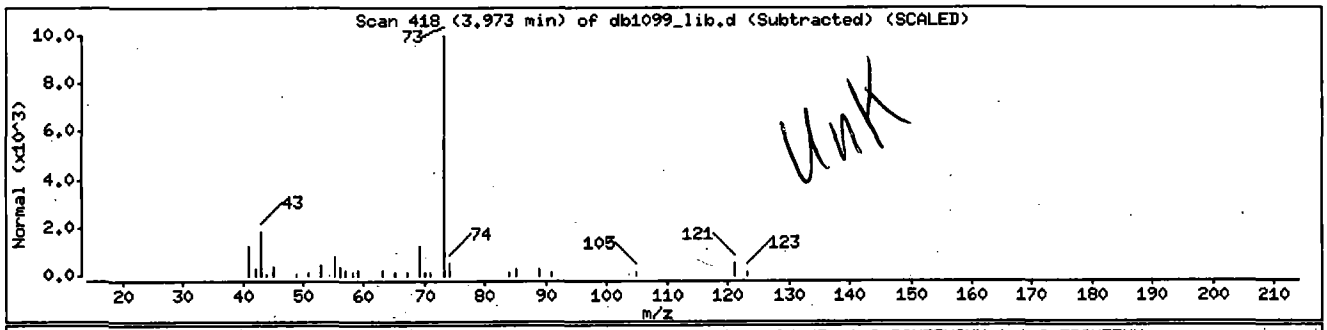
Volume Injected (uL): 1.0

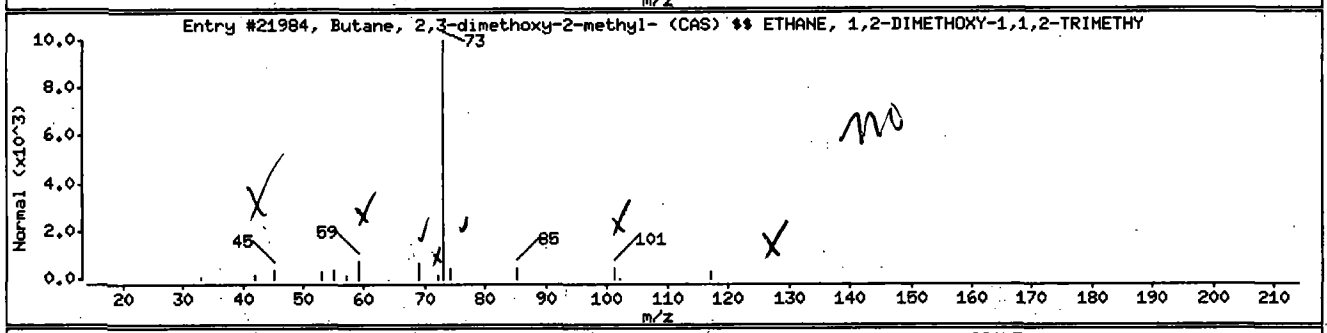
Operator: ceb05247

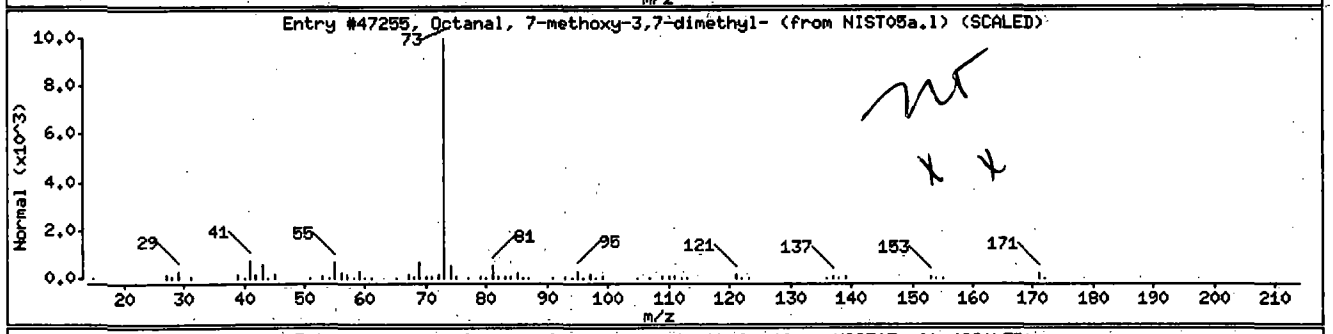
Column phase: J&W DB-5MS

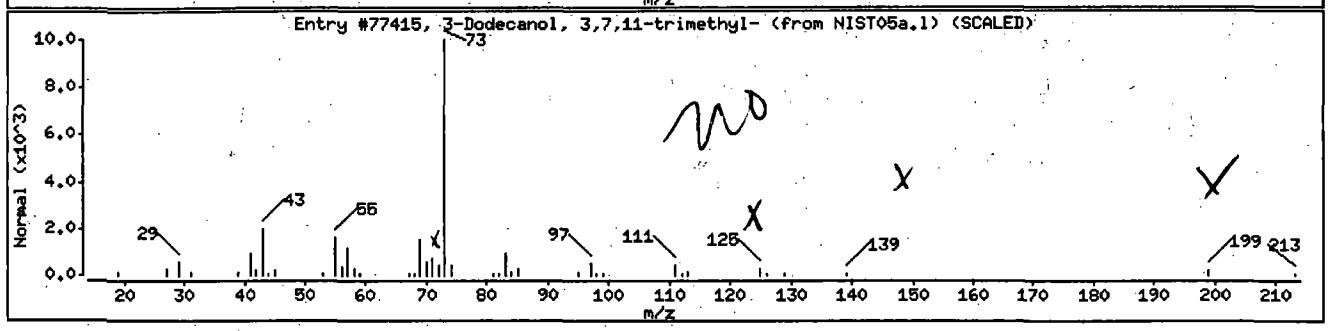
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	28	C7H16O2	132
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	42	C11H22O2	186
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	36	C15H32O	228









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

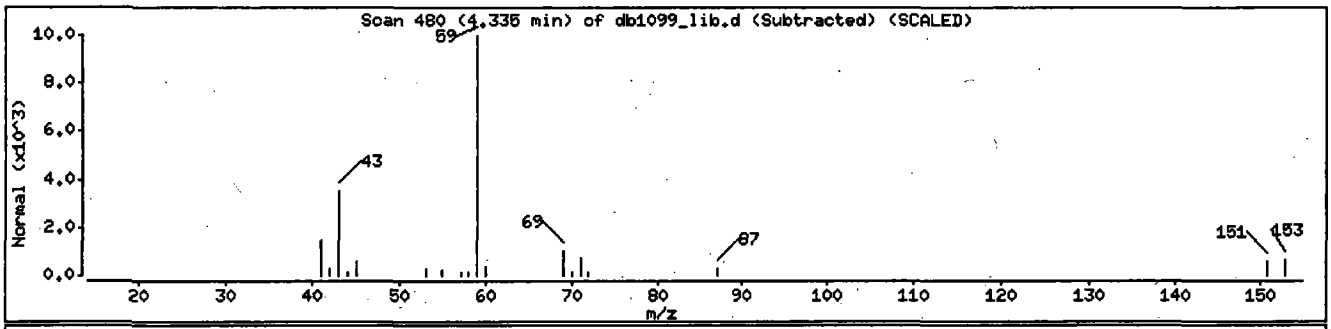
Volume Injected (uL): 1.0

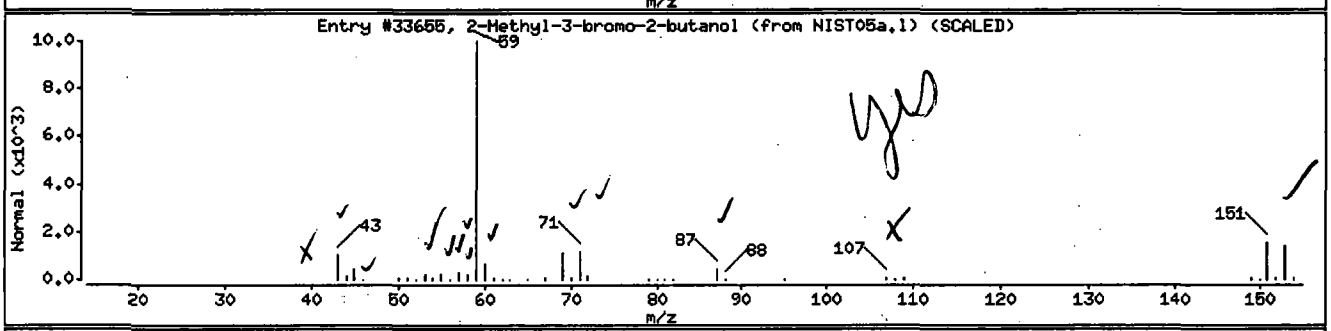
Operator: ceb05247

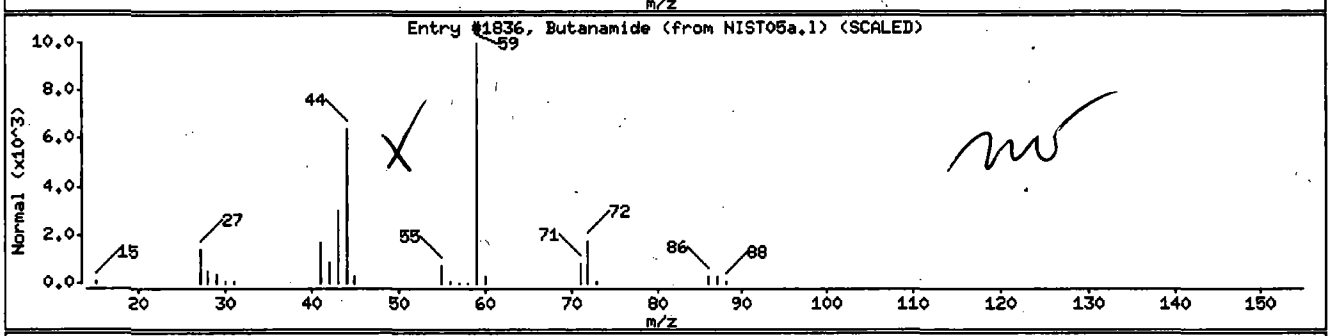
Column phase: J&W DB-5MS

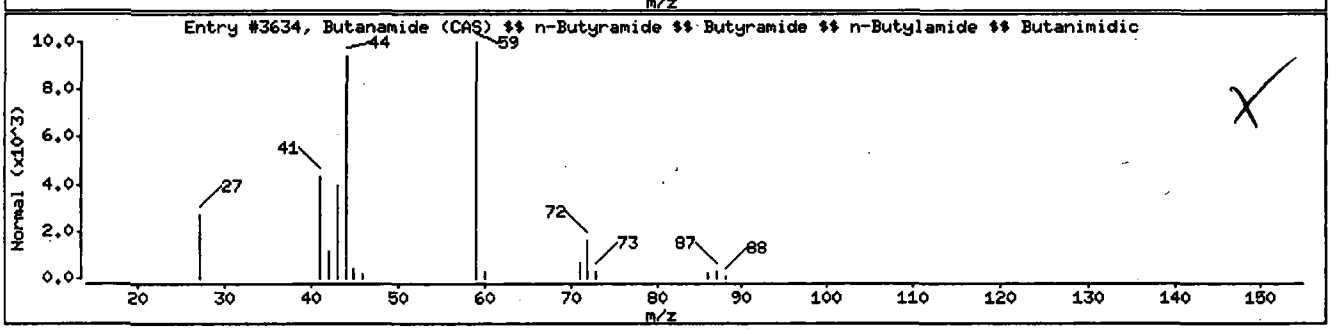
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Methyl-3-bromo-2-butanol	2588-77-4	NIST05a.l	33655	64	C5H11BrO	166
Butanamide	541-35-5	NIST05a.l	1836	64	C4H9NO	87
Butanamide (CAS) $$ n-Butyramide $$ Buty	541-35-5	WILEY275.l	3634	64	C4H9NO	87









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

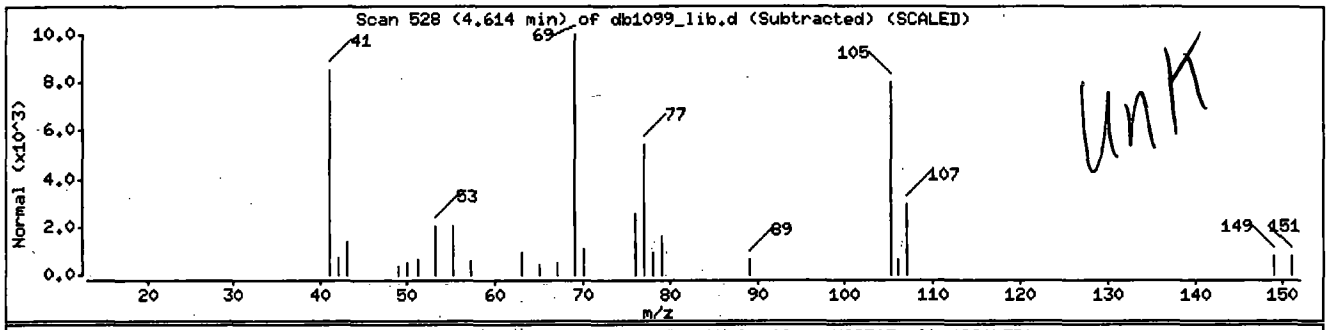
Volume Injected (uL): 1.0

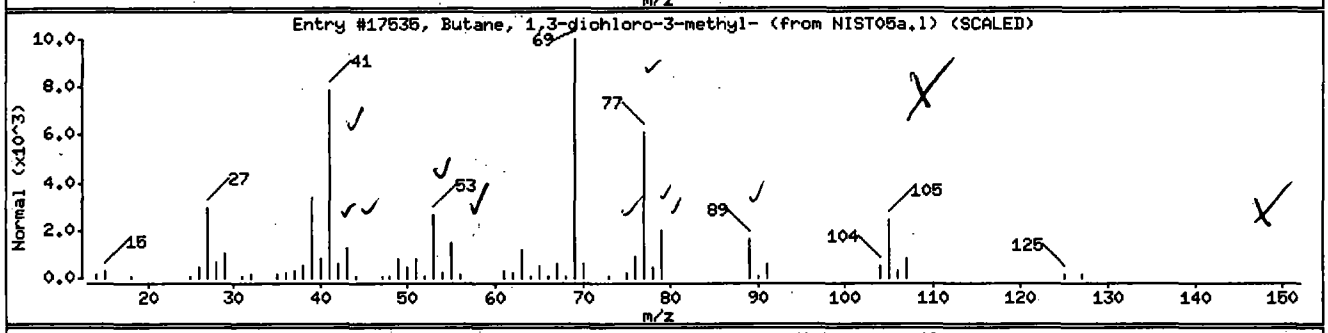
Operator: ceb05247

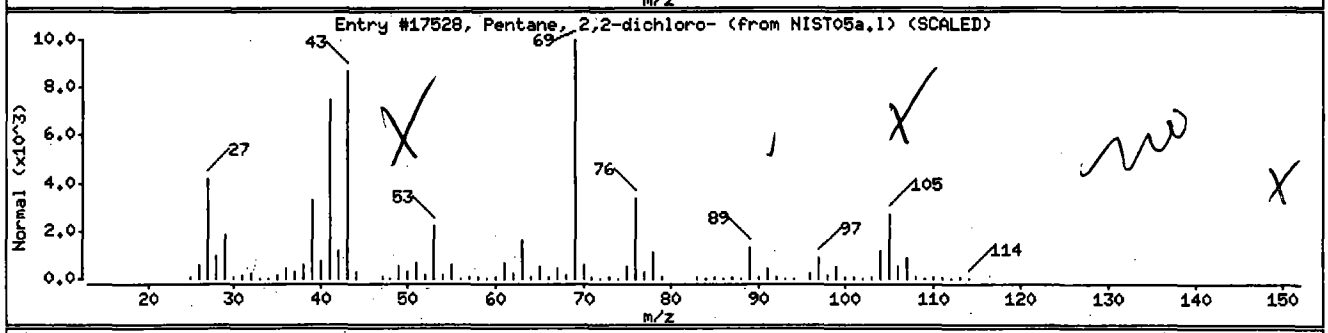
Column phase: J&W DB-5MS

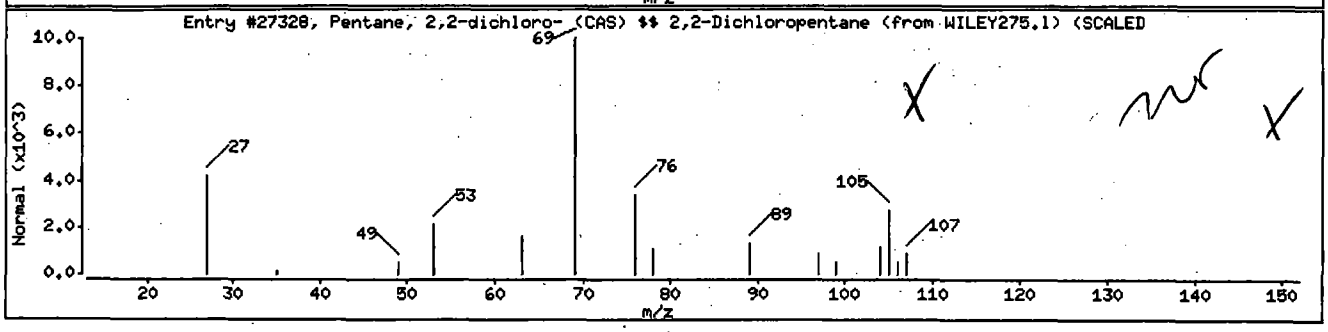
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 1,3-dichloro-3-methyl-	624-96-4	NIST05a.l	17535	42	C5H10Cl2	140
Pentane, 2,2-dichloro-	34887-14-4	NIST05a.l	17528	42	C5H10Cl2	140
Pentane, 2,2-dichloro- (CAS) ** 2,2-Dich	34887-14-4	WILEY275.l	27328	42	C5H10Cl2	140









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

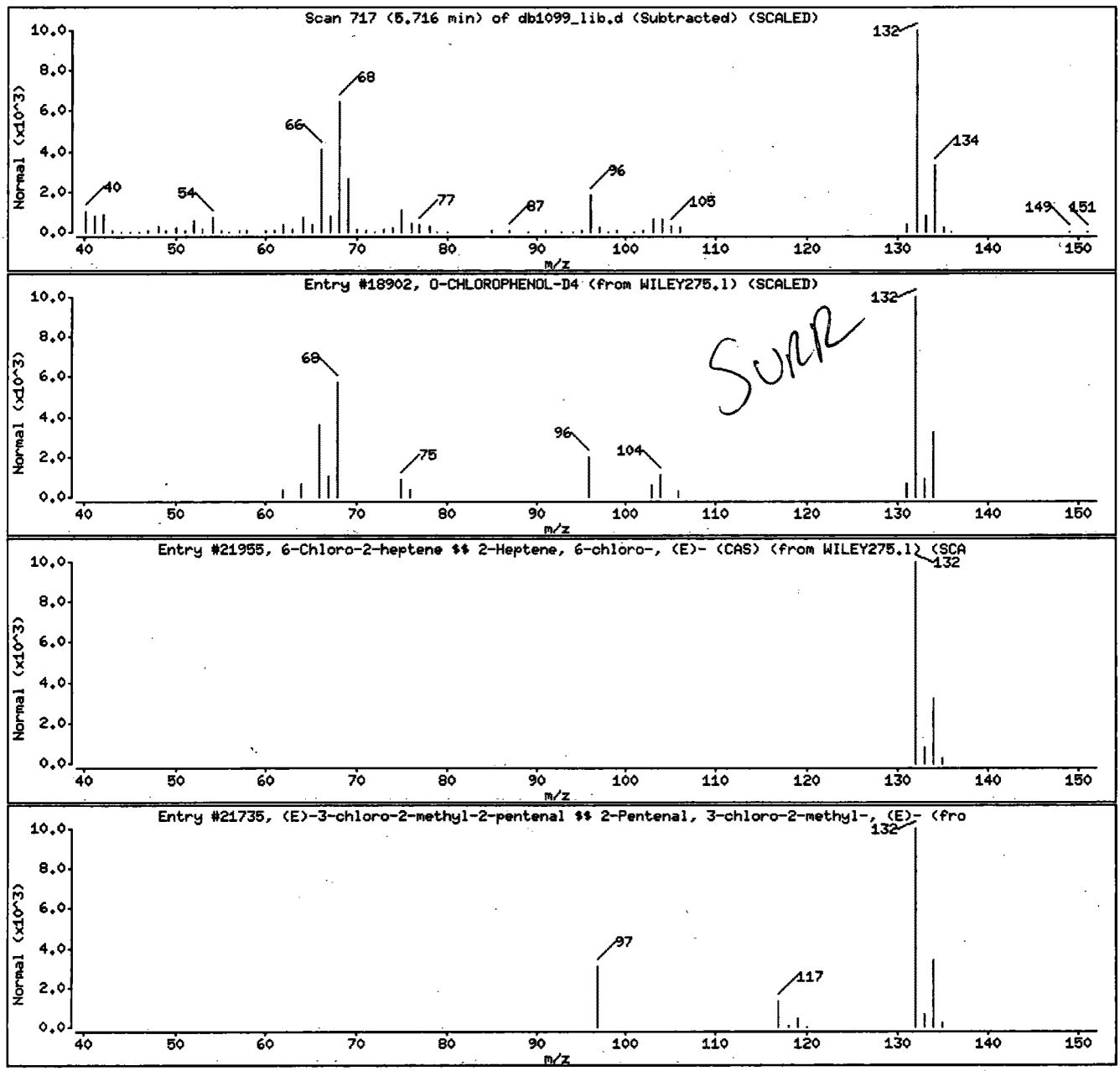
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

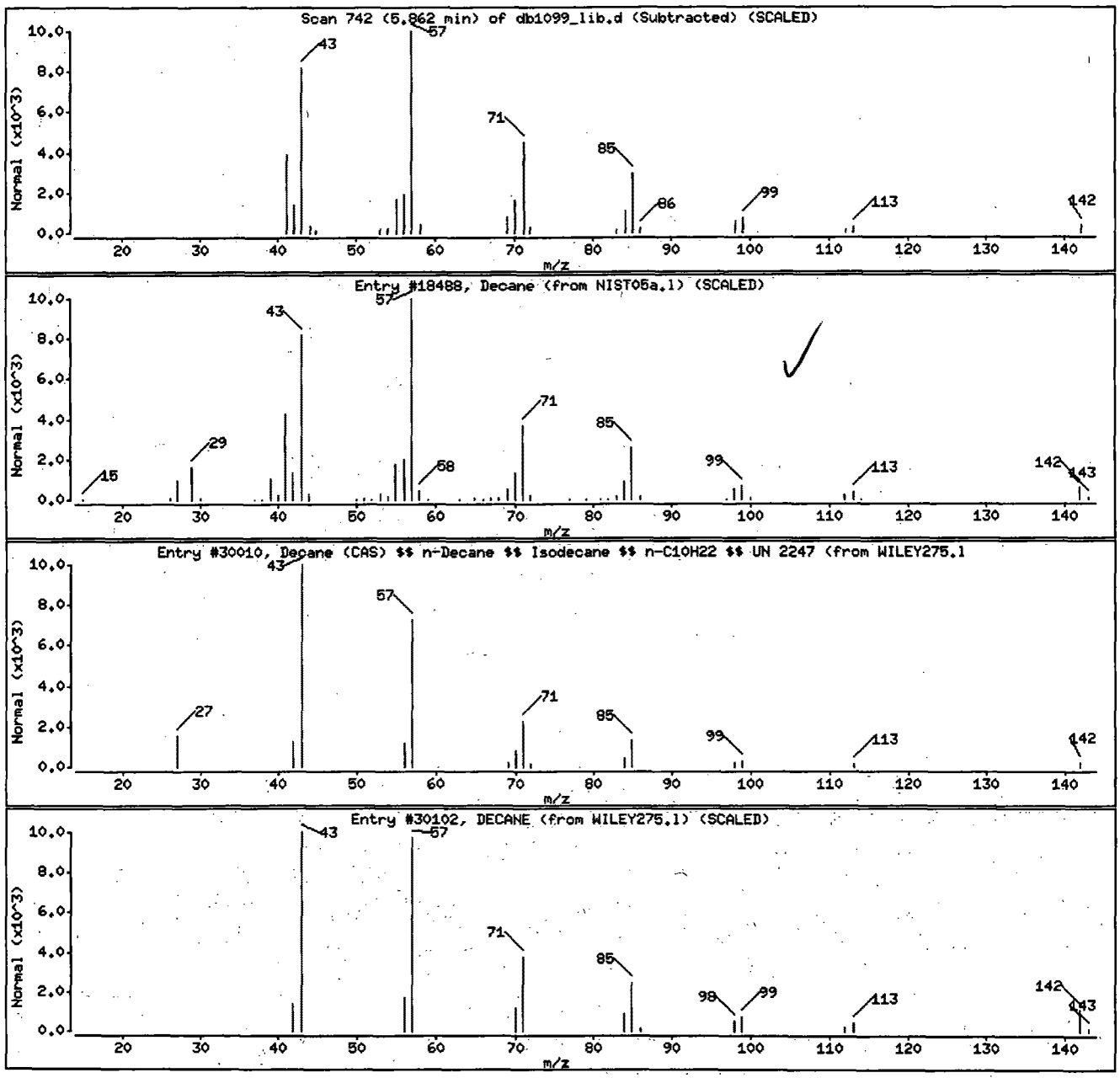
Client ID: H9021 Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18488	96	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30010	91	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

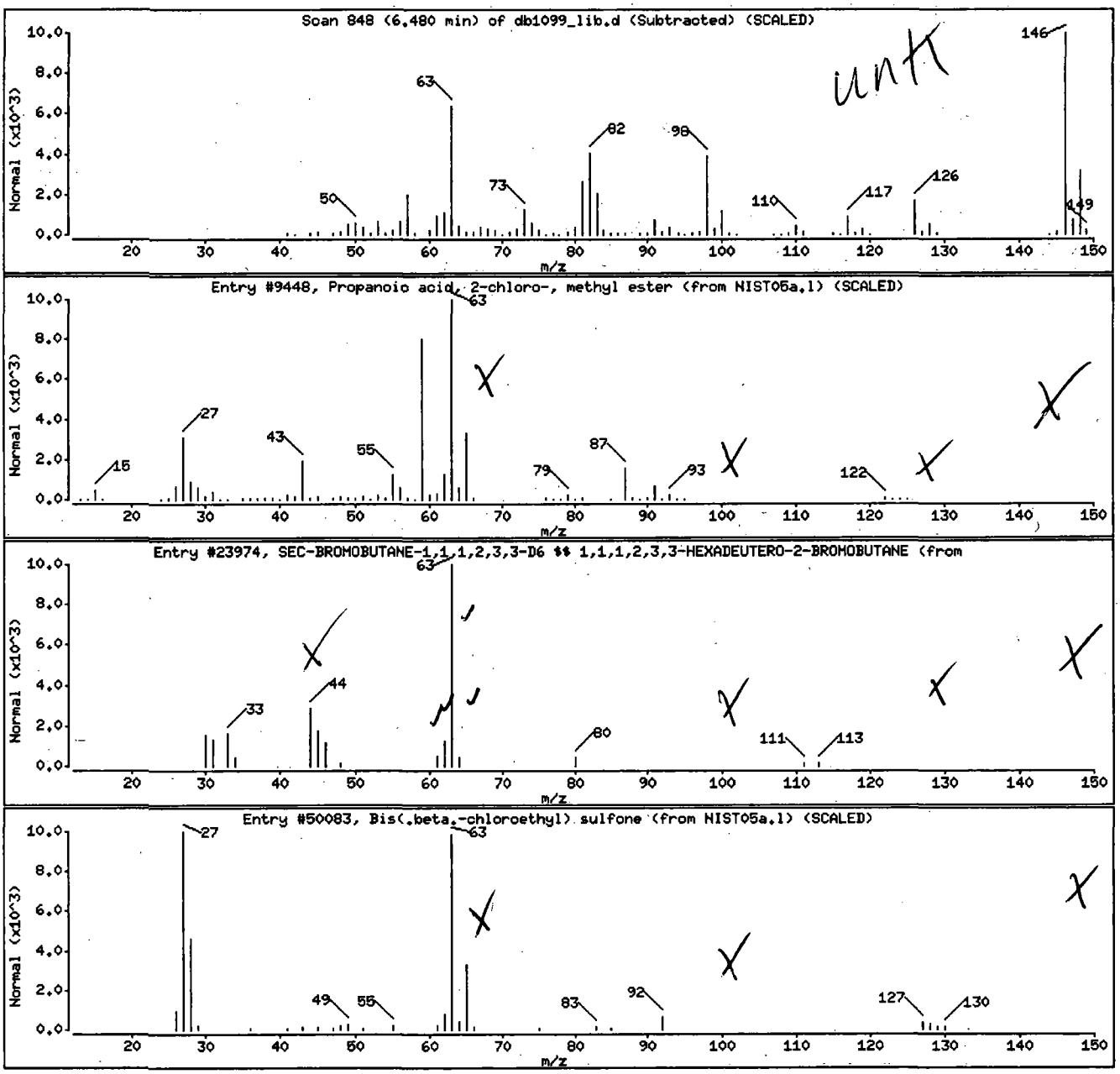
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	38	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 ** 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Bis(.beta.-chloroethyl) sulfone	471-03-4	NIST05a.l	50083	17	C4H8Cl2O2S	190



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

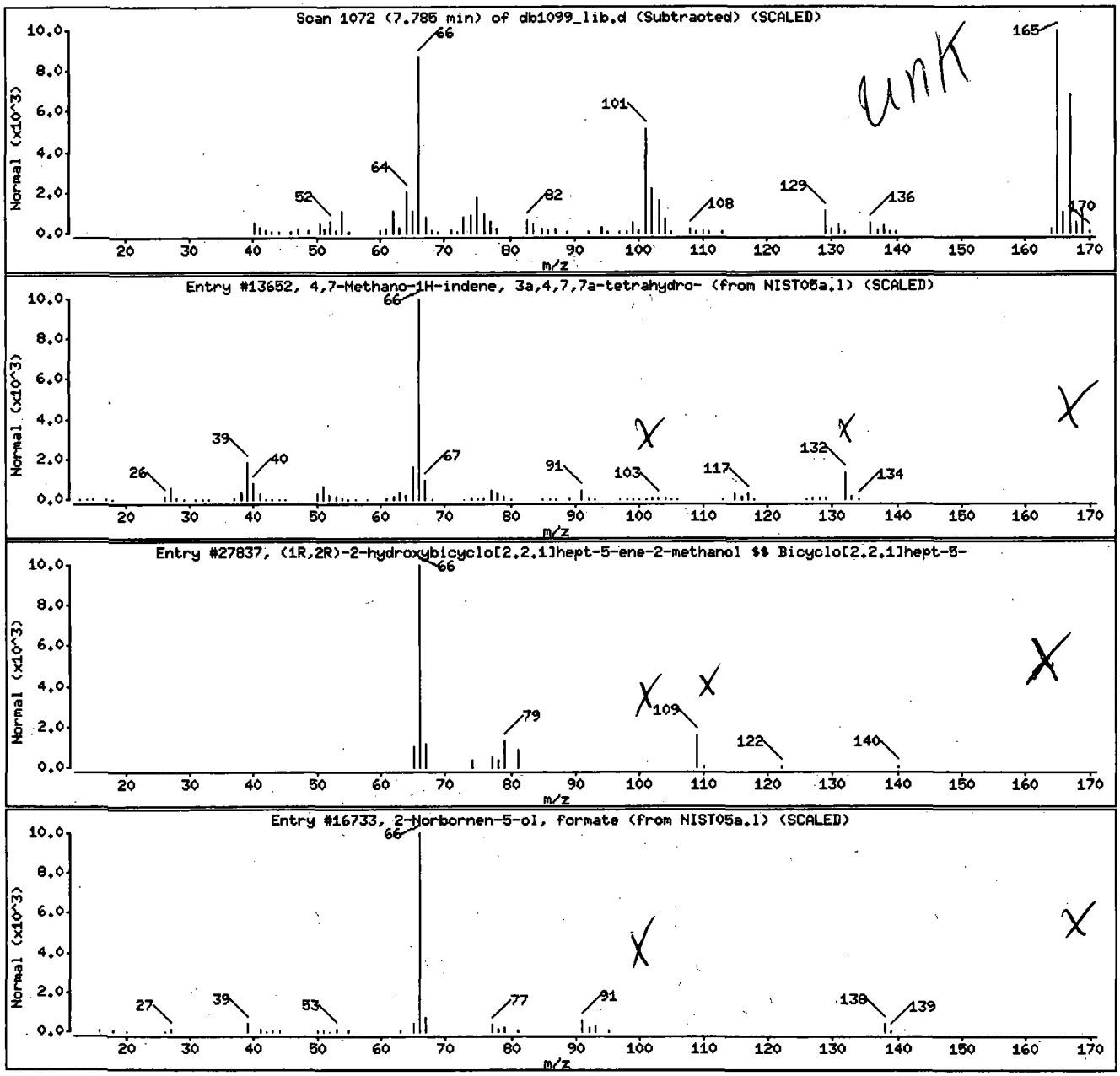
Client ID: H9021 Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	43	C10H12	132
(1R,2R)-2-hydroxybicyclo[2.2.1]hept-5-en	116697-44-0	WILEY275.l	27837	47	C8H12O2	140
2-Norbornen-5-ol, formate	1000142-76-9	NIST05a.l	16733	46	C8H10O2	138



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

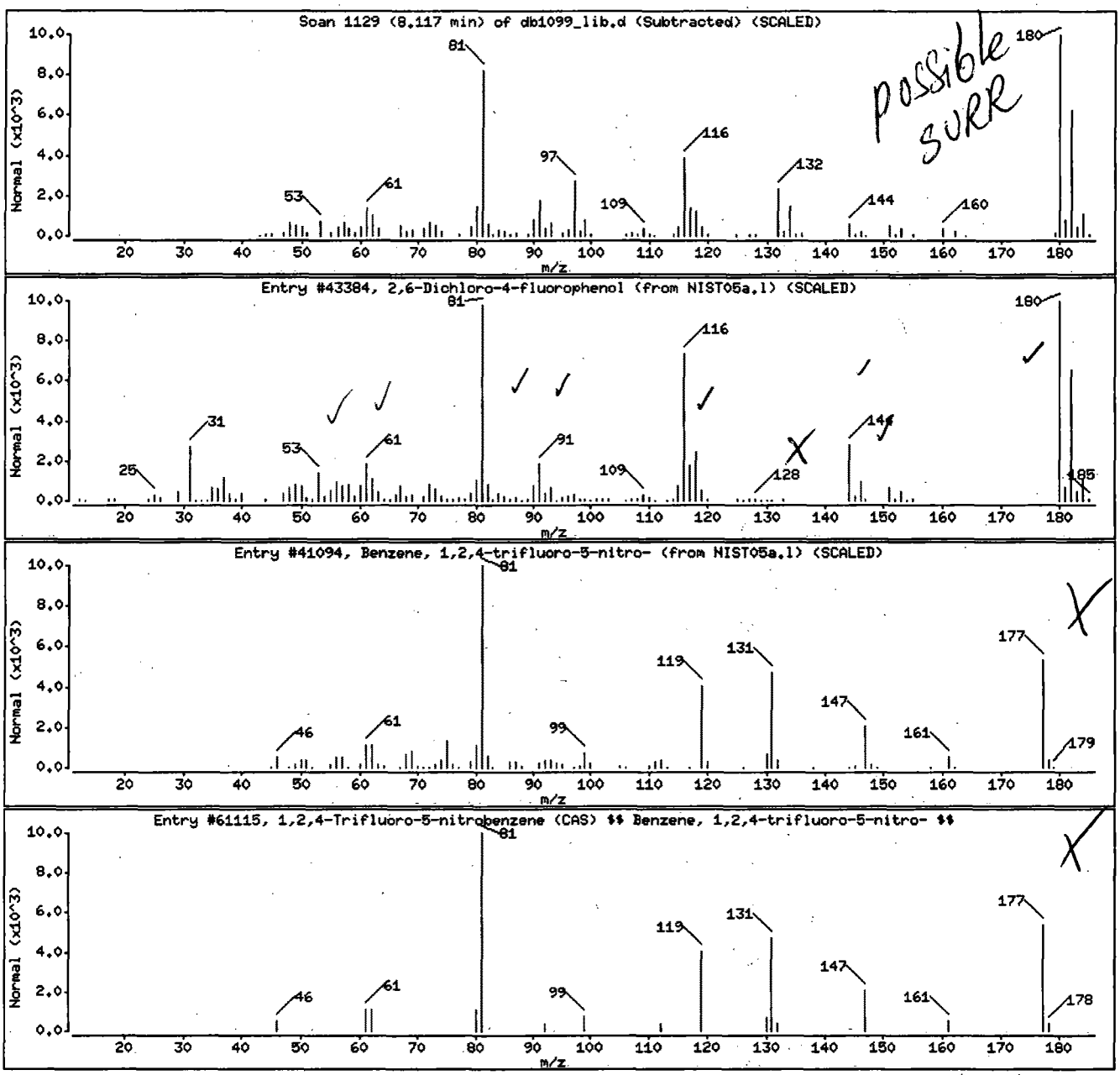
Client ID: H9021 Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43384	53	C6H3Cl2FO	180
Benzene, 1,2,4-trifluoro-5-nitro-	2105-61-5	NIST05a.l	41094	12	C6H2F3NO2	177
1,2,4-Trifluoro-5-nitrobenzene (CAS) $$	2105-61-5	WILEY275.l	61115	12	C6H2F3NO2	177



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

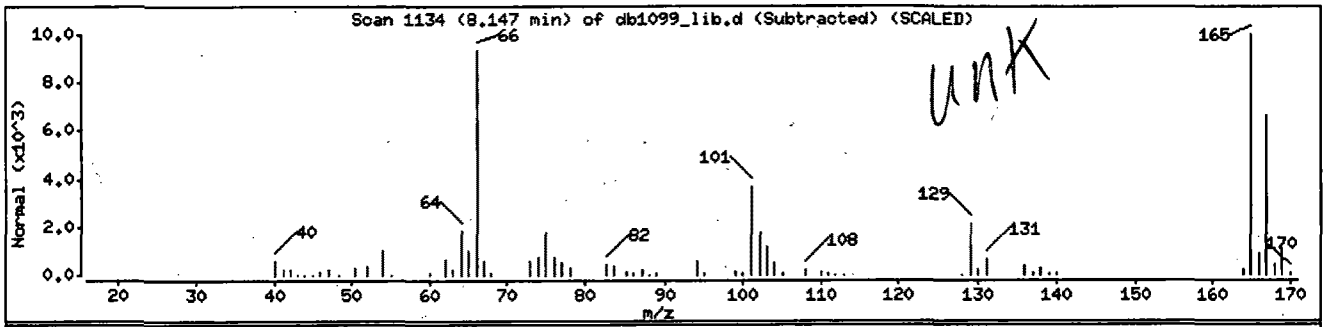
Volume Injected (uL): 1.0

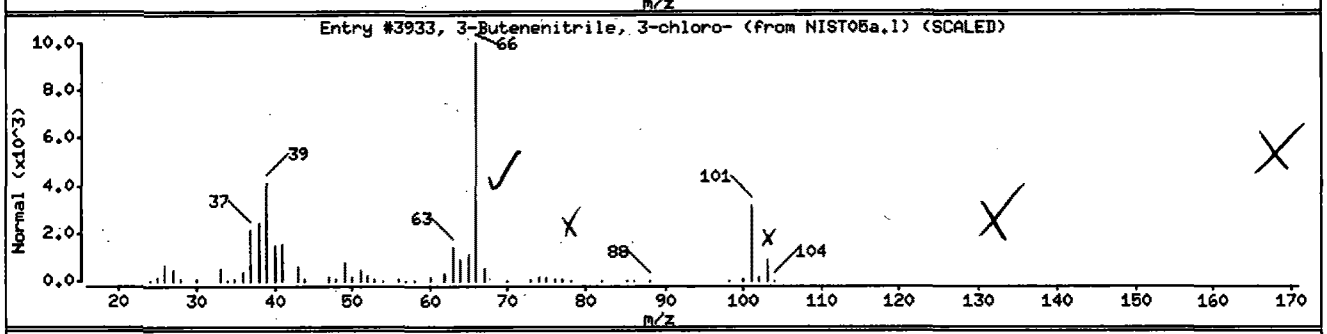
Operator: ceb05247

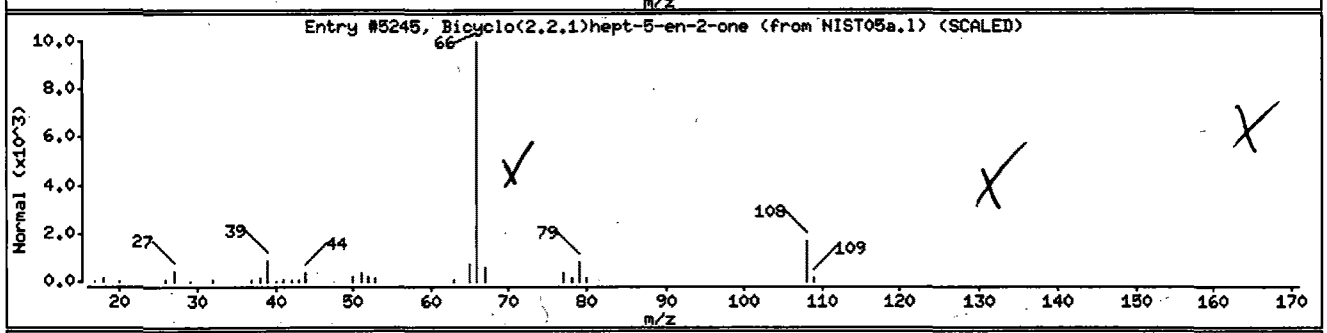
Column phase: J&W DB-5MS

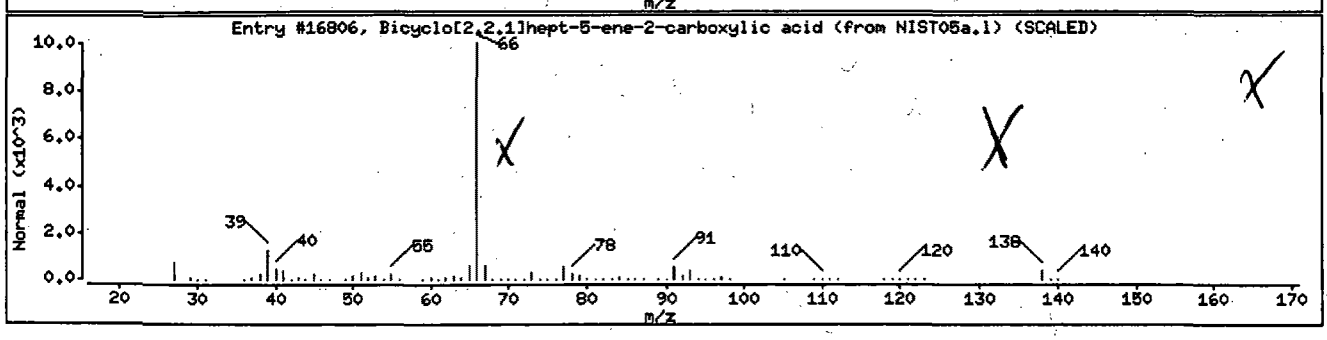
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	40	C4H4ClN	101
Bicyclo(2.2.1)hept-5-en-2-one	694-98-4	NIST05a.l	5245	49	C7H8O	108
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb24a.b/db1099_lib.d

Date : 25-FEB-2014 04:19

Client ID: H9021

Instrument: HP19760.i

Sample Info: H9021;7369306;1;0;SAMPLE;;;

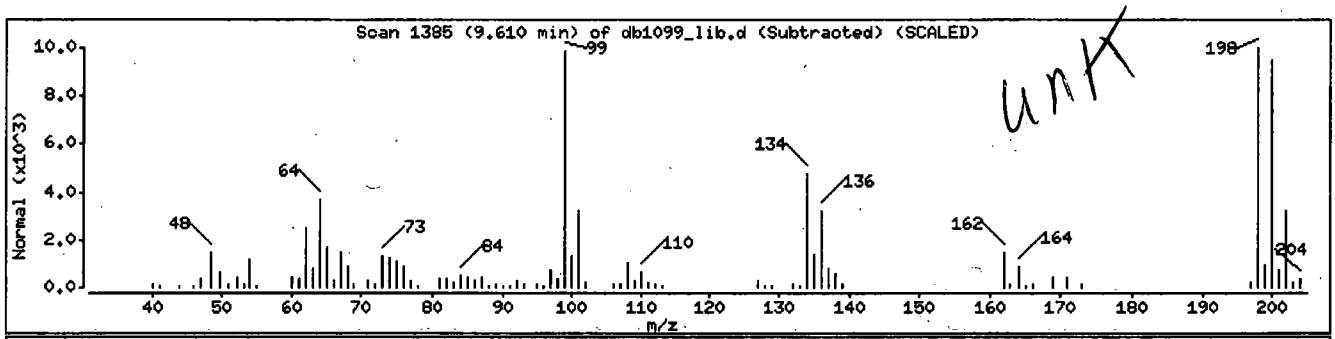
Volume Injected (uL): 1.0

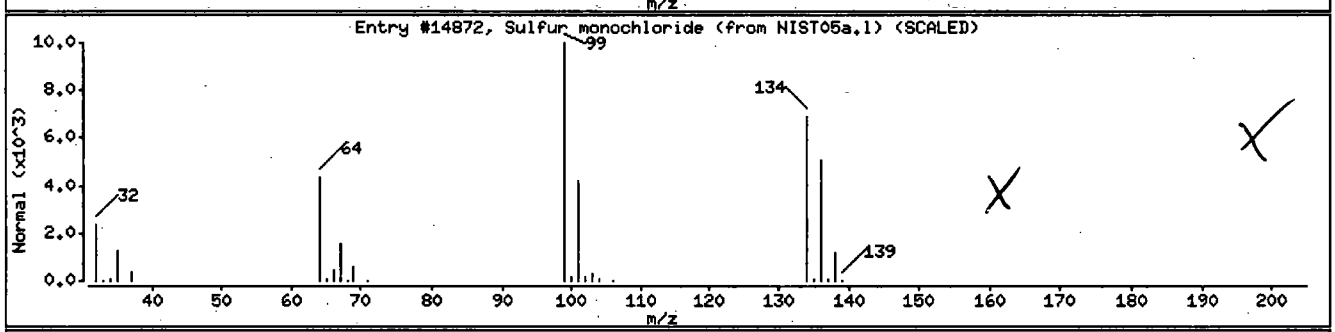
Operator: ceb05247

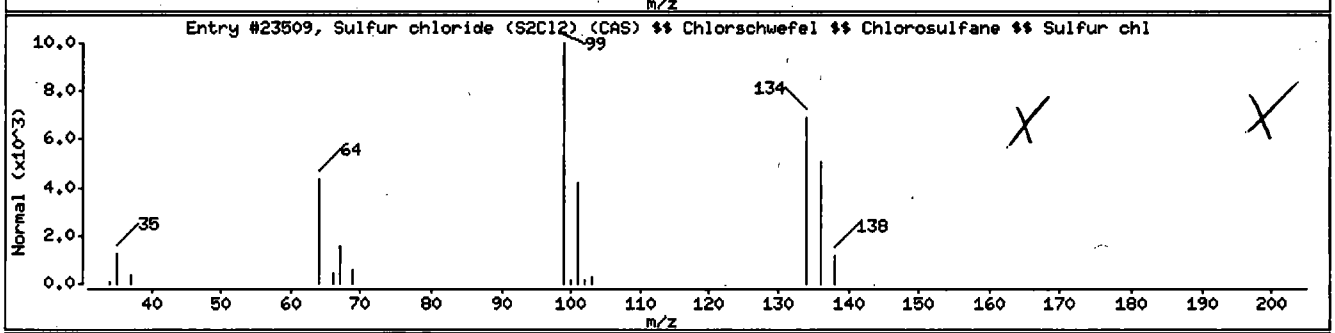
Column phase: J&W DB-5MS

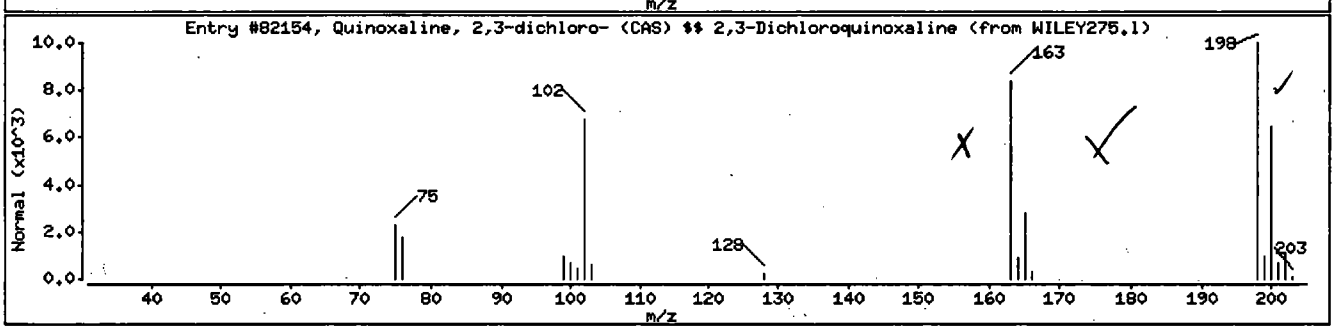
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	Cl2S2	134
Sulfur chloride (S2Cl2) (CAS) $$ Chlorsc	10025-67-9	WILEY275.l	23509	38	Cl2S2	134
Quinoxaline, 2,3-dichloro- (CAS) $$ 2,3-	2213-63-0	WILEY275.l	82154	37	C8H4Cl2N2	198



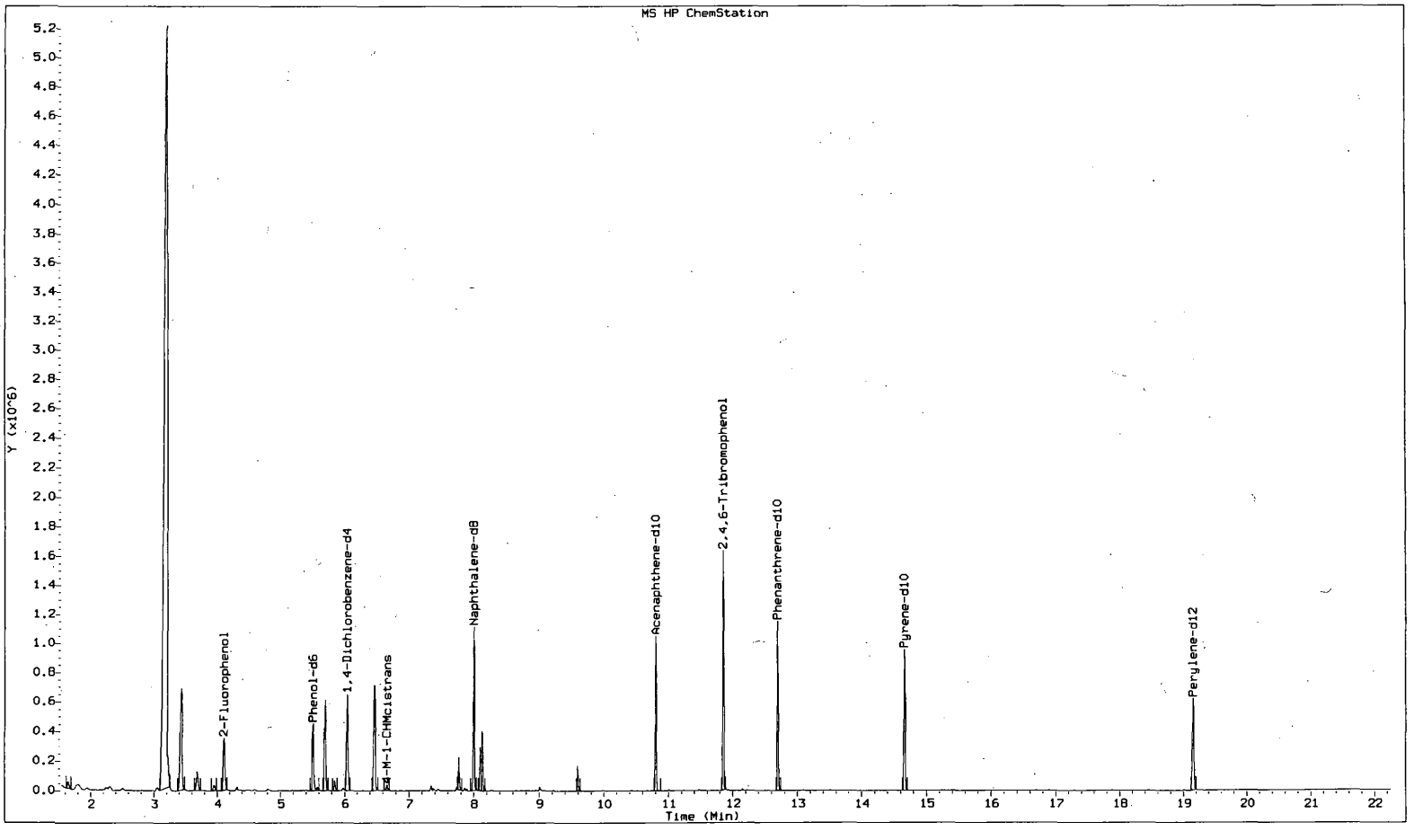






Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:36.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb25a.b/db1180_lib.d
Operator : ceb05247
Acquired : 26-FEB-2014 04:53
Instrument : HP19760.i
Sample Name: H1011;7369317;1;0;SAMPLE;;;
Misc Info : 14051WAO;WL13463;;1034;1000;0;db1172;13166;
Vial Number: 21



Lancaster Labs

Data file : /chem/HP19760.i/14feb25a.b/db1180_lib.d
Lab Smp Id: 7369317 Client Smp ID: H1011
Inj Date : 26-FEB-2014 04:53
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H1011;7369317;1;0;SAMPLE;;;
Misc Info : 14051WAO;WL13463;;1034;1000;0;db1172;13166;
Comment : Max. number of TICs to report is 50, 12 TICs were found initially.
Method : /chem/HP19760.i/14feb25a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 15:23 ajs00193 Quant Type: ISTD
Cal Date : 25-FEB-2014 21:43 Cal File: db1164_lib.d
Als bottle: 21
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1034.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.042	938710	10.000
* 48 Naphthalene-d8	8.001	1391479	10.000
* 83 Acenaphthene-d10	10.804	1219525	10.000

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro- (CAS) $$ Bromodi				CAS #: 75-27-4			
1.642	92534	0.98575395	0.95334	83	WILEY275.1	46493	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

RT	AREA	CONCENTRATIONS ON-COL(ng/ul)	FINAL(ug/L)	QUAL	QUANT LIBRARY	LIB ENTRY	CPND #
1,1-Dimethyl-3-chloropropanol				CAS #: 1985-88-2			
3.204	18123764	193.070838	186.72228	83	NIST05a.l	9464	21
Butane, 2,3-dichloro-2-methyl-				CAS #: 507-45-9			
3.431	1350261	14.3842141	13.91123	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-				CAS #: 2419-74-1			
3.688	263435	2.80635295	2.71407	32	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$				CAS #: 74421-00-4			
3.956	63245	0.67374250	0.65158	38	WILEY275.l	21984	21(L)
O-CHLOROPHENOL-D4				CAS #: 0-00-0			
5.698	861025	9.17241809	8.87081	91	WILEY275.l	18902	21
Decane				CAS #: 124-18-5			
5.850	95711	1.01959934	0.98607	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester				CAS #: 17639-93-9			
6.462	1170897	12.4734587	12.06330	35	NIST05a.l	9448	21(L)
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy				CAS #: 77-73-6			
7.773	268220	1.92758803	1.86420	25	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol				CAS #: 392-71-2			
8.100	346098	2.48726923	2.40548	60	NIST05a.l	43384	48
3-Butenenitrile, 3-chloro-				CAS #: 21031-46-9			
8.129	485409	3.48843895	3.37373	50	NIST05a.l	3933	48
Sulfur monochloride				CAS #: 10025-67-9			
9.598	186593	1.53004690	1.47973	18	NIST05a.l	14872	83(L)

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

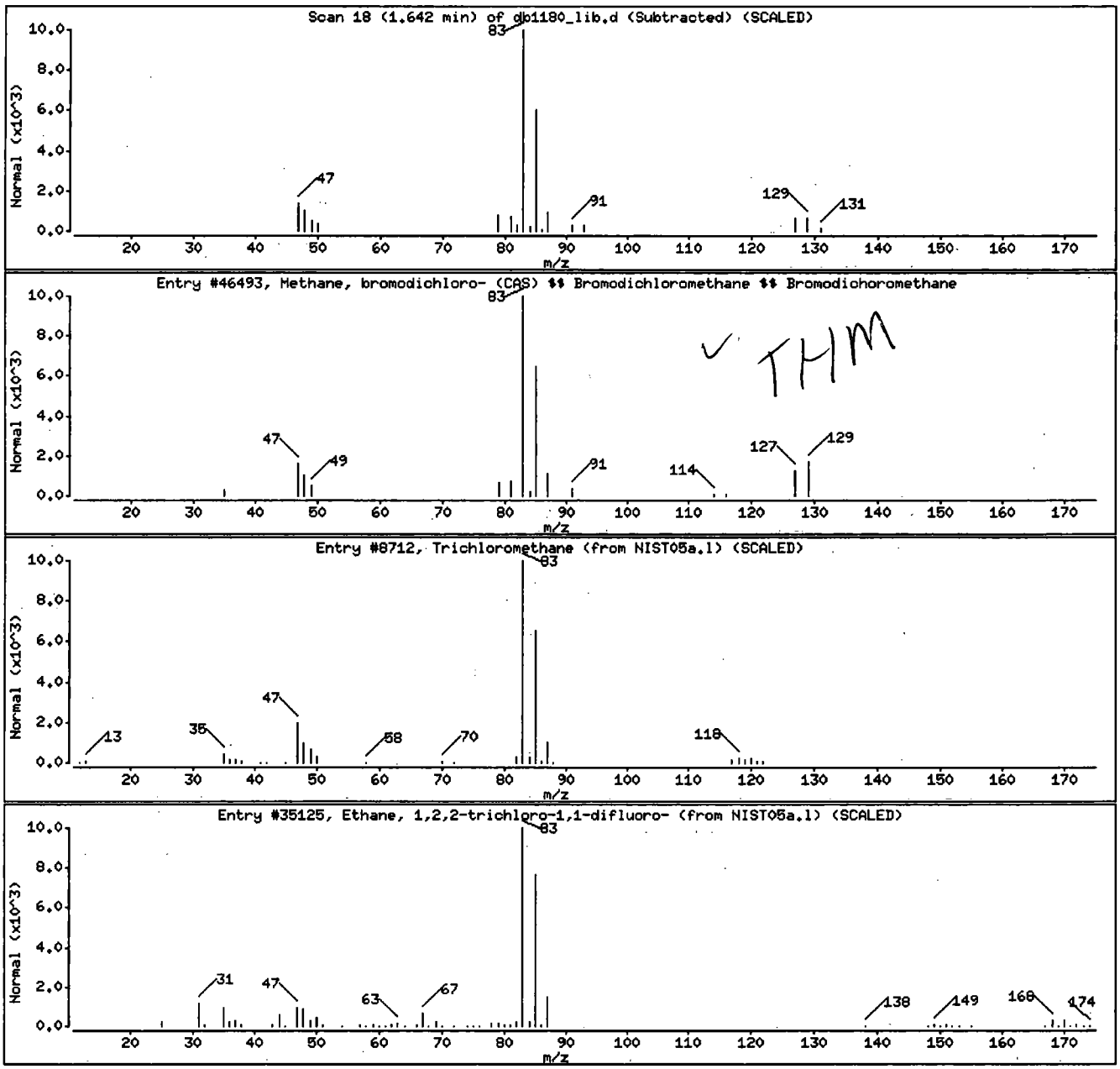
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46493	83	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118
Ethane, 1,2,2-trichloro-1,1-difluoro-	354-21-2	NIST05a.l	35125	72	C2HCl3F2	168



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

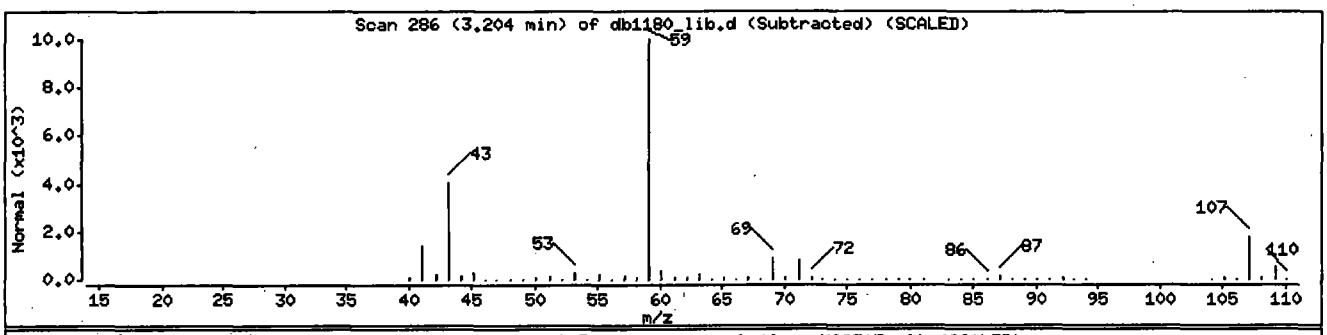
Volume Injected (uL): 1.0

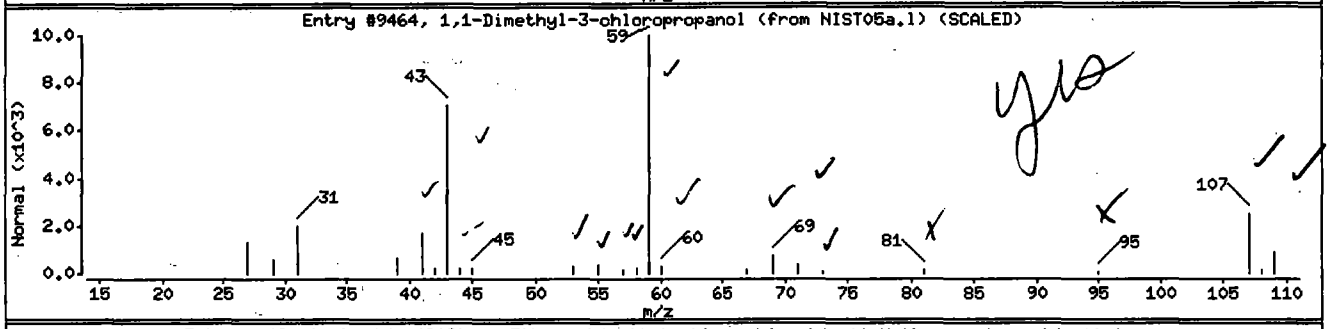
Operator: ceb05247

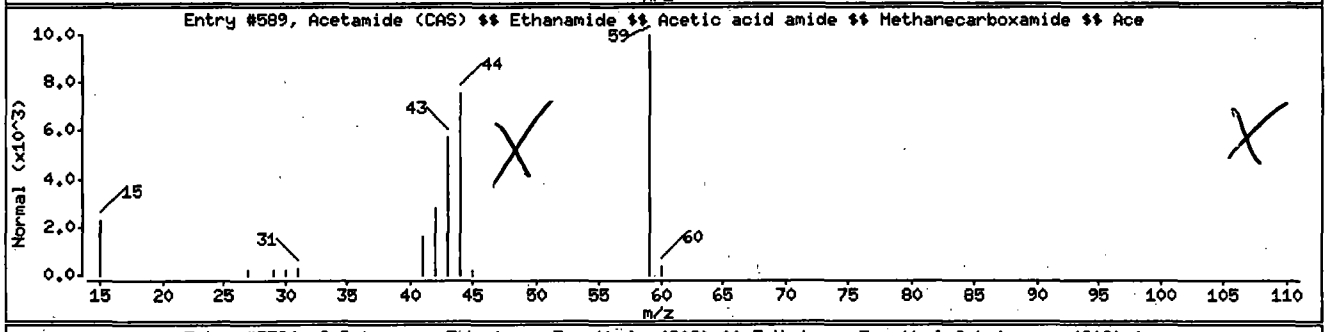
Column phase: J&W DB-5MS

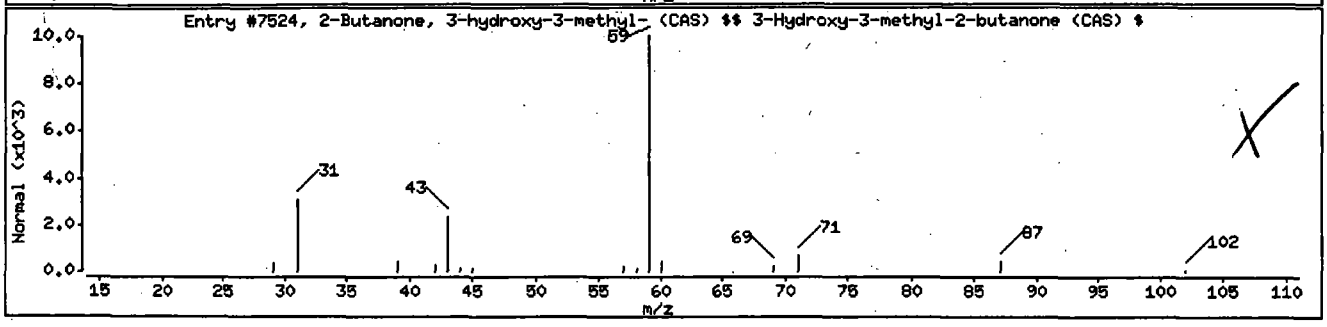
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	83	C5H11Cl0	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	589	42	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	40	C5H10O2	102









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

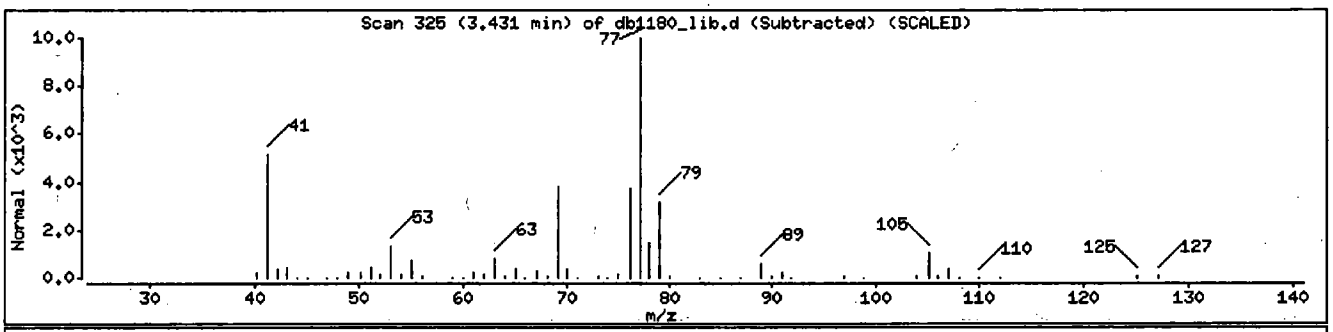
Volume Injected (uL): 1.0

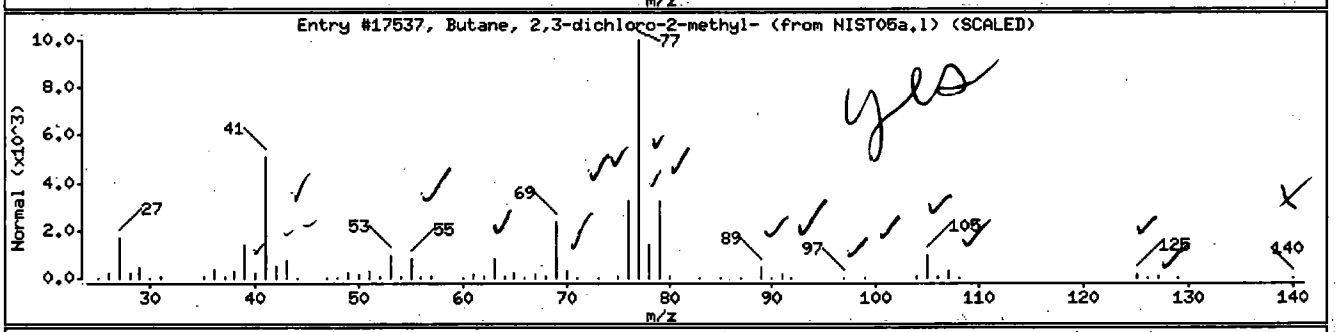
Operator: ceb05247

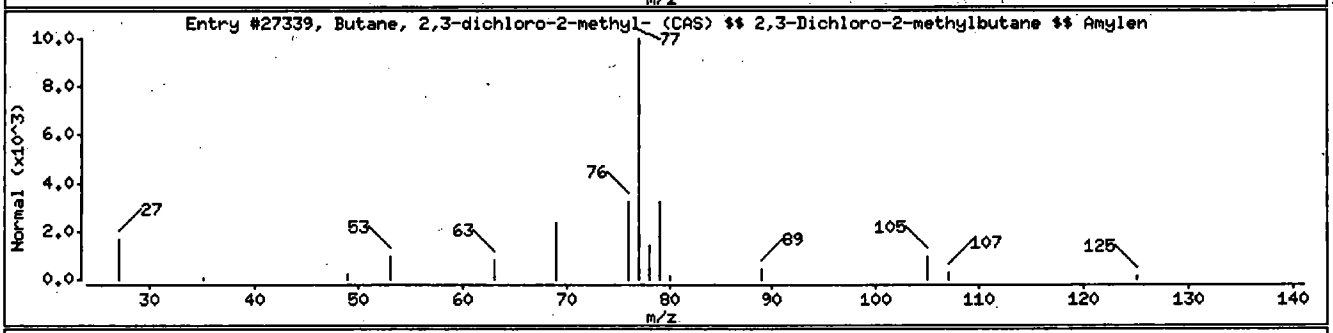
Column phase: J&W DB-5MS

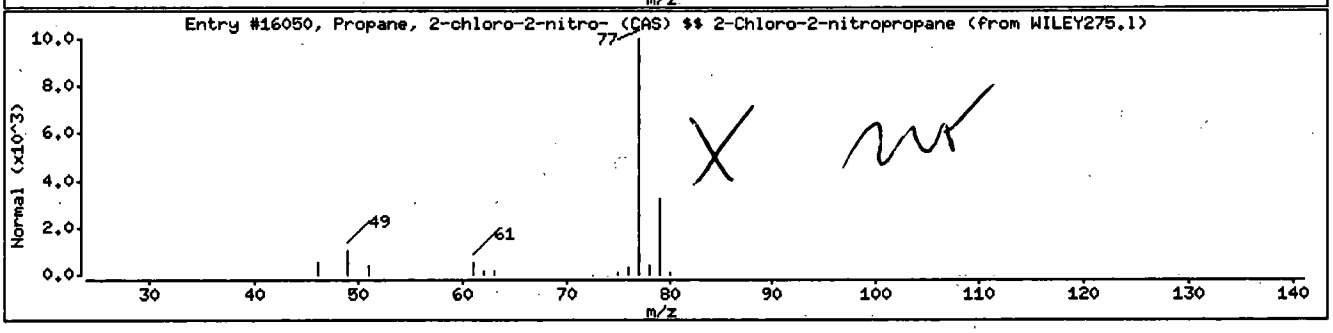
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

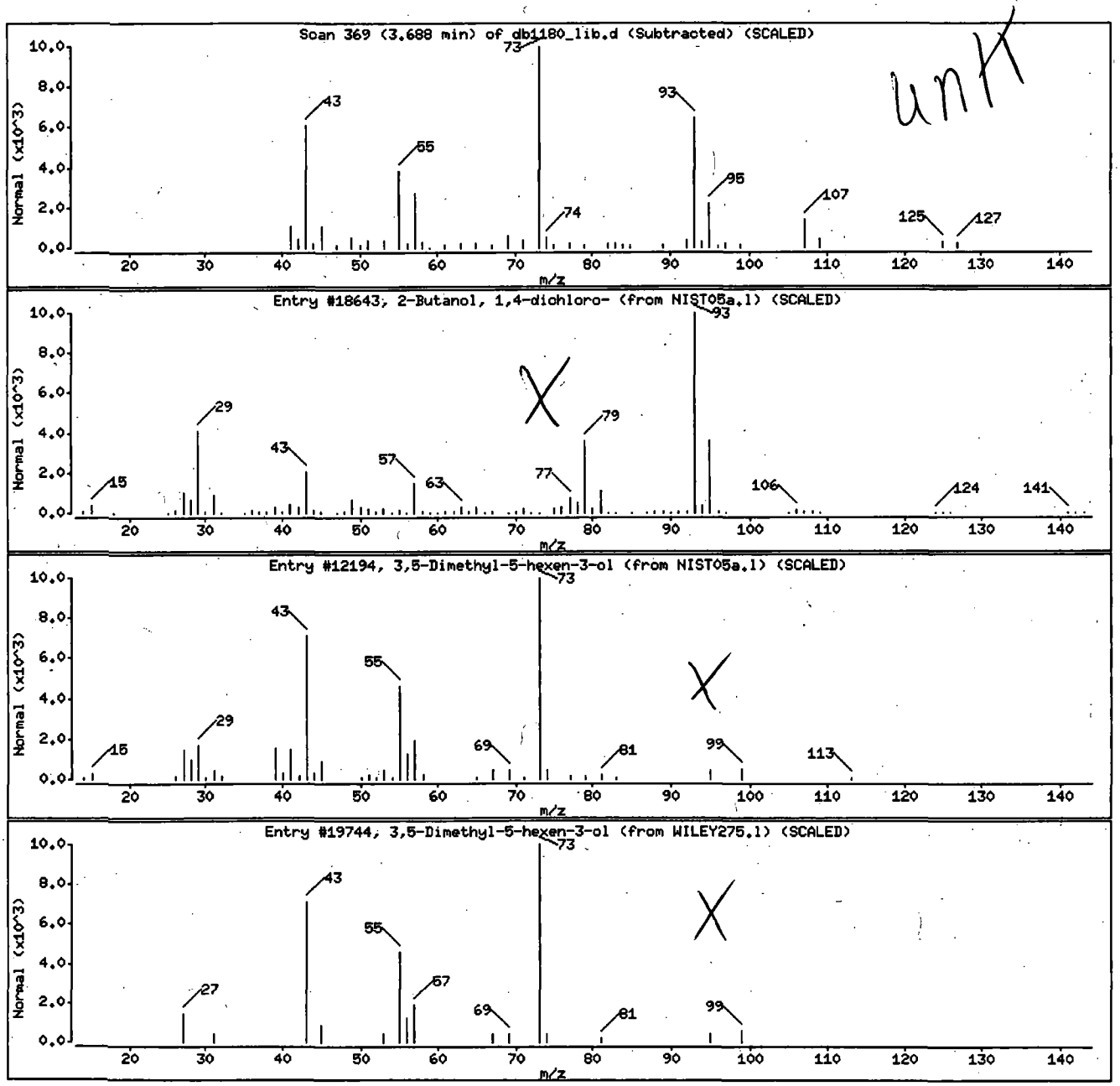
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	32	C4H8Cl2O	142
3,5-Dimethyl-5-hexen-3-ol	1569-46-6	NIST05a.l	12194	12	C8H16O	128
3,5-Dimethyl-5-hexen-3-ol	0-00-0	WILEY275.l	19744	12	C8H16O	128



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

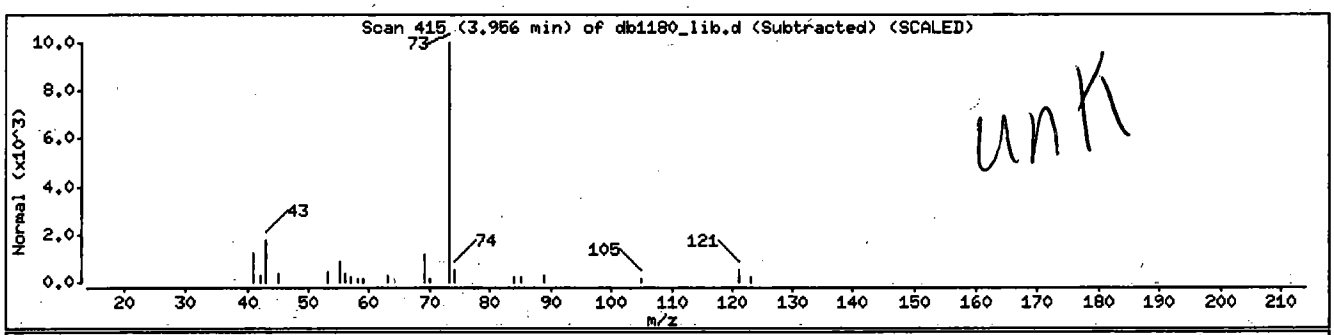
Volume Injected (uL): 1.0

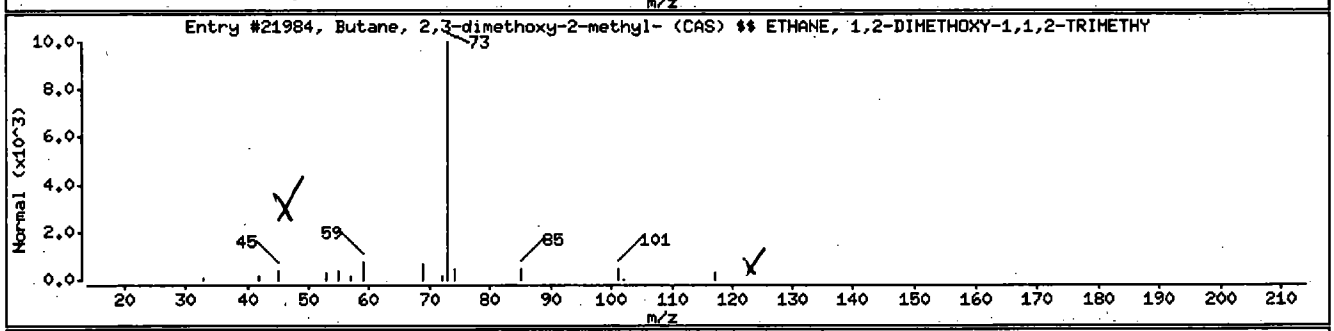
Operator: ceb05247

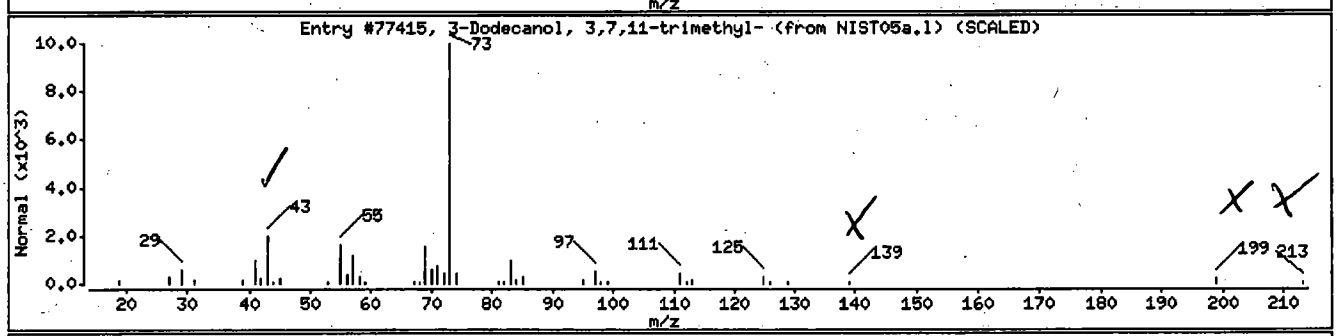
Column phase: J&W DB-5MS

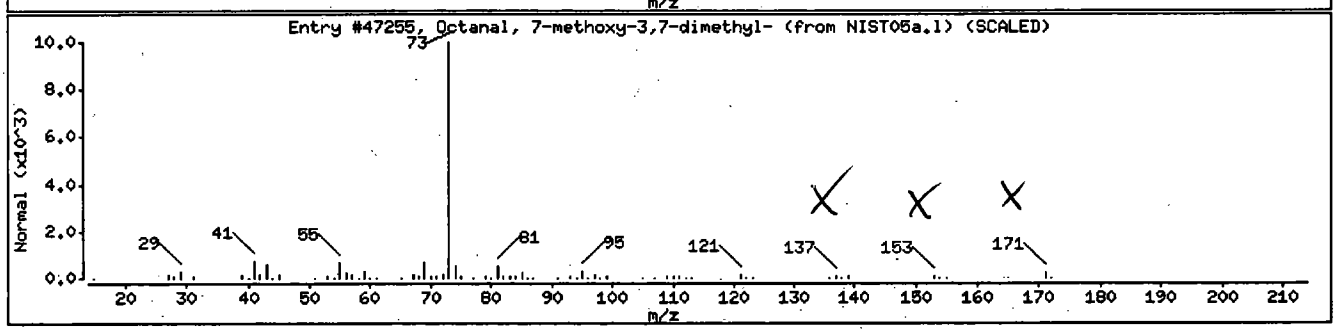
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	38	C7H16O2	132
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	38	C15H32O	228
Octanal, 7-methoxy-3,7-dimethyl-	3613-30-7	NIST05a.l	47255	38	C11H22O2	186









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

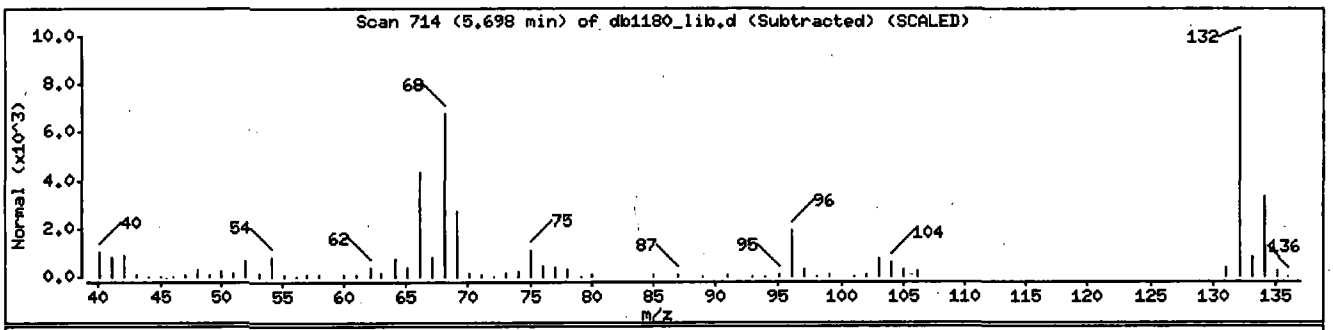
Client ID: H1011 Instrument: HP19760.i

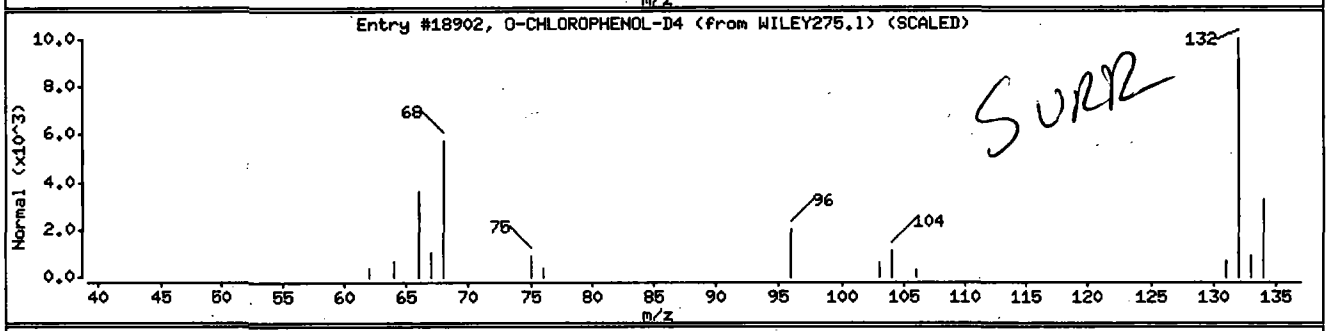
Sample Info: H1011;7369317;1;0;SAMPLE;;;

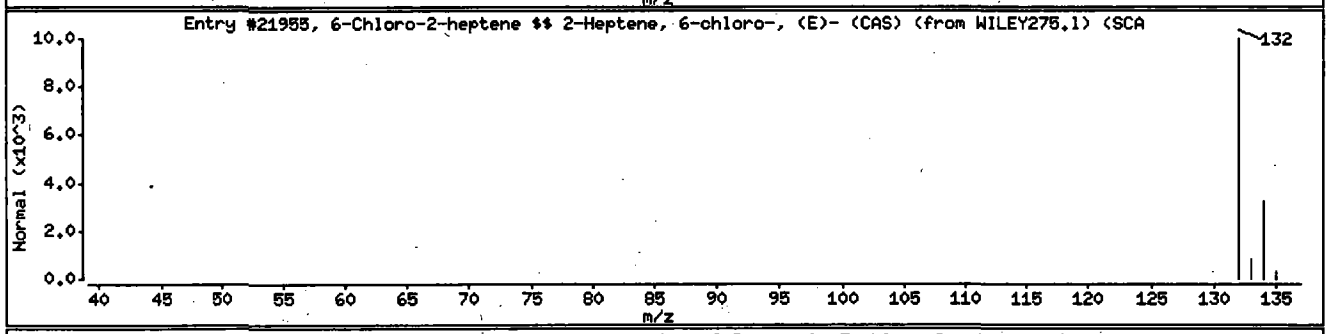
Volume Injected (uL): 1.0 Operator: ceb05247

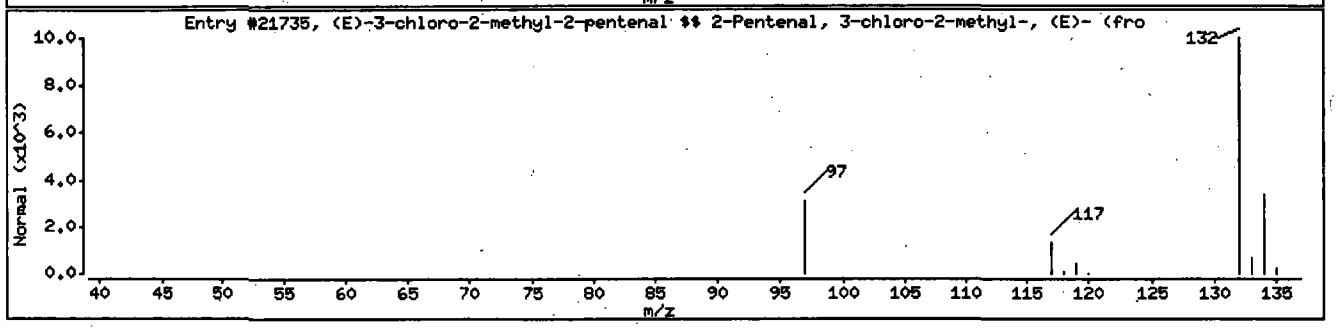
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match .	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

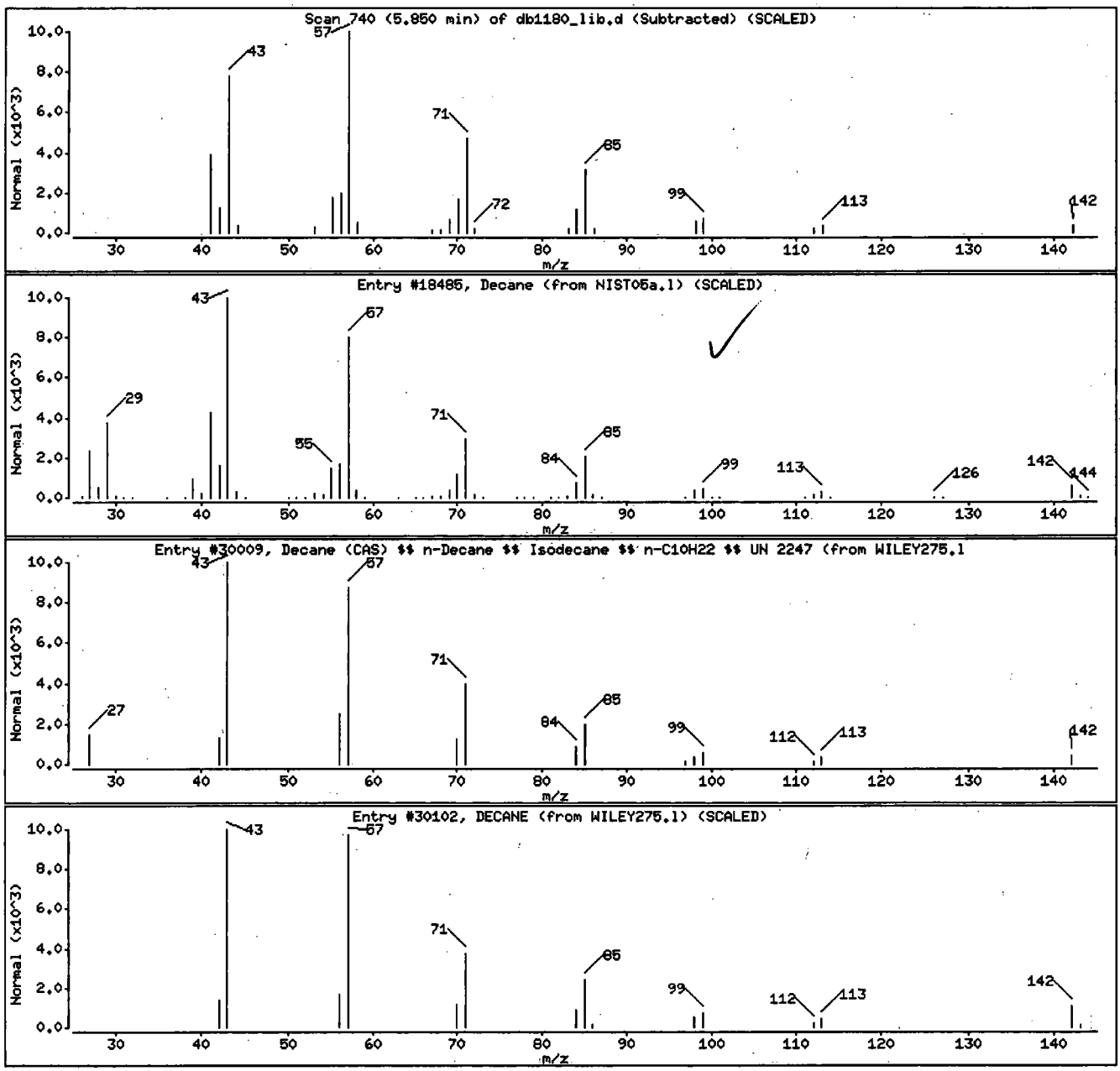
Client ID: H1011 Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30009	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	90	C10H22	142



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

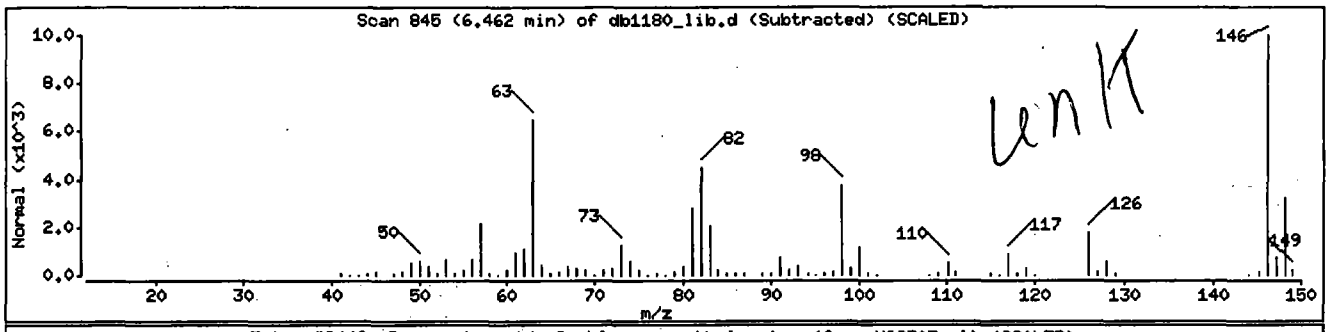
Volume Injected (uL): 1.0

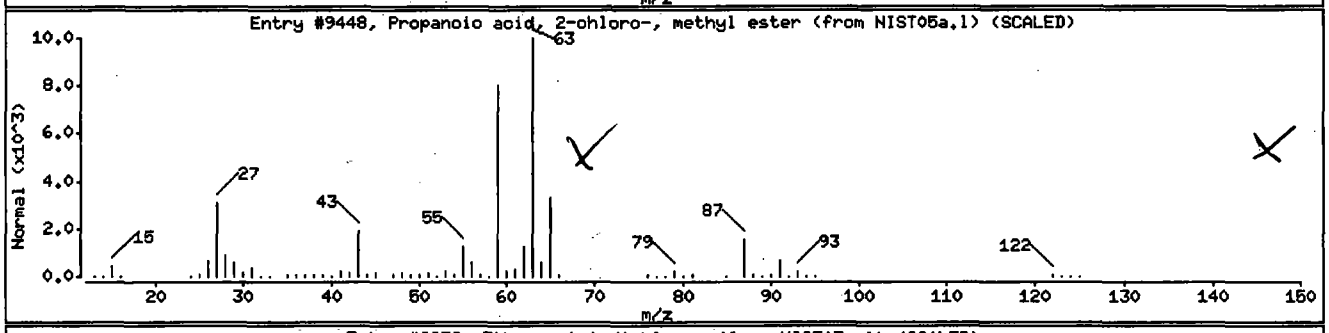
Operator: ceb05247

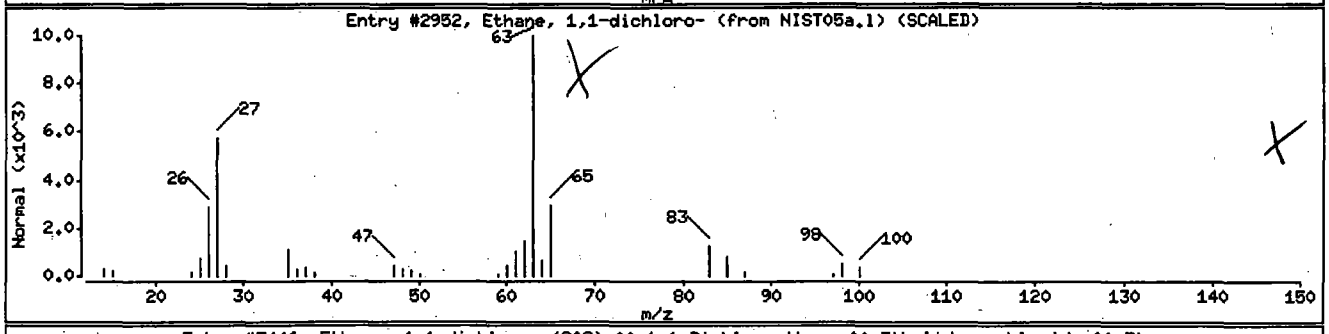
Column phase: J&W DB-5MS

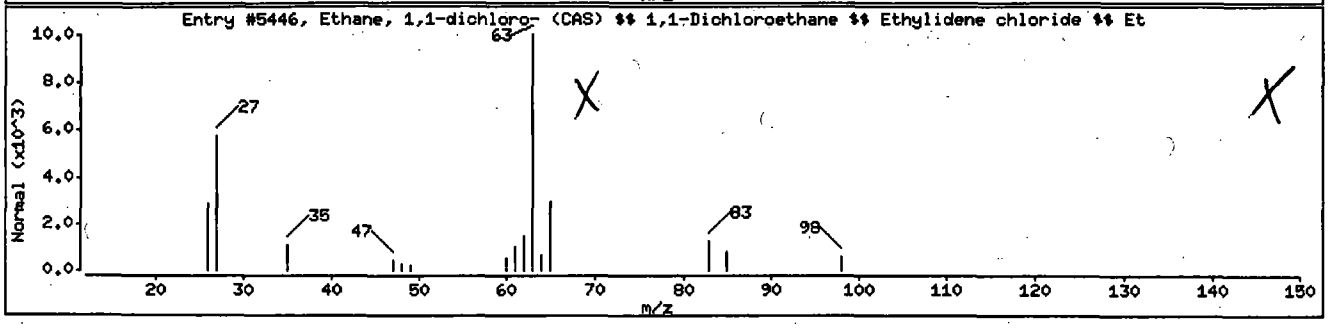
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2952	37	C2H4Cl2	98
Ethane, 1,1-dichloro- (CAS) $$ 1,1-Dichl	75-34-3	WILEY275.l	5446	37	C2H4Cl2	98









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

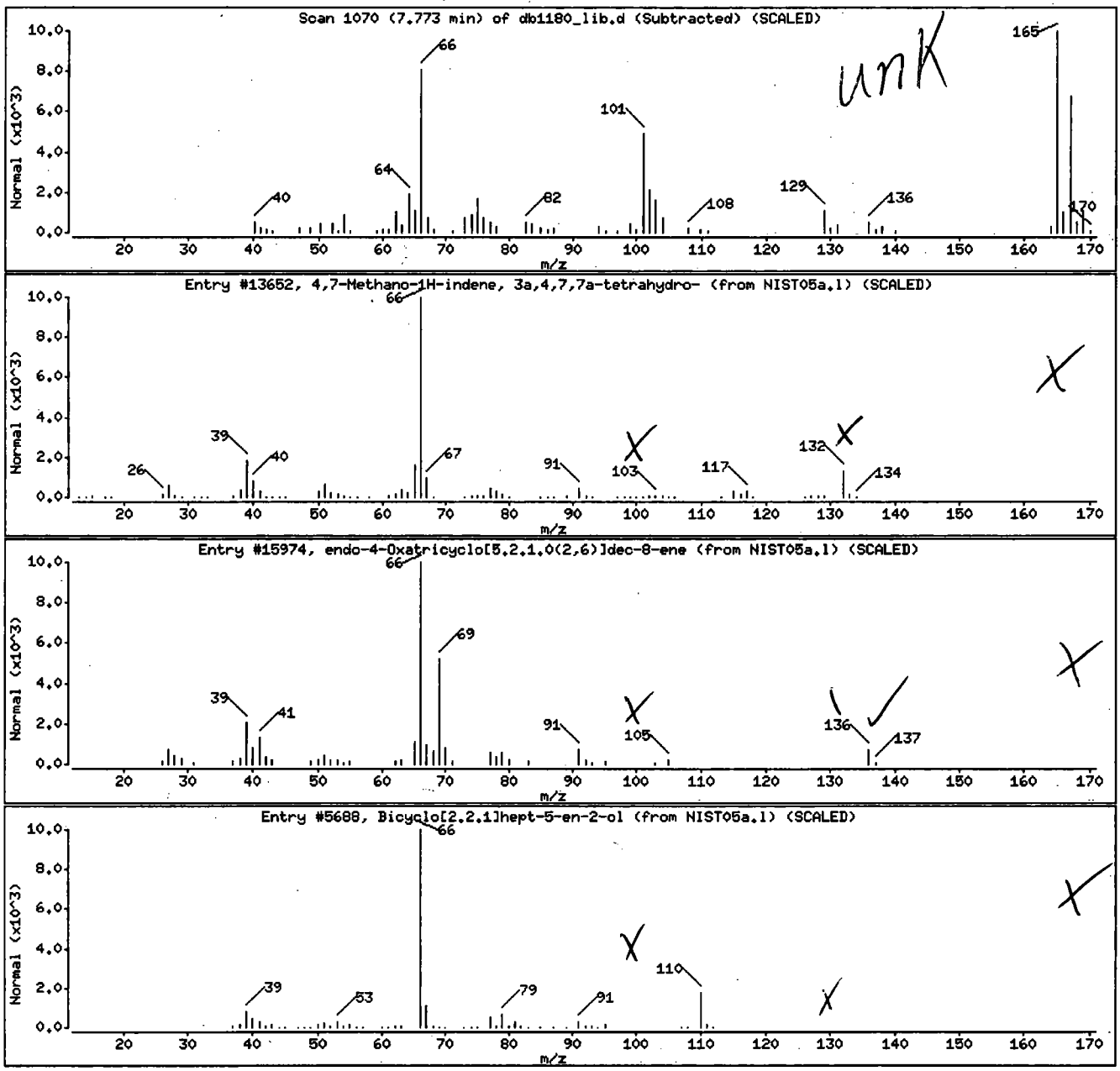
Client ID: H1011 Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	26	C10H12	132
endo-4-Oxatricyclo[5.2.1.0(2,6)]dec-8-en	1528-23-0	NIST05a.l	15974	46	C9H12O	136
Bicyclo[2.2.1]hept-5-en-2-ol	13080-90-5	NIST05a.l	5688	46	C7H10O	110



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

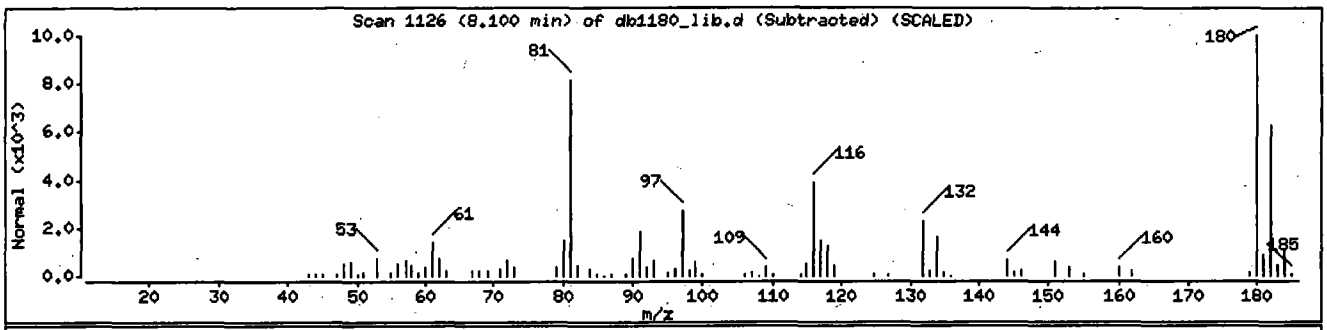
Volume Injected (uL): 1.0

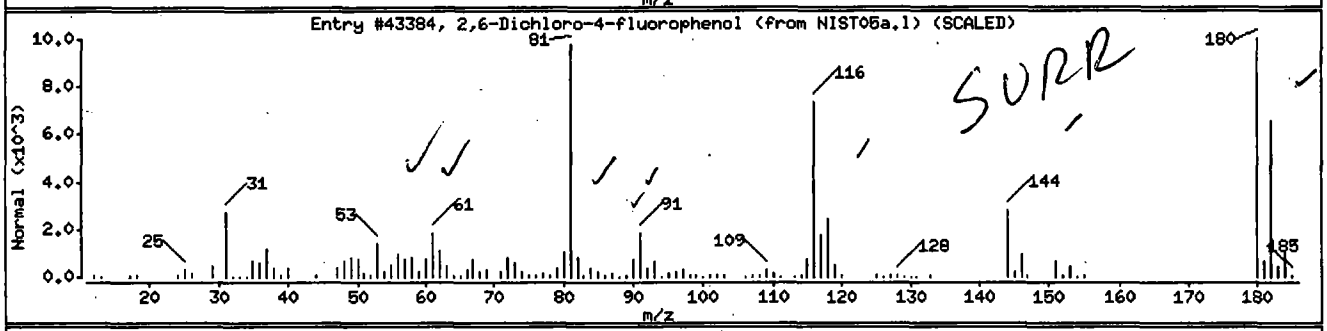
Operator: ceb05247

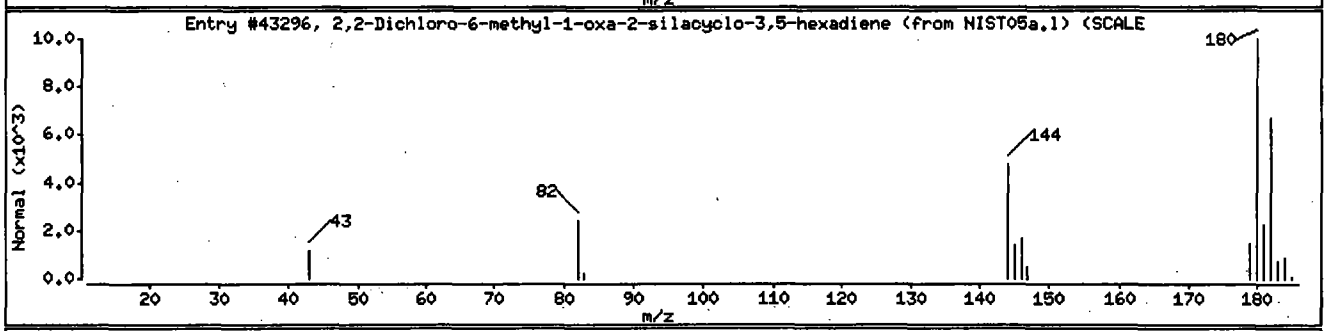
Column phase: J&W DB-5MS

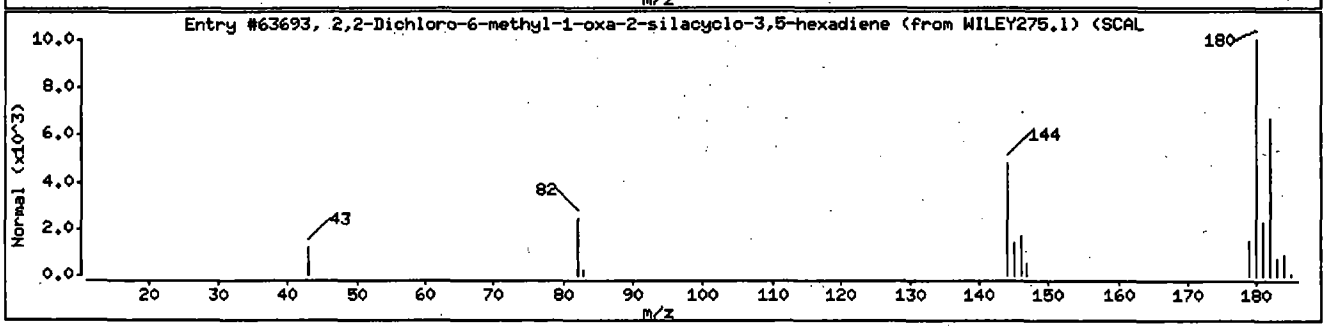
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43384	60	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	27	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	27	C5H6Cl2OSi	180









Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

Client ID: H1011

Instrument: HP19760.i

Sample Info: H1011;7369317;1;0;SAMPLE;;;

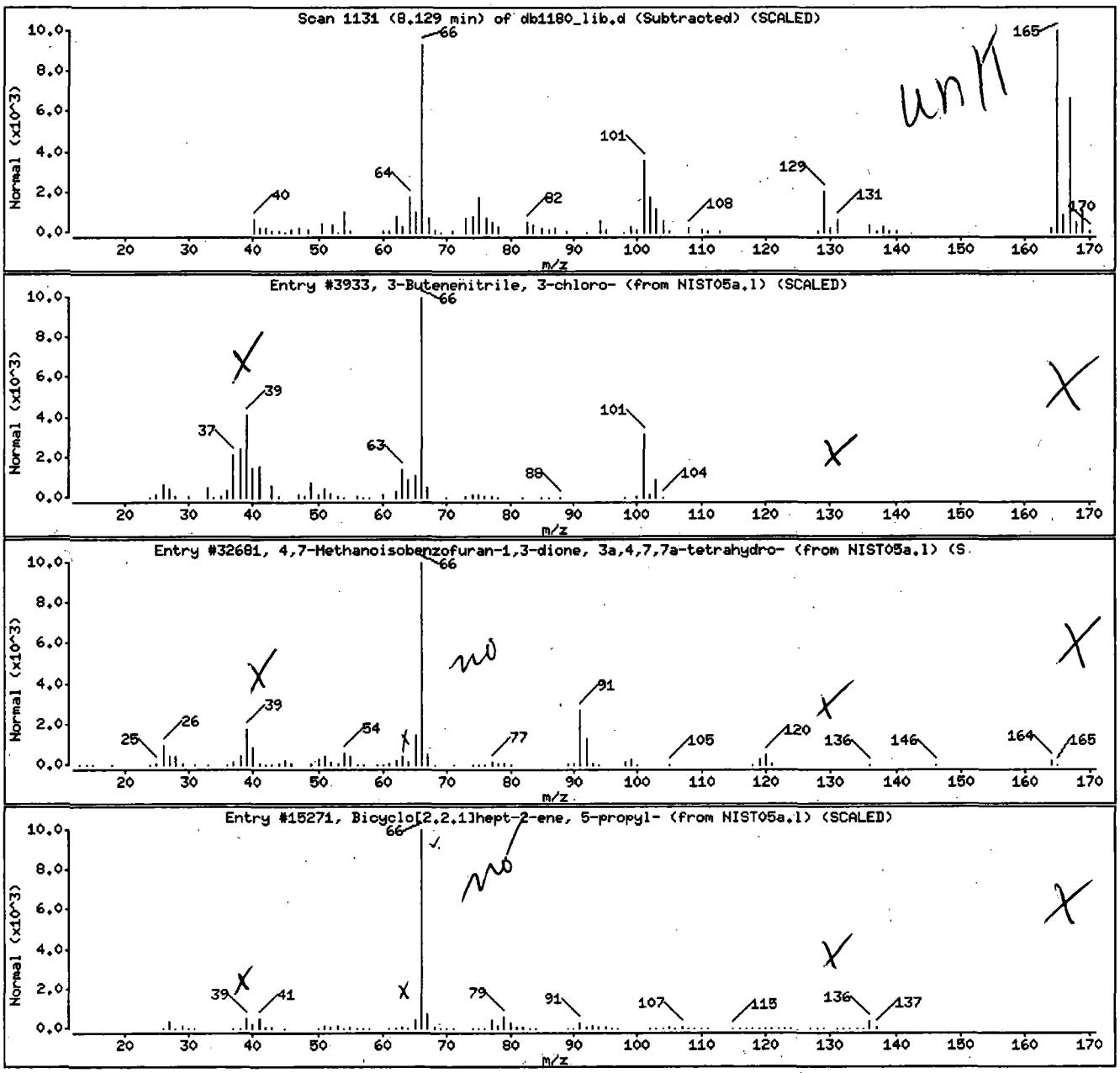
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	50	C4H4ClN	101
4,7-Methanoisobenzofuran-1,3-dione, 3a,4	826-62-0	NIST05a.l	32681	49	C9H8O3	164
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	22094-80-0	NIST05a.l	15271	49	C10H16	136



Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb25a.b/db1180_lib.d

Date : 26-FEB-2014 04:53

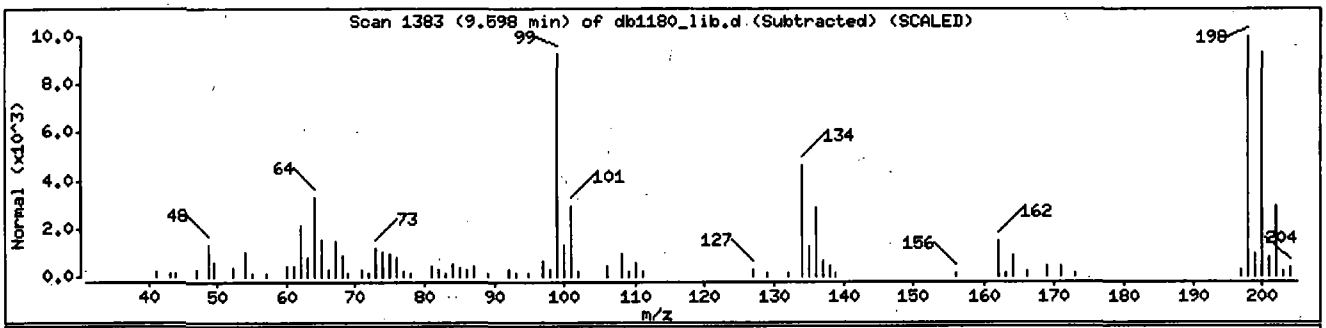
Client ID: H1011 Instrument: HP19760.i

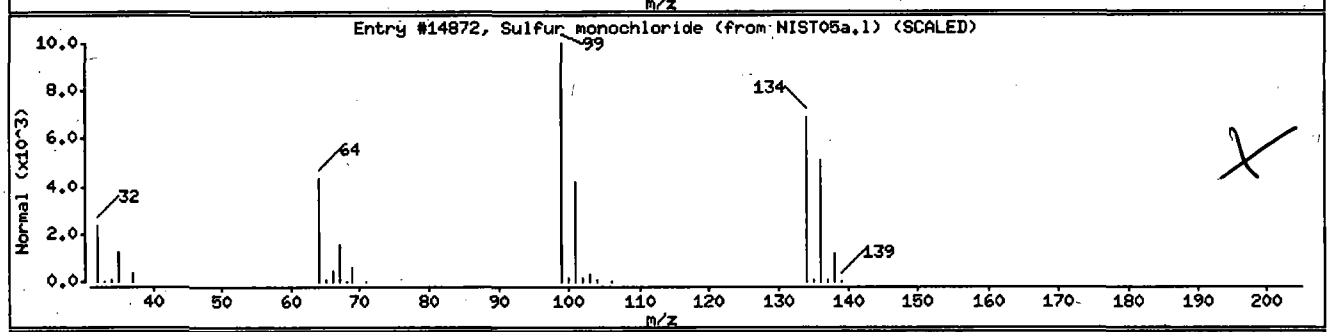
Sample Info: H1011;7369317;1;0;SAMPLE;;;

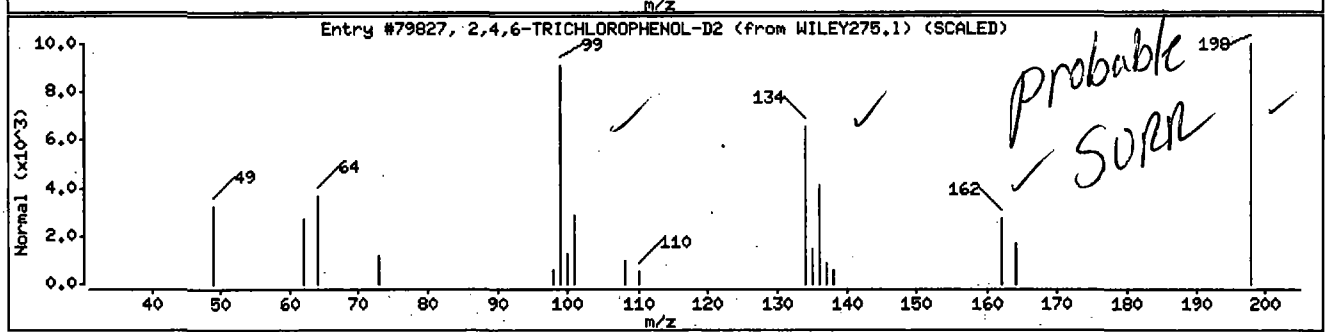
Volume Injected (uL): 1.0 Operator: ceb05247

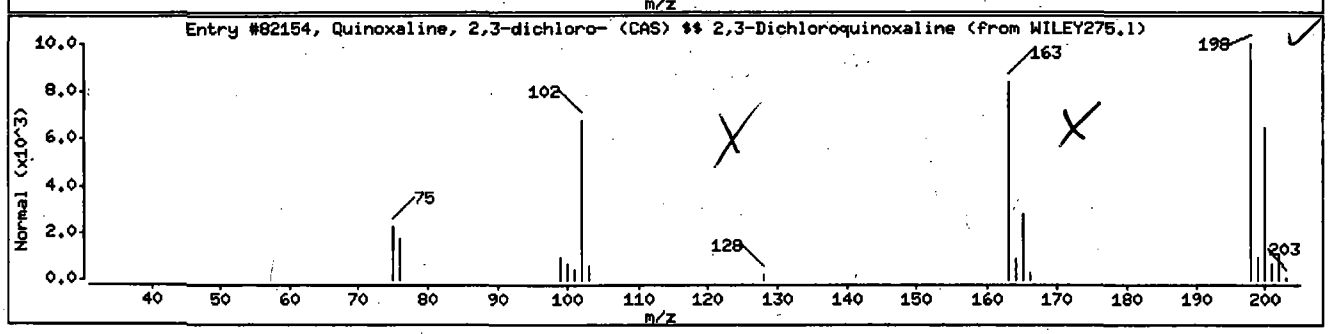
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	18	Cl2S2	134
2,4,6-TRICHLOROPHENOL-D2	0-00-0	WILEY275.l	79827	38	C6HD2Cl3O	198
Quinoxaline, 2,3-dichloro- (CAS) $$ 2,3-	2213-63-0	WILEY275.l	82154	37	C8H4Cl2N2	198



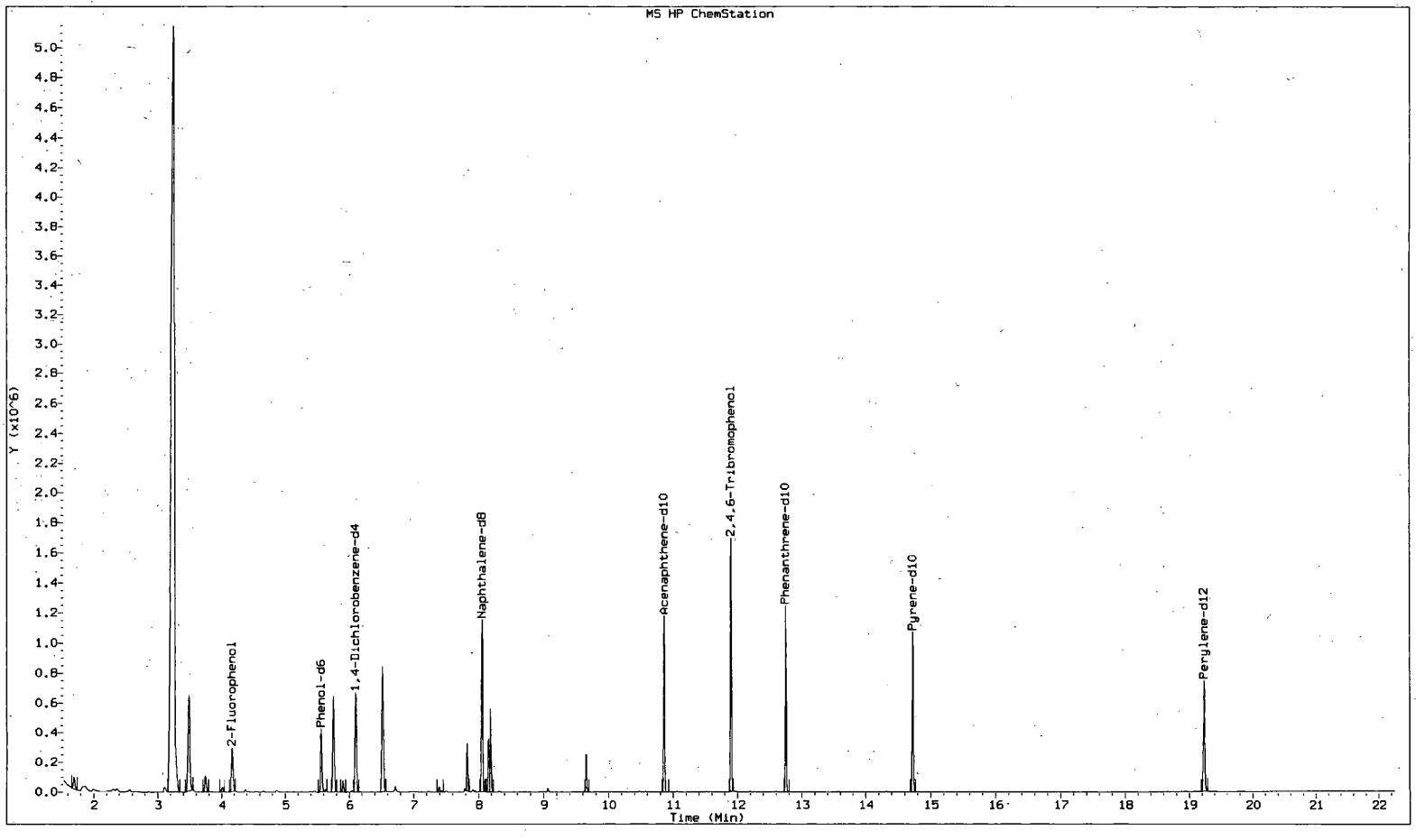






Digitally signed by Andrew J. Strebel on 03/02/2014 at 15:53.
Target 3.5 esignature user ID: ajs00193

File : /chem/HP19760.i/14feb21a.b/db0996_lib.d
Operator : ceb05247
Acquired : 22-FEB-2014 01:43
Instrument : HP19760.i
Sample Name: H1021;7369321;1;0;SAMPLE;;;
Misc Info : 14051WAP;WL13463;;1052;1000;0;db0982;13166;
Vial Number: 17



Lancaster Labs

Data file : /chem/HP19760.i/14feb21a.b/db0996_lib.d
Lab Smp Id: 7369321 Client Smp ID: H1021
Inj Date : 22-FEB-2014 01:43
Operator : ceb05247 Inst ID: HP19760.i
Smp Info : H1021;7369321;1;0;SAMPLE;;;
Misc Info : 14051WAP;WL13463;;1052;1000;0;db0982;13166;
Comment : Max. number of TICs to report is 50, 13 TICs were found initially.
Method : /chem/HP19760.i/14feb21a.b/8270_WVA_lib.m
Meth Date : 02-Mar-2014 14:02 ajs00193 Quant Type: ISTD
Cal Date : 11-FEB-2014 17:36 Cal File: db0387.d
Als bottle: 17
Dil Factor: 1.00000
Integrator: Falcon Compound Sublist: house_lib-376.sub
Target Version: 3.50
Processing Host: d26cs01

Concentration Formula: Amt * DF * Uf * Vt/(Vo) * CpndVariable

Name	Value	Description
DF	1.00000	Dilution Factor
Uf	1.00000	ng unit correction factor
Vt	1000.00000	Volume of final extract (uL)
Vo	1052.00000	Volume of sample extracted (mL)

Cpnd Variable Local Compound Variable

ISTD	RT	AREA	AMOUNT
* 21 1,4-Dichlorobenzene-d4	6.101	991399	10.000
* 48 Naphthalene-d8	8.059	1520973	10.000
* 83 Acenaphthene-d10	10.863	1328084	10.000

CONCENTRATIONS					QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
Methane, bromodichloro-				CAS #: 75-27-4			
1.694	144031	1.45280661	1.38099	90	NIST05a.1	31323	21

Digitally signed by Andrew J. Strebel on 03/02/2014 at 16:21.
Target 3.5 esignature user ID: ajs00193

		CONCENTRATIONS			QUANT		
RT	AREA	ON-COL(ng/ul)	FINAL(ug/L)	QUAL	LIBRARY	LIB ENTRY	CPND #
====	====	==========	==========	====	=======	=========	======
1,1-Dimethyl-3-chloropropanol					CAS #: 1985-88-2		
3.256	17649256	178.023568	169.22392	9	NIST05a.l	9464	21(L)
Butane, 2,3-dichloro-2-methyl-					CAS #: 507-45-9		
3.489	1325267	13.3676372	12.70687	83	NIST05a.l	17537	21
2-Butanol, 1,4-dichloro-					CAS #: 2419-74-1		
3.746	195875	1.97573959	1.87807	37	NIST05a.l	18643	21
Butane, 2,3-dimethoxy-2-methyl-					CAS #: 74421-00-4		
4.014	58404	0.58910634	0.55998	33	NIST05a.l	13998	21
O-CHLOROPHENOL-D4					CAS #: 0-00-0		
5.757	950792	9.59039320	9.11634	91	WILEY275.l	18902	21
Decane					CAS #: 124-18-5		
5.902	112153	1.13125809	1.07534	95	NIST05a.l	18485	21
Propanoic acid, 2-chloro-, methyl ester					CAS #: 17639-93-9		
6.520	1298171	13.0943240	12.44707	35	NIST05a.l	9448	21
Cyclopentasiloxane, decamethyl-					CAS #: 541-02-6		
7.394	53722	0.35320881	0.33574	83	NIST05a.l	161016	48
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy					CAS #: 77-73-6		
7.826	383996	2.52467601	2.39988	43	NIST05a.l	13652	48(L)
2,6-Dichloro-4-fluorophenol					CAS #: 392-71-2		
8.158	405090	2.66335896	2.53171	60	NIST05a.l	43384	48
3-Butenenitrile, 3-chloro-					CAS #: 21031-46-9		
8.187	683215	4.49195949	4.26992	40	NIST05a.l	3933	48(L)
Sulfur monochloride					CAS #: 10025-67-9		
9.650	302983	2.28135388	2.16858	38	NIST05a.l	14872	83

QC Flag Legend

L - Operator selected an alternate library search match.

Digitally signed by Andrew J. Strebel on 03/02/2014 at 16:21.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

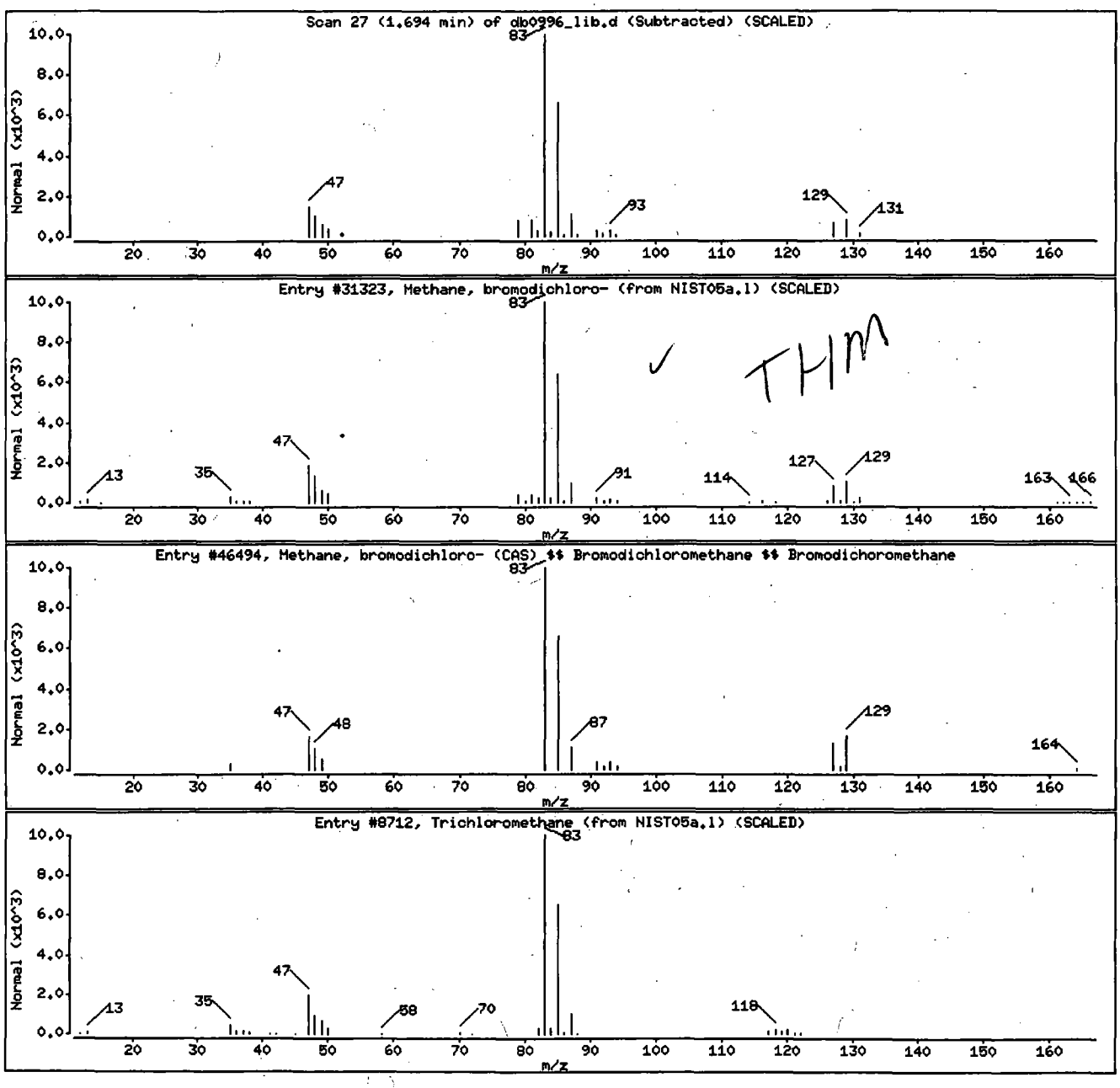
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Methane, bromodichloro-	75-27-4	NIST05a.l	31323	90	CHBrCl2	162
Methane, bromodichloro- (CAS) $$ Bromodi	75-27-4	WILEY275.l	46494	83	CHBrCl2	162
Trichloromethane	67-66-3	NIST05a.l	8712	78	CHCl3	118



Digitally signed by Andrew J. Strebel on 03/02/2014 at 16:21.
Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

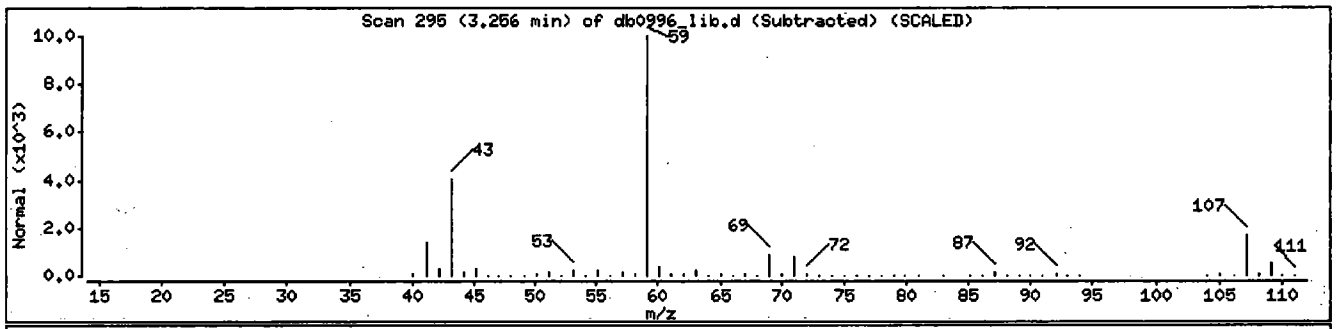
Volume Injected (uL): 1.0

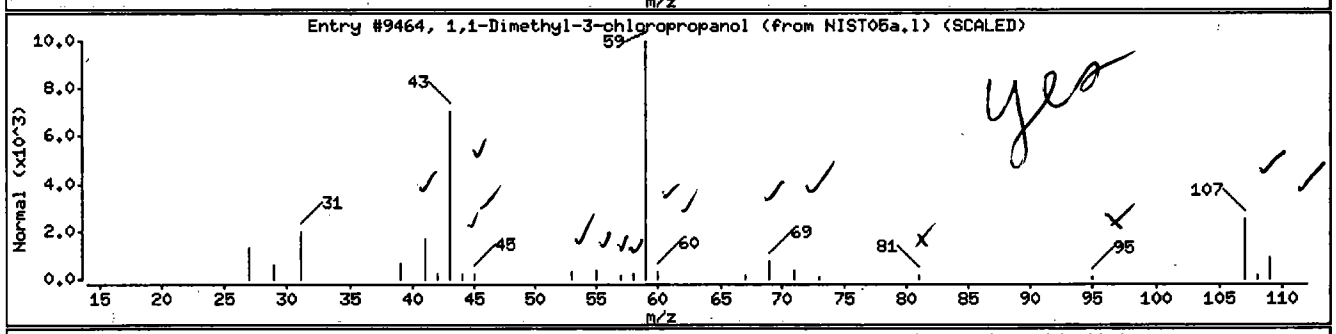
Operator: ceb05247

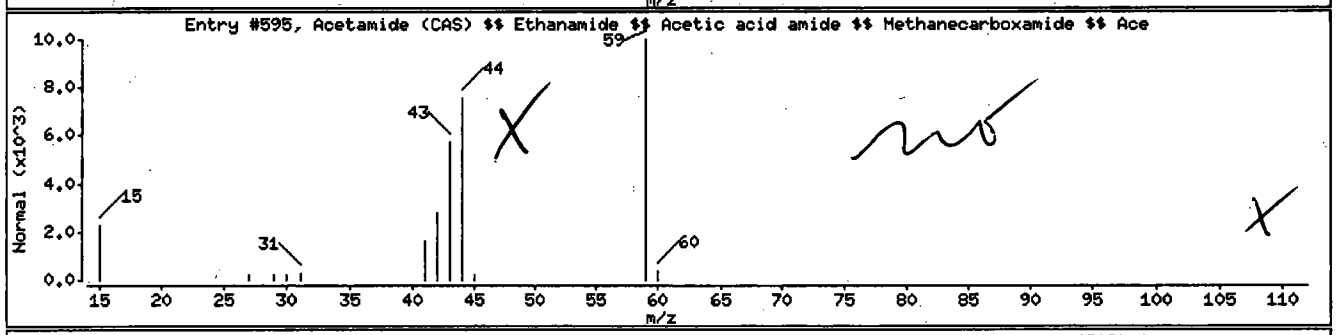
Column phase: J&W DB-5MS

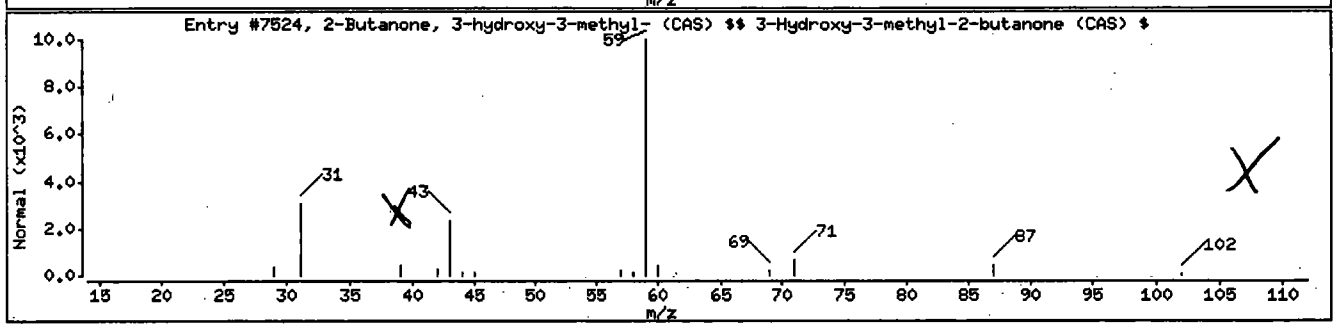
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
1,1-Dimethyl-3-chloropropanol	1985-88-2	NIST05a.l	9464	9	C5H11ClO	122
Acetamide (CAS) $$ Ethanamide $$ Acetic	60-35-5	WILEY275.l	595	45	C2H5NO	59
2-Butanone, 3-hydroxy-3-methyl- (CAS) $$	115-22-0	WILEY275.l	7524	42	C5H10O2	102









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

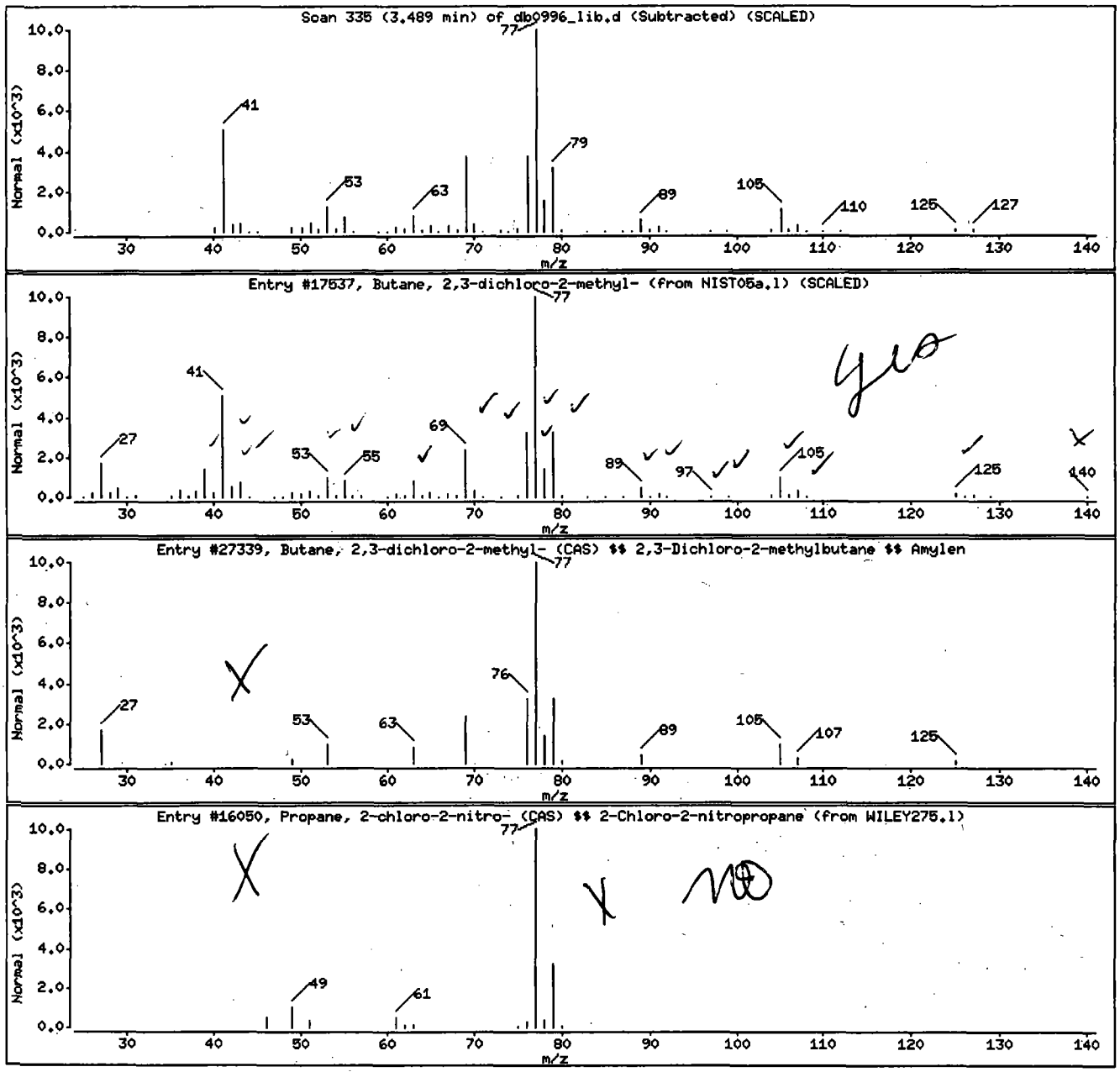
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dichloro-2-methyl-	507-45-9	NIST05a.l	17537	83	C5H10Cl2	140
Butane, 2,3-dichloro-2-methyl- (CAS) $$	507-45-9	WILEY275.l	27339	83	C5H10Cl2	140
Propane, 2-chloro-2-nitro- (CAS) $$ 2-Ch	594-71-8	WILEY275.l	16050	33	C3H6ClNO2	123



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Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

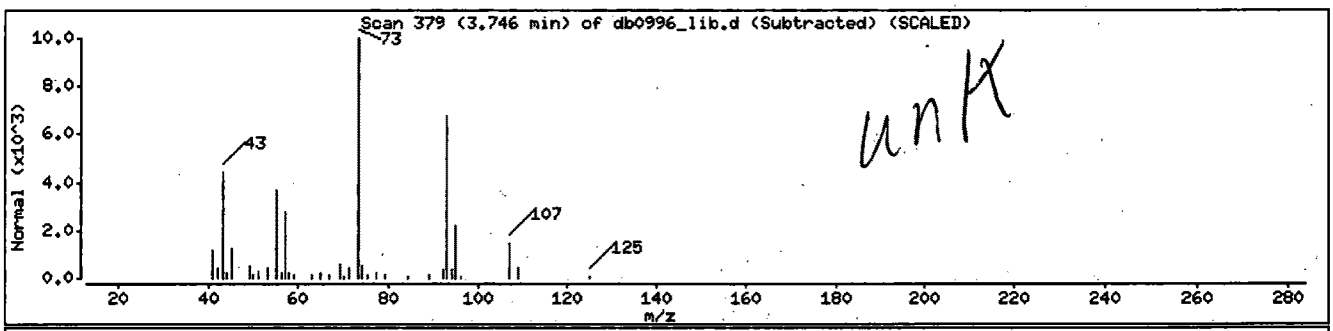
Client ID: H1021 Instrument: HP19760.i

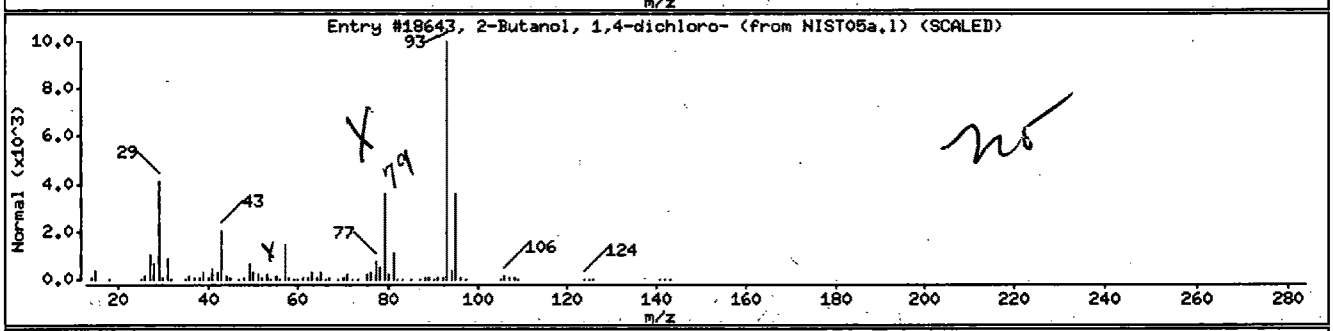
Sample Info: H1021;7369321;1;0;SAMPLE;;;

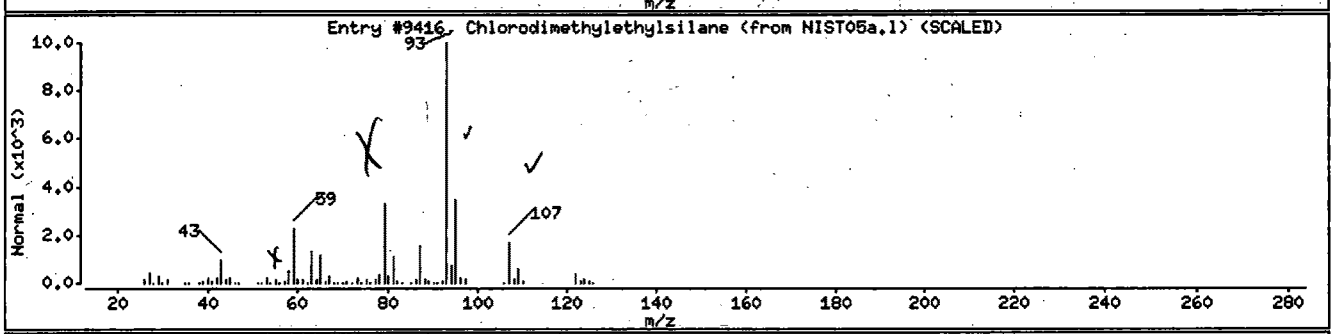
Volume Injected (uL): 1.0 Operator: ceb05247

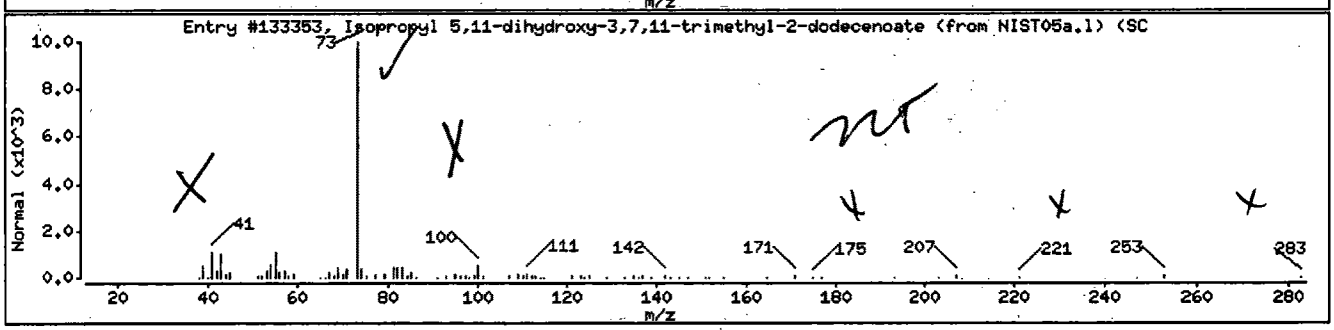
Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2-Butanol, 1,4-dichloro-	2419-74-1	NIST05a.l	18643	37	C4H8Cl2O	142
Chlorodimethylethylsilane	6917-76-6	NIST05a.l	9416	33	C4H11ClSi	122
Isopropyl 5,11-dihydroxy-3,7,11-trimethy	1000223-34-1	NIST05a.l	133353	9	C18H34O4	314









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

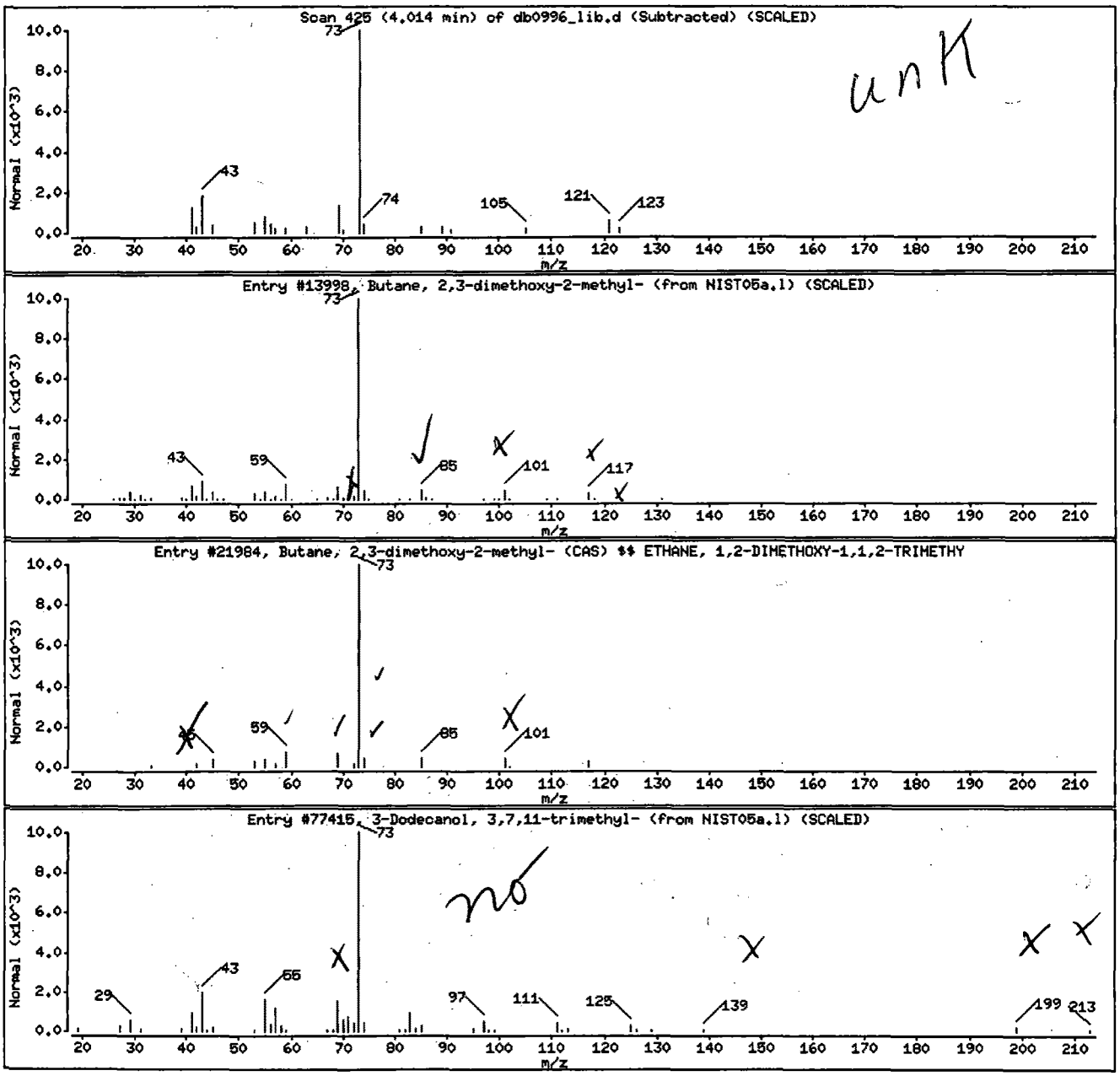
Client ID: H1021 Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Butane, 2,3-dimethoxy-2-methyl-	74421-00-4	NIST05a.l	13998	33	C7H16O2	132
Butane, 2,3-dimethoxy-2-methyl- (CAS) $$	74421-00-4	WILEY275.l	21984	33	C7H16O2	132
3-Dodecanol, 3,7,11-trimethyl-	7278-65-1	NIST05a.l	77415	9	C15H32O	228



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

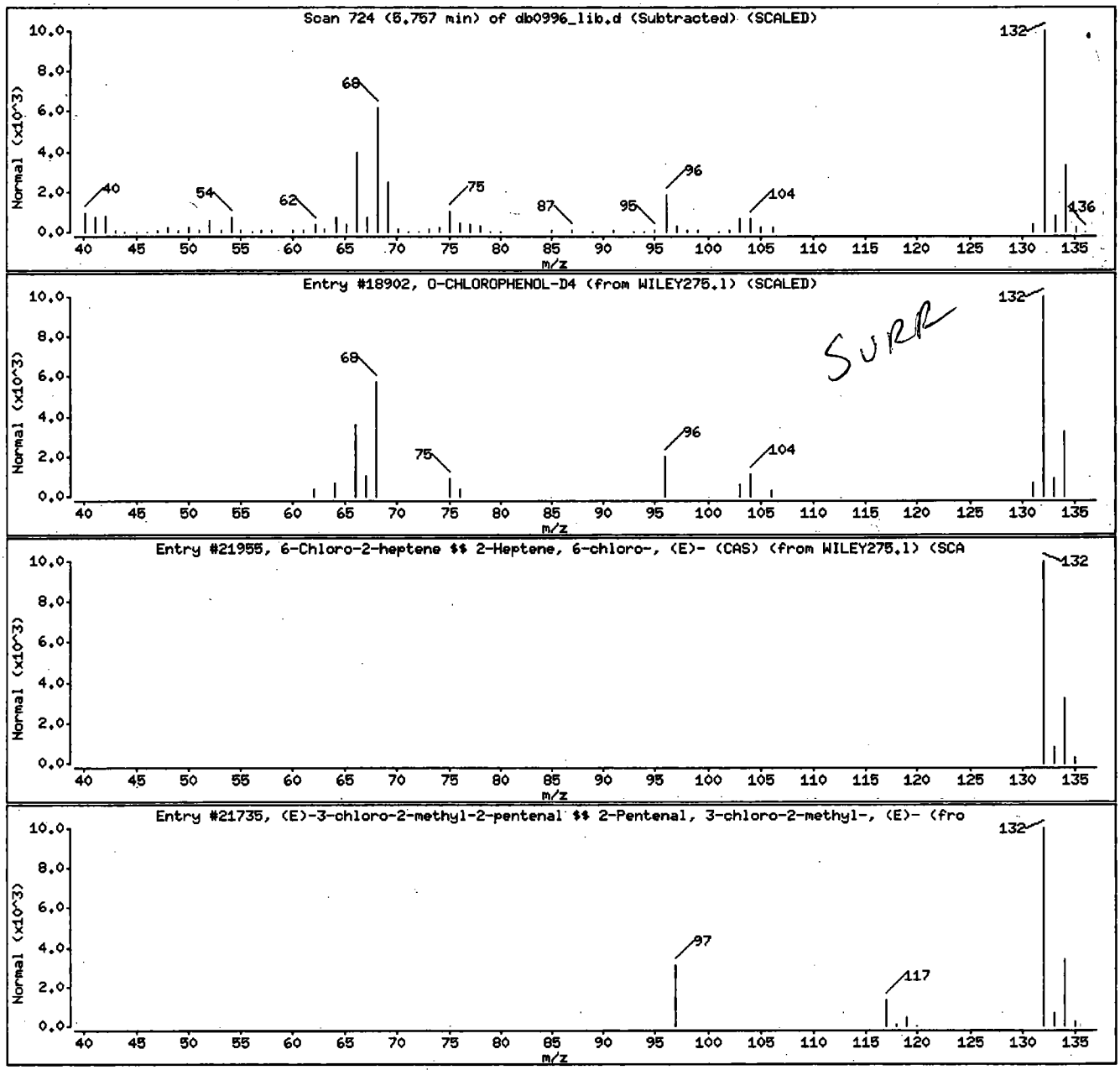
Client ID: H1021 Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

Volume Injected (uL): 1.0 Operator: ceb05247

Column phase: J&W DB-5MS Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
O-CHLOROPHENOL-D4	0-00-0	WILEY275.1	18902	91	C6HD4ClO	132
6-Chloro-2-heptene $$ 2-Heptene, 6-chlor	92639-28-6	WILEY275.1	21955	83	C7H13Cl	132
(E)-3-chloro-2-methyl-2-pentenal $$ 2-Pe	31357-76-3	WILEY275.1	21735	72	C6H9ClO	132



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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

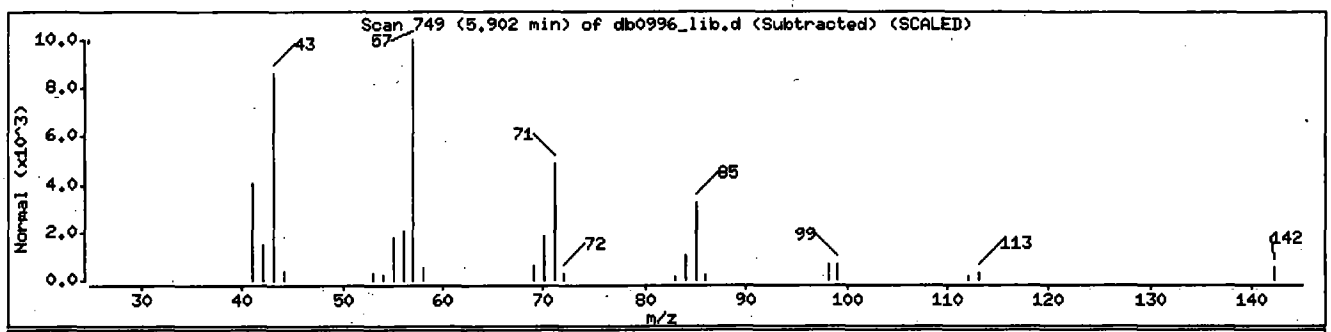
Volume Injected (uL): 1.0

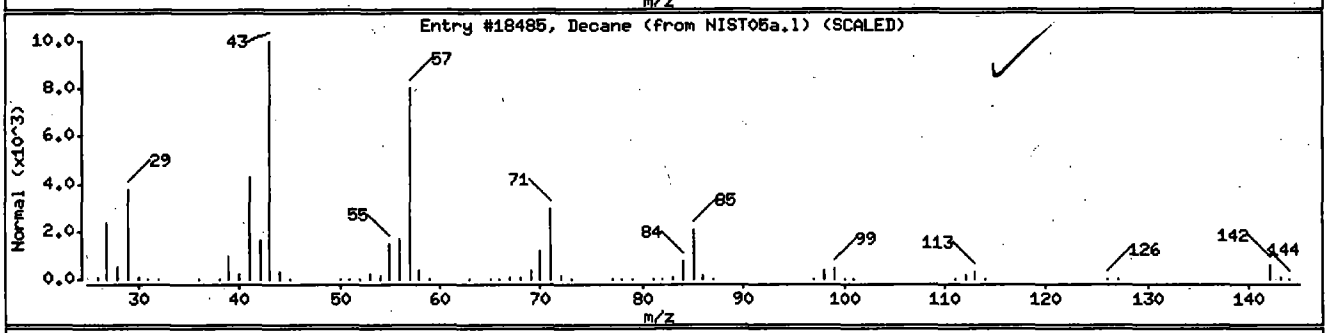
Operator: ceb05247

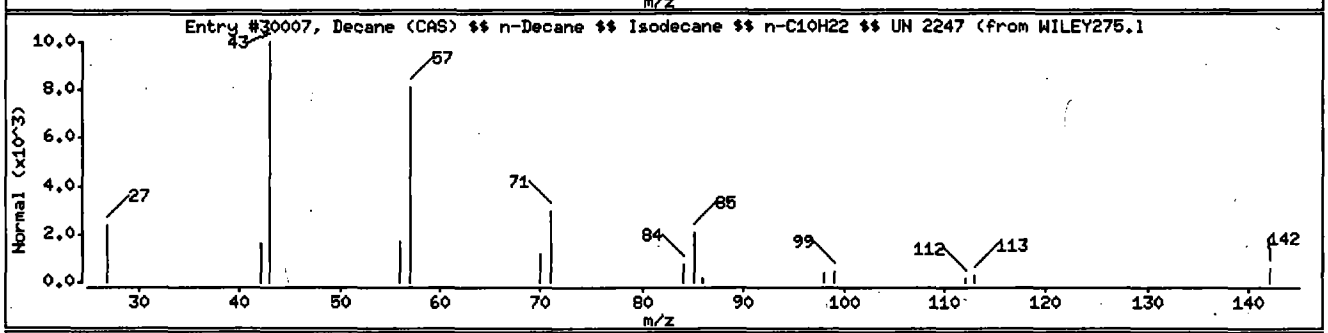
Column phase: J&W DB-5MS

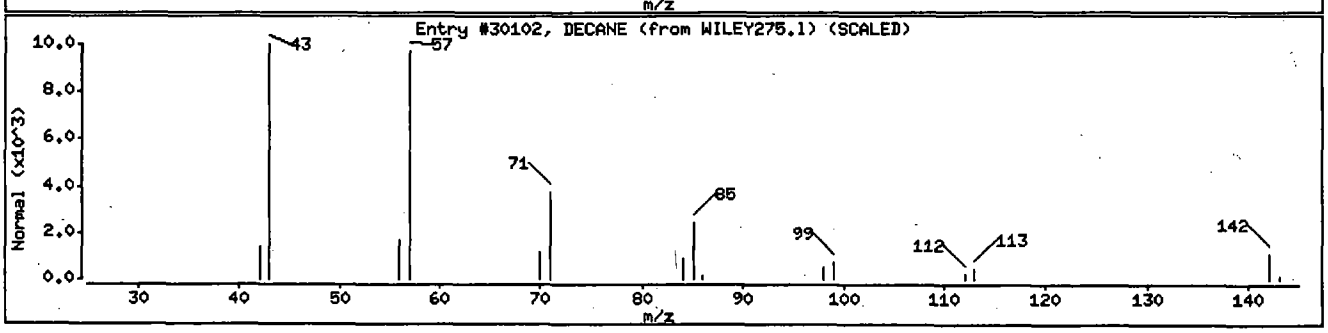
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Decane	124-18-5	NIST05a.l	18485	95	C10H22	142
Decane (CAS) $$ n-Decane $$ Isodecane $$	124-18-5	WILEY275.l	30007	95	C10H22	142
DECANE	0-00-0	WILEY275.l	30102	91	C10H22	142









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

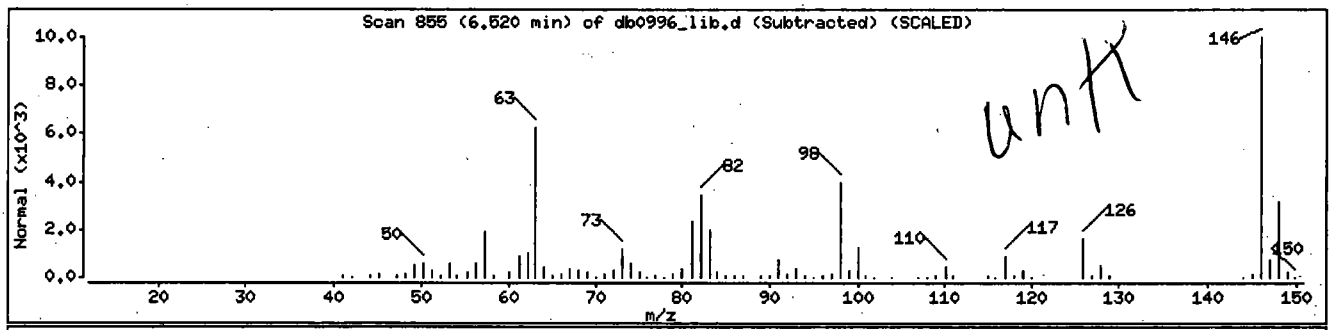
Volume Injected (uL): 1.0

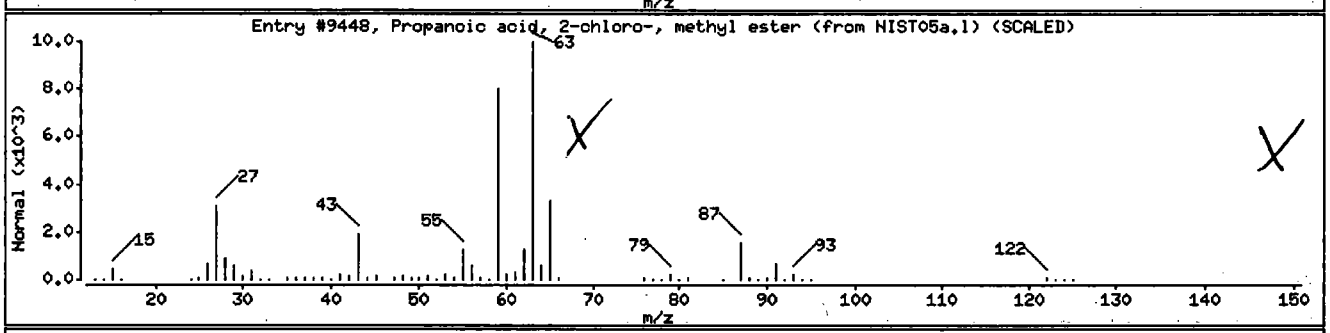
Operator: ceb05247

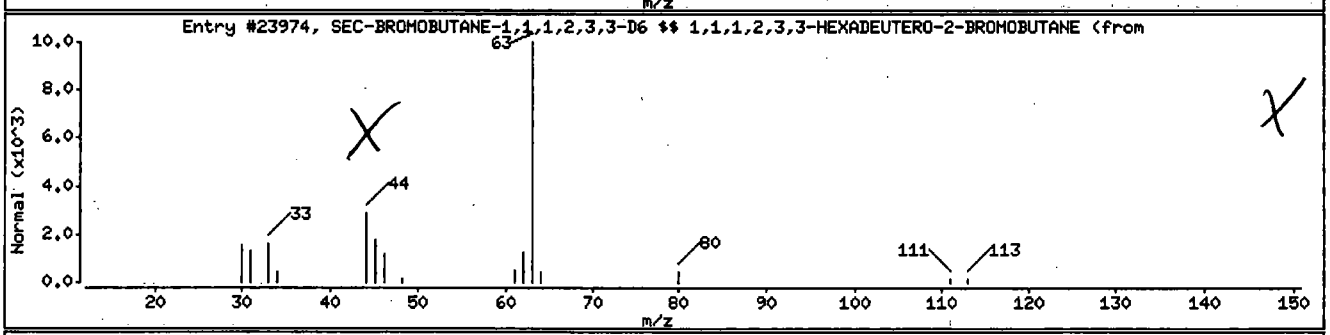
Column phase: J&W DB-5MS

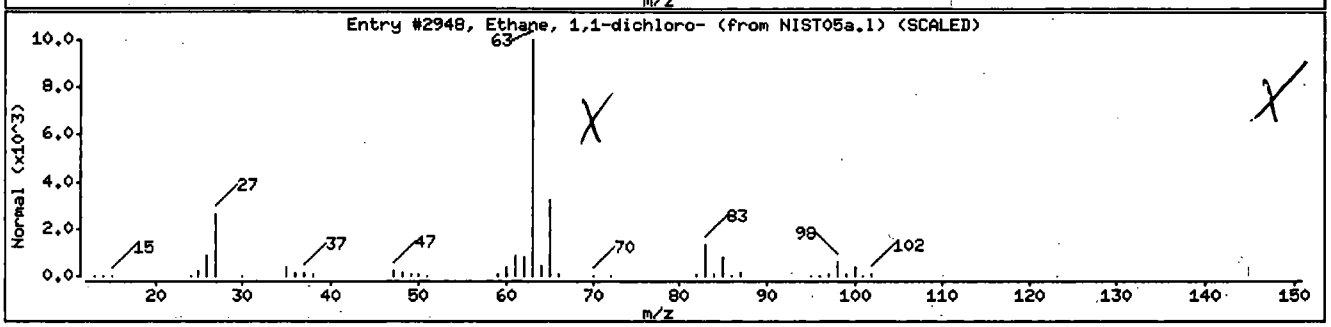
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Propanoic acid, 2-chloro-, methyl ester	17639-93-9	NIST05a.l	9448	35	C4H7ClO2	122
SEC-BROMOBUTANE-1,1,1,2,3,3-D6 $$ 1,1,1,	53966-37-3	WILEY275.l	23974	25	C4H3D6Br	142
Ethane, 1,1-dichloro-	75-34-3	NIST05a.l	2948	23	C2H4Cl2	98









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Target 3.5 esignature user ID: ajs00193

Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

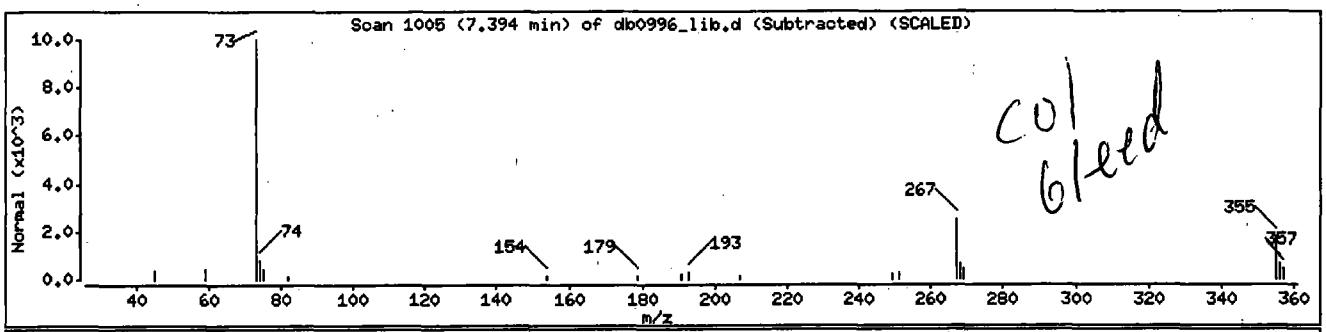
Volume Injected (uL): 1.0

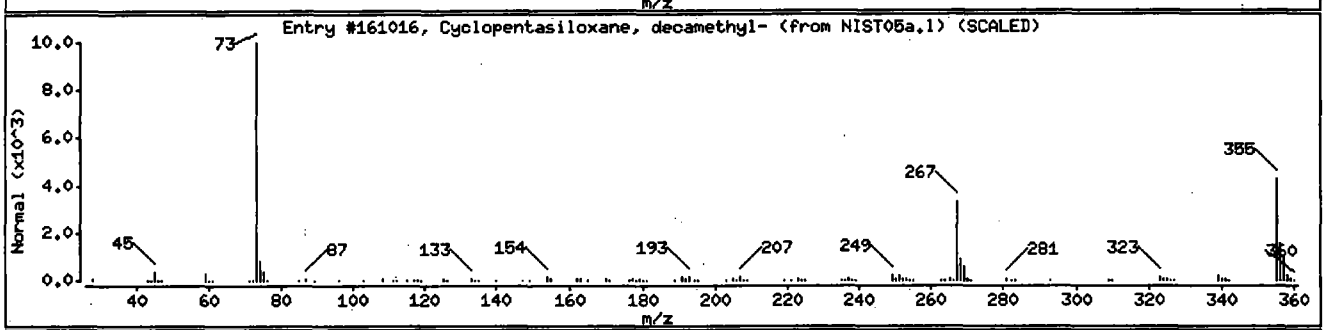
Operator: ceb05247

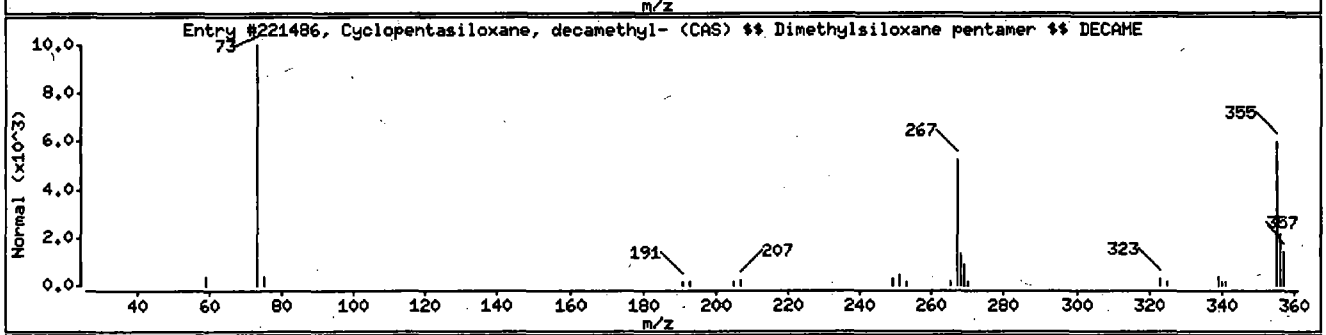
Column phase: J&W DB-5MS

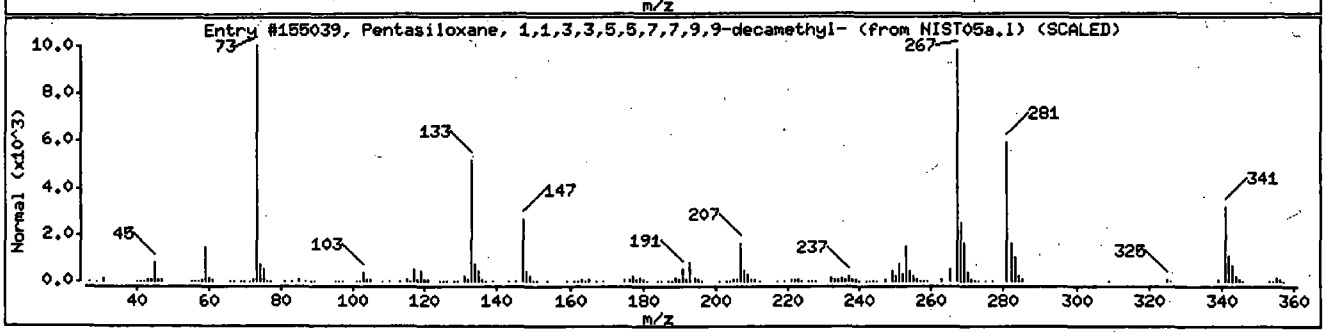
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Cyclopentasiloxane, decamethyl-	541-02-6	NIST05a.l	161016	83	C10H30O5Si5	370
Cyclopentasiloxane, decamethyl- (CAS) $$	541-02-6	WILEY275.l	221486	83	C10H30O5Si5	370
Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decam	995-83-5	NIST05a.l	155039	45	C10H32O4Si5	366









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Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

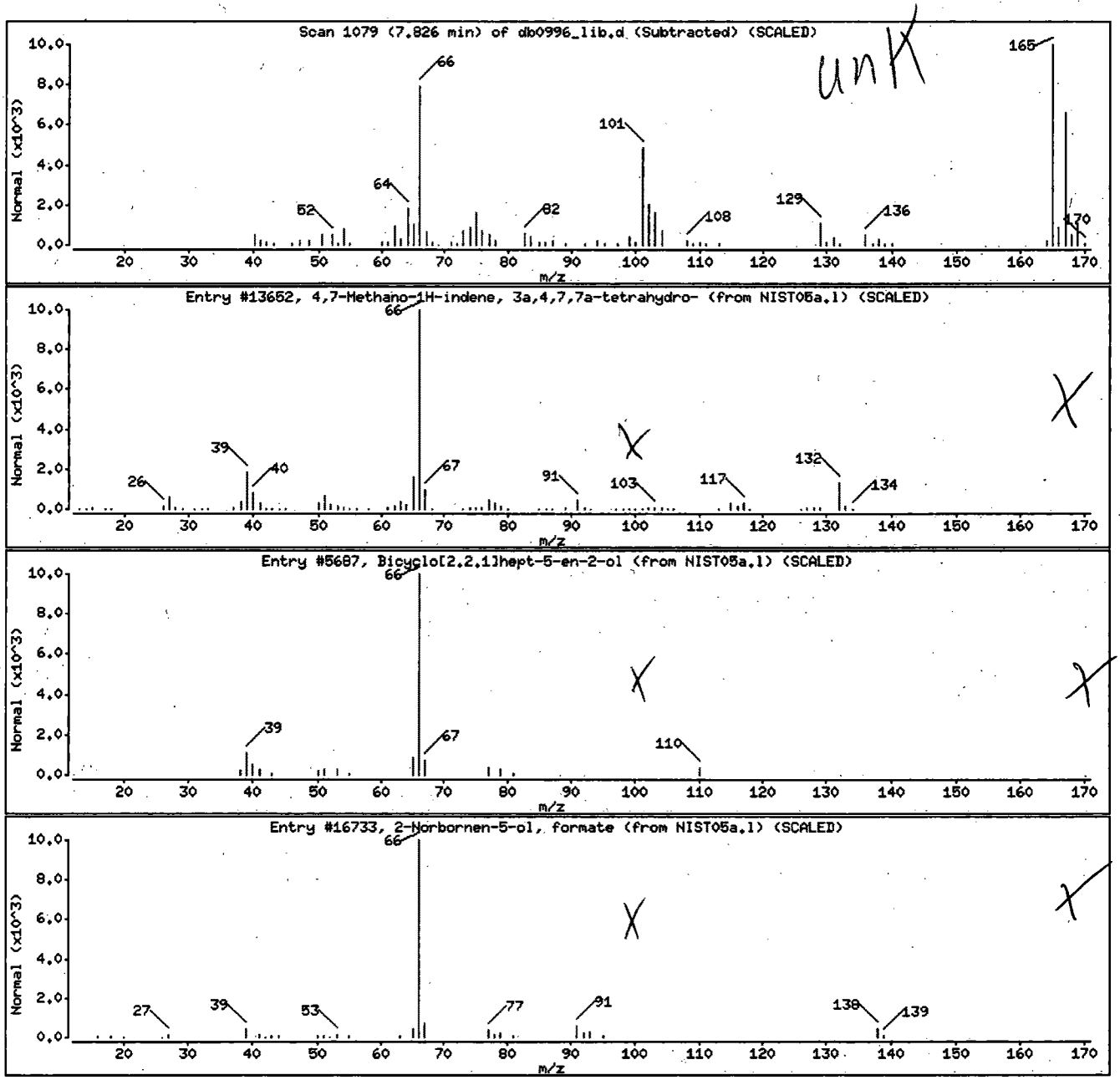
Volume Injected (uL): 1.0

Operator: ceb05247

Column phase: J&W DB-5MS

Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
4,7-Methano-1H-indene, 3a,4,7,7a-tetrahy	77-73-6	NIST05a.l	13652	43	C10H12	132
Bicyclo[2.2.1]hept-5-en-2-ol	13080-90-5	NIST05a.l	5687	46	C7H10O	110
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	46	C8H10O2	138



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Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

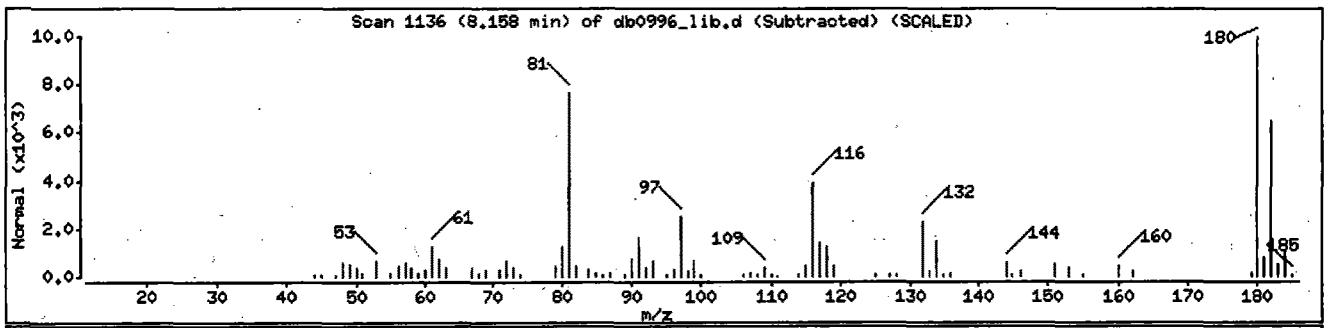
Volume Injected (uL): 1.0

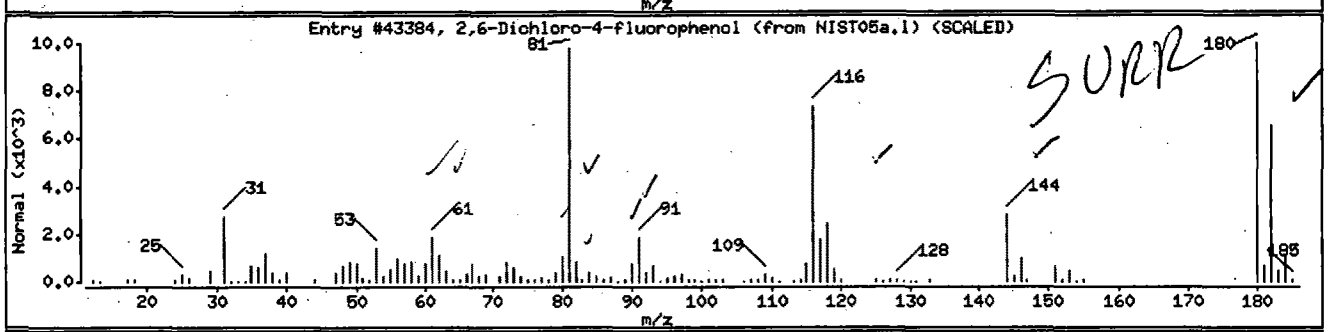
Operator: ceb05247

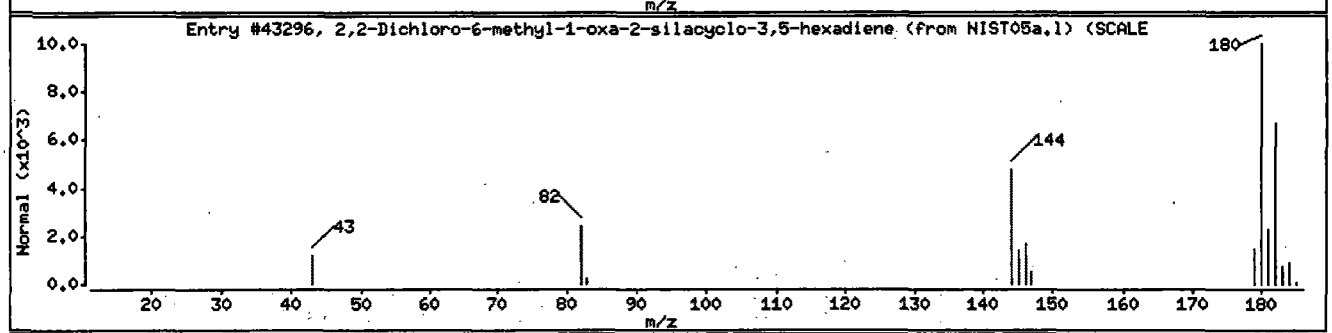
Column phase: J&W DB-5MS

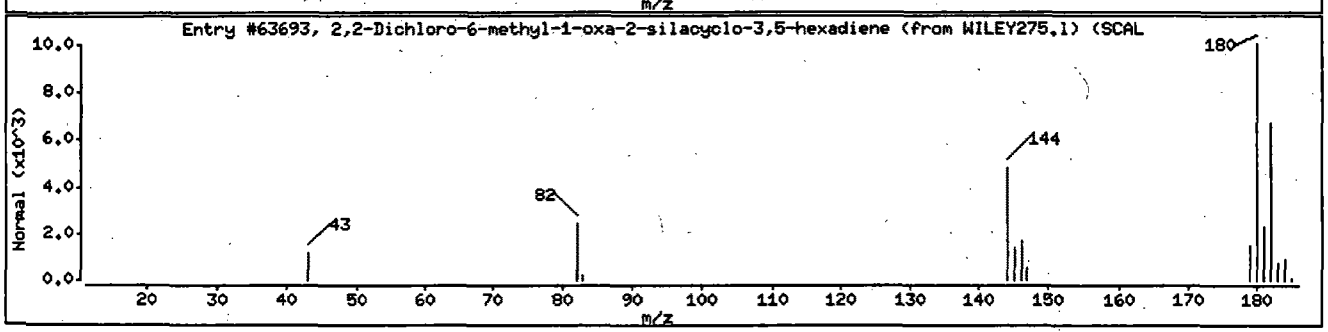
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
2,6-Dichloro-4-fluorophenol	392-71-2	NIST05a.l	43384	60	C6H3Cl2FO	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	NIST05a.l	43296	27	C5H6Cl2OSi	180
2,2-Dichloro-6-methyl-1-oxa-2-silacyclo-	67608-54-2	WILEY275.l	63693	27	C5H6Cl2OSi	180









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Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

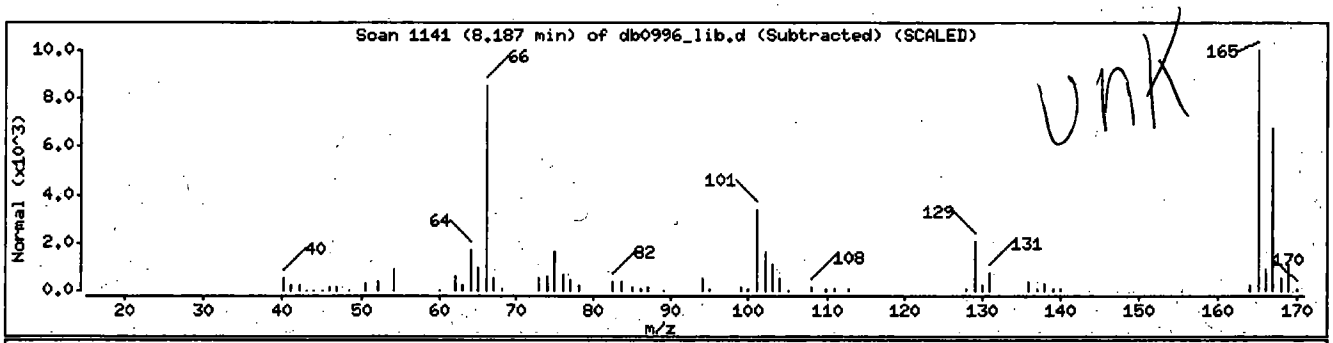
Volume Injected (uL): 1.0

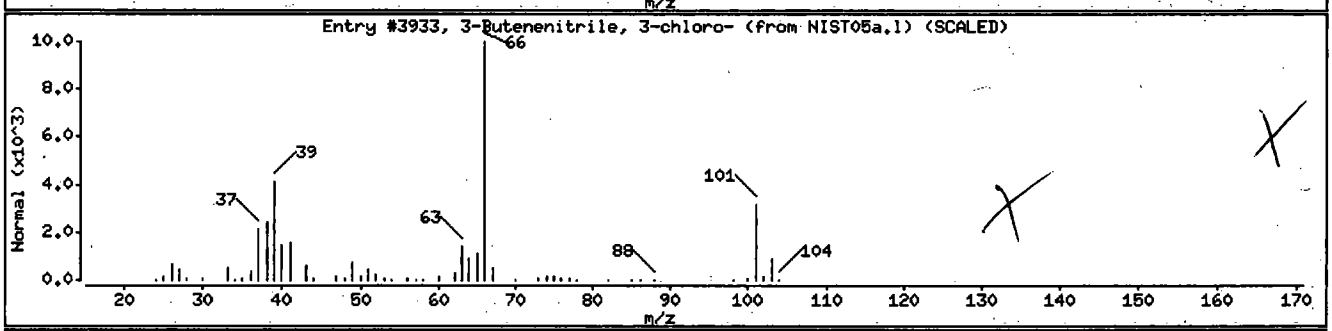
Operator: ceb05247

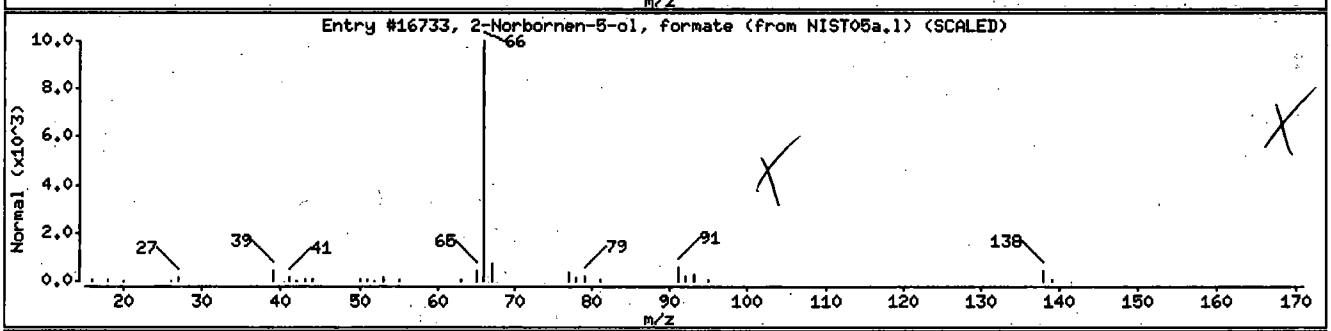
Column phase: J&W DB-5MS

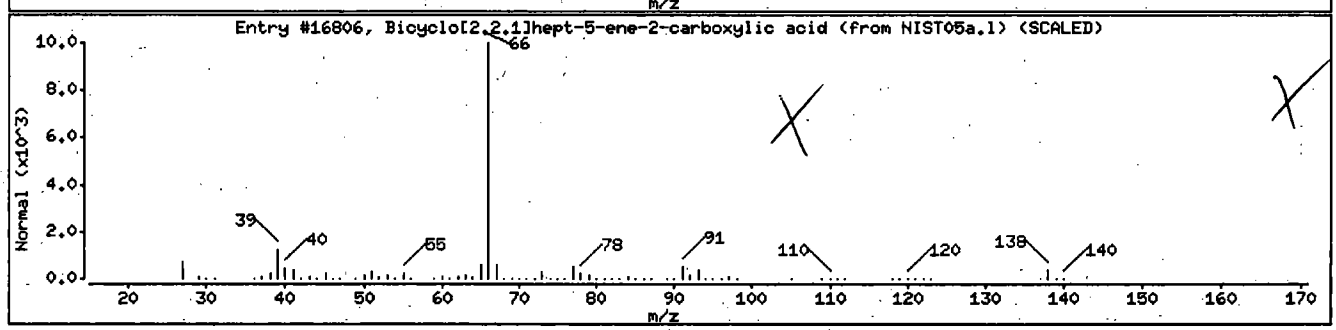
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
3-Butenenitrile, 3-chloro-	21031-46-9	NIST05a.l	3933	40	C4H4ClN	101
2-Norbornen-5-ol, formate	1000142-75-9	NIST05a.l	16733	47	C8H10O2	138
Bicyclo[2.2.1]hept-5-ene-2-carboxylic ac	120-74-1	NIST05a.l	16806	47	C8H10O2	138









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Data File: /chem/HP19760.i/14feb21a.b/db0996_lib.d

Date : 22-FEB-2014 01:43

Client ID: H1021

Instrument: HP19760.i

Sample Info: H1021;7369321;1;0;SAMPLE;;;

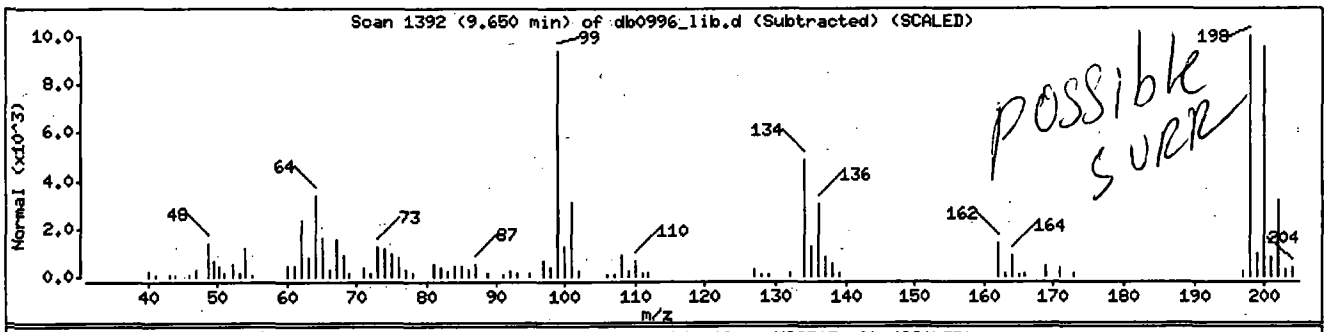
Volume Injected (uL): 1.0

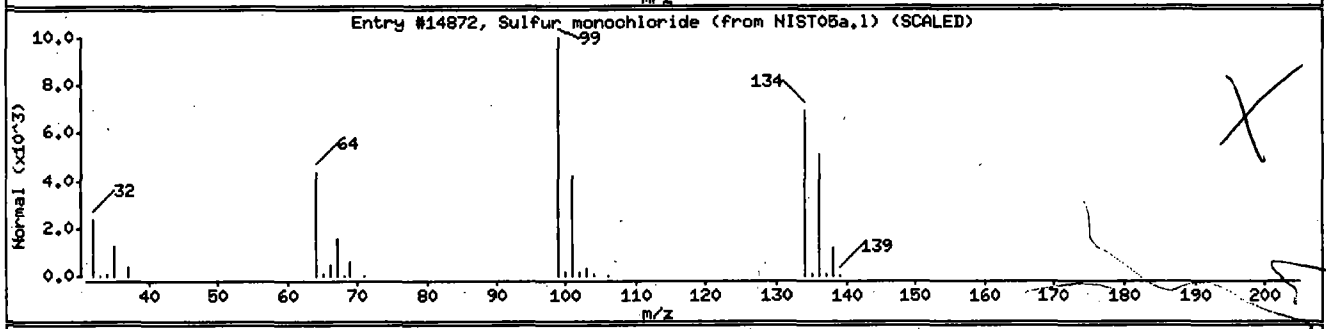
Operator: ceb05247

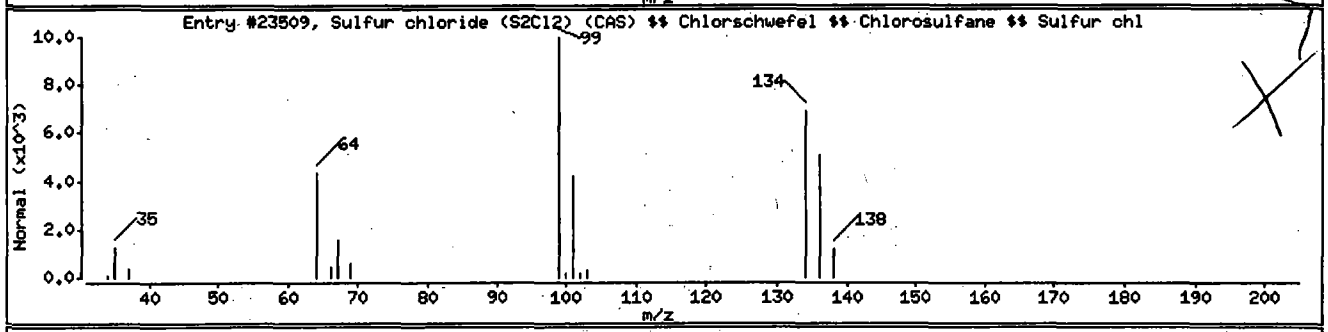
Column phase: J&W DB-5MS

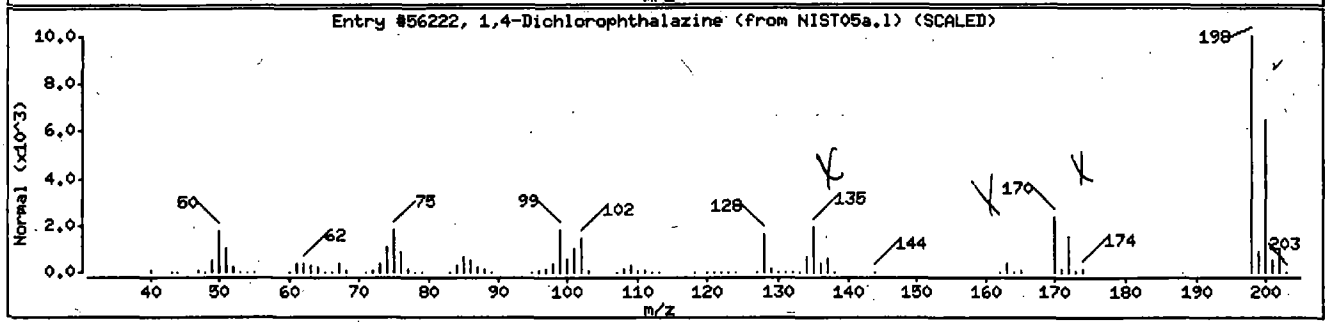
Column diameter: 0.18

Library Search Compound Match	CAS Number	Library	Entry	Quality	Formula	Weight
Sulfur monochloride	10025-67-9	NIST05a.l	14872	38	C12S2	134
Sulfur chloride (S2Cl2) (CAS) $$ Chlorso	10025-67-9	WILEY275.l	23509	38	C12S2	134
1,4-Dichlorophthalazine	4752-10-7	NIST05a.l	56222	35	C8H4Cl2N2	198









Digitally signed by Andrew J. Strebel on 03/02/2014 at 16:21.
Target 3.5 esignature user ID: ajs00193

Warner, Sue

From: Warner, Sue
Sent: Thursday, April 10, 2014 4:54 PM
To: Caporale, Cynthia
Subject: RE: WVTAP Data

Cindy,

I have looked at the first sample and they are reporting some surrogates as TICs. It appears that they have spiked the samples with an unusual surrogate mix, in addition to the traditional surrogates. I've searched vendor catalogs for such a mix and can't find one. I did find one of the unusual surrogates- 2-chlorophenol-d4. If it is OK with you, I'm going to contact Bill Arguto and ask him to ask the lab to identify which surrogates were spiked, so that these are not reported as TICs.

Sue

Ex. 5 - Deliberative

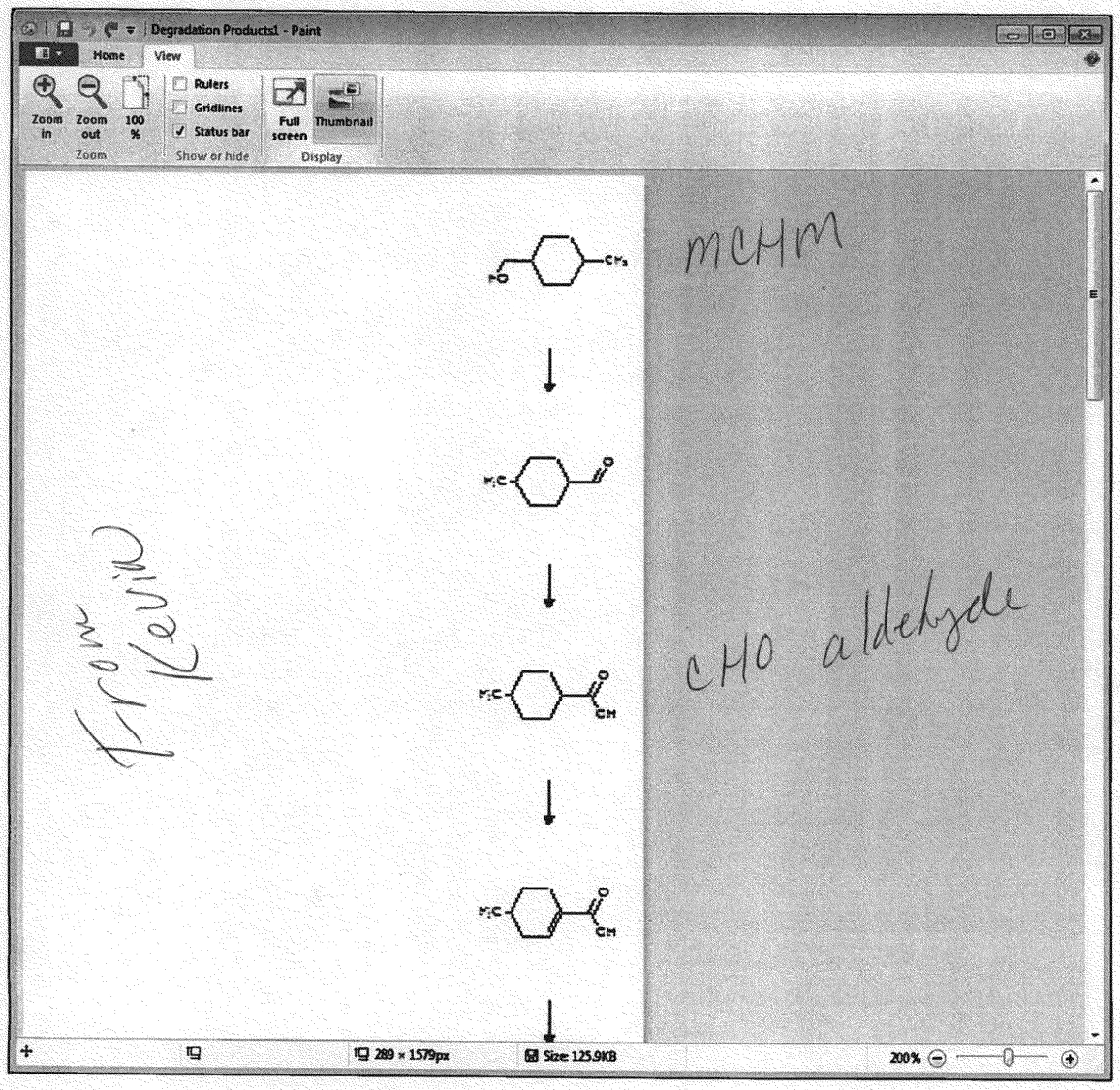
From: Caporale, Cynthia
Sent: Thursday, April 10, 2014 10:09 AM
To: Warner, Sue
Subject: WVTAP Data
Importance: High

Sue,

Would you send a note or call Bill Arguto (cc: Victoria Binetti) on exactly which data set you are reviewing for TICs? Bill is going to try and find the sampling location for that data set.

Cindy

Freedom_0006097_0434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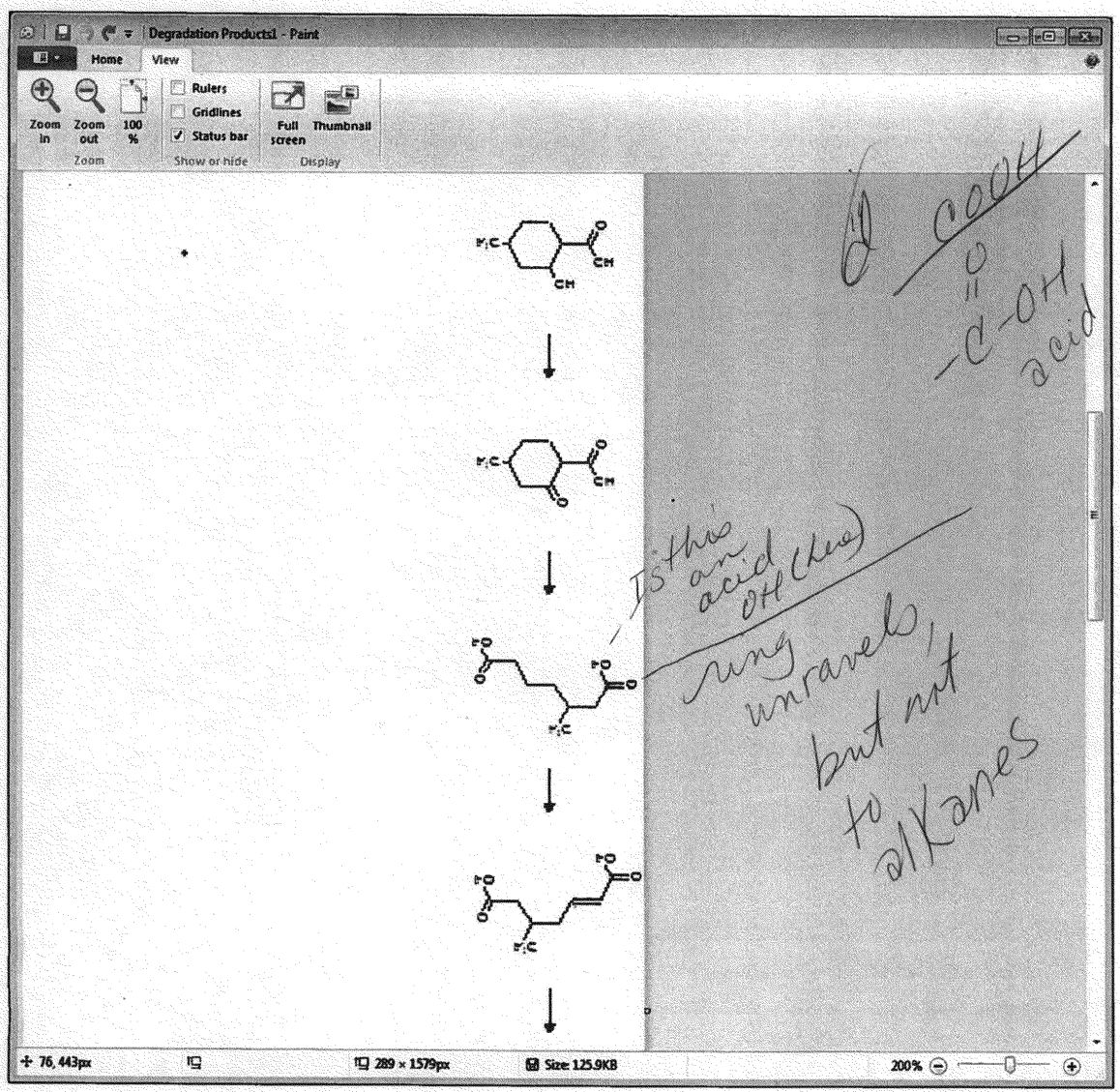
MCHM
CHO aldehyde
From Kevin



~~COOH~~

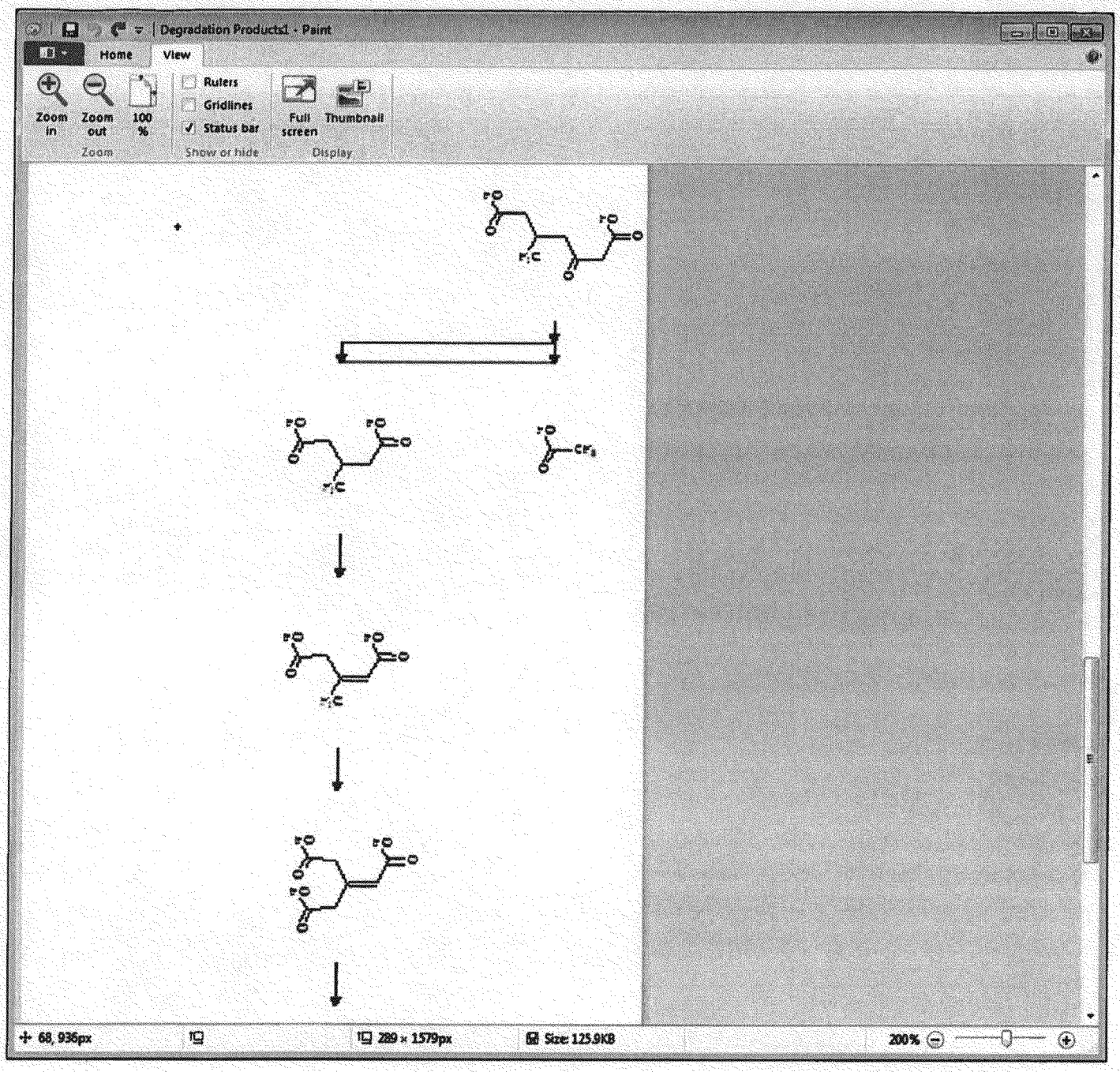
$-\overset{O}{\overset{\|}{C}}-OH$ acid

Is this an acid OH (here)

ring unravels, but not to alkanes

$H\overset{H}{\underset{H}{C}}-\overset{O}{\overset{\|}{C}}-OH$

acetic acid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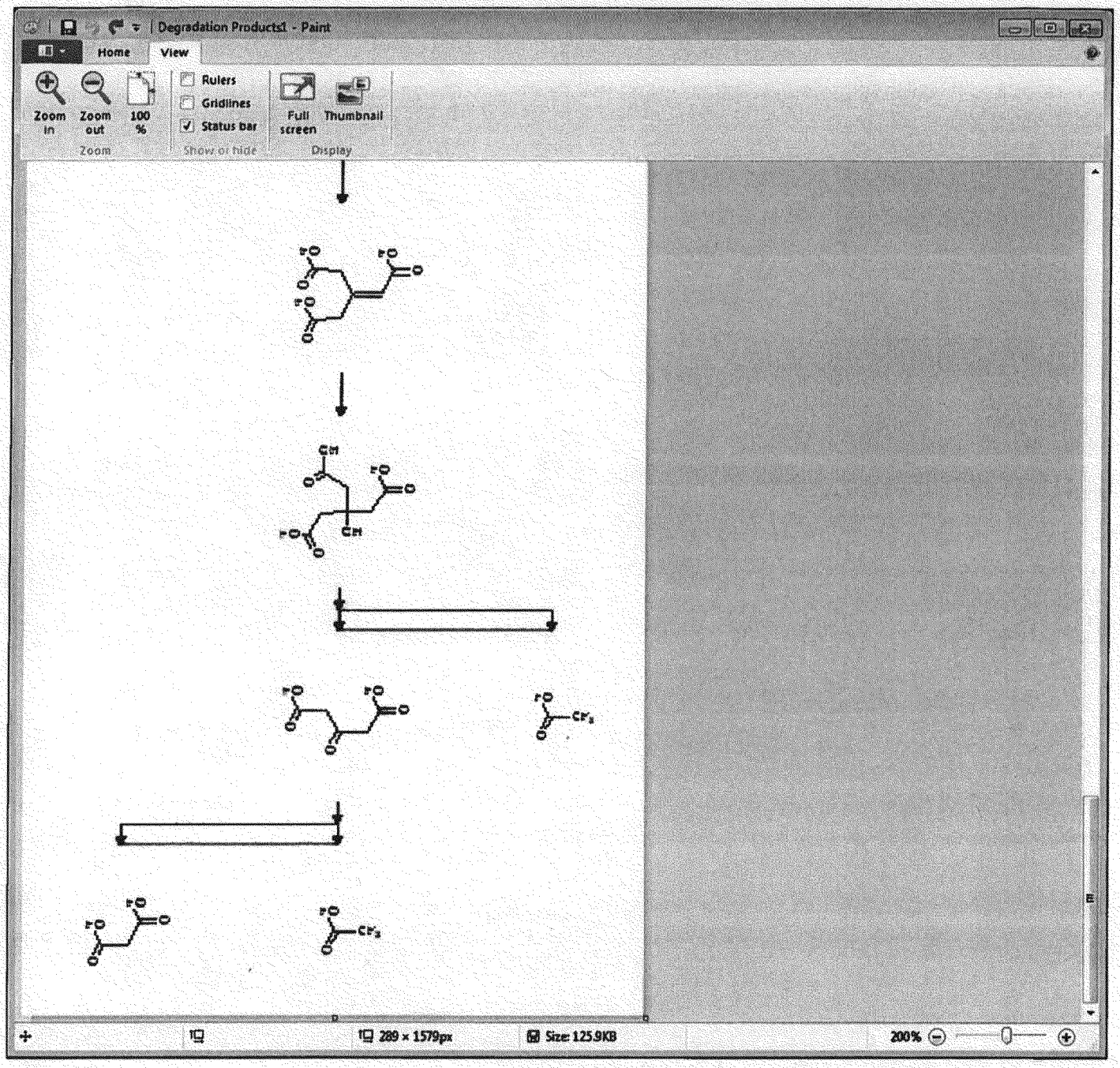
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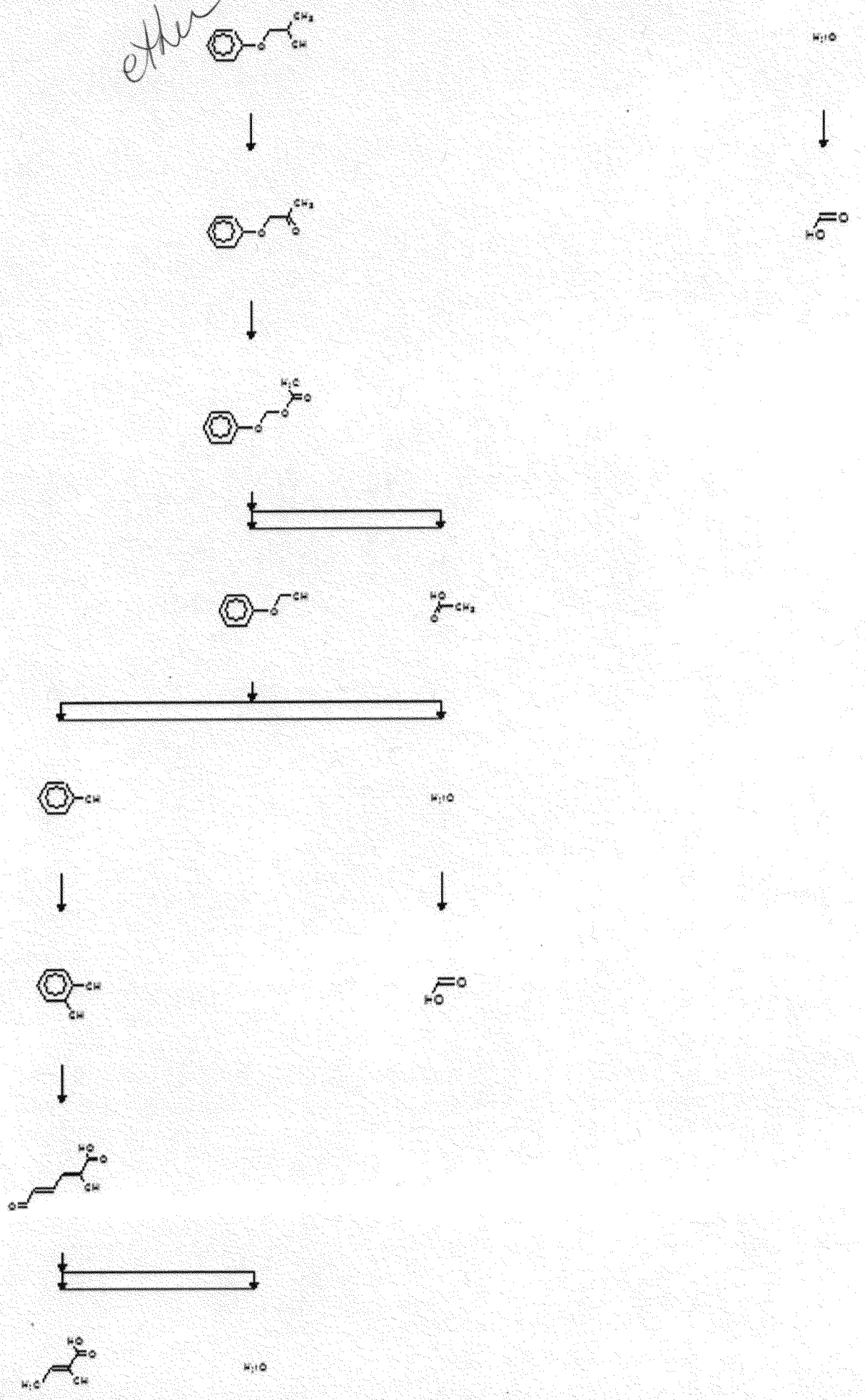
PPH

ether



Ex. 5 - Deliberative

Compound	CAS number	Comment
1,1-Dimethyl-3-chloropropanol	1985-88-2 ✓	Largest peak
MCHM isomer	3937-49-3 ✓	MCHM
Bromodichloromethane	75-27-4 ✓	THM
Dibromochloromethane X X	~~75-25-2~~ ✓ 124-48-1	THM
Dichloronitromethane	76-06-2 ✓	
Toluene	108-88-3 ✓	VOA
1,1,2,2-Tetrachloroethane	79-34-5 ✓	VOA
2-Chloro-3-methyl-1-butene	17773-64-7 ✓	
2,3-Dichloro-2-methylbutane	507-45-9 ✓	
2-Methyl-3-bromo-2-butanol	2588-77-4 ✓	
Decane	124-18-5 ✓	Alkane
1-Methyldecyl benzene	4536-88-3 ✓	
2,2-Dimethoxybutane	3453-99-4 ✓	

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill_011214_1112014_c

Method: Spill_011214_1112014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill_011214_1112014_c.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
16	Sample	1112014_c016	N/A	Milliken 900	1/12/2014 5:46:29 AM	

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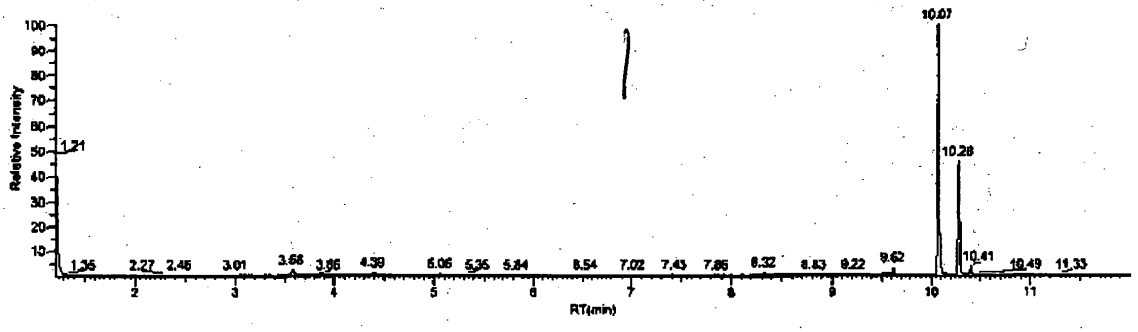

Internal Standards	RT	Quan Peak	Response			Injected Conc	Units	Calculated Conc	Units
fluorobenzene(ISTD)	4.39	96.00 mz	330214			5.000	ug/L	5.000	ug/L
Surrogates	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
4-bromofluorobenzene(surr)	8.32	95.00 mz	133216	Average RF	0.403	3.847	ug/L	3.847	ug/L
1,2-dichlorobenzene_d4(surr)	9.62	152.00 mz	172038	Average RF	0.521	5.075	ug/L	5.075	ug/L
Target Compounds	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
dichlorodifluoromethane	1.22	85.00 mz	171	Average RF	0.001	0.007	ug/L	0.007	ug/L
chloromethane	1.30	50.00 mz	117	Average RF	0.000	0.002	ug/L	0.002	ug/L
vinylchloride	N/F	62.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromomethane	1.52	94.00 mz	1337	Average RF	0.004	0.068	ug/L	0.068	ug/L
chloroethane	1.61	64.00 mz	177	Average RF	0.001	0.007	ug/L	0.007	ug/L
trichlorofluoromethane	1.71	101.00 mz	101	Average RF	0.000	0.003	ug/L	0.003	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill_011214_1112014_c

Method: Spill_011214_1112014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill_011214_1112014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,1-dichloroethane	1.99	61.00 mz	126	Average RF	0.000	0.002	ug/L	0.002	ug/L
methylene_chloride	N/F	84.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1-dichloroethane	2.81	63.00 mz	513	Average RF	0.002	0.007	ug/L	0.007	ug/L
cis-1,2-dichloroethene	3.25	96.00 mz	237	Average RF	0.001	0.009	ug/L	0.009	ug/L
2,2-dichloropropane	N/F	77.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromochloromethane	3.36	128.00 mz	137	Average RF	0.000	0.015	ug/L	0.015	ug/L
carbon_tetrachloride	3.56	117.00 mz	4840	Average RF	0.015	0.185	ug/L	0.185	ug/L
chloroform	3.58	83.00 mz	612114	Average RF	1.854	8.800	ug/L	8.800	ug/L
1,1,1-trichloroethane	3.63	97.00 mz	922	Average RF	0.003	0.024	ug/L	0.024	ug/L
1,1-dichloropropene	3.75	75.00 mz	391	Average RF	0.001	0.007	ug/L	0.007	ug/L
benzene	N/F	78.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2-dichloroethane	4.22	62.00 mz	161	Average RF	0.000	0.003	ug/L	0.003	ug/L
trichloroethene	4.39	95.00 mz	32641	Average RF	0.099	1.067	ug/L	1.067	ug/L
dibromomethane	4.86	93.00 mz	145	Average RF	0.000	0.007	ug/L	0.007	ug/L
1,2-dichloropropane	N/F	63.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromodichloromethane	5.06	83.00 mz	190367	Average RF	0.576	3.803	ug/L	3.803	ug/L
cis-1,3-dichloropropene	5.53	75.00 mz	129	Average RF	0.000	0.002	ug/L	0.002	ug/L
toluene	5.73	92.00 mz	83	Average RF	0.000	0.001	ug/L	0.001	ug/L
tetrachloroethene	5.98	166.00 mz	99	Average RF	0.000	0.003	ug/L	0.003	ug/L
trans-1,3-dichloropropene	6.20	75.00 mz	935	Average RF	0.003	0.012	ug/L	0.012	ug/L
1,1,2-trichloroethane	6.31	83.00 mz	306	Average RF	0.001	0.011	ug/L	0.011	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill_011214_1112014_c

Method: Spill_011214_1112014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill_011214_1112014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
dibromochloromethane	6.53	129.00 mz	23027	Average RF	0.070	0.834	ug/L	0.834	ug/L
1,3-dichloropropane	6.55	76.00 mz	10187	Average RF	0.031	0.120	ug/L	0.120	ug/L
1,2-dibromoethane	6.69	107.00 mz	228	Average RF	0.001	0.007	ug/L	0.007	ug/L
chlorobenzene	7.17	112.00 mz	45	Average RF	0.000	0.001	ug/L	0.001	ug/L
ethylbenzene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,1,2-tetrachloroethane	7.28	131.00 mz	176	Average RF	0.001	0.010	ug/L	0.010	ug/L
m&p-xylene	7.39	106.00 mz	42	Average RF	0.000	0.001	ug/L	0.001	ug/L
o-xylene	7.77	106.00 mz	38	Average RF	0.000	0.001	ug/L	0.001	ug/L
styrene	N/F	104.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromoform	7.85	173.00 mz	1148	Average RF	0.003	0.035	ug/L	0.035	ug/L
isopropylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromobenzene	8.32	156.00 mz	121	Average RF	0.000	0.003	ug/L	0.003	ug/L
n-propylbenzene	8.41	91.00 mz	709	Average RF	0.002	0.004	ug/L	0.004	ug/L
1,1,2,2-tetrachloroethane	8.48	83.00 mz	284	Average RF	0.001	0.005	ug/L	0.005	ug/L
2-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,3-trichloropropane	8.55	75.00 mz	98	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,3,5-trimethylbenzene	8.84	105.00 mz	564	Average RF	0.002	0.005	ug/L	0.005	ug/L
4-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
tert-butylbenzene	8.84	119.00 mz	171	Average RF	0.001	0.002	ug/L	0.002	ug/L
1,2,4-trimethylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
sec-butylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
p-isopropyltoluene	9.20	119.00 mz	287	Average RF	0.001	0.003	ug/L	0.003	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill_011214_1112014_c

Method: Spill_011214_1112014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill_011214_1112014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,3-dichlorobenzene	N/F	146.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,4-dichlorobenzene	N/F	146.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
n-butylbenzene	9.58	91.00 mz	29263	Average RF	0.089	0.216	ug/L	0.216	ug/L
1,2-dichlorobenzene	9.55	146.00 mz	304	Average RF	0.001	0.004	ug/L	0.004	ug/L
4-methylcyclohexanemethanol	10.08	55.11 mz	18473227	Ext Curve	55.943	3090.489	ug/L	3090.489	ug/L
check later	10.28	75.00 mz	40551	Average RF	0.123	1.582	ug/L	1.582	ug/L
4-(methoxymethyl)cyclohexanemethanol	10.28	55.11 mz	7868817	Ext Curve	23.829	1316.418	ug/L	1316.418	ug/L
hexachlorobutadiene	10.78	225.00 mz	7	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,2,4-trichlorobenzene	10.82	180.00 mz	320	Average RF	0.001	0.006	ug/L	0.006	ug/L
naphthalene	11.11	128.00 mz	11254	Average RF	0.034	0.101	ug/L	0.101	ug/L
1,2,3-trichlorobenzene	11.18	180.00 mz	102	Average RF	0.000	0.002	ug/L	0.002	ug/L

Manually Integrated

TIC Summary Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill_011214_1112014_c

Method: Spill_011214_1112014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill_011214_1112014

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
16	Sample	1112014_c016	N/A	Milliken 900	1/12/2014 5:46:29 AM	

Internal Standards

Internal Standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
fluorobenzene(ISTD)	1	4.39	1178294	5.000	ug/L	5.000	ug/L

Qualitatively-identified Compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag
Carbon dioxide	1	1.25	2859362	11.285	ug/L	11.285	ug/L	
Ethyne, fluoro-	1	4.65	131604	0.558	ug/L	0.558	ug/L	

$HC \equiv CF$

Manually Integrated [ ] Flag legend: P = Library entry selected manually

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: EPAMethod524_List_1102014_k

Method: EPAMethod524_List_1102014_k_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_EPAMethod524_List_1102014_k.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
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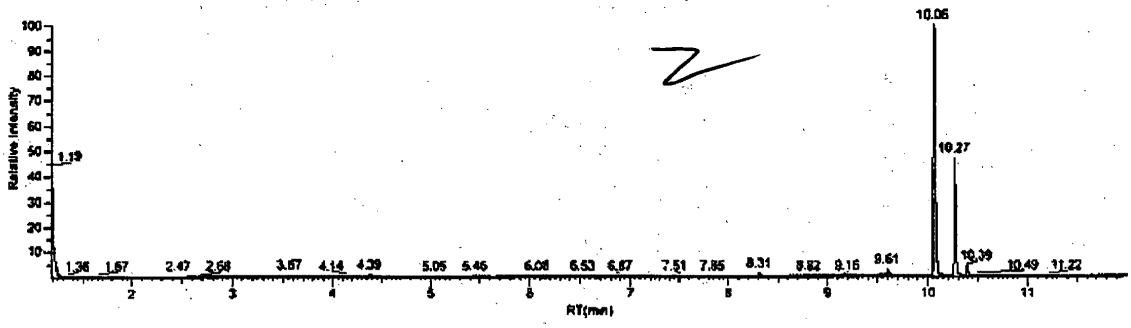

Internal Standards	RT	Quan Peak	Response			Injected Conc	Units	Calculated Conc	Units
fluorobenzene(ISTD)	4.39	96.00 mz	297845			5.000	ug/L	5.000	ug/L
Surrogates	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
4-bromofluorobenzene(surr)	8.31	95.00 mz	145628	Average RF	0.489	4.662	ug/L	4.662	ug/L
1,2-dichlorobenzene_d4(surr)	9.61	152.00 mz	203405	Average RF	0.683	6.652	ug/L	6.652	ug/L
Target Compounds	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
dichlorodifluoromethane	1.21	85.00 mz	297	Average RF	0.001	0.014	ug/L	0.014	ug/L
chloromethane	1.30	50.00 mz	449	Average RF	0.002	0.011	ug/L	0.011	ug/L
vinylchloride	N/F	62.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromomethane	1.53	94.00 mz	2948	Average RF	0.010	0.166	ug/L	0.166	ug/L
chloroethane	1.60	64.00 mz	703	Average RF	0.002	0.033	ug/L	0.033	ug/L
trichlorofluoromethane	1.69	101.00 mz	87	Average RF	0.000	0.003	ug/L	0.003	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: EPAMethod524_List_1102014_k

Method: EPAMethod524_List_1102014_k_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_EPAMethod524_List_1102014_k.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,1-dichloroethene	2.00	61.00 mz	216	Average RF	0.001	0.004	ug/L	0.004	ug/L
methylene_chloride	N/F	84.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1-dichloroethane	2.82	63.00 mz	965	Average RF	0.003	0.015	ug/L	0.015	ug/L
cis-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
2,2-dichloropropane	N/F	77.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromochloromethane	3.43	128.00 mz	36	Average RF	0.000	0.004	ug/L	0.004	ug/L
chloroform	N/F	83.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
carbon_tetrachloride	3.57	117.00 mz	913	Average RF	0.003	0.039	ug/L	0.039	ug/L
1,1,1-trichloroethane	3.66	97.00 mz	180	Average RF	0.001	0.005	ug/L	0.005	ug/L
1,1-dichloropropene	3.76	75.00 mz	120	Average RF	0.000	0.002	ug/L	0.002	ug/L
benzene	N/F	78.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2-dichloroethane	4.39	62.00 mz	10018	Average RF	0.034	0.174	ug/L	0.174	ug/L
trichloroethene	4.39	95.00 mz	26551	Average RF	0.069	0.962	ug/L	0.962	ug/L
dibromomethane	4.81	93.00 mz	159	Average RF	0.001	0.009	ug/L	0.009	ug/L
1,2-dichloropropane	N/F	63.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromodichloromethane	4.98	83.00 mz	143	Average RF	0.000	0.003	ug/L	0.003	ug/L
cis-1,3-dichloropropene	5.56	75.00 mz	145	Average RF	0.000	0.002	ug/L	0.002	ug/L
toluene	5.80	92.00 mz	65	Average RF	0.000	0.001	ug/L	0.001	ug/L
tetrachloroethene	6.07	166.00 mz	86	Average RF	0.000	0.003	ug/L	0.003	ug/L
trans-1,3-dichloropropene	N/F	75.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,2-trichloroethane	6.37	83.00 mz	92	Average RF	0.000	0.004	ug/L	0.004	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: EPAMethod524_List_1102014_k

Method: EPAMethod524_List_1102014_k_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_EPAMethod524_List_1102014_k.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
dibromochloromethane	6.48	129.00 mz	122	Average RF	0.000	0.005	ug/L	0.005	ug/L
1,3-dichloropropane	6.54	76.00 mz	4557	Average RF	0.015	0.059	ug/L	0.059	ug/L
1,2-dibromoethane	6.68	107.00 mz	194	Average RF	0.001	0.007	ug/L	0.007	ug/L
chlorobenzene	7.24	112.00 mz	74	Average RF	0.000	0.001	ug/L	0.001	ug/L
ethylbenzene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,1,2-tetrachloroethane	7.25	131.00 mz	248	Average RF	0.001	0.015	ug/L	0.015	ug/L
m&p-xylene	7.41	106.00 mz	847	Average RF	0.003	0.018	ug/L	0.018	ug/L
o-xylene	7.79	106.00 mz	188	Average RF	0.001	0.004	ug/L	0.004	ug/L
bromoform	7.80	173.00 mz	24	Average RF	0.000	0.001	ug/L	0.001	ug/L
styrene	7.85	104.00 mz	7938	Average RF	0.027	0.107	ug/L	0.107	ug/L
isopropylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromobenzene	8.37	156.00 mz	134	Average RF	0.000	0.003	ug/L	0.003	ug/L
n-propylbenzene	8.42	91.00 mz	322	Average RF	0.001	0.002	ug/L	0.002	ug/L
1,1,2,2-tetrachloroethane	8.50	83.00 mz	298	Average RF	0.001	0.006	ug/L	0.006	ug/L
2-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,3-trichloropropane	8.60	75.00 mz	72	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,3,5-trimethylbenzene	8.64	105.00 mz	72	Average RF	0.000	0.001	ug/L	0.001	ug/L
4-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
tert-butylbenzene	N/F	119.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,4-trimethylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
sec-butylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
p-isopropyltoluene	N/F	119.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: EPAMethod524_List_1102014_k

Method: EPAMethod524_List_1102014_k_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_EPAMethod524_List_1102014_k.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,3-dichlorobenzene	9.15	146.00 mz	38	Average RF	0.000	0.000	ug/L	0.000	ug/L
1,4-dichlorobenzene	9.25	146.00 mz	91	Average RF	0.000	0.001	ug/L	0.001	ug/L
n-butylbenzene	9.57	91.00 mz	23440	Average RF	0.079	0.192	ug/L	0.192	ug/L
1,2-dichlorobenzene	9.58	146.00 mz	204	Average RF	0.001	0.003	ug/L	0.003	ug/L
4-methylcyclohexanemethanol	10.06	55.11 mz	24887529	Ext Curve	63.559	4616.068	ug/L	4616.068	ug/L
check later	10.27	75.00 mz	58671	Average RF	0.197	2.538	ug/L	2.538	ug/L
4-(methoxymethyl)cyclohexanemethanol	10.27	55.11 mz	11871672	Ext Curve	39.859	2201.924	ug/L	2201.924	ug/L
hexachlorobutadiene	10.80	225.00 mz	11	Average RF	0.000	0.002	ug/L	0.002	ug/L
1,2,4-trichlorobenzene	10.78	180.00 mz	198	Average RF	0.001	0.004	ug/L	0.004	ug/L
naphthalene	11.08	128.00 mz	38	Average RF	0.000	0.000	ug/L	0.000	ug/L
1,2,3-trichlorobenzene	11.23	180.00 mz	43	Average RF	0.000	0.001	ug/L	0.001	ug/L

Manually Integrated

TIC Summary Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: EPAMethod524_List_1102014_k

Method: EPAMethod524_List_1102014_k_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_EPAMethod524_List_1

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
22	Plant Eff Charleston	192014_a022	N/A		1/9/2014 9:36:29 PM	

Internal Standards

Internal Standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
fluorobenzene(ISTD)	1	4.39	977091	5.000	ug/L	5.000	ug/L

Qualitatively-identified Compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag
Carbon dioxide	1	1.25	341261	1.746	ug/L	1.746	ug/L	
Methane, bromodichloro-	1	5.05	264230	1.352	ug/L	1.352	ug/L	
Octodrine	1	9.84	139524	0.714	ug/L	0.714	ug/L	

Ex. 5 - Deliberative

Manually integrated [ ] Flag legend: P = Library entry selected manually

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill 4_1132014_c

Method: Spill 4_1132014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill 4_1132014_c.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
9	Sample	1132014_c009	N/A	Thurmond St Zone 13 011314 1358	1/14/2014 11:22:54 AM	

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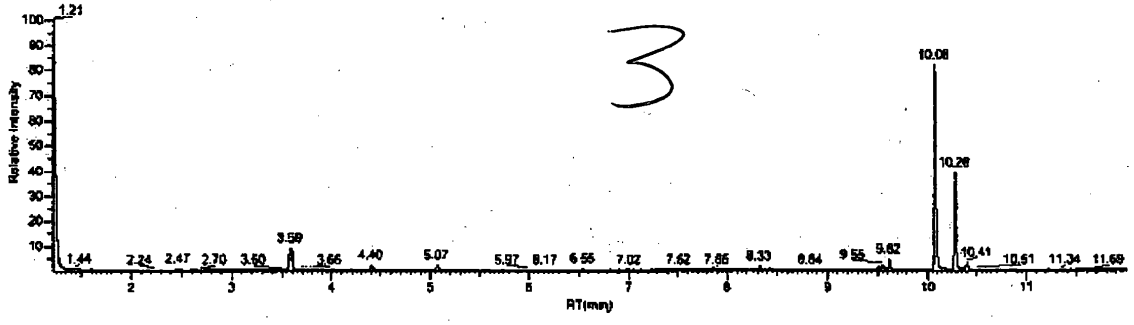

3

Internal Standards	RT	Quan Peak	Response			Injected Conc	Units	Calculated Conc	Units
fluorobenzene(ISTD)	4.40	96.00 mz	292227			5.000	ug/L	5.000	ug/L
Surrogates	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
4-bromofluorobenzene(surr)	8.33	95.00 mz	105010	Average RF	0.359	4.349	ug/L	4.349	ug/L
1,2-dichlorobenzene_d4(surr)	9.62	152.00 mz	176226	Average RF	0.603	7.259	ug/L	7.259	ug/L
Target Compounds	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
dichlorodifluoromethane	1.23	85.00 mz	316	Average RF	0.001	0.019	ug/L	0.019	ug/L
chloromethane	1.32	50.00 mz	155	Average RF	0.001	0.005	ug/L	0.005	ug/L
vinylchloride	N/F	62.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromomethane	1.56	94.00 mz	565	Average RF	0.002	0.040	ug/L	0.040	ug/L
chloroethane	1.61	64.00 mz	1107	Average RF	0.004	0.065	ug/L	0.065	ug/L
trichlorofluoromethane	1.71	101.00 mz	142	Average RF	0.000	0.006	ug/L	0.006	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill 4_1132014_c

Method: Spill 4_1132014_c_EPAMethod524_List
EPAMethod524_List
Cal File: EPAMethod524_List_1102014_gcalibration_Spill 4_1132014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,1-dichloroethene	1.99	61.00 mz	460	Average RF	0.002	0.011	ug/L	0.011	ug/L
methylene_chloride	N/F	84.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1-dichloroethane	2.83	63.00 mz	211	Average RF	0.001	0.004	ug/L	0.004	ug/L
cis-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
2,2-dichloropropane	N/F	77.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromochloromethane	3.37	128.00 mz	82	Average RF	0.000	0.010	ug/L	0.010	ug/L
carbon_tetrachloride	3.59	117.00 mz	14064	Average RF	0.048	0.745	ug/L	0.745	ug/L
chloroform	3.59	83.00 mz	1519503	Average RF	5.200	39.306	ug/L	39.306	ug/L
1,1,1-trichloroethane	3.65	97.00 mz	134	Average RF	0.000	0.005	ug/L	0.005	ug/L
1,1-dichloropropene	3.75	75.00 mz	83	Average RF	0.000	0.002	ug/L	0.002	ug/L
benzene	N/F	78.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2-dichloroethane	4.23	62.00 mz	563	Average RF	0.002	0.012	ug/L	0.012	ug/L
trichloroethene	4.40	95.00 mz	33507	Average RF	0.115	1.516	ug/L	1.516	ug/L
dibromomethane	4.81	93.00 mz	55	Average RF	0.000	0.004	ug/L	0.004	ug/L
1,2-dichloropropane	N/F	63.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromodichloromethane	5.07	83.00 mz	300011	Average RF	1.027	8.046	ug/L	8.046	ug/L
cis-1,3-dichloropropene	5.58	75.00 mz	64	Average RF	0.000	0.001	ug/L	0.001	ug/L
toluene	5.76	92.00 mz	79	Average RF	0.000	0.001	ug/L	0.001	ug/L
tetrachloroethene	N/F	166.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,3-dichloropropene	6.18	75.00 mz	721	Average RF	0.002	0.013	ug/L	0.013	ug/L
1,1,2-trichloroethane	6.29	83.00 mz	318	Average RF	0.001	0.015	ug/L	0.015	ug/L

Manually Integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill 4_1132014_c

Method: Spill 4_1132014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill 4_1132014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
dibromochloromethane	6.45	129.00 mz	149	Average RF	0.001	0.007	ug/L	0.007	ug/L
1,3-dichloropropane	6.55	76.00 mz	17488	Average RF	0.060	0.291	ug/L	0.291	ug/L
1,2-dibromoethane	6.75	107.00 mz	283	Average RF	0.001	0.012	ug/L	0.012	ug/L
chlorobenzene	7.17	112.00 mz	97	Average RF	0.000	0.002	ug/L	0.002	ug/L
ethylbenzene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,1,2-tetrachloroethane	7.29	131.00 mz	102	Average RF	0.000	0.008	ug/L	0.008	ug/L
m&p-xylene	7.42	106.00 mz	483	Average RF	0.002	0.013	ug/L	0.013	ug/L
o-xylene	7.81	106.00 mz	375	Average RF	0.001	0.011	ug/L	0.011	ug/L
styrene	N/F	104.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromoform	7.85	173.00 mz	1618	Average RF	0.006	0.094	ug/L	0.094	ug/L
isopropylbenzene	8.05	105.00 mz	675	Average RF	0.002	0.008	ug/L	0.008	ug/L
bromobenzene	8.33	156.00 mz	262	Average RF	0.001	0.008	ug/L	0.008	ug/L
n-propylbenzene	8.42	91.00 mz	1079	Average RF	0.004	0.008	ug/L	0.008	ug/L
1,1,2,2-tetrachloroethane	8.53	83.00 mz	149	Average RF	0.001	0.004	ug/L	0.004	ug/L
2-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,3-trichloropropane	8.63	75.00 mz	166	Average RF	0.001	0.003	ug/L	0.003	ug/L
1,3,5-trimethylbenzene	8.59	105.00 mz	153	Average RF	0.001	0.002	ug/L	0.002	ug/L
4-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
tert-butylbenzene	8.87	119.00 mz	15	Average RF	0.000	0.000	ug/L	0.000	ug/L
1,2,4-trimethylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
sec-butylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
p-isopropyltoluene	9.20	119.00 mz	348	Average RF	0.001	0.005	ug/L	0.005	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill 4_1132014_c

Method: Spill 4_1132014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill 4_1132014_c.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,3-dichlorobenzene	9.17	146.00 mz	46	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,4-dichlorobenzene	9.25	146.00 mz	27	Average RF	0.000	0.000	ug/L	0.000	ug/L
n-butylbenzene	9.55	91.00 mz	35484	Average RF	0.121	0.361	ug/L	0.361	ug/L
1,2-dichlorobenzene	9.55	146.00 mz	33	Average RF	0.000	0.001	ug/L	0.001	ug/L
4-methylcyclohexanemethanol	10.08	55.11 mz	8655068	Ext Curve	29.618	1989.554	ug/L	1989.554	ug/L
check later	10.28	75.00 mz	21017	Average RF	0.072	1.175	ug/L	1.175	ug/L
4-(methoxymethyl)cyclohexanemethanol	10.28	55.11 mz	4137884	Ext Curve	14.160	951.182	ug/L	951.182	ug/L
hexachlorobutadiene	10.81	225.00 mz	12	Average RF	0.000	0.003	ug/L	0.003	ug/L
1,2,4-trichlorobenzene	10.81	180.00 mz	53	Average RF	0.000	0.001	ug/L	0.001	ug/L
naphthalene	11.07	128.00 mz	205	Average RF	0.001	0.003	ug/L	0.003	ug/L
1,2,3-trichlorobenzene	11.23	180.00 mz	58	Average RF	0.000	0.002	ug/L	0.002	ug/L

Manually integrated

TIC Summary Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill 4_1132014_c

Method: Spill 4_1132014_c_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill 4_1132014_c.cal

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
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Internal Standards

Internal Standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
fluorobenzene(ISTD)	1	4.40	1077793	5.000	ug/L	5.000	ug/L

Qualitatively-identified Compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag

Manually integrated [ ] Flag legend: P = Library entry selected manually

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Vial Pos	Sample_ID	File Name	Level	Sample Name	File Date	Comment
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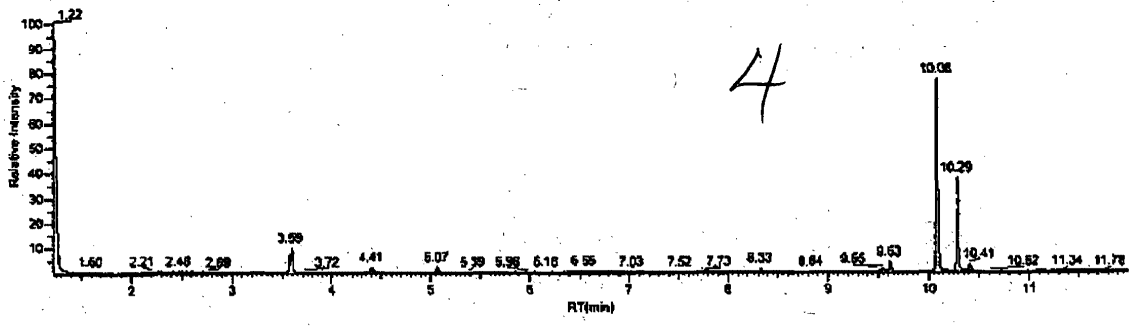


4

Internal Standards	RT	Quan Peak	Response			Injected Conc	Units	Calculated Conc	Units
fluorobenzene(ISTD)	4.41	96.00 mz	307829			5.000	ug/L	5.000	ug/L
Surrogates	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
4-bromofluorobenzene(surr)	8.33	95.00 mz	102739	Average RF	0.334	4.039	ug/L	4.039	ug/L
1,2-dichlorobenzene_d4(surr)	9.62	152.00 mz	159231	Average RF	0.517	6.227	ug/L	6.227	ug/L
Target Compounds	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
dichlorodifluoromethane	1.25	85.00 mz	237	Average RF	0.001	0.013	ug/L	0.013	ug/L
chloromethane	1.31	50.00 mz	533	Average RF	0.002	0.015	ug/L	0.015	ug/L
vinylchloride	N/F	62.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromomethane	1.55	94.00 mz	460	Average RF	0.001	0.031	ug/L	0.031	ug/L
chloroethane	1.81	64.00 mz	2271	Average RF	0.007	0.126	ug/L	0.126	ug/L
trichlorofluoromethane	1.89	101.00 mz	126	Average RF	0.000	0.005	ug/L	0.005	ug/L

Manually Integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,1-dichloroethene	N/F	61.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
methylene_chloride	N/F	84.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1-dichloroethane	2.80	63.00 mz	246	Average RF	0.001	0.005	ug/L	0.005	ug/L
cis-1,2-dichloroethene	3.21	96.00 mz	212	Average RF	0.001	0.010	ug/L	0.010	ug/L
2,2-dichloropropane	N/F	77.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromochloromethane	3.48	128.00 mz	64	Average RF	0.000	0.009	ug/L	0.009	ug/L
carbon_tetrachloride	3.58	117.00 mz	11596	Average RF	0.038	0.583	ug/L	0.583	ug/L
chloroform	3.59	83.00 mz	1646950	Average RF	5.350	40.443	ug/L	40.443	ug/L
1,1,1-trichloroethane	3.64	97.00 mz	135	Average RF	0.000	0.005	ug/L	0.005	ug/L
1,1-dichloropropene	3.73	75.00 mz	87	Average RF	0.000	0.002	ug/L	0.002	ug/L
benzene	N/F	78.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2-dichloroethane	4.12	62.00 mz	67	Average RF	0.000	0.001	ug/L	0.001	ug/L
trichloroethene	4.41	95.00 mz	31742	Average RF	0.103	1.363	ug/L	1.363	ug/L
dibromomethane	4.83	93.00 mz	57	Average RF	0.000	0.004	ug/L	0.004	ug/L
1,2-dichloropropane	N/F	63.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromodichloromethane	5.07	83.00 mz	287225	Average RF	0.933	7.313	ug/L	7.313	ug/L
cis-1,3-dichloropropene	5.57	75.00 mz	57	Average RF	0.000	0.001	ug/L	0.001	ug/L
toluene	5.86	92.00 mz	697	Average RF	0.002	0.012	ug/L	0.012	ug/L
tetrachloroethene	6.18	166.00 mz	17631	Average RF	0.057	0.608	ug/L	0.608	ug/L
trans-1,3-dichloropropene	N/F	75.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,2-trichloroethane	6.34	83.00 mz	115	Average RF	0.000	0.005	ug/L	0.005	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cell File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
dibromochloromethane	6.54	129.00 mz	34113	Average RF	0.111	1.613	ug/L	1.613	ug/L
1,3-dichloropropane	6.56	76.00 mz	12544	Average RF	0.041	0.198	ug/L	0.198	ug/L
1,2-dibromoethane	6.66	107.00 mz	216	Average RF	0.001	0.009	ug/L	0.009	ug/L
chlorobenzene	7.25	112.00 mz	40	Average RF	0.000	0.001	ug/L	0.001	ug/L
ethylbenzene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,1,2-tetrachloroethane	7.27	131.00 mz	110	Average RF	0.000	0.008	ug/L	0.008	ug/L
m&p-xylene	7.40	106.00 mz	158	Average RF	0.001	0.004	ug/L	0.004	ug/L
o-xylene	7.75	106.00 mz	52	Average RF	0.000	0.001	ug/L	0.001	ug/L
styrene	N/F	104.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromoform	7.86	173.00 mz	1446	Average RF	0.005	0.080	ug/L	0.080	ug/L
isopropylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromobenzene	8.35	156.00 mz	30	Average RF	0.000	0.001	ug/L	0.001	ug/L
n-propylbenzene	8.41	91.00 mz	224	Average RF	0.001	0.002	ug/L	0.002	ug/L
1,1,2,2-tetrachloroethane	8.51	83.00 mz	94	Average RF	0.000	0.002	ug/L	0.002	ug/L
2-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,3-trichloropropane	8.61	75.00 mz	154	Average RF	0.001	0.003	ug/L	0.003	ug/L
1,3,5-trimethylbenzene	8.64	105.00 mz	97	Average RF	0.000	0.001	ug/L	0.001	ug/L
4-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
tert-butylbenzene	8.87	119.00 mz	113	Average RF	0.000	0.002	ug/L	0.002	ug/L
1,2,4-trimethylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
sec-butylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
p-isopropyltoluene	N/F	119.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,3-dichlorobenzene	9.17	146.00 mz	132	Average RF	0.000	0.002	ug/L	0.002	ug/L
1,4-dichlorobenzene	N/F	146.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
n-butylbenzene	9.55	91.00 mz	24510	Average RF	0.080	0.237	ug/L	0.237	ug/L
1,2-dichlorobenzene	9.56	146.00 mz	35	Average RF	0.000	0.001	ug/L	0.001	ug/L
4-methylcyclohexanemethanol	10.08	55.11 mz	8148030	Ext Curve	26.469	1778.069	ug/L	1778.069	ug/L
check later	10.29	75.00 mz	20135	Average RF	0.065	1.068	ug/L	1.068	ug/L
4-(methoxymethyl)cyclohexanemethanol	10.29	55.11 mz	3784010	Ext Curve	12.293	825.749	ug/L	825.749	ug/L
hexachlorobutadiene	10.79	225.00 mz	57	Average RF	0.000	0.012	ug/L	0.012	ug/L
1,2,4-trichlorobenzene	10.85	180.00 mz	96	Average RF	0.000	0.002	ug/L	0.002	ug/L
naphthalene	11.11	128.00 mz	802	Average RF	0.003	0.010	ug/L	0.010	ug/L
1,2,3-trichlorobenzene	N/F	180.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L

Manually integrated

TIC Summary Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
51	Sample	1132014_a051	N/A	Zone 13 Rt 17 Mifflin Rd	01/14/2014 7:13:07 AM	

Internal Standards

Internal Standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
fluorobenzene(ISTD)	1	4.41	1107528	5.000	ug/L	5.000	ug/L

Qualitatively-Identified Compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag

Manually integrated [ ] Flag legend: P = Library entry selected manually

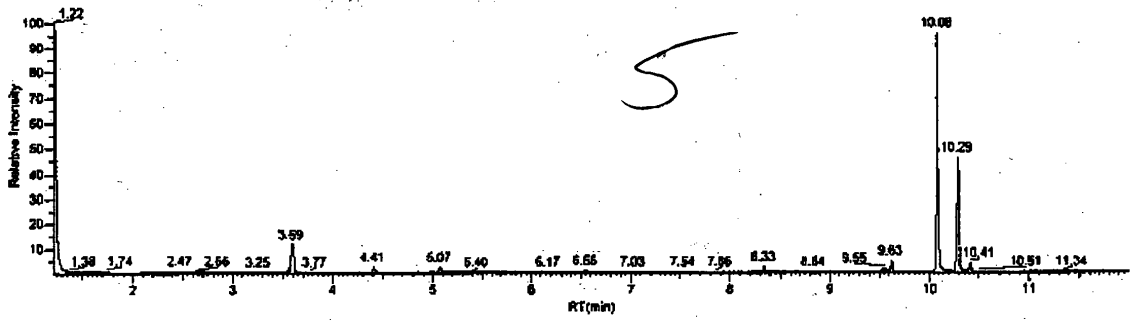
Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
49	Sample	1132014_a049	N/A	Hyd #6014 Zone 10 011314 1630	1/14/2014 6:23:03 AM	

C:\ThermoTraceFinder3.0\EFS\Projects\2014\Jan\Spill3_1132014_a\Data\1132014_a049.raw



Internal Standards	RT	Quan Peak	Response			Injected Conc	Units	Calculated Conc	Units
fluorobenzene(ISTD)	4.41	96.00 mz	253424			5.000	ug/L	5.000	ug/L
Surrogates	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
4-bromofluorobenzene(surr)	8.33	95.00 mz	92187	Average RF	0.364	4.402	ug/L	4.402	ug/L
1,2-dichlorobenzene_d4(surr)	9.62	152.00 mz	140507	Average RF	0.554	6.674	ug/L	6.674	ug/L
Target Compounds	**RT**	**Quan Peak**	**Response**	**Curve Type**	**Average RF/ Response Ratio**	**Injected Conc**	**Units**	**Calculated Conc**	**Units**
dichlorodifluoromethane	1.24	85.00 mz	221	Average RF	0.001	0.015	ug/L	0.015	ug/L
chloromethane	1.31	50.00 mz	401	Average RF	0.002	0.013	ug/L	0.013	ug/L
vinylchloride	N/F	62.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromomethane	1.53	94.00 mz	542	Average RF	0.002	0.044	ug/L	0.044	ug/L
chloroethane	1.61	64.00 mz	1826	Average RF	0.007	0.123	ug/L	0.123	ug/L
trichlorofluoromethane	1.71	101.00 mz	31	Average RF	0.000	0.002	ug/L	0.002	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,1-dichloroethene	1.99	61.00 mz	561	Average RF	0.002	0.016	ug/L	0.016	ug/L
methylene_chloride	N/F	84.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
trans-1,2-dichloroethene	N/F	96.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1-dichloroethene	2.83	63.00 mz	929	Average RF	0.004	0.021	ug/L	0.021	ug/L
cis-1,2-dichloroethene	3.24	96.00 mz	250	Average RF	0.001	0.015	ug/L	0.015	ug/L
2,2-dichloropropane	N/F	77.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromochloromethane	3.63	128.00 mz	100	Average RF	0.000	0.016	ug/L	0.016	ug/L
carbon_tetrachloride	3.59	117.00 mz	13061	Average RF	0.052	0.799	ug/L	0.799	ug/L
chloroform	3.59	83.00 mz	1551615	Average RF	6.123	46.282	ug/L	46.282	ug/L
1,1,1-trichloroethane	3.83	97.00 mz	312	Average RF	0.001	0.013	ug/L	0.013	ug/L
1,1-dichloropropene	3.76	75.00 mz	221	Average RF	0.001	0.006	ug/L	0.006	ug/L
benzene	N/F	78.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2-dichloroethane	4.14	62.00 mz	54	Average RF	0.000	0.001	ug/L	0.001	ug/L
trichloroethene	4.41	95.00 mz	25834	Average RF	0.102	1.347	ug/L	1.347	ug/L
dibromomethane	4.83	93.00 mz	171	Average RF	0.001	0.014	ug/L	0.014	ug/L
1,2-dichloropropane	N/F	63.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromodichloromethane	5.07	83.00 mz	250129	Average RF	0.987	7.736	ug/L	7.736	ug/L
cis-1,3-dichloropropene	5.60	75.00 mz	84	Average RF	0.000	0.002	ug/L	0.002	ug/L
toluene	5.74	92.00 mz	143	Average RF	0.001	0.003	ug/L	0.003	ug/L
tetrachloroethene	6.08	166.00 mz	34	Average RF	0.000	0.001	ug/L	0.001	ug/L
trans-1,3-dichloropropene	6.06	75.00 mz	3277	Average RF	0.013	0.066	ug/L	0.066	ug/L
1,1,2-trichloroethane	6.32	83.00 mz	162	Average RF	0.001	0.009	ug/L	0.009	ug/L

Manually Integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
dibromochloromethane	6.54	129.00 mz	29440	Average RF	0.116	1.691	ug/L	1.691	ug/L
1,3-dichloropropane	6.58	76.00 mz	9585	Average RF	0.038	0.184	ug/L	0.184	ug/L
1,2-dibromoethane	6.64	107.00 mz	234	Average RF	0.001	0.012	ug/L	0.012	ug/L
chlorobenzene	N/F	112.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
ethylbenzene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,1,1,2-tetrachloroethane	7.28	131.00 mz	52	Average RF	0.000	0.005	ug/L	0.005	ug/L
m&p-xylene	7.40	106.00 mz	108	Average RF	0.000	0.003	ug/L	0.003	ug/L
o-xylene	7.78	106.00 mz	120	Average RF	0.000	0.004	ug/L	0.004	ug/L
styrene	N/F	104.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromoform	7.86	173.00 mz	2107	Average RF	0.008	0.141	ug/L	0.141	ug/L
isopropylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
bromobenzene	8.33	156.00 mz	203	Average RF	0.001	0.007	ug/L	0.007	ug/L
n-propylbenzene	8.44	91.00 mz	96	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,1,2,2-tetrachloroethane	8.52	83.00 mz	182	Average RF	0.001	0.005	ug/L	0.005	ug/L
2-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
1,2,3-trichloropropane	8.61	75.00 mz	114	Average RF	0.000	0.002	ug/L	0.002	ug/L
1,3,5-trimethylbenzene	8.65	105.00 mz	187	Average RF	0.001	0.003	ug/L	0.003	ug/L
4-chlorotoluene	N/F	91.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
tert-butylbenzene	8.88	119.00 mz	16	Average RF	0.000	0.000	ug/L	0.000	ug/L
1,2,4-trimethylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
sec-butylbenzene	N/F	105.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
p-isopropyltoluene	N/F	119.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L

Manually integrated

Quantitation Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Target Compounds	RT	Quan Peak	Response	Curve Type	Average RF/ Response Ratio	Injected Conc	Units	Calculated Conc	Units
1,3-dichlorobenzene	9.17	146.00 mz	38	Average RF	0.000	0.001	ug/L	0.001	ug/L
1,4-dichlorobenzene	N/F	146.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
n-butylbenzene	9.55	91.00 mz	24385	Average RF	0.096	0.286	ug/L	0.286	ug/L
1,2-dichlorobenzene	9.58	146.00 mz	64	Average RF	0.000	0.001	ug/L	0.001	ug/L
4-methylcyclohexanemethanol	10.08	55.11 mz	8486771	Ext Curve	33.488	2249.568	ug/L	2249.568	ug/L
check later	10.29	75.00 mz	18416	Average RF	0.073	1.187	ug/L	1.187	ug/L
4-(methoxymethyl)cyclohexanemethanol	10.29	55.11 mz	3777645	Ext Curve	14.907	1001.384	ug/L	1001.384	ug/L
hexachlorobutadiene	10.76	225.00 mz	6	Average RF	0.000	0.002	ug/L	0.002	ug/L
1,2,4-trichlorobenzene	N/F	180.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L
naphthalene	11.11	128.00 mz	906	Average RF	0.004	0.013	ug/L	0.013	ug/L
1,2,3-trichlorobenzene	N/F	180.00 mz	N/F	N/F	N/F	N/F	ug/L	N/F	ug/L

Manually Integrated

TIC Summary Report

Lab Name: Huntington Water
Instrument: Thermo Scientific Instrument
User:
Batch: Spill3_1132014_a

Method: Spill3_1132014_a_EPAMethod524_List
EPAMethod524_List
Cali File: EPAMethod524_List_1102014_gcalibration_Spill3_1132014_a.calx

Vial Pos	Sample ID	File Name	Level	Sample Name	File Date	Comment
49	Sample	1132014_a049	N/A	Hyd #6014 Zone 10 011314	1/14/2014 6:23:03 AM	

Internal Standards

Internal Standard	ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units
fluorobenzene(ISTD)	1	4.41	951122	5.000	ug/L	5.000	ug/L

Qualitatively-identified Compounds

Compound	Uses ISTD#	RT	Response	Injected Conc	Injected Units	Sample Conc	Sample Units	Flag

Manually Integrated [ ] Flag legend: P = Library entry selected manually

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Warner, Sue

From: Hedrick, Elizabeth
Sent: Tuesday, February 11, 2014 3:34 PM
To: Poff, Kevin; Magnuson, Matthew; Arguto, William; Gray, Wendy; Weber, Eric; Caporale, Cynthia; binetti, victoria; Warner, Sue
Cc: Allgeier, Steve
Subject: RE: EPI Suite prediction for MCMH. RE: MCHM DEGREDATION DISCUSSION Call in Number
Attachments: Possible Degradation Products 021114.docx

Thanks for sharing the EPISuite data and QSAR predicted degradation products. I had promised to share my armchair chemist's thoughts which aren't too far off from QSAR on some of the final oxidation products.

Elizabeth

Water Security Division
Office of Ground Water and Drinking Water
U.S. Environmental Protection Agency
26 West Martin Luther King Drive
MS 140
Cincinnati, Ohio 45268
Ph (513) 569-7296
Fax (513) 569-7191

From: Poff, Kevin
Sent: Tuesday, February 11, 2014 11:27 AM
To: Magnuson, Matthew; Arguto, William; Gray, Wendy; Weber, Eric; Caporale, Cynthia; binetti, victoria; Hedrick, Elizabeth; Warner, Sue
Cc: Allgeier, Steve; R3 ESC-LB; Sayles, Gregory; Lindquist, Alan
Subject: RE: EPI Suite prediction for MCMH. RE: MCHM DEGREDATION DISCUSSION Call in Number

In addition to the EPISuite data , I attached the QSAR modeling that was run on MCHM and diPPH using the EPIsuite and CATABOL interfaces. The degradation products show chemical structures and probabilities of that particular degradation pathway.

From: Magnuson, Matthew
Sent: Tuesday, February 11, 2014 10:30 AM
To: Arguto, William; Gray, Wendy; Weber, Eric; Caporale, Cynthia; binetti, victoria; Hedrick, Elizabeth; Warner, Sue
Cc: Allgeier, Steve; R3 ESC-LB; Sayles, Gregory; Lindquist, Alan
Subject: EPI Suite prediction for MCMH. RE: MCHM DEGREDATION DISCUSSION Call in Number

As discussed on the call, here is the printout of EPI Suite predictions for MCHM.

From: Arguto, William
Sent: Tuesday, February 11, 2014 6:57 AM
To: Gray, Wendy; Magnuson, Matthew; Weber, Eric; Caporale, Cynthia; binetti, victoria; Hedrick, Elizabeth; Warner, Sue
Cc: Allgeier, Steve; R3 ESC-LB
Subject: MCHM DEGREDATION DISCUSSION Call in Number
Importance: High

The call in number for the conference call is

Ex. 6 - Personal Privacy

Freedom_0006097_0471

Conference Code Ex. 6 - Personal Privacy

Thanks
Bill

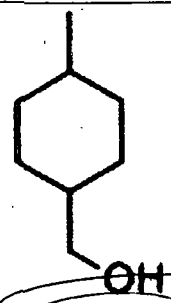
Freedom_0006097_0472

Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
Crude MCHM	4-methylcyclohexane methanol	68 to 89%	100-49-2	128.21	180-202°C
	4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158.25	?°C
	methyl 4-methylcyclohexanecarboxylate	5%	51181-40-9	156.22	191.7 °C
	dimethyl 1,4-cyclohexanedicarboxylate	1%	94-60-0	200.23	132 °C (technical grade)
	methanol	1%	67-56-1	32.04	64.7 °C
	1,4-cyclohexanedimethanol	1-2%	105-08-8	144.21	283 °C
DOWANOL™ DIPPH Glycol Ether	Dipropylene glycol phenyl ether or (methyl-2-phenoxyethoxy)propanol	>60%	51730-94-0	210.27	280 °C
	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152.19	242.7 °C

* Eric Weber, ORD/NERL/ERD, 2/4/2014

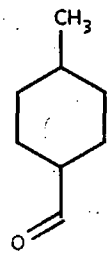
** source dependent

Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
4-methylcyclohexanemethanol	68 to 89%	100-49-2	128.21	180-202°C



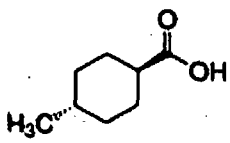
NOTE: The following information has not been peer-reviewed nor does it represent the views of the Agency.

Oxidation of primary alcohol ➔ 4-methyl cyclohexane -1-carbaldehyde (Fig 1). CAS RN: 33242-79-4. Formula: C8H14O. MW: 126.19, B.P. : 202-205 °C.



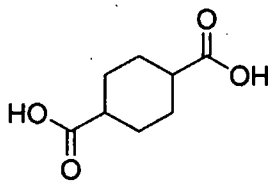
(Fig 1)

Further oxidation of an aldehyde yields a carboxylic acid. A stepwise oxidation (as opposed to oxidation of methyl group and opening of the ring)might result in 4-Methyl-1-cyclohexanecarboxylic acid (Fig 2). CAS No.: 13064-83-0 (Fig 2). Formula: CH3C6H10CO2H. MW: 142.20. A powder in pure form. This compound is a napthenic acid (NA) and has been used to study biodegradation kinetics of NAs. NAs in the oil refinery business refer to naturally occurring complex mixtures of alkyl-substituted cycloaliphatic carboxylic acids that concentrate in the tailings from extraction of oil from tar sands. The most interesting thing I read with respect to the NAs was one study that found different biodegradation rates between cis- and trans- isomers (Canadian Water Resources Journal, Biodegradation Kinetics of Geometric Isomers of Model Naphthenic Acids in Athabasca River Water J.V. Headley , K.M. Peru , S. Tanapat & G. Putz, Published online: 23 Jan 2013, http://www.tandfonline.com/doi/abs/10.4296/cwrj2701025).



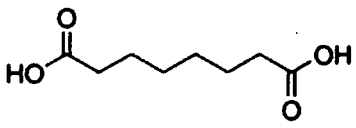
(Fig 2)

If KMnO4 did not open the cyclohexane ring to yield monocarboxylic acids or a dicarboxylic acid you might in theory get 1,4 cyclohexanedicarboxylic acid (Fig 3), CAS No. 1076-97-7, a compound with very low water solubility unless deprotonated at more basic pH resulting in a soluble carboxylate.



(Fig 3)

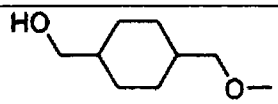
Alkaline KMnO4 would likely open the cyclohexane ring to give a dicarboxylic acid the octanedioic acid (Fig 4) or perhaps smaller acids such as acetic or oxalic acid. Smaller carboxylic acids are formic (C=1), acetic (C=2), propranoic (C=3) and dicarboxylic acids oxalic (C=2), malonic (C=3) succinic (C=4) up to C=5 are soluble in water.



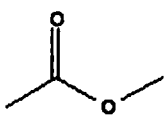
(Fig 4)

In general, open chain carboxylic acids might be the ultimate products of alkaline KMnO4 oxidation of MCHM. KMnO4 prefers to oxidize double bonds so MCHM may not have been oxidized at all by KMnO4 in river water treatment. Chlorination may not be sufficient to make carboxylic acids but small soluble carboxylic acids, produced by KMnO4 or free radicals, that make it to chlorination could be halogenated. Depending on pH before the chlorination step, the larger dicarboxylic acids may be removed as precipitates.

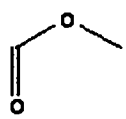
Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP
4-(methoxymethyl)cyclohexanemethanol	4-22%	98955-27-2	158.25	?°C



In theory, oxidation of primary alcohol and ether groups might result in small open chain carboxylic acids and perhaps acetates such as methyl acetate (Fig 5) or methyl formate (Fig 6). I would trust the QSAR predictions more on this one.



(Fig 5)



(Fig 6)

Some EPA Methods

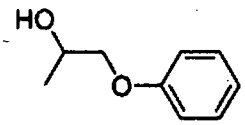
EPA 556.1 DETERMINATION OF CARBONYL COMPOUNDS IN DRINKING WATER BY FAST GAS CHROMATOGRAPHY, 1999. A place to start to detect aldehydes and ketones.

EPA 522 DETERMINATION OF 1,4-DIOXANE IN DRINKING WATER BY SOLID PHASE EXTRACTION (SPE) AND GAS CHROMATOGRAPHY/MASS SPECTROMETRY (GC/MS) WITH SELECTED ION MONITORING (SIM), 2008. A place to start for ethers.

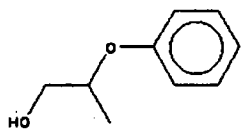
EPA Method 611—Haloethers.

Commercial Product	Component Chemicals	Component Chemical Distribution*	CAS #	MW	BP**
DOWANOL™ DiPPH Glycol Ether	propylene glycol phenyl ether or 1-phenoxy-2-propanol	<25%	770-35-4	152.19	242.7 °C

PPh



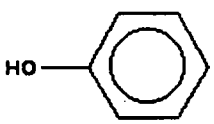
secondary alcohol, major isomer, CAS No.: 770-35-4



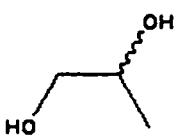
primary alcohol, the minor isomer, CAS No.: 4169-04-4

The EPA's EPIWIN/APO model is reported to estimate atmospheric photodegradation half-life of PPh at 3.45 hrs based on 12 hours of sunlight and avg OH radical concentration of 1.5E6 OH/cm^3. Free radical oxidation might result in phenol (Fig and propylene glycol. (I attempted writing out the free radical reaction and terminated it there.) I also found literature indicating that acidic KMnO4 could oxidize phenyl glycol ether to phenol and carboxylic acids. Another source indicated propylene glycol (Fig 8) oxidation to oxalic (Fig 9) and carbonic acids (Fig 10).

Phenol (Fig 7). Formula: C6H6O. Molecular weight: 94.1112. CAS No.: 108-95-2



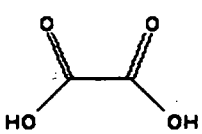
(Fig 7)



(Fig 8)

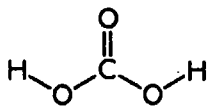
Propylene glycol (Fig 8). CAS No.: 57-55-6. Formula: C3H8O2. Molecular weight: 76.0944

Oxalic acid (Fig 9): CAS No: 144-62-7. Molecular weight: 90.03



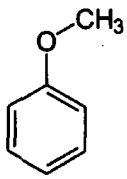
(Fig 9)

Carbonic acid (Fig 10):



(Fig 10)

Biological methylation of phenol to anisole (Fig 11) is reported in the literature. Anisole (methoxy benzene) CAS No.: 100-66-3. Formula: C7H8O. Molecular weight: 108.1378. Article on halogenated anisoles in the environment: Fresenius J Anal Chem (2001) 371 :598–606, "Halogenated methyl-phenyl ethers (anisoles) in the environment: Determination of vapor pressures, aqueous solubilities, Henry's law constants, and gas/water- (Kgw), n-octanol/water- (Kow) and gas/n-octanol (Kgo) partition coefficients."



(Fig 11)

Oxidation of phenol with KMnO4 is reported to produce benzoquinones (Fig 12).

(Fig 12)

I found one article that reported using PPh as a model compound for chlorination. Environ. Sci. Technol. 2004, 38, 4019-4025, "Transformation of Aromatic Ether and Amine-Containing Pharmaceuticals during Chlorine Disinfection." Researchers looked at chlorination of pharmaceuticals using PPh (1-phenoxy-2-propanol) as a model compound. Used RP-HPLC , 30%HEPES buffer/70%acetonitrile and UV detection at 275. The point might be that if PPh survives drinking water pre-treatment, it may halogenate.

Ex. 5 - Deliberative

Ex. 5 - Deliberative

Warner, Sue

From: Warner, Sue
Sent: Tuesday, March 18, 2014 4:03 PM
To: Caporale, Cynthia; Gundersen, Jennifer
Subject: RE: Charleston DW GC/MS Data Request

I reviewed the data sent by Ex. 6 - Personal Privacy from Battelle and the only compounds detected were the cis and trans isomers of MCHM.

From: Ex. 6 - Personal Privacy
Sent: Friday, March 14, 2014 4:36 PM
To: Warner, Sue
Subject: RE: Charleston DW GC/MS Data Request

Sue, the data are attached. I want to apologize for the delay. Our instruments were Agilent 5973 MDSs. NIST 02 was used to identify the few peaks that are present in the chromatograms. Our matches to NIST were not good; however, we used a standard of 4-MCHM provided to us with our first set of samples to create a calibration curve for analysis. So we compared spectra and retention times to the calibration standards. Autotunes were run prior to each set of samples on each instrument. All tunes passed using the criteria in the Agilent manual. The method was provided to us by the Ohio CST unit. I do not know where they got it. The handwritten comments on the reference method were made by Battelle to adapt the GC-FID method to the Mass Spec. Please let me know if you have any questions.

Thanks,

Ex. 6 - Personal Privacy
Principal Research Scientist
Hazard Characterization
CBRNE Defense Threat Assessment Group
Ex. 6 - Personal Privacy

Battelle
505 King Ave
Columbus, Ohio 43201
http://www.battelle.org

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From: Warner, Sue [mailto:Warner.Sue@epa.gov]
Sent: Friday, March 14, 2014 8:57 AM
To: Ex. 6 - Personal Privacy
Cc: 'Mark.LeChevallier@amwater.com'; 'Walt Ivey'; binetti, victoria; Arguto, William; Caporale, Cynthia
Subject: RE: Charleston DW GC/MS Data Request

Hi Julie,

basketball

I'm just checking on the status of the data request. Please let me know if you have any questions.

Thanks.

Sue

From: Ex. 6 - Personal Privacy
Sent: Tuesday, March 04, 2014 11:53 AM
To: Arguto, William; Warner, Sue; Caporale, Cynthia
Cc: Ex. 6 - Personal Privacy; 'Walt Ivey'; binetti, victoria
Subject: RE: Charleston DW GC/MS Data Request

I have been on travel the last two weeks but I will be back in the office next week. I can assemble the requested information early next week. I anticipate no issues in getting you the requested data.

Thank you,
Julie

-----Original Message-----
From: Arguto, William [Arguto.William@epa.gov]
Sent: Tuesday, March 04, 2014 11:39 AM Eastern Standard Time
To: Warner, Sue; Ex. 6 - Personal Privacy N; Caporale, Cynthia
Cc: Ex. 6 - Personal Privacy; Walt Ivey; binetti, victoria
Subject: RE: Charleston DW GC/MS Data Request

/ Sue

Thank you for pursuing this information and please let me know of any delays in processing this request. This information will be important in increasing our understanding of any additional DBP formation in the distribution system and is the one piece of actual results that will add to the theoretical discussions we have on this chemical and its potential to form DBPs. This request has been discussed and supported by the West Virginia Department of Health and Human Resources and the American Water Co who are also cc'd on this email.

If you have any additional questions please call me at 215-814-3367

William Arguto
U.S. EPA Region 3
Drinking Water Branch Chief

From: Warner, Sue
Sent: Tuesday, February 25, 2014 1:04 PM
To: Ex. 6 - Personal Privacy N; Caporale, Cynthia
Cc: Arguto, William
Subject: RE: Charleston DW GC/MS Data Request

Julie,

Freedom_0006097_0482

We're asking - is
there a name. who
talked to press. a details

WV Spill 9-10 tomorrow

Ex. 6 - Personal Privacy

Ex. 5 - Deliberative

Ex. 6 - Personal Privacy
Principal Research Scientist
Hazard Characterization
CBRNE Defense Threat Assessment Group
Ex. 6 - Personal Privacy
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From: Caporale, Cynthia [mailto:Caporale.Cynthia@epa.gov]
Sent: Friday, February 14, 2014 2:47 PM
To: Ex. 6 - Personal Privacy
Cc: Warner, Sue
Subject: Charleston DW GC/MS Data Request

Ms Ex. 6 - Personal Privacy

I am the USEPA R3 Lab Manager and I am working with our Drinking Water Program managers to review existing GC/MS data that may have been acquired by laboratories during the initial days of the Charleston Drinking Water Incident.

Did your laboratory run the drinking water samples using GC/MS in full-scan for any of the drinking water samples (pre- and post-treatment)? If so, we would be interested in the raw data from some of the sample analysis. Below is the specific information we are seeking.

VOC and SVOC GC/MS raw data files, including a TIC report processed against the NIST or similar library, which includes the chromatogram and spectra for the 20 largest TICs, for the following samples that were been analyzed using a full scan rather than targeted MCHM scan:

- Approximately 4 of the highest quantitative results for MCHM at locations in the distribution system
- Plant finished water sample showing high quantitative result for MCHM

Please clarify the instrument type, method used (Drinking water versus SW-846 type protocol), and preservative/quench agent.

Please feel free to contact me for more information or if you have any questions.

Thanks,
Cindy

Cynthia Caporale, Chief
OASQA Laboratory Branch
U.S. EPA Region III

GCWW

Warner, Sue

From: Fromme, Bill [Bill.Fromme@gcww.cincinnati-oh.gov]
Sent: Monday, March 31, 2014 1:18 PM
To: Warner, Sue
Cc: Caporale, Cynthia; Swertfeger, Jeff; Whitteberry, Bruce; Selar, Niranjan
Subject: RE: Charleston, WV Drinking Water Samples- TIC Reports and Possible Degradation Products
Attachments: Spill_TIC_send_033114.pdf; Spill_TIC_Upriver_send_033114.pdf; Spill_TIC_Tank_Std_send_033114.pdf; Spill_TIC_Fisher_Std_send_033114.pdf

Ex. 5 - Deliberative

Hi Sue,
I have attached four pdfs:

1) There are two chromatograms in the first attached pdf (Spill_TIC_send_033114).

I have summarized them in the Table below.

TIC Name	Location Description	Collection Date & Time	Acq on (Analysis Date)
Beckjord-0815	Ohio River (app 10 miles upriver of Intake)	01/15/2014 @08:15 AM	15-Jan-2014
BECK-0815-01152014	Ohio River (app 10 miles upriver of Intake). Duplicate of sample Beckjord-0815	01/15/2014 @08:15 AM	17-Jan-2014

The samples were collected on Jan 15th in duplicate from the Beckjord Power Station (which is located approximately 10 miles upstream of our Intake)

We used Method 524.3.
Each chromatogram shows three peaks from Internal Standards and three peaks from Surrogates.
The peaks from the 4-Methylcyclohexane Methanol are marked in yellow on the chromatogram.

We were unsure of the effect of a preservative on this compound and consequently did not use any when the samples were collected.
The sample named BECK-0815-01152014 is a duplicate of the sample named Beckjord-0815.
The sample named Beckjord-0815 was analyzed on Jan 15th.
The duplicate sample named BECK-0815-01152014 was analyzed on Jan 17th.
The 4-Methylcyclohexane Methanol was not detected in the duplicate sample after 2 days without preservative.

2) The second pdf (Spill_TIC_Upriver_send_033114) are two chromatograms of samples that came from upriver and are at a higher concentration. They were not collected by GCWW. I do not have any additional information on them at this time.
3) The third pdf (Spill_Tank_Std_send_033114) is a standard we made from material that was taken out of the tank that leaked.
4) The fourth pdf (Spill_TIC_Fisher_Std_send_033114) is a standard we made from compound we obtained through Fisher Scientific.

Thanks!

From: Warner, Sue [mailto:Warner.Sue@epa.gov]
Sent: Friday, March 28, 2014 3:32 PM
To: Fromme, Bill
Cc: Caporale, Cynthia
Subject: RE: Charleston, WV Drinking Water Samples- TIC Reports and Possible Degradation Products

Thank you very much.

From: Fromme, Bill [mailto:Bill.Fromme@gcww.cincinnati-oh.gov]
Sent: Friday, March 28, 2014 3:31 PM
To: Warner, Sue
Cc: Caporale, Cynthia
Subject: RE: Charleston, WV Drinking Water Samples- TIC Reports and Possible Degradation Products

Hi Sue,
We will send chromatograms Monday.
Thanks!

From: Warner, Sue [mailto:Warner.Sue@epa.gov]
Sent: Friday, March 28, 2014 1:17 PM
To: Fromme, Bill
Cc: Caporale, Cynthia
Subject: FW: Charleston, WV Drinking Water Samples- TIC Reports and Possible Degradation Products

Mr. Fromme,

Below is the message I sent to Mr. Swertfeger and the string of emails associated with it. Thank you very much for your assistance in this matter. Please let me know if you have any questions.

Sue Warner
Chemist
Office of Analytical Services and Quality Assurance
U.S. Environmental Protection Agency
Environmental Science Center
701 Mapes Road
Ft. Meade, MD 20755-5350
(410) 305-2658
Fax(410) 305-3096

From: Warner, Sue
Sent: Friday, March 28, 2014 1:05 PM
To: 'Jeff.Swertfeger@gcww.cincinnati-oh.gov'
Cc: Caporale, Cynthia
Subject: Charleston, WV Drinking Water Samples- TIC Reports and Possible Degradation Products

Mr. Swertfeger,

I am following up on the original data request from 2/28/14. Do you have any tentatively identified compound (TIC) reports run using the NIST or similar library for any Charleston, WV drinking water samples taken around the time of the original spill? You don't have to assess or review the data. You can send it to us and we

will review the TIC data. Thank you very much for your assistance in this matter. Please let me know if you have any questions.

Sue Warner
Chemist
Office of Analytical Services and Quality Assurance
U.S. Environmental Protection Agency
Environmental Science Center
701 Mapes Road
Ft. Meade, MD 20755-5350
(410) 305-2658
Fax(410) 305-3096

From: Swertfeger, Jeff [mailto:Jeff.Swertfeger@gcww.cincinnati-oh.gov]
Sent: Friday, February 28, 2014 4:20 PM
To: Caporale, Cynthia
Cc: Warner, Sue
Subject: RE: Degradation Products

Sure, we can share what we have. We did not identify any by-product compounds though, we just saw the MCHM decrease pretty rapidly in our unpreserved samples.

If you want to talk, let us know a few times next week when you are available and we will let you know what works for us.

From: Caporale, Cynthia [mailto:Caporale.Cynthia@epa.gov]
Sent: Friday, February 28, 2014 11:25 AM
To: Swertfeger, Jeff
Cc: Warner, Sue
Subject: Degradation Products

Mr. Swertfeger,

I was given your name from Elizabeth Hedrick, EPA Water Security Division, and she informed me that you had some information on the degradation products being observed in some of the Charleston, WV Drinking Water samples. We are trying to obtain some of that information, as well, so if you are willing to share the "TIC" report please let me know.

Thanks,
Cindy

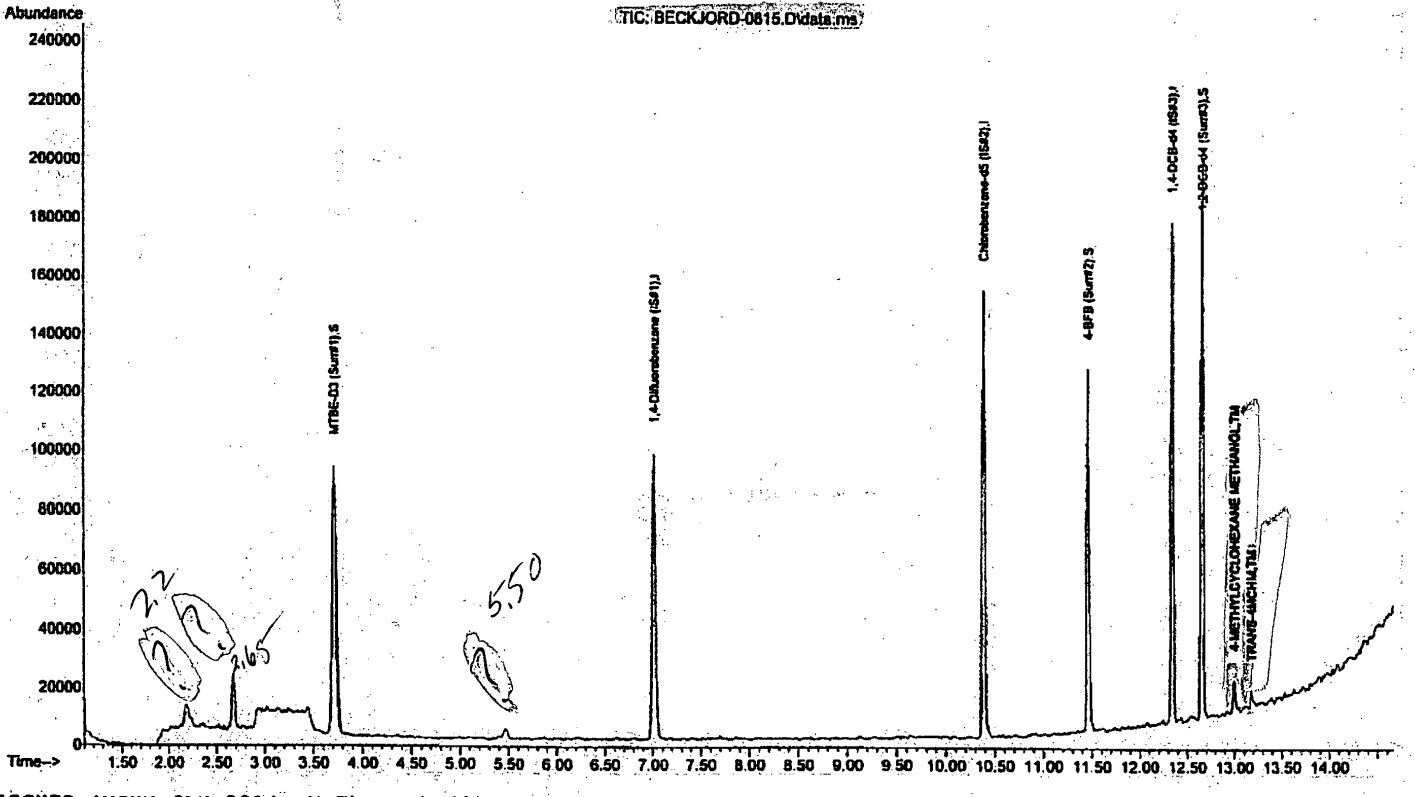
Cynthia Caporale, Chief
OASQA Laboratory Branch
U.S. EPA Region III
Environmental Science Center
Fort Meade, MD
(410) 305-2732
Fax: (410) 305-3095

Freedom_0006097_0488

Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\JAN_2014\RMTP_SPILL\
Data File : BECKJORD-0815.D
Acq On : 15 Jan 2014 9:04 am
Operator : NSELAR
Sample : BECKJORD-0815
Misc : 01/15/2014 @08:15am
ALS Vial : 1 Sample Multiplier: 1

Quant Time: Feb 27 14:10:55 2014
Quant Method : D:\msdchem\1\2014_METHODS\FISCHER_4MCHM_JAN_2014_.M
Quant Title : Method 524.3
QLast Update : Tue Jan 14 16:18:12 2014
Response via : Initial Calibration



FISCHER_4MCHM_JAN_2014_.M Thu Feb 27 14:11:58 2014 AGILENT5975

Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\SPILL_011714\
Data File : BECK-0815-01152014.D
Acq On : 17 Jan 2014 3:02 pm
Operator : NSELAR
Sample : BECK-0815-01152014
Misc :
ALS Vial : 7 Sample Multiplier: 1

Quant Time: Feb 27 13:55:52 2014
Quant Method : D:\msdchem\1\2014_METHODS\FISCHER_4MCHM_JAN_2014_.M
Quant Title : Method 524.3
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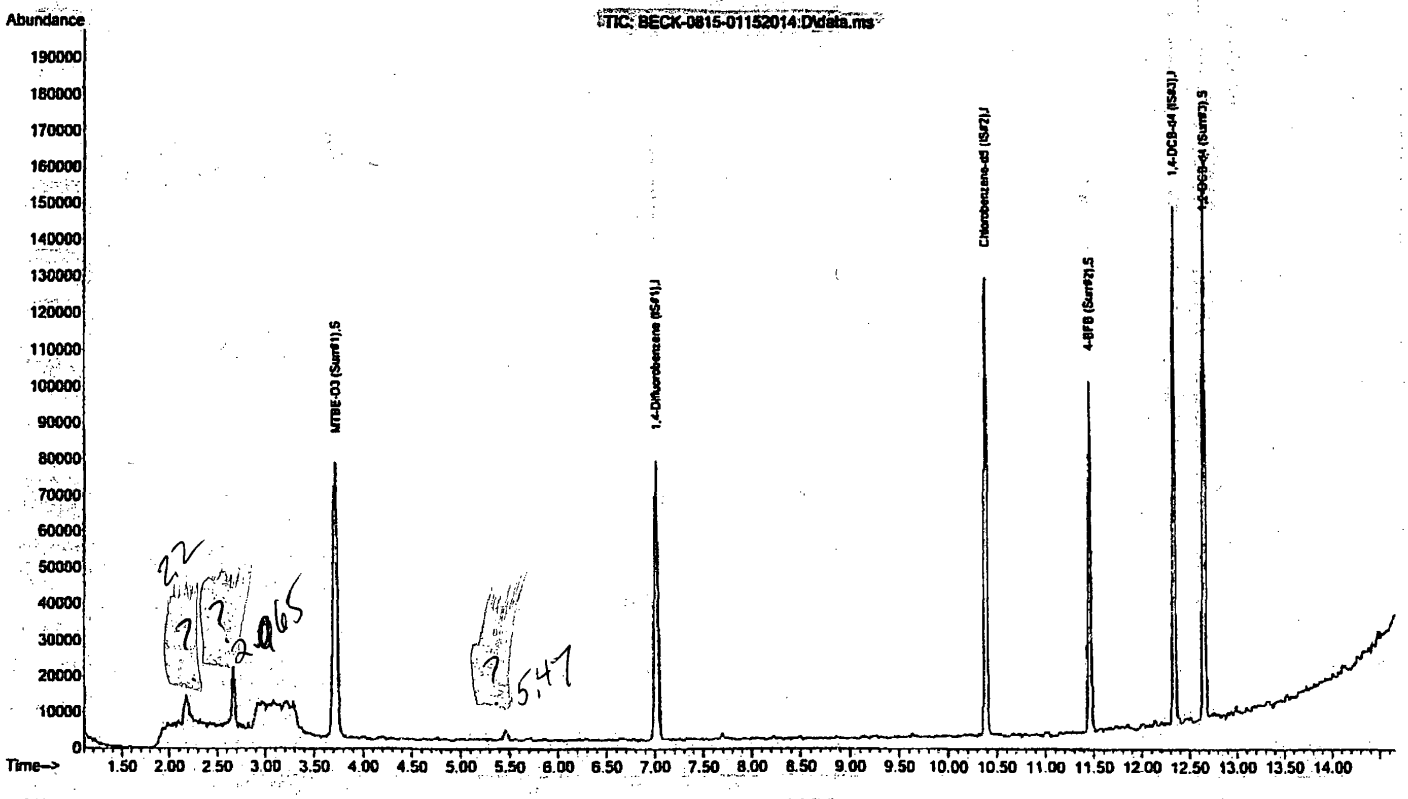
Response via : Initial Calibration



FISCHER_4MCHM_JAN_2014_.M Thu Feb 27 13:56:10 2014 AGILENT5975 Page: 2

Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\JAN_2014\ORSANCO_KRMO_011014\
Data File : 3221363.D
Acq On : 12 Jan 2014 10:50 am
Operator : htodd
Sample : 3221363
Misc : SHULTE
ALS Vial : 24 Sample Multiplier: 1

Quant Time: Mar 31 10:16:54 2014
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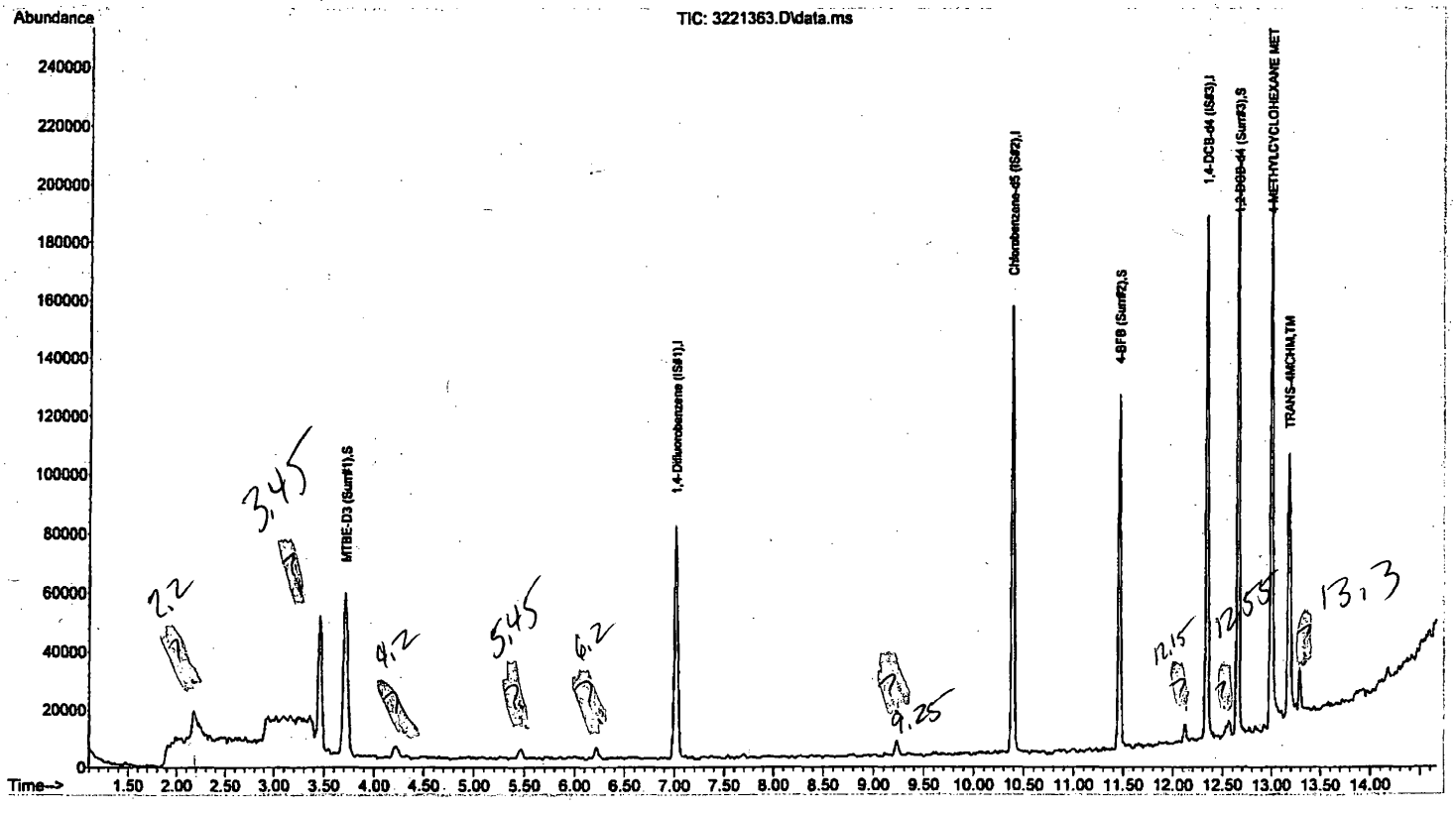
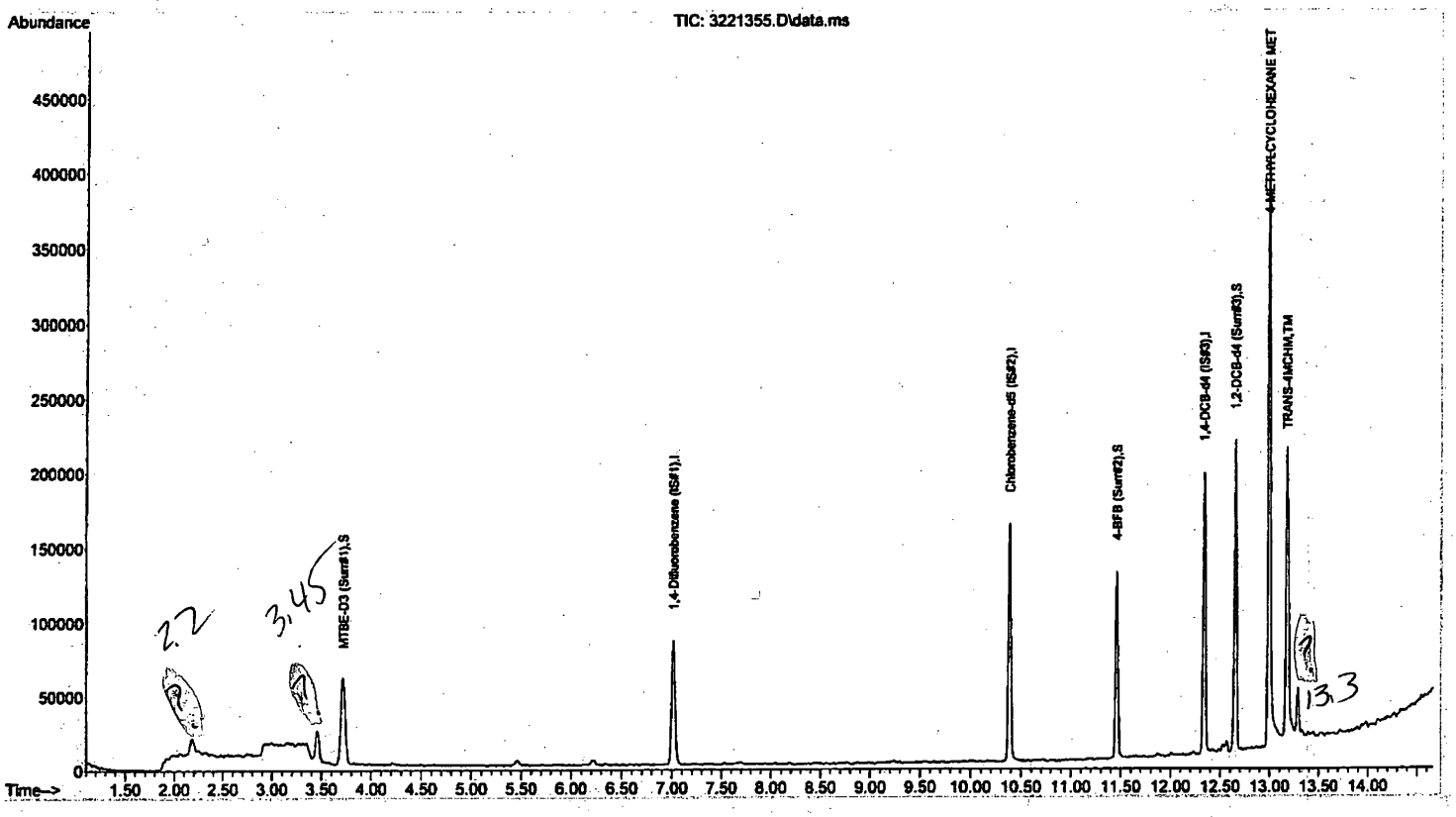
Response via : Initial Calibration



Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\JAN_2014\ORSANCO_KRMO_011014\
Data File : 3221355.D
Acq On : 12 Jan 2014 10:01 am
Operator : htodd
Sample : 3221355
Misc : SHULTE
ALS Vial : 22 Sample Multiplier: 1

Quant Time: Mar 31 10:23:41 2014
Quant Method : D:\msdchem\1\2014_METHODS\FISCHER_4MCHM_JAN_2014_.M
Quant Title : Method 524.3
QLast Update : Tue Jan 14 16:18:12 2014
Response via : Initial Calibration

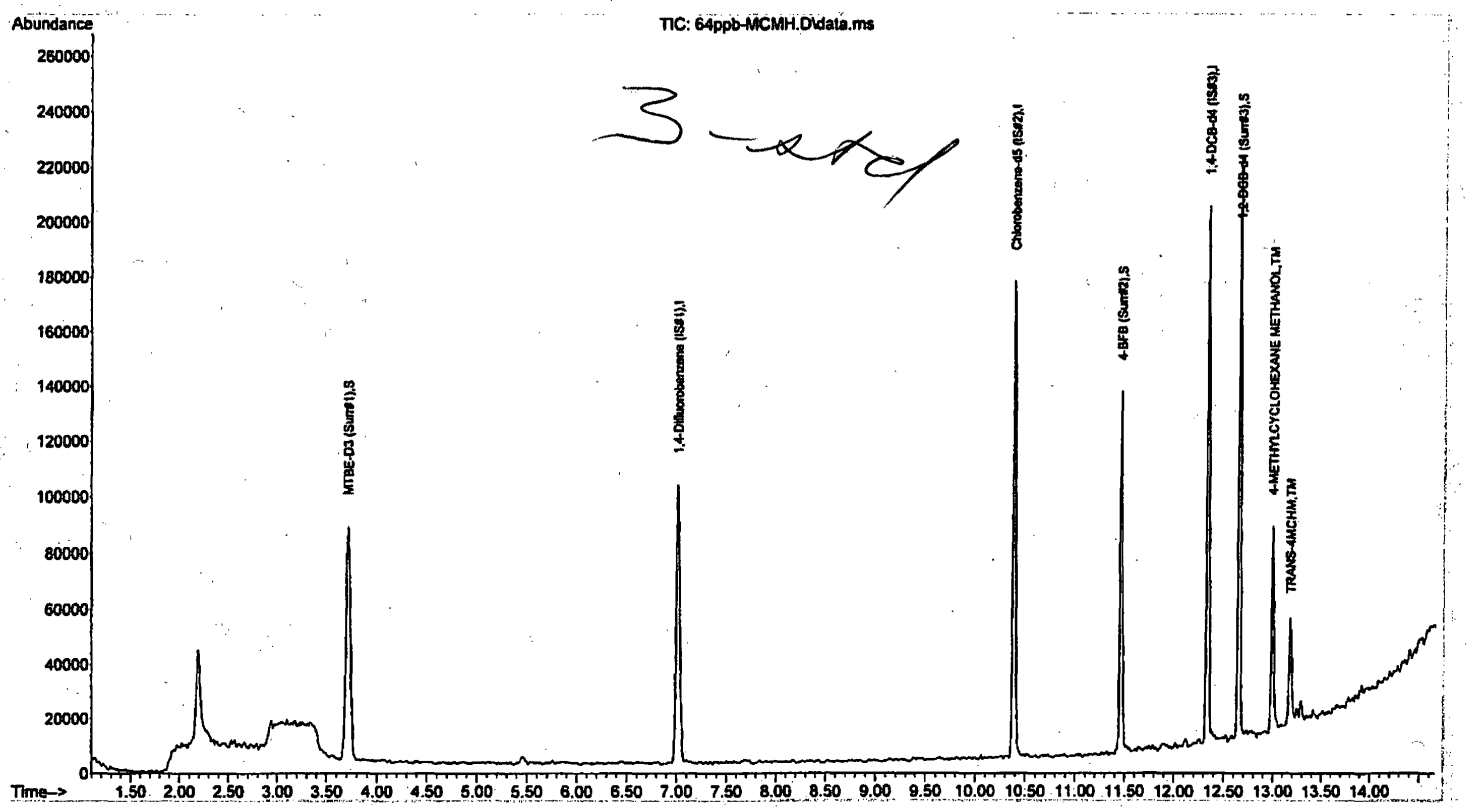


FISCHER_4MCHM_JAN_2014_.M Mon Mar 31 10:30:54 2014 AGILENT5975 Page: 2

Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\JAN_2014\WV-SPILL-01102014\
Data File : 64ppb-MCMH.D
Acq On : 10 Jan 2014 10:41 pm
Operator : NSELAR
Sample : 64ppb-MCMH
Misc :
ALS Vial : 10 Sample Multiplier: 1

Quant Time: Mar 31 10:34:41 2014
Quant Method : D:\msdchem\1\2014_METHODS\FISCHER_4MCHM_JAN_2014_.M
Quant Title : Method 524.3
QLast Update : Tue Jan 14 16:18:12 2014
Response via : Initial Calibration



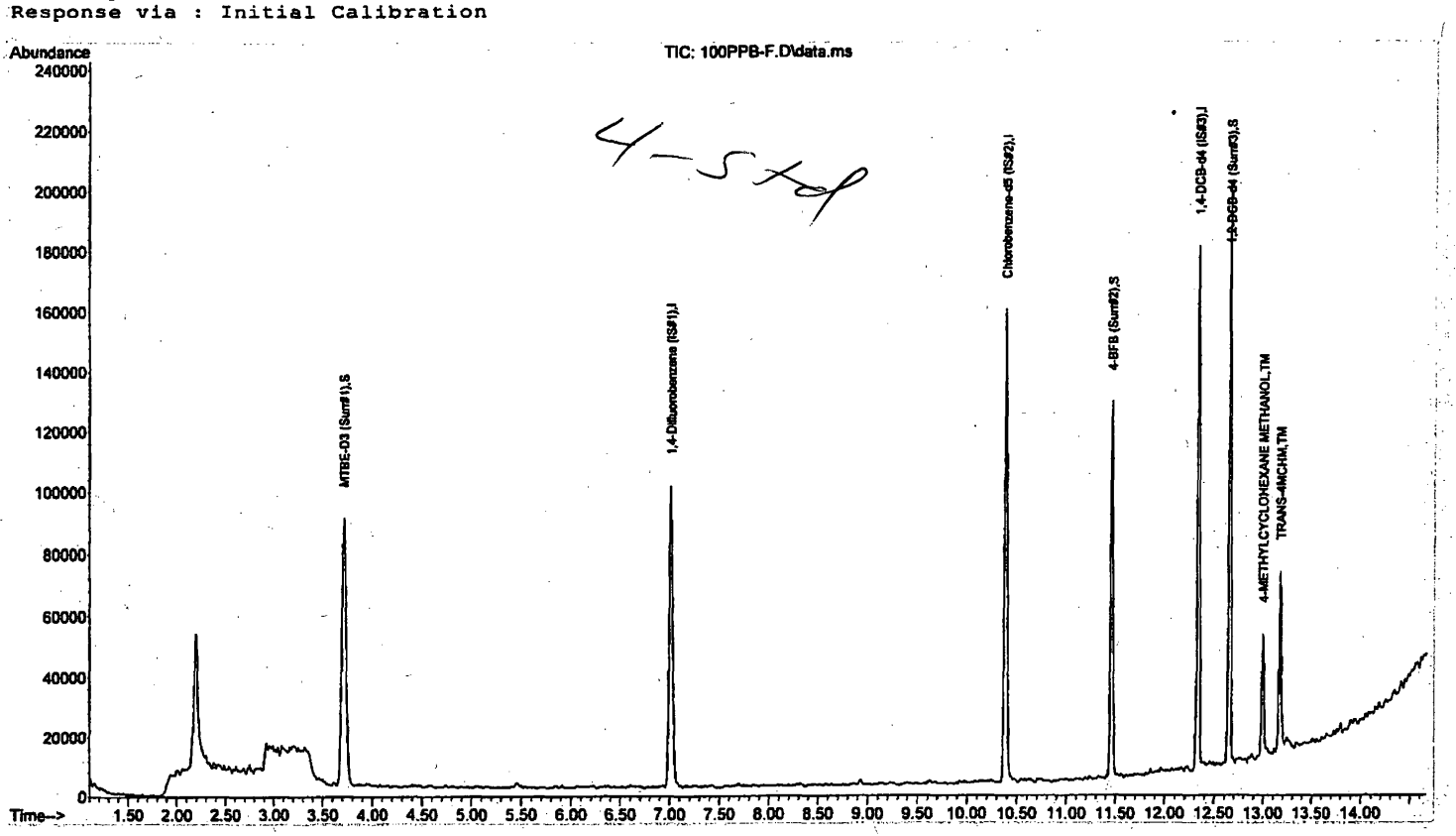
3-ad

FISCHER_4MCHM_JAN_2014_.M Mon Mar 31 10:35:31 2014 AGILENT5975 Page: 2

Quantitation Report (QT Reviewed)

Data Path : D:\msdchem\1\DATA\2014\JAN_2014\JERRY-SCHULTY\
Data File : 100PPB-F.D
Acq On : 13 Jan 2014 1:15 pm
Operator : NSELAR
Sample : 100PPB-F
Misc :
ALS Vial : 13 Sample Multiplier: 1

Quant Time: Mar 31 10:31:48 2014
Quant Method : D:\msdchem\1\2014_METHODS\FISCHER_4MCHM_JAN_2014_.M
Quant Title : Method 524.3
QLast Update : Tue Jan 14 16:18:12 2014
Response via : Initial Calibration



FISCHER_4MCHM_JAN_2014_.M Mon Mar 31 10:32:04 2014 AGILENT5975 Page: 2